

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID : 8QKF

Title: SmtB protein of Mycobacterium smegmatis

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Deposited on : 2023-09-15

Resolution : 1.88 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.13 \end{array}$

EDS: 3.0

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

CCP4 : 9.0.002 (Gargrove)

Density-Fitness : 1.0.11

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

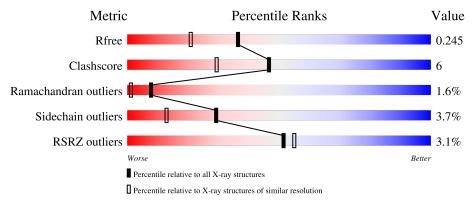
Validation Pipeline (wwPDB-VP) : 2.38.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	164625	1090 (1.88-1.88)
Clashscore	180529	1144 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

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 <=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	120	68%	12%	 18%
1	В	120	70%	7%	22%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1587 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 ArsR family transcriptional regulator.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	99	Total 759		N 143	O 137	S 1	0	0	0
1	В	94	Total 727	C 456		O 132	S 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	LYS	GLN	conflict	UNP A0A653FM47
В	53	LYS	GLN	conflict	UNP A0A653FM47

• Molecule 2 is water.

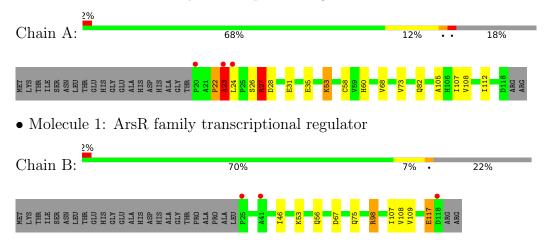
M	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	2	A	59	Total O 59 59	0	0
2	2	В	42	Total O 42 42	0	0



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: ArsR family transcriptional regulator





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	42.29Å 72.48Å 82.23Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.11 - 1.88	Depositor
Resolution (A)	41.11 - 1.88	EDS
% Data completeness	95.9 (41.11-1.88)	Depositor
(in resolution range)	96.0 (41.11-1.88)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.96 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
D D.	0.194 , 0.244	Depositor
R, R_{free}	0.204 , 0.245	DCC
R_{free} test set	1022 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 50.9	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1587	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.90% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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		
WIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.83	0/771	1.03	1/1050 (0.1%)	
1	В	0.75	0/737	0.91	1/1001 (0.1%)	
All	All	0.79	0/1508	0.97	2/2051 (0.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	98	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	23	ALA	N-CA-CB	5.63	117.98	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	PRO	Peptide
1	A	26	SER	Peptide

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	asvmmetric	unit.	whereas S	Svmm-	Clashes	lists s	vmmetr	v-related	clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	759	0	791	12	0
1	В	727	0	756	6	0
2	A	59	0	0	3	0
2	В	42	0	0	1	0
All	All	1587	0	1547	17	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 6.

All (17) 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:58:CYS:HB3	2:A:244:HOH:O	1.54	1.07
1:A:82:GLN:OE1	2:A:201:HOH:O	1.97	0.82
1:B:53:LYS:HE2	1:B:109:VAL:HG21	1.73	0.70
1:A:68:VAL:HG23	1:A:73:VAL:HG23	1.78	0.65
1:B:117:GLU:OE1	1:B:117:GLU:N	2.34	0.60
1:A:22:PRO:HB2	1:A:23:ALA:HB3	1.84	0.59
1:A:22:PRO:HB2	1:A:23:ALA:CB	2.36	0.55
1:A:27:ARG:HB2	2:A:254:HOH:O	2.07	0.54
1:B:53:LYS:HD3	2:B:210:HOH:O	2.10	0.50
1:A:108:VAL:O	1:A:112:ILE:HG12	2.13	0.48
1:A:58:CYS:SG	1:A:60:HIS:CE1	3.07	0.47
1:A:107:ILE:HG23	1:B:107:ILE:HG23	1.96	0.46
1:A:27:ARG:HD2	1:A:27:ARG:HA	1.80	0.43
1:A:53:LYS:HD3	1:A:105:ALA:CB	2.49	0.42
1:A:31:GLU:O	1:A:35:GLU:HG3	2.20	0.42
1:B:56:GLN:HG2	1:B:98:ARG:HB3	2.02	0.42
1:B:46:ILE:HG23	1:B:108:VAL:HG13	2.03	0.41

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	\mathbf{s}
1	A	97/120 (81%)	92 (95%)	2 (2%)	3 (3%)	3 0	
1	В	92/120 (77%)	90 (98%)	2 (2%)	0	100 100	
All	All	189/240 (79%)	182 (96%)	4 (2%)	3 (2%)	8 1	

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ALA
1	A	27	ARG
1	A	24	LEU

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	82/99 (83%)	79 (96%)	3 (4%)	29 13
1	В	79/99 (80%)	76 (96%)	3 (4%)	28 12
All	All	161/198 (81%)	155 (96%)	6 (4%)	29 13

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	28	ASP
1	A	53	LYS
1	В	67	ASP
1	В	75	GLN
1	В	117	GLU

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	82	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	99/120 (82%)	0.19	3 (3%) 52 56	37, 48, 89, 104	0
1	В	94/120 (78%)	0.39	3 (3%) 50 53	39, 54, 86, 117	0
All	All	193/240 (80%)	0.28	6 (3%) 51 55	37, 52, 89, 117	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	PRO	3.7
1	A	23	ALA	3.2
1	В	25	PRO	2.6
1	A	24	LEU	2.3
1	В	118	ASP	2.1
1	В	41	ALA	2.1

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)

There are no ligands in this entry.



6.5 Other polymers (i)

There are no such residues in this entry.

