wwPDB NMR Structure Validation Summary Report

Dec 19, 2023 – 02:55 AM EST

PDB ID	:	2MV8
BMRB ID	:	25250
Title	:	Solution structure of Ovis Aries PrP with mutation delta190-197
Authors	:	Munoz, C.; Egalon, A.; Beringue, V.; Rezaei, H.; Dron, M.; Sizun, C.
Deposited on	:	2014-09-25

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

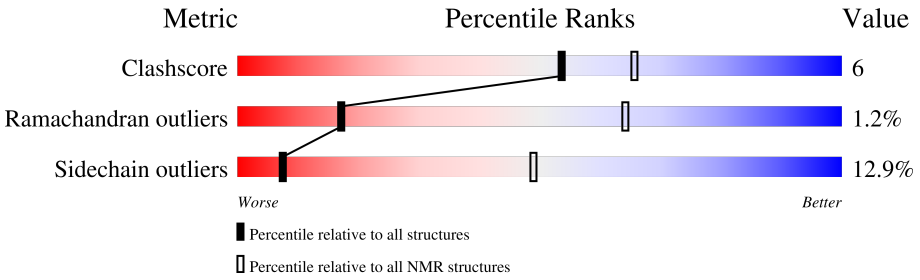
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 is 87%.

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	146	51% 11% 31% 8%

2 Ensemble composition and analysis

This entry contains 20 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:131-A:189, A:198-A:228 (90)	0.73	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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2105 atoms, of which 1028 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	135	2105	669	1028	195	204	9	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	MET	-	expression tag	UNP Q712V9
A	82	GLY	-	expression tag	UNP Q712V9
A	83	SER	-	expression tag	UNP Q712V9
A	84	SER	-	expression tag	UNP Q712V9
A	85	HIS	-	expression tag	UNP Q712V9
A	86	HIS	-	expression tag	UNP Q712V9
A	87	HIS	-	expression tag	UNP Q712V9
A	88	HIS	-	expression tag	UNP Q712V9
A	89	HIS	-	expression tag	UNP Q712V9
A	90	HIS	-	expression tag	UNP Q712V9
A	91	SER	-	expression tag	UNP Q712V9
A	92	SER	-	expression tag	UNP Q712V9
A	93	GLY	-	expression tag	UNP Q712V9
A	94	LEU	-	expression tag	UNP Q712V9
A	95	VAL	-	expression tag	UNP Q712V9
A	96	PRO	-	expression tag	UNP Q712V9
A	97	ARG	-	expression tag	UNP Q712V9
A	98	GLY	-	expression tag	UNP Q712V9
A	99	SER	-	expression tag	UNP Q712V9
A	100	HIS	-	expression tag	UNP Q712V9
A	101	MET	-	expression tag	UNP Q712V9
A	102	SER	-	expression tag	UNP Q712V9
A	?	-	HIS	deletion	UNP Q712V9
A	?	-	THR	deletion	UNP Q712V9
A	?	-	VAL	deletion	UNP Q712V9
A	?	-	THR	deletion	UNP Q712V9
A	?	-	THR	deletion	UNP Q712V9
A	?	-	THR	deletion	UNP Q712V9
A	?	-	THR	deletion	UNP Q712V9
A	?	-	LYS	deletion	UNP Q712V9

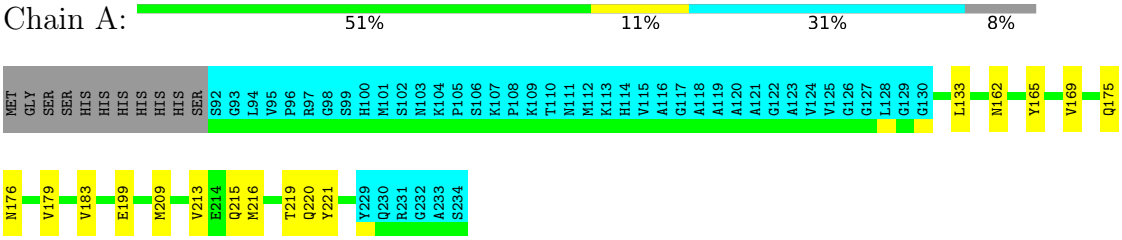
4 Residue-property plots

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: Major prion protein

Chain A:

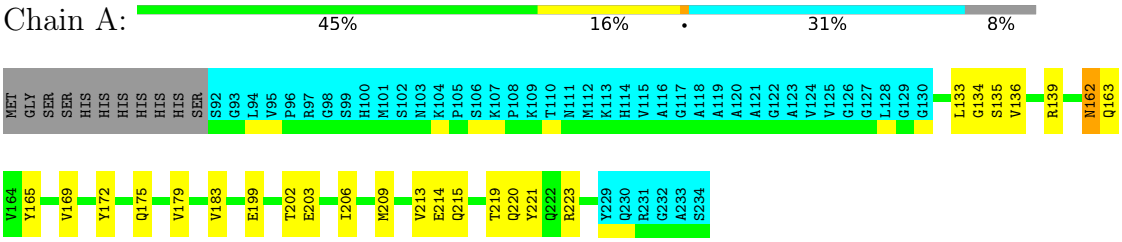


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 6. Colouring as in section 4.1 above.

• Molecule 1: Major prion protein

Chain A:



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
CYANA	structure calculation	3.0
CYANA	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1609
Number of shifts mapped to atoms	1590
Number of unparsed shifts	0
Number of shifts with mapping errors	19
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality

6.1 Standard geometry

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

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	773	716	716	8±2
All	All	15460	14320	14320	164

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 6.

5 of 50 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:169:VAL:HG21	1:A:221:TYR:CE1	0.69	2.23	9	12
1:A:133:LEU:HD22	1:A:165:TYR:CE2	0.67	2.24	10	13
1:A:169:VAL:HG21	1:A:221:TYR:CD1	0.66	2.26	6	4
1:A:175:GLN:O	1:A:179:VAL:HG23	0.64	1.92	15	19
1:A:133:LEU:HD13	1:A:165:TYR:CE2	0.64	2.28	13	4

6.3 Torsion angles

6.3.1 Protein backbone

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	90/146 (62%)	84±1 (94±1%)	5±1 (5±2%)	1±1 (1±1%)	17 64
All	All	1800/2920 (62%)	1683 (94%)	96 (5%)	21 (1%)	17 64

All 4 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	134	GLY	9
1	A	172	TYR	8
1	A	201	PHE	3
1	A	174	ASN	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	86/125 (69%)	75±2 (87±3%)	11±2 (13±3%)	7 49
All	All	1720/2500 (69%)	1498 (87%)	222 (13%)	7 49

5 of 40 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	215	GLN	20
1	A	220	GLN	17
1	A	199	GLU	16
1	A	219	THR	14
1	A	176	ASN	11

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

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1609
Number of shifts mapped to atoms	1590
Number of unparsed shifts	0
Number of shifts with mapping errors	19
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 19) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	83	SER	CA	58.05	0.25	1
1	A	83	SER	CB	63.95	0.25	1
1	A	83	SER	C	174.52	0.25	1
1	A	84	SER	N	117.83	0.15	1
1	A	84	SER	H	8.48	0.02	1
1	A	84	SER	CA	58.19	0.25	1
1	A	84	SER	HA	4.41	0.02	1
1	A	84	SER	HB2	3.79	0.02	2
1	A	84	SER	HB3	3.8	0.02	2
1	A	90	HIS	CA	55.62	0.25	1
1	A	90	HIS	CB	29.99	0.25	1
1	A	91	SER	N	118.19	0.15	1
1	A	91	SER	H	8.47	0.02	1
1	A	91	SER	CA	58.1	0.25	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	91	SER	HA	4.46	0.02	1
1	A	91	SER	CB	63.8	0.25	1
1	A	91	SER	HB2	3.83	0.02	2
1	A	91	SER	HB3	3.83	0.02	2
1	A	91	SER	C	174.41	0.25	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	138	-0.02 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	121	0.23 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	124	0.04 ± 0.10	None needed (< 0.5 ppm)
^{15}N	125	0.04 ± 0.13	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1115 atoms were assigned a chemical shift out of a possible 1289. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	421/447 (94%)	170/180 (94%)	170/180 (94%)	81/87 (93%)
Sidechain	589/699 (84%)	400/446 (90%)	174/214 (81%)	15/39 (38%)
Aromatic	105/143 (73%)	55/67 (82%)	50/74 (68%)	0/2 (0%)
Overall	1115/1289 (87%)	625/693 (90%)	394/468 (84%)	96/128 (75%)

7.1.4 Statistically unusual chemical shifts

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	186	THR	HG1	6.16	0.08 – 2.19	23.8

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: