



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 06:07 AM EDT

PDB ID : 5SX7 / pdb_00005sx7
Title : Crystal structure of catalase-peroxidase KatG of B. pseudomallei at pH 8.5
Authors : Loewen, P.C.
Deposited on : 2016-08-09
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 ⓘ 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 ⓘ](#)) 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

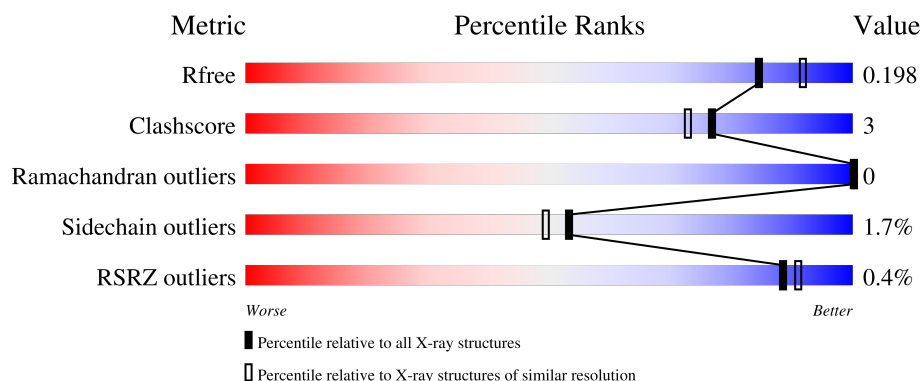
1 Overall quality at a glance

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 $\leq 5\%$. 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	% 88% 9% ..
1	B	728	 88% 9% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	TRS	A	807	-	X	-	-

2 Entry composition [i](#)

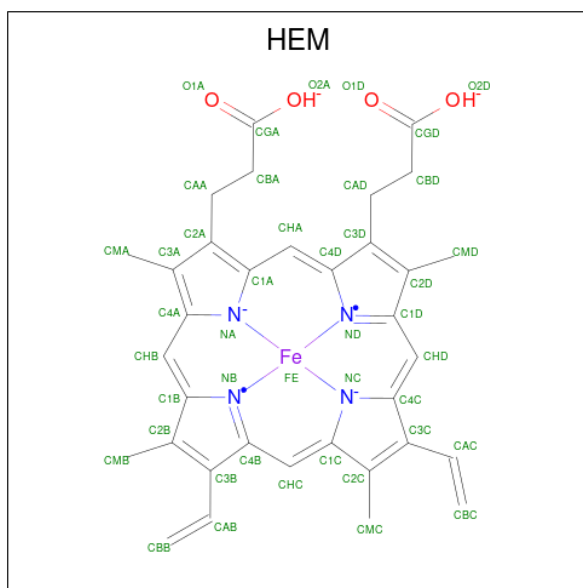
There are 7 unique types of molecules in this entry. The entry contains 12705 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	713	Total	C	N	O	S	0	7	0
			5538	3497	983	1044	14			
1	B	713	Total	C	N	O	S	0	6	0
			5539	3498	986	1041	14			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

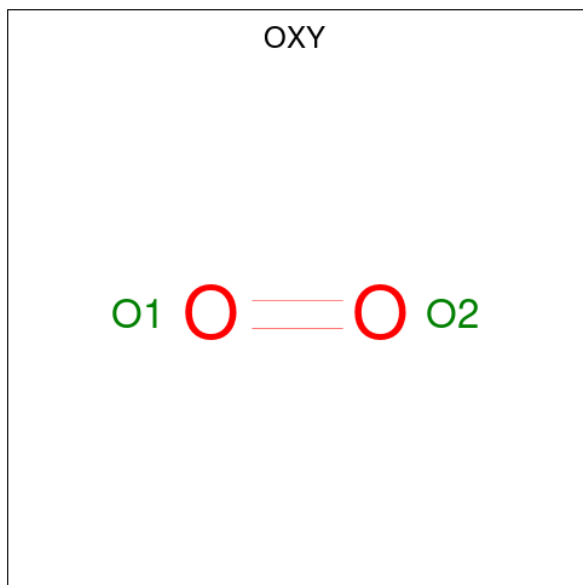


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

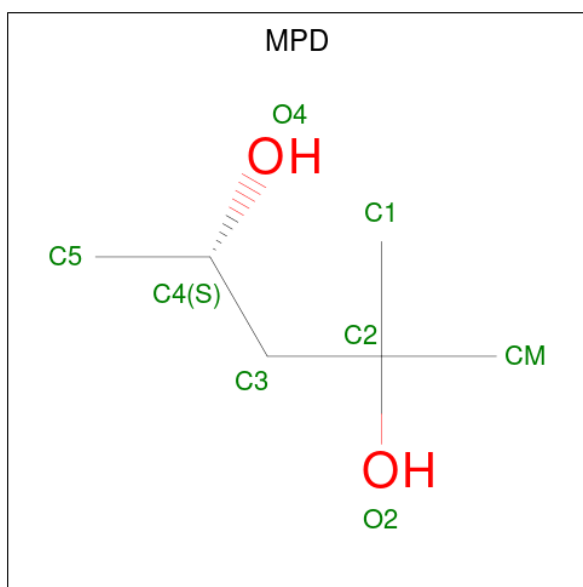
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



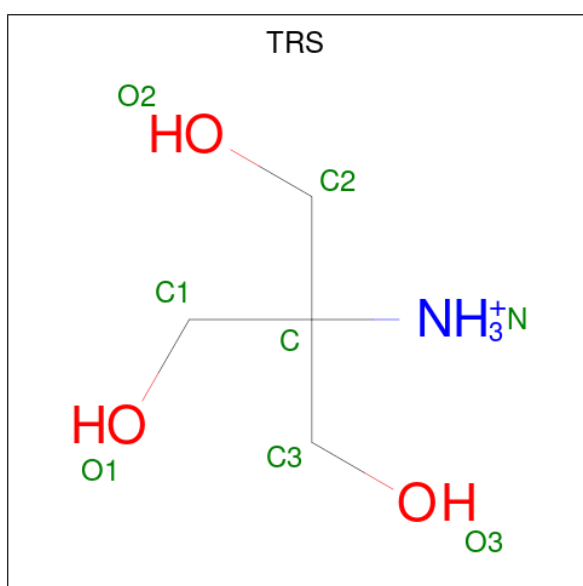
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 2	O 2	0	0
4	B	1	Total 2	O 2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	B	1	Total	C	N	O	0	0
			8	4	1	3		
6	B	1	Total	C	N	O	0	0
			8	4	1	3		

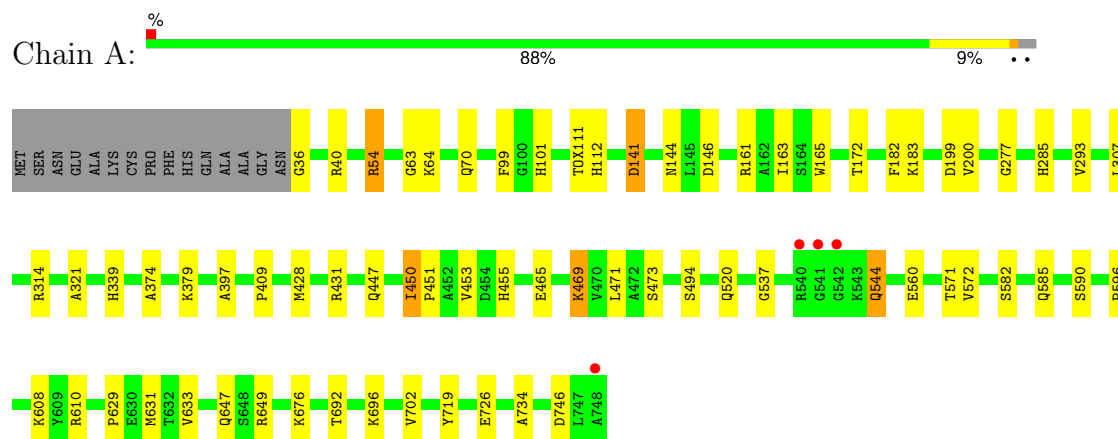
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	709	Total	O	0	0
			709	709		
7	B	763	Total	O	0	0
			763	763		

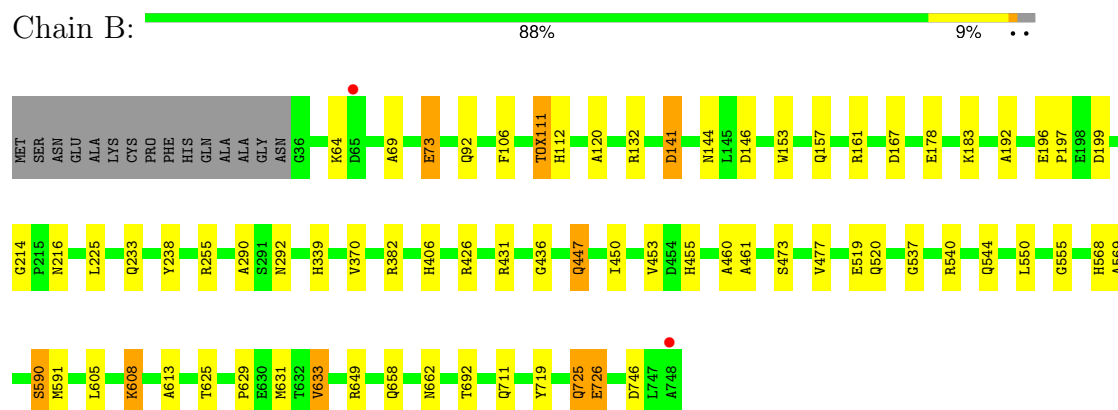
3 Residue-property plots [i](#)

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



• Molecule 1: Catalase-peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.41Å 114.95Å 174.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 20.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-1.95) 91.0 (20.00-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.151 , 0.189 0.164 , 0.198	Depositor DCC
R_{free} test set	6673 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12705	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TOX, MPD, TRS, HEM, 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	1.58	32/5683 (0.6%)	1.20	4/7724 (0.1%)
1	B	1.57	38/5686 (0.7%)	1.19	10/7727 (0.1%)
All	All	1.57	70/11369 (0.6%)	1.19	14/15451 (0.1%)

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	ASP	C-O	8.29	1.34	1.23
1	A	453	VAL	C-O	-8.26	1.14	1.24
1	A	101	HIS	C-O	8.11	1.33	1.23
1	A	285	HIS	C-O	7.80	1.32	1.23
1	A	726	GLU	CG-CD	7.65	1.71	1.52
1	B	450	ILE	C-O	-7.62	1.16	1.23
1	A	726	GLU	CD-OE1	7.26	1.39	1.25
1	A	428	MET	C-O	-6.89	1.15	1.24
1	B	519	GLU	CA-CB	6.80	1.64	1.53
1	B	692	THR	C-O	-6.77	1.15	1.24
1	A	450	ILE	C-O	-6.66	1.17	1.23
1	A	676	LYS	CA-C	-6.66	1.45	1.52
1	A	200	VAL	N-CA	6.45	1.53	1.46
1	B	537	GLY	C-O	-6.45	1.16	1.24
1	A	596	PRO	CA-C	-6.40	1.46	1.53
1	A	494	SER	CA-C	6.36	1.60	1.52
1	B	370	VAL	C-O	-6.34	1.17	1.24
1	A	36	GLY	N-CA	6.29	1.55	1.45
1	A	314	ARG	C-O	-6.27	1.18	1.24
1	A	165	TRP	CA-C	6.25	1.61	1.52
1	A	307	LEU	N-CA	-6.18	1.38	1.45
1	A	473	SER	C-O	-6.15	1.16	1.24
1	B	746	ASP	C-O	-6.09	1.16	1.24
1	B	477	VAL	N-CA	6.04	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	157	GLN	N-CA	-6.04	1.39	1.46
1	A	277	GLY	C-O	-6.00	1.16	1.23
1	A	746	ASP	C-O	-6.00	1.16	1.24
1	A	63	GLY	N-CA	5.95	1.53	1.45
1	B	216	ASN	CA-C	5.93	1.60	1.53
1	B	153	TRP	CA-C	5.88	1.60	1.52
1	B	436	GLY	C-O	-5.84	1.16	1.24
1	B	225	LEU	C-O	-5.80	1.17	1.24
1	B	658	GLN	CD-NE2	-5.79	1.21	1.33
1	B	447	GLN	CA-C	5.68	1.60	1.52
1	B	132	ARG	CZ-NH1	5.66	1.40	1.32
1	B	555	GLY	N-CA	5.65	1.52	1.45
1	A	163	ILE	C-O	5.62	1.29	1.24
1	A	726	GLU	CD-OE2	5.58	1.35	1.25
1	A	397	ALA	N-CA	-5.54	1.39	1.46
1	B	106	PHE	C-O	-5.53	1.17	1.24
1	B	233	GLN	N-CA	5.53	1.52	1.45
1	B	461	ALA	N-CA	5.53	1.53	1.46
1	B	453	VAL	C-O	-5.52	1.17	1.24
1	B	746	ASP	CA-CB	5.51	1.63	1.53
1	B	631	MET	C-O	5.49	1.30	1.24
1	B	214	GLY	C-O	5.48	1.31	1.24
1	A	631	MET	C-O	5.44	1.30	1.24
1	A	293	VAL	C-O	-5.40	1.18	1.24
1	B	382	ARG	CZ-NH1	5.38	1.40	1.32
1	B	199	ASP	N-CA	5.37	1.53	1.46
1	B	608	LYS	N-CA	5.35	1.53	1.46
1	B	167	ASP	CG-OD2	5.34	1.35	1.25
1	B	426	ARG	CZ-NH2	5.30	1.40	1.33
1	B	519	GLU	C-N	-5.30	1.27	1.33
1	B	192	ALA	N-CA	5.28	1.52	1.46
1	A	537	GLY	C-O	-5.27	1.17	1.24
1	B	92	GLN	CD-NE2	-5.24	1.22	1.33
1	B	292	ASN	N-CA	-5.24	1.39	1.46
1	A	734	ALA	N-CA	-5.21	1.40	1.46
1	B	161	ARG	CA-CB	5.21	1.62	1.53
1	B	550	LEU	CA-CB	5.21	1.61	1.53
1	A	321	ALA	C-O	-5.18	1.17	1.23
1	B	625	THR	CA-CB	5.18	1.61	1.53
1	A	182	PHE	C-O	-5.16	1.18	1.24
1	B	183	LYS	C-O	-5.14	1.17	1.24
1	A	172	THR	CA-C	5.08	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	ARG	CA-C	-5.06	1.46	1.53
1	B	473	SER	C-O	-5.01	1.17	1.24
1	A	451	PRO	C-O	-5.00	1.17	1.23
1	A	702	VAL	C-O	5.00	1.30	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	726	GLU	CB-CG-CD	7.63	125.57	112.60
1	B	725	GLN	CB-CG-CD	6.18	123.10	112.60
1	B	519	GLU	CB-CG-CD	-5.67	102.95	112.60
1	A	54	ARG	CG-CD-NE	-5.66	99.56	112.00
1	A	692	THR	N-CA-C	5.62	120.41	113.50
1	B	64	LYS	CB-CA-C	-5.61	101.48	110.79
1	B	633[A]	VAL	CB-CA-C	-5.60	104.58	112.14
1	B	633[B]	VAL	CB-CA-C	-5.60	104.58	112.14
1	A	70	GLN	CA-CB-CG	5.38	124.85	114.10
1	B	73	GLU	CB-CA-C	-5.35	100.72	110.63
1	B	153	TRP	CA-C-N	-5.34	113.12	119.05
1	B	153	TRP	C-N-CA	-5.34	113.12	119.05
1	B	460	ALA	N-CA-C	5.05	116.78	111.28
1	B	120	ALA	N-CA-C	5.05	116.47	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	5538	0	5333	29	0
1	B	5539	0	5345	30	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	1	0
5	A	16	0	28	1	0
5	B	16	0	28	7	0
6	A	16	0	24	1	0
6	B	16	0	24	0	0
7	A	709	0	0	11	1
7	B	763	0	0	9	1
All	All	12705	0	10842	64	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 3.

All (64) 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:339[B]:HIS:CE1	7:A:901:HOH:O	1.95	1.19
1:A:339[B]:HIS:ND1	7:A:901:HOH:O	1.85	1.09
1:B:255[A]:ARG:HD3	7:B:1008:HOH:O	1.70	0.92
1:B:339[A]:HIS:HE1	1:B:406:HIS:HA	1.37	0.87
1:A:560:GLU:OE1	7:A:902:HOH:O	1.93	0.87
6:A:807:TRS:H22	7:B:1466:HOH:O	1.79	0.82
1:A:339[B]:HIS:HE1	7:A:1229:HOH:O	1.67	0.77
4:B:804:OXY:O2	7:B:901:HOH:O	2.03	0.75
1:B:339[A]:HIS:CE1	1:B:406:HIS:HA	2.19	0.75
5:B:805:MPD:O4	5:B:805:MPD:C1	2.41	0.69
5:B:805:MPD:O4	5:B:805:MPD:H12	1.94	0.67
1:B:711[A]:GLN:NE2	7:B:905:HOH:O	2.30	0.63
1:B:178:GLU:OE1	7:B:902:HOH:O	2.16	0.62
1:B:69:ALA:O	1:B:73:GLU:HG2	2.01	0.61
1:B:569:ALA:H	5:B:806:MPD:CM	2.16	0.59
1:A:339[B]:HIS:CG	1:A:409:PRO:HB3	2.40	0.57
1:A:339[B]:HIS:CD2	1:A:409:PRO:HB3	2.39	0.56
1:B:726:GLU:OE1	5:B:806:MPD:H13	2.06	0.55
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.42	0.54
1:B:455:HIS:CE1	1:B:544:GLN:HG3	2.44	0.53
1:A:54:ARG:NE	1:A:199:ASP:OD2	2.39	0.51
1:A:455:HIS:CE1	1:A:544:GLN:HG3	2.46	0.51
1:B:290:ALA:HB2	5:B:805:MPD:H52	1.92	0.50
1:A:633[A]:VAL:HG22	1:A:719:TYR:CZ	2.47	0.49
1:B:633[B]:VAL:HG13	1:B:719:TYR:CZ	2.48	0.49
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:LEU:HD11	1:B:613:ALA:HB2	1.95	0.48
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.14	0.48
1:B:725:GLN:NE2	7:B:926:HOH:O	2.47	0.48
1:A:560:GLU:HG3	1:A:572:VAL:HG23	1.94	0.48
1:A:431:ARG:HG3	7:A:1091:HOH:O	2.14	0.47
5:A:804:MPD:H52	7:A:1572:HOH:O	2.14	0.47
1:A:465:GLU:OE2	1:A:469:LYS:HE3	2.15	0.47
1:B:290:ALA:CB	5:B:805:MPD:H52	2.44	0.46
1:B:662:ASN:H	1:B:725:GLN:HE22	1.63	0.46
1:A:339[A]:HIS:HB2	7:A:1408:HOH:O	2.15	0.46
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.15	0.46
1:A:629:PRO:O	1:A:633[A]:VAL:HG23	2.16	0.45
1:A:339[B]:HIS:CE1	1:A:409:PRO:HB3	2.51	0.45
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE1	2.51	0.45
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.17	0.45
1:B:591:MET:HE2	7:B:903:HOH:O	2.17	0.45
1:A:339[B]:HIS:CE1	7:A:1229:HOH:O	2.52	0.45
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.47	0.45
1:A:99:PHE:CD2	1:A:374:ALA:HA	2.52	0.45
1:A:339[A]:HIS:HB2	7:A:1138:HOH:O	2.17	0.44
1:A:696:LYS:HE2	7:A:1015:HOH:O	2.17	0.44
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	3.01	0.43
1:A:465:GLU:O	1:A:469:LYS:HD3	2.19	0.43
1:B:633[B]:VAL:CG1	1:B:719:TYR:CZ	3.02	0.42
1:B:568:HIS:HA	5:B:806:MPD:HM2	2.00	0.42
1:A:183:LYS:HB3	1:A:183:LYS:HE2	1.90	0.42
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.19	0.42
1:B:111:TOX:H9	1:B:238:TYR:OH	2.19	0.42
1:B:431:ARG:HG3	7:B:1043:HOH:O	2.19	0.42
1:A:571:THR:OG1	7:A:903:HOH:O	2.21	0.42
1:B:633[B]:VAL:HG13	1:B:719:TYR:CE1	2.54	0.41
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.95	0.41
1:B:196:GLU:HB2	1:B:197:PRO:HD2	2.03	0.41
1:B:112:HIS:CE1	1:B:141:ASP:O	2.74	0.41
1:B:590:SER:OG	7:B:903:HOH:O	2.22	0.41
1:A:647:GLN:CD	1:A:647:GLN:N	2.79	0.40
1:A:112:HIS:CE1	1:A:141:ASP:O	2.74	0.40
1:A:582:SER:OG	1:A:585:GLN:HG3	2.22	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:1558:HOH:O	7:B:1618:HOH:O[4_445]	1.80	0.40

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	716/728 (98%)	708 (99%)	8 (1%)	0	100	100
1	B	716/728 (98%)	707 (99%)	9 (1%)	0	100	100
All	All	1432/1456 (98%)	1415 (99%)	17 (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	555/560 (99%)	542 (98%)	13 (2%)	44	38
1	B	555/560 (99%)	549 (99%)	6 (1%)	65	64
All	All	1110/1120 (99%)	1091 (98%)	19 (2%)	53	49

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	64	LYS
1	A	141	ASP

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Mol	Chain	Res	Type
1	A	161	ARG
1	A	379	LYS
1	A	450	ILE
1	A	469	LYS
1	A	520	GLN
1	A	544	GLN
1	A	590	SER
1	A	608	LYS
1	A	610	ARG
1	A	649	ARG
1	B	141	ASP
1	B	520	GLN
1	B	590	SER
1	B	608	LYS
1	B	649	ARG
1	B	726	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	520	GLN
1	B	45	ASN
1	B	520	GLN
1	B	725	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	A	111[A]	2	14,17,18	2.84	7 (50%)	12,23,25	3.10	7 (58%)
1	TOX	B	111	1,2	14,17,18	2.04	4 (28%)	12,23,25	2.60	8 (66%)
1	TOX	A	111[B]	-	14,17,18	2.84	7 (50%)	12,23,25	3.10	7 (58%)

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	A	111[A]	2	-	2/5/8/10	0/2/2/2
1	TOX	B	111	1,2	-	2/5/8/10	0/2/2/2
1	TOX	A	111[B]	-	-	2/5/8/10	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[A]	TOX	CD2-CE2	5.44	1.48	1.41
1	A	111[B]	TOX	CD2-CE2	5.44	1.48	1.41
1	B	111	TOX	O-C	4.55	1.37	1.20
1	A	111[A]	TOX	O-C	4.15	1.35	1.20
1	A	111[B]	TOX	O-C	4.15	1.35	1.20
1	A	111[A]	TOX	O1-NE1	3.88	1.44	1.39
1	A	111[B]	TOX	O1-NE1	3.88	1.44	1.39
1	A	111[A]	TOX	CE2-NE1	-3.45	1.33	1.39
1	A	111[B]	TOX	CE2-NE1	-3.45	1.33	1.39
1	A	111[A]	TOX	CE3-CD2	-3.27	1.35	1.39
1	A	111[B]	TOX	CE3-CD2	-3.27	1.35	1.39
1	B	111	TOX	CD1-CG	3.25	1.43	1.36
1	B	111	TOX	CD2-CE2	2.96	1.45	1.41
1	A	111[A]	TOX	CH2-CZ2	2.94	1.43	1.38
1	A	111[B]	TOX	CH2-CZ2	2.94	1.43	1.38
1	B	111	TOX	CD2-CG	2.84	1.48	1.44
1	A	111[A]	TOX	CH2-CZ3	2.34	1.43	1.38
1	A	111[B]	TOX	CH2-CZ3	2.34	1.43	1.38

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[A]	TOX	CZ2-CE2-CD2	-5.65	115.65	121.95
1	A	111[B]	TOX	CZ2-CE2-CD2	-5.65	115.65	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[A]	TOX	CZ2-CE2-NE1	5.46	138.06	129.37
1	A	111[B]	TOX	CZ2-CE2-NE1	5.46	138.06	129.37
1	A	111[A]	TOX	CZ3-CH2-CZ2	-4.21	115.04	120.24
1	A	111[B]	TOX	CZ3-CH2-CZ2	-4.21	115.04	120.24
1	B	111	TOX	CD2-CG-CD1	3.91	109.89	106.34
1	B	111	TOX	CE2-CD2-CG	-3.88	103.82	107.39
1	A	111[A]	TOX	CH2-CZ2-CE2	3.64	125.62	118.28
1	A	111[B]	TOX	CH2-CZ2-CE2	3.64	125.62	118.28
1	B	111	TOX	CZ2-CE2-NE1	3.46	134.89	129.37
1	B	111	TOX	CB-CG-CD1	-3.07	122.40	126.67
1	A	111[A]	TOX	CB-CG-CD1	3.06	130.92	126.67
1	A	111[B]	TOX	CB-CG-CD1	3.06	130.92	126.67
1	B	111	TOX	CZ2-CE2-CD2	-2.95	118.66	121.95
1	B	111	TOX	CZ3-CH2-CZ2	-2.81	116.78	120.24
1	B	111	TOX	CH2-CZ2-CE2	2.45	123.22	118.28
1	B	111	TOX	CE3-CD2-CG	2.17	137.09	133.85
1	A	111[A]	TOX	CE2-CD2-CG	-2.06	105.50	107.39
1	A	111[B]	TOX	CE2-CD2-CG	-2.06	105.50	107.39
1	A	111[A]	TOX	CB-CG-CD2	-2.01	122.83	126.70
1	A	111[B]	TOX	CB-CG-CD2	-2.01	122.83	126.70

There are no chirality outliers.

All (6) 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	TOX	N-CA-CB-CG
1	B	111	TOX	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	111	TOX	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	HEM	B	802	1	50,50,50	1.70	9 (18%)	67,82,82	1.63	11 (16%)
4	OXY	A	803	-	1,1,1	0.26	0	-		
6	TRS	B	807	-	7,7,7	1.13	1 (14%)	9,9,9	1.00	1 (11%)
6	TRS	A	806	-	7,7,7	0.75	0	9,9,9	0.70	0
6	TRS	A	807	-	7,7,7	0.90	0	9,9,9	2.16	4 (44%)
2	HEM	A	801	1	50,50,50	1.83	11 (22%)	67,82,82	1.65	12 (17%)
5	MPD	B	806	-	7,7,7	1.18	1 (14%)	9,10,10	2.17	3 (33%)
4	OXY	B	804	-	1,1,1	0.02	0	-		
5	MPD	B	805	-	7,7,7	0.53	0	9,10,10	1.51	1 (11%)
6	TRS	B	801	-	7,7,7	1.09	0	9,9,9	2.02	4 (44%)
5	MPD	A	805	-	7,7,7	0.64	0	9,10,10	1.20	1 (11%)
5	MPD	A	804	-	7,7,7	0.61	0	9,10,10	1.37	1 (11%)

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
2	HEM	B	802	1	-	3/14/54/54	-
6	TRS	B	807	-	-	3/9/9/9	-
6	TRS	A	806	-	-	1/9/9/9	-
6	TRS	A	807	-	-	6/9/9/9	-
2	HEM	A	801	1	-	2/14/54/54	-
5	MPD	B	806	-	-	2/5/5/5	-
6	TRS	B	801	-	-	3/9/9/9	-
5	MPD	B	805	-	-	3/5/5/5	-
5	MPD	A	805	-	-	3/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	A	804	-	-	0/5/5/5	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	HEM	C1B-NB	-5.48	1.30	1.40
2	A	801	HEM	C1B-NB	-5.10	1.31	1.40
2	A	801	HEM	C4D-C3D	5.04	1.53	1.45
2	A	801	HEM	FE-NB	4.56	2.08	1.94
2	B	802	HEM	FE-NB	4.45	2.08	1.94
2	A	801	HEM	FE-NC	3.83	2.07	1.95
2	B	802	HEM	CHC-C1C	3.49	1.45	1.38
2	A	801	HEM	C1A-NA	3.22	1.45	1.39
2	B	802	HEM	C4D-ND	-2.91	1.35	1.40
2	A	801	HEM	CMC-C2C	-2.78	1.45	1.50
2	A	801	HEM	O1A-CGA	2.72	1.31	1.22
2	A	801	HEM	C4D-ND	-2.67	1.35	1.40
2	B	802	HEM	FE-NC	2.58	2.03	1.95
2	A	801	HEM	FE-NA	2.43	2.03	1.95
5	B	806	MPD	O2-C2	2.35	1.50	1.44
2	A	801	HEM	CHA-C1A	-2.21	1.34	1.39
2	B	802	HEM	C1B-C2B	-2.19	1.40	1.44
6	B	807	TRS	C2-C	2.19	1.58	1.53
2	B	802	HEM	C1D-ND	-2.16	1.34	1.38
2	A	801	HEM	CHD-C4C	2.11	1.42	1.38
2	B	802	HEM	O1A-CGA	2.10	1.28	1.22
2	B	802	HEM	FE-NA	2.05	2.01	1.95

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C3B-C2B-C1B	5.72	110.70	106.41
2	A	801	HEM	C4B-C3B-C2B	-4.99	102.69	107.28
2	B	802	HEM	CHC-C4B-NB	4.65	129.43	124.42
5	B	806	MPD	O2-C2-C1	4.33	121.50	107.99
2	B	802	HEM	CHA-C4D-ND	3.88	129.16	124.37
6	B	801	TRS	O3-C3-C	-3.78	100.33	110.88
2	B	802	HEM	CAA-CBA-CGA	-3.77	103.67	113.67
2	B	802	HEM	C3B-C4B-NB	-3.63	106.86	109.47
6	A	807	TRS	C2-C-C1	-3.56	101.18	110.66
2	B	802	HEM	C1B-NB-C4B	3.44	109.28	105.21
2	B	802	HEM	O2D-CGD-CBD	3.40	124.74	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	HEM	CHC-C1C-NC	-3.33	120.83	124.45
6	A	807	TRS	C2-C-N	3.28	116.53	108.17
5	B	805	MPD	CM-C2-C1	-3.26	103.33	110.63
2	A	801	HEM	CHC-C1C-NC	3.22	127.96	124.45
5	B	806	MPD	C1-C2-C3	-2.98	97.32	110.20
2	B	802	HEM	CHA-C4D-C3D	-2.81	120.04	125.23
6	A	807	TRS	O2-C2-C	-2.76	103.18	110.88
2	A	801	HEM	CMD-C2D-C1D	2.74	129.32	125.03
2	A	801	HEM	C4C-NC-C1C	2.70	110.23	105.82
2	A	801	HEM	O1D-CGD-CBD	-2.57	114.94	123.09
6	A	807	TRS	C3-C-C1	2.50	117.32	110.66
5	B	806	MPD	O2-C2-CM	-2.50	100.19	107.99
5	A	804	MPD	CM-C2-C3	2.48	120.90	110.20
2	A	801	HEM	C2A-C1A-NA	-2.47	107.42	110.15
2	A	801	HEM	O2D-CGD-CBD	2.45	121.75	114.00
2	A	801	HEM	CAA-CBA-CGA	-2.45	107.17	113.67
2	B	802	HEM	CHD-C4C-NC	-2.42	121.82	124.45
2	A	801	HEM	CBA-CAA-C2A	2.41	119.18	112.53
2	A	801	HEM	CHA-C4D-ND	2.37	127.30	124.37
2	A	801	HEM	C2D-C1D-ND	2.31	112.57	109.90
6	B	801	TRS	C2-C-N	-2.24	102.46	108.17
6	B	801	TRS	O1-C1-C	-2.23	104.67	110.88
2	B	802	HEM	CAB-C3B-C2B	2.23	135.67	128.43
6	B	807	TRS	C3-C-N	2.20	113.79	108.17
6	B	801	TRS	C1-C-N	2.14	113.63	108.17
2	B	802	HEM	C1A-CHA-C4D	-2.09	121.33	126.25
5	A	805	MPD	C1-C2-C3	2.01	118.88	110.20

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	805	MPD	C2-C3-C4-C5
5	B	805	MPD	C1-C2-C3-C4
6	A	807	TRS	C1-C-C2-O2
6	A	807	TRS	C3-C-C2-O2
6	A	807	TRS	N-C-C2-O2
6	B	801	TRS	N-C-C1-O1
6	B	807	TRS	C2-C-C3-O3
5	A	805	MPD	C1-C2-C3-C4
5	B	805	MPD	CM-C2-C3-C4
5	B	806	MPD	CM-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
6	A	807	TRS	C1-C-C3-O3
6	A	807	TRS	C2-C-C3-O3
6	B	801	TRS	C1-C-C3-O3
6	B	807	TRS	C1-C-C3-O3
6	A	807	TRS	N-C-C3-O3
6	B	807	TRS	N-C-C3-O3
2	B	802	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	802	HEM	CAA-CBA-CGA-O1A
6	A	806	TRS	C2-C-C3-O3
6	B	801	TRS	C2-C-C3-O3
2	A	801	HEM	CAA-CBA-CGA-O1A
5	B	805	MPD	O2-C2-C3-C4
5	A	805	MPD	CM-C2-C3-C4
5	B	806	MPD	C1-C2-C3-C4
2	B	802	HEM	CAD-CBD-CGD-O2D

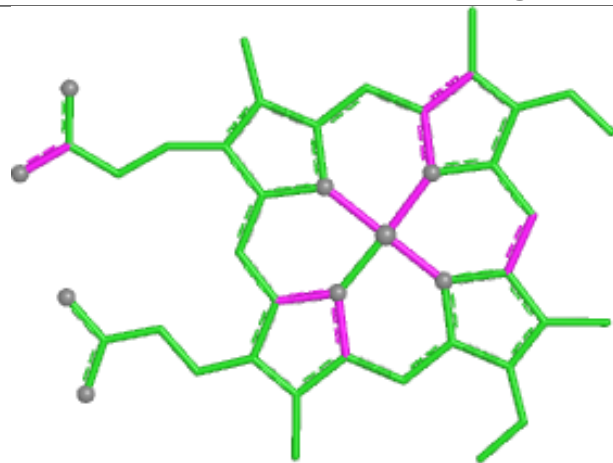
There are no ring outliers.

5 monomers are involved in 10 short contacts:

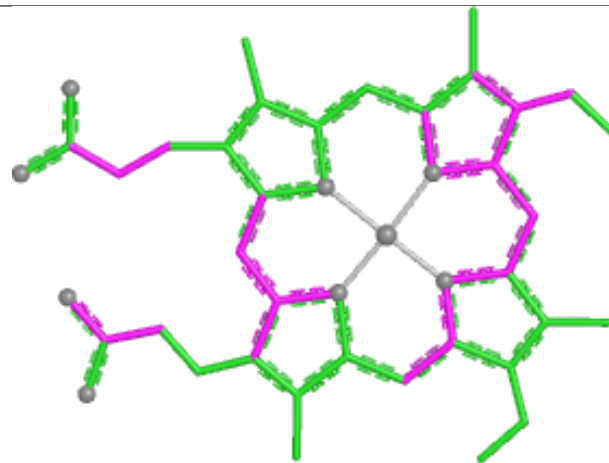
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	807	TRS	1	0
5	B	806	MPD	3	0
4	B	804	OXY	1	0
5	B	805	MPD	4	0
5	A	804	MPD	1	0

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

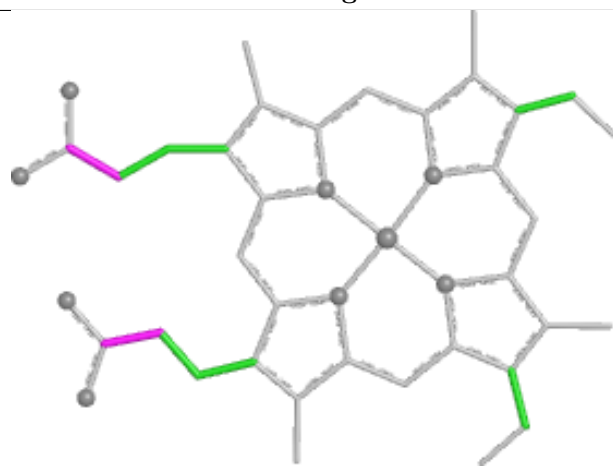
Ligand HEM B 802



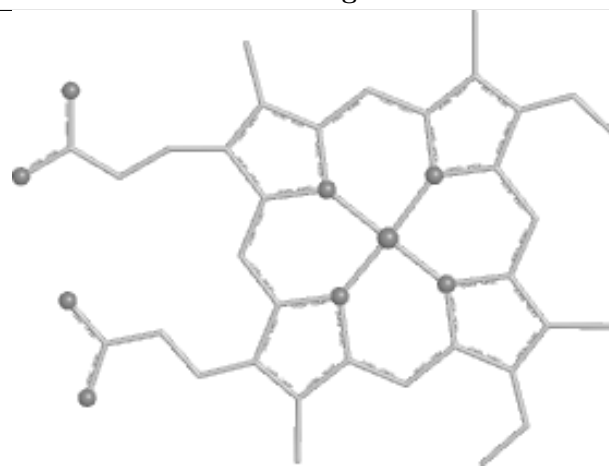
Bond lengths



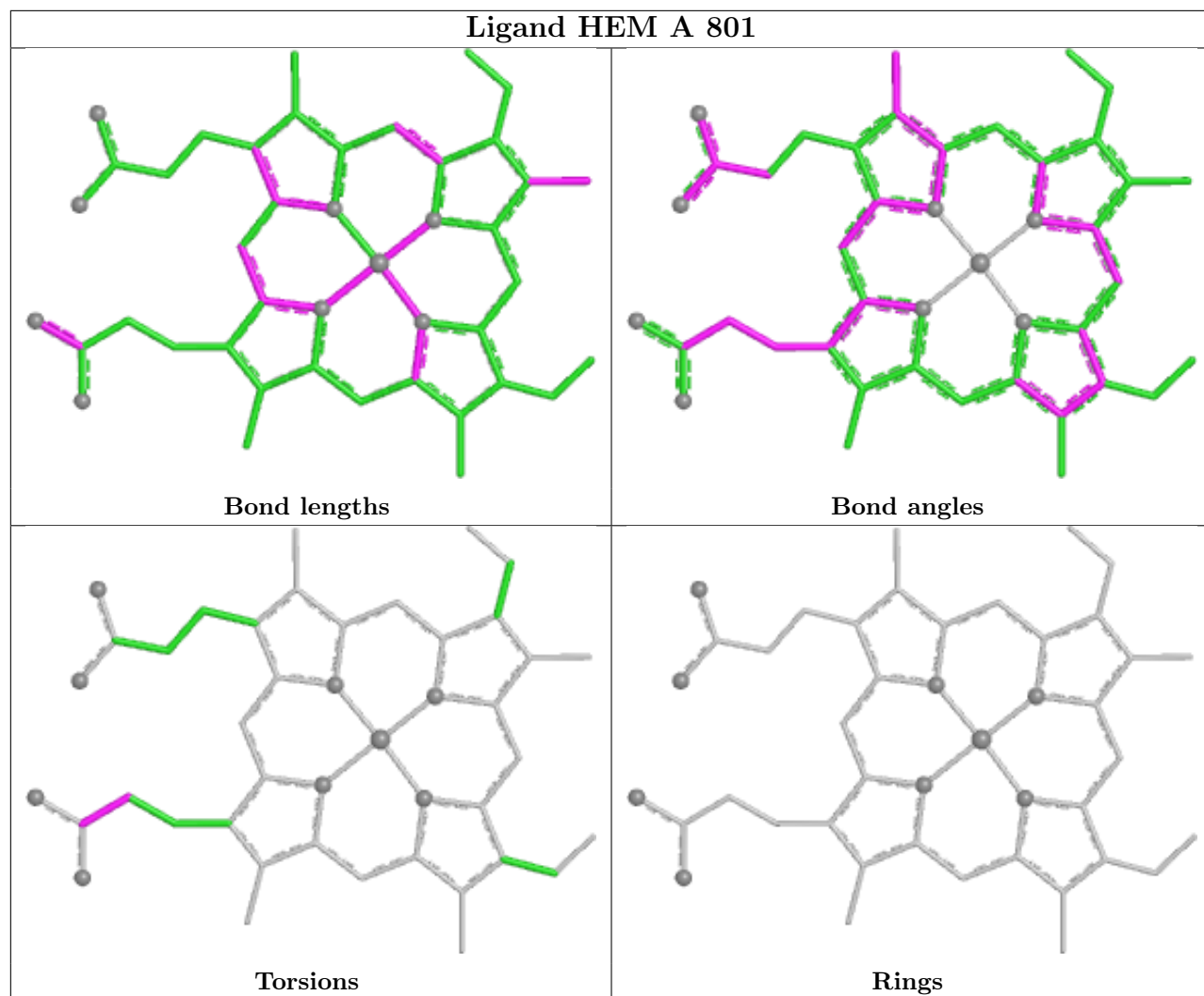
Bond angles



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	712/728 (97%)	-0.39	4 (0%) 85 89	9, 19, 35, 67	6 (0%)
1	B	712/728 (97%)	-0.53	2 (0%) 90 92	9, 18, 32, 59	6 (0%)
All	All	1424/1456 (97%)	-0.46	6 (0%) 88 91	9, 18, 33, 67	12 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	GLY	3.1
1	A	748	ALA	2.8
1	B	748	ALA	2.4
1	A	542	GLY	2.2
1	A	540	ARG	2.1
1	B	65	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	0.05	12,16,21,22	2
1	TOX	A	111[B]	16/17	0.97	0.05	12,16,19,22	2
1	TOX	B	111	16/17	0.97	0.06	13,14,25,28	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

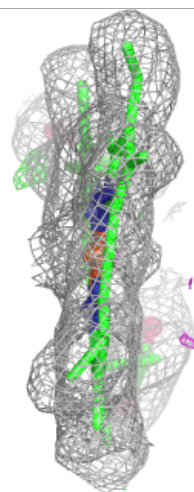
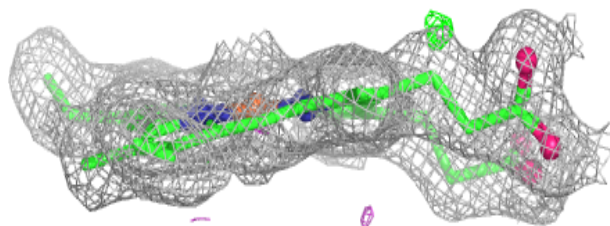
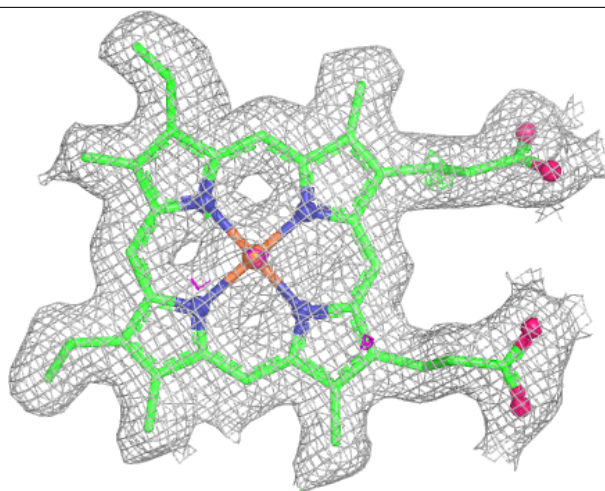
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

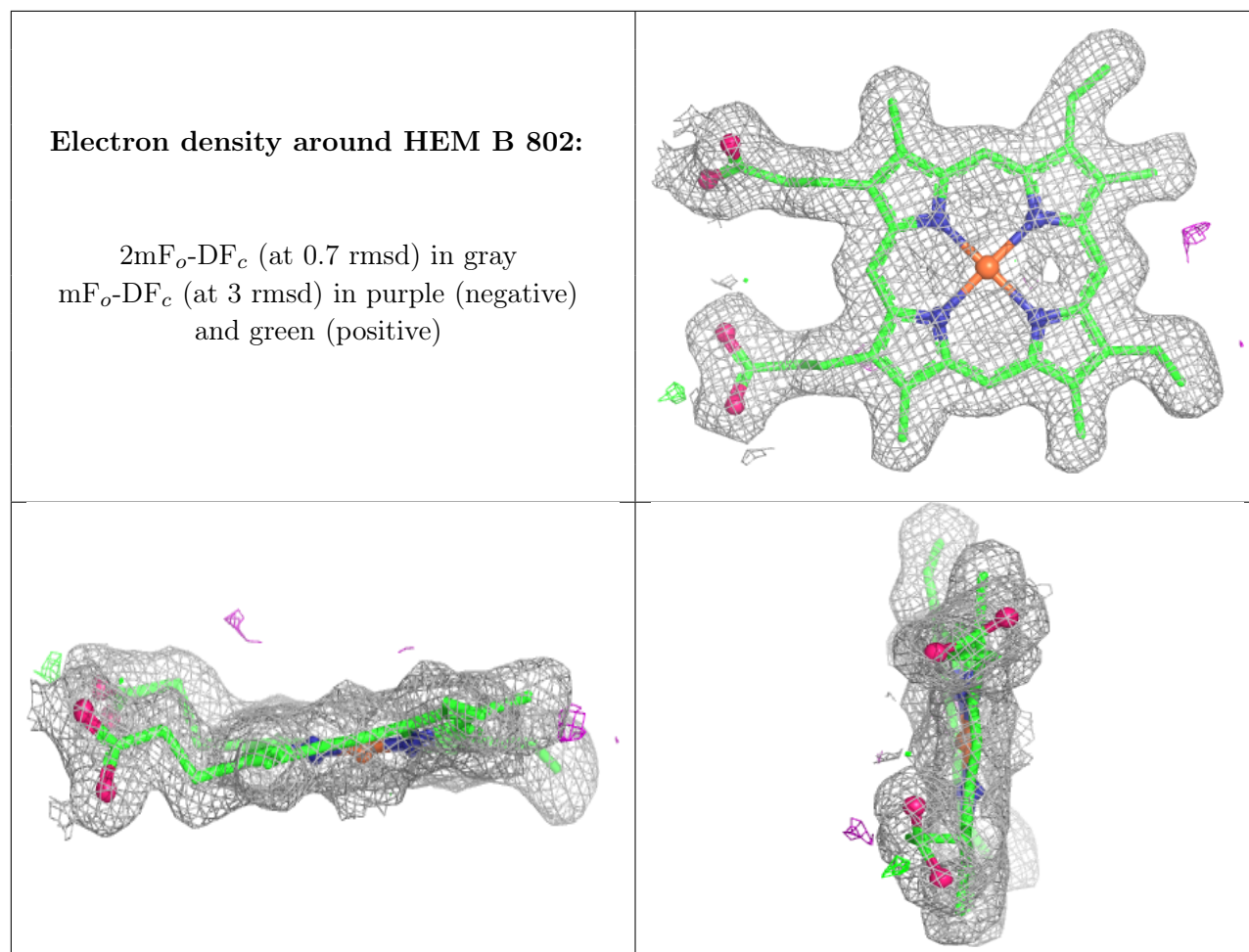
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MPD	B	806	8/8	0.80	0.21	44,54,58,64	0
5	MPD	A	805	8/8	0.85	0.15	45,48,57,59	0
5	MPD	B	805	8/8	0.86	0.14	39,47,57,60	0
6	TRS	B	801	8/8	0.87	0.13	33,43,48,48	0
6	TRS	A	807	8/8	0.88	0.10	39,43,47,47	0
5	MPD	A	804	8/8	0.90	0.14	47,52,64,67	0
4	OXY	B	804	2/2	0.95	0.17	27,27,27,35	0
6	TRS	A	806	8/8	0.97	0.06	24,27,27,30	0
4	OXY	A	803	2/2	0.97	0.15	30,30,30,36	0
3	NA	A	802	1/1	0.97	0.10	20,20,20,20	0
6	TRS	B	807	8/8	0.97	0.06	17,19,19,20	0
3	NA	B	803	1/1	0.98	0.08	16,16,16,16	0
2	HEM	A	801	43/43	0.99	0.05	14,15,16,18	0
2	HEM	B	802	43/43	0.99	0.04	13,13,14,15	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 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.