Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 02:54 AM EDT

PDB ID	:	5SYL
Title	:	B. pseudomallei KatG with KCN bound
Authors	:	Loewen, P.C.
Deposited on	:	2016-08-11
Resolution	:	1.95 Å(reported)

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

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

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

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

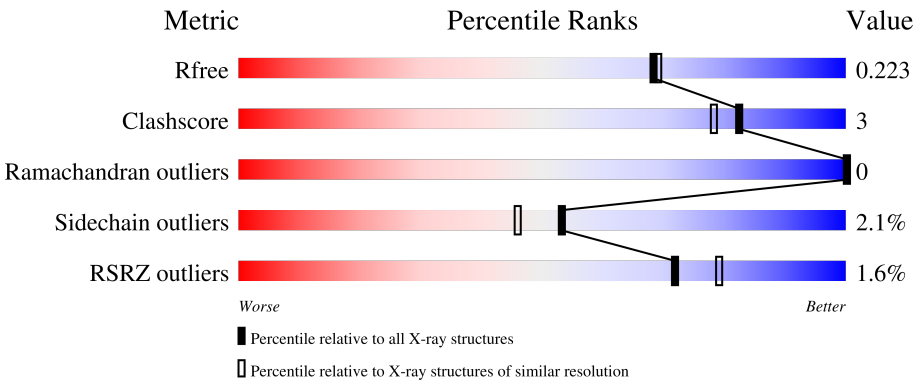
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	728	2% 89% 9% • •
1	B	728	% 89% 9% • •

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12683 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 Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	713	5523	3489	984	1036	14	0	3	0
1	B	713	5554	3511	990	1039	14	0	9	0

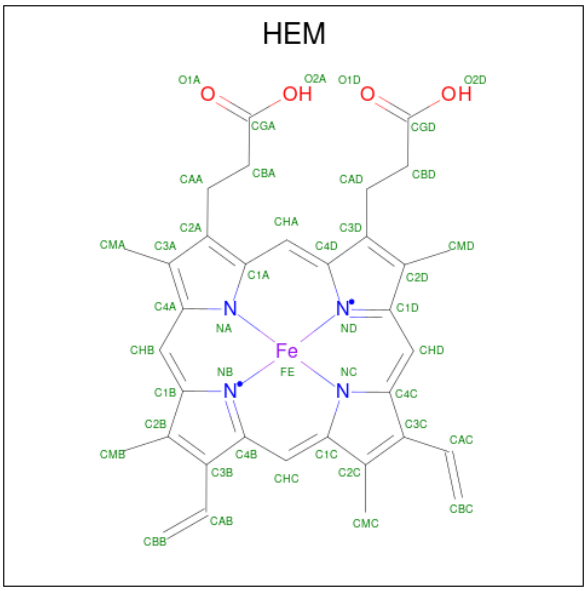
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

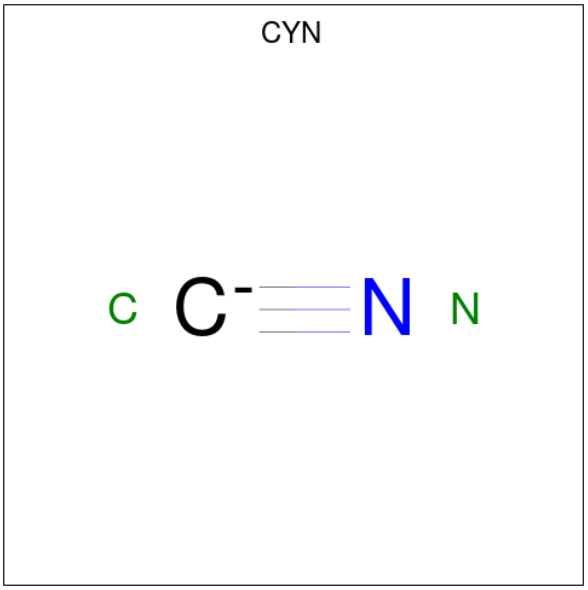
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

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



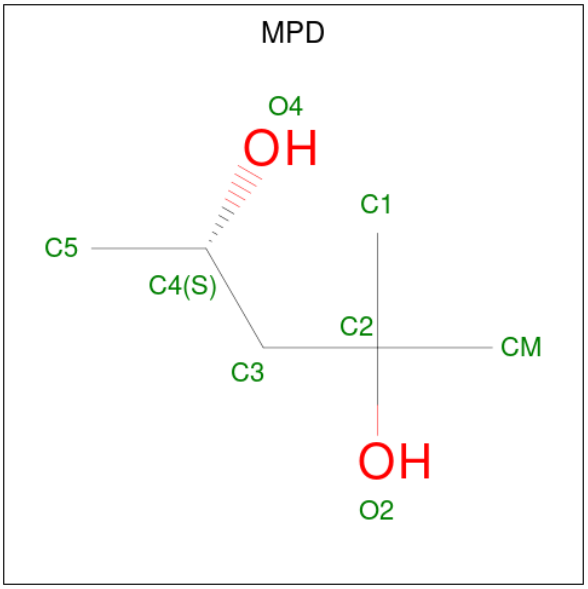
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
4	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	B	1	43	34	1	4	4	0	0

- Molecule 5 is CYANIDE ION (three-letter code: CYN) (formula: CN).



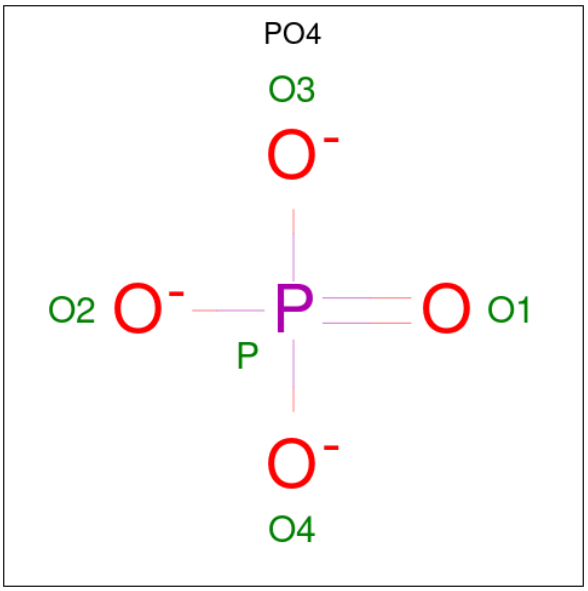
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
5	A	1	2	1	1	0	0
			Total	C	N		
5	B	1	2	1	1	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	A	1	8	6	2		0	0
			Total	C	O			
6	A	1	8	6	2		0	0
			Total	C	O			
6	B	1	8	6	2		0	0
			Total	C	O			
6	B	1	8	6	2		0	0
			Total	C	O			
6	B	1	8	6	2		0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O P 5 4 1	0	0

- Molecule 8 is water.

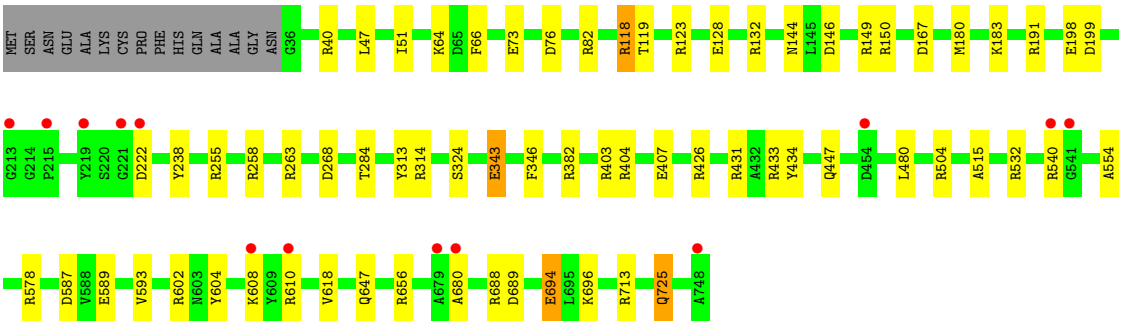
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	743	Total O 743 743	0	0
8	B	724	Total O 724 724	0	0

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.

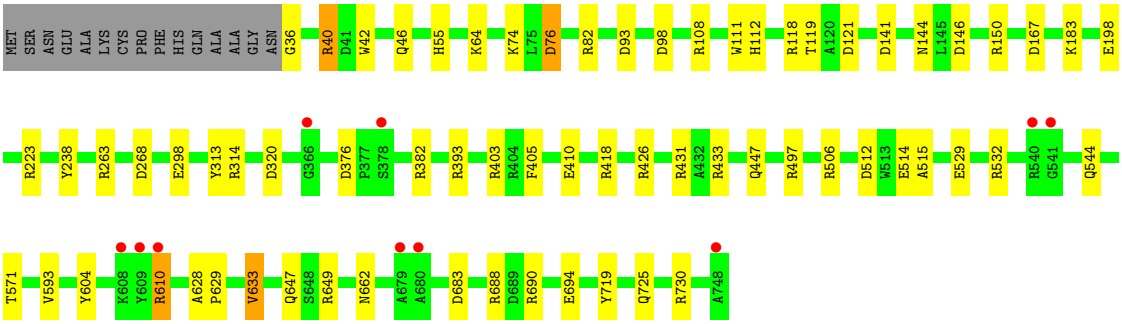
- Molecule 1: Catalase-peroxidase

Chain A:



- Molecule 1: Catalase-peroxidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.11Å 114.23Å 175.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 44.70 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-1.95) 98.9 (44.70-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.177 , 0.216 0.186 , 0.223	Depositor DCC
R_{free} test set	7279 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	16.2	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12683	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: MPD, PO4, NA, HEM, CYN, CL

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	1.15	10/5674 (0.2%)	1.08	34/7714 (0.4%)
1	B	1.13	7/5725 (0.1%)	1.08	33/7782 (0.4%)
All	All	1.14	17/11399 (0.1%)	1.08	67/15496 (0.4%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	GLU	CD-OE2	7.22	1.33	1.25
1	B	514	GLU	CD-OE2	-6.47	1.18	1.25
1	A	407	GLU	CD-OE1	6.17	1.32	1.25
1	A	725	GLN	CG-CD	6.12	1.65	1.51
1	A	238	TYR	CE1-CZ	6.06	1.46	1.38
1	A	532	ARG	NE-CZ	-5.95	1.25	1.33
1	B	529	GLU	CG-CD	5.77	1.60	1.51
1	A	407	GLU	CG-CD	5.52	1.60	1.51
1	B	410	GLU	CG-CD	5.47	1.60	1.51
1	B	36	GLY	N-CA	5.43	1.54	1.46
1	B	42	TRP	CE3-CZ3	5.31	1.47	1.38
1	A	694	GLU	CD-OE1	5.28	1.31	1.25
1	A	66	PHE	CG-CD1	-5.23	1.30	1.38
1	A	198	GLU	CD-OE2	5.17	1.31	1.25
1	B	298	GLU	CD-OE2	5.06	1.31	1.25
1	A	324	SER	CB-OG	5.04	1.48	1.42
1	A	128	GLU	CD-OE2	-5.04	1.20	1.25

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	532	ARG	NE-CZ-NH2	-10.11	115.24	120.30
1	A	76	ASP	CB-CG-OD2	-8.58	110.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	B	433	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	656	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	512[A]	ASP	CB-CG-OD2	7.67	125.20	118.30
1	B	512[B]	ASP	CB-CG-OD2	7.67	125.20	118.30
1	A	123	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	B	76	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	A	132	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	A	150	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	433	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	132	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	578	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	258	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	167	ASP	CB-CG-OD1	6.64	124.28	118.30
1	B	82	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	149	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	382	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	82	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	404	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	82	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	602	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	376	ASP	CB-CG-OD1	6.08	123.77	118.30
1	B	382	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	404	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	222	ASP	CB-CG-OD1	5.94	123.65	118.30
1	B	532	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	118	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	587	ASP	CB-CG-OD1	5.86	123.58	118.30
1	B	150	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	688	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	263	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	504	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	167	ASP	CB-CG-OD1	5.76	123.49	118.30
1	B	108	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	713	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	191	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	B	98	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	376	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	199	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	B	76	ASP	CB-CG-OD1	5.56	123.30	118.30
1	B	426	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	320	ASP	CB-CG-OD1	-5.50	113.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	180	MET	CG-SD-CE	5.42	108.88	100.20
1	B	393	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	343	GLU	CA-CB-CG	5.41	125.30	113.40
1	B	610	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	683	ASP	CB-CG-OD2	-5.37	113.46	118.30
1	B	497	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	426	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	504	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	382	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	268	ASP	CB-CG-OD1	5.33	123.09	118.30
1	B	223	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	B	418	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	689	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	121	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	222	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	B	688	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	B	263	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	529	GLU	OE1-CD-OE2	-5.17	117.10	123.30
1	A	434	TYR	CB-CG-CD1	5.11	124.06	121.00
1	B	403	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	405	PHE	CB-CG-CD1	5.04	124.33	120.80
1	B	93	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5523	0	5345	19	0
1	B	5554	0	5396	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	43	0	30	1	0
4	B	43	0	30	0	0
5	A	2	0	0	0	0
5	B	2	0	0	1	0
6	A	16	0	28	3	0
6	B	24	0	42	8	0
7	B	5	0	0	0	0
8	A	743	0	0	10	0
8	B	724	0	0	10	0
All	All	12683	0	10871	56	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 3.

All (56) 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)
6:B:807:MPD:H53	6:B:807:MPD:H12	1.50	0.91
1:A:119[B]:THR:HG21	8:A:1181:HOH:O	1.75	0.86
1:B:506:ARG:HE	6:B:805:MPD:H12	1.37	0.85
1:B:119[B]:THR:HG22	1:B:593:VAL:HG11	1.59	0.83
6:A:806:MPD:O4	6:A:806:MPD:O2	1.98	0.80
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.64	0.79
1:B:55:HIS:HD2	8:B:1189:HOH:O	1.67	0.78
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	1.87	0.75
6:B:805:MPD:H52	6:B:805:MPD:H11	1.68	0.75
1:B:730[A]:ARG:HD2	8:B:1479:HOH:O	1.87	0.73
1:B:544:GLN:OE1	8:B:901:HOH:O	2.10	0.70
6:B:806:MPD:H11	6:B:806:MPD:C5	2.25	0.67
6:A:805:MPD:H53	6:A:805:MPD:H11	1.78	0.65
1:A:343:GLU:HG3	8:A:1497:HOH:O	1.98	0.63
1:A:343:GLU:CG	8:A:1497:HOH:O	2.49	0.60
1:B:662:ASN:H	1:B:725:GLN:HE22	1.52	0.58
1:A:593:VAL:HG13	8:A:1008:HOH:O	2.02	0.57
6:B:806:MPD:H11	6:B:806:MPD:H52	1.86	0.57
1:B:119[B]:THR:CG2	1:B:593:VAL:HG11	2.34	0.55
1:A:255[A]:ARG:HG2	8:A:972:HOH:O	2.08	0.54
6:B:807:MPD:H53	6:B:807:MPD:C1	2.31	0.53
6:B:806:MPD:HM2	6:B:806:MPD:H53	1.91	0.53
1:B:76:ASP:OD2	8:B:902:HOH:O	2.19	0.53
6:A:806:MPD:HO2	6:A:806:MPD:HO4	1.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.93	0.51
1:A:47:LEU:O	8:A:901:HOH:O	2.19	0.51
1:B:649[A]:ARG:HD3	8:B:1105:HOH:O	2.10	0.50
1:A:647:GLN:HG2	8:A:909:HOH:O	2.12	0.50
1:B:112:HIS:NE2	5:B:804:CYN:N	2.51	0.50
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.11	0.50
1:B:119[B]:THR:HG23	8:B:1104:HOH:O	2.13	0.48
1:B:431:ARG:HD3	8:B:1340:HOH:O	2.14	0.47
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.18	0.44
1:A:515:ALA:HB2	1:A:604:TYR:CE2	2.52	0.44
1:B:629:PRO:O	1:B:633[B]:VAL:HG12	2.18	0.44
1:B:119[B]:THR:CG2	1:B:593:VAL:HG21	2.48	0.44
1:B:515:ALA:HB2	1:B:604:TYR:CE2	2.53	0.44
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.18	0.44
1:A:313:TYR:CE2	1:A:314:ARG:HD3	2.52	0.43
1:B:111:TRP:HZ3	1:B:238:TYR:HH	1.63	0.43
1:A:343:GLU:HG2	8:A:1497:HOH:O	2.18	0.43
1:B:119[B]:THR:HG21	8:B:1555:HOH:O	2.18	0.43
1:B:690:ARG:HD2	8:B:1478:HOH:O	2.19	0.43
1:A:680:ALA:HB3	8:A:1209:HOH:O	2.19	0.43
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.54	0.42
1:A:696:LYS:NZ	8:A:904:HOH:O	2.36	0.42
6:B:805:MPD:H13	8:B:1533:HOH:O	2.19	0.42
1:A:284:THR:HG22	4:A:803:HEM:HAA1	2.01	0.42
1:B:628:ALA:HB3	1:B:629:PRO:HD3	2.02	0.41
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE2	2.54	0.41
1:B:40[A]:ARG:HH11	1:B:40[A]:ARG:HA	1.85	0.41
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.20	0.41
1:A:346:PHE:CE1	1:A:403:ARG:NH2	2.89	0.41
1:B:313:TYR:CE2	1:B:314:ARG:HD3	2.55	0.41
1:A:51:ILE:HD11	1:A:618:VAL:HG12	2.03	0.41
1:A:480:LEU:HD22	1:A:554:ALA:HB1	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	714/728 (98%)	706 (99%)	8 (1%)	0	100	100
1	B	720/728 (99%)	712 (99%)	8 (1%)	0	100	100
All	All	1434/1456 (98%)	1418 (99%)	16 (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	553/561 (99%)	542 (98%)	11 (2%)	55	48
1	B	559/561 (100%)	545 (98%)	14 (2%)	47	38
All	All	1112/1122 (99%)	1087 (98%)	25 (2%)	53	44

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	64	LYS
1	A	73	GLU
1	A	118	ARG
1	A	183	LYS
1	A	540	ARG
1	A	589	GLU
1	A	608	LYS
1	A	610	ARG
1	A	694	GLU
1	A	725	GLN
1	B	40[A]	ARG
1	B	40[B]	ARG
1	B	46	GLN

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Mol	Chain	Res	Type
1	B	64	LYS
1	B	74	LYS
1	B	118	ARG
1	B	141	ASP
1	B	183	LYS
1	B	571	THR
1	B	610	ARG
1	B	633[A]	VAL
1	B	633[B]	VAL
1	B	647	GLN
1	B	694	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	HIS
1	A	737	ASN
1	B	55	HIS
1	B	650	HIS
1	B	711	GLN
1	B	725	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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
6	MPD	A	805	-	7,7,7	0.57	0	9,10,10	1.28	0
6	MPD	B	805	-	7,7,7	1.41	1 (14%)	9,10,10	1.61	2 (22%)
7	PO4	B	808	-	4,4,4	1.00	0	6,6,6	0.92	0
5	CYN	B	804	-	0,1,1	-	-	-		
4	HEM	B	801	1	41,50,50	1.53	6 (14%)	45,82,82	2.10	18 (40%)
6	MPD	B	806	-	7,7,7	0.53	0	9,10,10	1.49	2 (22%)
5	CYN	A	804	-	0,1,1	-	-	-		
6	MPD	A	806	-	7,7,7	0.64	0	9,10,10	1.09	0
4	HEM	A	803	1	41,50,50	1.36	6 (14%)	45,82,82	2.10	18 (40%)
6	MPD	B	807	-	7,7,7	0.78	0	9,10,10	1.43	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
6	MPD	A	805	-	-	1/5/5/5	-
6	MPD	B	805	-	-	4/5/5/5	-
4	HEM	B	801	1	-	3/12/54/54	-
6	MPD	B	806	-	-	1/5/5/5	-
6	MPD	A	806	-	-	3/5/5/5	-
4	HEM	A	803	1	-	2/12/54/54	-
6	MPD	B	807	-	-	3/5/5/5	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	HEM	C1B-NB	-5.50	1.30	1.40
4	A	803	HEM	C4B-NB	-3.83	1.30	1.38
6	B	805	MPD	C3-C2	3.30	1.62	1.53
4	A	803	HEM	C1B-NB	-3.17	1.34	1.40
4	B	801	HEM	C1D-ND	-3.13	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	HEM	C4D-ND	-3.05	1.35	1.40
4	B	801	HEM	O1D-CGD	2.93	1.31	1.22
4	B	801	HEM	CAA-C2A	-2.88	1.47	1.52
4	A	803	HEM	C1D-ND	-2.79	1.33	1.38
4	B	801	HEM	CHB-C1B	2.54	1.41	1.35
4	A	803	HEM	FE-NB	2.30	2.08	1.96
4	B	801	HEM	FE-NB	2.17	2.07	1.96
4	A	803	HEM	O1A-CGA	2.03	1.28	1.22

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	HEM	CHC-C4B-NB	5.51	130.42	124.43
4	A	803	HEM	C1B-NB-C4B	5.09	110.33	105.07
4	B	801	HEM	C2C-C3C-C4C	-4.43	103.81	106.90
4	A	803	HEM	C2C-C3C-C4C	4.16	109.80	106.90
4	B	801	HEM	CHC-C4B-NB	4.11	128.90	124.43
4	B	801	HEM	C4B-C3B-C2B	-3.80	104.10	107.11
4	B	801	HEM	CHA-C4D-ND	3.71	128.97	124.38
4	B	801	HEM	C1B-NB-C4B	3.35	108.54	105.07
4	A	803	HEM	CMA-C3A-C4A	-3.24	123.48	128.46
4	A	803	HEM	O2A-CGA-CBA	3.24	124.43	114.03
4	B	801	HEM	CMA-C3A-C4A	-3.15	123.62	128.46
4	B	801	HEM	C3B-C2B-C1B	3.08	108.77	106.49
4	B	801	HEM	CMD-C2D-C1D	3.04	129.66	125.04
4	B	801	HEM	CHA-C4D-C3D	-2.94	119.80	125.33
4	B	801	HEM	CMA-C3A-C2A	2.82	130.26	124.94
4	B	801	HEM	CBD-CAD-C3D	2.75	120.27	112.63
6	B	806	MPD	C5-C4-C3	2.75	124.64	111.69
4	A	803	HEM	C4C-CHD-C1D	2.66	126.06	122.56
6	B	805	MPD	O2-C2-CM	-2.62	99.66	108.08
4	A	803	HEM	O2D-CGD-CBD	2.62	122.44	114.03
6	B	805	MPD	O4-C4-C3	2.52	121.54	111.36
4	B	801	HEM	O2D-CGD-CBD	2.50	122.06	114.03
4	B	801	HEM	CMB-C2B-C1B	2.45	128.77	125.04
4	A	803	HEM	CHC-C4B-C3B	-2.45	120.83	124.57
4	A	803	HEM	O2A-CGA-O1A	-2.44	117.22	123.30
4	A	803	HEM	C4B-CHC-C1C	2.43	125.77	122.56
4	B	801	HEM	CMB-C2B-C3B	-2.42	122.38	128.30
4	A	803	HEM	CMD-C2D-C1D	2.41	128.71	125.04
6	B	806	MPD	O4-C4-C5	-2.40	99.00	109.38
4	B	801	HEM	C2D-C1D-ND	2.36	112.71	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	HEM	CAA-CBA-CGA	-2.31	107.30	113.76
4	A	803	HEM	CMC-C2C-C3C	2.26	128.91	124.68
4	A	803	HEM	CHB-C1B-NB	2.23	127.13	124.38
4	A	803	HEM	C3C-C4C-NC	-2.22	106.74	110.94
4	B	801	HEM	CMC-C2C-C3C	2.17	128.74	124.68
4	A	803	HEM	CMA-C3A-C2A	2.14	128.98	124.94
4	A	803	HEM	O1D-CGD-CBD	-2.13	116.24	123.08
4	A	803	HEM	CBB-CAB-C3B	-2.12	117.10	127.62
4	B	801	HEM	O1D-CGD-CBD	-2.08	116.39	123.08
4	B	801	HEM	CAB-C3B-C2B	2.07	135.41	128.60

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	805	MPD	C1-C2-C3-C4
6	B	805	MPD	O2-C2-C3-C4
6	B	806	MPD	C2-C3-C4-C5
6	B	807	MPD	C1-C2-C3-C4
6	B	807	MPD	O2-C2-C3-C4
6	A	805	MPD	C2-C3-C4-C5
6	A	806	MPD	C2-C3-C4-C5
6	A	806	MPD	C2-C3-C4-O4
6	B	805	MPD	CM-C2-C3-C4
4	B	801	HEM	CAA-CBA-CGA-O2A
6	A	806	MPD	O2-C2-C3-C4
4	A	803	HEM	CAA-CBA-CGA-O1A
4	A	803	HEM	CAA-CBA-CGA-O2A
4	B	801	HEM	CAA-CBA-CGA-O1A
6	B	805	MPD	C2-C3-C4-C5
6	B	807	MPD	C2-C3-C4-C5
4	B	801	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	805	MPD	1	0
6	B	805	MPD	3	0
5	B	804	CYN	1	0
6	B	806	MPD	3	0

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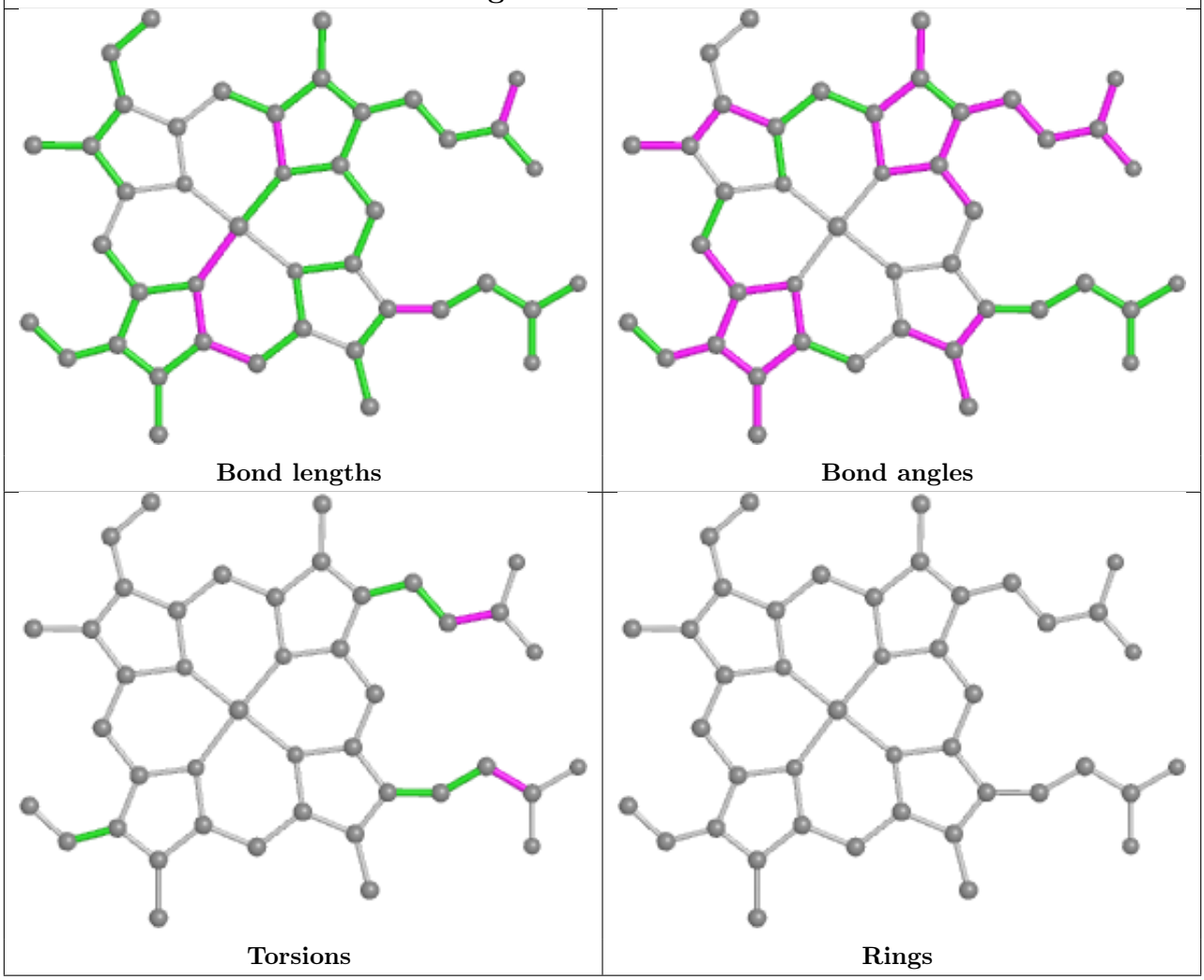
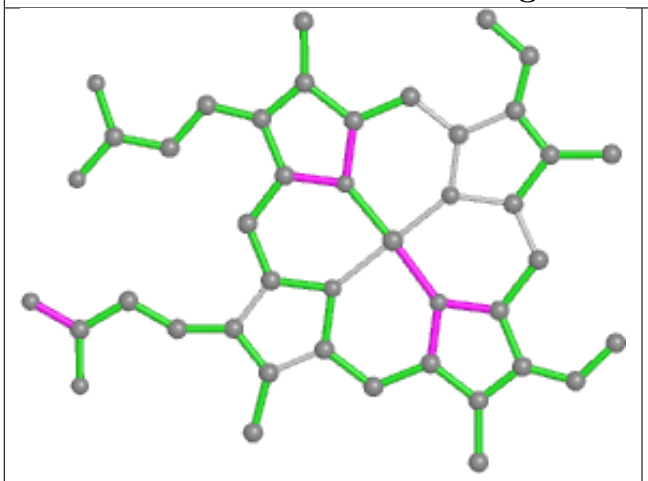
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	806	MPD	2	0
4	A	803	HEM	1	0
6	B	807	MPD	2	0

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

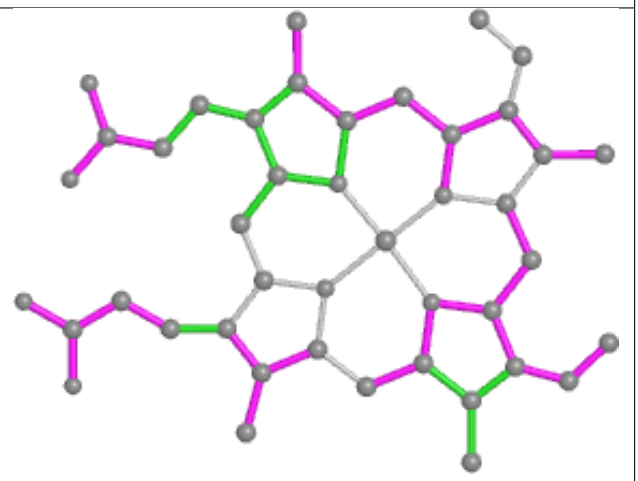
Ligand HEM B 801



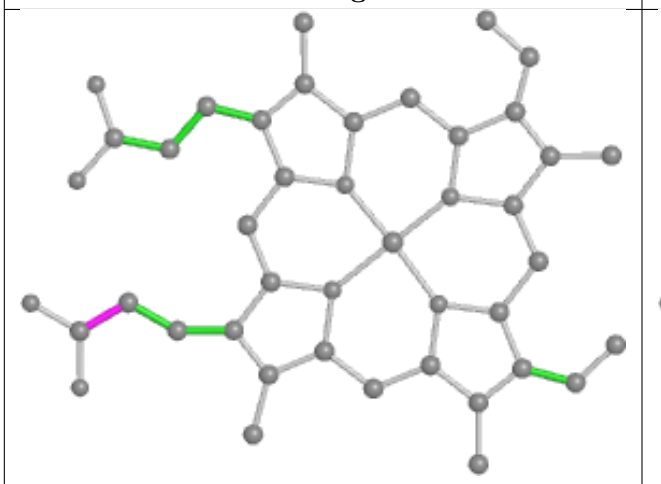
Ligand HEM A 803



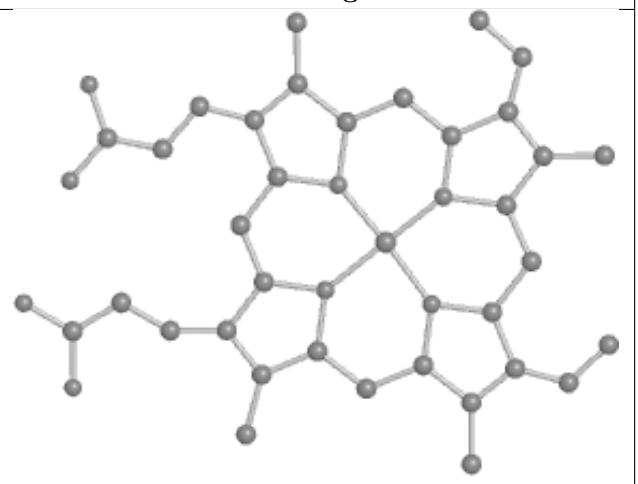
Bond lengths



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	713/728 (97%)	-0.32	13 (1%)	68	76	9, 17, 36, 76	0
1	B	713/728 (97%)	-0.34	10 (1%)	75	82	10, 16, 32, 74	0
All	All	1426/1456 (97%)	-0.33	23 (1%)	72	79	9, 17, 35, 76	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	5.4
1	A	748	ALA	4.5
1	A	541	GLY	4.2
1	A	540	ARG	4.0
1	A	610	ARG	3.6
1	B	679	ALA	3.6
1	B	540	ARG	3.5
1	A	608	LYS	3.5
1	B	610	ARG	3.1
1	B	541	GLY	3.0
1	B	680	ALA	2.8
1	A	215	PRO	2.8
1	A	680	ALA	2.7
1	B	609	TYR	2.5
1	B	378	SER	2.5
1	B	608	LYS	2.4
1	A	219	TYR	2.3
1	A	454	ASP	2.3
1	A	221	GLY	2.1
1	A	222	ASP	2.1
1	A	679	ALA	2.1
1	A	213	GLY	2.1
1	B	366	GLY	2.1

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)

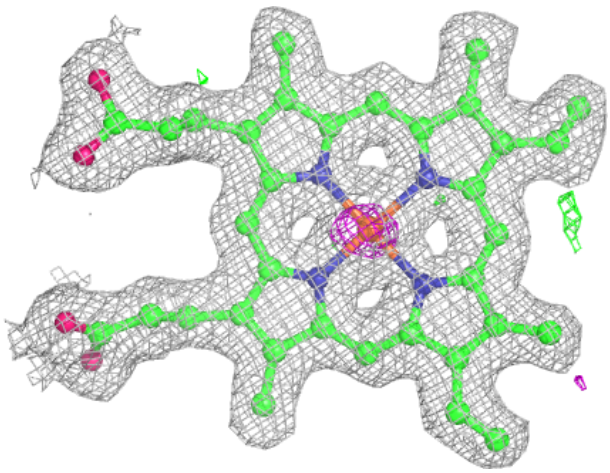
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

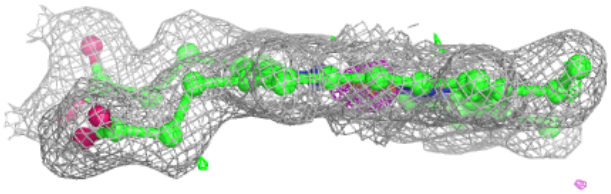
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MPD	B	805	8/8	0.83	0.24	40,47,49,51	0
6	MPD	A	806	8/8	0.89	0.16	42,45,47,49	0
6	MPD	A	805	8/8	0.89	0.17	36,40,43,46	0
6	MPD	B	807	8/8	0.89	0.18	36,43,45,46	0
6	MPD	B	806	8/8	0.91	0.18	27,34,40,41	0
7	PO4	B	808	5/5	0.93	0.21	40,51,56,57	0
3	CL	B	803	1/1	0.98	0.05	31,31,31,31	0
4	HEM	A	803	43/43	0.98	0.09	11,13,14,16	0
4	HEM	B	801	43/43	0.98	0.13	10,12,13,15	0
2	NA	B	802	1/1	0.99	0.03	13,13,13,13	0
3	CL	A	802	1/1	0.99	0.04	29,29,29,29	0
5	CYN	A	804	2/2	0.99	0.07	15,15,15,15	0
5	CYN	B	804	2/2	0.99	0.11	16,16,16,17	0
2	NA	A	801	1/1	0.99	0.03	12,12,12,12	0

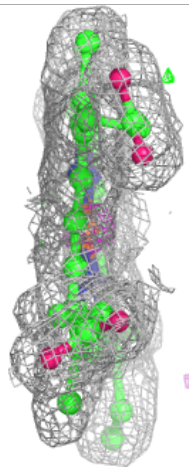
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM A 803:

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

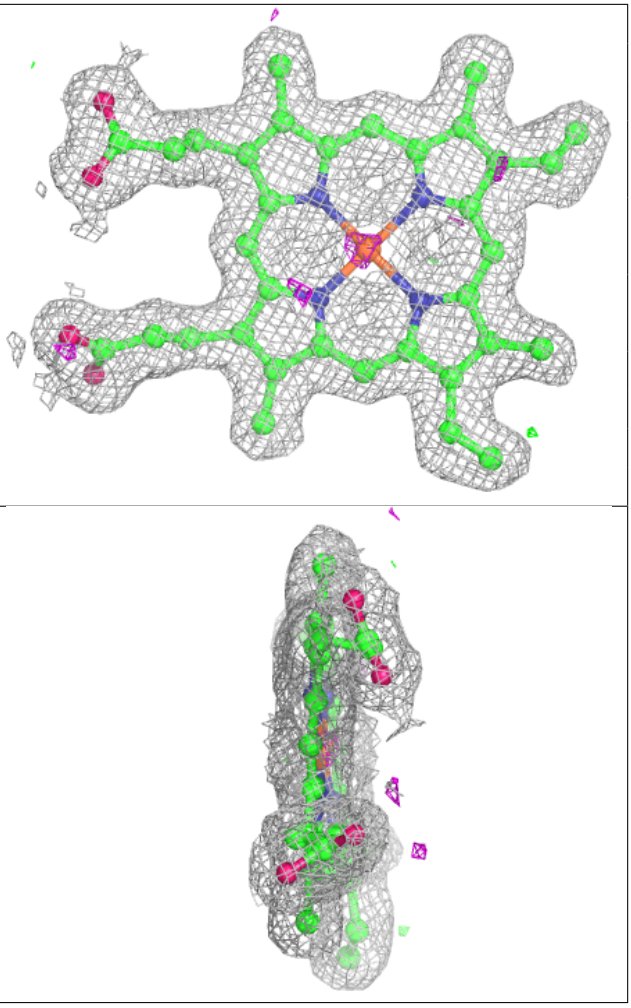






Electron density around HEM B 801:

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.