



wwPDB EM Map/Model Validation Report i

Apr 10, 2016 – 01:41 PM BST

PDB ID : 3J1T
EMDB ID: : EMD-5439
Title : High affinity dynein microtubule binding domain - tubulin complex
Authors : Redwine, W.B.; Hernandez-Lopez, R.; Zou, S.; Huang, J.; Reck-Peterson, S.L.;
Leschziner, A.E.
Deposited on : 2012-06-25
Resolution : 9.70 Å(reported)
Based on PDB ID : 3ERR, 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>

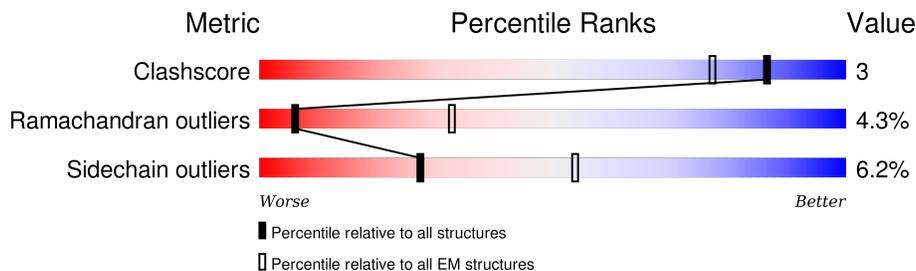
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 9.70 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
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 ≥ 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	164	
2	B	451	
3	C	427	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8091 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 Cytoplasmic dynein 1 heavy chain 1, seryl t-RNA synthetase chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	164	1308	820	227	252	9	0	0

- Molecule 2 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	439	3423	2163	582	656	22	0	0

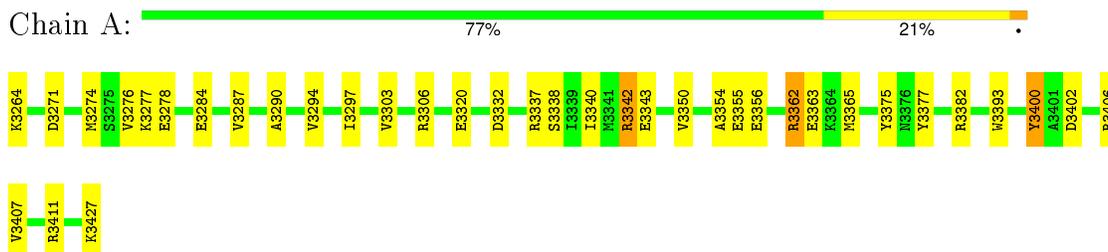
- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	427	3360	2110	576	648	26	0	0

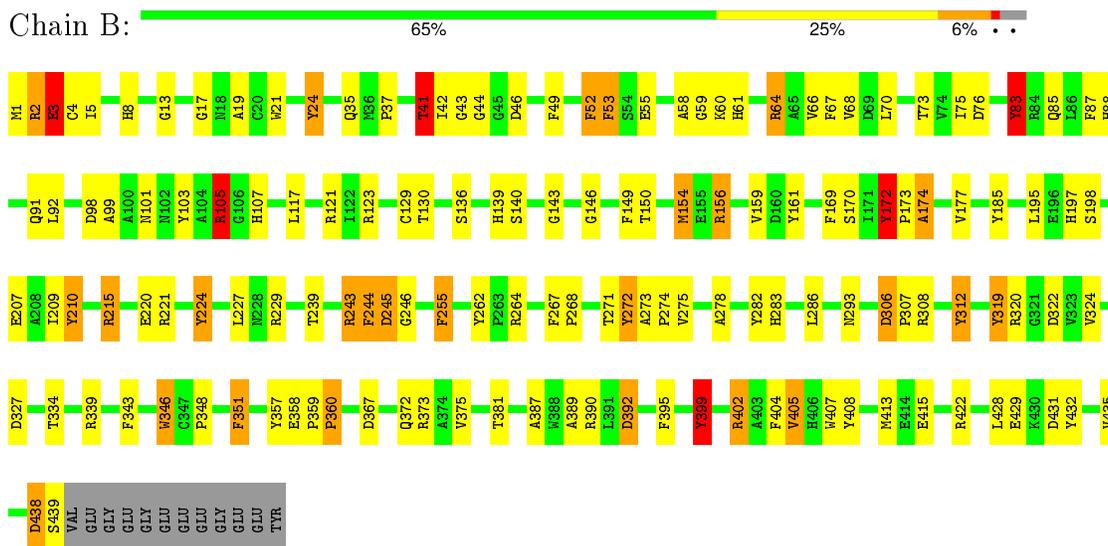
3 Residue-property plots

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.

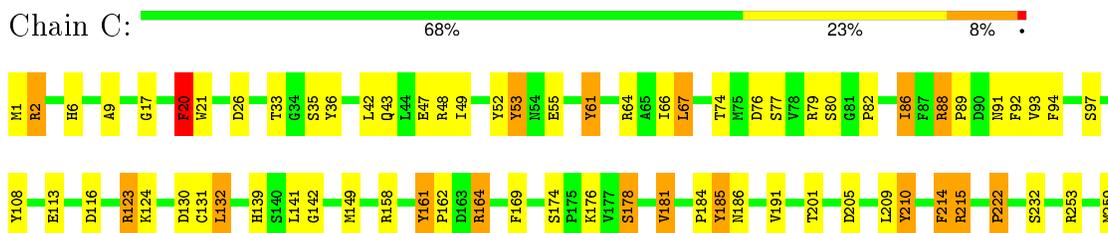
- Molecule 1: Cytoplasmic dynein 1 heavy chain 1, seryl t-RNA synthetase chimera



- Molecule 2: Tubulin alpha-1B chain



- Molecule 3: Tubulin beta-2B chain





4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	10419	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	phase and amplitude correction using Fre-align	Depositor
Microscope	FEI Tecnai F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	62000	Depositor
Image detector	Kodak SO-163 film	Depositor

5 Model quality i

5.1 Standard geometry i

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	1.66	9/1325 (0.7%)	1.90	28/1783 (1.6%)
2	B	1.62	23/3501 (0.7%)	2.08	100/4752 (2.1%)
3	C	1.64	25/3435 (0.7%)	1.97	82/4652 (1.8%)
All	All	1.63	57/8261 (0.7%)	2.01	210/11187 (1.9%)

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	4
2	B	0	18
3	C	0	27
All	All	0	49

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3427	LYS	C-OXT	-12.07	1.00	1.23
3	C	437	ASP	C-OXT	-12.06	1.00	1.23
1	A	3427	LYS	C-O	-12.05	1.00	1.23
3	C	437	ASP	C-O	-12.05	1.00	1.23
2	B	439	SER	C-O	-12.02	1.00	1.23

The worst 5 of 210 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	ARG	NE-CZ-NH2	-20.97	109.81	120.30
2	B	422	ARG	NE-CZ-NH1	18.36	129.48	120.30
2	B	2	ARG	NE-CZ-NH1	16.95	128.78	120.30
3	C	64	ARG	NE-CZ-NH1	15.31	127.95	120.30
3	C	214	PHE	CB-CG-CD1	-15.02	110.28	120.80

There are no chirality outliers.

5 of 49 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3337	ARG	Sidechain
1	A	3342	ARG	Sidechain
1	A	3356	GLU	Peptide
1	A	3362	ARG	Sidechain
2	B	24	TYR	Sidechain

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	1308	0	1342	3	0
2	B	3423	0	3324	24	0
3	C	3360	0	3241	16	0
All	All	8091	0	7907	42	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 3.

The worst 5 of 42 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)
3:C:259:MET:HB3	3:C:268:PHE:CZ	2.27	0.69
3:C:6:HIS:HE1	3:C:17:GLY:HA2	1.65	0.60
1:A:3338:SER:HB2	3:C:162:PRO:HG3	1.88	0.55
3:C:6:HIS:CE1	3:C:17:GLY:HA2	2.42	0.54
3:C:86:ILE:H	3:C:86:ILE:HD13	1.73	0.54

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
2	B	437/451 (97%)	372 (85%)	42 (10%)	23 (5%)	2	29
3	C	425/427 (100%)	364 (86%)	40 (9%)	21 (5%)	3	31
All	All	1024/1042 (98%)	888 (87%)	92 (9%)	44 (4%)	6	34

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	ALA
2	B	129	CYS
2	B	245	ASP
2	B	264	ARG
3	C	178	SER

5.3.2 Protein sidechains [i](#)

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	146/146 (100%)	141 (97%)	5 (3%)	44	75
2	B	368/377 (98%)	344 (94%)	24 (6%)	21	58
3	C	368/368 (100%)	342 (93%)	26 (7%)	18	55
All	All	882/891 (99%)	827 (94%)	55 (6%)	27	60

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	399	TYR
3	C	49	ILE
3	C	413	MET
2	B	402	ARG
2	B	415	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	283	HIS
3	C	433	GLN
3	C	28	HIS
2	B	88	HIS
3	C	336	GLN

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](#)

There are no ligands in this entry.

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.