



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:31 PM UTC

PDB ID : 1QLZ / pdb_00001qlz
Title : Human prion protein
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 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

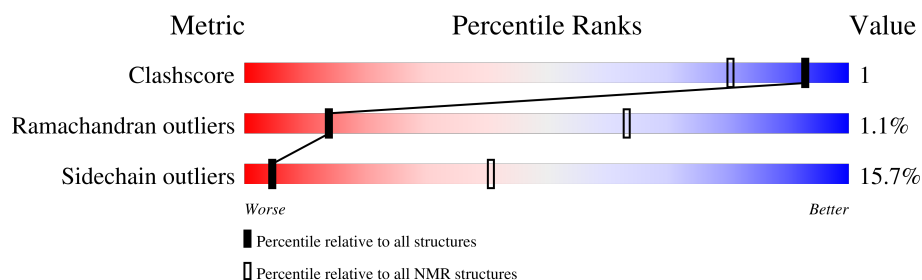
1 Overall quality at a glance

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	210	

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 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:228 (101)	0.73	19

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

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
1	A	104	Total	C	H	N	O	S	0
			1688	544	811	153	171	9	

There are 2 discrepancies between the modelled and reference sequences:

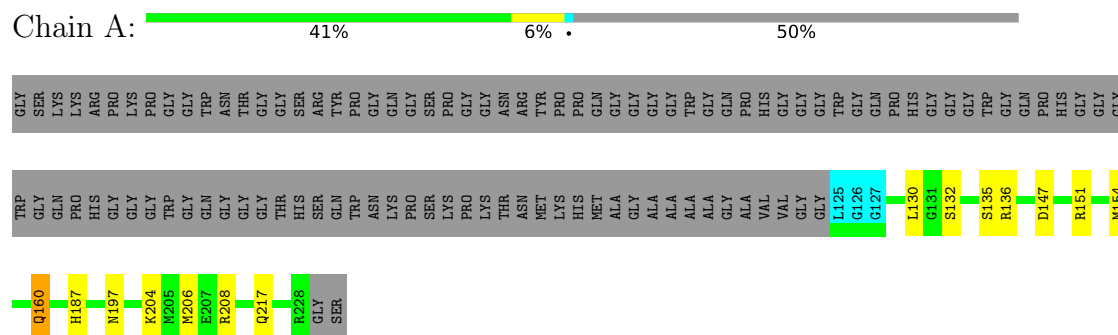
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	cloning artifact	UNP P04156
A	22	SER	-	cloning artifact	UNP P04156

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

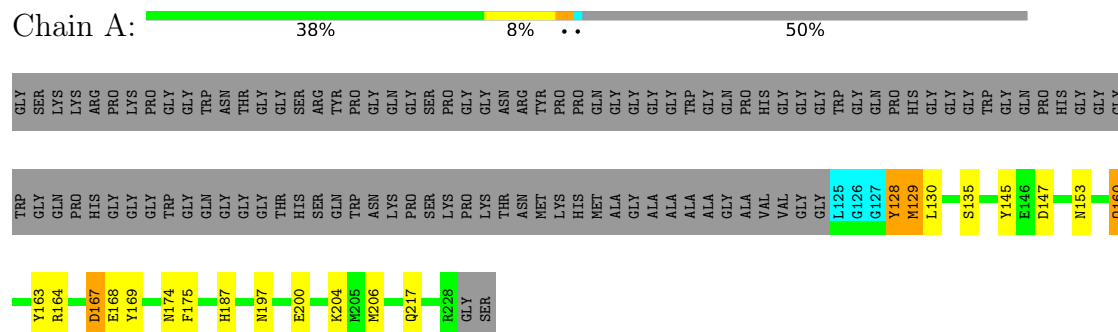


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

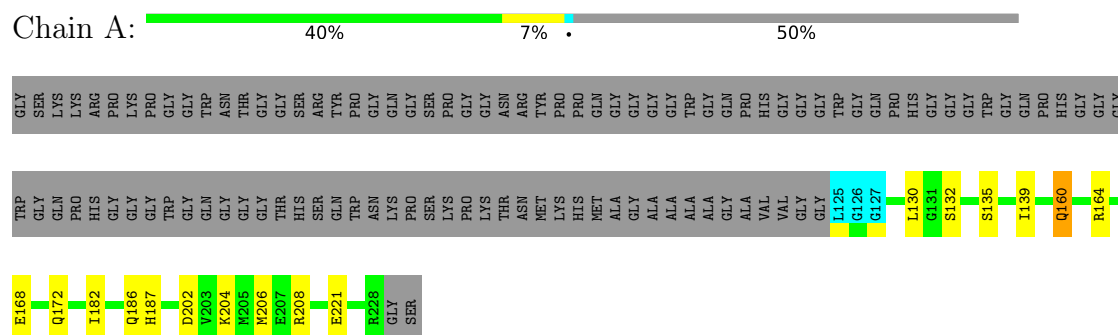
4.2.1 Score per residue for model 1

• Molecule 1: PRION PROTEIN



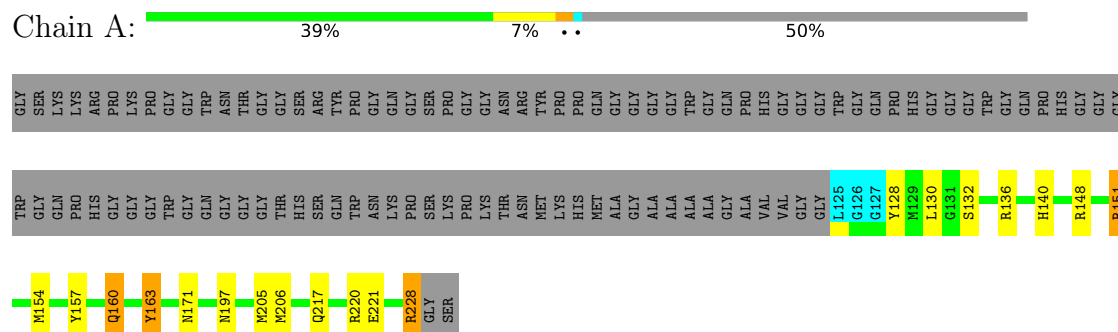
4.2.2 Score per residue for model 2

• Molecule 1: PRION PROTEIN



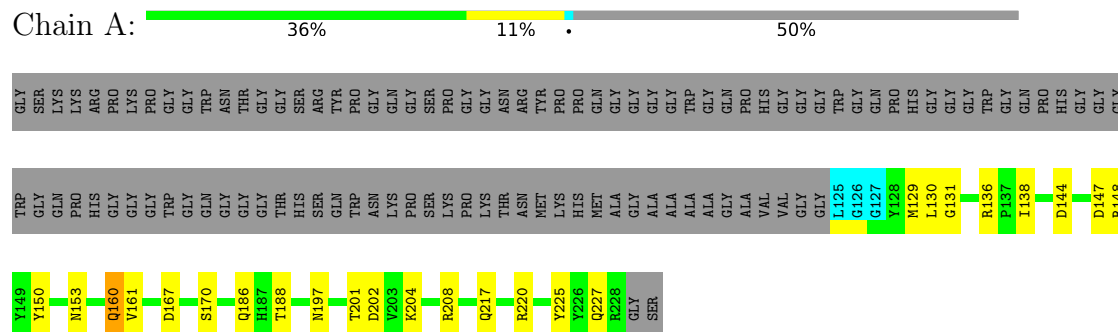
4.2.3 Score per residue for model 3

• Molecule 1: PRION PROTEIN



4.2.4 Score per residue for model 4

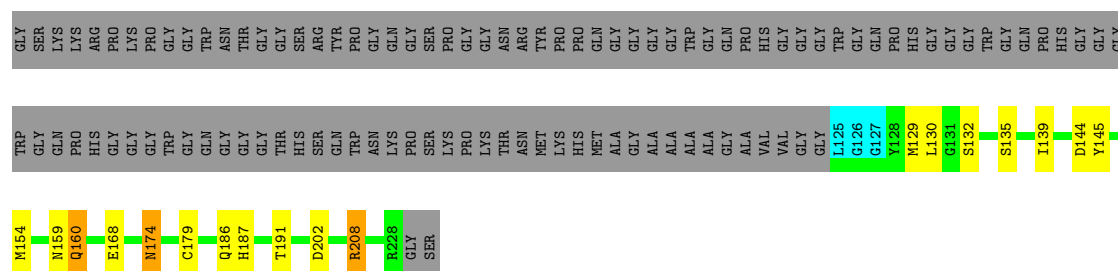
• Molecule 1: PRION PROTEIN



4.2.5 Score per residue for model 5

• Molecule 1: PRION PROTEIN

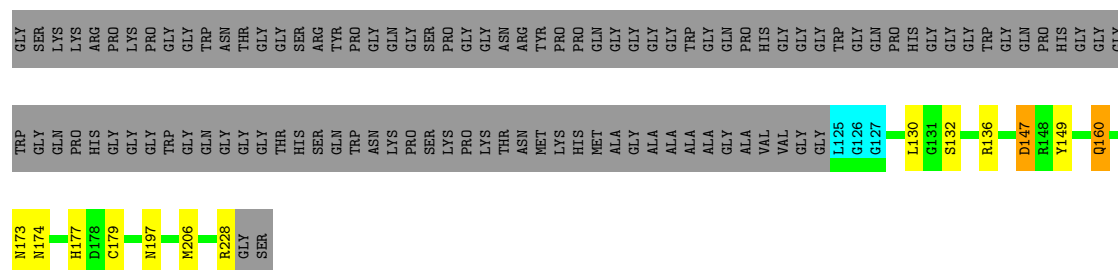
Chain A:  40% 7% .. 50%



4.2.6 Score per residue for model 6

- Molecule 1: PRION PROTEIN

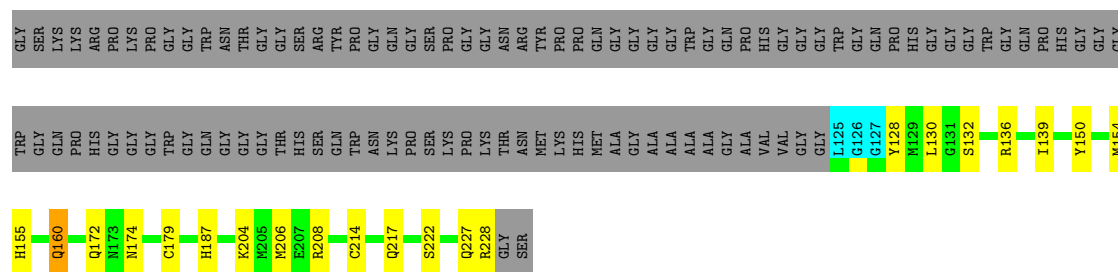
Chain A:  42% 5% .. 50%



4.2.7 Score per residue for model 7

- Molecule 1: PRION PROTEIN

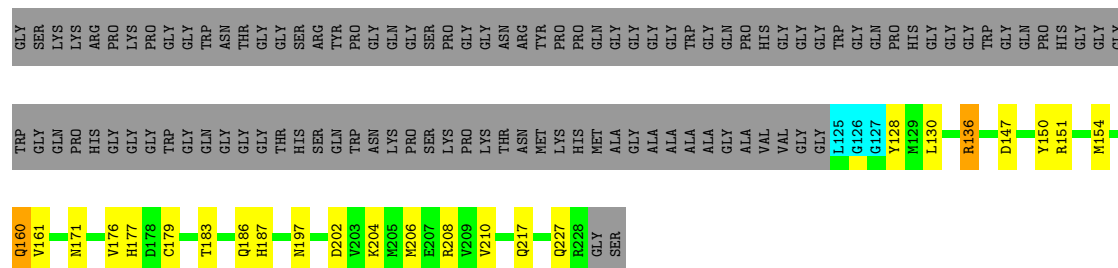
Chain A:  38% 10% . 50%



4.2.8 Score per residue for model 8

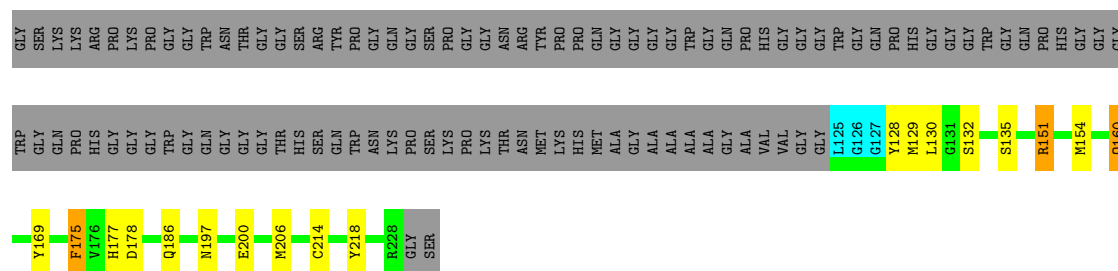
- Molecule 1: PRION PROTEIN

Chain A:  37% 10% .. 50%



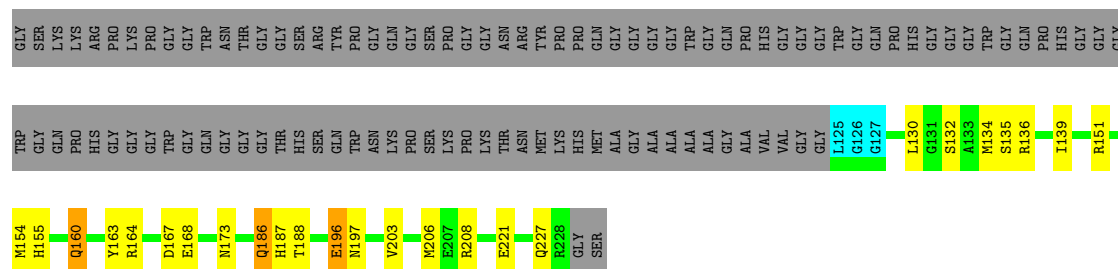
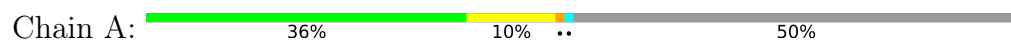
4.2.9 Score per residue for model 9

- Molecule 1: PRION PROTEIN



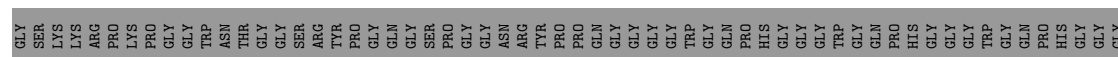
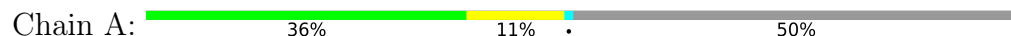
4.2.10 Score per residue for model 10

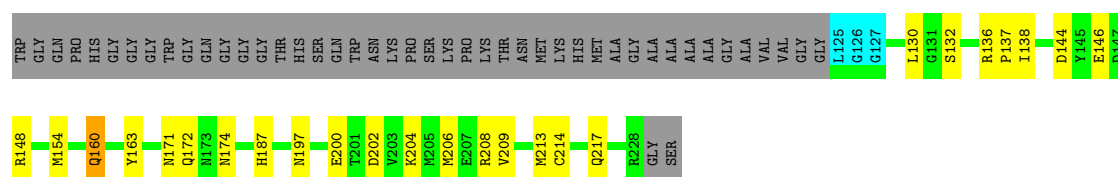
- Molecule 1: PRION PROTEIN



4.2.11 Score per residue for model 11

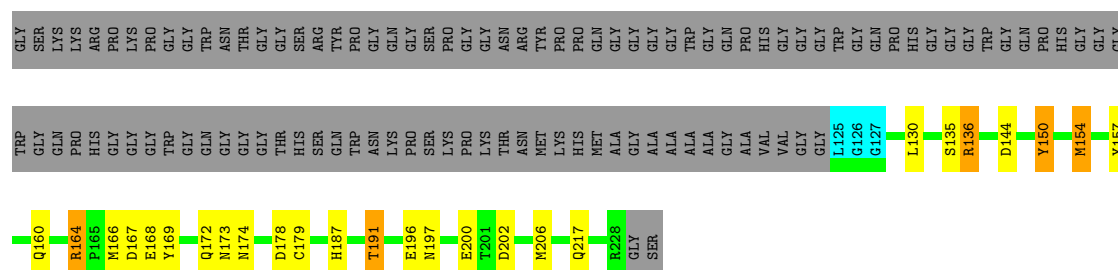
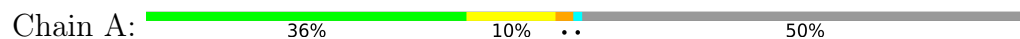
- Molecule 1: PRION PROTEIN





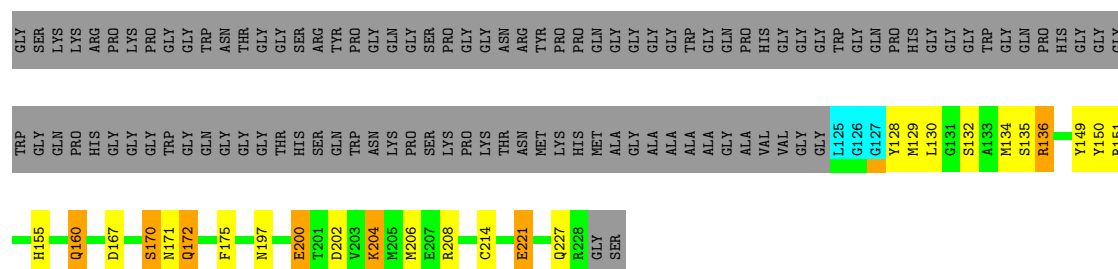
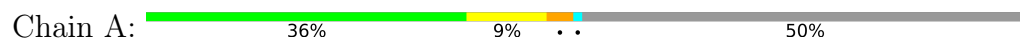
4.2.12 Score per residue for model 12

- Molecule 1: PRION PROTEIN



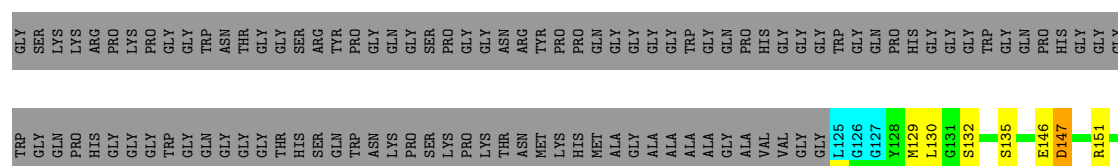
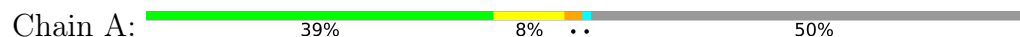
4.2.13 Score per residue for model 13

- Molecule 1: PRION PROTEIN



4.2.14 Score per residue for model 14

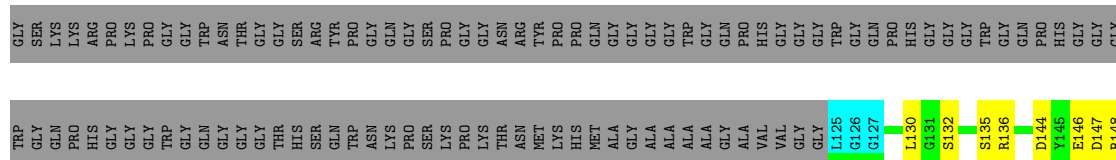
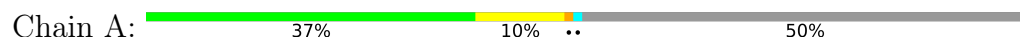
- Molecule 1: PRION PROTEIN





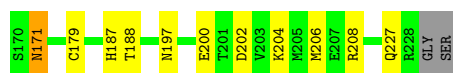
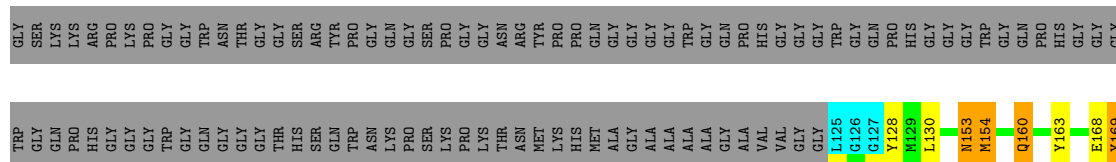
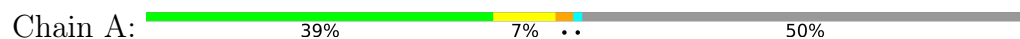
4.2.15 Score per residue for model 15

- Molecule 1: PRION PROTEIN



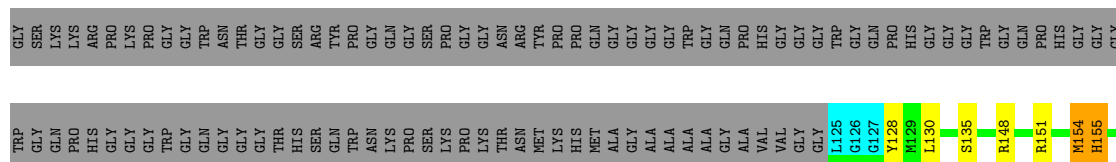
4.2.16 Score per residue for model 16

- Molecule 1: PRION PROTEIN



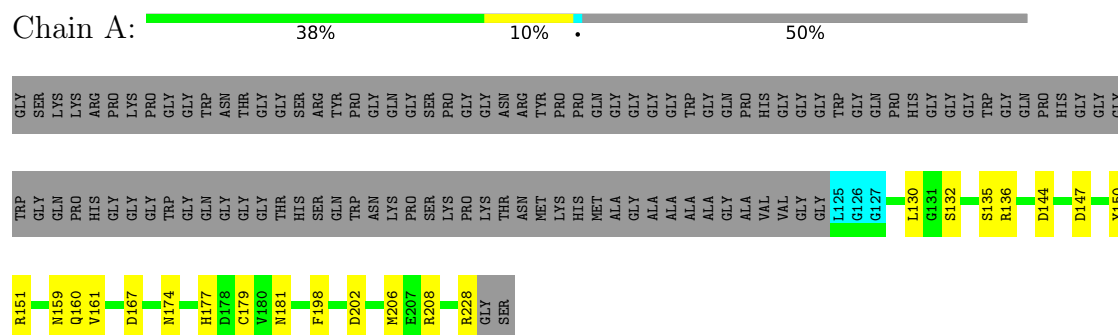
4.2.17 Score per residue for model 17

- Molecule 1: PRION PROTEIN



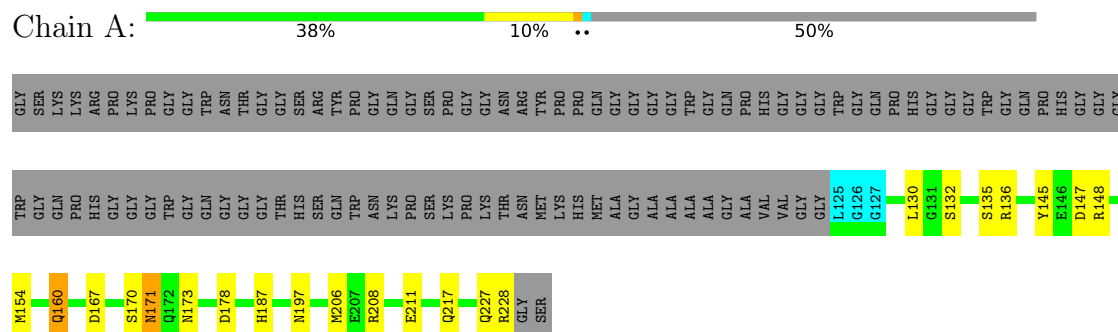
4.2.18 Score per residue for model 18

• Molecule 1: PRION PROTEIN



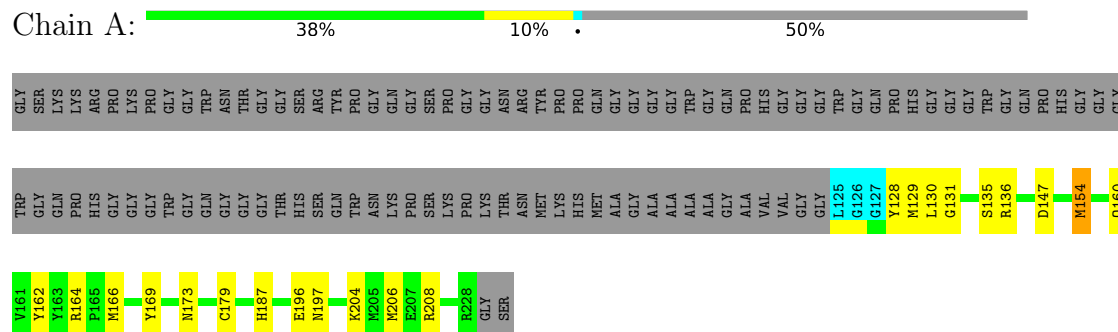
4.2.19 Score per residue for model 19 (medoid)

• Molecule 1: PRION PROTEIN



4.2.20 Score per residue for model 20

• Molecule 1: PRION PROTEIN



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: *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	0.70±0.02	0±0/881 (0.0± 0.0%)	1.43±0.04	2±2/1189 (0.2± 0.2%)
All	All	0.70	0/17620 (0.0%)	1.43	47/23780 (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	1.7±1.3
All	All	0	34

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	178	ASP	CA-CB-CG	11.57	124.17	112.60	12	1
1	A	159	ASN	CA-CB-CG	7.75	120.36	112.60	5	1
1	A	202	ASP	CA-CB-CG	7.49	120.08	112.60	5	8
1	A	147	ASP	CA-CB-CG	7.44	120.04	112.60	14	4
1	A	173	ASN	CA-CB-CG	7.06	119.66	112.60	6	1
1	A	153	ASN	CA-CB-CG	6.31	118.91	112.60	16	2
1	A	128	TYR	CA-CB-CG	6.27	125.18	113.90	1	1
1	A	155	HIS	CA-C-N	6.11	129.29	120.38	17	1
1	A	155	HIS	C-N-CA	6.11	129.29	120.38	17	1
1	A	144	ASP	CA-C-N	6.00	129.12	120.79	4	1
1	A	144	ASP	C-N-CA	6.00	129.12	120.79	4	1
1	A	171	ASN	CA-CB-CG	5.83	118.42	112.60	16	1
1	A	221	GLU	CA-C-N	5.65	128.12	120.44	13	1
1	A	221	GLU	C-N-CA	5.65	128.12	120.44	13	1
1	A	174	ASN	CA-CB-CG	5.64	118.24	112.60	5	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	167	ASP	CA-CB-CG	5.59	118.19	112.60	19	1
1	A	203	VAL	N-CA-C	-5.56	105.30	110.53	10	1
1	A	186	GLN	OE1-CD-NE2	-5.55	117.05	122.60	10	1
1	A	197	ASN	CA-CB-CG	5.53	118.13	112.60	14	1
1	A	146	GLU	CA-C-N	5.33	127.36	120.44	14	2
1	A	146	GLU	C-N-CA	5.33	127.36	120.44	14	2
1	A	201	THR	CA-C-N	5.32	127.73	120.54	4	1
1	A	201	THR	C-N-CA	5.32	127.73	120.54	4	1
1	A	200	GLU	CB-CG-CD	5.22	121.48	112.60	13	1
1	A	177	HIS	CB-CG-CD2	-5.20	124.45	131.20	9	1
1	A	155	HIS	CB-CG-CD2	-5.17	124.49	131.20	13	1
1	A	175	PHE	CA-CB-CG	5.14	118.94	113.80	13	1
1	A	168	GLU	CA-C-N	5.07	131.23	121.54	16	1
1	A	168	GLU	C-N-CA	5.07	131.23	121.54	16	1
1	A	140	HIS	CB-CG-CD2	-5.07	124.61	131.20	3	1
1	A	202	ASP	CA-C-N	5.06	127.12	120.60	11	1
1	A	202	ASP	C-N-CA	5.06	127.12	120.60	11	1
1	A	167	ASP	CA-C-N	5.01	131.12	121.54	12	1
1	A	167	ASP	C-N-CA	5.01	131.12	121.54	12	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	151	ARG	Sidechain	4
1	A	136	ARG	Sidechain	4
1	A	145	TYR	Sidechain	3
1	A	164	ARG	Sidechain	3
1	A	157	TYR	Sidechain	3
1	A	208	ARG	Sidechain	3
1	A	228	ARG	Sidechain	2
1	A	149	TYR	Sidechain	2
1	A	134	MET	Peptide	2
1	A	148	ARG	Sidechain	2
1	A	169	TYR	Sidechain	2
1	A	163	TYR	Peptide	1
1	A	220	ARG	Sidechain	1
1	A	198	PHE	Sidechain	1
1	A	162	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	861	794	797	2±1
All	All	17220	15880	15940	47

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:151:ARG:HG3	1:A:154:MET:HE3	0.70	1.60	3	4
1:A:130:LEU:HD11	1:A:160:GLN:HB2	0.62	1.72	18	20
1:A:217:GLN:HA	1:A:220:ARG:CG	0.54	2.32	15	1
1:A:209:VAL:HG12	1:A:213:MET:HE2	0.53	1.81	11	1
1:A:200:GLU:HG2	1:A:204:LYS:HE3	0.52	1.82	13	1
1:A:175:PHE:CD2	1:A:218:TYR:CE1	0.48	3.01	9	1
1:A:183:THR:HB	1:A:210:VAL:HG11	0.48	1.84	8	1
1:A:129:MET:HE1	1:A:163:TYR:CZ	0.48	2.44	1	1
1:A:130:LEU:HD12	1:A:161:VAL:O	0.47	2.10	4	4
1:A:161:VAL:HG12	1:A:210:VAL:HG13	0.47	1.85	8	1
1:A:191:THR:HG22	1:A:196:GLU:CG	0.45	2.42	12	1
1:A:172:GLN:CD	1:A:172:GLN:H	0.44	2.18	14	1
1:A:217:GLN:HA	1:A:220:ARG:HG3	0.43	1.91	15	1
1:A:150:TYR:CZ	1:A:154:MET:SD	0.43	3.11	12	1
1:A:136:ARG:HG3	1:A:154:MET:HE2	0.42	1.91	11	2
1:A:200:GLU:CG	1:A:204:LYS:HE3	0.42	2.43	13	1
1:A:136:ARG:CD	1:A:154:MET:HE3	0.41	2.45	20	1
1:A:176:VAL:HA	1:A:179:CYS:SG	0.40	2.56	8	1
1:A:129:MET:HE1	1:A:163:TYR:CE1	0.40	2.52	1	1
1:A:137:PRO:HD2	1:A:209:VAL:HG13	0.40	1.94	11	1
1:A:130:LEU:HD21	1:A:160:GLN:NE2	0.40	2.32	16	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	100/210 (48%)	90±3 (90±3%)	9±2 (9±2%)	1±1 (1±1%)	14	63
All	All	2000/4200 (48%)	1793 (90%)	186 (9%)	21 (1%)	14	63

All 11 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	167	ASP	4
1	A	172	GLN	3
1	A	131	GLY	2
1	A	171	ASN	2
1	A	169	TYR	2
1	A	170	SER	2
1	A	154	MET	2
1	A	196	GLU	1
1	A	166	MET	1
1	A	155	HIS	1
1	A	132	SER	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	96/159 (60%)	81±2 (84±3%)	15±2 (16±3%)	4	41
All	All	1920/3180 (60%)	1619 (84%)	301 (16%)	4	41

All 59 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	160	GLN	17
1	A	206	MET	17
1	A	197	ASN	16
1	A	135	SER	13
1	A	187	HIS	13
1	A	132	SER	12
1	A	208	ARG	12
1	A	204	LYS	10
1	A	217	GLN	10
1	A	128	TYR	9
1	A	136	ARG	9
1	A	174	ASN	8
1	A	129	MET	7
1	A	147	ASP	7
1	A	186	GLN	7
1	A	227	GLN	7
1	A	154	MET	7
1	A	179	CYS	7
1	A	200	GLU	6
1	A	163	TYR	6
1	A	150	TYR	6
1	A	168	GLU	5
1	A	171	ASN	5
1	A	144	ASP	5
1	A	167	ASP	4
1	A	139	ILE	4
1	A	164	ARG	4
1	A	172	GLN	4
1	A	221	GLU	4
1	A	148	ARG	4
1	A	228	ARG	4
1	A	177	HIS	4
1	A	214	CYS	4
1	A	173	ASN	4
1	A	169	TYR	3
1	A	188	THR	3
1	A	155	HIS	3
1	A	151	ARG	3
1	A	153	ASN	2
1	A	175	PHE	2
1	A	138	ILE	2
1	A	170	SER	2
1	A	191	THR	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	178	ASP	2
1	A	196	GLU	2
1	A	182	ILE	1
1	A	205	MET	1
1	A	202	ASP	1
1	A	220	ARG	1
1	A	225	TYR	1
1	A	222	SER	1
1	A	146	GLU	1
1	A	194	LYS	1
1	A	219	GLU	1
1	A	223	GLN	1
1	A	159	ASN	1
1	A	181	ASN	1
1	A	211	GLU	1
1	A	166	MET	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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided