Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:34 AM GMT

PDB ID	:	2ASB
Title	:	Structure of a Mycobacterium tuberculosis NusA-RNA complex
Authors	:	Beuth, B.; Pennell, S.; Arnvig, K.B.; Martin, S.R.; Taylor, I.A.
Deposited on	:	2005-08-23
Resolution	:	1.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

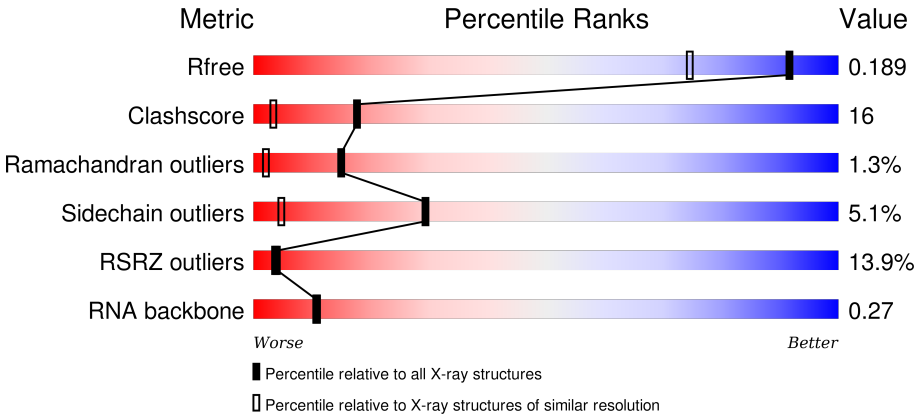
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.50 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}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)
RNA backbone	2183	1046 (2.70-0.62)

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. 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	B	11	36% 55% 9%
2	A	251	13% 75% 12% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2183 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 RNA chain called ribosomal RNA (5'- GAACUCAAUAG -3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	11	Total	C	N	O	P	0	0	0
			233	106	45	72	10			

- Molecule 2 is a protein called Transcription elongation protein nusA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	226	Total	C	N	O	S	0	0	0
			1690	1045	323	318	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	348	LEU	-	CLONING ARTIFACT	UNP P0A5M2
A	349	GLU	-	CLONING ARTIFACT	UNP P0A5M2
A	350	HIS	-	EXPRESSION TAG	UNP P0A5M2
A	351	HIS	-	EXPRESSION TAG	UNP P0A5M2
A	352	HIS	-	EXPRESSION TAG	UNP P0A5M2
A	353	HIS	-	EXPRESSION TAG	UNP P0A5M2
A	354	HIS	-	EXPRESSION TAG	UNP P0A5M2
A	355	HIS	-	EXPRESSION TAG	UNP P0A5M2

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	213	Total	O	0	0
			213	213		
3	B	47	Total	O	0	0
			47	47		

3 Residue-property plots (i)

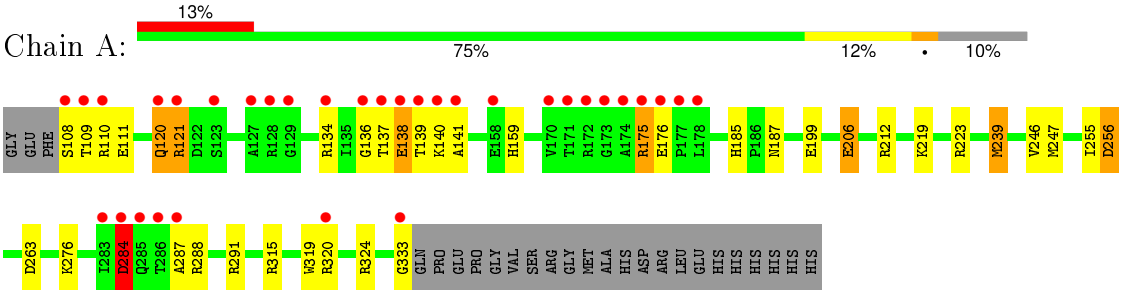
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ribosomal RNA (5'- GAACUCAAUAG -3')

Chain B:

- Molecule 2: Transcription elongation protein nusA

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	71.42Å 71.42Å 115.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 27.93 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-1.50) 97.2 (27.93-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.188 , 0.222 0.190 , 0.189	Depositor DCC
R_{free} test set	2352 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 51.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 47086 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2183	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	B	1.05	0/261	1.76	5/405 (1.2%)
2	A	0.56	0/1714	0.85	4/2325 (0.2%)
All	All	0.65	0/1975	1.04	9/2730 (0.3%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	11	G	O4'-C1'-N9	-7.79	101.97	108.20
1	B	10	A	O4'-C1'-N9	-7.19	102.45	108.20
1	B	3	A	O5'-P-OP2	-7.09	99.32	105.70
2	A	256	ASP	CB-CG-OD1	6.71	124.33	118.30
2	A	212	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	3	A	N9-C4-C5	5.64	108.06	105.80
2	A	284	ASP	CB-CG-OD2	5.51	123.26	118.30
2	A	263	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	9	U	P-O3'-C3'	5.21	125.95	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	B	233	0	121	1	0
2	A	1690	0	1732	59	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	213	0	0	16	4
3	B	47	0	0	7	1
All	All	2183	0	1853	60	4

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 16.

All (60) 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)
2:A:120:GLN:OE1	2:A:134:ARG:HB2	1.09	1.26
2:A:137:THR:HG21	3:A:392:HOH:O	1.46	1.11
2:A:138:GLU:HG2	2:A:139:THR:HG23	1.34	1.08
2:A:120:GLN:OE1	2:A:134:ARG:CB	2.04	1.06
2:A:108:SER:O	2:A:138:GLU:HB3	1.63	0.97
2:A:206:GLU:OE1	2:A:223:ARG:NE	1.98	0.97
2:A:284:ASP:OD1	2:A:287:ALA:HB3	1.70	0.91
2:A:121:ARG:HH11	2:A:121:ARG:CG	1.84	0.91
2:A:121:ARG:H	2:A:159:HIS:HD2	1.12	0.91
2:A:291:ARG:HD3	2:A:324:ARG:NH1	1.84	0.91
2:A:284:ASP:OD1	2:A:287:ALA:CB	2.21	0.88
2:A:185:HIS:HD2	2:A:187:ASN:H	1.17	0.87
2:A:134:ARG:NH2	3:A:517:HOH:O	2.08	0.87
3:B:1110:HOH:O	2:A:320:ARG:HD3	1.78	0.83
2:A:121:ARG:NH1	2:A:121:ARG:HG2	1.97	0.79
2:A:108:SER:N	2:A:139:THR:HG1	1.81	0.79
2:A:111:GLU:OE1	3:A:554:HOH:O	2.01	0.78
2:A:320:ARG:HG3	3:A:479:HOH:O	1.85	0.75
2:A:138:GLU:CG	2:A:139:THR:HG23	2.16	0.74
2:A:121:ARG:H	2:A:159:HIS:CD2	2.02	0.74
2:A:121:ARG:HH11	2:A:121:ARG:HG2	1.51	0.73
1:B:1:G:N2	3:B:1162:HOH:O	2.21	0.72
2:A:284:ASP:OD1	2:A:287:ALA:N	2.20	0.71
2:A:320:ARG:CG	3:A:479:HOH:O	2.40	0.70
2:A:206:GLU:OE1	2:A:223:ARG:CZ	2.41	0.69
2:A:284:ASP:OD2	3:A:558:HOH:O	2.10	0.68
2:A:288:ARG:HD2	2:A:319:TRP:NE1	2.10	0.67
2:A:121:ARG:HH11	2:A:121:ARG:HG3	1.61	0.65
2:A:315:ARG:NH2	3:A:417:HOH:O	2.31	0.64
2:A:333:GLY:O	3:A:568:HOH:O	2.15	0.63
2:A:320:ARG:NE	3:A:533:HOH:O	2.34	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:121:ARG:N	2:A:159:HIS:HD2	1.93	0.58
2:A:134:ARG:CZ	3:A:517:HOH:O	2.50	0.56
2:A:185:HIS:CD2	2:A:187:ASN:H	2.09	0.56
2:A:291:ARG:CD	2:A:324:ARG:NH1	2.64	0.56
2:A:185:HIS:HE1	3:A:382:HOH:O	1.89	0.55
2:A:108:SER:HB3	2:A:138:GLU:OE1	2.07	0.55
2:A:246:VAL:HG12	2:A:255:ILE:HD11	1.90	0.54
2:A:206:GLU:OE1	2:A:223:ARG:NH2	2.42	0.53
2:A:109:THR:HG22	2:A:110:ARG:N	2.25	0.51
3:B:1225:HOH:O	2:A:247:MET:HE1	2.11	0.50
2:A:134:ARG:NE	3:A:517:HOH:O	2.44	0.49
3:B:1110:HOH:O	2:A:320:ARG:HB3	2.11	0.49
3:B:1225:HOH:O	2:A:247:MET:CE	2.60	0.49
2:A:109:THR:HG22	2:A:110:ARG:H	1.78	0.48
3:B:1079:HOH:O	2:A:239:MET:HE3	2.13	0.48
2:A:288:ARG:HD2	2:A:319:TRP:CE2	2.49	0.48
2:A:219:LYS:HG2	2:A:256:ASP:HB2	1.98	0.46
2:A:324:ARG:HG2	3:A:552:HOH:O	2.16	0.45
2:A:138:GLU:O	2:A:139:THR:HG22	2.16	0.45
2:A:291:ARG:CZ	2:A:324:ARG:HH22	2.31	0.43
2:A:284:ASP:HB2	3:A:462:HOH:O	2.18	0.43
2:A:284:ASP:OD1	2:A:287:ALA:CA	2.65	0.43
2:A:108:SER:N	2:A:138:GLU:HG2	2.34	0.42
3:B:1110:HOH:O	2:A:320:ARG:CD	2.51	0.41
2:A:320:ARG:HG2	3:A:479:HOH:O	2.13	0.41
2:A:315:ARG:NH1	3:A:567:HOH:O	2.13	0.41
2:A:291:ARG:HD3	2:A:324:ARG:HH12	1.76	0.41
2:A:138:GLU:C	2:A:139:THR:CG2	2.89	0.41
2:A:288:ARG:HD2	2:A:319:TRP:CD1	2.56	0.41

All (4) 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)
3:A:442:HOH:O	3:A:442:HOH:O[5_756]	1.87	0.33
2:A:175:ARG:NH2	3:A:426:HOH:O[7_645]	1.91	0.29
3:B:1085:HOH:O	3:A:482:HOH:O[7_555]	2.09	0.11
2:A:199:GLU:CD	3:A:540:HOH:O[6_565]	2.16	0.04

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
2	A	224/251 (89%)	211 (94%)	10 (4%)	3 (1%)	15 2

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	138	GLU
2	A	141	ALA
2	A	136	GLY

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
2	A	178/199 (89%)	169 (95%)	9 (5%)	29 5

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	120	GLN
2	A	121	ARG
2	A	140	LYS
2	A	175	ARG
2	A	176	GLU
2	A	206	GLU
2	A	239	MET
2	A	276	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	284	ASP

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

Mol	Chain	Res	Type
2	A	159	HIS
2	A	161	ASN
2	A	185	HIS
2	A	187	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	10/11 (90%)	3 (30%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	7	A
1	B	8	A
1	B	10	A

There are no RNA pucker outliers to report.

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

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	B	11/11 (100%)	-0.25	0 100 100	18, 20, 25, 28	0
2	A	226/251 (90%)	1.12	33 (14%) 3 3	11, 19, 49, 66	0
All	All	237/262 (90%)	1.06	33 (13%) 4 4	11, 19, 49, 66	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	174	ALA	17.2
2	A	139	THR	15.6
2	A	137	THR	14.8
2	A	136	GLY	13.5
2	A	173	GLY	12.3
2	A	140	LYS	10.9
2	A	175	ARG	8.9
2	A	138	GLU	8.6
2	A	108	SER	8.0
2	A	286	THR	7.6
2	A	172	ARG	7.0
2	A	176	GLU	6.7
2	A	141	ALA	6.5
2	A	283	ILE	6.3
2	A	171	THR	5.4
2	A	333	GLY	4.4
2	A	123	SER	3.8
2	A	284	ASP	3.7
2	A	285	GLN	3.6
2	A	121	ARG	3.4
2	A	110	ARG	3.4
2	A	177	PRO	3.3
2	A	127	ALA	3.2
2	A	178	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	287	ALA	3.2
2	A	120	GLN	3.2
2	A	320	ARG	2.9
2	A	109	THR	2.9
2	A	134	ARG	2.5
2	A	128	ARG	2.4
2	A	158	GLU	2.3
2	A	170	VAL	2.1
2	A	129	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.