Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 12:28 PM EST

PDB ID	:	5KQQ
Title	:	Crystal structure of the W153F variant of catalase-peroxidase from B. pseudomallei treated
Authors	:	Loewen, P.C.
Deposited on	:	2016-07-06
Resolution	:	1.87 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:

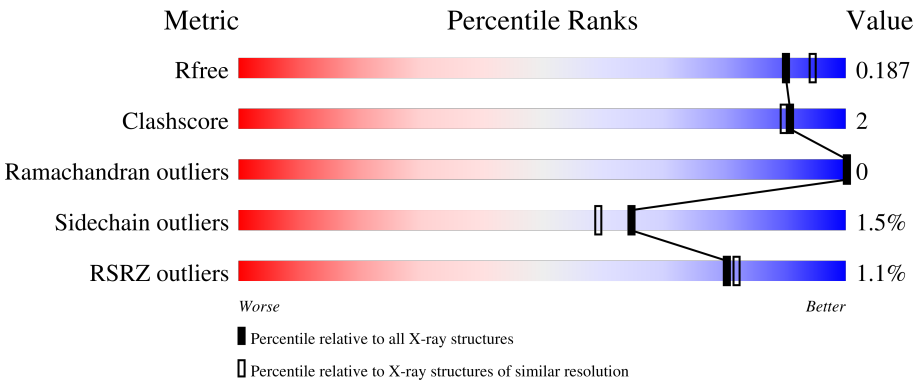
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	% 89% 8% • •
1	B	728	% 88% 9% • •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12673 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.

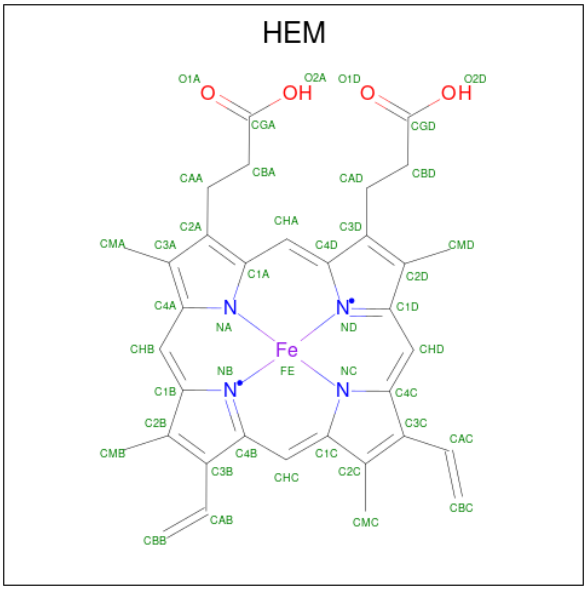
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	713	5547	3500	989	1044	14	0	6	0
1	B	713	5586	3523	993	1056	14	0	11	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	PHE	TRP	engineered mutation	UNP Q3JNW6
B	153	PHE	TRP	engineered mutation	UNP Q3JNW6

- Molecule 2 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		
2	A	1	43	34	1	4	4	0	0

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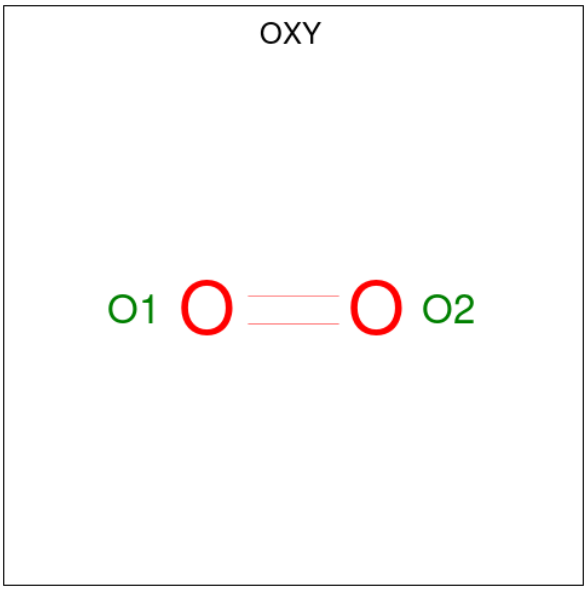
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

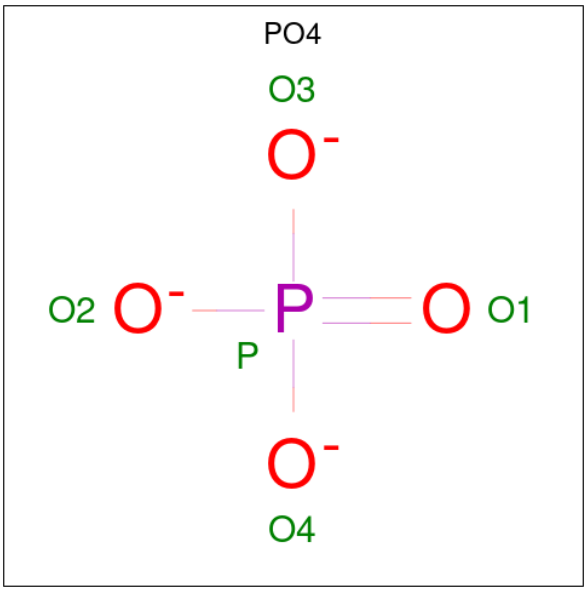
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0
			Total	Na		
3	B	1	1	1	0	0

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



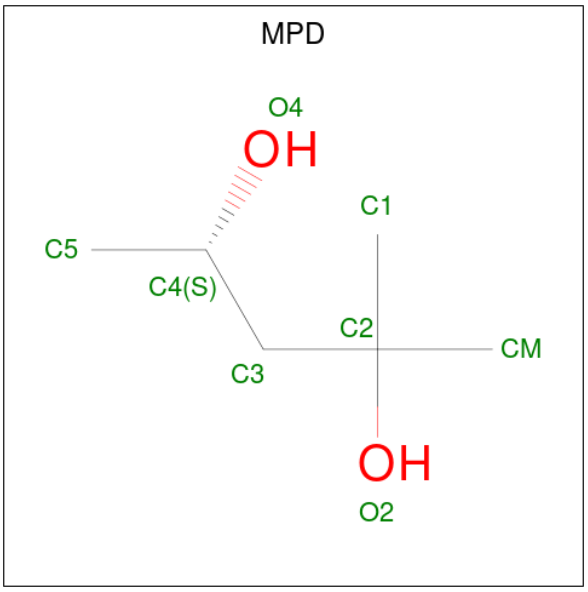
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	1	2	2	0	0
			Total	O		
4	B	1	2	2	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 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
6	A	1	Total C O 8 6 2	0	0

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

- Molecule 7 is water.

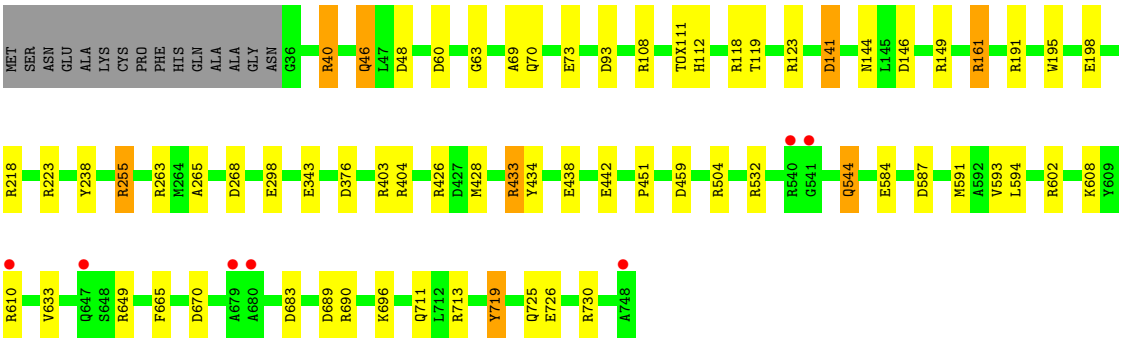
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	710	710	710	0	1
			Total	O		
7	B	704	704	704	0	2

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.

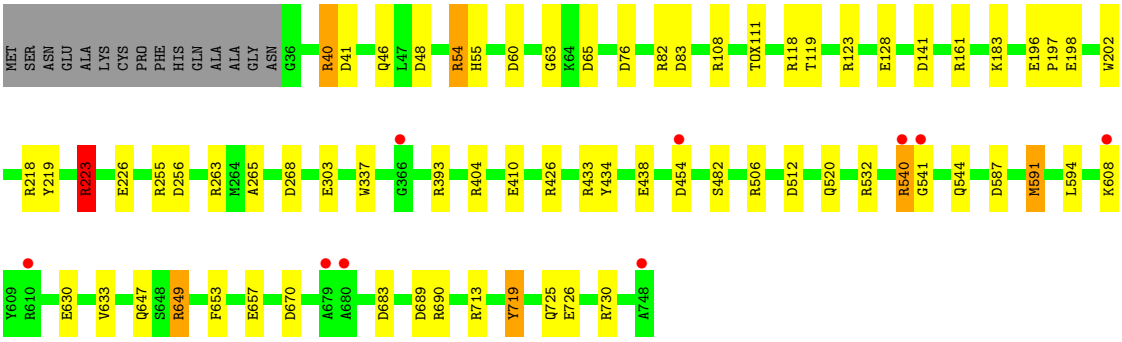
• Molecule 1: Catalase-peroxidase

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	100.92Å 116.13Å 175.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.90 – 1.87 48.45 – 1.87	Depositor EDS
% Data completeness (in resolution range)	90.2 (96.90-1.87) 90.2 (48.45-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.143 , 0.175 0.157 , 0.187	Depositor DCC
R_{free} test set	7599 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12673	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 3.61% 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, TOX, HEM, PO4, NA, OXY

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	1.29	20/5671 (0.4%)	1.29	51/7705 (0.7%)
1	B	1.29	26/5716 (0.5%)	1.19	49/7765 (0.6%)
All	All	1.29	46/11387 (0.4%)	1.24	100/15470 (0.6%)

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	GLU	CG-CD	8.72	1.65	1.51
1	B	198	GLU	CG-CD	8.22	1.64	1.51
1	A	544	GLN	CD-OE1	8.06	1.41	1.24
1	A	725	GLN	CD-NE2	7.96	1.52	1.32
1	A	434	TYR	CE2-CZ	-7.76	1.28	1.38
1	B	730	ARG	CZ-NH1	7.72	1.43	1.33
1	A	434	TYR	CG-CD1	-7.58	1.29	1.39
1	A	442	GLU	CD-OE2	-7.39	1.17	1.25
1	B	512	ASP	CG-OD2	6.86	1.41	1.25
1	B	725	GLN	CD-NE2	6.80	1.49	1.32
1	B	63	GLY	N-CA	6.66	1.56	1.46
1	B	438	GLU	CD-OE1	-6.62	1.18	1.25
1	B	410	GLU	CG-CD	6.61	1.61	1.51
1	B	337	TRP	CE3-CZ3	6.50	1.49	1.38
1	B	434	TYR	CG-CD1	-6.45	1.30	1.39
1	A	725	GLN	CG-CD	6.34	1.65	1.51
1	A	161	ARG	CZ-NH1	6.23	1.41	1.33
1	A	343	GLU	CD-OE1	6.19	1.32	1.25
1	B	128	GLU	CD-OE1	-5.91	1.19	1.25
1	A	195	TRP	CG-CD1	5.88	1.45	1.36
1	B	730	ARG	CZ-NH2	5.80	1.40	1.33
1	A	63	GLY	N-CA	5.78	1.54	1.46
1	B	82	ARG	CZ-NH2	-5.68	1.25	1.33
1	A	161	ARG	CD-NE	-5.67	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	438	GLU	CD-OE2	5.60	1.31	1.25
1	B	226	GLU	CG-CD	5.56	1.60	1.51
1	B	202	TRP	CZ3-CH2	5.52	1.48	1.40
1	B	196	GLU	CG-CD	5.51	1.60	1.51
1	B	303	GLU	CD-OE2	-5.51	1.19	1.25
1	A	298	GLU	CD-OE2	5.46	1.31	1.25
1	B	219	TYR	CE1-CZ	5.42	1.45	1.38
1	A	255[A]	ARG	CZ-NH2	-5.37	1.26	1.33
1	A	255[B]	ARG	CZ-NH2	-5.37	1.26	1.33
1	B	482	SER	CA-CB	5.31	1.60	1.52
1	B	197	PRO	N-CA	-5.29	1.38	1.47
1	B	630	GLU	CD-OE2	5.21	1.31	1.25
1	B	544	GLN	CD-NE2	5.20	1.45	1.32
1	B	719	TYR	CD2-CE2	5.15	1.47	1.39
1	B	719	TYR	CE2-CZ	5.14	1.45	1.38
1	A	725	GLN	CD-OE1	5.13	1.35	1.24
1	B	196	GLU	CB-CG	-5.11	1.42	1.52
1	A	719	TYR	CD2-CE2	5.10	1.47	1.39
1	B	719	TYR	CZ-OH	5.06	1.46	1.37
1	B	410	GLU	CD-OE2	5.06	1.31	1.25
1	A	584	GLU	CG-CD	5.03	1.59	1.51
1	A	504	ARG	CZ-NH1	-5.00	1.26	1.33

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	255[A]	ARG	NE-CZ-NH2	-23.01	108.79	120.30
1	A	255[B]	ARG	NE-CZ-NH2	-23.01	108.79	120.30
1	A	161	ARG	NE-CZ-NH2	-18.68	110.96	120.30
1	A	255[A]	ARG	NE-CZ-NH1	16.64	128.62	120.30
1	A	255[B]	ARG	NE-CZ-NH1	16.64	128.62	120.30
1	A	161	ARG	NE-CZ-NH1	14.30	127.45	120.30
1	B	512	ASP	CB-CG-OD1	-11.76	107.72	118.30
1	B	161	ARG	NE-CZ-NH1	11.32	125.96	120.30
1	B	404	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	A	404	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	B	649	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	A	649	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	B	713	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	A	263	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	B	198	GLU	OE1-CD-OE2	-9.15	112.32	123.30
1	A	404	ARG	NE-CZ-NH2	-8.94	115.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	198	GLU	OE1-CD-OE2	-8.82	112.71	123.30
1	B	40	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	60	ASP	CB-CG-OD2	-8.34	110.79	118.30
1	B	108	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	B	393	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	B	40	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	B	226	GLU	OE1-CD-OE2	-7.60	114.18	123.30
1	B	404	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	649	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	713	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	B	123	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	433	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	670	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	B	268	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	108	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	60	ASP	CB-CG-OD1	7.21	124.78	118.30
1	B	83	ASP	CB-CG-OD2	7.19	124.77	118.30
1	B	48	ASP	CB-CG-OD1	7.12	124.71	118.30
1	B	512	ASP	CB-CG-OD2	7.12	124.71	118.30
1	A	713	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	263	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	B	719	TYR	CB-CG-CD1	-7.00	116.80	121.00
1	A	123	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	65	ASP	CB-CG-OD2	-6.88	112.10	118.30
1	A	198	GLU	CG-CD-OE1	6.84	131.99	118.30
1	A	434	TYR	CB-CG-CD1	6.82	125.09	121.00
1	B	268	ASP	CB-CG-OD2	-6.82	112.17	118.30
1	A	433	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	A	191	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	A	683	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	40	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	A	532	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	376	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	A	690	ARG	NE-CZ-NH1	-6.43	117.09	120.30
1	A	149	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	255[A]	ARG	CG-CD-NE	-6.38	98.40	111.80
1	A	255[B]	ARG	CG-CD-NE	-6.38	98.40	111.80
1	B	60	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	48	ASP	CB-CG-OD1	6.26	123.93	118.30
1	B	82	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	198	GLU	CG-CD-OE1	6.18	130.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	689	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	719	TYR	CB-CG-CD1	-6.12	117.33	121.00
1	B	263	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	B	587	ASP	CB-CG-OD1	5.94	123.65	118.30
1	B	161	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	B	506	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	587	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	B	433	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	218	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	602	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	60	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	689	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	690	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	A	218	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	719	TYR	CB-CG-CD2	5.53	124.32	121.00
1	A	268	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	683	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	665	PHE	CB-CG-CD1	-5.47	116.97	120.80
1	B	532	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	541	GLY	N-CA-C	-5.44	99.49	113.10
1	A	93	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	434	TYR	CB-CG-CD1	5.39	124.23	121.00
1	B	670	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	A	690	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	B	649	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	108	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	403	ARG	CG-CD-NE	-5.23	100.82	111.80
1	B	41	ASP	CB-CG-OD1	5.21	122.98	118.30
1	A	426[A]	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	426[B]	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	587	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	459	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	454	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	256	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	725	GLN	CB-CG-CD	5.08	124.82	111.60
1	B	689	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	B	591	MET	CG-SD-CE	-5.07	92.09	100.20
1	B	683	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	B	540	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	B	653	PHE	CB-CG-CD1	5.02	124.31	120.80
1	A	46	GLN	CA-CB-CG	5.00	124.41	113.40
1	B	223	ARG	NE-CZ-NH1	-5.00	117.80	120.30

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	5547	0	5352	16	0
1	B	5586	0	5381	17	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	16	0	28	3	0
6	B	8	0	14	1	0
7	A	710	0	0	6	1
7	B	704	0	0	9	1
All	All	12673	0	10835	38	1

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 2.

All (38) 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:119[B]:THR:HG21	7:B:1169:HOH:O	1.63	0.96
1:A:119[B]:THR:HG21	7:A:1149:HOH:O	1.64	0.96
1:B:255[B]:ARG:HG2	7:B:1531:HOH:O	1.73	0.88
1:B:520:GLN:HG3	7:B:916:HOH:O	1.78	0.83
1:B:726[B]:GLU:CD	7:B:911:HOH:O	2.16	0.82
1:B:46:GLN:NE2	7:B:901:HOH:O	2.03	0.67
1:A:711:GLN:OE1	7:A:902:HOH:O	2.15	0.64
6:A:805:MPD:CM	6:A:805:MPD:O4	2.46	0.63
1:B:647:GLN:HG2	7:B:918:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:805:MPD:O4	6:A:805:MPD:HM1	2.00	0.61
1:B:76:ASP:OD1	7:B:902:HOH:O	2.16	0.60
1:A:255[A]:ARG:NH2	7:A:903:HOH:O	2.20	0.56
1:A:593:VAL:HG13	7:A:918:HOH:O	2.06	0.55
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.43	0.54
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.92	0.53
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.42	0.50
1:A:161:ARG:NH2	7:A:908:HOH:O	2.39	0.50
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.94	0.50
1:B:647:GLN:NE2	7:B:918:HOH:O	2.45	0.49
4:B:803:OXY:O2	7:B:904:HOH:O	2.20	0.48
1:A:69:ALA:O	1:A:73:GLU:HG3	2.13	0.47
1:A:726[B]:GLU:HG2	1:A:730:ARG:HH12	1.80	0.46
1:B:591:MET:SD	1:B:594:LEU:HD12	2.55	0.46
1:A:696:LYS:HE2	7:A:1080:HOH:O	2.15	0.46
1:A:591:MET:SD	1:A:594:LEU:HD12	2.56	0.46
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.17	0.45
6:A:806:MPD:H11	6:A:806:MPD:C5	2.46	0.45
1:A:70:GLN:HE21	1:A:70:GLN:HB2	1.59	0.44
1:B:540:ARG:HA	1:B:540:ARG:NH1	2.32	0.44
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.48	0.44
1:B:119[A]:THR:CG2	1:B:265:ALA:HB2	2.47	0.44
1:B:649:ARG:HH22	1:B:657[B]:GLU:CD	2.21	0.43
1:B:223:ARG:HH11	1:B:223:ARG:HD2	1.67	0.43
6:B:805:MPD:O4	6:B:805:MPD:H12	2.19	0.43
1:B:426[B]:ARG:HA	1:B:426[B]:ARG:HD2	1.82	0.42
1:A:112:HIS:CE1	1:A:141:ASP:O	2.73	0.41
1:A:428:MET:O	1:A:433:ARG:HD3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1151:HOH:O	7:B:1290:HOH:O[2_444]	1.99	0.21

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	715/728 (98%)	705 (99%)	10 (1%)	0	100	100
1	B	720/728 (99%)	711 (99%)	9 (1%)	0	100	100
All	All	1435/1456 (99%)	1416 (99%)	19 (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	554/560 (99%)	545 (98%)	9 (2%)	62	56
1	B	559/560 (100%)	552 (99%)	7 (1%)	69	64
All	All	1113/1120 (99%)	1097 (99%)	16 (1%)	65	62

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	118	ARG
1	A	141	ASP
1	A	223	ARG
1	A	451	PRO
1	A	544	GLN
1	A	608	LYS

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Mol	Chain	Res	Type
1	A	610	ARG
1	B	40	ARG
1	B	54	ARG
1	B	118	ARG
1	B	141	ASP
1	B	183	LYS
1	B	223	ARG
1	B	608	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	247	ASN
1	B	227	ASN
1	B	406	HIS
1	B	647	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	TOX	B	111[B]	-	10,17,18	2.50	5 (50%)	10,23,25	1.33	1 (10%)
1	TOX	A	111[A]	2	10,17,18	2.22	6 (60%)	10,23,25	2.22	4 (40%)
1	TOX	B	111[A]	2	10,17,18	2.50	5 (50%)	10,23,25	1.33	1 (10%)
1	TOX	A	111[B]	-	10,17,18	2.22	6 (60%)	10,23,25	2.22	4 (40%)

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
1	TOX	B	111[B]	-	-	2/4/8/10	0/2/2/2
1	TOX	A	111[A]	2	-	2/4/8/10	0/2/2/2
1	TOX	B	111[A]	2	-	2/4/8/10	0/2/2/2
1	TOX	A	111[B]	-	-	2/4/8/10	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	O-C	4.55	1.38	1.19
1	B	111[B]	TOX	O-C	4.55	1.38	1.19
1	A	111[A]	TOX	O-C	3.87	1.35	1.19
1	A	111[B]	TOX	O-C	3.87	1.35	1.19
1	A	111[A]	TOX	CD1-NE1	-3.52	1.35	1.39
1	A	111[B]	TOX	CD1-NE1	-3.52	1.35	1.39
1	B	111[A]	TOX	CZ2-CE2	-3.24	1.34	1.41
1	B	111[B]	TOX	CZ2-CE2	-3.24	1.34	1.41
1	B	111[A]	TOX	CD1-NE1	-3.20	1.36	1.39
1	B	111[B]	TOX	CD1-NE1	-3.20	1.36	1.39
1	B	111[A]	TOX	CH2-CZ3	2.92	1.45	1.38
1	B	111[B]	TOX	CH2-CZ3	2.92	1.45	1.38
1	B	111[A]	TOX	CA-N	-2.77	1.39	1.48
1	B	111[B]	TOX	CA-N	-2.77	1.39	1.48
1	A	111[A]	TOX	CZ3-CE3	2.25	1.41	1.36
1	A	111[B]	TOX	CZ3-CE3	2.25	1.41	1.36
1	A	111[A]	TOX	CZ2-CE2	-2.25	1.36	1.41
1	A	111[B]	TOX	CZ2-CE2	-2.25	1.36	1.41
1	A	111[A]	TOX	CA-N	-2.22	1.41	1.48
1	A	111[B]	TOX	CA-N	-2.22	1.41	1.48
1	A	111[A]	TOX	CE3-CD2	-2.18	1.37	1.42
1	A	111[B]	TOX	CE3-CD2	-2.18	1.37	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111[A]	TOX	CZ2-CE2-CD2	-4.01	115.49	120.94
1	A	111[B]	TOX	CZ2-CE2-CD2	-4.01	115.49	120.94
1	A	111[A]	TOX	CH2-CZ2-CE2	2.69	124.60	119.44
1	A	111[B]	TOX	CH2-CZ2-CE2	2.69	124.60	119.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111[A]	TOX	CB-CG-CD1	2.53	131.09	127.97
1	A	111[B]	TOX	CB-CG-CD1	2.53	131.09	127.97
1	A	111[A]	TOX	CZ3-CE3-CD2	-2.47	117.47	120.89
1	A	111[B]	TOX	CZ3-CE3-CD2	-2.47	117.47	120.89
1	B	111[A]	TOX	CZ2-CE2-CD2	-2.10	118.08	120.94
1	B	111[B]	TOX	CZ2-CE2-CD2	-2.10	118.08	120.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111[A]	TOX	N-CA-CB-CG
1	A	111[A]	TOX	C-CA-CB-CG
1	A	111[B]	TOX	N-CA-CB-CG
1	A	111[B]	TOX	C-CA-CB-CG
1	B	111[A]	TOX	N-CA-CB-CG
1	B	111[A]	TOX	C-CA-CB-CG
1	B	111[B]	TOX	N-CA-CB-CG
1	B	111[B]	TOX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PO4	B	804	-	4,4,4	0.70	0	6,6,6	2.16	2 (33%)
6	MPD	B	805	-	7,7,7	0.73	0	9,10,10	1.45	2 (22%)
2	HEM	A	801	1	41,50,50	1.47	5 (12%)	45,82,82	1.92	15 (33%)
6	MPD	A	806	-	7,7,7	0.65	0	9,10,10	1.80	2 (22%)
4	OXY	B	803	-	1,1,1	0.99	0	-		
2	HEM	B	801	1	41,50,50	1.64	9 (21%)	45,82,82	1.74	12 (26%)
4	OXY	A	803	-	1,1,1	0.41	0	-		
6	MPD	A	805	-	7,7,7	0.56	0	9,10,10	0.88	0
5	PO4	A	804	-	4,4,4	1.29	0	6,6,6	2.71	3 (50%)

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	B	805	-	-	3/5/5/5	-
2	HEM	A	801	1	-	2/12/54/54	-
6	MPD	A	806	-	-	4/5/5/5	-
2	HEM	B	801	1	-	2/12/54/54	-
6	MPD	A	805	-	-	0/5/5/5	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1B-NB	-4.57	1.32	1.40
2	B	801	HEM	CHB-C1B	3.80	1.44	1.35
2	A	801	HEM	C1B-NB	-3.61	1.34	1.40
2	A	801	HEM	CHB-C1B	3.59	1.44	1.35
2	B	801	HEM	C1A-NA	3.53	1.43	1.36
2	A	801	HEM	CAA-C2A	2.83	1.56	1.52
2	A	801	HEM	CMD-C2D	-2.47	1.45	1.50
2	A	801	HEM	FE-NB	2.40	2.08	1.96
2	B	801	HEM	FE-NB	2.37	2.08	1.96
2	B	801	HEM	C4B-NB	-2.32	1.34	1.38
2	B	801	HEM	O1D-CGD	2.31	1.29	1.22
2	B	801	HEM	CBA-CGA	2.30	1.55	1.50
2	B	801	HEM	C3D-C2D	2.24	1.41	1.36
2	B	801	HEM	C4A-NA	2.01	1.40	1.36

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	804	PO4	O3-P-O1	-5.01	92.56	110.89
2	B	801	HEM	C4B-C3B-C2B	-4.66	103.41	107.11
2	A	801	HEM	CMA-C3A-C4A	-4.61	121.38	128.46
2	B	801	HEM	CAA-CBA-CGA	-4.52	101.08	113.76
2	A	801	HEM	C4A-C3A-C2A	4.45	110.09	107.00
5	B	804	PO4	O3-P-O2	3.84	120.31	107.97
2	A	801	HEM	CHC-C4B-NB	3.81	128.57	124.43
2	A	801	HEM	C1B-NB-C4B	3.72	108.91	105.07
6	A	806	MPD	C5-C4-C3	3.64	128.86	111.69
5	B	804	PO4	O2-P-O1	-3.37	98.58	110.89
2	A	801	HEM	O1A-CGA-CBA	-3.22	112.73	123.08
2	A	801	HEM	O2D-CGD-CBD	3.03	123.78	114.03
2	B	801	HEM	CHA-C4D-ND	3.00	128.09	124.38
5	A	804	PO4	O4-P-O1	3.00	121.86	110.89
2	B	801	HEM	CAD-CBD-CGD	2.95	119.96	113.60
2	B	801	HEM	CHB-C1B-NB	2.94	128.01	124.38
5	A	804	PO4	O4-P-O3	2.83	117.06	107.97
6	B	805	MPD	C1-C2-C3	2.82	123.08	109.96
6	A	806	MPD	CM-C2-C1	-2.80	104.74	110.57
2	A	801	HEM	CBA-CAA-C2A	2.56	117.00	112.62
2	A	801	HEM	CAD-C3D-C4D	2.55	129.12	124.66
2	A	801	HEM	O1D-CGD-CBD	-2.50	115.04	123.08
2	A	801	HEM	CAA-CBA-CGA	-2.49	106.78	113.76
2	A	801	HEM	CHB-C1B-NB	2.48	127.45	124.38
6	B	805	MPD	O2-C2-C1	-2.47	100.16	108.08
2	A	801	HEM	C3B-C2B-C1B	2.43	108.29	106.49
2	B	801	HEM	C2D-C1D-ND	2.34	112.69	109.88
2	A	801	HEM	O2A-CGA-CBA	2.33	121.52	114.03
2	B	801	HEM	CHA-C4D-C3D	-2.26	121.08	125.33
2	A	801	HEM	CBD-CAD-C3D	2.23	118.81	112.63
2	B	801	HEM	CBB-CAB-C3B	-2.14	116.99	127.62
2	A	801	HEM	C4B-C3B-C2B	-2.07	105.47	107.11
2	B	801	HEM	CMB-C2B-C1B	-2.07	121.89	125.04
2	B	801	HEM	CHB-C1B-C2B	-2.04	121.09	126.72
2	B	801	HEM	CAD-C3D-C4D	2.03	128.21	124.66
2	B	801	HEM	CBD-CAD-C3D	2.03	118.26	112.63

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	806	MPD	C2-C3-C4-C5
6	B	805	MPD	C1-C2-C3-C4
6	B	805	MPD	O2-C2-C3-C4
6	A	806	MPD	C1-C2-C3-C4
6	B	805	MPD	CM-C2-C3-C4
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
6	A	806	MPD	O2-C2-C3-C4
2	A	801	HEM	CAA-CBA-CGA-O1A
6	A	806	MPD	C2-C3-C4-O4

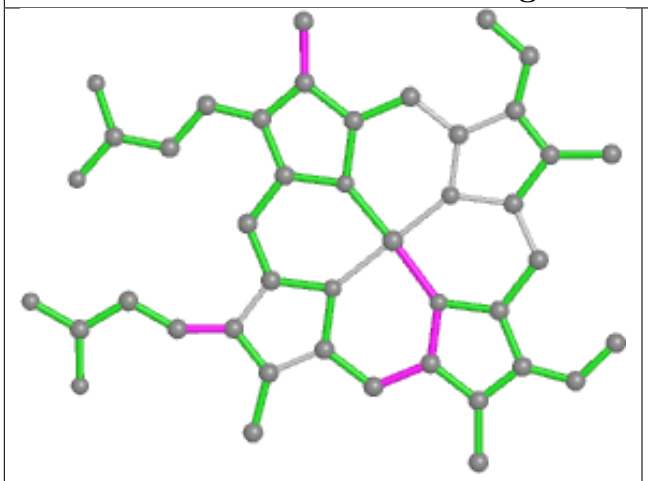
There are no ring outliers.

4 monomers are involved in 5 short contacts:

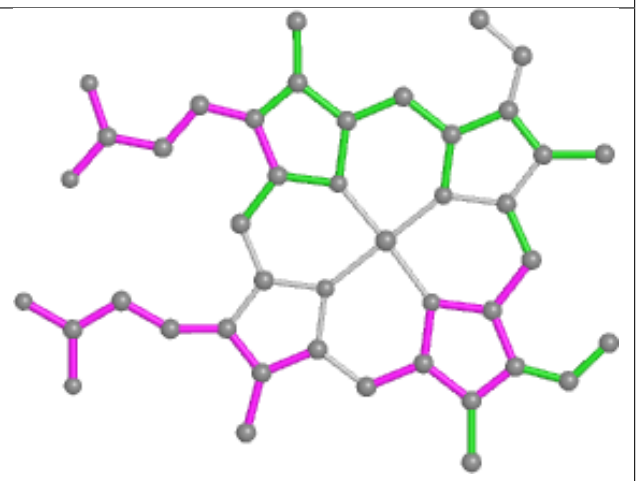
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	805	MPD	1	0
6	A	806	MPD	1	0
4	B	803	OXY	1	0
6	A	805	MPD	2	0

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.

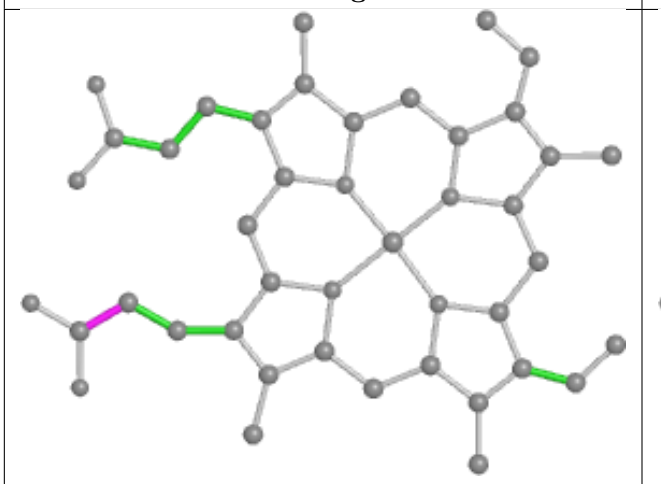
Ligand HEM A 801



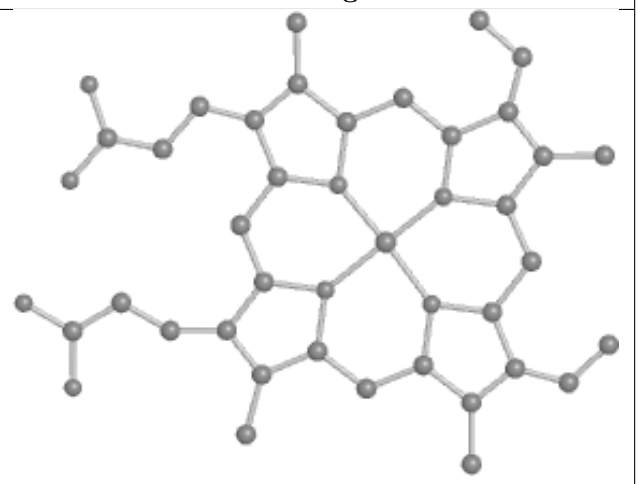
Bond lengths



Bond angles

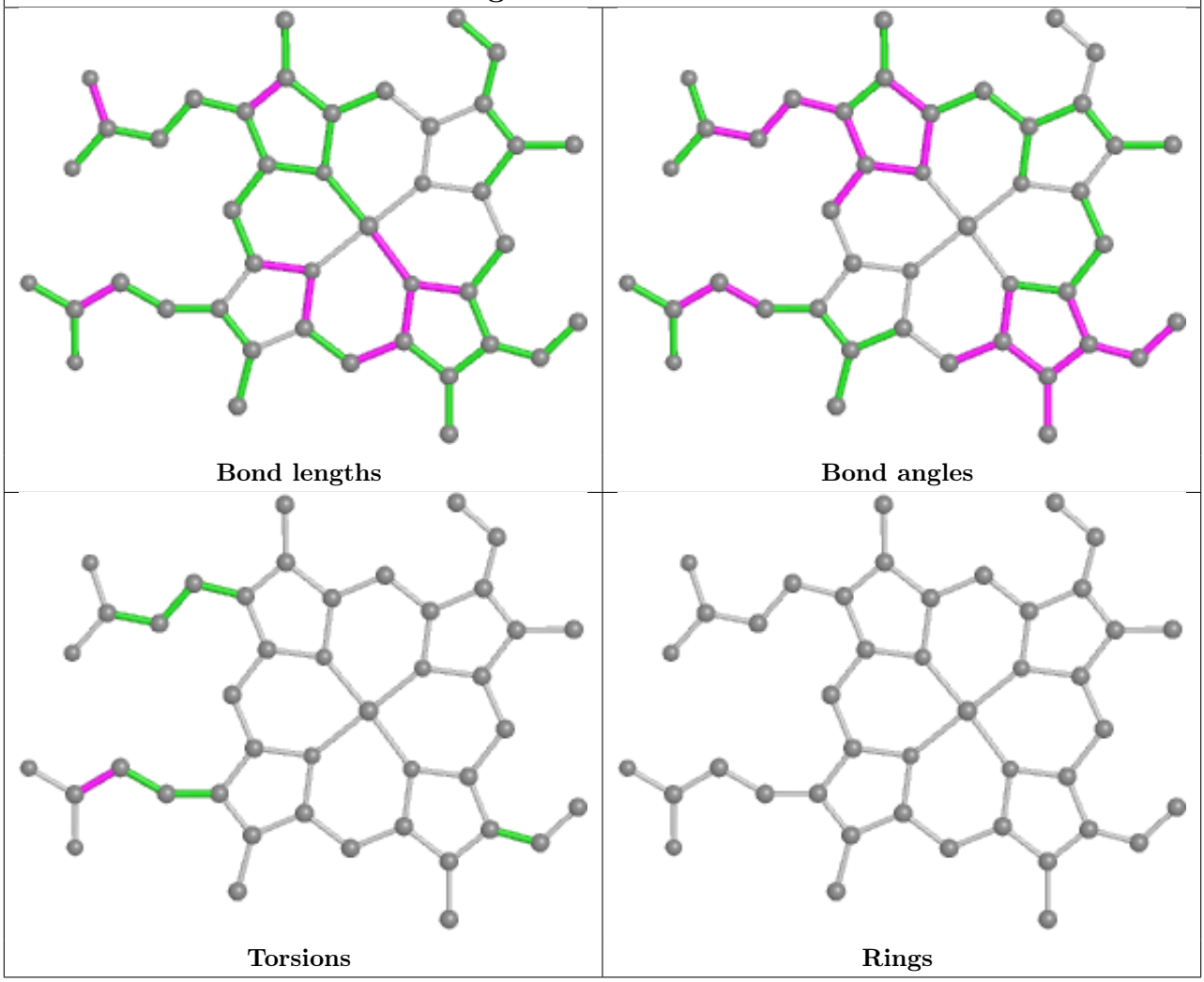


Torsions



Rings

Ligand HEM B 801



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	712/728 (97%)	-0.50	7 (0%)	82	83	15, 23, 40, 87	0
1	B	712/728 (97%)	-0.46	9 (1%)	77	79	15, 22, 40, 84	0
All	All	1424/1456 (97%)	-0.48	16 (1%)	80	82	15, 22, 40, 87	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	ARG	4.5
1	B	608	LYS	4.3
1	B	748	ALA	4.1
1	A	748	ALA	3.6
1	B	679	ALA	3.5
1	B	610	ARG	3.3
1	B	540	ARG	3.2
1	B	680	ALA	2.9
1	B	366	GLY	2.7
1	A	679	ALA	2.5
1	A	541	GLY	2.5
1	B	541	GLY	2.4
1	A	610	ARG	2.4
1	A	680	ALA	2.3
1	A	647	GLN	2.1
1	B	454	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	TOX	A	111[A]	16/17	0.97	0.11	15,17,22,22	2
1	TOX	A	111[B]	16/17	0.97	0.11	15,17,18,22	2
1	TOX	B	111[A]	16/17	0.98	0.12	15,16,23,23	1
1	TOX	B	111[B]	16/17	0.98	0.12	15,16,19,23	1

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

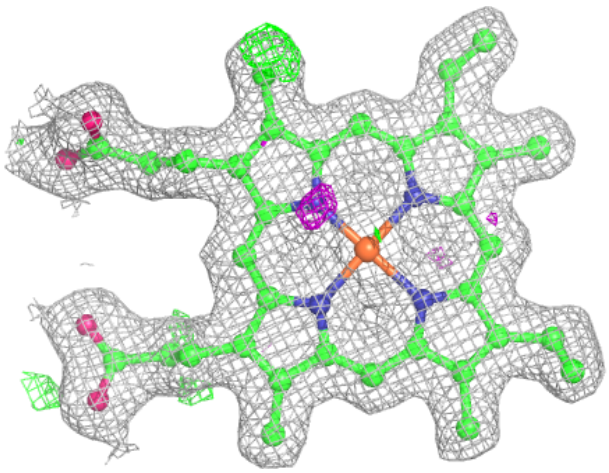
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

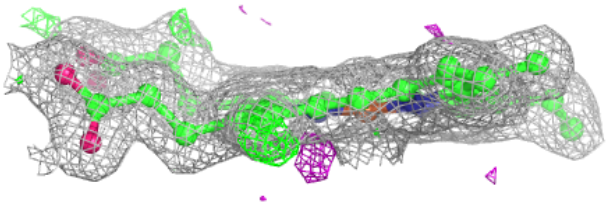
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MPD	A	805	8/8	0.90	0.17	57,67,71,73	0
6	MPD	B	805	8/8	0.92	0.13	54,59,62,63	0
6	MPD	A	806	8/8	0.93	0.15	43,45,52,57	0
4	OXY	A	803	2/2	0.93	0.18	34,34,34,39	0
4	OXY	B	803	2/2	0.94	0.15	32,32,32,35	0
5	PO4	B	804	5/5	0.95	0.22	46,55,64,67	0
5	PO4	A	804	5/5	0.96	0.12	45,58,63,68	0
2	HEM	B	801	43/43	0.99	0.11	15,17,19,21	0
2	HEM	A	801	43/43	0.99	0.09	15,17,20,21	0
3	NA	B	802	1/1	1.00	0.06	20,20,20,20	0
3	NA	A	802	1/1	1.00	0.08	18,18,18,18	0

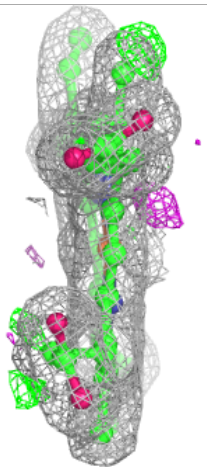
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM 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)

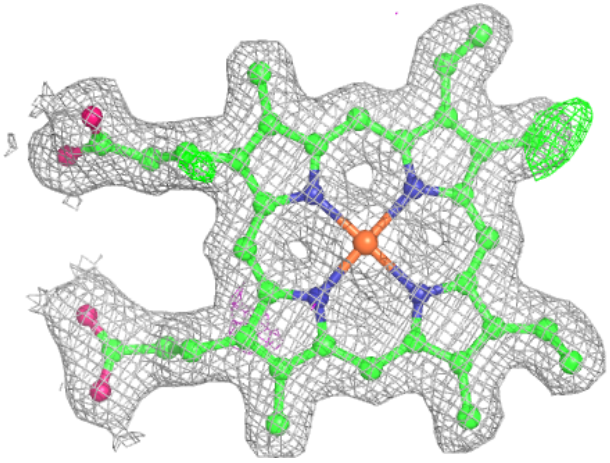


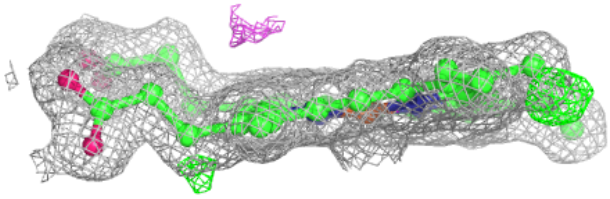


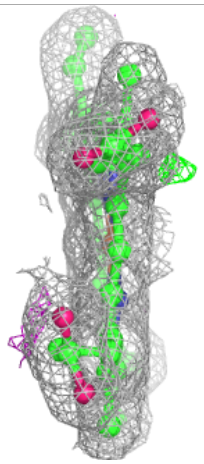


Electron density around HEM A 801:

$2mF_o$-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.