



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2026 – 10:48 PM EDT

PDB ID : 5KQ0 / pdb_00005kq0
Title : Crystal structure of the A290D variant of catalase-peroxidase from *B. pseudo-mallei*
Authors : Loewen, P.C.
Deposited on : 2016-07-05
Resolution : 1.80 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

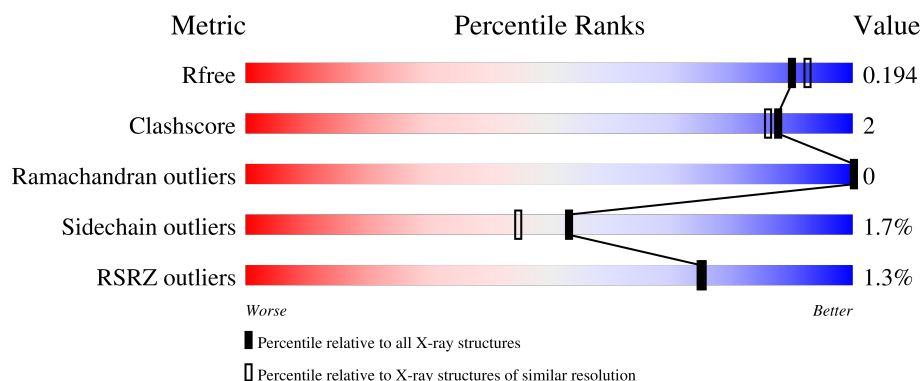
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	% 86% 11% ..
1	B	728	% 87% 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
4	CL	B	803	-	-	X	-
7	MPD	A	808	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12876 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.

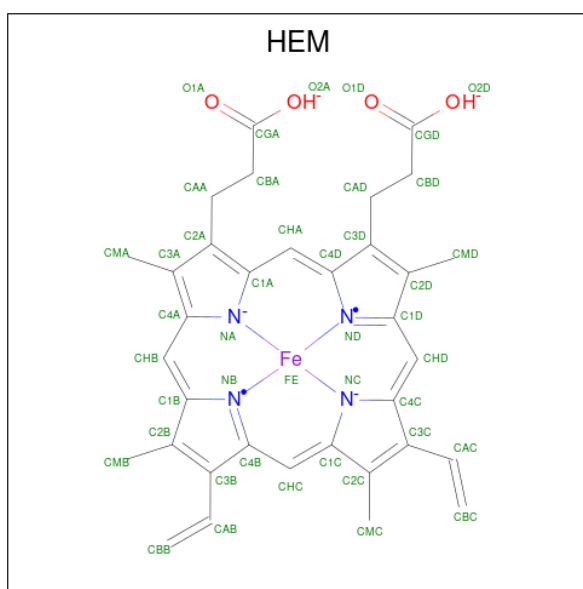
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	7	0
			5570	3513	992	1051	14			
1	B	713	Total	C	N	O	S	0	5	0
			5545	3500	986	1045	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	ASP	ALA	engineered mutation	UNP Q3JNW6
B	290	ASP	ALA	engineered mutation	UNP Q3JNW6

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



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 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).



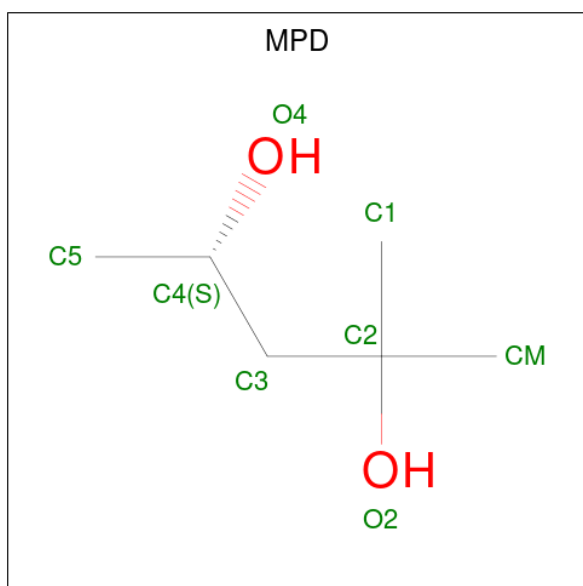
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	B	1	Total	O		
			2	2	0	0

- 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		

Continued on next page...

Continued from previous page...

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		

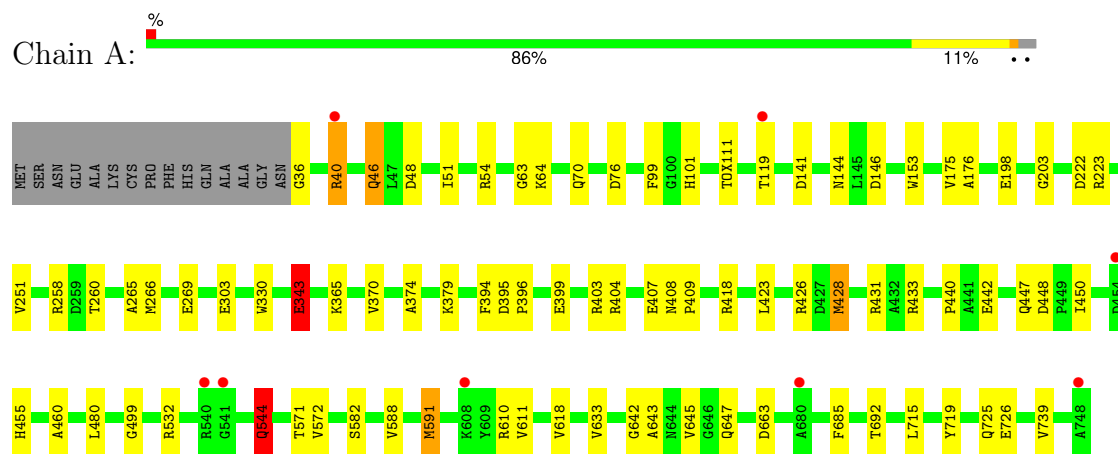
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	803	Total	O	0	0
			803	803		
8	B	822	Total	O	0	0
			822	822		

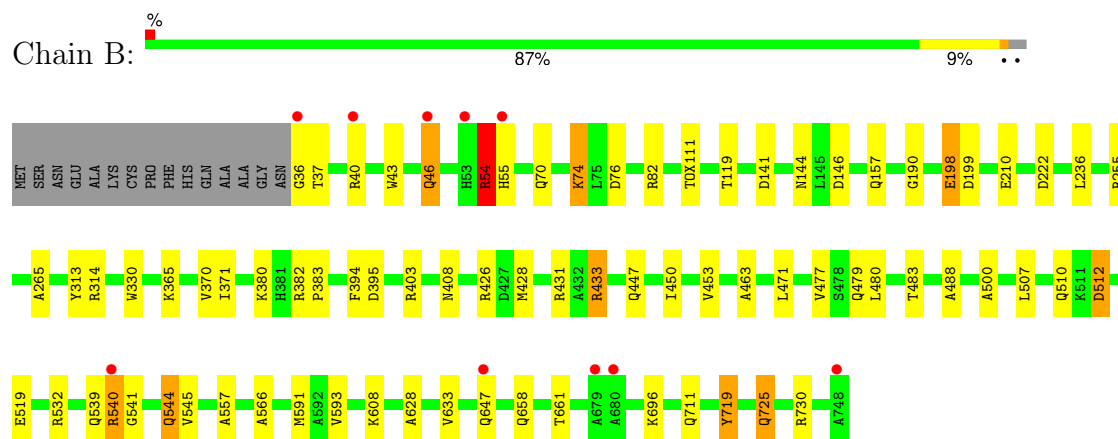
3 Residue-property plots [i](#)

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	100.76Å 113.49Å 174.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.14 – 1.80 95.14 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (95.14-1.80) 98.3 (95.14-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.152 , 0.185 0.164 , 0.194	Depositor DCC
R_{free} test set	9092 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12876	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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, OXY, PO4, HEM, MPD, NA, 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	1.72	49/5696 (0.9%)	1.28	17/7740 (0.2%)
1	B	1.71	45/5674 (0.8%)	1.30	16/7712 (0.2%)
All	All	1.72	94/11370 (0.8%)	1.29	33/15452 (0.2%)

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	512	ASP	CG-OD2	11.57	1.47	1.25
1	A	544	GLN	CD-OE1	9.32	1.41	1.23
1	B	544	GLN	CD-NE2	8.99	1.52	1.33
1	A	365	LYS	N-CA	8.75	1.57	1.46
1	B	557	ALA	N-CA	-8.73	1.35	1.46
1	B	532	ARG	CD-NE	-8.64	1.34	1.46
1	A	499	GLY	C-O	8.46	1.31	1.23
1	A	739	VAL	CA-CB	-7.92	1.45	1.54
1	A	203	GLY	C-O	7.36	1.29	1.23
1	B	479	GLN	N-CA	-7.20	1.37	1.46
1	B	512	ASP	CB-CG	7.11	1.69	1.52
1	B	453	VAL	C-O	-7.05	1.16	1.24
1	A	642	GLY	N-CA	6.76	1.54	1.45
1	B	480	LEU	CA-C	6.75	1.61	1.52
1	B	190	GLY	C-O	-6.73	1.17	1.24
1	A	448	ASP	C-O	6.67	1.26	1.23
1	A	571	THR	N-CA	-6.65	1.38	1.46
1	A	399	GLU	C-O	-6.61	1.16	1.24
1	B	82	ARG	CZ-NH2	-6.59	1.24	1.33
1	A	448	ASP	N-CA	6.55	1.52	1.46
1	B	477	VAL	N-CA	6.52	1.54	1.46
1	B	43	TRP	CA-CB	6.48	1.60	1.53
1	B	730	ARG	CZ-NH2	6.46	1.41	1.33
1	B	383	PRO	C-O	6.38	1.31	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	715	LEU	CA-C	-6.37	1.44	1.52
1	A	63	GLY	N-CA	6.33	1.53	1.45
1	A	40	ARG	N-CA	6.27	1.53	1.46
1	A	260	THR	N-CA	6.24	1.53	1.46
1	A	303	GLU	C-O	-6.22	1.16	1.24
1	B	222	ASP	CA-C	6.15	1.60	1.53
1	A	175	VAL	N-CA	-6.10	1.38	1.46
1	A	269	GLU	CA-C	6.00	1.60	1.52
1	A	395	ASP	CA-C	-6.00	1.46	1.52
1	B	725	GLN	CD-NE2	5.94	1.45	1.33
1	B	370	VAL	CA-C	5.92	1.61	1.52
1	B	532	ARG	CZ-NH1	-5.91	1.24	1.32
1	A	222	ASP	CA-C	5.90	1.60	1.53
1	B	210	GLU	C-O	5.90	1.30	1.23
1	A	370	VAL	CA-C	5.89	1.61	1.52
1	B	37	THR	C-O	-5.69	1.17	1.23
1	A	572	VAL	C-O	-5.65	1.17	1.24
1	A	269	GLU	N-CA	-5.61	1.39	1.46
1	A	36	GLY	N-CA	5.60	1.54	1.45
1	A	692	THR	CA-C	-5.60	1.45	1.52
1	B	711	GLN	CD-NE2	-5.57	1.21	1.33
1	B	545	VAL	N-CA	5.56	1.52	1.46
1	B	450	ILE	C-O	-5.55	1.18	1.24
1	B	510	GLN	CA-C	-5.51	1.45	1.52
1	A	442	GLU	C-O	-5.51	1.17	1.23
1	B	507	LEU	CA-C	-5.50	1.46	1.52
1	A	266	MET	CA-CB	-5.50	1.44	1.53
1	A	404	ARG	CA-C	5.50	1.59	1.52
1	B	488	ALA	N-CA	5.50	1.53	1.46
1	A	409	PRO	C-O	5.47	1.31	1.24
1	B	365	LYS	N-CA	5.46	1.53	1.46
1	A	423	LEU	CA-C	5.43	1.60	1.52
1	A	258	ARG	N-CA	-5.41	1.39	1.46
1	B	658	GLN	CD-NE2	-5.40	1.22	1.33
1	A	450	ILE	CA-C	5.39	1.57	1.52
1	B	157	GLN	N-CA	-5.38	1.39	1.46
1	A	223	ARG	CZ-NH1	5.37	1.40	1.32
1	A	260	THR	CA-CB	-5.36	1.45	1.53
1	A	645	VAL	CA-CB	-5.36	1.48	1.54
1	A	343	GLU	N-CA	5.34	1.52	1.46
1	A	394	PHE	N-CA	5.32	1.53	1.46
1	B	566	ALA	C-O	-5.31	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	433	ARG	CZ-NH2	-5.29	1.26	1.33
1	A	418	ARG	CZ-NH2	-5.27	1.26	1.33
1	B	483	THR	CA-CB	5.27	1.61	1.53
1	B	628	ALA	C-O	-5.27	1.19	1.24
1	A	532	ARG	CD-NE	-5.26	1.38	1.46
1	B	500	ALA	N-CA	5.25	1.53	1.46
1	A	460	ALA	CA-C	-5.25	1.46	1.52
1	A	408	ASN	CA-CB	-5.25	1.47	1.53
1	B	371	ILE	N-CA	5.25	1.53	1.46
1	A	379	LYS	C-O	5.24	1.30	1.23
1	A	440	PRO	N-CA	-5.23	1.40	1.47
1	B	463	ALA	C-O	5.22	1.30	1.24
1	B	46	GLN	CG-CD	5.22	1.65	1.52
1	B	314	ARG	C-O	-5.19	1.19	1.24
1	A	582	SER	CA-C	-5.17	1.45	1.53
1	A	101	HIS	C-O	-5.16	1.18	1.23
1	A	176	ALA	N-CA	-5.12	1.40	1.46
1	B	236	LEU	C-O	-5.12	1.17	1.23
1	A	480	LEU	N-CA	-5.10	1.40	1.46
1	B	54	ARG	CA-C	-5.08	1.46	1.53
1	A	588	VAL	N-CA	-5.08	1.40	1.46
1	B	719	TYR	N-CA	5.06	1.52	1.46
1	A	685	PHE	N-CA	-5.04	1.39	1.46
1	B	408	ASN	N-CA	-5.04	1.41	1.46
1	B	471	LEU	CB-CG	5.03	1.63	1.53
1	A	153	TRP	CA-CB	5.02	1.60	1.53
1	B	36	GLY	N-CA	5.01	1.53	1.45
1	B	313	TYR	CA-CB	5.00	1.59	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	591	MET	CG-SD-CE	-9.89	79.14	100.90
1	A	343	GLU	CA-CB-CG	8.22	130.54	114.10
1	B	426	ARG	NE-CZ-NH1	-6.29	115.21	121.50
1	A	403	ARG	CG-CD-NE	-6.27	98.20	112.00
1	A	70	GLN	CA-CB-CG	6.23	126.57	114.10
1	B	330	TRP	N-CA-C	6.20	118.11	111.36
1	A	643	ALA	N-CA-C	6.13	120.37	113.01
1	B	46	GLN	CB-CG-CD	6.13	123.02	112.60
1	B	395	ASP	N-CA-C	-6.06	102.02	109.65
1	B	403	ARG	CG-CD-NE	-5.93	98.95	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	VAL	N-CA-C	5.92	116.10	110.42
1	A	46	GLN	CB-CG-CD	5.80	122.47	112.60
1	A	48	ASP	N-CA-C	5.77	118.20	107.99
1	B	512	ASP	CB-CG-OD1	-5.77	105.14	118.40
1	B	539	GLN	O-C-N	5.71	129.42	122.96
1	B	532	ARG	CG-CD-NE	-5.67	99.52	112.00
1	B	512	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	330	TRP	N-CA-C	5.66	117.53	111.36
1	A	343	GLU	CB-CG-CD	5.62	122.16	112.60
1	B	46	GLN	N-CA-C	-5.59	102.61	110.50
1	A	46	GLN	N-CA-C	-5.58	102.63	110.50
1	A	46	GLN	N-CA-CB	5.56	118.18	110.17
1	B	46	GLN	N-CA-CB	5.55	118.17	110.17
1	B	70	GLN	CA-CB-CG	-5.54	103.03	114.10
1	A	404	ARG	NE-CZ-NH2	-5.42	114.32	119.20
1	A	591	MET	CA-CB-CG	5.31	124.72	114.10
1	A	396	PRO	N-CA-C	5.22	120.78	113.53
1	B	394	PHE	N-CA-C	5.18	119.60	113.28
1	B	541	GLY	N-CA-C	-5.17	101.60	112.45
1	A	663	ASP	N-CA-C	5.08	117.48	111.33
1	A	407	GLU	CG-CD-OE1	5.07	130.05	118.40
1	A	54	ARG	CG-CD-NE	-5.03	100.93	112.00
1	B	450	ILE	CB-CA-C	-5.02	105.00	110.37

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	5570	0	5369	18	0
1	B	5545	0	5354	24	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	1	0
4	B	1	0	0	2	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	3	0
7	B	8	0	14	0	0
8	A	803	0	0	3	0
8	B	822	0	0	9	0
All	All	12876	0	10839	45	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 (45) 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:540:ARG:NE	1:B:540:ARG:HA	1.86	0.89
7:A:806:MPD:O4	7:A:806:MPD:H12	1.82	0.79
1:B:512:ASP:OD1	8:B:901:HOH:O	1.99	0.79
1:B:540:ARG:HA	1:B:540:ARG:CZ	2.22	0.69
1:B:519:GLU:OE1	8:B:902:HOH:O	2.11	0.68
1:A:76:ASP:OD2	8:A:903:HOH:O	2.12	0.65
1:B:198:GLU:OE1	8:B:903:HOH:O	2.15	0.65
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.32	0.63
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.81	0.63
7:A:806:MPD:O4	7:A:806:MPD:C1	2.45	0.63
1:B:540:ARG:NE	1:B:540:ARG:CA	2.52	0.61
1:B:198:GLU:HG2	4:B:803:CL:CL	2.40	0.59
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.86	0.59
1:A:343:GLU:HG2	8:A:1494:HOH:O	2.03	0.58
1:A:725:GLN:NE2	1:A:726[A]:GLU:HG3	2.18	0.58
1:B:647:GLN:HG2	8:B:969:HOH:O	2.05	0.56
1:B:76:ASP:OD2	8:B:904:HOH:O	2.18	0.56
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.10	0.51
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.11	0.50
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.42	0.49
1:B:74:LYS:HD3	8:B:1421:HOH:O	2.11	0.49
1:B:661:THR:HA	1:B:725:GLN:HE22	1.76	0.49
1:A:119[A]:THR:HG22	1:A:265:ALA:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ASP:HB3	8:B:942:HOH:O	2.14	0.48
1:B:540:ARG:HA	1:B:540:ARG:HE	1.73	0.47
1:A:725:GLN:HE21	1:A:726[A]:GLU:HG3	1.80	0.46
1:B:255:ARG:HB2	8:B:1627:HOH:O	2.15	0.46
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.16	0.45
7:A:807:MPD:HM1	7:A:807:MPD:O4	2.16	0.45
1:A:610:ARG:HG3	1:A:611:VAL:HG23	2.00	0.44
1:B:119[A]:THR:CG2	1:B:265:ALA:HB2	2.48	0.44
1:B:198:GLU:CG	4:B:803:CL:CL	3.02	0.44
1:A:633[A]:VAL:HG22	1:A:719:TYR:CZ	2.51	0.43
1:A:426[B]:ARG:NH2	8:A:931:HOH:O	2.51	0.43
1:A:51:ILE:HD11	1:A:618:VAL:HG12	2.00	0.43
1:B:428:MET:O	1:B:433:ARG:HD3	2.20	0.41
1:A:428:MET:O	1:A:433:ARG:HD3	2.21	0.41
1:A:647:GLN:CD	1:A:647:GLN:N	2.79	0.41
1:B:119[B]:THR:HG23	1:B:593:VAL:HG11	2.02	0.41
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.19	0.41
1:B:647:GLN:HA	1:B:647:GLN:NE2	2.36	0.41
1:A:99:PHE:CD2	1:A:374:ALA:HA	2.55	0.41
1:A:198:GLU:HG3	4:A:803:CL:CL	2.58	0.40
1:B:382:ARG:HD2	8:B:953:HOH:O	2.21	0.40
1:A:455:HIS:CE1	1:A:544:GLN:HG3	2.57	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	717/728 (98%)	702 (98%)	15 (2%)	0	100	100
1	B	715/728 (98%)	705 (99%)	10 (1%)	0	100	100
All	All	1432/1456 (98%)	1407 (98%)	25 (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	557/561 (99%)	549 (99%)	8 (1%)	59	52
1	B	555/561 (99%)	544 (98%)	11 (2%)	48	38
All	All	1112/1122 (99%)	1093 (98%)	19 (2%)	53	45

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

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	64	LYS
1	A	141	ASP
1	A	343	GLU
1	A	428	MET
1	A	544	GLN
1	A	591	MET
1	B	40	ARG
1	B	46	GLN
1	B	54	ARG
1	B	74	LYS
1	B	141	ASP
1	B	198	GLU
1	B	380	LYS
1	B	540	ARG
1	B	544	GLN
1	B	608	LYS
1	B	696	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	247	ASN
1	A	520	GLN
1	A	711	GLN
1	B	406	HIS
1	B	520	GLN
1	B	544	GLN
1	B	647	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	1	14,17,18	2.02	7 (50%)	12,23,25	2.78	5 (41%)
1	TOX	A	111	1,2	14,17,18	2.39	7 (50%)	12,23,25	2.17	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	-	4/5/8/10	0/2/2/2
1	TOX	A	111	1,2	-	2/5/8/10	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-CG	4.09	1.50	1.44
1	B	111	TOX	CE3-CD2	-3.93	1.34	1.39
1	A	111	TOX	O-C	3.51	1.33	1.20
1	A	111	TOX	CD1-CG	3.44	1.43	1.36
1	A	111	TOX	CH2-CZ3	2.95	1.44	1.38
1	B	111	TOX	CZ3-CE3	-2.69	1.34	1.38
1	A	111	TOX	CE2-NE1	-2.54	1.35	1.39
1	B	111	TOX	CD2-CG	2.40	1.47	1.44
1	B	111	TOX	CH2-CZ3	2.39	1.43	1.38
1	B	111	TOX	O-C	2.35	1.28	1.20
1	B	111	TOX	CH2-CZ2	2.25	1.42	1.38
1	B	111	TOX	O1-NE1	-2.13	1.36	1.39
1	A	111	TOX	O1-NE1	2.05	1.41	1.39
1	A	111	TOX	CD2-CE2	2.02	1.43	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	TOX	CH2-CZ3-CE3	5.64	127.20	120.24
1	B	111	TOX	CZ3-CH2-CZ2	-5.47	113.48	120.24
1	A	111	TOX	CE3-CD2-CE2	4.57	124.51	119.24
1	B	111	TOX	CZ2-CE2-NE1	3.15	134.39	129.37
1	A	111	TOX	CE2-CD2-CG	-2.86	104.76	107.39
1	B	111	TOX	CB-CG-CD1	-2.68	122.94	126.67
1	A	111	TOX	CZ2-CE2-CD2	-2.64	119.01	121.95
1	B	111	TOX	CB-CG-CD2	2.63	131.75	126.70
1	A	111	TOX	CZ3-CE3-CD2	-2.54	115.20	119.80
1	A	111	TOX	CZ2-CE2-NE1	2.31	133.04	129.37
1	A	111	TOX	CE3-CD2-CG	-2.19	130.59	133.85

There are no chirality outliers.

All (6) 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
1	B	111	TOX	CA-CB-CG-CD2
1	B	111	TOX	CA-CB-CG-CD1

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	B	801	1	50,50,50	1.81	14 (28%)	67,82,82	2.20	29 (43%)
7	MPD	A	807	-	7,7,7	0.66	0	9,10,10	1.19	0
6	PO4	B	805	-	4,4,4	0.89	0	6,6,6	2.24	2 (33%)
7	MPD	A	808	-	7,7,7	0.99	0	9,10,10	2.66	4 (44%)
2	HEM	A	801	1	50,50,50	2.11	16 (32%)	67,82,82	1.97	21 (31%)
5	OXY	B	804	-	1,1,1	0.37	0	-	-	-
7	MPD	B	806	-	7,7,7	0.96	0	9,10,10	2.05	3 (33%)
7	MPD	A	806	-	7,7,7	0.92	0	9,10,10	1.08	1 (11%)
6	PO4	A	805	-	4,4,4	0.58	0	6,6,6	1.65	2 (33%)
5	OXY	A	804	-	1,1,1	0.40	0	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	801	1	-	2/14/54/54	-
7	MPD	A	807	-	-	0/5/5/5	-
7	MPD	A	808	-	-	5/5/5/5	-
2	HEM	A	801	1	-	2/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MPD	B	806	-	-	3/5/5/5	-
7	MPD	A	806	-	-	3/5/5/5	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C4B-NB	-6.13	1.26	1.38
2	A	801	HEM	FE-NB	5.52	2.11	1.94
2	A	801	HEM	C4D-ND	-4.77	1.32	1.40
2	B	801	HEM	CHD-C1D	4.13	1.48	1.39
2	A	801	HEM	CHB-C4A	3.77	1.47	1.39
2	B	801	HEM	C1C-NC	-3.54	1.32	1.39
2	B	801	HEM	C1B-NB	-3.51	1.34	1.40
2	A	801	HEM	C1B-NB	-3.49	1.34	1.40
2	B	801	HEM	FE-NA	3.40	2.06	1.95
2	B	801	HEM	C1A-NA	-3.34	1.33	1.39
2	B	801	HEM	CHC-C4B	-3.03	1.32	1.39
2	B	801	HEM	CHB-C1B	2.90	1.44	1.38
2	A	801	HEM	C1D-ND	-2.72	1.33	1.38
2	A	801	HEM	CHA-C1A	-2.72	1.33	1.39
2	B	801	HEM	FE-NB	2.70	2.03	1.94
2	A	801	HEM	FE-NA	2.59	2.03	1.95
2	B	801	HEM	CBA-CGA	2.51	1.56	1.50
2	B	801	HEM	CHA-C4D	-2.39	1.33	1.38
2	B	801	HEM	CMB-C2B	2.37	1.55	1.50
2	A	801	HEM	C3B-C4B	2.36	1.49	1.44
2	A	801	HEM	CHD-C4C	2.35	1.43	1.38
2	B	801	HEM	O2A-CGA	-2.34	1.23	1.30
2	A	801	HEM	O1A-CGA	2.32	1.29	1.22
2	A	801	HEM	FE-ND	2.32	2.02	1.94
2	A	801	HEM	C1A-NA	2.07	1.43	1.39
2	A	801	HEM	C1D-C2D	2.06	1.48	1.44
2	B	801	HEM	CHB-C4A	-2.05	1.34	1.39
2	A	801	HEM	C3C-C4C	-2.05	1.42	1.46
2	B	801	HEM	O1D-CGD	2.04	1.28	1.22
2	A	801	HEM	O1D-CGD	2.03	1.28	1.22

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	808	MPD	O4-C4-C3	-5.43	89.76	111.35
2	A	801	HEM	CAD-C3D-C4D	5.06	133.52	124.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CHA-C4D-ND	4.92	130.45	124.37
2	A	801	HEM	CHB-C1B-NB	4.70	130.19	124.37
2	A	801	HEM	CHD-C1D-ND	4.51	129.27	124.42
7	B	806	MPD	CM-C2-C1	4.39	120.45	110.63
2	B	801	HEM	O1A-CGA-CBA	-4.29	109.50	123.09
2	B	801	HEM	CHD-C4C-C3C	-4.07	118.35	125.21
2	B	801	HEM	C4C-CHD-C1D	-4.00	117.51	126.02
2	B	801	HEM	C4C-C3C-C2C	-3.93	103.41	106.81
2	B	801	HEM	CMD-C2D-C1D	3.84	131.04	125.03
2	B	801	HEM	CHB-C4A-NA	3.81	130.77	123.86
7	A	808	MPD	C5-C4-C3	3.75	129.08	111.67
6	B	805	PO4	O2-P-O1	-3.64	98.09	110.95
6	B	805	PO4	O3-P-O2	3.62	119.17	107.91
2	A	801	HEM	C4B-C3B-C2B	-3.54	104.02	107.28
2	A	801	HEM	CHB-C4A-NA	-3.54	117.44	123.86
2	B	801	HEM	C1D-C2D-C3D	-3.52	103.28	106.98
2	A	801	HEM	CAA-CBA-CGA	-3.51	104.36	113.67
2	B	801	HEM	CHD-C1D-C2D	-3.37	119.70	125.03
2	B	801	HEM	CAA-CBA-CGA	-3.29	104.93	113.67
2	B	801	HEM	C2D-C1D-ND	3.17	113.57	109.90
2	B	801	HEM	CBD-CAD-C3D	3.11	121.13	112.53
7	B	806	MPD	O2-C2-C3	-3.03	97.94	109.27
2	B	801	HEM	CMA-C3A-C4A	-2.97	120.90	125.42
2	B	801	HEM	CHD-C4C-NC	2.93	127.65	124.45
2	B	801	HEM	CAA-C2A-C1A	2.93	130.66	124.94
2	A	801	HEM	C3A-C4A-NA	2.90	114.79	110.14
2	B	801	HEM	O2A-CGA-CBA	2.87	123.07	114.00
2	B	801	HEM	C3A-C4A-NA	-2.85	105.58	110.14
7	A	808	MPD	O2-C2-CM	-2.79	99.30	107.99
2	A	801	HEM	CHC-C1C-NC	2.73	127.43	124.45
2	A	801	HEM	C3D-C4D-ND	2.67	113.10	110.17
2	A	801	HEM	CHB-C1B-C2B	-2.62	119.50	126.95
2	A	801	HEM	C4D-C3D-C2D	-2.62	103.08	106.89
2	B	801	HEM	CHC-C4B-NB	2.62	127.24	124.42
2	B	801	HEM	CHA-C4D-C3D	-2.61	120.41	125.23
2	A	801	HEM	CHD-C4C-NC	-2.55	121.67	124.45
2	A	801	HEM	CMD-C2D-C1D	-2.52	121.09	125.03
2	A	801	HEM	C1B-NB-C4B	2.52	108.19	105.21
2	B	801	HEM	C4D-ND-C1D	-2.52	102.23	105.21
2	B	801	HEM	CHD-C1D-ND	-2.48	121.76	124.42
2	A	801	HEM	C4D-ND-C1D	2.47	108.14	105.21
2	A	801	HEM	CAD-C3D-C2D	-2.45	123.27	127.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CMA-C3A-C2A	2.45	130.82	125.62
2	B	801	HEM	CMC-C2C-C1C	2.43	129.00	124.73
2	B	801	HEM	C4A-NA-C1A	2.34	109.63	105.82
7	B	806	MPD	O4-C4-C3	-2.33	102.08	111.35
2	B	801	HEM	O1D-CGD-CBD	-2.31	115.76	123.09
2	B	801	HEM	CAA-C2A-C3A	-2.30	121.92	127.07
6	A	805	PO4	O4-P-O1	-2.29	102.87	110.95
2	A	801	HEM	C2B-C1B-NB	-2.27	107.23	109.84
2	A	801	HEM	C3B-C2B-C1B	-2.19	104.77	106.41
2	A	801	HEM	CAA-C2A-C1A	2.18	129.19	124.94
2	B	801	HEM	C4B-C3B-C2B	-2.14	105.32	107.28
2	B	801	HEM	C3D-C4D-ND	-2.13	107.83	110.17
2	B	801	HEM	O2D-CGD-CBD	2.13	120.74	114.00
2	A	801	HEM	C3C-C2C-C1C	-2.13	105.03	107.05
6	A	805	PO4	O4-P-O3	2.11	114.47	107.91
7	A	808	MPD	O2-C2-C1	2.01	114.27	107.99
7	A	806	MPD	O4-C4-C3	-2.01	103.35	111.35
2	A	801	HEM	C4C-C3C-C2C	2.00	108.55	106.81

There are no chirality outliers.

All (15) torsion outliers are listed below:

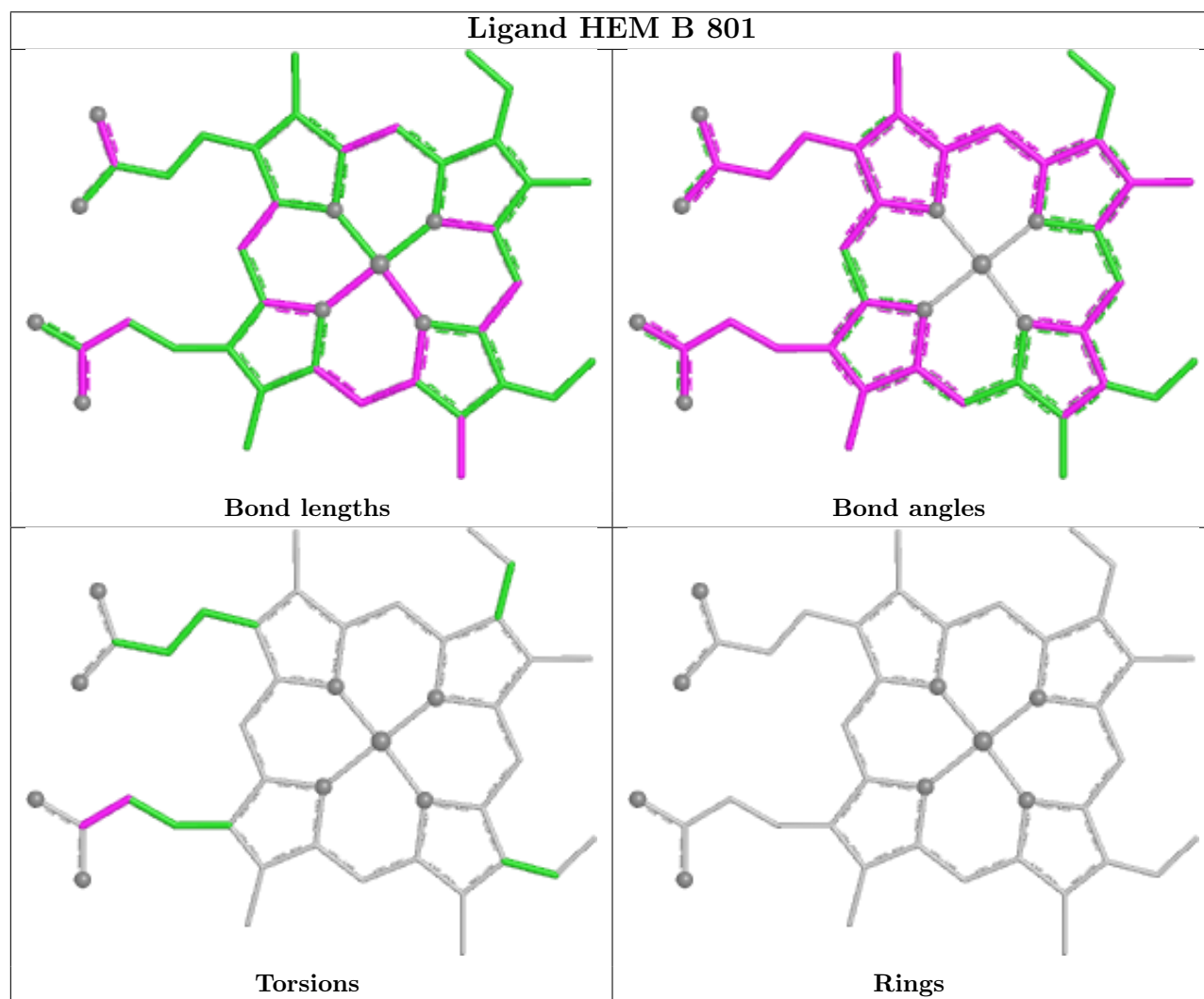
Mol	Chain	Res	Type	Atoms
7	A	806	MPD	C1-C2-C3-C4
7	A	806	MPD	O2-C2-C3-C4
7	A	808	MPD	O2-C2-C3-C4
7	A	808	MPD	C2-C3-C4-O4
7	B	806	MPD	O2-C2-C3-C4
7	A	808	MPD	C1-C2-C3-C4
7	A	808	MPD	CM-C2-C3-C4
7	A	808	MPD	C2-C3-C4-C5
7	B	806	MPD	C2-C3-C4-C5
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O1A
7	B	806	MPD	C2-C3-C4-O4
7	A	806	MPD	CM-C2-C3-C4

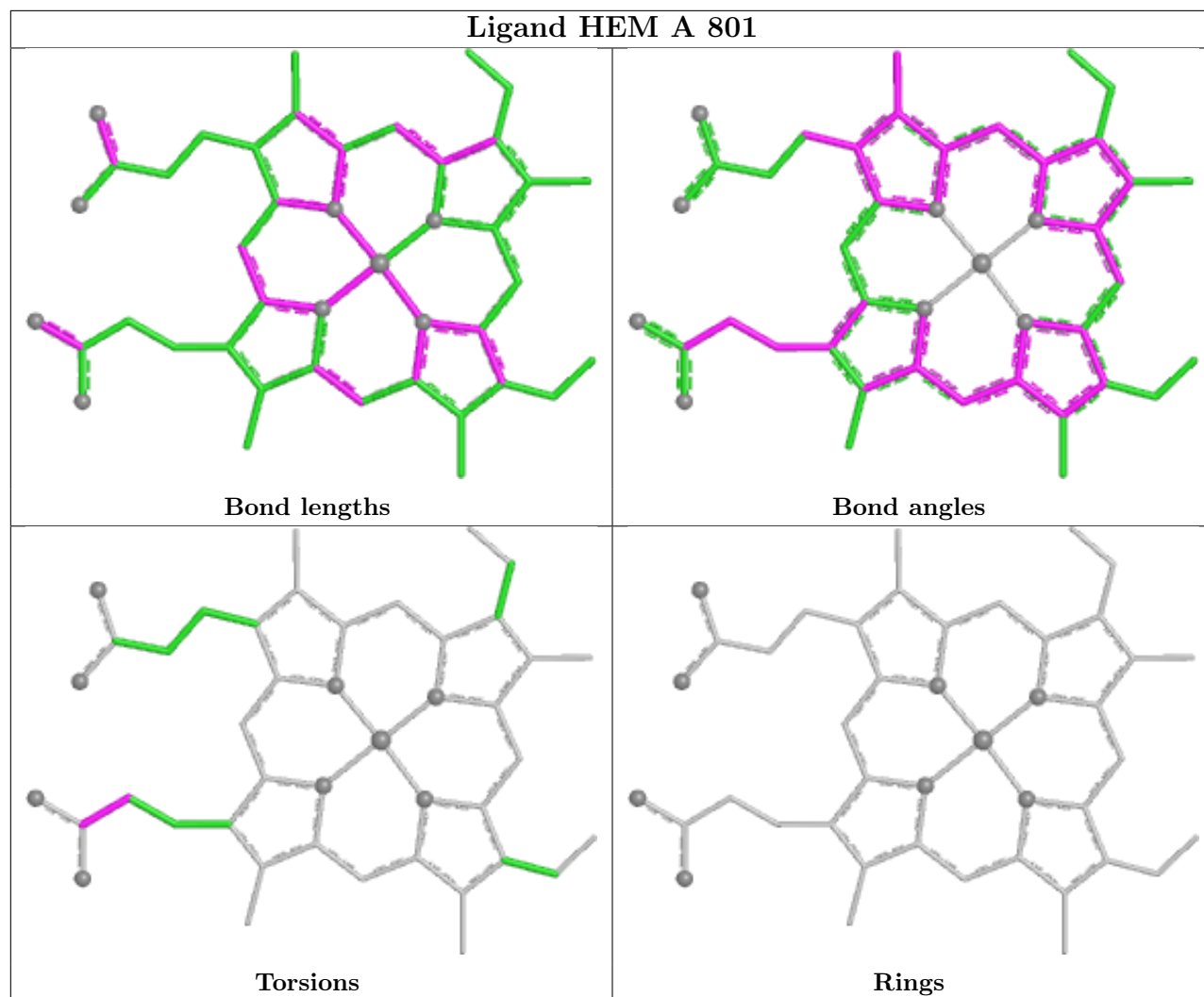
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	807	MPD	1	0
7	A	806	MPD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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%)	-0.34	8 (1%) 78 78	9, 22, 39, 80	7 (0%)
1	B	712/728 (97%)	-0.37	10 (1%) 73 73	8, 22, 39, 82	5 (0%)
All	All	1424/1456 (97%)	-0.36	18 (1%) 75 75	8, 22, 39, 82	12 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	4.6
1	A	748	ALA	3.6
1	B	40	ARG	3.3
1	A	608	LYS	3.3
1	B	647	GLN	3.0
1	A	680	ALA	2.8
1	A	40	ARG	2.7
1	B	679	ALA	2.7
1	A	541	GLY	2.7
1	B	46	GLN	2.6
1	A	454	ASP	2.6
1	B	540	ARG	2.4
1	B	55	HIS	2.4
1	B	36	GLY	2.4
1	B	680	ALA	2.2
1	A	119[A]	THR	2.2
1	B	53	HIS	2.1
1	A	540	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($\text{\AA}^2$)	Q<0.9
1	TOX	A	111	16/17	0.97	0.06	16,17,27,32	0
1	TOX	B	111	16/17	0.98	0.04	15,18,25,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

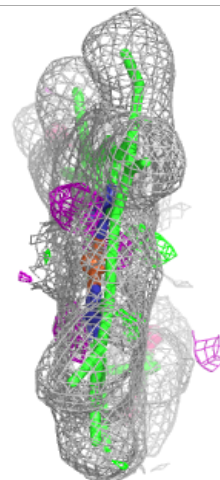
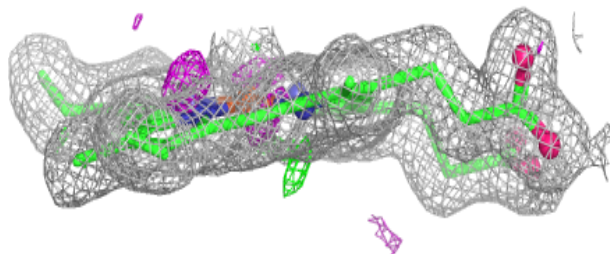
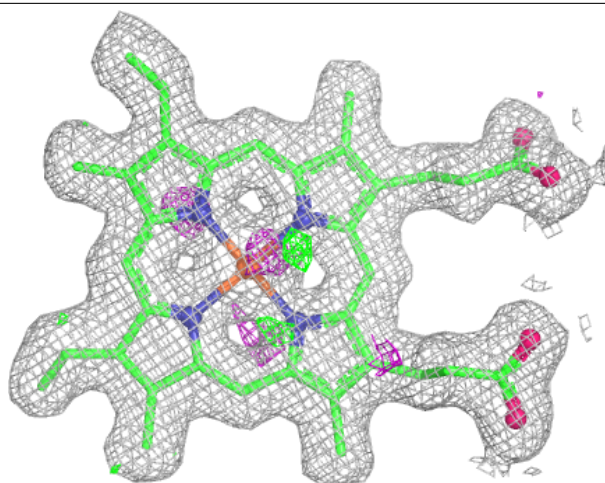
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	PO4	A	805	5/5	0.75	0.15	53,73,94,94	0
7	MPD	A	808	8/8	0.86	0.15	38,40,54,58	0
7	MPD	A	807	8/8	0.88	0.20	60,70,74,75	0
7	MPD	A	806	8/8	0.88	0.16	32,40,56,59	0
7	MPD	B	806	8/8	0.88	0.20	55,59,71,71	0
6	PO4	B	805	5/5	0.89	0.10	41,55,60,60	0
5	OXY	B	804	2/2	0.90	0.21	38,38,38,38	0
5	OXY	A	804	2/2	0.93	0.20	38,38,38,38	0
4	CL	B	803	1/1	0.96	0.09	37,37,37,37	0
4	CL	A	803	1/1	0.97	0.06	36,36,36,36	0
2	HEM	A	801	43/43	0.98	0.05	14,17,19,20	0
2	HEM	B	801	43/43	0.98	0.05	14,16,18,20	0
3	NA	A	802	1/1	0.99	0.05	17,17,17,17	0
3	NA	B	802	1/1	1.00	0.03	18,18,18,18	0

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

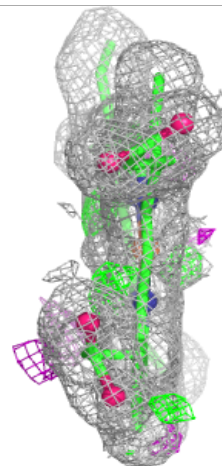
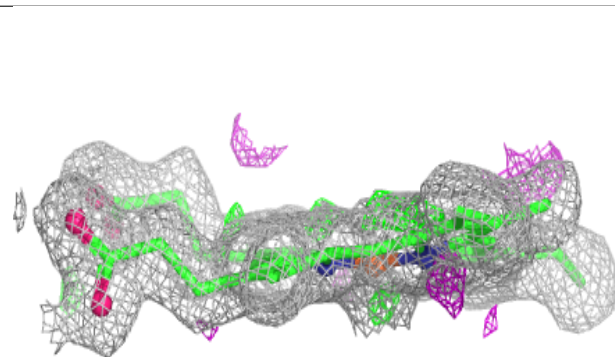
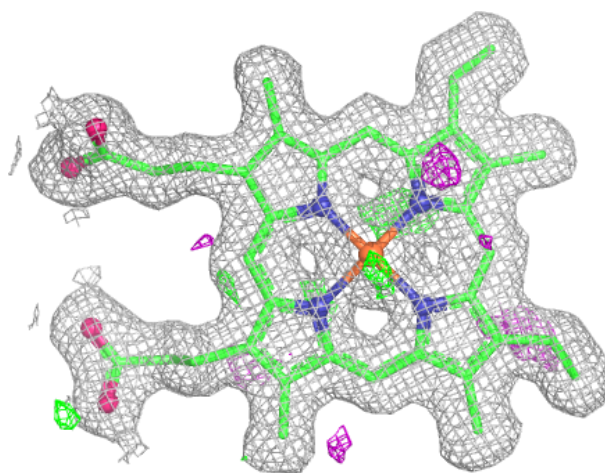
Electron density around HEM A 801:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.