



wwPDB X-ray Structure Validation Summary Report

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PDB ID : 3OTV
Title : Crystal structure of the intracellular domain of Rv3910 from Mycobacterium tuberculosis
Authors : Gee, C.L.; Alber, T.
Deposited on : 2010-09-14
Resolution : 3.09 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

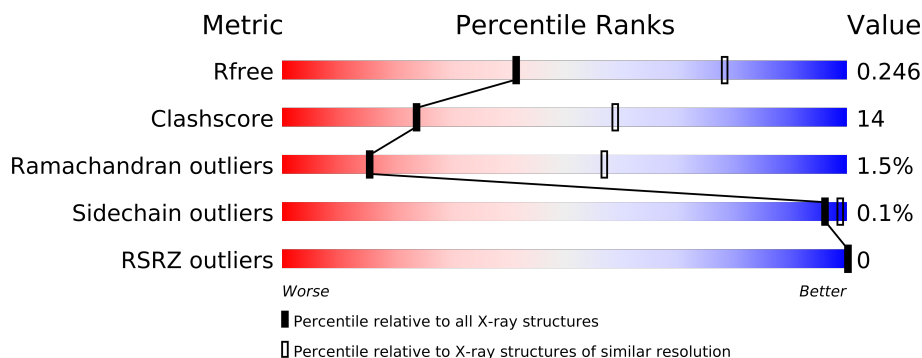
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.09 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}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	285	
1	B	285	
1	C	285	
1	D	285	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7513 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROBABLE CONSERVED TRANSMEMBRANE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	63	0	0
			1890	1182	350	355	3			
1	B	244	Total	C	N	O	S	34	0	0
			1815	1135	336	341	3			
1	C	257	Total	C	N	O	S	60	0	0
			1911	1193	353	362	3			
1	D	248	Total	C	N	O	S	64	0	0
			1837	1150	338	346	3			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	O	0	0
			7	7		
2	B	28	Total	O	0	0
			28	28		
2	C	11	Total	O	0	0
			11	11		
2	D	14	Total	O	0	0
			14	14		

M256	Q257	Q258	V262	A263	ASP	ARG	THR	GLU	VAL	LEU	GLY	PRO	PRO	ILE	ASP	GLU	ALA	PRO	VAL	SER	ALA	ALA	ALA	PRO	PRO	ARG	A138	D139	V146	A147	I150	D161	H152	P153	L166	A167	Y168	P169	A170	P173	M176	P177	I184	L188	A201	G202	V203	E211	R212	D213	Q217	P218	I219	D223	I224	D225	R226	Q231	A234	V235	A236	A237	R238	Q241	G242	D243	G244	A249	L252
ALA	ASP	ALA	LEU	ARG	GLU	PRO	ASP	ARG	GLU	SER	SER	ALA	PRO	PRO	ASP	ASP	V16	A22	R23	I24	R30	L31	F34	H35	G36	G37	V38	P39	F43	T58	F59	V60	D61	P62	R77	T84	D85	K86	V89	A90	R91	E107	I128	R129	A130	M131	A137																						

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.04Å 59.69Å 145.06Å 90.00° 97.21° 90.00°	Depositor
Resolution (Å)	40.81 – 3.09 40.81 – 3.09	Depositor EDS
% Data completeness (in resolution range)	87.3 (40.81-3.09) 87.4 (40.81-3.09)	Depositor EDS
R_{merge}	0.63	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.189 , 0.248 0.187 , 0.246	Depositor DCC
R_{free} test set	827 reflections (5.18%)	DCC
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 15986 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7513	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.47	0/1924	0.65	0/2630
1	B	0.49	0/1849	0.72	0/2527
1	C	0.47	0/1945	0.67	0/2659
1	D	0.44	0/1871	0.64	0/2559
All	All	0.47	0/7589	0.67	0/10375

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1890	0	1912	55	0
1	B	1815	0	1833	62	0
1	C	1911	0	1922	47	0
1	D	1837	0	1853	44	0
2	A	7	0	0	0	0
2	B	28	0	0	1	0
2	C	11	0	0	0	0
2	D	14	0	0	0	0
All	All	7513	0	7520	207	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 207 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:VAL:HG12	1:A:17:GLN:H	1.12	1.09
1:B:131:MET:CE	1:B:184:ILE:HG23	2.08	0.84
1:A:16:VAL:HG12	1:A:17:GLN:N	1.93	0.84
1:B:113:SER:OG	1:B:116:GLU:HG3	1.77	0.83
1:C:40:PRO:HG3	1:C:66:LEU:HD11	1.63	0.81

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	252/285 (88%)	224 (89%)	22 (9%)	6 (2%)	9	43
1	B	242/285 (85%)	222 (92%)	18 (7%)	2 (1%)	27	74
1	C	255/285 (90%)	240 (94%)	14 (6%)	1 (0%)	43	84
1	D	246/285 (86%)	224 (91%)	16 (6%)	6 (2%)	9	43
All	All	995/1140 (87%)	910 (92%)	70 (7%)	15 (2%)	15	57

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	ALA
1	C	170	ALA
1	B	170	ALA
1	D	170	ALA
1	A	200	GLU

5.3.2 Protein sidechains ⓘ

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	196/221 (89%)	196 (100%)	0	100	100
1	B	188/221 (85%)	187 (100%)	1 (0%)	94	98
1	C	198/221 (90%)	198 (100%)	0	100	100
1	D	190/221 (86%)	190 (100%)	0	100	100
All	All	772/884 (87%)	771 (100%)	1 (0%)	96	99

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	53	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	ASN
1	C	257	GLN
1	D	132	GLN
1	D	257	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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, 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	254/285 (89%)	-0.16	0 100 100	34, 62, 96, 115	13 (5%)
1	B	244/285 (85%)	-0.28	0 100 100	35, 51, 74, 105	8 (3%)
1	C	257/285 (90%)	-0.18	0 100 100	35, 61, 92, 101	13 (5%)
1	D	248/285 (87%)	-0.26	0 100 100	36, 61, 85, 96	13 (5%)
All	All	1003/1140 (87%)	-0.22	0 100 100	34, 58, 90, 115	47 (4%)

There are no RSRZ outliers to report.

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 carbohydrates 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.