Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 09:24 PM EDT

PDB ID	:	1ITK / pdb_00001itk
Title	:	Crystal structure of catalase-peroxidase from Haloarcula marismortui
Authors	:	Yamada, Y.; Fujiwara, T.; Sato, T.; Igarashi, N.; Tanaka, N.
Deposited on	:	2002-01-18
Resolution	:	2.00 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:

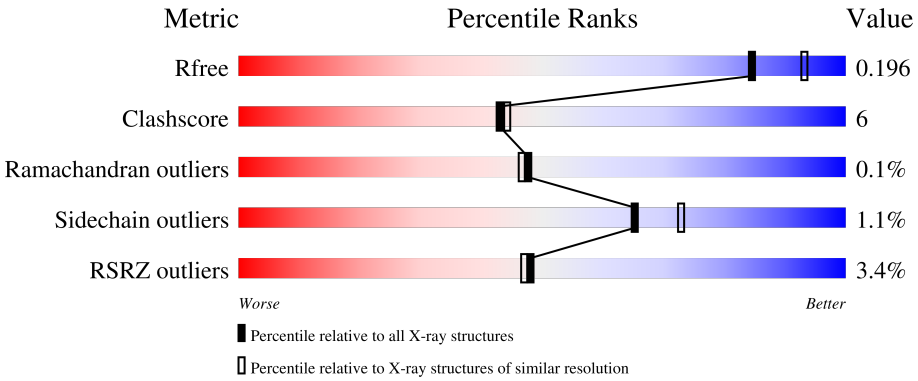
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	731	4% 82% 14%
1	B	731	3% 83% 14%

2 Entry composition (i)

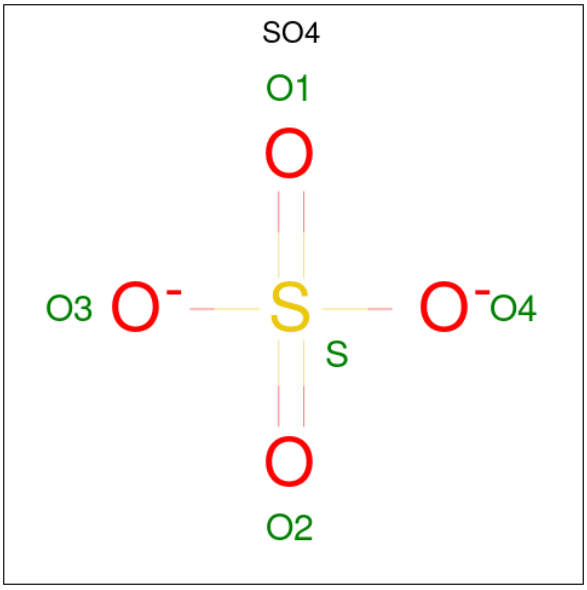
There are 6 unique types of molecules in this entry. The entry contains 12691 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	707	Total	C	N	O	S	0	0	0
			5567	3482	932	1134	19			
1	B	714	Total	C	N	O	S	0	0	0
			5611	3506	941	1145	19			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

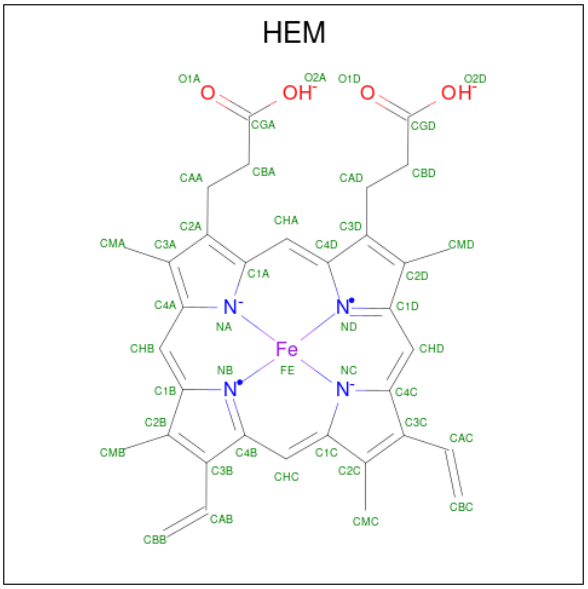
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	12	Total Cl 12 12	0	0
3	B	4	Total Cl 4 4	0	0

- Molecule 4 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total X 1 1	0	0
4	B	5	Total X 5 5	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 6 is water.

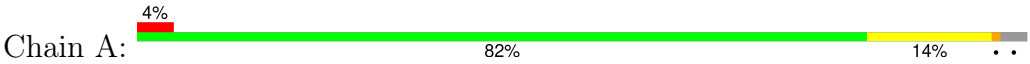
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	776	Total	O	0	0
			776	776		
6	B	599	Total	O	0	0
			599	599		

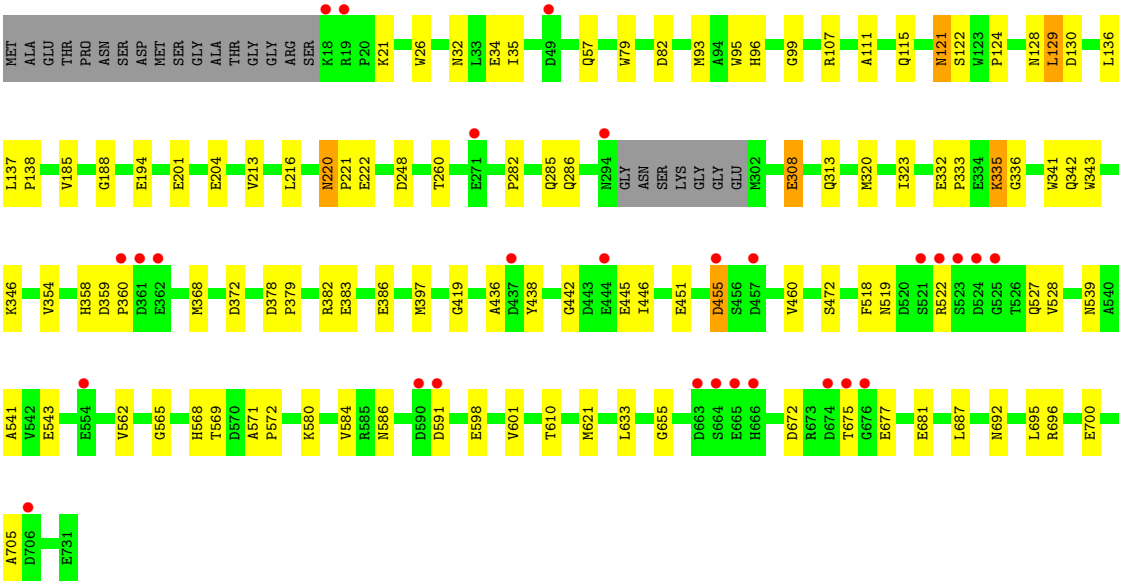
3 Residue-property plots (i)

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

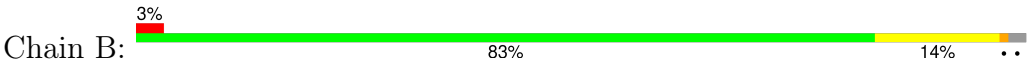
Chain A:

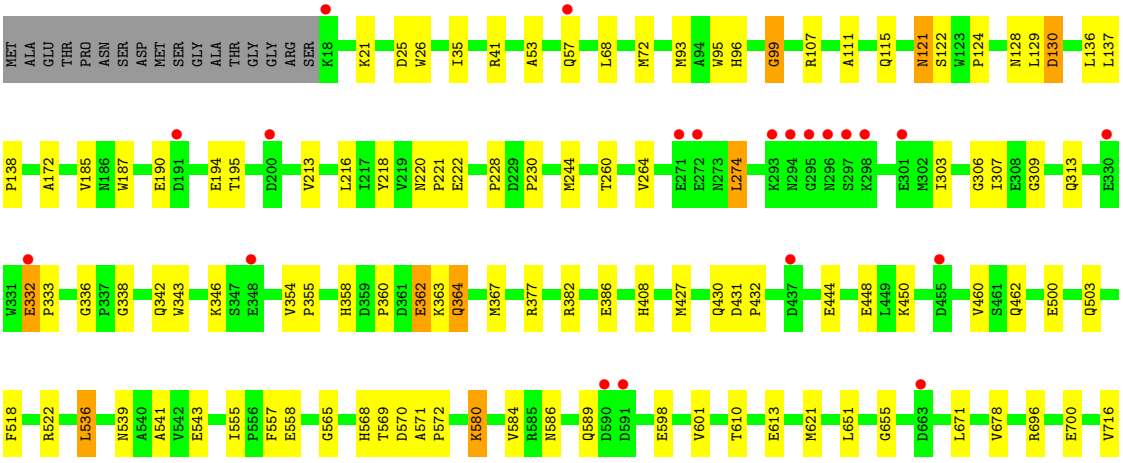




- Molecule 1: catalase-peroxidase

Chain B:






E731

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	317.63Å 82.14Å 75.10Å 90.00° 100.24° 90.00°	Depositor
Resolution (Å)	34.10 – 2.00 34.10 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.10-2.00) 99.8 (34.10-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.43 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.182 , 0.203 0.175 , 0.196	Depositor DCC
R_{free} test set	6458 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12691	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: UNX, HEM, CL, SO4

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	0.34	0/5702	0.90	23/7749 (0.3%)
1	B	0.32	0/5747	0.86	13/7809 (0.2%)
All	All	0.33	0/11449	0.88	36/15558 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	THR	N-CA-C	-7.76	103.27	112.89
1	A	99	GLY	N-CA-C	7.28	122.48	114.40
1	B	260	THR	N-CA-C	-6.91	104.32	112.89
1	A	111	ALA	N-CA-C	6.85	119.58	111.71
1	A	308	GLU	N-CA-C	6.45	119.66	108.76
1	A	378	ASP	N-CA-C	-6.44	101.53	109.65
1	A	580	LYS	N-CA-C	-6.41	105.61	113.50
1	A	129	LEU	N-CA-C	-6.39	105.44	113.18
1	B	129	LEU	N-CA-C	-6.38	105.47	113.18
1	A	419	GLY	CA-C-N	6.07	126.18	119.87
1	A	419	GLY	C-N-CA	6.07	126.18	119.87
1	B	569	THR	N-CA-C	6.03	118.22	108.34
1	A	655	GLY	N-CA-C	-5.98	108.09	114.67
1	B	99	GLY	N-CA-C	5.97	121.03	114.40
1	B	655	GLY	N-CA-C	-5.80	108.29	114.67
1	A	79	TRP	CA-C-N	5.77	126.10	119.93
1	A	79	TRP	C-N-CA	5.77	126.10	119.93
1	B	111	ALA	N-CA-C	5.76	119.12	111.75
1	B	580	LYS	N-CA-C	-5.75	106.42	113.50
1	A	472	SER	N-CA-C	5.65	119.65	112.87
1	B	115	GLN	N-CA-C	-5.63	105.67	112.54
1	A	569	THR	N-CA-C	5.61	117.53	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	GLN	N-CA-C	-5.58	105.73	112.54
1	A	188	GLY	CA-C-N	5.52	125.22	119.64
1	A	188	GLY	C-N-CA	5.52	125.22	119.64
1	B	130	ASP	N-CA-C	-5.45	105.50	111.82
1	A	248	ASP	N-CA-C	5.32	116.76	111.07
1	B	332	GLU	CA-C-N	5.29	125.23	119.78
1	B	332	GLU	C-N-CA	5.29	125.23	119.78
1	A	359	ASP	CA-C-N	5.22	125.52	119.47
1	A	359	ASP	C-N-CA	5.22	125.52	119.47
1	A	687	LEU	N-CA-C	5.14	118.82	112.54
1	A	610	THR	N-CA-C	-5.12	103.16	110.59
1	B	500	GLU	CA-C-N	5.10	126.21	119.84
1	B	500	GLU	C-N-CA	5.10	126.21	119.84
1	A	705	ALA	N-CA-C	5.07	117.20	111.11

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	5567	0	5203	64	0
1	B	5611	0	5243	72	0
2	A	20	0	0	0	0
2	B	10	0	0	0	0
3	A	12	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	0	0
4	B	5	0	0	0	0
5	A	43	0	30	0	0
5	B	43	0	30	0	0
6	A	776	0	0	4	0
6	B	599	0	0	2	0
All	All	12691	0	10506	135	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 6.

All (135) 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:A:565:GLY:H	1:A:568:HIS:HD2	1.16	0.89
1:B:313:GLN:HA	1:B:354:VAL:HG22	1.55	0.88
1:B:565:GLY:H	1:B:568:HIS:HD2	1.22	0.86
1:B:427:MET:H	1:B:430:GLN:HE21	1.23	0.84
1:A:692:ASN:HD22	1:A:695:LEU:H	1.26	0.79
1:B:35:ILE:HD11	1:B:601:VAL:HG12	1.66	0.77
1:A:121:ASN:HD22	1:A:122:SER:N	1.84	0.74
1:B:53:ALA:O	1:B:57:GLN:HG2	1.88	0.73
1:A:633:LEU:HD23	1:A:681:GLU:HG2	1.70	0.73
1:B:462:GLN:HE21	1:B:503:GLN:HE22	1.36	0.72
1:A:519:ASN:HD21	1:A:528:VAL:H	1.41	0.68
1:B:121:ASN:HD22	1:B:122:SER:N	1.90	0.68
1:B:427:MET:H	1:B:430:GLN:NE2	1.92	0.68
1:B:462:GLN:HE21	1:B:503:GLN:NE2	1.91	0.68
1:A:358:HIS:O	1:A:360:PRO:HD3	1.93	0.67
1:B:336:GLY:HA3	1:B:342:GLN:NE2	2.09	0.67
1:A:220:ASN:C	1:A:220:ASN:HD22	2.03	0.67
1:A:201:GLU:HB2	1:A:204:GLU:HG3	1.77	0.66
1:A:675:THR:HG23	1:A:677:GLU:H	1.60	0.65
1:B:172:ALA:H	1:B:408:HIS:HE1	1.44	0.64
1:A:35:ILE:HD11	1:A:601:VAL:HG12	1.80	0.64
1:A:220:ASN:ND2	1:A:222:GLU:H	1.96	0.64
1:B:571:ALA:HB3	1:B:572:PRO:HD3	1.80	0.63
1:B:213:VAL:HB	1:B:216:LEU:HD12	1.80	0.63
1:A:672:ASP:CG	1:A:675:THR:HG22	2.25	0.62
1:A:397:MET:HA	1:A:397:MET:HE2	1.82	0.62
1:A:518:PHE:O	1:A:522:ARG:HG2	2.00	0.62
1:B:220:ASN:HD22	1:B:220:ASN:C	2.10	0.60
1:A:565:GLY:H	1:A:568:HIS:CD2	2.08	0.60
1:B:565:GLY:H	1:B:568:HIS:CD2	2.13	0.59
1:A:137:LEU:HB3	1:A:138:PRO:HD3	1.86	0.58
1:B:124:PRO:HG2	1:B:194:GLU:HG3	1.85	0.58
1:A:696:ARG:O	1:A:700:GLU:HG3	2.03	0.58
1:B:21:LYS:HD3	1:B:26:TRP:CE2	2.39	0.58
1:B:450:LYS:CG	1:B:536:LEU:HD22	2.34	0.58
1:B:539:ASN:O	1:B:543:GLU:HG3	2.04	0.58
1:A:633:LEU:CD2	1:A:681:GLU:HG2	2.34	0.57
1:A:220:ASN:HD22	1:A:221:PRO:N	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:LEU:HD23	1:B:678:VAL:HA	1.86	0.57
1:A:21:LYS:HD3	1:A:26:TRP:CE2	2.40	0.56
1:B:444:GLU:O	1:B:448:GLU:HG3	2.06	0.56
1:A:539:ASN:O	1:A:543:GLU:HG3	2.06	0.55
1:B:41:ARG:O	1:B:41:ARG:HD2	2.06	0.55
1:B:358:HIS:O	1:B:360:PRO:HD3	2.07	0.55
1:B:274:LEU:HD11	1:B:303:ILE:HB	1.89	0.55
1:A:320:MET:HE1	1:A:323:ILE:HD12	1.89	0.54
1:A:571:ALA:HB3	1:A:572:PRO:HD3	1.88	0.54
1:A:82:ASP:OD2	1:A:358:HIS:HE1	1.90	0.54
1:B:333:PRO:HG3	1:B:343:TRP:CH2	2.43	0.53
1:B:431:ASP:N	1:B:432:PRO:HD3	2.23	0.53
1:A:368:MET:HG3	1:A:372:ASP:HB2	1.90	0.53
1:B:382:ARG:O	1:B:386:GLU:HG2	2.09	0.53
1:B:93:MET:HE1	1:B:136:LEU:HD11	1.89	0.53
1:A:308:GLU:H	1:A:342:GLN:HE22	1.56	0.53
1:B:220:ASN:ND2	1:B:222:GLU:H	2.06	0.53
1:A:313:GLN:HA	1:A:354:VAL:HG22	1.91	0.52
1:B:228:PRO:O	1:B:230:PRO:HD3	2.10	0.52
1:B:121:ASN:HD22	1:B:121:ASN:C	2.17	0.52
1:B:536:LEU:HG	1:B:557:PHE:CZ	2.46	0.51
1:B:671:LEU:CD2	1:B:678:VAL:HG22	2.40	0.51
1:A:442:GLY:O	1:A:446:ILE:HG13	2.11	0.51
1:B:696:ARG:O	1:B:700:GLU:HG3	2.11	0.51
1:B:450:LYS:HG2	1:B:536:LEU:HD22	1.93	0.50
1:B:95:TRP:HZ3	1:B:218:TYR:HH	1.60	0.50
1:B:584:VAL:HG13	1:B:621:MET:HG2	1.93	0.50
1:A:32:ASN:OD1	1:A:34:GLU:HG2	2.12	0.50
1:A:282:PRO:HD2	1:A:285:GLN:NE2	2.26	0.49
1:B:220:ASN:HD22	1:B:221:PRO:N	2.11	0.49
1:B:121:ASN:C	1:B:121:ASN:ND2	2.71	0.49
1:A:584:VAL:HG13	1:A:621:MET:HG2	1.93	0.49
1:B:41:ARG:CD	1:B:41:ARG:C	2.86	0.49
1:B:95:TRP:CD1	1:B:96:HIS:HD2	2.30	0.49
1:A:382:ARG:O	1:A:386:GLU:HG2	2.12	0.49
1:B:128:ASN:HA	1:B:130:ASP:OD2	2.13	0.48
1:A:107:ARG:HD3	1:A:185:VAL:HG22	1.96	0.48
1:A:360:PRO:HG2	6:A:2768:HOH:O	2.13	0.48
1:B:555:ILE:HG12	1:B:716:VAL:HG13	1.95	0.48
1:B:68:LEU:O	1:B:72:MET:HG2	2.13	0.48
1:B:462:GLN:NE2	1:B:503:GLN:HE22	2.07	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:LYS:HG2	1:B:589:GLN:NE2	2.29	0.47
1:A:335:LYS:HG2	6:A:2529:HOH:O	2.14	0.47
1:A:121:ASN:HD22	1:A:121:ASN:C	2.17	0.47
1:A:335:LYS:HE3	1:A:341:TRP:CE2	2.49	0.47
1:A:220:ASN:HD22	1:A:222:GLU:H	1.61	0.47
1:A:598:GLU:HG2	6:A:2769:HOH:O	2.13	0.47
1:B:107:ARG:HD3	1:B:185:VAL:HG22	1.96	0.47
1:B:264:VAL:HG22	1:B:309:GLY:O	2.14	0.47
1:B:518:PHE:O	1:B:522:ARG:HG2	2.14	0.47
1:A:451:GLU:O	1:A:455:ASP:HB2	2.15	0.46
1:B:367:MET:O	1:B:367:MET:HE3	2.15	0.46
1:B:671:LEU:HD21	1:B:678:VAL:HG22	1.98	0.46
1:A:121:ASN:C	1:A:121:ASN:ND2	2.73	0.46
1:B:137:LEU:HB3	1:B:138:PRO:HD3	1.98	0.46
1:B:362:GLU:HA	1:B:362:GLU:OE1	2.16	0.46
1:A:121:ASN:ND2	1:A:122:SER:N	2.60	0.46
1:B:610:THR:OG1	1:B:613:GLU:HG3	2.16	0.46
1:A:333:PRO:HD3	1:A:343:TRP:CZ3	2.52	0.45
1:B:355:PRO:HA	1:B:363:LYS:HD3	1.99	0.45
1:A:95:TRP:CD1	1:A:96:HIS:HD2	2.33	0.45
1:A:82:ASP:OD2	1:A:358:HIS:CE1	2.69	0.45
1:B:343:TRP:CD1	1:B:343:TRP:N	2.84	0.45
1:A:128:ASN:HA	1:A:130:ASP:OD2	2.17	0.45
1:B:558:GLU:HB2	6:B:2023:HOH:O	2.16	0.44
1:A:220:ASN:C	1:A:220:ASN:ND2	2.74	0.44
1:A:121:ASN:HD22	1:A:122:SER:H	1.64	0.44
1:B:190:GLU:HG2	1:B:195:THR:O	2.17	0.43
1:A:93:MET:HE1	1:A:136:LEU:HD11	2.00	0.43
1:B:41:ARG:HD2	1:B:41:ARG:C	2.43	0.43
1:B:220:ASN:HD22	1:B:222:GLU:H	1.66	0.43
1:B:264:VAL:HG21	1:B:307:ILE:HG22	1.99	0.43
1:A:436:ALA:HB2	1:A:562:VAL:HG12	2.01	0.43
1:A:438:TYR:CG	1:A:527:GLN:HB2	2.54	0.43
1:A:124:PRO:HG2	1:A:194:GLU:HG3	2.01	0.43
1:B:185:VAL:HG11	1:B:187:TRP:CZ2	2.54	0.43
1:B:570:ASP:OD1	1:B:572:PRO:HD2	2.19	0.43
1:A:32:ASN:ND2	1:A:35:ILE:HG23	2.34	0.42
1:A:332:GLU:CG	1:A:346:LYS:HE2	2.48	0.42
1:A:343:TRP:N	1:A:343:TRP:CD1	2.86	0.42
1:B:306:GLY:O	1:B:338:GLY:HA3	2.19	0.42
1:B:598:GLU:HG2	6:B:2339:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:PRO:HB2	1:B:377:ARG:HG3	2.00	0.42
1:B:580:LYS:HA	1:B:589:GLN:HE21	1.83	0.42
1:A:336:GLY:HA3	1:A:342:GLN:NE2	2.35	0.41
1:B:99:GLY:O	1:B:244:MET:HE1	2.19	0.41
1:A:379:PRO:O	1:A:383:GLU:HG3	2.20	0.41
1:A:672:ASP:CB	1:A:675:THR:HG22	2.51	0.41
1:A:213:VAL:HB	1:A:216:LEU:HD12	2.03	0.41
1:B:460:VAL:HG13	1:B:541:ALA:HB1	2.03	0.41
1:A:129:LEU:HD23	1:A:129:LEU:HA	1.88	0.41
1:B:332:GLU:OE2	1:B:346:LYS:HA	2.20	0.41
1:B:364:GLN:OE1	1:B:364:GLN:HA	2.21	0.41
1:A:286:GLN:NE2	1:B:651:LEU:HD11	2.36	0.40
1:A:285:GLN:NE2	6:A:2146:HOH:O	2.33	0.40
1:A:460:VAL:HG13	1:A:541:ALA:HB1	2.02	0.40
1:A:445:GLU:OE1	1:A:445:GLU:N	2.55	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	703/731 (96%)	680 (97%)	22 (3%)	1 (0%)	48	46
1	B	712/731 (97%)	693 (97%)	19 (3%)	0	100	100
All	All	1415/1462 (97%)	1373 (97%)	41 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	591	ASP

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	584/602 (97%)	578 (99%)	6 (1%)	68	75
1	B	588/602 (98%)	581 (99%)	7 (1%)	63	70
All	All	1172/1204 (97%)	1159 (99%)	13 (1%)	65	73

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	121	ASN
1	A	220	ASN
1	A	335	LYS
1	A	455	ASP
1	A	586	ASN
1	B	25	ASP
1	B	121	ASN
1	B	274	LEU
1	B	362	GLU
1	B	364	GLN
1	B	536	LEU
1	B	586	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	121	ASN
1	A	206	GLN
1	A	220	ASN
1	A	285	GLN
1	A	286	GLN
1	A	324	ASN
1	A	342	GLN
1	A	352	ASN

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Mol	Chain	Res	Type
1	A	358	HIS
1	A	389	GLN
1	A	513	ASN
1	A	515	GLN
1	A	519	ASN
1	A	544	GLN
1	A	568	HIS
1	A	586	ASN
1	A	589	GLN
1	A	692	ASN
1	B	57	GLN
1	B	121	ASN
1	B	206	GLN
1	B	220	ASN
1	B	286	GLN
1	B	294	ASN
1	B	296	ASN
1	B	324	ASN
1	B	342	GLN
1	B	352	ASN
1	B	389	GLN
1	B	398	ASN
1	B	408	HIS
1	B	430	GLN
1	B	493	GLN
1	B	503	GLN
1	B	515	GLN
1	B	527	GLN
1	B	568	HIS
1	B	586	ASN
1	B	589	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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 30 ligands modelled in this entry, 16 are monoatomic and 6 are unknown - leaving 8 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	$\#\|Z\| > 2$
2	SO4	A	733	-	4,4,4	0.37	0	6,6,6	0.11	0
2	SO4	B	733	-	4,4,4	0.37	0	6,6,6	0.07	0
2	SO4	B	732	-	4,4,4	0.37	0	6,6,6	0.06	0
2	SO4	A	734	-	4,4,4	0.37	0	6,6,6	0.07	0
2	SO4	A	735	-	4,4,4	0.37	0	6,6,6	0.14	0
5	HEM	A	800	1,6	50,50,50	2.55	12 (24%)	67,82,82	6.45	46 (68%)
5	HEM	B	800	1	50,50,50	2.50	12 (24%)	67,82,82	6.34	41 (61%)
2	SO4	A	732	-	4,4,4	0.36	0	6,6,6	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	B	800	1	-	3/14/54/54	-
5	HEM	A	800	1,6	-	4/14/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	800	HEM	FE-NC	8.32	2.22	1.95
5	A	800	HEM	FE-NA	7.72	2.20	1.95
5	A	800	HEM	FE-NB	6.89	2.16	1.94
5	B	800	HEM	FE-NB	6.88	2.16	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	FE-NC	6.86	2.17	1.95
5	B	800	HEM	FE-NA	6.71	2.17	1.95
5	A	800	HEM	FE-ND	6.47	2.14	1.94
5	B	800	HEM	CBC-CAC	5.32	1.56	1.30
5	A	800	HEM	CBC-CAC	5.23	1.55	1.30
5	B	800	HEM	CBB-CAB	5.17	1.55	1.30
5	A	800	HEM	CBB-CAB	5.09	1.54	1.30
5	B	800	HEM	CBD-CGD	-4.14	1.41	1.50
5	B	800	HEM	FE-ND	4.13	2.07	1.94
5	A	800	HEM	CBD-CGD	-4.01	1.41	1.50
5	B	800	HEM	CBA-CGA	-3.91	1.41	1.50
5	A	800	HEM	CBA-CGA	-3.90	1.41	1.50
5	A	800	HEM	O1A-CGA	2.48	1.30	1.22
5	B	800	HEM	C4D-ND	-2.35	1.36	1.40
5	B	800	HEM	O1A-CGA	2.35	1.29	1.22
5	A	800	HEM	CBD-CAD	2.17	1.59	1.51
5	A	800	HEM	C4D-ND	-2.15	1.36	1.40
5	B	800	HEM	CBD-CAD	2.11	1.59	1.51
5	A	800	HEM	CAC-C3C	2.05	1.52	1.47
5	B	800	HEM	CAC-C3C	2.05	1.52	1.47

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	800	HEM	CHD-C1D-ND	-18.12	104.92	124.42
5	A	800	HEM	CHC-C4B-NB	-15.04	108.24	124.42
5	B	800	HEM	CHC-C4B-NB	-14.63	108.68	124.42
5	B	800	HEM	CHC-C1C-NC	-14.30	108.88	124.45
5	B	800	HEM	C1C-CHC-C4B	14.25	156.30	126.02
5	A	800	HEM	CHD-C4C-NC	-13.95	109.27	124.45
5	B	800	HEM	CHD-C4C-NC	-13.57	109.68	124.45
5	A	800	HEM	C4C-CHD-C1D	13.40	154.50	126.02
5	A	800	HEM	CHD-C4C-C3C	13.29	147.62	125.21
5	B	800	HEM	CHD-C1D-ND	-13.15	110.27	124.42
5	A	800	HEM	C1D-C2D-C3D	-12.35	93.99	106.98
5	B	800	HEM	CHA-C4D-ND	-11.80	109.77	124.37
5	A	800	HEM	C2D-C1D-ND	11.58	123.29	109.90
5	B	800	HEM	C4C-CHD-C1D	11.45	150.36	126.02
5	B	800	HEM	CHB-C1B-NB	-11.44	110.21	124.37
5	A	800	HEM	CHA-C4D-ND	-11.41	110.26	124.37
5	A	800	HEM	C4A-CHB-C1B	11.00	152.11	126.25
5	A	800	HEM	C1C-CHC-C4B	10.89	149.17	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	800	HEM	C1A-CHA-C4D	10.87	151.82	126.25
5	B	800	HEM	C4A-CHB-C1B	10.45	150.81	126.25
5	A	800	HEM	CHB-C1B-NB	-10.41	111.49	124.37
5	B	800	HEM	C3B-C2B-C1B	-9.91	98.97	106.41
5	A	800	HEM	C1A-CHA-C4D	9.86	149.43	126.25
5	A	800	HEM	C4C-C3C-C2C	9.03	114.64	106.81
5	B	800	HEM	CHC-C4B-C3B	8.97	142.98	125.07
5	B	800	HEM	CHC-C1C-C2C	8.95	144.09	125.49
5	B	800	HEM	O2A-CGA-O1A	-8.48	101.52	123.33
5	B	800	HEM	CHD-C4C-C3C	8.44	139.43	125.21
5	A	800	HEM	CHC-C4B-C3B	8.14	141.32	125.07
5	B	800	HEM	C1D-C2D-C3D	-7.72	98.86	106.98
5	B	800	HEM	CHA-C1A-NA	-7.59	110.09	123.86
5	A	800	HEM	CHA-C4D-C3D	7.52	139.10	125.23
5	A	800	HEM	CHA-C1A-C2A	7.42	141.53	125.30
5	B	800	HEM	C2D-C1D-ND	7.39	118.45	109.90
5	B	800	HEM	CHA-C4D-C3D	7.34	138.77	125.23
5	A	800	HEM	CHB-C4A-NA	-7.09	111.01	123.86
5	B	800	HEM	C2B-C1B-NB	6.82	117.68	109.84
5	B	800	HEM	CHA-C1A-C2A	6.74	140.05	125.30
5	B	800	HEM	O2D-CGD-O1D	-6.68	106.15	123.33
5	B	800	HEM	CHB-C4A-NA	-6.52	112.04	123.86
5	B	800	HEM	CAA-CBA-CGA	-6.39	96.72	113.67
5	A	800	HEM	C4D-ND-C1D	-6.26	97.79	105.21
5	A	800	HEM	CAA-C2A-C1A	-6.13	112.96	124.94
5	B	800	HEM	C4B-C3B-C2B	6.13	112.92	107.28
5	A	800	HEM	C3B-C2B-C1B	-5.89	101.99	106.41
5	A	800	HEM	CAC-C3C-C4C	-5.82	110.92	124.82
5	A	800	HEM	CHA-C1A-NA	-5.66	113.59	123.86
5	A	800	HEM	C4D-C3D-C2D	5.39	114.75	106.89
5	A	800	HEM	C2B-C1B-NB	5.08	115.67	109.84
5	A	800	HEM	C2A-C1A-NA	-5.01	104.60	110.15
5	A	800	HEM	C4A-C3A-C2A	-4.63	101.51	106.82
5	B	800	HEM	O1D-CGD-CBD	4.60	137.68	123.09
5	A	800	HEM	C1A-C2A-C3A	4.40	113.67	106.87
5	A	800	HEM	CAA-CBA-CGA	-4.34	102.15	113.67
5	A	800	HEM	CHD-C1D-C2D	4.28	131.78	125.03
5	A	800	HEM	CHC-C1C-NC	-4.16	119.92	124.45
5	B	800	HEM	CMD-C2D-C1D	4.10	131.44	125.03
5	B	800	HEM	O1A-CGA-CBA	3.95	135.62	123.09
5	B	800	HEM	CHD-C1D-C2D	3.82	131.06	125.03
5	B	800	HEM	C4D-ND-C1D	-3.81	100.70	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	800	HEM	CAA-C2A-C1A	-3.67	117.77	124.94
5	A	800	HEM	C3C-C2C-C1C	-3.65	103.59	107.05
5	B	800	HEM	CHB-C4A-C3A	3.62	137.92	127.43
5	A	800	HEM	CMD-C2D-C3D	3.32	135.13	126.15
5	A	800	HEM	CMD-C2D-C1D	3.32	130.22	125.03
5	A	800	HEM	CAD-C3D-C2D	-3.23	121.81	127.87
5	A	800	HEM	CHC-C1C-C2C	3.23	132.20	125.49
5	A	800	HEM	C4C-NC-C1C	3.22	111.06	105.82
5	B	800	HEM	CAA-C2A-C3A	3.16	134.16	127.07
5	B	800	HEM	CMC-C2C-C1C	-3.05	119.36	124.73
5	A	800	HEM	CHB-C4A-C3A	3.00	136.15	127.43
5	B	800	HEM	C4D-C3D-C2D	2.97	111.21	106.89
5	A	800	HEM	CBA-CAA-C2A	2.93	120.63	112.53
5	A	800	HEM	O2A-CGA-O1A	-2.92	115.83	123.33
5	B	800	HEM	CAD-C3D-C4D	-2.82	119.79	124.70
5	B	800	HEM	CMB-C2B-C3B	2.81	135.24	128.43
5	A	800	HEM	CAA-C2A-C3A	2.81	133.37	127.07
5	B	800	HEM	O2A-CGA-CBA	2.81	122.86	114.00
5	A	800	HEM	C4B-C3B-C2B	2.77	109.83	107.28
5	B	800	HEM	C1B-NB-C4B	-2.61	102.12	105.21
5	A	800	HEM	CMA-C3A-C2A	2.60	131.14	125.62
5	A	800	HEM	C1B-NB-C4B	-2.37	102.40	105.21
5	B	800	HEM	C3C-C2C-C1C	2.33	109.25	107.05
5	A	800	HEM	O2D-CGD-CBD	2.31	121.28	114.00
5	A	800	HEM	CAD-CBD-CGD	2.23	119.58	113.67
5	B	800	HEM	CAC-C3C-C4C	-2.18	119.60	124.82
5	A	800	HEM	CHB-C1B-C2B	2.06	132.81	126.95

There are no chirality outliers.

All (7) torsion outliers are listed below:

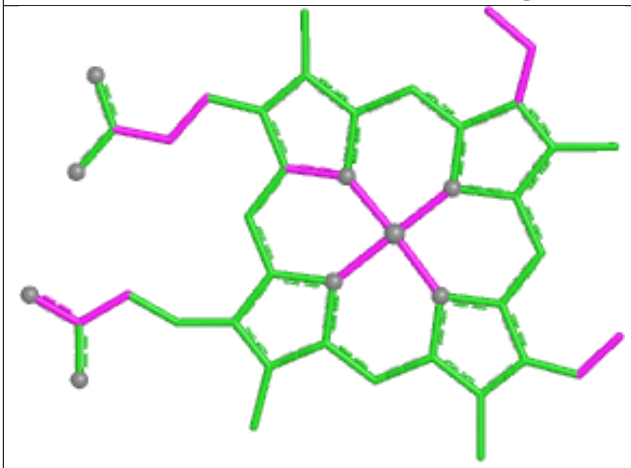
Mol	Chain	Res	Type	Atoms
5	A	800	HEM	C2B-C3B-CAB-CBB
5	A	800	HEM	C2C-C3C-CAC-CBC
5	B	800	HEM	CAA-CBA-CGA-O2A
5	B	800	HEM	CAA-CBA-CGA-O1A
5	A	800	HEM	CAA-CBA-CGA-O2A
5	A	800	HEM	CAA-CBA-CGA-O1A
5	B	800	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

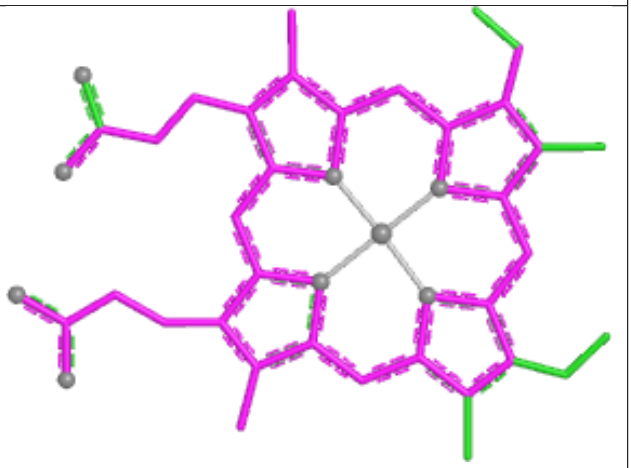
No monomer is involved in short contacts.

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.

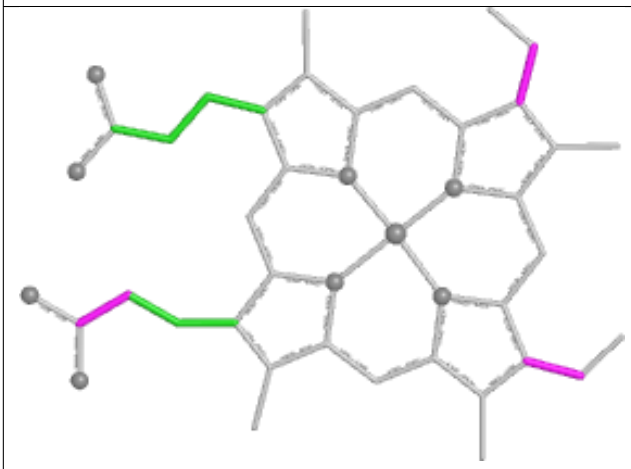
Ligand HEM A 800



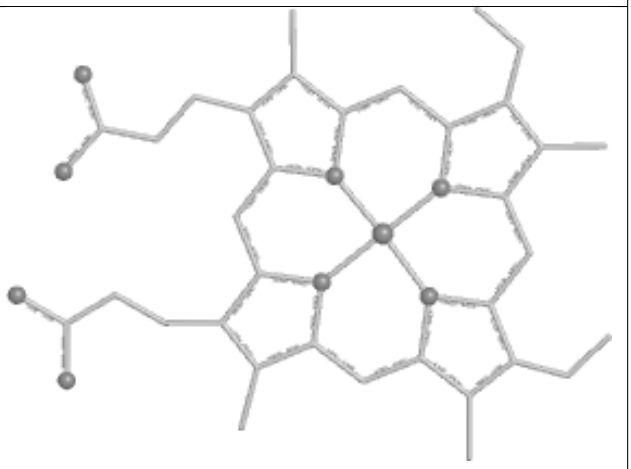
Bond lengths



Bond angles

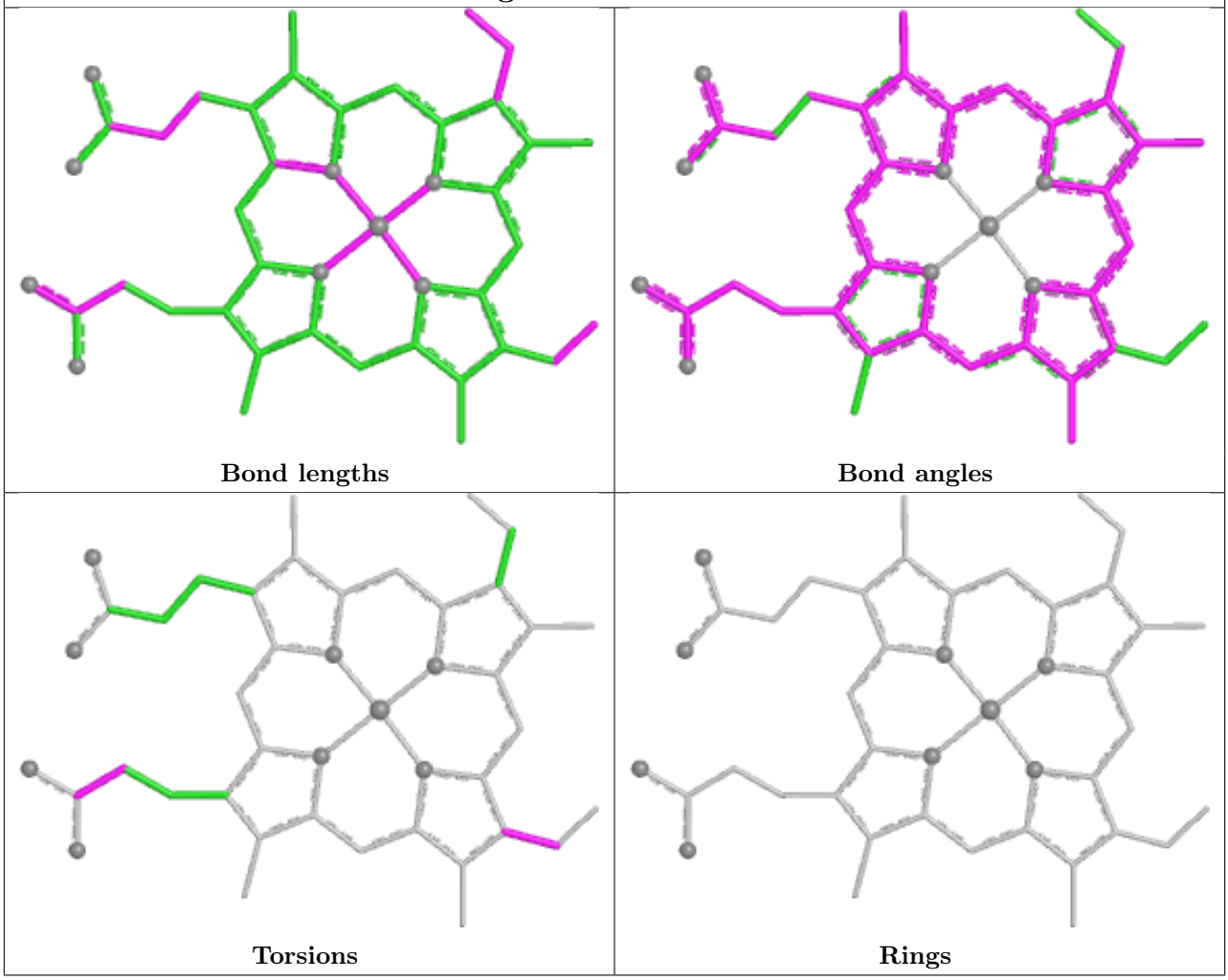


Torsions



Rings

Ligand HEM B 800



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	707/731 (96%)	-0.18	28 (3%) 42 41	10, 18, 41, 56	0
1	B	714/731 (97%)	0.11	21 (2%) 53 52	14, 25, 43, 58	0
All	All	1421/1462 (97%)	-0.04	49 (3%) 48 47	10, 22, 42, 58	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	437	ASP	4.9
1	B	590	ASP	4.9
1	A	591	ASP	4.5
1	A	590	ASP	4.3
1	B	591	ASP	3.5
1	A	675	THR	3.5
1	A	664	SER	3.4
1	B	18	LYS	3.3
1	A	663	ASP	3.2
1	A	294	ASN	3.1
1	B	294	ASN	3.1
1	A	18	LYS	3.1
1	A	271	GLU	3.1
1	A	362	GLU	3.1
1	A	361	ASP	3.0
1	A	523	SER	2.9
1	A	676	GLY	2.9
1	B	200	ASP	2.9
1	B	293	LYS	2.9
1	B	295	GLY	2.9
1	B	271	GLU	2.8
1	B	297	SER	2.7
1	B	663	ASP	2.7
1	A	437	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	524	ASP	2.7
1	B	330	GLU	2.6
1	B	272	GLU	2.6
1	B	296	ASN	2.5
1	A	457	ASP	2.5
1	A	554	GLU	2.5
1	A	522	ARG	2.5
1	A	525	GLY	2.4
1	A	444	GLU	2.4
1	A	665	GLU	2.4
1	B	191	ASP	2.4
1	A	49	ASP	2.3
1	B	57	GLN	2.3
1	A	674	ASP	2.3
1	A	19	ARG	2.2
1	A	706	ASP	2.2
1	A	521	SER	2.2
1	B	298	LYS	2.2
1	B	348	GLU	2.2
1	B	332	GLU	2.1
1	B	455	ASP	2.1
1	A	455	ASP	2.1
1	B	301	GLU	2.0
1	A	666	HIS	2.0
1	A	360	PRO	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)

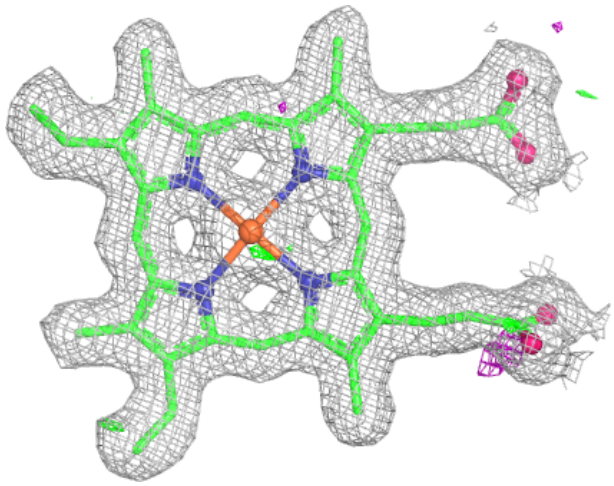
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

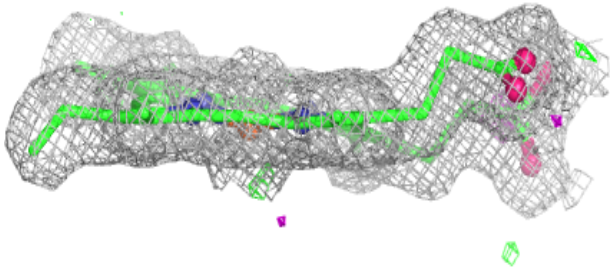
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	UNX	B	2020	1/1	0.84	0.54	44,44,44,44	0
2	SO4	A	734	5/5	0.87	0.13	56,57,58,58	0
2	SO4	B	733	5/5	0.89	0.11	67,67,68,68	0
4	UNX	B	2022	1/1	0.89	0.45	35,35,35,35	0
4	UNX	B	2021	1/1	0.91	0.44	28,28,28,28	0
2	SO4	A	735	5/5	0.92	0.15	38,40,45,45	0
4	UNX	A	2017	1/1	0.94	0.42	25,25,25,25	0
2	SO4	B	732	5/5	0.94	0.14	49,50,50,50	0
2	SO4	A	732	5/5	0.95	0.09	44,45,46,47	0
2	SO4	A	733	5/5	0.95	0.13	35,37,40,41	0
4	UNX	B	2018	1/1	0.96	0.57	29,29,29,29	0
3	CL	B	2016	1/1	0.98	0.04	24,24,24,24	0
5	HEM	A	800	43/43	0.98	0.05	8,12,14,16	0
5	HEM	B	800	43/43	0.98	0.07	19,22,24,26	0
3	CL	A	2012	1/1	0.99	0.11	28,28,28,28	0
3	CL	A	2014	1/1	0.99	0.03	20,20,20,20	0
3	CL	B	2008	1/1	0.99	0.06	25,25,25,25	0
3	CL	B	2015	1/1	0.99	0.04	19,19,19,19	0
3	CL	A	2001	1/1	0.99	0.02	16,16,16,16	0
3	CL	A	2002	1/1	0.99	0.03	18,18,18,18	0
3	CL	A	2004	1/1	0.99	0.03	22,22,22,22	0
4	UNX	B	2019	1/1	0.99	0.42	31,31,31,31	0
3	CL	A	2005	1/1	0.99	0.02	20,20,20,20	0
3	CL	A	2006	1/1	0.99	0.12	28,28,28,28	0
3	CL	A	2009	1/1	0.99	0.06	24,24,24,24	0
3	CL	A	2010	1/1	0.99	0.04	27,27,27,27	0
3	CL	A	2011	1/1	0.99	0.08	28,28,28,28	0
3	CL	B	2003	1/1	1.00	0.03	18,18,18,18	0
3	CL	A	2013	1/1	1.00	0.02	16,16,16,16	0
3	CL	A	2007	1/1	1.00	0.03	22,22,22,22	0

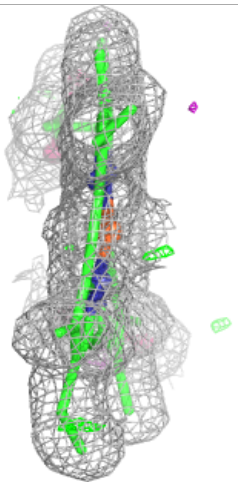
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM A 800:

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

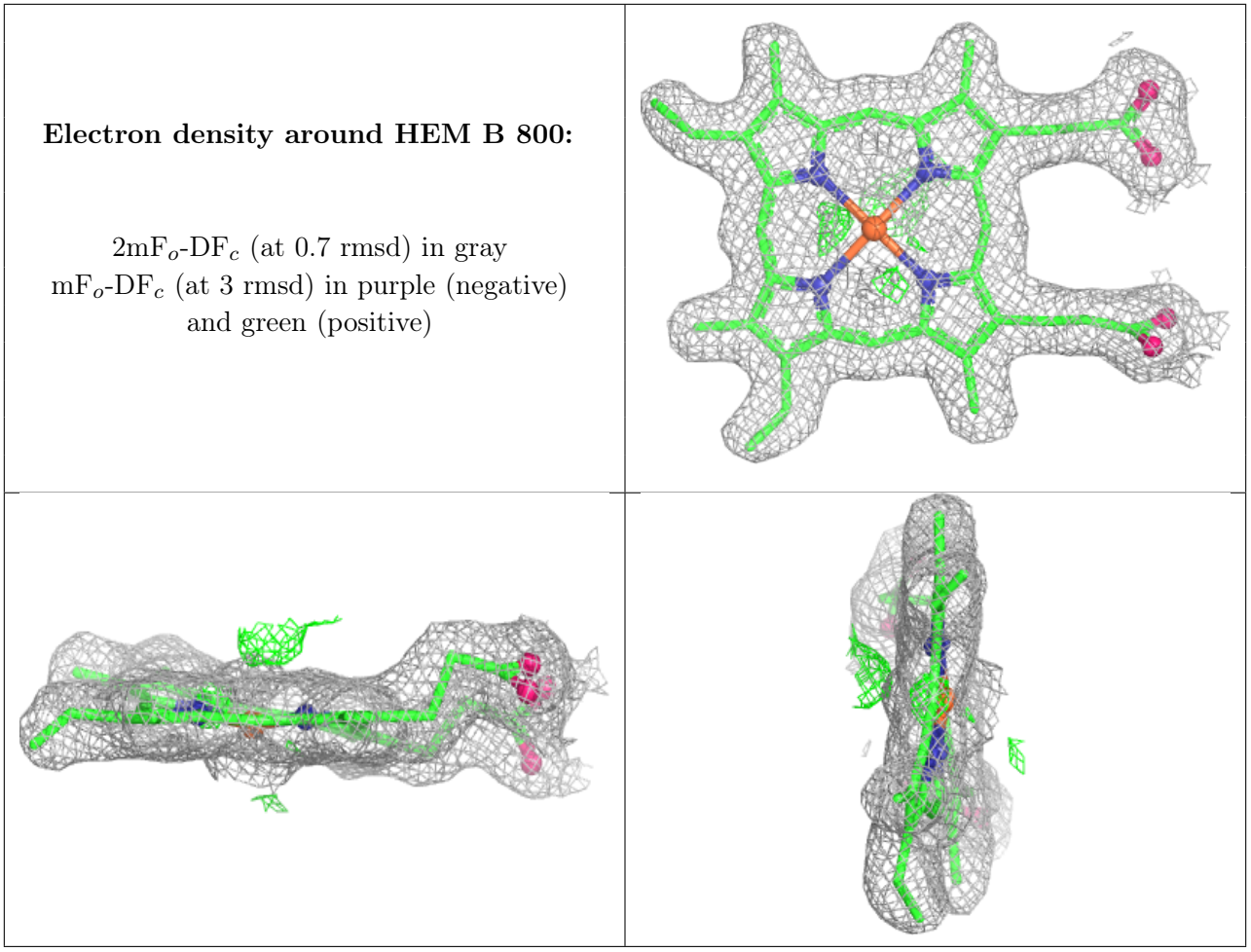






Electron density around HEM B 800:

$2mF_o$-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.