



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 07:25 AM EDT

PDB ID : 5KQ6 / pdb_00005kq6
Title : Crystal structure of the A359D variant of catalase-peroxidase from *B. pseudo-mallei*
Authors : Loewen, P.C.
Deposited on : 2016-07-05
Resolution : 1.62 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

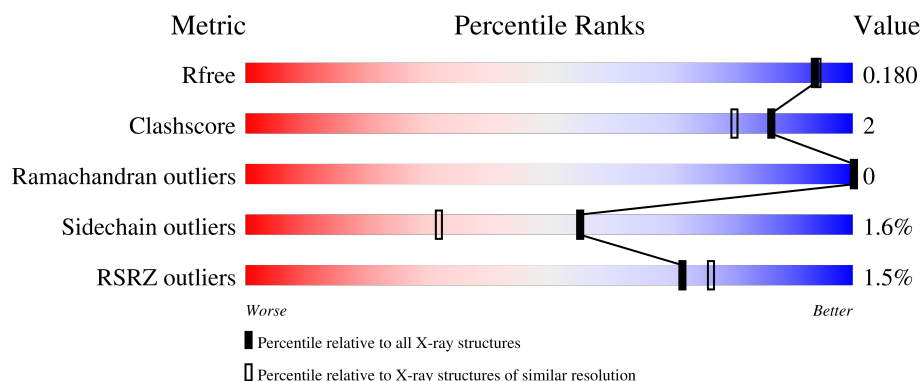
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

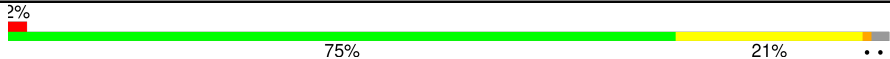
The reported resolution of this entry is 1.62 Å.

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	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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	
1	B	728	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PO4	B	805	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12835 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.

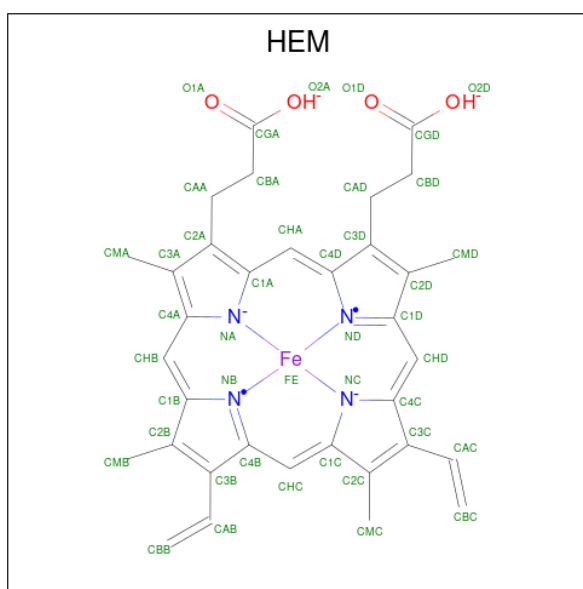
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	8	0
			5568	3512	992	1050	14			
1	B	713	Total	C	N	O	S	0	7	0
			5552	3504	986	1048	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ASP	ALA	engineered mutation	UNP Q3JNW6
B	359	ASP	ALA	engineered mutation	UNP Q3JNW6

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



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

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

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

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

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

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

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



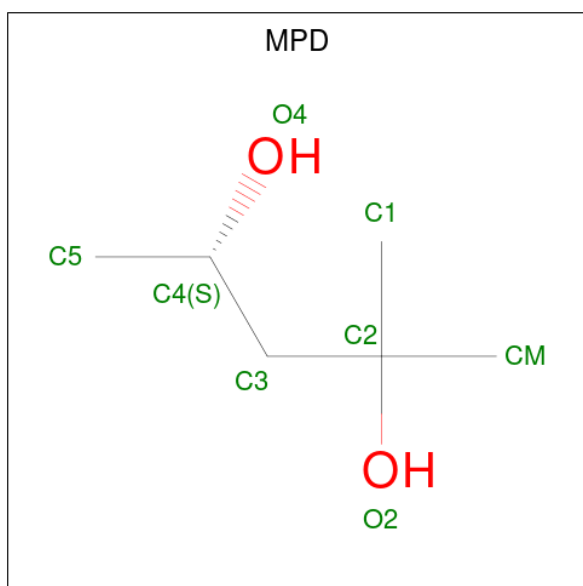
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	B	1	Total	O		
			2	2	0	0

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



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

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



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

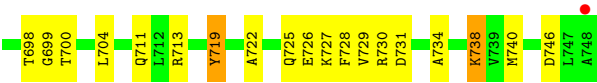
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	794	Total	O	0	0
			794	794		
8	B	785	Total	O	0	0
			785	785		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.58Å 115.79Å 174.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.80 – 1.62 47.80 – 1.62	Depositor EDS
% Data completeness (in resolution range)	97.5 (47.80-1.62) 97.5 (47.80-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.144 , 0.170 0.158 , 0.180	Depositor DCC
R_{free} test set	12728 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.5	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	12835	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, NA, HEM, PO4, CL, MPD, OXY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.03	147/5696 (2.6%)	1.57	44/7740 (0.6%)
1	B	2.03	128/5683 (2.3%)	1.57	47/7724 (0.6%)
All	All	2.03	275/11379 (2.4%)	1.57	91/15464 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (275) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	544	GLN	CD-OE1	14.13	1.50	1.23
1	B	453	VAL	C-O	-10.79	1.11	1.24
1	B	512	ASP	CG-OD2	10.44	1.45	1.25
1	B	540	ARG	C-O	10.17	1.36	1.23
1	B	568	HIS	CA-C	9.49	1.64	1.52
1	A	588	VAL	N-CA	-9.02	1.35	1.46
1	A	377	PRO	C-O	-9.01	1.11	1.24
1	B	532	ARG	CD-NE	-8.62	1.34	1.46
1	A	294	GLY	C-O	8.58	1.32	1.23
1	A	711	GLN	CD-NE2	-8.52	1.15	1.33
1	B	725	GLN	CD-NE2	8.41	1.50	1.33
1	A	676	LYS	CA-C	-8.26	1.44	1.52
1	B	596	PRO	CA-CB	-8.17	1.45	1.54
1	A	74	LYS	N-CA	-8.14	1.35	1.46
1	B	370	VAL	N-CA	-8.10	1.37	1.46
1	A	453	VAL	C-O	-8.08	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	363	VAL	C-O	8.00	1.31	1.24
1	A	588	VAL	CA-CB	7.95	1.64	1.54
1	B	728	PHE	CA-C	7.81	1.63	1.52
1	A	351	GLU	C-O	7.77	1.33	1.24
1	B	418	ARG	CZ-NH2	-7.68	1.23	1.33
1	B	299	ALA	CA-C	-7.67	1.42	1.52
1	B	694	GLU	CA-C	7.66	1.62	1.52
1	B	544	GLN	CD-NE2	7.62	1.49	1.33
1	A	375	PHE	C-O	-7.61	1.14	1.24
1	A	479	GLN	C-N	-7.60	1.23	1.33
1	B	365	LYS	N-CA	7.56	1.55	1.46
1	B	529	GLU	CA-C	7.51	1.62	1.52
1	A	540	ARG	C-O	7.43	1.33	1.23
1	B	532	ARG	CZ-NH1	-7.41	1.22	1.32
1	B	82	ARG	CZ-NH2	-7.34	1.24	1.33
1	A	67	ASN	CG-ND2	-7.32	1.17	1.33
1	A	499	GLY	C-O	7.30	1.31	1.23
1	B	448	ASP	N-CA	7.21	1.51	1.46
1	A	407	GLU	CD-OE1	7.20	1.39	1.25
1	B	679	ALA	N-CA	7.19	1.54	1.46
1	B	631	MET	C-O	7.15	1.32	1.24
1	B	571[A]	THR	C-O	7.13	1.32	1.24
1	B	571[B]	THR	C-O	7.13	1.32	1.24
1	B	179	SER	C-O	7.11	1.32	1.24
1	A	731	ASP	CA-C	7.11	1.62	1.52
1	B	408	ASN	CA-CB	-7.04	1.45	1.53
1	A	434	TYR	CB-CG	-6.99	1.36	1.51
1	A	736	TRP	N-CA	6.98	1.54	1.46
1	A	531	ILE	N-CA	6.98	1.54	1.46
1	B	46	GLN	CG-CD	6.95	1.69	1.52
1	A	161	ARG	CD-NE	-6.87	1.36	1.46
1	A	545	VAL	C-O	-6.87	1.16	1.24
1	A	227	ASN	CA-C	-6.86	1.46	1.53
1	A	462	ASP	CA-CB	-6.84	1.42	1.53
1	B	571[A]	THR	C-N	6.84	1.39	1.32
1	B	571[B]	THR	C-N	6.84	1.39	1.32
1	B	455	HIS	CA-C	6.83	1.59	1.52
1	B	746	ASP	N-CA	6.82	1.55	1.46
1	B	100	GLY	N-CA	-6.82	1.34	1.45
1	B	591	MET	SD-CE	-6.81	1.62	1.79
1	A	725	GLN	CG-CD	6.80	1.69	1.52
1	A	82	ARG	CZ-NH2	-6.75	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	532	ARG	N-CA	-6.73	1.38	1.46
1	B	722	ALA	C-N	-6.73	1.25	1.33
1	A	708	SER	CA-C	-6.71	1.45	1.52
1	B	711	GLN	CD-NE2	-6.71	1.19	1.33
1	A	492	ARG	N-CA	6.71	1.54	1.46
1	A	199	ASP	C-O	6.70	1.31	1.23
1	B	606	LYS	N-CA	6.68	1.54	1.46
1	B	344	ASN	C-O	6.66	1.31	1.24
1	A	502	GLY	CA-C	-6.66	1.43	1.52
1	B	196	GLU	CB-CG	-6.65	1.32	1.52
1	B	740	MET	CA-CB	-6.65	1.42	1.53
1	A	692	THR	CB-CG2	-6.64	1.30	1.52
1	A	703	ASP	CG-OD2	6.60	1.37	1.25
1	B	606	LYS	CA-C	-6.59	1.43	1.52
1	A	362	TRP	CA-C	-6.56	1.44	1.52
1	A	458	ILE	CA-CB	-6.54	1.47	1.54
1	B	569	ALA	C-O	6.54	1.31	1.23
1	A	552	VAL	N-CA	6.53	1.54	1.46
1	B	426	ARG	CZ-NH2	6.53	1.42	1.33
1	A	47	LEU	CB-CG	-6.53	1.40	1.53
1	B	593	VAL	CA-C	-6.49	1.44	1.52
1	A	462	ASP	N-CA	6.47	1.54	1.46
1	B	49	LEU	CB-CG	-6.46	1.40	1.53
1	A	95	TRP	N-CA	6.46	1.55	1.46
1	A	727	LYS	C-N	-6.45	1.25	1.33
1	A	527	THR	N-CA	-6.43	1.38	1.46
1	B	46	GLN	CD-OE1	6.42	1.35	1.23
1	B	688	ARG	N-CA	6.42	1.53	1.45
1	A	46	GLN	N-CA	6.42	1.54	1.45
1	B	63	GLY	N-CA	6.40	1.53	1.45
1	A	536	ASN	CA-C	6.39	1.61	1.52
1	A	61	PRO	C-O	-6.37	1.16	1.24
1	B	572	VAL	N-CA	-6.37	1.40	1.46
1	A	266	MET	CA-C	6.36	1.60	1.52
1	A	688	ARG	CA-C	-6.35	1.45	1.52
1	A	446	TRP	NE1-CE2	-6.33	1.30	1.37
1	B	46	GLN	N-CA	6.33	1.53	1.45
1	A	725	GLN	N-CA	6.33	1.54	1.46
1	B	725	GLN	N-CA	6.30	1.53	1.46
1	A	417	ALA	N-CA	6.28	1.54	1.46
1	B	443	VAL	CA-C	-6.26	1.45	1.52
1	A	730	ARG	N-CA	-6.25	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	375	PHE	N-CA	6.22	1.54	1.46
1	A	456	PRO	CA-C	6.20	1.60	1.52
1	A	711	GLN	CD-OE1	6.20	1.35	1.23
1	A	685	PHE	N-CA	-6.19	1.38	1.46
1	B	727	LYS	N-CA	-6.18	1.39	1.46
1	B	423	LEU	N-CA	6.16	1.53	1.46
1	B	541	GLY	C-O	6.14	1.34	1.24
1	A	196	GLU	CB-CG	-6.13	1.34	1.52
1	A	544	GLN	CA-C	6.13	1.60	1.52
1	B	55	HIS	CA-CB	6.13	1.62	1.53
1	A	454	ASP	CB-CG	6.12	1.67	1.52
1	A	679	ALA	N-CA	6.12	1.53	1.46
1	B	512	ASP	CB-CG	6.11	1.67	1.52
1	B	448	ASP	CA-C	-6.10	1.49	1.53
1	A	199	ASP	CA-C	-6.09	1.45	1.53
1	B	47	LEU	CB-CG	-6.08	1.41	1.53
1	A	398	TYR	N-CA	6.07	1.54	1.46
1	B	640	VAL	C-O	-6.05	1.16	1.24
1	B	572	VAL	C-N	-6.03	1.25	1.33
1	B	689	ASP	CG-OD2	-5.99	1.14	1.25
1	B	268	ASP	N-CA	-5.97	1.39	1.46
1	B	293	VAL	CA-C	-5.96	1.45	1.52
1	A	567	GLY	CA-C	-5.96	1.43	1.51
1	A	56	SER	CA-C	-5.93	1.45	1.53
1	A	473	SER	C-O	-5.93	1.16	1.24
1	A	343	GLU	C-O	5.92	1.31	1.24
1	B	698	THR	N-CA	-5.92	1.38	1.45
1	B	620	LYS	CA-CB	-5.90	1.44	1.53
1	A	503	ALA	C-O	5.90	1.31	1.23
1	A	343	GLU	CD-OE1	5.89	1.36	1.25
1	A	428	MET	CG-SD	-5.88	1.66	1.80
1	A	62	MET	C-N	-5.88	1.24	1.33
1	B	438	GLU	CD-OE2	5.87	1.36	1.25
1	A	203	GLY	N-CA	5.86	1.51	1.45
1	A	46	GLN	CG-CD	5.86	1.66	1.52
1	B	151	LEU	N-CA	5.85	1.53	1.46
1	A	196	GLU	N-CA	-5.82	1.40	1.45
1	A	556	CYS	CA-C	5.82	1.60	1.52
1	A	259	ASP	CA-C	5.80	1.60	1.52
1	B	267	ASN	C-O	5.79	1.31	1.23
1	B	514	GLU	CA-CB	5.79	1.62	1.53
1	A	64	LYS	C-O	-5.78	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	387	THR	C-O	5.78	1.30	1.24
1	B	699	GLY	N-CA	5.78	1.51	1.45
1	A	407	GLU	CG-CD	5.77	1.66	1.52
1	A	162	ALA	CA-C	-5.77	1.44	1.52
1	A	96	PRO	C-O	5.77	1.30	1.23
1	A	602	ARG	CZ-NH2	-5.76	1.25	1.33
1	B	302	ILE	CB-CG1	-5.75	1.42	1.53
1	B	704	LEU	CA-C	-5.74	1.44	1.52
1	B	268	ASP	C-N	-5.74	1.26	1.33
1	A	120	ALA	C-O	5.73	1.30	1.24
1	B	564	LYS	CA-C	5.72	1.60	1.52
1	B	540	ARG	CA-C	-5.72	1.46	1.52
1	A	376	ASP	N-CA	5.71	1.53	1.46
1	A	471	LEU	CA-CB	-5.70	1.43	1.53
1	B	537	GLY	N-CA	5.67	1.53	1.45
1	B	42	TRP	N-CA	-5.67	1.39	1.46
1	B	410	GLU	CG-CD	5.67	1.66	1.52
1	A	46	GLN	CA-CB	5.65	1.62	1.53
1	A	430	PRO	N-CA	5.64	1.54	1.47
1	B	602	ARG	CZ-NH2	-5.63	1.26	1.33
1	A	656	ARG	CD-NE	5.62	1.54	1.46
1	A	746	ASP	N-CA	5.61	1.53	1.46
1	A	203	GLY	C-O	5.60	1.27	1.23
1	A	471	LEU	CA-C	5.60	1.60	1.52
1	A	444	LEU	N-CA	-5.59	1.39	1.46
1	A	519	GLU	N-CA	5.58	1.53	1.46
1	A	736	TRP	C-N	5.57	1.41	1.33
1	A	476	THR	N-CA	-5.57	1.39	1.45
1	B	550	LEU	N-CA	-5.56	1.39	1.46
1	B	719	TYR	N-CA	5.55	1.53	1.46
1	A	670	ASP	CA-CB	5.54	1.59	1.53
1	A	317	LYS	N-CA	5.54	1.52	1.46
1	A	428	MET	N-CA	5.53	1.53	1.46
1	A	101	HIS	C-O	-5.51	1.17	1.23
1	B	67	ASN	CG-ND2	-5.51	1.21	1.33
1	A	345	LEU	CA-C	5.50	1.59	1.52
1	B	223	ARG	CZ-NH1	5.50	1.40	1.32
1	B	289	PRO	N-CA	-5.50	1.40	1.47
1	B	596	PRO	C-N	-5.49	1.27	1.33
1	B	676	LYS	C-O	-5.49	1.17	1.24
1	A	571	THR	CA-C	5.48	1.59	1.52
1	A	349	GLU	C-O	-5.48	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	585	GLN	CD-OE1	5.48	1.33	1.23
1	B	643	ALA	N-CA	-5.47	1.39	1.46
1	B	690	ARG	CD-NE	-5.47	1.38	1.46
1	B	713	ARG	NE-CZ	-5.46	1.27	1.33
1	B	132	ARG	CZ-NH1	5.45	1.40	1.32
1	A	564	LYS	C-O	5.44	1.30	1.24
1	A	636	GLY	N-CA	5.44	1.52	1.45
1	B	61	PRO	N-CA	-5.43	1.40	1.47
1	A	516	ASN	N-CA	-5.43	1.39	1.46
1	B	80	VAL	C-O	5.43	1.30	1.24
1	A	49	LEU	N-CA	-5.42	1.39	1.46
1	B	203	GLY	CA-C	5.42	1.57	1.52
1	A	449	PRO	C-O	-5.42	1.17	1.23
1	B	299	ALA	N-CA	5.40	1.53	1.46
1	A	608	LYS	N-CA	5.40	1.53	1.46
1	B	692	THR	N-CA	5.39	1.53	1.46
1	B	572	VAL	CA-CB	5.39	1.61	1.54
1	B	371	ILE	N-CA	5.39	1.53	1.46
1	A	695	LEU	N-CA	5.39	1.52	1.46
1	B	54	ARG	CA-C	-5.39	1.45	1.53
1	A	237	ILE	C-O	5.38	1.29	1.24
1	B	92	GLN	CD-NE2	-5.37	1.22	1.33
1	A	91	SER	CA-C	-5.37	1.45	1.52
1	B	731	ASP	N-CA	-5.37	1.39	1.46
1	A	264	MET	CA-CB	5.36	1.60	1.53
1	A	370	VAL	CA-C	5.36	1.58	1.52
1	B	427	ASP	CG-OD2	5.35	1.35	1.25
1	A	447	GLN	C-O	-5.34	1.16	1.24
1	A	656	ARG	CA-CB	-5.34	1.46	1.53
1	B	376	ASP	CA-C	-5.34	1.46	1.52
1	A	438	GLU	N-CA	5.34	1.52	1.46
1	B	67	ASN	CA-C	5.34	1.59	1.52
1	B	36	GLY	N-CA	5.33	1.54	1.45
1	A	249	ASP	N-CA	-5.33	1.39	1.46
1	B	466	LEU	N-CA	5.32	1.52	1.46
1	A	137	ASN	N-CA	-5.32	1.39	1.46
1	B	468	ALA	N-CA	-5.31	1.39	1.46
1	A	649	ARG	CZ-NH1	5.30	1.40	1.32
1	A	225	LEU	CA-CB	5.29	1.61	1.53
1	A	247	ASN	CG-ND2	-5.29	1.22	1.33
1	B	496	LYS	CE-NZ	-5.28	1.33	1.49
1	A	382	ARG	CA-C	5.27	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	364	ALA	N-CA	5.26	1.52	1.46
1	B	622	GLN	C-O	5.26	1.30	1.24
1	A	710	SER	CA-C	-5.24	1.45	1.52
1	A	134	ALA	CA-C	-5.23	1.47	1.53
1	B	90	THR	CA-CB	-5.22	1.45	1.52
1	B	734	ALA	N-CA	-5.21	1.40	1.46
1	A	172	THR	C-O	5.21	1.30	1.24
1	A	173	GLY	CA-C	5.21	1.57	1.52
1	A	698	THR	C-O	-5.21	1.17	1.23
1	B	446	TRP	CD2-CE2	5.20	1.50	1.41
1	B	660	LEU	C-O	5.20	1.30	1.23
1	A	551	ILE	C-N	-5.19	1.27	1.33
1	A	443	VAL	CA-C	-5.18	1.46	1.52
1	A	694	GLU	CA-C	5.18	1.59	1.52
1	A	365	LYS	N-CA	5.18	1.52	1.46
1	A	431	ARG	N-CA	5.17	1.52	1.46
1	A	178	GLU	C-O	5.17	1.30	1.24
1	B	700	THR	N-CA	-5.17	1.39	1.45
1	A	70	GLN	N-CA	5.16	1.52	1.46
1	A	347	GLY	N-CA	5.16	1.52	1.45
1	A	442	GLU	N-CA	5.16	1.52	1.46
1	A	731	ASP	N-CA	-5.15	1.39	1.46
1	A	652	VAL	C-N	5.15	1.40	1.33
1	A	532	ARG	CD-NE	-5.13	1.39	1.46
1	B	157	GLN	N-CA	-5.13	1.40	1.46
1	A	43	TRP	CA-CB	5.12	1.59	1.53
1	B	524	VAL	CA-C	-5.12	1.46	1.52
1	A	191	ARG	CA-C	5.11	1.59	1.52
1	A	121	ASP	CA-C	-5.10	1.45	1.52
1	B	56	SER	C-N	-5.10	1.26	1.33
1	B	726	GLU	CA-C	-5.09	1.46	1.52
1	A	429	GLY	C-O	-5.09	1.17	1.24
1	A	695	LEU	CA-C	-5.08	1.46	1.52
1	A	453	VAL	C-N	-5.07	1.26	1.33
1	A	570	VAL	CA-CB	5.07	1.63	1.55
1	B	463	ALA	CA-C	-5.07	1.46	1.52
1	B	711	GLN	CD-OE1	5.05	1.33	1.23
1	B	204	SER	CA-CB	5.05	1.61	1.53
1	A	108	ARG	CA-C	-5.05	1.46	1.52
1	B	599	ASP	C-O	-5.04	1.18	1.23
1	B	738	LYS	N-CA	-5.03	1.40	1.46
1	A	335	THR	CA-CB	-5.03	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	ARG	C-O	-5.03	1.17	1.23
1	B	159	TYR	CA-CB	-5.02	1.45	1.53
1	B	370	VAL	CA-C	5.02	1.59	1.52
1	B	448	ASP	C-O	5.02	1.26	1.23
1	B	318	GLY	C-O	5.01	1.30	1.24
1	B	570	VAL	CA-CB	-5.01	1.48	1.55
1	A	79	ALA	N-CA	-5.00	1.40	1.46

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	541	GLY	N-CA-C	-8.86	96.07	112.37
1	B	46	GLN	N-CA-C	-8.80	98.09	110.50
1	A	196	GLU	O-C-N	8.24	127.67	121.65
1	B	529	GLU	N-CA-C	-8.15	102.37	111.82
1	A	46	GLN	N-CA-C	-7.98	99.25	110.50
1	A	544	GLN	CG-CD-NE2	-7.62	104.97	116.40
1	B	47	LEU	N-CA-CB	-7.51	99.35	110.17
1	A	439	VAL	N-CA-C	7.48	116.28	108.95
1	B	428	MET	CA-CB-CG	-7.44	99.22	114.10
1	A	407	GLU	CG-CD-OE1	7.42	135.48	118.40
1	A	47	LEU	N-CA-CB	-7.25	99.73	110.17
1	B	569	ALA	N-CA-C	-7.23	98.77	110.20
1	A	431	ARG	NE-CZ-NH2	7.10	125.59	119.20
1	B	48	ASP	N-CA-C	7.10	121.60	107.62
1	B	223	ARG	CA-CB-CG	-7.01	100.08	114.10
1	B	729	VAL	O-C-N	-6.99	115.09	121.87
1	B	46	GLN	CA-CB-CG	6.87	127.84	114.10
1	B	66	PHE	CA-C-N	-6.84	113.08	123.07
1	B	66	PHE	C-N-CA	-6.84	113.08	123.07
1	A	55	HIS	CB-CA-C	6.66	121.70	111.39
1	A	431	ARG	NE-CZ-NH1	-6.49	115.01	121.50
1	A	541	GLY	N-CA-C	-6.40	106.40	115.43
1	A	46	GLN	CA-CB-CG	6.37	126.85	114.10
1	A	594	LEU	CA-C-O	6.29	126.89	119.28
1	A	736	TRP	CA-C-O	6.25	127.17	120.55
1	B	310	LYS	CG-CD-CE	6.24	125.66	111.30
1	A	73	GLU	CB-CG-CD	6.22	123.17	112.60
1	B	725	GLN	CB-CG-CD	6.13	123.03	112.60
1	A	736	TRP	O-C-N	-6.10	115.65	122.12
1	A	571	THR	OG1-CB-CG2	-6.05	97.20	109.30
1	A	47	LEU	CA-C-O	-6.04	114.98	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	539	GLN	O-C-N	5.99	129.68	122.85
1	B	374	ALA	N-CA-C	5.95	118.55	111.71
1	B	479	GLN	N-CA-C	5.92	117.81	111.36
1	B	550	LEU	N-CA-C	5.87	118.46	111.71
1	B	175	VAL	N-CA-C	-5.84	104.82	110.72
1	B	434	TYR	CA-CB-CG	5.80	124.35	113.90
1	B	353	THR	CA-CB-OG1	-5.79	100.91	109.60
1	A	161	ARG	NE-CZ-NH1	5.77	127.27	121.50
1	A	462	ASP	N-CA-C	-5.76	104.91	111.07
1	B	445	LEU	O-C-N	-5.75	116.03	122.12
1	A	382	ARG	O-C-N	5.71	127.81	121.53
1	A	429	GLY	O-C-N	5.68	127.45	121.77
1	B	478	SER	CA-C-O	5.65	126.54	120.55
1	B	554	ALA	N-CA-C	5.65	118.20	111.71
1	A	439	VAL	CA-C-O	-5.64	114.46	119.71
1	A	454	ASP	N-CA-CB	-5.63	101.92	111.20
1	A	69	ALA	N-CA-C	5.62	117.41	111.28
1	A	57	SER	N-CA-C	-5.61	105.69	112.54
1	B	690	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	A	48	ASP	N-CA-C	5.56	118.57	107.62
1	B	512	ASP	CB-CG-OD1	-5.52	105.70	118.40
1	A	690	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	B	609	TYR	N-CA-C	-5.50	101.05	109.41
1	A	212	SER	O-C-N	5.50	129.18	122.75
1	B	123	ARG	NE-CZ-NH2	-5.49	114.25	119.20
1	A	182	PHE	O-C-N	5.47	129.75	123.29
1	B	62	MET	CA-C-N	-5.46	114.36	120.53
1	B	62	MET	C-N-CA	-5.46	114.36	120.53
1	A	649	ARG	NE-CZ-NH2	-5.46	114.29	119.20
1	A	710	SER	N-CA-C	5.45	118.14	111.82
1	B	569	ALA	CA-C-N	-5.44	114.40	122.23
1	B	569	ALA	C-N-CA	-5.44	114.40	122.23
1	B	310	LYS	CB-CG-CD	-5.36	98.97	111.30
1	A	628	ALA	O-C-N	5.33	125.72	120.71
1	A	592	ALA	N-CA-C	5.33	117.84	111.71
1	B	512	ASP	CA-CB-CG	5.30	117.91	112.60
1	B	649	ARG	NE-CZ-NH2	-5.28	114.44	119.20
1	A	594	LEU	O-C-N	-5.28	115.09	122.37
1	B	345	LEU	O-C-N	5.28	127.71	122.12
1	A	46	GLN	CA-C-O	5.28	127.31	121.56
1	A	690	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	B	57	SER	N-CA-C	-5.27	106.11	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	GLN	N-CA-CB	5.27	117.76	110.17
1	B	46	GLN	CA-C-O	5.17	127.19	121.56
1	A	319	ALA	N-CA-C	5.15	118.67	112.38
1	B	54	ARG	CA-C-N	-5.15	115.33	122.74
1	B	54	ARG	C-N-CA	-5.15	115.33	122.74
1	A	423	LEU	O-C-N	5.14	127.44	122.09
1	B	678	THR	CA-C-N	5.14	127.13	120.44
1	B	678	THR	C-N-CA	5.14	127.13	120.44
1	A	554	ALA	N-CA-C	5.14	116.88	111.28
1	A	412	PHE	CA-CB-CG	5.13	118.93	113.80
1	B	46	GLN	CG-CD-OE1	5.13	131.07	120.80
1	B	206	LYS	CG-CD-CE	5.10	123.04	111.30
1	A	608	LYS	N-CA-CB	5.07	118.44	110.23
1	A	66	PHE	CA-C-O	5.05	126.82	121.16
1	A	108	ARG	NE-CZ-NH1	5.05	126.55	121.50
1	B	46	GLN	CB-CG-CD	5.03	121.16	112.60
1	A	46	GLN	N-CA-CB	5.02	117.40	110.17
1	B	46	GLN	O-C-N	-5.02	116.94	122.86

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	199	ASP	Mainchain
1	B	514	GLU	Sidechain

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	5568	0	5365	15	0
1	B	5552	0	5353	22	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	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	24	0	42	7	0
7	B	8	0	14	3	0
8	A	794	0	0	7	2
8	B	785	0	0	11	2
All	All	12835	0	10834	47	2

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 (47) 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)
7:A:807:MPD:H52	7:A:807:MPD:H11	1.38	1.05
1:A:119[B]:THR:HG21	8:A:1080:HOH:O	1.62	0.97
1:B:569:ALA:O	1:B:570:VAL:HG23	1.65	0.95
1:B:198[A]:GLU:OE1	8:B:901:HOH:O	1.83	0.94
1:B:76:ASP:OD2	8:B:902:HOH:O	1.89	0.89
1:B:119[B]:THR:HG21	8:B:1142:HOH:O	1.77	0.83
1:B:540:ARG:NE	1:B:540:ARG:HA	1.94	0.83
5:B:804:OXY:O2	8:B:903:HOH:O	1.99	0.81
1:B:647:GLN:HG2	8:B:990:HOH:O	1.80	0.80
1:B:65:ASP:HB2	8:B:930:HOH:O	1.80	0.80
1:B:512:ASP:OD1	8:B:904:HOH:O	2.00	0.77
1:B:569:ALA:O	1:B:570:VAL:CG2	2.33	0.75
7:A:808:MPD:O4	7:A:808:MPD:HM2	1.87	0.73
7:A:807:MPD:H11	7:A:807:MPD:C5	2.11	0.71
1:B:431:ARG:CD	8:B:1511:HOH:O	2.39	0.70
1:B:540:ARG:NE	1:B:540:ARG:CA	2.57	0.67
1:B:431:ARG:HD2	8:B:1511:HOH:O	1.98	0.63
1:A:696:LYS:NZ	8:A:903:HOH:O	2.32	0.61
1:B:540:ARG:HA	1:B:540:ARG:CZ	2.35	0.56
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.91	0.53
1:B:591:MET:SD	1:B:594:LEU:HD12	2.48	0.53
1:A:226:GLU:OE1	1:A:610:ARG:NH2	2.43	0.52
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.39	0.51
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:806:MPD:CM	7:B:806:MPD:H52	2.42	0.48
7:B:806:MPD:H52	7:B:806:MPD:HM2	1.96	0.47
7:A:807:MPD:C1	8:A:1165:HOH:O	2.62	0.47
7:A:807:MPD:HM2	8:A:1514:HOH:O	2.15	0.47
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.98	0.46
1:A:726[B]:GLU:HG2	1:A:730:ARG:HH12	1.81	0.46
1:B:607:GLY:C	1:B:608:LYS:HE2	2.41	0.45
1:A:426[B]:ARG:HA	1:A:426[B]:ARG:HD2	1.65	0.45
7:A:808:MPD:O4	7:A:808:MPD:CM	2.62	0.44
1:B:324:SER:C	7:B:806:MPD:H53	2.43	0.44
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.17	0.44
1:A:70:GLN:NE2	8:A:929:HOH:O	2.50	0.44
1:A:591:MET:SD	1:A:594:LEU:HD12	2.58	0.44
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.18	0.43
7:A:807:MPD:H11	8:A:1165:HOH:O	2.18	0.43
1:B:431:ARG:HD3	8:B:1511:HOH:O	2.13	0.43
1:B:738:LYS:NZ	8:B:925:HOH:O	2.51	0.43
1:A:54:ARG:HB2	1:A:55:HIS:CD2	2.54	0.43
1:A:336[B]:GLN:HG3	8:A:922:HOH:O	2.19	0.42
1:A:119[A]:THR:HG21	1:A:265:ALA:HB2	2.02	0.42
1:A:198:GLU:HG3	4:A:803:CL:CL	2.58	0.41
1:A:455:HIS:CE1	1:A:544:GLN:HG3	2.55	0.41
1:A:726[B]:GLU:CG	1:A:730:ARG:HH12	2.34	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1227:HOH:O	8:B:954:HOH:O[2_444]	2.18	0.02
8:A:1538:HOH:O	8:B:1351:HOH:O[4_445]	2.19	0.01

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%)	704 (98%)	13 (2%)	0	100	100
1	B	716/728 (98%)	704 (98%)	12 (2%)	0	100	100
All	All	1433/1456 (98%)	1408 (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	37
1	B	556/561 (99%)	545 (98%)	11 (2%)	48	24
All	All	1113/1122 (99%)	1094 (98%)	19 (2%)	55	29

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	183	LYS
1	A	379	LYS
1	A	544	GLN
1	A	608	LYS
1	B	40	ARG
1	B	46	GLN
1	B	54	ARG
1	B	141	ASP
1	B	379	LYS
1	B	496	LYS
1	B	571[A]	THR
1	B	571[B]	THR

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Mol	Chain	Res	Type
1	B	608	LYS
1	B	649	ARG
1	B	730	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	HIS
1	A	520	GLN
1	A	568	HIS
1	A	647	GLN
1	A	741	ASN
1	B	406	HIS
1	B	520	GLN
1	B	544	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TOX	A	111[A]	2	14,17,18	1.95	4 (28%)	12,23,25	1.73	3 (25%)
1	TOX	A	111[B]	-	14,17,18	1.95	4 (28%)	12,23,25	1.73	3 (25%)
1	TOX	B	111[A]	2	14,17,18	2.55	6 (42%)	12,23,25	2.05	5 (41%)
1	TOX	B	111[B]	-	14,17,18	2.55	6 (42%)	12,23,25	2.05	5 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TOX	A	111[A]	2	-	2/5/8/10	0/2/2/2
1	TOX	A	111[B]	-	-	2/5/8/10	0/2/2/2
1	TOX	B	111[A]	2	-	3/5/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	3/5/8/10	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	CZ2-CE2	-5.69	1.30	1.39
1	B	111[B]	TOX	CZ2-CE2	-5.69	1.30	1.39
1	B	111[A]	TOX	CD2-CG	5.08	1.52	1.44
1	B	111[B]	TOX	CD2-CG	5.08	1.52	1.44
1	A	111[A]	TOX	O1-NE1	3.62	1.43	1.39
1	A	111[B]	TOX	O1-NE1	3.62	1.43	1.39
1	A	111[A]	TOX	CD2-CG	3.22	1.49	1.44
1	A	111[B]	TOX	CD2-CG	3.22	1.49	1.44
1	A	111[A]	TOX	CE3-CD2	-3.11	1.35	1.39
1	A	111[B]	TOX	CE3-CD2	-3.11	1.35	1.39
1	B	111[A]	TOX	O-C	2.90	1.31	1.20
1	B	111[B]	TOX	O-C	2.90	1.31	1.20
1	A	111[A]	TOX	O-C	2.70	1.30	1.20
1	A	111[B]	TOX	O-C	2.70	1.30	1.20
1	B	111[A]	TOX	O1-NE1	2.48	1.42	1.39
1	B	111[B]	TOX	O1-NE1	2.48	1.42	1.39
1	B	111[A]	TOX	CA-N	-2.45	1.41	1.48
1	B	111[B]	TOX	CA-N	-2.45	1.41	1.48
1	B	111[A]	TOX	CH2-CZ3	2.25	1.43	1.38
1	B	111[B]	TOX	CH2-CZ3	2.25	1.43	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111[A]	TOX	CE2-CD2-CG	-3.98	103.73	107.39
1	B	111[B]	TOX	CE2-CD2-CG	-3.98	103.73	107.39
1	A	111[A]	TOX	CZ2-CE2-NE1	3.96	135.68	129.37
1	A	111[B]	TOX	CZ2-CE2-NE1	3.96	135.68	129.37
1	B	111[A]	TOX	CZ3-CE3-CD2	-3.30	113.83	119.80
1	B	111[B]	TOX	CZ3-CE3-CD2	-3.30	113.83	119.80
1	A	111[A]	TOX	CZ2-CE2-CD2	-2.84	118.78	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[B]	TOX	CZ2-CE2-CD2	-2.84	118.78	121.95
1	B	111[A]	TOX	CE3-CD2-CE2	2.82	122.48	119.24
1	B	111[B]	TOX	CE3-CD2-CE2	2.82	122.48	119.24
1	B	111[A]	TOX	CH2-CZ3-CE3	2.78	123.67	120.24
1	B	111[B]	TOX	CH2-CZ3-CE3	2.78	123.67	120.24
1	A	111[A]	TOX	CD2-CG-CD1	-2.73	103.87	106.34
1	A	111[B]	TOX	CD2-CG-CD1	-2.73	103.87	106.34
1	B	111[A]	TOX	CZ3-CH2-CZ2	-2.00	117.77	120.24
1	B	111[B]	TOX	CZ3-CH2-CZ2	-2.00	117.77	120.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111[A]	TOX	N-CA-CB-CG
1	A	111[A]	TOX	C-CA-CB-CG
1	A	111[B]	TOX	N-CA-CB-CG
1	A	111[B]	TOX	C-CA-CB-CG
1	B	111[A]	TOX	N-CA-CB-CG
1	B	111[A]	TOX	C-CA-CB-CG
1	B	111[B]	TOX	N-CA-CB-CG
1	B	111[B]	TOX	C-CA-CB-CG
1	B	111[A]	TOX	CA-CB-CG-CD1
1	B	111[B]	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
6	PO4	B	805	-	4,4,4	2.22	3 (75%)	6,6,6	1.62	2 (33%)
5	OXY	A	804	-	1,1,1	0.64	0	-		
7	MPD	A	806	-	7,7,7	1.69	1 (14%)	9,10,10	2.86	5 (55%)
7	MPD	B	806	-	7,7,7	1.06	0	9,10,10	1.56	1 (11%)
5	OXY	B	804	-	1,1,1	0.62	0	-		
7	MPD	A	807	-	7,7,7	1.15	1 (14%)	9,10,10	1.94	4 (44%)
2	HEM	A	801	1	50,50,50	1.79	14 (28%)	67,82,82	1.84	14 (20%)
6	PO4	A	805	-	4,4,4	1.91	1 (25%)	6,6,6	2.18	2 (33%)
2	HEM	B	801	1	50,50,50	2.08	14 (28%)	67,82,82	2.13	19 (28%)
7	MPD	A	808	-	7,7,7	0.87	0	9,10,10	2.23	4 (44%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MPD	A	806	-	-	0/5/5/5	-
7	MPD	B	806	-	-	3/5/5/5	-
7	MPD	A	807	-	-	3/5/5/5	-
2	HEM	A	801	1	-	2/14/54/54	-
2	HEM	B	801	1	-	3/14/54/54	-
7	MPD	A	808	-	-	3/5/5/5	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1B-NB	-5.61	1.30	1.40
2	A	801	HEM	FE-NB	4.71	2.09	1.94
2	B	801	HEM	C3C-C4C	-4.54	1.38	1.46
2	B	801	HEM	C1C-NC	-4.50	1.31	1.39
2	B	801	HEM	C1B-C2B	-4.23	1.35	1.44
7	A	806	MPD	C5-C4	3.92	1.67	1.51
2	A	801	HEM	C4A-NA	-3.92	1.32	1.39
2	B	801	HEM	FE-NB	3.85	2.06	1.94
6	A	805	PO4	P-O3	-3.48	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C4A-C3A	3.32	1.50	1.43
2	A	801	HEM	CMD-C2D	-3.23	1.44	1.50
2	B	801	HEM	CMB-C2B	3.09	1.57	1.50
2	A	801	HEM	C3B-C4B	3.07	1.50	1.44
2	A	801	HEM	C4D-C3D	3.04	1.50	1.45
2	B	801	HEM	CHB-C1B	3.04	1.44	1.38
6	B	805	PO4	P-O2	-3.02	1.45	1.54
2	A	801	HEM	FE-NC	2.96	2.04	1.95
2	A	801	HEM	FE-NA	2.94	2.04	1.95
2	A	801	HEM	CHD-C4C	-2.94	1.32	1.38
2	B	801	HEM	C3D-C2D	2.80	1.42	1.36
2	B	801	HEM	C1D-ND	-2.76	1.33	1.38
2	B	801	HEM	FE-NC	2.70	2.04	1.95
2	A	801	HEM	C1B-NB	-2.70	1.35	1.40
2	B	801	HEM	C3B-C2B	-2.59	1.31	1.37
2	A	801	HEM	O1A-CGA	2.57	1.30	1.22
2	A	801	HEM	O1D-CGD	2.56	1.30	1.22
6	B	805	PO4	P-O1	2.42	1.56	1.50
2	B	801	HEM	CHD-C4C	2.38	1.43	1.38
2	A	801	HEM	C1D-C2D	2.36	1.49	1.44
2	B	801	HEM	C2A-C3A	-2.35	1.32	1.38
2	A	801	HEM	C1A-NA	2.34	1.44	1.39
7	A	807	MPD	O2-C2	2.18	1.50	1.44
6	B	805	PO4	P-O3	-2.13	1.48	1.54
2	A	801	HEM	CHB-C1B	2.10	1.42	1.38

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C3B-C2B-C1B	7.76	112.24	106.41
2	A	801	HEM	C4B-C3B-C2B	-5.71	102.03	107.28
2	B	801	HEM	C3B-C4B-NB	-5.56	105.48	109.47
2	A	801	HEM	C3B-C2B-C1B	5.32	110.41	106.41
7	A	806	MPD	O2-C2-C1	-4.86	92.83	107.99
2	B	801	HEM	C2A-C1A-NA	4.64	115.30	110.15
2	A	801	HEM	CHC-C1C-NC	4.46	129.31	124.45
7	A	806	MPD	O4-C4-C3	-4.40	93.84	111.35
2	A	801	HEM	C2D-C1D-ND	4.13	114.68	109.90
2	B	801	HEM	CAD-C3D-C4D	4.01	131.69	124.70
2	B	801	HEM	CHA-C4D-ND	3.90	129.20	124.37
7	B	806	MPD	CM-C2-C1	3.83	119.21	110.63
2	B	801	HEM	CMB-C2B-C1B	-3.83	119.05	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	808	MPD	O2-C2-CM	-3.79	96.16	107.99
7	A	807	MPD	CM-C2-C1	-3.77	102.19	110.63
7	A	806	MPD	C5-C4-C3	3.65	128.62	111.67
7	A	808	MPD	CM-C2-C1	3.51	118.48	110.63
2	A	801	HEM	CAA-CBA-CGA	-3.44	104.55	113.67
6	A	805	PO4	O4-P-O1	-3.37	99.03	110.95
2	A	801	HEM	CHA-C4D-ND	-3.35	120.22	124.37
2	A	801	HEM	CHD-C1D-ND	-3.30	120.87	124.42
2	B	801	HEM	CHA-C1A-NA	-3.29	117.89	123.86
2	B	801	HEM	C4A-NA-C1A	-3.22	100.58	105.82
2	A	801	HEM	C1B-NB-C4B	3.13	108.91	105.21
2	B	801	HEM	C4B-C3B-C2B	-3.05	104.47	107.28
2	A	801	HEM	C1D-C2D-C3D	-2.88	103.95	106.98
2	B	801	HEM	CAD-C3D-C2D	-2.82	122.58	127.87
2	B	801	HEM	CHC-C4B-NB	2.81	127.45	124.42
6	A	805	PO4	O4-P-O3	-2.76	99.32	107.91
2	B	801	HEM	CHA-C4D-C3D	-2.70	120.26	125.23
2	A	801	HEM	C4D-ND-C1D	-2.69	102.02	105.21
6	B	805	PO4	O2-P-O1	-2.69	101.45	110.95
2	B	801	HEM	C4D-ND-C1D	2.68	108.38	105.21
2	A	801	HEM	CMB-C2B-C1B	-2.60	120.97	125.03
2	B	801	HEM	O1A-CGA-CBA	-2.57	114.94	123.09
7	A	808	MPD	O2-C2-C3	2.41	118.27	109.27
2	B	801	HEM	CMA-C3A-C2A	2.39	130.69	125.62
7	A	806	MPD	CM-C2-C3	2.37	120.43	110.20
2	B	801	HEM	CBD-CAD-C3D	2.34	118.99	112.53
6	B	805	PO4	O3-P-O2	2.32	115.12	107.91
7	A	807	MPD	C5-C4-C3	2.31	122.42	111.67
2	A	801	HEM	O1A-CGA-CBA	-2.30	115.80	123.09
7	A	806	MPD	O2-C2-C3	2.28	117.78	109.27
2	A	801	HEM	O2A-CGA-CBA	2.27	121.16	114.00
2	B	801	HEM	C1B-NB-C4B	2.25	107.87	105.21
2	B	801	HEM	CAD-CBD-CGD	2.23	119.57	113.67
7	A	807	MPD	O4-C4-C5	-2.21	99.96	109.45
2	A	801	HEM	C4C-NC-C1C	2.20	109.41	105.82
7	A	807	MPD	O4-C4-C3	-2.09	103.04	111.35
2	B	801	HEM	CHB-C4A-NA	2.03	127.54	123.86
7	A	808	MPD	CM-C2-C3	-2.01	101.53	110.20

There are no chirality outliers.

All (14) torsion outliers are listed below:

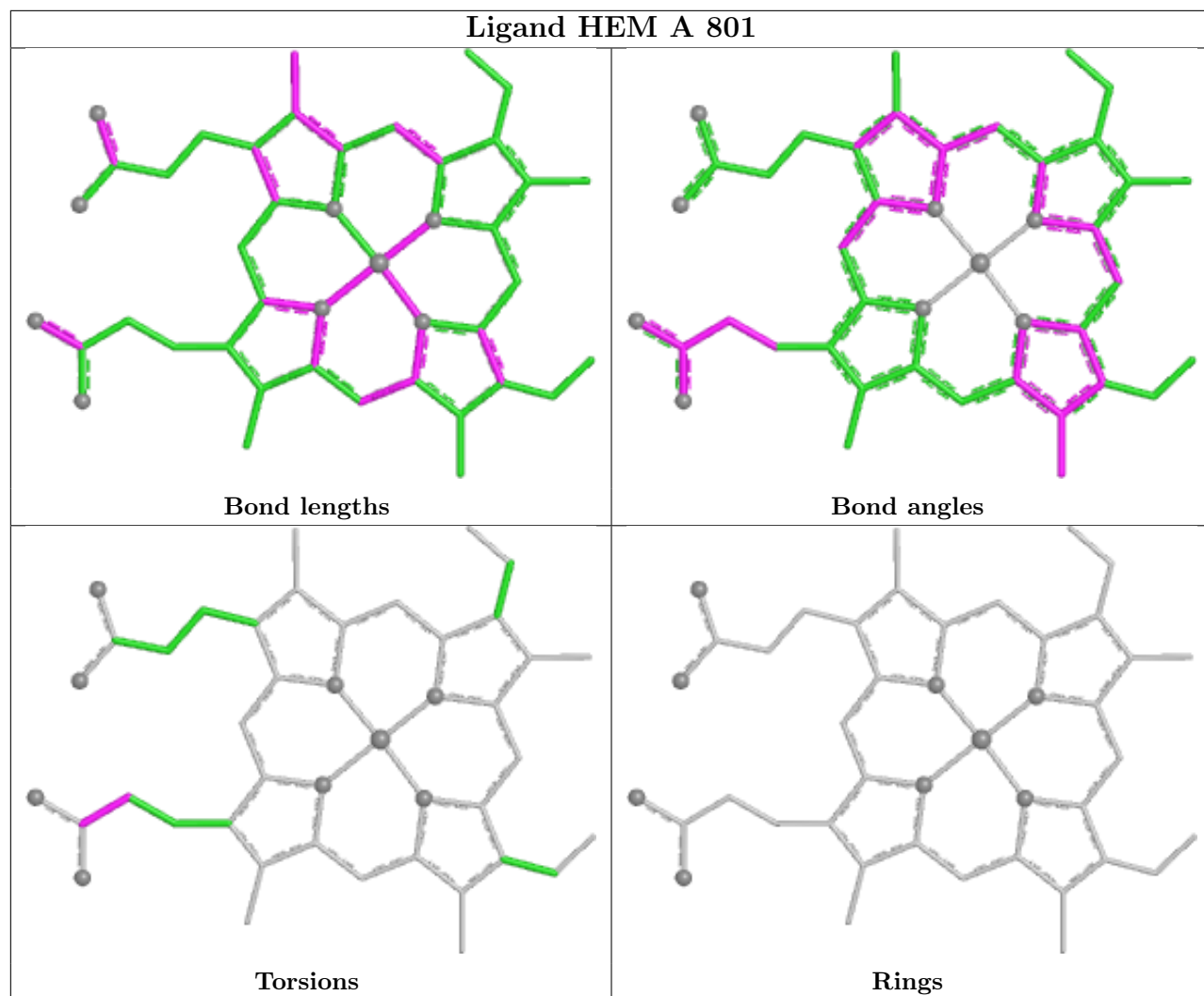
Mol	Chain	Res	Type	Atoms
7	A	807	MPD	C1-C2-C3-C4
7	A	807	MPD	C2-C3-C4-O4
7	A	808	MPD	C2-C3-C4-C5
7	B	806	MPD	O2-C2-C3-C4
7	B	806	MPD	C2-C3-C4-C5
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAA-CBA-CGA-O2A
7	A	808	MPD	C2-C3-C4-O4
7	B	806	MPD	C2-C3-C4-O4
7	A	807	MPD	CM-C2-C3-C4
7	A	808	MPD	C1-C2-C3-C4
2	B	801	HEM	CAD-CBD-CGD-O2D

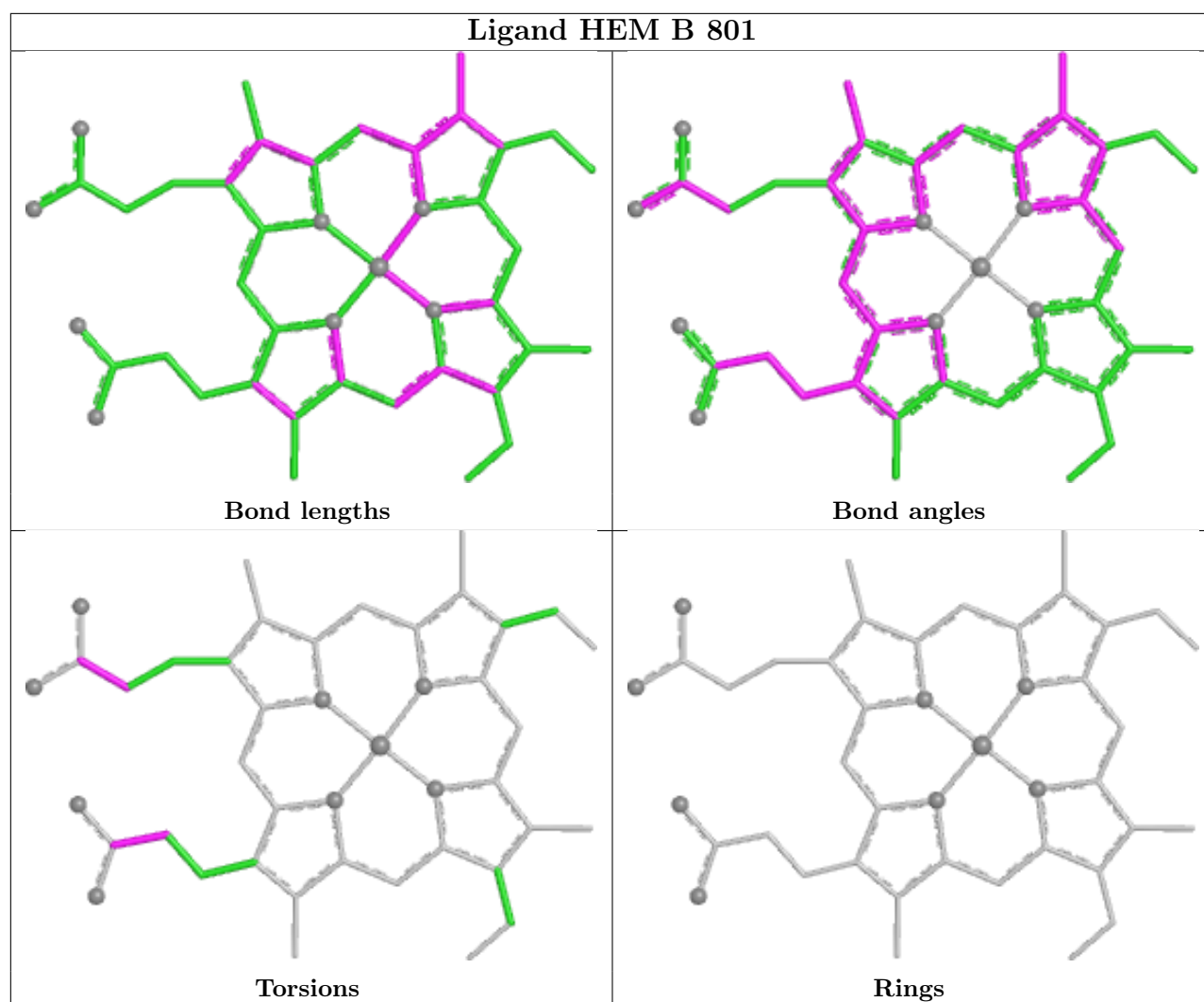
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	806	MPD	3	0
5	B	804	OXY	1	0
7	A	807	MPD	5	0
7	A	808	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

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	712/728 (97%)	-0.33	11 (1%)	72 76	8, 21, 37, 79	7 (0%)
1	B	712/728 (97%)	-0.36	11 (1%)	72 76	8, 20, 38, 90	6 (0%)
All	All	1424/1456 (97%)	-0.35	22 (1%)	72 76	8, 20, 38, 90	13 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	6.2
1	A	748	ALA	5.3
1	B	55	HIS	3.5
1	A	608	LYS	2.9
1	B	40	ARG	2.9
1	A	610	ARG	2.6
1	B	608	LYS	2.5
1	B	65	ASP	2.5
1	B	568	HIS	2.5
1	A	40	ARG	2.4
1	A	379	LYS	2.2
1	B	679	ALA	2.2
1	A	55	HIS	2.1
1	A	609	TYR	2.1
1	B	46	GLN	2.1
1	B	691	ALA	2.1
1	A	64	LYS	2.1
1	A	540	ARG	2.0
1	A	119[A]	THR	2.0
1	A	255[A]	ARG	2.0
1	B	609	TYR	2.0
1	B	610	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TOX	A	111[A]	16/17	0.98	0.04	13,15,27,28	1
1	TOX	A	111[B]	16/17	0.98	0.04	13,15,19,27	1
1	TOX	B	111[A]	16/17	0.98	0.04	14,15,24,26	0
1	TOX	B	111[B]	16/17	0.98	0.04	14,15,17,26	1

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

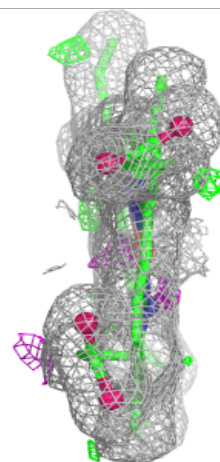
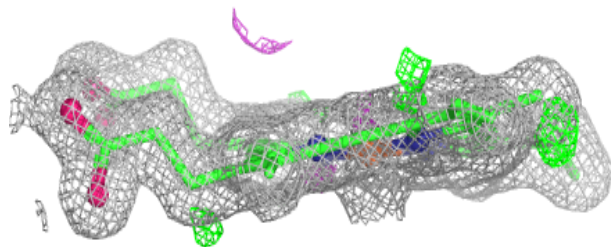
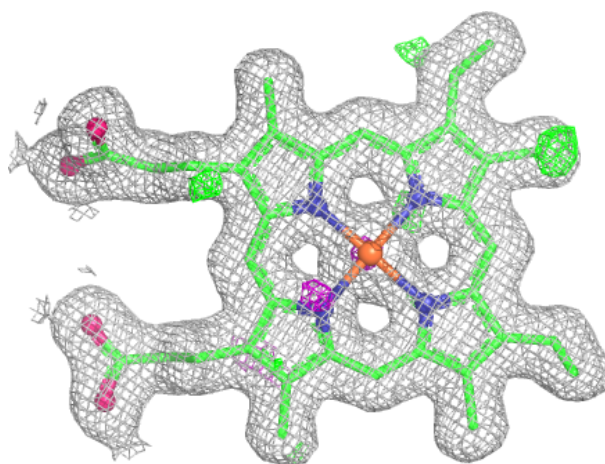
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

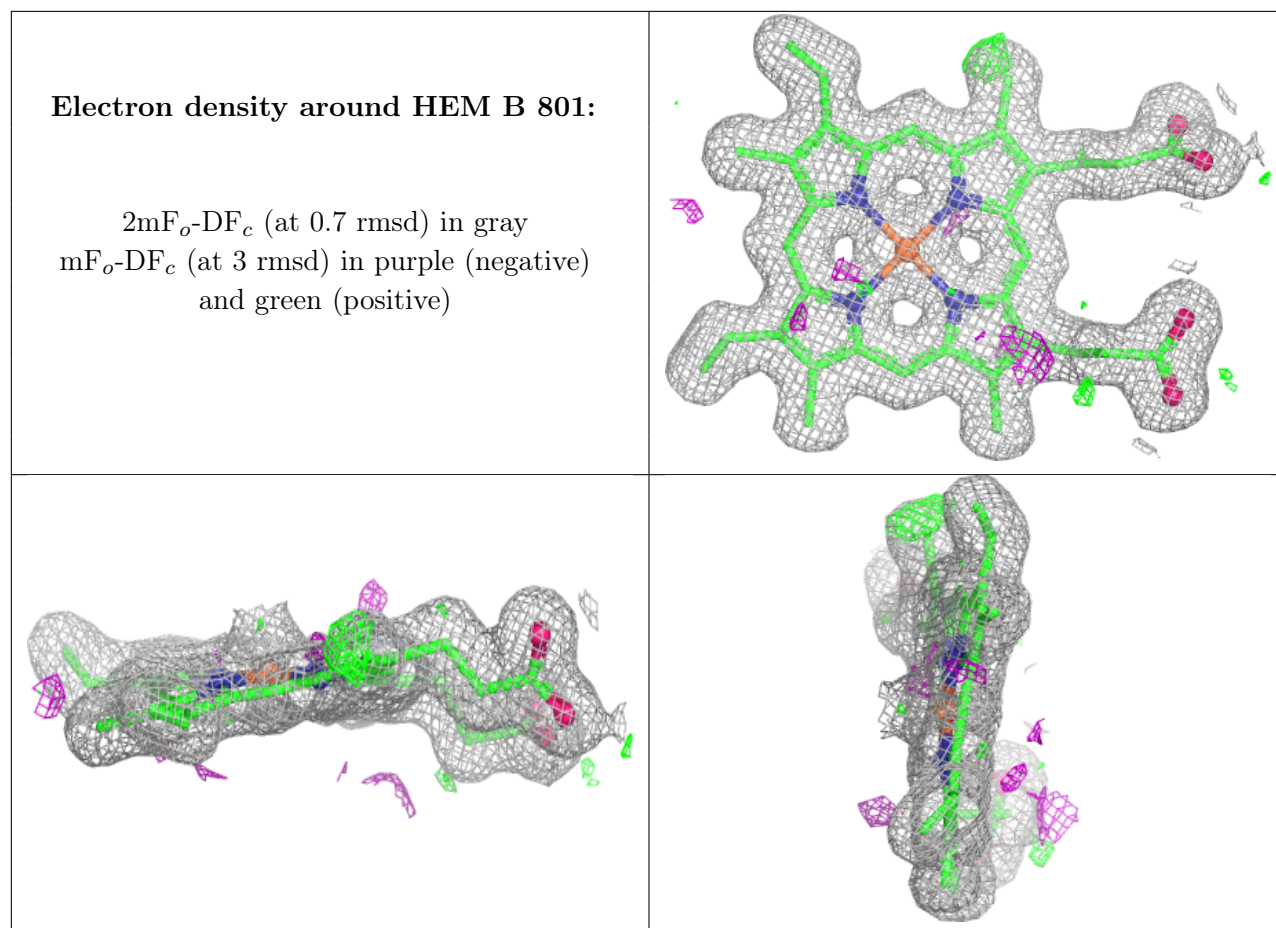
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MPD	A	806	8/8	0.77	0.27	49,59,62,67	0
7	MPD	B	806	8/8	0.81	0.22	53,55,61,67	0
7	MPD	A	808	8/8	0.83	0.22	57,68,73,73	0
5	OXY	A	804	2/2	0.89	0.28	30,30,30,40	0
7	MPD	A	807	8/8	0.91	0.13	34,40,58,58	0
4	CL	A	803	1/1	0.92	0.12	39,39,39,39	0
6	PO4	A	805	5/5	0.94	0.07	40,44,63,64	0
6	PO4	B	805	5/5	0.94	0.08	40,50,51,63	0
5	OXY	B	804	2/2	0.94	0.21	28,28,28,36	0
2	HEM	A	801	43/43	0.99	0.04	14,16,19,20	0
4	CL	B	803	1/1	0.99	0.08	26,26,26,26	1
2	HEM	B	801	43/43	0.99	0.04	13,15,18,20	0
3	NA	A	802	1/1	0.99	0.04	18,18,18,18	0
3	NA	B	802	1/1	0.99	0.04	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)





6.5 Other polymers ⓘ

There are no such residues in this entry.