



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 08:22 pm BST

PDB ID : 1QM1
Title : Human prion protein fragment 90-230
Authors : Zahn, R.; Liu, A.; Luhrs, T.; Wuthrich, K.
Deposited on : 1999-09-20

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 ⓘ symbol.

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 : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

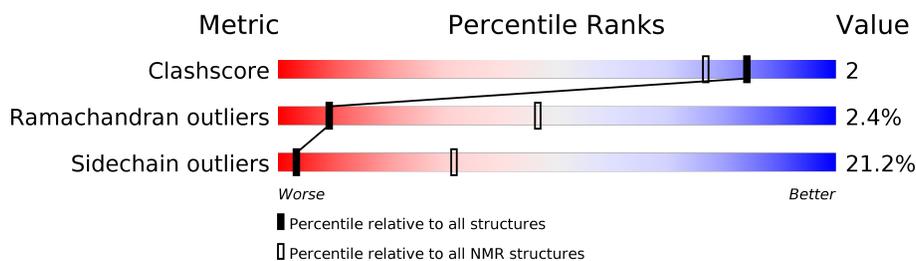
1 Overall quality at a glance i

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 ≥ 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	143	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 19 as representative.

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:129-A:166, A:172-A:228 (95)	0.45	11

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1688 atoms, of which 811 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PRION PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	104	1688	544	811	153	171	9	0

There are 2 discrepancies between the modelled and reference sequences:

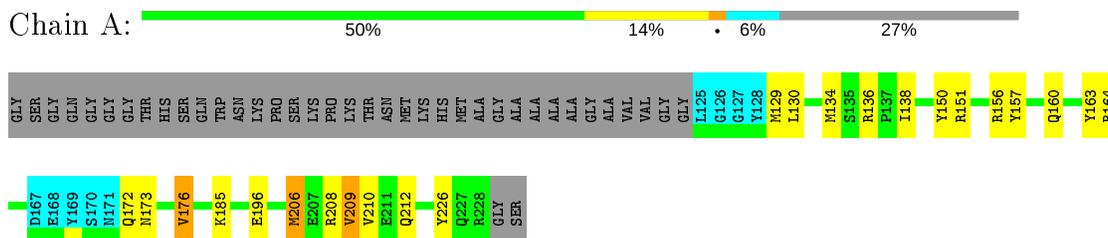
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLY	-	cloning artifact	UNP P04156
A	89	SER	-	cloning artifact	UNP P04156

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: PRION PROTEIN

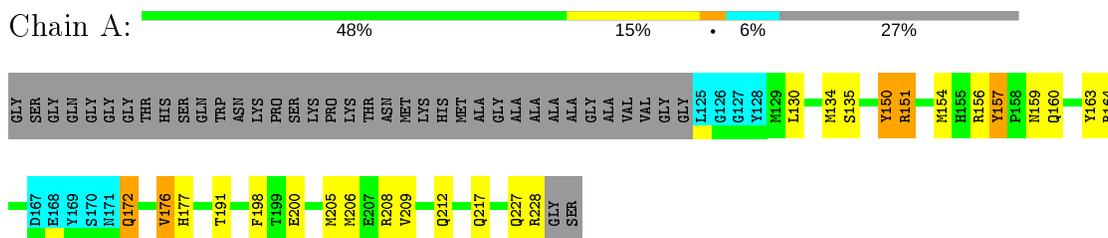


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

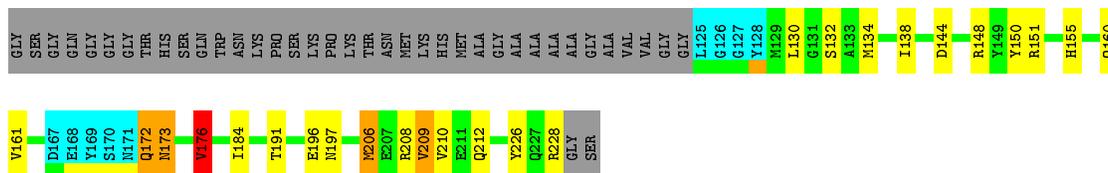
- Molecule 1: PRION PROTEIN



4.2.2 Score per residue for model 2

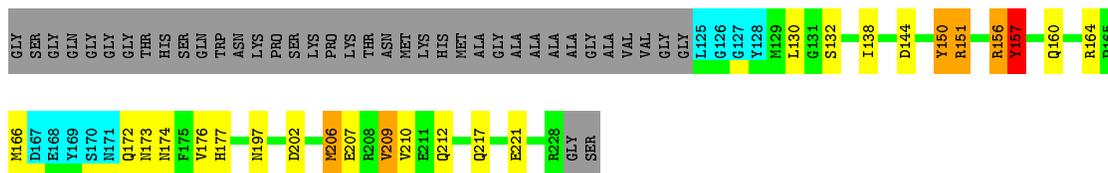
- Molecule 1: PRION PROTEIN





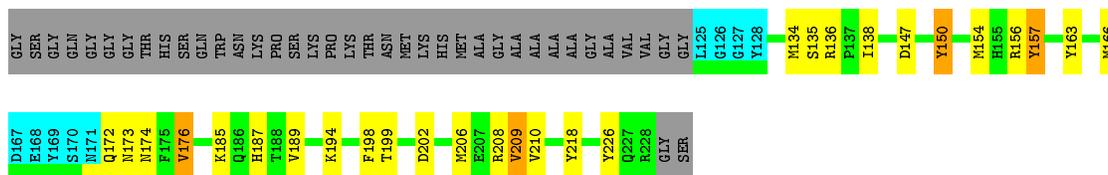
4.2.3 Score per residue for model 3

- Molecule 1: PRION PROTEIN



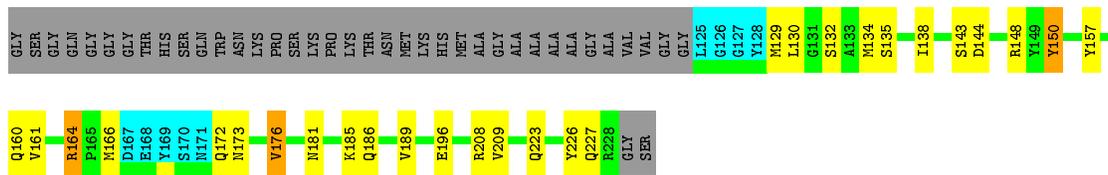
4.2.4 Score per residue for model 4

- Molecule 1: PRION PROTEIN



4.2.5 Score per residue for model 5

- Molecule 1: PRION PROTEIN

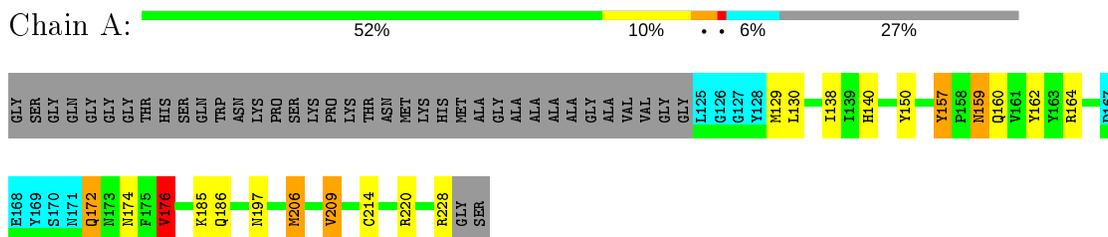


4.2.6 Score per residue for model 6

- Molecule 1: PRION PROTEIN

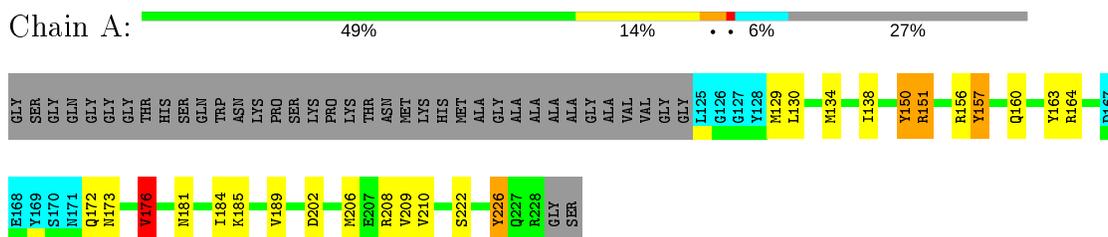
4.2.10 Score per residue for model 10

- Molecule 1: PRION PROTEIN



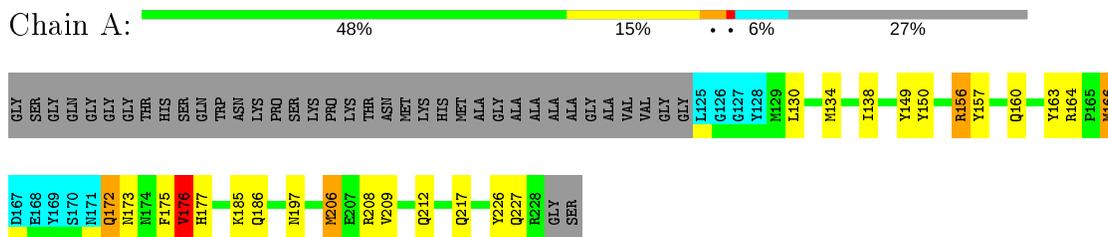
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: PRION PROTEIN



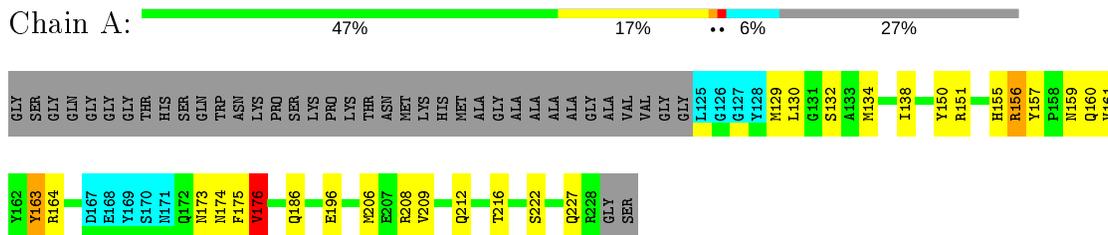
4.2.12 Score per residue for model 12

- Molecule 1: PRION PROTEIN



4.2.13 Score per residue for model 13

- Molecule 1: PRION PROTEIN



5 Refinement protocol and experimental data overview i

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
OPALP	refinement	
DYANA	structure solution	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	806	755	758	4±2
All	All	16120	15100	15160	72

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:LEU:HD11	1:A:160:GLN:HB3	0.93	1.41	18	18
1:A:185:LYS:O	1:A:189:VAL:HG23	0.58	1.98	11	7
1:A:173:ASN:HA	1:A:176:VAL:HG23	0.57	1.75	14	10
1:A:191:THR:HG22	1:A:196:GLU:HB3	0.52	1.82	6	3
1:A:206:MET:O	1:A:210:VAL:HG23	0.51	2.05	19	8
1:A:184:ILE:CG1	1:A:210:VAL:HG21	0.49	2.37	11	5
1:A:130:LEU:HD12	1:A:161:VAL:O	0.48	2.08	13	5
1:A:176:VAL:HG12	1:A:214:CYS:HB2	0.48	1.86	10	1
1:A:136:ARG:HH12	1:A:209:VAL:CG2	0.48	2.22	9	1
1:A:191:THR:HG21	1:A:198:PHE:CE2	0.47	2.45	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:THR:HG21	1:A:198:PHE:CZ	0.46	2.46	7	2
1:A:130:LEU:HD13	1:A:162:TYR:CD1	0.45	2.47	19	1
1:A:176:VAL:O	1:A:180:VAL:HG23	0.44	2.11	9	1
1:A:130:LEU:HD13	1:A:162:TYR:CE1	0.44	2.47	10	1
1:A:156:ARG:CG	1:A:157:TYR:H	0.43	2.27	3	1
1:A:172:GLN:CD	1:A:172:GLN:H	0.42	2.18	10	1
1:A:139:ILE:HD11	1:A:212:GLN:HG3	0.42	1.90	6	2
1:A:136:ARG:HH12	1:A:209:VAL:HG21	0.41	1.75	9	1
1:A:137:PRO:HG2	1:A:209:VAL:HG23	0.40	1.93	17	1
1:A:150:TYR:CD1	1:A:157:TYR:CD2	0.40	3.09	11	1

5.2 Torsion angles [i](#)

5.2.1 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	94/143 (66%)	85±2 (90±2%)	7±2 (7±2%)	2±1 (2±1%)	9	46
All	All	1880/2860 (66%)	1695 (90%)	140 (7%)	45 (2%)	9	46

All 10 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	138	ILE	16
1	A	172	GLN	10
1	A	157	TYR	8
1	A	166	MET	4
1	A	196	GLU	2
1	A	132	SER	1
1	A	159	ASN	1
1	A	136	ARG	1
1	A	198	PHE	1
1	A	135	SER	1

5.2.2 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	90/120 (75%)	71±3 (79±4%)	19±3 (21±4%)	3 31
All	All	1800/2400 (75%)	1419 (79%)	381 (21%)	3 31

All 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	176	VAL	19
1	A	209	VAL	18
1	A	150	TYR	18
1	A	206	MET	18
1	A	157	TYR	15
1	A	208	ARG	13
1	A	164	ARG	13
1	A	172	GLN	12
1	A	212	GLN	12
1	A	156	ARG	11
1	A	226	TYR	11
1	A	144	ASP	10
1	A	163	TYR	10
1	A	202	ASP	10
1	A	186	GLN	10
1	A	217	GLN	10
1	A	129	MET	10
1	A	197	ASN	9
1	A	151	ARG	9
1	A	185	LYS	8
1	A	132	SER	8
1	A	134	MET	8
1	A	227	GLN	7
1	A	174	ASN	7
1	A	159	ASN	7
1	A	196	GLU	6
1	A	207	GLU	6
1	A	135	SER	6
1	A	228	ARG	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	136	ARG	5
1	A	173	ASN	5
1	A	149	TYR	5
1	A	181	ASN	4
1	A	178	ASP	4
1	A	155	HIS	4
1	A	143	SER	3
1	A	140	HIS	3
1	A	194	LYS	3
1	A	154	MET	3
1	A	177	HIS	3
1	A	187	HIS	3
1	A	166	MET	2
1	A	188	THR	2
1	A	175	PHE	2
1	A	200	GLU	2
1	A	199	THR	2
1	A	222	SER	2
1	A	153	ASN	2
1	A	211	GLU	1
1	A	223	GLN	1
1	A	147	ASP	1
1	A	216	THR	1
1	A	221	GLU	1
1	A	179	CYS	1
1	A	191	THR	1
1	A	192	THR	1
1	A	138	ILE	1
1	A	214	CYS	1
1	A	193	THR	1
1	A	190	THR	1
1	A	152	GLU	1
1	A	148	ARG	1
1	A	225	TYR	1

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

No chemical shift data were provided