



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 04:54 PM BST

PDB ID : 5KQI
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.

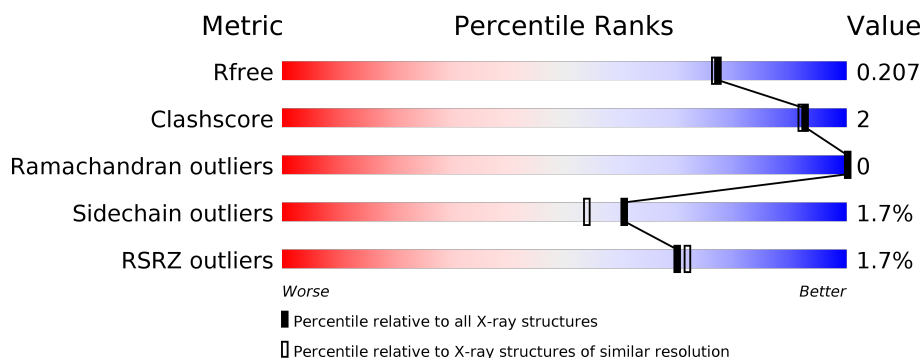
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

i

X-RAY DIFFRACTION

A.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

Mol	Chain	Length	Quality of chain
1	A	728	<div> <div> <div></div> <div>2%</div> </div> <div> <div></div> <div>88%</div> </div> <div> <div></div> <div>9%</div> </div> <div> <div></div> <div>••</div> </div> </div>
1	B	728	<div> <div> <div></div> <div>%</div> </div> <div> <div></div> <div>87%</div> </div> <div> <div></div> <div>10%</div> </div> <div> <div></div> <div>••</div> </div> </div>

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.

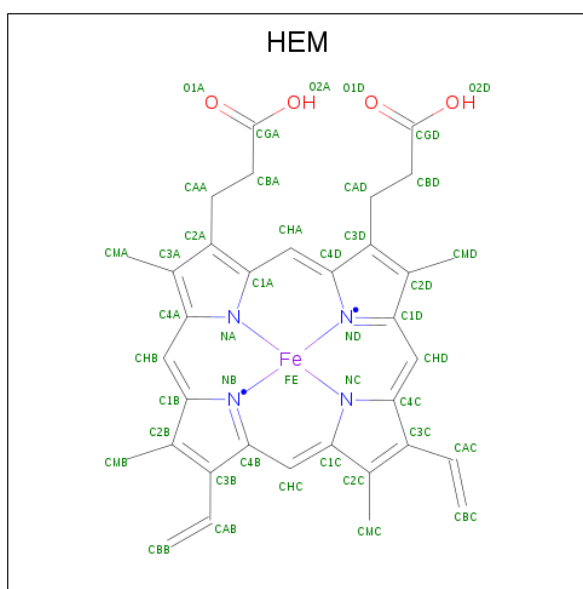
- Molecule 1 is a protein called Catalase-peroxidase.

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 (three-letter code: 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

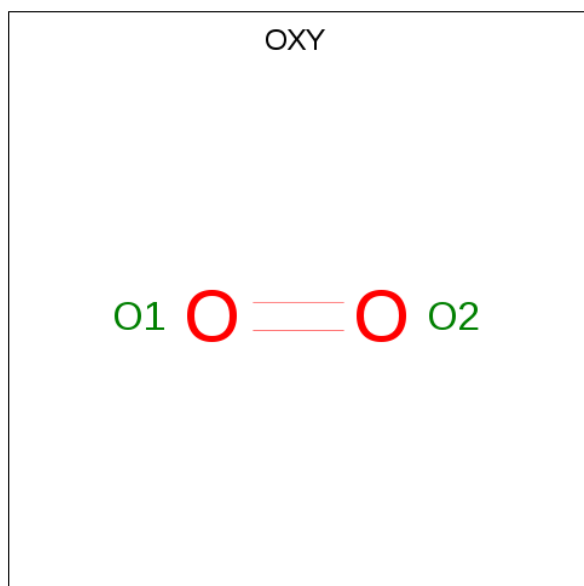
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

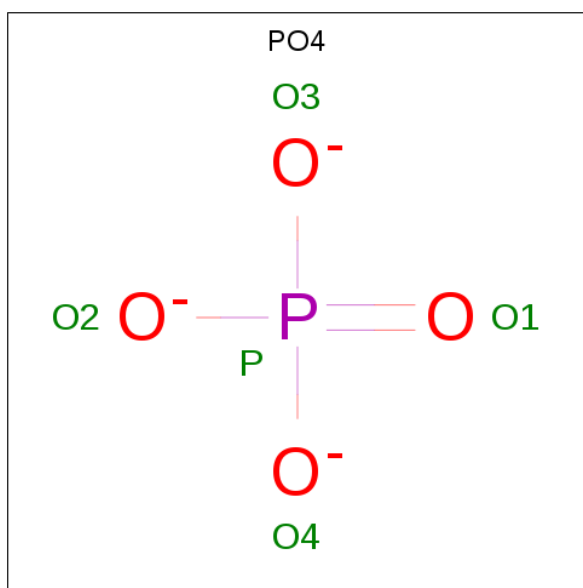
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl		
			1	1	0	0
4	A	1	Total	Cl		
			1	1	0	0

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



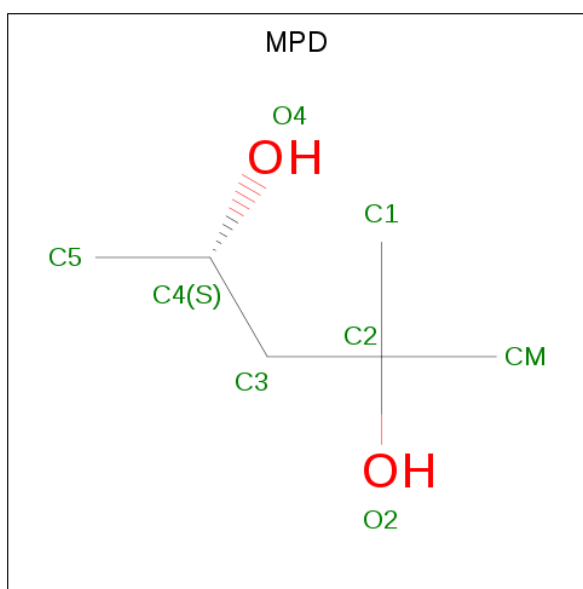
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	B	1	Total	O		
			2	2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: 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 (three-letter code: MPD) (formula: $\text{C}_6\text{H}_{14}\text{O}_2$).



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

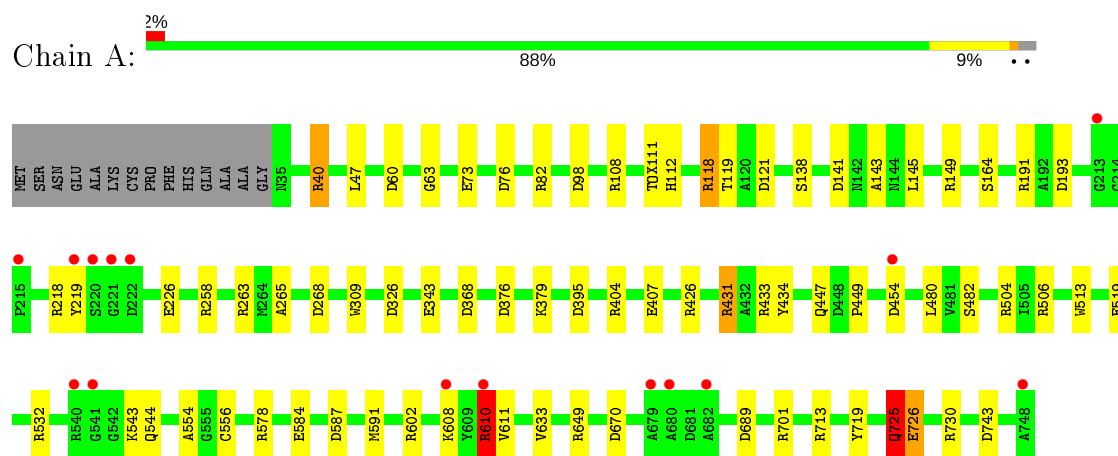
- Molecule 8 is water.

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

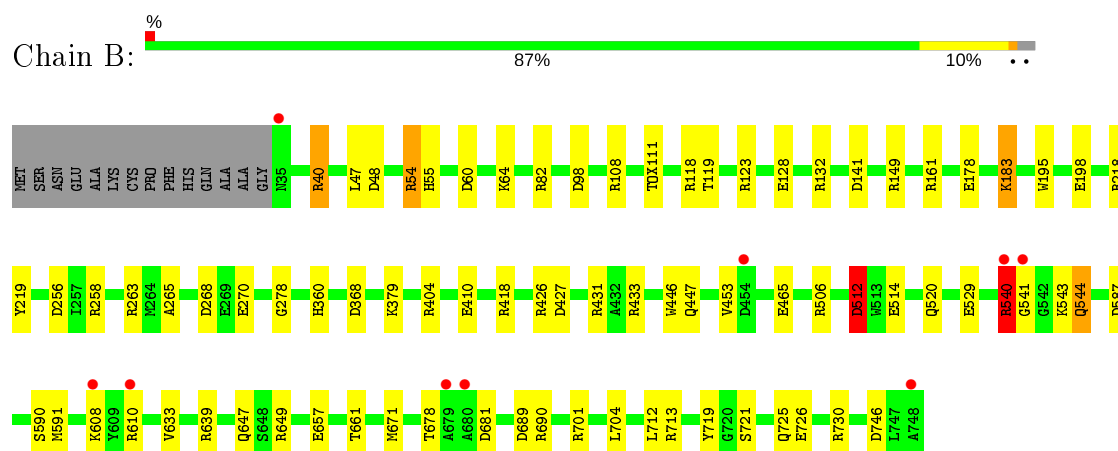
3 Residue-property plots [i](#)

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	100.79Å 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 0.174 , 0.207	Depositor DCC
R_{free} test set	8160 reflections (4.92%)	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 , 42.5	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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.43	24/5701 (0.4%)	1.28	57/7747 (0.7%)
1	B	1.43	22/5688 (0.4%)	1.25	46/7731 (0.6%)
All	All	1.43	46/11389 (0.4%)	1.26	103/15478 (0.7%)

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	GLU	CD-OE1	10.69	1.37	1.25
1	B	726	GLU	CD-OE2	10.45	1.37	1.25
1	A	434	TYR	CE1-CZ	-8.32	1.27	1.38
1	A	407	GLU	CG-CD	8.04	1.64	1.51
1	A	426[A]	ARG	CZ-NH2	7.92	1.43	1.33
1	A	426[B]	ARG	CZ-NH2	7.92	1.43	1.33
1	B	410	GLU	CD-OE2	7.64	1.34	1.25
1	B	529	GLU	CG-CD	7.42	1.63	1.51
1	B	726	GLU	CG-CD	7.31	1.62	1.51
1	B	721	SER	CA-CB	7.05	1.63	1.52
1	A	343	GLU	CD-OE1	6.96	1.33	1.25
1	A	519	GLU	CD-OE1	6.87	1.33	1.25
1	B	410	GLU	CG-CD	6.81	1.62	1.51
1	A	725	GLN	CG-CD	6.80	1.66	1.51
1	B	730[A]	ARG	CZ-NH1	6.77	1.41	1.33
1	A	108	ARG	CZ-NH1	-6.72	1.24	1.33
1	A	726[A]	GLU	CG-CD	6.54	1.61	1.51
1	A	726[B]	GLU	CG-CD	6.54	1.61	1.51
1	B	218	ARG	CZ-NH1	6.31	1.41	1.33
1	A	584	GLU	CG-CD	6.28	1.61	1.51
1	A	73	GLU	CG-CD	6.18	1.61	1.51
1	A	454	ASP	CB-CG	6.18	1.64	1.51
1	B	514	GLU	CD-OE1	-6.06	1.19	1.25
1	B	446	TRP	CE3-CZ3	-6.02	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	657	GLU	CD-OE2	5.97	1.32	1.25
1	A	482	SER	CB-OG	5.88	1.49	1.42
1	B	453	VAL	C-O	-5.83	1.12	1.23
1	B	512	ASP	CG-OD2	5.79	1.38	1.25
1	A	164	SER	CA-CB	-5.64	1.44	1.52
1	B	278	GLY	C-O	5.64	1.32	1.23
1	A	193	ASP	CB-CG	5.54	1.63	1.51
1	B	195	TRP	CE3-CZ3	5.39	1.47	1.38
1	A	138	SER	CB-OG	-5.37	1.35	1.42
1	A	449	PRO	N-CA	-5.36	1.38	1.47
1	B	590	SER	CB-OG	-5.30	1.35	1.42
1	A	219	TYR	CE1-CZ	5.27	1.45	1.38
1	A	63	GLY	N-CA	5.23	1.53	1.46
1	A	513	TRP	CE3-CZ3	-5.19	1.29	1.38
1	B	219	TYR	CG-CD2	-5.18	1.32	1.39
1	B	544	GLN	CD-NE2	5.14	1.45	1.32
1	B	465	GLU	CG-CD	5.12	1.59	1.51
1	B	418	ARG	CZ-NH2	-5.09	1.26	1.33
1	A	513	TRP	CE2-CZ2	-5.02	1.31	1.39
1	B	746	ASP	CB-CG	5.02	1.62	1.51
1	B	270	GLU	CD-OE1	5.02	1.31	1.25
1	A	556	CYS	CB-SG	5.00	1.90	1.82

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	701	ARG	NE-CZ-NH1	11.53	126.06	120.30
1	A	149	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	B	433	ARG	NE-CZ-NH1	10.25	125.42	120.30
1	A	149	ARG	NE-CZ-NH2	-10.01	115.29	120.30
1	A	649	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	A	426[A]	ARG	NE-CZ-NH1	-9.89	115.35	120.30
1	A	426[B]	ARG	NE-CZ-NH1	-9.89	115.35	120.30
1	B	258	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	A	649	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	A	433	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	A	82	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	B	713	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	A	713	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	B	108	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	B	368	ASP	CB-CG-OD1	8.57	126.01	118.30
1	B	649	ARG	NE-CZ-NH2	-8.33	116.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	B	40	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	B	506	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	B	132	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	A	82	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	591	MET	CG-SD-CE	-7.63	87.99	100.20
1	B	591	MET	CG-SD-CE	-7.56	88.10	100.20
1	B	149	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	689	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	A	602	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	191	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	376	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	B	268	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	532	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	433	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	404	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	506	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	426	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	B	433	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	B	541	GLY	N-CA-C	-7.00	95.60	113.10
1	A	578	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	B	649	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	82	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	161[A]	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	B	161[B]	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	B	689	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	404	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	404	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	368	ASP	CB-CG-OD1	-6.67	112.30	118.30
1	B	713	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	587	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	258	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	123	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	427	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	B	540	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	218	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	B	418	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	587	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	395	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	584	GLU	CG-CD-OE1	6.28	130.86	118.30
1	A	98	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	40	ARG	NE-CZ-NH1	6.10	123.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	407	GLU	CG-CD-OE1	6.10	130.50	118.30
1	B	543	LYS	CD-CE-NZ	-6.10	97.67	111.70
1	A	730	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	98	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	512	ASP	CB-CG-OD1	-6.06	112.85	118.30
1	A	47	LEU	CB-CG-CD1	-6.03	100.75	111.00
1	A	584	GLU	OE1-CD-OE2	-6.03	116.07	123.30
1	B	183	LYS	CB-CG-CD	5.97	127.13	111.60
1	B	690	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	A	60	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	268	ASP	CB-CG-OD1	5.87	123.59	118.30
1	B	256	ASP	CB-CG-OD1	5.87	123.59	118.30
1	A	610	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	60	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	A	730	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	602	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	268	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	A	368	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	48	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	121	ASP	CB-CG-OD1	5.66	123.40	118.30
1	A	263	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	60	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	108	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	587	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	671	MET	CG-SD-CE	-5.55	91.32	100.20
1	A	670	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	701	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	543	LYS	CD-CE-NZ	-5.46	99.14	111.70
1	B	263	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	639	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	743	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	73	GLU	OE1-CD-OE2	-5.26	116.99	123.30
1	B	610	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	704	LEU	CB-CG-CD2	5.22	119.87	111.00
1	A	76	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	191	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	123	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	118	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	60	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	112	HIS	N-CA-CB	-5.14	101.34	110.60
1	A	431	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	B	270	GLU	CG-CD-OE1	5.11	128.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	LEU	CB-CG-CD1	-5.11	102.32	111.00
1	B	712	LEU	CB-CG-CD2	5.04	119.56	111.00
1	A	326	ASP	CB-CG-OD1	-5.03	113.78	118.30

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	10	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	5	0
8	B	644	0	0	10	0
All	All	12535	0	10848	34	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 (34) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H11	7:A:807:MPD:H53	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
1:A:726[A]:GLU:HG3	8:A:1321:HOH:O	2.12	0.49
7:A:806:MPD:HM1	7:A:806:MPD:O4	2.14	0.48
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: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:C1	7:A:807:MPD:H53	2.51	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	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%)	549 (99%)	8 (1%)	67	62
1	B	556/560 (99%)	545 (98%)	11 (2%)	55	47
All	All	1113/1120 (99%)	1094 (98%)	19 (2%)	60	54

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

Mol	Chain	Res	Type
1	A	40	ARG
1	A	118	ARG
1	A	141	ASP
1	A	379	LYS
1	A	544	GLN
1	A	608	LYS
1	A	610	ARG
1	A	725	GLN

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Mol	Chain	Res	Type
1	B	40	ARG
1	B	54	ARG
1	B	64	LYS
1	B	118	ARG
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

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

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

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	A	111	1,2	10,17,18	3.01	3 (30%)	10,23,25	1.61	3 (30%)
1	TOX	B	111	1,2	10,17,18	2.28	4 (40%)	10,23,25	1.62	3 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TOX	A	111	1,2	-	2/4/8/10	0/2/2/2
1	TOX	B	111	1,2	-	2/4/8/10	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	TOX	CD1-NE1	-8.02	1.31	1.39
1	B	111	TOX	O-C	4.48	1.37	1.19
1	A	111	TOX	O-C	3.19	1.32	1.19
1	B	111	TOX	CZ2-CE2	-2.98	1.35	1.41
1	B	111	TOX	CB-CA	-2.83	1.47	1.53
1	B	111	TOX	CE3-CD2	-2.58	1.37	1.42
1	A	111	TOX	CH2-CZ3	2.08	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	TOX	CB-CG-CD2	3.12	131.10	126.25
1	A	111	TOX	CZ3-CH2-CZ2	-2.82	116.48	120.44
1	B	111	TOX	CB-CG-CD1	-2.81	124.49	127.97
1	A	111	TOX	CB-CA-C	2.24	115.67	111.47
1	B	111	TOX	CZ2-CE2-CD2	-2.22	117.92	120.94
1	A	111	TOX	CZ3-CE3-CD2	2.02	123.69	120.89

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 monosaccharides 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
6	PO4	B	805	-	4,4,4	1.53	1 (25%)	6,6,6	0.81	0
7	MPD	A	808	-	7,7,7	1.19	1 (14%)	9,10,10	2.82	2 (22%)
6	PO4	A	805	-	4,4,4	1.17	0	6,6,6	1.63	2 (33%)
5	OXY	A	804	-	1,1,1	0.09	0	-		
2	HEM	B	801	1	27,50,50	1.72	7 (25%)	17,82,82	2.71	7 (41%)
2	HEM	A	801	1	27,50,50	1.49	2 (7%)	17,82,82	2.40	6 (35%)
7	MPD	A	807	-	7,7,7	0.82	0	9,10,10	1.93	3 (33%)
7	MPD	A	806	-	7,7,7	0.79	0	9,10,10	1.64	2 (22%)
7	MPD	B	806	-	7,7,7	0.56	0	9,10,10	2.24	4 (44%)
5	OXY	B	804	-	1,1,1	0.58	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
7	MPD	A	808	-	-	1/5/5/5	-
7	MPD	B	806	-	-	3/5/5/5	-
2	HEM	B	801	1	-	0/6/54/54	-
2	HEM	A	801	1	-	0/6/54/54	-
7	MPD	A	807	-	-	1/5/5/5	-
7	MPD	A	806	-	-	2/5/5/5	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3B-C2B	-4.91	1.33	1.40
2	A	801	HEM	C1A-NA	4.22	1.44	1.36
2	B	801	HEM	C4A-NA	3.58	1.43	1.36
2	B	801	HEM	CAA-C2A	-3.05	1.47	1.52
2	A	801	HEM	C3C-CAC	2.87	1.53	1.47
2	B	801	HEM	C3C-C2C	-2.68	1.36	1.40
6	B	805	PO4	P-O3	-2.26	1.47	1.54
2	B	801	HEM	C2A-C3A	-2.18	1.31	1.37
2	B	801	HEM	C1B-C2B	2.10	1.47	1.42
7	A	808	MPD	C1-C2	2.04	1.58	1.52
2	B	801	HEM	C1C-C2C	-2.02	1.38	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CAA-CBA-CGA	-6.40	101.94	112.67
7	A	808	MPD	O2-C2-CM	-5.86	89.27	108.08
7	A	808	MPD	CM-C2-C1	5.74	122.54	110.57
2	B	801	HEM	CBD-CAD-C3D	5.03	121.75	112.48
2	B	801	HEM	CAD-CBD-CGD	4.62	120.42	112.67
2	B	801	HEM	C4C-C3C-C2C	-4.40	103.82	106.90
7	A	807	MPD	CM-C2-C1	-4.04	102.15	110.57
2	A	801	HEM	C1D-C2D-C3D	3.95	109.75	107.00
2	B	801	HEM	C1D-C2D-C3D	-3.64	104.46	107.00
2	B	801	HEM	CAA-CBA-CGA	-3.58	106.67	112.67
2	A	801	HEM	CBD-CAD-C3D	3.56	119.03	112.48
7	B	806	MPD	C1-C2-C3	3.45	126.03	109.96
7	B	806	MPD	O2-C2-C3	-3.45	96.84	109.80
7	A	806	MPD	O4-C4-C3	-3.35	97.84	111.36
2	A	801	HEM	CAD-CBD-CGD	3.01	117.73	112.67
2	B	801	HEM	C4A-C3A-C2A	2.99	109.08	107.00
2	B	801	HEM	CBA-CAA-C2A	2.86	117.76	112.49
6	A	805	PO4	O3-P-O1	2.81	121.19	110.89
7	B	806	MPD	O2-C2-CM	2.79	117.03	108.08
7	B	806	MPD	CM-C2-C1	-2.71	104.93	110.57
7	A	807	MPD	O2-C2-C1	2.62	116.49	108.08
7	A	806	MPD	O4-C4-C5	2.37	119.66	109.38
7	A	807	MPD	C5-C4-C3	2.36	122.79	111.69
6	A	805	PO4	O4-P-O1	-2.22	102.78	110.89
2	A	801	HEM	C3C-C4C-NC	-2.20	106.78	110.94
2	A	801	HEM	CMD-C2D-C1D	-2.13	125.19	128.46

There are no chirality outliers.

All (7) torsion outliers are listed below:

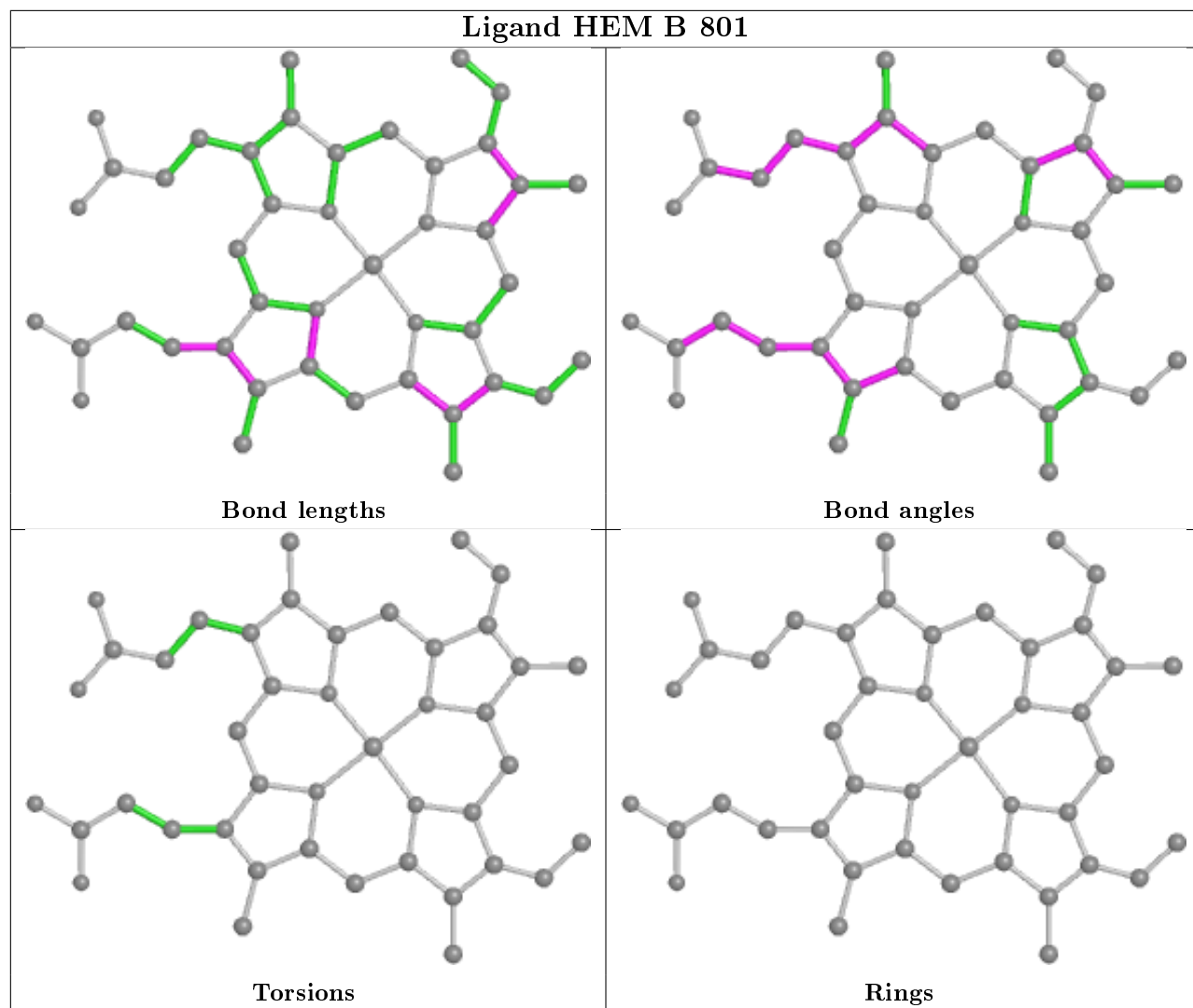
Mol	Chain	Res	Type	Atoms
7	B	806	MPD	C1-C2-C3-C4
7	B	806	MPD	O2-C2-C3-C4
7	A	806	MPD	C1-C2-C3-C4
7	B	806	MPD	CM-C2-C3-C4
7	A	808	MPD	O2-C2-C3-C4
7	A	806	MPD	O2-C2-C3-C4
7	A	807	MPD	C2-C3-C4-C5

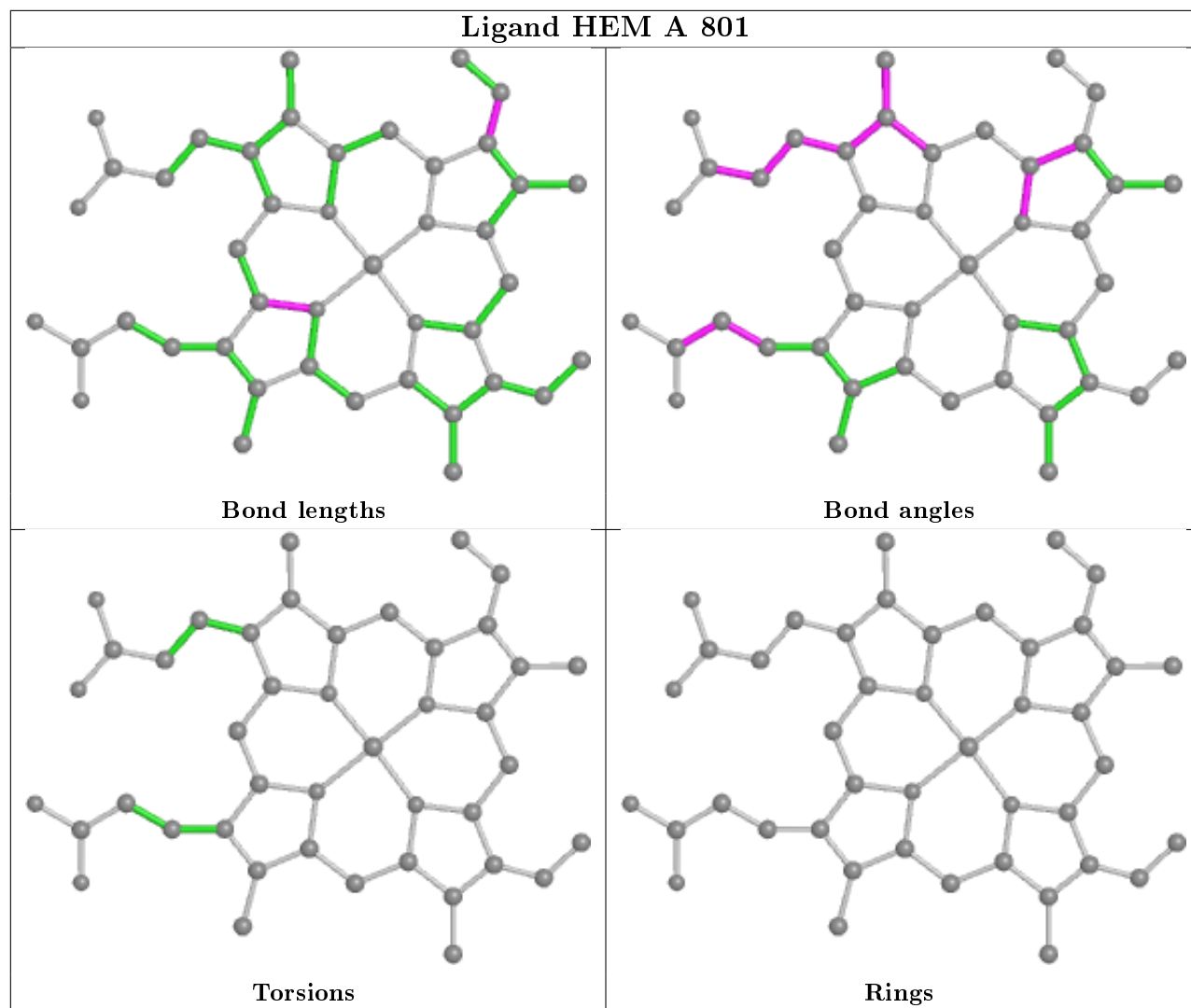
There are no ring outliers.

3 monomers are involved in 6 short contacts:

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

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.27	15 (2%) 63 65	16, 25, 45, 84	0
1	B	713/728 (97%)	-0.38	9 (1%) 77 79	17, 24, 44, 84	0
All	All	1426/1456 (97%)	-0.33	24 (1%) 70 72	16, 24, 45, 84	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	5.5
1	A	540	ARG	5.0
1	B	748	ALA	5.0
1	A	679	ALA	4.2
1	A	541	GLY	3.7
1	A	610	ARG	3.6
1	B	540	ARG	3.1
1	A	680	ALA	2.8
1	A	608	LYS	2.8
1	A	213	GLY	2.5
1	B	610	ARG	2.5
1	A	454	ASP	2.4
1	B	35	ASN	2.4
1	B	608	LYS	2.4
1	A	219	TYR	2.3
1	A	220	SER	2.3
1	B	680	ALA	2.3
1	B	679	ALA	2.3
1	A	222	ASP	2.2
1	A	215	PRO	2.2
1	A	682	ALA	2.2
1	A	221	GLY	2.1
1	B	454	ASP	2.1
1	B	541	GLY	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(\AA^2)	Q<0.9
1	TOX	A	111	16/17	0.97	0.09	15,19,28,30	0
1	TOX	B	111	16/17	0.98	0.11	15,18,27,29	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

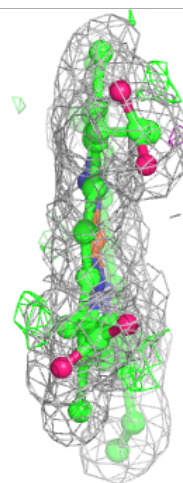
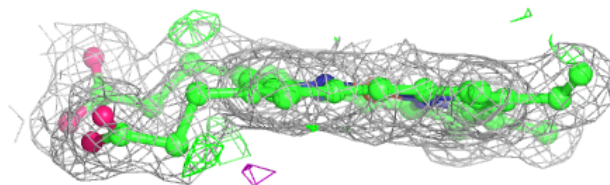
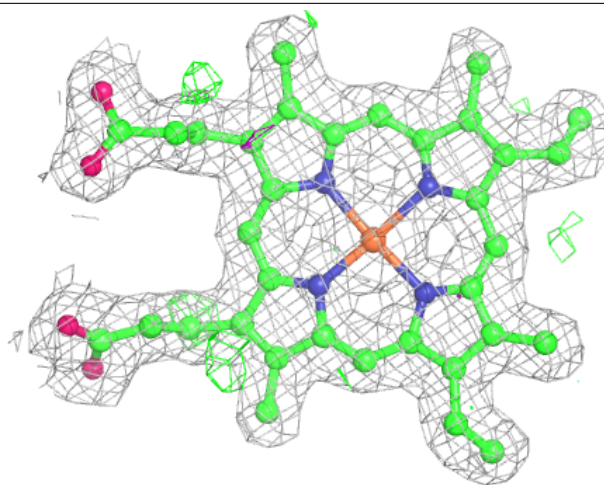
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

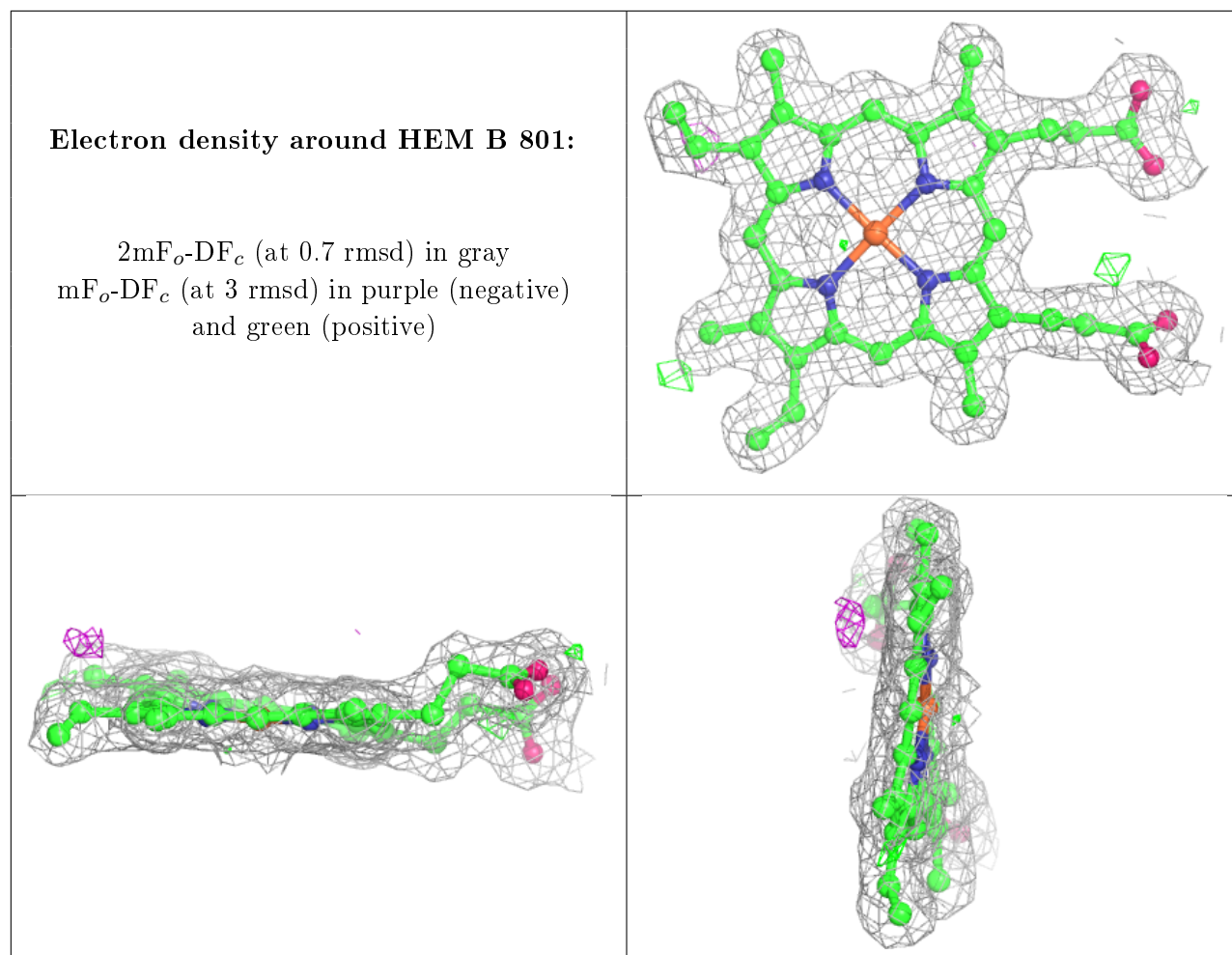
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MPD	B	806	8/8	0.81	0.18	49,57,60,63	0
7	MPD	A	807	8/8	0.83	0.18	48,53,67,68	0
7	MPD	A	808	8/8	0.84	0.35	66,71,76,77	0
6	PO4	A	805	5/5	0.91	0.19	59,76,86,89	0
6	PO4	B	805	5/5	0.92	0.25	52,64,70,74	0
7	MPD	A	806	8/8	0.92	0.19	58,66,72,73	0
5	OXY	A	804	2/2	0.94	0.24	47,47,47,54	0
4	CL	A	803	1/1	0.97	0.10	45,45,45,45	0
3	NA	A	802	1/1	0.98	0.07	20,20,20,20	0
5	OXY	B	804	2/2	0.98	0.08	31,31,31,33	0
2	HEM	A	801	43/43	0.98	0.09	17,21,24,25	0
2	HEM	B	801	43/43	0.99	0.10	16,19,21,23	0
3	NA	B	802	1/1	0.99	0.06	20,20,20,20	0
4	CL	B	803	1/1	0.99	0.07	28,28,28,28	1

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.