



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:23 PM UTC

PDB ID : 5KQI / pdb_00005kqi
Title : Crystal structure of the L326D variant of catalase-peroxidase from *B. pseudo-mallei*
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 ⓘ 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

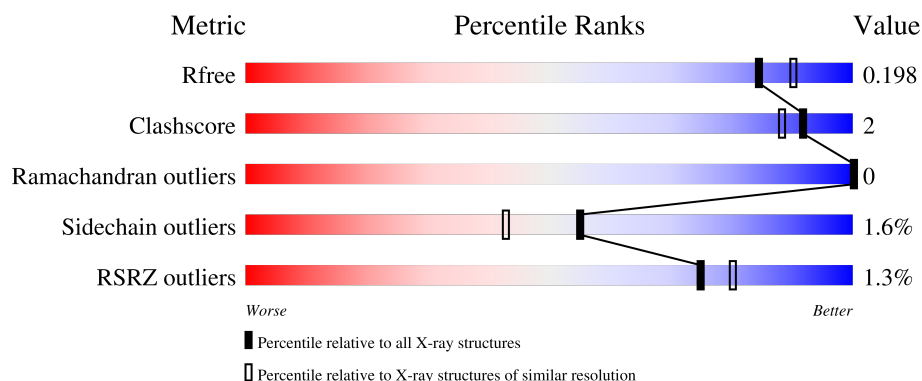
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	% 84% 13% ..
1	B	728	2% 84% 13% ..

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12535 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	714	Total	C	N	O	S	0	7	0
			5572	3513	994	1051	14			
1	B	714	Total	C	N	O	S	0	7	0
			5556	3505	988	1049	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	ASP	LEU	engineered mutation	UNP Q3JNW6
B	326	ASP	LEU	engineered mutation	UNP Q3JNW6

- 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		

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

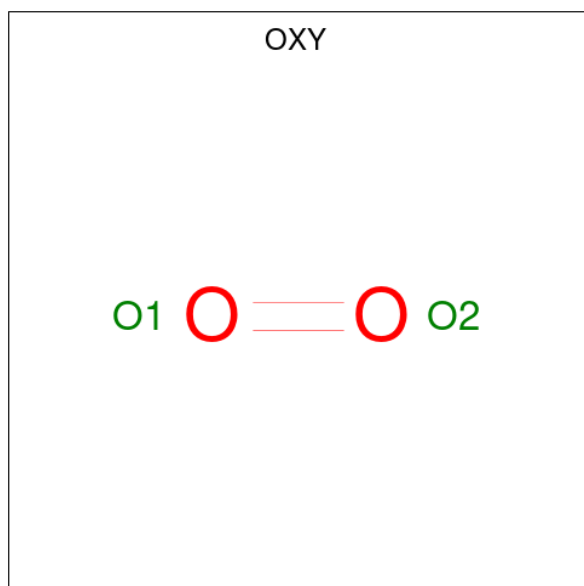
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



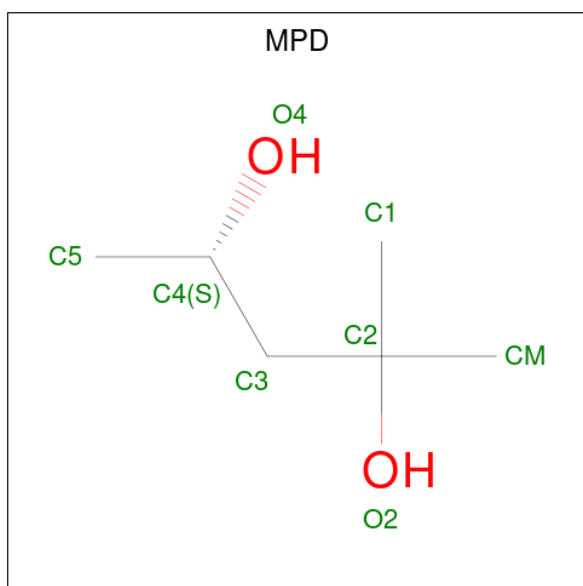
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	B	1	Total	O		
			2	2	0	0

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



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

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

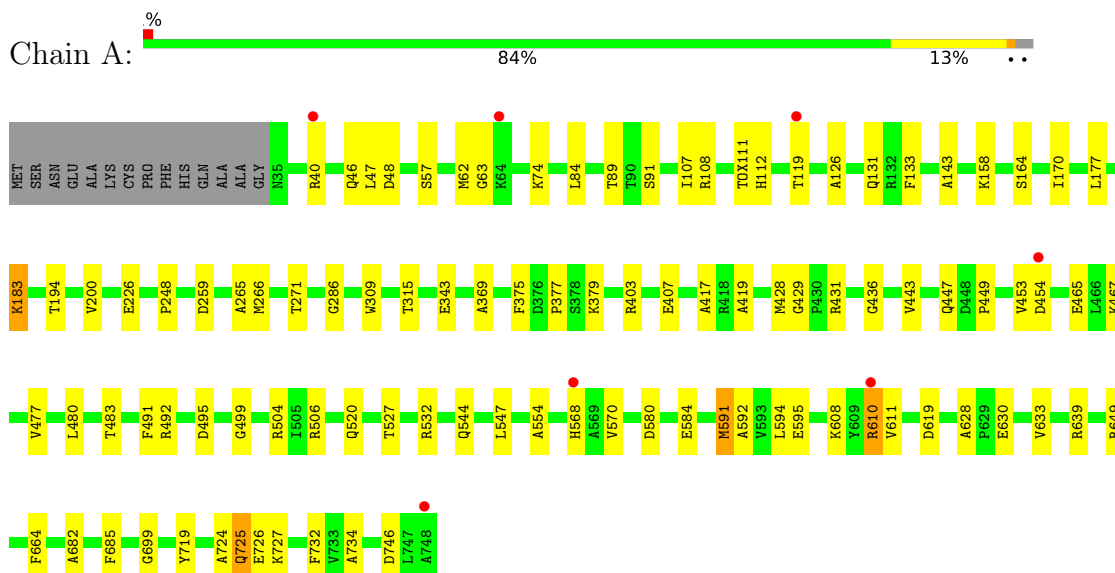
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	627	Total	O	0	0
			627	627		
8	B	644	Total	O	0	0
			644	644		

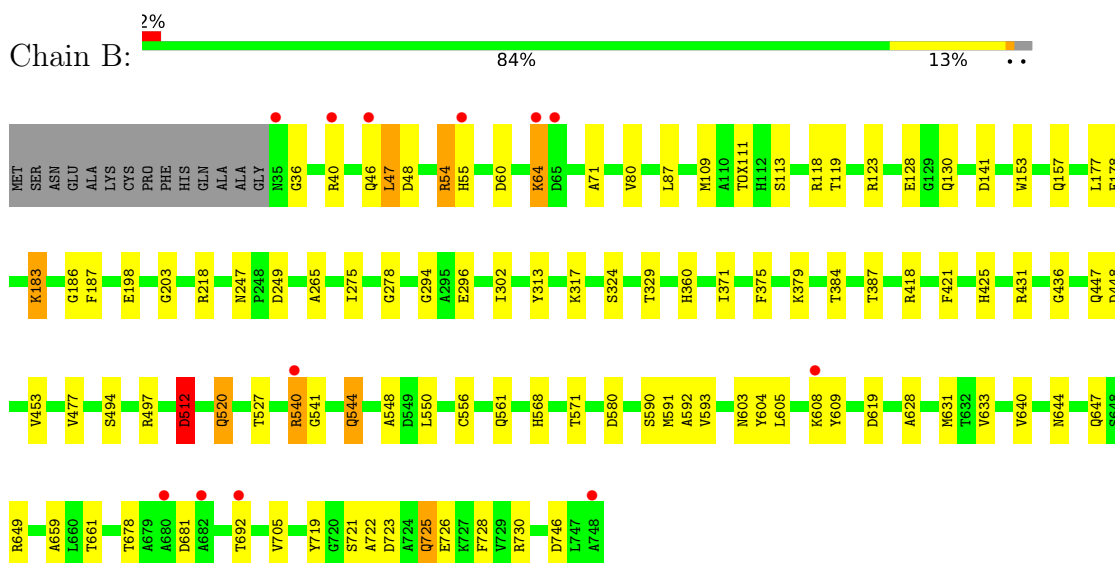
3 Residue-property plots

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	100.79Å 115.23Å 174.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.42 – 1.87 48.42 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.42-1.87) 98.8 (48.42-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.164 , 0.198 (Not available) , 0.198	Depositor DCC
R_{free} test set	8161 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12535	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, OXY, NA, TOX, MPD, PO4, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.77	69/5701 (1.2%)	1.34	14/7747 (0.2%)
1	B	1.78	73/5688 (1.3%)	1.34	22/7731 (0.3%)
All	All	1.78	142/11389 (1.2%)	1.34	36/15478 (0.2%)

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	453	VAL	C-O	-9.90	1.12	1.24
1	B	448	ASP	C-O	9.49	1.28	1.23
1	A	259	ASP	CA-C	7.51	1.62	1.52
1	B	387	THR	N-CA	-7.46	1.37	1.46
1	A	453	VAL	C-O	-7.45	1.15	1.24
1	A	449	PRO	N-CA	-7.45	1.38	1.47
1	B	278	GLY	C-O	7.39	1.32	1.23
1	B	512	ASP	CG-OD2	7.01	1.38	1.25
1	A	107	ILE	N-CA	6.95	1.54	1.46
1	A	315	THR	C-O	-6.89	1.15	1.24
1	A	194	THR	N-CA	6.88	1.53	1.45
1	A	568	HIS	C-O	-6.88	1.16	1.24
1	A	746	ASP	C-O	-6.83	1.15	1.24
1	B	448	ASP	N-CA	6.83	1.51	1.46
1	A	63	GLY	N-CA	6.81	1.53	1.45
1	A	619	ASP	N-CA	6.78	1.54	1.46
1	A	126	ALA	N-CA	-6.61	1.37	1.46
1	A	465	GLU	C-O	-6.58	1.16	1.24
1	A	403	ARG	CA-C	-6.57	1.44	1.52
1	A	443	VAL	C-O	-6.56	1.16	1.24
1	B	568	HIS	CA-C	6.54	1.60	1.52
1	B	692	THR	C-O	-6.54	1.15	1.24
1	A	495	ASP	N-CA	6.53	1.54	1.46
1	B	730[A]	ARG	CZ-NH1	6.50	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	746	ASP	C-O	-6.48	1.16	1.24
1	B	580	ASP	C-O	-6.42	1.16	1.24
1	B	87	LEU	N-CA	-6.42	1.38	1.46
1	A	419	ALA	C-N	-6.41	1.25	1.33
1	A	407	GLU	CD-OE1	6.35	1.37	1.25
1	B	118	ARG	C-O	6.34	1.31	1.24
1	B	294	GLY	C-O	6.33	1.30	1.23
1	B	644	ASN	C-O	-6.32	1.16	1.23
1	A	449	PRO	C-O	-6.29	1.16	1.23
1	B	425	HIS	C-O	-6.29	1.15	1.24
1	A	664	PHE	N-CA	-6.26	1.38	1.46
1	B	203	GLY	C-O	6.26	1.28	1.23
1	A	343	GLU	C-O	-6.23	1.17	1.24
1	B	60	ASP	C-O	-6.22	1.16	1.24
1	B	722	ALA	C-O	-6.22	1.16	1.24
1	B	726	GLU	CD-OE2	6.21	1.37	1.25
1	B	218	ARG	N-CA	-6.17	1.38	1.46
1	A	499	GLY	C-O	6.16	1.30	1.24
1	B	619	ASP	N-CA	6.16	1.53	1.46
1	A	248	PRO	CA-C	-6.13	1.47	1.53
1	B	123	ARG	N-CA	-6.13	1.37	1.45
1	B	721	SER	CA-CB	6.13	1.63	1.53
1	B	71	ALA	C-O	6.12	1.31	1.24
1	B	448	ASP	CA-C	-6.11	1.48	1.53
1	B	218	ARG	CZ-NH1	6.07	1.41	1.32
1	A	108	ARG	CZ-NH1	-6.02	1.24	1.32
1	B	604	TYR	N-CA	-5.99	1.38	1.46
1	A	377	PRO	C-O	-5.98	1.16	1.24
1	B	561	GLN	C-O	5.96	1.31	1.24
1	B	592	ALA	CA-C	-5.95	1.44	1.52
1	A	491	PHE	CA-C	-5.95	1.45	1.52
1	B	544	GLN	CD-NE2	5.93	1.45	1.33
1	B	527	THR	N-CA	-5.92	1.39	1.46
1	B	421	PHE	N-CA	-5.90	1.39	1.46
1	A	699	GLY	N-CA	5.87	1.51	1.45
1	B	728	PHE	CA-C	5.86	1.60	1.52
1	A	725	GLN	CG-CD	5.85	1.66	1.52
1	A	492	ARG	N-CA	5.84	1.53	1.46
1	A	639	ARG	C-O	5.76	1.30	1.24
1	B	186	GLY	N-CA	5.75	1.52	1.44
1	B	590	SER	C-O	-5.75	1.17	1.24
1	B	375	PHE	CA-CB	-5.75	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	725	GLN	CD-NE2	5.72	1.45	1.33
1	B	628	ALA	CA-C	-5.70	1.46	1.52
1	A	628	ALA	N-CA	-5.67	1.41	1.46
1	B	187	PHE	N-CA	-5.64	1.39	1.46
1	B	512	ASP	C-O	-5.63	1.16	1.24
1	A	57	SER	C-O	-5.62	1.16	1.24
1	A	91	SER	C-O	-5.62	1.17	1.23
1	B	497	ARG	N-CA	5.62	1.52	1.45
1	A	375	PHE	C-O	-5.57	1.17	1.24
1	B	109	MET	C-O	5.57	1.30	1.24
1	B	313	TYR	CA-C	-5.57	1.46	1.52
1	B	721	SER	C-O	-5.56	1.16	1.23
1	A	133	PHE	N-CA	5.55	1.52	1.45
1	A	580	ASP	C-O	-5.55	1.17	1.24
1	A	271	THR	C-O	-5.55	1.17	1.24
1	A	170	ILE	N-CA	-5.54	1.39	1.46
1	A	532	ARG	N-CA	-5.53	1.39	1.46
1	B	371	ILE	C-O	5.52	1.31	1.24
1	A	286	GLY	N-CA	5.52	1.53	1.45
1	B	249	ASP	N-CA	5.51	1.52	1.46
1	B	477	VAL	CA-CB	-5.50	1.48	1.54
1	B	593	VAL	N-CA	5.50	1.53	1.46
1	A	164	SER	CA-CB	-5.50	1.44	1.53
1	A	732	PHE	CA-C	5.44	1.59	1.52
1	A	492	ARG	C-O	5.43	1.30	1.24
1	B	425	HIS	CA-C	5.43	1.59	1.52
1	B	329	THR	C-O	5.42	1.30	1.24
1	B	659	ALA	CA-CB	-5.40	1.45	1.53
1	B	418	ARG	CZ-NH2	-5.39	1.26	1.33
1	A	200	VAL	C-O	-5.39	1.18	1.24
1	A	727	LYS	C-O	5.39	1.30	1.24
1	B	659	ALA	N-CA	-5.38	1.39	1.46
1	B	80	VAL	N-CA	-5.37	1.40	1.46
1	A	527	THR	N-CA	-5.36	1.39	1.46
1	A	630	GLU	N-CA	5.29	1.52	1.46
1	A	84	LEU	CA-CB	-5.29	1.45	1.53
1	A	477	VAL	CA-CB	-5.27	1.48	1.54
1	B	631	MET	C-N	-5.26	1.26	1.33
1	B	296	GLU	N-CA	5.26	1.54	1.45
1	A	158	LYS	C-O	-5.25	1.18	1.24
1	B	556	CYS	CA-CB	5.25	1.61	1.53
1	A	436	GLY	C-N	-5.23	1.29	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	506	ARG	CZ-NH2	-5.23	1.26	1.33
1	B	384	THR	CA-C	5.23	1.59	1.52
1	B	609	TYR	CA-C	-5.23	1.46	1.52
1	A	266	MET	CA-C	5.22	1.58	1.52
1	A	594	LEU	C-O	-5.22	1.17	1.24
1	A	89	THR	CB-OG1	-5.20	1.35	1.43
1	A	47	LEU	CB-CG	-5.20	1.43	1.53
1	A	131	GLN	N-CA	-5.17	1.39	1.46
1	B	324	SER	C-O	-5.17	1.17	1.24
1	A	428	MET	C-O	-5.16	1.17	1.24
1	A	369	ALA	N-CA	-5.16	1.40	1.46
1	A	570	VAL	C-O	-5.13	1.18	1.23
1	B	640	VAL	C-O	-5.13	1.17	1.24
1	B	571[A]	THR	C-O	5.13	1.30	1.24
1	B	571[B]	THR	C-O	5.13	1.30	1.24
1	A	595	GLU	CA-C	5.12	1.58	1.52
1	B	36	GLY	N-CA	5.10	1.52	1.45
1	A	682	ALA	C-O	5.10	1.30	1.24
1	B	275	ILE	CA-CB	-5.10	1.48	1.54
1	A	74	LYS	C-O	-5.09	1.17	1.24
1	A	483	THR	CA-CB	5.08	1.61	1.53
1	B	436	GLY	C-O	-5.07	1.17	1.24
1	A	454	ASP	CB-CG	5.07	1.64	1.52
1	B	705	VAL	N-CA	-5.06	1.40	1.46
1	A	734	ALA	N-CA	-5.06	1.40	1.46
1	B	548	ALA	N-CA	5.06	1.52	1.46
1	A	685	PHE	N-CA	-5.05	1.39	1.45
1	B	302	ILE	CB-CG1	-5.05	1.43	1.53
1	A	417	ALA	C-O	-5.04	1.18	1.24
1	B	64	LYS	C-O	-5.03	1.17	1.24
1	A	520	GLN	C-O	-5.02	1.18	1.24
1	B	605	LEU	C-O	-5.02	1.18	1.23
1	B	603	ASN	C-O	-5.02	1.17	1.23
1	A	547	LEU	N-CA	-5.02	1.40	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	GLN	N-CA-C	-9.43	97.81	110.55
1	A	46	GLN	N-CA-C	-8.91	98.52	110.55
1	B	541	GLY	N-CA-C	-8.03	95.60	112.45
1	B	183	LYS	CB-CG-CD	6.88	127.13	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	520	GLN	CB-CG-CD	6.55	123.73	112.60
1	B	247	ASN	CB-CA-C	6.30	118.45	109.38
1	B	494	SER	N-CA-C	6.07	117.56	111.07
1	A	177	LEU	N-CA-C	6.01	118.32	111.11
1	B	48	ASP	N-CA-C	5.92	119.27	107.62
1	A	591	MET	CG-SD-CE	-5.87	87.99	100.90
1	B	591	MET	CG-SD-CE	-5.82	88.10	100.90
1	B	153	TRP	CA-C-N	-5.76	112.66	119.05
1	B	153	TRP	C-N-CA	-5.76	112.66	119.05
1	B	47	LEU	N-CA-CB	-5.73	101.58	110.29
1	A	429	GLY	O-C-N	5.70	127.47	121.77
1	B	157	GLN	N-CA-C	5.68	117.48	111.28
1	B	130	GLN	N-CA-C	5.62	119.61	112.87
1	B	550	LEU	N-CA-C	5.57	117.36	111.28
1	A	62	MET	CA-C-N	-5.46	112.64	121.05
1	A	62	MET	C-N-CA	-5.46	112.64	121.05
1	A	584	GLU	CG-CD-OE1	5.42	130.86	118.40
1	B	177	LEU	N-CA-C	5.41	117.60	111.11
1	A	112	HIS	N-CA-CB	-5.39	101.34	110.50
1	B	723	ASP	N-CA-C	-5.35	105.98	112.88
1	A	592	ALA	N-CA-C	5.30	117.75	111.33
1	A	724	ALA	N-CA-C	5.30	119.84	113.17
1	B	317	LYS	CA-C-O	-5.27	115.59	121.23
1	A	407	GLU	CG-CD-OE1	5.26	130.50	118.40
1	A	48	ASP	N-CA-C	5.22	117.91	107.62
1	B	113	SER	O-C-N	5.22	127.44	122.07
1	B	571[A]	THR	CA-C-N	-5.18	118.28	123.04
1	B	571[A]	THR	C-N-CA	-5.18	118.28	123.04
1	B	571[B]	THR	CA-C-N	-5.18	118.28	123.04
1	B	571[B]	THR	C-N-CA	-5.18	118.28	123.04
1	A	183	LYS	CB-CG-CD	5.17	123.19	111.30
1	A	47	LEU	N-CA-CB	-5.14	102.29	110.06

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	5572	0	5372	12	0
1	B	5556	0	5360	18	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	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	24	0	42	5	0
7	B	8	0	14	1	0
8	A	627	0	0	6	0
8	B	644	0	0	10	0
All	All	12535	0	10848	36	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 2.

All (36) 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:198[A]:GLU:OE1	8:B:901:HOH:O	1.69	1.09
1:B:119[B]:THR:HG21	8:B:1101:HOH:O	1.71	0.90
1:B:647:GLN:HG2	8:B:1117:HOH:O	1.75	0.87
1:B:360:HIS:ND1	8:B:902:HOH:O	2.10	0.84
1:B:512:ASP:OD1	8:B:903:HOH:O	2.10	0.70
7:A:807:MPD:HM2	8:A:1373:HOH:O	1.96	0.65
1:B:520:GLN:CG	8:B:1058:HOH:O	2.46	0.62
1:B:520:GLN:HG3	8:B:1058:HOH:O	1.98	0.62
1:B:47:LEU:O	8:B:904:HOH:O	2.19	0.54
7:A:807:MPD:H53	7:A:807:MPD:H11	1.90	0.54
7:A:807:MPD:CM	8:A:1373:HOH:O	2.52	0.53
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.45	0.51
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.11	0.51
1:B:520:GLN:HG2	8:B:1058:HOH:O	2.11	0.50
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.95	0.49
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.96	0.49
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.43	0.49
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726[A]:GLU:HG3	8:A:1321:HOH:O	2.12	0.49
7:A:806:MPD:O4	7:A:806:MPD:HM1	2.14	0.48
1:A:467:LYS:NZ	8:A:909:HOH:O	2.35	0.47
1:B:661:THR:HA	1:B:725:GLN:HE22	1.79	0.46
1:B:540:ARG:NE	1:B:540:ARG:HA	2.31	0.46
1:B:119[A]:THR:CG2	1:B:265:ALA:HB2	2.45	0.46
1:A:504:ARG:HD3	1:A:591:MET:HE3	2.00	0.44
1:B:128:GLU:OE1	1:B:198[A]:GLU:OE2	2.36	0.43
1:B:678:THR:OG1	1:B:681:ASP:O	2.33	0.42
7:B:806:MPD:O4	7:B:806:MPD:H12	2.19	0.42
1:A:226:GLU:OE1	1:A:610:ARG:NH2	2.52	0.42
1:A:725:GLN:HB2	8:A:1401:HOH:O	2.20	0.41
1:A:143:ALA:HA	1:A:309:TRP:CZ3	2.56	0.41
1:A:480:LEU:HD22	1:A:554:ALA:HB1	2.02	0.41
1:B:178:GLU:OE1	8:B:905:HOH:O	2.22	0.41
1:A:504:ARG:HD2	8:A:941:HOH:O	2.20	0.41
1:A:610:ARG:HG3	1:A:611:VAL:HG23	2.02	0.40
7:A:807:MPD:H53	7:A:807:MPD:C1	2.51	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	718/728 (99%)	710 (99%)	8 (1%)	0	100	100
1	B	717/728 (98%)	708 (99%)	9 (1%)	0	100	100
All	All	1435/1456 (99%)	1418 (99%)	17 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	557/560 (100%)	550 (99%)	7 (1%)	61	50
1	B	556/560 (99%)	545 (98%)	11 (2%)	48	33
All	All	1113/1120 (99%)	1095 (98%)	18 (2%)	55	43

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	183	LYS
1	A	379	LYS
1	A	544	GLN
1	A	608	LYS
1	A	610	ARG
1	A	649	ARG
1	B	40	ARG
1	B	54	ARG
1	B	64	LYS
1	B	141	ASP
1	B	183	LYS
1	B	379	LYS
1	B	512	ASP
1	B	540	ARG
1	B	544	GLN
1	B	608	LYS
1	B	649	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	92	GLN
1	A	339	HIS
1	B	406	HIS

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Mol	Chain	Res	Type
1	B	520	GLN
1	B	544	GLN
1	B	737	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	2,1	14,17,18	2.88	5 (35%)	12,23,25	2.25	4 (33%)
1	TOX	A	111	2,1	14,17,18	1.99	5 (35%)	12,23,25	1.98	5 (41%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	TOX	CE2-NE1	-5.73	1.29	1.39
1	B	111	TOX	CD2-CE2	5.35	1.48	1.41
1	B	111	TOX	O-C	4.70	1.37	1.20
1	A	111	TOX	CD2-CG	3.70	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	TOX	O-C	3.34	1.32	1.20
1	A	111	TOX	CZ2-CE2	3.21	1.44	1.39
1	B	111	TOX	CB-CA	-2.96	1.47	1.53
1	B	111	TOX	CZ2-CE2	-2.88	1.35	1.39
1	A	111	TOX	CE2-NE1	-2.54	1.35	1.39
1	A	111	TOX	CH2-CZ3	2.40	1.43	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	TOX	CZ2-CE2-NE1	5.29	137.79	129.37
1	B	111	TOX	CZ2-CE2-CD2	-3.61	117.92	121.95
1	A	111	TOX	CZ2-CE2-NE1	3.41	134.79	129.37
1	A	111	TOX	CZ3-CH2-CZ2	-3.04	116.48	120.24
1	A	111	TOX	CZ2-CE2-CD2	-3.03	118.56	121.95
1	A	111	TOX	CE2-CD2-CG	-2.38	105.20	107.39
1	B	111	TOX	CD2-CG-CD1	-2.34	104.22	106.34
1	B	111	TOX	CB-CG-CD2	2.29	131.10	126.70
1	A	111	TOX	CZ3-CE3-CD2	2.16	123.69	119.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111	TOX	N-CA-CB-CG
1	A	111	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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	A	801	1	50,50,50	1.91	11 (22%)	67,82,82	1.73	14 (20%)
5	OXY	A	804	-	1,1,1	0.04	0	-		
7	MPD	A	806	-	7,7,7	0.83	0	9,10,10	1.64	2 (22%)
7	MPD	A	807	-	7,7,7	0.84	0	9,10,10	1.90	3 (33%)
2	HEM	B	801	1	50,50,50	1.91	11 (22%)	67,82,82	1.96	20 (29%)
5	OXY	B	804	-	1,1,1	0.48	0	-		
7	MPD	A	808	-	7,7,7	1.20	1 (14%)	9,10,10	2.77	2 (22%)
6	PO4	A	805	-	4,4,4	1.24	1 (25%)	6,6,6	1.69	2 (33%)
6	PO4	B	805	-	4,4,4	1.60	2 (50%)	6,6,6	0.84	0
7	MPD	B	806	-	7,7,7	0.60	0	9,10,10	2.26	4 (44%)

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	A	801	1	-	3/14/54/54	-
7	MPD	A	806	-	-	3/5/5/5	-
7	MPD	A	807	-	-	2/5/5/5	-
2	HEM	B	801	1	-	2/14/54/54	-
7	MPD	A	808	-	-	2/5/5/5	-
7	MPD	B	806	-	-	3/5/5/5	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1B-NB	-6.20	1.29	1.40
2	A	801	HEM	C1B-NB	-5.61	1.30	1.40
2	A	801	HEM	FE-NB	5.14	2.10	1.94
2	B	801	HEM	C3C-C4C	-4.58	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	FE-NB	4.00	2.07	1.94
2	B	801	HEM	C4D-ND	-3.94	1.33	1.40
2	A	801	HEM	C1C-NC	-3.88	1.32	1.39
2	A	801	HEM	FE-NA	3.82	2.07	1.95
2	B	801	HEM	C1C-C2C	-3.71	1.38	1.45
2	B	801	HEM	C1A-NA	-3.34	1.33	1.39
2	A	801	HEM	FE-NC	3.31	2.06	1.95
2	B	801	HEM	CHA-C4D	-3.06	1.32	1.38
2	A	801	HEM	CBA-CGA	3.05	1.57	1.50
2	B	801	HEM	C2A-C3A	-2.95	1.31	1.38
2	A	801	HEM	C1A-NA	2.78	1.44	1.39
2	A	801	HEM	C3C-C2C	2.74	1.42	1.37
2	A	801	HEM	CMB-C2B	2.69	1.56	1.50
2	A	801	HEM	C1B-C2B	-2.47	1.39	1.44
2	A	801	HEM	CAC-C3C	2.36	1.53	1.47
6	B	805	PO4	P-O3	-2.34	1.47	1.54
2	B	801	HEM	CBD-CAD	-2.19	1.44	1.51
7	A	808	MPD	C1-C2	2.16	1.58	1.52
6	B	805	PO4	P-O1	2.11	1.55	1.50
6	A	805	PO4	P-O1	2.09	1.55	1.50
2	B	801	HEM	C4A-NA	2.08	1.43	1.39
2	B	801	HEM	CHC-C1C	2.05	1.42	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CHC-C4B-NB	6.25	131.15	124.42
7	A	808	MPD	O2-C2-CM	-6.00	89.27	107.99
7	A	808	MPD	CM-C2-C1	5.32	122.54	110.63
2	A	801	HEM	C3B-C2B-C1B	5.06	110.21	106.41
2	B	801	HEM	C1B-NB-C4B	4.75	110.84	105.21
2	A	801	HEM	C4B-C3B-C2B	-4.69	102.97	107.28
2	A	801	HEM	CAA-CBA-CGA	-4.42	101.94	113.67
2	B	801	HEM	C2A-C1A-NA	4.10	114.70	110.15
2	A	801	HEM	C3D-C4D-ND	3.87	114.42	110.17
7	A	807	MPD	CM-C2-C1	-3.79	102.15	110.63
7	B	806	MPD	C1-C2-C3	3.67	126.03	110.20
2	A	801	HEM	C2A-C1A-NA	-3.67	106.08	110.15
2	B	801	HEM	C3B-C4B-NB	-3.57	106.91	109.47
2	B	801	HEM	C4C-C3C-C2C	-3.45	103.82	106.81
7	A	806	MPD	O4-C4-C3	-3.40	97.84	111.35
2	B	801	HEM	CBD-CAD-C3D	3.33	121.75	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	806	MPD	O2-C2-C3	-3.32	96.84	109.27
2	A	801	HEM	C1B-NB-C4B	3.25	109.05	105.21
2	B	801	HEM	CHA-C1A-NA	-3.22	118.02	123.86
7	B	806	MPD	O2-C2-CM	2.90	117.03	107.99
6	A	805	PO4	O3-P-O1	2.90	121.19	110.95
2	B	801	HEM	C3B-C2B-C1B	2.86	108.56	106.41
2	A	801	HEM	O2A-CGA-CBA	2.84	122.98	114.00
2	B	801	HEM	CAA-C2A-C1A	2.82	130.45	124.94
2	B	801	HEM	O1A-CGA-CBA	-2.75	114.38	123.09
2	B	801	HEM	C2B-C1B-NB	-2.74	106.69	109.84
7	A	807	MPD	O2-C2-C1	2.73	116.49	107.99
2	A	801	HEM	CHA-C4D-ND	-2.69	121.04	124.37
2	B	801	HEM	CAA-CBA-CGA	-2.64	106.67	113.67
2	A	801	HEM	C1D-C2D-C3D	2.63	109.75	106.98
2	A	801	HEM	C4D-C3D-C2D	-2.61	103.10	106.89
2	A	801	HEM	C4C-NC-C1C	2.55	109.97	105.82
7	B	806	MPD	CM-C2-C1	-2.55	104.93	110.63
2	B	801	HEM	CAD-CBD-CGD	2.54	120.42	113.67
2	B	801	HEM	C3C-C2C-C1C	2.49	109.40	107.05
2	B	801	HEM	O2A-CGA-CBA	2.42	121.64	114.00
2	B	801	HEM	C1D-C2D-C3D	-2.40	104.46	106.98
7	A	807	MPD	C5-C4-C3	2.39	122.79	111.67
7	A	806	MPD	O4-C4-C5	2.37	119.66	109.45
2	A	801	HEM	CBD-CAD-C3D	2.35	119.03	112.53
2	B	801	HEM	C4B-C3B-C2B	-2.33	105.14	107.28
6	A	805	PO4	O4-P-O1	-2.31	102.78	110.95
2	B	801	HEM	C4A-NA-C1A	-2.28	102.11	105.82
2	A	801	HEM	O1D-CGD-CBD	-2.26	115.94	123.09
2	B	801	HEM	O1D-CGD-CBD	-2.22	116.06	123.09
2	A	801	HEM	C4D-ND-C1D	-2.06	102.77	105.21
2	B	801	HEM	O2D-CGD-CBD	2.02	120.38	114.00

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	808	MPD	C2-C3-C4-C5
7	B	806	MPD	C1-C2-C3-C4
7	B	806	MPD	O2-C2-C3-C4
7	A	806	MPD	C1-C2-C3-C4
7	B	806	MPD	CM-C2-C3-C4
2	B	801	HEM	CAA-CBA-CGA-O1A

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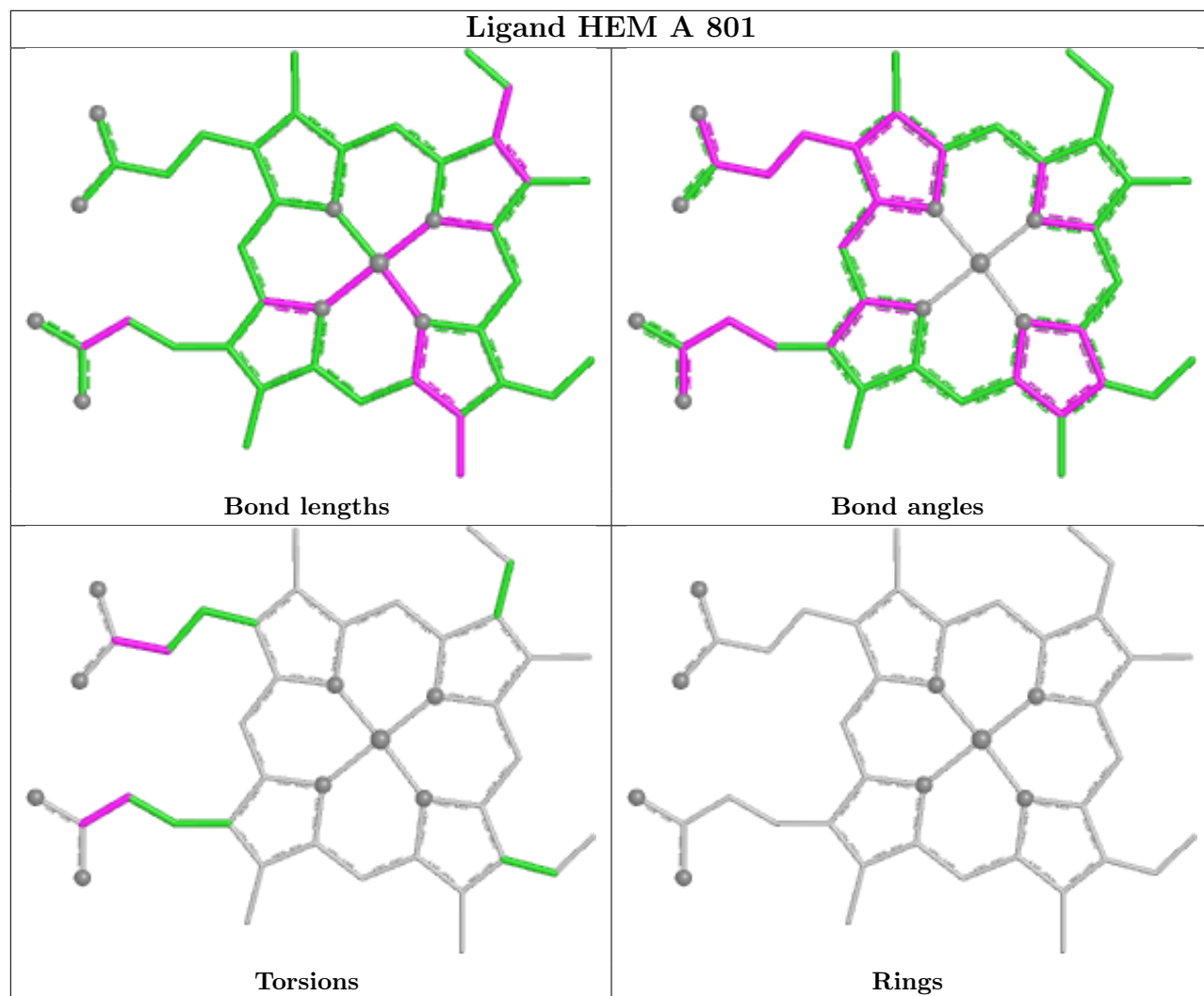
Mol	Chain	Res	Type	Atoms
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
7	A	806	MPD	O2-C2-C3-C4
7	A	807	MPD	O2-C2-C3-C4
7	A	806	MPD	CM-C2-C3-C4
7	A	807	MPD	C1-C2-C3-C4
7	A	808	MPD	C1-C2-C3-C4
2	A	801	HEM	CAD-CBD-CGD-O2D

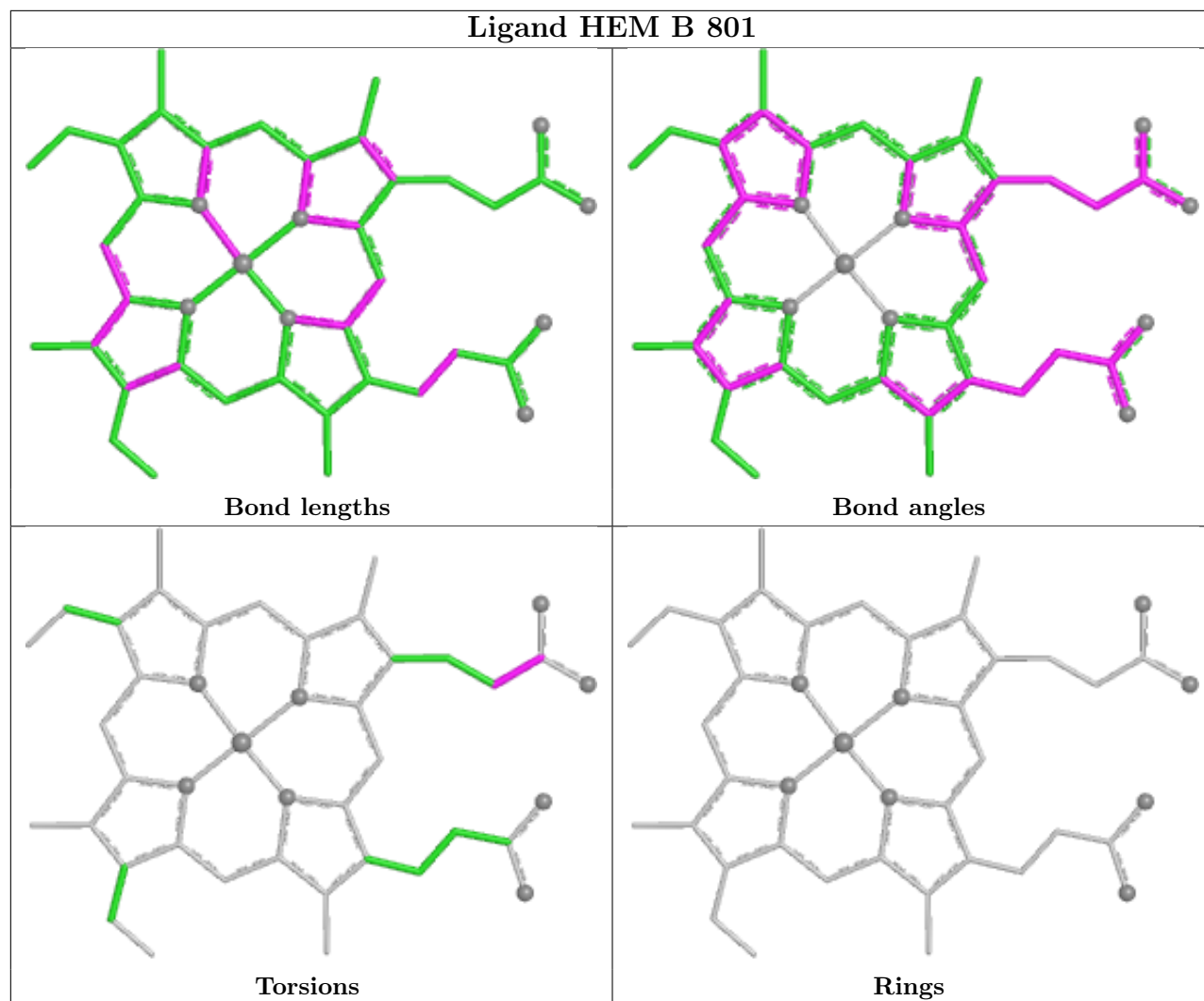
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	806	MPD	1	0
7	A	807	MPD	4	0
7	B	806	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	713/728 (97%)	-0.24	7 (0%) 79 83	9, 25, 45, 84	7 (0%)
1	B	713/728 (97%)	-0.31	12 (1%) 69 74	9, 24, 44, 84	6 (0%)
All	All	1426/1456 (97%)	-0.27	19 (1%) 75 80	9, 24, 45, 84	13 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	5.8
1	B	748	ALA	5.3
1	A	64	LYS	2.9
1	B	680	ALA	2.9
1	A	119[A]	THR	2.8
1	B	40	ARG	2.7
1	B	65	ASP	2.6
1	B	682	ALA	2.6
1	B	35	ASN	2.6
1	B	55	HIS	2.5
1	B	540	ARG	2.5
1	B	692	THR	2.5
1	B	608	LYS	2.4
1	A	610	ARG	2.4
1	A	454	ASP	2.3
1	B	64	LYS	2.3
1	A	568	HIS	2.3
1	B	46	GLN	2.2
1	A	40	ARG	2.1

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	16/17	0.98	0.05	15,19,28,30	0
1	TOX	B	111	16/17	0.98	0.05	15,18,27,29	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

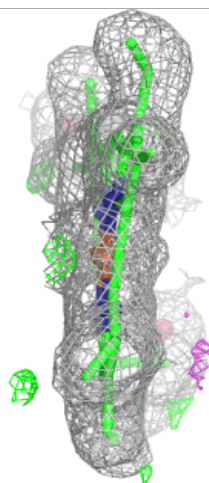
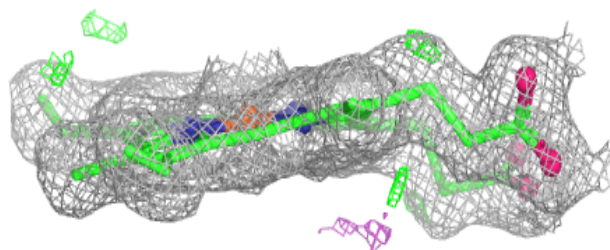
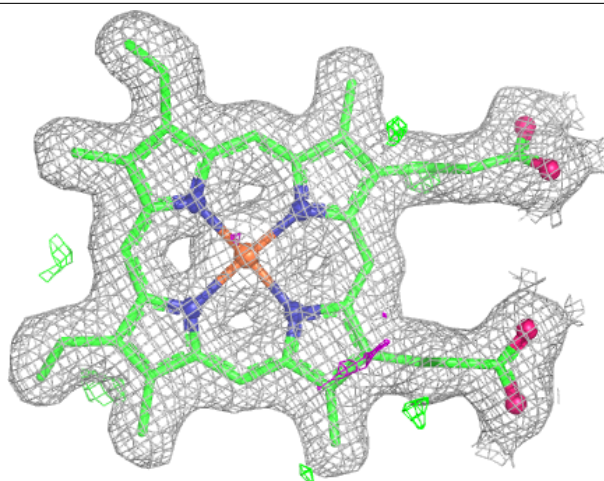
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

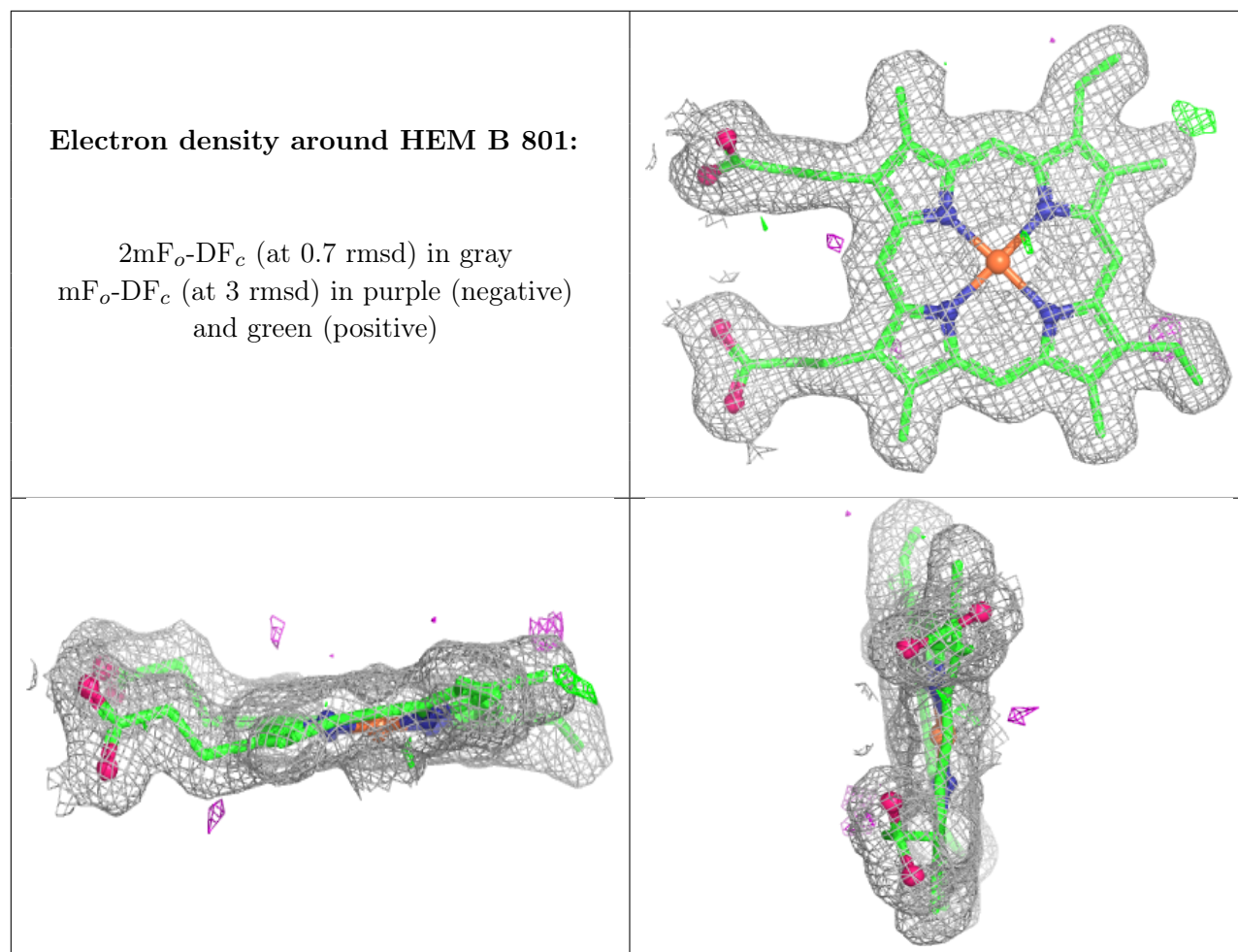
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MPD	A	808	8/8	0.76	0.26	66,71,76,77	0
6	PO4	A	805	5/5	0.84	0.12	59,76,86,89	0
7	MPD	A	807	8/8	0.85	0.18	48,53,67,68	0
7	MPD	A	806	8/8	0.86	0.19	58,66,72,73	0
7	MPD	B	806	8/8	0.86	0.18	49,57,60,63	0
6	PO4	B	805	5/5	0.89	0.11	52,64,70,74	0
5	OXY	A	804	2/2	0.92	0.24	47,47,47,54	0
4	CL	A	803	1/1	0.95	0.09	45,45,45,45	0
5	OXY	B	804	2/2	0.97	0.17	31,31,31,33	0
3	NA	A	802	1/1	0.98	0.07	20,20,20,20	0
2	HEM	A	801	43/43	0.98	0.06	17,21,24,25	0
4	CL	B	803	1/1	0.99	0.05	28,28,28,28	1
3	NA	B	802	1/1	0.99	0.06	20,20,20,20	0
2	HEM	B	801	43/43	0.99	0.05	16,19,21,23	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.