



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:56 PM BST

PDB ID : 4ATX
EMDB ID: : EMD-2098
Title : Rigor kinesin motor domain with an ordered neck-linker, docked on tubulin dimer, modelled into the 8A cryo-EM map of doublecortin- microtubules decorated with kinesin
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Deposited on : 2012-05-10
Resolution : 8.20 Å(reported)
Based on PDB ID : 2XRP, 1BG2

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

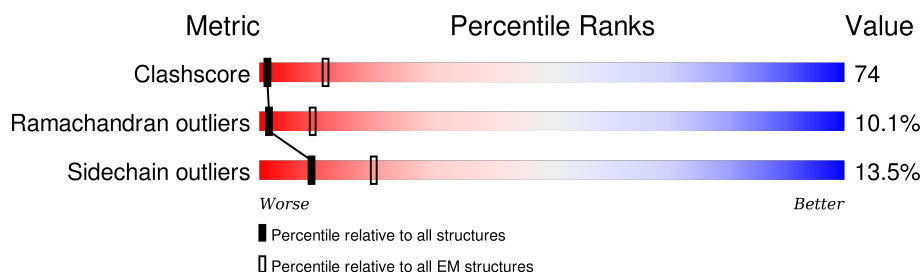
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.20 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	445	
2	B	452	
3	C	340	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9183 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 BETA-2B CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ALA	THR	CONFLICT	UNP Q6B856
A	172	VAL	MET	CONFLICT	UNP Q6B856
A	298	ALA	SER	CONFLICT	UNP Q6B856
A	318	VAL	ILE	CONFLICT	UNP Q6B856

- Molecule 2 is a protein called TUBULIN ALPHA-1D CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	429	Total	C	N	O	S	0	0
			3334	2114	569	630	21		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	ILE	VAL	CONFLICT	UNP Q2HJ86
B	114	ILE	LEU	CONFLICT	UNP Q2HJ86
B	136	SER	LEU	CONFLICT	UNP Q2HJ86
B	137	VAL	ILE	CONFLICT	UNP Q2HJ86
B	265	GLY	ILE	CONFLICT	UNP Q2HJ86
B	358	GLU	GLN	CONFLICT	UNP Q2HJ86
B	437	VAL	MET	CONFLICT	UNP Q2HJ86
B	450	GLU	ASP	CONFLICT	UNP Q2HJ86

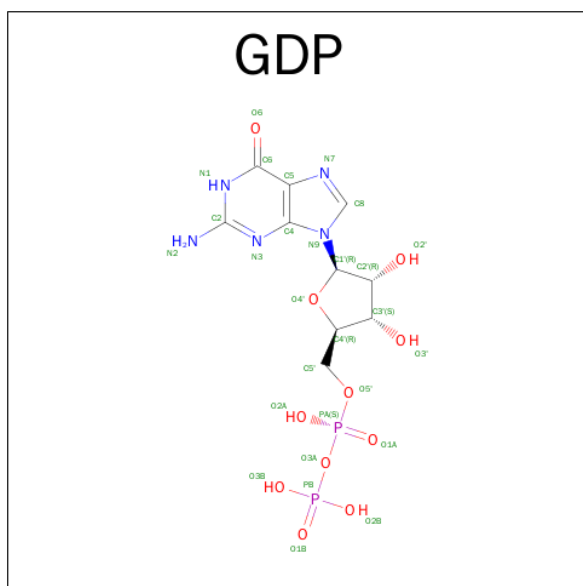
- Molecule 3 is a protein called KINESIN-1 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	310	Total	C	N	O	S	0	1
			2438	1517	420	485	16		

There is a discrepancy between the modelled and reference sequences:

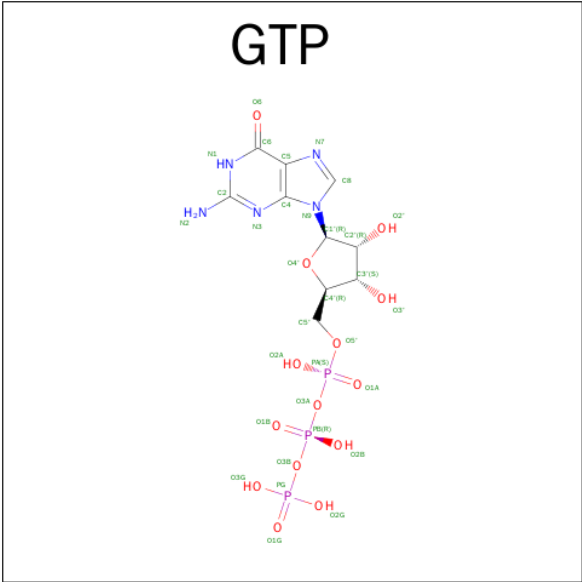
Chain	Residue	Modelled	Actual	Comment	Reference
C	92	ASN	THR	ENGINEERED MUTATION	UNP Q2PQA9

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

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

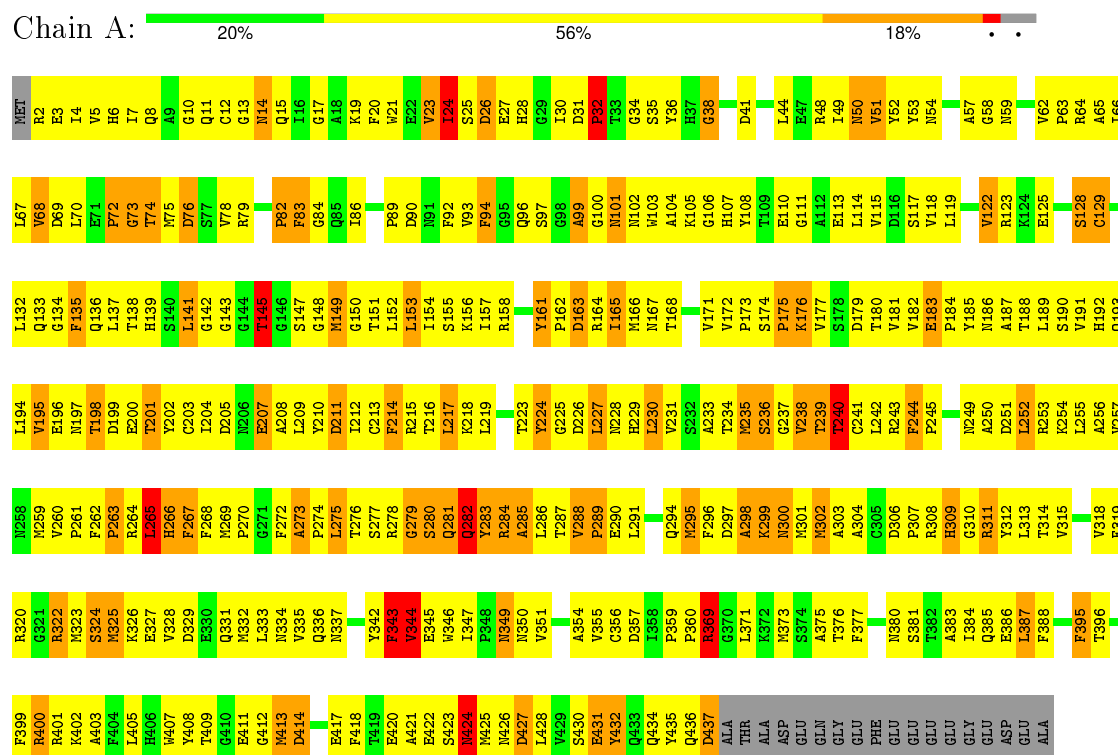


Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			32	10	5	14	3	

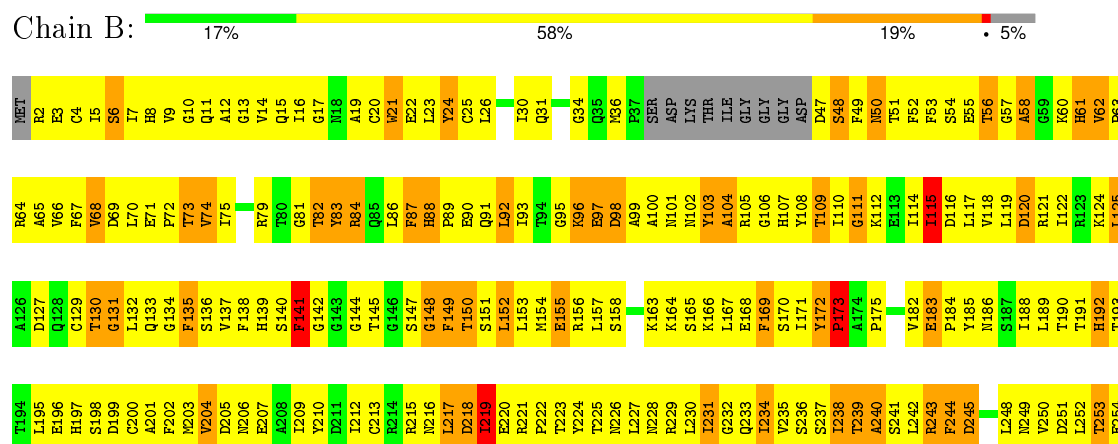
3 Residue-property plots

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: TUBULIN BETA-2B CHAIN



• Molecule 2: TUBULIN ALPHA-1D CHAIN



4 Experimental information

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	DONE WITH FREALIGN	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	760	Depositor
Maximum defocus (nm)	2900	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

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	0.51	0/3426	0.76	2/4642 (0.0%)
2	B	0.82	3/3410 (0.1%)	0.77	3/4629 (0.1%)
3	C	0.95	1/2477 (0.0%)	1.17	8/3339 (0.2%)
All	All	0.76	4/9313 (0.0%)	0.89	13/12610 (0.1%)

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
3	C	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	92	LEU	C-N	27.96	1.98	1.34
2	B	298	PRO	C-N	17.31	1.73	1.34
2	B	68	VAL	C-N	14.35	1.67	1.34
3	C	29	TYR	CB-CG	-5.01	1.44	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	307	TYR	CA-CB-CG	-11.33	91.87	113.40
3	C	307	TYR	CB-CG-CD1	-10.06	114.96	121.00
3	C	29	TYR	CB-CG-CD2	-7.39	116.57	121.00
2	B	68	VAL	O-C-N	-7.10	111.34	122.70
2	B	298	PRO	O-C-N	-6.72	111.94	122.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	16	ARG	Sidechain
3	C	27	ASP	Peptide
3	C	28	LYS	Peptide
3	C	30	VAL	Peptide
3	C	305	SER	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	3351	0	3229	547	0
2	B	3334	0	3223	633	0
3	C	2438	0	2397	186	0
4	A	28	0	12	1	0
5	B	32	0	12	5	0
All	All	9183	0	8873	1343	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 74.

The worst 5 of 1343 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:296:PHE:CE1	2:B:341:ILE:HD11	1.32	1.63
2:B:5:ILE:HG12	2:B:64:ARG:NH1	1.27	1.42
2:B:57:GLY:HA3	2:B:58:ALA:CB	1.45	1.42
2:B:298:PRO:C	2:B:299:ALA:N	1.73	1.40
2:B:3:GLU:CG	2:B:51:THR:HA	1.57	1.34

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	424/445 (95%)	274 (65%)	94 (22%)	56 (13%)	0	7
2	B	423/452 (94%)	279 (66%)	87 (21%)	57 (14%)	0	7
3	C	306/340 (90%)	295 (96%)	8 (3%)	3 (1%)	19	65
All	All	1153/1237 (93%)	848 (74%)	189 (16%)	116 (10%)	1	14

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	24	ILE
1	A	32	PRO
1	A	50	ASN
1	A	82	PRO

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	367/381 (96%)	307 (84%)	60 (16%)	3	20
2	B	354/378 (94%)	295 (83%)	59 (17%)	3	19
3	C	279/303 (92%)	263 (94%)	16 (6%)	25	62
All	All	1000/1062 (94%)	865 (86%)	135 (14%)	9	27

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	20	CYS
2	B	98	ASP
3	C	134	TYR
2	B	21	TRP
2	B	74	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	436	GLN
2	B	50	ASN
3	C	156	HIS
2	B	15	GLN
2	B	61	HIS

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](#)

2 ligands are modelled in this entry.

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	GDP	A	600	-	24,30,30	2.65	8 (33%)	26,47,47	3.30	9 (34%)
5	GTP	B	500	-	26,34,34	1.61	4 (15%)	29,54,54	2.40	7 (24%)

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	GDP	A	600	-	-	0/12/32/32	0/3/3/3
5	GTP	B	500	-	-	0/18/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GDP	PB-O2B	-4.21	1.40	1.54
5	B	500	GTP	PB-O2B	-2.12	1.46	1.55
5	B	500	GTP	O4'-C1'	2.07	1.44	1.41
4	A	600	GDP	O3'-C3'	2.09	1.47	1.43
4	A	600	GDP	C5-C4	2.43	1.46	1.40

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	GDP	C6-C5-C4	-9.95	109.49	120.86
5	B	500	GTP	C5-C6-N1	-7.75	113.39	123.52
4	A	600	GDP	N2-C2-N1	-5.70	107.80	117.20
4	A	600	GDP	N3-C2-N1	-5.37	120.25	127.56
5	B	500	GTP	N3-C2-N1	-3.48	122.82	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GDP	1	0
5	B	500	GTP	5	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.