



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:36 am GMT

PDB ID : 3J8X
EMDB ID: : EMD-6187
Title : High-resolution structure of no-nucleotide kinesin on microtubules
Authors : Shang, Z.; Zhou, K.; Xu, C.; Csencsits, R.; Cochran, J.C.; Sindelar, C.V.
Deposited on : 2014-11-20
Resolution : 5.00 Å(reported)
Based on PDB ID : 4HNA

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at 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.

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) : recalc29047

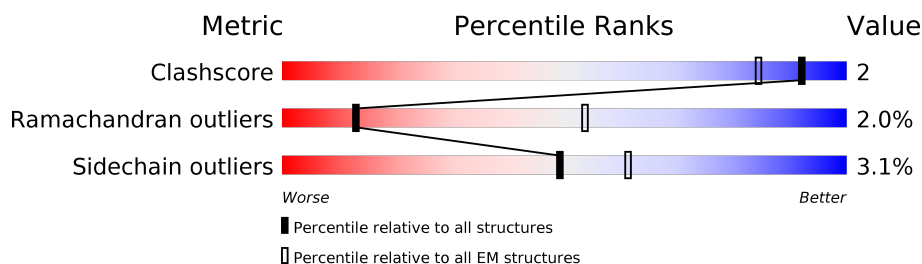
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 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
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	K	349	
2	A	451	
3	B	445	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9295 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 Kinesin-1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	316	Total	C	N	O	S	0	0
			2474	1543	423	498	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	7	SER	CYS	CONFLICT	UNP P33176
K	168	ALA	CYS	CONFLICT	UNP P33176
K	174	SER	CYS	CONFLICT	UNP P33176
K	330	SER	CYS	CONFLICT	UNP P33176

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		

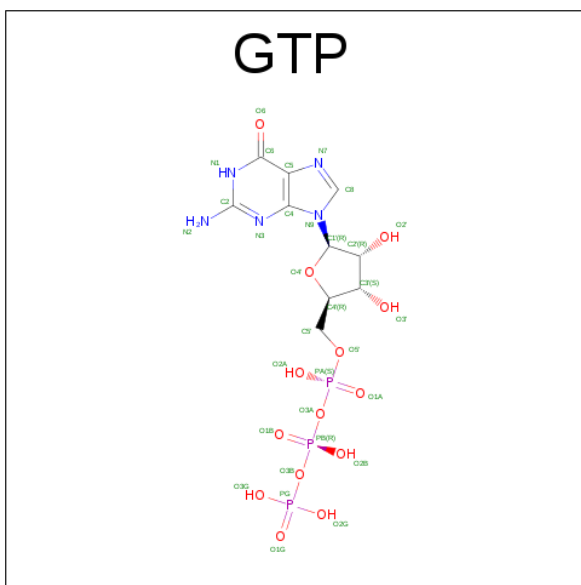
- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	431	Total	C	N	O	S	0	0
			3389	2126	580	657	26		

There is a discrepancy between the modelled and reference sequences:

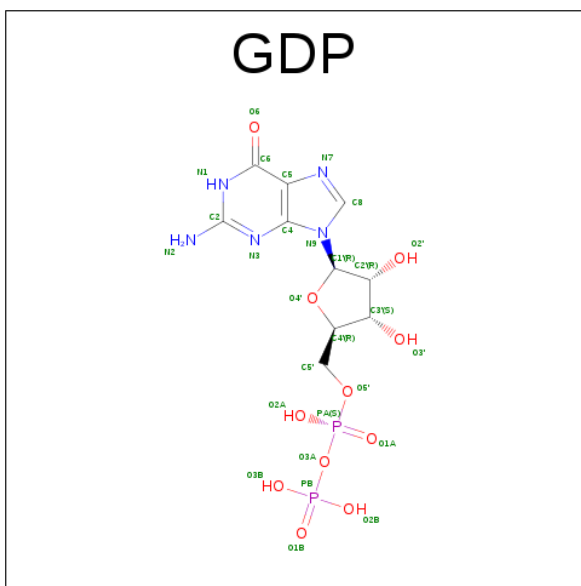
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	SER	CYS	CONFLICT	UNP F2Z5B2

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).

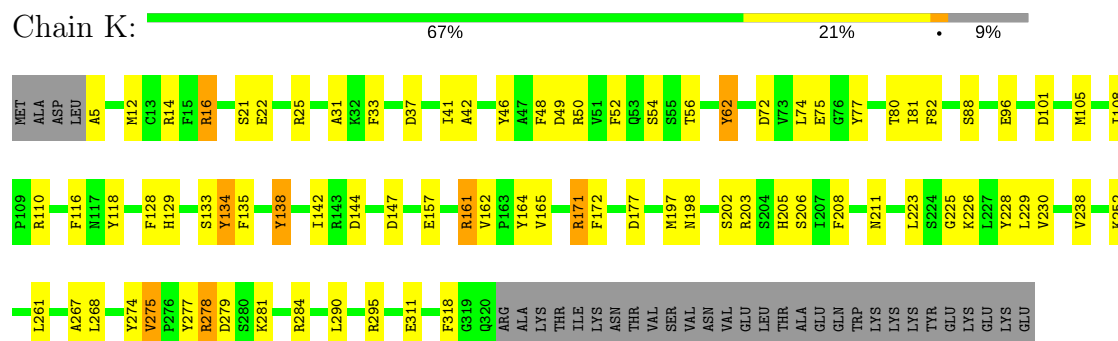


Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total 28	C 10	N 5	O 11 P 2	0

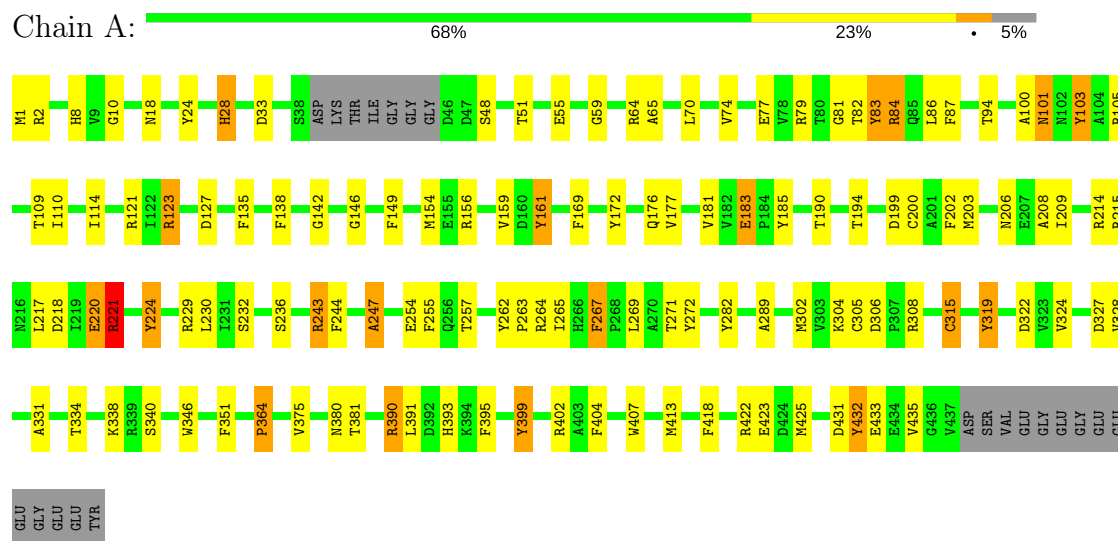
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

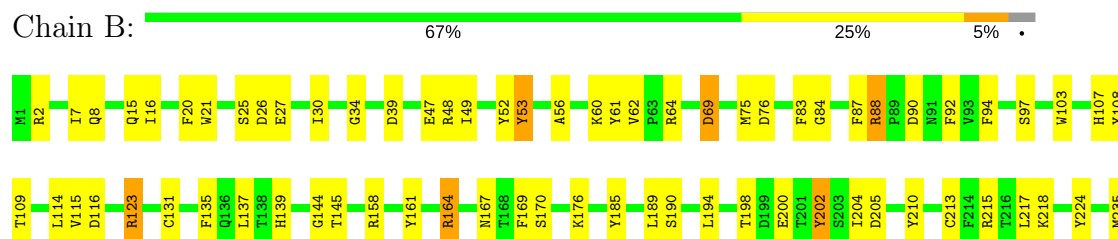
• Molecule 1: Kinesin-1 heavy chain

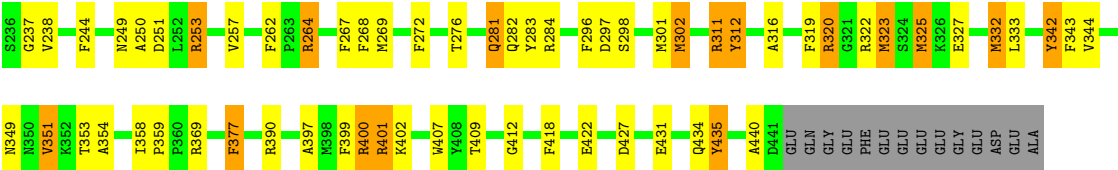


• Molecule 2: Tubulin alpha-1B chain



• Molecule 3: Tubulin beta-2B chain





4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	120783	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	done within FREALIGN	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 (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, 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	K	1.64	15/2513 (0.6%)	1.96	67/3389 (2.0%)
2	A	1.64	21/3450 (0.6%)	2.01	92/4685 (2.0%)
3	B	1.61	16/3464 (0.5%)	2.06	119/4692 (2.5%)
All	All	1.63	52/9427 (0.6%)	2.02	278/12766 (2.2%)

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	K	0	10
2	A	1	19
3	B	0	18
All	All	1	47

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	412	GLY	CA-C	-7.85	1.39	1.51
1	K	277	TYR	CG-CD2	7.84	1.49	1.39
2	A	282	TYR	CG-CD2	7.35	1.48	1.39
1	K	206	SER	CA-CB	7.00	1.63	1.52
2	A	305	CYS	CB-SG	6.45	1.93	1.82

The worst 5 of 278 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	278	ARG	NE-CZ-NH2	-17.75	111.43	120.30
2	A	272	TYR	CB-CG-CD2	-17.55	110.47	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	243	ARG	NE-CZ-NH1	17.17	128.88	120.30
3	B	108	TYR	CB-CG-CD1	16.12	130.68	121.00
1	K	25	ARG	NE-CZ-NH1	15.52	128.06	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	46	ASP	CA

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	110	ARG	Sidechain
1	K	129	HIS	Sidechain
1	K	16	ARG	Sidechain
1	K	62	TYR	Sidechain
1	K	75	GLU	Peptide

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	K	2474	0	2434	6	0
2	A	3372	0	3287	16	0
3	B	3389	0	3266	13	0
4	A	32	0	12	0	0
5	B	28	0	12	0	0
All	All	9295	0	9011	31	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.

The worst 5 of 31 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:A:208:ALA:HB2	2:A:304:LYS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:332:MET:HG3	3:B:351:VAL:HG11	1.87	0.56
2:A:407:TRP:CE3	3:B:257:VAL:HG22	2.41	0.55
3:B:69:ASP:HA	3:B:145:THR:HG21	1.87	0.55
3:B:30:ILE:HD11	3:B:49:ILE:HD11	1.90	0.53

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	K	314/349 (90%)	273 (87%)	39 (12%)	2 (1%)	28	70
2	A	428/451 (95%)	374 (87%)	44 (10%)	10 (2%)	7	44
3	B	429/445 (96%)	367 (86%)	51 (12%)	11 (3%)	6	41
All	All	1171/1245 (94%)	1014 (87%)	134 (11%)	23 (2%)	13	47

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	220	GLU
3	B	84	GLY
3	B	282	GLN
3	B	349	ASN
2	A	59	GLY

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	K	279/311 (90%)	272 (98%)	7 (2%)	53	77
2	A	364/379 (96%)	352 (97%)	12 (3%)	43	70
3	B	372/383 (97%)	360 (97%)	12 (3%)	44	71
All	All	1015/1073 (95%)	984 (97%)	31 (3%)	49	71

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	221	ARG
2	A	381	THR
3	B	332	MET
2	A	230	LEU
2	A	413	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	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	GTP	A	600	-	27,34,34	1.93	7 (25%)	27,54,54	3.18	10 (37%)
5	GDP	B	501	-	25,30,30	1.94	6 (24%)	26,47,47	3.20	7 (26%)

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	600	-	-	0/18/38/38	0/3/3/3
5	GDP	B	501	-	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	GDP	C2'-C1'	-6.30	1.43	1.53
5	B	501	GDP	C8-N7	-3.23	1.28	1.34
4	A	600	GTP	PG-O3B	-2.32	1.56	1.60
5	B	501	GDP	C2-N2	-2.23	1.29	1.34
5	B	501	GDP	O6-C6	-2.06	1.19	1.24

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	GDP	C5-C6-N1	-9.11	110.51	123.48
4	A	600	GTP	C5-C6-N1	-8.50	111.38	123.48
4	A	600	GTP	C6-C5-C4	-5.70	115.18	120.84
5	B	501	GDP	N3-C2-N1	-5.12	119.99	127.46
5	B	501	GDP	O4'-C4'-C3'	-3.52	98.17	105.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.