wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 1, 2017 – 05:26 PM EDT

PDB ID : 5W3F
EMDB ID: : EMD-8755
Title : Yeast tubulin polymerized with GTP in vitro
Authors : Howes, S.C.; Geyer, E.A.; LaFrance, B.; Zhang, R.; Kellogg, E.H.; Westermann, S.; Rice, L.M.; Nogales, E.
Deposited on : unknown
Resolution : 3.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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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 3.70 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.
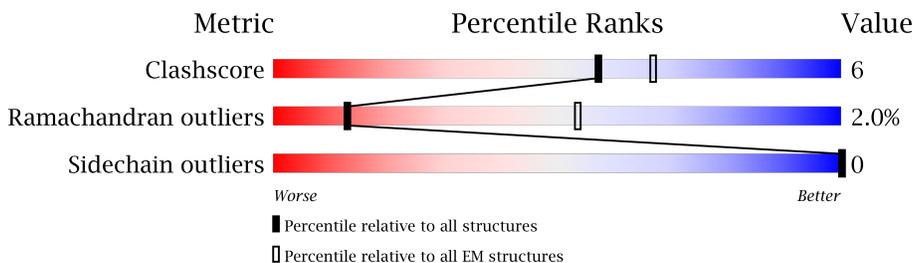
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	447	84% 13% ··
2	B	457	84% 9% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GTP	A	502	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13367 atoms, of which 6525 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 Tubulin alpha-1 chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	440	6766	2167	3328	585	667	19	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	427	6540	2098	3197	571	653	21	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	A	1	1	1	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	32	10	5	14	3	0

- Molecule 5 is G U A N O S I N E - 5 ' - D I P H O S P H A T E (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	B	1	28	10	5	11	2	0
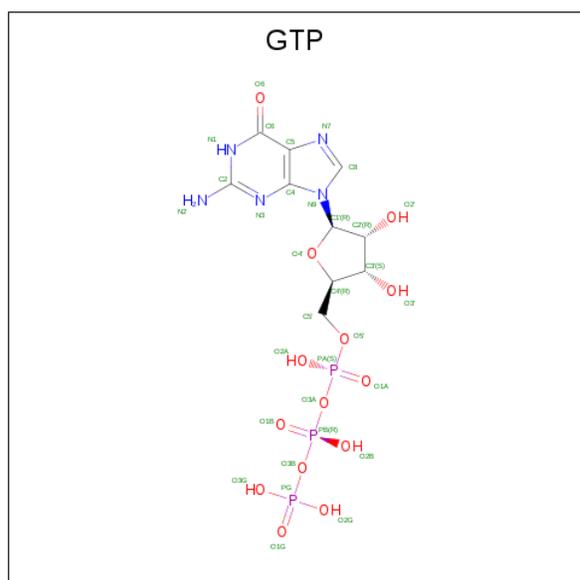
3 Residue-property plots ⓘ

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: Tubulin alpha-1 chain
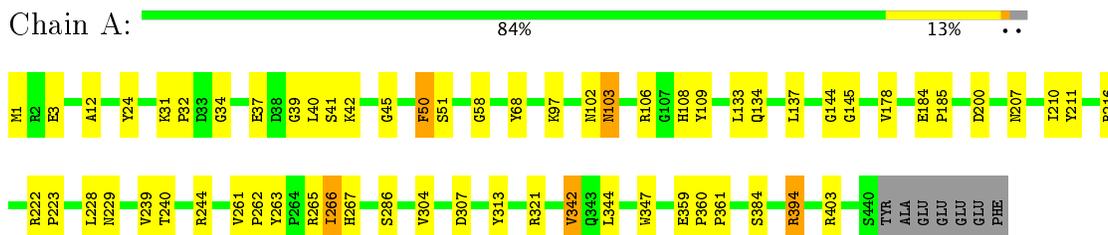
Chain A:

• Molecule 2: Tubulin beta chain

Chain B:
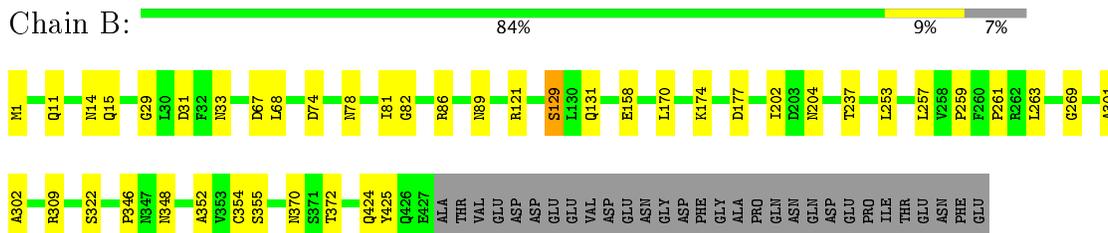
4   Experimental information ⓘ

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-29.85°, rise=10.4 Å, axial sym=C1	Depositor
Number of segments used	42871	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	28	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: GDP, GTP, MG

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	A	0.88	0/3514	1.22	25/4766 (0.5%)
2	B	0.23	0/3416	0.38	0/4627
All	All	0.65	0/6930	0.91	25/9393 (0.3%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	222	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	A	106	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	A	58	GLY	C-N-CA	10.11	146.97	121.70
1	A	244	ARG	NE-CZ-NH2	9.81	125.20	120.30
1	A	384	SER	C-N-CA	9.63	145.76	121.70

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	3438	3328	3337	51	0
2	B	3343	3197	3208	28	0
3	A	1	0	0	0	0
4	A	32	0	12	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	28	0	12	7	0
All	All	6842	6525	6569	78	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 6.

The worst 5 of 78 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:B:204:ASN:ND2	5:B:600:GDP:O2'	1.86	1.06
1:A:1:MET:CE	1:A:134:GLN:HG2	2.00	0.91
1:A:102:ASN:HA	1:A:103:ASN:HB2	1.53	0.91
1:A:1:MET:HE2	1:A:134:GLN:HG2	1.56	0.86
1:A:228:LEU:CD2	4:A:502:GTP:N2	2.41	0.83

There are no symmetry-related clashes.

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 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	A	438/447 (98%)	401 (92%)	29 (7%)	8 (2%)	10	52
2	B	425/457 (93%)	365 (86%)	51 (12%)	9 (2%)	8	49
All	All	863/904 (96%)	766 (89%)	80 (9%)	17 (2%)	13	50

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	103	ASN
1	A	240	THR

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Mol	Chain	Res	Type
1	A	266	ILE
2	B	237	THR

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 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	A	375/381 (98%)	375 (100%)	0	100	100
2	B	366/392 (93%)	366 (100%)	0	100	100
All	All	741/773 (96%)	741 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
2	B	348	ASN
2	B	370	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)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\#|Z| > 2$
4	GTP	A	502	3	27,34,34	1.50	2 (7%)	27,54,54	2.16	5 (18%)
5	GDP	B	600	-	25,30,30	2.62	8 (32%)	26,47,47	3.64	9 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	502	3	-	0/18/38/38	0/3/3/3
5	GDP	B	600	-	-	0/12/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	600	GDP	PB-O2B	-3.53	1.40	1.54
5	B	600	GDP	O3'-C3'	2.15	1.47	1.43
5	B	600	GDP	PB-O3B	2.22	1.64	1.54
5	B	600	GDP	C5-C4	2.42	1.46	1.40
5	B	600	GDP	C8-N7	3.40	1.41	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	600	GDP	C6-C5-C4	-11.33	109.58	120.84
4	A	502	GTP	C5-C6-N1	-7.13	113.34	123.48
5	B	600	GDP	N2-C2-N1	-5.92	107.77	117.24
5	B	600	GDP	C4-C5-N7	-5.06	104.52	109.41
5	B	600	GDP	N3-C2-N1	-4.97	120.20	127.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	GTP	12	0
5	B	600	GDP	7	0

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.