



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 09:13 am BST

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 X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.11  
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

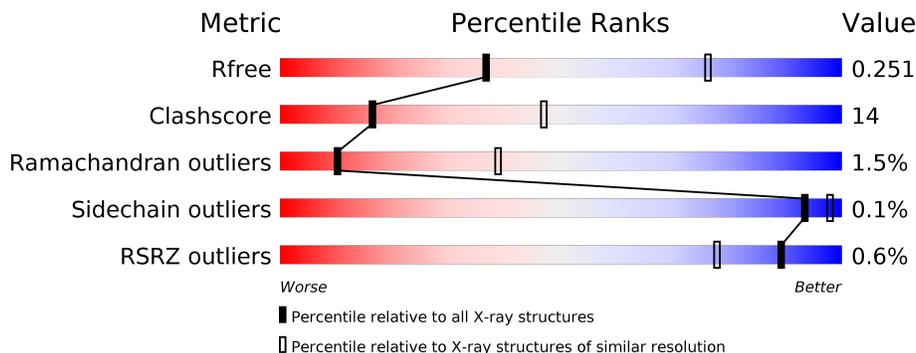
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	285	<p>63% 25% 11%</p>
1	B	285	<p>60% 25% 14%</p>
1	C	285	<p>68% 21% 10%</p>
1	D	285	<p>64% 22% 13%</p>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7513 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 PROBABLE CONSERVED TRANSMEMBRANE PROTEIN.

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

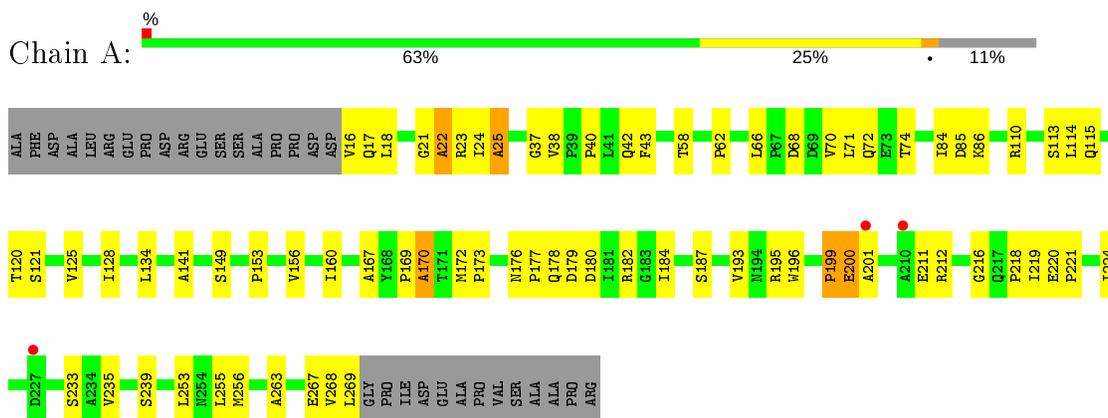
- Molecule 2 is water.

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

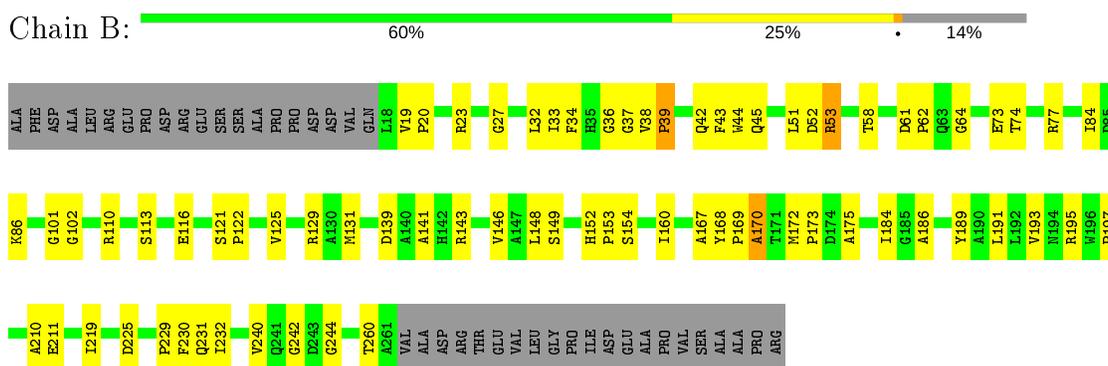
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

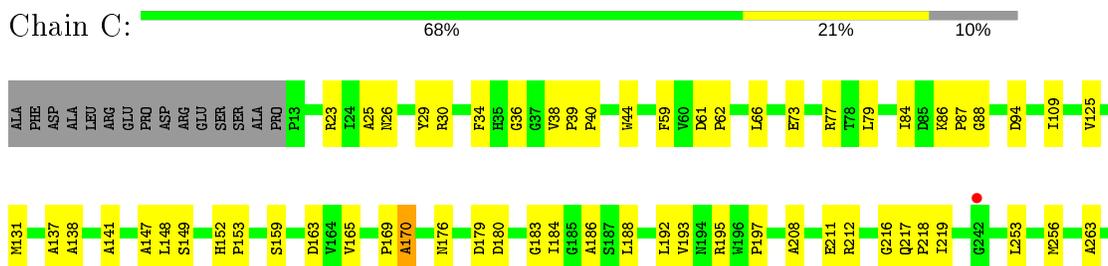
- Molecule 1: PROBABLE CONSERVED TRANSMEMBRANE PROTEIN



- Molecule 1: PROBABLE CONSERVED TRANSMEMBRANE PROTEIN



- Molecule 1: PROBABLE CONSERVED TRANSMEMBRANE PROTEIN



T266  
E267  
V268  
I269  
GLY  
PRO  
ILE  
ASP  
GLU  
ALA  
PRO  
VAL  
SER  
ALA  
ALA  
PRO  
PRO  
ARG

● Molecule 1: PROBABLE CONSERVED TRANSMEMBRANE PROTEIN

Chain D: %

ALA  
PHE  
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  
I84  
D85  
K86  
V89  
A90  
R91  
E107  
I128  
R129  
A130  
M131  
A137

A138  
D139  
V146  
A147  
I150  
H151  
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

M256  
Q257  
Q258  
V262  
A263  
ASP  
ARG  
THR  
GLU  
VAL  
LEU  
GLY  
PRO  
ILE  
ASP  
GLU  
ALA  
PRO  
VAL  
SER  
ALA  
ALA  
PRO  
ARG

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 3.12Å)	Xtrriage
Refinement program	ELVES, PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.189 , 0.248 0.188 , 0.251	Depositor DCC
$R_{free}$ test set	829 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtrriage
Anisotropy	0.122	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7513	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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	0.47	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 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	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

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 14.

The worst 5 of 207 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: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 [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	252/285 (88%)	224 (89%)	22 (9%)	6 (2%)	6 27
1	B	242/285 (85%)	222 (92%)	18 (7%)	2 (1%)	19 54
1	C	255/285 (90%)	240 (94%)	14 (6%)	1 (0%)	34 69
1	D	246/285 (86%)	224 (91%)	16 (6%)	6 (2%)	6 27
All	All	995/1140 (87%)	910 (92%)	70 (7%)	15 (2%)	10 39

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 [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	196/221 (89%)	196 (100%)	0	100	100
1	B	188/221 (85%)	187 (100%)	1 (0%)	88	94
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%)	93	98

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	254/285 (89%)	-0.20	3 (1%) 79 61	34, 62, 96, 115	13 (5%)
1	B	244/285 (85%)	-0.40	0 100 100	35, 51, 74, 105	8 (3%)
1	C	257/285 (90%)	-0.25	1 (0%) 92 84	35, 61, 92, 101	13 (5%)
1	D	248/285 (87%)	-0.35	2 (0%) 86 72	36, 61, 85, 96	13 (5%)
All	All	1003/1140 (87%)	-0.30	6 (0%) 89 78	34, 58, 90, 115	47 (4%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	ASP	3.1
1	C	242	GLY	2.7
1	D	262	VAL	2.4
1	A	201	ALA	2.1
1	D	202	GLY	2.1

### 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.