



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 10:28 am BST

PDB ID : 5KSF
Title : Crystal structure of the D141A variant of the catalase-peroxidase from *B. pseudomallei* treated with acetate
Authors : Loewen, P.C.
Deposited on : 2016-07-08
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

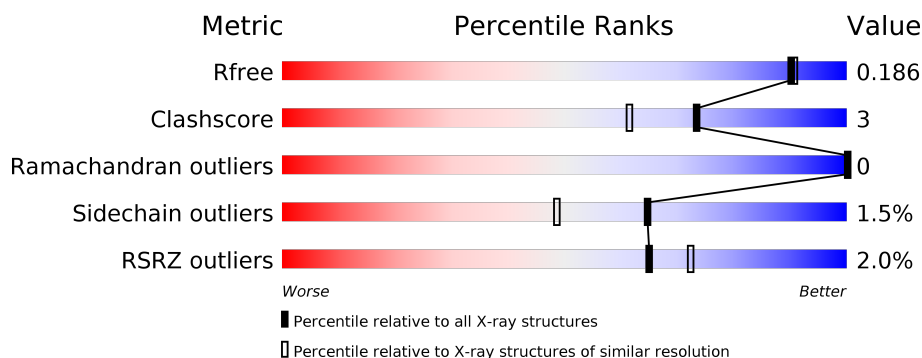
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 on 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	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>••</div> </div> </div>
1	B	728	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>••</div> </div> </div>

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	OXY	A	804	-	-	X	-
5	OXY	B	804	-	-	X	-
6	ACT	A	805	-	-	X	-
6	ACT	B	805	-	-	X	-
7	MPD	B	806	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12667 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	6	0
			5538	3500	985	1039	14			
1	B	713	Total	C	N	O	S	0	9	0
			5548	3508	990	1036	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	ASP	engineered mutation	UNP Q3JNW6
B	141	ALA	ASP	engineered mutation	UNP Q3JNW6

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



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

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

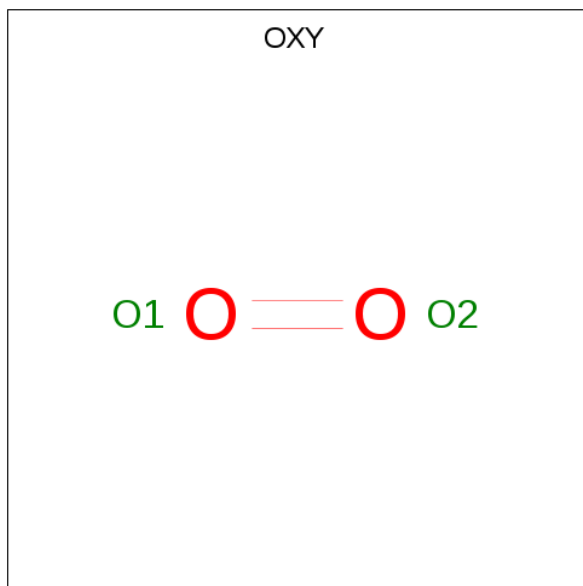
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

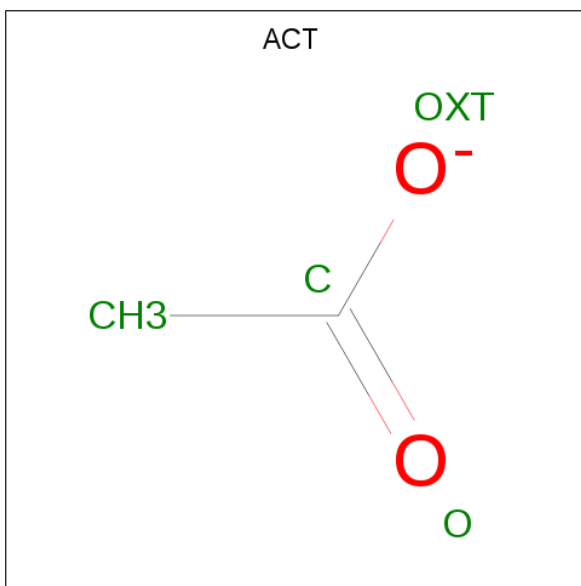
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl		
			1	1	0	0
4	A	1	Total	Cl		
			1	1	0	0

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



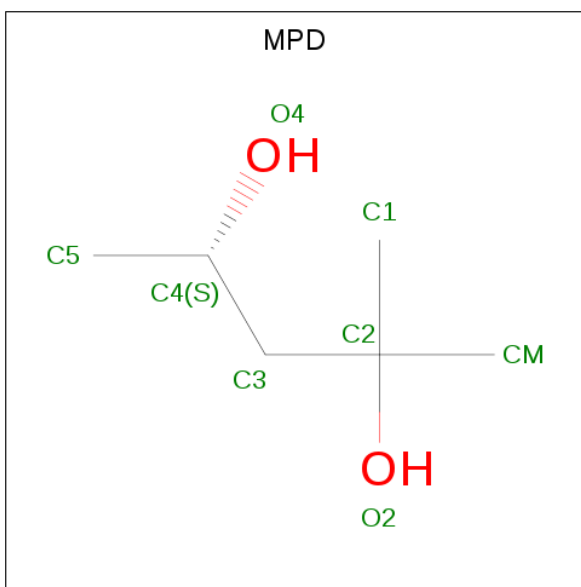
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	B	1	Total	O		
			2	2	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: 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		
7	B	1	Total	C	O	0	0
			8	6	2		

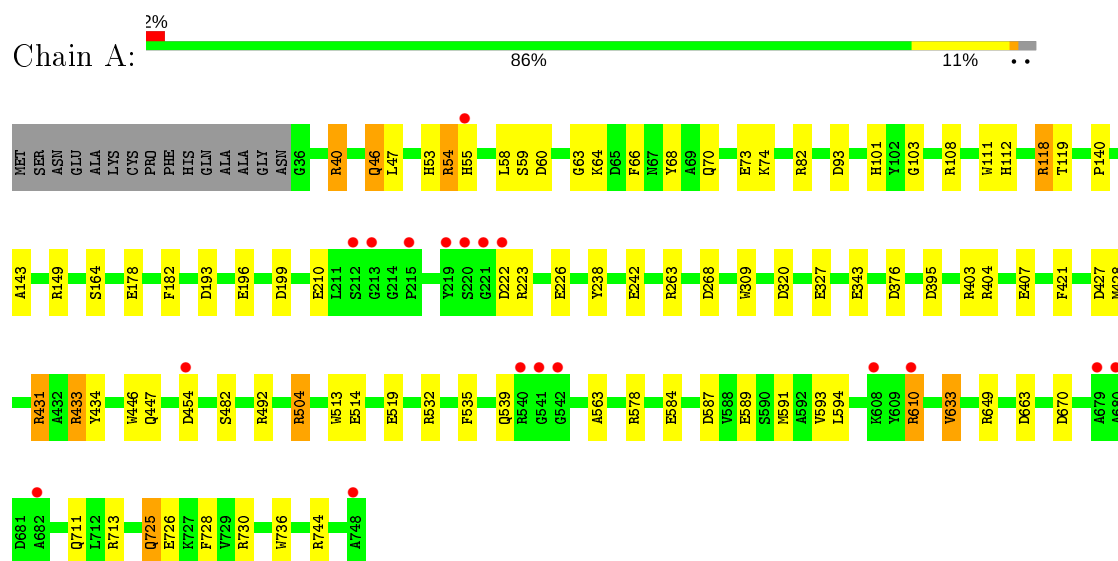
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	717	Total	O	0	0
			717	717		
8	B	722	Total	O	0	0
			722	722		

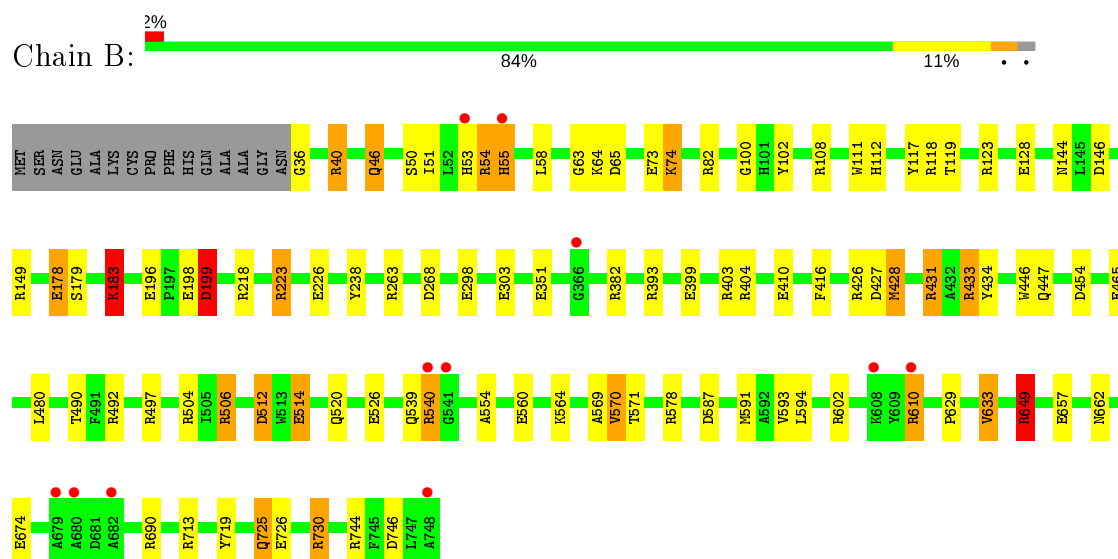
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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	100.69Å 115.47Å 174.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 1.75 48.37 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.38-1.75) 99.4 (48.37-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.148 , 0.175 0.160 , 0.186	Depositor DCC
R_{free} test set	10207 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12667	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: MPD, OXY, CL, NA, ACT, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.56	41/5698 (0.7%)	1.33	54/7746 (0.7%)
1	B	1.56	41/5714 (0.7%)	1.38	67/7768 (0.9%)
All	All	1.56	82/11412 (0.7%)	1.36	121/15514 (0.8%)

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	A	0	2
1	B	0	3
All	All	0	5

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	178	GLU	CD-OE2	10.72	1.37	1.25
1	A	407[A]	GLU	CD-OE1	10.69	1.37	1.25
1	A	407[B]	GLU	CD-OE1	10.69	1.37	1.25
1	B	178	GLU	CD-OE1	10.38	1.37	1.25
1	B	726	GLU	CD-OE1	10.14	1.36	1.25
1	A	589	GLU	CD-OE1	10.05	1.36	1.25
1	A	196	GLU	CG-CD	8.87	1.65	1.51
1	B	198	GLU	CD-OE2	8.65	1.35	1.25
1	B	196	GLU	CG-CD	8.58	1.64	1.51
1	A	728	PHE	CG-CD2	-8.51	1.25	1.38
1	A	407[A]	GLU	CG-CD	8.37	1.64	1.51
1	A	407[B]	GLU	CG-CD	8.37	1.64	1.51
1	B	410	GLU	CG-CD	8.31	1.64	1.51
1	A	726	GLU	CG-CD	8.20	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ARG	CZ-NH2	-8.17	1.22	1.33
1	B	512	ASP	CG-OD2	8.08	1.44	1.25
1	B	602	ARG	CZ-NH2	-8.03	1.22	1.33
1	A	725	GLN	CG-CD	8.00	1.69	1.51
1	B	434	TYR	CE2-CZ	-7.77	1.28	1.38
1	B	540	ARG	C-O	7.66	1.38	1.23
1	A	589	GLU	CG-CD	7.57	1.63	1.51
1	A	633	VAL	CB-CG1	-7.55	1.36	1.52
1	B	226	GLU	CD-OE2	-7.32	1.17	1.25
1	B	226	GLU	CG-CD	7.20	1.62	1.51
1	A	584	GLU	CG-CD	7.05	1.62	1.51
1	A	178	GLU	CD-OE1	-7.00	1.18	1.25
1	B	726	GLU	CG-CD	6.86	1.62	1.51
1	B	63	GLY	N-CA	6.68	1.56	1.46
1	A	726	GLU	CD-OE1	6.67	1.32	1.25
1	B	434	TYR	CE1-CZ	-6.64	1.29	1.38
1	B	512	ASP	CB-CG	6.64	1.65	1.51
1	A	327	GLU	CD-OE1	6.61	1.32	1.25
1	B	128	GLU	CD-OE2	-6.59	1.18	1.25
1	B	399	GLU	CD-OE2	6.47	1.32	1.25
1	A	519	GLU	CD-OE1	6.44	1.32	1.25
1	B	434	TYR	CG-CD1	-6.43	1.30	1.39
1	B	674	GLU	CG-CD	6.42	1.61	1.51
1	A	589	GLU	CD-OE2	6.42	1.32	1.25
1	A	434	TYR	CE2-CZ	-6.41	1.30	1.38
1	B	560	GLU	CD-OE2	6.18	1.32	1.25
1	A	736	TRP	CG-CD1	-6.11	1.28	1.36
1	B	123	ARG	CZ-NH2	6.10	1.41	1.33
1	B	102	TYR	CG-CD1	-6.05	1.31	1.39
1	B	226	GLU	CB-CG	-6.03	1.40	1.52
1	B	446	TRP	CZ2-CH2	-5.98	1.25	1.37
1	A	711	GLN	CD-NE2	-5.94	1.18	1.32
1	A	532	ARG	NE-CZ	-5.88	1.25	1.33
1	B	36	GLY	N-CA	5.80	1.54	1.46
1	A	63	GLY	N-CA	5.78	1.54	1.46
1	A	563	ALA	N-CA	-5.77	1.34	1.46
1	A	73	GLU	CG-CD	5.74	1.60	1.51
1	B	465	GLU	CD-OE1	5.74	1.31	1.25
1	A	482	SER	CB-OG	5.72	1.49	1.42
1	A	649	ARG	CZ-NH2	5.70	1.40	1.33
1	A	446	TRP	CG-CD1	5.65	1.44	1.36
1	B	526	GLU	CG-CD	5.62	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	PHE	CG-CD1	-5.59	1.30	1.38
1	A	421	PHE	CG-CD2	-5.57	1.30	1.38
1	B	351	GLU	CD-OE1	5.54	1.31	1.25
1	A	454	ASP	CB-CG	5.44	1.63	1.51
1	A	242	GLU	CD-OE2	5.44	1.31	1.25
1	A	70	GLN	CG-CD	5.38	1.63	1.51
1	B	196	GLU	CB-CG	-5.38	1.42	1.52
1	A	59	SER	C-O	-5.34	1.13	1.23
1	A	164	SER	CA-CB	-5.33	1.45	1.52
1	B	179	SER	C-O	5.32	1.33	1.23
1	B	746	ASP	CB-CG	5.30	1.62	1.51
1	A	327	GLU	CG-CD	5.26	1.59	1.51
1	A	514	GLU	CD-OE1	-5.24	1.19	1.25
1	B	46	GLN	CG-CD	5.19	1.62	1.51
1	B	416	PHE	CG-CD1	-5.18	1.30	1.38
1	B	454	ASP	CB-CG	5.17	1.62	1.51
1	B	657	GLU	CD-OE1	5.16	1.31	1.25
1	A	513	TRP	CE3-CZ3	-5.16	1.29	1.38
1	A	226	GLU	CG-CD	5.14	1.59	1.51
1	A	726	GLU	CD-OE2	5.13	1.31	1.25
1	B	298	GLU	CD-OE2	5.11	1.31	1.25
1	B	117	TYR	CE1-CZ	-5.11	1.31	1.38
1	B	100	GLY	N-CA	-5.09	1.38	1.46
1	B	303	GLU	CD-OE2	-5.05	1.20	1.25
1	B	725	GLN	CD-OE1	5.01	1.34	1.24
1	A	504	ARG	CZ-NH1	-5.01	1.26	1.33

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	512	ASP	CB-CG-OD1	-14.33	105.40	118.30
1	A	40	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	B	123	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	B	149	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	404	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	B	403	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	B	427	ASP	CB-CG-OD2	-9.78	109.50	118.30
1	B	730[B]	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	B	40	ARG	NE-CZ-NH1	9.49	125.04	120.30
1	A	376	ASP	CB-CG-OD2	-9.43	109.81	118.30
1	A	730	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	B	226	GLU	OE1-CD-OE2	-9.14	112.33	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	GLU	OE1-CD-OE2	8.97	134.06	123.30
1	B	578	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	B	218	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	A	108	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	A	149	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	B	82	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	B	223	ARG	NE-CZ-NH1	-8.77	115.92	120.30
1	B	730[B]	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	B	690	ARG	NE-CZ-NH2	8.45	124.53	120.30
1	A	670	ASP	CB-CG-OD2	-8.33	110.81	118.30
1	A	93	ASP	CB-CG-OD1	8.31	125.78	118.30
1	B	649[A]	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	B	649[B]	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	A	633	VAL	CG1-CB-CG2	-8.03	98.05	110.90
1	B	504	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B	149	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	B	54	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	B	744	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	B	428	MET	CA-CB-CG	-7.75	100.13	113.30
1	A	713	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	149	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	82	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	713	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	A	404	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	B	123	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	B	54	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	744	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	B	199	ASP	CB-CG-OD1	-7.31	111.72	118.30
1	B	393	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	A	587	ASP	CB-CG-OD1	7.26	124.83	118.30
1	B	713	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	434	TYR	CB-CG-CD1	7.17	125.30	121.00
1	B	108	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	433	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	713	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	B	587	ASP	CB-CG-OD1	7.05	124.64	118.30
1	A	54	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	B	610	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	B	82	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	492	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	B	633[A]	VAL	CG1-CB-CG2	-6.87	99.90	110.90
1	B	633[B]	VAL	CG1-CB-CG2	-6.87	99.90	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	514	GLU	OE1-CD-OE2	-6.86	115.07	123.30
1	B	108	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	B	512	ASP	CB-CG-OD2	6.79	124.42	118.30
1	A	108	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	407[A]	GLU	CG-CD-OE1	6.78	131.86	118.30
1	A	407[B]	GLU	CG-CD-OE1	6.78	131.86	118.30
1	A	66	PHE	CB-CG-CD2	-6.78	116.06	120.80
1	B	434	TYR	CB-CG-CD1	6.78	125.07	121.00
1	A	222	ASP	CB-CG-OD1	6.71	124.34	118.30
1	B	178	GLU	CG-CD-OE2	-6.70	104.90	118.30
1	A	403	ARG	CG-CD-NE	6.67	125.80	111.80
1	B	492	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	433	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	B	65	ASP	CB-CG-OD2	-6.57	112.38	118.30
1	B	73	GLU	OE1-CD-OE2	6.50	131.10	123.30
1	A	54	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	A	60	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	578	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	B	223	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	B	403	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	560	GLU	OE1-CD-OE2	6.27	130.82	123.30
1	B	268	ASP	CB-CG-OD1	6.19	123.87	118.30
1	B	570	VAL	CG1-CB-CG2	-6.16	101.04	110.90
1	A	193	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	B	587	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	431	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	A	320	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	A	46	GLN	CA-CB-CG	5.95	126.48	113.40
1	B	382	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	506	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	532	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	B	564	LYS	CD-CE-NZ	-5.88	98.16	111.70
1	B	382	ARG	CG-CD-NE	-5.86	99.50	111.80
1	A	263	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	433	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	47	LEU	N-CA-CB	-5.77	98.85	110.40
1	B	51	ILE	CG1-CB-CG2	-5.75	98.74	111.40
1	A	584	GLU	OE1-CD-OE2	-5.74	116.41	123.30
1	A	210	GLU	OE1-CD-OE2	-5.68	116.49	123.30
1	B	431	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	A	223	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	395	ASP	CB-CG-OD1	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	610	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	B	497	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	663	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	268	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	B	55	HIS	CB-CA-C	5.43	121.26	110.40
1	B	46	GLN	CA-CB-CG	5.43	125.34	113.40
1	A	93	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	55	HIS	CB-CA-C	5.39	121.19	110.40
1	A	504	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	118	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	263	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	540	ARG	CB-CA-C	5.31	121.02	110.40
1	A	343	GLU	CG-CD-OE1	5.28	128.86	118.30
1	A	427	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	B	490	THR	CA-CB-CG2	-5.22	105.09	112.40
1	A	182	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	A	395	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	B	183	LYS	CD-CE-NZ	5.08	123.39	111.70
1	B	74	LYS	CB-CA-C	-5.07	100.27	110.40
1	B	263	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	B	404	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	40	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	68	TYR	CB-CG-CD1	-5.02	117.98	121.00
1	A	376	ASP	OD1-CG-OD2	5.01	132.82	123.30
1	B	427	ASP	OD1-CG-OD2	5.00	132.81	123.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	539	GLN	Peptide
1	A	74	LYS	Mainchain
1	B	199	ASP	Mainchain
1	B	514	GLU	Sidechain
1	B	539	GLN	Peptide

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	5538	0	5366	19	0
1	B	5548	0	5386	39	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	3	0
5	B	2	0	0	2	0
6	A	4	0	3	6	0
6	B	4	0	3	3	0
7	A	16	0	28	5	0
7	B	24	0	42	10	0
8	A	717	0	0	2	0
8	B	722	0	0	13	0
All	All	12667	0	10888	72	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:ARG:HE	7:B:806:MPD:H12	1.24	0.98
1:A:101:HIS:HD2	1:A:103:GLY:H	1.14	0.90
1:B:55:HIS:HD2	8:B:1315:HOH:O	1.55	0.87
1:B:112:HIS:NE2	6:B:805:ACT:C	2.38	0.87
1:A:119[B]:THR:HG21	8:A:950:HOH:O	1.75	0.85
1:A:112:HIS:NE2	6:A:805:ACT:C	2.41	0.83
5:B:804:OXY:O2	6:B:805:ACT:H1	1.80	0.81
7:B:806:MPD:H51	8:B:1327:HOH:O	1.86	0.75
7:B:806:MPD:H13	8:B:1508:HOH:O	1.86	0.75
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.69	0.74
1:B:520[B]:GLN:HG3	8:B:1408:HOH:O	1.88	0.72
1:A:101:HIS:CD2	1:A:103:GLY:H	2.04	0.70
1:B:512:ASP:OD1	8:B:902:HOH:O	2.10	0.68
5:B:804:OXY:O1	6:B:805:ACT:H1	1.93	0.67
7:B:806:MPD:C1	7:B:806:MPD:H52	2.25	0.67
1:A:101:HIS:HD2	1:A:103:GLY:N	1.90	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.79	0.65
1:B:506:ARG:HE	7:B:806:MPD:C1	2.07	0.63
7:B:807:MPD:O2	7:B:807:MPD:C5	2.49	0.61
1:A:58:LEU:HB3	1:B:53[A]:HIS:HD2	1.65	0.61
1:B:569:ALA:O	1:B:570:VAL:HG23	2.01	0.60
1:B:50[B]:SER:HA	1:B:53[B]:HIS:CD2	2.38	0.58
7:B:806:MPD:H52	7:B:806:MPD:H11	1.87	0.55
1:B:119[B]:THR:HG23	8:B:1161:HOH:O	2.06	0.55
5:A:804:OXY:O1	6:A:805:ACT:CH3	2.55	0.54
7:A:806:MPD:H11	7:A:806:MPD:H52	1.89	0.54
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	2.08	0.53
1:B:569:ALA:O	1:B:570:VAL:CG2	2.56	0.53
1:B:506:ARG:NE	7:B:806:MPD:H12	2.08	0.53
7:A:806:MPD:C5	7:A:806:MPD:HM2	2.38	0.53
1:B:426[A]:ARG:NE	8:B:903:HOH:O	2.14	0.53
1:B:53[B]:HIS:O	1:B:53[B]:HIS:ND1	2.43	0.52
1:B:53[B]:HIS:CD2	8:B:1184:HOH:O	2.63	0.52
7:A:807:MPD:O4	7:A:807:MPD:O2	2.18	0.51
1:A:140:PRO:HB3	7:A:807:MPD:H31	1.92	0.51
1:A:504:ARG:HD2	8:A:928:HOH:O	2.10	0.50
1:A:112:HIS:CE1	6:A:805:ACT:H2	2.46	0.50
1:B:178:GLU:OE2	1:B:183:LYS:HE2	2.12	0.49
1:B:119[B]:THR:CG2	8:B:1161:HOH:O	2.60	0.48
5:A:804:OXY:O1	6:A:805:ACT:H2	2.14	0.48
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE2	2.49	0.48
1:B:111:TRP:HZ3	1:B:238:TYR:HH	1.59	0.47
1:A:54:ARG:NE	1:A:199:ASP:OD2	2.47	0.47
1:B:74:LYS:HB2	8:B:1222:HOH:O	2.14	0.46
1:A:111:TRP:HZ3	1:A:238:TYR:HH	1.59	0.45
1:B:591:MET:SD	1:B:594:LEU:HD12	2.57	0.45
1:A:591:MET:SD	1:A:594:LEU:HD12	2.57	0.45
1:B:662:ASN:H	1:B:725:GLN:HE22	1.65	0.45
1:B:512:ASP:HB2	8:B:1334:HOH:O	2.17	0.45
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	3.00	0.45
7:A:806:MPD:H52	7:A:806:MPD:HM2	1.99	0.44
1:B:426[B]:ARG:HD2	1:B:426[B]:ARG:HA	1.74	0.44
1:A:112:HIS:NE2	6:A:805:ACT:O	2.49	0.44
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.17	0.44
1:B:54:ARG:HB3	1:B:55:HIS:ND1	2.32	0.44
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.18	0.43
1:B:428:MET:O	1:B:433:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.54	0.43
1:B:649[A]:ARG:HG2	8:B:1337:HOH:O	2.19	0.43
1:B:54:ARG:NE	1:B:199:ASP:OD2	2.47	0.42
1:B:53[B]:HIS:CG	1:B:53[B]:HIS:O	2.72	0.42
1:A:143:ALA:HA	1:A:309:TRP:CH2	2.54	0.42
1:A:119[B]:THR:CG2	1:A:593:VAL:HG11	2.48	0.42
7:B:806:MPD:H52	7:B:806:MPD:H12	2.01	0.42
1:A:53:HIS:HA	1:B:58:LEU:HD13	2.02	0.41
7:B:807:MPD:O2	7:B:807:MPD:H53	2.19	0.41
1:B:480:LEU:HD22	1:B:554:ALA:HB1	2.02	0.41
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.21	0.40
5:A:804:OXY:O2	6:A:805:ACT:H2	2.21	0.40
1:A:428:MET:O	1:A:433:ARG:HD3	2.21	0.40
1:B:223:ARG:HD2	1:B:223:ARG:HH11	1.62	0.40
1:B:74:LYS:HE3	8:B:1251:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	717/728 (98%)	707 (99%)	10 (1%)	0	100	100
1	B	719/728 (99%)	705 (98%)	14 (2%)	0	100	100
All	All	1436/1456 (99%)	1412 (98%)	24 (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	555/560 (99%)	548 (99%)	7 (1%)	69	54
1	B	557/560 (100%)	546 (98%)	11 (2%)	55	34
All	All	1112/1120 (99%)	1094 (98%)	18 (2%)	65	45

All (18) 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	118	ARG
1	A	610	ARG
1	A	633	VAL
1	A	725	GLN
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	118	ARG
1	B	183	LYS
1	B	540	ARG
1	B	571	THR
1	B	610	ARG
1	B	649[A]	ARG
1	B	649[B]	ARG
1	B	730[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	227	ASN
1	A	247	ASN
1	B	46	GLN
1	B	55	HIS
1	B	227	ASN
1	B	544	GLN
1	B	647	GLN

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Mol	Chain	Res	Type
1	B	650	HIS
1	B	725	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	ACT	A	805	-	1,3,3	2.72	1 (100%)	0,3,3	0.00	-
5	OXY	B	804	-	1,1,1	0.49	0	-		
5	OXY	A	804	-	1,1,1	0.12	0	-		
7	MPD	B	807	-	7,7,7	0.57	0	9,10,10	1.92	4 (44%)
7	MPD	A	807	-	7,7,7	1.00	0	9,10,10	1.61	2 (22%)
7	MPD	A	806	-	7,7,7	0.61	0	9,10,10	1.46	3 (33%)
7	MPD	B	806	-	7,7,7	1.59	2 (28%)	9,10,10	1.22	1 (11%)
2	HEM	A	801	1	27,50,50	1.86	9 (33%)	17,82,82	2.83	9 (52%)
7	MPD	B	808	-	7,7,7	1.17	1 (14%)	9,10,10	1.60	2 (22%)
2	HEM	B	801	1	27,50,50	1.66	6 (22%)	17,82,82	2.63	9 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	B	805	-	1,3,3	7.66	1 (100%)	0,3,3	0.00	-

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	-	-	2/5/5/5	-
7	MPD	B	807	-	-	3/5/5/5	-
7	MPD	A	807	-	-	0/5/5/5	-
7	MPD	B	806	-	-	3/5/5/5	-
2	HEM	A	801	1	-	0/6/54/54	-
7	MPD	B	808	-	-	1/5/5/5	-
2	HEM	B	801	1	-	0/6/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	805	ACT	CH3-C	7.66	1.58	1.48
2	B	801	HEM	C4A-NA	4.94	1.46	1.36
2	B	801	HEM	C3B-C2B	-4.22	1.34	1.40
2	A	801	HEM	CMD-C2D	-3.54	1.44	1.51
2	A	801	HEM	CMA-C3A	3.44	1.58	1.51
2	A	801	HEM	C3B-CAB	-3.43	1.41	1.47
2	A	801	HEM	C3C-CAC	3.01	1.54	1.47
7	B	806	MPD	C3-C2	3.00	1.61	1.53
6	A	805	ACT	CH3-C	2.72	1.52	1.48
2	A	801	HEM	CAD-C3D	-2.69	1.47	1.52
2	A	801	HEM	CMB-C2B	2.52	1.57	1.51
2	B	801	HEM	C3C-C2C	-2.50	1.36	1.40
2	A	801	HEM	C1A-CHA	-2.47	1.34	1.41
7	B	808	MPD	C1-C2	2.39	1.59	1.52
2	A	801	HEM	C4B-CHC	-2.32	1.34	1.41
7	B	806	MPD	C1-C2	2.22	1.59	1.52
2	B	801	HEM	CAD-C3D	-2.12	1.48	1.52
2	B	801	HEM	C4D-C3D	2.10	1.47	1.42
2	B	801	HEM	C4A-CHB	-2.02	1.35	1.41
2	A	801	HEM	C1A-NA	2.01	1.40	1.36

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CAA-CBA-CGA	-7.23	100.55	112.67
2	B	801	HEM	CAA-CBA-CGA	-5.85	102.86	112.67
2	B	801	HEM	CAD-CBD-CGD	4.33	119.94	112.67
2	A	801	HEM	CMA-C3A-C4A	-3.76	122.68	128.46
2	A	801	HEM	CAD-CBD-CGD	3.71	118.89	112.67
2	B	801	HEM	C4C-C3C-C2C	-3.70	104.32	106.90
2	B	801	HEM	CMA-C3A-C4A	-3.63	122.89	128.46
2	A	801	HEM	CMB-C2B-C3B	3.44	131.11	124.68
7	A	807	MPD	O4-C4-C3	-3.06	99.01	111.36
2	B	801	HEM	CBD-CAD-C3D	3.00	118.01	112.48
2	A	801	HEM	C3C-C4C-NC	-2.92	105.43	110.94
7	B	808	MPD	O2-C2-C3	-2.91	98.88	109.80
7	B	807	MPD	O4-C4-C3	-2.80	100.06	111.36
7	B	807	MPD	O2-C2-C1	-2.74	99.30	108.08
2	B	801	HEM	CMA-C3A-C2A	2.67	129.98	124.94
7	B	807	MPD	C5-C4-C3	2.63	124.06	111.69
2	B	801	HEM	C1D-C2D-C3D	-2.51	105.25	107.00
2	A	801	HEM	C1D-C2D-C3D	-2.49	105.26	107.00
7	B	808	MPD	CM-C2-C1	-2.48	105.41	110.57
7	A	806	MPD	O4-C4-C3	-2.39	101.73	111.36
2	B	801	HEM	CBA-CAA-C2A	2.36	116.83	112.49
7	A	807	MPD	O4-C4-C5	2.21	118.97	109.38
2	A	801	HEM	CBA-CAA-C2A	2.20	116.54	112.49
7	A	806	MPD	O4-C4-C5	-2.19	99.88	109.38
7	B	807	MPD	CM-C2-C1	2.18	115.13	110.57
7	B	806	MPD	C1-C2-C3	2.12	119.81	109.96
2	A	801	HEM	CMA-C3A-C2A	2.07	128.85	124.94
7	A	806	MPD	C5-C4-C3	2.06	121.41	111.69
2	B	801	HEM	CMB-C2B-C3B	2.03	128.48	124.68
2	A	801	HEM	CMD-C2D-C3D	2.03	128.78	124.94

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	807	MPD	C2-C3-C4-C5
7	A	806	MPD	C2-C3-C4-O4
7	B	806	MPD	O2-C2-C3-C4
7	A	806	MPD	C2-C3-C4-C5
7	B	806	MPD	C2-C3-C4-C5
7	B	808	MPD	C2-C3-C4-C5
7	B	806	MPD	C1-C2-C3-C4
7	B	807	MPD	O2-C2-C3-C4

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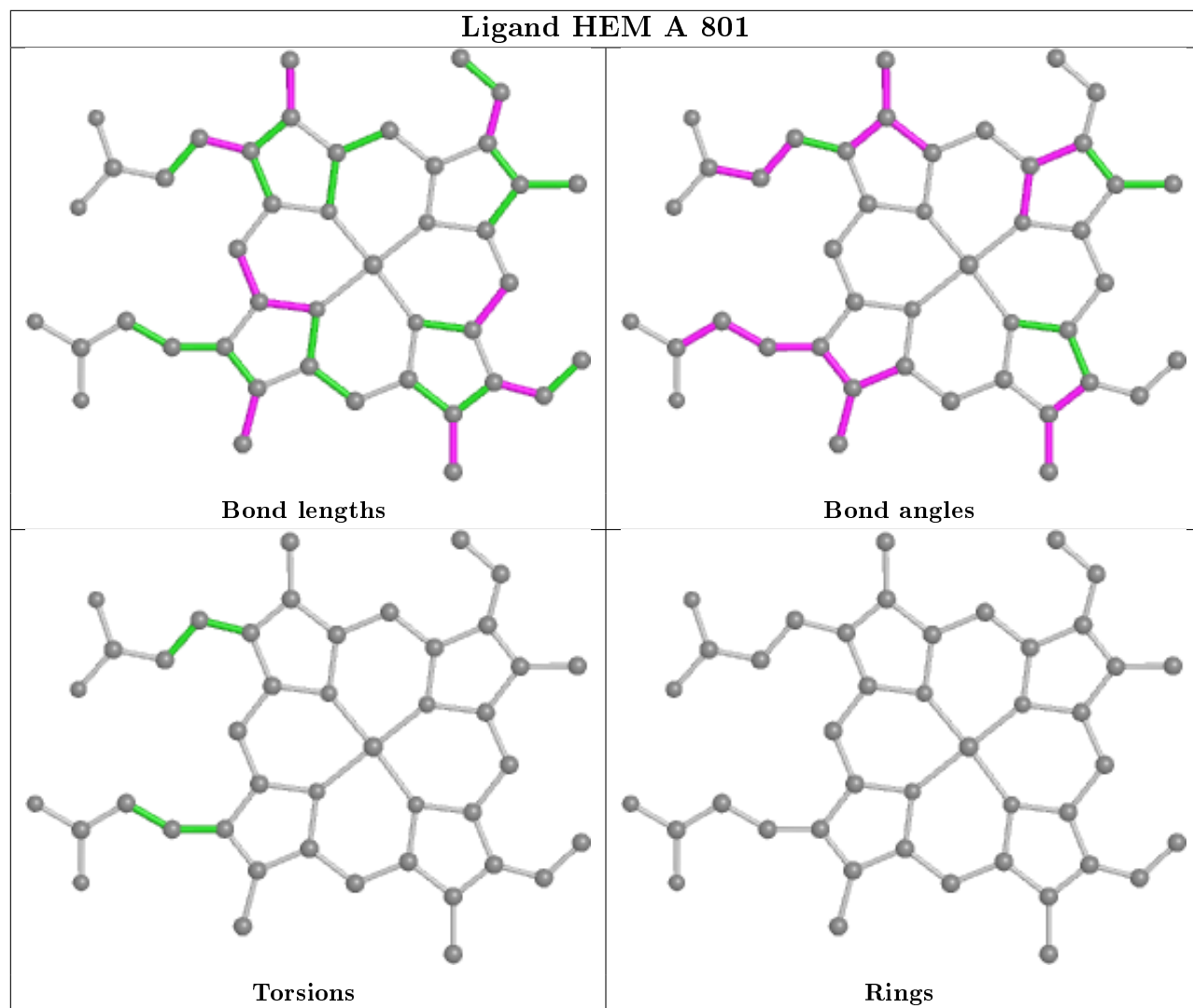
Mol	Chain	Res	Type	Atoms
7	B	807	MPD	C2-C3-C4-O4

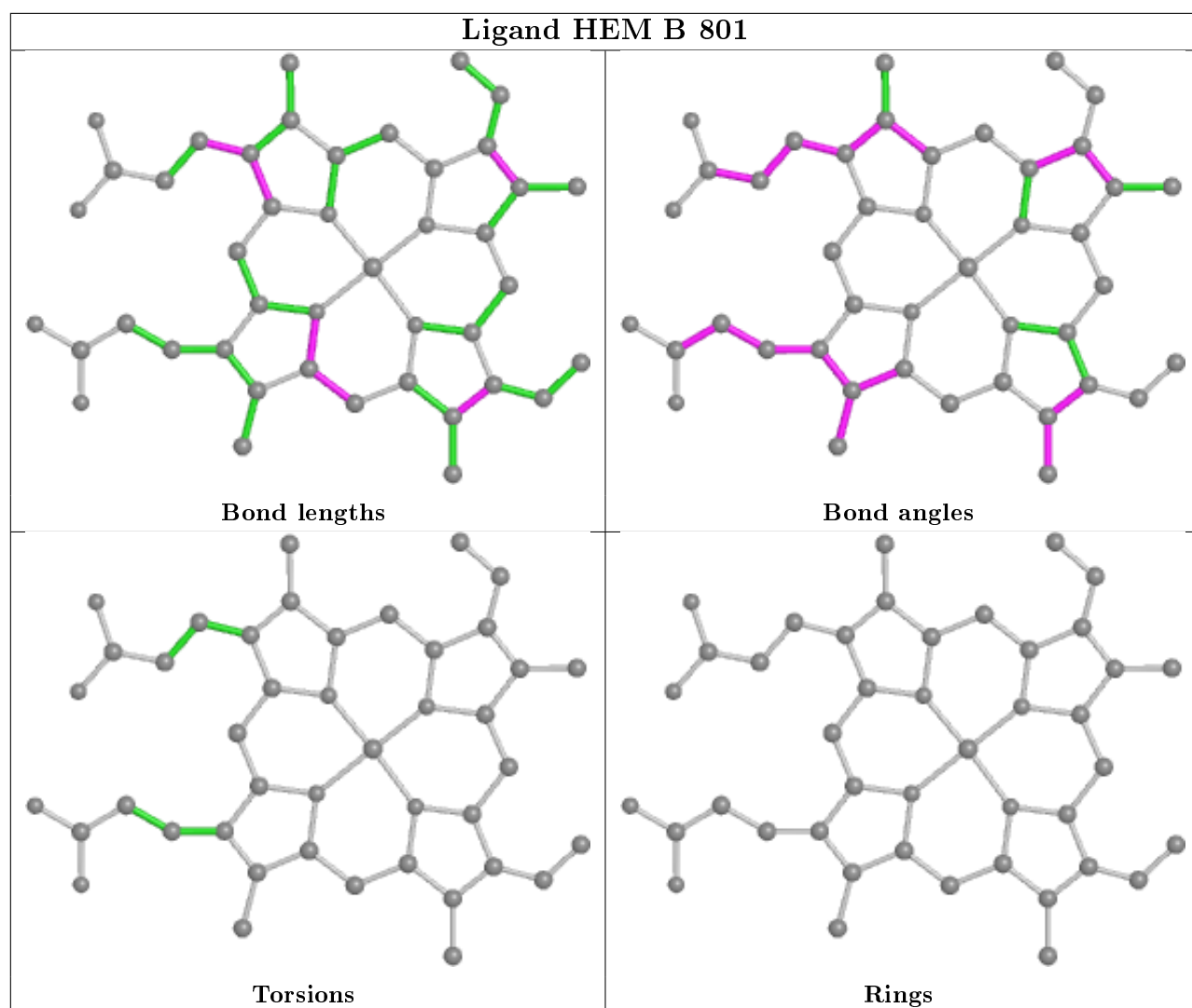
There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	805	ACT	6	0
5	B	804	OXY	2	0
5	A	804	OXY	3	0
7	B	807	MPD	2	0
7	A	807	MPD	2	0
7	A	806	MPD	3	0
7	B	806	MPD	8	0
6	B	805	ACT	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	713/728 (97%)	-0.34	18 (2%) 57 63	17, 25, 45, 92	0
1	B	713/728 (97%)	-0.38	11 (1%) 73 80	17, 24, 46, 90	0
All	All	1426/1456 (97%)	-0.36	29 (2%) 65 72	17, 24, 46, 92	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	7.0
1	B	748	ALA	6.3
1	B	680	ALA	4.5
1	B	610	ARG	4.4
1	A	680	ALA	3.8
1	A	540	ARG	3.7
1	A	679	ALA	3.5
1	B	679	ALA	3.5
1	B	540	ARG	3.5
1	B	541	GLY	3.3
1	B	53[A]	HIS	3.2
1	B	682	ALA	3.1
1	A	608	LYS	3.0
1	A	541	GLY	3.0
1	A	55	HIS	2.9
1	A	610	ARG	2.8
1	A	682	ALA	2.8
1	A	219	TYR	2.7
1	A	221	GLY	2.7
1	A	215	PRO	2.7
1	B	608	LYS	2.7
1	A	454	ASP	2.7
1	B	55	HIS	2.6
1	A	213	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	220	SER	2.6
1	B	366	GLY	2.4
1	A	222	ASP	2.3
1	A	542	GLY	2.2
1	A	212	SER	2.1

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 carbohydrates in this entry.

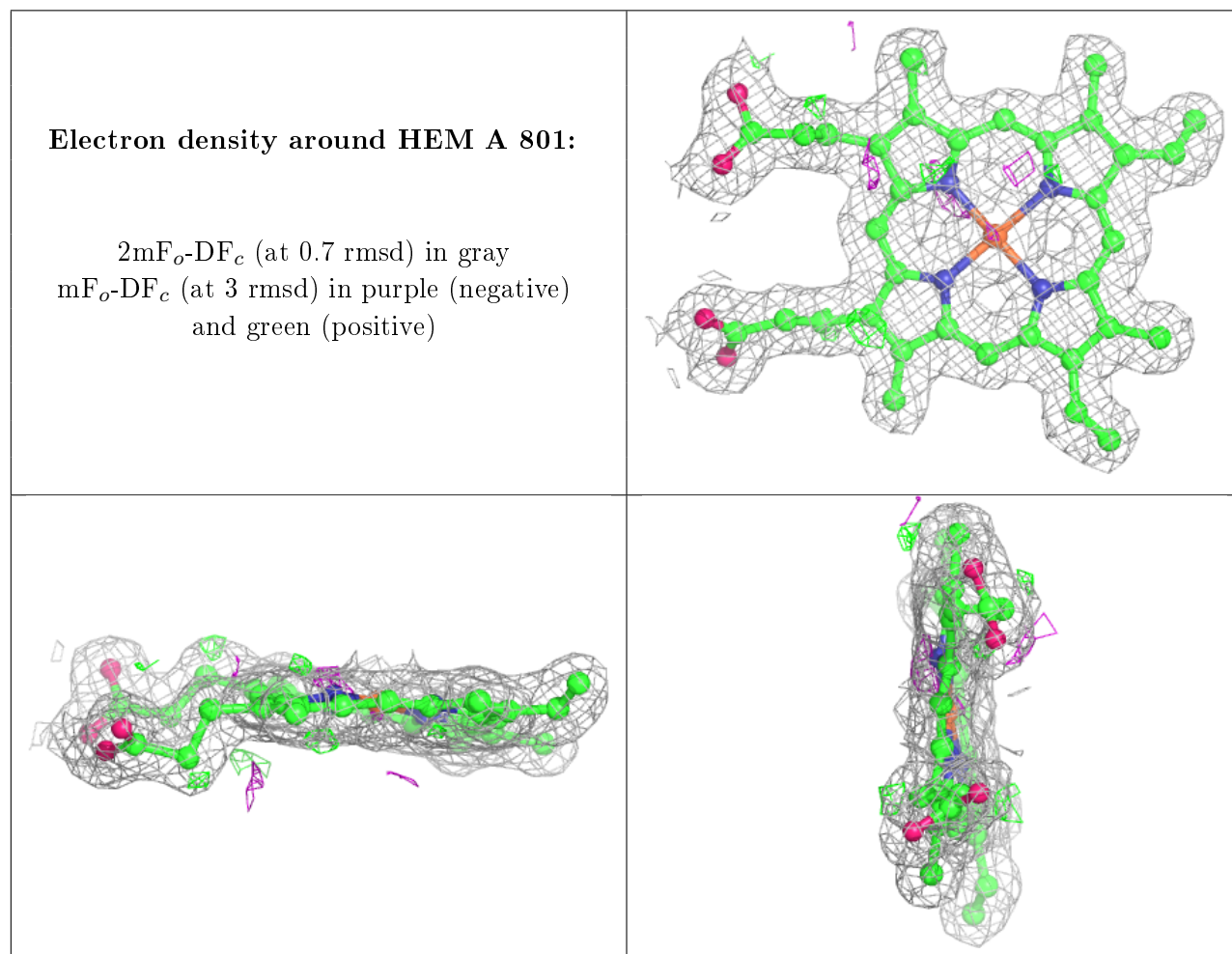
6.4 Ligands [i](#)

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	B	808	8/8	0.75	0.25	60,75,79,80	0
7	MPD	A	807	8/8	0.86	0.20	51,62,83,83	0
6	ACT	B	805	4/4	0.88	0.17	33,35,39,42	0
7	MPD	B	807	8/8	0.90	0.19	62,70,75,81	0
7	MPD	B	806	8/8	0.90	0.19	32,43,48,48	0
7	MPD	A	806	8/8	0.91	0.13	48,52,60,61	0
6	ACT	A	805	4/4	0.93	0.14	40,43,45,51	0
5	OXY	A	804	2/2	0.93	0.14	42,42,42,47	0
5	OXY	B	804	2/2	0.95	0.10	37,37,37,37	0
2	HEM	A	801	43/43	0.98	0.08	18,21,26,28	0
3	NA	A	802	1/1	0.99	0.04	22,22,22,22	0
3	NA	B	802	1/1	0.99	0.03	21,21,21,21	0
4	CL	A	803	1/1	0.99	0.04	38,38,38,38	0
2	HEM	B	801	43/43	0.99	0.09	16,18,22,25	0
4	CL	B	803	1/1	0.99	0.04	37,37,37,37	0

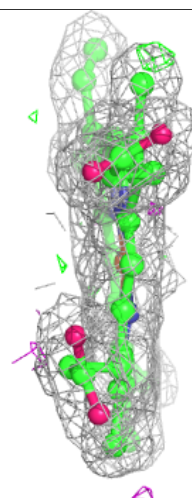
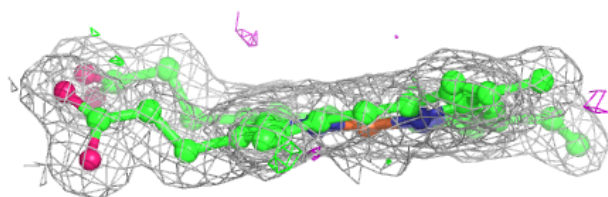
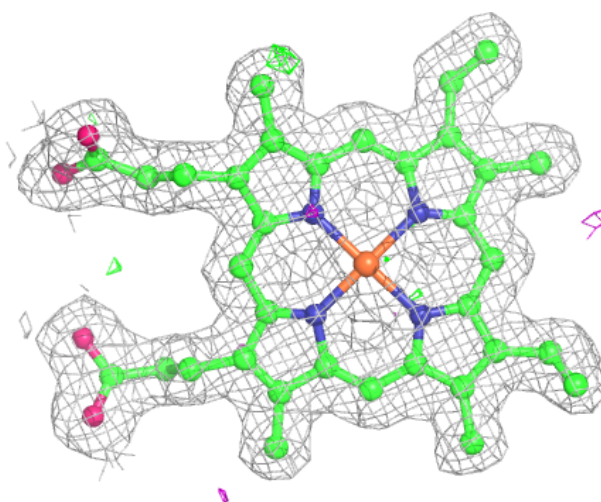
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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 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.