



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:12 am BST

PDB ID : 5SX6
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 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

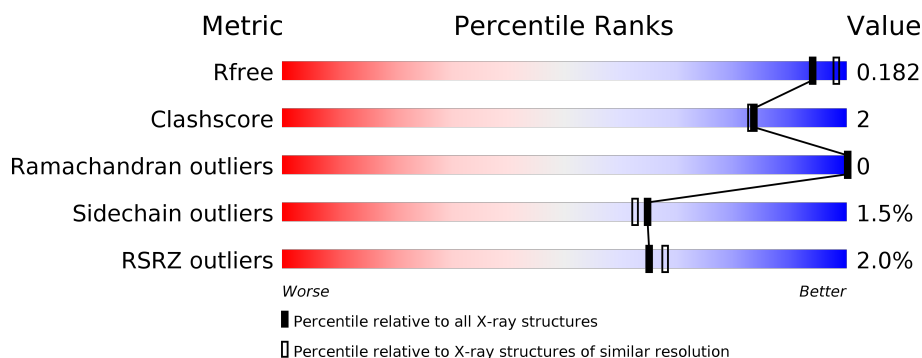
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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>87%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	728	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>12%</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
6	TRS	A	807	-	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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

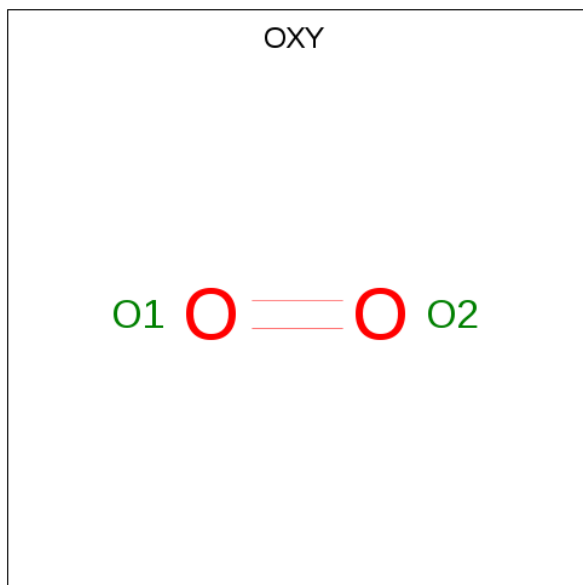


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



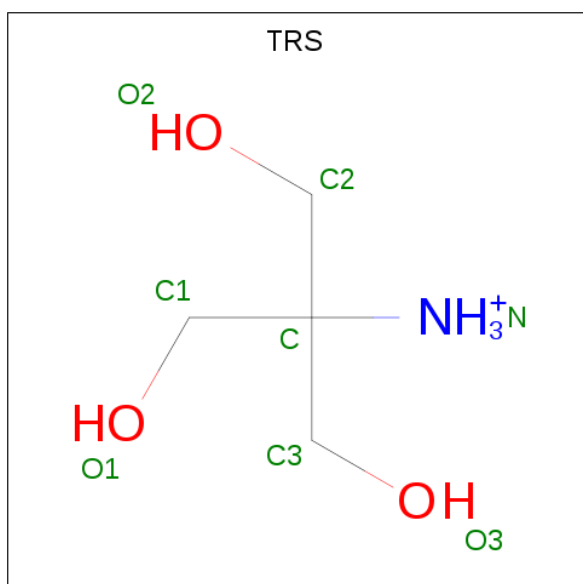
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			2	2		
4	B	1	Total	O	0	0
			2	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: 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 (three-letter code: 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		

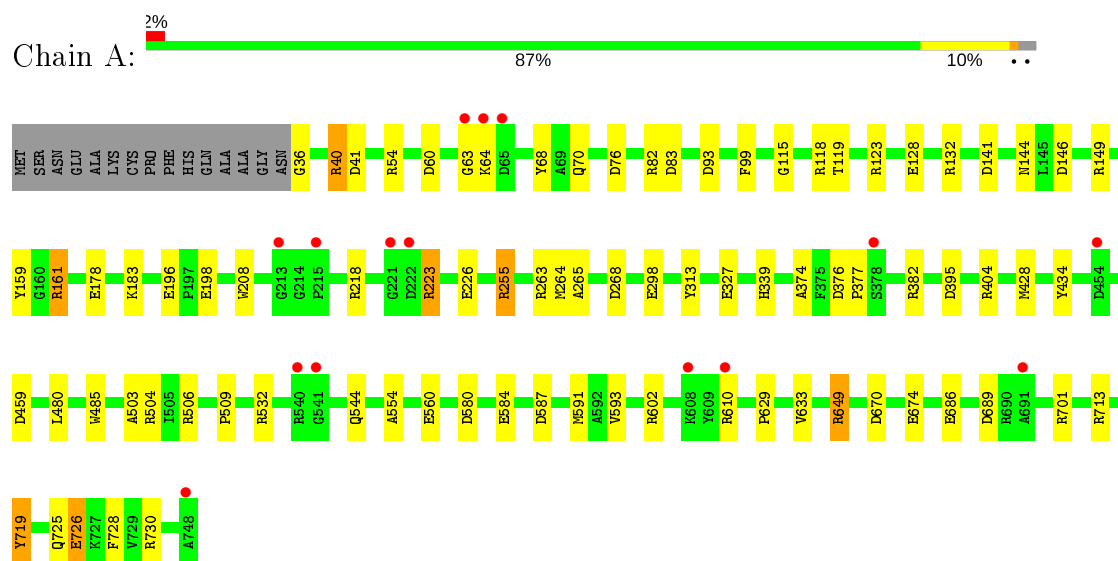
- Molecule 7 is water.

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

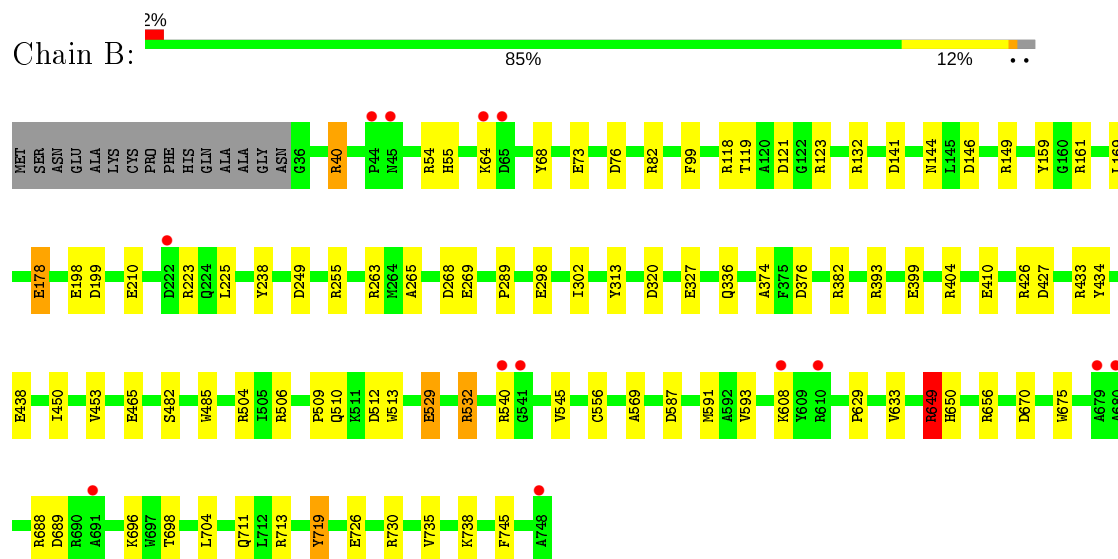
3 Residue-property plots [i](#)

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	100.53Å 114.80Å 174.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 19.92 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.90) 99.8 (19.92-1.90)	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 (4.97%)	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 , 51.7	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: TOX, OXY, NA, MPD, HEM, TRS

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	1.49	33/5702 (0.6%)	1.31	58/7748 (0.7%)
1	B	1.45	37/5740 (0.6%)	1.30	58/7798 (0.7%)
All	All	1.47	70/11442 (0.6%)	1.31	116/15546 (0.7%)

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	726	GLU	CD-OE2	14.74	1.41	1.25
1	A	726	GLU	CG-CD	13.95	1.72	1.51
1	B	726	GLU	CG-CD	9.20	1.65	1.51
1	A	584	GLU	CG-CD	8.89	1.65	1.51
1	B	382	ARG	CZ-NH1	8.33	1.43	1.33
1	B	410	GLU	CG-CD	8.06	1.64	1.51
1	B	532	ARG	CD-NE	-8.04	1.32	1.46
1	A	382	ARG	CZ-NH1	7.97	1.43	1.33
1	A	726	GLU	CD-OE1	7.78	1.34	1.25
1	A	532	ARG	CD-NE	-7.68	1.33	1.46
1	A	198	GLU	CG-CD	7.43	1.63	1.51
1	B	198	GLU	CG-CD	7.21	1.62	1.51
1	B	210	GLU	CD-OE2	7.04	1.33	1.25
1	A	725	GLN	CD-NE2	6.90	1.50	1.32
1	B	198	GLU	CD-OE1	6.83	1.33	1.25
1	A	198	GLU	CD-OE1	6.78	1.33	1.25
1	B	298	GLU	CD-OE1	6.77	1.33	1.25
1	B	82	ARG	CZ-NH2	-6.76	1.24	1.33
1	B	529[A]	GLU	CD-OE1	-6.57	1.18	1.25
1	B	529[B]	GLU	CD-OE1	-6.57	1.18	1.25
1	B	426[A]	ARG	CZ-NH2	6.51	1.41	1.33
1	B	426[B]	ARG	CZ-NH2	6.51	1.41	1.33
1	A	674	GLU	CG-CD	6.46	1.61	1.51
1	B	556	CYS	CB-SG	6.46	1.93	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	68	TYR	CE2-CZ	6.27	1.46	1.38
1	B	313	TYR	CG-CD1	6.26	1.47	1.39
1	A	560	GLU	CD-OE2	-6.21	1.18	1.25
1	A	602	ARG	CZ-NH2	-5.94	1.25	1.33
1	B	512	ASP	CG-OD2	5.92	1.39	1.25
1	A	327	GLU	CD-OE1	5.85	1.32	1.25
1	A	485	TRP	CG-CD1	5.81	1.44	1.36
1	A	36	GLY	N-CA	5.80	1.54	1.46
1	B	327	GLU	CG-CD	5.80	1.60	1.51
1	A	208	TRP	CZ3-CH2	5.78	1.49	1.40
1	B	675	TRP	CZ3-CH2	-5.75	1.30	1.40
1	B	485	TRP	CE3-CZ3	5.75	1.48	1.38
1	A	63	GLY	C-O	5.73	1.32	1.23
1	A	128	GLU	CD-OE1	5.70	1.31	1.25
1	A	730	ARG	CG-CD	5.58	1.66	1.51
1	B	238	TYR	CE1-CZ	5.57	1.45	1.38
1	B	438	GLU	CD-OE1	-5.56	1.19	1.25
1	A	532	ARG	NE-CZ	-5.54	1.25	1.33
1	A	728	PHE	CG-CD2	-5.54	1.30	1.38
1	B	178	GLU	CG-CD	5.54	1.60	1.51
1	A	584	GLU	CB-CG	5.50	1.62	1.52
1	A	313	TYR	CE2-CZ	5.47	1.45	1.38
1	A	503	ALA	C-O	5.43	1.33	1.23
1	A	159	TYR	CG-CD2	5.42	1.46	1.39
1	B	745	PHE	CG-CD2	-5.39	1.30	1.38
1	B	73[A]	GLU	CG-CD	5.37	1.60	1.51
1	B	73[B]	GLU	CG-CD	5.37	1.60	1.51
1	A	377	PRO	C-O	-5.34	1.12	1.23
1	A	686	GLU	CG-CD	5.34	1.59	1.51
1	B	269	GLU	CG-CD	5.33	1.59	1.51
1	B	159	TYR	CE1-CZ	5.32	1.45	1.38
1	B	399	GLU	CD-OE1	5.31	1.31	1.25
1	A	68	TYR	CE1-CZ	5.30	1.45	1.38
1	A	298	GLU	CG-CD	5.29	1.59	1.51
1	B	532	ARG	NE-CZ	-5.26	1.26	1.33
1	A	226	GLU	CG-CD	5.22	1.59	1.51
1	B	719	TYR	CZ-OH	5.19	1.46	1.37
1	B	726	GLU	CD-OE1	5.15	1.31	1.25
1	B	410	GLU	CD-OE1	5.11	1.31	1.25
1	B	532	ARG	CZ-NH2	-5.10	1.26	1.33
1	A	63	GLY	N-CA	5.09	1.53	1.46
1	A	313	TYR	CG-CD1	5.08	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	336	GLN	CG-CD	5.08	1.62	1.51
1	B	465	GLU	CD-OE2	5.02	1.31	1.25
1	B	482	SER	CA-CB	5.01	1.60	1.52
1	A	719	TYR	CE1-CZ	5.00	1.45	1.38

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH2	-27.44	106.58	120.30
1	B	532	ARG	NE-CZ-NH2	-22.40	109.10	120.30
1	A	532	ARG	NE-CZ-NH1	19.18	129.89	120.30
1	B	532	ARG	NE-CZ-NH1	17.61	129.10	120.30
1	B	393	ARG	NE-CZ-NH2	-12.17	114.21	120.30
1	B	82	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	B	263	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	A	382	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	A	161[A]	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	A	161[B]	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	A	649	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	A	649	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	A	60	ASP	CB-CG-OD2	-9.38	109.86	118.30
1	A	268	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	A	532	ARG	CD-NE-CZ	8.77	135.87	123.60
1	B	532	ARG	CD-NE-CZ	8.54	135.55	123.60
1	B	713	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	A	76	ASP	CB-CG-OD2	-8.46	110.69	118.30
1	B	704	LEU	CB-CG-CD2	8.22	124.98	111.00
1	A	404	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	B	54	ARG	CG-CD-NE	-8.18	94.62	111.80
1	A	587	ASP	CB-CG-OD1	7.82	125.33	118.30
1	B	268	ASP	CB-CG-OD1	7.81	125.33	118.30
1	B	149	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	B	382	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	B	132	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	584	GLU	OE1-CD-OE2	-7.70	114.06	123.30
1	B	506	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	263	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	A	434	TYR	CB-CG-CD1	7.46	125.48	121.00
1	A	93	ASP	CB-CG-OD1	7.42	124.98	118.30
1	B	433	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	376	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	A	701	ARG	NE-CZ-NH1	7.16	123.88	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	713	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	B	54	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	688	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	649	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	198	GLU	OE1-CD-OE2	-6.72	115.24	123.30
1	A	670	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	B	198	GLU	OE1-CD-OE2	-6.63	115.34	123.30
1	B	689	ASP	CB-CG-OD1	6.61	124.24	118.30
1	A	40	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	54	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	689	ASP	CB-CG-OD1	6.54	124.18	118.30
1	B	670	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	268	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	268	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	A	60	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	532	ARG	CG-CD-NE	-6.33	98.52	111.80
1	A	459	ASP	CB-CG-OD1	6.30	123.97	118.30
1	B	225	LEU	CB-CG-CD2	-6.29	100.31	111.00
1	B	688	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	376	ASP	CB-CG-OD2	-6.28	112.64	118.30
1	A	730	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	199	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	A	149	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	149	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	689	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	B	427	ASP	CB-CG-OD1	-6.14	112.77	118.30
1	B	161[A]	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	B	161[B]	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	506	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	82	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	198	GLU	CG-CD-OE1	6.04	130.39	118.30
1	A	196	GLU	OE1-CD-OE2	-5.97	116.14	123.30
1	A	587	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	198	GLU	CG-CD-OE1	5.88	130.07	118.30
1	B	263	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	404	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	B	54	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	123	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	532	ARG	CG-CD-NE	-5.77	99.69	111.80
1	A	428	MET	CG-SD-CE	5.74	109.39	100.20
1	A	504	ARG	NE-CZ-NH1	5.73	123.17	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	A	123	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	602	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	529[A]	GLU	OE1-CD-OE2	-5.64	116.54	123.30
1	B	529[B]	GLU	OE1-CD-OE2	-5.64	116.54	123.30
1	A	726	GLU	CG-CD-OE2	5.62	129.53	118.30
1	B	504	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	713	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	726	GLU	OE1-CD-OE2	-5.56	116.63	123.30
1	B	540	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	434	TYR	CB-CG-CD1	5.48	124.29	121.00
1	B	506	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	404	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	689	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	161[A]	ARG	CG-CD-NE	5.33	122.98	111.80
1	A	161[B]	ARG	CG-CD-NE	5.33	122.98	111.80
1	B	320	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	504	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	545	VAL	CG1-CB-CG2	-5.27	102.47	110.90
1	B	656	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	A	395	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	726	GLU	CB-CG-CD	5.27	128.42	114.20
1	B	121	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	183	LYS	CD-CE-NZ	5.25	123.77	111.70
1	B	587	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	132	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	735	VAL	CG1-CB-CG2	-5.19	102.60	110.90
1	A	54	ARG	CG-CD-NE	-5.15	100.98	111.80
1	A	83	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	218	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	70	GLN	CA-CB-CG	5.13	124.69	113.40
1	A	41	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	249	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	40	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	730	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	B	169	LEU	CB-CG-CD2	5.08	119.64	111.00
1	B	450	ILE	CA-CB-CG1	-5.07	101.37	111.00
1	A	198	GLU	CA-CB-CG	5.03	124.47	113.40
1	A	255[A]	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	A	255[B]	ARG	NE-CZ-NH1	-5.02	117.79	120.30

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	30	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	53	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 (53) 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:HM1	5:A:804:MPD:O4	1.74	0.84
5:A:804:MPD:CM	5:A:804:MPD:O4	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:C5	5:A:805:MPD:H11	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H52	5:A:805:MPD:H11	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:119[A]:THR:CG2	1:A:265:ALA:HB2	2.48	0.44
1:A:99:PHE:CD2	1:A:374:ALA:HA	2.53	0.44
1:B:650:HIS:HD2	1:B:698:THR:OG1	2.00	0.44
1:B:738:LYS:NZ	7:B:914:HOH:O	2.40	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:804:MPD:H12	5:B:804:MPD:O4	2.21	0.40
1:B:302:ILE:HG21	1:B:302:ILE:HD13	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 [i](#)

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%)	59	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	561/560 (100%)	553 (99%)	8 (1%)	67	65
All	All	1118/1120 (100%)	1100 (98%)	18 (2%)	65	60

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	64	LYS
1	A	118	ARG
1	A	141	ASP
1	A	161[A]	ARG
1	A	161[B]	ARG
1	A	223	ARG
1	A	610	ARG
1	A	649	ARG
1	A	726	GLU
1	B	40	ARG
1	B	64	LYS
1	B	118	ARG
1	B	141	ASP
1	B	223	ARG
1	B	289	PRO
1	B	608	LYS
1	B	649	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	247	ASN
1	B	55	HIS
1	B	216	ASN
1	B	227	ASN
1	B	650	HIS

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	A	111[B]	-	10,17,18	2.76	5 (50%)	10,23,25	2.51	3 (30%)
1	TOX	B	111[A]	2	10,17,18	2.67	5 (50%)	10,23,25	1.83	3 (30%)
1	TOX	A	111[A]	2	10,17,18	2.76	5 (50%)	10,23,25	2.51	3 (30%)
1	TOX	B	111[B]	-	10,17,18	2.67	5 (50%)	10,23,25	1.83	3 (30%)

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	A	111[B]	-	-	2/4/8/10	0/2/2/2
1	TOX	B	111[A]	2	-	2/4/8/10	0/2/2/2
1	TOX	A	111[A]	2	-	2/4/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	2/4/8/10	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[B]	TOX	CD1-NE1	-5.58	1.33	1.39
1	A	111[A]	TOX	CD1-NE1	-5.58	1.33	1.39
1	B	111[A]	TOX	CD1-NE1	-5.12	1.34	1.39
1	B	111[B]	TOX	CD1-NE1	-5.12	1.34	1.39
1	B	111[A]	TOX	O-C	3.49	1.33	1.19
1	B	111[B]	TOX	O-C	3.49	1.33	1.19
1	A	111[B]	TOX	O-C	3.48	1.33	1.19
1	A	111[A]	TOX	O-C	3.48	1.33	1.19
1	B	111[A]	TOX	CZ3-CE3	3.48	1.44	1.36
1	B	111[B]	TOX	CZ3-CE3	3.48	1.44	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[B]	TOX	CH2-CZ3	3.28	1.46	1.38
1	A	111[A]	TOX	CH2-CZ3	3.28	1.46	1.38
1	B	111[A]	TOX	CA-N	-3.25	1.38	1.48
1	B	111[B]	TOX	CA-N	-3.25	1.38	1.48
1	A	111[B]	TOX	CH2-CZ2	2.63	1.42	1.36
1	A	111[A]	TOX	CH2-CZ2	2.63	1.42	1.36
1	A	111[B]	TOX	CZ3-CE3	2.46	1.42	1.36
1	A	111[A]	TOX	CZ3-CE3	2.46	1.42	1.36
1	B	111[A]	TOX	CH2-CZ3	2.12	1.43	1.38
1	B	111[B]	TOX	CH2-CZ3	2.12	1.43	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[B]	TOX	CZ2-CE2-CD2	-5.30	113.72	120.94
1	A	111[A]	TOX	CZ2-CE2-CD2	-5.30	113.72	120.94
1	A	111[B]	TOX	CZ3-CE3-CD2	-3.98	115.37	120.89
1	A	111[A]	TOX	CZ3-CE3-CD2	-3.98	115.37	120.89
1	B	111[A]	TOX	CH2-CZ2-CE2	3.10	125.39	119.44
1	B	111[B]	TOX	CH2-CZ2-CE2	3.10	125.39	119.44
1	A	111[B]	TOX	CE3-CD2-CG	-2.83	129.22	134.42
1	A	111[A]	TOX	CE3-CD2-CG	-2.83	129.22	134.42
1	B	111[A]	TOX	CZ3-CH2-CZ2	-2.59	116.81	120.44
1	B	111[B]	TOX	CZ3-CH2-CZ2	-2.59	116.81	120.44
1	B	111[A]	TOX	CZ2-CE2-CD2	-2.45	117.61	120.94
1	B	111[B]	TOX	CZ2-CE2-CD2	-2.45	117.61	120.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	A	111[A]	TOX	N-CA-CB-CG
1	A	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 carbohydrates 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	A	807	-	7,7,7	1.25	0	9,9,9	2.59	6 (66%)
6	TRS	B	806	-	7,7,7	1.29	1 (14%)	9,9,9	1.86	2 (22%)
5	MPD	A	805	-	7,7,7	0.49	0	9,10,10	1.47	2 (22%)
5	MPD	B	805	-	7,7,7	0.86	0	9,10,10	1.10	0
6	TRS	A	806	-	7,7,7	1.53	2 (28%)	9,9,9	1.95	4 (44%)
2	HEM	B	801	1	27,50,50	1.47	4 (14%)	17,82,82	2.20	7 (41%)
2	HEM	A	801	1	27,50,50	1.28	4 (14%)	17,82,82	2.09	7 (41%)
6	TRS	B	807	-	7,7,7	1.18	1 (14%)	9,9,9	1.31	3 (33%)
5	MPD	A	804	-	7,7,7	0.64	0	9,10,10	1.30	1 (11%)
5	MPD	B	804	-	7,7,7	0.43	0	9,10,10	1.30	0
4	OXY	A	803	-	1,1,1	0.20	0	-	-	-
4	OXY	B	803	-	1,1,1	0.79	0	-	-	-

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	A	807	-	-	5/9/9/9	-
6	TRS	B	806	-	-	5/9/9/9	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	A	805	-	-	3/5/5/5	-
5	MPD	B	805	-	-	1/5/5/5	-
6	TRS	A	806	-	-	0/9/9/9	-
2	HEM	B	801	1	-	0/6/54/54	-
2	HEM	A	801	1	-	0/6/54/54	-
6	TRS	B	807	-	-	0/9/9/9	-
5	MPD	A	804	-	-	0/5/5/5	-
5	MPD	B	804	-	-	2/5/5/5	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C1A-NA	4.21	1.44	1.36
2	B	801	HEM	C4B-NB	-3.89	1.28	1.36
2	B	801	HEM	C3B-C2B	-3.42	1.35	1.40
2	B	801	HEM	CAD-C3D	-3.25	1.46	1.52
6	A	806	TRS	O1-C1	2.91	1.51	1.42
6	A	806	TRS	C1-C	2.75	1.61	1.53
6	B	806	TRS	C-N	2.63	1.58	1.49
2	B	801	HEM	C1C-C2C	2.43	1.48	1.42
2	A	801	HEM	C4D-C3D	2.18	1.47	1.42
2	A	801	HEM	C3B-C2B	-2.17	1.37	1.40
6	B	807	TRS	O1-C1	2.11	1.49	1.42
2	A	801	HEM	C1D-ND	2.00	1.40	1.36

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CAA-CBA-CGA	-4.93	104.40	112.67
2	B	801	HEM	CMB-C2B-C3B	4.38	132.86	124.68
6	A	807	TRS	C3-C-C1	4.23	123.94	110.81
6	A	807	TRS	O1-C1-C	-3.98	98.38	111.00
2	A	801	HEM	C1D-C2D-C3D	-3.83	104.33	107.00
6	B	806	TRS	C3-C-N	3.55	118.58	107.98
2	B	801	HEM	CMA-C3A-C4A	-3.40	123.24	128.46
6	A	806	TRS	C1-C-N	3.32	117.90	107.98
2	B	801	HEM	CMA-C3A-C2A	3.15	130.87	124.94
2	B	801	HEM	CAD-CBD-CGD	2.92	117.57	112.67
5	A	805	MPD	C5-C4-C3	2.90	125.38	111.69
2	B	801	HEM	CAA-CBA-CGA	-2.86	107.88	112.67
2	A	801	HEM	CMB-C2B-C3B	2.75	129.83	124.68
6	A	806	TRS	C3-C-N	-2.70	99.92	107.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	807	TRS	O2-C2-C	-2.65	102.60	111.00
2	A	801	HEM	CMC-C2C-C3C	2.53	129.41	124.68
2	A	801	HEM	CBD-CAD-C3D	2.52	117.12	112.48
6	A	806	TRS	O1-C1-C	2.50	118.91	111.00
6	A	807	TRS	C2-C-N	2.48	115.39	107.98
2	A	801	HEM	C3C-C4C-NC	-2.47	106.28	110.94
5	A	805	MPD	O4-C4-C3	-2.45	101.45	111.36
6	B	807	TRS	O1-C1-C	2.34	118.40	111.00
6	A	807	TRS	C1-C-N	-2.32	101.06	107.98
6	A	807	TRS	C3-C-C2	-2.25	103.84	110.81
2	B	801	HEM	CBD-CAD-C3D	2.18	116.50	112.48
6	B	806	TRS	C2-C-N	2.17	114.45	107.98
6	B	807	TRS	C3-C-C2	-2.14	104.18	110.81
2	B	801	HEM	C4C-C3C-C2C	2.12	108.38	106.90
6	A	806	TRS	C2-C-N	-2.11	101.69	107.98
2	A	801	HEM	CBA-CAA-C2A	2.05	116.27	112.49
6	B	807	TRS	C2-C-C1	2.05	117.17	110.81
5	A	804	MPD	CM-C2-C3	2.01	119.30	109.96

There are no chirality outliers.

All (16) torsion outliers are listed below:

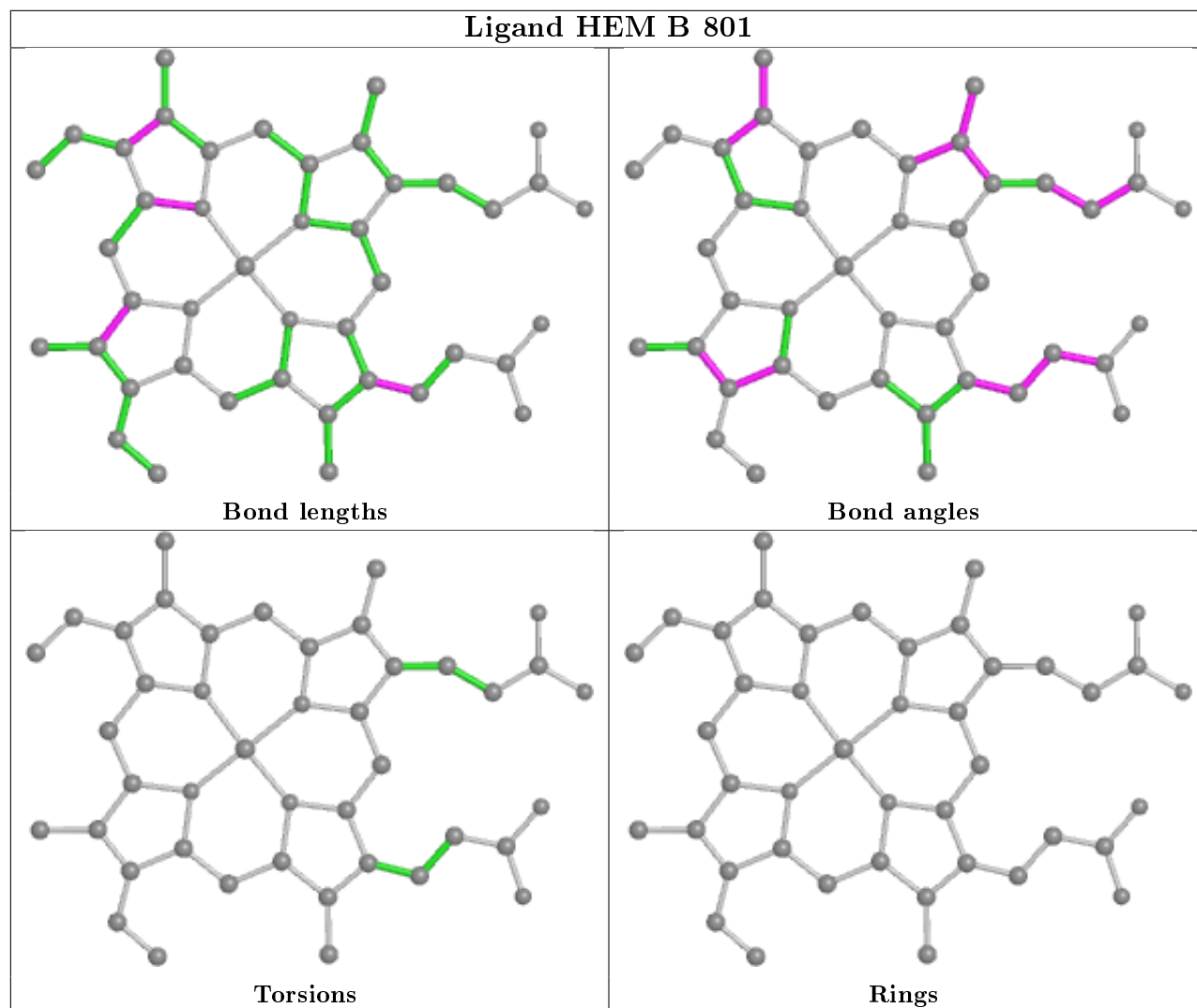
Mol	Chain	Res	Type	Atoms
5	A	805	MPD	C2-C3-C4-C5
6	A	807	TRS	C2-C-C1-O1
6	A	807	TRS	C3-C-C1-O1
6	A	807	TRS	N-C-C1-O1
5	B	804	MPD	O2-C2-C3-C4
6	B	806	TRS	C3-C-C2-O2
6	B	806	TRS	C1-C-C2-O2
6	B	806	TRS	N-C-C2-O2
6	B	806	TRS	N-C-C3-O3
6	A	807	TRS	C1-C-C2-O2
6	A	807	TRS	N-C-C2-O2
5	A	805	MPD	C1-C2-C3-C4
5	B	805	MPD	CM-C2-C3-C4
5	B	804	MPD	C1-C2-C3-C4
6	B	806	TRS	C1-C-C3-O3
5	A	805	MPD	O2-C2-C3-C4

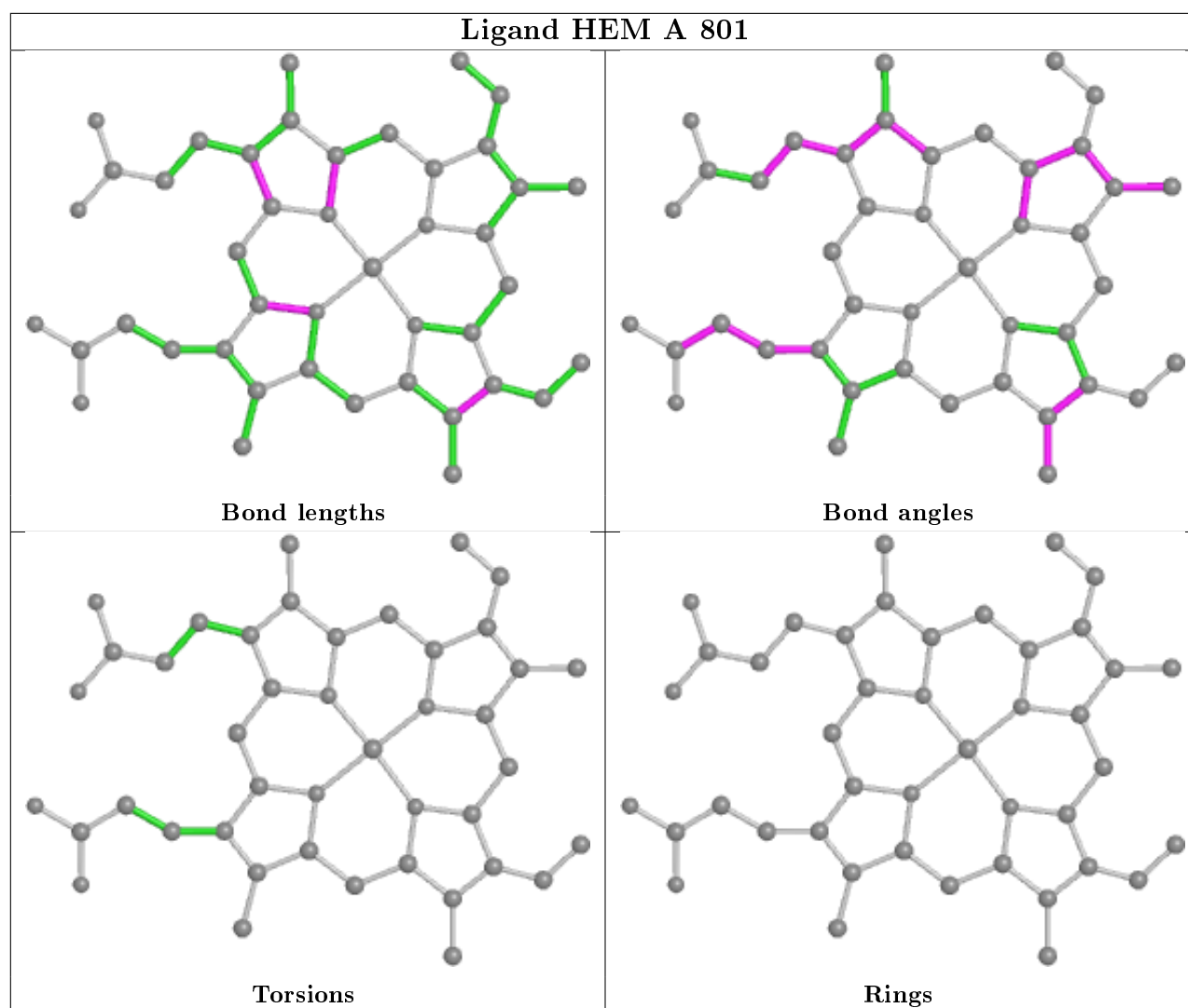
There are no ring outliers.

4 monomers are involved in 8 short contacts:

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.39	15 (2%) 63 66	15, 23, 40, 77	0
1	B	712/728 (97%)	-0.48	13 (1%) 68 71	14, 21, 38, 72	0
All	All	1424/1456 (97%)	-0.44	28 (1%) 65 68	14, 22, 40, 77	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	7.3
1	B	748	ALA	6.2
1	B	679	ALA	4.5
1	A	540	ARG	4.3
1	A	541	GLY	4.2
1	A	610	ARG	4.1
1	B	610	ARG	3.6
1	B	65	ASP	3.4
1	B	680	ALA	3.3
1	A	65	ASP	3.2
1	A	222	ASP	3.2
1	A	608	LYS	3.1
1	B	64	LYS	3.1
1	B	44	PRO	3.0
1	B	540	ARG	2.9
1	A	64	LYS	2.9
1	A	378	SER	2.8
1	A	454	ASP	2.8
1	A	221	GLY	2.8
1	A	215	PRO	2.8
1	B	608	LYS	2.7
1	B	541	GLY	2.5
1	B	691	ALA	2.3
1	B	45	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	213	GLY	2.3
1	A	63	GLY	2.3
1	A	691	ALA	2.3
1	B	222	ASP	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TOX	A	111[B]	16/17	0.95	0.10	16,20,23,25	2
1	TOX	B	111[A]	16/17	0.95	0.09	15,17,19,20	2
1	TOX	A	111[A]	16/17	0.95	0.10	16,20,23,25	2
1	TOX	B	111[B]	16/17	0.95	0.09	15,17,19,20	2

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
5	MPD	B	805	8/8	0.82	0.19	38,52,54,66	0
6	TRS	B	806	8/8	0.83	0.23	43,53,57,64	0
6	TRS	A	807	8/8	0.84	0.21	46,50,52,58	0
5	MPD	A	804	8/8	0.89	0.17	59,66,73,74	0
5	MPD	A	805	8/8	0.92	0.16	43,51,60,63	0
5	MPD	B	804	8/8	0.93	0.14	52,56,62,63	0
4	OXY	B	803	2/2	0.93	0.24	31,31,31,36	0
4	OXY	A	803	2/2	0.94	0.28	41,41,41,45	0
6	TRS	B	807	8/8	0.96	0.09	24,28,31,32	0
6	TRS	A	806	8/8	0.96	0.13	28,35,38,42	0

Continued on next page...

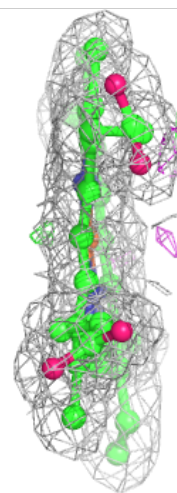
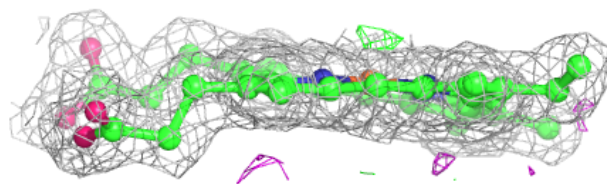
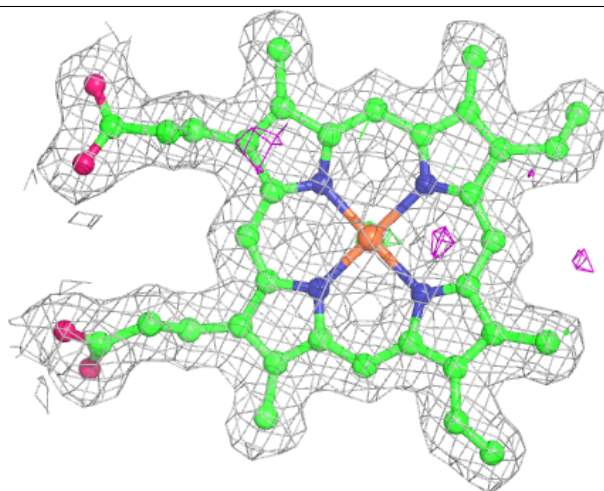
Continued from previous page...

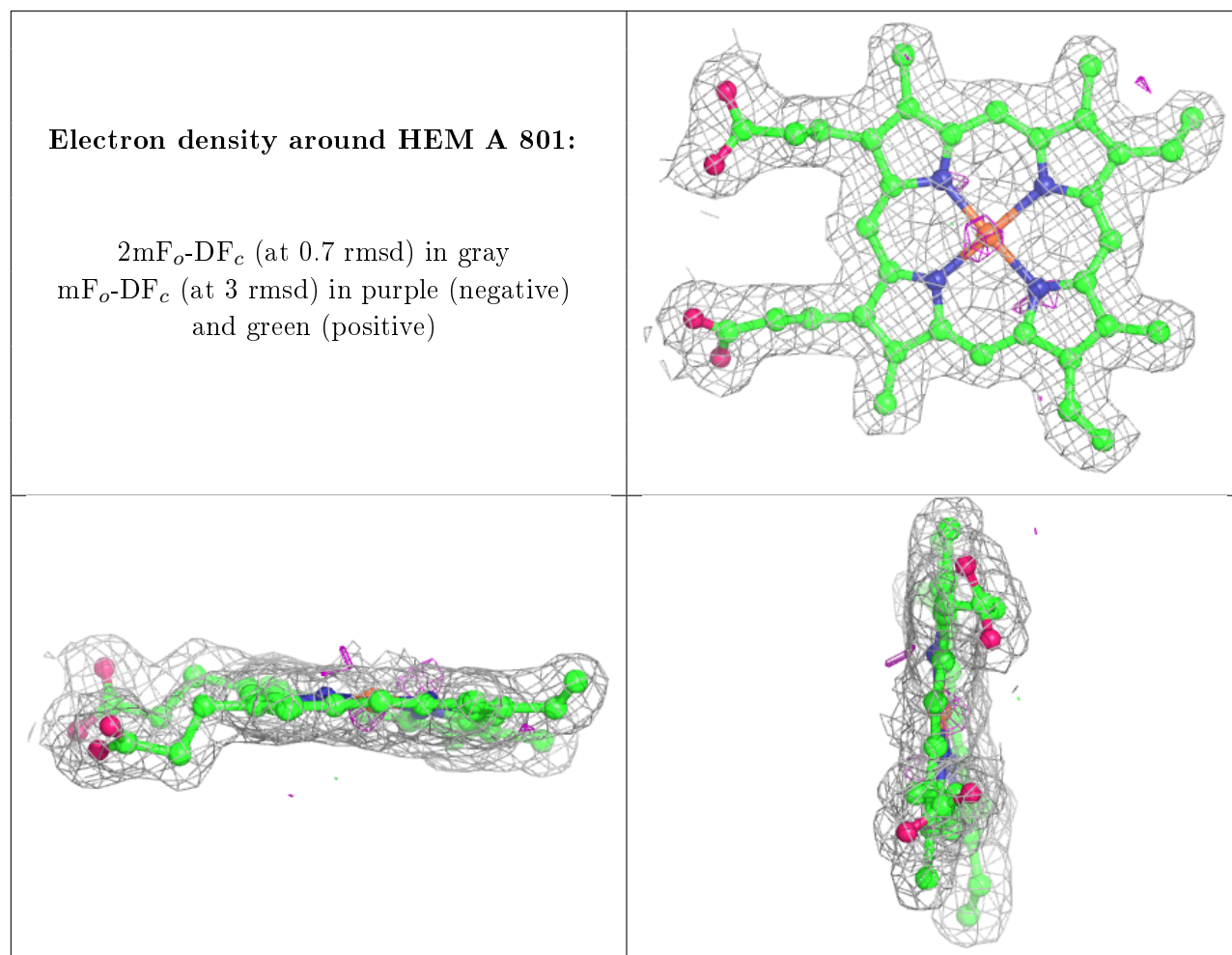
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	B	802	1/1	0.99	0.15	23,23,23,23	0
3	NA	A	802	1/1	0.99	0.14	24,24,24,24	0
2	HEM	B	801	43/43	0.99	0.06	13,15,17,19	0
2	HEM	A	801	43/43	0.99	0.05	16,19,22,23	0

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.