



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:52 PM BST

PDB ID : 3JAO  
EMDB ID: : EMD-6312  
Title : Ciliary microtubule doublet  
Authors : Maheshwari, A.; Obbineni, J.M.; Bui, K.H.; Shibata, K.; Toyoshima, Y.Y.;  
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Deposited on : 2015-06-18  
Resolution : 23.00 Å(reported)  
Based on PDB ID : 3J6E

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

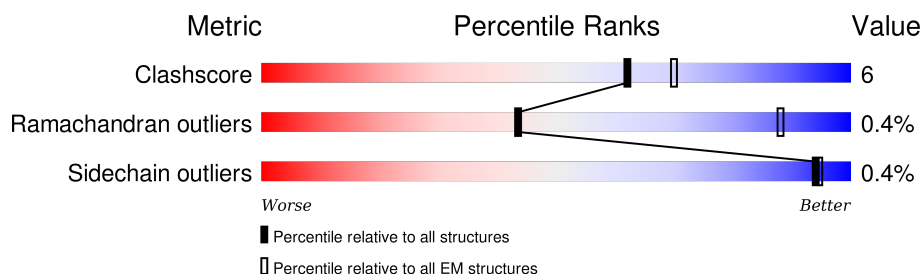
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 23.00 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	A	451	 79% 14% • 5%
2	B	445	 77% 17% • •

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6774 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.

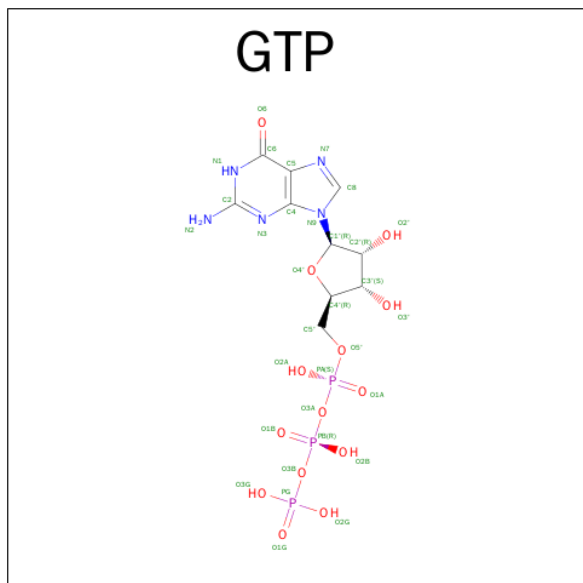
- Molecule 1 is a protein called Tubulin alpha 1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	428	3349	2121	570	637	21	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	426	3351	2105	575	646	25	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

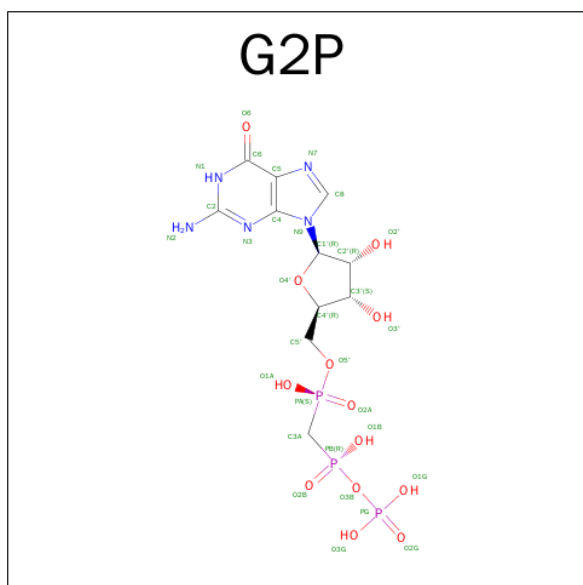


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	32	10	5	14	3	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	

- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			32	11	5	13	3	

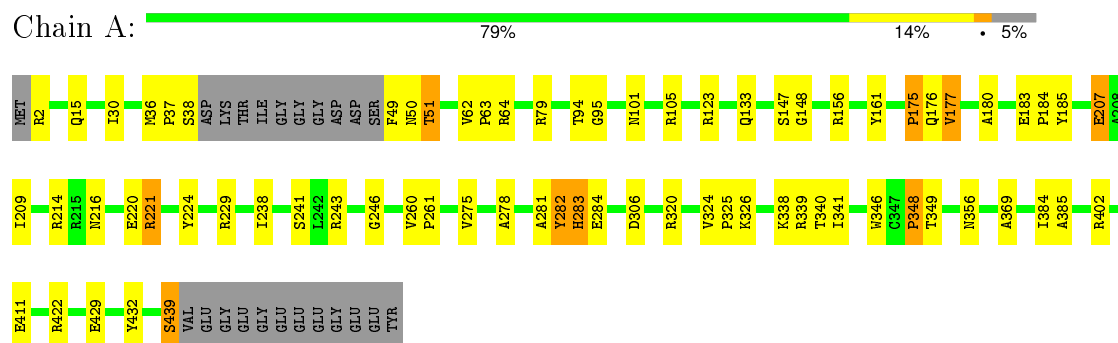
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	4	Total	O	0
			4	4	
6	B	4	Total	O	0
			4	4	

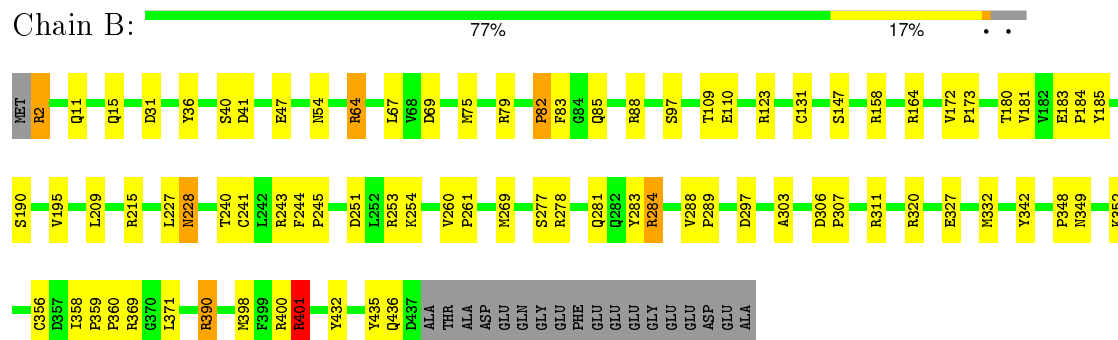
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 1A chain



#### • Molecule 2: Tubulin beta chain



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	10700	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	67000	Depositor
Image detector	CCD	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: GTP, MG, G2P

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	1.13	15/3426 (0.4%)	1.42	37/4651 (0.8%)
2	B	0.94	1/3426 (0.0%)	1.45	44/4642 (0.9%)
All	All	1.04	16/6852 (0.2%)	1.44	81/9293 (0.9%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	ASN	N-CA	-10.24	1.25	1.46
1	A	349	THR	CA-C	-8.04	1.32	1.52
1	A	340	THR	N-CA	-7.79	1.30	1.46
1	A	37	PRO	N-CA	-6.96	1.35	1.47
1	A	339	ARG	CA-C	-6.60	1.35	1.52

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	88	ARG	NE-CZ-NH1	18.64	129.62	120.30
2	B	401	ARG	NE-CZ-NH1	16.80	128.70	120.30
1	A	105	ARG	NE-CZ-NH2	-14.72	112.94	120.30
2	B	401	ARG	NE-CZ-NH2	-14.23	113.18	120.30
2	B	253	ARG	NE-CZ-NH1	14.01	127.31	120.30

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	3349	0	3254	34	0
2	B	3351	0	3229	41	0
3	A	32	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	32	0	13	4	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
All	All	6774	0	6508	73	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 73 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:228:ASN:HD21	5:B:501:G2P:H1	1.13	0.97
1:A:341:ILE:HG13	1:A:341:ILE:O	1.67	0.92
2:B:401:ARG:HD3	2:B:401:ARG:N	2.07	0.69
1:A:439:SER:O	1:A:439:SER:OG	2.05	0.66
1:A:177:VAL:HG23	1:A:207:GLU:OE1	1.95	0.66

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	424/451 (94%)	405 (96%)	18 (4%)	1 (0%)	52	86
2	B	424/445 (95%)	411 (97%)	11 (3%)	2 (0%)	34	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	848/896 (95%)	816 (96%)	29 (3%)	3 (0%)	43 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	PRO
2	B	97	SER
2	B	47	GLU

### 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	A	360/377 (96%)	359 (100%)	1 (0%)	94 96
2	B	367/381 (96%)	365 (100%)	2 (0%)	92 96
All	All	727/758 (96%)	724 (100%)	3 (0%)	94 96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
2	B	352	LYS
2	B	401	ARG

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

Mol	Chain	Res	Type
1	A	31	GLN
2	B	8	GLN
2	B	192	HIS

### 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 ⓘ

Of 4 ligands modelled in this entry, 2 are 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	$\# Z  > 2$
3	GTP	A	501	4	26,34,34	1.37	3 (11%)	29,54,54	2.33	5 (17%)
5	G2P	B	501	4	29,34,34	5.92	25 (86%)	32,54,54	4.83	20 (62%)

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
3	GTP	A	501	4	-	0/18/38/38	0/3/3/3
5	G2P	B	501	4	-	0/15/38/38	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	G2P	PB-C3A	-19.24	1.60	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	G2P	PA-O1A	-6.24	1.41	1.56
5	B	501	G2P	O2'-C2'	-6.12	1.28	1.43
5	B	501	G2P	C8-N7	-5.01	1.25	1.34
5	B	501	G2P	PA-C3A	-4.81	1.75	1.80

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	G2P	N3-C2-N1	-11.04	112.54	127.56
3	A	501	GTP	C5-C6-N1	-7.73	113.41	123.52
5	B	501	G2P	O4'-C4'-C3'	-7.61	89.73	105.16
5	B	501	G2P	C1'-N9-C4	-6.16	119.93	126.81
5	B	501	G2P	C5-C6-N1	-5.56	116.25	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	G2P	4	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.