



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:44 PM BST

PDB ID : 3J2U
EMDB ID: : EMD-5565
Title : Kinesin-13 KLP10A HD in complex with CS-tubulin and a microtubule
Authors : Asenjo, A.B.; Chatterjee, C.; Tan, D.; DePaoli, V.; Rice, W.J.; Diaz-Avalos, R.; Silvestry, M.; Sosa, H.
Deposited on : 2013-01-10
Resolution : 10.80 Å(reported)
Based on PDB ID : 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

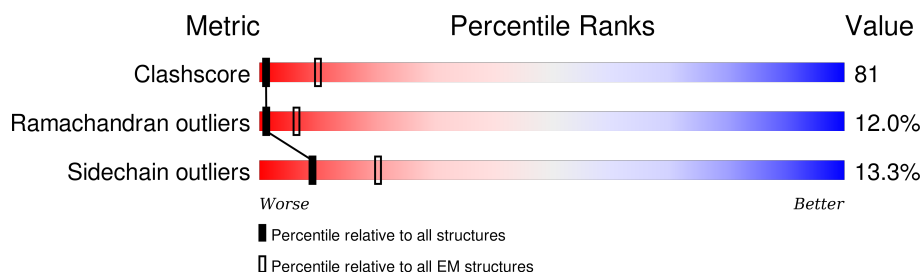
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.80 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	K	374	
2	A	451	
2	C	451	
3	B	445	
3	D	445	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15575 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-like protein Klp10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	309	Total	C	N	O	S	0	0
			2419	1525	432	446	16		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	242	MET	-	EXPRESSION TAG	UNP Q960Z0
K	243	ARG	-	EXPRESSION TAG	UNP Q960Z0
K	244	GLY	-	EXPRESSION TAG	UNP Q960Z0
K	245	SER	-	EXPRESSION TAG	UNP Q960Z0
K	246	HIS	-	EXPRESSION TAG	UNP Q960Z0
K	247	HIS	-	EXPRESSION TAG	UNP Q960Z0
K	248	HIS	-	EXPRESSION TAG	UNP Q960Z0
K	249	HIS	-	EXPRESSION TAG	UNP Q960Z0
K	250	HIS	-	EXPRESSION TAG	UNP Q960Z0
K	251	HIS	-	EXPRESSION TAG	UNP Q960Z0
K	252	GLY	-	EXPRESSION TAG	UNP Q960Z0
K	253	MET	-	EXPRESSION TAG	UNP Q960Z0
K	254	ALA	-	EXPRESSION TAG	UNP Q960Z0
K	255	SER	-	EXPRESSION TAG	UNP Q960Z0
K	256	MET	-	EXPRESSION TAG	UNP Q960Z0
K	257	THR	-	EXPRESSION TAG	UNP Q960Z0
K	258	GLY	-	EXPRESSION TAG	UNP Q960Z0
K	259	GLY	-	EXPRESSION TAG	UNP Q960Z0
K	260	GLN	-	EXPRESSION TAG	UNP Q960Z0
K	261	GLN	-	EXPRESSION TAG	UNP Q960Z0
K	262	MET	-	EXPRESSION TAG	UNP Q960Z0
K	263	GLY	-	EXPRESSION TAG	UNP Q960Z0
K	264	ARG	-	EXPRESSION TAG	UNP Q960Z0
K	265	ASP	-	EXPRESSION TAG	UNP Q960Z0
K	266	LEU	-	EXPRESSION TAG	UNP Q960Z0
K	267	TYR	-	EXPRESSION TAG	UNP Q960Z0
K	268	ASP	-	EXPRESSION TAG	UNP Q960Z0
K	269	ASP	-	EXPRESSION TAG	UNP Q960Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
K	270	ASP	-	EXPRESSION TAG	UNP Q960Z0
K	271	ASP	-	EXPRESSION TAG	UNP Q960Z0
K	272	LYS	-	EXPRESSION TAG	UNP Q960Z0
K	273	ASP	-	EXPRESSION TAG	UNP Q960Z0
K	274	PRO	-	EXPRESSION TAG	UNP Q960Z0
K	275	SER	-	EXPRESSION TAG	UNP Q960Z0
K	276	SER	-	EXPRESSION TAG	UNP Q960Z0
K	277	ARG	-	EXPRESSION TAG	UNP Q960Z0
K	278	SER	-	EXPRESSION TAG	UNP Q960Z0

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

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

There are 10 discrepancies between the modelled and reference sequences:

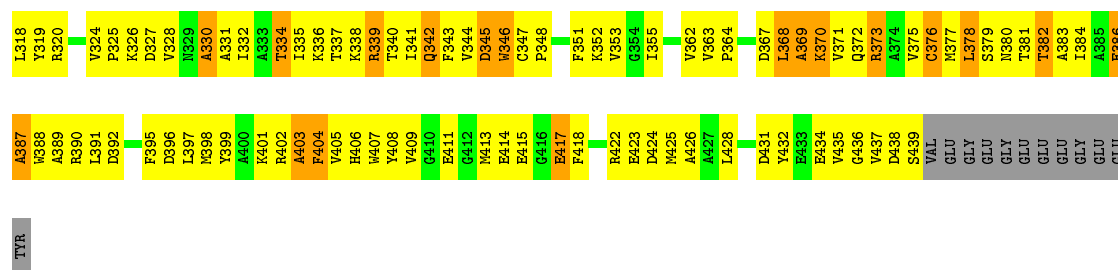
Chain	Residue	Modelled	Actual	Comment	Reference
A	136	SER	LEU	CONFLICT	UNP P81947
A	232	GLY	SER	CONFLICT	UNP P81947
A	265	GLY	ILE	CONFLICT	UNP P81947
A	340	THR	SER	CONFLICT	UNP P81947
A	358	GLU	GLN	CONFLICT	UNP P81947
C	136	SER	LEU	CONFLICT	UNP P81947
C	232	GLY	SER	CONFLICT	UNP P81947
C	265	GLY	ILE	CONFLICT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

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

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

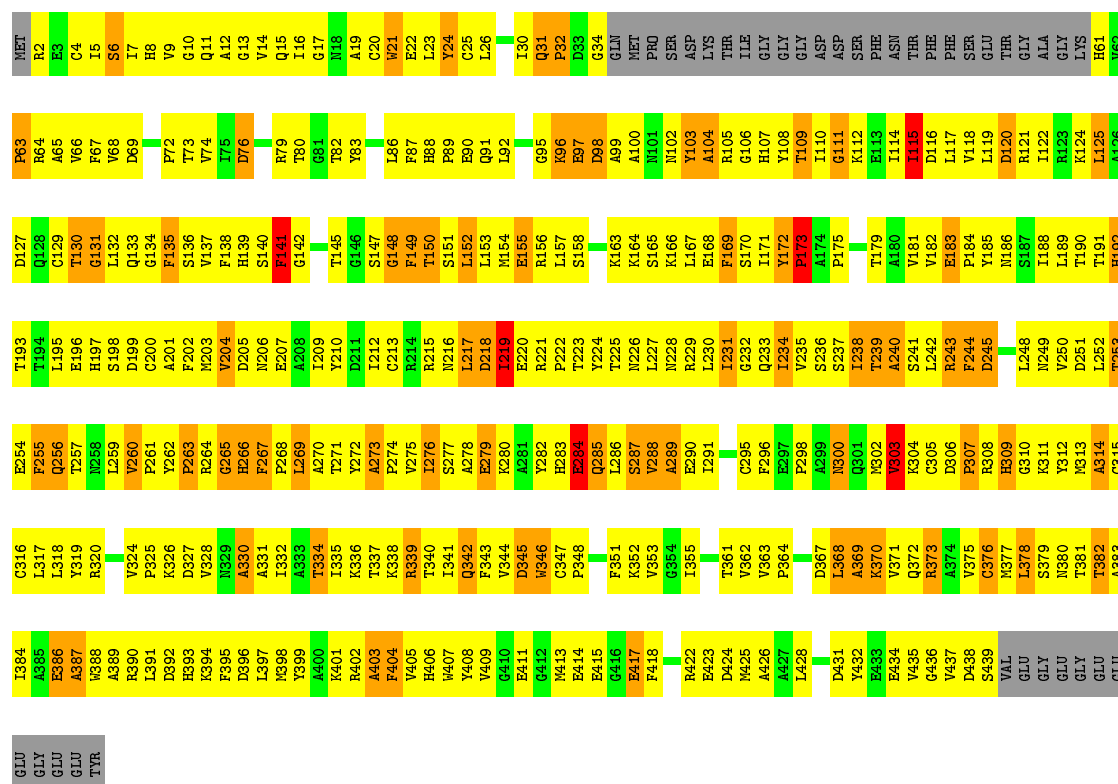
There are 12 discrepancies between the modelled and reference sequences:

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
B	450	GLY	GLU	CONFLICT	UNP Q6B856
B	451	GLU	GLY	CONFLICT	UNP Q6B856
D	57	ALA	THR	CONFLICT	UNP Q6B856
D	172	VAL	MET	CONFLICT	UNP Q6B856
D	298	ALA	SER	CONFLICT	UNP Q6B856
D	318	VAL	ILE	CONFLICT	UNP Q6B856
D	450	GLY	GLU	CONFLICT	UNP Q6B856
D	451	GLU	GLY	CONFLICT	UNP Q6B856



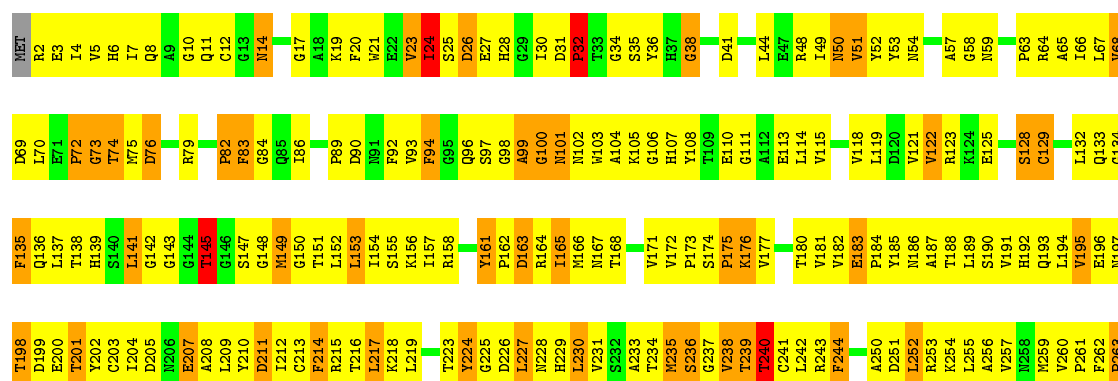
• Molecule 2: Tubulin alpha-1A chain

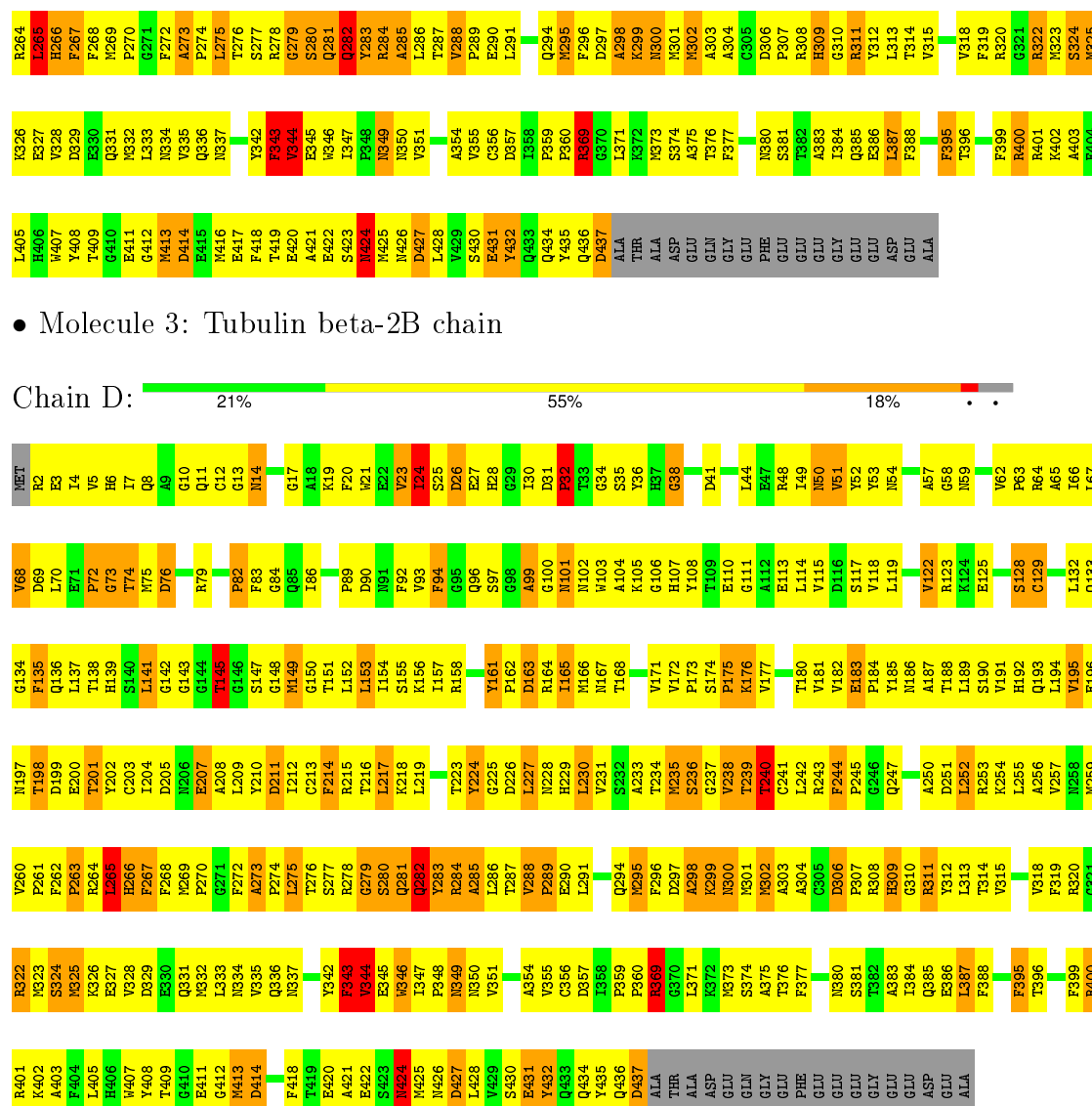
Chain C: 17% 56% 17% 9%



• Molecule 3: Tubulin beta-2B chain

Chain B: 21% 55% 18%





4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	54584	Depositor
Resolution determination method	FSC calculated from two independently re-fined maps at 0.143 cut-off.	Depositor
CTF correction method	each particle	Depositor
Microscope	JEOL 3200FSC, FEI TECNAI F20	Depositor
Voltage (kV)	300, 200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided, Not provided	Depositor
Minimum defocus (nm)	Not provided, Not provided	Depositor
Maximum defocus (nm)	Not provided, Not provided	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	Not provided	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	K	0.93	0/2453	1.10	1/3290 (0.0%)
2	A	0.51	0/3300	0.73	0/4482
2	C	0.51	0/3300	0.73	0/4482
3	B	0.51	0/3426	0.76	2/4642 (0.0%)
3	D	0.51	0/3426	0.76	2/4642 (0.0%)
All	All	0.59	0/15905	0.81	5/21538 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	235	MET	CG-SD-CE	6.08	109.92	100.20
3	B	235	MET	CG-SD-CE	6.07	109.92	100.20
1	K	384	GLY	N-CA-C	-5.47	99.43	113.10
3	D	217	LEU	N-CA-C	-5.36	96.54	111.00
3	B	217	LEU	N-CA-C	-5.35	96.56	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2419	0	2487	389	0
2	A	3227	0	3143	520	0
2	C	3227	0	3143	569	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3351	0	3229	563	0
3	D	3351	0	3229	568	0
All	All	15575	0	15231	2506	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 81.

The worst 5 of 2506 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)
1:K:444:ASP:HA	3:B:419:THR:CG2	1.37	1.48
1:K:444:ASP:N	3:B:416:MET:HE1	1.26	1.43
1:K:444:ASP:N	3:B:416:MET:CE	1.87	1.37
1:K:444:ASP:CA	3:B:419:THR:CG2	2.01	1.35
2:C:407:TRP:CZ2	3:D:257:VAL:HA	1.60	1.34

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	303/374 (81%)	285 (94%)	12 (4%)	6 (2%)	9	51
2	A	408/451 (90%)	265 (65%)	84 (21%)	59 (14%)	0	6
2	C	408/451 (90%)	266 (65%)	83 (20%)	59 (14%)	0	6
3	B	424/445 (95%)	274 (65%)	94 (22%)	56 (13%)	0	7
3	D	424/445 (95%)	274 (65%)	94 (22%)	56 (13%)	0	7
All	All	1967/2166 (91%)	1364 (69%)	367 (19%)	236 (12%)	1	8

5 of 236 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	501	GLN
1	K	503	SER
1	K	506	ILE
2	A	96	LYS
2	A	97	GLU

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	K	269/323 (83%)	261 (97%)	8 (3%)	48	77
2	A	347/377 (92%)	298 (86%)	49 (14%)	4	26
2	C	347/377 (92%)	298 (86%)	49 (14%)	4	26
3	B	367/381 (96%)	308 (84%)	59 (16%)	3	20
3	D	367/381 (96%)	307 (84%)	60 (16%)	3	20
All	All	1697/1839 (92%)	1472 (87%)	225 (13%)	9	28

5 of 225 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	324	SER
2	C	125	LEU
3	D	306	ASP
3	B	344	VAL
3	B	432	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	331	GLN
2	C	11	GLN
3	D	337	ASN
3	B	334	ASN
3	B	349	ASN

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.