wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:00 PM BST

PDB ID	:	4UY0
EMDB ID:	:	EMD-2771
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	:	2014-08-27
Resolution	:	7.70 Å(reported)
Based on PDB ID	:	4HNA

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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

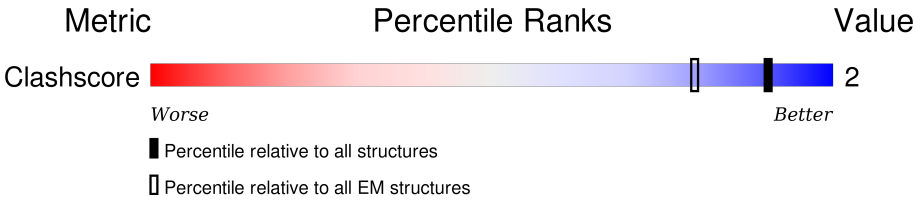
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.70 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	114402	924

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	451	91% 9%
2	B	426	100%
3	C	340	97% • •

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 1329 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-1B CHAIN.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
1	A	412	412	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 TUBULIN BETA-2B CHAIN.

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

There are 4 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

- Molecule 3 is a protein called KINESIN HEAVY CHAIN ISOFORM 5A.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
3	C	333	333	333	0	333

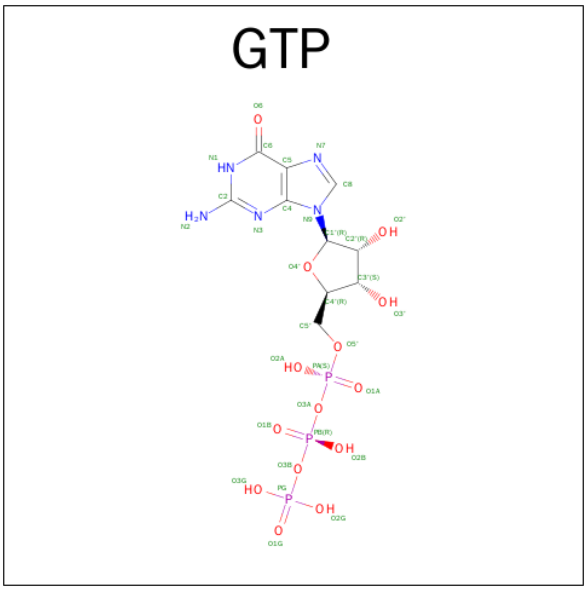
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

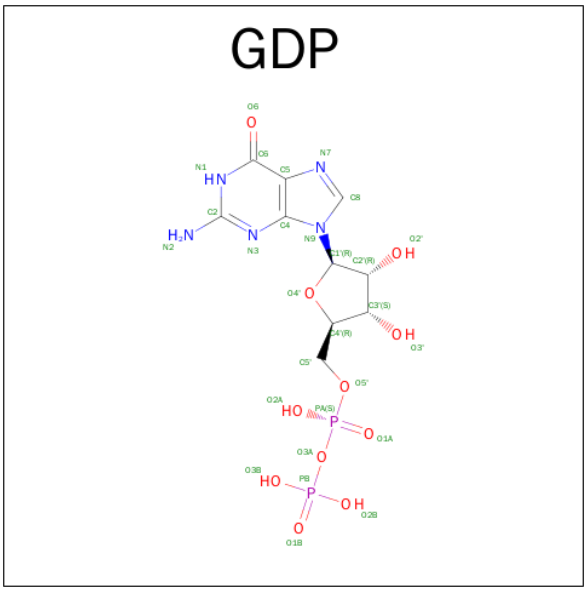
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	A	1	1	1	0
			Total	Mg	
5	C	1	1	1	0

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



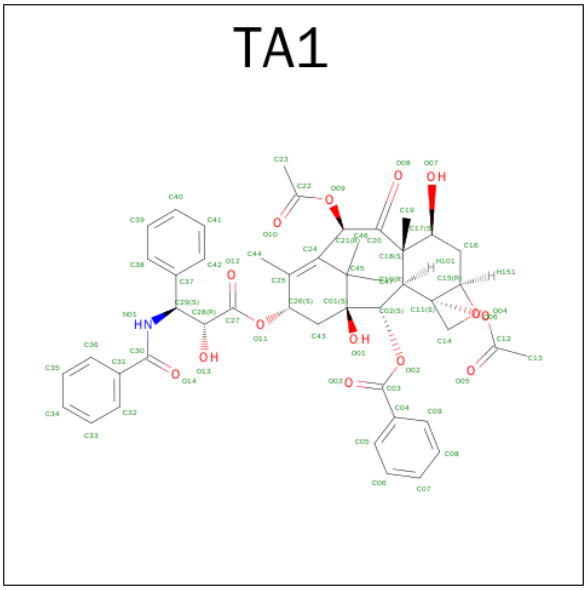
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	32	10	5	14	3	0

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



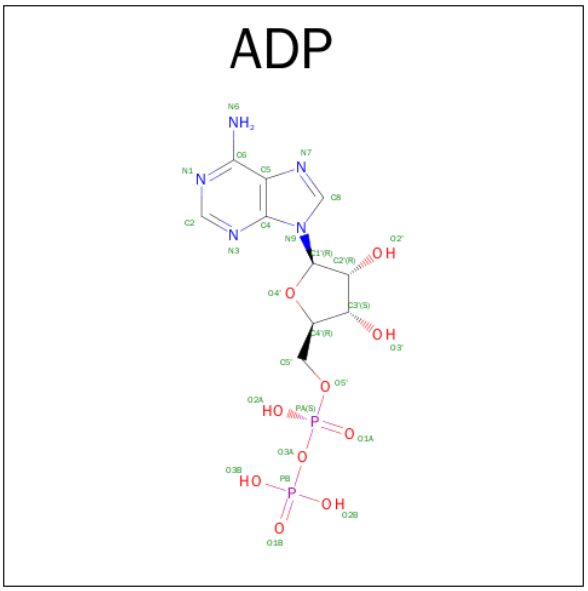
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	B	1	28	10	5	11	2	0

- Molecule 8 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).



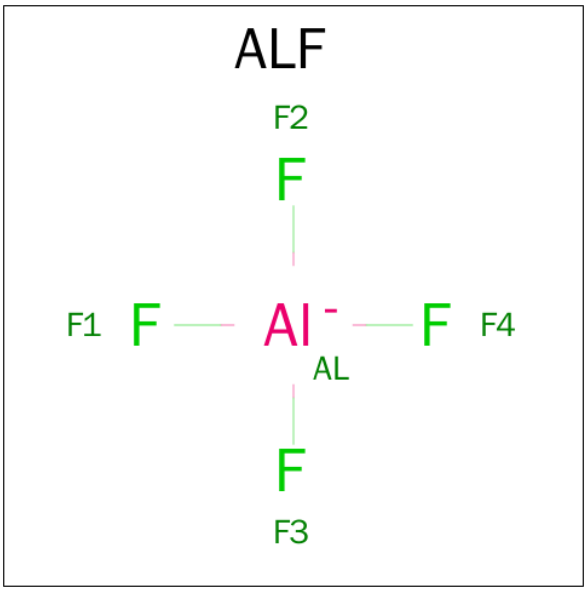
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	B	1	62	47	1	14	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



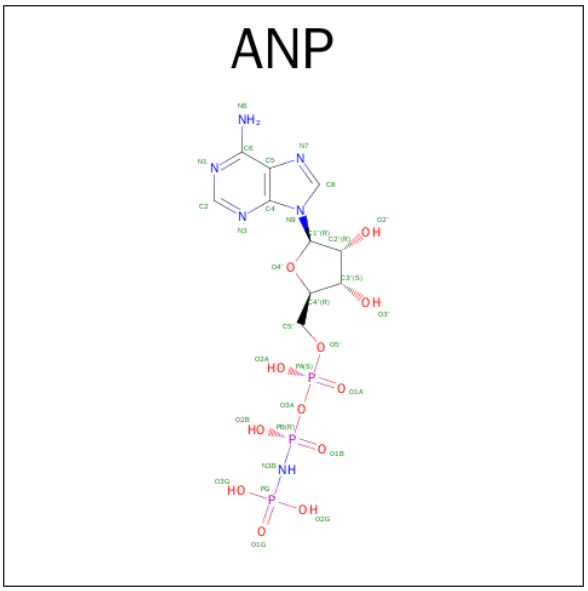
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	C	1	27	10	5	10	2	0

- Molecule 10 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Al	F	
10	C	1	5	1	4	0

- Molecule 11 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms		AltConf
			Total	N	
11	C	1	1	1	0

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 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-1B CHAIN

Chain A: 91% 9%

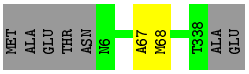
- Molecule 2: TUBULIN BETA-2B CHAIN

Chain B: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: KINESIN HEAVY CHAIN ISOFORM 5A

Chain C: 97%



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	FREALIGN, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN ULTRASCAN 4000 (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, ZN, TA1, ADP, ALF, MG, GTP, ANP

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 (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	412	0	0	0	0
2	B	426	0	0	0	0
3	C	333	0	0	1	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
5	C	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
9	C	27	0	12	0	0
10	C	5	0	0	0	0
11	C	1	0	0	0	0
All	All	1329	0	87	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:67:ALA:CA	3:C:68:MET:CA	2.78	0.61
8:B:1428:TA1:C26	8:B:1428:TA1:H463	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 9 ligands modelled in this entry, 1 is modelled with single atom and 3 are monoatomic - leaving 5 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	26,34,34	1.35	1 (3%)	29,54,54	2.28	4 (13%)
7	GDP	B	1427	-	24,30,30	2.65	8 (33%)	26,47,47	3.29	8 (30%)
8	TA1	B	1428	-	68,68,68	1.93	20 (29%)	102,105,105	1.31	8 (7%)
9	ADP	C	1339	10,5	24,29,29	0.72	1 (4%)	23,45,45	0.73	0
10	ALF	C	1341	9	0,4,4	0.00	-	0,6,6	0.00	-

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
9	ADP	C	1339	10,5	-	0/12/32/32	0/3/3/3
10	ALF	C	1341	9	-	0/0/0/0	0/0/0/0

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1428	TA1	C08-C07	-4.97	1.25	1.38
7	B	1427	GDP	PB-O2B	-4.19	1.40	1.54
8	B	1428	TA1	C04-C03	-2.32	1.44	1.49
9	C	1339	ADP	C8-N7	-2.19	1.30	1.34
8	B	1428	TA1	C10-C02	2.01	1.62	1.57

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1427	GDP	C6-C5-C4	-9.89	109.56	120.86
6	A	1415	GTP	C5-C6-N1	-7.77	113.37	123.52
7	B	1427	GDP	N2-C2-N1	-5.71	107.78	117.20
7	B	1427	GDP	N3-C2-N1	-5.36	120.27	127.56
8	B	1428	TA1	C06-C05-C04	-4.83	114.59	120.35

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.