



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:17 am BST

PDB ID : 4KL7
Title : Crystal structure of the catalytic domain of RpfB from Mycobacterium tuberculosis
Authors : Squeglia, F.; Romano, M.; Ruggiero, A.; Berisio, R.
Deposited on : 2013-05-07
Resolution : 1.45 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2918 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 Resuscitation-promoting factor RpfB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	80	Total 598	C 373	N 111	O 112	S 2	0	0	0
1	B	80	Total 598	C 373	N 111	O 112	S 2	0	0	0
1	C	80	Total 598	C 373	N 111	O 112	S 2	0	0	0
1	D	80	Total 598	C 373	N 111	O 112	S 2	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

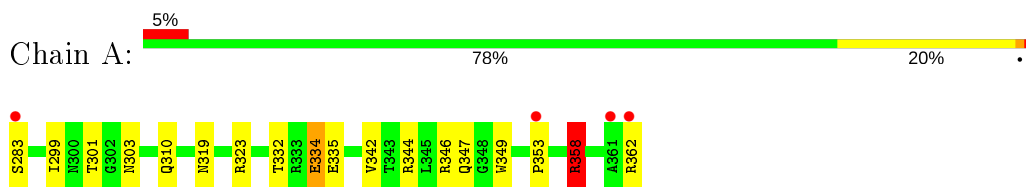
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total 136	O 136	0	0
3	B	137	Total 137	O 137	0	0
3	C	120	Total 120	O 120	0	0
3	D	123	Total 123	O 123	0	0

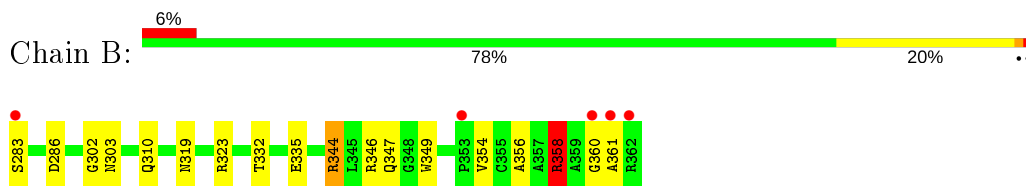
3 Residue-property plots [i](#)

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.

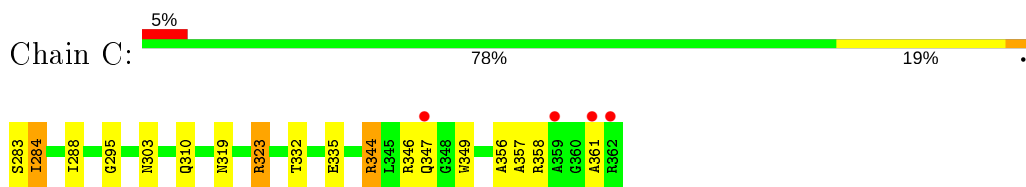
- Molecule 1: Resuscitation-promoting factor RpfB



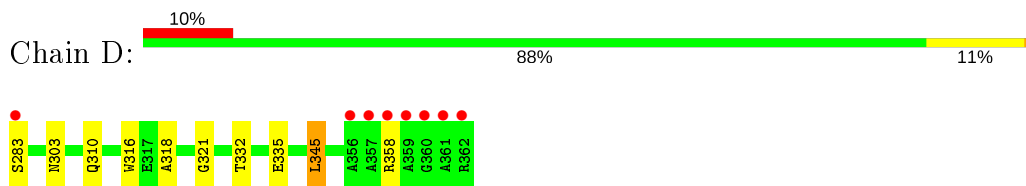
- Molecule 1: Resuscitation-promoting factor RpfB



- Molecule 1: Resuscitation-promoting factor RpfB



- Molecule 1: Resuscitation-promoting factor RpfB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.43Å 51.59Å 66.59Å 90.00° 104.06° 90.00°	Depositor
Resolution (Å)	25.33 – 1.45 25.33 – 1.45	Depositor EDS
% Data completeness (in resolution range)	82.2 (25.33-1.45) 82.2 (25.33-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.24 (at 1.45Å)	Xtrriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.145 , 0.192 0.154 , 0.200	Depositor DCC
R_{free} test set	2112 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtrriage
Anisotropy	0.631	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2918	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.85% 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: SO4

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	0.88	2/613 (0.3%)	0.96	4/835 (0.5%)
1	B	0.74	0/613	0.82	3/835 (0.4%)
1	C	0.75	0/613	0.87	3/835 (0.4%)
1	D	0.74	0/613	0.72	0/835
All	All	0.78	2/2452 (0.1%)	0.85	10/3340 (0.3%)

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	GLU	CG-CD	6.71	1.62	1.51
1	A	358	ARG	CB-CG	5.22	1.66	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	ARG	NE-CZ-NH1	-10.82	114.89	120.30
1	C	358	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	A	346	ARG	CD-NE-CZ	6.61	132.85	123.60
1	C	358	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	B	358	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	346	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	A	353	PRO	N-CA-C	5.66	126.81	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	C	323	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	344	ARG	NE-CZ-NH2	-5.31	117.64	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	283	SER	Peptide

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	598	0	549	15	0
1	B	598	0	549	20	0
1	C	598	0	549	24	0
1	D	598	0	549	13	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	136	0	0	6	0
3	B	137	0	0	9	0
3	C	120	0	0	8	0
3	D	123	0	0	3	0
All	All	2918	0	2196	71	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 15.

All (71) 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:C:344:ARG:CZ	3:C:510:HOH:O	2.05	1.02
1:A:332:THR:HG21	3:A:726:HOH:O	1.70	0.90
1:D:332:THR:HG23	1:D:335:GLU:H	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:ILE:HD11	1:C:288:ILE:HD11	1.59	0.84
1:B:332:THR:HG23	1:B:335:GLU:H	1.44	0.83
1:B:332:THR:HG21	3:B:525:HOH:O	1.81	0.80
1:A:334:GLU:HG2	3:A:774:HOH:O	1.84	0.77
1:A:349:TRP:HE1	1:A:362:ARG:HB2	1.50	0.76
1:C:332:THR:HG23	1:C:335:GLU:H	1.50	0.76
1:D:332:THR:HG21	3:D:449:HOH:O	1.83	0.76
1:A:347:GLN:NE2	3:A:829:HOH:O	2.19	0.76
1:C:284:ILE:CD1	1:C:288:ILE:CD1	2.65	0.74
1:C:332:THR:HG21	3:C:487:HOH:O	1.88	0.74
1:D:358:ARG:NH2	3:D:500:HOH:O	2.21	0.72
1:C:284:ILE:HD11	1:C:288:ILE:CD1	2.21	0.70
1:D:345:LEU:HD23	1:D:345:LEU:O	1.94	0.67
1:A:332:THR:HG23	1:A:335:GLU:H	1.59	0.67
1:C:295:GLY:O	3:C:499:HOH:O	2.11	0.67
1:B:360:GLY:HA2	3:B:611:HOH:O	1.95	0.66
1:B:347:GLN:NE2	3:B:635:HOH:O	2.28	0.65
1:B:303:ASN:HD21	1:B:310:GLN:HE22	1.45	0.64
1:A:303:ASN:HD21	1:A:310:GLN:HE22	1.45	0.63
1:C:344:ARG:HD2	1:C:349:TRP:CZ2	2.36	0.61
1:B:358:ARG:NH2	3:B:546:HOH:O	2.35	0.60
1:B:283:SER:HA	3:B:528:HOH:O	2.02	0.58
1:B:347:GLN:HG3	3:B:635:HOH:O	2.03	0.58
1:B:360:GLY:CA	3:B:611:HOH:O	2.50	0.57
1:B:283:SER:HB2	1:B:286:ASP:OD2	2.04	0.57
1:C:284:ILE:CD1	1:C:288:ILE:HD11	2.29	0.57
1:A:323:ARG:NH2	3:A:828:HOH:O	2.38	0.55
1:C:303:ASN:HD21	1:C:310:GLN:HE22	1.55	0.55
1:C:284:ILE:CD1	1:C:288:ILE:HD12	2.36	0.55
1:D:332:THR:HG22	1:D:335:GLU:CG	2.37	0.55
1:C:344:ARG:NE	3:C:510:HOH:O	2.32	0.54
1:A:349:TRP:NE1	1:A:362:ARG:HB2	2.21	0.54
1:B:349:TRP:CG	1:B:361:ALA:HB1	2.43	0.53
1:C:319:ASN:ND2	1:C:346:ARG:HH11	2.07	0.52
1:C:347:GLN:NE2	3:C:507:HOH:O	2.41	0.52
1:C:284:ILE:HD13	1:C:284:ILE:O	2.09	0.52
1:B:354:VAL:HG12	1:B:358:ARG:HD3	1.93	0.50
1:C:332:THR:CG2	1:C:335:GLU:H	2.22	0.49
1:D:283:SER:N	3:D:511:HOH:O	2.45	0.49
1:A:332:THR:OG1	1:A:334:GLU:OE1	2.25	0.49
1:C:349:TRP:CD2	1:C:361:ALA:HB1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ARG:HD2	1:B:302:GLY:O	2.13	0.48
1:D:345:LEU:CD2	1:D:345:LEU:O	2.60	0.48
1:B:303:ASN:HD21	1:B:310:GLN:NE2	2.10	0.48
1:B:332:THR:HG22	1:B:335:GLU:CG	2.44	0.48
1:B:356:ALA:HB1	1:B:361:ALA:HB2	1.95	0.47
1:A:283:SER:N	3:A:804:HOH:O	2.46	0.47
1:D:303:ASN:HD21	1:D:310:GLN:HE22	1.63	0.47
1:B:354:VAL:N	3:B:501:HOH:O	2.38	0.47
1:C:323:ARG:NH1	3:C:426:HOH:O	2.48	0.46
3:C:499:HOH:O	1:D:318:ALA:HB2	2.14	0.46
1:A:332:THR:HG22	1:A:335:GLU:CG	2.46	0.46
1:C:349:TRP:CG	1:C:361:ALA:HB1	2.51	0.45
1:C:332:THR:HG22	1:C:335:GLU:CG	2.46	0.45
1:B:323:ARG:HD2	3:B:585:HOH:O	2.16	0.45
1:C:284:ILE:HD13	1:C:284:ILE:C	2.37	0.45
1:C:356:ALA:HB1	1:C:361:ALA:HB2	2.00	0.44
1:D:332:THR:CG2	1:D:335:GLU:H	2.20	0.44
1:B:319:ASN:HD22	1:B:346:ARG:HH11	1.66	0.43
1:C:357:ALA:HB3	3:C:459:HOH:O	2.18	0.43
1:A:362:ARG:O	3:A:782:HOH:O	2.22	0.43
1:D:316:TRP:CE2	1:D:321:GLY:HA3	2.55	0.42
1:D:345:LEU:CD2	1:D:345:LEU:C	2.88	0.42
1:D:332:THR:HG22	1:D:335:GLU:CD	2.39	0.42
1:A:299:ILE:HG12	1:A:301:THR:HG23	2.01	0.41
1:A:319:ASN:HD22	1:A:342:VAL:HG12	1.85	0.40
1:C:284:ILE:HD13	1:C:288:ILE:CD1	2.48	0.40
1:B:354:VAL:CG1	1:B:358:ARG:HD3	2.52	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	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
1	B	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
1	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
1	D	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
All	All	312/320 (98%)	301 (96%)	11 (4%)	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	51/52 (98%)	49 (96%)	2 (4%)	32	4
1	B	51/52 (98%)	49 (96%)	2 (4%)	32	4
1	C	51/52 (98%)	49 (96%)	2 (4%)	32	4
1	D	51/52 (98%)	50 (98%)	1 (2%)	55	22
All	All	204/208 (98%)	197 (97%)	7 (3%)	37	6

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	ARG
1	A	358	ARG
1	B	344	ARG
1	B	358	ARG
1	C	284	ILE
1	C	344	ARG
1	D	345	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	GLN

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Mol	Chain	Res	Type
1	A	319	ASN
1	A	347	GLN
1	B	310	GLN
1	B	319	ASN
1	C	310	GLN
1	C	319	ASN
1	C	347	GLN
1	D	310	GLN
1	D	319	ASN

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	601	-	4,4,4	0.14	0	6,6,6	0.43	0
2	SO4	B	401	-	4,4,4	0.23	0	6,6,6	0.44	0

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

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	80/80 (100%)	0.17	4 (5%) 28 31	11, 15, 27, 41	0
1	B	80/80 (100%)	0.30	5 (6%) 20 22	11, 15, 30, 48	0
1	C	80/80 (100%)	0.22	4 (5%) 28 31	10, 14, 29, 50	0
1	D	80/80 (100%)	0.44	8 (10%) 7 8	12, 17, 42, 52	0
All	All	320/320 (100%)	0.28	21 (6%) 18 20	10, 15, 32, 52	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	361	ALA	11.1
1	D	359	ALA	9.3
1	B	361	ALA	8.5
1	D	360	GLY	8.2
1	B	362	ARG	8.0
1	B	360	GLY	6.6
1	A	362	ARG	6.0
1	D	283	SER	5.4
1	D	362	ARG	5.2
1	C	362	ARG	4.9
1	D	358	ARG	3.7
1	A	361	ALA	3.6
1	A	353	PRO	3.2
1	B	353	PRO	2.9
1	B	283	SER	2.8
1	A	283	SER	2.7
1	C	359	ALA	2.6
1	D	357	ALA	2.6
1	C	347	GLN	2.5
1	D	361	ALA	2.3
1	D	356	ALA	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](#)

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(\AA^2)	Q<0.9
2	SO4	A	601	5/5	0.99	0.06	15,15,17,17	0
2	SO4	B	401	5/5	0.99	0.13	16,18,24,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.