



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5EBC / pdb\_00005ebc  
Title : Crystal structure of EccB1 of Mycobacterium tuberculosis in spacegroup P21 (state III)  
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Deposited on : 2015-10-19  
Resolution : 3.00 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](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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

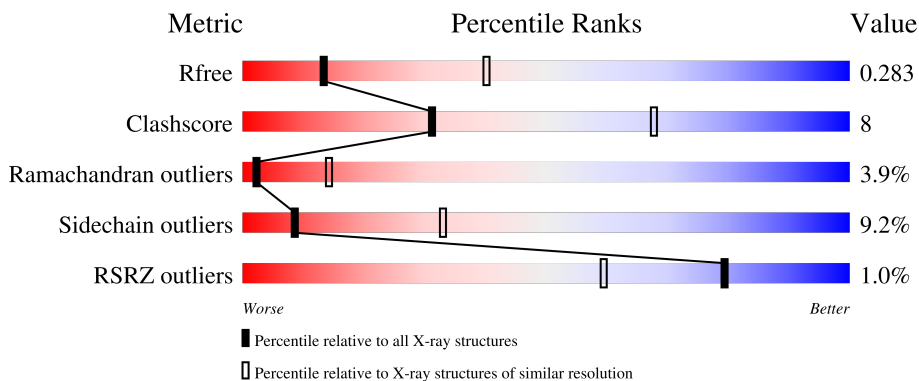
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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  $\geq 3$ , 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	432	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 2853 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 ESX-1 secretion system protein eccB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	384	2852	1810	483	547	12	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP P9WNR7
A	-21	GLY	-	expression tag	UNP P9WNR7
A	-20	SER	-	expression tag	UNP P9WNR7
A	-19	SER	-	expression tag	UNP P9WNR7
A	-18	HIS	-	expression tag	UNP P9WNR7
A	-17	HIS	-	expression tag	UNP P9WNR7
A	-16	HIS	-	expression tag	UNP P9WNR7
A	-15	HIS	-	expression tag	UNP P9WNR7
A	-14	HIS	-	expression tag	UNP P9WNR7
A	-13	HIS	-	expression tag	UNP P9WNR7
A	-12	SER	-	expression tag	UNP P9WNR7
A	-11	SER	-	expression tag	UNP P9WNR7
A	-10	GLY	-	expression tag	UNP P9WNR7
A	-9	LEU	-	expression tag	UNP P9WNR7
A	-8	GLU	-	expression tag	UNP P9WNR7
A	-7	VAL	-	expression tag	UNP P9WNR7
A	-6	LEU	-	expression tag	UNP P9WNR7
A	-5	PHE	-	expression tag	UNP P9WNR7
A	-4	GLN	-	expression tag	UNP P9WNR7
A	-3	GLY	-	expression tag	UNP P9WNR7
A	-2	PRO	-	expression tag	UNP P9WNR7
A	-1	HIS	-	expression tag	UNP P9WNR7
A	0	MET	-	expression tag	UNP P9WNR7

- 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		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	31.61Å 120.21Å 61.26Å 90.00° 102.92° 90.00°	Depositor
Resolution (Å)	30.28 – 3.00 30.28 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.28-3.00) 93.2 (30.28-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, $R_{free}$	0.232 , 0.286 0.231 , 0.283	Depositor DCC
$R_{free}$ test set	862 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.5	Xtrriage
Anisotropy	0.662	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 84.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.086 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2853	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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](#)

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	0.31	0/2924	0.81	7/4017 (0.2%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	VAL	N-CA-C	-5.86	107.56	113.47
1	A	241	VAL	CA-C-N	5.54	126.77	119.84
1	A	241	VAL	C-N-CA	5.54	126.77	119.84
1	A	88	THR	CA-C-N	5.28	131.20	121.70
1	A	88	THR	C-N-CA	5.28	131.20	121.70
1	A	253	TYR	CA-C-N	5.21	126.36	119.84
1	A	253	TYR	C-N-CA	5.21	126.36	119.84

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	2852	0	2858	47	0
2	A	1	0	0	0	0
All	All	2853	0	2858	47	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 8.

All (47) 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:161:MET:HE1	1:A:275:TRP:HB2	1.64	0.80
1:A:153:ARG:HD3	1:A:154:PRO:HD2	1.71	0.71
1:A:271:PRO:HD2	1:A:294:ARG:HA	1.75	0.67
1:A:201:THR:HG23	1:A:203:LYS:H	1.60	0.67
1:A:137:LEU:HD12	1:A:154:PRO:HD3	1.79	0.65
1:A:71:GLY:HA2	1:A:72:SER:HB2	1.82	0.60
1:A:88:THR:HB	1:A:89:SER:HB2	1.84	0.60
1:A:109:PRO:HA	1:A:291:LEU:HA	1.86	0.57
1:A:118:VAL:HG12	1:A:125:TRP:HB2	1.86	0.57
1:A:17:LEU:O	1:A:19:GLY:N	2.37	0.56
1:A:227:ARG:NH2	1:A:235:VAL:O	2.39	0.55
1:A:25:TYR:OH	1:A:389:HIS:ND1	2.39	0.55
1:A:145:SER:OG	1:A:146:MET:SD	2.63	0.54
1:A:171:TRP:HA	1:A:171:TRP:CE3	2.42	0.54
1:A:309:GLN:HB3	1:A:312:GLY:HA3	1.90	0.53
1:A:193:ILE:HD11	1:A:212:PRO:HD3	1.91	0.52
1:A:160:GLY:HA3	1:A:373:LEU:HD21	1.93	0.51
1:A:266:SER:O	1:A:270:ASP:N	2.44	0.51
1:A:146:MET:O	1:A:148:ILE:N	2.41	0.50
1:A:173:LEU:HD22	1:A:226:LEU:HG	1.95	0.49
1:A:240:MET:HE3	1:A:244:LEU:HD22	1.96	0.48
1:A:81:THR:HB	1:A:93:GLN:HG3	1.95	0.47
1:A:166:PRO:HB2	1:A:168:MET:HE2	1.96	0.46
1:A:107:ILE:HA	1:A:293:GLY:HA3	1.97	0.46
1:A:13:LEU:HD11	1:A:64:TYR:HE1	1.81	0.45
1:A:144:SER:HA	1:A:148:ILE:O	2.17	0.45
1:A:356:LYS:HA	1:A:356:LYS:HD2	1.76	0.44
1:A:222:THR:OG1	1:A:255:SER:OG	2.34	0.44
1:A:202:ASP:HB3	1:A:203:LYS:NZ	2.32	0.44
1:A:277:TRP:CE3	1:A:367:PRO:HD3	2.52	0.44
1:A:1:GLY:HA3	1:A:2:THR:O	2.18	0.43
1:A:87:SER:OG	1:A:88:THR:N	2.51	0.43
1:A:251:ARG:HA	1:A:251:ARG:HD3	1.81	0.43
1:A:117:LEU:HD22	1:A:154:PRO:HB3	2.00	0.42
1:A:90:PRO:HG2	1:A:156:PRO:HG2	2.01	0.42
1:A:351:ASN:OD1	1:A:354:THR:OG1	2.25	0.42
1:A:44:LYS:H	1:A:44:LYS:HG2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:HA	1:A:174:PRO:HD3	1.95	0.41
1:A:275:TRP:CZ2	1:A:288:SER:HB2	2.55	0.41
1:A:325:ALA:HB1	1:A:335:GLU:HG3	2.02	0.41
1:A:116:VAL:HG21	1:A:273:LEU:HD13	2.01	0.41
1:A:337:MET:HE3	1:A:363:PRO:HG3	2.03	0.41
1:A:171:TRP:HB3	1:A:172:GLN:H	1.65	0.41
1:A:146:MET:SD	1:A:146:MET:N	2.94	0.41
1:A:170:PRO:HB2	1:A:172:GLN:HG2	2.03	0.41
1:A:111:GLN:HG2	1:A:114:GLU:OE1	2.21	0.40
1:A:84:ARG:HB3	1:A:87:SER:HB2	2.03	0.40

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	380/432 (88%)	326 (86%)	39 (10%)	15 (4%)	<b>2</b> <b>14</b>

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	350	PRO
1	A	18	SER
1	A	2	THR
1	A	147	GLY
1	A	149	PRO
1	A	171	TRP
1	A	254	PRO
1	A	139	ASP
1	A	69	SER
1	A	255	SER

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Mol	Chain	Res	Type
1	A	281	ALA
1	A	107	ILE
1	A	89	SER
1	A	60	PRO

### 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	315/355 (89%)	286 (91%)	29 (9%)	<b>8</b> 33

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	6	THR
1	A	32	LEU
1	A	43	VAL
1	A	56	THR
1	A	81	THR
1	A	91	VAL
1	A	92	VAL
1	A	94	THR
1	A	96	VAL
1	A	103	ILE
1	A	117	LEU
1	A	118	VAL
1	A	126	ILE
1	A	137	LEU
1	A	142	LEU
1	A	146	MET
1	A	148	ILE
1	A	171	TRP
1	A	187	LEU
1	A	192	VAL
1	A	193	ILE

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Mol	Chain	Res	Type
1	A	240	MET
1	A	241	VAL
1	A	244	LEU
1	A	265	VAL
1	A	288	SER
1	A	310	ILE
1	A	351	ASN

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	284	GLN
1	A	287	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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](#)

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	384/432 (88%)	0.19	4 (1%) 79 59	29, 75, 121, 152	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	ASP	2.7
1	A	171	TRP	2.5
1	A	149	PRO	2.2
1	A	15	VAL	2.0

### 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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CA	A	501	1/1	0.66	0.18	100,100,100,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.