



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2016 – 11:35 AM EDT

PDB ID : 5L02
Title : S324T variant of B. pseudomallei KatG
Authors : Loewen, P.C.
Deposited on : 2016-07-26
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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

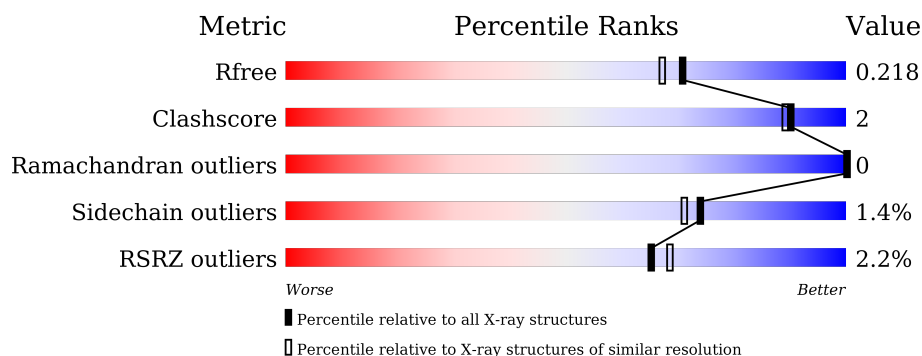
1 Overall quality at a glance

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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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. 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>3%</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>87%</div> <div>10%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MPD	A	804	-	-	-	X
5	MPD	B	804	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12604 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.

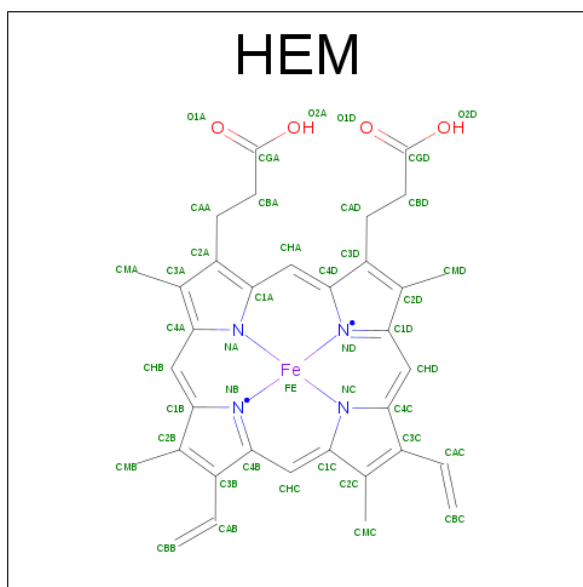
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	9	0
			5585	3521	998	1052	14			
1	B	713	Total	C	N	O	S	0	9	0
			5582	3519	999	1050	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	THR	SER	engineered mutation	UNP Q3JNW6
B	324	THR	SER	engineered mutation	UNP Q3JNW6

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



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

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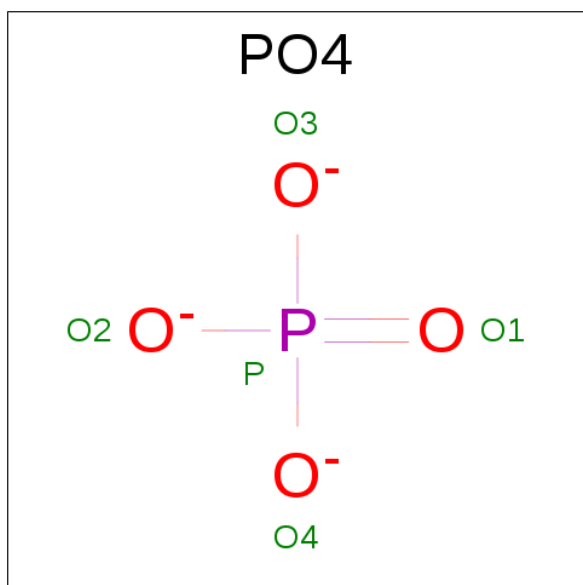
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

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

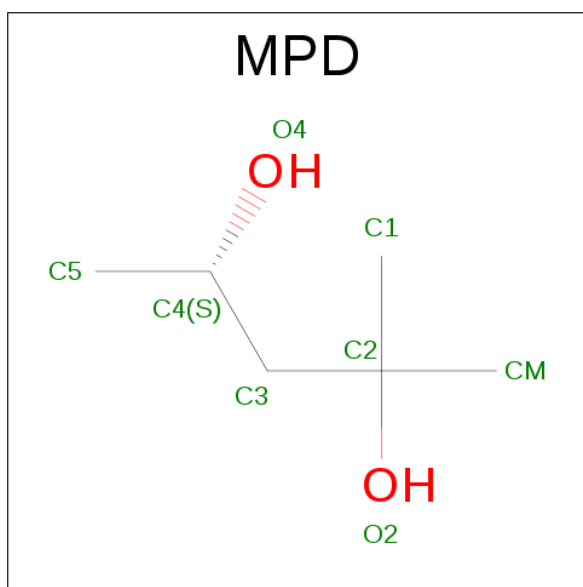
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na		
			1	1	0	0
3	A	1	Total	Na		
			1	1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- 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		

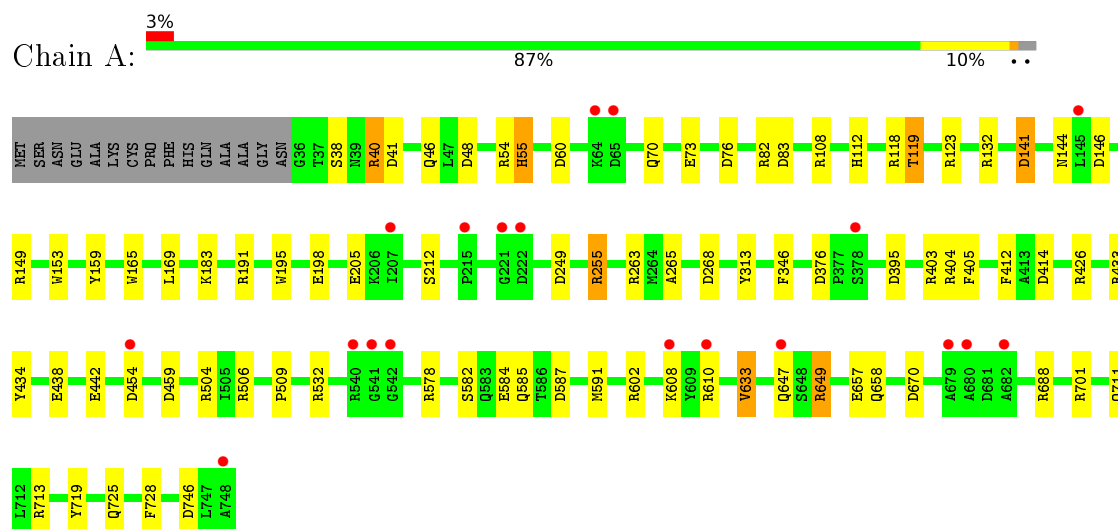
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	660	Total	O	0	0
			660	660		
6	B	655	Total	O	0	0
			655	655		

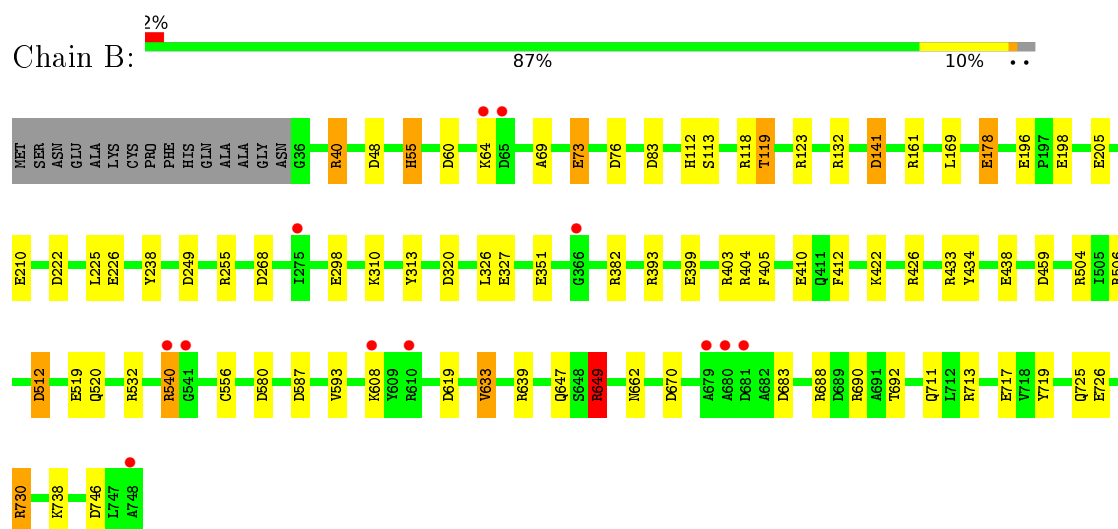
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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	100.50 Å 114.63 Å 174.93 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.05 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-1.90) 99.1 (29.05-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 1.91 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.173 , 0.211 0.184 , 0.218	Depositor DCC
R_{free} test set	7879 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.6	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	0.96	EDS
Total number of atoms	12604	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 3.09% 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: NA, TOX, PO4, HEM, 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	1.33	26/5711 (0.5%)	1.26	61/7760 (0.8%)
1	B	1.34	23/5704 (0.4%)	1.24	53/7749 (0.7%)
All	All	1.34	49/11415 (0.4%)	1.25	114/15509 (0.7%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	726	GLU	CG-CD	10.19	1.67	1.51
1	B	512	ASP	CG-OD2	8.11	1.44	1.25
1	B	532	ARG	CD-NE	-8.01	1.32	1.46
1	B	196	GLU	CG-CD	7.84	1.63	1.51
1	B	746	ASP	CB-CG	7.50	1.67	1.51
1	A	584	GLU	CG-CD	7.43	1.63	1.51
1	A	532	ARG	CD-NE	-7.17	1.34	1.46
1	A	728	PHE	CG-CD2	-6.56	1.28	1.38
1	B	438	GLU	CD-OE2	6.48	1.32	1.25
1	B	556	CYS	CB-SG	6.44	1.93	1.82
1	B	399	GLU	CD-OE1	6.33	1.32	1.25
1	A	73	GLU	CG-CD	6.21	1.61	1.51
1	B	327	GLU	CG-CD	6.17	1.61	1.51
1	A	153	TRP	CG-CD1	-6.15	1.28	1.36
1	A	532	ARG	NE-CZ	-6.08	1.25	1.33
1	A	159	TYR	CE1-CZ	6.04	1.46	1.38
1	B	119[A]	THR	CB-CG2	-5.90	1.32	1.52
1	B	119[B]	THR	CB-CG2	-5.90	1.32	1.52
1	A	746	ASP	CB-CG	5.83	1.64	1.51
1	A	313	TYR	CE2-CZ	5.79	1.46	1.38
1	A	195	TRP	CE3-CZ3	5.78	1.48	1.38
1	B	161	ARG	NE-CZ	5.74	1.40	1.33
1	B	351	GLU	CD-OE1	5.69	1.31	1.25
1	B	178	GLU	CG-CD	5.67	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	442	GLU	CD-OE2	-5.65	1.19	1.25
1	B	210	GLU	CD-OE2	5.62	1.31	1.25
1	B	746	ASP	C-O	-5.51	1.12	1.23
1	A	82	ARG	CZ-NH2	-5.49	1.25	1.33
1	A	119[A]	THR	CB-CG2	-5.47	1.34	1.52
1	A	119[B]	THR	CB-CG2	-5.47	1.34	1.52
1	A	657[A]	GLU	CD-OE2	-5.41	1.19	1.25
1	A	657[B]	GLU	CD-OE2	-5.41	1.19	1.25
1	B	717	GLU	CD-OE1	5.39	1.31	1.25
1	B	506	ARG	CZ-NH2	-5.36	1.26	1.33
1	A	438	GLU	CD-OE2	5.36	1.31	1.25
1	A	602	ARG	CZ-NH2	-5.33	1.26	1.33
1	A	212	SER	CB-OG	-5.31	1.35	1.42
1	B	113	SER	CB-OG	5.31	1.49	1.42
1	B	313	TYR	CG-CD1	5.28	1.46	1.39
1	B	205	GLU	CD-OE1	5.27	1.31	1.25
1	A	38	SER	CA-CB	5.23	1.60	1.52
1	B	327	GLU	CD-OE1	5.18	1.31	1.25
1	A	658	GLN	CD-NE2	-5.17	1.20	1.32
1	A	313	TYR	CG-CD1	5.14	1.45	1.39
1	A	688	ARG	CZ-NH2	-5.07	1.26	1.33
1	A	434	TYR	CE1-CZ	-5.05	1.31	1.38
1	B	226	GLU	CG-CD	5.05	1.59	1.51
1	A	165	TRP	CE2-CZ2	5.03	1.48	1.39
1	A	205	GLU	CG-CD	5.03	1.59	1.51

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH2	-29.96	105.32	120.30
1	B	532	ARG	NE-CZ-NH2	-23.27	108.67	120.30
1	B	532	ARG	NE-CZ-NH1	19.00	129.80	120.30
1	A	532	ARG	NE-CZ-NH1	17.32	128.96	120.30
1	B	393	ARG	NE-CZ-NH2	-12.63	113.98	120.30
1	B	506	ARG	NE-CZ-NH1	10.47	125.54	120.30
1	B	433	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	B	132	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	B	512	ASP	CB-CG-OD1	-9.18	110.04	118.30
1	A	40	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	A	376	ASP	CB-CG-OD2	-9.03	110.17	118.30
1	A	633	VAL	CG1-CB-CG2	-9.01	96.49	110.90
1	A	713	ARG	NE-CZ-NH1	8.95	124.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ASP	CB-CG-OD1	8.56	126.01	118.30
1	A	433	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	B	268	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	A	454	ASP	CB-CG-OD2	8.26	125.73	118.30
1	B	633	VAL	CG1-CB-CG2	-8.21	97.77	110.90
1	B	688	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	B	619	ASP	CB-CG-OD1	-8.09	111.02	118.30
1	A	191	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	268	ASP	CB-CG-OD2	-7.76	111.31	118.30
1	B	713	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	B	48	ASP	CB-CG-OD1	7.69	125.22	118.30
1	A	713	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	B	249	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	191	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	434	TYR	CB-CG-CD1	7.45	125.47	121.00
1	B	123	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	B	726	GLU	OE1-CD-OE2	-7.33	114.50	123.30
1	A	132	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	B	268	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	60	ASP	CB-CG-OD1	7.27	124.85	118.30
1	A	578	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	512	ASP	CB-CG-OD2	7.19	124.77	118.30
1	A	587	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	149	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	395	ASP	CB-CG-OD1	7.03	124.63	118.30
1	B	683	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	B	320	ASP	CB-CG-OD1	-6.93	112.07	118.30
1	B	506	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	A	649	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	649	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	506	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	B	404	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	504	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	183	LYS	CD-CE-NZ	6.75	127.23	111.70
1	A	255	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	532	ARG	CD-NE-CZ	6.73	133.02	123.60
1	B	426	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	B	60	ASP	CB-CG-OD1	6.65	124.28	118.30
1	B	40	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	A	404	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	198[A]	GLU	OE1-CD-OE2	-6.44	115.57	123.30
1	A	198[B]	GLU	OE1-CD-OE2	-6.44	115.57	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	GLU	OE1-CD-OE2	6.42	131.01	123.30
1	A	249	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	A	198[A]	GLU	CG-CD-OE1	6.38	131.06	118.30
1	A	198[B]	GLU	CG-CD-OE1	6.38	131.06	118.30
1	B	587	ASP	CB-CG-OD1	6.35	124.01	118.30
1	A	670	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	83	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	504	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	649	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	688	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	83	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	532	ARG	CG-CD-NE	-6.18	98.83	111.80
1	A	255	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	426[A]	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	A	426[B]	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	B	169	LEU	CB-CG-CD2	6.14	121.44	111.00
1	A	263	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	123	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	433	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	A	602	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	73	GLU	OE1-CD-OE2	-5.94	116.17	123.30
1	B	670	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	532	ARG	CD-NE-CZ	5.89	131.84	123.60
1	B	688	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	434	TYR	CB-CG-CD1	5.86	124.51	121.00
1	A	40	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	602	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	249	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	198	GLU	OE1-CD-OE2	-5.80	116.34	123.30
1	A	54	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	198	GLU	CG-CD-OE1	5.72	129.75	118.30
1	B	161	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	587	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	222	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	70	GLN	CA-CB-CG	5.51	125.52	113.40
1	B	639	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	580	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	41	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	55	HIS	CB-CA-C	5.36	121.13	110.40
1	B	225	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	B	55	HIS	CB-CA-C	5.36	121.12	110.40
1	B	60	ASP	CB-CG-OD2	-5.34	113.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	730[A]	ARG	CA-CB-CG	5.29	125.05	113.40
1	B	730[B]	ARG	CA-CB-CG	5.29	125.05	113.40
1	A	404	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	504	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	459	ASP	CB-CG-OD1	5.24	123.01	118.30
1	B	532	ARG	CG-CD-NE	-5.22	100.83	111.80
1	A	108	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	532	ARG	NH1-CZ-NH2	5.17	125.09	119.40
1	A	701	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	310	LYS	CD-CE-NZ	-5.08	100.02	111.70
1	A	169	LEU	CB-CG-CD2	5.06	119.60	111.00
1	B	619	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	414	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	506	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	B	382	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	B	326	LEU	CA-CB-CG	-5.01	103.78	115.30

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	5585	0	5388	16	0
1	B	5582	0	5381	29	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	5	0	0	0	0
4	B	5	0	0	0	0
5	A	16	0	28	5	0
5	B	8	0	14	2	0
6	A	660	0	0	6	0
6	B	655	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12604	0	10871	51	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 2.

All (51) 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:520:GLN:HG3	6:B:956:HOH:O	1.62	0.97
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.65	0.79
1:A:711[B]:GLN:OE1	6:A:901:HOH:O	2.00	0.78
1:B:119[B]:THR:HG23	6:B:955:HOH:O	1.83	0.78
1:B:540:ARG:HA	1:B:540:ARG:NE	2.00	0.77
1:A:255:ARG:NH2	6:A:904:HOH:O	2.18	0.76
5:B:804:MPD:HM2	5:B:804:MPD:H52	1.67	0.74
1:B:55:HIS:HD2	6:B:1307:HOH:O	1.69	0.74
1:B:512:ASP:OD1	6:B:901:HOH:O	2.10	0.69
5:A:805:MPD:H52	5:A:805:MPD:H11	1.73	0.69
1:B:519:GLU:OE1	6:B:902:HOH:O	2.11	0.68
5:A:805:MPD:C5	5:A:805:MPD:H11	2.23	0.68
1:A:55:HIS:HD2	6:A:1325:HOH:O	1.75	0.68
1:A:76:ASP:OD1	6:A:903:HOH:O	2.11	0.68
1:B:178:GLU:OE1	6:B:903:HOH:O	2.13	0.65
1:B:76:ASP:OD1	6:B:904:HOH:O	2.15	0.62
5:B:804:MPD:CM	5:B:804:MPD:H52	2.32	0.59
5:A:804:MPD:CM	5:A:804:MPD:O4	2.51	0.59
1:B:119[B]:THR:HG21	6:B:1485:HOH:O	2.04	0.57
1:B:410:GLU:HB2	6:B:1379:HOH:O	2.03	0.56
1:B:647:GLN:HG2	6:B:1275:HOH:O	2.06	0.56
1:B:69:ALA:O	1:B:73:GLU:HG2	2.06	0.56
1:B:540:ARG:HE	1:B:540:ARG:HA	1.71	0.55
1:B:540:ARG:CA	1:B:540:ARG:NE	2.69	0.55
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.37	0.55
1:A:647:GLN:HG2	6:A:1211:HOH:O	2.08	0.54
1:A:633:VAL:CG2	1:A:719:TYR:CZ	2.92	0.53
1:A:46:GLN:NE2	1:B:298:GLU:O	2.43	0.51
1:B:633:VAL:CG2	1:B:719:TYR:CZ	2.94	0.51
1:B:711[A]:GLN:NE2	6:B:913:HOH:O	2.44	0.51
1:B:692:THR:HG21	6:B:905:HOH:O	2.11	0.50
1:B:255:ARG:HD3	6:B:1256:HOH:O	2.11	0.50
1:B:405:PHE:HB3	1:B:412:PHE:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:804:MPD:HM1	5:A:804:MPD:O4	2.13	0.48
1:A:582:SER:OG	1:A:585:GLN:HG3	2.14	0.48
1:B:403[B]:ARG:NH1	6:B:922:HOH:O	2.47	0.47
1:B:255:ARG:CD	6:B:1256:HOH:O	2.65	0.45
5:A:805:MPD:H52	5:A:805:MPD:C1	2.44	0.45
1:B:112:HIS:CE1	1:B:141:ASP:O	2.71	0.44
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.17	0.44
1:A:405:PHE:HB3	1:A:412:PHE:HB2	1.98	0.43
1:B:662:ASN:H	1:B:725:GLN:HE22	1.65	0.43
1:A:346:PHE:CD2	1:A:403[A]:ARG:CZ	3.01	0.43
1:A:112:HIS:CE1	1:A:141:ASP:O	2.72	0.43
1:B:649:ARG:HG2	6:B:1367:HOH:O	2.18	0.42
1:A:725:GLN:HG3	6:A:1164:HOH:O	2.19	0.42
1:B:738:LYS:NZ	6:B:938:HOH:O	2.52	0.42
1:A:119[A]:THR:HG21	1:A:265:ALA:HB2	2.02	0.41
1:B:422:LYS:NZ	6:B:949:HOH:O	2.54	0.40
1:A:509:PRO:HD2	1:A:591:MET:HG2	2.02	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	719/728 (99%)	709 (99%)	10 (1%)	0	100	100
1	B	718/728 (99%)	706 (98%)	12 (2%)	0	100	100
All	All	1437/1456 (99%)	1415 (98%)	22 (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	558/560 (100%)	552 (99%)	6 (1%)	80	79
1	B	557/560 (100%)	547 (98%)	10 (2%)	66	61
All	All	1115/1120 (100%)	1099 (99%)	16 (1%)	74	71

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	118	ARG
1	A	141	ASP
1	A	608	LYS
1	A	610	ARG
1	A	649	ARG
1	B	40	ARG
1	B	64	LYS
1	B	118	ARG
1	B	141	ASP
1	B	540	ARG
1	B	608	LYS
1	B	649	ARG
1	B	690	ARG
1	B	730[A]	ARG
1	B	730[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	B	647	GLN
1	B	650	HIS
1	B	725	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	1,2	10,17,18	2.26	6 (60%)	9,23,25	1.50	2 (22%)
1	TOX	B	111[A]	2	10,17,18	3.28	3 (30%)	9,23,25	1.95	3 (33%)
1	TOX	B	111[B]	-	10,17,18	3.28	3 (30%)	9,23,25	1.95	3 (33%)

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	1,2	-	0/3/8/10	0/2/2/2
1	TOX	B	111[A]	2	-	0/3/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	0/3/8/10	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	CD1-NE1	-8.78	1.31	1.39
1	B	111[B]	TOX	CD1-NE1	-8.78	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	TOX	CE3-CD2	-2.86	1.36	1.42
1	A	111	TOX	CZ2-CE2	-2.51	1.35	1.41
1	B	111[A]	TOX	CD2-CE2	2.09	1.44	1.41
1	B	111[B]	TOX	CD2-CE2	2.09	1.44	1.41
1	A	111	TOX	CZ3-CH2	2.20	1.43	1.38
1	A	111	TOX	CH2-CZ2	2.26	1.41	1.36
1	A	111	TOX	O-C	3.29	1.35	1.19
1	A	111	TOX	CD2-CE2	3.56	1.46	1.41
1	B	111[A]	TOX	O-C	4.82	1.42	1.19
1	B	111[B]	TOX	O-C	4.82	1.42	1.19

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111[A]	TOX	O-C-CA	-4.28	114.26	125.72
1	B	111[B]	TOX	O-C-CA	-4.28	114.26	125.72
1	A	111	TOX	O-C-CA	-2.85	118.08	125.72
1	B	111[A]	TOX	CZ2-CE2-CD2	-2.67	117.22	120.58
1	B	111[B]	TOX	CZ2-CE2-CD2	-2.67	117.22	120.58
1	A	111	TOX	CZ3-CH2-CZ2	-2.37	117.02	120.45
1	B	111[A]	TOX	CB-CG-CD1	-2.07	125.41	127.97
1	B	111[B]	TOX	CB-CG-CD1	-2.07	125.41	127.97

There are no chirality outliers.

There are no torsion outliers.

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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	A	801	1	24,50,50	1.37	3 (12%)	16,82,82	2.18	7 (43%)
4	PO4	A	803	-	4,4,4	0.60	0	6,6,6	0.26	0
5	MPD	A	804	-	6,7,7	0.82	0	6,10,10	1.39	0
5	MPD	A	805	-	6,7,7	1.06	0	6,10,10	1.14	0
2	HEM	B	801	1	24,50,50	2.22	7 (29%)	16,82,82	2.07	6 (37%)
4	PO4	B	803	-	4,4,4	0.57	0	6,6,6	0.43	0
5	MPD	B	804	-	6,7,7	0.70	0	6,10,10	0.97	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
2	HEM	A	801	1	-	0/6/54/54	0/0/8/8
4	PO4	A	803	-	-	0/0/0/0	0/0/0/0
5	MPD	A	804	-	-	0/5/5/5	0/0/0/0
5	MPD	A	805	-	-	0/5/5/5	0/0/0/0
2	HEM	B	801	1	-	0/6/54/54	0/0/8/8
4	PO4	B	803	-	-	0/0/0/0	0/0/0/0
5	MPD	B	804	-	-	0/5/5/5	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3B-C2B	-7.47	1.30	1.40
2	A	801	HEM	C1B-NB	-3.84	1.31	1.36
2	B	801	HEM	C1C-NC	-3.79	1.31	1.36
2	B	801	HEM	C2A-C3A	-3.49	1.27	1.37
2	B	801	HEM	CAA-C2A	-3.26	1.46	1.52
2	B	801	HEM	CAD-C3D	-2.90	1.48	1.52
2	A	801	HEM	C1C-NC	-2.82	1.33	1.36
2	B	801	HEM	C1B-NB	-2.21	1.33	1.36
2	A	801	HEM	CAA-C2A	-2.12	1.48	1.52
2	B	801	HEM	C4C-NC	2.16	1.39	1.36

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CMA-C3A-C4A	-3.90	121.69	128.31
2	B	801	HEM	C3B-CAB-CBB	-3.32	119.72	126.40
2	A	801	HEM	C3B-CAB-CBB	-3.28	119.80	126.40
2	A	801	HEM	CAA-CBA-CGA	-3.06	106.83	112.78
2	B	801	HEM	CMA-C3A-C4A	-2.90	123.38	128.31
2	A	801	HEM	C3C-C4C-NC	-2.47	106.28	110.94
2	B	801	HEM	CAA-CBA-CGA	-2.09	108.72	112.78
2	A	801	HEM	CMA-C3A-C2A	2.42	130.31	125.24
2	A	801	HEM	CAD-CBD-CGD	2.61	117.86	112.78
2	B	801	HEM	CAD-CBD-CGD	3.11	118.83	112.78
2	B	801	HEM	CMB-C2B-C3B	3.16	131.26	125.09
2	B	801	HEM	CBD-CAD-C3D	3.18	118.05	112.47
2	A	801	HEM	CBD-CAD-C3D	4.04	119.56	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

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

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%)	-0.18	19 (2%) 58 61	17, 26, 46, 83	0
1	B	712/728 (97%)	-0.27	12 (1%) 73 76	17, 25, 43, 79	0
All	All	1424/1456 (97%)	-0.22	31 (2%) 65 68	17, 25, 45, 83	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	5.8
1	A	748	ALA	5.5
1	A	540	ARG	4.8
1	B	679	ALA	4.7
1	A	610	ARG	4.6
1	A	541	GLY	4.6
1	B	610	ARG	4.1
1	B	608	LYS	4.0
1	B	540	ARG	3.8
1	A	221	GLY	3.7
1	B	680	ALA	3.6
1	A	608	LYS	3.5
1	A	65	ASP	3.2
1	B	65	ASP	3.2
1	A	64	LYS	3.0
1	A	542	GLY	2.7
1	B	541	GLY	2.6
1	A	222	ASP	2.6
1	B	64	LYS	2.5
1	A	215	PRO	2.5
1	A	454	ASP	2.5
1	B	275	ILE	2.4
1	A	378	SER	2.4
1	B	366	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	679	ALA	2.3
1	A	682	ALA	2.2
1	A	145	LEU	2.2
1	A	207	ILE	2.1
1	B	681	ASP	2.1
1	A	647	GLN	2.0
1	A	680	ALA	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	TOX	B	111[A]	16/17	0.97	0.13	-	17,19,28,31	1
1	TOX	B	111[B]	16/17	0.97	0.13	-	17,19,23,28	1
1	TOX	A	111	16/17	0.97	0.16	-	17,23,34,37	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	MPD	B	804	8/8	0.83	0.20	9.67	60,67,77,82	0
5	MPD	A	804	8/8	0.86	0.21	6.59	63,69,71,74	0
2	HEM	A	801	43/43	0.98	0.14	1.08	19,22,25,26	0
2	HEM	B	801	43/43	0.99	0.13	0.32	17,18,20,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	A	802	1/1	0.98	0.04	-1.62	21,21,21,21	0
3	NA	B	802	1/1	1.00	0.05	-4.68	22,22,22,22	0
5	MPD	A	805	8/8	0.91	0.17	-	49,54,58,60	0
4	PO4	A	803	5/5	0.96	0.15	-	50,60,65,66	0
4	PO4	B	803	5/5	0.94	0.16	-	40,55,56,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.