



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2026 – 11:38 PM EDT

PDB ID : 5KSF / pdb_00005ksf
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 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

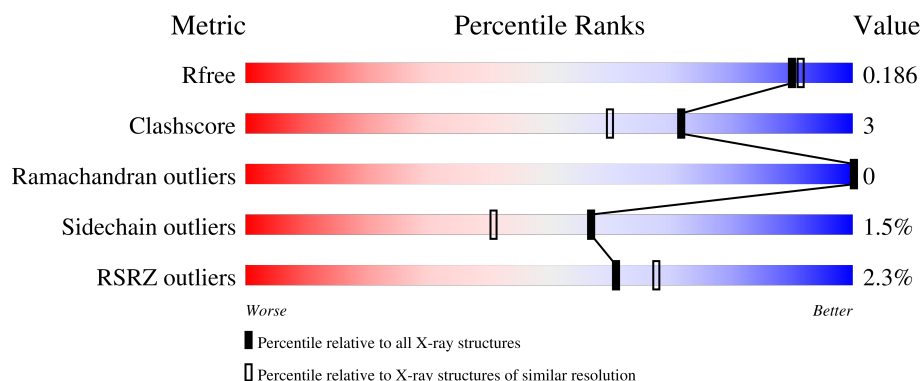
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 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	OXY	A	804	-	-	X	-
5	OXY	B	804	-	-	X	-
6	ACT	A	805	-	-	X	-
6	ACT	B	805	-	X	X	-
7	MPD	B	806	-	-	X	-
7	MPD	B	807	-	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.

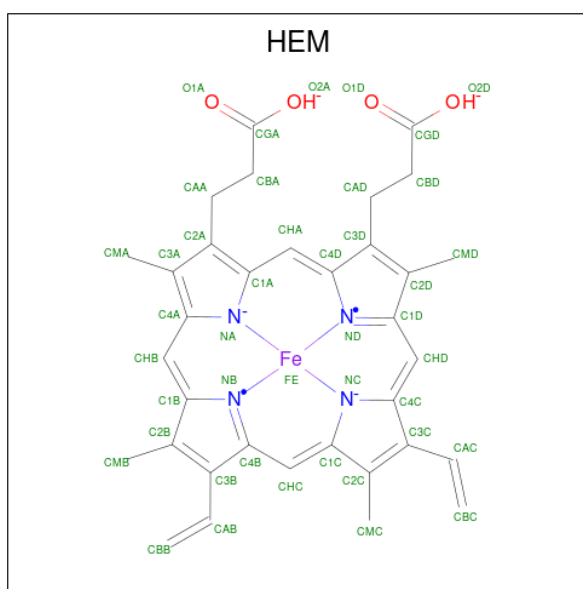
- Molecule 1 is a protein called Catalase-peroxidase.

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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

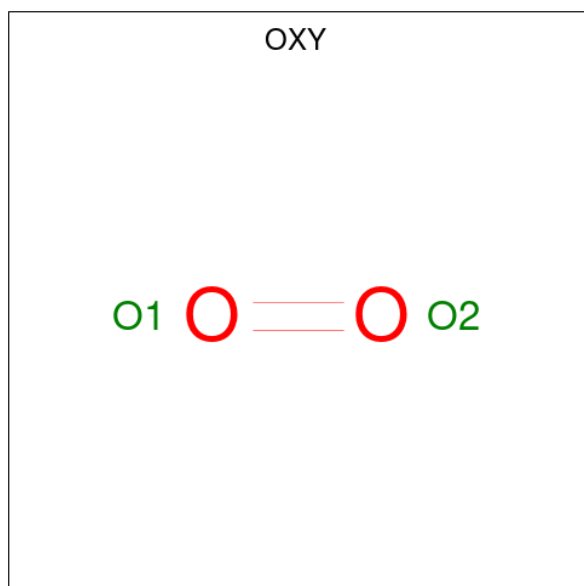
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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

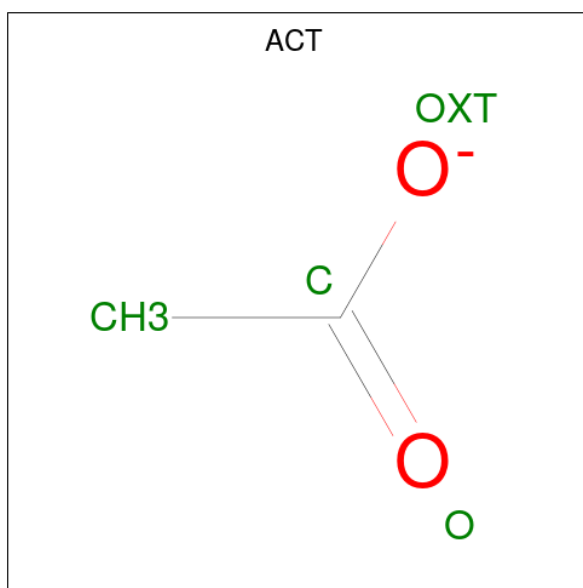
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl		
			1	1	0	0
4	B	1	Total	Cl		
			1	1	0	0

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



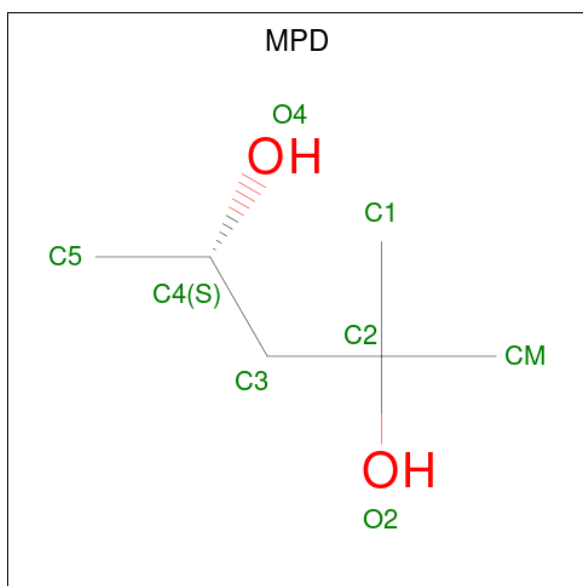
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	B	1	Total	O		
			2	2	0	0

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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 (CCD ID: MPD) (formula: $\text{C}_6\text{H}_{14}\text{O}_2$).



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

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

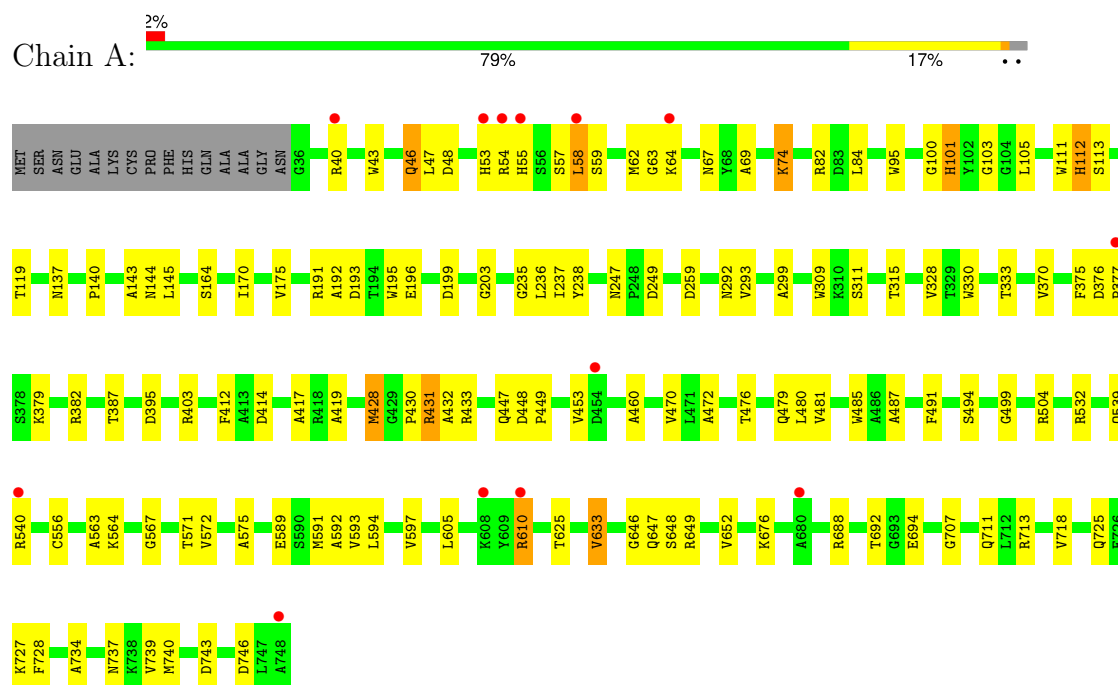
- Molecule 8 is water.

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

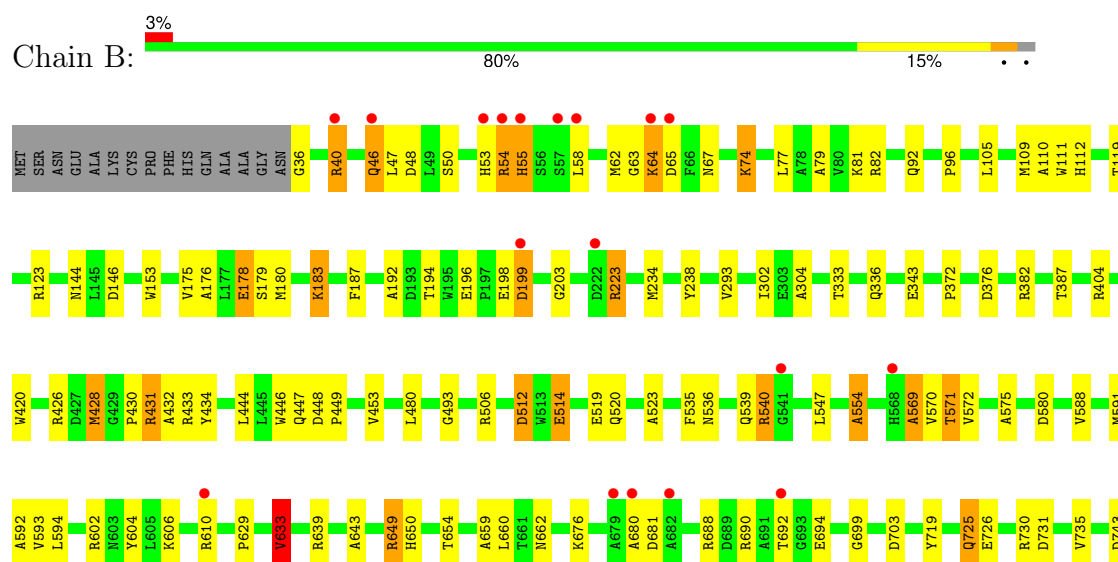
3 Residue-property plots

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	100.69Å 115.47Å 174.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 1.75 48.38 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.38-1.75) 99.4 (48.38-1.75)	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	10214 reflections (4.99%)	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 , 40.0	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: OXY, CL, NA, HEM, ACT, MPD

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	1.90	112/5698 (2.0%)	1.43	25/7746 (0.3%)
1	B	1.91	98/5714 (1.7%)	1.45	32/7768 (0.4%)
All	All	1.91	210/11412 (1.8%)	1.44	57/15514 (0.4%)

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 (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	694	GLU	CA-C	9.89	1.65	1.52
1	B	512	ASP	CG-OD2	9.78	1.44	1.25
1	B	540	ARG	C-O	9.60	1.38	1.23
1	A	563	ALA	N-CA	-9.39	1.34	1.46
1	A	203	GLY	C-O	8.82	1.30	1.23
1	A	82	ARG	CZ-NH2	-8.48	1.22	1.33
1	B	453	VAL	C-O	-8.34	1.14	1.24
1	B	602	ARG	CZ-NH2	-8.34	1.22	1.33
1	B	63	GLY	N-CA	8.33	1.56	1.45
1	A	688	ARG	CA-C	-8.31	1.43	1.52
1	A	59	SER	C-O	-8.26	1.13	1.24
1	B	179	SER	C-O	7.97	1.33	1.24
1	B	536	ASN	N-CA	-7.72	1.36	1.46
1	A	625	THR	CA-CB	7.70	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	74	LYS	CA-C	7.57	1.63	1.52
1	A	718	VAL	C-O	7.45	1.32	1.24
1	B	343	GLU	C-O	7.34	1.32	1.24
1	A	63	GLY	N-CA	7.30	1.54	1.45
1	A	711	GLN	CD-NE2	-7.26	1.18	1.33
1	B	535	PHE	CA-C	-7.25	1.43	1.52
1	B	633[A]	VAL	CA-CB	7.04	1.63	1.54
1	B	633[B]	VAL	CA-CB	7.04	1.63	1.54
1	A	725	GLN	CG-CD	6.96	1.69	1.52
1	A	532	ARG	NE-CZ	-6.95	1.25	1.33
1	A	676	LYS	CA-C	-6.92	1.45	1.52
1	B	333	THR	CA-C	6.91	1.61	1.52
1	A	480	LEU	CA-C	6.91	1.61	1.52
1	B	430	PRO	C-O	6.90	1.31	1.23
1	A	193	ASP	C-O	6.90	1.32	1.23
1	B	654	THR	N-CA	-6.89	1.37	1.45
1	A	315	THR	C-O	-6.67	1.15	1.24
1	B	420	TRP	CA-C	6.66	1.61	1.52
1	A	95	TRP	N-CA	6.61	1.55	1.46
1	B	449	PRO	CA-C	6.58	1.61	1.52
1	A	575	ALA	C-O	-6.57	1.17	1.24
1	B	192	ALA	N-CA	6.55	1.54	1.46
1	A	69	ALA	CA-C	-6.54	1.44	1.52
1	B	680	ALA	N-CA	6.54	1.54	1.46
1	A	494	SER	CA-C	6.53	1.61	1.52
1	B	681	ASP	CA-C	6.53	1.59	1.52
1	B	67	ASN	CA-C	6.51	1.60	1.52
1	A	328	VAL	C-O	6.51	1.30	1.24
1	A	113	SER	C-O	6.48	1.31	1.24
1	B	293	VAL	N-CA	6.47	1.54	1.46
1	B	40	ARG	N-CA	6.46	1.54	1.46
1	A	430	PRO	C-O	6.44	1.31	1.23
1	B	448	ASP	CA-CB	-6.37	1.48	1.52
1	B	178	GLU	CD-OE2	6.37	1.37	1.25
1	B	592	ALA	CA-C	-6.36	1.43	1.52
1	B	703	ASP	N-CA	-6.33	1.38	1.46
1	A	647	GLN	CA-C	6.28	1.61	1.53
1	B	448	ASP	N-CA	6.25	1.50	1.46
1	A	414	ASP	N-CA	6.22	1.53	1.46
1	B	376	ASP	N-CA	6.22	1.54	1.46
1	B	47	LEU	CB-CG	-6.21	1.41	1.53
1	A	330	TRP	N-CA	-6.21	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	MET	N-CA	6.20	1.54	1.46
1	A	236	LEU	CA-C	6.20	1.61	1.53
1	B	178	GLU	CD-OE1	6.17	1.37	1.25
1	A	311	SER	CA-C	6.13	1.59	1.52
1	A	728	PHE	CG-CD2	-6.12	1.25	1.38
1	A	203	GLY	N-CA	6.12	1.51	1.45
1	A	692	THR	N-CA	6.09	1.54	1.46
1	A	740	MET	C-O	-6.08	1.16	1.24
1	A	417	ALA	CA-C	6.08	1.60	1.52
1	A	299	ALA	N-CA	6.05	1.54	1.46
1	A	556	CYS	CA-C	6.03	1.60	1.52
1	B	726	GLU	CD-OE1	6.03	1.36	1.25
1	B	725	GLN	CD-OE1	6.02	1.34	1.23
1	A	382	ARG	CA-C	6.00	1.60	1.52
1	A	532	ARG	CD-NE	5.99	1.54	1.46
1	A	62	MET	C-N	-5.99	1.24	1.33
1	A	589	GLU	CD-OE1	5.98	1.36	1.25
1	B	643	ALA	N-CA	-5.98	1.38	1.46
1	B	676	LYS	C-O	-5.93	1.17	1.24
1	B	446	TRP	CZ2-CH2	-5.93	1.25	1.37
1	A	448	ASP	C-O	5.93	1.26	1.23
1	B	203	GLY	N-CA	5.92	1.51	1.45
1	B	304	ALA	N-CA	5.90	1.54	1.46
1	B	79	ALA	C-O	5.90	1.30	1.24
1	A	74	LYS	CA-C	5.90	1.60	1.52
1	B	187	PHE	N-CA	-5.89	1.39	1.46
1	A	491	PHE	C-O	5.88	1.30	1.23
1	A	460	ALA	C-O	5.85	1.31	1.24
1	B	523	ALA	C-O	5.84	1.30	1.24
1	A	572	VAL	N-CA	-5.83	1.39	1.46
1	A	743	ASP	CG-OD2	5.83	1.36	1.25
1	A	739	VAL	CA-CB	-5.82	1.47	1.54
1	A	137	ASN	N-CA	-5.82	1.38	1.46
1	B	387	THR	C-O	5.81	1.30	1.24
1	A	46	GLN	N-CA	5.80	1.53	1.45
1	B	123	ARG	CZ-NH2	5.79	1.41	1.33
1	A	692	THR	CA-C	-5.78	1.45	1.52
1	A	376	ASP	N-CA	5.77	1.53	1.46
1	A	292	ASN	CA-C	5.77	1.60	1.52
1	A	540	ARG	C-O	5.77	1.31	1.23
1	A	491	PHE	CA-C	-5.76	1.45	1.52
1	A	47	LEU	CB-CG	-5.76	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	646	GLY	C-O	-5.75	1.16	1.23
1	B	36	GLY	N-CA	5.75	1.54	1.45
1	A	375	PHE	C-O	-5.72	1.17	1.24
1	B	659	ALA	N-CA	-5.72	1.39	1.46
1	A	67	ASN	CA-C	5.72	1.59	1.52
1	A	370	VAL	C-O	-5.72	1.17	1.24
1	A	259	ASP	CA-C	5.72	1.60	1.52
1	B	493	GLY	C-N	-5.71	1.26	1.33
1	B	105	LEU	CA-C	5.70	1.60	1.52
1	B	431	ARG	N-CA	5.69	1.53	1.46
1	A	105	LEU	N-CA	-5.68	1.39	1.46
1	A	564	LYS	C-O	5.67	1.30	1.24
1	B	575	ALA	C-O	-5.67	1.19	1.25
1	A	648	SER	N-CA	-5.67	1.38	1.46
1	A	237	ILE	C-O	5.66	1.30	1.24
1	A	247	ASN	CG-ND2	-5.66	1.21	1.33
1	B	372	PRO	CA-C	-5.65	1.45	1.52
1	A	377	PRO	C-O	-5.64	1.16	1.24
1	B	434	TYR	N-CA	5.64	1.53	1.46
1	B	606	LYS	N-CA	5.64	1.53	1.46
1	B	175	VAL	CA-C	5.63	1.60	1.52
1	B	176	ALA	CA-CB	-5.63	1.44	1.53
1	A	175	VAL	CA-C	5.63	1.60	1.52
1	A	453	VAL	C-O	-5.63	1.17	1.24
1	B	65	ASP	CG-OD1	5.61	1.35	1.25
1	B	650	HIS	CA-CB	-5.60	1.44	1.53
1	B	431	ARG	C-O	5.59	1.31	1.24
1	A	145	LEU	N-CA	5.59	1.53	1.46
1	B	431	ARG	CD-NE	5.57	1.54	1.46
1	A	101	HIS	ND1-CE1	5.57	1.38	1.32
1	B	77	LEU	CA-CB	-5.55	1.44	1.53
1	B	731	ASP	N-CA	-5.53	1.39	1.46
1	A	571	THR	CA-C	5.52	1.59	1.52
1	B	64	LYS	CA-C	5.51	1.60	1.52
1	A	734	ALA	N-CA	-5.50	1.39	1.46
1	A	737	ASN	CA-C	5.50	1.59	1.52
1	B	699	GLY	N-CA	5.50	1.51	1.45
1	B	336	GLN	CA-C	-5.49	1.45	1.52
1	B	46	GLN	N-CA	5.49	1.53	1.45
1	A	84	LEU	C-O	-5.49	1.17	1.24
1	A	100	GLY	C-O	-5.48	1.16	1.23
1	B	512	ASP	CB-CG	5.46	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	604	TYR	C-O	5.46	1.30	1.24
1	B	446	TRP	NE1-CE2	-5.42	1.31	1.37
1	A	476	THR	N-CA	-5.42	1.39	1.45
1	A	743	ASP	C-O	5.40	1.31	1.24
1	A	649	ARG	CZ-NH2	5.39	1.40	1.33
1	A	592	ALA	CA-CB	5.35	1.61	1.53
1	A	293	VAL	C-O	-5.33	1.18	1.24
1	A	479	GLN	C-N	-5.33	1.26	1.33
1	B	96	PRO	CA-CB	5.33	1.61	1.53
1	B	434	TYR	CA-C	-5.33	1.45	1.52
1	A	191	ARG	N-CA	5.33	1.52	1.46
1	B	575	ALA	CA-CB	-5.31	1.46	1.53
1	B	694	GLU	N-CA	-5.31	1.39	1.46
1	A	387	THR	CA-C	5.31	1.59	1.52
1	A	403	ARG	N-CA	-5.31	1.39	1.46
1	B	82	ARG	CZ-NH2	-5.30	1.26	1.33
1	A	403	ARG	CD-NE	5.29	1.53	1.46
1	B	547	LEU	N-CA	-5.29	1.39	1.46
1	B	660	LEU	C-O	5.29	1.30	1.23
1	B	110	ALA	C-O	5.28	1.30	1.24
1	A	449	PRO	CA-C	5.28	1.59	1.52
1	A	196	GLU	CG-CD	5.28	1.65	1.52
1	B	743	ASP	N-CA	-5.28	1.39	1.46
1	B	639	ARG	CD-NE	-5.26	1.38	1.46
1	A	448	ASP	N-CA	5.26	1.50	1.46
1	A	694	GLU	CA-C	5.26	1.59	1.52
1	A	57	SER	C-O	-5.25	1.17	1.24
1	A	688	ARG	N-CA	5.19	1.52	1.45
1	B	404	ARG	N-CA	-5.19	1.40	1.46
1	A	487	ALA	N-CA	-5.18	1.40	1.46
1	A	610	ARG	CA-CB	5.18	1.61	1.53
1	A	499	GLY	C-O	5.17	1.29	1.23
1	B	746	ASP	C-O	-5.17	1.17	1.24
1	A	170	ILE	C-O	5.16	1.30	1.24
1	B	198	GLU	CD-OE2	5.16	1.35	1.25
1	A	192	ALA	N-CA	5.15	1.52	1.46
1	B	203	GLY	C-O	5.14	1.27	1.23
1	B	92	GLN	C-O	5.14	1.29	1.23
1	A	419	ALA	C-N	-5.13	1.27	1.33
1	A	247	ASN	C-O	5.13	1.30	1.24
1	B	67	ASN	CG-ND2	-5.13	1.22	1.33
1	A	481	VAL	C-O	5.12	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	MET	C-O	5.11	1.29	1.24
1	B	196	GLU	CG-CD	5.11	1.64	1.52
1	A	485	TRP	CA-C	-5.11	1.46	1.52
1	A	431	ARG	N-CA	5.11	1.52	1.46
1	A	195	TRP	C-O	-5.10	1.17	1.24
1	A	746	ASP	N-CA	5.10	1.52	1.46
1	B	234	MET	CA-CB	-5.10	1.45	1.53
1	A	727	LYS	C-N	-5.09	1.27	1.33
1	A	333	THR	CA-C	5.09	1.58	1.52
1	B	692	THR	CA-C	-5.09	1.46	1.52
1	A	567	GLY	CA-C	-5.08	1.44	1.51
1	A	652	VAL	CA-C	-5.08	1.46	1.52
1	B	572	VAL	C-N	-5.08	1.26	1.33
1	B	580	ASP	C-O	-5.06	1.17	1.24
1	A	164	SER	CA-CB	-5.06	1.45	1.53
1	B	180	MET	CA-CB	-5.06	1.45	1.53
1	B	571	THR	CA-CB	5.06	1.62	1.53
1	B	688	ARG	N-CA	5.06	1.52	1.45
1	A	713	ARG	N-CA	-5.05	1.39	1.46
1	B	746	ASP	N-CA	5.05	1.52	1.46
1	A	249	ASP	CA-C	5.04	1.59	1.52
1	B	514	GLU	C-O	-5.04	1.18	1.24
1	B	588	VAL	N-CA	-5.04	1.40	1.46
1	A	428	MET	CG-SD	-5.03	1.68	1.80
1	A	235	GLY	CA-C	5.02	1.58	1.51
1	B	444	LEU	N-CA	-5.02	1.39	1.45
1	A	472	ALA	N-CA	5.01	1.52	1.46
1	A	597	VAL	N-CA	-5.00	1.40	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	GLN	N-CA-C	-7.71	99.63	110.50
1	B	46	GLN	N-CA-C	-7.40	100.76	110.53
1	B	62	MET	CA-C-N	-7.27	112.31	120.53
1	B	62	MET	C-N-CA	-7.27	112.31	120.53
1	A	47	LEU	N-CA-CB	-7.27	98.85	109.83
1	B	428	MET	CA-CB-CG	-6.99	100.13	114.10
1	A	432	ALA	N-CA-C	6.94	119.69	111.71
1	A	62	MET	CA-C-N	-6.66	113.00	120.53
1	A	62	MET	C-N-CA	-6.66	113.00	120.53
1	B	569	ALA	N-CA-C	-6.55	98.95	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	514	GLU	N-CA-C	6.53	119.23	111.33
1	B	432	ALA	N-CA-C	6.42	119.09	111.71
1	A	48	ASP	N-CA-C	6.40	119.14	108.20
1	B	55	HIS	CB-CA-C	6.37	121.26	111.39
1	A	55	HIS	CB-CA-C	6.32	121.19	111.39
1	A	470	VAL	N-CA-C	-6.28	104.63	110.53
1	A	403	ARG	CG-CD-NE	6.27	125.80	112.00
1	B	48	ASP	N-CA-C	6.25	118.89	108.20
1	A	46	GLN	CA-CB-CG	6.19	126.48	114.10
1	A	707	GLY	O-C-N	6.13	127.80	121.97
1	A	395	ASP	N-CA-C	-6.01	102.21	109.72
1	A	417	ALA	N-CA-C	-5.99	104.83	111.36
1	B	690	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	A	112	HIS	N-CA-C	5.89	118.49	111.71
1	B	178	GLU	CG-CD-OE2	-5.87	104.90	118.40
1	A	633	VAL	CG1-CB-CG2	-5.80	98.05	110.80
1	B	47	LEU	N-CA-CB	-5.77	101.48	109.97
1	B	571	THR	CA-C-N	-5.76	117.74	123.04
1	B	571	THR	C-N-CA	-5.76	117.74	123.04
1	B	46	GLN	N-CA-CB	5.73	118.55	110.36
1	A	58	LEU	CA-C-O	-5.70	114.84	120.82
1	B	382	ARG	CG-CD-NE	-5.68	99.50	112.00
1	B	46	GLN	CB-CG-CD	5.68	122.25	112.60
1	B	512	ASP	CB-CG-OD1	-5.65	105.40	118.40
1	B	46	GLN	CA-CB-CG	5.62	125.34	114.10
1	B	223	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	A	412	PHE	CA-CB-CG	5.58	119.38	113.80
1	B	554	ALA	CA-C-N	5.56	126.11	119.94
1	B	554	ALA	C-N-CA	5.56	126.11	119.94
1	B	571	THR	CB-CA-C	5.55	119.87	109.71
1	A	592	ALA	N-CA-C	5.52	118.01	111.33
1	B	153	TRP	CA-C-N	-5.47	112.98	119.05
1	B	153	TRP	C-N-CA	-5.47	112.98	119.05
1	B	333	THR	O-C-N	5.46	125.81	121.17
1	A	727	LYS	N-CA-C	5.42	117.18	111.28
1	A	144	ASN	CA-CB-CG	-5.39	107.21	112.60
1	B	194	THR	N-CA-C	-5.35	101.63	109.81
1	A	46	GLN	CB-CG-CD	5.34	121.68	112.60
1	A	46	GLN	N-CA-CB	5.30	117.81	110.17
1	B	735	VAL	N-CA-C	5.30	116.03	110.62
1	B	302	ILE	CB-CA-C	5.28	119.27	112.14
1	B	54	ARG	N-CA-C	-5.08	102.46	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	605	LEU	CB-CA-C	-5.07	103.23	110.62
1	A	43	TRP	CA-C-N	-5.06	114.61	119.87
1	A	43	TRP	C-N-CA	-5.06	114.61	119.87
1	B	535	PHE	N-CA-C	5.04	116.47	111.07
1	B	519	GLU	CB-CA-C	-5.03	102.31	110.85

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	40	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	14	0
All	All	12667	0	10888	73	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 (73) 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:H52	7:B:806:MPD:C1	2.25	0.67
1:A:101:HIS:HD2	1:A:103:GLY:N	1.90	0.66
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:C5	7:B:807:MPD:O2	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:H52	7:A:806:MPD:H11	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:HM2	7:A:806:MPD:C5	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:53[B]:HIS:O	1:B:53[B]:HIS:CG	2.72	0.42
1:B:54:ARG:NE	1:B:199:ASP:OD2	2.47	0.42
1:A:119[B]:THR:CG2	1:A:593:VAL:HG11	2.48	0.42
1:A:143:ALA:HA	1:A:309:TRP:CH2	2.54	0.42
7:B:806:MPD:H12	7:B:806:MPD:H52	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:B:81:LYS:NZ	8:B:906:HOH:O	2.34	0.40
1:A:428:MET:O	1:A:433:ARG:HD3	2.21	0.40
1:B:74:LYS:HE3	8:B:1251:HOH:O	2.20	0.40
1:B:111:TRP:HZ3	1:B:238:TYR:HH	1.68	0.40
1:B:223:ARG:HH11	1:B:223:ARG:HD2	1.62	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%)	549 (99%)	6 (1%)	65	52
1	B	557/560 (100%)	545 (98%)	12 (2%)	45	26
All	All	1112/1120 (99%)	1094 (98%)	18 (2%)	57	38

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	379	LYS
1	A	610	ARG
1	A	633	VAL
1	B	40	ARG
1	B	46	GLN

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Mol	Chain	Res	Type
1	B	64	LYS
1	B	183	LYS
1	B	540	ARG
1	B	571	THR
1	B	610	ARG
1	B	633[A]	VAL
1	B	633[B]	VAL
1	B	649[A]	ARG
1	B	649[B]	ARG
1	B	730[B]	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	101	HIS
1	A	247	ASN
1	A	647	GLN
1	A	737	ASN
1	B	55	HIS
1	B	544	GLN
1	B	650	HIS
1	B	725	GLN

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 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
5	OXY	A	804	-	1,1,1	0.07	0	-		
6	ACT	B	805	-	3,3,3	3.46	3 (100%)	3,3,3	4.22	2 (66%)
7	MPD	A	806	-	7,7,7	0.63	0	9,10,10	1.48	3 (33%)
7	MPD	B	806	-	7,7,7	1.54	2 (28%)	9,10,10	1.25	1 (11%)
2	HEM	A	801	1	50,50,50	1.95	16 (32%)	67,82,82	1.78	14 (20%)
6	ACT	A	805	-	3,3,3	2.28	1 (33%)	3,3,3	1.25	0
7	MPD	A	807	-	7,7,7	1.04	1 (14%)	9,10,10	1.64	2 (22%)
2	HEM	B	801	1	50,50,50	1.72	11 (22%)	67,82,82	1.58	13 (19%)
5	OXY	B	804	-	1,1,1	0.40	0	-		
7	MPD	B	807	-	7,7,7	0.61	0	9,10,10	1.95	5 (55%)
7	MPD	B	808	-	7,7,7	1.22	1 (14%)	9,10,10	1.56	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
7	MPD	A	806	-	-	4/5/5/5	-
7	MPD	B	806	-	-	3/5/5/5	-
2	HEM	A	801	1	-	2/14/54/54	-
7	MPD	A	807	-	-	1/5/5/5	-
2	HEM	B	801	1	-	2/14/54/54	-
7	MPD	B	807	-	-	5/5/5/5	-
7	MPD	B	808	-	-	1/5/5/5	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C1B-NB	-4.62	1.32	1.40
2	A	801	HEM	FE-NB	4.56	2.08	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1C-NC	-4.18	1.31	1.39
2	A	801	HEM	CMA-C3A	3.92	1.58	1.50
6	B	805	ACT	O-C	3.91	1.39	1.22
6	B	805	ACT	OXT-C	3.87	1.48	1.30
6	A	805	ACT	O-C	3.83	1.38	1.22
2	A	801	HEM	C4A-NA	-3.76	1.32	1.39
2	B	801	HEM	C1A-NA	-3.71	1.32	1.39
2	B	801	HEM	C4A-NA	3.57	1.46	1.39
2	A	801	HEM	FE-NC	3.36	2.06	1.95
2	A	801	HEM	CMB-C2B	3.31	1.57	1.50
2	A	801	HEM	CMD-C2D	-3.16	1.44	1.50
2	B	801	HEM	C1B-NB	-2.96	1.35	1.40
2	B	801	HEM	CHA-C1A	2.88	1.45	1.39
7	B	806	MPD	C3-C2	2.62	1.61	1.54
2	B	801	HEM	C4C-NC	2.61	1.44	1.39
7	B	808	MPD	C1-C2	2.54	1.59	1.52
2	A	801	HEM	C1C-NC	-2.51	1.34	1.39
2	B	801	HEM	FE-NB	2.50	2.02	1.94
2	B	801	HEM	CHD-C4C	-2.49	1.33	1.38
2	A	801	HEM	CAC-C3C	2.47	1.54	1.47
2	A	801	HEM	CAB-C3B	-2.41	1.41	1.47
6	B	805	ACT	CH3-C	2.39	1.58	1.49
2	B	801	HEM	C4D-ND	-2.38	1.36	1.40
2	A	801	HEM	CHA-C1A	-2.36	1.34	1.39
7	B	806	MPD	C1-C2	2.35	1.59	1.52
2	A	801	HEM	C2A-C3A	-2.31	1.32	1.38
2	A	801	HEM	FE-NA	2.28	2.02	1.95
2	B	801	HEM	C4B-NB	-2.28	1.34	1.38
2	A	801	HEM	CHB-C4A	2.23	1.44	1.39
2	B	801	HEM	CHC-C1C	2.11	1.42	1.38
7	A	807	MPD	C5-C4	2.05	1.60	1.51
2	A	801	HEM	CHC-C4B	-2.04	1.34	1.39
2	A	801	HEM	C3B-C2B	2.00	1.41	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	805	ACT	O-C-CH3	-5.45	100.18	122.53
2	A	801	HEM	CAA-CBA-CGA	-4.95	100.55	113.67
6	B	805	ACT	OXT-C-CH3	4.87	135.49	115.05
2	A	801	HEM	CHC-C1C-NC	4.10	128.92	124.45
2	A	801	HEM	C4B-C3B-C2B	-4.08	103.53	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CAA-CBA-CGA	-4.07	102.86	113.67
2	A	801	HEM	C4C-NC-C1C	3.97	112.29	105.82
2	A	801	HEM	O2A-CGA-CBA	3.72	125.77	114.00
2	B	801	HEM	CHA-C4D-ND	3.59	128.81	124.37
2	B	801	HEM	CHC-C4B-NB	3.25	127.92	124.42
2	B	801	HEM	CHA-C4D-C3D	-3.13	119.46	125.23
7	A	807	MPD	O4-C4-C3	-3.10	99.01	111.35
2	A	801	HEM	C4D-ND-C1D	-2.94	101.73	105.21
2	B	801	HEM	C4C-C3C-C2C	-2.88	104.32	106.81
7	B	807	MPD	O4-C4-C3	-2.84	100.06	111.35
7	B	807	MPD	O2-C2-C1	-2.79	99.30	107.99
7	B	808	MPD	O2-C2-C3	-2.78	98.88	109.27
2	A	801	HEM	O1A-CGA-CBA	-2.76	114.34	123.09
2	B	801	HEM	C1C-CHC-C4B	-2.72	120.24	126.02
2	A	801	HEM	CMB-C2B-C1B	-2.72	120.79	125.03
7	B	807	MPD	C5-C4-C3	2.67	124.06	111.67
2	A	801	HEM	C2D-C1D-ND	2.55	112.85	109.90
2	A	801	HEM	CAD-C3D-C2D	-2.52	123.15	127.87
7	A	806	MPD	O4-C4-C3	-2.42	101.73	111.35
2	B	801	HEM	CAD-CBD-CGD	2.37	119.94	113.67
2	A	801	HEM	C2A-C1A-NA	-2.36	107.53	110.15
2	B	801	HEM	C2A-C1A-NA	2.35	112.75	110.15
7	B	808	MPD	CM-C2-C1	-2.33	105.41	110.63
2	B	801	HEM	C1A-CHA-C4D	-2.27	120.92	126.25
7	B	806	MPD	C1-C2-C3	2.23	119.81	110.20
2	A	801	HEM	C2B-C1B-NB	2.23	112.40	109.84
7	A	806	MPD	O4-C4-C5	-2.22	99.88	109.45
2	B	801	HEM	C3A-C4A-NA	-2.22	106.58	110.14
7	A	807	MPD	O4-C4-C5	2.21	118.97	109.45
2	A	801	HEM	CAD-C3D-C4D	2.16	128.46	124.70
2	A	801	HEM	CHB-C1B-NB	-2.14	121.72	124.37
2	B	801	HEM	CHD-C4C-C3C	-2.10	121.66	125.21
2	B	801	HEM	CHC-C1C-NC	-2.10	122.16	124.45
7	A	806	MPD	C5-C4-C3	2.10	121.41	111.67
7	B	807	MPD	O2-C2-C3	2.06	116.98	109.27
2	B	801	HEM	CMA-C3A-C2A	2.05	129.98	125.62
7	B	807	MPD	CM-C2-C1	2.01	115.13	110.63

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

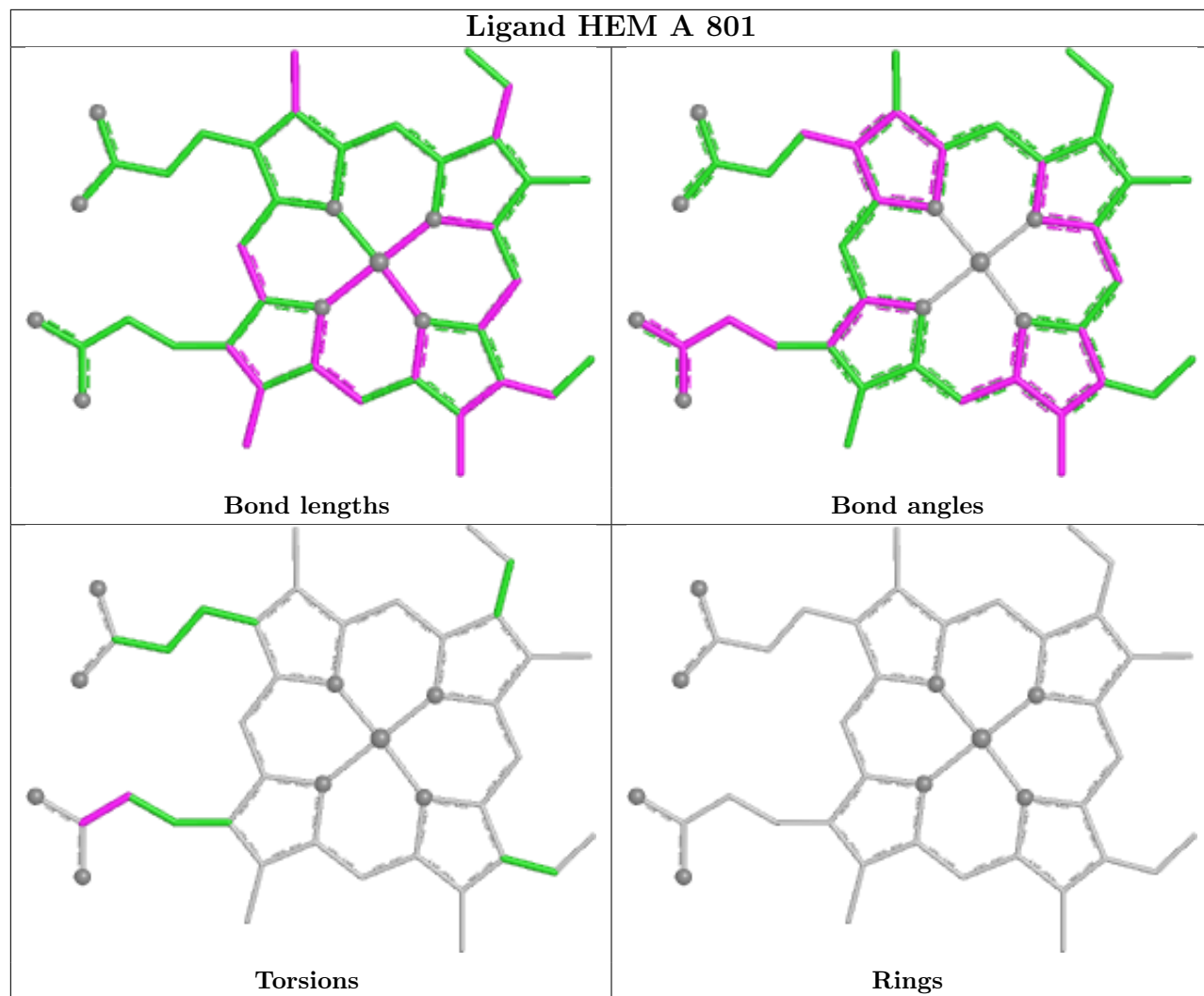
There are no ring outliers.

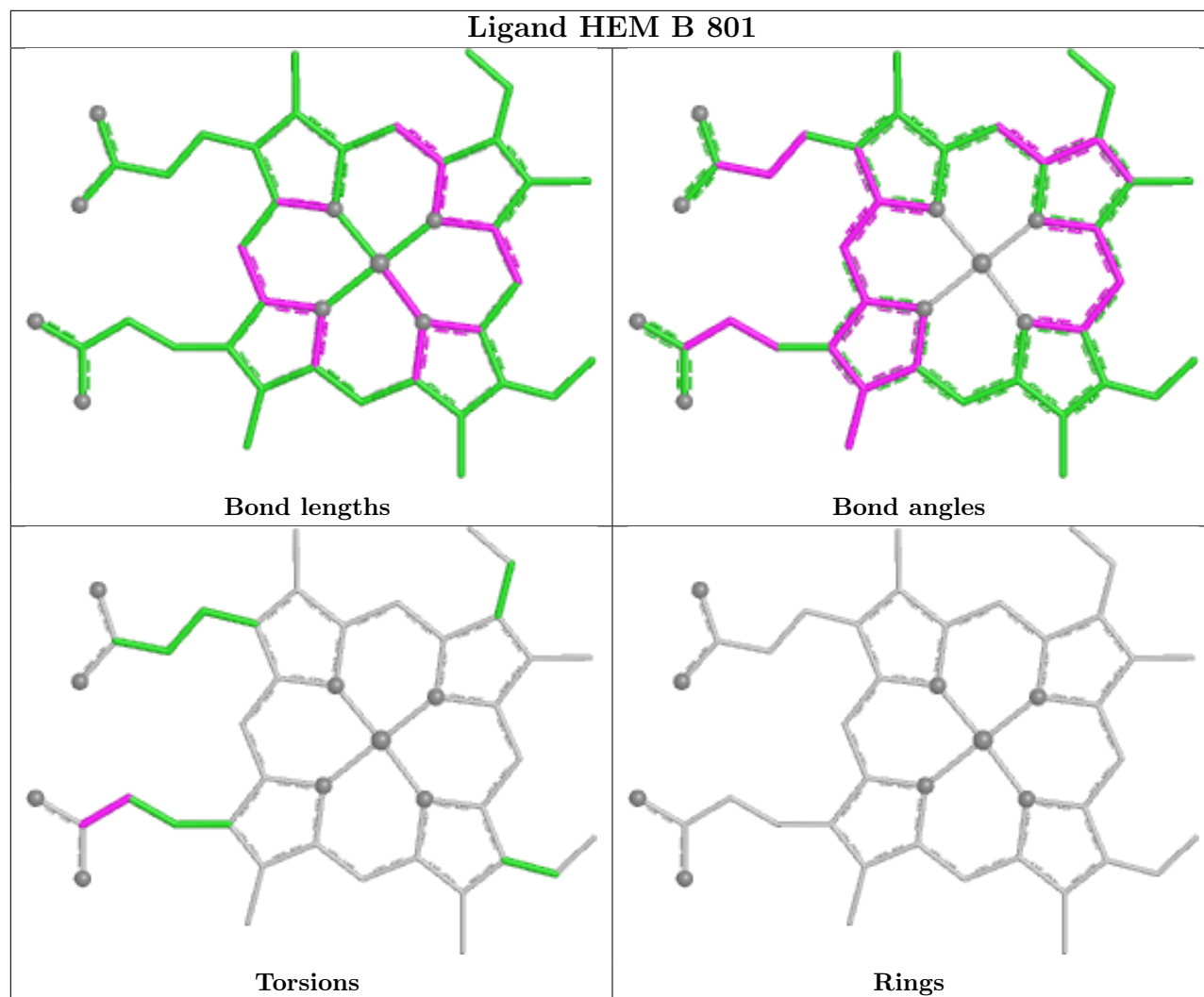
8 monomers are involved in 24 short contacts:

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

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

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	713/728 (97%)	-0.18	13 (1%) 67 74	14, 24, 45, 92	6 (0%)
1	B	713/728 (97%)	-0.25	20 (2%) 55 61	13, 24, 46, 90	8 (1%)
All	All	1426/1456 (97%)	-0.21	33 (2%) 61 67	13, 24, 46, 92	14 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	5.7
1	B	748	ALA	5.6
1	A	53	HIS	5.2
1	A	55	HIS	4.9
1	B	53[A]	HIS	4.3
1	B	55	HIS	4.3
1	B	679	ALA	3.6
1	B	64	LYS	3.5
1	A	610	ARG	3.4
1	B	610	ARG	3.4
1	B	680	ALA	3.2
1	A	64	LYS	3.2
1	A	54	ARG	3.0
1	B	568	HIS	3.0
1	A	58	LEU	2.9
1	B	40	ARG	2.8
1	A	680	ALA	2.7
1	B	65	ASP	2.6
1	B	222	ASP	2.6
1	B	58	LEU	2.4
1	B	747	LEU	2.4
1	A	608	LYS	2.4
1	B	57	SER	2.3
1	A	40	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	199	ASP	2.3
1	B	692	THR	2.2
1	A	454	ASP	2.2
1	B	682	ALA	2.2
1	B	54	ARG	2.1
1	B	541	GLY	2.1
1	B	46	GLN	2.1
1	A	540	ARG	2.1
1	A	377	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

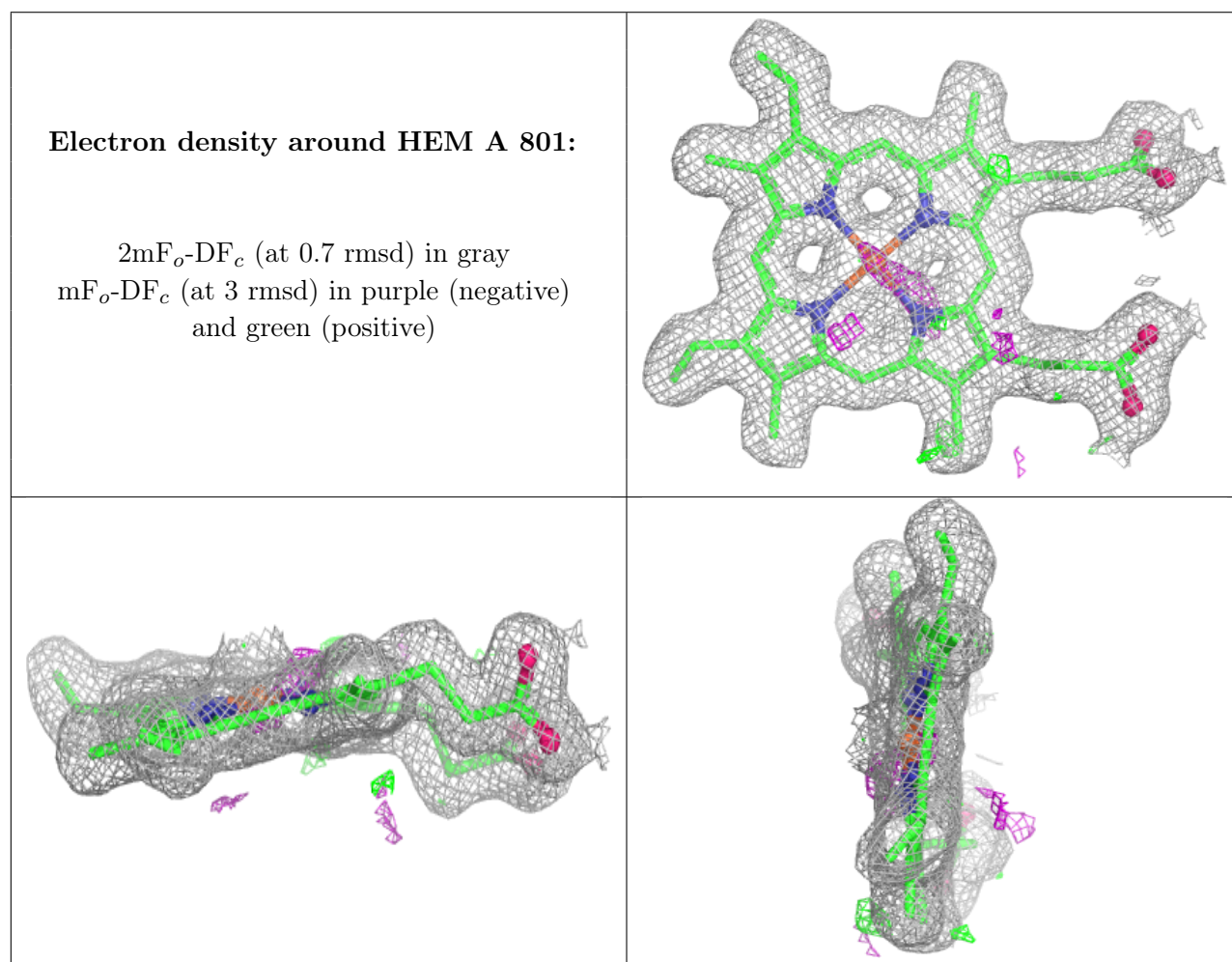
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MPD	B	808	8/8	0.71	0.33	60,75,79,80	0
7	MPD	A	807	8/8	0.83	0.22	51,62,83,83	0
7	MPD	B	807	8/8	0.86	0.24	62,70,75,81	0
7	MPD	B	806	8/8	0.88	0.14	32,43,48,48	0
6	ACT	B	805	4/4	0.89	0.15	33,35,39,42	0
7	MPD	A	806	8/8	0.90	0.14	48,52,60,61	0
6	ACT	A	805	4/4	0.91	0.14	40,43,45,51	0
5	OXY	B	804	2/2	0.92	0.12	37,37,37,37	0
5	OXY	A	804	2/2	0.93	0.15	42,42,42,47	0
4	CL	B	803	1/1	0.97	0.10	37,37,37,37	0
4	CL	A	803	1/1	0.97	0.13	38,38,38,38	0
2	HEM	A	801	43/43	0.98	0.06	18,21,26,28	0
3	NA	B	802	1/1	0.99	0.07	21,21,21,21	0
2	HEM	B	801	43/43	0.99	0.05	16,18,22,25	0

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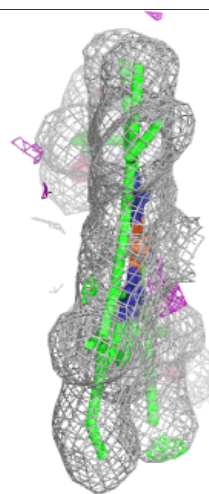
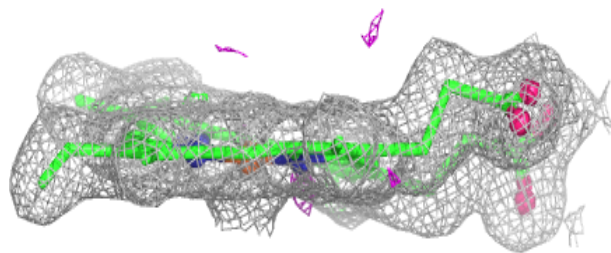
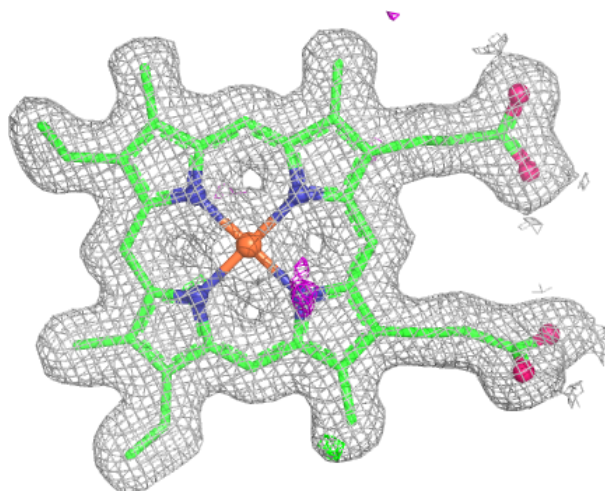
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	802	1/1	0.99	0.06	22,22,22,22	0

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 [i](#)

There are no such residues in this entry.