



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1PN5  
Title : NMR structure of the NALP1 Pyrin domain (PYD)  
Authors : Hiller, S.; Kohl, A.; Fiorito, F.; Herrmann, T.; Wider, G.; Tschopp, J.; Grutter, M.G.; Wuthrich, K.  
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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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

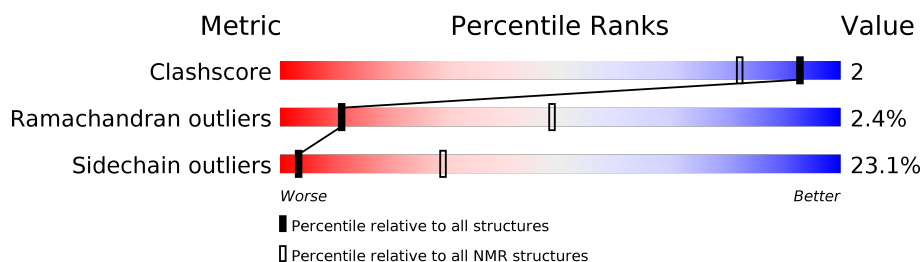
# 1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	159	<div> <div></div> <div>36%</div> <div>6%</div> <div>•</div> <div>16%</div> <div>42%</div> </div>

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 17 as representative, based on the following criterion: *aesthetic reasons*.

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:64-A:90, A:105-A:145 (68)	0.42	19

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 1 single-model cluster was found.

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

### 3 Entry composition

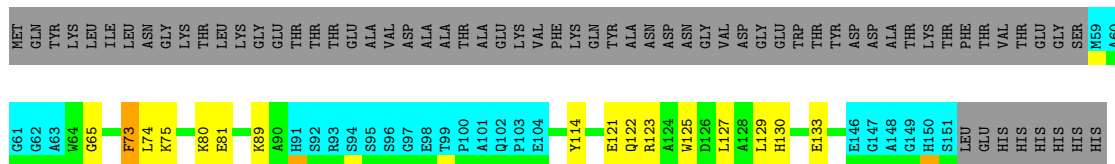
There is only 1 type of molecule in this entry. The entry contains 1411 atoms, of which 693 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NACHT-, LRR- and PYD-containing protein 2.

Mol	Chain	Residues	Atoms						Trace
1	A	93	Total	C	H	N	O	S	0
			1411	449	693	127	137	5	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING MET	UNP P06654
A	2	GLN	THR	ENGINEERED	UNP P06654
A	57	GLY	-	SEE REMARK 999	UNP P06654
A	58	SER	-	SEE REMARK 999	UNP P06654
A	152	LEU	-	EXPRESSION TAG	UNP Q9C000
A	153	GLU	-	EXPRESSION TAG	UNP Q9C000
A	154	HIS	-	EXPRESSION TAG	UNP Q9C000
A	155	HIS	-	EXPRESSION TAG	UNP Q9C000
A	156	HIS	-	EXPRESSION TAG	UNP Q9C000
A	157	HIS	-	EXPRESSION TAG	UNP Q9C000
A	158	HIS	-	EXPRESSION TAG	UNP Q9C000
A	159	HIS	-	EXPRESSION TAG	UNP Q9C000



## 5 Refinement protocol and experimental data overview

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

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
DYANA	structure solution	
CANDID	structure solution	
ATNOS	structure solution	
ATNOS	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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.62±0.01	0±0/564 (0.0±0.0%)	1.09±0.04	1±1/760 (0.1±0.1%)
All	All	0.62	0/11280 (0.0%)	1.09	11/15200 (0.1%)

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	0.7±0.8
All	All	0	14

There are no bond-length outliers.

5 of 8 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	85	LEU	CB-CG-CD1	6.83	122.62	111.00	3	1
1	A	66	ARG	NE-CZ-NH2	-6.03	117.28	120.30	14	1
1	A	111	VAL	CA-CB-CG2	5.95	119.82	110.90	20	1
1	A	119	TYR	CB-CG-CD1	-5.82	117.51	121.00	3	1
1	A	138	ARG	NE-CZ-NH2	-5.62	117.49	120.30	14	3

There are no chirality outliers.

5 of 10 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	66	ARG	Sidechain	2
1	A	119	TYR	Sidechain	2
1	A	123	ARG	Sidechain	2

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*Continued from previous page...*

Mol	Chain	Res	Type	Group	Models (Total)
1	A	82	PHE	Sidechain	2
1	A	90	ALA	Peptide	1

## 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	552	550	550	2±1
All	All	11040	11000	11000	36

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 2.

5 of 27 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:PHE:CE2	1:A:140:LEU:HD21	0.68	2.23	1	6
1:A:81:GLU:HA	1:A:85:LEU:HD13	0.62	1.71	13	1
1:A:125:TRP:CD1	1:A:129:LEU:HD11	0.57	2.34	5	2
1:A:73:PHE:CZ	1:A:140:LEU:HD21	0.57	2.35	8	2
1:A:137:LEU:N	1:A:137:LEU:HD22	0.54	2.16	2	1

## 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	68/159 (43%)	58±3 (85±4%)	8±3 (12±4%)	2±1 (2±1%)	11	48
All	All	1360/3180 (43%)	1162 (85%)	166 (12%)	32 (2%)	11	48

5 of 7 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	122	GLN	15
1	A	90	ALA	7
1	A	65	GLY	5
1	A	77	GLU	2
1	A	89	LYS	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	55/126 (44%)	42±3 (77±5%)	13±3 (23±5%)	3	29
All	All	1100/2520 (44%)	846 (77%)	254 (23%)	3	29

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	73	PHE	19
1	A	74	LEU	15
1	A	80	LYS	14
1	A	127	LEU	13
1	A	89	LYS	12

### 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

No chemical shift data were provided