



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 12, 2018 – 06:39 AM EDT

PDB ID : 3J4T
EMDB ID: : EMD-5763
Title : Helical model of TubZ-Bt two-stranded filament
Authors : Agard, D.A.; Montabana, E.A.
Deposited on : 2013-10-04
Resolution : 10.80 Å(reported)
Based on PDB ID : 2XKA

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

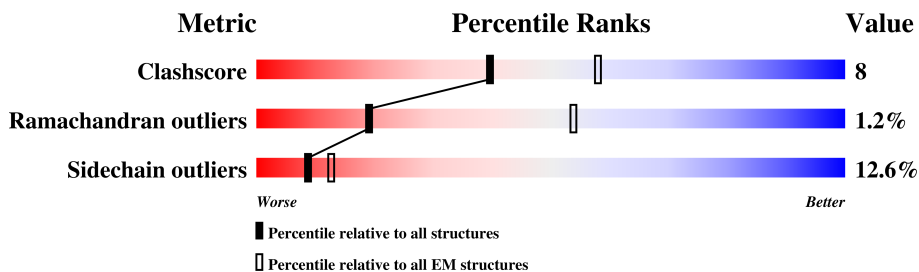
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.80 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	F	490	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3274 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 FtsZ/tubulin-related protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	414	Total	C	N	O	S	0	0
			3274	2060	561	640	13		

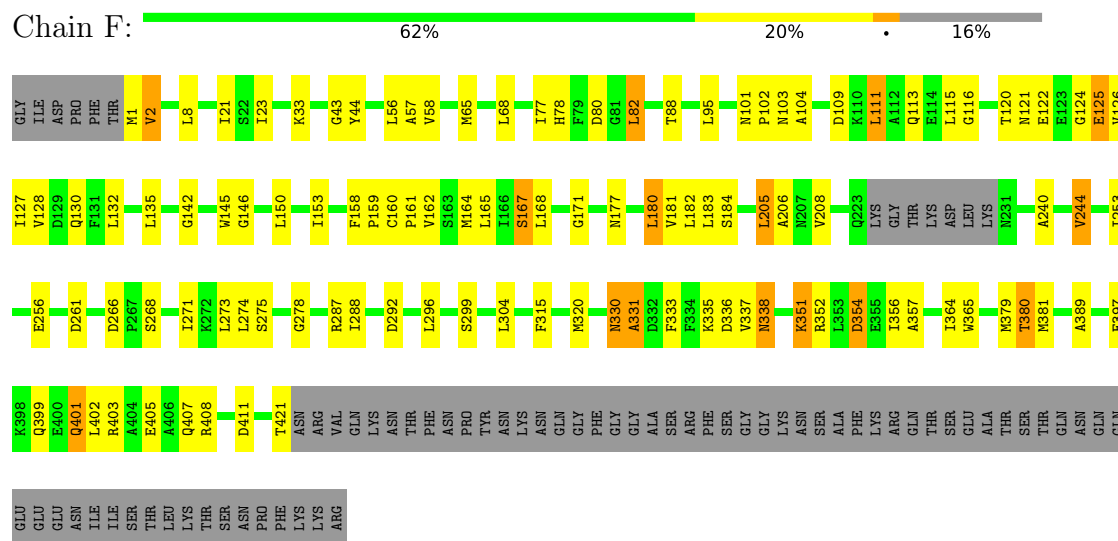
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	GLY	-	EXPRESSION TAG	UNP Q8KNP3
F	-4	ILE	-	EXPRESSION TAG	UNP Q8KNP3
F	-3	ASP	-	EXPRESSION TAG	UNP Q8KNP3
F	-2	PRO	-	EXPRESSION TAG	UNP Q8KNP3
F	-1	PHE	-	EXPRESSION TAG	UNP Q8KNP3
F	0	THR	-	EXPRESSION TAG	UNP Q8KNP3
F	2	VAL	LEU	SEE REMARK 999	UNP Q8KNP3

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. 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. 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: FtsZ/tubulin-related protein



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-168.15849°, rise=22.04811 Å, axial sym=C1	Depositor
Number of segments used	Not provided	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Whole Micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	62000	Depositor
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	F	0.60	1/3336 (0.0%)	0.68	0/4510

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	125	GLU	CG-CD	5.01	1.59	1.51

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	F	3274	0	3187	54	0
All	All	3274	0	3187	54	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 (54) 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:F:23:ILE:HD12	1:F:274:LEU:HD12	1.60	0.84
1:F:116:GLY:O	1:F:120:THR:OG1	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:ILE:HD13	1:F:296:LEU:HD12	1.70	0.73
1:F:183:LEU:HD22	1:F:381:MET:HE3	1.74	0.68
1:F:288:ILE:CD1	1:F:296:LEU:HD12	2.26	0.65
1:F:177:ASN:O	1:F:181:VAL:HG13	1.99	0.63
1:F:122:GLU:OE2	1:F:122:GLU:HA	2.01	0.60
1:F:23:ILE:CD1	1:F:274:LEU:HD12	2.30	0.60
1:F:56:LEU:HD22	1:F:77:ILE:CD1	2.32	0.59
1:F:56:LEU:HD22	1:F:77:ILE:HD11	1.84	0.59
1:F:153:ILE:HG22	1:F:158:PHE:CD1	2.39	0.57
1:F:21:ILE:HG22	1:F:253:ILE:HD13	1.87	0.57
1:F:401:GLN:HG2	1:F:402:LEU:N	2.20	0.57
1:F:160:CYS:HB2	1:F:161:PRO:CD	2.39	0.53
1:F:336:ASP:OD1	1:F:338:ASN:HB2	2.09	0.52
1:F:315:PHE:HA	1:F:379:MET:HE3	1.92	0.51
1:F:330:ASN:CG	1:F:331:ALA:N	2.64	0.51
1:F:380:THR:HG23	1:F:381:MET:N	2.25	0.51
1:F:2:VAL:HG22	1:F:43:GLY:HA3	1.94	0.50
1:F:261:ASP:OD2	1:F:364:ILE:HD11	2.11	0.50
1:F:135:LEU:HD22	1:F:142:GLY:O	2.11	0.50
1:F:2:VAL:HG23	1:F:44:TYR:CD1	2.46	0.49
1:F:121:ASN:HB2	1:F:125:GLU:O	2.13	0.48
1:F:315:PHE:CD2	1:F:379:MET:CE	2.96	0.48
1:F:320:MET:HG3	1:F:357:ALA:O	2.13	0.48
1:F:402:LEU:HA	1:F:405:GLU:HB2	1.95	0.48
1:F:33:LYS:HE3	1:F:167:SER:CB	2.44	0.47
1:F:57:ALA:O	1:F:65:MET:HE1	2.14	0.47
1:F:160:CYS:HB2	1:F:161:PRO:HD2	1.97	0.47
1:F:33:LYS:HE3	1:F:167:SER:HB3	1.97	0.47
1:F:168:LEU:HD21	1:F:183:LEU:HD11	1.98	0.46
1:F:101:ASN:O	1:F:104:ALA:HB2	2.16	0.46
1:F:271:ILE:O	1:F:275:SER:OG	2.23	0.46
1:F:315:PHE:HA	1:F:379:MET:CE	2.45	0.46
1:F:183:LEU:HD13	1:F:381:MET:HE1	1.98	0.46
1:F:162:VAL:O	1:F:205:LEU:HD23	2.15	0.45
1:F:351:LYS:HD2	1:F:356:ILE:HD13	1.99	0.45
1:F:126:VAL:HG21	1:F:159:PRO:CB	2.47	0.45
1:F:109:ASP:O	1:F:113:GLN:HB2	2.18	0.44
1:F:183:LEU:HD22	1:F:381:MET:CE	2.47	0.44
1:F:101:ASN:HA	1:F:102:PRO:HD3	1.87	0.43
1:F:121:ASN:HB3	1:F:124:GLY:H	1.84	0.43
1:F:180:LEU:HD21	1:F:389:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:VAL:HG11	1:F:145:TRP:CH2	2.54	0.43
1:F:240:ALA:O	1:F:244:VAL:HG13	2.19	0.42
1:F:82:LEU:HD21	1:F:95:LEU:CD1	2.49	0.42
1:F:352:ARG:NH2	1:F:354:ASP:OD1	2.51	0.42
1:F:111:LEU:HA	1:F:111:LEU:HD23	1.83	0.42
1:F:82:LEU:HD13	1:F:82:LEU:HA	1.95	0.41
1:F:153:ILE:HG22	1:F:158:PHE:HD1	1.82	0.41
1:F:164:MET:HB2	1:F:208:VAL:HG22	2.03	0.41
1:F:146:GLY:HA2	1:F:164:MET:HE1	2.02	0.41
1:F:183:LEU:HB3	1:F:381:MET:HE1	2.03	0.41
1:F:206:ALA:O	1:F:278:GLY:HA2	2.21	0.41

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 PDB entries followed by that with respect to all EM entries.

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	F	410/490 (84%)	382 (93%)	23 (6%)	5 (1%)	14 56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	338	ASN
1	F	331	ALA
1	F	333	PHE
1	F	127	ILE
1	F	171	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 PDB entries followed by that with respect to all EM entries.

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	F	357/423 (84%)	312 (87%)	45 (13%)	5 23

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1	MET
1	F	2	VAL
1	F	8	LEU
1	F	68	LEU
1	F	78	HIS
1	F	80	ASP
1	F	82	LEU
1	F	88	THR
1	F	103	ASN
1	F	111	LEU
1	F	115	LEU
1	F	128	VAL
1	F	130	GLN
1	F	132	LEU
1	F	150	LEU
1	F	165	LEU
1	F	167	SER
1	F	180	LEU
1	F	182	LEU
1	F	184	SER
1	F	205	LEU
1	F	244	VAL
1	F	256	GLU
1	F	266	ASP
1	F	268	SER
1	F	273	LEU
1	F	287	ARG
1	F	292	ASP
1	F	299	SER
1	F	304	LEU

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Mol	Chain	Res	Type
1	F	330	ASN
1	F	335	LYS
1	F	337	VAL
1	F	351	LYS
1	F	354	ASP
1	F	365	TRP
1	F	380	THR
1	F	397	GLU
1	F	399	GLN
1	F	401	GLN
1	F	403	ARG
1	F	407	GLN
1	F	408	ARG
1	F	411	ASP
1	F	421	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.