



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:37 PM BST

PDB ID : 2HXF
Title : KIF1A head-microtubule complex structure in amppnp-form
Authors : Kikkawa, M.; Hirokawa, N.
Deposited on : 2006-08-03
Resolution : 10.00 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) : trunk27241

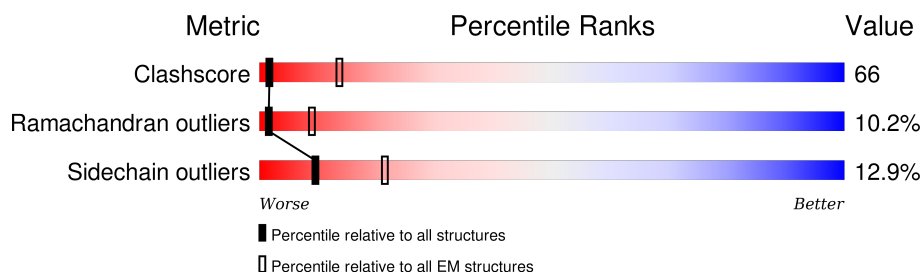
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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	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	C	394	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9279 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 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		

- Molecule 2 is a protein called Tubulin beta chain.

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

- Molecule 3 is a protein called Kinesin-like protein KIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	324	Total	C	N	O	S	0	0
			2546	1581	446	505	14		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	MET	-	CLONING ARTIFACT	UNP P33173
C	-14	ALA	-	CLONING ARTIFACT	UNP P33173
C	-13	SER	-	CLONING ARTIFACT	UNP P33173
C	-12	MET	-	CLONING ARTIFACT	UNP P33173
C	-11	THR	-	CLONING ARTIFACT	UNP P33173
C	-10	GLY	-	CLONING ARTIFACT	UNP P33173
C	-9	GLY	-	CLONING ARTIFACT	UNP P33173
C	-8	GLN	-	CLONING ARTIFACT	UNP P33173
C	-7	GLN	-	CLONING ARTIFACT	UNP P33173
C	-6	MET	-	CLONING ARTIFACT	UNP P33173
C	-5	GLY	-	CLONING ARTIFACT	UNP P33173
C	-4	ARG	-	CLONING ARTIFACT	UNP P33173
C	-3	ASP	-	CLONING ARTIFACT	UNP P33173
C	-2	PRO	-	CLONING ARTIFACT	UNP P33173
C	-1	ILE	-	CLONING ARTIFACT	UNP P33173

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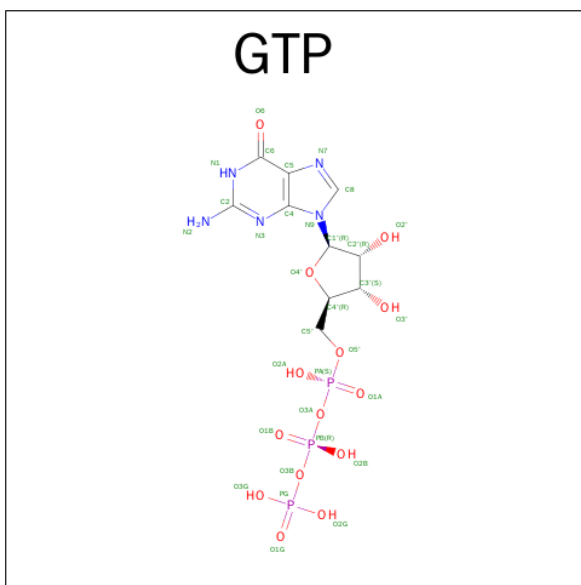
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ASN	-	CLONING ARTIFACT	UNP P33173
C	1	MET	-	CLONING ARTIFACT	UNP P33173
C	2	PRO	-	CLONING ARTIFACT	UNP P33173
C	202	ALA	PRO	ENGINEERED	UNP P33173
C	356	ASN	-	LINKER	UNP P33173
C	357	THR	-	LINKER	UNP P33173
C	358	VAL	-	LINKER	UNP P33173
C	359	SER	-	LINKER	UNP P33173
C	360	VAL	-	LINKER	UNP P33173
C	361	ASN	-	LINKER	UNP P33173
C	362	LEU	-	LINKER	UNP P33173
C	363	GLU	-	LINKER	UNP P33173
C	364	LEU	-	LINKER	UNP P33173
C	365	THR	-	LINKER	UNP P33173
C	366	ALA	-	LINKER	UNP P33173
C	367	GLU	-	LINKER	UNP P33173
C	368	GLU	-	LINKER	UNP P33173
C	369	TRP	-	LINKER	UNP P33173
C	370	LYS	-	LINKER	UNP P33173
C	371	LYS	-	LINKER	UNP P33173
C	372	LYS	-	LINKER	UNP P33173
C	373	HIS	-	EXPRESSION TAG	UNP P33173
C	374	HIS	-	EXPRESSION TAG	UNP P33173
C	375	HIS	-	EXPRESSION TAG	UNP P33173
C	376	HIS	-	EXPRESSION TAG	UNP P33173
C	377	HIS	-	EXPRESSION TAG	UNP P33173
C	378	HIS	-	EXPRESSION TAG	UNP P33173

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

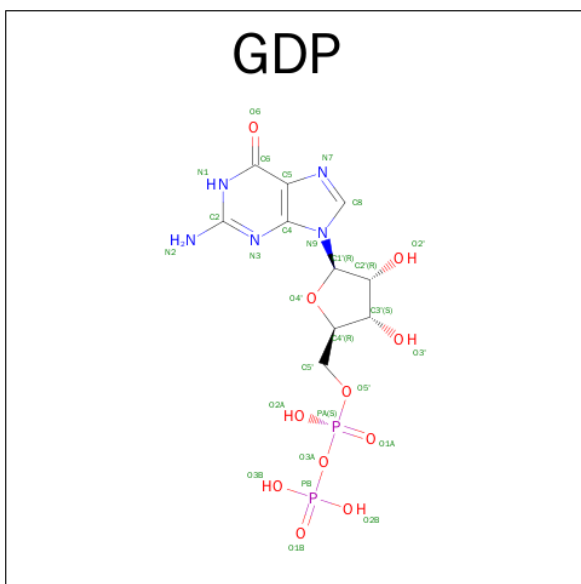
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0

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



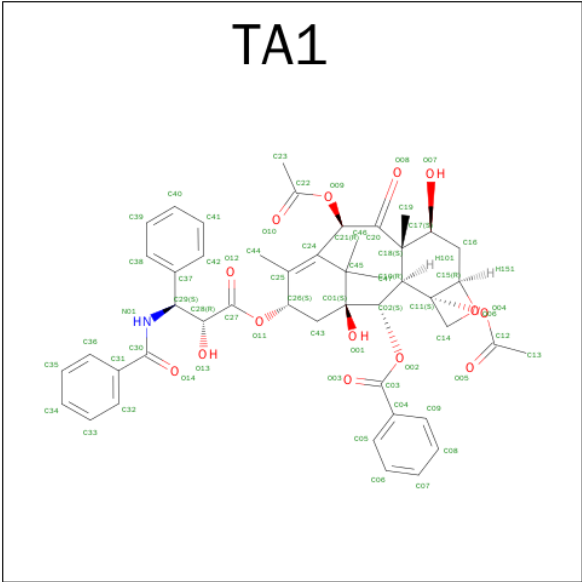
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



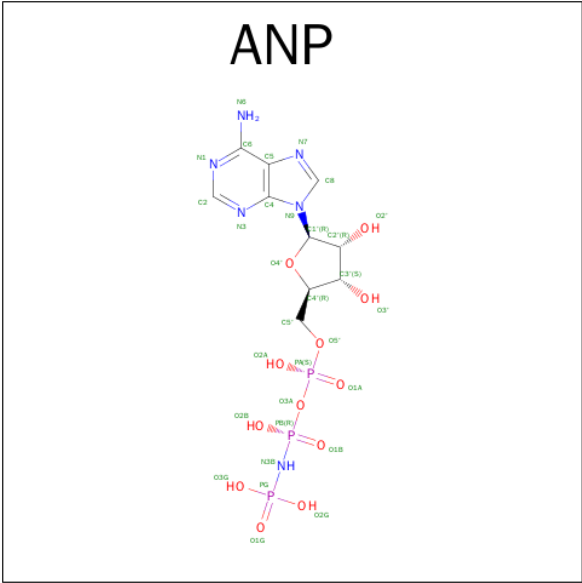
Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

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



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

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	N	O	P	0
			31	10	6	12	3	

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	each filament	Depositor
Microscope	JEM-2010F	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	11000	Depositor
Maximum defocus (nm)	33000	Depositor
Magnification	40000	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, ANP, 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	0.50	0/3300	0.73	0/4482
2	B	0.51	0/3426	0.76	2/4642 (0.0%)
3	C	0.46	0/2585	0.80	3/3491 (0.1%)
All	All	0.49	0/9311	0.76	5/12615 (0.0%)

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	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	213	THR	CA-CB-CG2	-13.59	93.38	112.40
3	C	155	ARG	NE-CZ-NH2	-8.47	116.07	120.30
2	B	235	MET	CG-SD-CE	6.09	109.95	100.20
3	C	155	ARG	CD-NE-CZ	-6.03	115.16	123.60
2	B	217	LEU	N-CA-C	-5.36	96.53	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	155	ARG	Sidechain
3	C	74	TYR	Sidechain

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	3141	566	0
2	B	3351	0	3227	569	0
3	C	2546	0	2507	132	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	12	5	0
6	B	28	0	12	1	0
7	B	62	0	51	5	0
8	C	31	0	13	0	0
All	All	9279	0	8963	1206	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 66.

The worst 5 of 1206 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:204:THR:CA	3:C:205:VAL:HB	1.63	1.27
1:A:414:GLU:HB2	3:C:253:GLU:O	1.32	1.25
1:A:409:VAL:HG12	3:C:272:ASN:CB	1.69	1.23
2:B:234:THR:HG21	2:B:270:PRO:HB2	1.23	1.17
1:A:243:ARG:NH2	1:A:252:LEU:H	1.45	1.14

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%)	266 (65%)	83 (20%)	59 (14%)	0	6
2	B	424/445 (95%)	273 (64%)	95 (22%)	56 (13%)	0	7
3	C	316/394 (80%)	309 (98%)	5 (2%)	2 (1%)	30	74
All	All	1148/1290 (89%)	848 (74%)	183 (16%)	117 (10%)	1	13

5 of 117 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	C	286/345 (83%)	266 (93%)	20 (7%)	19	56
All	All	1000/1103 (91%)	871 (87%)	129 (13%)	9	28

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	101	ASN
2	B	203	CYS
3	C	229	ARG
2	B	129	CYS
2	B	153	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	101	ASN
2	B	136	GLN
3	C	162	ASN
2	B	102	ASN
2	B	139	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	500	4	26,34,34	1.35	1 (3%)	29,54,54	2.28	4 (13%)
6	GDP	B	600	-	24,30,30	2.66	8 (33%)	26,47,47	3.29	8 (30%)
7	TA1	B	601	-	68,68,68	1.93	20 (29%)	102,105,105	1.31	8 (7%)
8	ANP	C	1500	4	29,33,33	2.06	8 (27%)	26,52,52	3.59	13 (50%)

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	500	4	-	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
8	ANP	C	1500	4	-	0/13/38/38	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	601	TA1	C08-C07	-4.94	1.25	1.38
6	B	600	GDP	PB-O2B	-4.19	1.40	1.54
8	C	1500	ANP	PB-O2B	-3.80	1.46	1.56
8	C	1500	ANP	PG-O2G	-3.78	1.46	1.56
8	C	1500	ANP	PB-O1B	-3.61	1.42	1.46

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	GDP	C6-C5-C4	-9.88	109.56	120.86
8	C	1500	ANP	O5'-PA-O1A	-7.77	77.41	109.21
5	A	500	GTP	C5-C6-N1	-7.76	113.38	123.52
8	C	1500	ANP	N3-C2-N1	-7.11	123.28	128.87
8	C	1500	ANP	O2A-PA-O5'	-6.03	79.49	108.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	GTP	5	0
6	B	600	GDP	1	0
7	B	601	TA1	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.