



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 05:20 PM EDT

PDB ID : 5SX1 / pdb_00005sx1
Title : Crystal structure of D141E variant of B. pseudomallei KatG
Authors : Loewen, P.C.
Deposited on : 2016-08-09
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

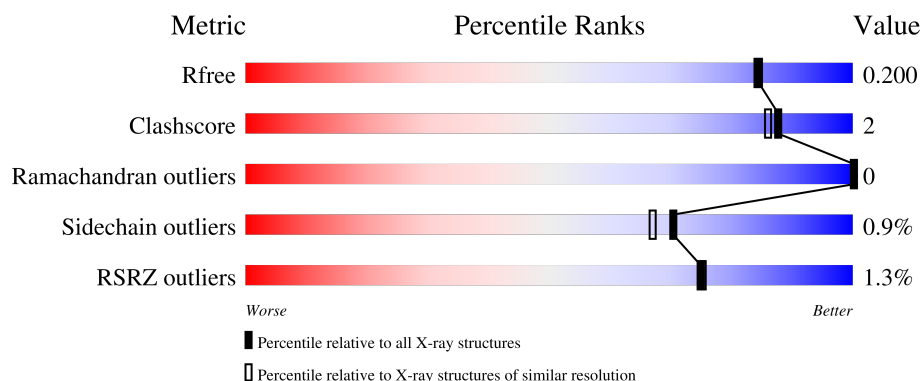
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

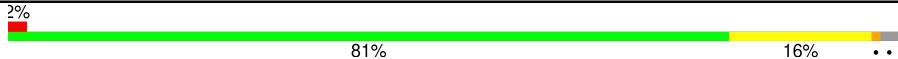
The reported resolution of this entry is 1.80 Å.

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	
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
5	MPD	B	805	-	X	-	-
6	PO4	A	807	-	X	-	-
6	PO4	B	806	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12789 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.

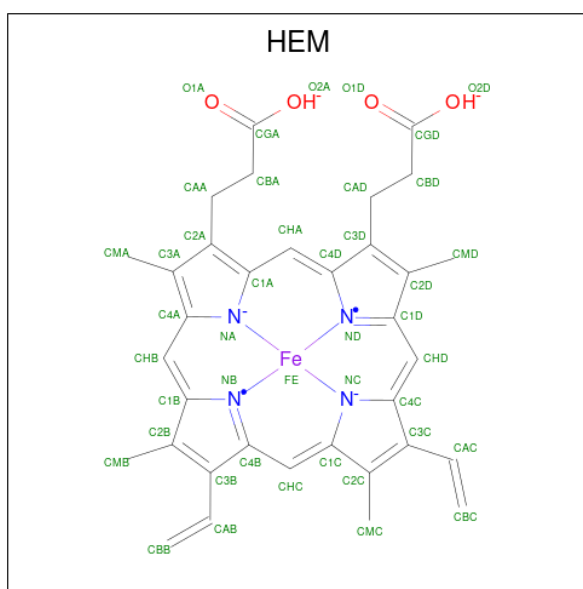
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	5	0
			5532	3497	985	1036	14			
1	B	713	Total	C	N	O	S	0	6	0
			5528	3491	983	1040	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	GLU	ASP	engineered mutation	UNP Q3JNW6
B	141	GLU	ASP	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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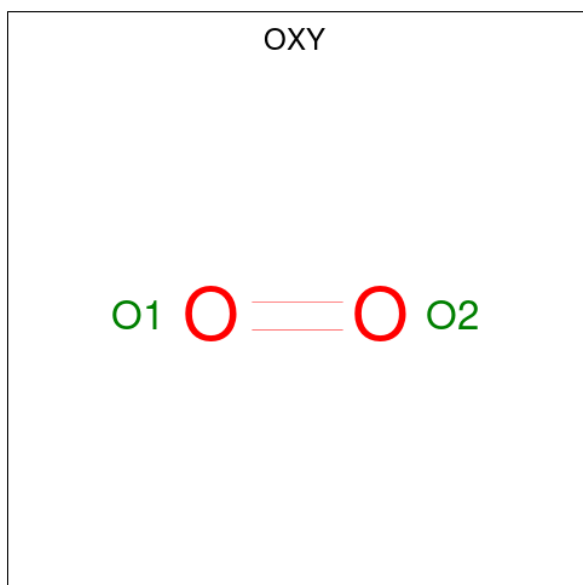
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

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

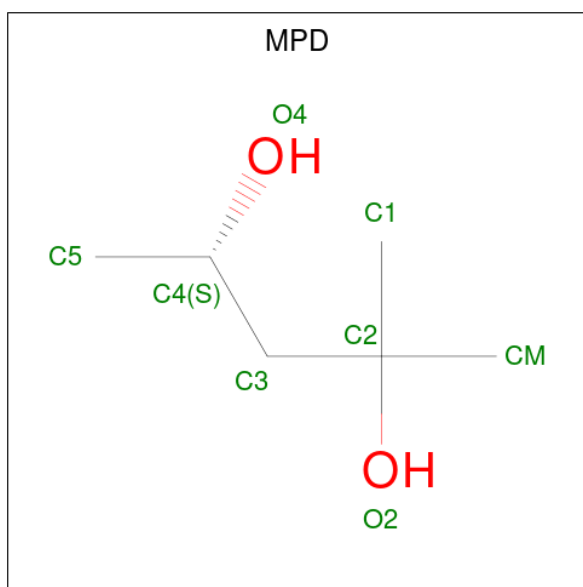
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na		
			1	1	0	0
3	B	1	Total	Na		
			1	1	0	0

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



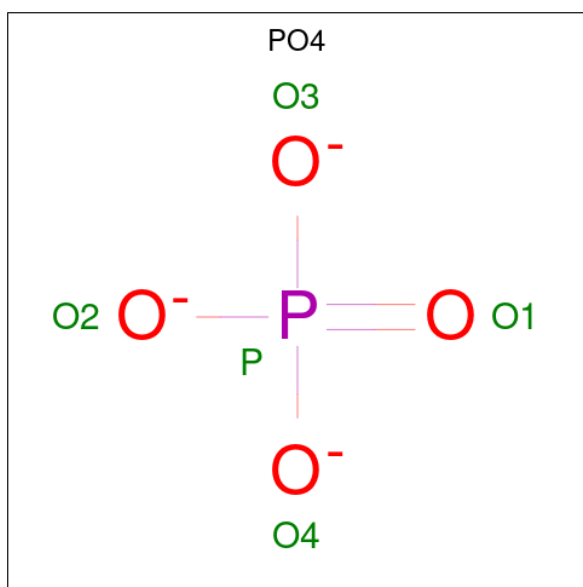
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O		
			2	2	0	0
4	A	1	Total	O		
			2	2	0	0
4	B	1	Total	O		
			2	2	0	0
4	B	1	Total	O		
			2	2	0	0
4	B	1	Total	O		
			2	2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

- 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		

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

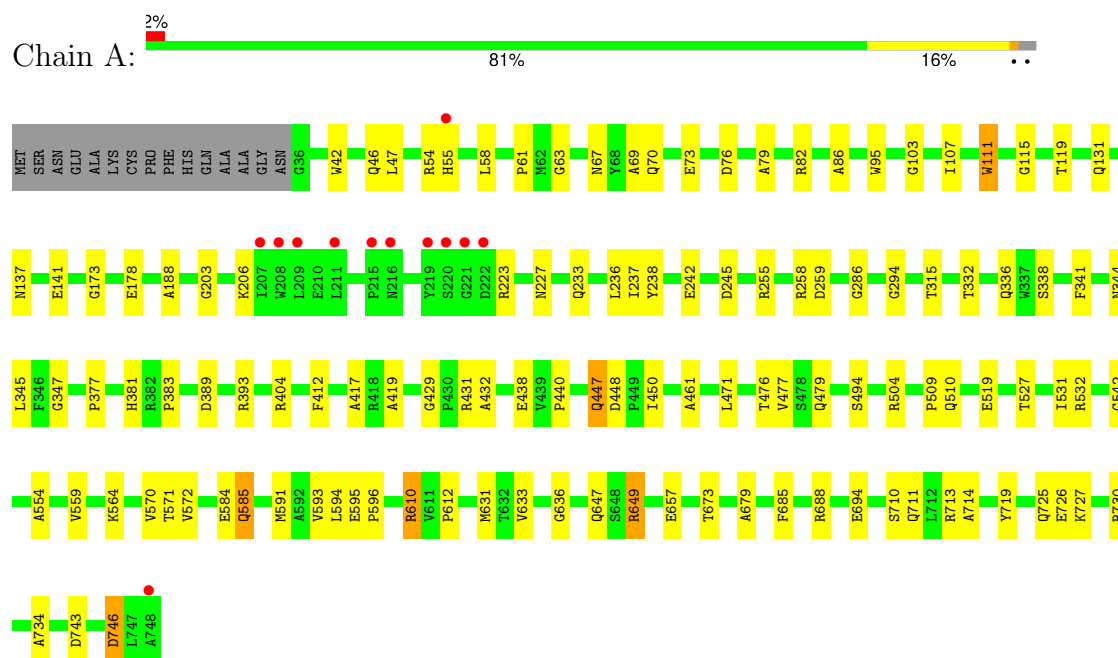
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	819	Total	O	0	0
			819	819		
7	B	778	Total	O	0	0
			778	778		

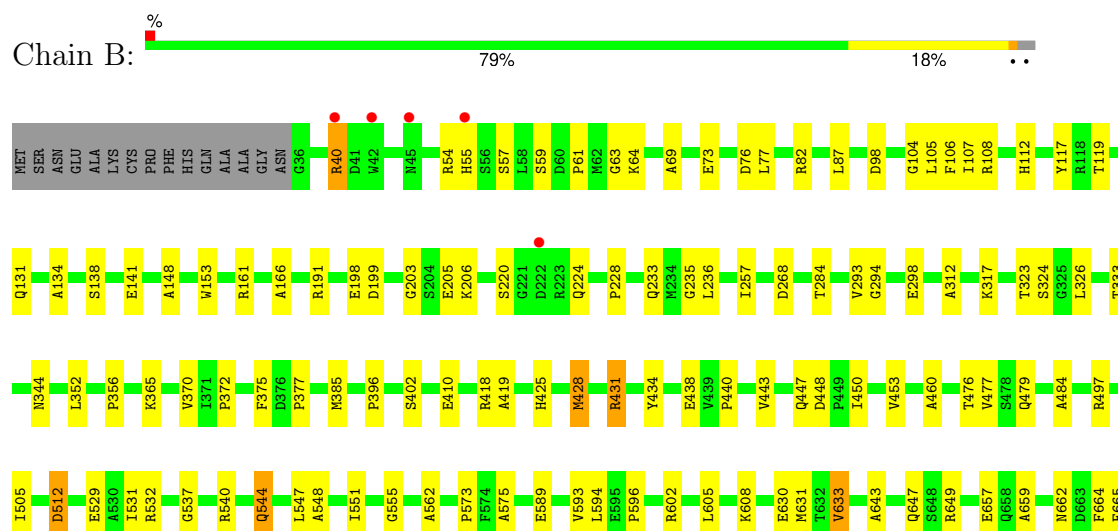
3 Residue-property plots [i](#)

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	100.74Å 116.20Å 175.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-1.80) 99.0 (20.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.155 , 0.191 0.167 , 0.200	Depositor DCC
R_{free} test set	9292 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12789	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: PO4, HEM, MPD, OXY, NA

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	1.97	100/5690 (1.8%)	1.42	21/7734 (0.3%)
1	B	1.96	106/5696 (1.9%)	1.43	30/7743 (0.4%)
All	All	1.97	206/11386 (1.8%)	1.43	51/15477 (0.3%)

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 (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	GLY	C-O	11.47	1.32	1.23
1	B	686	GLU	C-N	-11.45	1.27	1.33
1	B	294	GLY	C-O	10.43	1.34	1.23
1	A	532	ARG	CD-NE	-9.53	1.32	1.46
1	B	532	ARG	CD-NE	-9.35	1.33	1.46
1	A	344	ASN	C-O	8.39	1.34	1.24
1	B	575	ALA	CA-CB	-8.27	1.43	1.53
1	B	512	ASP	CG-OD2	8.22	1.41	1.25
1	A	725	GLN	CG-CD	8.19	1.72	1.52
1	A	688	ARG	CA-C	-8.13	1.43	1.52
1	B	460	ALA	CA-C	-8.03	1.42	1.52
1	B	233	GLN	N-CA	7.93	1.56	1.45
1	A	448	ASP	CA-CB	7.92	1.58	1.52
1	B	573	PRO	CA-C	7.89	1.62	1.52
1	B	697	TRP	CA-C	-7.88	1.42	1.52
1	A	294	GLY	C-O	7.71	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	529	GLU	CA-C	7.59	1.62	1.52
1	B	63	GLY	N-CA	7.57	1.55	1.45
1	B	643	ALA	N-CA	-7.50	1.36	1.46
1	B	544	GLN	CD-OE1	7.37	1.37	1.23
1	B	664	PHE	CA-C	7.24	1.62	1.52
1	B	532	ARG	NE-CZ	-7.18	1.25	1.33
1	A	315	THR	C-O	-7.17	1.14	1.24
1	A	714	ALA	C-O	7.16	1.32	1.24
1	B	82	ARG	CZ-NH2	-7.11	1.24	1.33
1	A	636	GLY	N-CA	7.07	1.54	1.45
1	B	730	ARG	CZ-NH1	7.03	1.42	1.32
1	A	76	ASP	CA-C	7.02	1.61	1.52
1	B	206	LYS	N-CA	7.02	1.54	1.46
1	B	203	GLY	C-O	6.97	1.29	1.23
1	B	746	ASP	C-O	-6.88	1.15	1.24
1	B	575	ALA	C-O	-6.88	1.18	1.25
1	A	336	GLN	CD-NE2	6.82	1.47	1.33
1	B	497	ARG	N-CA	6.76	1.54	1.45
1	B	738	LYS	N-CA	-6.75	1.38	1.46
1	B	476	THR	CA-C	6.71	1.62	1.53
1	B	370	VAL	N-CA	-6.70	1.39	1.46
1	B	54	ARG	CA-C	-6.67	1.44	1.53
1	A	476	THR	N-CA	-6.63	1.37	1.45
1	A	245	ASP	CG-OD1	6.60	1.37	1.25
1	B	402	SER	N-CA	-6.59	1.38	1.46
1	B	714	ALA	CA-C	6.57	1.61	1.52
1	A	673	THR	N-CA	-6.56	1.38	1.46
1	A	236	LEU	CA-C	6.56	1.61	1.52
1	A	532	ARG	NE-CZ	-6.53	1.25	1.33
1	A	725	GLN	N-CA	6.51	1.54	1.46
1	A	494	SER	CA-C	6.51	1.61	1.52
1	B	725	GLN	N-CA	6.49	1.54	1.46
1	A	95	TRP	N-CA	6.44	1.55	1.46
1	A	137	ASN	N-CA	-6.40	1.37	1.46
1	A	477	VAL	N-CA	6.39	1.53	1.46
1	B	453	VAL	C-O	-6.36	1.16	1.24
1	B	138	SER	N-CA	6.34	1.53	1.46
1	B	293	VAL	C-O	-6.34	1.17	1.24
1	B	98	ASP	C-O	6.33	1.31	1.23
1	B	425	HIS	CA-C	6.30	1.60	1.52
1	A	734	ALA	N-CA	-6.29	1.38	1.46
1	B	551	ILE	CA-C	6.26	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	602	ARG	CZ-NH2	-6.25	1.25	1.33
1	B	365	LYS	N-CA	6.25	1.54	1.46
1	A	726	GLU	CG-CD	6.24	1.67	1.52
1	A	612	PRO	CA-C	6.22	1.60	1.52
1	A	440	PRO	N-CA	-6.20	1.39	1.47
1	B	531	ILE	N-CA	6.19	1.53	1.46
1	B	59	SER	C-O	-6.19	1.16	1.24
1	A	531	ILE	N-CA	6.18	1.53	1.46
1	B	317	LYS	N-CA	6.17	1.53	1.46
1	B	537	GLY	C-O	-6.17	1.16	1.23
1	B	396	PRO	CA-CB	6.16	1.63	1.53
1	B	385	MET	C-O	6.14	1.31	1.23
1	A	432	ALA	N-CA	-6.13	1.38	1.46
1	A	61	PRO	N-CA	-6.12	1.39	1.47
1	A	447	GLN	CA-C	6.11	1.63	1.52
1	B	694	GLU	CA-C	6.11	1.60	1.52
1	A	685	PHE	N-CA	-6.09	1.38	1.46
1	A	237	ILE	C-O	6.08	1.29	1.24
1	B	352	LEU	CA-C	-6.07	1.44	1.52
1	B	326	LEU	C-O	6.06	1.31	1.23
1	B	431	ARG	N-CA	6.06	1.53	1.46
1	A	404	ARG	CA-C	6.04	1.60	1.52
1	A	203	GLY	N-CA	6.02	1.51	1.45
1	B	679	ALA	N-CA	6.02	1.53	1.46
1	A	338	SER	C-O	5.95	1.30	1.23
1	A	259	ASP	CA-C	5.95	1.60	1.52
1	A	341	PHE	CA-C	5.94	1.60	1.52
1	B	548	ALA	N-CA	5.93	1.53	1.46
1	A	173	GLY	CA-C	5.92	1.58	1.52
1	B	630	GLU	N-CA	5.91	1.53	1.46
1	A	286	GLY	N-CA	5.86	1.53	1.45
1	B	664	PHE	N-CA	-5.86	1.39	1.46
1	B	505	ILE	N-CA	-5.84	1.39	1.46
1	B	692	THR	N-CA	5.81	1.53	1.46
1	A	571	THR	CA-C	5.80	1.59	1.52
1	B	323	THR	N-CA	-5.79	1.41	1.46
1	A	79	ALA	CA-C	5.78	1.60	1.52
1	A	63	GLY	N-CA	5.77	1.52	1.45
1	B	657	GLU	CA-C	5.73	1.60	1.52
1	B	235	GLY	C-N	5.72	1.41	1.33
1	A	419	ALA	C-N	-5.69	1.26	1.33
1	A	178	GLU	CA-C	-5.69	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	GLN	C-O	5.68	1.30	1.24
1	B	333	THR	CA-CB	-5.68	1.46	1.53
1	A	730	ARG	N-CA	-5.67	1.39	1.46
1	A	393	ARG	CZ-NH2	5.65	1.40	1.33
1	A	494	SER	N-CA	-5.65	1.39	1.46
1	A	572	VAL	N-CA	-5.64	1.39	1.46
1	B	659	ALA	N-CA	-5.61	1.39	1.46
1	A	471	LEU	C-O	-5.58	1.17	1.24
1	A	103	GLY	N-CA	5.57	1.52	1.45
1	A	332	THR	N-CA	5.56	1.53	1.46
1	A	417	ALA	C-O	-5.55	1.17	1.24
1	A	479	GLN	C-N	-5.55	1.26	1.33
1	A	743	ASP	C-O	5.53	1.31	1.24
1	A	584	GLU	CG-CD	5.53	1.65	1.52
1	A	510	GLN	C-O	5.51	1.30	1.24
1	A	70	GLN	CG-CD	5.51	1.65	1.52
1	B	153	TRP	CA-CB	5.51	1.61	1.53
1	B	410	GLU	CG-CD	5.51	1.65	1.52
1	A	532	ARG	CZ-NH2	-5.49	1.26	1.33
1	B	134	ALA	CA-CB	-5.49	1.44	1.53
1	A	233	GLN	N-CA	5.49	1.52	1.45
1	A	223	ARG	CA-C	5.48	1.60	1.53
1	B	106	PHE	C-N	-5.47	1.27	1.33
1	B	372	PRO	CA-C	-5.47	1.45	1.52
1	B	55	HIS	C-O	-5.46	1.15	1.23
1	B	148	ALA	CA-C	-5.46	1.45	1.52
1	B	596	PRO	C-O	5.45	1.28	1.24
1	B	377	PRO	N-CA	5.43	1.54	1.47
1	B	375	PHE	CA-CB	-5.43	1.44	1.53
1	A	206	LYS	N-CA	5.42	1.53	1.46
1	A	554	ALA	N-CA	-5.42	1.39	1.46
1	B	220	SER	N-CA	5.42	1.52	1.45
1	B	419	ALA	CA-C	5.41	1.60	1.52
1	A	519	GLU	N-CA	5.39	1.52	1.46
1	B	205	GLU	N-CA	5.39	1.52	1.46
1	A	504	ARG	CZ-NH1	-5.38	1.25	1.32
1	B	665	PHE	C-N	-5.38	1.27	1.33
1	B	477	VAL	N-CA	5.35	1.52	1.46
1	B	605	LEU	C-O	-5.35	1.17	1.23
1	A	531	ILE	CA-CB	-5.34	1.48	1.54
1	A	542	GLY	C-O	-5.33	1.16	1.24
1	B	236	LEU	CA-C	5.33	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	324	SER	C-O	-5.32	1.17	1.24
1	A	649	ARG	CZ-NH1	5.31	1.40	1.32
1	A	694	GLU	CA-C	5.31	1.59	1.52
1	B	531	ILE	CA-C	-5.31	1.46	1.52
1	A	461	ALA	CA-C	5.31	1.59	1.52
1	A	82	ARG	CZ-NH2	-5.30	1.26	1.33
1	A	258	ARG	N-CA	-5.29	1.40	1.46
1	B	191	ARG	C-O	-5.29	1.17	1.23
1	A	341	PHE	N-CA	-5.28	1.40	1.46
1	A	347	GLY	N-CA	5.28	1.52	1.45
1	B	734	ALA	N-CA	-5.28	1.40	1.46
1	B	55	HIS	CA-CB	5.28	1.61	1.53
1	B	105	LEU	CA-C	5.27	1.59	1.52
1	A	383	PRO	C-O	5.27	1.30	1.23
1	B	443	VAL	CA-C	-5.27	1.46	1.52
1	B	257	ILE	N-CA	-5.26	1.40	1.46
1	A	746	ASP	C-O	-5.26	1.17	1.24
1	A	42	TRP	CA-C	5.25	1.59	1.52
1	B	344	ASN	C-O	5.25	1.30	1.24
1	A	115	GLY	CA-C	5.25	1.60	1.51
1	B	448	ASP	N-CA	5.23	1.50	1.46
1	B	284	THR	C-N	-5.23	1.26	1.33
1	B	594	LEU	N-CA	-5.22	1.39	1.46
1	B	418	ARG	CZ-NH1	-5.21	1.25	1.32
1	A	381	HIS	CA-C	-5.21	1.46	1.52
1	A	58	LEU	N-CA	5.21	1.52	1.46
1	B	448	ASP	CA-C	-5.20	1.49	1.53
1	A	438	GLU	CD-OE2	5.19	1.35	1.25
1	A	141	GLU	CG-CD	5.19	1.65	1.52
1	A	188	ALA	CA-CB	-5.17	1.44	1.53
1	B	555	GLY	N-CA	5.17	1.52	1.45
1	A	559	VAL	N-CA	5.17	1.52	1.46
1	B	161	ARG	NE-CZ	5.14	1.38	1.33
1	A	594	LEU	N-CA	-5.14	1.39	1.46
1	A	679	ALA	N-CA	5.14	1.52	1.46
1	B	268	ASP	C-O	5.14	1.30	1.24
1	A	242	GLU	N-CA	5.13	1.52	1.46
1	A	377	PRO	C-O	-5.13	1.17	1.24
1	A	570	VAL	N-CA	5.11	1.51	1.46
1	B	428[A]	MET	CA-CB	5.10	1.62	1.53
1	B	428[B]	MET	CA-CB	5.10	1.62	1.53
1	B	547	LEU	CA-C	5.09	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	440	PRO	N-CA	-5.09	1.41	1.47
1	B	484	ALA	CA-C	5.09	1.59	1.52
1	B	104	GLY	C-N	5.08	1.40	1.33
1	A	67	ASN	CG-ND2	-5.07	1.22	1.33
1	B	312	ALA	N-CA	5.07	1.52	1.46
1	B	375	PHE	CA-C	5.07	1.59	1.52
1	A	345	LEU	CA-C	5.07	1.59	1.52
1	B	726	GLU	CG-CD	5.06	1.64	1.52
1	A	527	THR	N-CA	-5.05	1.40	1.46
1	A	595	GLU	C-O	-5.05	1.17	1.24
1	A	79	ALA	CA-CB	-5.05	1.45	1.53
1	A	657	GLU	CA-C	5.05	1.59	1.52
1	A	727	LYS	C-N	-5.05	1.27	1.33
1	B	562	ALA	N-CA	-5.05	1.39	1.46
1	A	141	GLU	CD-OE1	5.04	1.34	1.25
1	B	166	ALA	N-CA	5.04	1.52	1.46
1	B	107	ILE	CA-CB	-5.04	1.48	1.54
1	A	477	VAL	C-O	5.03	1.29	1.24
1	B	356	PRO	C-O	-5.03	1.17	1.24
1	A	107	ILE	N-CA	5.01	1.52	1.46
1	A	585[A]	GLN	C-O	-5.01	1.17	1.24
1	A	585[B]	GLN	C-O	-5.01	1.17	1.24

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH2	-14.81	105.87	119.20
1	B	532	ARG	NE-CZ-NH2	-12.37	108.07	119.20
1	A	532	ARG	NE-CZ-NH1	7.88	129.38	121.50
1	B	532	ARG	CD-NE-CZ	7.59	135.02	124.40
1	A	532	ARG	CD-NE-CZ	7.39	134.75	124.40
1	A	450	ILE	CB-CA-C	-7.35	103.00	110.13
1	B	460	ALA	N-CA-C	7.12	119.04	111.28
1	B	532	ARG	NE-CZ-NH1	6.93	128.43	121.50
1	B	631	MET	N-CA-C	-6.46	104.16	111.07
1	B	633	VAL	CG1-CB-CG2	-6.33	96.87	110.80
1	A	86	ALA	N-CA-C	6.25	118.10	111.28
1	A	727	LYS	N-CA-C	6.20	118.04	111.28
1	B	153	TRP	CA-C-N	-6.10	112.20	118.85
1	B	153	TRP	C-N-CA	-6.10	112.20	118.85
1	A	710	SER	N-CA-C	6.06	118.85	111.82
1	B	77	LEU	N-CA-C	-5.80	105.09	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	CG-CD-NE	-5.66	99.56	112.00
1	B	87	LEU	N-CA-C	5.66	117.44	111.28
1	B	450	ILE	CA-CB-CG1	-5.62	100.85	110.40
1	A	389	ASP	N-CA-C	-5.61	105.08	111.14
1	B	61	PRO	N-CA-C	-5.60	106.40	114.18
1	A	479	GLN	N-CA-C	5.59	117.38	111.28
1	A	412	PHE	CA-CB-CG	5.55	119.35	113.80
1	B	57	SER	N-CA-C	-5.54	105.78	112.54
1	B	676	LYS	N-CA-C	5.54	117.20	108.23
1	A	429	GLY	O-C-N	5.53	127.30	121.77
1	B	532	ARG	CG-CD-NE	-5.52	99.86	112.00
1	B	713	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	A	54	ARG	CB-CA-C	-5.46	99.11	110.40
1	A	55	HIS	CB-CA-C	5.39	119.75	111.39
1	A	47	LEU	N-CA-CB	-5.37	102.07	109.97
1	A	131	GLN	N-CA-C	-5.36	106.00	112.54
1	A	631	MET	N-CA-C	-5.33	105.47	111.28
1	B	664	PHE	N-CA-C	-5.33	105.47	111.28
1	B	54	ARG	CA-C-N	-5.33	115.07	122.74
1	B	54	ARG	C-N-CA	-5.33	115.07	122.74
1	B	370	VAL	N-CA-C	5.30	119.21	113.43
1	B	450	ILE	CA-C-O	-5.28	116.24	119.51
1	A	596	PRO	CB-CA-C	5.25	116.28	111.87
1	B	112	HIS	N-CA-C	5.21	117.87	111.82
1	B	690	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	713	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	B	131	GLN	N-CA-C	-5.17	106.23	112.54
1	B	108	ARG	NE-CZ-NH1	5.16	126.66	121.50
1	B	333	THR	O-C-N	5.13	125.53	121.17
1	B	198	GLU	CG-CD-OE1	5.13	130.20	118.40
1	A	610	ARG	CB-CA-C	-5.11	102.17	110.85
1	A	450	ILE	CA-C-O	-5.07	116.36	119.51
1	B	40	ARG	CA-CB-CG	5.06	124.22	114.10
1	B	479	GLN	N-CA-C	5.06	116.79	111.28
1	B	438	GLU	N-CA-C	5.04	118.75	112.59

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	117	TYR	Sidechain
1	B	199	ASP	Mainchain

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	5532	0	5363	15	0
1	B	5528	0	5339	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	4	0	0	0	0
4	B	6	0	0	1	0
5	A	16	0	28	3	0
5	B	8	0	14	4	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	819	0	0	8	1
7	B	778	0	0	11	1
All	All	12789	0	10804	43	1

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 (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:NH2	7:A:903:HOH:O	2.05	0.89
1:B:119:THR:HG21	7:B:1017:HOH:O	1.74	0.85
1:B:76:ASP:OD2	7:B:901:HOH:O	2.02	0.77
1:A:119:THR:HG21	7:A:1101:HOH:O	1.89	0.71
1:B:512:ASP:OD1	7:B:902:HOH:O	2.14	0.64
1:A:647:GLN:HG2	7:A:1488:HOH:O	1.98	0.64
1:B:141:GLU:OE2	4:B:807:OXY:O1	2.18	0.60
1:B:76:ASP:OD1	7:B:903:HOH:O	2.17	0.60
5:B:805:MPD:CM	5:B:805:MPD:H52	2.31	0.60
5:A:805:MPD:CM	5:A:805:MPD:O4	2.51	0.59
1:B:662:ASN:H	1:B:725:GLN:HE22	1.53	0.55
1:B:540:ARG:NE	1:B:540:ARG:HA	2.23	0.54
1:B:512:ASP:HB2	7:B:1396:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ALA:O	1:A:73:GLU:HG3	2.08	0.53
1:A:711:GLN:OE1	7:A:905:HOH:O	2.18	0.51
1:B:647:GLN:HG2	7:B:1138:HOH:O	2.12	0.50
5:B:805:MPD:H52	5:B:805:MPD:HM1	1.94	0.50
1:B:431:ARG:CD	7:B:1497:HOH:O	2.59	0.50
1:B:633:VAL:CG2	1:B:719:TYR:CZ	2.95	0.50
1:A:119:THR:HG23	1:A:593:VAL:HG11	1.94	0.49
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.96	0.49
1:A:746:ASP:HB3	7:A:1531:HOH:O	2.12	0.49
1:A:111:TRP:HZ3	1:A:238:TYR:HH	1.57	0.48
1:A:564:LYS:HE2	7:A:1478:HOH:O	2.13	0.48
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.14	0.48
5:A:806:MPD:H53	5:A:806:MPD:H11	1.97	0.47
1:B:730:ARG:HD2	7:B:1495:HOH:O	2.15	0.46
1:B:69:ALA:O	1:B:73:GLU:HG2	2.16	0.45
1:B:709:HIS:CE1	1:B:711[B]:GLN:HB2	2.51	0.45
1:A:585[A]:GLN:NE2	7:A:931:HOH:O	2.50	0.45
1:A:509:PRO:HD2	1:A:591:MET:HG2	2.00	0.43
1:B:428[B]:MET:HE2	1:B:434:TYR:CD1	2.53	0.43
1:B:589:GLU:HG2	7:B:944:HOH:O	2.18	0.43
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.18	0.42
1:B:725:GLN:NE2	7:B:931:HOH:O	2.53	0.42
1:B:119:THR:HG23	1:B:593:VAL:HG11	2.01	0.42
1:B:540:ARG:NE	1:B:540:ARG:CA	2.82	0.42
1:A:46:GLN:NE2	1:B:298:GLU:O	2.53	0.41
5:A:806:MPD:HM2	7:A:1025:HOH:O	2.18	0.41
1:B:431:ARG:HD2	7:B:1497:HOH:O	2.21	0.41
1:A:633[A]:VAL:HG22	1:A:719:TYR:CZ	2.55	0.41
5:B:805:MPD:H52	5:B:805:MPD:HM2	2.02	0.41
5:B:805:MPD:CM	5:B:805:MPD:C5	2.97	0.40

All (1) 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)
7:A:1321:HOH:O	7:B:1069:HOH:O[2_444]	2.11	0.09

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	716/728 (98%)	710 (99%)	6 (1%)	0	100	100
1	B	717/728 (98%)	708 (99%)	9 (1%)	0	100	100
All	All	1433/1456 (98%)	1418 (99%)	15 (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	555/561 (99%)	551 (99%)	4 (1%)	76	73
1	B	556/561 (99%)	550 (99%)	6 (1%)	65	60
All	All	1111/1122 (99%)	1101 (99%)	10 (1%)	70	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	TRP
1	A	227	ASN
1	A	610	ARG
1	A	649	ARG
1	B	40	ARG
1	B	64	LYS
1	B	228	PRO
1	B	544	GLN

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

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	46	GLN
1	A	247	ASN
1	A	339	HIS
1	A	539	GLN
1	A	711	GLN
1	B	520	GLN
1	B	650	HIS
1	B	725	GLN
1	B	737	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OXY	B	803	-	1,1,1	0.34	0	-		
5	MPD	A	805	-	7,7,7	0.66	0	9,10,10	1.66	3 (33%)
2	HEM	B	801	1,4	50,50,50	1.65	12 (24%)	67,82,82	1.66	16 (23%)
6	PO4	A	807	-	4,4,4	2.15	1 (25%)	6,6,6	1.96	4 (66%)
6	PO4	B	806	-	4,4,4	1.89	2 (50%)	6,6,6	2.01	2 (33%)
4	OXY	A	803	-	1,1,1	0.11	0	-		
4	OXY	B	804	2	1,1,1	0.18	0	-		
4	OXY	B	807	-	1,1,1	0.57	0	-		
4	OXY	A	804	-	1,1,1	0.45	0	-		
2	HEM	A	801	1	50,50,50	1.79	13 (26%)	67,82,82	1.39	11 (16%)
5	MPD	B	805	-	7,7,7	1.04	1 (14%)	9,10,10	2.89	4 (44%)
5	MPD	A	806	-	7,7,7	0.99	0	9,10,10	2.12	3 (33%)

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
5	MPD	A	805	-	-	2/5/5/5	-
2	HEM	B	801	1,4	-	3/14/54/54	-
5	MPD	B	805	-	-	4/5/5/5	-
2	HEM	A	801	1	-	3/14/54/54	-
5	MPD	A	806	-	-	3/5/5/5	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1B-NB	-4.87	1.31	1.40
2	A	801	HEM	C1C-NC	-4.36	1.31	1.39
2	B	801	HEM	C1C-NC	-4.13	1.31	1.39
2	A	801	HEM	C1B-NB	-3.57	1.34	1.40
6	A	807	PO4	P-O4	-3.49	1.44	1.54
2	A	801	HEM	FE-NB	3.44	2.05	1.94
2	A	801	HEM	O1A-CGA	3.28	1.32	1.22
2	A	801	HEM	CBD-CGD	-3.10	1.43	1.50
2	A	801	HEM	C1A-NA	3.07	1.45	1.39
2	A	801	HEM	FE-NA	3.04	2.05	1.95
2	B	801	HEM	CHC-C1C	-2.95	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	806	PO4	P-O3	-2.94	1.46	1.54
2	A	801	HEM	FE-NC	2.70	2.04	1.95
2	A	801	HEM	O1D-CGD	2.69	1.30	1.22
2	B	801	HEM	CHB-C1B	2.65	1.43	1.38
2	A	801	HEM	CAD-C3D	-2.57	1.44	1.51
2	A	801	HEM	C4D-ND	2.55	1.44	1.40
2	B	801	HEM	FE-NA	2.44	2.03	1.95
2	B	801	HEM	C3B-C4B	2.42	1.49	1.44
2	A	801	HEM	CBC-CAC	2.41	1.41	1.30
2	B	801	HEM	CHD-C4C	2.32	1.42	1.38
6	B	806	PO4	P-O2	-2.26	1.48	1.54
2	B	801	HEM	CMD-C2D	-2.22	1.46	1.50
2	B	801	HEM	FE-NB	2.21	2.01	1.94
2	B	801	HEM	O1A-CGA	2.21	1.29	1.22
5	B	805	MPD	C3-C2	-2.20	1.47	1.54
2	A	801	HEM	C3B-C2B	2.18	1.41	1.37
2	B	801	HEM	C4A-NA	-2.16	1.35	1.39
2	B	801	HEM	O1D-CGD	2.15	1.29	1.22

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	805	MPD	O4-C4-C3	-6.03	87.36	111.35
2	B	801	HEM	C2B-C1B-NB	5.16	115.77	109.84
5	B	805	MPD	O2-C2-C3	-4.81	91.29	109.27
5	A	806	MPD	O4-C4-C3	-4.18	94.73	111.35
2	A	801	HEM	CAA-CBA-CGA	-3.70	103.86	113.67
6	B	806	PO4	O4-P-O1	-3.34	99.15	110.95
5	A	806	MPD	CM-C2-C1	-3.16	103.55	110.63
2	B	801	HEM	CAA-CBA-CGA	-3.09	105.48	113.67
2	B	801	HEM	CHD-C4C-NC	2.99	127.71	124.45
2	A	801	HEM	C3C-C2C-C1C	-2.99	104.22	107.05
2	B	801	HEM	C3B-C2B-C1B	-2.87	104.26	106.41
6	B	806	PO4	O3-P-O2	2.80	116.62	107.91
2	A	801	HEM	O2A-CGA-CBA	2.78	122.80	114.00
2	B	801	HEM	C2D-C1D-ND	2.74	113.07	109.90
2	B	801	HEM	C1A-C2A-C3A	-2.73	102.64	106.87
2	A	801	HEM	C4B-C3B-C2B	-2.63	104.86	107.28
5	B	805	MPD	CM-C2-C1	2.62	116.50	110.63
5	A	806	MPD	C5-C4-C3	2.59	123.69	111.67
2	B	801	HEM	O2D-CGD-O1D	-2.57	116.73	123.33
2	A	801	HEM	C1B-NB-C4B	2.54	108.21	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CAD-C3D-C4D	2.52	129.09	124.70
2	A	801	HEM	CBD-CAD-C3D	2.49	119.41	112.53
6	A	807	PO4	O4-P-O1	2.46	119.64	110.95
6	A	807	PO4	O3-P-O1	-2.44	102.33	110.95
5	A	805	MPD	O2-C2-C1	2.37	115.38	107.99
2	A	801	HEM	CMB-C2B-C1B	2.37	128.74	125.03
5	A	805	MPD	CM-C2-C1	-2.36	105.34	110.63
2	B	801	HEM	CAD-C3D-C2D	-2.36	123.45	127.87
2	A	801	HEM	O1D-CGD-CBD	-2.35	115.62	123.09
2	B	801	HEM	CHB-C4A-NA	2.33	128.09	123.86
2	B	801	HEM	C1D-C2D-C3D	-2.33	104.53	106.98
2	B	801	HEM	CMA-C3A-C4A	2.33	128.96	125.42
6	A	807	PO4	O4-P-O2	-2.31	100.72	107.91
5	B	805	MPD	O4-C4-C5	2.30	119.34	109.45
2	B	801	HEM	O2D-CGD-CBD	2.28	121.19	114.00
2	A	801	HEM	CHB-C4A-NA	-2.25	119.77	123.86
2	B	801	HEM	CHB-C4A-C3A	-2.25	120.89	127.43
2	A	801	HEM	O1A-CGA-CBA	-2.21	116.07	123.09
2	B	801	HEM	O1A-CGA-CBA	-2.11	116.41	123.09
2	B	801	HEM	C4C-CHD-C1D	-2.10	121.57	126.02
5	A	805	MPD	CM-C2-C3	2.09	119.19	110.20
2	A	801	HEM	CMA-C3A-C2A	2.08	130.04	125.62
6	A	807	PO4	O2-P-O1	2.02	118.11	110.95

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

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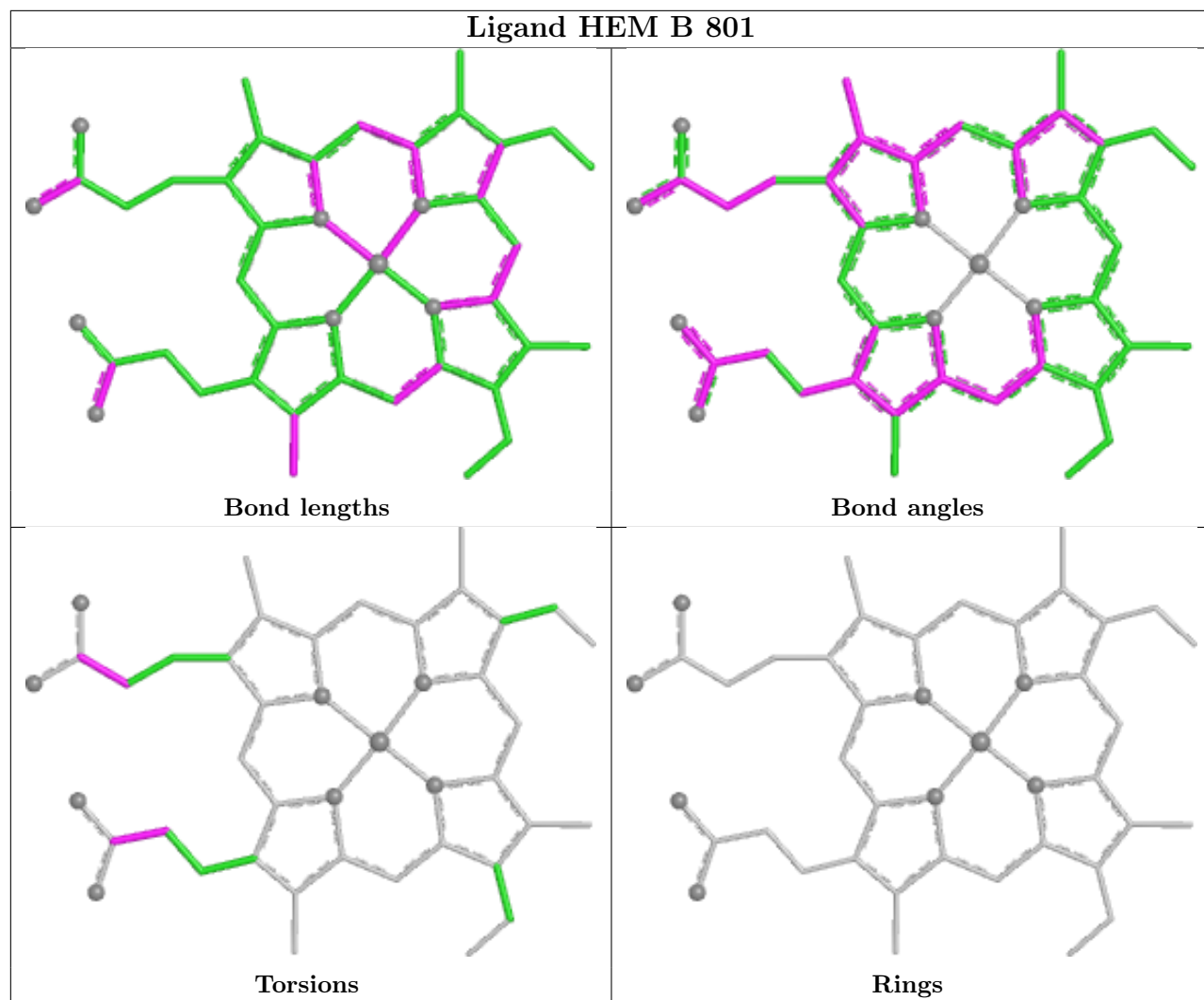
Mol	Chain	Res	Type	Atoms
2	B	801	HEM	CAD-CBD-CGD-O2D

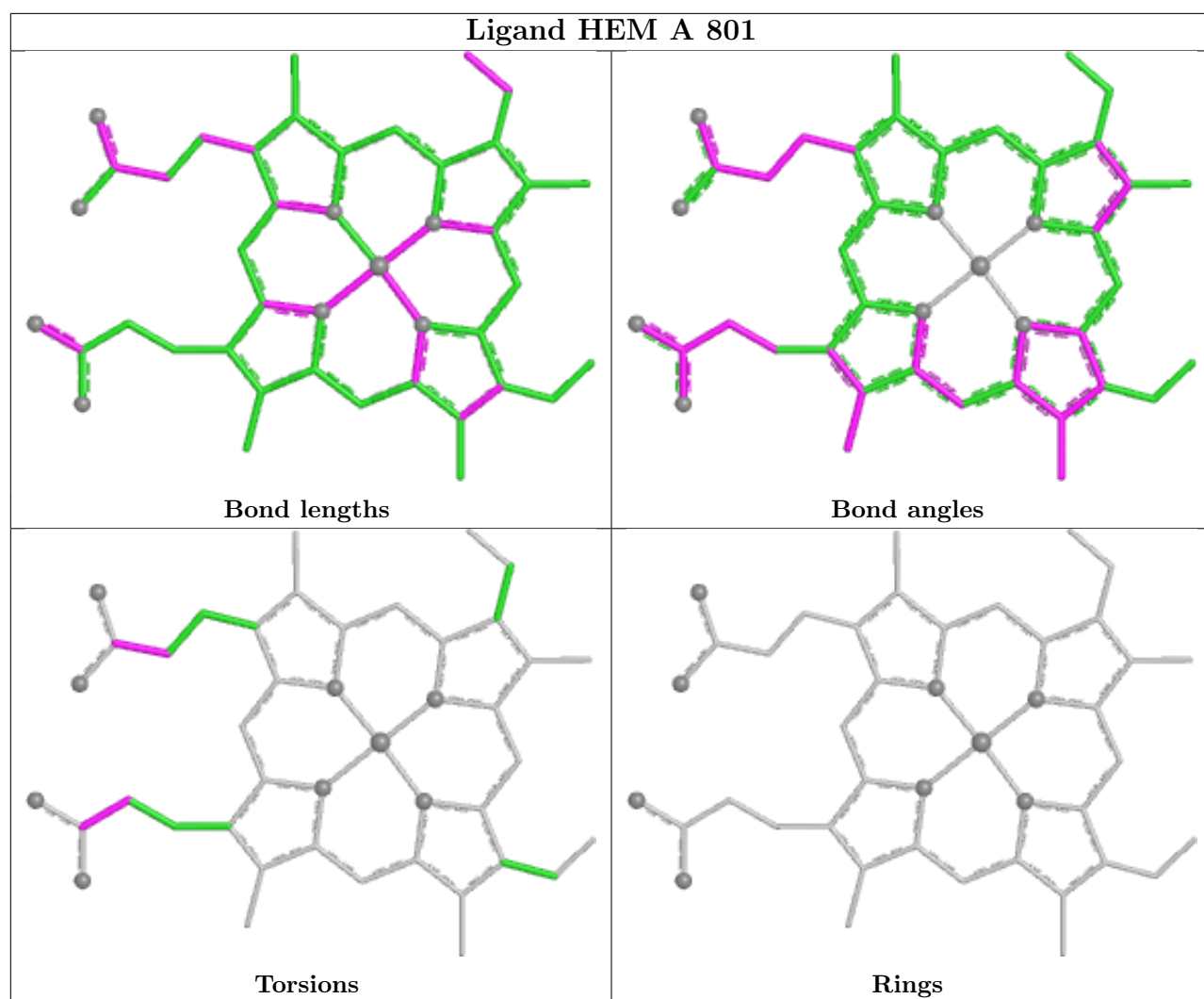
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	805	MPD	1	0
4	B	807	OXY	1	0
5	B	805	MPD	4	0
5	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	713/728 (97%)	-0.40	12 (1%) 69 69	8, 19, 44, 78	5 (0%)
1	B	713/728 (97%)	-0.49	6 (0%) 82 83	10, 18, 39, 87	6 (0%)
All	All	1426/1456 (97%)	-0.44	18 (1%) 75 75	8, 19, 40, 87	11 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	6.5
1	A	748	ALA	4.0
1	A	211	LEU	3.4
1	B	55	HIS	3.1
1	A	219	TYR	2.9
1	A	221	GLY	2.9
1	B	40	ARG	2.8
1	A	208	TRP	2.6
1	A	220	SER	2.6
1	B	222	ASP	2.6
1	A	215	PRO	2.5
1	A	216	ASN	2.4
1	B	42	TRP	2.4
1	A	222	ASP	2.3
1	A	55	HIS	2.2
1	A	207	ILE	2.2
1	A	209	LEU	2.1
1	B	45[A]	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

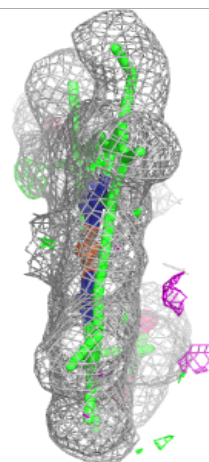
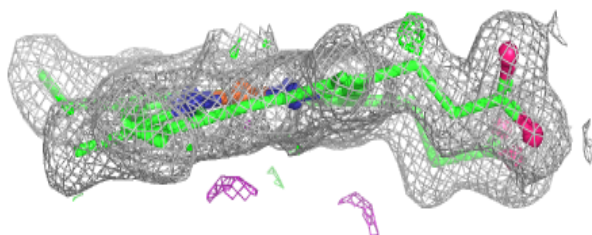
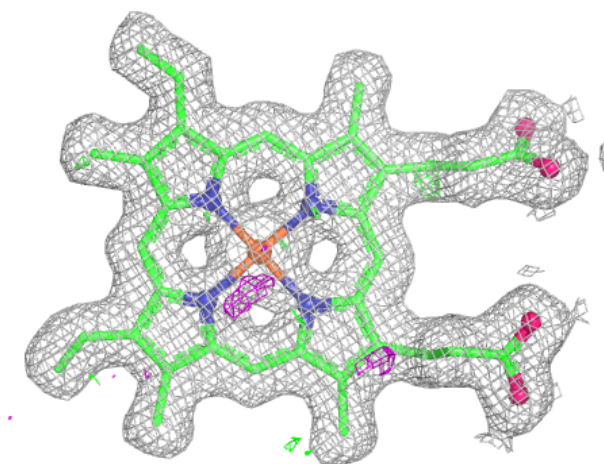
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MPD	A	805	8/8	0.80	0.20	52,62,73,74	0
5	MPD	B	805	8/8	0.80	0.20	53,59,65,66	0
4	OXY	A	804	2/2	0.84	0.18	33,33,33,44	0
5	MPD	A	806	8/8	0.86	0.14	33,38,50,53	0
4	OXY	B	804	2/2	0.87	0.21	39,39,39,50	0
4	OXY	B	807	2/2	0.89	0.18	30,30,30,38	0
6	PO4	B	806	5/5	0.92	0.09	42,48,49,61	0
4	OXY	A	803	2/2	0.94	0.25	35,35,35,44	0
6	PO4	A	807	5/5	0.95	0.07	41,51,56,62	0
4	OXY	B	803	2/2	0.96	0.18	25,25,25,41	0
3	NA	A	802	1/1	0.99	0.05	17,17,17,17	0
3	NA	B	802	1/1	0.99	0.04	15,15,15,15	0
2	HEM	A	801	43/43	0.99	0.04	12,14,19,19	0
2	HEM	B	801	43/43	0.99	0.04	11,13,15,18	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.

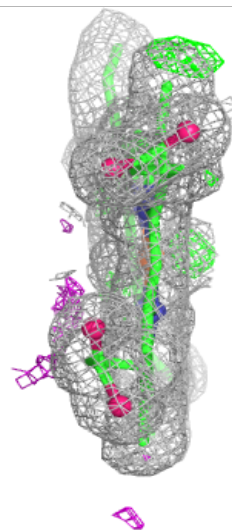
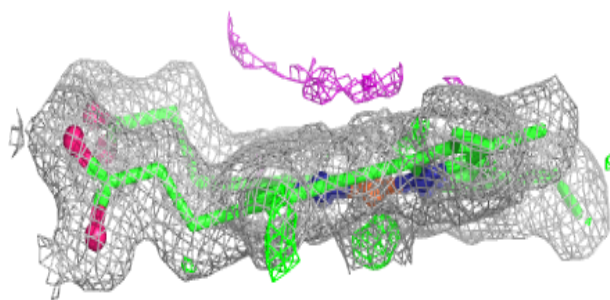
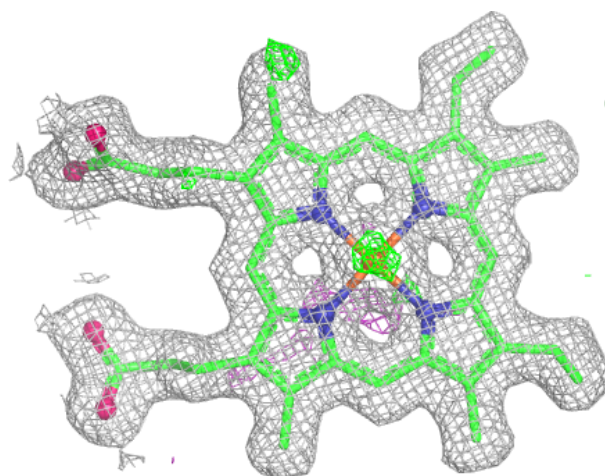
Electron density around HEM A 801:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.