

# wwPDB X-ray Structure Validation Summary Report (i)

#### Feb 22, 2022 - 12:11 am GMT

PDB ID	:	7R22
Title	:	Crystal structure of protein Mab3862 from Mycobacterium abscessus
Authors	:	Kim, S.Y.; Eun, H.J.; Lee, J.Y.; Lee, B.J.; Blundell, T.L.
Deposited on		
Resolution	:	2.73 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

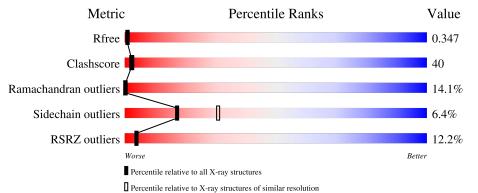
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 2.73 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1271(2.76-2.72)
Clashscore	141614	1322(2.76-2.72)
Ramachandran outliers	138981	1297(2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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				
			8%				
1	А	151	27%	28%	7% •	33%	



## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 780 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	А	101	Total 780	C 477	N 153	0 147	${ m Se} \ 3$	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MET	-	initiating methionine	UNP A0A418LEB3
А	2	ASN	-	expression tag	UNP A0A418LEB3
А	3	THR	-	expression tag	UNP A0A418LEB3
А	4	ILE	-	expression tag	UNP A0A418LEB3
А	5	HIS	-	expression tag	UNP A0A418LEB3
А	6	HIS	-	expression tag	UNP A0A418LEB3
А	7	HIS	-	expression tag	UNP A0A418LEB3
А	8	HIS	-	expression tag	UNP A0A418LEB3
А	9	HIS	-	expression tag	UNP A0A418LEB3
А	10	HIS	-	expression tag	UNP A0A418LEB3
А	11	ASN	-	expression tag	UNP A0A418LEB3
А	12	THR	-	expression tag	UNP A0A418LEB3
А	13	SER	-	expression tag	UNP A0A418LEB3
А	14	GLY	-	expression tag	UNP A0A418LEB3
А	15	SER	-	expression tag	UNP A0A418LEB3
А	16	GLY	-	expression tag	UNP A0A418LEB3
А	17	GLY	-	expression tag	UNP A0A418LEB3
А	18	GLY	-	expression tag	UNP A0A418LEB3
А	19	GLY	-	expression tag	UNP A0A418LEB3
А	20	GLY	-	expression tag	UNP A0A418LEB3
А	21	ARG	-	expression tag	UNP A0A418LEB3
А	22	LEU	-	expression tag	UNP A0A418LEB3
А	23	VAL	-	expression tag	UNP A0A418LEB3
А	24	PRO	-	expression tag	UNP A0A418LEB3
А	25	ARG	-	expression tag	UNP A0A418LEB3
А	26	GLY	-	expression tag	UNP A0A418LEB3
А	27	SER	-	expression tag	UNP A0A418LEB3

There are 39 discrepancies between the modelled and reference sequences:

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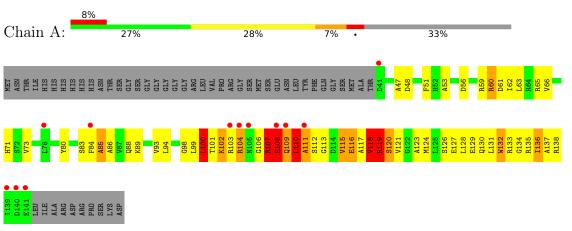
Chain	Residue	Modelled	Actual	Comment	Reference
А	28	MET	-	expression tag	UNP A0A418LEB3
А	29	SER	-	expression tag	UNP A0A418LEB3
А	30	GLU	-	expression tag	UNP A0A418LEB3
А	31	ASN	-	expression tag	UNP A0A418LEB3
А	32	LEU	-	expression tag	UNP A0A418LEB3
А	33	TYR	-	expression tag	UNP A0A418LEB3
А	34	PHE	-	expression tag	UNP A0A418LEB3
А	35	GLN	-	expression tag	UNP A0A418LEB3
А	36	GLY	-	expression tag	UNP A0A418LEB3
А	37	SER	-	expression tag	UNP A0A418LEB3
А	38	MET	-	expression tag	UNP A0A418LEB3
А	39	ALA	-	expression tag	UNP A0A418LEB3

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# 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 41 3 2	Depositor
Cell constants	106.89Å 106.89Å 106.89Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	47.80 - 2.73	Depositor
Resolution (A)	47.80 - 2.73	EDS
% Data completeness	75.5 (47.80-2.73)	Depositor
(in resolution range)	66.0(47.80-2.73)	EDS
R <sub>merge</sub>	0.12	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.90 (at 2.73 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
D D	0.299 , $0.347$	Depositor
$R, R_{free}$	0.300 , $0.347$	DCC
$R_{free}$ test set	451 reflections $(10.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	94.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$ L  > = 0.40, < L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	780	wwPDB-VP
Average B, all atoms $(Å^2)$	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 10.86% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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		
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.61	0/784	1.00	4/1047~(0.4%)	

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 mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	100	LEU	CA-CB-CG	7.00	131.40	115.30
1	А	108	GLU	C-N-CA	5.80	136.20	121.70
1	А	118	VAL	N-CA-C	5.64	126.23	111.00
1	А	110	LEU	CA-CB-CG	5.06	126.95	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	110	LEU	Peptide
1	А	119	ARG	Peptide
1	А	83	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 asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	780	0	781	62	0
All	All	780	0	781	62	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 40.

The worst 5 of 62 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:128:LEU:O	1:A:132:TRP:HB2	1.73	0.89
1:A:108:GLU:HA	1:A:109:GLN:HB2	1.55	0.88
1:A:86:ALA:HA	1:A:89:LYS:HE3	1.57	0.85
1:A:71:HIS:HB3	1:A:107:ARG:HG2	1.56	0.85
1:A:101:THR:O	1:A:109:GLN:HB3	1.77	0.85

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		Analysed				
1	А	99/151~(66%)	68~(69%)	17 (17%)	14 (14%)	0 0

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	85	ALA
1	А	109	GLN
1	А	115	VAL
1	А	119	ARG

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Mol	Chain	Res	Type
1	А	120	SER

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	78/117~(67%)	73~(94%)	5 (6%)	17 31

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	48	ASP
1	А	102	LYS
1	А	104	ARG
1	А	107	ARG
1	А	132	TRP

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

Mol	Chain	Res	Type
1	А	105	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)

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	< <b>RSRZ</b> >	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	98/151~(64%)	0.72	12 (12%) 4 4	76, 90, 134, 151	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	140	ASP	5.8
1	А	139	ILE	5.1
1	А	103	ARG	4.0
1	А	41	ASP	3.9
1	А	105	ASN	3.8

#### 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.

