wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:55 PM BST

PDB ID	:	4AQW
EMDB ID:	:	EMD-2078
Title	:	Model of human kinesin-5 motor domain (1II6, 3HQD) and mammalian tubulin heterodimer (1JFF) docked into the 9.5-angstrom cryo-EM map of microtubule-bound kinesin-5 motor domain in the rigor state.
Authors	:	Goulet, A.; Behnke-Parks, W.M.; Sindelar, C.V.; Rosenfeld, S.S.; Moores, C.A.
Deposited on	:	2012-04-19
Resolution	:	9.50 Å(reported)
Based on PDB ID	:	1II6,3HQD,1JFF

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

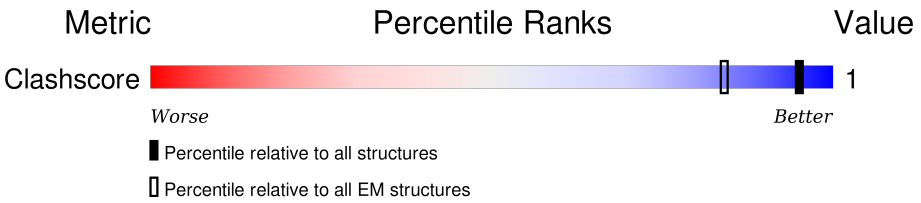
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 9.50 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	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	452	91% 9%
2	B	445	96% .
3	C	373	94% 6%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 1311 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-1D CHAIN.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ILE	VAL	CONFLICT	UNP Q2HJ86
A	114	ILE	LEU	CONFLICT	UNP Q2HJ86
A	136	SER	LEU	CONFLICT	UNP Q2HJ86
A	137	VAL	ILE	CONFLICT	UNP Q2HJ86
A	265	GLY	ILE	CONFLICT	UNP Q2HJ86
A	358	GLU	GLN	CONFLICT	UNP Q2HJ86
A	437	VAL	MET	CONFLICT	UNP Q2HJ86

- 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	57	ALA	THR	CONFLICT	UNP Q6B856
B	172	VAL	MET	CONFLICT	UNP Q6B856
B	298	ALA	SER	CONFLICT	UNP Q6B856
B	318	VAL	ILE	CONFLICT	UNP Q6B856

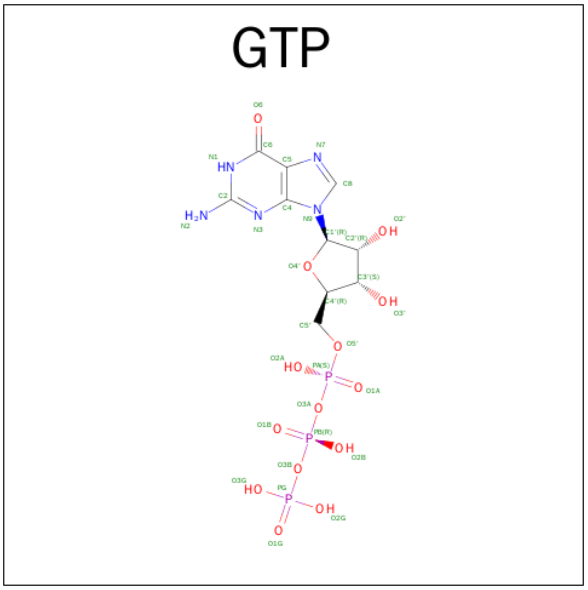
- Molecule 3 is a protein called KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms		AltConf	Trace
			Total	C		
3	C	350	350	350	0	350

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	25	VAL	CYS	ENGINEERED MUTATION	UNP P52732
C	43	SER	CYS	ENGINEERED MUTATION	UNP P52732
C	87	ALA	CYS	ENGINEERED MUTATION	UNP P52732
C	99	ALA	CYS	ENGINEERED MUTATION	UNP P52732
C	126	CYS	THR	ENGINEERED MUTATION	UNP P52732
C	368	HIS	-	EXPRESSION TAG	UNP P52732
C	369	HIS	-	EXPRESSION TAG	UNP P52732
C	370	HIS	-	EXPRESSION TAG	UNP P52732
C	371	HIS	-	EXPRESSION TAG	UNP P52732
C	372	HIS	-	EXPRESSION TAG	UNP P52732
C	373	HIS	-	EXPRESSION TAG	UNP P52732

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



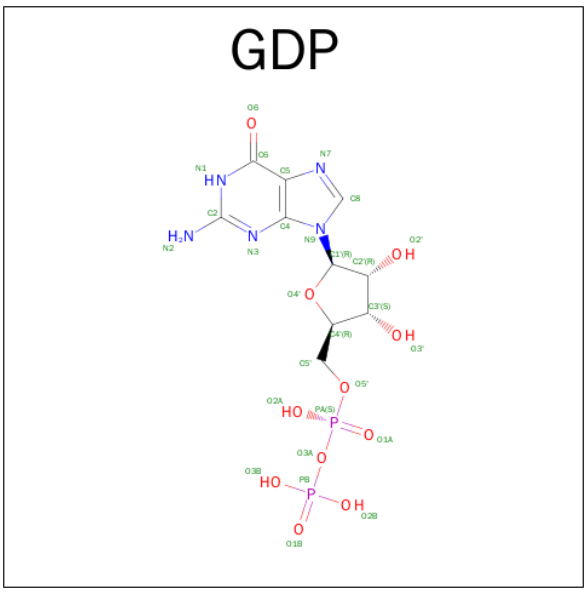
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	32	10	5	14	3	0

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

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

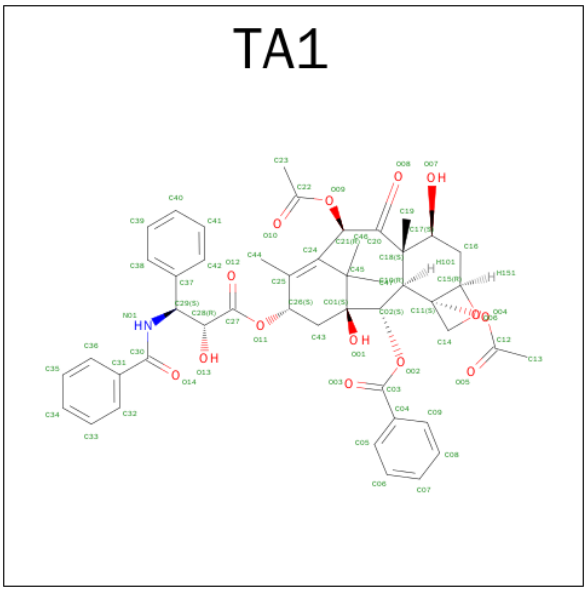
- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:

$C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 7 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).



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

3 Residue-property plots (i)

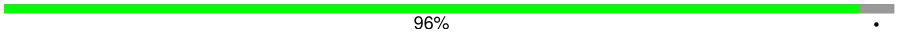
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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-1D CHAIN

Chain A:

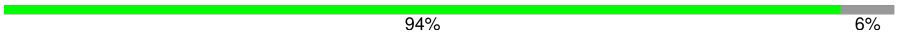
- Molecule 2: TUBULIN BETA-2B CHAIN

Chain B:



- Molecule 3: KINESIN-LIKE PROTEIN KIF11

Chain C:



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	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	18	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 FILM	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, TA1

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	350	0	0	0	0
4	A	32	0	12	0	0
5	A	1	0	0	0	0
6	B	28	0	12	0	0
7	B	62	0	51	2	0
All	All	1311	0	75	2	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 1.

All (2) 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)
7:B:601:TA1:H261	7:B:601:TA1:H463	1.80	0.63
7:B:601:TA1:C26	7:B:601:TA1:H463	2.46	0.44

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 4 ligands modelled in this entry, 1 is 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
4	GTP	A	500	5	26,34,34	1.37	2 (7%)	29,54,54	2.32	4 (13%)
6	GDP	B	600	-	24,30,30	2.77	8 (33%)	26,47,47	3.31	9 (34%)
7	TA1	B	601	-	68,68,68	1.94	19 (27%)	102,105,105	1.31	9 (8%)

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	500	5	-	0/18/38/38	0/3/3/3
6	GDP	B	600	-	-	0/12/32/32	0/3/3/3
7	TA1	B	601	-	-	0/41/127/127	0/5/7/7

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	601	TA1	C07-C06	-4.99	1.25	1.38
6	B	600	GDP	PB-O2B	-4.21	1.40	1.54
7	B	601	TA1	C04-C03	-2.35	1.44	1.49
4	A	500	GTP	PB-O2B	-2.13	1.46	1.55
7	B	601	TA1	C10-C02	2.05	1.62	1.57
7	B	601	TA1	C18-C20	2.09	1.62	1.56
7	B	601	TA1	C01-C45	2.14	1.66	1.56
7	B	601	TA1	C11-C10	2.14	1.61	1.55
6	B	600	GDP	O3'-C3'	2.15	1.48	1.43
7	B	601	TA1	C37-C29	2.16	1.54	1.51
7	B	601	TA1	C16-C15	2.18	1.56	1.52
6	B	600	GDP	C5-C4	2.38	1.45	1.40
7	B	601	TA1	C43-C26	2.42	1.58	1.52
7	B	601	TA1	C26-C25	2.42	1.56	1.51
7	B	601	TA1	C43-C01	2.85	1.60	1.54
7	B	601	TA1	C46-C45	2.95	1.60	1.53
7	B	601	TA1	C25-C24	3.03	1.39	1.34
6	B	600	GDP	C8-N7	3.36	1.41	1.34
7	B	601	TA1	C45-C24	3.38	1.61	1.54
7	B	601	TA1	O02-C03	3.40	1.41	1.34
7	B	601	TA1	C32-C31	3.53	1.45	1.39
6	B	600	GDP	O6-C6	4.08	1.34	1.24
7	B	601	TA1	C18-C10	4.16	1.69	1.57
6	B	600	GDP	PB-O1B	4.16	1.64	1.50
7	B	601	TA1	C09-C04	4.50	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	GTP	C6-N1	4.83	1.41	1.33
7	B	601	TA1	C08-C09	5.72	1.50	1.38
6	B	600	GDP	O4'-C1'	5.95	1.49	1.41
6	B	600	GDP	C2-N1	7.29	1.49	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	600	GDP	C6-C5-C4	-9.94	109.50	120.86
4	A	500	GTP	C5-C6-N1	-7.81	113.31	123.52
6	B	600	GDP	N2-C2-N1	-5.72	107.77	117.20
6	B	600	GDP	N3-C2-N1	-5.37	120.25	127.56
7	B	601	TA1	C08-C09-C04	-4.79	114.63	120.35
7	B	601	TA1	C09-C04-C03	-3.93	111.52	120.38
4	A	500	GTP	N3-C2-N1	-3.57	122.70	127.56
6	B	600	GDP	C1'-N9-C4	-2.65	123.85	126.81
7	B	601	TA1	O04-C11-C14	-2.48	101.78	108.08
4	A	500	GTP	C6-C5-C4	-2.14	118.41	120.86
7	B	601	TA1	C06-C05-C04	-2.02	117.94	120.35
6	B	600	GDP	O2'-C2'-C3'	2.25	119.12	111.86
6	B	600	GDP	O3B-PB-O2B	2.38	116.19	107.44
7	B	601	TA1	O01-C01-C43	2.51	113.38	106.82
7	B	601	TA1	C17-C18-C20	2.58	109.87	102.14
7	B	601	TA1	C45-C01-C02	3.05	115.16	111.64
6	B	600	GDP	C2'-C3'-C4'	3.22	109.23	102.64
7	B	601	TA1	C05-C04-C03	3.52	128.31	120.38
6	B	600	GDP	C4'-O4'-C1'	4.19	114.08	109.64
7	B	601	TA1	C07-C06-C05	5.20	127.43	120.20
4	A	500	GTP	C6-N1-C2	7.56	124.73	115.88
6	B	600	GDP	N2-C2-N3	7.60	131.97	117.72

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
7	B	601	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.