



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 02:26 PM UTC

PDB ID : 1DWZ / pdb_00001dwz
Title : Bovine prion protein fragment 121-230
Authors : Lopez-Garcia, F.; Zahn, R.; Riek, R.; Billeter, M.; Wuthrich, K.
Deposited on : 1999-12-15

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

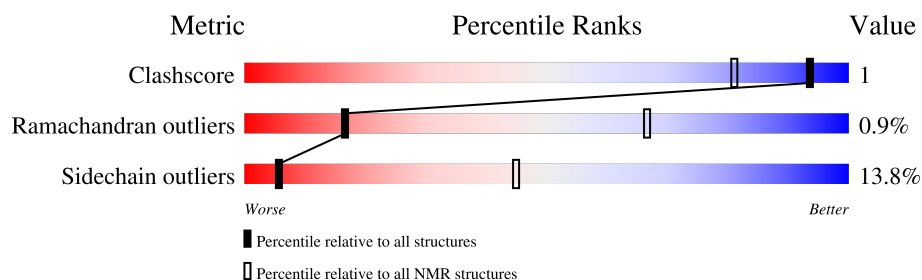
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	112	79% 10% • 7%

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 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:128-A:227 (100)	0.80	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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1675 atoms, of which 806 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PRION PROTEIN.

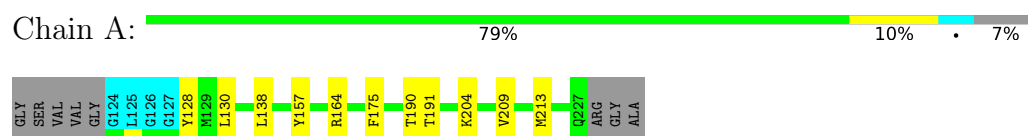
Mol	Chain	Residues	Atoms							Trace
1	A	104	Total	C	H	N	O	S		0
			1675	540	806	151	170	8		

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: PRION PROTEIN

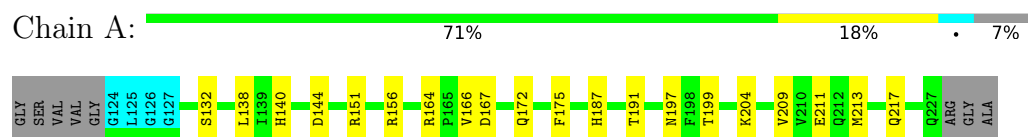


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

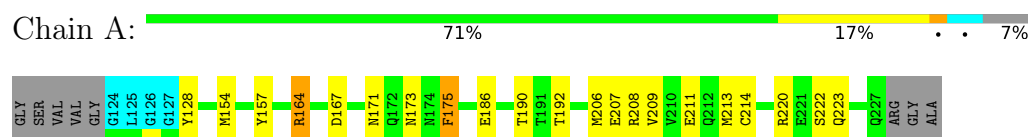
4.2.1 Score per residue for model 1

• Molecule 1: PRION PROTEIN



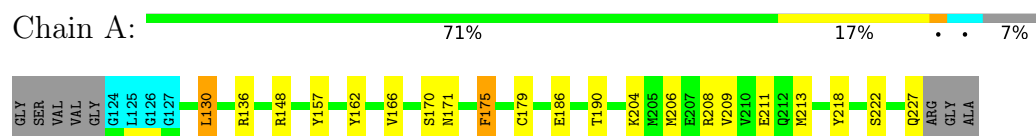
4.2.2 Score per residue for model 2

• Molecule 1: PRION PROTEIN



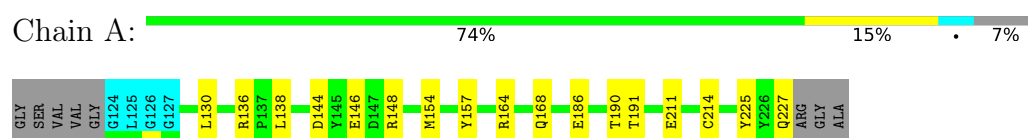
4.2.3 Score per residue for model 3

- Molecule 1: PRION PROTEIN



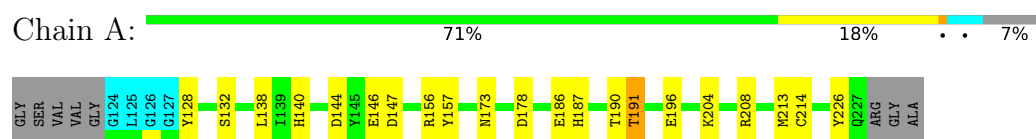
4.2.4 Score per residue for model 4

- Molecule 1: PRION PROTEIN



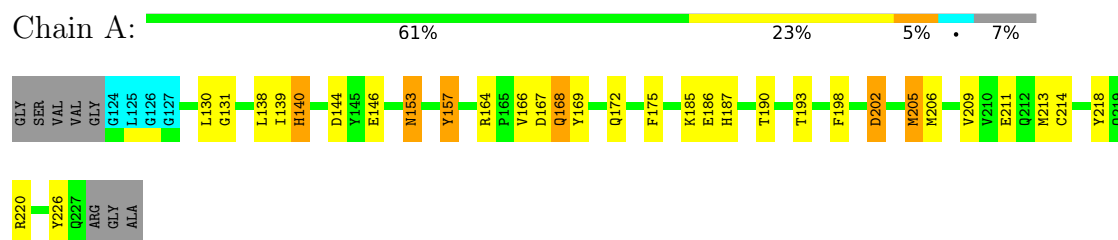
4.2.5 Score per residue for model 5

- Molecule 1: PRION PROTEIN



4.2.6 Score per residue for model 6

- Molecule 1: PRION PROTEIN



4.2.7 Score per residue for model 7

- Molecule 1: PRION PROTEIN





4.2.8 Score per residue for model 8

- Molecule 1: PRION PROTEIN

Chain A: 80% 9% 7%



4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: PRION PROTEIN

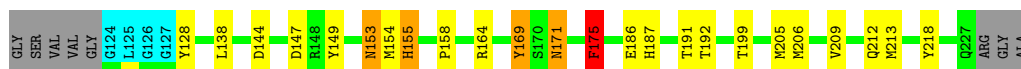
Chain A: 75% 12% 7%



4.2.10 Score per residue for model 10

- Molecule 1: PRION PROTEIN

Chain A: 68% 17% 7%



4.2.11 Score per residue for model 11

- Molecule 1: PRION PROTEIN

Chain A: 72% 16% 7%



4.2.12 Score per residue for model 12

- Molecule 1: PRION PROTEIN

Chain A: 71% 17% 7%



4.2.13 Score per residue for model 13

- Molecule 1: PRION PROTEIN

Chain A: 69% 18% 7%



4.2.14 Score per residue for model 14

- Molecule 1: PRION PROTEIN

Chain A: 68% 20% 7%



4.2.15 Score per residue for model 15

- Molecule 1: PRION PROTEIN

Chain A: 72% 15% 7%



4.2.16 Score per residue for model 16

- Molecule 1: PRION PROTEIN

Chain A: 72% 16% 7%



4.2.17 Score per residue for model 17

- Molecule 1: PRION PROTEIN

Chain A: 71% 17% 7%



4.2.18 Score per residue for model 18

- Molecule 1: PRION PROTEIN

Chain A: 73% 15% 7%



4.2.19 Score per residue for model 19

- Molecule 1: PRION PROTEIN

Chain A: 71% 17% 7%



4.2.20 Score per residue for model 20

- Molecule 1: PRION PROTEIN

Chain A: 76% 13% 7%



5 Refinement protocol and experimental data overview ⓘ

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

Of the 50 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.

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.69±0.01	0±0/869 (0.0± 0.0%)	1.42±0.05	2±2/1175 (0.2± 0.1%)
All	All	0.69	0/17380 (0.0%)	1.42	40/23500 (0.2%)

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	3.0±1.6
All	All	0	60

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	167	ASP	CA-CB-CG	7.36	119.96	112.60	2	2
1	A	171	ASN	CA-CB-CG	6.82	119.42	112.60	13	1
1	A	136	ARG	CD-NE-CZ	6.65	133.71	124.40	12	1
1	A	153	ASN	CA-CB-CG	6.37	118.97	112.60	10	2
1	A	166	VAL	CA-C-N	6.20	128.91	120.54	1	3
1	A	166	VAL	C-N-CA	6.20	128.91	120.54	1	3
1	A	178	ASP	CA-CB-CG	6.20	118.80	112.60	11	1
1	A	187	HIS	CB-CG-CD2	-6.12	123.24	131.20	10	4
1	A	209	VAL	CA-CB-CG1	5.58	119.89	110.40	15	1
1	A	191	THR	CA-C-N	5.53	128.01	120.54	5	2
1	A	191	THR	C-N-CA	5.53	128.01	120.54	5	2
1	A	209	VAL	CA-CB-CG2	5.51	119.77	110.40	9	1
1	A	197	ASN	CA-CB-CG	5.37	117.97	112.60	13	1
1	A	196	GLU	CA-C-N	5.35	131.41	121.62	11	1
1	A	196	GLU	C-N-CA	5.35	131.41	121.62	11	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	184	VAL	CA-C-O	-5.33	115.58	121.29	14	1
1	A	225	TYR	CA-C-N	5.32	127.72	120.54	19	1
1	A	225	TYR	C-N-CA	5.32	127.72	120.54	19	1
1	A	202	ASP	CA-CB-CG	5.32	117.92	112.60	6	1
1	A	191	THR	CA-CB-CG2	5.25	119.43	110.50	9	2
1	A	187	HIS	CA-CB-CG	-5.22	108.58	113.80	10	1
1	A	181	ASN	CA-CB-CG	-5.10	107.50	112.60	11	1
1	A	177	HIS	CB-CG-CD2	-5.08	124.59	131.20	18	1
1	A	155	HIS	CB-CG-CD2	-5.04	124.64	131.20	18	2
1	A	173	ASN	CA-CB-CG	-5.02	107.58	112.60	12	1
1	A	145	TYR	CA-C-N	5.00	127.49	120.28	7	1
1	A	145	TYR	C-N-CA	5.00	127.49	120.28	7	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	157	TYR	Sidechain	15
1	A	128	TYR	Sidechain	7
1	A	151	ARG	Sidechain	5
1	A	156	ARG	Sidechain	5
1	A	175	PHE	Sidechain	5
1	A	164	ARG	Sidechain	4
1	A	208	ARG	Sidechain	4
1	A	148	ARG	Sidechain	3
1	A	220	ARG	Sidechain	2
1	A	225	TYR	Sidechain	2
1	A	171	ASN	Peptide	1
1	A	136	ARG	Sidechain	1
1	A	226	TYR	Sidechain	1
1	A	163	TYR	Sidechain	1
1	A	149	TYR	Sidechain	1
1	A	150	TYR	Sidechain	1
1	A	153	ASN	Peptide	1
1	A	218	TYR	Sidechain	1

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	849	786	786	2±2
All	All	16980	15720	15720	44

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:209:VAL:HG12	1:A:213:MET:HE2	0.72	1.58	10	8
1:A:138:LEU:HD11	1:A:151:ARG:HE	0.72	1.43	14	1
1:A:209:VAL:CG1	1:A:213:MET:HE2	0.65	2.22	2	11
1:A:150:TYR:OH	1:A:209:VAL:HG21	0.57	2.00	17	1
1:A:130:LEU:HD11	1:A:160:GLN:HB3	0.56	1.77	20	2
1:A:201:THR:HG22	1:A:205:MET:SD	0.54	2.43	17	1
1:A:166:VAL:HG12	1:A:218:TYR:CE1	0.53	2.39	9	1
1:A:175:PHE:CE2	1:A:218:TYR:HB2	0.52	2.38	18	2
1:A:138:LEU:HD11	1:A:151:ARG:NE	0.51	2.17	14	1
1:A:215:ILE:HG22	1:A:219:GLN:HE21	0.48	1.67	17	1
1:A:140:HIS:CD2	1:A:140:HIS:H	0.45	2.27	6	1
1:A:175:PHE:CZ	1:A:218:TYR:HB2	0.45	2.46	10	3
1:A:215:ILE:HG23	1:A:219:GLN:NE2	0.44	2.28	7	1
1:A:158:PRO:O	1:A:213:MET:HE1	0.44	2.13	10	2
1:A:191:THR:HG21	1:A:198:PHE:CZ	0.43	2.48	17	1
1:A:157:TYR:OH	1:A:205:MET:HE2	0.43	2.14	6	1
1:A:130:LEU:HD23	1:A:162:TYR:CE1	0.43	2.48	3	1
1:A:156:ARG:HH12	1:A:196:GLU:CD	0.42	2.22	9	1
1:A:175:PHE:CE1	1:A:218:TYR:HB2	0.42	2.49	13	1
1:A:209:VAL:CG1	1:A:213:MET:HE3	0.41	2.45	8	1
1:A:198:PHE:CD2	1:A:202:ASP:HB3	0.40	2.52	6	1
1:A:150:TYR:CE2	1:A:154:MET:HE3	0.40	2.51	13	1

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	99/112 (88%)	91±2 (92±2%)	7±2 (7±2%)	1±1 (1±1%)	16	66
All	All	1980/2240 (88%)	1816 (92%)	146 (7%)	18 (1%)	16	66

All 12 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	171	ASN	3
1	A	128	TYR	3
1	A	154	MET	2
1	A	167	ASP	2
1	A	172	GLN	1
1	A	131	GLY	1
1	A	166	VAL	1
1	A	168	GLN	1
1	A	220	ARG	1
1	A	169	TYR	1
1	A	132	SER	1
1	A	170	SER	1

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	95/100 (95%)	82±4 (86±4%)	13±4 (14±4%)	6	45
All	All	1900/2000 (95%)	1637 (86%)	263 (14%)	6	45

All 65 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	190	THR	15
1	A	138	LEU	14
1	A	204	LYS	12
1	A	144	ASP	9
1	A	211	GLU	9
1	A	186	GLU	9
1	A	130	LEU	9
1	A	164	ARG	8
1	A	227	GLN	8
1	A	191	THR	8
1	A	199	THR	7
1	A	214	CYS	7
1	A	175	PHE	6
1	A	206	MET	6
1	A	146	GLU	6
1	A	205	MET	6
1	A	209	VAL	6
1	A	132	SER	5
1	A	140	HIS	5
1	A	173	ASN	5
1	A	179	CYS	5
1	A	168	GLN	5
1	A	223	GLN	4
1	A	136	ARG	4
1	A	169	TYR	4
1	A	172	GLN	4
1	A	192	THR	3
1	A	220	ARG	3
1	A	222	SER	3
1	A	154	MET	3
1	A	178	ASP	3
1	A	213	MET	3
1	A	185	LYS	3
1	A	193	THR	3
1	A	166	VAL	3
1	A	171	ASN	3
1	A	148	ARG	3
1	A	187	HIS	3
1	A	197	ASN	2
1	A	217	GLN	2
1	A	207	GLU	2
1	A	170	SER	2
1	A	225	TYR	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	147	ASP	2
1	A	139	ILE	2
1	A	153	ASN	2
1	A	226	TYR	2
1	A	155	HIS	2
1	A	149	TYR	2
1	A	151	ARG	2
1	A	219	GLN	2
1	A	189	VAL	2
1	A	196	GLU	1
1	A	157	TYR	1
1	A	201	THR	1
1	A	143	SER	1
1	A	212	GLN	1
1	A	177	HIS	1
1	A	221	GLU	1
1	A	208	ARG	1
1	A	174	ASN	1
1	A	160	GLN	1
1	A	128	TYR	1
1	A	215	ILE	1
1	A	135	SER	1

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 oligosaccharides 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