

Full wwPDB NMR Structure Validation Report (i)

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PDB ID : 7M3U

Title: Solution NMR Structure of PawS-Derived Peptide PDP-24

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This is a Full wwPDB NMR Structure Validation 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 following versions of software and data (see references (i)) were used in the production of this report:

MolProbity : FAILED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

RCI : FAILED
PANAV : FAILED
ShiftChecker : FAILED

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.27

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.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:9 (8)	0.08	18		
2	A:12-A:25 (14)	0.12	1		

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 5 clusters and 2 single-model clusters were found.

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 387 atoms, of which 175 are hydrogens and 0 are deuteriums.

 \bullet Molecule 1 is a protein called PawS-Derived Peptide PDP-24.

Mol	Chain	Residues	Atoms				Trace		
1	Λ	97	Total	С	Н	N	О	S	0
	1 A	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	138	175	35	35	4		



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: PawS-Derived Peptide PDP-24

Chain A: 81% 19%

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: PawS-Derived Peptide PDP-24

Chain A: 81% 19%



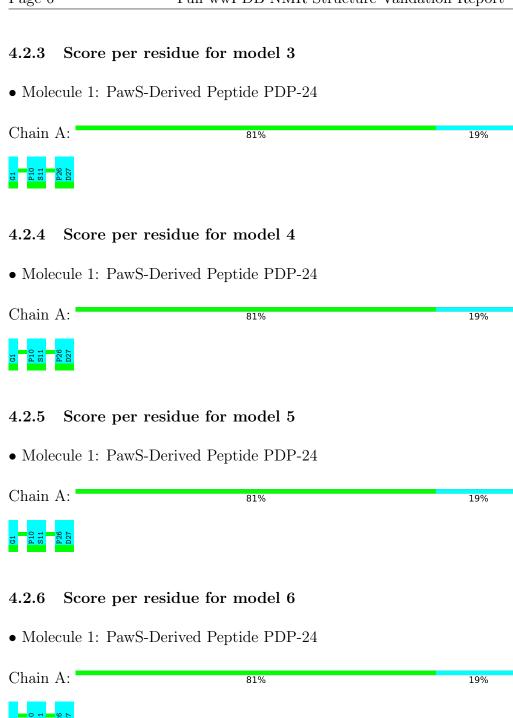
4.2.2 Score per residue for model 2

• Molecule 1: PawS-Derived Peptide PDP-24

Chain A: 81% 19%

G1 P10 S11 P26 D27





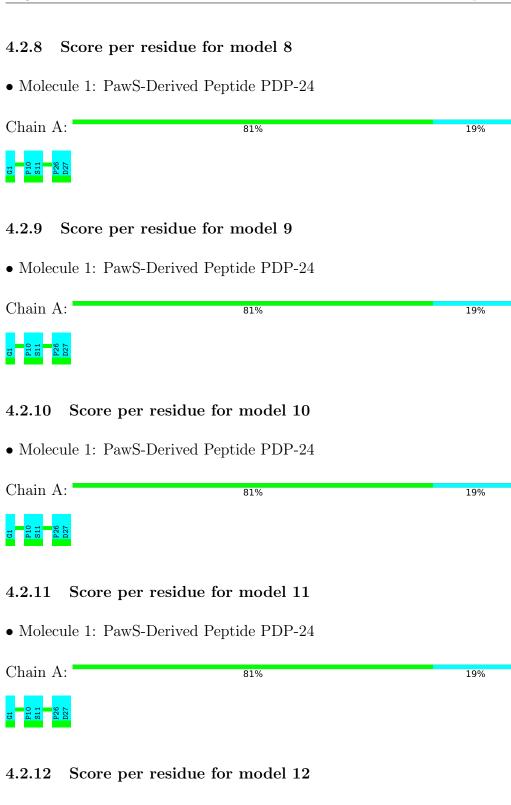


4.2.7 Score per residue for model 7

• Molecule 1: PawS-Derived Peptide PDP-24



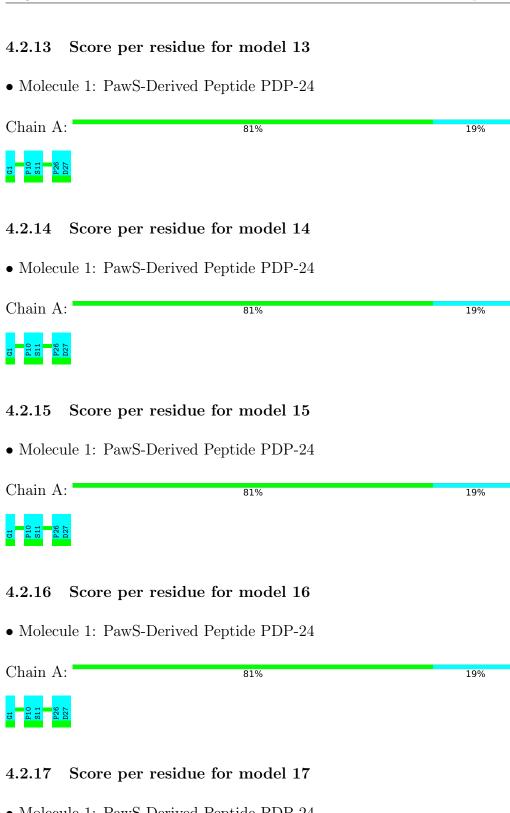




• Molecule 1: PawS-Derived Peptide PDP-24







• Molecule 1: PawS-Derived Peptide PDP-24





4.2.18	Score	per	residue	for	model	18

• Molecule 1: PawS-Derived Peptide PDP-24

Chain A: 81% 19%



4.2.19 Score per residue for model 19

• Molecule 1: PawS-Derived Peptide PDP-24

Chain A: 81% 19%



4.2.20 Score per residue for model 20

• Molecule 1: PawS-Derived Peptide PDP-24





Refinement protocol and experimental data overview (i) 5



The models were refined using the following method: simulated annealing, simulated annealing, simulated annealing.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: structures with the least restraint violations.

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

Software name	Classification	Version
CNS	refinement	
CNS	structure calculation	
CYANA	structure calculation	

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts (i)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA (i)

MolProbity failed to run properly - this section will have to be empty.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

MolProbity failed to run properly - this section will have to be empty.

6.5 Carbohydrates (i)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry (i)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers (i)

MolProbity failed to run properly - this section will have to be empty.



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

