



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 10:34 pm GMT

PDB ID : 4KBJ
Title : Structure of Mtb RNAP Beta subunit B1 and B2 domains
Authors : Gulten, G.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2013-04-23
Resolution : 2.45 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
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

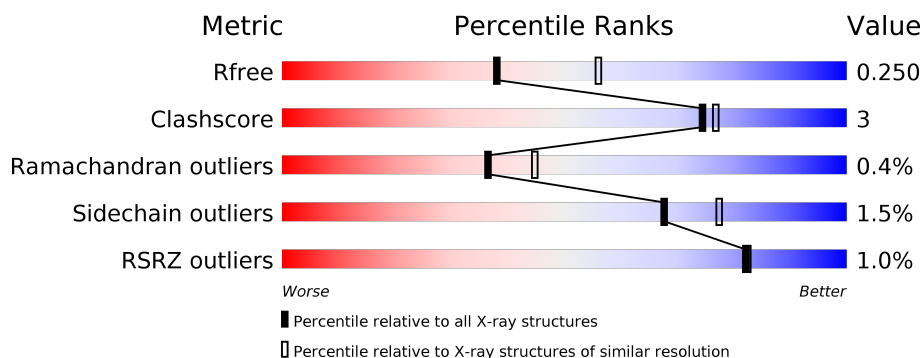
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	111664	1259 (2.48-2.44)
Clashscore	122126	1323 (2.48-2.44)
Ramachandran outliers	120053	1314 (2.48-2.44)
Sidechain outliers	120020	1314 (2.48-2.44)
RSRZ outliers	108989	1238 (2.48-2.44)

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 $\leq 5\%$. 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	409	
1	B	409	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6225 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 DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3044	1915	527	589	13			
1	B	386	Total	C	N	O	S	0	0	0
			3053	1920	530	590	13			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP P0A680
A	-20	GLY	-	EXPRESSION TAG	UNP P0A680
A	-19	SER	-	EXPRESSION TAG	UNP P0A680
A	-18	SER	-	EXPRESSION TAG	UNP P0A680
A	-17	HIS	-	EXPRESSION TAG	UNP P0A680
A	-16	HIS	-	EXPRESSION TAG	UNP P0A680
A	-15	HIS	-	EXPRESSION TAG	UNP P0A680
A	-14	HIS	-	EXPRESSION TAG	UNP P0A680
A	-13	HIS	-	EXPRESSION TAG	UNP P0A680
A	-12	HIS	-	EXPRESSION TAG	UNP P0A680
A	-11	SER	-	EXPRESSION TAG	UNP P0A680
A	-10	SER	-	EXPRESSION TAG	UNP P0A680
A	-9	GLY	-	EXPRESSION TAG	UNP P0A680
A	-8	LEU	-	EXPRESSION TAG	UNP P0A680
A	-7	VAL	-	EXPRESSION TAG	UNP P0A680
A	-6	PRO	-	EXPRESSION TAG	UNP P0A680
A	-5	ARG	-	EXPRESSION TAG	UNP P0A680
A	-4	GLY	-	EXPRESSION TAG	UNP P0A680
A	-3	SER	-	EXPRESSION TAG	UNP P0A680
A	-2	HIS	-	EXPRESSION TAG	UNP P0A680
A	-1	MET	-	EXPRESSION TAG	UNP P0A680
A	0	MET	-	EXPRESSION TAG	UNP P0A680
B	-21	MET	-	EXPRESSION TAG	UNP P0A680
B	-20	GLY	-	EXPRESSION TAG	UNP P0A680
B	-19	SER	-	EXPRESSION TAG	UNP P0A680

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	SER	-	EXPRESSION TAG	UNP P0A680
B	-17	HIS	-	EXPRESSION TAG	UNP P0A680
B	-16	HIS	-	EXPRESSION TAG	UNP P0A680
B	-15	HIS	-	EXPRESSION TAG	UNP P0A680
B	-14	HIS	-	EXPRESSION TAG	UNP P0A680
B	-13	HIS	-	EXPRESSION TAG	UNP P0A680
B	-12	HIS	-	EXPRESSION TAG	UNP P0A680
B	-11	SER	-	EXPRESSION TAG	UNP P0A680
B	-10	SER	-	EXPRESSION TAG	UNP P0A680
B	-9	GLY	-	EXPRESSION TAG	UNP P0A680
B	-8	LEU	-	EXPRESSION TAG	UNP P0A680
B	-7	VAL	-	EXPRESSION TAG	UNP P0A680
B	-6	PRO	-	EXPRESSION TAG	UNP P0A680
B	-5	ARG	-	EXPRESSION TAG	UNP P0A680
B	-4	GLY	-	EXPRESSION TAG	UNP P0A680
B	-3	SER	-	EXPRESSION TAG	UNP P0A680
B	-2	HIS	-	EXPRESSION TAG	UNP P0A680
B	-1	MET	-	EXPRESSION TAG	UNP P0A680
B	0	MET	-	EXPRESSION TAG	UNP P0A680

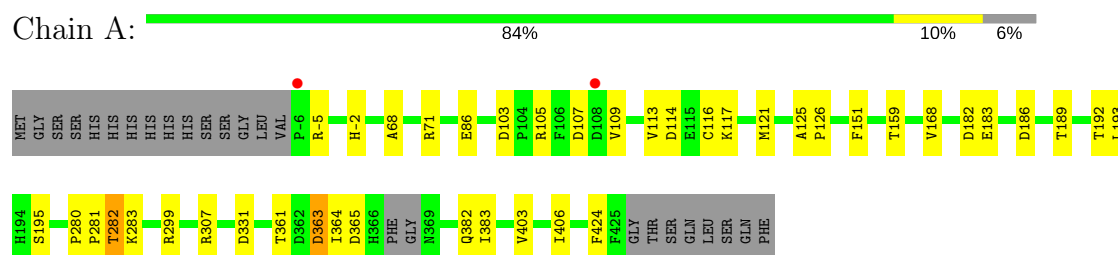
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	64	Total O 64 64	0	0
2	B	64	Total O 64 64	0	0

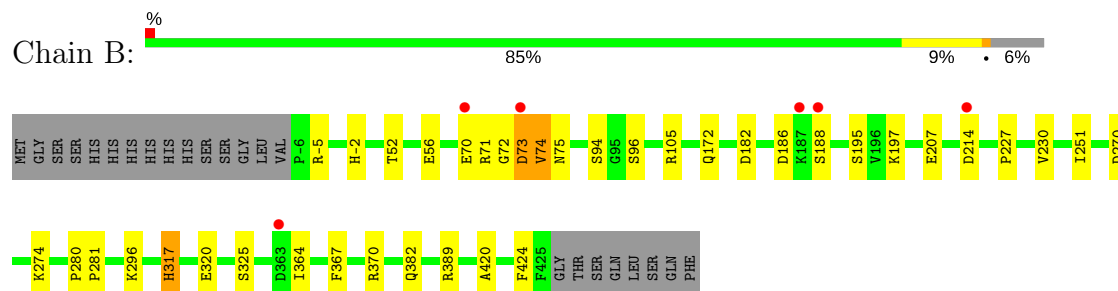
3 Residue-property plots [i](#)

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: DNA-directed RNA polymerase subunit beta



- Molecule 1: DNA-directed RNA polymerase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.18Å 123.91Å 135.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 2.45 49.51 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.51-2.45) 99.7 (49.51-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.214 , 0.263 0.205 , 0.250	Depositor DCC
R_{free} test set	1702 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6225	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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](#)

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	0.23	0/3097	0.41	0/4189
1	B	0.23	0/3107	0.42	0/4204
All	All	0.23	0/6204	0.42	0/8393

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	3044	0	3041	22	0
1	B	3053	0	3049	23	0
2	A	64	0	0	0	0
2	B	64	0	0	1	0
All	All	6225	0	6090	42	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 3.

All (42) 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:-2:HIS:HE1	1:B:-5:ARG:H	1.29	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASP:O	1:A:365:ASP:N	2.34	0.61
1:B:94:SER:HB2	1:B:96:SER:H	1.69	0.58
1:A:159:THR:HG22	1:A:168:VAL:HG22	1.86	0.56
1:B:227:PRO:HG2	1:B:230:VAL:HG23	1.88	0.56
1:B:-5:ARG:NH2	1:B:172:GLN:OE1	2.38	0.56
1:A:-2:HIS:CE1	1:B:-5:ARG:H	2.19	0.55
1:B:70:GLU:HG3	1:B:71:ARG:H	1.71	0.55
1:A:114:ASP:OD1	1:A:114:ASP:N	2.41	0.54
1:B:182:ASP:OD1	1:B:195:SER:OG	2.20	0.54
1:A:86:GLU:O	1:A:299:ARG:NH1	2.40	0.50
1:A:282:THR:OG1	1:A:283:LYS:N	2.48	0.47
1:B:186:ASP:OD2	1:B:188:SER:OG	2.31	0.47
1:A:107:ASP:HB2	1:A:126:PRO:HG2	1.98	0.46
1:B:270:ASP:OD1	1:B:274:LYS:NZ	2.49	0.46
1:A:116:CYS:HA	1:A:121:MET:HB3	1.98	0.45
1:A:151:PHE:HE2	1:A:383:ILE:HD11	1.81	0.45
1:A:307:ARG:HH22	1:A:331:ASP:CG	2.20	0.45
1:B:74:VAL:HG22	1:B:75:ASN:H	1.81	0.45
1:A:403:VAL:HA	1:A:406:ILE:HD12	1.99	0.45
1:A:109:VAL:HG12	1:A:125:ALA:HB2	1.98	0.44
1:A:-5:ARG:H	1:B:-2:HIS:HE1	1.63	0.44
1:A:68:ALA:HA	1:A:71:ARG:HG2	1.98	0.44
1:B:296:LYS:HD3	1:B:296:LYS:HA	1.83	0.44
1:B:280:PRO:HA	1:B:281:PRO:HD3	1.78	0.43
1:B:317:HIS:HB3	1:B:320:GLU:HB2	2.01	0.43
1:B:389:ARG:NH1	2:B:528:HOH:O	2.51	0.43
1:A:382:GLN:HG3	1:A:424:PHE:CD1	2.54	0.42
1:B:70:GLU:HG3	1:B:71:ARG:N	2.35	0.42
1:B:214:ASP:HB3	1:B:251:ILE:HG22	2.01	0.42
1:A:182:ASP:OD1	1:A:195:SER:OG	2.30	0.42
1:B:197:LYS:HG2	1:B:207:GLU:HG2	2.01	0.42
1:A:186:ASP:HB2	1:A:193:LEU:HD11	2.01	0.41
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.80	0.41
1:B:52:THR:O	1:B:56:GLU:HG2	2.19	0.41
1:B:382:GLN:NE2	1:B:420:ALA:O	2.52	0.41
1:A:113:VAL:HG12	1:A:117:LYS:HE3	2.03	0.41
1:B:382:GLN:HG3	1:B:424:PHE:HD1	1.85	0.41
1:B:72:GLY:HA2	1:B:73:ASP:HA	1.73	0.41
1:A:183:GLU:HB2	1:A:361:THR:HG21	2.03	0.40
1:A:103:ASP:OD1	1:A:105:ARG:NH1	2.55	0.40
1:B:270:ASP:O	1:B:274:LYS:HG2	2.22	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	380/409 (93%)	371 (98%)	8 (2%)	1 (0%)	43	52
1	B	384/409 (94%)	369 (96%)	13 (3%)	2 (0%)	31	37
All	All	764/818 (93%)	740 (97%)	21 (3%)	3 (0%)	36	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ILE
1	B	367	PHE
1	B	364	ILE

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	340/365 (93%)	336 (99%)	4 (1%)	74	82
1	B	340/365 (93%)	334 (98%)	6 (2%)	62	74
All	All	680/730 (93%)	670 (98%)	10 (2%)	67	77

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	THR
1	A	192	THR
1	A	282	THR
1	A	363	ASP
1	B	73	ASP
1	B	74	VAL
1	B	105	ARG
1	B	317	HIS
1	B	325	SER
1	B	370	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	B	-2	HIS

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

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, 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	384/409 (93%)	-0.20	2 (0%) 90 92	32, 50, 81, 100	0
1	B	386/409 (94%)	-0.18	6 (1%) 72 69	36, 52, 90, 113	0
All	All	770/818 (94%)	-0.19	8 (1%) 82 82	32, 51, 83, 113	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	LYS	4.8
1	B	70	GLU	2.7
1	B	363	ASP	2.7
1	A	-6	PRO	2.5
1	B	188	SER	2.3
1	A	108	ASP	2.3
1	B	73	ASP	2.1
1	B	214	ASP	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 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.