wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1U38
Title	:	Auto-inhibition Mechanism of X11s/Mints Family Scaffold Proteins Revealed by the Closed Conformation of the Tandem PDZ Domains
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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:

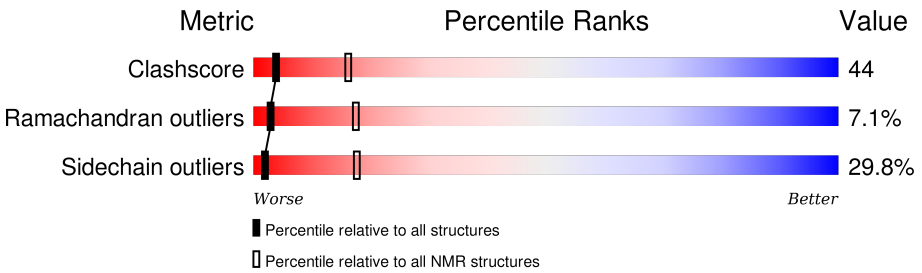
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	89	39% 45% 13% •
2	B	4	25% 75%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:17-A:105, B:-3-B:0 (93)	0.25	16

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 3 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1453 atoms, of which 751 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called amyloid beta A4 precursor protein-binding, family A, member 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1382	425	715	115	123	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLU	-	CLONING ARTIFACT	UNP Q02410
A	18	PHE	-	CLONING ARTIFACT	UNP Q02410

- Molecule 2 is a protein called PVYI.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	4	71	25	36	4	6	0

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: amyloid beta A4 precursor protein-binding, family A, member 1

Chain A: 39% 45% 13% •

E17 F18 K19 D20 V21 F22 K25 E29 I30 L31 G32 V33 V34 I35 V36 W40 G41 S42 I43 L44 P45 T46 V47 I48 I49 A50 N51 M52 M53 H54 E59 K60 S61 G62 K63 L64 N65 I66 G67 D68 Q69 I70 M71 S72 I73 T76 S77 L78 V79 G80 L81 P82 L83 S84 T85

C86 Q87 S88 I89 I90 K91 G92 L93 K94 R98 V99 K100 L101 N102 I103 V104 R105

- Molecule 2: PVYI

Chain B: 25% 75%

P-3 V-2 Y-1 I0

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

The representative model is number 16. Colouring as in section 4.1 above.

- Molecule 1: amyloid beta A4 precursor protein-binding, family A, member 1

Chain A: 44% 37% 16% •

E17 F18 K19 D20 V21 F22 K25 E29 I30 L31 G32 V33 V34 E37 W40 I43 L44 P45 T46 V47 I48 I49 M53 H54 G55 E59 K63 L64 N65 I66 G67 D68 Q69 I70 M71 S72 I73 T76 S77 L78 L81 P82 L83 S84 T85 I89 I90 L93

K94 N95 Q96 S97 R98 V99 K100 L101 N102 I103 V104 R105

- Molecule 2: PVYI

Chain B: 25% 75%

P-3
V-2
Y-1
I0

5 Refinement protocol and experimental data overview (i)

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

Of the 200 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
CNS	structure solution	1.1
CNS	refinement	1.1

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	667	715	713	61±5
2	B	35	36	38	11±1
All	All	14040	15020	15020	1265

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 44.

5 of 284 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:VAL:HG22	2:B:0:ILE:HD11	1.08	1.22	13	20
1:A:49:ILE:HG22	1:A:66:ILE:HD13	1.07	1.27	15	19
1:A:90:ILE:HG21	2:B:0:ILE:HD13	1.06	1.26	16	20
1:A:76:THR:HG21	1:A:89:ILE:HD12	0.95	1.33	19	13
1:A:73:ILE:HD12	1:A:78:LEU:HD11	0.88	1.43	13	12

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	87/89 (98%)	68±1 (78±2%)	13±2 (15±2%)	6±1 (7±1%)	3 18
2	B	2/4 (50%)	1±1 (70±33%)	0±1 (18±29%)	0±0 (12±22%)	1 7
All	All	1780/1860 (96%)	1388 (78%)	265 (15%)	127 (7%)	3 17

5 of 13 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	31	LEU	20
1	A	40	TRP	20
1	A	30	ILE	20
1	A	45	PRO	16
1	A	42	SER	15

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	76/76 (100%)	52±2 (69±2%)	24±2 (31±2%)	2 16
2	B	4/4 (100%)	4±0 (94±11%)	0±0 (6±11%)	27 72
All	All	1600/1600 (100%)	1124 (70%)	476 (30%)	2 18

5 of 51 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	30	ILE	20
1	A	101	LEU	20
1	A	22	PHE	20
1	A	33	VAL	20
1	A	48	ILE	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