wwPDB NMR Structure Validation Summary Report (i)

Apr 26, 2016 – 09:26 PM BST

PDB ID	:	2JRF
Title	:	Solution NMR structure of Tubulin polymerization-promoting protein family member 3 from Homo sapiens. Northeast Structural Genomics target HR387.
Authors	:	Aramini, J.M.; Rossi, P.; Shastry, R.; Nwosu, C.; Cunningham, K.; Xiao, R.; Liu, J.; Baran, M.C.; Rajan, P.K.; Acton, T.B.; Rost, B.; Montelione, G.T.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2007-06-25

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

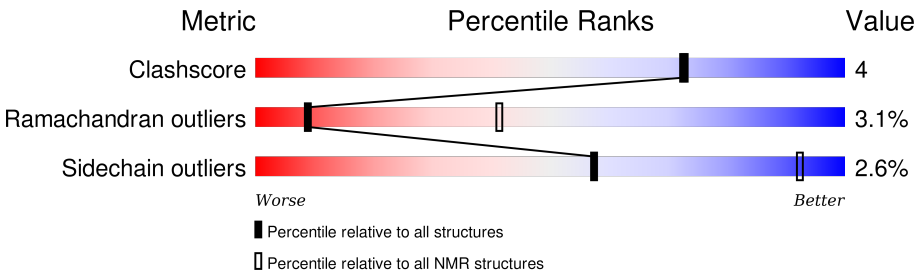
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 is 93%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	184	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:7-A:109 (103)	0.68	10

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 1 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2708 atoms, of which 1360 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tubulin polymerization-promoting protein family member 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	178	2708	838	1360	238	267	5	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ILE	MET	SEE REMARK 999	UNP Q9BW30
A	177	LEU	-	CLONING ARTIFACT	UNP Q9BW30
A	178	GLU	-	CLONING ARTIFACT	UNP Q9BW30
A	179	HIS	-	CLONING ARTIFACT	UNP Q9BW30
A	180	HIS	-	CLONING ARTIFACT	UNP Q9BW30
A	181	HIS	-	CLONING ARTIFACT	UNP Q9BW30
A	182	HIS	-	CLONING ARTIFACT	UNP Q9BW30
A	183	HIS	-	CLONING ARTIFACT	UNP Q9BW30
A	184	HIS	-	CLONING ARTIFACT	UNP Q9BW30

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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 polymerization-promoting protein family member 3

Chain A: 53% • 41% •

M1 A2 A3 S4 T5 D6 R15 C42 T53 I57 E107 N110 V111 G112 V113 T114 K115 A116 K117 T118 G119 G120 A121 V122 D123 R124 L125 T126 D127 T128 S129 R130 Y131 T132 G133 S134 H135 K136 E137 R138 F139 D140 E141 S142 G143 K144 G145 K146 G147 I148 A149 G150 R151 Q152

D153 I154 L155 D156 D157 S158 G159 Y160 V161 S162 A163 Y164 K165 N166 A167 G168 T169 Y170 D171 A172 K173 V174 K175 K176 L177 E178 HIS HIS HIS HIS HIS HIS

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 10. Colouring as in section 4.1 above.

- Molecule 1: Tubulin polymerization-promoting protein family member 3

Chain A: 46% 10% 41% •

M1 A2 A3 S4 T5 D6 I7 A8 G9 H20 N31 N34 C42 K43 V44 T53 D54 I57 G64 N71 R86 F87 K88 G89 V103 E107 P108 A109 N110 V111 G112 V113 T114 K115 A116 K117 T118 G119 G120 A121 V122 D123 R124 L125 T126 D127 T128 S129 R130

Y131 T132 G133 S134 H135 K136 E137 R138 F139 D140 E141 S142 G143 K144 G145 K146 G147 I148 A149 G150 R151 Q152 D153 I154 L155 D156 D157 S158 G159 Y160 V161 S162 A163 Y164 K165 N166 A167 G168 T169 Y170 D171 A172 K173 V174 K175 K176 L177 E178 HIS HIS HIS HIS HIS HIS

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
AutoStructure	structure solution	2.1.1
X-PLOR NIH	structure solution	2.11.2
X-PLOR NIH	refinement	2.11.2
CNS	refinement	1.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 15329
Number of chemical shift lists	1
Total number of shifts	2048
Number of shifts mapped to atoms	2048
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	790	808	807	7±3
All	All	15800	16160	16140	134

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 4.

5 of 90 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:CYS:SG	1:A:102:LEU:HB3	0.86	2.10	14	2
1:A:17:PHE:HB3	1:A:30:MET:SD	0.78	2.18	13	1
1:A:39:CYS:SG	1:A:55:VAL:HG11	0.63	2.34	2	1
1:A:39:CYS:HA	1:A:42:CYS:SG	0.62	2.34	4	2
1:A:42:CYS:HA	1:A:106:LYS:HE2	0.61	1.71	15	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	103/184 (56%)	91±4 (88±4%)	9±3 (9±3%)	3±2 (3±2%)	9 41
All	All	2060/3680 (56%)	1811 (88%)	186 (9%)	63 (3%)	9 41

5 of 24 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	109	ALA	5
1	A	26	SER	5
1	A	20	HIS	5
1	A	65	LYS	4
1	A	25	ALA	4

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	82/145 (57%)	80±2 (97±2%)	2±2 (3±2%)	57 92
All	All	1640/2900 (57%)	1597 (97%)	43 (3%)	57 92

5 of 29 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	107	GLU	5
1	A	74	GLU	4
1	A	43	LYS	2
1	A	15	ARG	2
1	A	17	PHE	2

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 carbohydrates 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)

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 15329

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2048
Number of shifts mapped to atoms	2048
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	176	-0.37 ± 0.07	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	157	0.13 ± 0.04	None needed (< 0.5 ppm)
$^{13}C'$	175	-0.29 ± 0.09	None needed (< 0.5 ppm)
^{15}N	170	-0.36 ± 0.14	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 1158 atoms were assigned a chemical shift out of a possible 1251. 11 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	509/511 (100%)	203/204 (100%)	206/206 (100%)	100/101 (99%)
Sidechain	581/658 (88%)	358/387 (93%)	217/240 (90%)	6/31 (19%)

Continued on next page...

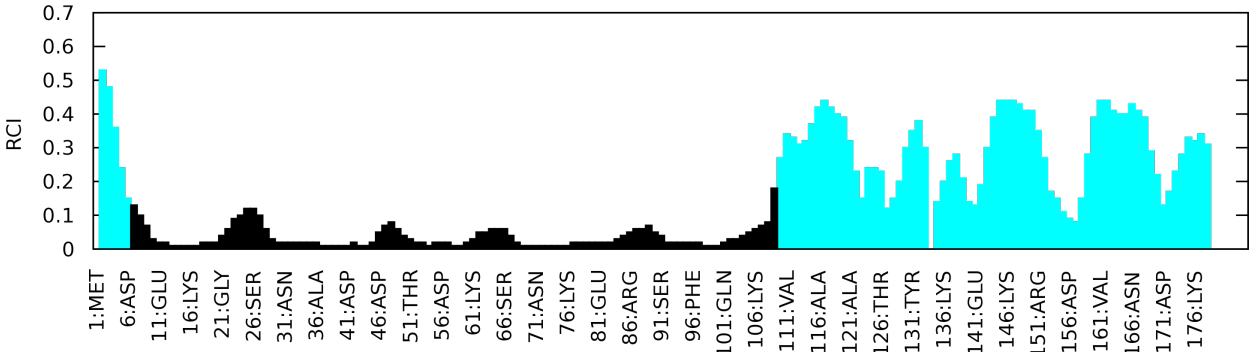
Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	68/82 (83%)	37/44 (84%)	30/35 (86%)	1/3 (33%)
Overall	1158/1251 (93%)	598/635 (94%)	453/481 (94%)	107/135 (79%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A: