wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1E41
Title	:	Death domain from human FADD/MORT1
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Deposited on	:	2000-06-27

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
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:

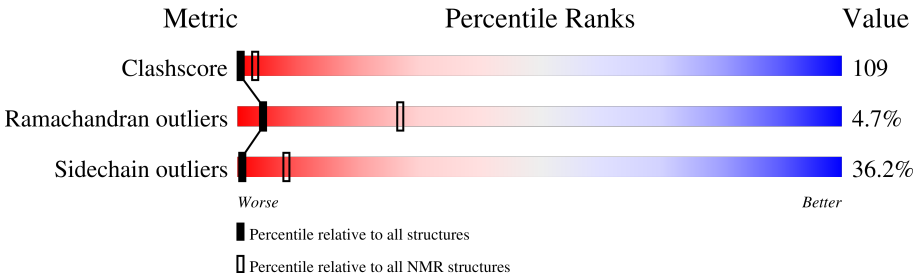
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson 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	104	6% 58% 19% • 16%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 25 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:96-A:182 (87)	0.91	25

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, 6, 7, 11, 14, 17, 18, 21, 22, 23, 25
2	8, 10, 12, 13, 15, 16, 20, 24
3	9, 19

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1654 atoms, of which 825 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FADD PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	104	1654	502	825	161	161	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, 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: FADD PROTEIN

Chain A: 6% 58% 19% • 16%

G89 S90 H91 M92 G93 E94 E95 D96 L97 C98 A99 A100 F101 N102 V103 I104 C105 D106 N107 V108 G109 K110 D111 W112 R113 R114 L115 A116 R117 Q118 L119 K120 V121 S122 D123 T124 K125 I126 D127 S128 I129 E130 D131 R132 Y133 P134 R135 N136 L137 T138 E139 R140 V141 R142 E143 S144 L145 R146 I147 W148

K149 N150 T151 E152 K153 E154 N155 A156 T157 V158 A159 H160 L161 V162 G163 A164 L165 R166 S167 C168 Q169 M170 N171 L172 V173 A174 D175 L176 V177 Q178 E179 V180 Q181 Q182 A183 R184 D185 L186 Q187 N188 R189 S190 G191 A192

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

The representative model is number 25. Colouring as in section 4.1 above.

• Molecule 1: FADD PROTEIN

Chain A: 13% 41% 26% • 16%

G89 S90 H91 M92 G93 E94 E95 D96 L97 C98 A99 A100 F101 N102 V103 I104 C105 D106 N107 V108 G109 K110 D111 W112 R113 R114 L115 A116 R117 Q118 L119 K120 D123 T124 K125 I126 D127 S128 I129 E130 P134 R135 N136 L137 T138 E139 R140 V141 R142 E143 S144 L145 R146 I147 W148 K149 N150 T151

E152 K153 E154 N155 A156 T157 V158 A159 H160 L161 V162 G163 A164 L165 R166 S167 C168 Q169 M170 N171 L172 V173 A174 D175 L176 V177 Q178 E179 V180 Q181 Q182 A183 R184 D185 L186 Q187 N188 R189 S190 G191 A192

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *SIMULATED ANNEALING FROM RANDOM CHAIN STARTING CONFORMERS*.

Of the 100 calculated structures, 25 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION AND GOOD NON-BONDED CONTACTS*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851
NMRPipe	structure solution	
ANSIG	structure solution	
X-PLOR	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	8.6±0.6
All	All	0	215

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

5 of 9 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	117	ARG	Sidechain	25
1	A	146	ARG	Sidechain	25
1	A	113	ARG	Sidechain	24
1	A	114	ARG	Sidechain	24
1	A	132	ARG	Sidechain	24

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	703	711	711	154±14
All	All	17575	17775	17775	3848

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 109.

5 of 1099 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:VAL:O	1:A:176:LEU:HD23	1.23	1.32	18	22
1:A:103:VAL:HG21	1:A:177:VAL:HG22	1.09	1.12	3	25
1:A:100:ALA:CB	1:A:161:LEU:HD21	1.06	1.79	12	2
1:A:100:ALA:HB1	1:A:161:LEU:HD22	1.06	1.09	24	9
1:A:103:VAL:HG23	1:A:176:LEU:HD11	1.05	1.21	23	3

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	87/104 (84%)	68±3 (78±4%)	15±3 (18±4%)	4±1 (5±1%)	4	27
All	All	2175/2600 (84%)	1688 (78%)	384 (18%)	103 (5%)	4	27

5 of 16 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	120	LYS	23
1	A	145	LEU	20
1	A	108	VAL	15
1	A	153	LYS	9
1	A	110	LYS	9

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	78/90 (87%)	50±4 (64±5%)	28±4 (36±5%)	1	8
All	All	1950/2250 (87%)	1244 (64%)	706 (36%)	1	8

5 of 68 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	138	THR	25
1	A	180	VAL	25
1	A	148	TRP	24
1	A	176	LEU	24
1	A	177	VAL	24

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