



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 4QRA / pdb_00004qra
Title : Structure and specificity of L-D-Transpeptidase from Mycobacterium tuberculosis and antibiotic resistance: Calcium binding promotes dimer formation
Authors : Gokulan, K.; Varughese, K.I.
Deposited on : 2014-06-30
Resolution : 2.29 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

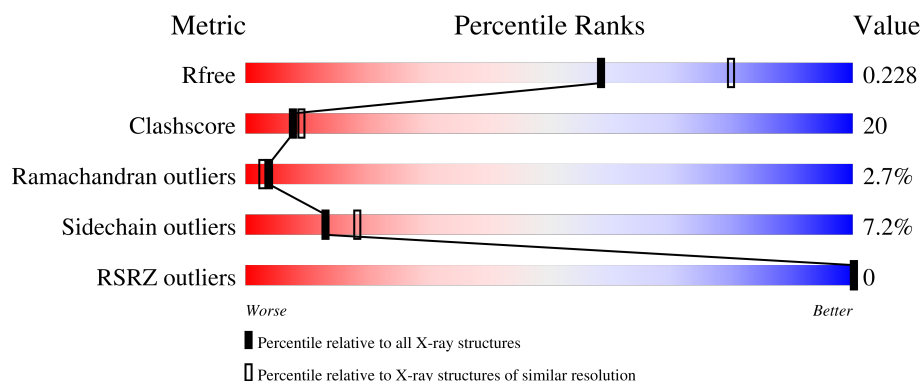
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	352	 73% 16% 5% • 5%
1	B	352	 76% 11% • • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5344 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 L,d-transpeptidase LdtB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2539	1590	445	496	8			
1	B	330	Total	C	N	O	S	0	0	0
			2507	1572	437	490	8			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	151	Total	O	0	0
			151	151		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.76Å 88.13Å 90.51Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	34.86 – 2.29 34.86 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.5 (34.86-2.29) 97.6 (34.86-2.29)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.49 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.182 , 0.226 0.190 , 0.228	Depositor DCC
R_{free} test set	1964 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.459 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5344	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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: CA

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	1.35	9/2603 (0.3%)	1.17	9/3561 (0.3%)
1	B	1.25	7/2571 (0.3%)	1.11	4/3518 (0.1%)
All	All	1.30	16/5174 (0.3%)	1.14	13/7079 (0.2%)

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	A	0	3
1	B	0	2
All	All	0	5

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	TRP	C-N	-28.97	0.95	1.33
1	A	399	ASP	C-O	-6.00	1.17	1.24
1	A	99	ARG	C-N	5.67	1.41	1.33
1	B	399	ASP	C-O	-5.46	1.17	1.24
1	A	100	PRO	N-CD	5.39	1.55	1.47

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	SER	N-CA-C	14.71	121.37	108.13
1	A	112	TRP	O-C-N	-12.98	107.43	123.27
1	B	95	ASN	N-CA-C	9.78	125.58	110.42
1	B	99	ARG	C-N-CD	-7.91	92.58	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ARG	CA-C-N	-6.74	112.82	119.76

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	VAL	Peptide
1	A	88	LEU	Peptide
1	A	94	VAL	Peptide
1	B	100	PRO	Peptide
1	B	121	ASN	Peptide

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	2539	0	2425	96	0
1	B	2507	0	2393	100	0
2	A	1	0	0	0	0
3	A	146	0	0	1	0
3	B	151	0	0	3	0
All	All	5344	0	4818	196	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 20.

The worst 5 of 196 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:104:ARG:HB3	1:B:112:TRP:CZ2	1.32	1.62
1:B:104:ARG:CB	1:B:112:TRP:CZ2	1.86	1.55
1:B:101:VAL:CG2	1:B:116:GLU:OE2	1.64	1.45
1:B:98:GLY:O	1:B:100:PRO:HD3	1.13	1.28
1:B:86:GLY:CA	1:B:87:VAL:HG12	1.65	1.25

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	330/352 (94%)	308 (93%)	14 (4%)	8 (2%)	4	4
1	B	326/352 (93%)	305 (94%)	11 (3%)	10 (3%)	3	2
All	All	656/704 (93%)	613 (93%)	25 (4%)	18 (3%)	4	3

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ALA
1	A	97	ASN
1	A	99	ARG
1	A	104	ARG
1	B	96	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	271/282 (96%)	254 (94%)	17 (6%)	16	23
1	B	268/282 (95%)	246 (92%)	22 (8%)	10	14
All	All	539/564 (96%)	500 (93%)	39 (7%)	13	18

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	110	LEU

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Mol	Chain	Res	Type
1	B	276	MET
1	B	113	SER
1	B	118	LEU
1	B	307	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	HIS
1	A	352	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	112:TRP	C	113:SER	N	0.95

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	334/352 (94%)	-1.24	0 100 100	19, 31, 105, 116	0
1	B	330/352 (93%)	-1.22	0 100 100	19, 31, 103, 114	0
All	All	664/704 (94%)	-1.23	0 100 100	19, 31, 104, 116	0

There are no RSRZ outliers to report.

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 oligosaccharides 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
2	CA	A	501	1/1	1.00	0.02	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.