wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1WJM
Title	:	Solution structure of pleckstrin homology domain of human beta III spectrin.
Authors	:	Sato, M.; Tochio, N.; Koshiba, S.; Inoue, M.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
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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:

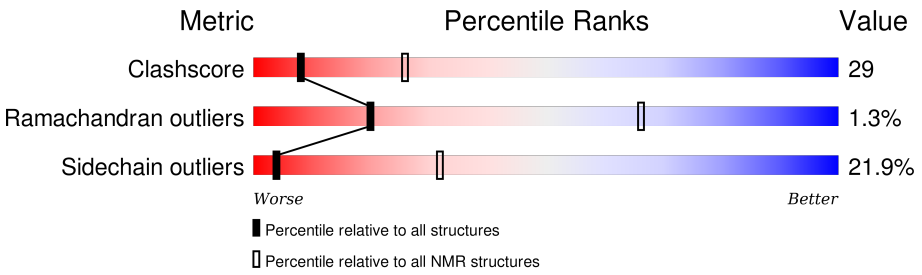
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 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	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	123	46% 35% 5% 15%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 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:8-A:75, A:82-A:118 (105)	0.23	2

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 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1860 atoms, of which 922 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called beta-spectrin III.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	123	1860	585	922	172	175	6	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP O15020
A	2	SER	-	CLONING ARTIFACT	UNP O15020
A	3	SER	-	CLONING ARTIFACT	UNP O15020
A	4	GLY	-	CLONING ARTIFACT	UNP O15020
A	5	SER	-	CLONING ARTIFACT	UNP O15020
A	6	SER	-	CLONING ARTIFACT	UNP O15020
A	7	GLY	-	CLONING ARTIFACT	UNP O15020
A	118	SER	-	CLONING ARTIFACT	UNP O15020
A	119	GLY	-	CLONING ARTIFACT	UNP O15020
A	120	PRO	-	CLONING ARTIFACT	UNP O15020
A	121	SER	-	CLONING ARTIFACT	UNP O15020
A	122	SER	-	CLONING ARTIFACT	UNP O15020
A	123	GLY	-	CLONING ARTIFACT	UNP O15020

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: beta-spectrin III

Chain A: 46% 35% 5% 15%

G1 S2 S3 G4 S5 S6 G7 M10 M13 L14 C15 R16 M20 E21 A22 K25 K26 A27 A28 V35 Y36 C37 V38 L39 R40 R41 G42 S43 L44 G45 F46 Y47 K48 D49 A50 V63 L67 A68 R69 V74 A75 F76 D77 Y78 R79 K80 R81 K82 H83 V84 F85

K93 L96 F97 Q98 A99 K100 E104 M105 S106 S107 W108 L109 R110 V111 V112 N113 A114 A115 S118 G119 P120 S121 S122 G123

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

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: beta-spectrin III

Chain A: 49% 31% 6% 15%

G1 S2 S3 G4 S5 S6 G7 M10 M13 L14 C15 R16 K25 K26 R30 Q33 N34 V35 Y36 C37 V38 L39 R40 R41 G42 S43 L44 G45 F46 Y47 K48 D49 A50 S54 V63 L67 A68 R69 A70 Q71 V74 A75 F76 D77 Y78 R79 K80 R81 K82 H83 V84

F85 K86 L87 K93 L96 F97 Q98 A99 E104 M105 S106 S107 W108 L109 R110 V111 V112 N113 A114 A115 S118 G119 P120 S121 S122 G123

5 Refinement protocol and experimental data overview (i)

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

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

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

Software name	Classification	Version
CYANA	structure solution	1.0.7
CYANA	refinement	1.0.7

No chemical shift data was provided. 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	813	809	809	47±6
All	All	16260	16180	16180	932

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 29.

5 of 193 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:HD22	1:A:111:VAL:HG12	0.99	1.32	11	20
1:A:107:SER:O	1:A:111:VAL:HG23	0.81	1.73	18	20
1:A:39:LEU:CD2	1:A:111:VAL:HG12	0.78	2.09	14	20
1:A:37:CYS:SG	1:A:44:LEU:HD11	0.77	2.18	10	18
1:A:10:MET:HB2	1:A:111:VAL:HG11	0.76	1.57	13	16

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	105/123 (85%)	87±2 (83±2%)	17±2 (16±2%)	1±1 (1±1%)	20 66
All	All	2100/2460 (85%)	1738 (83%)	335 (16%)	27 (1%)	20 66

5 of 10 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	28	ALA	5
1	A	118	SER	4
1	A	63	VAL	3
1	A	99	ALA	3
1	A	41	ARG	3

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	81/94 (86%)	63±2 (78±3%)	18±2 (22±3%)	4 32
All	All	1620/1880 (86%)	1266 (78%)	354 (22%)	4 32

5 of 43 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	15	CYS	20
1	A	25	LYS	20
1	A	37	CYS	20
1	A	107	SER	20
1	A	93	LYS	20

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)

No chemical shift data were provided