wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2DO9
Title	:	Solution structure of the Pyrin/PAAD-DAPIN domain in mouse NALP10 (NACHT, leucine rich repeat and PYD containing 10)
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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:

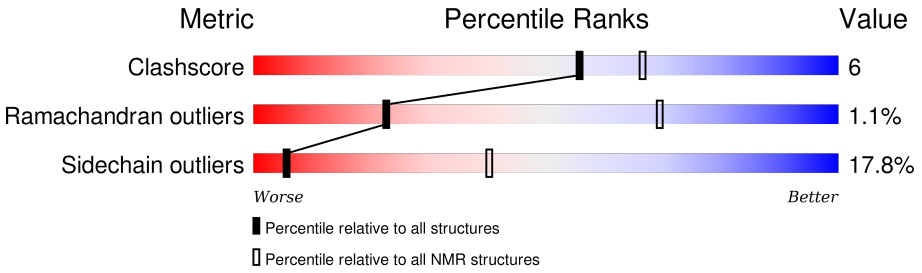
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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	115	59% 13% • 27%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 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:13-A:96 (84)	0.40	11

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 6 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1777 atoms, of which 883 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NACHT-, LRR- and PYD-containing protein 10.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	115	1777	556	883	157	176	5	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP Q8CCN1
A	2	SER	-	CLONING ARTIFACT	UNP Q8CCN1
A	3	SER	-	CLONING ARTIFACT	UNP Q8CCN1
A	4	GLY	-	CLONING ARTIFACT	UNP Q8CCN1
A	5	SER	-	CLONING ARTIFACT	UNP Q8CCN1
A	6	SER	-	CLONING ARTIFACT	UNP Q8CCN1
A	7	GLY	-	CLONING ARTIFACT	UNP Q8CCN1
A	110	SER	-	CLONING ARTIFACT	UNP Q8CCN1
A	111	GLY	-	CLONING ARTIFACT	UNP Q8CCN1
A	112	PRO	-	CLONING ARTIFACT	UNP Q8CCN1
A	113	SER	-	CLONING ARTIFACT	UNP Q8CCN1
A	114	SER	-	CLONING ARTIFACT	UNP Q8CCN1
A	115	GLY	-	CLONING ARTIFACT	UNP Q8CCN1

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: NACHT-, LRR- and PYD-containing protein 10

Chain A: 59% 13% • 27%

G1 S2 S3 G4 S5 S6 G7 M8 A9 L10 A11 R12 L24 K36 F37 H38 L39 H46 R49 L55 L60 K63 A70 Q71 E72 A73 V74 R75 V76 L86 M87 V90 C97 L98 N99 D100 Y101 R102 E103 I104 Y105 R106 E107 H108 V109 S110 G111 P112 S113

S114 G115

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

The representative model is number 11. Colouring as in section 4.1 above.

- Molecule 1: NACHT-, LRR- and PYD-containing protein 10

Chain A: 50% 22% • 27%

G1 S2 S3 G4 S5 S6 G7 M8 A9 L10 A11 R12 Q17 D26 E29 V42 T43 H46 R49 G50 E53 S54 L55 S56 K63 L64 I65 E72 V76 V77 S78 R79 S80 N85 L86 M87 E88 L89 V90 D91 Y92 L93 N94 C97 L98 N99 D100 Y101

R102 E103 I104 Y105 R106 E107 H108 V109 S110 G111 P112 S113 S114 G115

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
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	668	672	672	9±2
All	All	13360	13440	13440	171

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 6.

5 of 62 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:GLU:O	1:A:76:VAL:HG23	0.78	1.78	15	16
1:A:24:LEU:HD12	1:A:61:ALA:HB2	0.78	1.54	16	7
1:A:86:LEU:O	1:A:90:VAL:HG23	0.73	1.83	18	12
1:A:70:ALA:O	1:A:74:VAL:HG23	0.72	1.84	2	6
1:A:24:LEU:CD1	1:A:61:ALA:HB2	0.69	2.17	15	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	84/115 (73%)	76±1 (91±2%)	7±2 (8±2%)	1±1 (1±1%)	23 69
All	All	1680/2300 (73%)	1522 (91%)	140 (8%)	18 (1%)	23 69

5 of 6 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	46	HIS	5
1	A	48	ALA	4
1	A	49	ARG	4
1	A	50	GLY	3
1	A	55	LEU	1

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	74/98 (76%)	61±2 (82±3%)	13±2 (18±3%)	6 40
All	All	1480/1960 (76%)	1217 (82%)	263 (18%)	6 40

5 of 48 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	37	PHE	15
1	A	72	GLU	14
1	A	87	MET	13
1	A	63	LYS	12
1	A	59	ASP	9

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