



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 6POJ  
Title : STRUCTURAL REFINEMENT OF AQUAPORIN 1 VIA SSNMR  
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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

<https://www.wwpdb.org/validation/2017/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	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	NOT EXECUTED
PANAV	:	NOT EXECUTED
ShiftChecker	:	NOT EXECUTED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

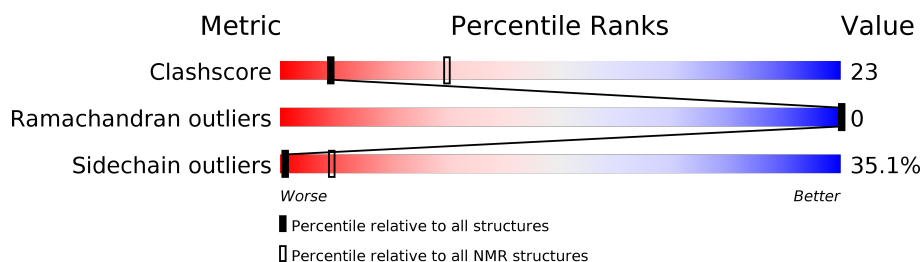
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLID-STATE 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  $\geq 3$ , 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	292	<div> <div></div> <div>31%</div> <div>25%</div> <div>43%</div> </div>

## 2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 9 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:12-A:32, A:48-A:84, A:93-A:116, A:125-A:156, A:168-A:201, A:211-A:227 (165)	0.15	9

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4417 atoms, of which 2216 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Aquaporin-1.

Mol	Chain	Residues	Atoms						Trace
1	A	292	Total	C	H	N	O	S	0
			4417	1406	2216	381	407	7	

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	ALA	-	expression tag	UNP P29972
A	271	LEU	-	expression tag	UNP P29972
A	272	GLU	-	expression tag	UNP P29972
A	273	GLN	-	expression tag	UNP P29972
A	274	LYS	-	expression tag	UNP P29972
A	275	LEU	-	expression tag	UNP P29972
A	276	ILE	-	expression tag	UNP P29972
A	277	SER	-	expression tag	UNP P29972
A	278	GLU	-	expression tag	UNP P29972
A	279	GLU	-	expression tag	UNP P29972
A	280	ASP	-	expression tag	UNP P29972
A	281	LEU	-	expression tag	UNP P29972
A	282	ASN	-	expression tag	UNP P29972
A	283	SER	-	expression tag	UNP P29972
A	284	ALA	-	expression tag	UNP P29972
A	285	VAL	-	expression tag	UNP P29972
A	286	ASP	-	expression tag	UNP P29972
A	287	HIS	-	expression tag	UNP P29972
A	288	HIS	-	expression tag	UNP P29972
A	289	HIS	-	expression tag	UNP P29972
A	290	HIS	-	expression tag	UNP P29972
A	291	HIS	-	expression tag	UNP P29972
A	292	HIS	-	expression tag	UNP P29972





## 5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 10 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
X-PLOR NIH	refinement	2.48
X-PLOR NIH	structure calculation	2.48

No chemical shift data was provided. Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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	1171	1233	1235	53±18
All	All	11710	12330	11115	528

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 23.

5 of 160 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:ALA:HB3	1:A:191:ILE:HG22	0.90	1.41	8	2
1:A:149:LEU:HD11	1:A:176:VAL:HG22	0.84	1.50	3	9
1:A:63:LEU:HD13	1:A:75:LEU:HD12	0.84	1.49	6	1
1:A:21:THR:HG23	1:A:75:LEU:O	0.71	1.85	3	7
1:A:109:THR:HG21	1:A:198:GLY:O	0.69	1.88	5	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	165/292 (57%)	111±72 (67±44%)	5±3 (3±2%)	0±0 (0±0%)	100	100
All	All	1155/2920 (40%)	1106 (96%)	49 (4%)	0 (0%)	100	100

There are no Ramachandran outliers.

### 6.3.2 Protein sidechains ⓘ

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	120/235 (51%)	47±38 (39±32%)	25±21 (21±17%)	3	32
All	All	720/2350 (31%)	467 (65%)	253 (35%)	1	9

5 of 82 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	60	ILE	6
1	A	21	THR	6
1	A	63	LEU	6
1	A	187	THR	6
1	A	22	THR	6

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.5 Carbohydrates ⓘ

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