



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:40 PM UTC

PDB ID : 5KSN / pdb_00005ksn
Title : Crystal structure of the S324G variant of catalase-peroxidase from *B. pseudo-mallei* with INH bound
Authors : Loewen, P.C.
Deposited on : 2016-07-08
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

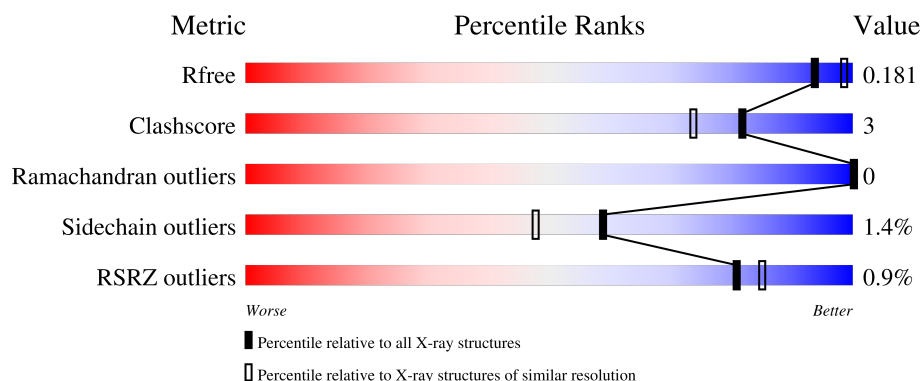
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	% 88% 9% ..
1	B	728	% 86% 10% ..

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	A	806	-	X	-	-
8	NIZ	A	809	-	X	-	-
8	NIZ	B	809	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12903 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	7	0
			5555	3508	989	1044	14			
1	B	713	Total	C	N	O	S	0	10	0
			5581	3523	994	1050	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	GLY	SER	engineered mutation	UNP Q3JNW6
B	324	GLY	SER	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	A	1	Total	O		
			2	2	0	0

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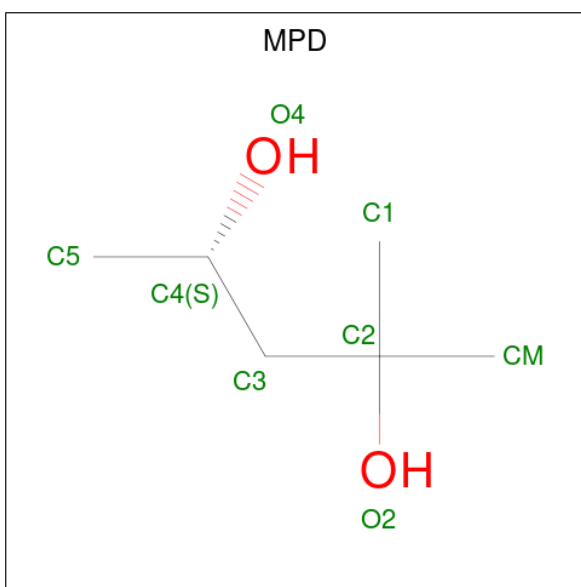
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			2	2		
5	B	1	Total	O	0	0
			2	2		

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



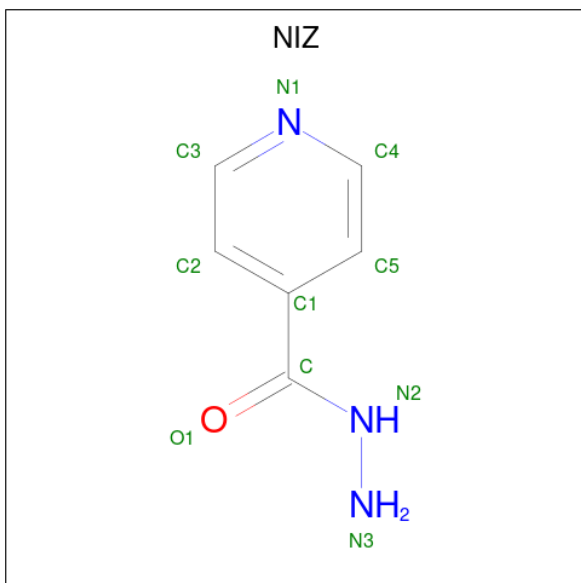
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

- 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		
7	A	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is pyridine-4-carbohydrazide (CCD ID: NIZ) (formula: $C_6H_7N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			10	6	3	1		
8	B	1	Total	C	N	O	0	0
			10	6	3	1		

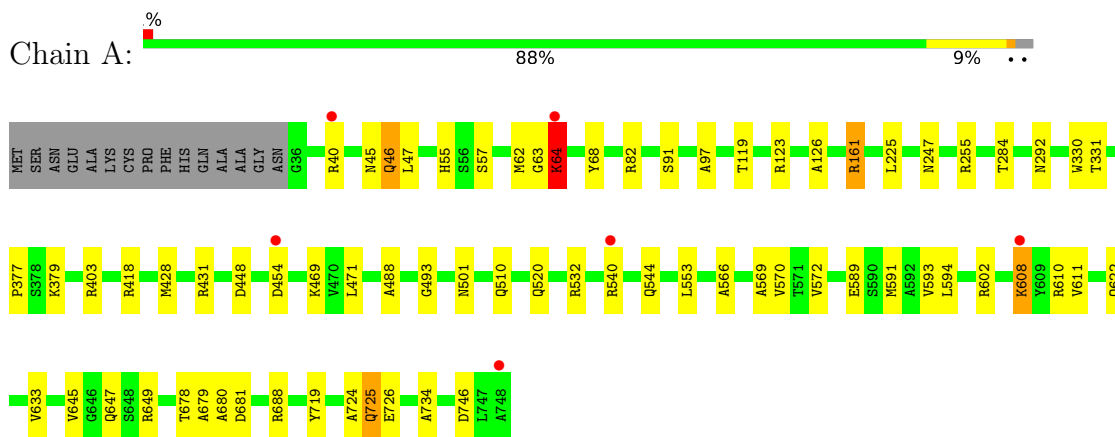
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	786	Total	O	0	0
			786	786		
9	B	821	Total	O	0	0
			821	821		

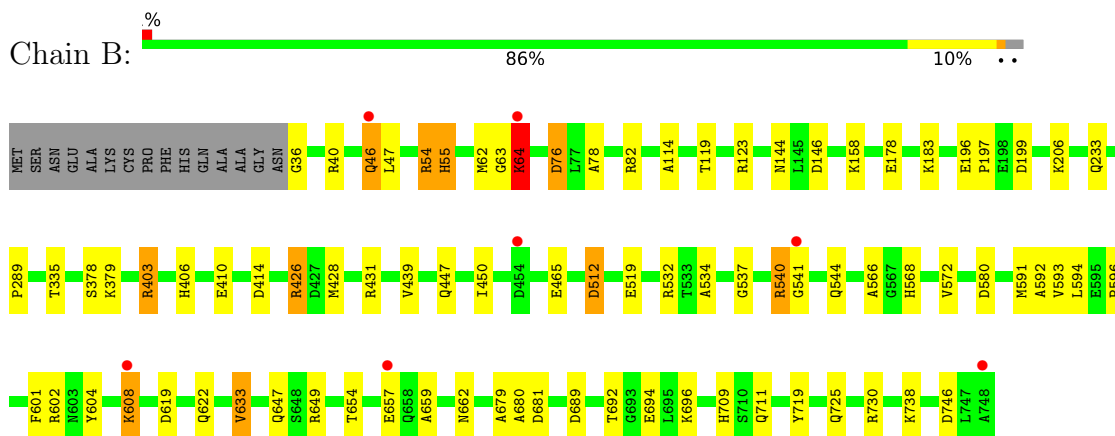
3 Residue-property plots [i](#)

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	100.43Å 115.28Å 174.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 1.87 48.05 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.05-1.87) 98.6 (48.05-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.141 , 0.171 0.154 , 0.181	Depositor DCC
R_{free} test set	8235 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12903	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.63	43/5706 (0.8%)	1.24	17/7757 (0.2%)
1	B	1.64	53/5735 (0.9%)	1.22	11/7795 (0.1%)
All	All	1.63	96/11441 (0.8%)	1.23	28/15552 (0.2%)

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	512	ASP	CG-OD2	8.89	1.42	1.25
1	B	426	ARG	CZ-NH2	8.71	1.44	1.33
1	B	199	ASP	C-O	7.83	1.33	1.23
1	B	746	ASP	C-O	-7.75	1.14	1.24
1	B	47	LEU	C-O	-7.58	1.14	1.23
1	B	532	ARG	CD-NE	-7.51	1.35	1.46
1	A	540	ARG	C-O	7.38	1.33	1.23
1	A	45	ASN	C-O	-7.31	1.14	1.24
1	B	47	LEU	CB-CG	-7.02	1.39	1.53
1	B	679	ALA	N-CA	6.91	1.54	1.46
1	B	540	ARG	C-O	6.90	1.32	1.23
1	A	47	LEU	CB-CG	-6.75	1.40	1.53
1	A	161	ARG	NE-CZ	6.73	1.40	1.33
1	A	688	ARG	CZ-NH2	-6.65	1.24	1.33
1	B	532	ARG	CZ-NH1	-6.65	1.23	1.32
1	B	63	GLY	N-CA	6.59	1.54	1.45
1	A	63	GLY	N-CA	6.56	1.53	1.45
1	A	431	ARG	CA-CB	6.48	1.64	1.53
1	B	659	ALA	CA-C	6.39	1.60	1.52
1	B	403	ARG	CA-C	-6.38	1.44	1.52
1	B	604	TYR	N-CA	-6.33	1.38	1.46
1	A	247	ASN	CG-ND2	-6.31	1.20	1.33
1	A	471	LEU	CA-C	6.29	1.61	1.52
1	A	428	MET	CG-SD	-6.28	1.65	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	589	GLU	C-O	-6.27	1.16	1.24
1	B	62	MET	N-CA	-6.27	1.37	1.45
1	A	64	LYS	C-O	-6.16	1.16	1.24
1	B	694	GLU	CA-C	6.11	1.60	1.52
1	B	692	THR	C-O	-6.08	1.16	1.24
1	A	46	GLN	CG-CD	6.06	1.67	1.52
1	A	97	ALA	C-O	6.05	1.31	1.23
1	A	746	ASP	C-O	-6.03	1.16	1.24
1	A	532	ARG	CA-C	6.01	1.60	1.52
1	B	541	GLY	C-O	6.01	1.34	1.24
1	A	55	HIS	C-O	-5.99	1.16	1.24
1	B	601	PHE	C-O	-5.95	1.16	1.24
1	A	331	THR	C-O	5.93	1.31	1.23
1	B	681	ASP	CA-C	5.89	1.59	1.52
1	B	46	GLN	C-O	5.89	1.31	1.23
1	B	82	ARG	CZ-NH2	-5.87	1.25	1.33
1	A	82	ARG	CZ-NH2	-5.86	1.25	1.33
1	B	114	ALA	C-O	5.77	1.31	1.24
1	A	488	ALA	C-O	-5.77	1.16	1.24
1	B	592	ALA	CA-C	-5.77	1.44	1.52
1	A	520	GLN	CA-C	5.75	1.60	1.52
1	B	537	GLY	C-O	-5.73	1.16	1.23
1	A	678	THR	C-O	5.70	1.31	1.23
1	B	289	PRO	N-CA	-5.70	1.40	1.47
1	B	596	PRO	CA-CB	-5.69	1.47	1.53
1	A	679	ALA	N-CA	5.63	1.53	1.46
1	B	410	GLU	CG-CD	5.58	1.66	1.52
1	A	724	ALA	CA-C	-5.58	1.44	1.52
1	A	493	GLY	CA-C	5.57	1.59	1.51
1	B	335	THR	N-CA	-5.51	1.39	1.46
1	B	76	ASP	CA-C	5.48	1.60	1.52
1	B	64	LYS	CA-CB	5.47	1.62	1.53
1	B	572	VAL	C-O	-5.46	1.17	1.24
1	B	619	ASP	CG-OD1	-5.43	1.15	1.25
1	B	534	ALA	CA-C	5.42	1.59	1.52
1	B	78	ALA	CA-C	5.40	1.59	1.52
1	A	566	ALA	C-O	-5.39	1.16	1.24
1	B	689	ASP	CG-OD2	-5.39	1.15	1.25
1	B	602	ARG	CZ-NH2	-5.38	1.26	1.33
1	B	738	LYS	N-CA	-5.38	1.40	1.46
1	B	233	GLN	N-CA	5.38	1.52	1.45
1	B	36	GLY	N-CA	5.35	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	LYS	C-O	-5.35	1.17	1.24
1	B	680	ALA	N-CA	5.35	1.53	1.46
1	B	414	ASP	CG-OD2	-5.35	1.15	1.25
1	B	568	HIS	CA-C	5.35	1.59	1.52
1	B	465	GLU	N-CA	-5.32	1.40	1.46
1	A	91	SER	C-O	-5.32	1.17	1.23
1	A	734	ALA	N-CA	-5.32	1.40	1.46
1	A	572	VAL	N-CA	-5.26	1.42	1.46
1	A	680	ALA	N-CA	5.25	1.52	1.46
1	A	292	ASN	CA-C	5.25	1.60	1.52
1	B	580	ASP	C-O	-5.25	1.17	1.24
1	A	448	ASP	CA-CB	5.25	1.56	1.52
1	A	126	ALA	C-O	5.24	1.30	1.24
1	A	501	ASN	CA-C	5.24	1.59	1.52
1	A	570	VAL	CA-C	-5.23	1.46	1.52
1	B	78	ALA	CA-CB	5.22	1.61	1.53
1	A	681	ASP	CA-C	5.19	1.58	1.52
1	B	439	VAL	C-O	-5.19	1.17	1.24
1	A	647	GLN	CD-NE2	5.19	1.44	1.33
1	A	377	PRO	C-O	-5.14	1.17	1.24
1	A	454	ASP	N-CA	5.14	1.51	1.46
1	B	63	GLY	C-O	5.13	1.29	1.23
1	A	418	ARG	CZ-NH1	-5.11	1.25	1.32
1	B	730	ARG	CZ-NH2	5.11	1.40	1.33
1	A	225	LEU	C-O	-5.10	1.17	1.24
1	B	55	HIS	C-O	-5.09	1.16	1.23
1	A	68	TYR	N-CA	5.09	1.52	1.46
1	A	510	GLN	CA-C	-5.09	1.46	1.52
1	B	158	LYS	N-CA	-5.02	1.40	1.46
1	B	566	ALA	C-O	-5.00	1.17	1.24

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	GLN	N-CA-C	-9.21	98.12	110.55
1	B	541	GLY	N-CA-C	-9.09	95.65	112.37
1	A	161	ARG	NE-CZ-NH1	8.36	129.86	121.50
1	A	47	LEU	N-CA-CB	-7.19	99.82	110.17
1	A	161	ARG	CD-NE-CZ	7.07	134.30	124.40
1	A	46	GLN	CA-CB-CG	6.93	127.95	114.10
1	B	46	GLN	N-CA-C	-6.41	102.07	110.53
1	B	54	ARG	N-CA-C	-5.89	102.60	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	LEU	CA-C-O	-5.87	114.72	121.47
1	B	47	LEU	N-CA-CB	-5.60	101.77	110.29
1	B	633[A]	VAL	CB-CA-C	-5.53	104.67	112.14
1	B	633[B]	VAL	CB-CA-C	-5.53	104.67	112.14
1	B	450	ILE	CA-C-O	-5.45	116.13	119.51
1	A	403	ARG	CG-CD-NE	-5.44	100.03	112.00
1	B	428	MET	CA-CB-CG	-5.42	103.26	114.10
1	A	569	ALA	N-CA-C	-5.42	99.90	108.73
1	A	62	MET	CA-C-N	-5.41	114.55	120.44
1	A	62	MET	C-N-CA	-5.41	114.55	120.44
1	A	330	TRP	N-CA-C	5.34	118.25	111.69
1	A	47	LEU	CA-C-O	-5.32	115.77	121.56
1	A	46	GLN	CA-C-O	5.31	128.08	121.81
1	A	161	ARG	NH1-CZ-NH2	-5.30	112.41	119.30
1	A	553	LEU	N-CA-C	5.27	117.02	111.28
1	B	206	LYS	CG-CD-CE	5.22	123.31	111.30
1	B	378	SER	N-CA-C	-5.19	106.63	113.17
1	A	520	GLN	CA-CB-CG	-5.16	103.78	114.10
1	A	46	GLN	CB-CG-CD	5.11	121.28	112.60
1	A	57	SER	N-CA-C	-5.08	106.19	112.38

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	5555	0	5368	22	0
1	B	5581	0	5391	29	0
2	A	43	0	30	1	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	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	0	0	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	16	0	28	3	0
7	B	16	0	28	1	0
8	A	10	0	7	0	0
8	B	10	0	7	1	0
9	A	786	0	0	5	1
9	B	821	0	0	13	1
All	All	12903	0	10889	56	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 3.

All (56) 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:725[A]:GLN:NE2	1:A:726[A]:GLU:HG3	1.45	1.30
1:B:622[A]:GLN:NE2	8:B:809:NIZ:O1	1.96	0.97
1:A:725[A]:GLN:NE2	1:A:726[A]:GLU:CG	2.30	0.94
1:A:119[B]:THR:HG21	9:A:1114:HOH:O	1.74	0.87
1:B:119[B]:THR:HG21	9:B:1087:HOH:O	1.73	0.87
1:B:403:ARG:NH1	9:B:903:HOH:O	2.07	0.86
1:B:647:GLN:HG2	9:B:928:HOH:O	1.76	0.85
1:A:544:GLN:OE1	9:A:901:HOH:O	2.02	0.75
1:B:519:GLU:OE1	9:B:902:HOH:O	2.05	0.75
1:A:725[A]:GLN:HE22	1:A:726[A]:GLU:HG3	1.50	0.73
1:A:593:VAL:HG13	9:A:988:HOH:O	1.90	0.72
1:B:178:GLU:OE1	9:B:904:HOH:O	2.08	0.71
1:A:725[A]:GLN:CD	1:A:726[A]:GLU:HG3	2.14	0.71
1:B:123:ARG:HH21	1:B:622[A]:GLN:HE21	1.39	0.69
1:B:76:ASP:OD1	9:B:905:HOH:O	2.12	0.67
7:A:807:MPD:HM1	7:A:807:MPD:O4	1.95	0.67
1:B:512:ASP:OD1	9:B:906:HOH:O	2.14	0.64
1:A:255[A]:ARG:NH2	9:A:902:HOH:O	2.11	0.64
1:B:657[A]:GLU:CD	9:B:926:HOH:O	2.39	0.64
1:A:123:ARG:HH21	1:A:622[A]:GLN:HE21	1.43	0.64
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.80	0.61
1:B:662:ASN:H	1:B:725:GLN:HE22	1.53	0.56
7:A:807:MPD:O4	7:A:807:MPD:CM	2.52	0.56
1:B:123:ARG:HH21	1:B:622[A]:GLN:NE2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725[A]:GLN:HE22	1:A:726[A]:GLU:CG	2.13	0.54
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.91	0.54
1:B:544:GLN:NE2	9:B:913:HOH:O	2.40	0.54
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.92	0.53
1:A:725[A]:GLN:NE2	9:A:903:HOH:O	2.22	0.52
1:B:46:GLN:NE2	9:B:901:HOH:O	1.96	0.52
1:A:608:LYS:HA	1:A:608:LYS:HE2	1.91	0.51
5:B:805:OXY:O1	9:B:908:HOH:O	2.19	0.51
1:B:696:LYS:HE2	9:B:973:HOH:O	2.12	0.50
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.48	0.49
1:B:608:LYS:HA	1:B:608:LYS:HE2	1.95	0.49
1:A:64:LYS:O	1:A:64:LYS:HE3	2.14	0.48
1:B:64:LYS:O	1:B:64:LYS:HE3	2.14	0.48
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.46	0.46
1:A:123:ARG:NH2	1:A:622[B]:GLN:OE1	2.49	0.46
1:B:196:GLU:HB2	1:B:197:PRO:HD2	1.98	0.45
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.17	0.45
7:B:807:MPD:O4	7:B:807:MPD:H12	2.17	0.44
1:B:119[B]:THR:HG23	1:B:593:VAL:HG11	1.98	0.44
1:B:591:MET:SD	1:B:594:LEU:HD12	2.57	0.44
1:B:426:ARG:HA	1:B:426:ARG:HD2	1.88	0.44
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.17	0.44
1:B:709:HIS:CE1	1:B:711[A]:GLN:HB2	2.53	0.44
7:A:808:MPD:H11	7:A:808:MPD:O4	2.18	0.43
1:A:610:ARG:HG2	1:A:611:VAL:HG23	2.02	0.41
1:A:633[A]:VAL:HG22	1:A:719:TYR:CZ	2.55	0.41
1:B:406:HIS:HD2	9:B:1408:HOH:O	2.02	0.41
1:A:591:MET:SD	1:A:594:LEU:HD12	2.61	0.41
1:A:602:ARG:HB3	1:A:645:VAL:HG23	2.03	0.41
1:B:654:THR:HG23	1:B:657[A]:GLU:HG3	2.02	0.40
1:A:284:THR:HG22	2:A:801:HEM:CAA	2.51	0.40
1:A:725[A]:GLN:NE2	1:A:726[A]:GLU:CD	2.79	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)
9:A:1251:HOH:O	9:B:1149:HOH:O[2_444]	2.01	0.19

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	721/728 (99%)	711 (99%)	10 (1%)	0	100	100
All	All	1439/1456 (99%)	1421 (99%)	18 (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	556/560 (99%)	546 (98%)	10 (2%)	51	38
1	B	559/560 (100%)	553 (99%)	6 (1%)	65	56
All	All	1115/1120 (100%)	1099 (99%)	16 (1%)	59	48

All (16) 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	161	ARG
1	A	379	LYS
1	A	469	LYS
1	A	608	LYS
1	A	649	ARG

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Mol	Chain	Res	Type
1	A	725[A]	GLN
1	A	725[B]	GLN
1	B	40	ARG
1	B	64	LYS
1	B	183	LYS
1	B	379	LYS
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	70	GLN
1	A	247	ASN
1	A	544	GLN
1	A	647	GLN
1	A	737	ASN
1	B	544	GLN
1	B	647	GLN
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 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	A	801	9,1	50,50,50	1.26	7 (14%)	67,82,82	1.59	12 (17%)
6	PO4	A	806	-	4,4,4	1.85	2 (50%)	6,6,6	2.60	2 (33%)
5	OXY	B	804	-	1,1,1	0.13	0	-		
7	MPD	B	808	-	7,7,7	0.76	0	9,10,10	1.64	4 (44%)
7	MPD	A	807	-	7,7,7	0.57	0	9,10,10	1.15	0
6	PO4	B	806	-	4,4,4	1.03	0	6,6,6	2.05	3 (50%)
7	MPD	B	807	-	7,7,7	0.55	0	9,10,10	1.45	1 (11%)
5	OXY	A	805	-	1,1,1	0.24	0	-		
5	OXY	B	805	-	1,1,1	0.17	0	-		
8	NIZ	A	809	-	10,10,10	2.91	4 (40%)	12,12,12	3.43	9 (75%)
8	NIZ	B	809	-	10,10,10	3.11	4 (40%)	12,12,12	3.17	8 (66%)
5	OXY	A	804	-	1,1,1	0.01	0	-		
2	HEM	B	801	9,1	50,50,50	1.62	10 (20%)	67,82,82	1.61	13 (19%)
7	MPD	A	808	-	7,7,7	0.76	0	9,10,10	1.70	2 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	801	9,1	-	2/14/54/54	-
7	MPD	B	808	-	-	4/5/5/5	-
7	MPD	A	807	-	-	0/5/5/5	-
7	MPD	B	807	-	-	3/5/5/5	-
8	NIZ	A	809	-	-	0/6/6/6	0/1/1/1
8	NIZ	B	809	-	-	0/6/6/6	0/1/1/1
2	HEM	B	801	9,1	-	3/14/54/54	-
7	MPD	A	808	-	-	1/5/5/5	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	809	NIZ	N3-N2	-7.30	1.31	1.41
8	B	809	NIZ	N3-N2	-6.55	1.32	1.41
2	B	801	HEM	C1B-NB	-4.79	1.32	1.40
8	B	809	NIZ	C5-C1	4.51	1.46	1.39
8	B	809	NIZ	C4-N1	4.45	1.46	1.33
2	B	801	HEM	FE-NB	3.68	2.06	1.94
2	B	801	HEM	C3C-C4C	-3.61	1.39	1.46
2	A	801	HEM	FE-NC	3.52	2.06	1.95
2	B	801	HEM	C2A-C3A	-3.34	1.30	1.38
8	A	809	NIZ	C4-N1	3.20	1.42	1.33
2	A	801	HEM	FE-NB	2.84	2.03	1.94
2	B	801	HEM	FE-NC	2.79	2.04	1.95
2	B	801	HEM	C1D-ND	-2.69	1.33	1.38
2	A	801	HEM	FE-NA	2.63	2.03	1.95
6	A	806	PO4	P-O4	-2.57	1.47	1.54
2	A	801	HEM	C1B-NB	-2.51	1.35	1.40
8	B	809	NIZ	C2-C3	2.45	1.43	1.38
2	A	801	HEM	C4A-NA	-2.45	1.35	1.39
2	B	801	HEM	C3B-C4B	2.42	1.49	1.44
8	A	809	NIZ	C1-C	-2.39	1.45	1.50
8	A	809	NIZ	O1-C	-2.39	1.17	1.23
2	B	801	HEM	O1D-CGD	2.36	1.29	1.22
2	A	801	HEM	CHC-C4B	-2.21	1.34	1.39
2	A	801	HEM	CAC-C3C	2.21	1.53	1.47
2	B	801	HEM	C1C-NC	-2.10	1.35	1.39
2	B	801	HEM	C4B-NB	-2.09	1.34	1.38
6	A	806	PO4	P-O1	2.02	1.55	1.50

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	809	NIZ	C1-C-N2	5.85	122.82	116.33
8	A	809	NIZ	O1-C-C1	-5.65	109.70	120.90
6	A	806	PO4	O4-P-O3	5.41	124.75	107.91
8	B	809	NIZ	C5-C4-N1	-5.41	114.38	123.60
8	A	809	NIZ	O1-C-N2	5.11	128.60	122.46
2	B	801	HEM	CHC-C4B-NB	4.19	128.93	124.42
8	A	809	NIZ	C5-C1-C2	4.17	123.87	118.57
8	A	809	NIZ	C1-C-N2	4.17	120.96	116.33
8	A	809	NIZ	C-N2-N3	4.14	127.99	121.50
2	A	801	HEM	C4B-C3B-C2B	-4.02	103.58	107.28
7	A	808	MPD	CM-C2-C1	-3.94	101.81	110.63
2	A	801	HEM	CHC-C4B-NB	3.89	128.61	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CAA-CBA-CGA	-3.78	103.63	113.67
8	B	809	NIZ	C3-C2-C1	-3.72	114.99	119.05
2	A	801	HEM	C3B-C2B-C1B	3.68	109.17	106.41
8	B	809	NIZ	O1-C-C1	-3.39	114.19	120.90
2	A	801	HEM	CMD-C2D-C1D	3.38	130.32	125.03
2	A	801	HEM	C3C-C2C-C1C	3.34	110.20	107.05
2	B	801	HEM	O2A-CGA-O1A	-3.24	114.99	123.33
8	A	809	NIZ	C5-C4-N1	-3.22	118.10	123.60
2	B	801	HEM	O2A-CGA-CBA	3.21	124.15	114.00
7	B	807	MPD	CM-C2-C1	-3.19	103.48	110.63
2	B	801	HEM	CMD-C2D-C1D	3.16	129.97	125.03
6	A	806	PO4	O4-P-O1	-3.15	99.82	110.95
6	B	806	PO4	O4-P-O1	-3.10	100.00	110.95
8	B	809	NIZ	C4-C5-C1	3.07	122.41	119.05
2	B	801	HEM	CHA-C4D-C3D	-2.94	119.80	125.23
8	B	809	NIZ	C4-N1-C3	2.92	123.53	116.86
8	B	809	NIZ	C-N2-N3	2.91	126.07	121.50
8	A	809	NIZ	C4-N1-C3	2.91	123.52	116.86
2	A	801	HEM	CAA-CBA-CGA	-2.75	106.38	113.67
2	B	801	HEM	C2D-C1D-ND	2.72	113.04	109.90
2	B	801	HEM	O1D-CGD-CBD	-2.69	114.58	123.09
7	B	808	MPD	O2-C2-C3	-2.51	99.87	109.27
2	B	801	HEM	C3D-C4D-ND	2.43	112.83	110.17
2	A	801	HEM	CMB-C2B-C1B	-2.43	121.24	125.03
7	B	808	MPD	CM-C2-C3	2.40	120.54	110.20
2	A	801	HEM	CHC-C4B-C3B	-2.38	120.33	125.07
2	A	801	HEM	C4C-NC-C1C	2.37	109.69	105.82
7	A	808	MPD	C1-C2-C3	2.32	120.20	110.20
7	B	808	MPD	O2-C2-C1	-2.29	100.86	107.99
2	A	801	HEM	CHC-C1C-NC	2.27	126.92	124.45
6	B	806	PO4	O4-P-O2	2.25	114.93	107.91
8	B	809	NIZ	C5-C1-C2	2.25	121.42	118.57
2	A	801	HEM	C3B-C4B-NB	2.20	111.05	109.47
8	A	809	NIZ	C3-C2-C1	-2.17	116.68	119.05
6	B	806	PO4	O3-P-O1	2.17	118.62	110.95
2	A	801	HEM	O1A-CGA-CBA	-2.16	116.25	123.09
2	B	801	HEM	C4D-ND-C1D	-2.15	102.66	105.21
7	B	808	MPD	O2-C2-CM	2.14	114.64	107.99
2	B	801	HEM	CHD-C1D-C2D	-2.13	121.67	125.03
8	A	809	NIZ	C2-C3-N1	-2.09	120.04	123.60
2	B	801	HEM	C1B-NB-C4B	2.07	107.65	105.21
2	B	801	HEM	C3B-C4B-NB	-2.05	108.00	109.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

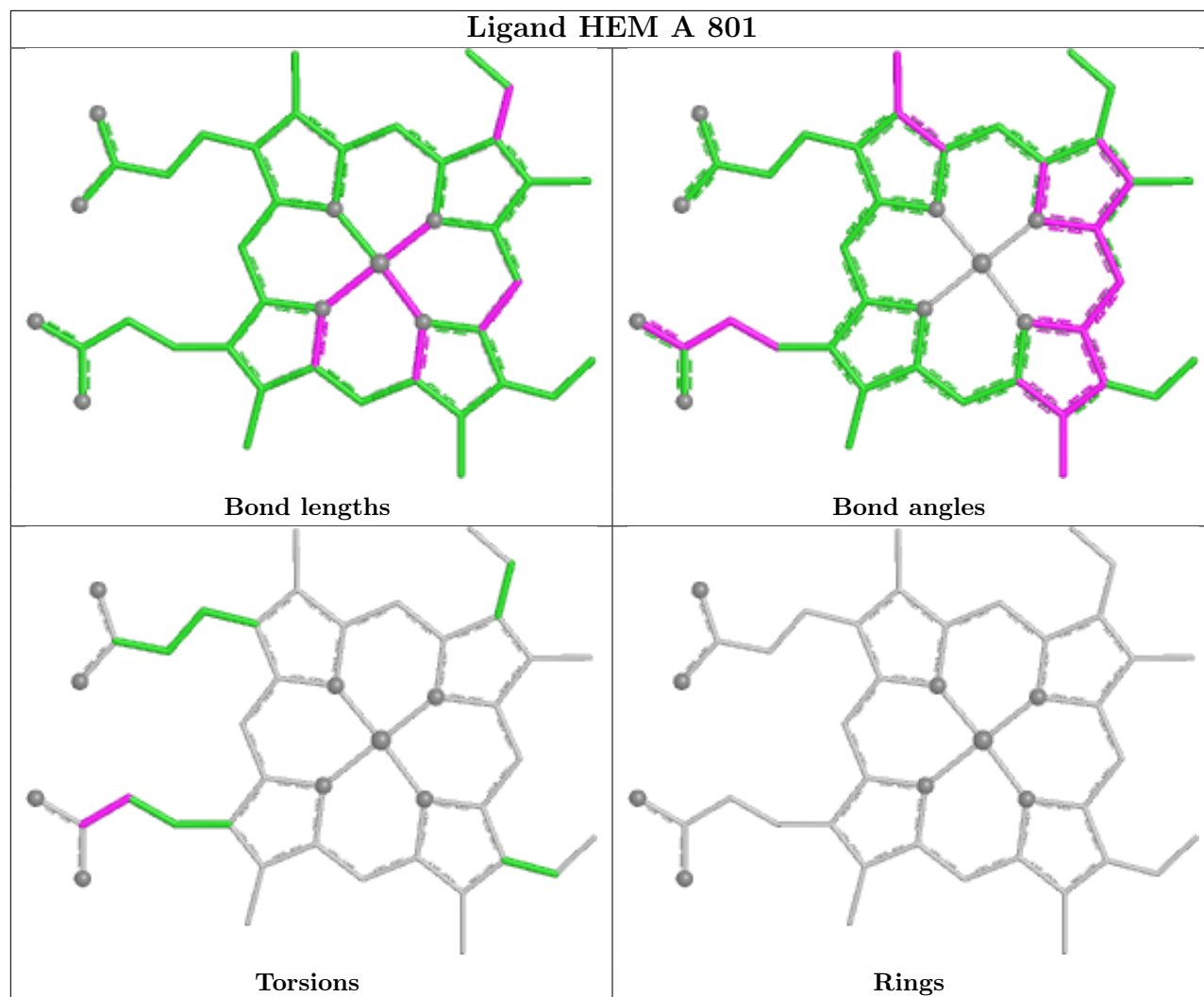
Mol	Chain	Res	Type	Atoms
7	B	807	MPD	C1-C2-C3-C4
7	B	807	MPD	O2-C2-C3-C4
7	B	808	MPD	O2-C2-C3-C4
7	B	808	MPD	CM-C2-C3-C4
7	B	807	MPD	CM-C2-C3-C4
2	B	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O2A
7	A	808	MPD	O2-C2-C3-C4
7	B	808	MPD	C2-C3-C4-O4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

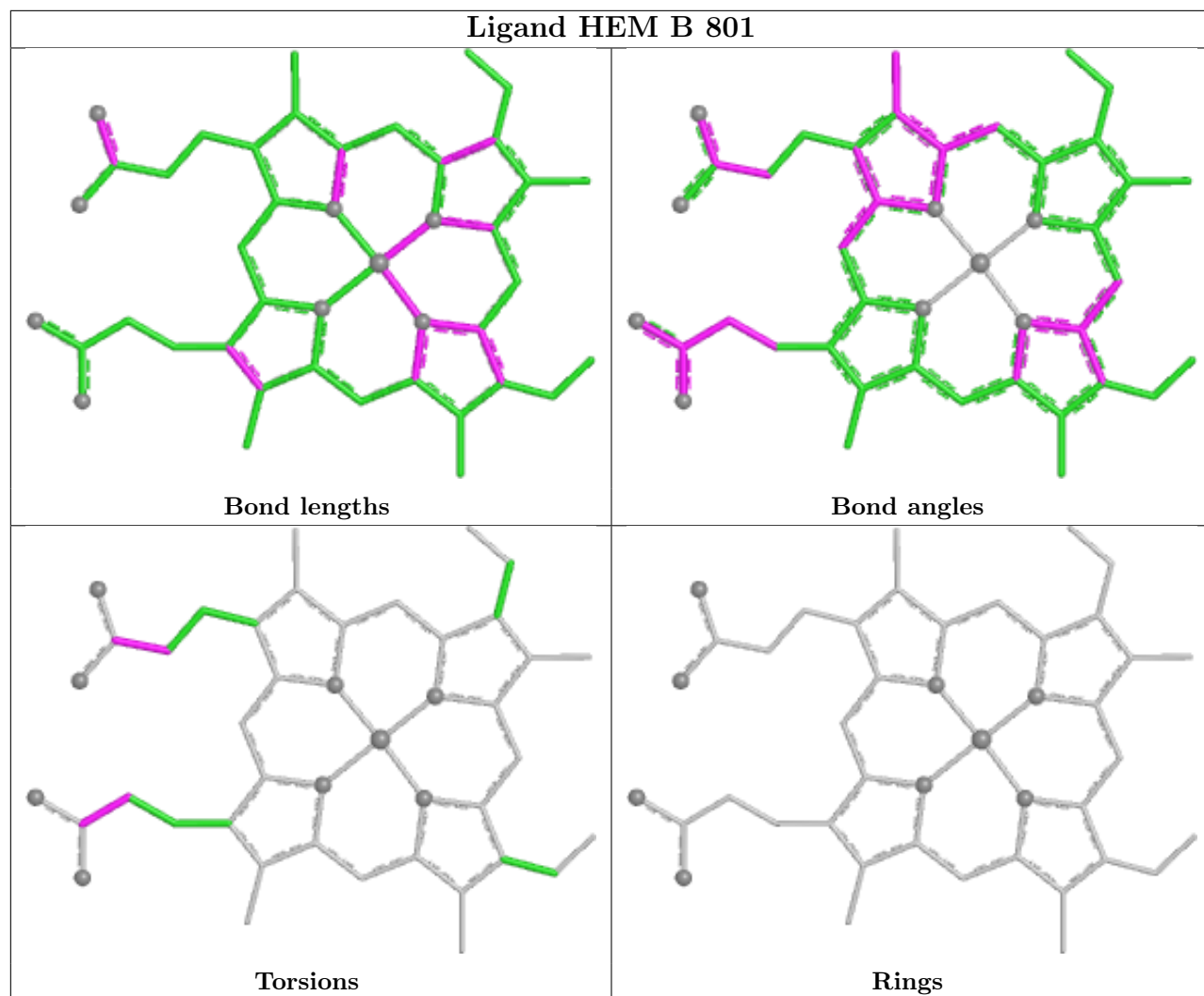
There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	1	0
7	A	807	MPD	2	0
7	B	807	MPD	1	0
5	B	805	OXY	1	0
8	B	809	NIZ	1	0
7	A	808	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 [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%)	-0.51	6 (0%) 82 86	7, 18, 35, 74	7 (0%)
1	B	713/728 (97%)	-0.55	7 (0%) 79 83	7, 17, 34, 67	10 (1%)
All	All	1426/1456 (97%)	-0.53	13 (0%) 81 85	7, 18, 34, 74	17 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	657[A]	GLU	4.5
1	B	748	ALA	4.5
1	A	748	ALA	4.4
1	B	64	LYS	3.6
1	A	540	ARG	2.9
1	A	608	LYS	2.4
1	B	541	GLY	2.4
1	B	454	ASP	2.3
1	B	46	GLN	2.3
1	A	64	LYS	2.2
1	B	608	LYS	2.1
1	A	40	ARG	2.1
1	A	454	ASP	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

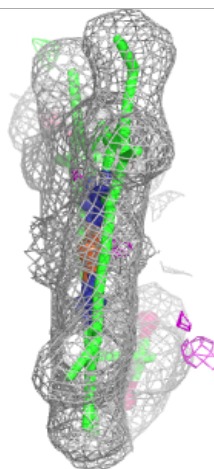
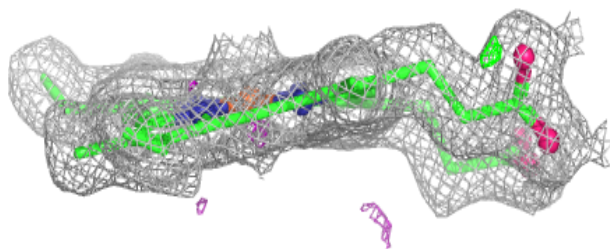
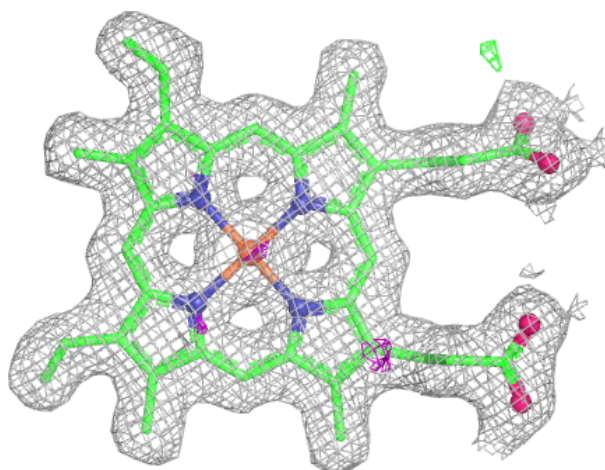
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

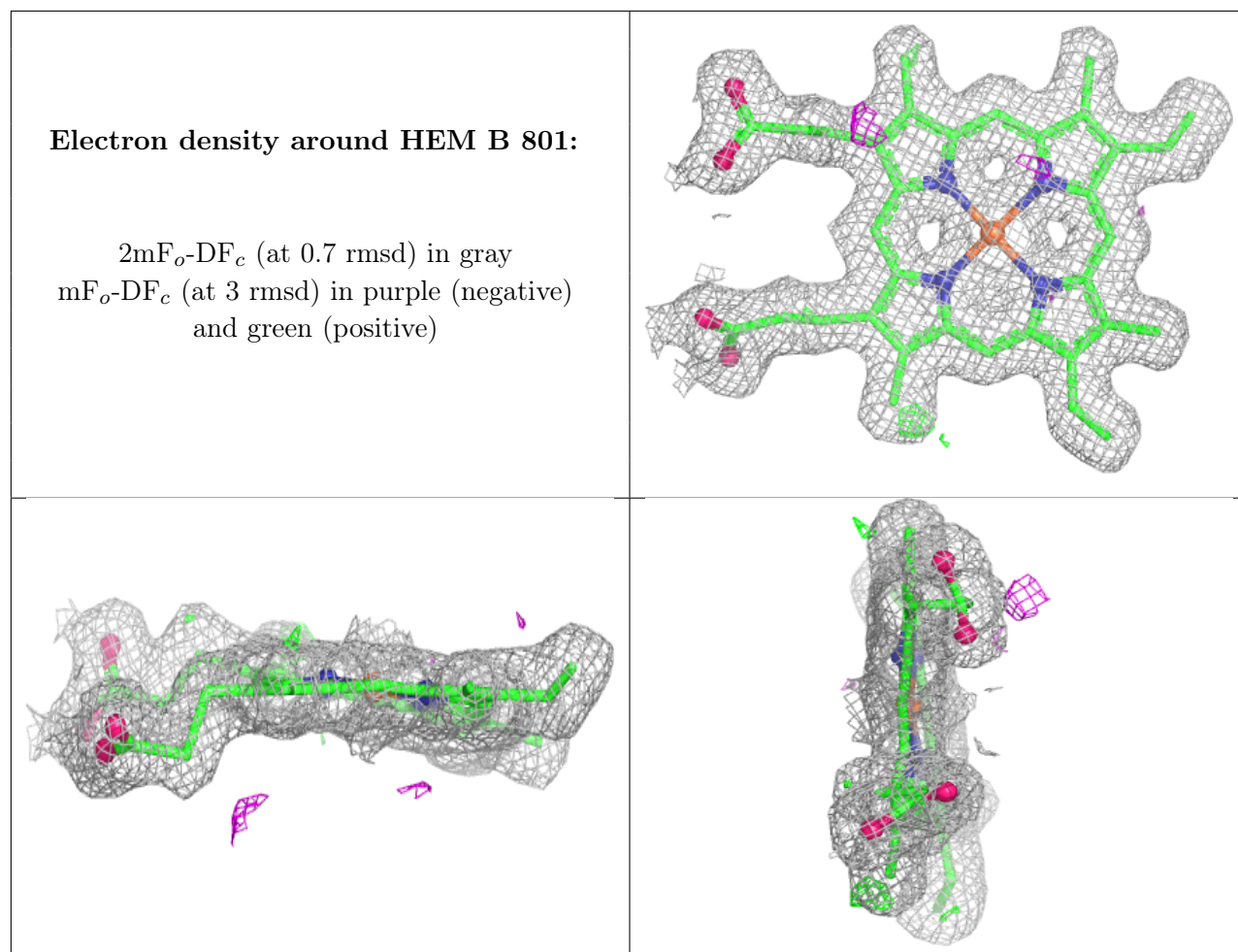
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NIZ	A	809	10/10	0.82	0.16	17,20,22,24	10
8	NIZ	B	809	10/10	0.90	0.10	21,24,29,29	10
6	PO4	A	806	5/5	0.91	0.10	40,50,59,59	0
7	MPD	A	808	8/8	0.92	0.12	35,40,54,56	0
7	MPD	B	808	8/8	0.92	0.13	40,43,45,47	0
6	PO4	B	806	5/5	0.92	0.10	39,50,56,61	0
7	MPD	A	807	8/8	0.92	0.18	50,58,59,64	0
7	MPD	B	807	8/8	0.93	0.13	39,42,47,48	0
5	OXY	B	805	2/2	0.94	0.17	31,31,31,39	0
5	OXY	A	805	2/2	0.95	0.14	32,32,32,38	0
5	OXY	B	804	2/2	0.97	0.17	24,24,24,27	0
5	OXY	A	804	2/2	0.97	0.17	25,25,25,33	0
3	NA	A	802	1/1	0.99	0.03	15,15,15,15	0
4	CL	A	803	1/1	0.99	0.05	25,25,25,25	0
4	CL	B	803	1/1	0.99	0.05	23,23,23,23	0
2	HEM	A	801	43/43	0.99	0.04	12,14,17,18	0
2	HEM	B	801	43/43	0.99	0.04	12,13,14,15	0
3	NA	B	802	1/1	1.00	0.06	14,14,14,14	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 [i](#)

There are no such residues in this entry.