



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:20 AM UTC

PDB ID : 5SX6 / pdb_00005sx6
Title : Crystal structure of the catalase-peroxidase KatG of *B. pseudomallei* at pH 6.5
Authors : Loewen, P.C.
Deposited on : 2016-08-09
Resolution : 1.90 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

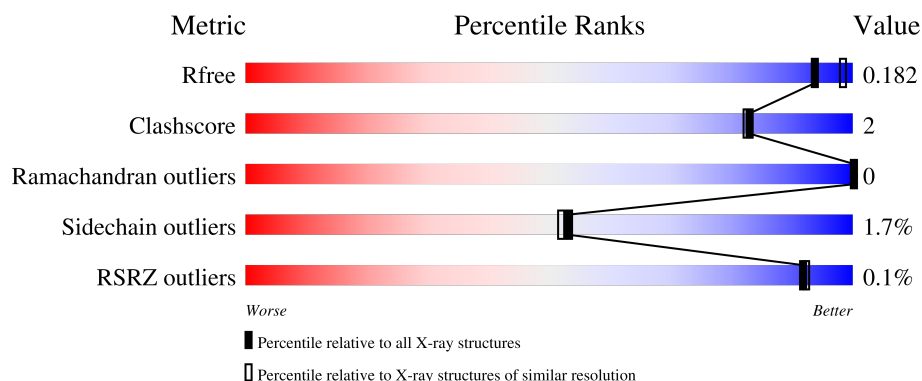
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	 84% 13% ..
1	B	728	 85% 12% ..

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	TRS	A	807	-	X	-	-
6	TRS	B	806	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12741 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	9	0
			5551	3505	990	1042	14			
1	B	713	Total	C	N	O	S	0	13	0
			5576	3521	994	1047	14			

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

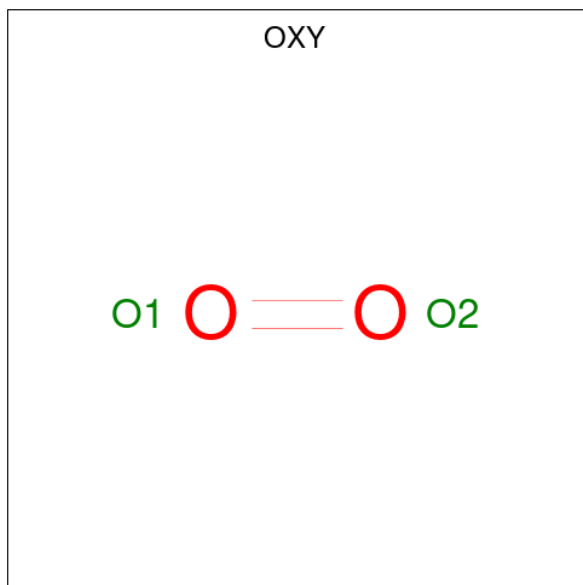


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

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



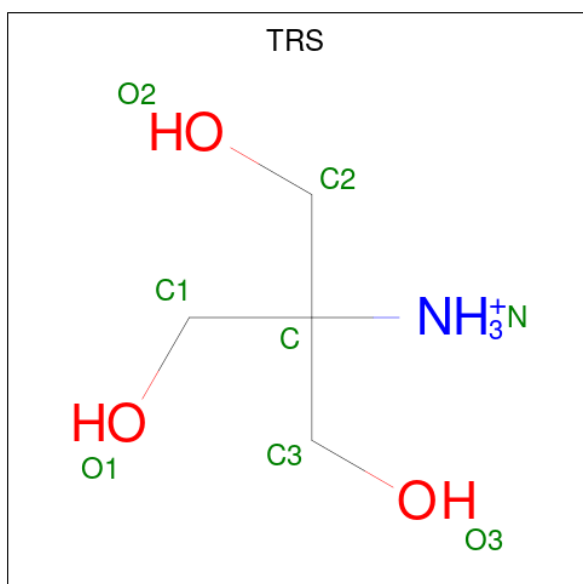
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 2	O 2	0	0
4	B	1	Total 2	O 2	0	0

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



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

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	B	1	Total	C	N	O	0	0
			8	4	1	3		
6	B	1	Total	C	N	O	0	0
			8	4	1	3		

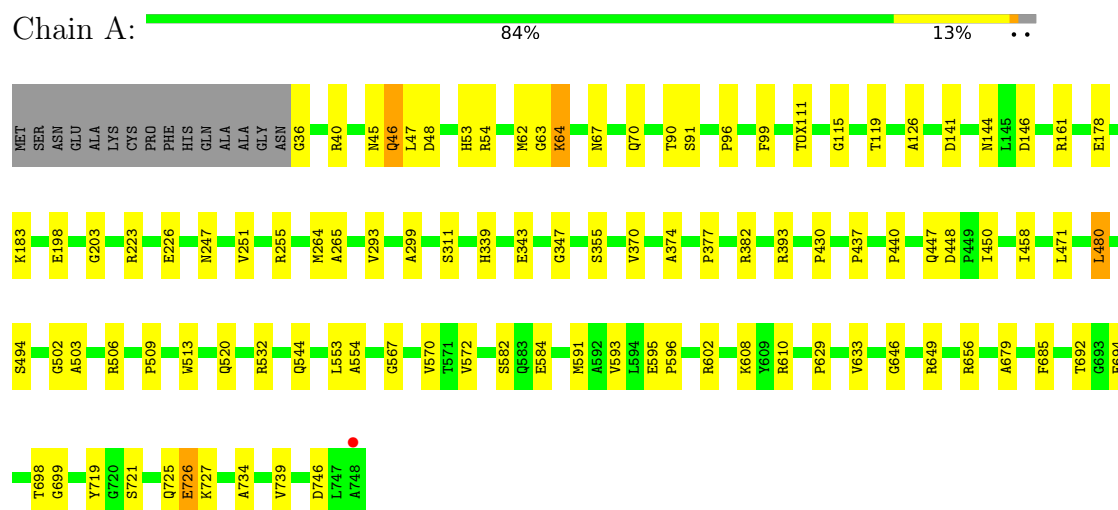
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	712	Total	O	0	0
			712	712		
7	B	746	Total	O	0	0
			746	746		

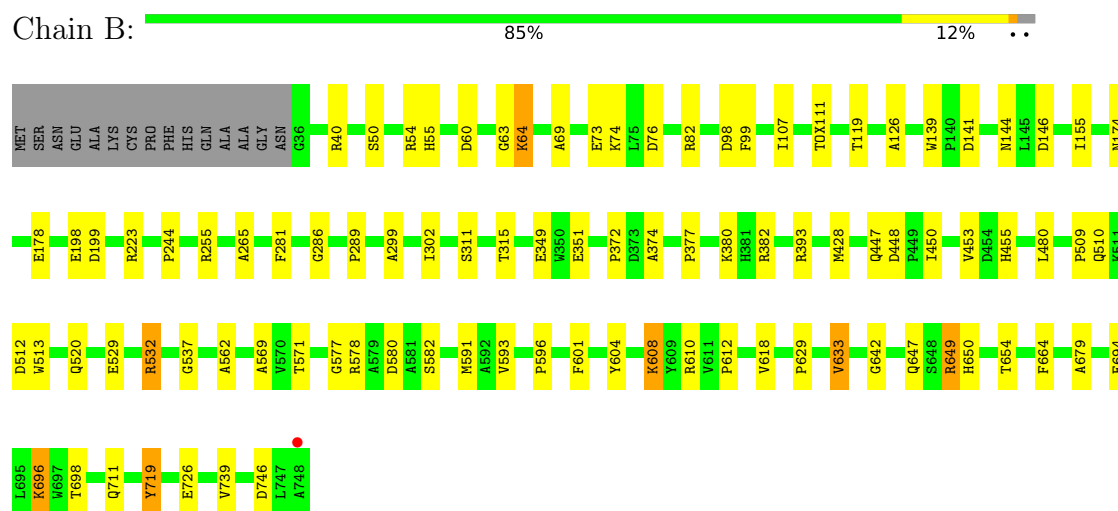
3 Residue-property plots

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	100.53Å 114.80Å 174.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.90) 99.7 (20.00-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.41 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.139 , 0.172 0.153 , 0.182	Depositor DCC
R_{free} test set	7888 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12741	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, NA, TRS, TOX, OXY, 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	1.81	68/5702 (1.2%)	1.31	17/7748 (0.2%)
1	B	1.76	56/5740 (1.0%)	1.33	16/7798 (0.2%)
All	All	1.79	124/11442 (1.1%)	1.32	33/15546 (0.2%)

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	532	ARG	CD-NE	-9.63	1.32	1.46
1	A	532	ARG	CD-NE	-9.19	1.33	1.46
1	A	458	ILE	CA-CB	-9.04	1.45	1.54
1	A	726	GLU	CD-OE2	8.69	1.41	1.25
1	A	377	PRO	C-O	-8.53	1.12	1.24
1	A	726	GLU	CG-CD	8.33	1.72	1.52
1	B	54	ARG	CA-C	-8.04	1.42	1.53
1	A	725	GLN	CD-NE2	8.02	1.50	1.33
1	B	382	ARG	CZ-NH1	7.95	1.43	1.32
1	B	746	ASP	C-O	-7.84	1.14	1.24
1	A	679	ALA	N-CA	7.65	1.55	1.46
1	A	503	ALA	C-O	7.64	1.33	1.23
1	A	382	ARG	CZ-NH1	7.62	1.43	1.32
1	A	699	GLY	CA-C	-7.17	1.44	1.51
1	B	512	ASP	CG-OD2	7.17	1.39	1.25
1	B	82	ARG	CZ-NH2	-7.07	1.24	1.33
1	B	562	ALA	N-CA	-7.03	1.37	1.46
1	B	480	LEU	CA-C	7.01	1.61	1.52
1	B	447	GLN	CA-C	6.96	1.62	1.52
1	A	183	LYS	CA-CB	6.93	1.62	1.53
1	B	679	ALA	N-CA	6.88	1.54	1.46
1	B	601	PHE	N-CA	-6.87	1.37	1.46
1	A	63	GLY	N-CA	6.80	1.53	1.45
1	A	471	LEU	CA-C	6.79	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	311	SER	CA-C	6.67	1.60	1.52
1	A	595	GLU	C-O	-6.67	1.15	1.24
1	B	455	HIS	C-O	6.58	1.29	1.24
1	A	299	ALA	CA-C	-6.58	1.44	1.52
1	A	532	ARG	NE-CZ	-6.55	1.25	1.33
1	A	203	GLY	C-O	6.46	1.29	1.23
1	A	430	PRO	C-O	6.42	1.31	1.23
1	A	734	ALA	N-CA	-6.39	1.38	1.46
1	B	377	PRO	C-O	-6.39	1.15	1.24
1	B	372	PRO	CA-C	-6.36	1.44	1.52
1	B	664	PHE	N-CA	-6.33	1.38	1.46
1	A	582	SER	CA-C	-6.31	1.44	1.53
1	B	64	LYS	CA-CB	6.30	1.63	1.53
1	A	602	ARG	CZ-NH2	-6.25	1.25	1.33
1	A	343	GLU	N-CA	6.23	1.53	1.46
1	B	532	ARG	NE-CZ	-6.22	1.26	1.33
1	B	60	ASP	C-O	-6.21	1.16	1.24
1	A	63	GLY	C-O	6.10	1.32	1.23
1	B	739	VAL	CA-C	6.09	1.60	1.52
1	A	721	SER	N-CA	-6.05	1.37	1.45
1	A	646	GLY	C-O	-5.97	1.15	1.23
1	A	572	VAL	C-O	-5.96	1.17	1.24
1	A	739	VAL	N-CA	5.94	1.53	1.46
1	B	199	ASP	C-O	5.94	1.31	1.23
1	A	91	SER	C-O	-5.93	1.16	1.23
1	B	299	ALA	CA-C	-5.93	1.44	1.52
1	B	571[A]	THR	C-O	-5.90	1.16	1.24
1	B	571[B]	THR	C-O	-5.90	1.16	1.24
1	A	64	LYS	C-O	-5.89	1.16	1.24
1	B	69	ALA	CA-C	-5.89	1.44	1.52
1	A	694	GLU	CA-C	5.85	1.60	1.52
1	A	656	ARG	NE-CZ	-5.85	1.26	1.33
1	A	727	LYS	N-CA	-5.84	1.39	1.46
1	B	604	TYR	N-CA	-5.81	1.39	1.46
1	A	513	TRP	CA-C	-5.79	1.45	1.52
1	B	582	SER	N-CA	5.78	1.52	1.45
1	B	694	GLU	CA-C	5.77	1.60	1.52
1	A	36	GLY	N-CA	5.75	1.54	1.45
1	B	448	ASP	N-CA	5.75	1.51	1.46
1	A	393	ARG	C-O	-5.74	1.16	1.24
1	A	67	ASN	CA-C	5.71	1.59	1.52
1	A	570	VAL	CA-C	-5.70	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	746	ASP	C-O	-5.69	1.16	1.24
1	A	596	PRO	CA-CB	-5.68	1.47	1.53
1	A	692	THR	CA-C	-5.66	1.45	1.52
1	A	494	SER	CA-C	5.64	1.59	1.52
1	B	596	PRO	CA-CB	-5.64	1.47	1.53
1	A	96	PRO	C-O	5.63	1.30	1.23
1	B	139	TRP	CA-CB	5.61	1.61	1.53
1	B	578	ARG	C-O	-5.61	1.16	1.23
1	A	437	PRO	C-O	5.60	1.30	1.24
1	A	54	ARG	N-CA	5.59	1.53	1.45
1	B	126	ALA	N-CA	5.55	1.53	1.46
1	B	654	THR	N-CA	-5.55	1.39	1.46
1	A	45	ASN	C-O	-5.54	1.16	1.24
1	B	608	LYS	C-O	-5.54	1.17	1.24
1	B	63	GLY	N-CA	5.53	1.52	1.45
1	B	174	ASN	N-CA	-5.49	1.39	1.46
1	B	726	GLU	CG-CD	5.48	1.65	1.52
1	B	577	GLY	C-O	-5.48	1.18	1.24
1	A	506	ARG	N-CA	5.46	1.53	1.46
1	B	596	PRO	C-N	-5.45	1.26	1.33
1	A	90	THR	C-O	5.42	1.30	1.23
1	B	618	VAL	N-CA	-5.41	1.39	1.46
1	B	532	ARG	CZ-NH2	-5.41	1.26	1.33
1	A	698	THR	N-CA	-5.41	1.38	1.45
1	A	355	SER	CA-CB	5.39	1.60	1.53
1	B	612	PRO	CA-C	5.38	1.59	1.52
1	A	370	VAL	C-O	-5.38	1.18	1.24
1	A	126	ALA	C-O	5.37	1.31	1.24
1	A	293	VAL	C-O	-5.36	1.18	1.24
1	A	53	HIS	N-CA	5.36	1.52	1.46
1	B	719	TYR	N-CA	5.30	1.53	1.46
1	A	685	PHE	N-CA	-5.30	1.39	1.46
1	A	584	GLU	CG-CD	5.30	1.65	1.52
1	B	537	GLY	N-CA	5.29	1.53	1.45
1	B	580	ASP	CG-OD1	5.25	1.35	1.25
1	A	251	VAL	CA-CB	5.24	1.60	1.54
1	A	584	GLU	C-O	-5.23	1.17	1.24
1	B	281	PHE	CA-C	-5.20	1.46	1.52
1	B	98	ASP	C-O	5.19	1.30	1.23
1	B	286	GLY	CA-C	5.18	1.59	1.51
1	B	155	ILE	N-CA	5.16	1.52	1.46
1	A	502	GLY	CA-C	-5.16	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	448	ASP	CA-CB	5.16	1.57	1.52
1	A	480	LEU	CA-C	5.15	1.59	1.52
1	B	315	THR	CB-OG1	5.15	1.51	1.43
1	B	380	LYS	CA-C	-5.15	1.46	1.52
1	A	570	VAL	C-O	-5.14	1.18	1.23
1	A	226	GLU	N-CA	5.12	1.52	1.46
1	A	311	SER	CA-C	5.12	1.58	1.52
1	B	642	GLY	N-CA	5.09	1.52	1.45
1	A	447	GLN	CA-C	5.08	1.59	1.52
1	B	349	GLU	C-O	-5.08	1.17	1.23
1	B	223	ARG	C-O	-5.06	1.17	1.23
1	A	347	GLY	N-CA	5.05	1.52	1.45
1	B	428	MET	C-N	-5.05	1.25	1.33
1	A	567	GLY	CA-C	-5.02	1.44	1.51
1	A	440	PRO	N-CA	-5.00	1.41	1.47
1	A	247	ASN	CG-ND2	-5.00	1.22	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH2	-14.02	106.58	119.20
1	B	532	ARG	NE-CZ-NH2	-11.22	109.10	119.20
1	A	726	GLU	CB-CG-CD	9.31	128.42	112.60
1	A	532	ARG	NE-CZ-NH1	8.39	129.89	121.50
1	A	450	ILE	CB-CA-C	-8.38	102.00	110.13
1	A	532	ARG	CD-NE-CZ	8.20	135.87	124.40
1	B	532	ARG	CD-NE-CZ	7.96	135.55	124.40
1	B	54	ARG	CG-CD-NE	-7.90	94.62	112.00
1	B	532	ARG	NE-CZ-NH1	7.60	129.10	121.50
1	B	633[A]	VAL	CB-CA-C	-6.15	103.73	112.22
1	B	633[B]	VAL	CB-CA-C	-6.15	103.73	112.22
1	A	520	GLN	CB-CG-CD	6.13	123.02	112.60
1	A	532	ARG	CG-CD-NE	-6.13	98.52	112.00
1	B	450	ILE	CB-CA-C	6.09	116.03	110.13
1	B	351	GLU	CB-CG-CD	-5.87	102.62	112.60
1	B	532	ARG	CG-CD-NE	-5.60	99.69	112.00
1	A	47	LEU	N-CA-CB	-5.56	101.80	109.97
1	B	393	ARG	NE-CZ-NH2	-5.54	114.21	119.20
1	B	450	ILE	CA-CB-CG1	-5.31	101.37	110.40
1	A	70	GLN	CA-CB-CG	5.30	124.69	114.10
1	B	50	SER	CA-CB-OG	-5.25	100.61	111.10
1	A	553	LEU	N-CA-C	5.23	116.98	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	GLU	CG-CD-OE1	5.21	130.39	118.40
1	A	198	GLU	CA-CB-CG	5.18	124.47	114.10
1	A	48	ASP	N-CA-C	5.16	117.03	108.20
1	B	107	ILE	N-CA-CB	5.13	116.55	110.55
1	A	198	GLU	CG-CD-OE1	5.07	130.07	118.40
1	B	244	PRO	CB-CA-C	-5.07	106.03	111.56
1	A	62	MET	CA-C-N	-5.07	114.92	120.44
1	A	62	MET	C-N-CA	-5.07	114.92	120.44
1	A	46	GLN	N-CA-C	-5.04	103.40	110.50
1	A	54	ARG	CG-CD-NE	-5.01	100.98	112.00
1	B	198	GLU	CA-CB-CG	5.00	124.11	114.10

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	5551	0	5365	18	0
1	B	5576	0	5394	31	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	2	0	0	0	0
4	B	2	0	0	0	0
5	A	16	0	28	4	0
5	B	16	0	28	4	0
6	A	16	0	24	0	0
6	B	16	0	23	0	0
7	A	712	0	0	4	2
7	B	746	0	0	15	2
All	All	12741	0	10922	54	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (54) 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:119[B]:THR:HG21	7:A:957:HOH:O	1.68	0.93
1:B:119[B]:THR:HG21	7:B:963:HOH:O	1.76	0.84
5:A:804:MPD:O4	5:A:804:MPD:HM1	1.74	0.84
5:A:804:MPD:O4	5:A:804:MPD:CM	2.28	0.79
1:A:544:GLN:OE1	7:A:903:HOH:O	2.09	0.71
1:B:76:ASP:OD1	7:B:903:HOH:O	2.09	0.69
1:B:255[A]:ARG:CD	7:B:916:HOH:O	2.47	0.63
1:B:569:ALA:H	5:B:805:MPD:CM	2.12	0.62
1:A:633[B]:VAL:CG1	1:A:719:TYR:CZ	2.82	0.62
5:A:805:MPD:H11	5:A:805:MPD:C5	2.33	0.58
1:B:569:ALA:H	5:B:805:MPD:HM3	1.68	0.58
1:A:629:PRO:O	1:A:633[A]:VAL:HG23	2.04	0.57
1:B:711[A]:GLN:NE2	7:B:909:HOH:O	2.30	0.56
1:A:178:GLU:OE1	7:A:904:HOH:O	2.18	0.56
1:B:255[B]:ARG:HG2	7:B:1602:HOH:O	2.06	0.55
1:B:255[A]:ARG:HD2	7:B:916:HOH:O	2.07	0.54
1:B:255[A]:ARG:HD3	7:B:916:HOH:O	2.07	0.53
1:B:55:HIS:HD2	7:B:1347:HOH:O	1.92	0.53
1:B:696:LYS:HE2	7:B:942:HOH:O	2.08	0.53
5:A:805:MPD:H11	5:A:805:MPD:H52	1.93	0.51
1:B:649:ARG:HG2	7:B:1239:HOH:O	2.09	0.50
1:B:633[B]:VAL:HG13	1:B:719:TYR:CZ	2.46	0.49
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	2.12	0.49
1:A:633[B]:VAL:HG11	1:A:719:TYR:CZ	2.48	0.48
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.96	0.48
1:A:509:PRO:HD2	1:A:591:MET:HG2	1.96	0.48
1:B:99:PHE:CD2	1:B:374:ALA:HA	2.51	0.46
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.51	0.45
1:A:633[B]:VAL:HG13	1:A:719:TYR:CE1	2.51	0.45
1:B:119[B]:THR:HG23	1:B:593:VAL:HG11	1.99	0.45
1:B:569:ALA:H	5:B:805:MPD:HM1	1.82	0.45
1:A:223:ARG:HB3	1:A:255[B]:ARG:NH2	2.31	0.44
1:A:115:GLY:O	1:A:264:MET:SD	2.75	0.44
1:B:55:HIS:CD2	7:B:1347:HOH:O	2.69	0.44
1:A:99:PHE:CD2	1:A:374:ALA:HA	2.53	0.44
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.48	0.44
1:B:650:HIS:HD2	1:B:698:THR:OG1	2.00	0.44
1:B:509:PRO:HD2	1:B:591:MET:HG2	2.00	0.44
1:B:255[B]:ARG:CG	7:B:1602:HOH:O	2.65	0.43
1:B:529[A]:GLU:OE2	1:B:532:ARG:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633[B]:VAL:CG1	1:A:719:TYR:CE1	3.01	0.43
1:B:178:GLU:OE1	7:B:904:HOH:O	2.21	0.43
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.18	0.43
1:A:339:HIS:HB2	7:A:1383:HOH:O	2.18	0.43
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.19	0.42
1:B:647:GLN:N	1:B:647:GLN:CD	2.79	0.41
1:B:510:GLN:HG2	1:B:513:TRP:CH2	2.55	0.41
1:B:453:VAL:HA	7:B:924:HOH:O	2.20	0.41
1:A:633[A]:VAL:HG22	1:A:719:TYR:CZ	2.55	0.41
1:B:119[A]:THR:CG2	1:B:265:ALA:HB2	2.51	0.41
1:A:480:LEU:HD22	1:A:554:ALA:HB1	2.02	0.40
5:B:804:MPD:O4	5:B:804:MPD:H12	2.21	0.40
1:B:73[B]:GLU:CD	7:B:910:HOH:O	2.64	0.40
1:B:302:ILE:HD13	1:B:302:ILE:HG21	1.86	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1103:HOH:O	7:B:1170:HOH:O[2_444]	2.07	0.13
7:A:1589:HOH:O	7:B:1573:HOH:O[4_445]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	722/728 (99%)	710 (98%)	12 (2%)	0	100	100
All	All	1440/1456 (99%)	1420 (99%)	20 (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	557/560 (100%)	547 (98%)	10 (2%)	51	50
1	B	561/560 (100%)	551 (98%)	10 (2%)	51	50
All	All	1118/1120 (100%)	1098 (98%)	20 (2%)	53	50

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	64	LYS
1	A	141	ASP
1	A	161[A]	ARG
1	A	161[B]	ARG
1	A	608	LYS
1	A	610	ARG
1	A	649	ARG
1	A	726	GLU
1	B	40	ARG
1	B	64	LYS
1	B	74	LYS
1	B	141	ASP
1	B	289	PRO
1	B	520	GLN
1	B	608	LYS
1	B	610	ARG
1	B	649	ARG
1	B	696	LYS

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

Mol	Chain	Res	Type
1	A	70	GLN
1	A	85	HIS

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Mol	Chain	Res	Type
1	A	520	GLN
1	A	737	ASN
1	B	55	HIS
1	B	216	ASN
1	B	650	HIS
1	B	737	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TOX	B	111[A]	2	14,17,18	2.66	6 (42%)	12,23,25	2.05	4 (33%)
1	TOX	B	111[B]	-	14,17,18	2.66	6 (42%)	12,23,25	2.05	4 (33%)
1	TOX	A	111[A]	2	14,17,18	3.32	7 (50%)	12,23,25	3.98	7 (58%)
1	TOX	A	111[B]	-	14,17,18	3.32	7 (50%)	12,23,25	3.98	7 (58%)

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

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[A]	TOX	O1-NE1	9.17	1.51	1.39
1	A	111[B]	TOX	O1-NE1	9.17	1.51	1.39
1	B	111[A]	TOX	O1-NE1	6.48	1.47	1.39
1	B	111[B]	TOX	O1-NE1	6.48	1.47	1.39
1	A	111[A]	TOX	CH2-CZ3	3.85	1.46	1.38
1	A	111[B]	TOX	CH2-CZ3	3.85	1.46	1.38
1	A	111[A]	TOX	CD2-CG	3.83	1.50	1.44
1	A	111[B]	TOX	CD2-CG	3.83	1.50	1.44
1	B	111[A]	TOX	O-C	3.66	1.33	1.20
1	B	111[B]	TOX	O-C	3.66	1.33	1.20
1	A	111[A]	TOX	O-C	3.64	1.33	1.20
1	A	111[B]	TOX	O-C	3.64	1.33	1.20
1	B	111[A]	TOX	CA-N	-3.47	1.38	1.48
1	B	111[B]	TOX	CA-N	-3.47	1.38	1.48
1	B	111[A]	TOX	CZ3-CE3	3.34	1.44	1.38
1	B	111[B]	TOX	CZ3-CE3	3.34	1.44	1.38
1	B	111[A]	TOX	CD1-CG	3.00	1.42	1.36
1	B	111[B]	TOX	CD1-CG	3.00	1.42	1.36
1	A	111[A]	TOX	CD2-CE2	2.56	1.44	1.41
1	A	111[B]	TOX	CD2-CE2	2.56	1.44	1.41
1	B	111[A]	TOX	CH2-CZ3	2.45	1.43	1.38
1	B	111[B]	TOX	CH2-CZ3	2.45	1.43	1.38
1	A	111[A]	TOX	CH2-CZ2	2.22	1.42	1.38
1	A	111[B]	TOX	CH2-CZ2	2.22	1.42	1.38
1	A	111[A]	TOX	CD1-CG	2.07	1.40	1.36
1	A	111[B]	TOX	CD1-CG	2.07	1.40	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[A]	TOX	CE3-CD2-CE2	8.11	128.59	119.24
1	A	111[B]	TOX	CE3-CD2-CE2	8.11	128.59	119.24
1	A	111[A]	TOX	CZ2-CE2-CD2	-7.37	113.72	121.95
1	A	111[B]	TOX	CZ2-CE2-CD2	-7.37	113.72	121.95
1	A	111[A]	TOX	CE2-CD2-CG	-5.66	102.18	107.39
1	A	111[B]	TOX	CE2-CD2-CG	-5.66	102.18	107.39
1	A	111[A]	TOX	CZ2-CE2-NE1	3.93	135.63	129.37
1	A	111[B]	TOX	CZ2-CE2-NE1	3.93	135.63	129.37
1	B	111[A]	TOX	CZ2-CE2-CD2	-3.88	117.61	121.95
1	B	111[B]	TOX	CZ2-CE2-CD2	-3.88	117.61	121.95
1	B	111[A]	TOX	CH2-CZ2-CE2	3.52	125.39	118.28
1	B	111[B]	TOX	CH2-CZ2-CE2	3.52	125.39	118.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[A]	TOX	CE3-CD2-CG	-3.11	129.22	133.85
1	A	111[B]	TOX	CE3-CD2-CG	-3.11	129.22	133.85
1	B	111[A]	TOX	CZ3-CH2-CZ2	-2.78	116.81	120.24
1	B	111[B]	TOX	CZ3-CH2-CZ2	-2.78	116.81	120.24
1	A	111[A]	TOX	CZ3-CE3-CD2	-2.45	115.37	119.80
1	A	111[B]	TOX	CZ3-CE3-CD2	-2.45	115.37	119.80
1	B	111[A]	TOX	CZ2-CE2-NE1	2.28	133.00	129.37
1	B	111[B]	TOX	CZ2-CE2-NE1	2.28	133.00	129.37
1	A	111[A]	TOX	CH2-CZ2-CE2	2.25	122.82	118.28
1	A	111[B]	TOX	CH2-CZ2-CE2	2.25	122.82	118.28

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111[A]	TOX	N-CA-CB-CG
1	A	111[A]	TOX	C-CA-CB-CG
1	A	111[B]	TOX	N-CA-CB-CG
1	A	111[B]	TOX	C-CA-CB-CG
1	B	111[A]	TOX	N-CA-CB-CG
1	B	111[A]	TOX	C-CA-CB-CG
1	B	111[B]	TOX	N-CA-CB-CG
1	B	111[B]	TOX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	TRS	B	806	-	7,7,7	1.38	1 (14%)	9,9,9	2.14	4 (44%)
5	MPD	B	805	-	7,7,7	0.90	0	9,10,10	1.08	0
5	MPD	A	805	-	7,7,7	0.51	0	9,10,10	1.51	2 (22%)
5	MPD	B	804	-	7,7,7	0.46	0	9,10,10	1.36	0
5	MPD	A	804	-	7,7,7	0.68	0	9,10,10	1.36	1 (11%)
2	HEM	B	801	1	50,50,50	1.91	13 (26%)	67,82,82	1.61	14 (20%)
6	TRS	B	807	-	7,7,7	1.28	1 (14%)	9,9,9	1.52	3 (33%)
6	TRS	A	807	-	7,7,7	1.41	2 (28%)	9,9,9	2.99	6 (66%)
6	TRS	A	806	-	7,7,7	1.70	2 (28%)	9,9,9	2.28	5 (55%)
4	OXY	A	803	-	1,1,1	0.14	0	-	-	-
4	OXY	B	803	-	1,1,1	0.67	0	-	-	-
2	HEM	A	801	1	50,50,50	1.63	11 (22%)	67,82,82	1.68	12 (17%)

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
6	TRS	B	806	-	-	6/9/9/9	-
5	MPD	B	805	-	-	2/5/5/5	-
5	MPD	A	805	-	-	3/5/5/5	-
5	MPD	B	804	-	-	3/5/5/5	-
5	MPD	A	804	-	-	0/5/5/5	-
2	HEM	B	801	1	-	2/14/54/54	-
6	TRS	B	807	-	-	1/9/9/9	-
6	TRS	A	807	-	-	5/9/9/9	-
6	TRS	A	806	-	-	0/9/9/9	-
2	HEM	A	801	1	-	2/14/54/54	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C4B-NB	-5.44	1.28	1.38
2	A	801	HEM	FE-NB	5.09	2.10	1.94
2	B	801	HEM	FE-NB	4.66	2.09	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C4D-ND	-4.26	1.32	1.40
2	B	801	HEM	C1B-NB	-3.72	1.33	1.40
2	B	801	HEM	C1C-NC	-3.68	1.32	1.39
2	B	801	HEM	FE-NC	3.63	2.07	1.95
2	A	801	HEM	FE-NC	3.43	2.06	1.95
2	A	801	HEM	FE-NA	3.30	2.06	1.95
6	A	806	TRS	C1-C	3.26	1.61	1.53
6	A	806	TRS	O1-C1	3.02	1.51	1.42
2	B	801	HEM	O1D-CGD	2.82	1.31	1.22
2	A	801	HEM	C1A-NA	2.77	1.44	1.39
6	B	806	TRS	C-N	2.76	1.58	1.49
2	A	801	HEM	C1B-NB	-2.72	1.35	1.40
2	B	801	HEM	C1A-C2A	2.52	1.49	1.44
2	B	801	HEM	O1A-CGA	2.51	1.30	1.22
2	A	801	HEM	C4A-NA	-2.30	1.35	1.39
2	B	801	HEM	C1B-C2B	-2.29	1.39	1.44
2	B	801	HEM	C4A-NA	-2.25	1.35	1.39
2	B	801	HEM	CHA-C4D	-2.23	1.34	1.38
6	B	807	TRS	O1-C1	2.19	1.49	1.42
2	A	801	HEM	CHB-C4A	2.17	1.44	1.39
2	A	801	HEM	C3C-C4C	2.11	1.49	1.46
2	A	801	HEM	O1D-CGD	2.09	1.28	1.22
2	A	801	HEM	CHB-C1B	2.06	1.42	1.38
2	B	801	HEM	CHB-C1B	2.05	1.42	1.38
6	A	807	TRS	C1-C	2.04	1.58	1.53
2	B	801	HEM	C4A-C3A	2.04	1.47	1.43
6	A	807	TRS	O3-C3	2.02	1.48	1.42

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C3B-C2B-C1B	5.89	110.83	106.41
6	A	807	TRS	C3-C-C1	4.99	123.94	110.66
2	A	801	HEM	C4B-C3B-C2B	-4.51	103.14	107.28
6	A	807	TRS	O1-C1-C	-4.48	98.38	110.88
6	B	806	TRS	C3-C-N	4.08	118.58	108.17
2	B	801	HEM	C3C-C2C-C1C	-4.08	103.19	107.05
2	A	801	HEM	C2A-C1A-NA	-3.88	105.85	110.15
6	A	806	TRS	C1-C-N	3.81	117.90	108.17
2	A	801	HEM	CMB-C2B-C1B	-3.79	119.12	125.03
2	B	801	HEM	C4D-ND-C1D	-3.69	100.84	105.21
2	A	801	HEM	CAA-CBA-CGA	-3.49	104.40	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	806	TRS	C3-C-N	-3.24	99.92	108.17
2	B	801	HEM	C2D-C1D-ND	3.06	113.44	109.90
6	A	807	TRS	O2-C2-C	-2.97	102.60	110.88
5	A	805	MPD	C5-C4-C3	2.95	125.38	111.67
2	B	801	HEM	C3D-C4D-ND	2.94	113.40	110.17
6	A	806	TRS	O1-C1-C	2.88	118.91	110.88
2	A	801	HEM	CHB-C1B-NB	2.87	127.92	124.37
6	A	807	TRS	C2-C-N	2.83	115.39	108.17
6	A	807	TRS	C1-C-N	-2.79	101.06	108.17
2	B	801	HEM	O2D-CGD-CBD	2.76	122.72	114.00
2	B	801	HEM	CHC-C4B-NB	2.75	127.38	124.42
6	B	807	TRS	O1-C1-C	2.70	118.40	110.88
2	A	801	HEM	C1B-NB-C4B	2.58	108.27	105.21
6	A	807	TRS	C3-C-C2	-2.56	103.84	110.66
6	A	806	TRS	C2-C-N	-2.54	101.69	108.17
2	A	801	HEM	C1D-C2D-C3D	-2.52	104.33	106.98
5	A	805	MPD	O4-C4-C3	-2.49	101.45	111.35
2	B	801	HEM	CMA-C3A-C2A	2.47	130.87	125.62
6	B	806	TRS	C2-C-N	2.46	114.45	108.17
6	B	807	TRS	C2-C-C1	2.45	117.17	110.66
6	B	807	TRS	C3-C-C2	-2.43	104.18	110.66
6	B	806	TRS	C1-C-N	-2.39	102.07	108.17
2	A	801	HEM	C2B-C1B-NB	-2.39	107.10	109.84
2	B	801	HEM	C3B-C2B-C1B	-2.29	104.69	106.41
2	B	801	HEM	CAA-C2A-C1A	2.29	129.41	124.94
2	A	801	HEM	CHC-C4B-NB	2.27	126.86	124.42
2	B	801	HEM	CAA-CBA-CGA	-2.18	107.88	113.67
6	B	806	TRS	C3-C-C1	-2.15	104.93	110.66
5	A	804	MPD	CM-C2-C3	2.11	119.30	110.20
2	A	801	HEM	CAC-C3C-C4C	-2.10	119.81	124.82
2	B	801	HEM	CHD-C1D-C2D	-2.09	121.73	125.03
2	B	801	HEM	O1D-CGD-CBD	-2.07	116.53	123.09
2	B	801	HEM	C4B-C3B-C2B	-2.06	105.39	107.28
2	A	801	HEM	CMD-C2D-C1D	2.03	128.21	125.03
6	A	806	TRS	C3-C-C1	2.02	116.03	110.66
2	B	801	HEM	C4D-C3D-C2D	-2.01	103.97	106.89

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	805	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	B	804	MPD	O2-C2-C3-C4
6	A	807	TRS	C2-C-C1-O1
6	A	807	TRS	C3-C-C1-O1
6	A	807	TRS	N-C-C1-O1
6	B	806	TRS	C3-C-C2-O2
6	A	807	TRS	C1-C-C2-O2
6	A	807	TRS	N-C-C2-O2
6	B	806	TRS	C1-C-C2-O2
6	B	806	TRS	N-C-C2-O2
6	B	806	TRS	N-C-C3-O3
5	A	805	MPD	C1-C2-C3-C4
5	B	804	MPD	C1-C2-C3-C4
5	B	805	MPD	CM-C2-C3-C4
6	B	806	TRS	C1-C-C3-O3
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O1A
6	B	807	TRS	C2-C-C1-O1
5	A	805	MPD	CM-C2-C3-C4
5	B	804	MPD	CM-C2-C3-C4
5	B	805	MPD	C1-C2-C3-C4
6	B	806	TRS	C2-C-C3-O3

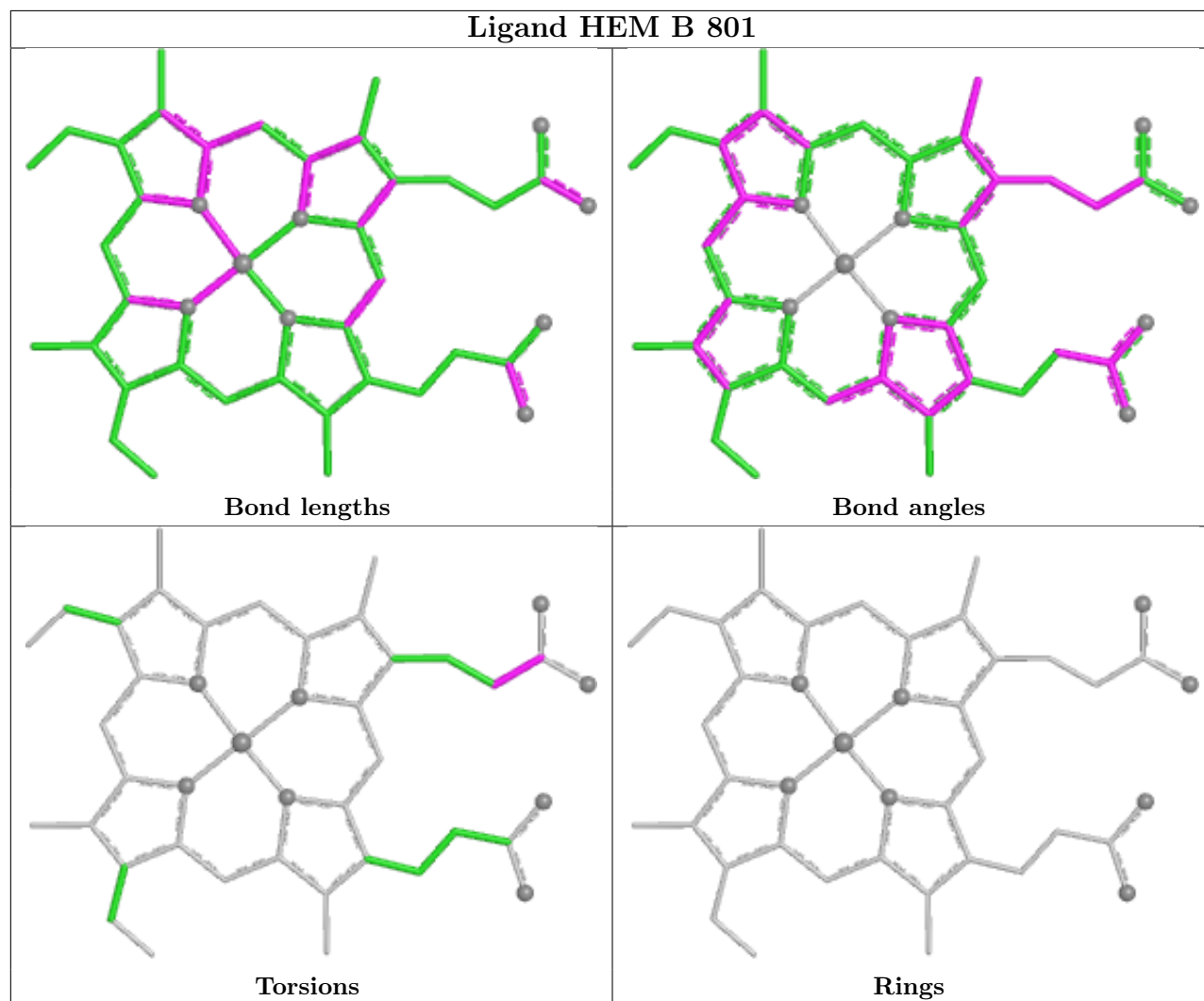
There are no ring outliers.

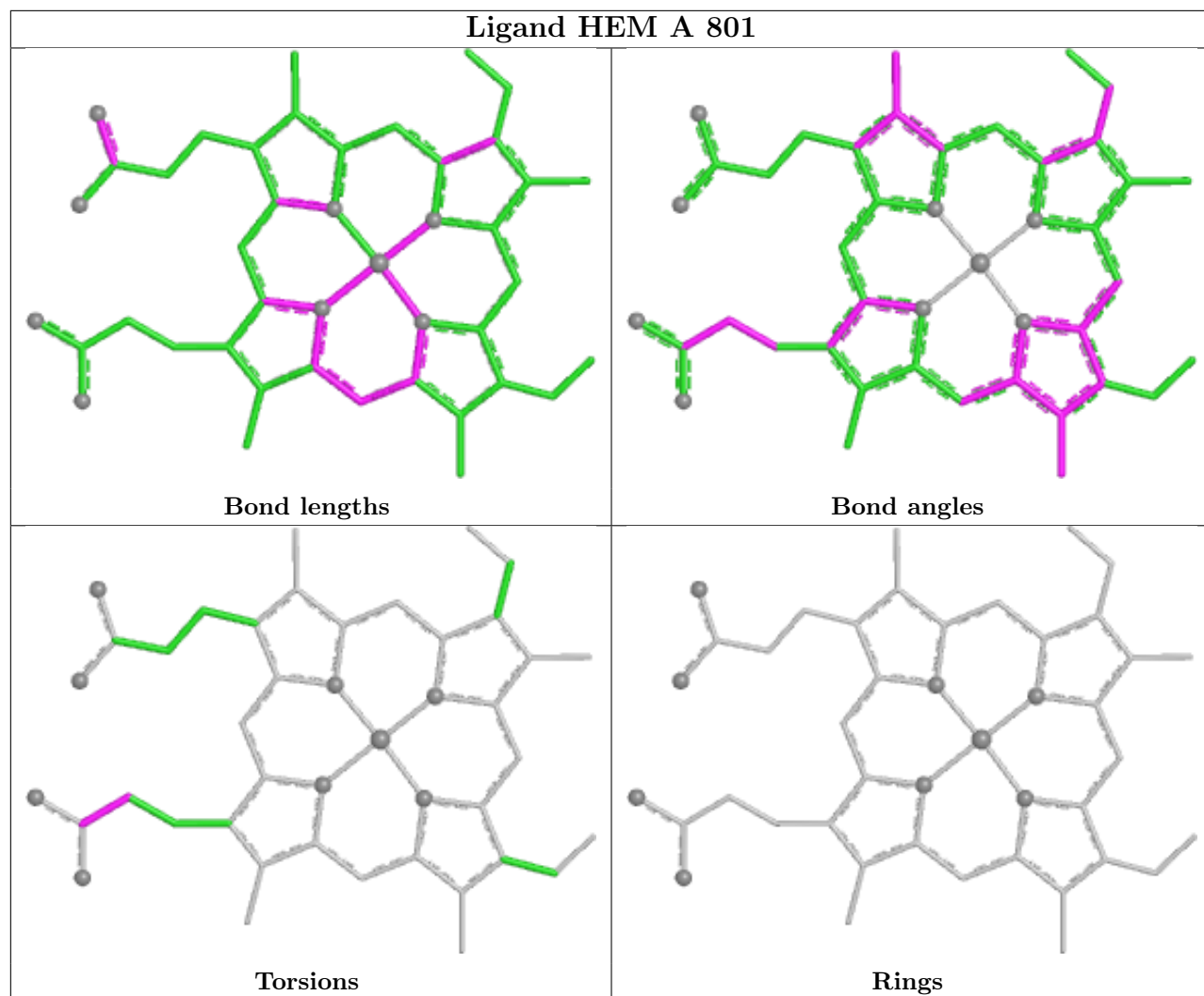
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	805	MPD	3	0
5	A	805	MPD	2	0
5	B	804	MPD	1	0
5	A	804	MPD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	712/728 (97%)	-0.46	1 (0%) 92 92	11, 23, 40, 77	8 (1%)
1	B	712/728 (97%)	-0.61	1 (0%) 92 92	11, 21, 38, 72	12 (1%)
All	All	1424/1456 (97%)	-0.54	2 (0%) 92 92	11, 22, 40, 77	20 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	3.9
1	A	748	ALA	3.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TOX	A	111[A]	16/17	0.96	0.06	16,20,23,25	2
1	TOX	A	111[B]	16/17	0.96	0.06	16,20,23,25	2
1	TOX	B	111[A]	16/17	0.97	0.05	15,17,19,20	2
1	TOX	B	111[B]	16/17	0.97	0.05	15,17,19,20	2

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

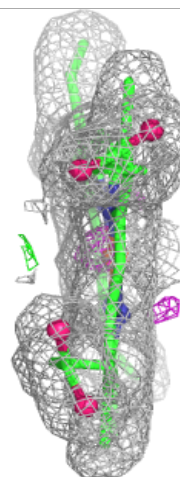
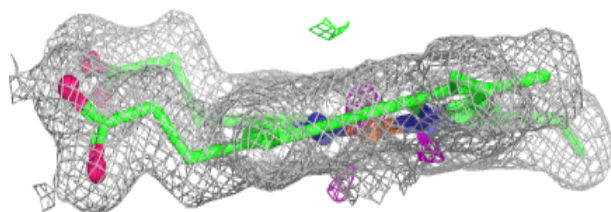
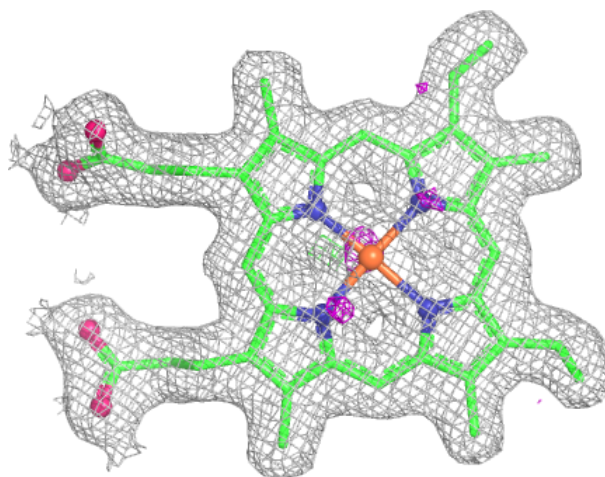
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

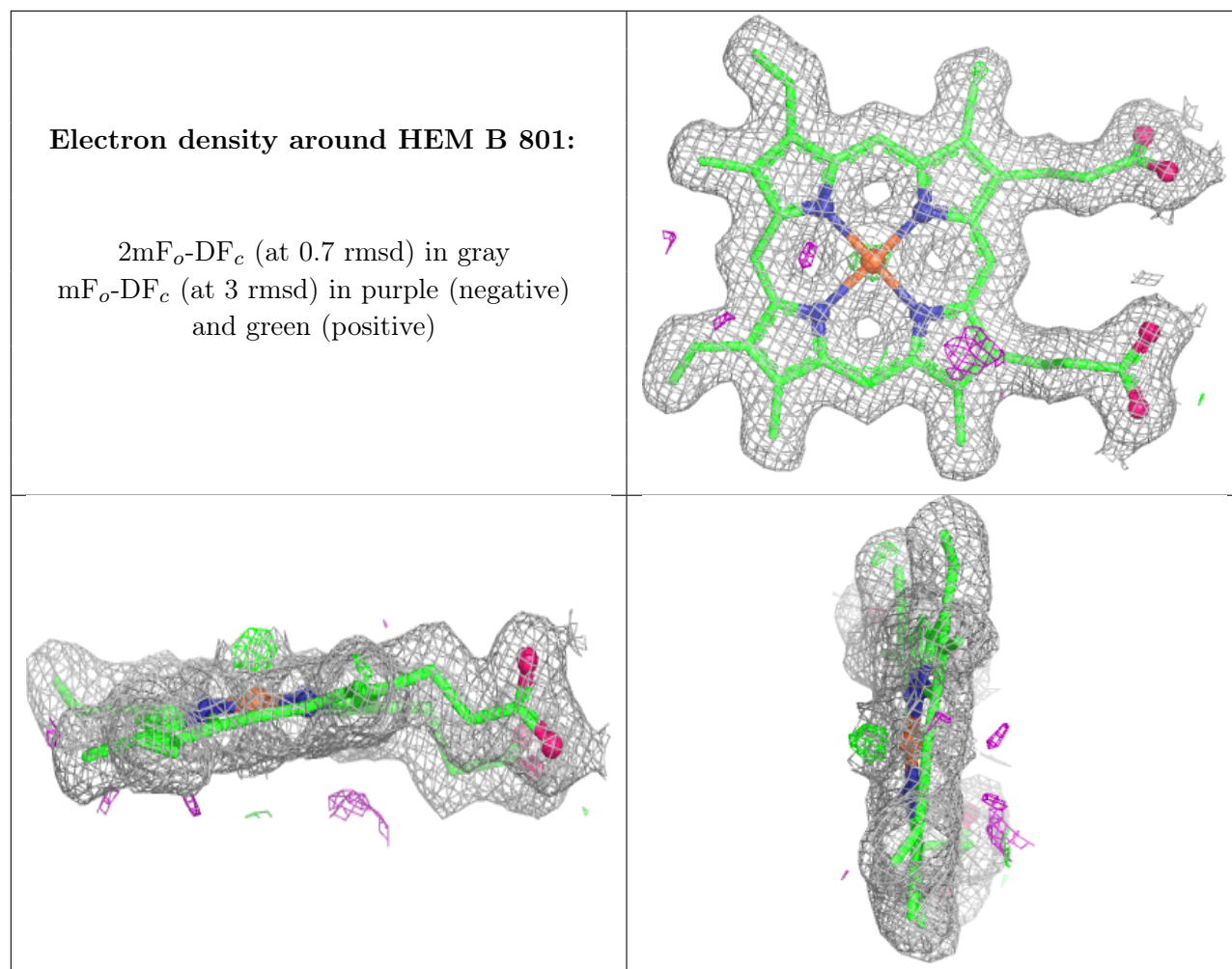
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MPD	B	805	8/8	0.80	0.15	38,52,54,66	0
6	TRS	A	807	8/8	0.81	0.13	46,50,52,58	0
6	TRS	B	806	8/8	0.84	0.14	43,53,57,64	0
5	MPD	A	805	8/8	0.88	0.14	43,51,60,63	0
5	MPD	A	804	8/8	0.89	0.17	59,66,73,74	0
4	OXY	B	803	2/2	0.89	0.21	31,31,31,36	0
5	MPD	B	804	8/8	0.89	0.16	52,56,62,63	0
4	OXY	A	803	2/2	0.92	0.19	41,41,41,45	0
6	TRS	A	806	8/8	0.95	0.07	28,35,38,42	0
6	TRS	B	807	8/8	0.96	0.08	24,28,31,32	0
3	NA	B	802	1/1	0.98	0.11	23,23,23,23	0
3	NA	A	802	1/1	0.99	0.12	24,24,24,24	0
2	HEM	A	801	43/43	0.99	0.05	16,19,22,23	0
2	HEM	B	801	43/43	0.99	0.04	13,15,17,19	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM A 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.