



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2022 – 01:03 am BST

PDB ID : 7OCU
Title : Mannitol-1-phosphate bound to the phosphatase domain of the bifunctional mannitol-1-phosphate dehydrogenase/phosphatase MtlD-N374A from *Acinetobacter baumannii*
Authors : Tam, H.K.; Mueller, V.; Pos, K.M.
Deposited on : 2021-04-28
Resolution : 2.70 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

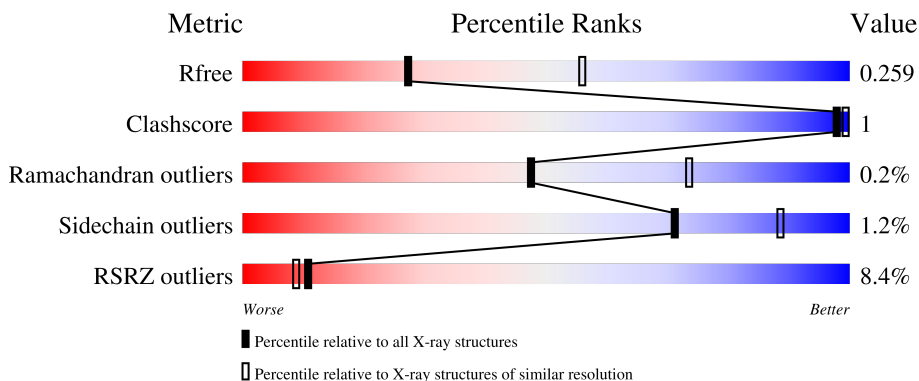
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	727	 6% (poor fit), 91% (0-3 outliers), 6% (not modelled)
1	B	727	 10% (poor fit), 91% (0-3 outliers), 7% (not modelled)

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	EPE	B	801	-	-	-	X

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 11157 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 Mannitol-1-phosphate dehydrogenase/phosphatase MtlD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	687	Total	C	N	O	S	0	1	0
			5546	3524	948	1041	33			
1	B	679	Total	C	N	O	S	0	0	0
			5482	3485	937	1028	32			

There are 28 discrepancies between the modelled and reference sequences:

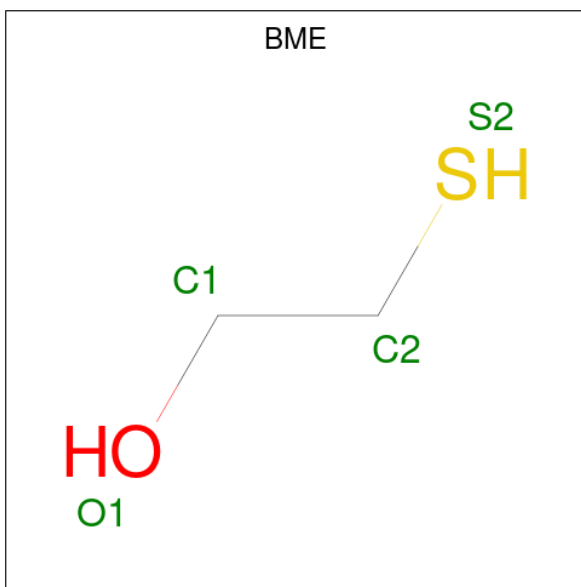
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP D0C7J2
A	2	VAL	-	expression tag	UNP D0C7J2
A	374	ALA	ASN	engineered mutation	UNP D0C7J2
A	717	ALA	-	expression tag	UNP D0C7J2
A	718	ALA	-	expression tag	UNP D0C7J2
A	719	ALA	-	expression tag	UNP D0C7J2
A	720	LEU	-	expression tag	UNP D0C7J2
A	721	GLU	-	expression tag	UNP D0C7J2
A	722	HIS	-	expression tag	UNP D0C7J2
A	723	HIS	-	expression tag	UNP D0C7J2
A	724	HIS	-	expression tag	UNP D0C7J2
A	725	HIS	-	expression tag	UNP D0C7J2
A	726	HIS	-	expression tag	UNP D0C7J2
A	727	HIS	-	expression tag	UNP D0C7J2
B	1	MET	-	initiating methionine	UNP D0C7J2
B	2	VAL	-	expression tag	UNP D0C7J2
B	374	ALA	ASN	engineered mutation	UNP D0C7J2
B	717	ALA	-	expression tag	UNP D0C7J2
B	718	ALA	-	expression tag	UNP D0C7J2
B	719	ALA	-	expression tag	UNP D0C7J2
B	720	LEU	-	expression tag	UNP D0C7J2
B	721	GLU	-	expression tag	UNP D0C7J2
B	722	HIS	-	expression tag	UNP D0C7J2
B	723	HIS	-	expression tag	UNP D0C7J2
B	724	HIS	-	expression tag	UNP D0C7J2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	725	HIS	-	expression tag	UNP D0C7J2
B	726	HIS	-	expression tag	UNP D0C7J2
B	727	HIS	-	expression tag	UNP D0C7J2

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

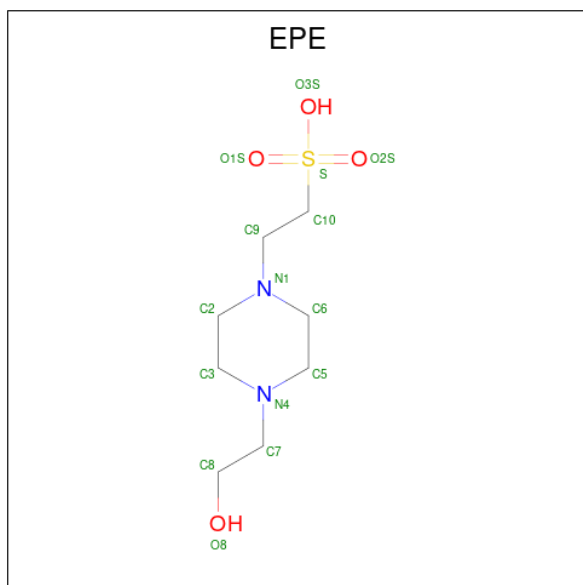


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

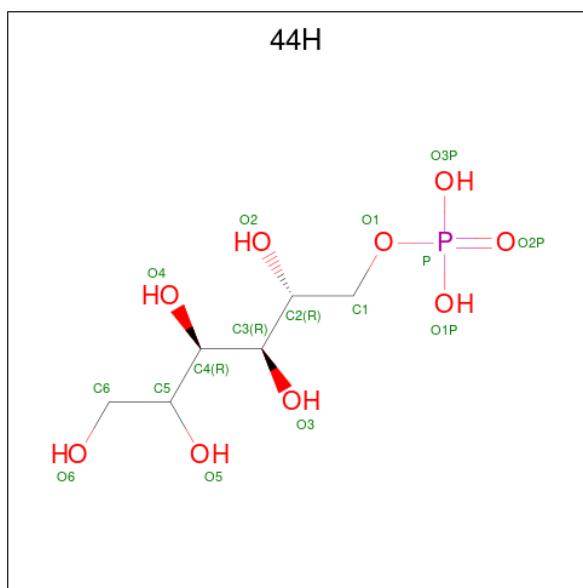
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	B	1	15	8	2	4	1	0	0

- Molecule 7 is D-Mannitol-1-phosphate (three-letter code: 44H) (formula: C₆H₁₅O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
7	B	1	16	6	9	1	0	0

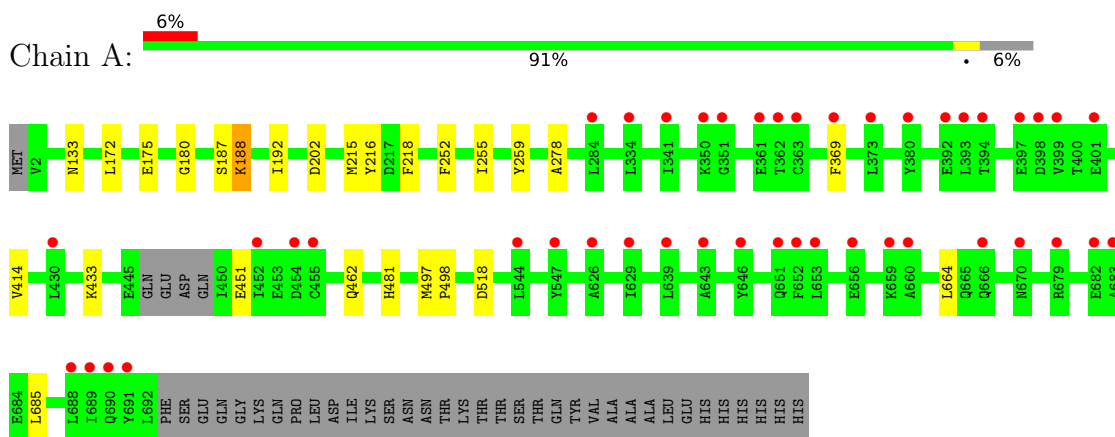
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	39	Total 39	O 39	0	0
8	B	36	Total 36	O 36	0	0

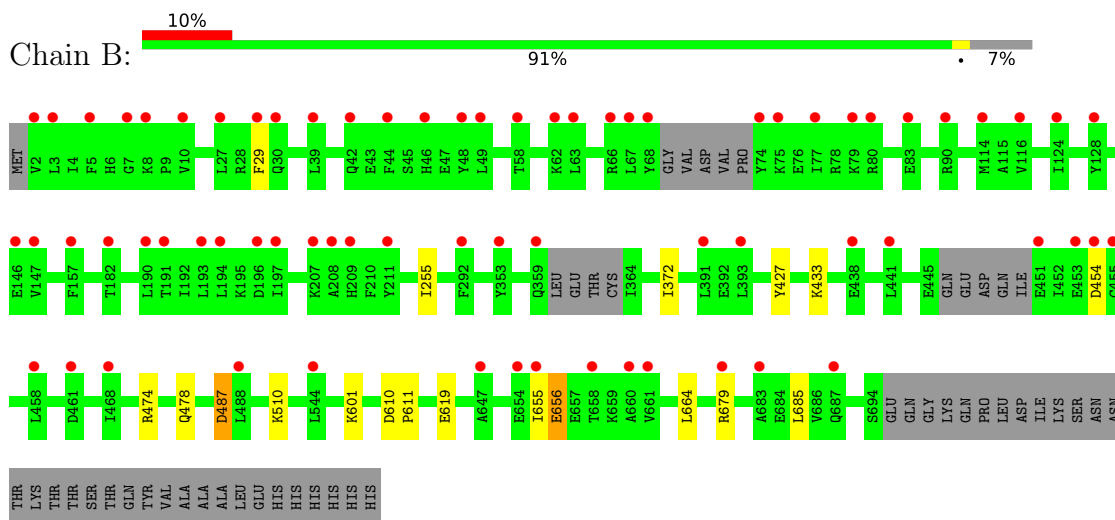
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Mannitol-1-phosphate dehydrogenase/phosphatase MtlD



- Molecule 1: Mannitol-1-phosphate dehydrogenase/phosphatase MtlD



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.44Å 157.43Å 219.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.49 – 2.70 48.49 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.49-2.70) 100.0 (48.49-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.227 , 0.264 0.227 , 0.259	Depositor DCC
R_{free} test set	2380 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	67.4	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	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	0.94	EDS
Total number of atoms	11157	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BME, 44H, SO4, EPE, CL

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	0.65	0/5651	0.69	0/7630
1	B	0.66	0/5584	0.69	0/7533
All	All	0.66	0/11235	0.69	0/15163

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5546	0	5524	10	0
1	B	5482	0	5458	7	0
2	A	4	0	6	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
5	A	1	0	0	0	0
6	B	15	0	17	0	0
7	B	16	0	0	0	0
8	A	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	36	0	0	0	0
All	All	11157	0	11005	16	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 1.

All (16) 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:255:ILE:HG21	1:B:372:ILE:HG21	1.86	0.58
1:B:664:LEU:CD1	1:B:685:LEU:HD23	2.41	0.51
1:B:433:LYS:NZ	1:B:487:ASP:O	2.41	0.49
1:A:172:LEU:HD22	1:A:192:ILE:HD11	1.94	0.48
1:A:175:GLU:HG2	1:A:180:GLY:C	2.34	0.48
1:B:474:ARG:O	1:B:478:GLN:HB2	2.15	0.47
1:A:664:LEU:HD11	1:A:685:LEU:HD23	1.97	0.46
1:A:259:TYR:CE2	1:A:414:VAL:HG13	2.51	0.46
1:B:655:ILE:O	1:B:656:GLU:HB2	2.17	0.45
1:A:255:ILE:HD11	1:A:414:VAL:HG11	2.00	0.43
1:A:252:PHE:HB2	1:A:278:ALA:HB1	2.02	0.42
1:B:610:ASP:N	1:B:611:PRO:HD3	2.34	0.42
1:A:192:ILE:HD13	1:A:218:PHE:CE1	2.55	0.42
1:A:497:MET:HB2	1:A:498:PRO:HD3	2.02	0.41
1:A:187:SER:O	1:A:188:LYS:HB2	2.21	0.40
1:A:462:GLN:HB2	1:B:427:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

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	684/727 (94%)	653 (96%)	30 (4%)	1 (0%)	51 78
1	B	671/727 (92%)	645 (96%)	24 (4%)	2 (0%)	41 66
All	All	1355/1454 (93%)	1298 (96%)	54 (4%)	3 (0%)	47 73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	B	656	GLU
1	B	454	ASP

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	606/641 (94%)	597 (98%)	9 (2%)	65 86
1	B	598/641 (93%)	592 (99%)	6 (1%)	76 91
All	All	1204/1282 (94%)	1189 (99%)	15 (1%)	71 88

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	202	ASP
1	A	215	MET
1	A	216	TYR
1	A	369	PHE
1	A	433	LYS
1	A	451	GLU
1	A	481	HIS
1	A	518	ASP
1	B	29	PHE
1	B	487	ASP
1	B	510	LYS
1	B	601	LYS

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Mol	Chain	Res	Type
1	B	619	GLU
1	B	679	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
7	44H	B	805	-	15,15,15	0.74	0	21,21,21	0.62	0
4	SO4	A	803	-	4,4,4	0.39	0	6,6,6	0.04	0
4	SO4	B	803	3	4,4,4	0.39	0	6,6,6	0.05	0
2	BME	A	801	-	3,3,3	0.14	0	1,2,2	0.08	0
6	EPE	B	801	-	15,15,15	1.27	2 (13%)	18,20,20	2.35	5 (27%)
4	SO4	B	804	-	4,4,4	0.39	0	6,6,6	0.05	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
7	44H	B	805	-	-	0/20/20/20	-
2	BME	A	801	-	-	0/1/1/1	-
6	EPE	B	801	-	-	6/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	801	EPE	O1S-S	3.24	1.54	1.45
6	B	801	EPE	C10-S	3.23	1.82	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	801	EPE	O2S-S-C10	7.53	115.98	106.92
6	B	801	EPE	O1S-S-C10	-3.49	102.72	106.92
6	B	801	EPE	O3S-S-O2S	2.87	118.29	111.27
6	B	801	EPE	O3S-S-O1S	-2.85	104.31	111.27
6	B	801	EPE	C6-N1-C2	2.43	114.29	108.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	801	EPE	S-C10-C9-N1
6	B	801	EPE	N4-C7-C8-O8
6	B	801	EPE	C10-C9-N1-C2
6	B	801	EPE	C10-C9-N1-C6
6	B	801	EPE	C9-C10-S-O1S
6	B	801	EPE	C9-C10-S-O2S

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	687/727 (94%)	0.65	44 (6%) 19 18	50, 88, 140, 163	0
1	B	679/727 (93%)	0.76	71 (10%) 6 4	59, 95, 152, 191	0
All	All	1366/1454 (93%)	0.71	115 (8%) 11 9	50, 92, 147, 191	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	ALA	6.1
1	B	455	CYS	5.6
1	B	191	THR	4.9
1	B	197	ILE	4.6
1	B	48	TYR	4.6
1	B	5	PHE	4.5
1	B	42	GLN	4.3
1	A	689	ILE	4.3
1	A	361	GLU	4.1
1	A	393	LEU	4.1
1	A	652	PHE	4.0
1	B	451	GLU	4.0
1	B	3	LEU	4.0
1	B	49	LEU	3.9
1	A	659	LYS	3.9
1	B	2	VAL	3.7
1	A	454	ASP	3.6
1	B	67	LEU	3.6
1	A	547	TYR	3.6
1	B	209	HIS	3.5
1	B	660	ALA	3.5
1	B	453	GLU	3.5
1	B	458	LEU	3.4
1	B	468	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	455	CYS	3.4
1	A	351	GLY	3.4
1	B	63	LEU	3.3
1	B	193	LEU	3.3
1	B	39	LEU	3.3
1	A	691	TYR	3.2
1	A	626	ALA	3.2
1	B	353	TYR	3.0
1	A	334	LEU	3.0
1	B	27	LEU	3.0
1	A	452	ILE	2.9
1	B	391	LEU	2.9
1	A	688	LEU	2.9
1	A	646	TYR	2.9
1	B	44	PHE	2.9
1	B	461	ASP	2.8
1	B	655	ILE	2.8
1	B	75	LYS	2.8
1	A	660	ALA	2.8
1	B	647	ALA	2.8
1	A	350	LYS	2.8
1	B	359	GLN	2.8
1	A	653	LEU	2.8
1	B	7	GLY	2.8
1	A	679	ARG	2.8
1	B	68	TYR	2.7
1	B	190	LEU	2.7
1	B	393	LEU	2.7
1	B	29	PHE	2.7
1	B	77	ILE	2.7
1	B	62	LYS	2.6
1	B	74	TYR	2.6
1	A	399	VAL	2.6
1	B	544	LEU	2.6
1	B	58	THR	2.6
1	B	211	TYR	2.5
1	B	292	PHE	2.5
1	B	194	LEU	2.5
1	B	157	PHE	2.5
1	A	397	GLU	2.5
1	A	398	ASP	2.5
1	B	116	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	454	ASP	2.5
1	A	666	GLN	2.4
1	B	46	HIS	2.4
1	B	147	VAL	2.4
1	A	682	GLU	2.4
1	A	651	GLN	2.4
1	B	90	ARG	2.4
1	A	544	LEU	2.4
1	A	656	GLU	2.4
1	A	629	ILE	2.4
1	A	670	ASN	2.4
1	A	683	ALA	2.4
1	B	488	LEU	2.4
1	B	679	ARG	2.3
1	A	284	LEU	2.3
1	B	80	ARG	2.3
1	B	661	VAL	2.3
1	B	83	GLU	2.2
1	B	146	GLU	2.2
1	B	207	LYS	2.2
1	B	10	VAL	2.2
1	B	683	ALA	2.2
1	A	369	PHE	2.2
1	B	654	GLU	2.2
1	A	639	LEU	2.2
1	B	196	ASP	2.1
1	B	8	LYS	2.1
1	A	430	LEU	2.1
1	B	66	ARG	2.1
1	A	394	THR	2.1
1	B	30	GLN	2.1
1	B	128	TYR	2.1
1	A	643	ALA	2.1
1	B	687	GLN	2.1
1	B	114	MET	2.1
1	A	401	GLU	2.1
1	A	373	LEU	2.1
1	A	380	TYR	2.1
1	B	79	LYS	2.0
1	B	124	ILE	2.0
1	A	362	THR	2.0
1	B	658	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	363	CYS	2.0
1	B	182	THR	2.0
1	A	341	ILE	2.0
1	A	392	GLU	2.0
1	B	438	GLU	2.0
1	A	690	GLN	2.0
1	B	441	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
6	EPE	B	801	15/15	0.74	0.46	112,115,118,120	0
4	SO4	B	803	5/5	0.83	0.13	132,132,132,133	0
4	SO4	B	804	5/5	0.87	0.17	103,103,104,104	0
3	MG	A	804	1/1	0.87	0.20	66,66,66,66	0
3	MG	B	802	1/1	0.89	0.15	104,104,104,104	0
4	SO4	A	803	5/5	0.90	0.16	122,122,123,123	0
2	BME	A	801	4/4	0.91	0.23	113,115,117,118	0
5	CL	A	805	1/1	0.94	0.24	67,67,67,67	0
3	MG	A	802	1/1	0.95	0.27	66,66,66,66	0
7	44H	B	805	16/16	0.95	0.16	61,63,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.