



wwPDB EM Map/Model Validation Report ⓘ

Oct 25, 2016 – 12:29 PM EDT

PDB ID : 5HNX
EMDB ID: : EMD-8059
Title : Structural basis of backwards motion in kinesin-14: minus-end directed nKn664 in the nucleotide-free state
Authors : Shigematsu, H.; Yokoyama, T.; Kikkawa, M.; Shirouzu, M.; Nitta, R.
Deposited on : 2016-01-19
Resolution : 6.60 Å(reported)

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) : rb-20027939

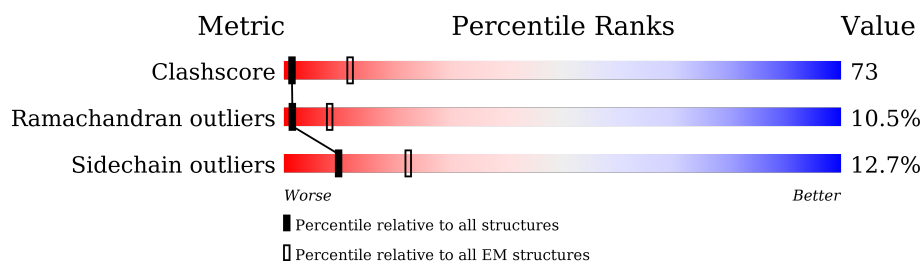
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 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	451	
2	B	445	
3	K	371	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GTP	A	502	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9198 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
1	A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	SER	LEU	conflict	UNP P81947
A	232	GLY	SER	conflict	UNP P81947
A	265	GLY	ILE	conflict	UNP P81947
A	340	THR	SER	conflict	UNP P81947
A	358	GLU	GLN	conflict	UNP P81947

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	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
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

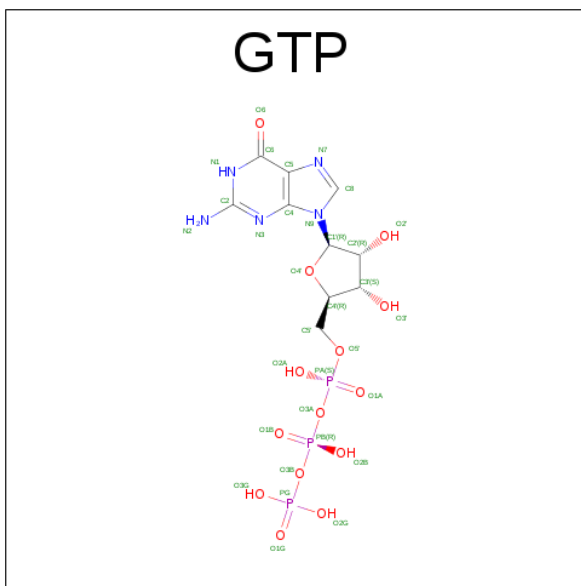
- Molecule 3 is a protein called Protein claret segregational,kinesin-1/kinesin-14,Protein claret segregational.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	320	Total	C	N	O	S	0	0
			2497	1567	432	485	13		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

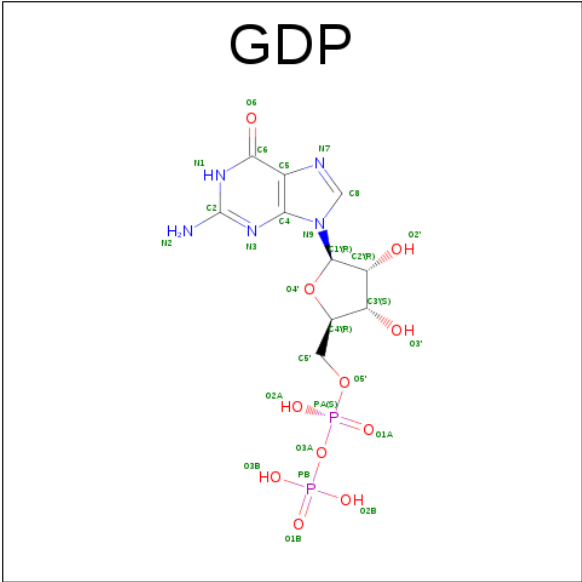
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

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



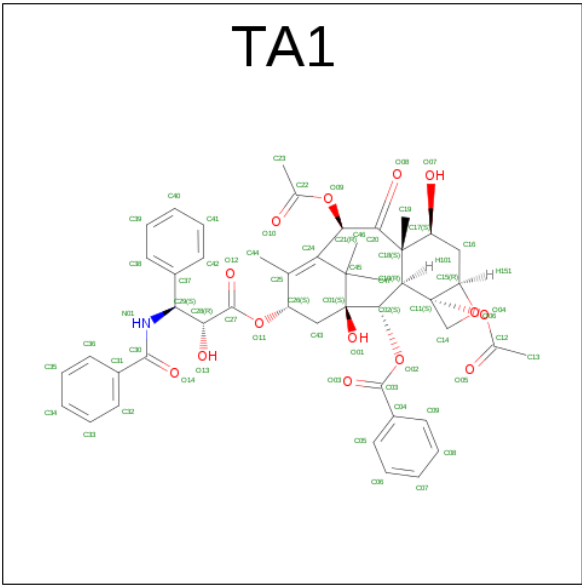
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

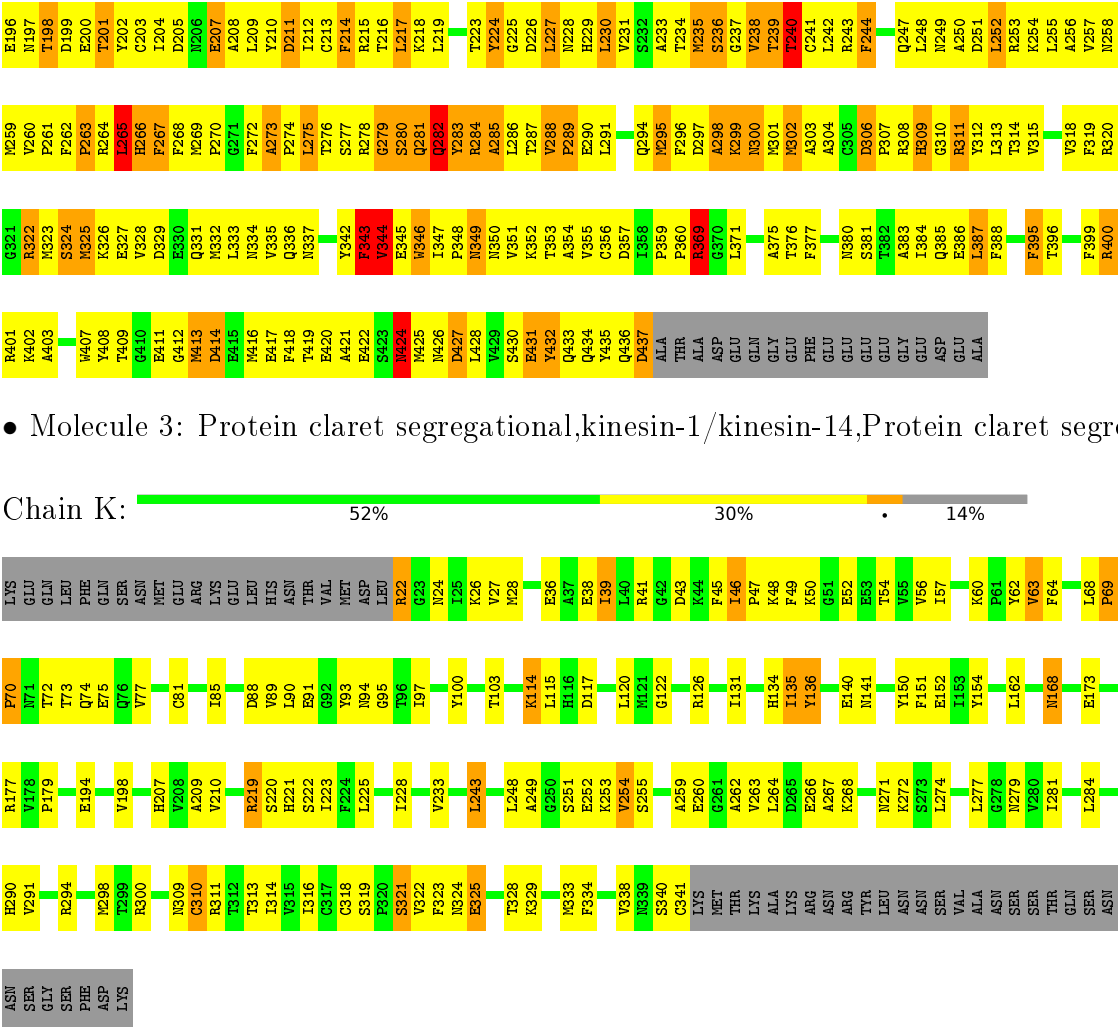
- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 7 is TAXOL (three-letter code: TA1) (formula: C₄₇H₅₁NO₁₄).





● Molecule 3: Protein claret segregational,kinesin-1/kinesin-14,Protein claret segregational

Chain K: 52% 30% 14%

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	229516	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.51	0/3300	0.73	0/4482
2	B	0.51	0/3426	0.76	2/4642 (0.0%)
3	K	0.91	2/2538 (0.1%)	0.99	7/3425 (0.2%)
All	All	0.64	2/9264 (0.0%)	0.82	9/12549 (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	K	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	69	PRO	N-CD	25.09	1.82	1.47
3	K	70	PRO	N-CD	21.14	1.77	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	168	ASN	O-C-N	-12.74	102.32	122.70
3	K	168	ASN	CA-C-N	8.09	134.99	117.20
3	K	69	PRO	CA-N-CD	-7.10	101.56	111.50
2	B	235	MET	CG-SD-CE	6.13	110.00	100.20
3	K	70	PRO	CA-N-CD	-5.67	103.56	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	168	ASN	Mainchain,Peptide
3	K	22	ARG	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	3227	0	3143	628	0
2	B	3351	0	3229	625	0
3	K	2497	0	2498	204	0
4	A	1	0	0	0	0
5	A	32	0	12	12	0
6	B	28	0	12	2	0
7	B	62	0	51	12	0
All	All	9198	0	8945	1321	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 73.

The worst 5 of 1321 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:416:MET:HE1	3:K:173:GLU:CB	1.39	1.47
1:A:108:TYR:CE2	3:K:255:SER:HB2	1.50	1.44
2:B:434:GLN:CD	3:K:290:HIS:HB2	1.38	1.42
2:B:416:MET:CE	3:K:173:GLU:HB2	1.46	1.42
3:K:70:PRO:CD	3:K:70:PRO:N	1.77	1.32

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	408/451 (90%)	265 (65%)	84 (21%)	59 (14%)	0	6
2	B	424/445 (95%)	273 (64%)	95 (22%)	56 (13%)	0	7
3	K	318/371 (86%)	287 (90%)	25 (8%)	6 (2%)	10	52
All	All	1150/1267 (91%)	825 (72%)	204 (18%)	121 (10%)	1	12

5 of 121 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	97	GLU
1	A	108	TYR
1	A	109	THR
1	A	141	PHE

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	347/377 (92%)	298 (86%)	49 (14%)	4	26
2	B	367/381 (96%)	307 (84%)	60 (16%)	3	20
3	K	280/330 (85%)	263 (94%)	17 (6%)	23	60
All	All	994/1088 (91%)	868 (87%)	126 (13%)	10	29

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	90	ASP
2	B	198	THR
3	K	140	GLU
2	B	101	ASN
2	B	145	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	101	ASN
2	B	139	HIS
3	K	207	HIS
2	B	102	ASN
2	B	107	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](#)

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	$\# Z > 2$
5	GTP	A	502	4	26,34,34	1.34	1 (3%)	29,54,54	2.28	4 (13%)
6	GDP	B	901	-	24,30,30	2.68	8 (33%)	26,47,47	3.30	8 (30%)
7	TA1	B	902	-	68,68,68	1.94	20 (29%)	102,105,105	1.31	8 (7%)

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
5	GTP	A	502	4	-	0/18/38/38	0/3/3/3
6	GDP	B	901	-	-	0/12/32/32	0/3/3/3
7	TA1	B	902	-	-	0/41/127/127	0/5/7/7

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	902	TA1	C08-C07	-4.96	1.25	1.38
6	B	901	GDP	PB-O2B	-4.22	1.40	1.54
7	B	902	TA1	C04-C03	-2.31	1.44	1.49
7	B	902	TA1	C10-C02	2.06	1.62	1.57
7	B	902	TA1	C18-C20	2.07	1.62	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	901	GDP	C6-C5-C4	-9.88	109.56	120.86
5	A	502	GTP	C5-C6-N1	-7.72	113.44	123.52
6	B	901	GDP	N2-C2-N1	-5.75	107.71	117.20
6	B	901	GDP	N3-C2-N1	-5.38	120.24	127.56
7	B	902	TA1	C06-C05-C04	-4.80	114.63	120.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	GTP	12	0
6	B	901	GDP	2	0
7	B	902	TA1	12	0

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.