Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 02:01 PM EDT

PDB ID	:	2L3L
Title	:	The solution structure of the N-terminal domain of human Tubulin Binding Cofactor C reveals a platform for the interaction with ab-tubulin
Authors	:	Garcia-Mayoral, M.F.; Castano, R.; Lopez-Fanarraga, M.L.; Zabala, J.C.; Rico, M.; Bruix, M.
Deposited on	:	2010-09-14

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

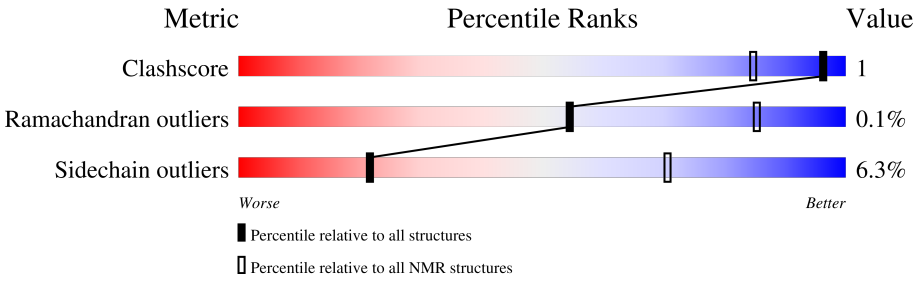
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	111	64% · 34%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:56-A:128 (73)	0.51	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 11, 13, 14, 16, 17, 18, 19, 20
2	10, 12
Single-model clusters	15

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1867 atoms, of which 941 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tubulin-specific chaperone C.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	111	1867	567	941	185	173	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP Q15814

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Tubulin-specific chaperone C

Chain A: 64% • 34%

M25 P26 E27 R28 L29 Q30 R31 R32 E33 Q34 E35 R36 Q37 L38 E39 V40 E41 R42 R43 K44 Q45 K46 R47 Q48 N49 Q50 E51 V52 E53 K54 E55 L91 D109 R129 G130 L131 Q132 P133 K134 K135

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Tubulin-specific chaperone C

Chain A: 60% 5% 34%

M25 P26 E27 R28 L29 Q30 R31 R32 E33 Q34 E35 R36 Q37 L38 E39 V40 E41 R42 R43 K44 Q45 K46 R47 Q48 N49 Q50 E51 V52 E53 K54 E55 R68 L91 K96 L120 R127 R128 R129 G130 L131 Q132 P133 K134 K135

4.2.2 Score per residue for model 2

• Molecule 1: Tubulin-specific chaperone C

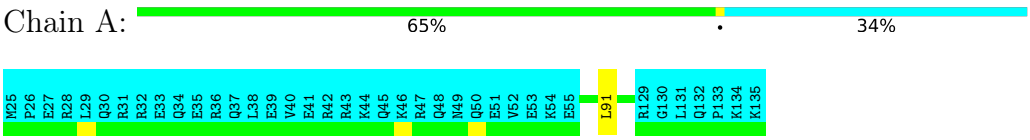
Chain A: 62% • • 34%

M25 P26 E27 R28 L29 Q30 R31 R32 E33 Q34 E35 R36 Q37 L38 E39 V40 E41 R42 R43 K44 Q45 K46 R47 Q48 N49 Q50 E51 V52 E53 K54 E55 V71 L91 D109 Q121 R129 G130 L131 Q132 P133 K134 K135

4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Tubulin-specific chaperone C

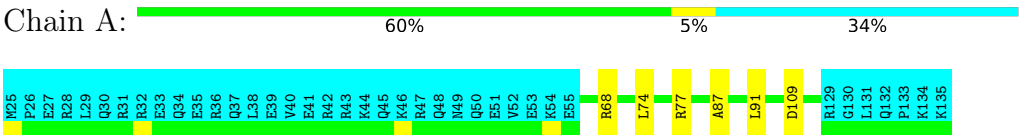
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Tubulin-specific chaperone C

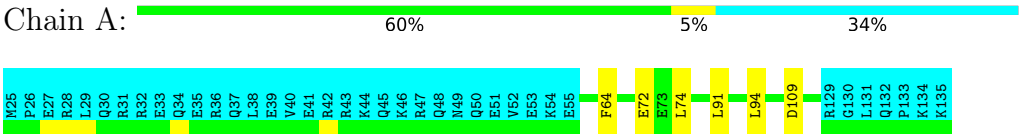
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Tubulin-specific chaperone C

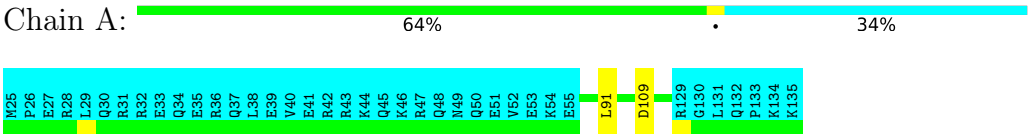
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Tubulin-specific chaperone C

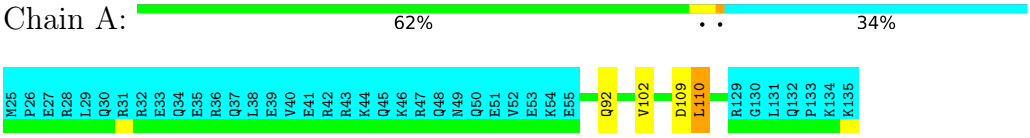
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Tubulin-specific chaperone C

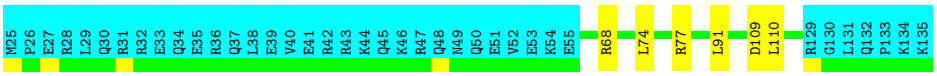
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: Tubulin-specific chaperone C

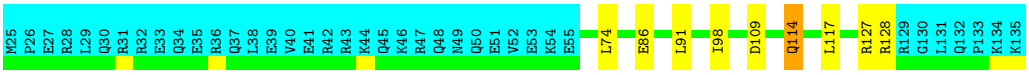
Chain A: 60% 5% 34%



4.2.9 Score per residue for model 9

- Molecule 1: Tubulin-specific chaperone C

Chain A: 58% 7% • 34%



4.2.10 Score per residue for model 10

- Molecule 1: Tubulin-specific chaperone C

Chain A: 59% 7% 34%

4.2.11 Score per residue for model 11

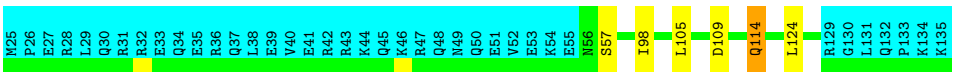
- Molecule 1: Tubulin-specific chaperone C

Chain A: 58% 8% 34%

4.2.12 Score per residue for model 12

- Molecule 1: Tubulin-specific chaperone C

Chain A: 60% 5% • 34%



4.2.13 Score per residue for model 13

- Molecule 1: Tubulin-specific chaperone C

Chain A: 64% • 34%

M25 P26 E27 R28 L29 Q30 R31 R32 E33 Q34 E35 R36 Q37 L38 E39 V40 E41 R42 R43 K44 Q45 K46 R47 Q48 N49 Q50 E51 V52 E53 K54 E55 E86 L91 R129 G130 L131 Q132 P133 K134 K135

4.2.14 Score per residue for model 14

- Molecule 1: Tubulin-specific chaperone C

Chain A: 61% 5% 34%

M25 P26 E27 R28 L29 Q30 R31 R32 E33 Q34 E35 R36 Q37 L38 E39 V40 E41 R42 R43 K44 Q45 K46 R47 Q48 N49 Q50 E51 V52 E53 K54 E55 E76 R77 A78 R83 L91 D109 R129 G130 L131 Q132 P133 K134 K135

4.2.15 Score per residue for model 15

- Molecule 1: Tubulin-specific chaperone C

Chain A: 60% 5% 34%

M25 P26 E27 R28 L29 Q30 R31 R32 E33 Q34 E35 R36 Q37 L38 E39 V40 E41 R42 R43 K44 Q45 K46 R47 Q48 N49 Q50 E51 V52 E53 K54 E55 R68 E72 L91 I98 L105 R111 R129 G130 L131 Q132 P133 K134 K135

4.2.16 Score per residue for model 16

- Molecule 1: Tubulin-specific chaperone C

Chain A: 58% 8% 34%

M25 P26 E27 R28 L29 Q30 R31 R32 E33 Q34 E35 R36 Q37 L38 E39 V40 E41 R42 R43 K44 Q45 K46 R47 Q48 N49 Q50 E51 V52 E53 K54 E55 F64 L74 A87 L91 L94 D109 E115 L124 R127 R128 R129 G130 L131 Q132 P133 K134 K135

4.2.17 Score per residue for model 17

- Molecule 1: Tubulin-specific chaperone C

Chain A: 60% 5% • 34%

M25 P26 E27 R28 L29 Q30 R31 R32 E33 Q34 E35 R36 Q37 L38 E39 V40 E41 R42 R43 K44 Q45 K46 R47 Q48 N49 Q50 E51 V52 E53 K54 E55 V71 L75 A88 S89 R90 L91 A123 R129 G130 L131 Q132 P133 K134 K135

4.2.18 Score per residue for model 18

- Molecule 1: Tubulin-specific chaperone C

Chain A: 62% • 34%

M25 P26 E27 R28 L29 Q30 R31 R32 E33 Q34 E35 R36 Q37 L38 E39 V40 E41 R42 R43 K44 Q45 K46 R47 Q48 M49 Q50 E51 V52 E53 K54 E55 R68 L91 D109 L110 R111 R129 G130 L131 Q132 P133 K134 K135

4.2.19 Score per residue for model 19

- Molecule 1: Tubulin-specific chaperone C

Chain A: 64% • 34%

M25 P26 E27 R28 L29 Q30 R31 R32 E33 Q34 E35 R36 Q37 L38 E39 V40 E41 R42 R43 K44 Q45 K46 R47 Q48 M49 Q50 E51 V52 E53 K54 E55 E76 L124 R129 G130 L131 Q132 P133 K134 K135

4.2.20 Score per residue for model 20

- Molecule 1: Tubulin-specific chaperone C

Chain A: 62% • 34%

M25 P26 E27 R28 L29 Q30 R31 R32 E33 Q34 E35 R36 Q37 L38 E39 V40 E41 R42 R43 K44 Q45 K46 R47 Q48 N49 Q50 E51 V52 E53 K54 E55 R66 L91 D109 L110 R129 G130 L131 Q132 P133 K134 K135

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.73±0.01	0±0/592 (0.0± 0.0%)	0.93±0.02	0±0/796 (0.0± 0.0%)
All	All	0.73	0/11840 (0.0%)	0.93	3/15920 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	111	ARG	NE-CZ-NH1	5.90	123.25	120.30	15	1
1	A	83	ARG	NE-CZ-NH1	5.73	123.16	120.30	14	1
1	A	127	ARG	NE-CZ-NH1	5.39	122.99	120.30	16	1

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	585	583	582	1±1
All	All	11700	11660	11640	18

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 1.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:LEU:HD22	1:A:87:ALA:HB2	0.73	1.58	4	2
1:A:98:ILE:HG21	1:A:114:GLN:HE22	0.68	1.49	12	2
1:A:102:VAL:HG23	1:A:110:LEU:HD21	0.51	1.82	7	1
1:A:75:LEU:HD13	1:A:123:ALA:HB3	0.51	1.82	17	1
1:A:68:ARG:HB2	1:A:120:LEU:HD11	0.47	1.86	1	1
1:A:64:PHE:CD2	1:A:94:LEU:HD22	0.47	2.45	5	3
1:A:67:GLU:HB2	1:A:94:LEU:HD21	0.46	1.88	10	2
1:A:71:VAL:HG22	1:A:90:ARG:HB3	0.46	1.88	17	1
1:A:98:ILE:HG23	1:A:105:LEU:HD12	0.45	1.88	12	2
1:A:75:LEU:HD21	1:A:124:LEU:HD23	0.45	1.89	10	1
1:A:71:VAL:HG11	1:A:91:LEU:HB3	0.42	1.91	2	1
1:A:88:ALA:HA	1:A:91:LEU:HD23	0.40	1.93	17	1

6.3 Torsion angles (i)

6.3.1 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 NMR 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	73/111 (66%)	72±1 (99±1%)	1±1 (1±1%)	0±0 (0±0%)	54	85
All	All	1460/2220 (66%)	1444 (99%)	15 (1%)	1 (0%)	54	85

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	78	ALA	1

6.3.2 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 NMR 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	57/94 (61%)	53±2 (94±3%)	4±2 (6±3%)	21	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1140/1880 (61%)	1068 (94%)	72 (6%)	21 70

All 23 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	91	LEU	17
1	A	109	ASP	14
1	A	68	ARG	4
1	A	74	LEU	4
1	A	110	LEU	4
1	A	124	LEU	4
1	A	127	ARG	2
1	A	128	ARG	2
1	A	77	ARG	2
1	A	72	GLU	2
1	A	86	GLU	2
1	A	114	GLN	2
1	A	117	LEU	2
1	A	76	GLU	2
1	A	96	LYS	1
1	A	121	GLN	1
1	A	92	GLN	1
1	A	95	GLN	1
1	A	100	ASP	1
1	A	57	SER	1
1	A	115	GLU	1
1	A	111	ARG	1
1	A	66	ARG	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided