



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 17, 2017 – 07:21 PM EDT

PDB ID : 5UCY  
EMDB ID: : EMD-8539  
Title : Cryo-EM map of protofilament of microtubule doublet  
Authors : Ichikawa, M.; Liu, D.; Kastiris, P.L.; Basu, K.; Bui, K.H.  
Deposited on : unknown  
Resolution : 4.60 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](mailto: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.

---

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

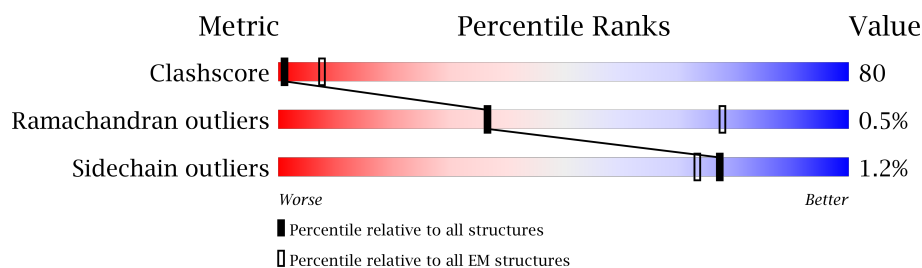
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.60 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  $\geq 3$ , 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	441	
2	B	429	

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
3	GTP	A	501	-	-	X	-
5	GDP	B	501	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8338 atoms, of which 1492 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.

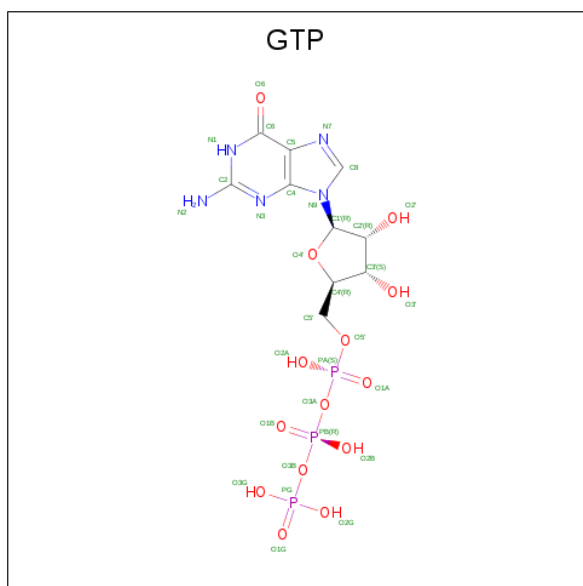
- Molecule 1 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	441	Total	C	H	N	O	S	0	0
			4165	2163	742	581	657	22		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	429	Total	C	H	N	O	S	0	0
			4104	2112	742	576	646	28		

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

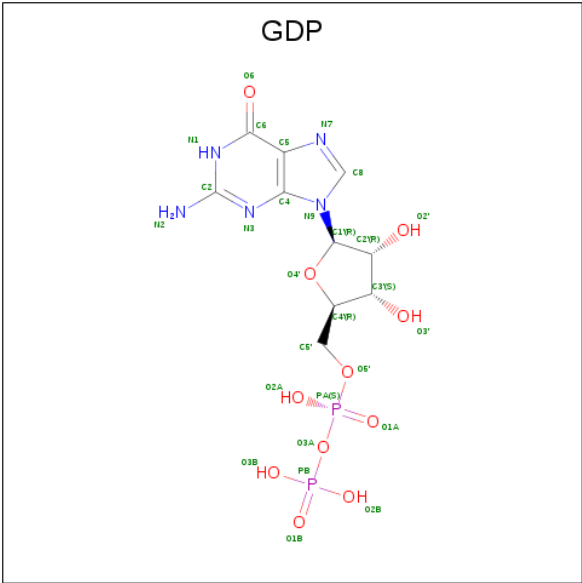


Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			35	10	3	5	14	3	

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

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

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).

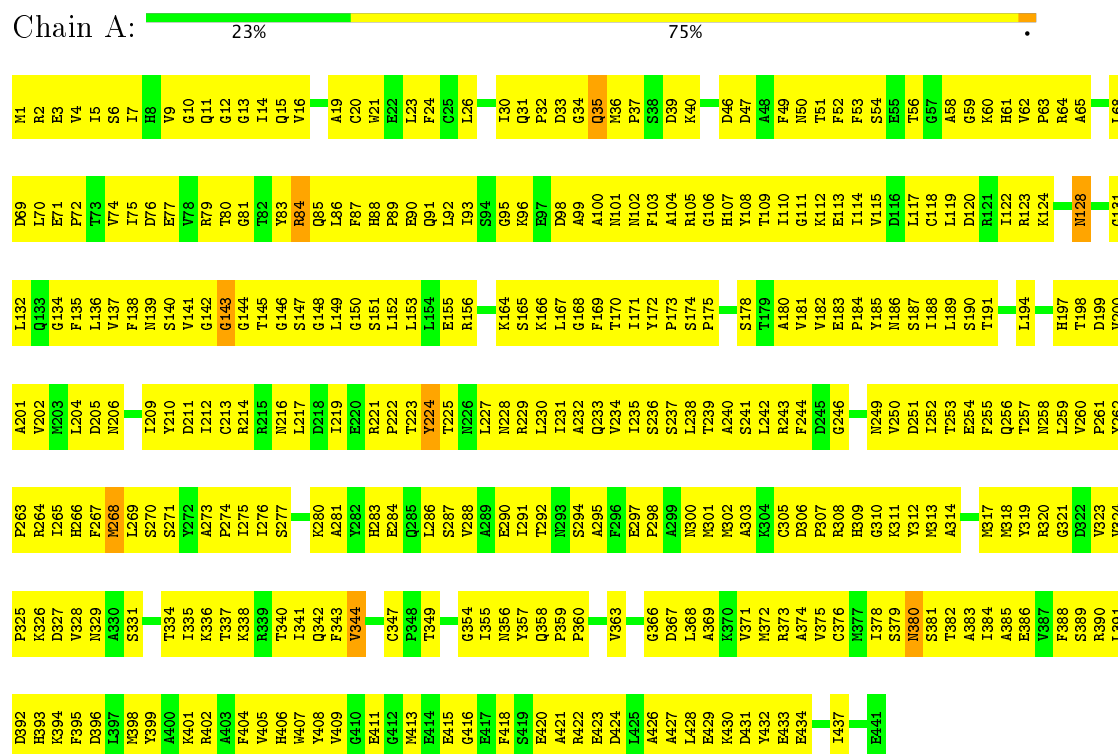


Mol	Chain	Residues	Atoms						AltConf
5	B	1	Total	C	H	N	O	P	0
			33	10	5	5	11	2	

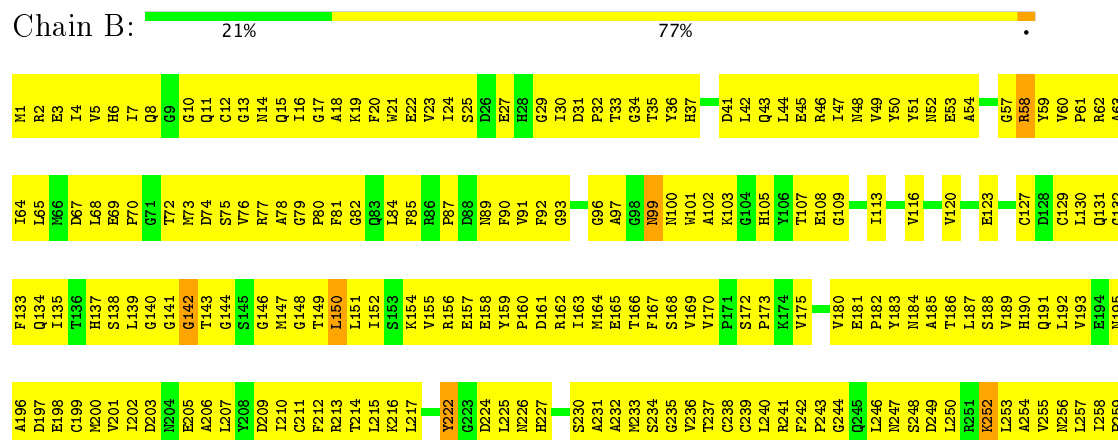
### 3 Residue-property plots

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 chain



#### • Molecule 2: Tubulin beta chain



F260	S322	F385
F261	I323	T386
R262	K324	A387
L263	E325	K388
R264	V326	F389
F265	D327	R390
F266	E328	R391
R267	Q329	K392
L268	M330	A393
G269	L331	F394
F270	N332	L395
A271	V333	
P272	Q334	Y398
L273	N335	T399
T274	K336	G400
S275	N337	E401
R276	S338	G402
G277	S339	N403
S278	Y340	D404
Q279	F341	E405
Q280	V342	M406
Y281	E343	E407
R282	M344	F408
A283	I345	T409
L284	P346	E410
T285	N347	A411
V286	N348	E412
P287	I349	S413
E288	K350	M414
L289	S351	N415
T290	S352	
Q291	I353	L418
Q292	C354	V419
M293	D355	S420
F294	I356	E421
D295	P357	Y422
A296	P358	
I297		Q426
N298	K362	
M299	M363	T429
N300	A364	
C301	V365	
A302	T366	
A303	F367	
D304	V368	
P305	G369	
R306	N370	
	S371	
	T372	
	A373	
	I374	
	Q375	
	E376	
	M377	
	F378	
	K379	
	L316	
	F317	
	R318	
	V381	
	A382	

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (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	0.58	1/3495 (0.0%)	0.61	0/4735
2	B	0.55	0/3435	0.66	3/4648 (0.1%)
All	All	0.57	1/6930 (0.0%)	0.64	3/9383 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	GLN	C-N	-8.21	1.15	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	252	LYS	CD-CE-NZ	8.19	130.54	111.70
2	B	150	LEU	CA-CB-CG	-5.54	102.55	115.30
2	B	58	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLY	Peptide
2	B	99	ASN	Peptide

## 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	A	3423	742	3353	545	0
2	B	3362	742	3244	558	0
3	A	32	3	9	41	0
4	A	1	0	0	1	0
5	B	28	5	11	20	0
All	All	6846	1492	6617	1078	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 80.

The worst 5 of 1078 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:12:CYS:HB2	5:B:501:GDP:C8	1.44	1.52
2:B:12:CYS:SG	5:B:501:GDP:C6	2.05	1.49
2:B:12:CYS:HB2	5:B:501:GDP:N7	1.19	1.46
2:B:12:CYS:SG	5:B:501:GDP:C5	2.08	1.42
1:A:12:GLY:CA	3:A:501:GTP:C5	2.17	1.26

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	439/441 (100%)	377 (86%)	59 (13%)	3 (1%)	25	68
2	B	427/429 (100%)	388 (91%)	38 (9%)	1 (0%)	51	85
All	All	866/870 (100%)	765 (88%)	97 (11%)	4 (0%)	37	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	PHE
1	A	344	VAL
1	A	143	GLY
2	B	142	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	A	371/371 (100%)	365 (98%)	6 (2%)	68	85
2	B	365/365 (100%)	362 (99%)	3 (1%)	85	92
All	All	736/736 (100%)	727 (99%)	9 (1%)	77	88

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	HIS
2	B	332	ASN
2	B	222	TYR
1	A	224	TYR
1	A	380	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	191	GLN
2	B	256	ASN
2	B	396	HIS
2	B	184	ASN
2	B	414	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	$\# Z  > 2$
3	GTP	A	501	1	27,34,34	1.24	4 (14%)	24,54,54	1.52	2 (8%)
5	GDP	B	501	2	25,30,30	1.29	4 (16%)	23,47,47	1.58	5 (21%)

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	1	-	0/18/38/38	0/3/3/3
5	GDP	B	501	2	-	0/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	GTP	O4'-C1'	2.19	1.44	1.41
5	B	501	GDP	O4'-C1'	2.35	1.44	1.41
3	A	501	GTP	C6-N1	2.53	1.40	1.36
3	A	501	GTP	C2-N1	2.55	1.40	1.36
5	B	501	GDP	C2-N1	2.66	1.40	1.36

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	GDP	C4-C5-N7	-2.40	107.09	109.41
3	A	501	GTP	C4'-O4'-C1'	-2.30	107.32	109.77
5	B	501	GDP	C2'-C3'-C4'	-2.30	98.15	102.62
5	B	501	GDP	C4'-O4'-C1'	-2.16	107.47	109.77
5	B	501	GDP	C5'-C4'-C3'	-2.10	107.28	115.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GTP	41	0
5	B	501	GDP	20	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	35:GLN	C	36:MET	N	1.15