



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3I7J
Title : Crystal Structure of a beta-lactamase (Mb2281c) from Mycobacterium bovis, Northeast Structural Genomics Consortium Target Mbr246
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Deposited on : 2009-07-08
Resolution : 2.20 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

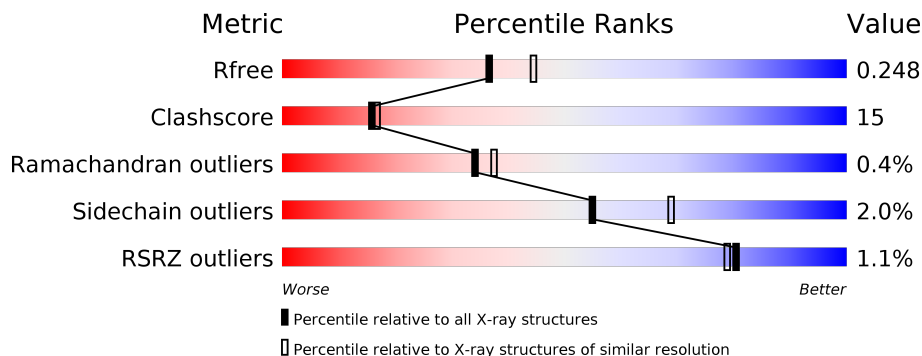
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	280	
1	B	280	

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 4387 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 beta-lactamase Mb2281c.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	273	2011	1274	350	381	2	4	0	0	0
1	B	272	2002	1269	349	378	2	4	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	LEU	-	expression tag	UNP Q7TYW1
A	274	GLU	-	expression tag	UNP Q7TYW1
A	275	HIS	-	expression tag	UNP Q7TYW1
A	276	HIS	-	expression tag	UNP Q7TYW1
A	277	HIS	-	expression tag	UNP Q7TYW1
A	278	HIS	-	expression tag	UNP Q7TYW1
A	279	HIS	-	expression tag	UNP Q7TYW1
A	280	HIS	-	expression tag	UNP Q7TYW1
B	273	LEU	-	expression tag	UNP Q7TYW1
B	274	GLU	-	expression tag	UNP Q7TYW1
B	275	HIS	-	expression tag	UNP Q7TYW1
B	276	HIS	-	expression tag	UNP Q7TYW1
B	277	HIS	-	expression tag	UNP Q7TYW1
B	278	HIS	-	expression tag	UNP Q7TYW1
B	279	HIS	-	expression tag	UNP Q7TYW1
B	280	HIS	-	expression tag	UNP Q7TYW1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	233	Total 233	O 233	0	0
2	B	141	Total 141	O 141	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.10Å 97.83Å 114.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 2.20 29.82 – 2.21	Depositor EDS
% Data completeness (in resolution range)	85.0 (19.88-2.20) 97.5 (29.82-2.21)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.2 & XtalView, REFMAC	Depositor
R, R_{free}	0.185 , 0.233 0.196 , 0.248	Depositor DCC
R_{free} test set	3540 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtrriage
Anisotropy	0.535	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4387	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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](#)

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	0.35	0/2058	0.62	0/2811
1	B	0.32	0/2049	0.56	0/2799
All	All	0.34	0/4107	0.59	0/5610

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	2011	0	1959	60	0
1	B	2002	0	1953	59	0
2	A	233	0	0	5	0
2	B	141	0	0	1	0
All	All	4387	0	3912	116	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 15.

The worst 5 of 116 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:112:GLN:HE21	1:A:119:PHE:H	1.09	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:GLY:H	1:B:219:ASN:HD22	1.14	0.88
1:A:216:GLY:H	1:A:219:ASN:HD22	1.22	0.85
1:B:84:MSE:HE3	1:B:85:HIS:NE2	1.95	0.81
1:B:216:GLY:H	1:B:219:ASN:ND2	1.82	0.79

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	271/280 (97%)	262 (97%)	8 (3%)	1 (0%)	34	37
1	B	270/280 (96%)	255 (94%)	14 (5%)	1 (0%)	34	37
All	All	541/560 (97%)	517 (96%)	22 (4%)	2 (0%)	34	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PHE
1	B	147	PHE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	203/205 (99%)	200 (98%)	3 (2%)	65	78
1	B	202/205 (98%)	197 (98%)	5 (2%)	47	60
All	All	405/410 (99%)	397 (98%)	8 (2%)	55	69

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	61	LEU
1	B	229	GLN
1	B	200	TRP
1	A	200	TRP
1	B	198	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	219	ASN
1	B	213	HIS
1	A	208	ASN
1	B	208	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 carbohydrates 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, 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	269/280 (96%)	-0.48	2 (0%) 87 86	7, 15, 27, 63	0
1	B	268/280 (95%)	-0.07	4 (1%) 73 72	12, 25, 41, 58	0
All	All	537/560 (95%)	-0.27	6 (1%) 80 79	7, 19, 38, 63	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	273	LEU	6.7
1	A	274	GLU	4.5
1	B	92	ARG	3.3
1	A	273	LEU	3.0
1	B	96	ARG	3.0

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 carbohydrates 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.