Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 07:24 pm BST

PDB ID	:	1DX1
Title	:	BOVINE PRION PROTEIN RESIDUES 23-230
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 (i) symbol.

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

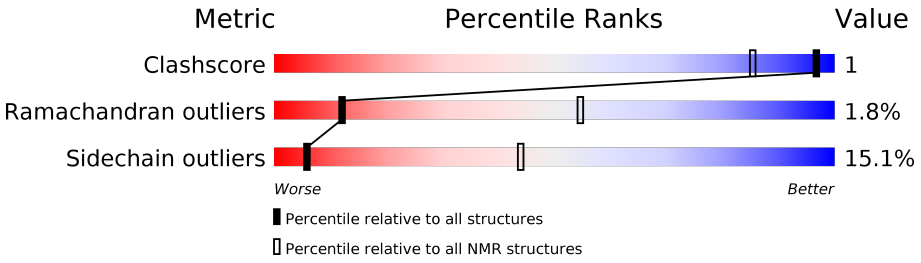
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	219	42% · 53%

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 3 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:125-A:227 (103)	0.59	18

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

3 Entry composition

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
			Total	C	H	N	O	S	
1	A	104	1675	540	806	151	170	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	cloning artifact	UNP P10279
A	13	SER	-	cloning artifact	UNP P10279

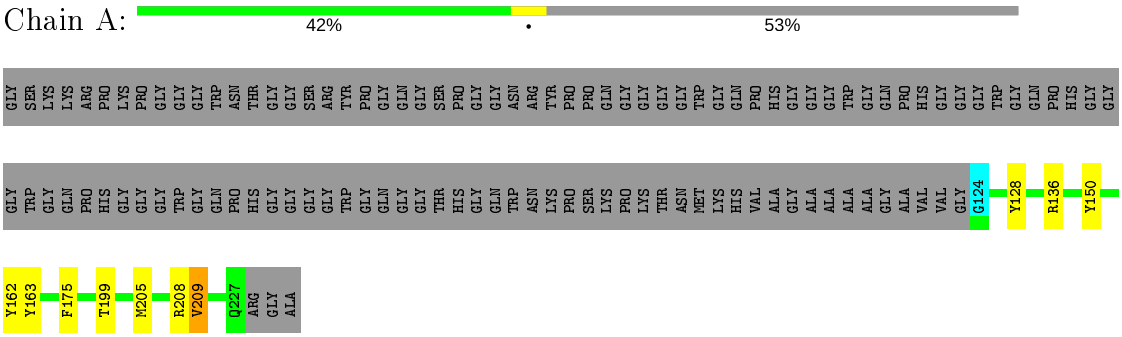
4 Residue-property plots

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

Chain A:



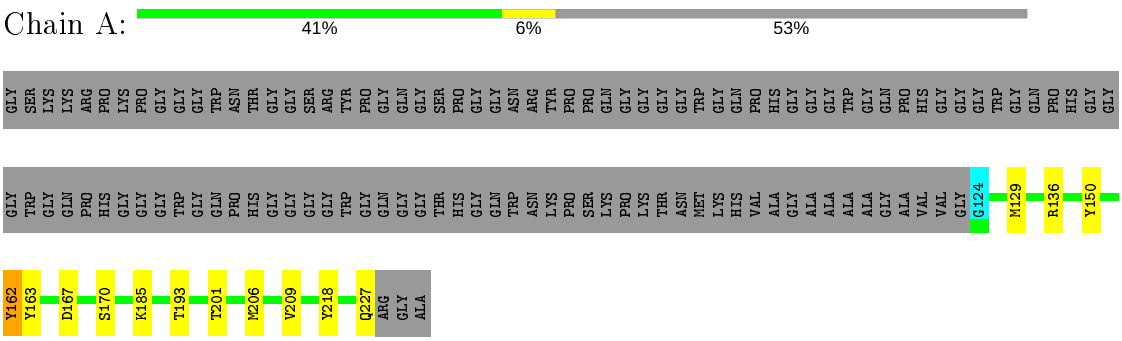
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: PRION PROTEIN

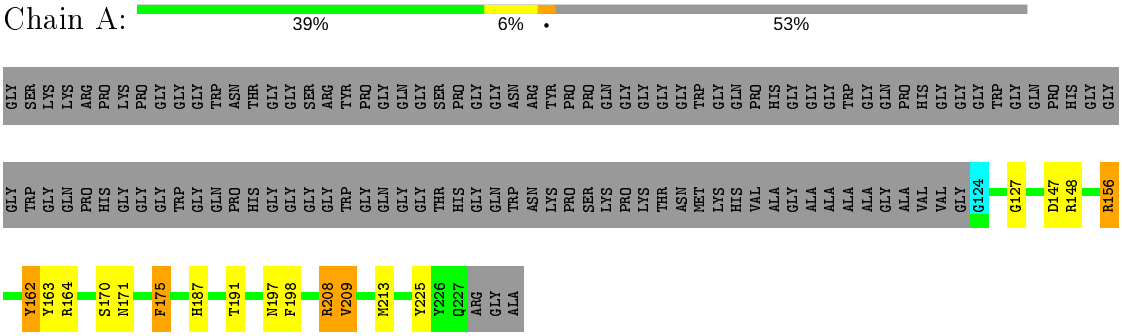
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: PRION PROTEIN

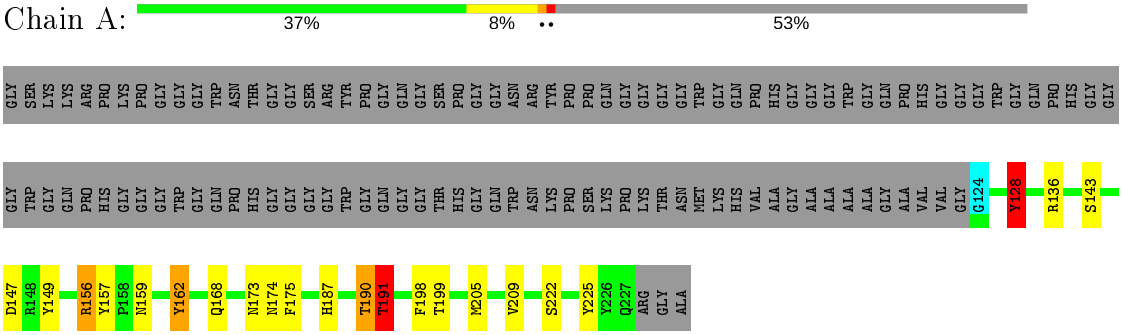
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: PRION PROTEIN

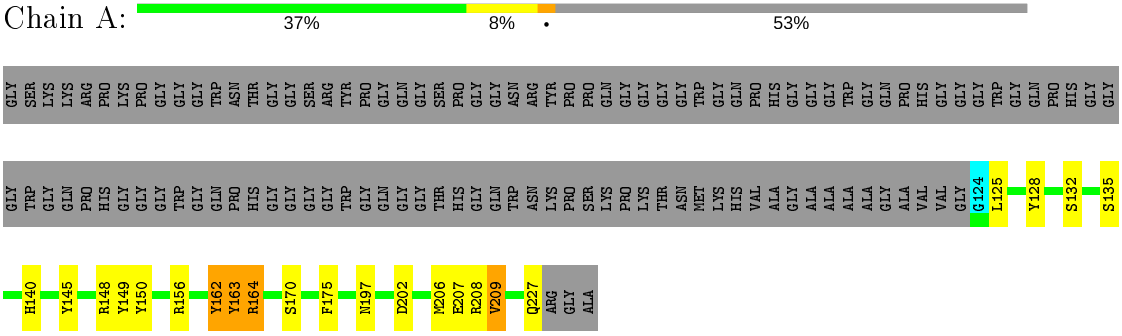
Chain A:



4.2.4 Score per residue for model 4

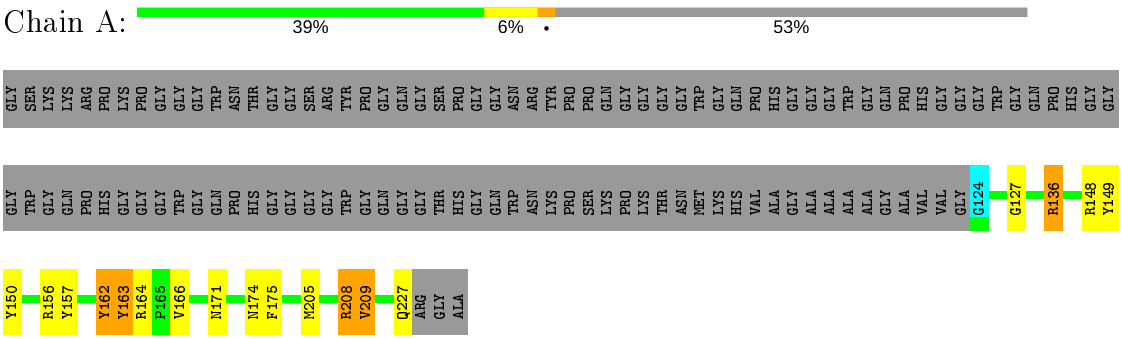
• Molecule 1: PRION PROTEIN

Chain A:



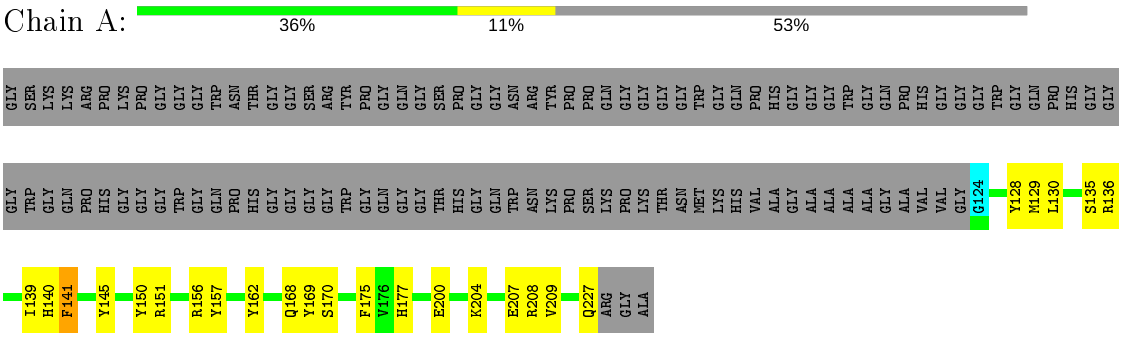
4.2.5 Score per residue for model 5

• Molecule 1: PRION PROTEIN



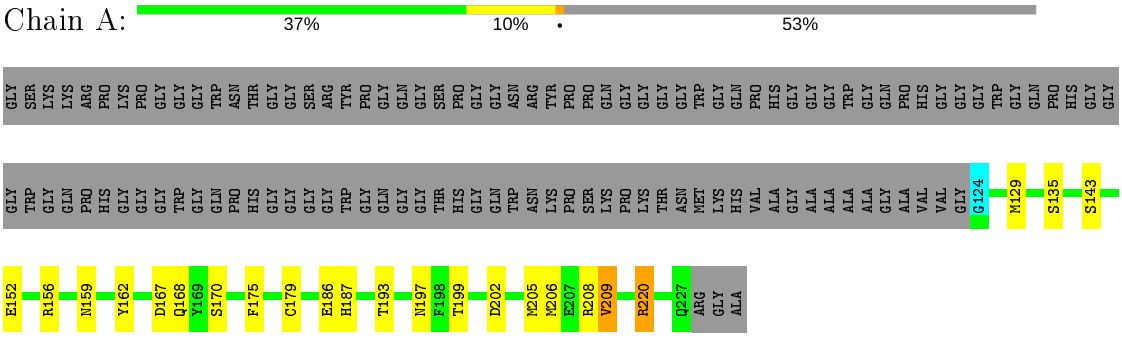
4.2.6 Score per residue for model 6

- Molecule 1: PRION PROTEIN



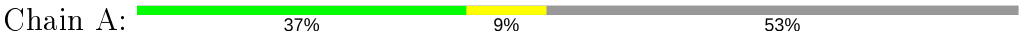
4.2.7 Score per residue for model 7

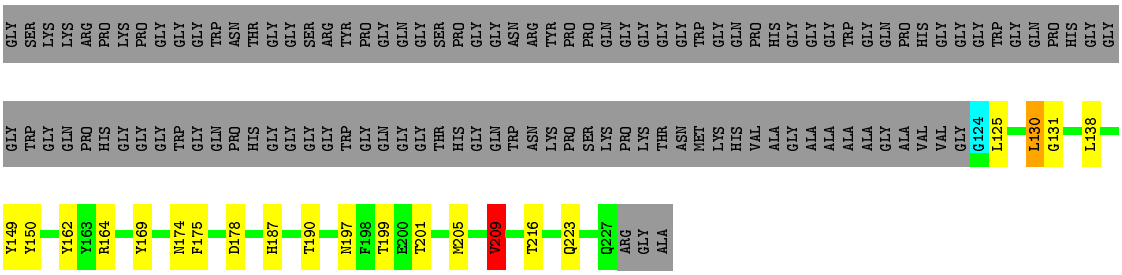
- Molecule 1: PRION PROTEIN



4.2.8 Score per residue for model 8

- Molecule 1: PRION PROTEIN

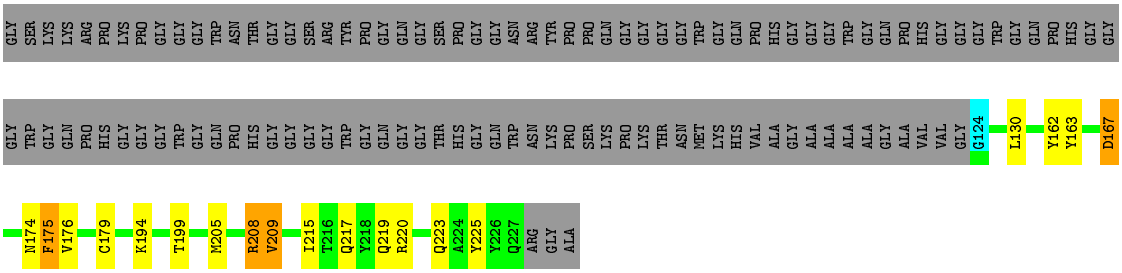




4.2.9 Score per residue for model 9

- Molecule 1: PRION PROTEIN

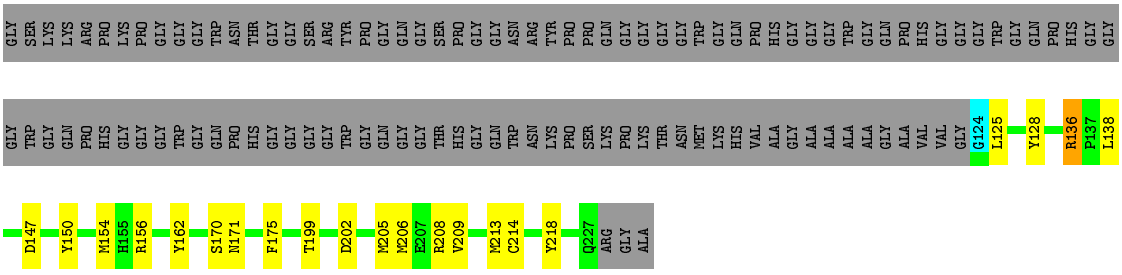
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: PRION PROTEIN

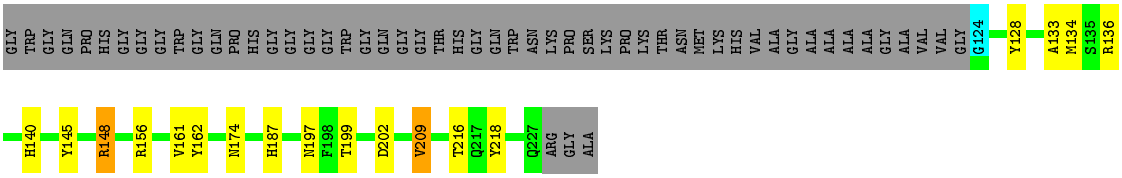
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: PRION PROTEIN

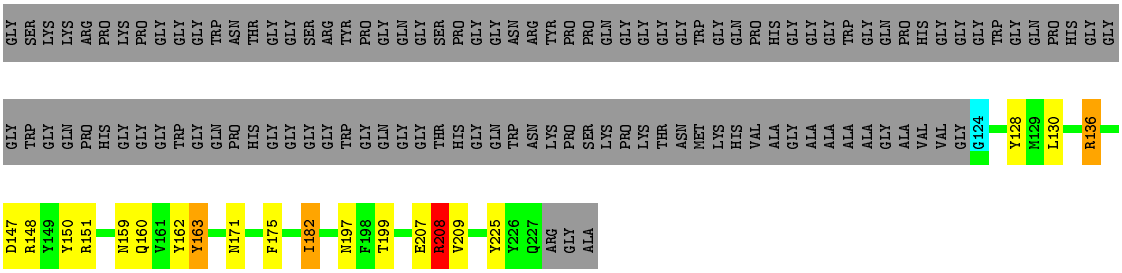
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: PRION PROTEIN

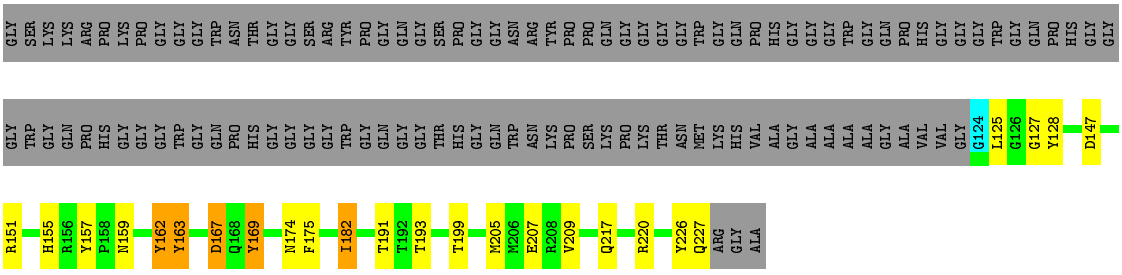
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: PRION PROTEIN

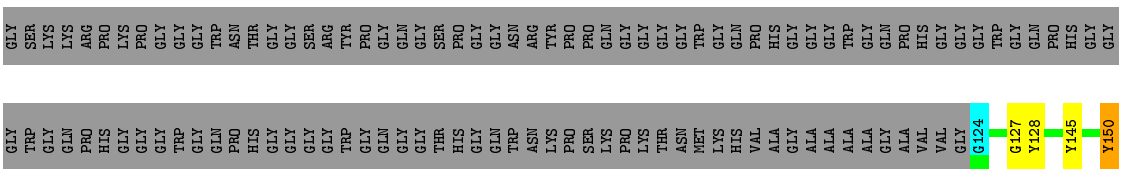
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: PRION PROTEIN

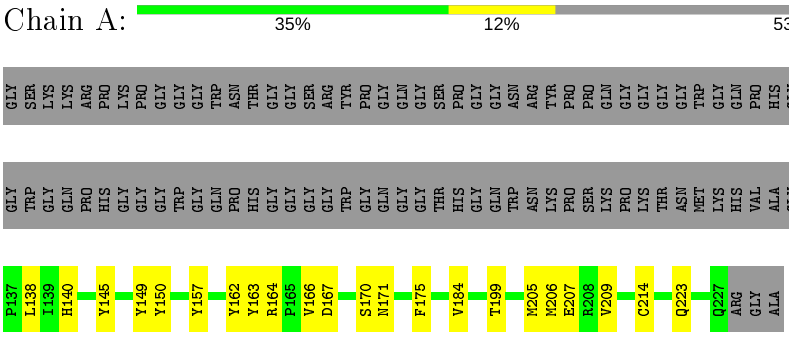
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: PRION PROTEIN

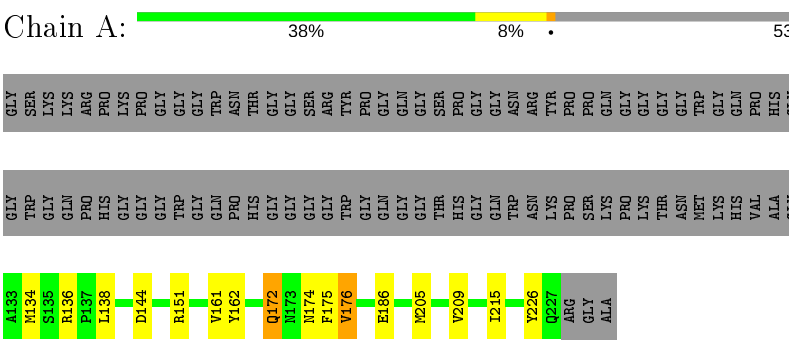
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: PRION PROTEIN

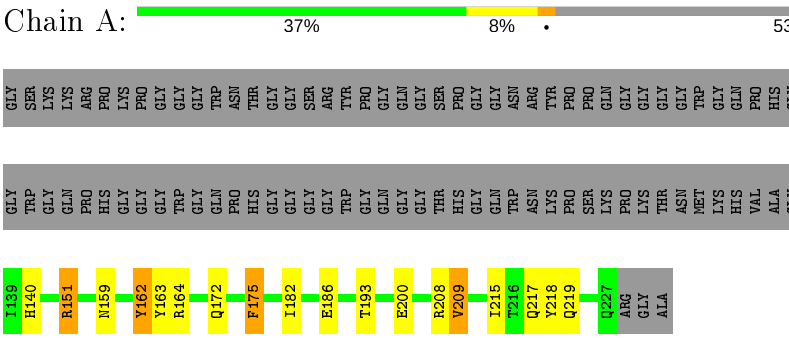
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: PRION PROTEIN

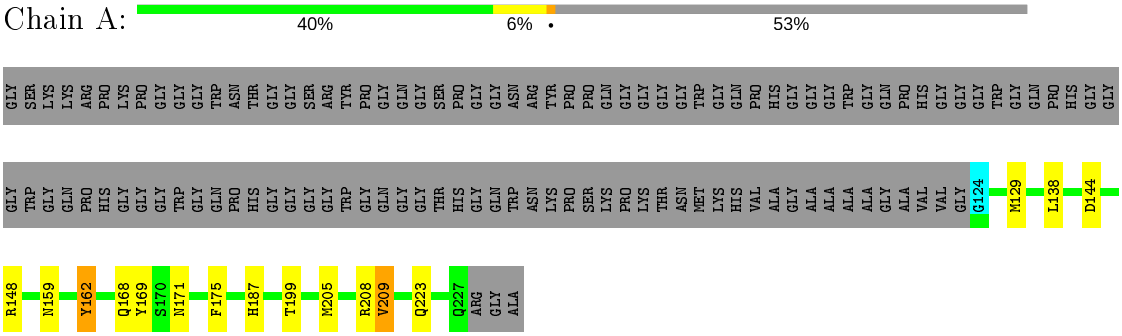
Chain A:



4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: PRION PROTEIN

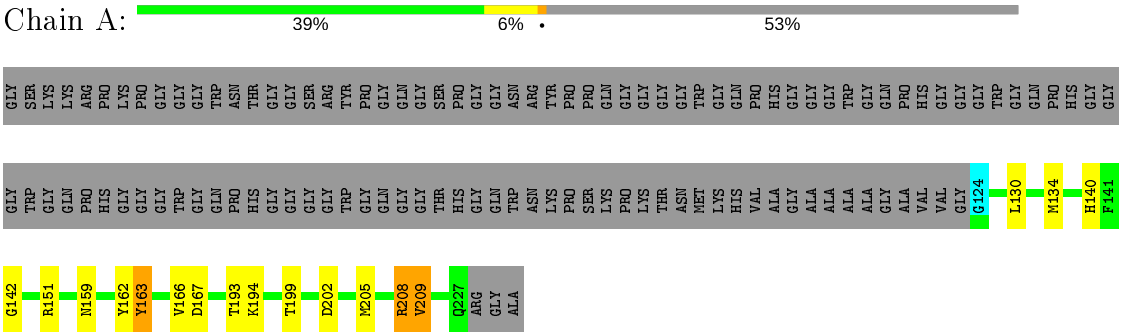
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: PRION PROTEIN

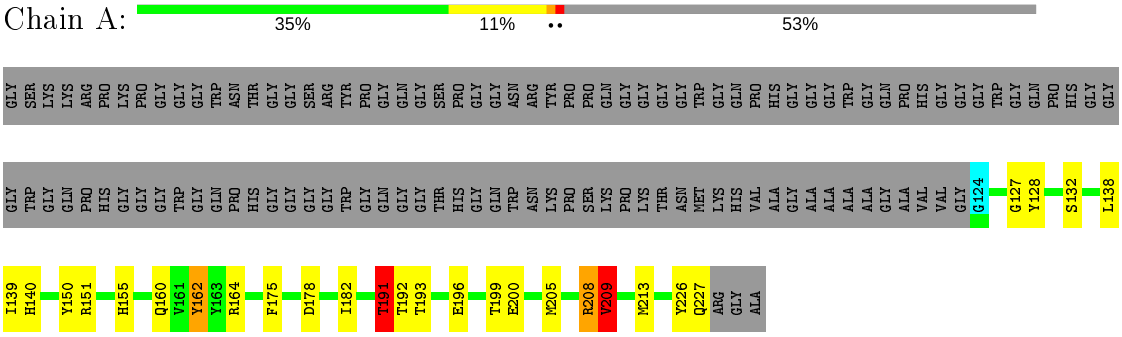
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: PRION PROTEIN

Chain A:



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. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	865	803	803	1±1
All	All	17300	16060	16060	24

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:206:MET:HA	1:A:209:VAL:HG22	0.69	1.64	14	2
1:A:201:THR:HG22	1:A:205:MET:SD	0.54	2.42	8	1
1:A:128:TYR:CE2	1:A:182:ILE:HG12	0.51	2.41	13	3
1:A:205:MET:O	1:A:209:VAL:HG22	0.50	2.07	8	1
1:A:206:MET:HA	1:A:209:VAL:CG2	0.50	2.36	10	2
1:A:172:GLN:O	1:A:176:VAL:HG13	0.50	2.06	16	1
1:A:191:THR:HG21	1:A:198:PHE:CE2	0.48	2.43	3	2
1:A:206:MET:HA	1:A:209:VAL:HG12	0.46	1.86	7	2
1:A:191:THR:HG23	1:A:192:THR:H	0.45	1.71	20	1
1:A:184:VAL:HG13	1:A:206:MET:SD	0.44	2.53	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:TYR:CE2	1:A:154:MET:CE	0.43	3.02	14	1
1:A:139:ILE:HD11	1:A:209:VAL:HA	0.43	1.91	20	1
1:A:209:VAL:HB	1:A:213:MET:SD	0.42	2.54	10	1
1:A:176:VAL:HG11	1:A:215:ILE:HG12	0.41	1.91	16	1
1:A:139:ILE:HB	1:A:141:PHE:CZ	0.41	2.50	6	1
1:A:215:ILE:HG22	1:A:219:GLN:HE21	0.41	1.74	9	2
1:A:130:LEU:HD22	1:A:131:GLY:N	0.40	2.32	8	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	102/219 (47%)	88±4 (86±4%)	12±3 (12±3%)	2±1 (2±1%)	12	54
All	All	2040/4380 (47%)	1762 (86%)	241 (12%)	37 (2%)	12	54

All 15 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	128	TYR	6
1	A	127	GLY	5
1	A	167	ASP	5
1	A	170	SER	4
1	A	171	ASN	3
1	A	166	VAL	3
1	A	168	GLN	2
1	A	125	LEU	2
1	A	132	SER	1
1	A	192	THR	1
1	A	142	GLY	1
1	A	172	GLN	1
1	A	191	THR	1
1	A	133	ALA	1
1	A	141	PHE	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	96/161 (60%)	82±3 (85±3%)	14±3 (15±3%)	6 44
All	All	1920/3220 (60%)	1631 (85%)	289 (15%)	6 44

All 66 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	162	TYR	20
1	A	175	PHE	17
1	A	209	VAL	17
1	A	199	THR	12
1	A	205	MET	12
1	A	208	ARG	11
1	A	163	TYR	9
1	A	159	ASN	8
1	A	136	ARG	8
1	A	138	LEU	7
1	A	174	ASN	7
1	A	140	HIS	7
1	A	130	LEU	6
1	A	187	HIS	6
1	A	227	GLN	6
1	A	193	THR	6
1	A	197	ASN	6
1	A	207	GLU	5
1	A	147	ASP	5
1	A	129	MET	5
1	A	135	SER	4
1	A	217	GLN	4
1	A	170	SER	4
1	A	223	GLN	4
1	A	169	TYR	4
1	A	125	LEU	4
1	A	226	TYR	4
1	A	186	GLU	4
1	A	164	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	168	GLN	3
1	A	134	MET	3
1	A	202	ASP	3
1	A	182	ILE	3
1	A	191	THR	3
1	A	200	GLU	3
1	A	167	ASP	3
1	A	190	THR	3
1	A	194	LYS	3
1	A	156	ARG	3
1	A	148	ARG	3
1	A	214	CYS	2
1	A	216	THR	2
1	A	178	ASP	2
1	A	171	ASN	2
1	A	143	SER	2
1	A	160	GLN	2
1	A	132	SER	2
1	A	161	VAL	2
1	A	179	CYS	2
1	A	225	TYR	2
1	A	213	MET	2
1	A	144	ASP	2
1	A	196	GLU	2
1	A	155	HIS	2
1	A	149	TYR	1
1	A	204	LYS	1
1	A	151	ARG	1
1	A	201	THR	1
1	A	222	SER	1
1	A	177	HIS	1
1	A	172	GLN	1
1	A	173	ASN	1
1	A	154	MET	1
1	A	152	GLU	1
1	A	185	LYS	1
1	A	206	MET	1

5.2.3 RNA

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains

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

5.4 Carbohydrates

There are no carbohydrates in this entry.

5.5 Ligand geometry

There are no ligands in this entry.

5.6 Other polymers

There are no such molecules in this entry.

5.7 Polymer linkage issues

There are no chain breaks in this entry.

6 Chemical shift validation

No chemical shift data were provided