Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 07:57 AM EDT

PDB ID	:	3ISF / pdb_00003isf
Title	:	Structure of non-mineralized Bfrb (as-isolated) from Pseudomonas aeruginosa to 2.07A Resolution
Authors	:	Lovell, S.; Weeratunga, S.K.; Battaile, K.P.; Rivera, M.
Deposited on	:	2009-08-25
Resolution	:	2.07 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:

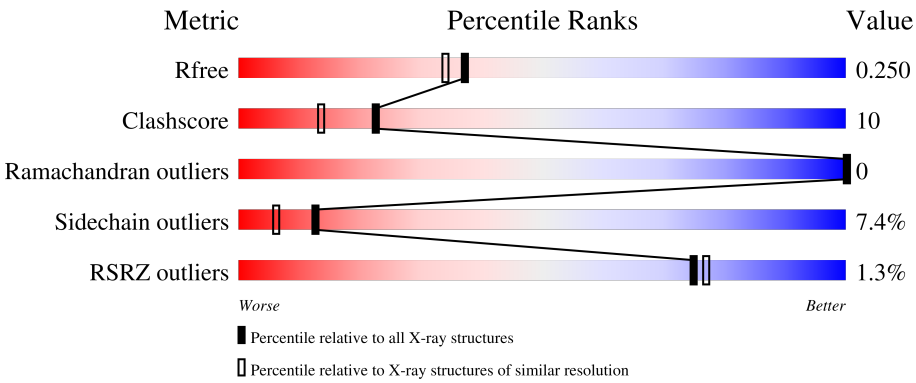
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.07 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}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	158	2% 84% 12%
1	B	158	% 77% 16%
1	C	158	% 82% 13%
1	D	158	2% 81% 15%
1	E	158	77% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	158	2% 77% 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8240 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.

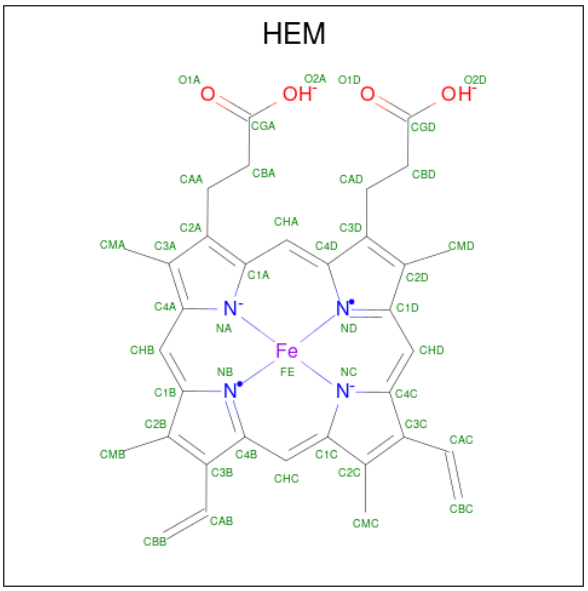
- Molecule 1 is a protein called Bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	155	1277	807	220	244	6	0	1	0
1	B	155	1281	810	221	244	6	0	1	0
1	C	156	1289	814	222	247	6	0	1	0
1	D	157	1294	817	223	247	7	0	0	0
1	E	155	1281	810	221	244	6	0	1	0
1	F	155	1281	810	221	244	6	0	1	0

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	E	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	F	1	43	34	1	4	4	0	0

- Molecule 4 is water.

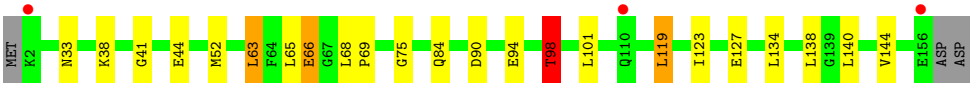
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	53	53	53	0	0
			Total	O		
4	B	59	59	59	0	0
			Total	O		
4	C	52	52	52	0	0
			Total	O		
4	D	58	58	58	0	0
			Total	O		
4	E	78	78	78	0	0
			Total	O		
4	F	63	63	63	0	0

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.

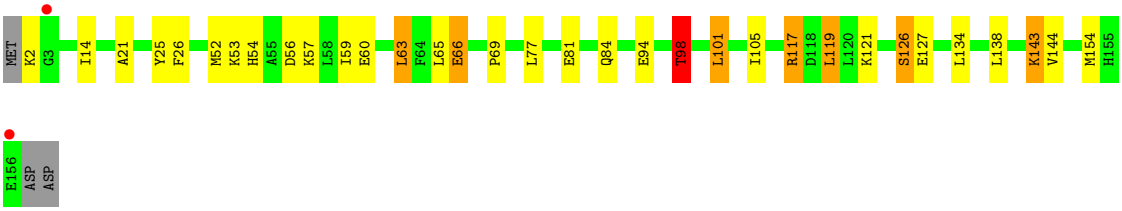
• Molecule 1: Bacterioferritin

Chain A:



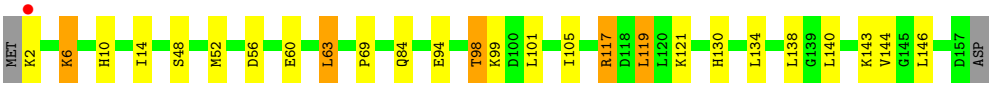
• Molecule 1: Bacterioferritin

Chain B:



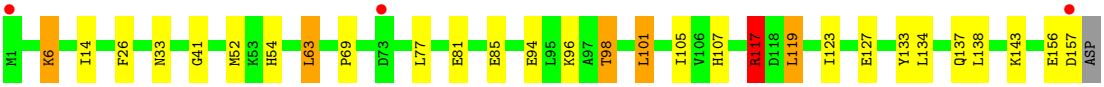
• Molecule 1: Bacterioferritin

Chain C:



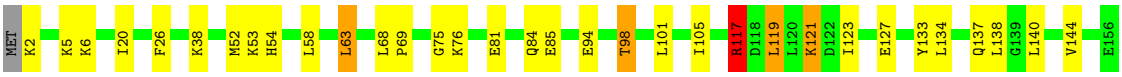
• Molecule 1: Bacterioferritin

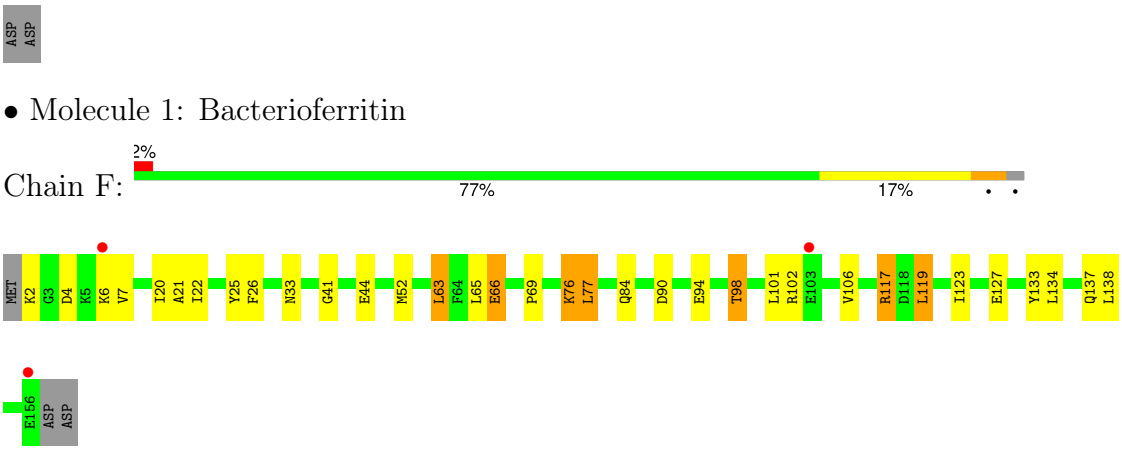
Chain D:



• Molecule 1: Bacterioferritin

Chain E:




ASP
ASP
• Molecule 1: Bacterioferritin
Chain F:
2%
77%
17%
MET
K2
G3
D4
K5
K6
V7
I20
A21
I22
Y25
F26
N33
G41
E44
M52
L63
F64
L65
E66
P69
K76
L77
Q84
D90
E94
T98
L101
R102
E103
V106
R117
D118
L119
I123
E127
Y133
L134
Q137
L138
E156
ASP
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	122.76Å 126.27Å 168.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.02 – 2.07 44.02 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.02-2.07) 99.4 (44.02-2.07)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.06Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0066	Depositor
R, R_{free}	0.198 , 0.245 0.210 , 0.250	Depositor DCC
R_{free} test set	3973 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.001 for -k,-h,-l 0.004 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.000 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.001 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.002 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8240	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.26	2/1301 (0.2%)	1.13	3/1751 (0.2%)
1	B	1.26	2/1305 (0.2%)	1.10	3/1755 (0.2%)
1	C	1.29	1/1313 (0.1%)	1.10	1/1766 (0.1%)
1	D	1.29	1/1315 (0.1%)	1.09	4/1768 (0.2%)
1	E	1.21	0/1305	1.11	5/1755 (0.3%)
1	F	1.24	0/1305	1.11	0/1755
All	All	1.26	6/7844 (0.1%)	1.11	16/10550 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	54	HIS	CA-C	6.13	1.60	1.52
1	B	59	ILE	C-O	5.51	1.30	1.24
1	A	98	THR	CB-CG2	-5.51	1.34	1.52
1	A	75	GLY	N-CA	5.29	1.51	1.44
1	C	146	LEU	CA-C	5.25	1.59	1.52
1	B	144	VAL	C-O	-5.24	1.18	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	117	ARG	NE-CZ-NH1	7.49	128.99	121.50
1	B	143	LYS	N-CA-C	7.21	119.14	111.28
1	A	68	LEU	CA-C-N	-7.04	112.72	119.76
1	A	68	LEU	C-N-CA	-7.04	112.72	119.76
1	C	143	LYS	N-CA-C	6.92	118.90	111.36
1	B	98	THR	N-CA-CB	-6.63	100.45	110.07
1	A	98	THR	N-CA-CB	-6.31	100.83	110.16
1	D	117	ARG	NE-CZ-NH2	-6.29	113.54	119.20
1	E	68	LEU	CA-C-N	-6.05	113.71	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	68	LEU	C-N-CA	-6.05	113.71	119.76
1	B	98	THR	CB-CA-C	5.97	120.33	110.90
1	E	117	ARG	CD-NE-CZ	5.93	132.71	124.40
1	D	117	ARG	CD-NE-CZ	5.77	132.48	124.40
1	E	53	LYS	N-CA-C	5.62	117.41	111.28
1	D	117	ARG	CB-CG-CD	5.42	123.77	111.30
1	E	117	ARG	NE-CZ-NH1	5.35	126.85	121.50

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	1277	0	1264	20	0
1	B	1281	0	1275	35	0
1	C	1289	0	1279	17	0
1	D	1294	0	1286	25	0
1	E	1281	0	1275	28	0
1	F	1281	0	1275	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	43	0	30	7	0
3	C	43	0	30	11	0
3	E	43	0	30	6	0
3	F	43	0	30	11	0
4	A	53	0	0	5	0
4	B	59	0	0	5	0
4	C	52	0	0	2	0
4	D	58	0	0	3	0
4	E	78	0	0	10	0
4	F	63	0	0	6	0
All	All	8240	0	7774	164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (164) 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:B:2:LYS:HG3	4:D:243:HOH:O	1.34	1.28
1:F:26:PHE:CE1	3:F:159:HEM:CBC	2.39	1.06
1:F:26:PHE:CZ	3:F:159:HEM:HBC2	1.99	0.98
1:D:98:THR:HG21	4:D:183:HOH:O	1.65	0.95
1:E:98:THR:HG21	4:E:177:HOH:O	1.67	0.94
1:B:119:LEU:C	1:B:119:LEU:HD23	1.93	0.94
1:B:119:LEU:HD23	1:B:119:LEU:O	1.72	0.90
1:F:26:PHE:CE1	3:F:159:HEM:HBC2	2.06	0.90
1:E:119:LEU:HD23	1:E:119:LEU:C	1.97	0.88
1:E:38:LYS:HD2	4:E:249:HOH:O	1.73	0.87
1:A:84:GLN:HG3	4:A:160:HOH:O	1.77	0.84
1:F:26:PHE:CE1	3:F:159:HEM:HBC1	2.12	0.83
1:A:98:THR:HG21	4:A:263:HOH:O	1.82	0.80
1:B:119:LEU:C	1:B:119:LEU:CD2	2.56	0.79
1:B:54:HIS:HD2	1:B:57:LYS:NZ	1.81	0.78
1:F:26:PHE:CD1	3:F:159:HEM:CBC	2.69	0.76
3:C:159:HEM:CBC	1:D:26:PHE:CE1	2.71	0.73
3:B:159:HEM:HBC2	3:B:159:HEM:HHD	1.71	0.71
1:A:65:LEU:O	1:A:66:GLU:HB2	1.90	0.71
1:B:117:ARG:HD3	4:B:164:HOH:O	1.90	0.71
1:F:63:LEU:HD13	1:F:69:PRO:HD3	1.73	0.70
1:E:84:GLN:HG3	4:E:335:HOH:O	1.90	0.70
1:B:105:ILE:HG23	1:B:117:ARG:HG3	1.73	0.70
1:F:26:PHE:CE2	3:F:159:HEM:HBC2	2.27	0.69
1:D:119:LEU:O	1:D:119:LEU:HD23	1.93	0.69
1:E:119:LEU:HD23	1:E:119:LEU:O	1.92	0.69
1:E:119:LEU:C	1:E:119:LEU:CD2	2.66	0.68
1:F:119:LEU:HD23	1:F:119:LEU:O	1.94	0.68
1:F:119:LEU:HD23	1:F:119:LEU:C	2.20	0.66
3:C:159:HEM:HBC2	1:D:26:PHE:CZ	2.30	0.66
1:A:119:LEU:HD23	1:A:119:LEU:C	2.20	0.65
1:F:119:LEU:C	1:F:119:LEU:CD2	2.70	0.65
1:D:119:LEU:HD23	1:D:119:LEU:C	2.22	0.64
1:A:119:LEU:HD23	1:A:119:LEU:O	1.96	0.64
1:F:25:TYR:OH	1:F:94:GLU:OE2	2.14	0.64
1:F:65:LEU:O	1:F:66:GLU:HB2	1.97	0.64
1:F:26:PHE:CZ	3:F:159:HEM:CBC	2.70	0.64
1:B:126[A]:SER:OG	4:B:182:HOH:O	2.16	0.63
1:C:63:LEU:HD13	1:C:69:PRO:CD	2.28	0.63
1:B:14:ILE:HD12	1:B:101:LEU:HD13	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:THR:CG2	4:E:177:HOH:O	2.34	0.63
1:A:63:LEU:HD13	1:A:69:PRO:CD	2.29	0.62
1:C:84:GLN:NE2	4:C:194:HOH:O	2.30	0.62
1:E:94:GLU:O	1:E:98:THR:HB	1.99	0.62
1:F:52:MET:HB3	3:F:159:HEM:CHB	2.28	0.62
1:B:143:LYS:HE2	4:E:343:HOH:O	1.98	0.62
1:A:119:LEU:C	1:A:119:LEU:CD2	2.73	0.62
1:E:52:MET:HB3	3:E:159:HEM:CHB	2.31	0.61
1:B:54:HIS:HD2	1:B:57:LYS:HZ3	1.48	0.61
1:B:143:LYS:CE	4:E:343:HOH:O	2.48	0.61
1:C:10:HIS:O	1:C:14:ILE:HG12	2.00	0.60
1:F:65:LEU:O	1:F:66:GLU:CB	2.49	0.60
1:F:63:LEU:HD13	1:F:69:PRO:CD	2.31	0.60
1:A:63:LEU:HD13	1:A:69:PRO:CG	2.32	0.60
3:C:159:HEM:HBC1	1:D:26:PHE:CE1	2.36	0.60
1:A:140:LEU:O	1:A:144:VAL:HG22	2.01	0.59
1:B:54:HIS:HD2	1:B:57:LYS:HZ1	1.50	0.59
1:C:6:LYS:HB2	1:C:6:LYS:HZ3	1.68	0.59
1:C:63:LEU:HD13	1:C:69:PRO:HD3	1.85	0.58
1:D:14:ILE:HD12	1:D:101:LEU:HD13	1.84	0.58
1:C:130:HIS:NE2	4:C:333:HOH:O	2.32	0.57
1:D:133:TYR:O	1:D:137:GLN:HG2	2.03	0.57
3:C:159:HEM:CMB	3:C:159:HEM:HBB2	2.33	0.57
1:A:123:ILE:O	1:A:127:GLU:HG2	2.04	0.57
1:C:105:ILE:HG23	1:C:117:ARG:HG3	1.86	0.57
1:A:38:LYS:HE2	4:A:260:HOH:O	2.04	0.57
1:C:48:SER:O	1:C:52:MET:HG3	2.05	0.57
1:E:63:LEU:HD13	1:E:69:PRO:HD3	1.88	0.56
1:F:133:TYR:O	1:F:137:GLN:HG2	2.07	0.55
1:B:65:LEU:O	1:B:66:GLU:HB2	2.06	0.55
1:D:63:LEU:HD13	1:D:69:PRO:HD3	1.88	0.55
1:D:119:LEU:HD21	1:D:123:ILE:HD11	1.87	0.55
1:B:94:GLU:O	1:B:98:THR:HB	2.07	0.55
1:D:119:LEU:C	1:D:119:LEU:CD2	2.80	0.55
1:A:65:LEU:O	1:A:66:GLU:CB	2.54	0.55
1:D:156:GLU:O	1:D:157:ASP:HB2	2.06	0.54
1:B:84:GLN:NE2	4:B:339:HOH:O	2.40	0.54
1:F:26:PHE:CD1	3:F:159:HEM:HBC2	2.41	0.54
1:A:98:THR:CG2	4:A:263:HOH:O	2.48	0.54
1:E:117:ARG:HD2	4:E:181:HOH:O	2.08	0.54
1:C:119:LEU:HD23	1:C:119:LEU:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLU:O	1:A:98:THR:HB	2.08	0.53
1:D:81:GLU:HG2	1:D:85:GLU:OE2	2.09	0.53
1:E:133:TYR:O	1:E:137:GLN:HG2	2.08	0.53
1:A:52:MET:HB3	3:B:159:HEM:CHD	2.38	0.53
3:C:159:HEM:CHB	1:D:52:MET:HB3	2.38	0.52
1:E:63:LEU:HD13	1:E:69:PRO:CD	2.39	0.52
1:B:63:LEU:HD13	1:B:69:PRO:HD3	1.92	0.52
1:C:94:GLU:O	1:C:98:THR:HB	2.10	0.52
1:B:63:LEU:HD13	1:B:69:PRO:CD	2.40	0.52
1:E:26:PHE:CE1	3:E:159:HEM:CBC	2.93	0.52
1:E:84:GLN:HG2	4:E:334:HOH:O	2.10	0.52
1:B:56:ASP:O	1:B:60:GLU:HG3	2.10	0.52
1:E:52:MET:HB3	3:E:159:HEM:C1B	2.45	0.52
1:E:140:LEU:O	1:E:144:VAL:HG22	2.10	0.52
1:C:119:LEU:CD2	1:C:119:LEU:C	2.84	0.51
1:E:52:MET:CE	3:E:159:HEM:NC	2.73	0.51
1:C:119:LEU:HD23	1:C:119:LEU:C	2.35	0.51
1:E:20:ILE:HD11	1:E:75:GLY:HA3	1.92	0.51
1:E:123:ILE:O	1:E:127:GLU:HG2	2.11	0.51
1:E:54:HIS:HE1	4:E:311:HOH:O	1.93	0.50
1:E:26:PHE:CZ	3:E:159:HEM:HBC2	2.46	0.50
1:F:44:GLU:OE2	1:F:90:ASP:OD2	2.29	0.50
1:B:2:LYS:HG2	1:B:66:GLU:OE2	2.12	0.50
1:D:98:THR:CG2	4:D:183:HOH:O	2.42	0.50
3:C:159:HEM:HBC2	3:C:159:HEM:HHD	1.92	0.50
1:A:63:LEU:HD13	1:A:69:PRO:HD3	1.94	0.49
1:F:94:GLU:OE1	1:F:127:GLU:OE1	2.30	0.49
1:F:123:ILE:O	1:F:127:GLU:HG2	2.11	0.49
1:B:26:PHE:CE1	3:B:159:HEM:CBC	2.95	0.49
1:B:94:GLU:OE1	1:B:127:GLU:OE1	2.30	0.49
3:B:159:HEM:CMB	3:B:159:HEM:HBB2	2.43	0.48
3:C:159:HEM:CMB	3:C:159:HEM:CBB	2.91	0.48
1:D:105:ILE:HG23	1:D:117:ARG:HG3	1.94	0.48
1:A:33:ASN:ND2	1:A:41:GLY:HA3	2.29	0.48
1:C:52:MET:HB3	3:C:159:HEM:CHD	2.44	0.48
3:C:159:HEM:CBC	1:D:26:PHE:CD1	2.96	0.47
1:B:54:HIS:HE1	4:B:182:HOH:O	1.97	0.47
1:D:33:ASN:ND2	1:D:41:GLY:HA3	2.30	0.47
1:F:33:ASN:ND2	1:F:41:GLY:HA3	2.30	0.47
1:E:52:MET:HE2	3:E:159:HEM:NC	2.28	0.47
1:B:21:ALA:HB1	1:B:25:TYR:CE2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ILE:O	1:D:127:GLU:HG2	2.15	0.47
1:F:4:ASP:HB3	1:F:7:VAL:HG23	1.97	0.47
3:C:159:HEM:CBC	1:D:26:PHE:CZ	2.95	0.47
1:F:20:ILE:HG23	1:F:77:LEU:HD12	1.97	0.47
1:B:117:ARG:HD2	4:B:180:HOH:O	2.14	0.47
1:C:56:ASP:O	1:C:60:GLU:HG3	2.15	0.47
1:F:76:LYS:O	4:F:185:HOH:O	2.20	0.46
1:B:65:LEU:O	1:B:66:GLU:CB	2.63	0.46
1:E:105:ILE:HG23	1:E:117:ARG:HG3	1.98	0.46
1:F:102:ARG:O	1:F:106:VAL:HG23	2.16	0.46
1:D:119:LEU:CD2	1:D:123:ILE:CD1	2.93	0.46
1:E:58:LEU:HA	1:E:58:LEU:HD23	1.78	0.45
1:F:117:ARG:HD3	4:F:195:HOH:O	2.16	0.45
4:A:326:HOH:O	1:D:143:LYS:HE3	2.17	0.45
1:D:94:GLU:O	1:D:98:THR:HB	2.16	0.45
1:B:121:LYS:O	1:B:121:LYS:HG2	2.17	0.45
1:F:117:ARG:HD2	4:F:196:HOH:O	2.16	0.45
1:A:44:GLU:OE2	1:A:90:ASP:OD2	2.36	0.44
3:F:159:HEM:O2A	4:F:359:HOH:O	2.21	0.44
1:B:54:HIS:CD2	1:B:57:LYS:HZ1	2.34	0.44
1:A:63:LEU:CD1	1:A:69:PRO:CD	2.96	0.44
1:F:94:GLU:O	1:F:98:THR:HB	2.18	0.44
1:E:81:GLU:HG2	1:E:85:GLU:OE2	2.18	0.44
1:D:63:LEU:HD13	1:D:69:PRO:CD	2.48	0.43
1:B:54:HIS:CD2	1:B:57:LYS:HZ3	2.33	0.43
1:B:52:MET:HB3	3:B:159:HEM:CHB	2.48	0.43
1:E:121:LYS:HB3	1:E:121:LYS:HE2	1.60	0.43
1:C:140:LEU:O	1:C:144:VAL:HG22	2.19	0.43
1:C:140:LEU:HA	1:C:140:LEU:HD23	1.82	0.43
1:B:53:LYS:O	1:B:57:LYS:HE3	2.20	0.42
1:B:154:MET:HE3	4:F:184:HOH:O	2.20	0.42
1:B:53:LYS:HE2	3:B:159:HEM:O1A	2.20	0.42
1:F:21:ALA:O	1:F:22:ILE:C	2.62	0.42
1:F:52:MET:HB3	3:F:159:HEM:C4A	2.56	0.41
1:B:26:PHE:CZ	3:B:159:HEM:HBC2	2.56	0.41
1:C:52:MET:HB3	3:C:159:HEM:C4C	2.56	0.41
1:F:76:LYS:HZ2	1:F:76:LYS:HG2	1.43	0.41
1:D:6:LYS:HB3	1:D:107:HIS:NE2	2.36	0.41
1:B:54:HIS:CD2	1:B:57:LYS:NZ	2.74	0.41
1:F:84:GLN:HB2	4:F:323:HOH:O	2.21	0.41
1:E:84:GLN:CG	4:E:334:HOH:O	2.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:HG3	1:A:84:GLN:H	1.63	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	154/158 (98%)	153 (99%)	1 (1%)	0	100	100
1	B	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
1	C	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	D	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	E	154/158 (98%)	154 (100%)	0	0	100	100
1	F	154/158 (98%)	153 (99%)	1 (1%)	0	100	100
All	All	926/948 (98%)	920 (99%)	6 (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	141/144 (98%)	134 (95%)	7 (5%)	22	14
1	B	142/144 (99%)	130 (92%)	12 (8%)	10	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	143/144 (99%)	132 (92%)	11 (8%)	12	5
1	D	143/144 (99%)	133 (93%)	10 (7%)	14	7
1	E	142/144 (99%)	130 (92%)	12 (8%)	10	4
1	F	142/144 (99%)	130 (92%)	12 (8%)	10	4
All	All	853/864 (99%)	789 (92%)	64 (8%)	13	6

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LEU
1	A	66	GLU
1	A	98	THR
1	A	101	LEU
1	A	119	LEU
1	A	134	LEU
1	A	138	LEU
1	B	63	LEU
1	B	66	GLU
1	B	77	LEU
1	B	81	GLU
1	B	98	THR
1	B	101	LEU
1	B	117	ARG
1	B	119	LEU
1	B	126[A]	SER
1	B	126[B]	SER
1	B	134	LEU
1	B	138	LEU
1	C	2	LYS
1	C	6	LYS
1	C	63	LEU
1	C	98	THR
1	C	99	LYS
1	C	101	LEU
1	C	117	ARG
1	C	119	LEU
1	C	121	LYS
1	C	134	LEU
1	C	138	LEU
1	D	6	LYS
1	D	63	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	77	LEU
1	D	96	LYS
1	D	98	THR
1	D	101	LEU
1	D	117	ARG
1	D	119	LEU
1	D	134	LEU
1	D	138	LEU
1	E	2	LYS
1	E	5	LYS
1	E	6	LYS
1	E	63	LEU
1	E	76	LYS
1	E	98	THR
1	E	101	LEU
1	E	117	ARG
1	E	119	LEU
1	E	121	LYS
1	E	134	LEU
1	E	138	LEU
1	F	2	LYS
1	F	6	LYS
1	F	63	LEU
1	F	66	GLU
1	F	76	LYS
1	F	77	LEU
1	F	98	THR
1	F	101	LEU
1	F	117	ARG
1	F	119	LEU
1	F	134	LEU
1	F	138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	46	HIS
1	A	54	HIS
1	A	88	GLN
1	A	130	HIS
1	A	137	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	155	HIS
1	B	33	ASN
1	B	54	HIS
1	B	84	GLN
1	B	130	HIS
1	C	33	ASN
1	C	54	HIS
1	C	130	HIS
1	C	137	GLN
1	D	33	ASN
1	D	54	HIS
1	D	88	GLN
1	D	112	HIS
1	D	130	HIS
1	E	33	ASN
1	E	46	HIS
1	E	54	HIS
1	E	130	HIS
1	E	142	GLN
1	F	10	HIS
1	F	33	ASN
1	F	54	HIS
1	F	112	HIS
1	F	137	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEM	C	159	1	50,50,50	1.93	10 (20%)	67,82,82	1.85	15 (22%)
3	HEM	E	159	1	50,50,50	2.23	11 (22%)	67,82,82	1.46	7 (10%)
3	HEM	F	159	1	50,50,50	2.09	8 (16%)	67,82,82	1.71	14 (20%)
3	HEM	B	159	1	50,50,50	1.93	10 (20%)	67,82,82	1.83	20 (29%)

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
3	HEM	C	159	1	-	5/14/54/54	-
3	HEM	E	159	1	-	3/14/54/54	-
3	HEM	F	159	1	-	4/14/54/54	-
3	HEM	B	159	1	-	5/14/54/54	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	159	HEM	FE-NB	9.15	2.23	1.94
3	F	159	HEM	C3D-C2D	8.03	1.54	1.36
3	E	159	HEM	C3D-C2D	8.00	1.54	1.36
3	B	159	HEM	C3D-C2D	6.93	1.51	1.36
3	C	159	HEM	C3D-C2D	6.58	1.51	1.36
3	C	159	HEM	FE-ND	6.20	2.14	1.94
3	F	159	HEM	FE-NB	5.96	2.13	1.94
3	B	159	HEM	FE-NB	5.64	2.12	1.94
3	F	159	HEM	FE-NA	4.99	2.11	1.95
3	E	159	HEM	FE-NA	4.86	2.11	1.95
3	B	159	HEM	FE-NA	4.48	2.09	1.95
3	C	159	HEM	FE-NA	4.30	2.09	1.95
3	F	159	HEM	FE-NC	4.29	2.09	1.95
3	F	159	HEM	FE-ND	4.22	2.07	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	159	HEM	FE-NB	3.59	2.06	1.94
3	E	159	HEM	CAC-C3C	3.30	1.56	1.47
3	B	159	HEM	FE-NC	3.24	2.05	1.95
3	C	159	HEM	C3C-C2C	-3.23	1.30	1.37
3	E	159	HEM	CAB-C3B	3.17	1.55	1.47
3	F	159	HEM	CAB-C3B	3.12	1.55	1.47
3	B	159	HEM	FE-ND	2.90	2.03	1.94
3	F	159	HEM	CAC-C3C	2.80	1.54	1.47
3	C	159	HEM	CMB-C2B	2.63	1.56	1.50
3	C	159	HEM	O2D-CGD	-2.53	1.22	1.30
3	E	159	HEM	FE-ND	2.48	2.02	1.94
3	B	159	HEM	C2A-C3A	-2.42	1.32	1.38
3	E	159	HEM	CMB-C2B	2.37	1.55	1.50
3	E	159	HEM	FE-NC	2.33	2.02	1.95
3	B	159	HEM	C1B-NB	-2.31	1.36	1.40
3	B	159	HEM	CMD-C2D	2.27	1.55	1.50
3	C	159	HEM	FE-NC	2.23	2.02	1.95
3	E	159	HEM	C2A-C3A	-2.17	1.33	1.38
3	C	159	HEM	C3B-C2B	-2.17	1.32	1.37
3	E	159	HEM	CMC-C2C	2.16	1.55	1.50
3	C	159	HEM	CAC-C3C	2.11	1.53	1.47
3	E	159	HEM	CMD-C2D	2.08	1.55	1.50
3	F	159	HEM	O2A-CGA	-2.07	1.24	1.30
3	B	159	HEM	C3C-C2C	-2.05	1.33	1.37
3	B	159	HEM	O2D-CGD	-2.01	1.24	1.30

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	159	HEM	C4D-ND-C1D	6.62	113.04	105.21
3	E	159	HEM	C4D-ND-C1D	6.58	113.00	105.21
3	C	159	HEM	C4D-ND-C1D	6.49	112.89	105.21
3	B	159	HEM	CHC-C1C-NC	4.91	129.80	124.45
3	B	159	HEM	C4D-ND-C1D	4.42	110.44	105.21
3	C	159	HEM	CAC-C3C-C4C	3.89	134.10	124.82
3	B	159	HEM	C2A-C1A-NA	-3.84	105.89	110.15
3	B	159	HEM	C3B-C2B-C1B	3.53	109.06	106.41
3	E	159	HEM	CBA-CAA-C2A	-3.43	103.04	112.53
3	B	159	HEM	CHA-C4D-ND	3.39	128.56	124.37
3	C	159	HEM	CBA-CAA-C2A	-3.38	103.18	112.53
3	B	159	HEM	CBD-CAD-C3D	-3.34	103.30	112.53
3	C	159	HEM	CAC-C3C-C2C	-3.34	117.58	128.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	159	HEM	CHC-C1C-NC	3.33	128.08	124.45
3	F	159	HEM	CBD-CAD-C3D	-3.26	103.52	112.53
3	C	159	HEM	CBD-CAD-C3D	-3.24	103.57	112.53
3	C	159	HEM	CHC-C1C-NC	3.17	127.91	124.45
3	B	159	HEM	CBA-CAA-C2A	-3.17	103.76	112.53
3	C	159	HEM	CBB-CAB-C3B	-3.13	111.87	127.53
3	F	159	HEM	C2A-C1A-NA	-3.13	106.68	110.15
3	F	159	HEM	CHA-C4D-ND	3.05	128.14	124.37
3	F	159	HEM	C3B-C2B-C1B	3.04	108.70	106.41
3	E	159	HEM	C3B-C2B-C1B	3.01	108.67	106.41
3	C	159	HEM	C2A-C1A-NA	-2.96	106.87	110.15
3	C	159	HEM	C3D-C4D-ND	-2.94	106.95	110.17
3	F	159	HEM	C3B-C4B-NB	-2.76	107.48	109.47
3	F	159	HEM	CBA-CAA-C2A	-2.74	104.96	112.53
3	C	159	HEM	CHC-C4B-NB	2.73	127.36	124.42
3	F	159	HEM	C1B-NB-C4B	2.64	108.34	105.21
3	F	159	HEM	C3D-C4D-ND	-2.64	107.28	110.17
3	B	159	HEM	CBB-CAB-C3B	-2.59	114.60	127.53
3	B	159	HEM	O2D-CGD-CBD	2.56	122.08	114.00
3	B	159	HEM	C4A-NA-C1A	2.51	109.92	105.82
3	B	159	HEM	C2B-C1B-NB	-2.49	106.97	109.84
3	E	159	HEM	CBD-CAD-C3D	-2.49	105.66	112.53
3	B	159	HEM	CMD-C2D-C1D	2.49	128.92	125.03
3	E	159	HEM	CHC-C1C-NC	2.47	127.14	124.45
3	C	159	HEM	CHD-C4C-C3C	2.45	129.33	125.21
3	B	159	HEM	C1B-NB-C4B	2.34	107.98	105.21
3	B	159	HEM	CAC-C3C-C4C	2.32	130.37	124.82
3	C	159	HEM	CAD-CBD-CGD	-2.32	107.51	113.67
3	E	159	HEM	C4C-C3C-C2C	2.31	108.81	106.81
3	B	159	HEM	CHD-C4C-C3C	2.30	129.08	125.21
3	B	159	HEM	CHC-C4B-NB	2.27	126.86	124.42
3	F	159	HEM	C4A-NA-C1A	2.25	109.49	105.82
3	B	159	HEM	O2A-CGA-O1A	-2.23	117.60	123.33
3	B	159	HEM	O2A-CGA-CBA	2.22	121.01	114.00
3	E	159	HEM	C2A-C1A-NA	-2.22	107.69	110.15
3	F	159	HEM	CHD-C1D-ND	2.22	126.81	124.42
3	B	159	HEM	C3C-C2C-C1C	2.19	109.12	107.05
3	C	159	HEM	C4B-C3B-C2B	2.19	109.29	107.28
3	B	159	HEM	CAC-C3C-C2C	-2.17	121.39	128.43
3	F	159	HEM	C3A-C4A-NA	-2.08	106.81	110.14
3	C	159	HEM	O2A-CGA-CBA	2.07	120.55	114.00
3	F	159	HEM	CHC-C4B-NB	2.04	126.62	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	159	HEM	CMC-C2C-C3C	-2.03	123.51	128.43

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	159	HEM	C4C-C3C-CAC-CBC
3	C	159	HEM	C4C-C3C-CAC-CBC
3	B	159	HEM	CAA-CBA-CGA-O2A
3	B	159	HEM	CAA-CBA-CGA-O1A
3	F	159	HEM	CAA-CBA-CGA-O1A
3	F	159	HEM	CAA-CBA-CGA-O2A
3	E	159	HEM	CAD-CBD-CGD-O2D
3	C	159	HEM	CAD-CBD-CGD-O2D
3	E	159	HEM	CAD-CBD-CGD-O1D
3	F	159	HEM	CAD-CBD-CGD-O2D
3	F	159	HEM	CAD-CBD-CGD-O1D
3	B	159	HEM	CAD-CBD-CGD-O2D
3	C	159	HEM	CAA-CBA-CGA-O2A
3	C	159	HEM	CAA-CBA-CGA-O1A
3	B	159	HEM	CAD-CBD-CGD-O1D
3	C	159	HEM	CAD-CBD-CGD-O1D
3	E	159	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

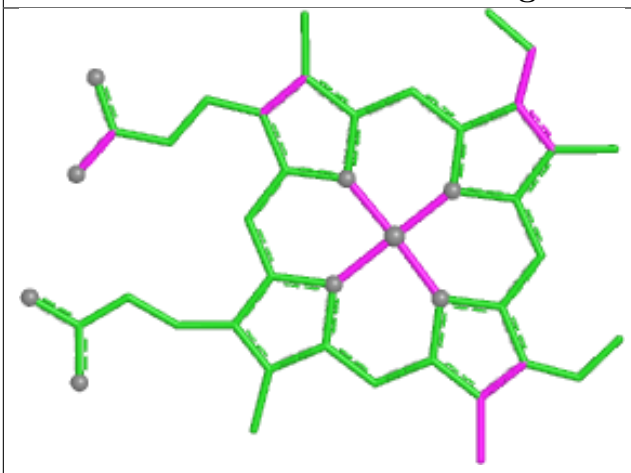
4 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	159	HEM	11	0
3	E	159	HEM	6	0
3	F	159	HEM	11	0
3	B	159	HEM	7	0

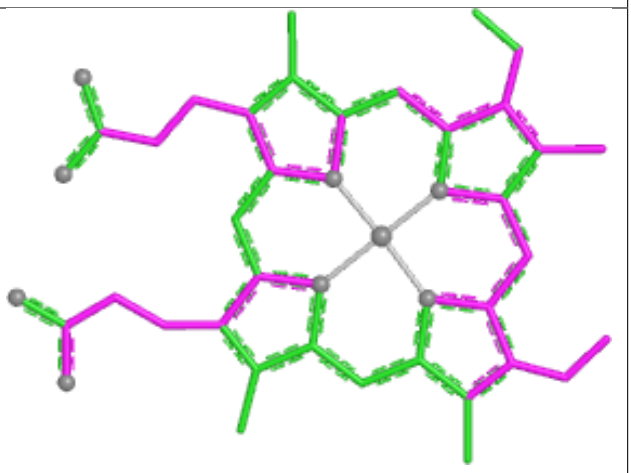
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

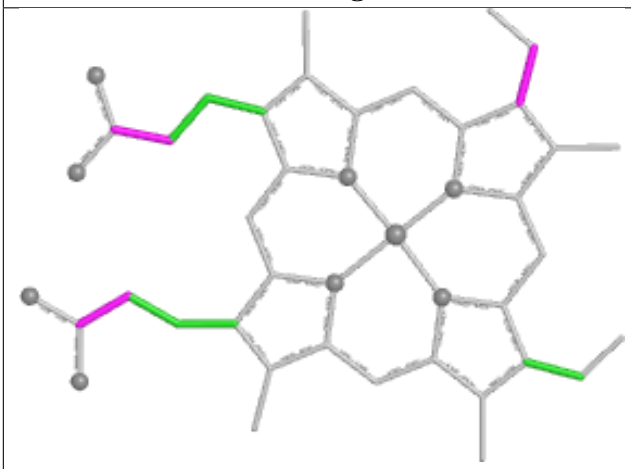
Ligand HEM C 159



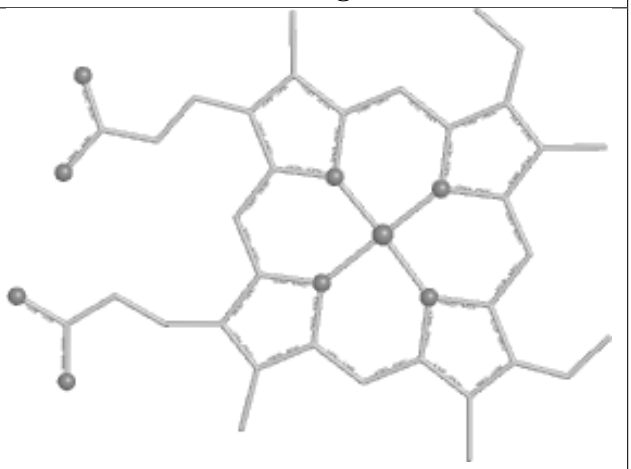
Bond lengths



Bond angles

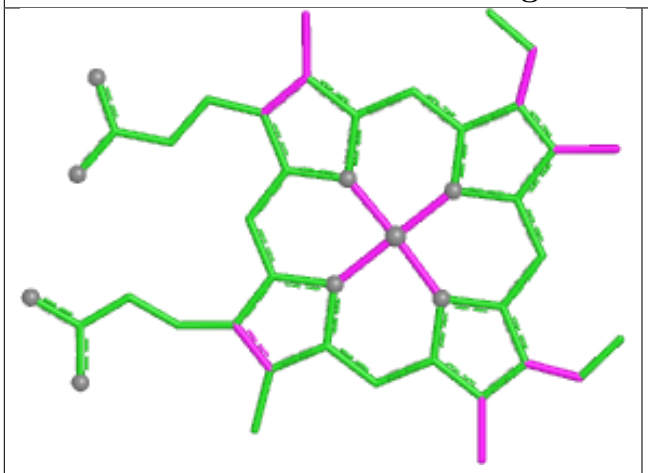


Torsions

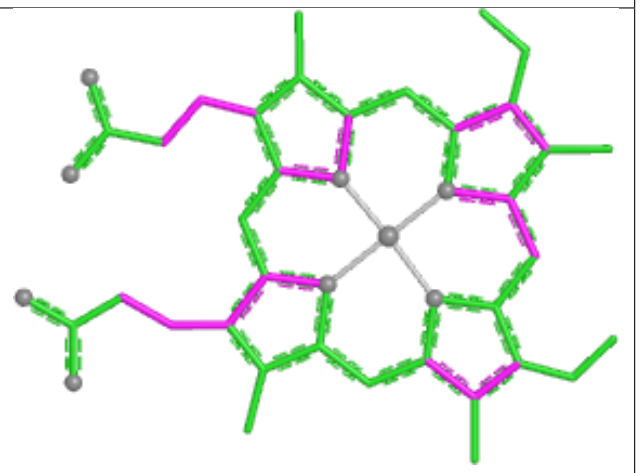


Rings

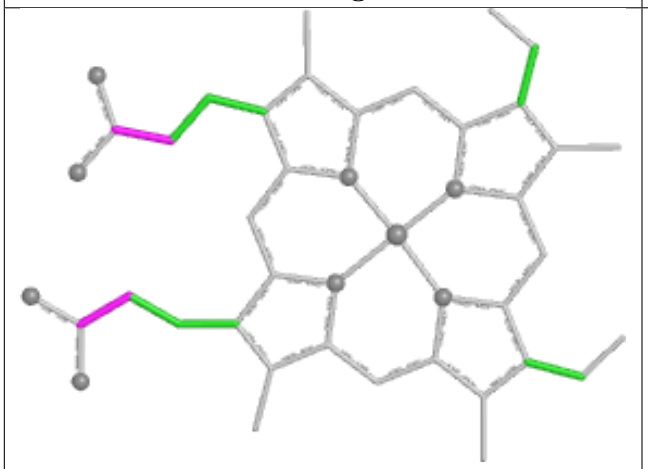
Ligand HEM E 159



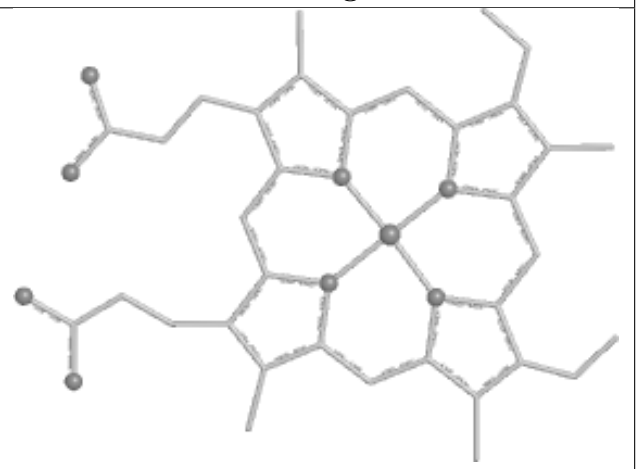
Bond lengths



Bond angles

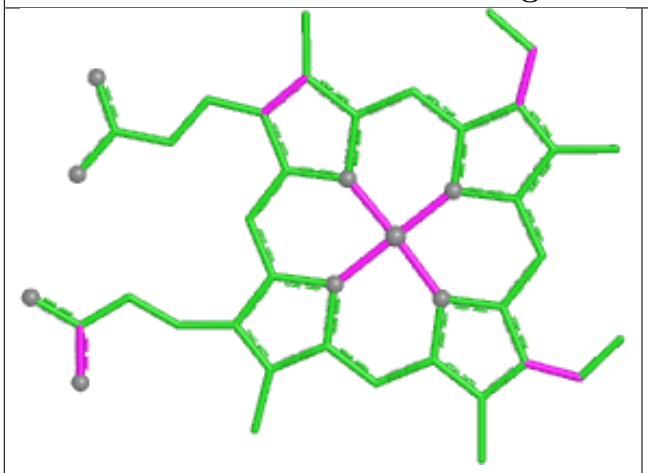


Torsions

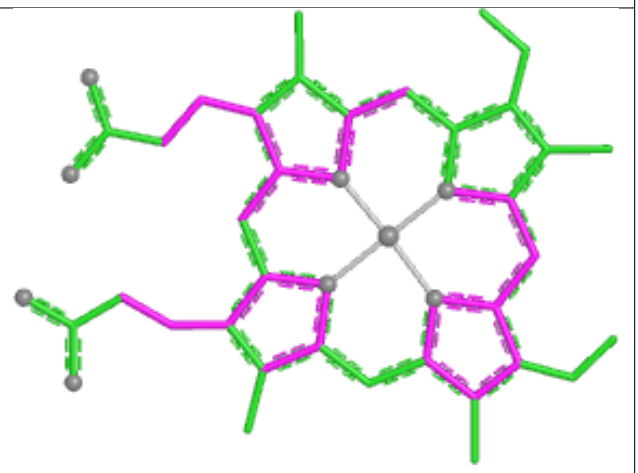


Rings

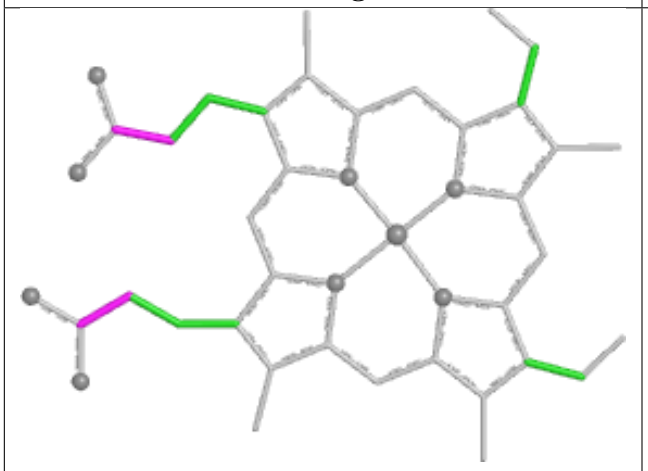
Ligand HEM F 159



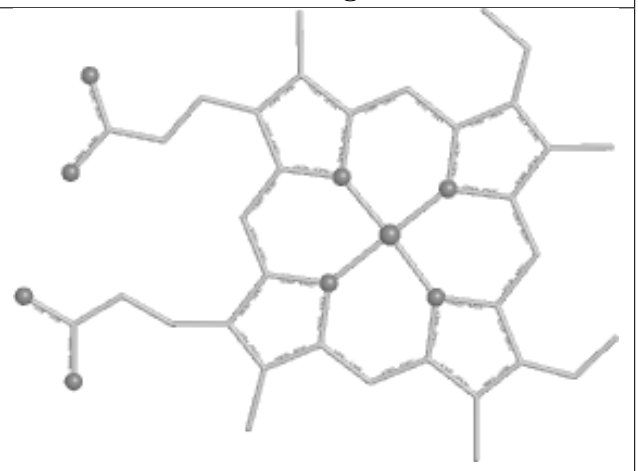
Bond lengths



Bond angles

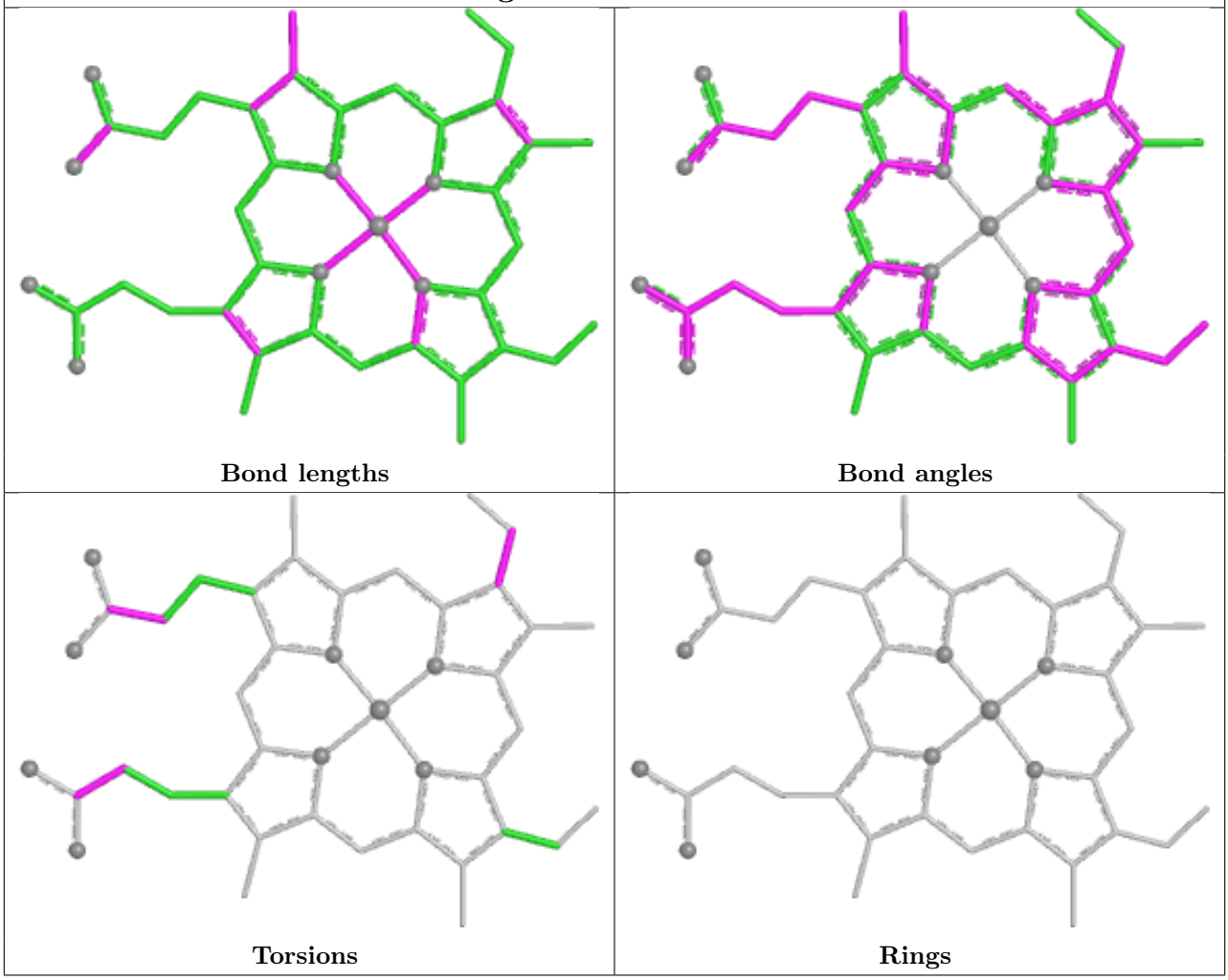


Torsions



Rings

Ligand HEM B 159



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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%)	0.44	3 (1%)	66	68	24, 39, 47, 52	1 (0%)
1	B	155/158 (98%)	0.30	2 (1%)	75	77	23, 37, 47, 54	1 (0%)
1	C	156/158 (98%)	0.45	1 (0%)	85	88	25, 38, 50, 57	1 (0%)
1	D	157/158 (99%)	0.43	3 (1%)	66	68	32, 38, 47, 63	0
1	E	155/158 (98%)	0.17	0	100	100	23, 36, 45, 55	1 (0%)
1	F	155/158 (98%)	0.41	3 (1%)	66	68	25, 39, 50, 57	1 (0%)
All	All	933/948 (98%)	0.37	12 (1%)	75	77	23, 38, 47, 63	5 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	3.5
1	D	73	ASP	2.7
1	F	103	GLU	2.3
1	D	157	ASP	2.3
1	B	156	GLU	2.3
1	C	2	LYS	2.3
1	B	3	GLY	2.2
1	A	2	LYS	2.2
1	A	110	GLN	2.1
1	F	156	GLU	2.0
1	F	6	LYS	2.0
1	A	156	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

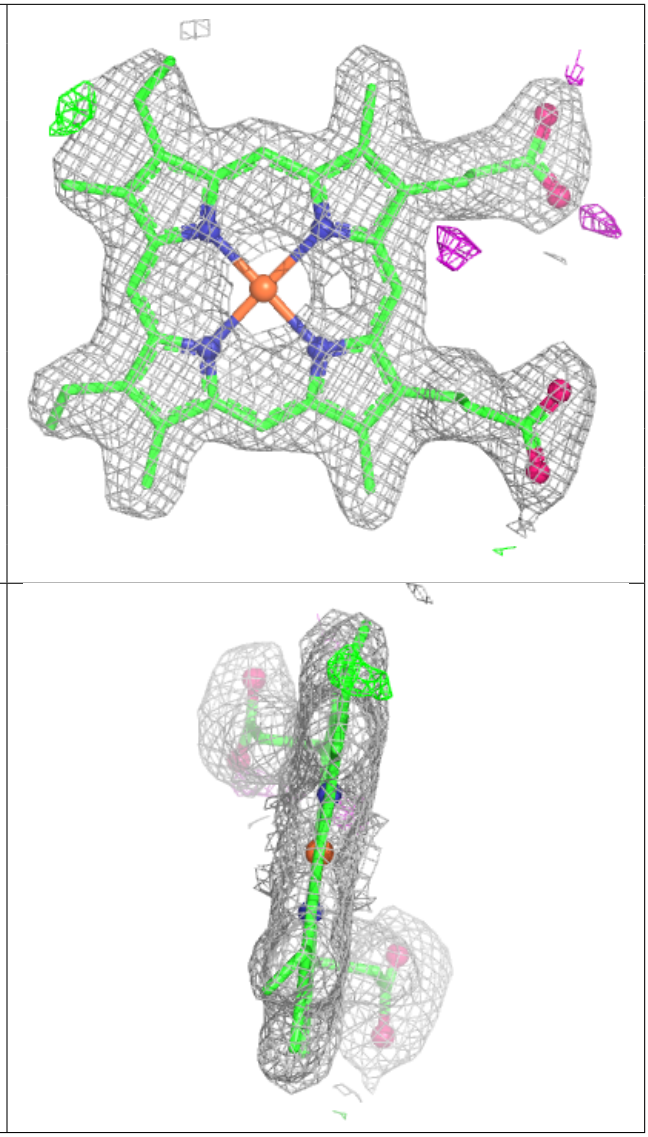
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEM	C	159	43/43	0.95	0.11	36,41,49,52	0
3	HEM	B	159	43/43	0.96	0.09	33,38,43,50	0
3	HEM	F	159	43/43	0.97	0.08	35,39,41,43	43
3	HEM	E	159	43/43	0.98	0.08	32,36,40,42	43
2	K	A	159	1/1	0.99	0.04	33,33,33,33	1
2	K	B	160	1/1	0.99	0.18	19,19,19,19	1

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

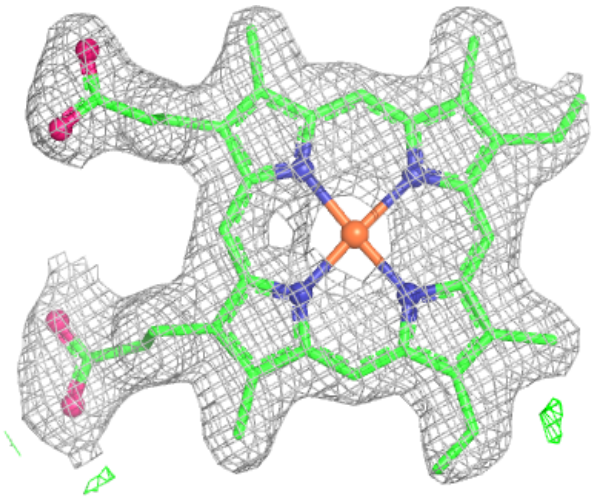
Electron density around HEM C 159:

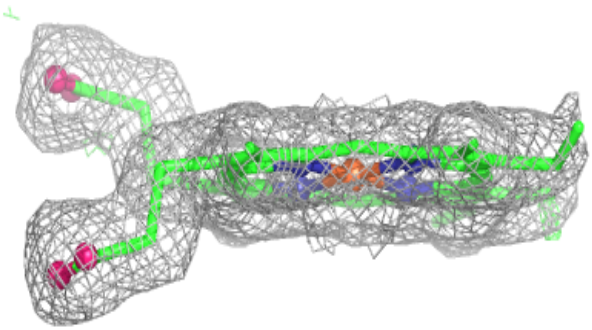
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

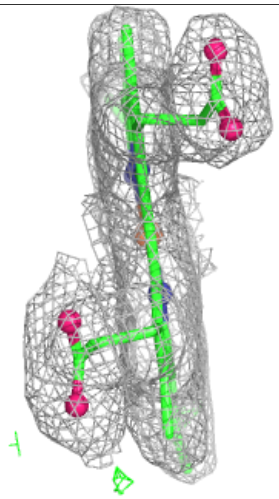


Electron density around HEM B 159:

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

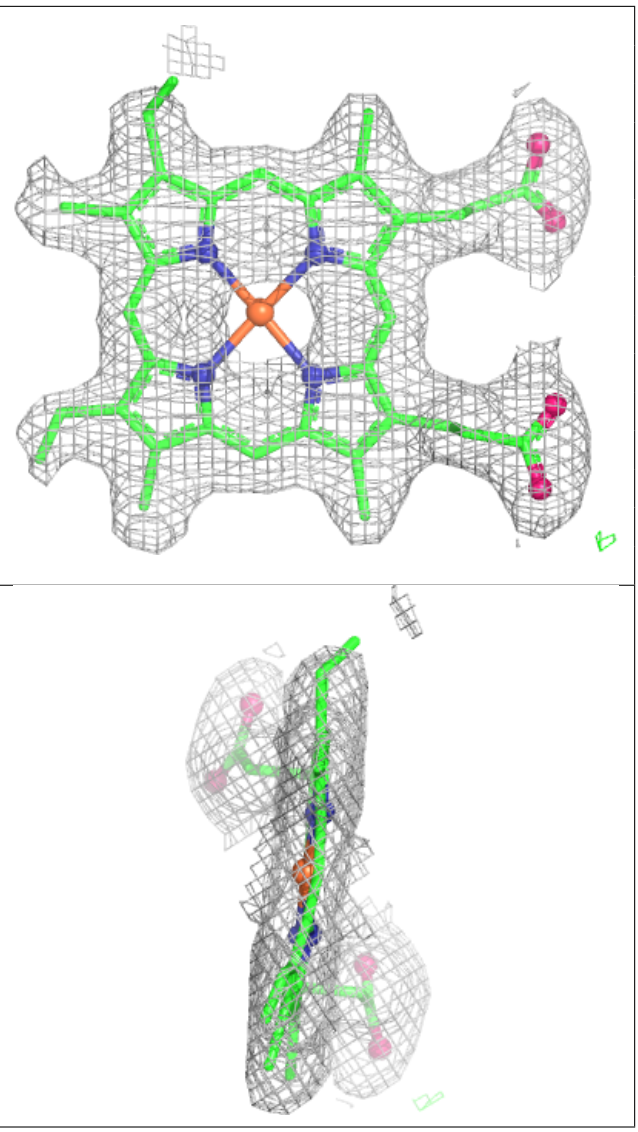






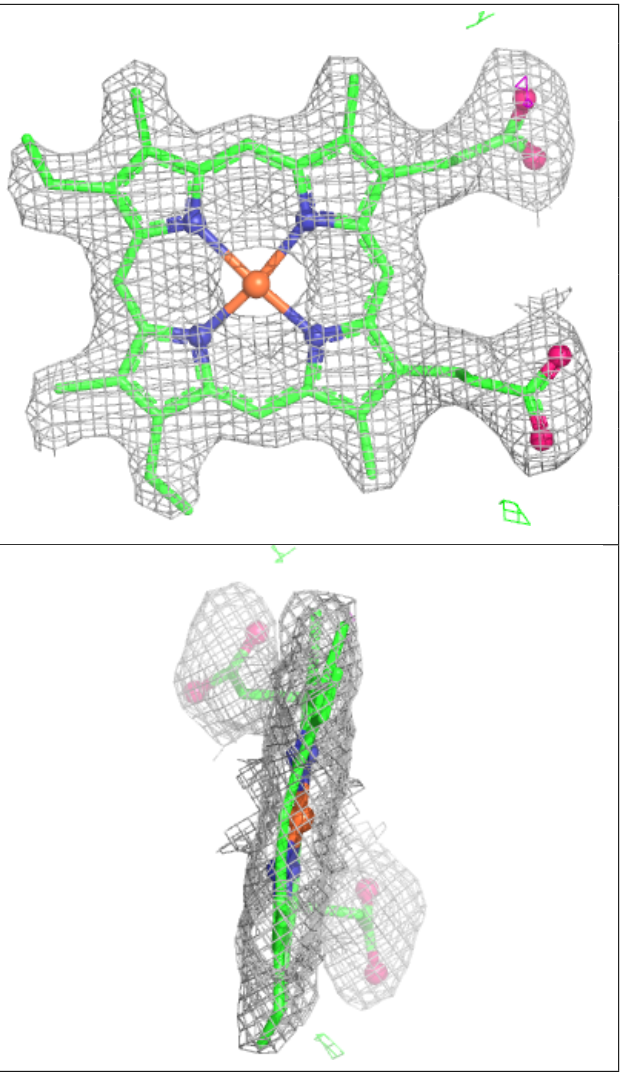
Electron density around HEM F 159:

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



Electron density around HEM E 159:

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



6.5 Other polymers (i)

There are no such residues in this entry.