



wwPDB NMR Structure Validation Summary Report ⓘ

Feb 14, 2022 – 08:47 AM EST

PDB ID : 1JKZ
Title : NMR Solution Structure of Pisum sativum defensin 1 (Psd1)
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Deposited on : 2001-07-13

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.26
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

2 Ensemble composition and analysis i

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 18 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:2-A:46 (45)	0.34	8

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, 7, 8, 9, 10, 12, 13, 16, 17, 18, 19, 20
2	5, 11, 14
3	6, 15

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 685 atoms, of which 326 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DEFENSE-RELATED PEPTIDE 1.

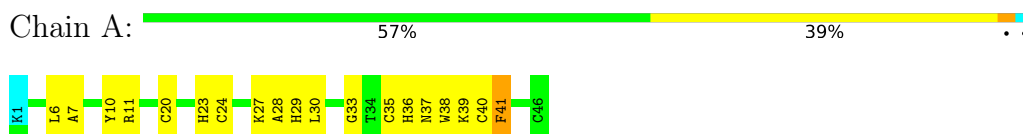
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	46	685	216	326	67	68	8	0

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.

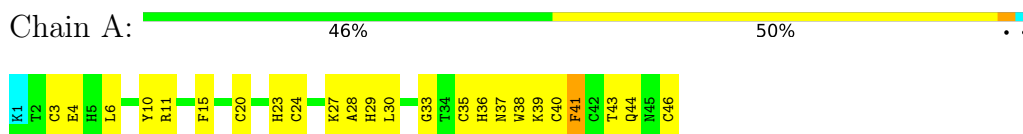
- Molecule 1: DEFENSE-RELATED PEPTIDE 1



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

The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: DEFENSE-RELATED PEPTIDE 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *THE STRUCTURE WAS CALCULATED USING TORSIONAL SIMULATED ANNEALING AND THEN MINIMIZED.*

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 SOLVE	structure solution	1.0
CNS SOLVE	refinement	1.0

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.

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	350	311	307	20±3
All	All	7000	6220	6140	400

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 102 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD11	1:A:39:LYS:CD	0.95	1.92	10	5
1:A:6:LEU:HD11	1:A:39:LYS:HD3	0.92	1.36	10	11
1:A:14:CYS:SG	1:A:20:CYS:SG	0.90	2.69	18	4
1:A:20:CYS:SG	1:A:35:CYS:SG	0.88	2.72	8	16
1:A:4:GLU:HG2	1:A:43:THR:HG22	0.83	1.48	7	5

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	44/46 (96%)	37±2 (84±5%)	6±2 (13±4%)	2±1 (4±1%)	6	34
All	All	880/920 (96%)	737 (84%)	111 (13%)	32 (4%)	6	34

All 3 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	29	HIS	20
1	A	37	ASN	11
1	A	19	SER	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	40/41 (98%)	39±1 (97±2%)	1±1 (3±2%)	40	87
All	All	800/820 (98%)	773 (97%)	27 (3%)	40	87

All 5 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	41	PHE	16
1	A	38	TRP	7
1	A	37	ASN	2
1	A	27	LYS	1
1	A	23	HIS	1

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

No chemical shift data were provided