



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2JOM  
Title : NMR structure of rabbit prion protein mutation I214V  
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Deposited on : 2007-03-14

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:

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	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

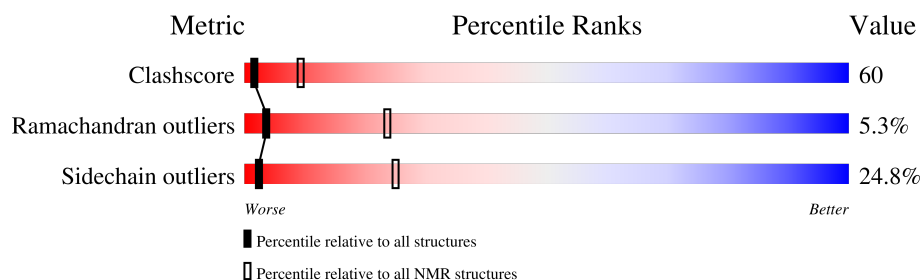
# 1 Overall quality at a glance

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	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	148	<div> <div></div> <div>17%</div> <div>41%</div> <div>13%</div> <div>29%</div> </div>

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:124-A:228 (105)	0.44	6

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 2 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1692 atoms, of which 819 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	105	Total	C	H	N	O	S	0
			1692	543	819	152	171	7	

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	MET	-	initiating methionine	UNP Q95211
A	90	HIS	-	expression tag	UNP Q95211
A	214	VAL	ILE	engineered mutation	UNP Q95211
A	229	LEU	-	expression tag	UNP Q95211
A	230	GLU	-	expression tag	UNP Q95211
A	231	HIS	-	expression tag	UNP Q95211
A	232	HIS	-	expression tag	UNP Q95211
A	233	HIS	-	expression tag	UNP Q95211
A	234	HIS	-	expression tag	UNP Q95211
A	235	HIS	-	expression tag	UNP Q95211
A	236	HIS	-	expression tag	UNP Q95211



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 15 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
ARIA	structure solution	
ARIA	refinement	

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.

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	0.1±0.3
All	All	0	2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	156	TYR	Peptide	2

### 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	873	819	815	102±8
All	All	13095	12285	12225	1523

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 60.

5 of 499 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:160:VAL:HG13	1:A:209:VAL:HG22	0.95	1.38	13	14
1:A:149:TYR:HA	1:A:152:ASN:HD22	0.92	1.20	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:ASP:HB2	1:A:221:SER:HA	0.92	1.36	12	13
1:A:179:VAL:HG11	1:A:210:GLU:HA	0.89	1.42	15	15
1:A:175:VAL:HG11	1:A:214:VAL:HG12	0.87	1.44	15	2

## 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	103/148 (70%)	80±2 (78±2%)	18±2 (17±2%)	5±1 (5±1%)	3	23
All	All	1545/2220 (70%)	1200 (78%)	263 (17%)	82 (5%)	3	23

5 of 14 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	131	SER	15
1	A	135	ARG	14
1	A	139	HIS	13
1	A	166	ASP	12
1	A	187	THR	12

### 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	96/126 (76%)	72±3 (75±3%)	24±3 (25±3%)	2	25
All	All	1440/1890 (76%)	1083 (75%)	357 (25%)	2	25

5 of 63 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	152	ASN	15
1	A	153	MET	15
1	A	160	VAL	15
1	A	171	GLN	15
1	A	183	VAL	15

### 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