wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2IB1
Title	:	Solution structure of p45 Death Domain
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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:

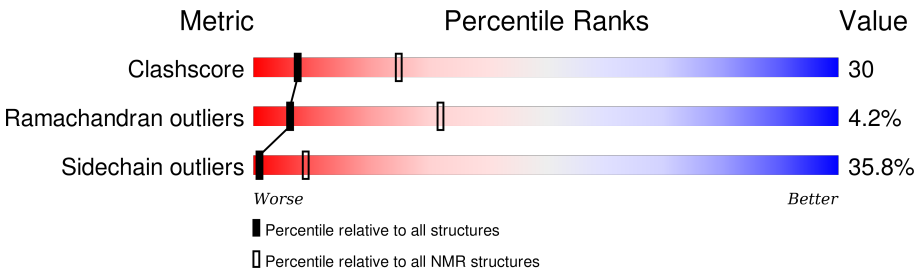
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	91	27% 57% 5% 10%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 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:138-A:219 (82)	0.74	4

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 and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1378 atoms, of which 681 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Death domain containing membrane protein NRADD.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	91	1378	429	681	123	140	5	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: Death domain containing membrane protein NRADD

Chain A: 27% 57% 5% 10%

P138 Q139 Q140 Q141 Q142 E143 E144 V145 Q146 R147 L148 L149 M150 M151 G152 E153 K156 G157 W158 Q159 E160 L161 A162 G163 H164 L165 G166 Y167 Q168 A169 V172 M175 Q179 M180 P181 A182 Y183 T184 L185 L186 R187 N188 W189 A190 A191 Q192 E193 G194 N195 R196 A197 T198 L199 R200 V201 L202

E203 D204 A205 L206 I209 G210 R211 E212 D213 V214 V215 Q216 V217 L218 S219 S220 P221 A222 E223 S224 S225 S226 V227 V228

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

The representative model is number 4. Colouring as in section 4.1 above.

- Molecule 1: Death domain containing membrane protein NRADD

Chain A: 36% 43% 10% • 10%

P138 Q139 Q140 E143 E144 V145 Q146 R147 L148 L149 M150 M151 A155 K156 G157 W158 Q159 E160 L165 G166 Y167 A171 V172 E173 T174 D178 Q179 M180 P181 A182 Y183 T184 L185 L186 R187 N188 W189 A190 A191 R196 L199 L202 E203 D204 A205 L206 A207 A208 I209 G210 R211 E212

D213 V214 V215 Q216 V217 L218 S219 S220 P221 A222 E223 S224 S225 S226 V227 V228

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: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	
CNS	refinement	

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	637	625	622	38±7
All	All	12740	12500	12440	754

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 30.

5 of 414 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:VAL:HG23	1:A:218:LEU:HD13	0.91	1.39	17	6
1:A:186:LEU:HD12	1:A:198:THR:HG22	0.88	1.45	13	1
1:A:158:TRP:CH2	1:A:176:ALA:HB2	0.85	2.07	14	8
1:A:165:LEU:HD23	1:A:189:TRP:CD1	0.80	2.12	7	6
1:A:158:TRP:CZ3	1:A:172:VAL:HG22	0.78	2.13	14	7

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	81/91 (89%)	67±2 (82±2%)	11±2 (13±3%)	3±1 (4±2%)	6 32
All	All	1620/1820 (89%)	1335 (82%)	217 (13%)	68 (4%)	6 32

5 of 14 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	180	MET	20
1	A	193	GLU	13
1	A	156	LYS	6
1	A	192	GLN	6
1	A	194	GLY	5

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	64/72 (89%)	41±4 (64±6%)	23±4 (36±6%)	1 9
All	All	1280/1440 (89%)	822 (64%)	458 (36%)	1 9

5 of 58 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	172	VAL	20
1	A	209	ILE	20
1	A	211	ARG	18
1	A	183	TYR	17
1	A	167	TYR	17

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