Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 06:51 PM EST

PDB ID	:	3TX4
Title	:	Crystal Structure of Mutant (C354A) M. tuberculosis LD-transpeptidase type 2
Authors	:	Erdemli, S.; Bianchet, M.A.; Gupta, R.; Lamichhane, G.; Amzel, L.M.
Deposited on	:	2011-09-22
Resolution	:	2.32 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 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:

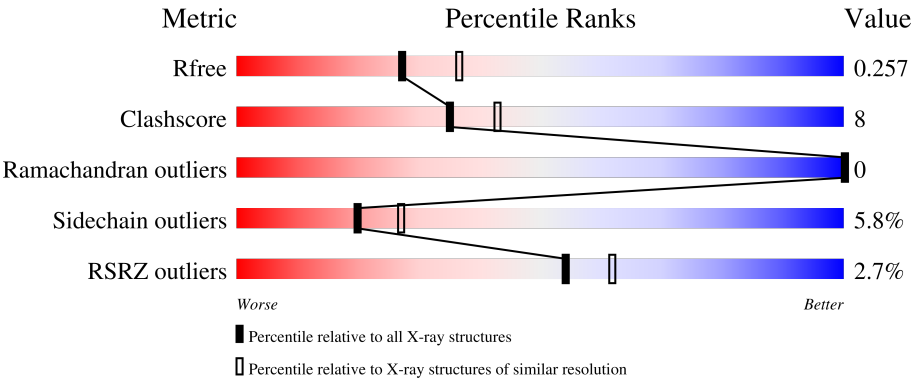
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 <=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	287	3% 77% 15% • 7%
1	B	287	% 75% 11% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4351 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 Mycobacterium Tuberculosis LD-transpeptidase type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	2	0
			2064	1303	358	397	6			
1	B	258	Total	C	N	O	S	0	2	0
			1993	1258	345	384	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	CYS	engineered mutation	UNP O53223
B	354	ALA	CYS	engineered mutation	UNP O53223

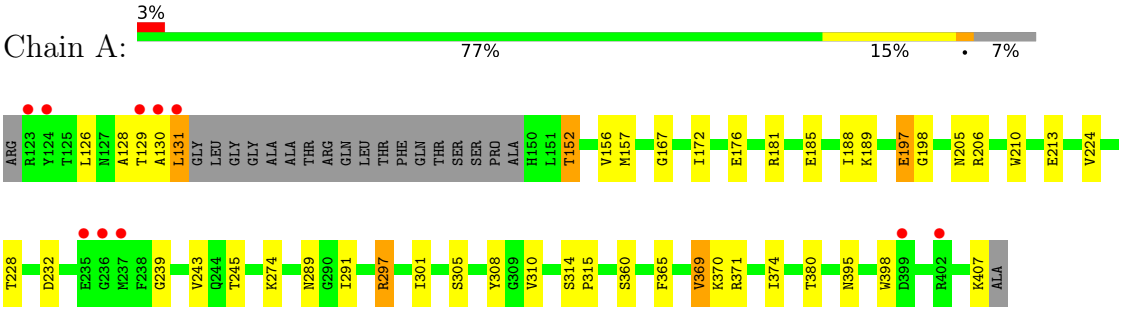
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total	O	0	0
			148	148		
2	B	146	Total	O	0	0
			146	146		

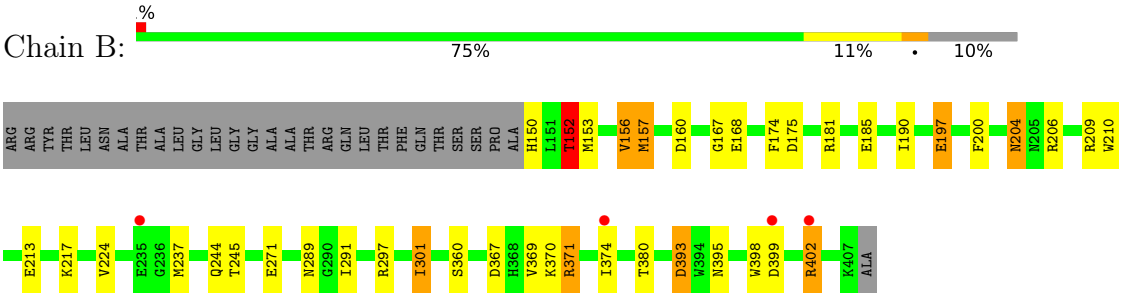
3 Residue-property plots (i)

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: Mycobacterium Tuberculosis LD-transpeptidase type 2



• Molecule 1: Mycobacterium Tuberculosis LD-transpeptidase type 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.78Å 121.03Å 122.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.71 – 2.32 28.44 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.71-2.32) 99.7 (28.44-2.32)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.210 , 0.266 0.201 , 0.257	Depositor DCC
R_{free} test set	1958 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.057 for -h,-l,-k 0.000 for l,-k,h 0.000 for -k,-h,-l 0.000 for k,-l,-h 0.000 for -l,h,-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4351	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

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	1.13	2/2123 (0.1%)	0.97	4/2904 (0.1%)
1	B	1.11	3/2055 (0.1%)	0.96	6/2810 (0.2%)
All	All	1.12	5/4178 (0.1%)	0.97	10/5714 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	TYR	CD1-CE1	6.45	1.49	1.39
1	B	271	GLU	CG-CD	5.98	1.60	1.51
1	B	197	GLU	CG-CD	5.77	1.60	1.51
1	A	197	GLU	CG-CD	5.13	1.59	1.51
1	B	197	GLU	CD-OE2	5.01	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	232	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	A	232	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	301	ILE	CB-CA-C	-5.94	99.72	111.60
1	A	130	ALA	N-CA-CB	-5.57	102.30	110.10
1	B	301	ILE	CB-CA-C	-5.52	100.56	111.60
1	B	370	LYS	CD-CE-NZ	5.51	124.37	111.70
1	B	152	THR	CB-CA-C	-5.42	96.96	111.60
1	B	399	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	367	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	160	ASP	CB-CG-OD1	5.01	122.81	118.30

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	2064	0	1963	37	0
1	B	1993	0	1898	28	0
2	A	148	0	0	5	1
2	B	146	0	0	4	0
All	All	4351	0	3861	65	1

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 8.

All (65) 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:289:ASN:HD21	1:B:380:THR:H	1.08	0.94
1:A:289:ASN:HD21	1:A:380:THR:H	1.13	0.94
1:B:204:ASN:HD22	1:B:206:ARG:H	1.14	0.94
1:A:152:THR:HG23	1:A:176:GLU:HB2	1.56	0.87
1:A:291:ILE:H	1:A:395:ASN:HD21	1.27	0.81
1:B:291:ILE:H	1:B:395:ASN:HD21	1.30	0.78
1:A:131:LEU:O	1:A:131:LEU:HD23	1.85	0.77
1:A:181:ARG:HH21	1:A:205:ASN:HD22	1.32	0.75
1:B:224:VAL:HB	1:B:245:THR:HG22	1.67	0.75
1:B:204:ASN:ND2	1:B:206:ARG:H	1.87	0.71
1:A:131:LEU:O	1:A:131:LEU:CG	2.36	0.71
1:B:289:ASN:HD21	1:B:380:THR:N	1.86	0.70
1:A:131:LEU:O	1:A:131:LEU:HG	1.91	0.70
1:A:228:THR:O	1:A:239:GLY:HA3	1.94	0.68
1:A:152:THR:CG2	1:A:176:GLU:HB2	2.26	0.65
1:A:297[A]:ARG:NH1	1:A:371:ARG:HG3	2.12	0.64
1:A:181:ARG:O	1:A:185:GLU:HG3	1.99	0.63
1:A:131:LEU:O	1:A:131:LEU:CD2	2.46	0.62
1:B:156:VAL:CG2	1:B:245:THR:HG21	2.31	0.61
1:B:157:MET:CE	1:B:371:ARG:HH12	2.14	0.60
1:A:128:ALA:HB2	1:A:156:VAL:HG13	1.83	0.60
1:A:167:GLY:HA3	1:A:374:ILE:HD11	1.82	0.60
1:B:152:THR:HG22	1:B:175:ASP:OD1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:VAL:HG12	1:A:243:VAL:HG11	1.83	0.59
1:B:181:ARG:O	1:B:185:GLU:HG3	2.05	0.57
1:B:297:ARG:NH1	1:B:369:VAL:O	2.37	0.56
1:A:181:ARG:HH21	1:A:205:ASN:ND2	2.04	0.55
1:A:314:SER:HB2	1:A:315:PRO:CD	2.36	0.55
1:A:371:ARG:HD2	2:A:508:HOH:O	2.07	0.55
1:B:244:GLN:HG3	2:B:624:HOH:O	2.06	0.54
1:A:156:VAL:HG12	1:A:243:VAL:CG1	2.38	0.54
1:B:289:ASN:ND2	1:B:380:THR:H	1.91	0.53
1:A:152:THR:HG23	1:A:176:GLU:CB	2.32	0.52
1:A:314:SER:HB2	1:A:315:PRO:HD2	1.91	0.52
1:B:204:ASN:HD22	1:B:206:ARG:N	1.96	0.52
1:A:213:GLU:HG3	1:A:398:TRP:CG	2.44	0.51
1:A:305:SER:HB2	1:A:310:VAL:HB	1.91	0.51
1:A:297[A]:ARG:NH2	1:A:297[A]:ARG:HB2	2.26	0.51
1:B:213:GLU:HG3	1:B:398:TRP:CG	2.46	0.50
1:B:360[B]:SER:HB3	2:B:501:HOH:O	2.10	0.50
1:A:371:ARG:CD	2:A:508:HOH:O	2.61	0.49
1:B:157:MET:HE2	1:B:371:ARG:HH12	1.78	0.48
1:B:167:GLY:HA3	1:B:374:ILE:HD11	1.96	0.48
1:B:371:ARG:HG2	2:B:509:HOH:O	2.13	0.47
1:A:198:GLY:HA3	1:A:210:TRP:CZ2	2.48	0.47
1:A:360:SER:OG	2:A:617:HOH:O	2.19	0.47
1:B:168:GLU:OE2	1:B:371:ARG:HD3	2.15	0.47
1:A:156:VAL:CG1	1:A:243:VAL:HG12	2.46	0.46
1:B:200:PHE:HA	1:B:209:ARG:O	2.16	0.46
1:B:152:THR:HG21	1:B:174:PHE:HB3	1.97	0.46
1:A:224:VAL:HB	1:A:245:THR:HG22	1.97	0.45
1:A:297[A]:ARG:HH11	1:A:371:ARG:HG3	1.79	0.45
1:A:371:ARG:NE	2:A:508:HOH:O	2.50	0.44
1:B:152:THR:CG2	1:B:175:ASP:OD1	2.65	0.44
1:A:172:ILE:HD13	1:A:188:ILE:HD13	2.00	0.43
1:B:402:ARG:HE	1:B:402:ARG:HB3	1.67	0.43
1:A:365:PHE:O	1:A:369:VAL:HB	2.19	0.43
1:B:393:ASP:OD1	1:B:393:ASP:N	2.52	0.42
1:B:190:ILE:HD13	1:B:210:TRP:CG	2.54	0.42
1:B:157:MET:HE1	1:B:371:ARG:HH12	1.83	0.42
1:A:314:SER:CB	1:A:315:PRO:CD	2.98	0.41
1:A:297[A]:ARG:HB2	1:A:297[A]:ARG:CZ	2.50	0.41
1:B:244:GLN:CG	2:B:624:HOH:O	2.65	0.40
1:A:156:VAL:CG1	1:A:243:VAL:CG1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LYS:HE3	2:A:513:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:644:HOH:O	2:A:644:HOH:O[7_455]	2.16	0.04

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	265/287 (92%)	256 (97%)	9 (3%)	0	100	100
1	B	258/287 (90%)	249 (96%)	9 (4%)	0	100	100
All	All	523/574 (91%)	505 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	219/231 (95%)	206 (94%)	13 (6%)	19	26
1	B	213/231 (92%)	200 (94%)	13 (6%)	18	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	432/462 (94%)	406 (94%)	26 (6%)	20 26

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	LEU
1	A	129	THR
1	A	131	LEU
1	A	152	THR
1	A	157	MET
1	A	189	LYS
1	A	197	GLU
1	A	206	ARG
1	A	274	LYS
1	A	297[A]	ARG
1	A	297[B]	ARG
1	A	369	VAL
1	A	407	LYS
1	B	150	HIS
1	B	152	THR
1	B	153	MET
1	B	156	VAL
1	B	157	MET
1	B	197	GLU
1	B	204	ASN
1	B	217	LYS
1	B	237	MET
1	B	301	ILE
1	B	371	ARG
1	B	393	ASP
1	B	402	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	289	ASN
1	A	361	ASN
1	A	379	ASN
1	A	395	ASN
1	B	204	ASN

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Mol	Chain	Res	Type
1	B	289	ASN
1	B	361	ASN
1	B	395	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	267/287 (93%)	0.01	10 (3%) 41 48	16, 25, 53, 100	0
1	B	258/287 (89%)	-0.10	4 (1%) 72 78	16, 25, 46, 57	0
All	All	525/574 (91%)	-0.05	14 (2%) 54 62	16, 25, 47, 100	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	TYR	6.1
1	B	399	ASP	3.3
1	A	131	LEU	3.1
1	A	123	ARG	2.8
1	B	402	ARG	2.8
1	A	130	ALA	2.6
1	A	236	GLY	2.4
1	A	399	ASP	2.3
1	A	235	GLU	2.3
1	A	237	MET	2.2
1	B	235	GLU	2.2
1	A	129	THR	2.2
1	A	402	ARG	2.1
1	B	374	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.