



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2016 – 05:08 PM EDT

PDB ID : 5SYV
Title : Crystal structure of Burkholderia pseudomallei KatG N240D variant
Authors : Loewen, P.C.
Deposited on : 2016-08-12
Resolution : 1.75 Å(reported)

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

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

A user guide is available at

<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

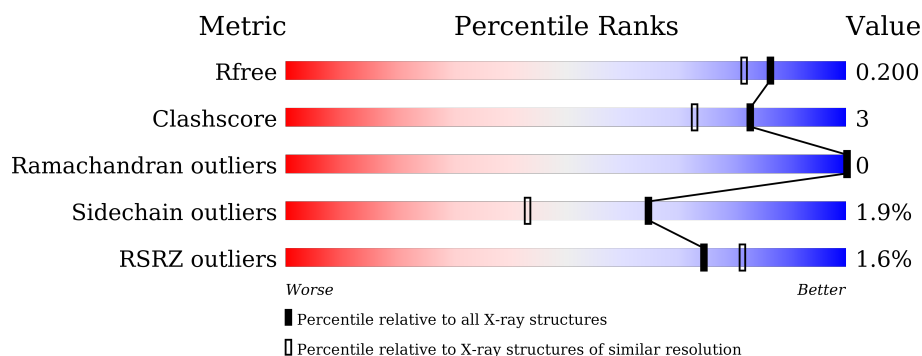
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>89%</div> <div>8%</div> <div>..</div> </div> </div>
1	B	728	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>7%</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	MPD	A	805	-	-	-	X
6	MPD	B	806	-	-	X	X
6	MPD	B	808	-	-	X	X

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.

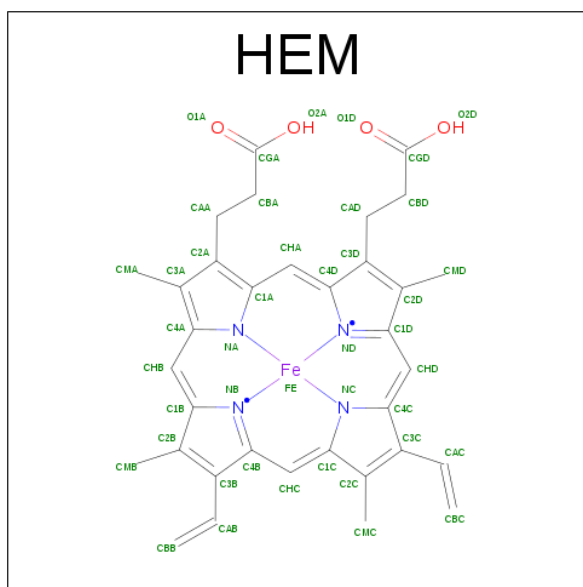
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total 5534	C 3494	N 986	O 1040	S 14	0	5	0
1	B	713	Total 5546	C 3505	N 986	O 1041	S 14	0	7	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	ASP	ASN	engineered mutation	UNP Q3JNW6
B	240	ASP	ASN	engineered mutation	UNP Q3JNW6

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



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

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

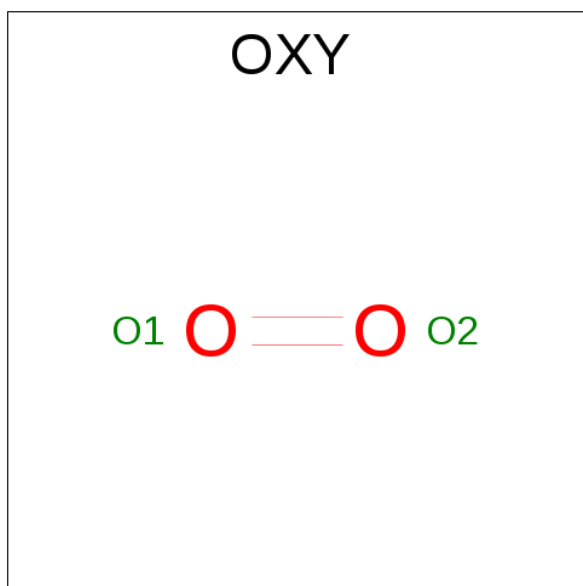
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

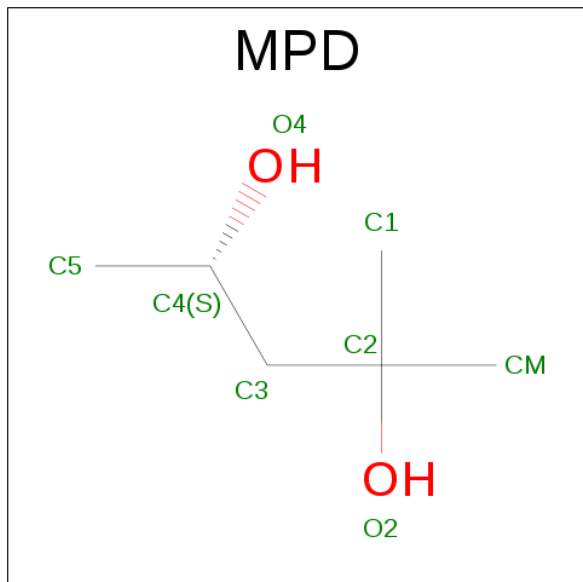
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl		
			1	1	0	0
4	A	1	Total	Cl		
			1	1	0	0

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



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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

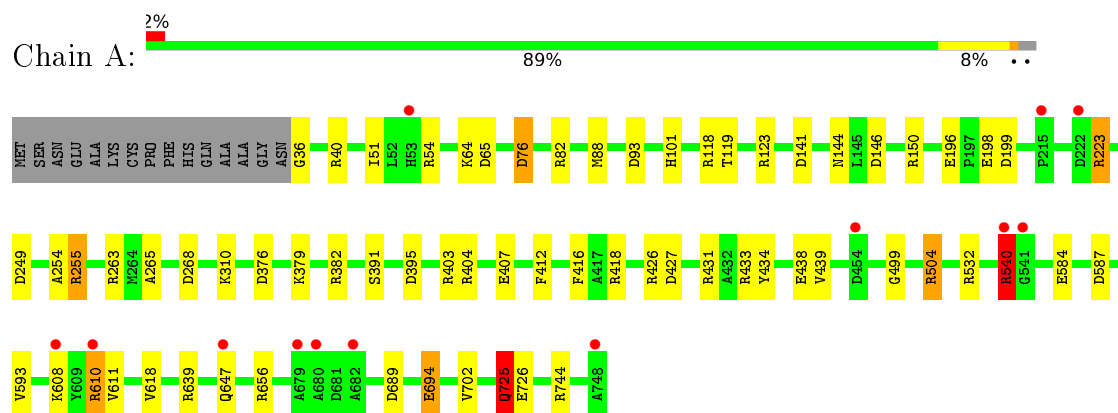
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	828	Total	O	0	0
			828	828		
8	B	804	Total	O	0	0
			804	804		

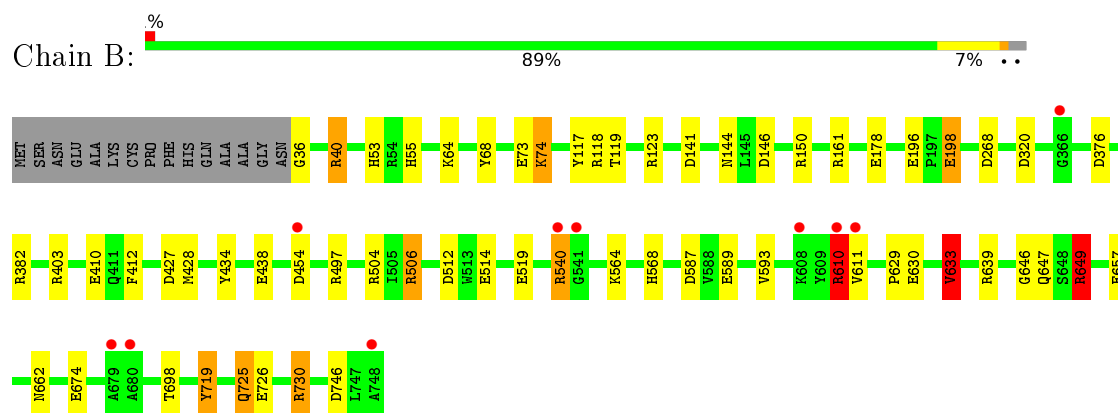
3 Residue-property plots [i](#)

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	100.79 Å 113.30 Å 174.52 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 1.75 47.52 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.00-1.75) 98.4 (47.52-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 1.75 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.159 , 0.190 0.170 , 0.200	Depositor DCC
R_{free} test set	9907 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12851	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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, CL, NA, PO4, MPD, 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	1.29	14/5668 (0.2%)	1.17	43/7702 (0.6%)
1	B	1.30	22/5692 (0.4%)	1.18	34/7735 (0.4%)
All	All	1.29	36/11360 (0.3%)	1.17	77/15437 (0.5%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	GLY	N-CA	8.56	1.58	1.46
1	A	438	GLU	CD-OE1	-7.96	1.16	1.25
1	B	198	GLU	CD-OE2	7.92	1.34	1.25
1	A	434	TYR	CE1-CZ	-7.48	1.28	1.38
1	A	196	GLU	CD-OE2	-7.21	1.17	1.25
1	B	730[A]	ARG	CZ-NH2	7.10	1.42	1.33
1	B	730[B]	ARG	CZ-NH2	7.10	1.42	1.33
1	B	410	GLU	CD-OE1	6.96	1.33	1.25
1	B	438	GLU	CD-OE1	-6.68	1.18	1.25
1	B	196	GLU	CD-OE2	-6.66	1.18	1.25
1	A	584	GLU	CG-CD	6.60	1.61	1.51
1	B	514	GLU	CD-OE2	-6.59	1.18	1.25
1	A	407	GLU	CG-CD	6.51	1.61	1.51
1	A	725	GLN	CG-CD	6.39	1.65	1.51
1	A	407	GLU	CD-OE1	6.33	1.32	1.25
1	A	532	ARG	NE-CZ	-6.13	1.25	1.33
1	B	657	GLU	CG-CD	6.03	1.60	1.51
1	B	726	GLU	CG-CD	6.01	1.60	1.51
1	B	410	GLU	CG-CD	5.84	1.60	1.51
1	B	519	GLU	CD-OE1	5.84	1.32	1.25
1	A	694	GLU	CD-OE1	5.74	1.31	1.25
1	B	519	GLU	CD-OE2	5.58	1.31	1.25
1	A	263	ARG	CZ-NH1	5.44	1.40	1.33
1	A	223	ARG	CZ-NH1	5.38	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	589	GLU	CD-OE1	5.30	1.31	1.25
1	B	674	GLU	CD-OE2	5.29	1.31	1.25
1	A	499	GLY	C-O	5.25	1.32	1.23
1	A	198	GLU	CD-OE2	5.16	1.31	1.25
1	B	68	TYR	CE1-CZ	5.16	1.45	1.38
1	B	117	TYR	CD1-CE1	-5.13	1.31	1.39
1	B	161	ARG	NE-CZ	5.13	1.39	1.33
1	A	427	ASP	CB-CG	5.11	1.62	1.51
1	B	73	GLU	CD-OE1	5.06	1.31	1.25
1	B	657	GLU	CD-OE1	5.02	1.31	1.25
1	B	725	GLN	CD-OE1	5.01	1.34	1.24
1	B	630	GLU	CD-OE1	-5.00	1.20	1.25

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	ARG	NE-CZ-NH1	11.03	125.81	120.30
1	A	404	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	B	504	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	B	403	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	A	249	ASP	CB-CG-OD2	-9.05	110.16	118.30
1	A	639	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	A	532	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	A	433	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	A	150	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	719	TYR	CB-CG-CD1	-7.25	116.65	121.00
1	B	268	ASP	CB-CG-OD1	7.24	124.82	118.30
1	A	540	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	649[A]	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	649[B]	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	65	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	B	434	TYR	CB-CG-CD1	7.03	125.22	121.00
1	A	407	GLU	OE1-CD-OE2	-6.97	114.93	123.30
1	A	689	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	123	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	B	161	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	A	376	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	B	639	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	404	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	B	497	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	B	587	ASP	CB-CG-OD1	6.65	124.29	118.30
1	B	587	ASP	CB-CG-OD2	-6.59	112.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	587	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	504	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	A	93	ASP	CB-CG-OD1	6.50	124.14	118.30
1	B	382	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	506	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	B	633[A]	VAL	CG1-CB-CG2	-6.31	100.80	110.90
1	B	633[B]	VAL	CG1-CB-CG2	-6.31	100.80	110.90
1	B	427	ASP	CB-CG-OD1	-6.21	112.72	118.30
1	A	268	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	418	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	656	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	B	730[A]	ARG	CB-CA-C	6.12	122.64	110.40
1	B	730[B]	ARG	CB-CA-C	6.12	122.64	110.40
1	B	506	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	150	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	610	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	255[A]	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	255[B]	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	702	VAL	CG1-CB-CG2	-5.80	101.62	110.90
1	A	268	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	395	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	431	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	A	382	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	412	PHE	CB-CG-CD1	5.56	124.69	120.80
1	B	376	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	B	512	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	123	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	150	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	40	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	698	THR	CA-CB-CG2	-5.32	104.95	112.40
1	A	412	PHE	CB-CG-CD2	-5.31	117.08	120.80
1	B	730[A]	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	730[B]	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	123	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	82	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	744	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	412	PHE	CB-CG-CD1	5.22	124.46	120.80
1	A	310	LYS	CD-CE-NZ	-5.21	99.71	111.70
1	B	382	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	320	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	B	746	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	263	ARG	NE-CZ-NH2	-5.09	117.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	VAL	CG1-CB-CG2	5.09	119.05	110.90
1	A	76	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	407	GLU	CG-CD-OE1	5.08	128.46	118.30
1	A	426[A]	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	426[B]	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	416	PHE	CB-CG-CD1	5.03	124.32	120.80
1	B	639	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	255[A]	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	255[B]	ARG	NE-CZ-NH1	5.02	122.81	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	5534	0	5348	25	0
1	B	5546	0	5377	25	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
5	A	2	0	0	0	0
5	B	2	0	0	1	0
6	A	16	0	28	4	0
6	B	24	0	42	16	0
7	B	5	0	0	0	0
8	A	828	0	0	10	1
8	B	804	0	0	10	1
All	All	12851	0	10855	69	1

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

All (69) 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:255[B]:ARG:HG2	8:A:1635:HOH:O	1.66	0.96
1:B:506:ARG:HE	6:B:808:MPD:H12	1.30	0.96
1:B:53:HIS:HB2	8:B:1529:HOH:O	1.74	0.88
1:A:119[B]:THR:HG21	8:A:1060:HOH:O	1.74	0.86
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.63	0.81
6:B:807:MPD:HM2	6:B:807:MPD:H53	1.69	0.74
6:B:808:MPD:H51	8:B:1380:HOH:O	1.86	0.74
6:B:806:MPD:C1	6:B:806:MPD:H53	2.19	0.73
1:A:540:ARG:HA	1:A:540:ARG:HE	1.55	0.72
1:B:564:LYS:HE3	8:B:1416:HOH:O	1.88	0.72
6:B:807:MPD:H11	6:B:807:MPD:C5	2.22	0.69
1:B:119[B]:THR:HG23	8:B:1187:HOH:O	1.93	0.69
1:B:178:GLU:OE1	8:B:901:HOH:O	2.11	0.68
6:B:808:MPD:H52	6:B:808:MPD:H11	1.76	0.66
1:B:730[A]:ARG:HD2	8:B:1586:HOH:O	1.95	0.66
1:B:568:HIS:ND1	8:B:903:HOH:O	2.29	0.66
5:B:804:OXY:O2	8:B:902:HOH:O	2.14	0.66
1:A:593:VAL:HG13	8:A:1031:HOH:O	1.95	0.65
6:B:806:MPD:H11	6:B:806:MPD:H53	1.78	0.65
1:A:51:ILE:HD11	1:A:618:VAL:HG12	1.78	0.64
1:A:255[A]:ARG:HG2	8:A:930:HOH:O	1.97	0.64
6:B:807:MPD:H11	6:B:807:MPD:H52	1.80	0.64
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.80	0.63
1:A:36:GLY:N	8:A:907:HOH:O	2.31	0.62
1:B:540:ARG:HA	1:B:540:ARG:NE	2.16	0.61
1:B:55:HIS:HD2	8:B:1259:HOH:O	1.83	0.60
6:A:806:MPD:H11	6:A:806:MPD:H53	1.83	0.58
1:B:506:ARG:NE	6:B:808:MPD:H12	2.13	0.58
6:A:805:MPD:HO4	6:A:805:MPD:HO2	1.47	0.57
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.40	0.56
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	2.06	0.56
1:A:76:ASP:OD2	8:A:904:HOH:O	2.18	0.55
6:B:808:MPD:H52	6:B:808:MPD:C1	2.39	0.53
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE2	2.43	0.52
1:A:540:ARG:NE	1:A:540:ARG:HA	2.23	0.52
6:A:806:MPD:H11	6:A:806:MPD:C5	2.40	0.52
6:B:806:MPD:H11	6:B:806:MPD:O4	2.10	0.51
1:A:255[B]:ARG:CD	8:A:1635:HOH:O	2.57	0.51
1:A:504:ARG:HD2	8:A:1028:HOH:O	2.11	0.51
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.41	0.50
6:B:806:MPD:HM2	6:B:806:MPD:O4	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ALA:HB2	1:A:391:SER:HB3	1.94	0.49
1:A:647:GLN:NE2	8:A:903:HOH:O	1.70	0.49
1:A:119[B]:THR:CG2	1:A:593:VAL:HG11	2.40	0.49
1:B:74:LYS:HA	1:B:74:LYS:HE2	1.94	0.49
1:A:725:GLN:HE22	1:A:726:GLU:HG2	1.77	0.48
1:A:725:GLN:NE2	1:A:726:GLU:HG2	2.30	0.47
6:B:806:MPD:H11	6:B:806:MPD:C5	2.43	0.47
6:B:808:MPD:H13	8:B:1575:HOH:O	2.14	0.46
1:A:540:ARG:HE	1:A:540:ARG:CA	2.22	0.46
6:B:807:MPD:HM2	6:B:807:MPD:C5	2.39	0.46
1:B:198:GLU:HG3	4:B:803:CL:CL	2.53	0.45
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.16	0.45
1:A:610:ARG:HD2	1:A:611:VAL:HG23	1.99	0.45
6:B:806:MPD:H53	6:B:806:MPD:H12	1.95	0.44
1:A:540:ARG:NE	1:A:540:ARG:CA	2.80	0.44
1:A:88:MET:HB3	1:A:101:HIS:CE1	2.53	0.44
1:B:662:ASN:H	1:B:725:GLN:HE22	1.66	0.43
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.18	0.42
1:B:649[A]:ARG:HD3	1:B:649[A]:ARG:HA	1.72	0.42
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.49	0.42
1:B:610:ARG:HD2	1:B:611:VAL:HG23	2.00	0.42
1:B:646:GLY:C	1:B:647:GLN:HG2	2.40	0.42
1:A:54:ARG:HE	1:A:199:ASP:CG	2.23	0.42
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	3.03	0.42
1:A:76:ASP:OD1	8:A:905:HOH:O	2.22	0.41
1:B:454:ASP:N	1:B:454:ASP:OD1	2.54	0.40
1:B:540:ARG:CA	1:B:540:ARG:NE	2.84	0.40
6:A:806:MPD:C1	6:A:806:MPD:C5	2.99	0.40

All (1) 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)
8:A:1711:HOH:O	8:B:1309:HOH:O[3_544]	2.16	0.04

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	714/728 (98%)	703 (98%)	11 (2%)	0	100	100
1	B	717/728 (98%)	706 (98%)	11 (2%)	0	100	100
All	All	1431/1456 (98%)	1409 (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	553/560 (99%)	542 (98%)	11 (2%)	63	39
1	B	556/560 (99%)	544 (98%)	12 (2%)	60	35
All	All	1109/1120 (99%)	1086 (98%)	23 (2%)	65	37

All (23) 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	223	ARG
1	A	379	LYS
1	A	540	ARG
1	A	608	LYS

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Mol	Chain	Res	Type
1	A	610	ARG
1	A	694	GLU
1	A	725	GLN
1	B	40	ARG
1	B	64	LYS
1	B	74	LYS
1	B	118	ARG
1	B	141	ASP
1	B	428	MET
1	B	540	ARG
1	B	610	ARG
1	B	633[A]	VAL
1	B	633[B]	VAL
1	B	649[A]	ARG
1	B	649[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	725	GLN
1	B	55	HIS
1	B	227	ASN
1	B	647	GLN
1	B	711	GLN
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[A]	2	10,17,18	2.63	4 (40%)	9,23,25	1.61	1 (11%)
1	TOX	A	111[B]	-	10,17,18	2.63	4 (40%)	9,23,25	1.61	1 (11%)
1	TOX	B	111	1,2	10,17,18	2.15	2 (20%)	9,23,25	2.87	5 (55%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[B]	TOX	CD1-NE1	-6.91	1.32	1.39
1	A	111[A]	TOX	CD1-NE1	-6.91	1.32	1.39
1	B	111	TOX	CD1-NE1	-5.62	1.34	1.39
1	A	111[B]	TOX	CE3-CD2	-2.71	1.36	1.42
1	A	111[A]	TOX	CE3-CD2	-2.71	1.36	1.42
1	A	111[B]	TOX	CZ3-CE3	2.08	1.41	1.36
1	A	111[A]	TOX	CZ3-CE3	2.08	1.41	1.36
1	A	111[B]	TOX	CH2-CZ2	2.47	1.42	1.36
1	A	111[A]	TOX	CH2-CZ2	2.47	1.42	1.36
1	B	111	TOX	CZ3-CH2	2.54	1.44	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	TOX	CB-CG-CD1	-4.78	122.06	127.97
1	B	111	TOX	CZ3-CE3-CD2	-4.32	114.88	120.88
1	A	111[B]	TOX	CZ2-CE2-CD2	-3.03	116.78	120.58
1	A	111[A]	TOX	CZ2-CE2-CD2	-3.03	116.78	120.58
1	B	111	TOX	CZ3-CH2-CZ2	-2.13	117.38	120.45
1	B	111	TOX	CE3-CD2-CE2	3.14	122.99	119.83
1	B	111	TOX	CH2-CZ3-CE3	3.24	125.13	120.45

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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	1.94	7 (29%)	16,82,82	2.15	7 (43%)
5	OXY	A	804	-	1,1,1	0.04	0	0,0,0	0.00	-
6	MPD	A	805	-	6,7,7	0.61	0	6,10,10	1.93	3 (50%)
6	MPD	A	806	-	6,7,7	1.27	0	6,10,10	1.38	1 (16%)
2	HEM	B	801	1	24,50,50	1.90	5 (20%)	16,82,82	2.15	7 (43%)
5	OXY	B	804	-	1,1,1	0.25	0	0,0,0	0.00	-
7	PO4	B	805	-	4,4,4	0.67	0	6,6,6	0.29	0
6	MPD	B	806	-	6,7,7	0.67	0	6,10,10	2.05	2 (33%)
6	MPD	B	807	-	6,7,7	0.66	0	6,10,10	1.44	1 (16%)
6	MPD	B	808	-	6,7,7	0.85	0	6,10,10	1.53	1 (16%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OXY	A	804	-	-	0/0/0/0	0/0/0/0
6	MPD	A	805	-	-	0/5/5/5	0/0/0/0
6	MPD	A	806	-	-	0/5/5/5	0/0/0/0
2	HEM	B	801	1	-	0/6/54/54	0/0/8/8
5	OXY	B	804	-	-	0/0/0/0	0/0/0/0
7	PO4	B	805	-	-	0/0/0/0	0/0/0/0
6	MPD	B	806	-	-	0/5/5/5	0/0/0/0
6	MPD	B	807	-	-	0/5/5/5	0/0/0/0
6	MPD	B	808	-	-	0/5/5/5	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3B-C2B	-5.20	1.33	1.40
2	B	801	HEM	C3C-C2C	-3.62	1.35	1.40
2	A	801	HEM	C4D-ND	-3.58	1.31	1.36
2	A	801	HEM	C1B-NB	-2.69	1.33	1.36
2	A	801	HEM	C3B-C2B	-2.33	1.37	1.40
2	B	801	HEM	C1C-NC	2.09	1.39	1.36
2	B	801	HEM	C4C-NC	2.72	1.40	1.36
2	A	801	HEM	C4C-NC	2.74	1.40	1.36
2	A	801	HEM	CMA-C3A	3.38	1.58	1.51
2	B	801	HEM	CAD-C3D	3.55	1.56	1.52
2	A	801	HEM	C1C-NC	3.76	1.41	1.36
2	A	801	HEM	CAD-C3D	4.22	1.57	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C3B-CAB-CBB	-3.85	118.65	126.40
2	A	801	HEM	CAA-CBA-CGA	-3.27	106.41	112.78
2	B	801	HEM	CAA-CBA-CGA	-3.16	106.63	112.78
2	A	801	HEM	C3B-CAB-CBB	-3.13	120.10	126.40
6	B	807	MPD	O4-C4-C5	-3.01	94.43	109.47
6	A	806	MPD	CM-C2-C1	-2.96	103.34	110.41
6	B	808	MPD	CM-C2-C1	-2.92	103.44	110.41
2	A	801	HEM	CMA-C3A-C4A	-2.46	124.13	128.31
6	B	806	MPD	O2-C2-C1	-2.42	99.12	108.01
6	A	805	MPD	O2-C2-C1	-2.38	99.25	108.01
2	B	801	HEM	C3C-C4C-NC	-2.34	106.53	110.94
2	B	801	HEM	CMA-C3A-C4A	-2.31	124.39	128.31
6	A	805	MPD	CM-C2-C1	-2.16	105.25	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C3B-C4B-NB	2.05	111.86	109.21
2	B	801	HEM	CMD-C2D-C3D	2.18	129.80	125.24
2	B	801	HEM	CAD-CBD-CGD	2.38	117.41	112.78
2	A	801	HEM	CBA-CAA-C2A	2.55	116.97	112.49
6	A	805	MPD	O2-C2-CM	3.26	120.00	108.01
2	A	801	HEM	CMA-C3A-C2A	3.33	132.19	125.24
2	B	801	HEM	CBD-CAD-C3D	3.68	118.93	112.47
6	B	806	MPD	CM-C2-C1	4.11	120.22	110.41
2	A	801	HEM	CBD-CAD-C3D	4.21	119.85	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	805	MPD	1	0
6	A	806	MPD	3	0
5	B	804	OXY	1	0
6	B	806	MPD	6	0
6	B	807	MPD	4	0
6	B	808	MPD	6	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%)	-0.38	13 (1%) 71 78	11, 16, 33, 71	0
1	B	712/728 (97%)	-0.39	10 (1%) 78 84	10, 16, 32, 88	0
All	All	1424/1456 (97%)	-0.38	23 (1%) 74 81	10, 16, 33, 88	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	540	ARG	5.8
1	B	610	ARG	4.9
1	B	679	ALA	4.5
1	A	540	ARG	3.9
1	A	748	ALA	3.8
1	A	679	ALA	3.6
1	A	608	LYS	3.5
1	B	608	LYS	3.3
1	A	610	ARG	3.2
1	A	680	ALA	3.0
1	B	680	ALA	3.0
1	A	541	GLY	3.0
1	B	748	ALA	2.9
1	A	454	ASP	2.4
1	A	222	ASP	2.4
1	B	541	GLY	2.3
1	A	682	ALA	2.3
1	A	215	PRO	2.2
1	B	611	VAL	2.2
1	A	647	GLN	2.1
1	B	366	GLY	2.1
1	B	454	ASP	2.1
1	A	53	HIS	2.1

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. 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	16/17	0.97	0.09	-	9,11,16,18	1
1	TOX	A	111[B]	16/17	0.97	0.10	-	11,11,13,14	2
1	TOX	A	111[A]	16/17	0.97	0.10	-	11,11,14,15	2

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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
6	MPD	A	805	8/8	0.85	0.17	8.33	46,51,63,67	0
6	MPD	B	806	8/8	0.83	0.18	8.11	42,47,53,55	0
6	MPD	B	808	8/8	0.89	0.13	3.34	30,34,35,35	0
6	MPD	B	807	8/8	0.92	0.13	1.85	24,28,38,40	0
2	HEM	B	801	43/43	0.98	0.09	0.40	11,12,14,15	0
2	HEM	A	801	43/43	0.98	0.08	0.14	9,10,13,14	0
3	NA	B	802	1/1	1.00	0.05	-2.26	12,12,12,12	0
4	CL	A	803	1/1	0.99	0.05	-2.35	26,26,26,26	0
3	NA	A	802	1/1	1.00	0.03	-4.62	12,12,12,12	0
4	CL	B	803	1/1	0.99	0.04	-4.75	24,24,24,24	0
6	MPD	A	806	8/8	0.85	0.15	-	29,31,42,44	0
7	PO4	B	805	5/5	0.87	0.19	-	30,46,53,55	0
5	OXY	A	804	2/2	0.96	0.15	-	34,34,34,43	0
5	OXY	B	804	2/2	0.93	0.12	-	25,25,25,29	0

6.5 Other polymers

There are no such residues in this entry.