



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 12:05 AM UTC

PDB ID : 5KQN / pdb_00005kqn
Title : Crystal structure of the H381S variant of catalase-peroxidase from *B. pseudo-mallei*
Authors : Loewen, P.C.
Deposited on : 2016-07-06
Resolution : 1.75 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

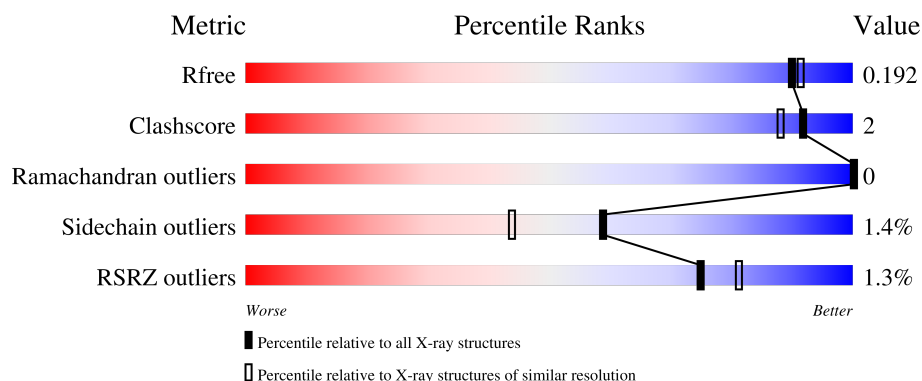
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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% 12% ..
1	B	728	% 83% 14% .

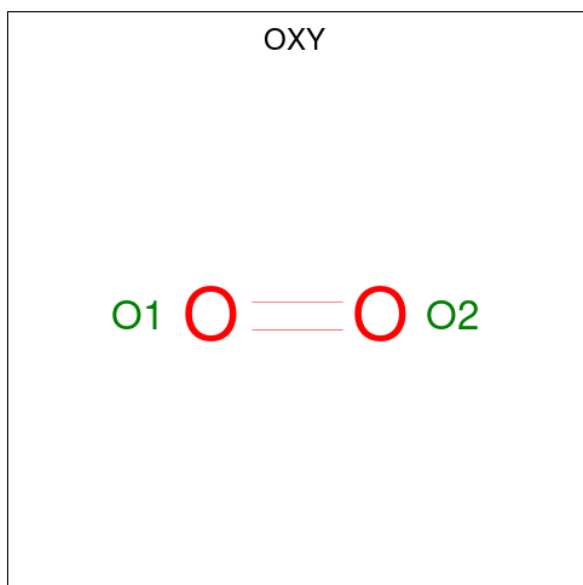
Continued from previous page...

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 OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

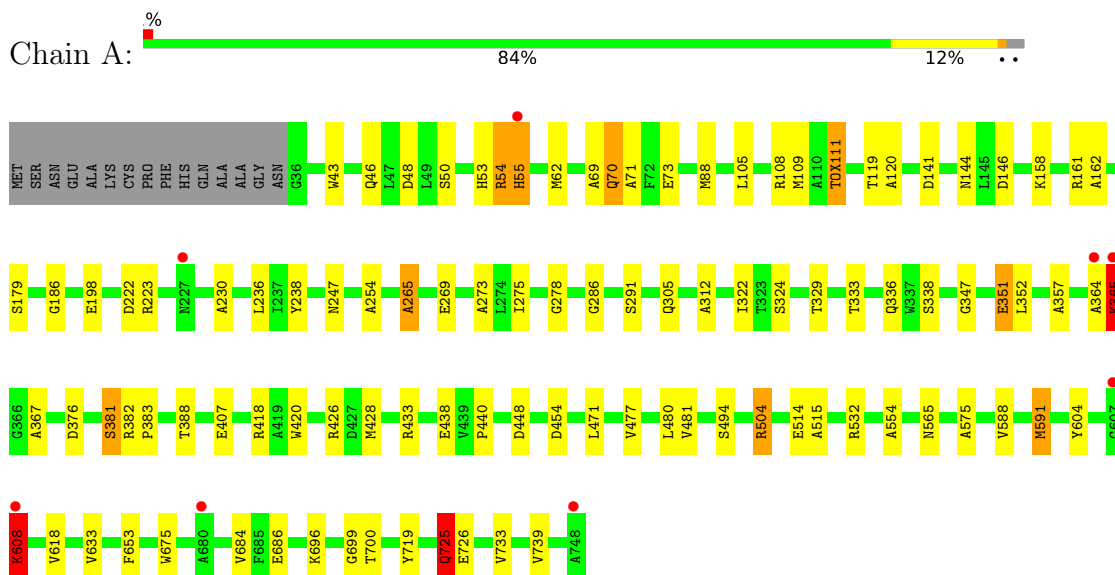
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	723	Total	O	0	0
			723	723		
6	B	724	Total	O	0	0
			724	724		

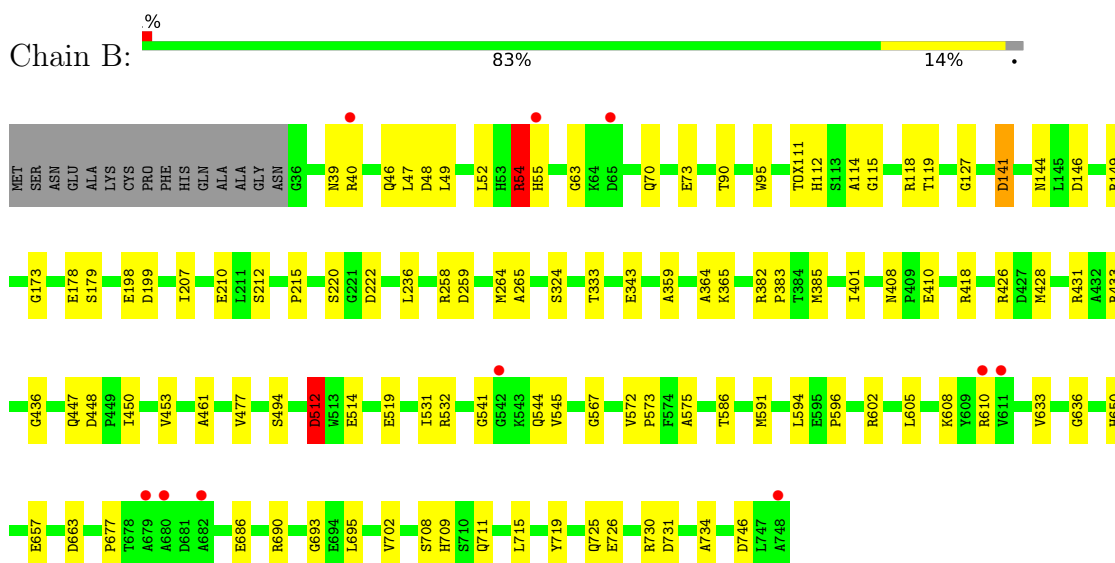
3 Residue-property plots

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	100.99Å 114.17Å 175.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.18 – 1.75 46.18 – 1.75	Depositor EDS
% Data completeness (in resolution range)	93.9 (46.18-1.75) 93.9 (46.18-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.153 , 0.182 0.164 , 0.192	Depositor DCC
R_{free} test set	9477 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12677	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 2.90% 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: MPD, NA, HEM, OXY, TOX

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	1.83	78/5688 (1.4%)	1.35	22/7729 (0.3%)
1	B	1.83	79/5677 (1.4%)	1.36	19/7715 (0.2%)
All	All	1.83	157/11365 (1.4%)	1.36	41/15444 (0.3%)

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	448	ASP	N-CA	12.11	1.55	1.46
1	B	512	ASP	CG-OD2	9.91	1.44	1.25
1	A	365	LYS	N-CA	9.04	1.57	1.46
1	B	708	SER	CA-C	-8.80	1.43	1.52
1	A	448	ASP	N-CA	8.15	1.52	1.46
1	B	596	PRO	C-O	8.15	1.30	1.24
1	A	329	THR	C-O	8.11	1.33	1.24
1	A	588	VAL	N-CA	-8.09	1.36	1.46
1	B	365	LYS	N-CA	7.80	1.55	1.46
1	B	453	VAL	C-O	-7.78	1.14	1.24
1	B	494	SER	CA-C	7.41	1.62	1.52
1	A	725	GLN	CG-CD	7.35	1.70	1.52
1	A	278	GLY	CA-C	7.30	1.60	1.52
1	A	514	GLU	CA-C	7.12	1.62	1.52
1	B	477	VAL	CA-C	-6.97	1.44	1.52
1	B	695	LEU	CA-C	-6.92	1.43	1.52
1	A	739	VAL	C-O	6.89	1.32	1.24
1	A	324	SER	CA-C	6.82	1.61	1.52
1	B	591	MET	SD-CE	-6.75	1.62	1.79
1	A	273	ALA	N-CA	-6.70	1.38	1.46
1	A	494	SER	CA-C	6.64	1.61	1.52
1	A	198	GLU	CG-CD	6.60	1.68	1.52
1	B	333	THR	N-CA	-6.60	1.39	1.46
1	B	711	GLN	CD-NE2	-6.58	1.19	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	343	GLU	N-CA	6.54	1.54	1.46
1	B	90	THR	CA-C	-6.52	1.45	1.53
1	B	215	PRO	C-O	-6.52	1.15	1.24
1	B	199	ASP	C-O	6.51	1.31	1.23
1	B	448	ASP	C-O	6.48	1.26	1.23
1	A	565	ASN	N-CA	-6.44	1.38	1.46
1	A	108	ARG	CA-C	6.42	1.60	1.52
1	A	407	GLU	CD-OE1	6.40	1.37	1.25
1	B	636	GLY	CA-C	-6.39	1.45	1.52
1	B	532	ARG	CD-NE	-6.38	1.37	1.46
1	A	684	VAL	C-O	6.37	1.30	1.24
1	B	677	PRO	C-O	6.36	1.31	1.23
1	B	702	VAL	CA-C	-6.36	1.44	1.52
1	A	161	ARG	CD-NE	-6.34	1.37	1.46
1	B	512	ASP	CB-CG	6.30	1.67	1.52
1	A	700	THR	N-CA	-6.29	1.38	1.45
1	B	63	GLY	N-CA	6.29	1.53	1.45
1	B	531	ILE	N-CA	6.29	1.53	1.46
1	B	734	ALA	N-CA	-6.13	1.39	1.46
1	A	618	VAL	C-O	-6.12	1.17	1.24
1	A	471	LEU	CA-C	6.12	1.60	1.52
1	A	223	ARG	CZ-NH2	6.11	1.41	1.33
1	B	544	GLN	CD-NE2	6.04	1.46	1.33
1	B	657	GLU	CA-C	6.03	1.60	1.52
1	A	477	VAL	CA-CB	-6.01	1.48	1.54
1	B	731	ASP	CA-C	6.00	1.60	1.52
1	A	418	ARG	NE-CZ	5.97	1.39	1.33
1	B	545	VAL	CA-CB	-5.96	1.47	1.54
1	B	436	GLY	N-CA	5.92	1.52	1.44
1	A	481	VAL	CA-CB	-5.92	1.47	1.54
1	B	179	SER	N-CA	-5.91	1.39	1.46
1	B	408	ASN	CA-CB	-5.89	1.46	1.53
1	B	477	VAL	N-CA	5.88	1.53	1.46
1	A	62	MET	C-N	-5.87	1.25	1.33
1	A	53	HIS	N-CA	5.86	1.53	1.46
1	A	322	ILE	CA-C	5.86	1.60	1.52
1	A	604	TYR	CA-C	-5.85	1.45	1.52
1	B	567	GLY	C-O	-5.85	1.16	1.24
1	A	62	MET	CA-C	5.83	1.60	1.52
1	B	385	MET	C-O	5.83	1.30	1.23
1	A	222	ASP	CA-C	5.82	1.60	1.53
1	A	686	GLU	CA-C	-5.82	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	ALA	C-O	5.81	1.31	1.24
1	B	709	HIS	CA-C	5.80	1.60	1.52
1	B	220	SER	C-O	5.79	1.30	1.23
1	B	95	TRP	CA-CB	5.77	1.60	1.53
1	B	711	GLN	CA-C	-5.77	1.45	1.52
1	B	198	GLU	CG-CD	5.77	1.66	1.52
1	B	258	ARG	CA-C	5.77	1.60	1.52
1	A	364	ALA	C-N	-5.76	1.26	1.34
1	A	440	PRO	N-CA	-5.75	1.40	1.47
1	A	388	THR	CB-CG2	-5.72	1.33	1.52
1	A	438	GLU	CA-C	-5.71	1.45	1.52
1	B	586	THR	C-O	5.71	1.30	1.23
1	B	222	ASP	CA-C	5.68	1.59	1.53
1	A	407	GLU	CG-CD	5.68	1.66	1.52
1	A	236	LEU	CA-C	5.67	1.59	1.52
1	B	426	ARG	CZ-NH2	5.66	1.40	1.33
1	B	726	GLU	CD-OE2	5.66	1.36	1.25
1	B	602	ARG	CZ-NH2	-5.66	1.26	1.33
1	A	675	TRP	C-O	5.65	1.30	1.24
1	B	591	MET	CB-CG	-5.64	1.35	1.52
1	A	247	ASN	CG-ND2	-5.64	1.21	1.33
1	B	359	ALA	N-CA	5.64	1.53	1.45
1	B	461	ALA	CA-C	5.63	1.60	1.52
1	A	454	ASP	CB-CG	5.62	1.66	1.52
1	A	381	SER	CB-OG	-5.62	1.30	1.42
1	B	650	HIS	CA-CB	-5.60	1.45	1.53
1	B	210	GLU	C-O	5.55	1.30	1.23
1	B	410	GLU	CG-CD	5.54	1.65	1.52
1	B	49	LEU	C-O	-5.53	1.16	1.24
1	B	52	LEU	C-O	5.53	1.31	1.24
1	B	746	ASP	CB-CG	5.53	1.65	1.52
1	B	572	VAL	C-N	-5.53	1.26	1.33
1	A	291	SER	CA-CB	5.51	1.63	1.53
1	A	109	MET	N-CA	-5.51	1.39	1.46
1	A	383	PRO	N-CA	5.50	1.53	1.47
1	A	88	MET	C-O	-5.49	1.17	1.24
1	A	230	ALA	N-CA	-5.46	1.40	1.46
1	B	383	PRO	C-O	5.46	1.30	1.23
1	A	158	LYS	CA-C	5.42	1.59	1.52
1	A	699	GLY	CA-C	-5.40	1.45	1.51
1	B	222	ASP	C-O	-5.39	1.16	1.23
1	B	594	LEU	C-O	5.37	1.31	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	364	ALA	CA-C	5.36	1.59	1.52
1	B	418	ARG	CZ-NH2	-5.34	1.26	1.33
1	A	105	LEU	CA-C	5.33	1.59	1.52
1	B	259	ASP	CA-C	5.33	1.59	1.52
1	A	186	GLY	N-CA	5.32	1.53	1.45
1	A	50	SER	CA-C	5.32	1.60	1.52
1	B	715	LEU	N-CA	5.31	1.52	1.46
1	B	693	GLY	CA-C	5.30	1.59	1.51
1	B	73	GLU	CA-CB	5.30	1.62	1.53
1	A	418	ARG	CZ-NH1	-5.29	1.25	1.32
1	B	212	SER	C-O	-5.29	1.16	1.23
1	A	532	ARG	CA-C	5.29	1.59	1.52
1	A	286	GLY	CA-C	5.28	1.59	1.51
1	A	376	ASP	N-CA	5.28	1.52	1.46
1	A	515	ALA	N-CA	5.28	1.52	1.46
1	B	401	ILE	CA-C	5.28	1.59	1.52
1	B	573	PRO	CA-C	5.26	1.59	1.52
1	B	382	ARG	CA-C	5.25	1.59	1.53
1	A	120	ALA	N-CA	5.25	1.52	1.46
1	A	364	ALA	CA-C	5.25	1.59	1.52
1	A	254	ALA	C-O	5.24	1.30	1.24
1	A	55	HIS	C-O	-5.24	1.16	1.23
1	A	733	VAL	CA-C	5.24	1.59	1.52
1	B	149	ARG	CZ-NH1	-5.23	1.25	1.32
1	A	269	GLU	C-O	5.23	1.30	1.24
1	B	514	GLU	CA-C	5.23	1.59	1.52
1	A	653	PHE	CA-CB	5.22	1.59	1.52
1	B	746	ASP	C-O	-5.22	1.17	1.24
1	A	305	GLN	CA-C	5.22	1.59	1.53
1	A	347	GLY	C-O	5.19	1.29	1.24
1	B	236	LEU	CA-C	5.19	1.59	1.52
1	A	365	LYS	CA-C	5.18	1.59	1.52
1	B	690	ARG	C-O	-5.17	1.17	1.24
1	B	118	ARG	N-CA	5.17	1.52	1.46
1	A	69	ALA	C-O	-5.17	1.18	1.24
1	A	223	ARG	C-O	5.17	1.30	1.23
1	A	357	ALA	C-O	-5.16	1.16	1.23
1	B	207	ILE	C-O	5.16	1.29	1.24
1	A	494	SER	CA-CB	-5.14	1.45	1.53
1	A	43	TRP	CA-C	5.14	1.58	1.52
1	A	46	GLN	N-CA	5.13	1.52	1.45
1	A	275	ILE	CA-C	-5.11	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	686	GLU	CA-CB	5.11	1.62	1.53
1	A	179	SER	C-O	5.07	1.30	1.24
1	B	127	GLY	C-O	-5.03	1.18	1.24
1	A	162	ALA	C-N	5.03	1.39	1.33
1	A	338	SER	C-O	5.01	1.29	1.23
1	A	367	ALA	CA-CB	5.01	1.61	1.53
1	B	173	GLY	C-N	-5.00	1.27	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	541	GLY	N-CA-C	-12.11	91.21	112.53
1	A	591	MET	CG-SD-CE	-8.49	82.22	100.90
1	B	591	MET	CG-SD-CE	-8.36	82.51	100.90
1	A	198	GLU	CG-CD-OE1	7.30	135.19	118.40
1	A	48	ASP	N-CA-C	7.04	120.23	108.20
1	B	198	GLU	CG-CD-OE1	6.96	134.41	118.40
1	B	693	GLY	N-CA-C	-6.89	105.81	115.32
1	A	265	ALA	N-CA-C	6.64	120.68	112.58
1	B	575	ALA	CA-C-N	-6.30	114.24	120.98
1	B	575	ALA	C-N-CA	-6.30	114.24	120.98
1	B	70	GLN	N-CA-C	6.04	117.87	111.28
1	A	365	LYS	CA-CB-CG	5.91	125.93	114.10
1	B	605	LEU	CB-CA-C	-5.91	101.04	110.14
1	A	70	GLN	CA-CB-CG	5.91	125.91	114.10
1	A	725	GLN	CB-CG-CD	5.90	122.63	112.60
1	B	127	GLY	N-CA-C	5.85	121.10	114.67
1	B	46	GLN	CB-CG-CD	5.85	122.54	112.60
1	B	198	GLU	CB-CG-CD	5.80	122.47	112.60
1	A	73	GLU	CB-CG-CD	5.80	122.45	112.60
1	A	333	THR	O-C-N	5.59	125.76	121.23
1	B	663	ASP	N-CA-C	5.55	118.05	111.33
1	A	46	GLN	N-CA-CB	5.48	118.06	110.17
1	A	247	ASN	CB-CA-C	5.43	117.19	109.38
1	A	575	ALA	CA-C-N	-5.41	115.16	120.52
1	A	575	ALA	C-N-CA	-5.41	115.16	120.52
1	B	114	ALA	N-CA-C	5.41	118.09	111.82
1	A	608	LYS	CB-CG-CD	5.39	123.70	111.30
1	A	381	SER	CB-CA-C	-5.38	98.73	111.65
1	B	39	ASN	CA-C-N	5.36	127.77	120.54
1	B	39	ASN	C-N-CA	5.36	127.77	120.54
1	A	591	MET	CA-CB-CG	5.32	124.73	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	SER	N-CA-CB	5.25	120.07	111.31
1	B	48	ASP	N-CA-C	5.21	117.10	108.20
1	A	504	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	B	450	ILE	CB-CA-C	-5.11	104.85	110.52
1	A	46	GLN	CB-CG-CD	5.07	121.22	112.60
1	A	420	TRP	N-CA-C	-5.05	105.85	111.36
1	A	71	ALA	N-CA-C	5.05	116.47	111.07
1	A	407	GLU	CB-CG-CD	5.03	121.16	112.60
1	B	54	ARG	N-CA-C	-5.02	103.78	110.55
1	B	46	GLN	N-CA-CB	5.01	117.38	110.17

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	5560	0	5371	17	0
1	B	5546	0	5366	16	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	24	0	42	1	0
5	B	8	0	14	2	0
6	A	723	0	0	5	0
6	B	724	0	0	8	0
All	All	12677	0	10853	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:A:119[B]:THR:HG21	6:A:999:HOH:O	1.82	0.80
1:B:119[B]:THR:HG21	6:B:1296:HOH:O	1.84	0.77
1:B:512:ASP:OD1	6:B:901:HOH:O	2.08	0.70
1:B:519:GLU:OE1	6:B:902:HOH:O	2.09	0.70
1:A:608:LYS:O	1:A:608:LYS:HD2	2.05	0.56
1:B:178:GLU:OE1	6:B:904:HOH:O	2.18	0.55
1:A:336[B]:GLN:HG3	6:A:1057:HOH:O	2.07	0.54
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.38	0.54
1:A:504:ARG:HD2	6:A:1082:HOH:O	2.10	0.52
1:A:365:LYS:HA	1:A:382:ARG:HH11	1.75	0.52
1:A:696:LYS:NZ	6:A:906:HOH:O	2.40	0.51
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.94	0.51
5:A:805:MPD:H52	5:A:805:MPD:H11	1.92	0.51
5:B:804:MPD:O4	5:B:804:MPD:H12	2.12	0.50
4:B:803:OXY:O2	6:B:903:HOH:O	2.18	0.49
1:B:428:MET:O	1:B:433:ARG:HD3	2.13	0.48
1:B:725:GLN:CD	6:B:1288:HOH:O	2.57	0.48
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.49	0.47
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.98	0.47
1:A:54:ARG:HB3	1:A:55:HIS:CD2	2.50	0.47
1:B:47:LEU:HB2	6:B:908:HOH:O	2.16	0.46
1:A:70:GLN:NE2	6:A:921:HOH:O	2.49	0.46
1:A:725:GLN:NE2	1:A:726[A]:GLU:HG3	2.30	0.46
1:A:426[B]:ARG:HA	1:A:426[B]:ARG:HD2	1.86	0.44
1:B:324:SER:O	5:B:804:MPD:H53	2.17	0.44
1:A:428:MET:O	1:A:433:ARG:HD3	2.18	0.44
1:B:512:ASP:HB2	6:B:1336:HOH:O	2.18	0.43
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.18	0.43
1:B:119[A]:THR:CG2	1:B:265:ALA:HB2	2.49	0.42
1:B:115:GLY:O	1:B:264:MET:HE1	2.20	0.42
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.20	0.42
1:A:480:LEU:HD22	1:A:554:ALA:HB1	2.01	0.41
1:B:112:HIS:CE1	1:B:141:ASP:O	2.73	0.41
1:A:351:GLU:HG3	1:A:352:LEU:N	2.36	0.41
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.21	0.40
1:A:111:TOX:H9	1:A:238:TYR:OH	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	717/728 (98%)	706 (98%)	11 (2%)	0	100	100
1	B	716/728 (98%)	703 (98%)	13 (2%)	0	100	100
All	All	1433/1456 (98%)	1409 (98%)	24 (2%)	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	556/560 (99%)	548 (99%)	8 (1%)	59	44
1	B	555/560 (99%)	548 (99%)	7 (1%)	61	46
All	All	1111/1120 (99%)	1096 (99%)	15 (1%)	59	44

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	141	ASP
1	A	351	GLU
1	A	365	LYS
1	A	381	SER
1	A	591	MET
1	A	608	LYS
1	A	725	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	40	ARG
1	B	54	ARG
1	B	141	ASP
1	B	512	ASP
1	B	608	LYS
1	B	610	ARG
1	B	730	ARG

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	737	ASN
1	B	227	ASN
1	B	406	HIS
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	1,2	14,17,18	2.45	7 (50%)	12,23,25	1.95	4 (33%)
1	TOX	A	111	1	14,17,18	2.64	7 (50%)	12,23,25	2.50	6 (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
1	TOX	B	111	1,2	-	3/5/8/10	0/2/2/2
1	TOX	A	111	1	-	4/5/8/10	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	TOX	CD2-CE2	4.96	1.47	1.41
1	B	111	TOX	CD2-CE2	4.45	1.46	1.41
1	A	111	TOX	CE3-CD2	-3.98	1.33	1.39
1	A	111	TOX	CE2-NE1	-3.90	1.32	1.39
1	B	111	TOX	O-C	3.83	1.34	1.20
1	A	111	TOX	O1-NE1	3.47	1.43	1.39
1	B	111	TOX	CE2-NE1	-3.40	1.33	1.39
1	B	111	TOX	CB-CA	3.17	1.60	1.53
1	A	111	TOX	CD1-CG	2.91	1.42	1.36
1	B	111	TOX	CE3-CD2	-2.79	1.35	1.39
1	A	111	TOX	CH2-CZ3	2.59	1.43	1.38
1	B	111	TOX	CZ2-CE2	-2.54	1.35	1.39
1	B	111	TOX	CH2-CZ3	2.27	1.43	1.38
1	A	111	TOX	O-C	2.09	1.27	1.20

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	TOX	CB-CG-CD2	4.55	135.45	126.70
1	A	111	TOX	CB-CG-CD1	-4.48	120.44	126.67
1	B	111	TOX	CZ2-CE2-NE1	3.96	135.68	129.37
1	A	111	TOX	CH2-CZ3-CE3	-2.86	116.71	120.24
1	A	111	TOX	CZ3-CH2-CZ2	2.71	123.58	120.24
1	B	111	TOX	CH2-CZ3-CE3	-2.70	116.90	120.24
1	A	111	TOX	CD2-CG-CD1	-2.48	104.10	106.34
1	B	111	TOX	CZ2-CE2-CD2	-2.26	119.42	121.95
1	A	111	TOX	CZ2-CE2-CD2	-2.24	119.45	121.95
1	B	111	TOX	CB-CG-CD1	-2.15	123.68	126.67

There are no chirality outliers.

All (7) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	B	111	TOX	C-CA-CB-CG
1	A	111	TOX	CA-CB-CG-CD2
1	A	111	TOX	CA-CB-CG-CD1
1	B	111	TOX	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	OXY	A	803	-	1,1,1	0.41	0	-		
2	HEM	A	801	1	50,50,50	1.60	10 (20%)	67,82,82	1.75	19 (28%)
5	MPD	B	804	-	7,7,7	0.57	0	9,10,10	1.65	3 (33%)
5	MPD	A	806	-	7,7,7	0.74	0	9,10,10	1.21	1 (11%)
5	MPD	A	805	-	7,7,7	0.68	0	9,10,10	2.12	3 (33%)
2	HEM	B	801	1	50,50,50	1.65	12 (24%)	67,82,82	1.40	9 (13%)
4	OXY	B	803	-	1,1,1	0.77	0	-		
5	MPD	A	804	-	7,7,7	0.69	0	9,10,10	1.58	2 (22%)

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	-
5	MPD	B	804	-	-	3/5/5/5	-
5	MPD	A	806	-	-	2/5/5/5	-
5	MPD	A	805	-	-	4/5/5/5	-
2	HEM	B	801	1	-	2/14/54/54	-
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	801	HEM	CMD-C2D	-4.00	1.42	1.50
2	A	801	HEM	FE-NA	3.70	2.07	1.95
2	A	801	HEM	FE-NC	3.64	2.07	1.95
2	B	801	HEM	C4D-ND	-3.49	1.34	1.40
2	A	801	HEM	C4D-ND	-3.35	1.34	1.40
2	A	801	HEM	C4A-NA	-3.32	1.33	1.39
2	B	801	HEM	C1B-NB	-3.02	1.35	1.40
2	A	801	HEM	C3C-C4C	2.96	1.51	1.46
2	B	801	HEM	FE-NC	2.89	2.04	1.95
2	A	801	HEM	CHD-C4C	-2.80	1.32	1.38
2	B	801	HEM	C1B-C2B	-2.78	1.38	1.44
2	B	801	HEM	O2D-CGD	-2.56	1.22	1.30
2	B	801	HEM	C3C-C4C	-2.54	1.41	1.46
2	B	801	HEM	C3C-C2C	-2.47	1.32	1.37
2	B	801	HEM	FE-NB	2.46	2.02	1.94
2	B	801	HEM	FE-NA	2.27	2.02	1.95
2	A	801	HEM	C1A-NA	-2.23	1.35	1.39
2	A	801	HEM	CHB-C1B	-2.21	1.34	1.38
2	B	801	HEM	C4D-C3D	2.04	1.48	1.45
2	A	801	HEM	CAD-C3D	2.03	1.56	1.51
2	B	801	HEM	FE-ND	2.02	2.01	1.94
2	A	801	HEM	CMC-C2C	2.01	1.54	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C3B-C2B-C1B	-4.65	102.92	106.41
2	A	801	HEM	CMA-C3A-C4A	4.63	132.47	125.42
5	A	805	MPD	O2-C2-CM	-4.41	94.24	107.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CHD-C4C-NC	-4.04	120.05	124.45
2	A	801	HEM	C4A-C3A-C2A	-4.01	102.23	106.82
2	B	801	HEM	CHC-C4B-NB	3.75	128.46	124.42
2	B	801	HEM	C3B-C4B-NB	-3.54	106.92	109.47
2	A	801	HEM	C2B-C1B-NB	3.19	113.51	109.84
2	A	801	HEM	O2A-CGA-CBA	3.12	123.85	114.00
2	B	801	HEM	O1A-CGA-CBA	-3.00	113.59	123.09
2	A	801	HEM	CHD-C1D-ND	2.97	127.62	124.42
5	A	804	MPD	O2-C2-C1	2.90	117.01	107.99
2	A	801	HEM	O1A-CGA-CBA	-2.88	113.97	123.09
2	A	801	HEM	CAA-CBA-CGA	-2.85	106.10	113.67
2	A	801	HEM	C3C-C2C-C1C	-2.81	104.39	107.05
5	A	804	MPD	O2-C2-CM	-2.79	99.28	107.99
2	B	801	HEM	CAC-C3C-C4C	-2.68	118.42	124.82
5	B	804	MPD	C1-C2-C3	2.68	121.75	110.20
5	A	806	MPD	O2-C2-CM	-2.65	99.73	107.99
5	A	805	MPD	CM-C2-C1	2.64	116.53	110.63
2	B	801	HEM	CAA-CBA-CGA	-2.59	106.80	113.67
2	A	801	HEM	CBD-CAD-C3D	2.55	119.58	112.53
5	A	805	MPD	O4-C4-C3	-2.53	101.27	111.35
5	B	804	MPD	O2-C2-C3	-2.52	99.83	109.27
2	A	801	HEM	C2A-C1A-NA	-2.49	107.39	110.15
2	A	801	HEM	C4B-C3B-C2B	2.43	109.52	107.28
2	A	801	HEM	CHC-C1C-C2C	-2.42	120.45	125.49
2	B	801	HEM	C1B-NB-C4B	2.40	108.05	105.21
5	B	804	MPD	O2-C2-CM	2.40	115.47	107.99
2	B	801	HEM	C4C-NC-C1C	-2.39	101.93	105.82
2	A	801	HEM	CHC-C1C-NC	2.34	127.00	124.45
2	B	801	HEM	C3C-C2C-C1C	-2.34	104.83	107.05
2	A	801	HEM	C1B-NB-C4B	-2.15	102.66	105.21
2	A	801	HEM	CAC-C3C-C4C	-2.13	119.72	124.82
2	A	801	HEM	CHB-C1B-NB	-2.13	121.73	124.37
2	A	801	HEM	C1D-C2D-C3D	-2.11	104.76	106.98
2	A	801	HEM	C4C-NC-C1C	2.10	109.24	105.82

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	805	MPD	C2-C3-C4-O4
5	A	806	MPD	C2-C3-C4-C5
5	B	804	MPD	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

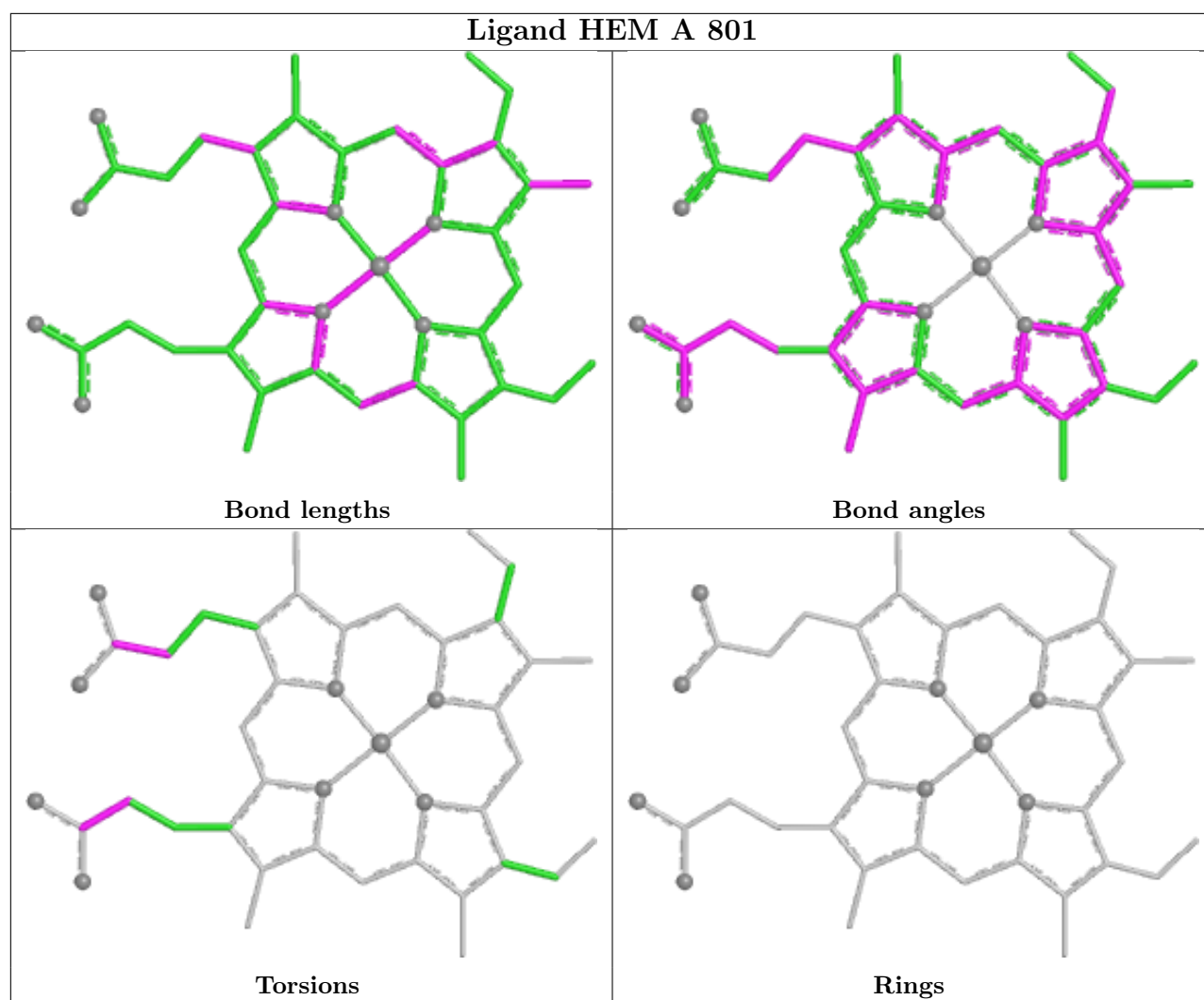
Mol	Chain	Res	Type	Atoms
5	B	804	MPD	O2-C2-C3-C4
5	A	805	MPD	CM-C2-C3-C4
5	B	804	MPD	CM-C2-C3-C4
5	A	805	MPD	C2-C3-C4-C5
2	B	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAA-CBA-CGA-O2A
5	A	806	MPD	C2-C3-C4-O4
5	A	805	MPD	C1-C2-C3-C4
2	A	801	HEM	CAD-CBD-CGD-O2D

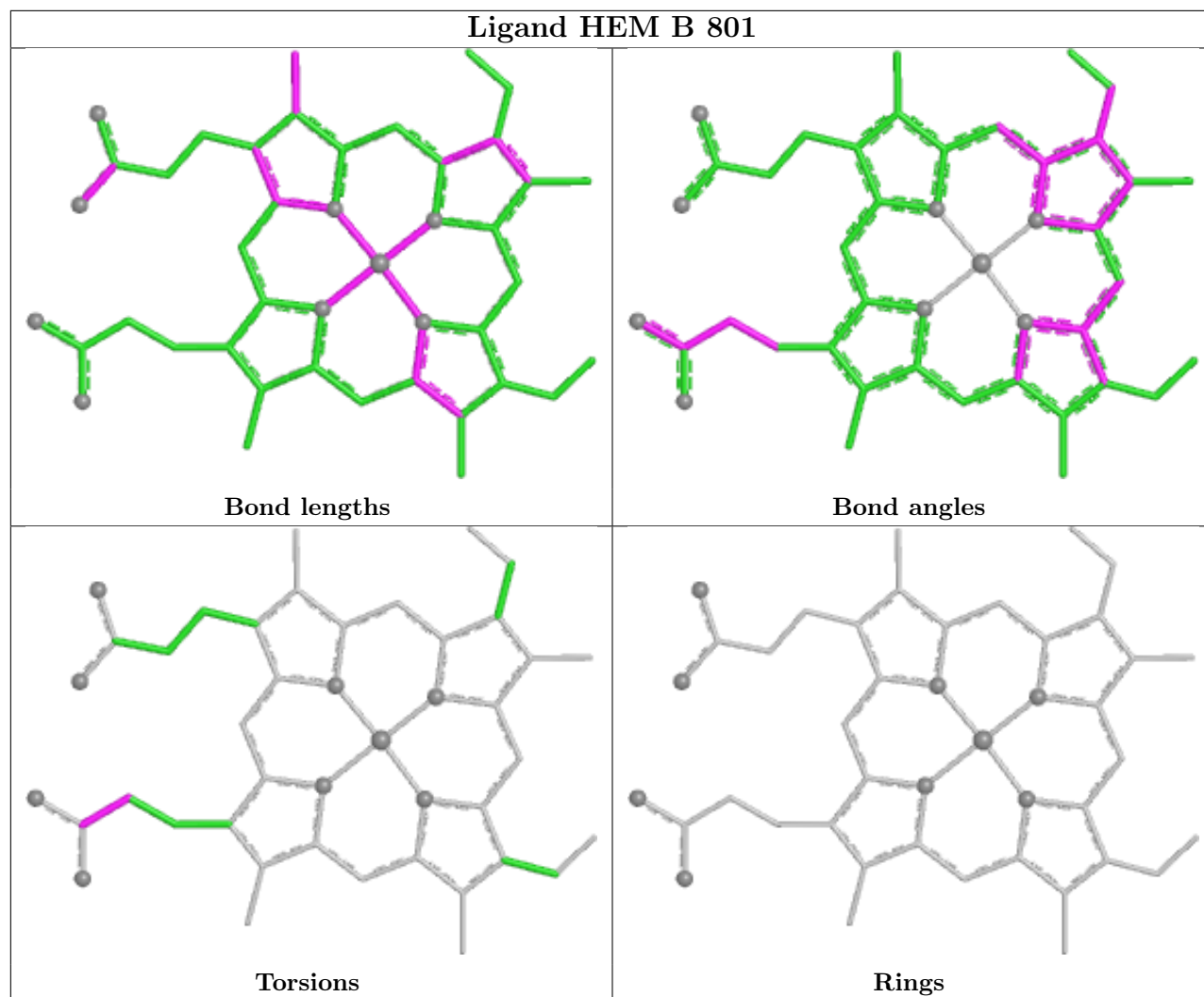
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	804	MPD	2	0
5	A	805	MPD	1	0
4	B	803	OXY	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	712/728 (97%)	-0.13	8 (1%) 78 83	10, 25, 43, 81	7 (0%)
1	B	712/728 (97%)	-0.23	10 (1%) 73 80	9, 24, 42, 82	6 (0%)
All	All	1424/1456 (97%)	-0.18	18 (1%) 75 81	9, 24, 43, 82	13 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	4.4
1	A	748	ALA	3.9
1	B	680	ALA	3.1
1	B	679	ALA	3.1
1	B	610	ARG	2.8
1	B	65	ASP	2.7
1	B	40	ARG	2.5
1	A	365	LYS	2.4
1	A	55	HIS	2.4
1	B	542	GLY	2.4
1	B	611	VAL	2.4
1	B	55	HIS	2.4
1	A	608	LYS	2.3
1	A	364	ALA	2.3
1	A	227	ASN	2.3
1	A	680	ALA	2.2
1	A	607	GLY	2.2
1	B	682	ALA	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($\text{\AA}^2$)	Q<0.9
1	TOX	A	111	16/17	0.98	0.05	16,19,26,30	2
1	TOX	B	111	16/17	0.98	0.05	17,19,31,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

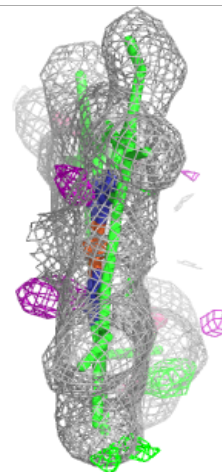
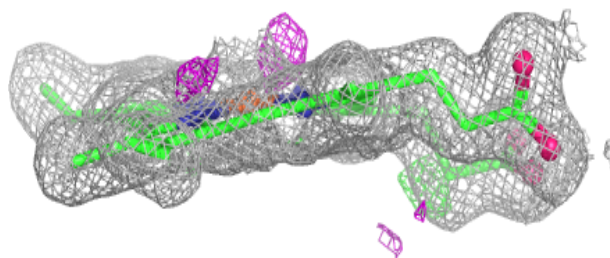
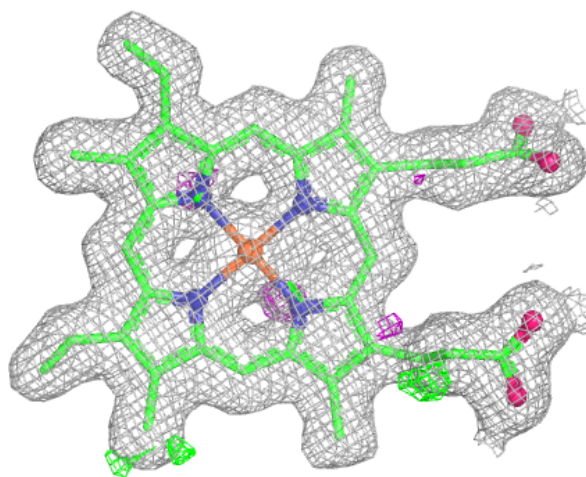
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MPD	A	804	8/8	0.85	0.19	58,67,73,73	0
5	MPD	A	806	8/8	0.85	0.19	73,80,84,85	0
5	MPD	B	804	8/8	0.89	0.17	53,60,68,68	0
5	MPD	A	805	8/8	0.90	0.13	39,45,66,68	0
4	OXY	B	803	2/2	0.91	0.16	36,36,36,37	0
4	OXY	A	803	2/2	0.93	0.17	34,34,34,45	0
2	HEM	A	801	43/43	0.98	0.05	17,19,22,26	0
2	HEM	B	801	43/43	0.99	0.04	18,19,21,27	0
3	NA	A	802	1/1	1.00	0.05	20,20,20,20	0
3	NA	B	802	1/1	1.00	0.04	21,21,21,21	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.

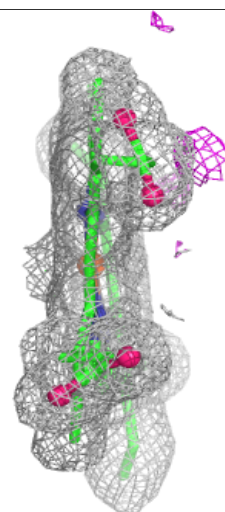
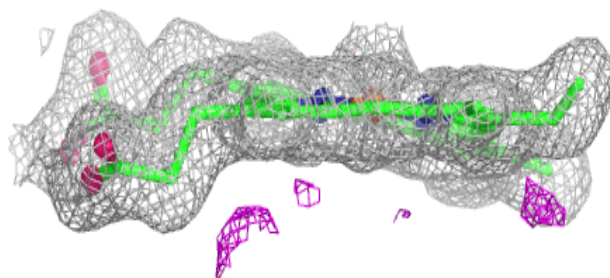
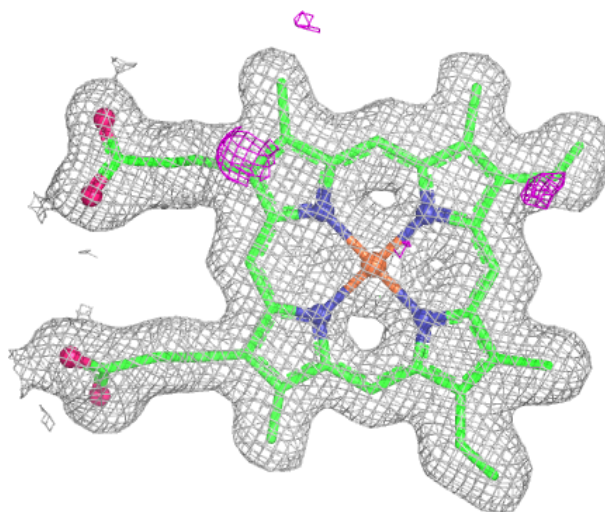
Electron density around HEM A 801:

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



Electron density around HEM B 801:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.