



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 20, 2017 – 08:46 AM EDT

PDB ID : 4UXY  
EMDB ID: : EMD-2770  
Title : Conserved mechanisms of microtubule-stimulated ADP release, ATP binding,  
and force generation in transport kinesins  
Authors : Atherton, J.; Farabella, I.; Yu, I.M.; Rosenfeld, S.S.; Houdusse, A.; Topf, M.;  
Moores, C.  
Deposited on : unknown  
Resolution : 6.50 Å(reported)  
Based on PDB ID : 4HNA

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](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.

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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

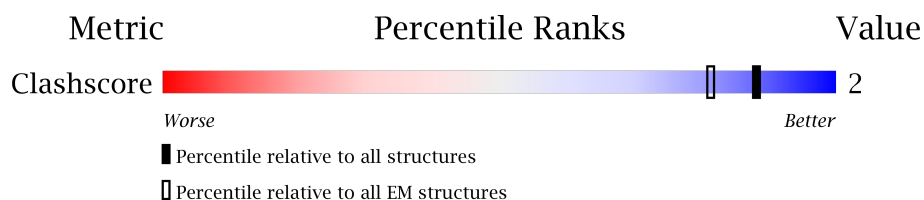
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


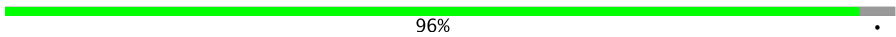
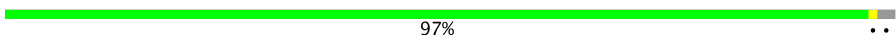
The reported resolution of this entry is 6.50 Å.

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

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	 91% 9%
2	B	445	 96% .
3	C	340	 97% ..

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 1294 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 ALPHA TUBULIN.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	412	Total 412	C 412	0	412

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	SER	LEU	conflict	UNP P81947
A	205	GLY	SER	conflict	UNP P81947
A	238	GLY	ILE	conflict	UNP P81947
A	313	THR	SER	conflict	UNP P81947
A	331	GLU	GLN	conflict	UNP P81947

- Molecule 2 is a protein called BETA TUBULIN.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	B	426	Total 426	C 426	0	426

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	54	ALA	THR	conflict	UNP Q6B856
B	169	VAL	MET	conflict	UNP Q6B856
B	295	ALA	SER	conflict	UNP Q6B856
B	315	VAL	ILE	conflict	UNP Q6B856
B	439	GLY	GLU	conflict	UNP Q6B856
B	440	GLU	GLY	conflict	UNP Q6B856

- Molecule 3 is a protein called KINESIN-1 MOTOR DOMAIN.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	C	332	Total 332	C 332	0	332

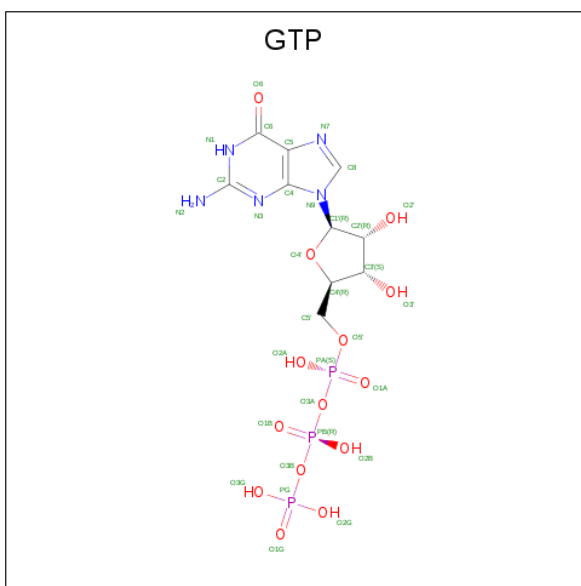
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



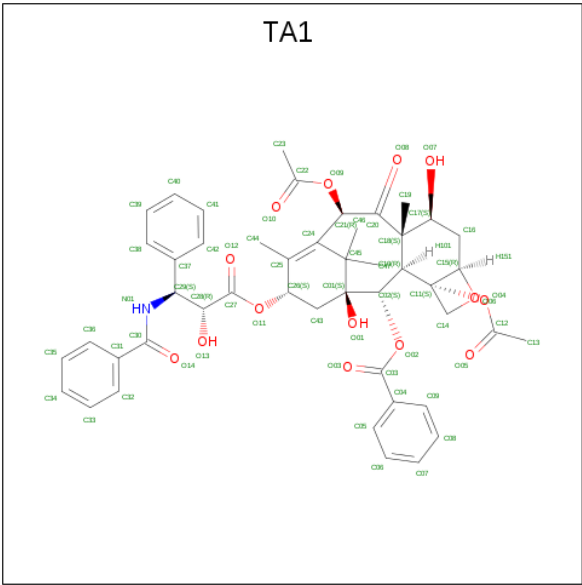
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 7 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
7	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 8 is TAXOL (three-letter code: TA1) (formula: C<sub>47</sub>H<sub>51</sub>NO<sub>14</sub>).



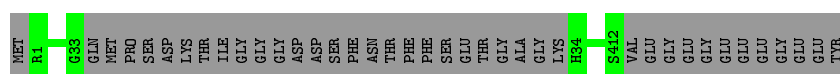
Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			62	47	1	14	

### 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.

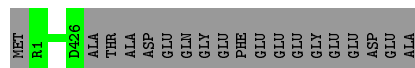
- Molecule 1: ALPHA TUBULIN

Chain A:  91% 9%



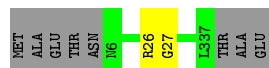
- Molecule 2: BETA TUBULIN

Chain B:  96% .



- Molecule 3: KINESIN-1 MOTOR DOMAIN

Chain C:  97% ..



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	186329	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	FREALIGN	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	100000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, ZN, TA1, 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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 ⓘ

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	412	0	0	0	0
2	B	426	0	0	0	0
3	C	332	0	0	1	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	32	0	12	0	0
7	B	28	0	12	0	0
8	B	62	0	51	2	0
All	All	1294	0	75	3	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 2.

All (3) 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)
8:B:1428:TA1:H261	8:B:1428:TA1:H463	1.80	0.62
3:C:26:ARG:CA	3:C:27:GLY:CA	2.88	0.51
8:B:1428:TA1:H463	8:B:1428:TA1:C26	2.46	0.43

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

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

### 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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
6	GTP	A	1415	5	27,34,34	1.51	2 (7%)	27,54,54	2.15	5 (18%)
7	GDP	B	1427	-	25,30,30	2.61	8 (32%)	26,47,47	3.64	9 (34%)
8	TA1	B	1428	-	68,68,68	1.98	20 (29%)	105,105,105	1.33	8 (7%)

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
6	GTP	A	1415	5	-	0/18/38/38	0/3/3/3
7	GDP	B	1427	-	-	0/12/32/32	0/3/3/3
8	TA1	B	1428	-	-	0/41/127/127	0/5/7/7

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1428	TA1	C08-C07	-5.13	1.25	1.38
7	B	1427	GDP	PB-O2B	-3.53	1.40	1.54
8	B	1428	TA1	C04-C03	-2.33	1.44	1.49
8	B	1428	TA1	C10-C02	2.02	1.62	1.57
8	B	1428	TA1	C41-C42	2.09	1.42	1.38
7	B	1427	GDP	O3'-C3'	2.14	1.47	1.43
8	B	1428	TA1	C16-C15	2.20	1.56	1.52
8	B	1428	TA1	C18-C20	2.20	1.62	1.56
7	B	1427	GDP	PB-O3B	2.22	1.63	1.54
8	B	1428	TA1	C37-C29	2.22	1.54	1.51
8	B	1428	TA1	C01-C45	2.23	1.66	1.56
8	B	1428	TA1	C11-C10	2.25	1.61	1.55
7	B	1427	GDP	C5-C4	2.40	1.45	1.40
8	B	1428	TA1	C26-C25	2.47	1.56	1.51
8	B	1428	TA1	C43-C26	2.51	1.58	1.52
8	B	1428	TA1	C43-C01	2.93	1.60	1.54
8	B	1428	TA1	C25-C24	3.02	1.39	1.34
8	B	1428	TA1	C46-C45	3.07	1.60	1.53
7	B	1427	GDP	C8-N7	3.43	1.41	1.34
8	B	1428	TA1	O02-C03	3.46	1.41	1.34
8	B	1428	TA1	C45-C24	3.48	1.61	1.54
8	B	1428	TA1	C36-C31	3.52	1.45	1.39
6	A	1415	GTP	PG-O3B	3.84	1.66	1.60
7	B	1427	GDP	O6-C6	4.10	1.34	1.24
8	B	1428	TA1	C18-C10	4.29	1.69	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1428	TA1	C05-C04	4.48	1.46	1.39
6	A	1415	GTP	C6-N1	4.80	1.41	1.33
8	B	1428	TA1	C06-C05	5.84	1.50	1.38
7	B	1427	GDP	O4'-C1'	6.11	1.49	1.41
7	B	1427	GDP	C2-N1	7.63	1.49	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1427	GDP	C6-C5-C4	-11.35	109.56	120.84
6	A	1415	GTP	C5-C6-N1	-7.10	113.37	123.48
7	B	1427	GDP	N2-C2-N1	-5.92	107.78	117.24
7	B	1427	GDP	C4-C5-N7	-5.01	104.57	109.41
7	B	1427	GDP	N3-C2-N1	-4.92	120.27	127.46
8	B	1428	TA1	C06-C05-C04	-4.90	114.59	120.35
8	B	1428	TA1	C05-C04-C03	-3.96	111.47	120.39
6	A	1415	GTP	N3-C2-N1	-3.21	122.78	127.46
8	B	1428	TA1	O04-C11-C14	-2.76	101.75	108.14
6	A	1415	GTP	C6-C5-C4	-2.43	118.43	120.84
6	A	1415	GTP	O5'-C5'-C4'	2.00	116.10	109.00
7	B	1427	GDP	O2'-C2'-C3'	2.30	119.20	111.83
8	B	1428	TA1	O01-C01-C43	2.46	113.37	106.86
8	B	1428	TA1	C45-C01-C02	2.65	115.17	111.85
8	B	1428	TA1	C17-C18-C20	2.83	109.80	102.33
7	B	1427	GDP	C2'-C3'-C4'	3.40	109.24	102.62
8	B	1428	TA1	C09-C04-C03	3.55	128.38	120.39
7	B	1427	GDP	C2-N3-C4	3.61	119.38	115.16
7	B	1427	GDP	C4'-O4'-C1'	4.01	114.04	109.77
8	B	1428	TA1	C07-C08-C09	5.16	127.30	120.21
6	A	1415	GTP	C6-N1-C2	5.98	124.67	116.06
7	B	1427	GDP	N2-C2-N3	7.69	131.94	117.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1428	TA1	2	0

## 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.