



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2018 – 12:34 PM EST

PDB ID : 1FO7
Title : HUMAN PRION PROTEIN MUTANT E200K FRAGMENT 90-231
Authors : Zhang, Y.; Swietnicki, W.; Zagorski, M.G.; Surewicz, W.K.; Soennichsen, F.D.
Deposited on : 2000-08-25

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

<http://wwpdb.org/validation/2016/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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20030736
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

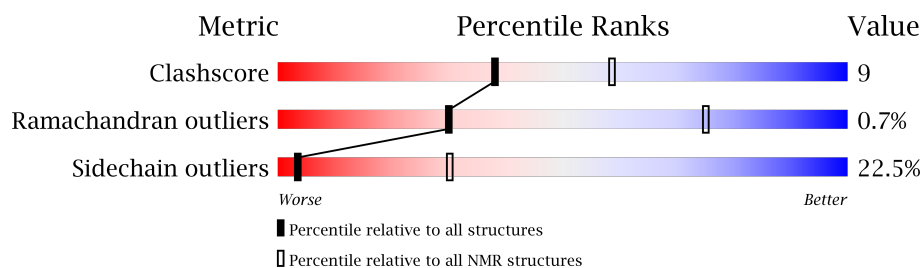
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	142	

2 Ensemble composition and analysis

This entry contains 30 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:127-A:165, A:173-A:222 (89)	0.18	4

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 5 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 17, 19, 22, 24, 28
2	3, 15, 20, 21, 25
3	18, 26, 27
4	16, 23
5	29, 30

3 Entry composition [i](#)

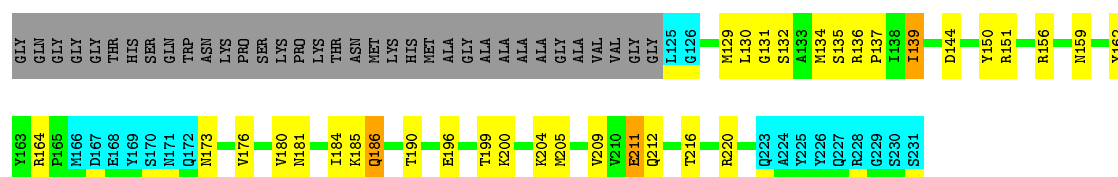
There is only 1 type of molecule in this entry. The entry contains 1731 atoms, of which 837 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PRION PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	107	Total	C	H	N	O	S	0
			1731	553	837	157	175	9	

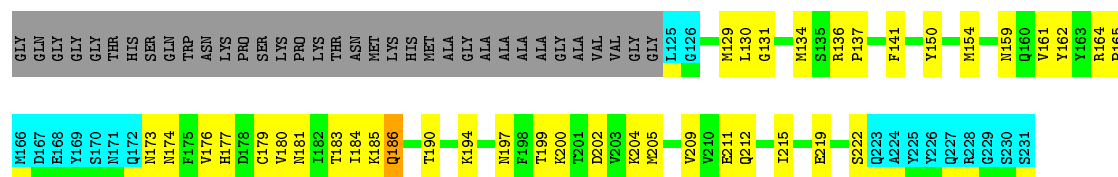
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	LYS	GLU	ENGINEERED MUTATION	UNP P04156



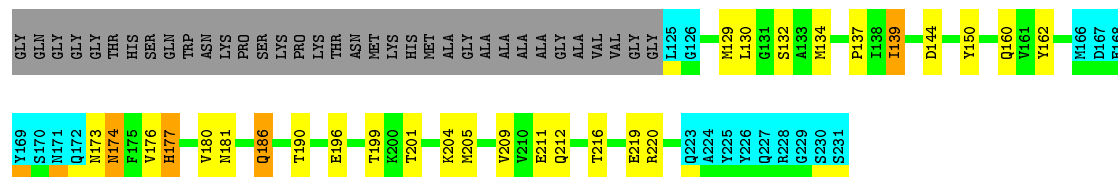
4.2.3 Score per residue for model 3

- Molecule 1: PRION PROTEIN



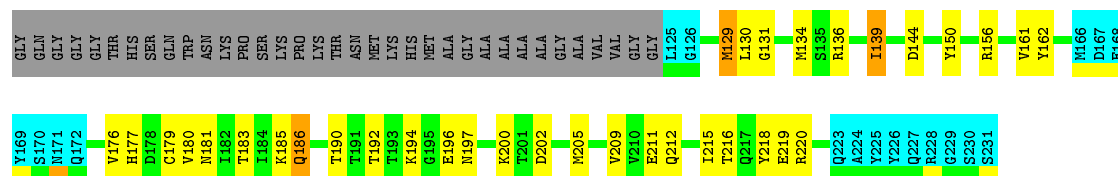
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: PRION PROTEIN



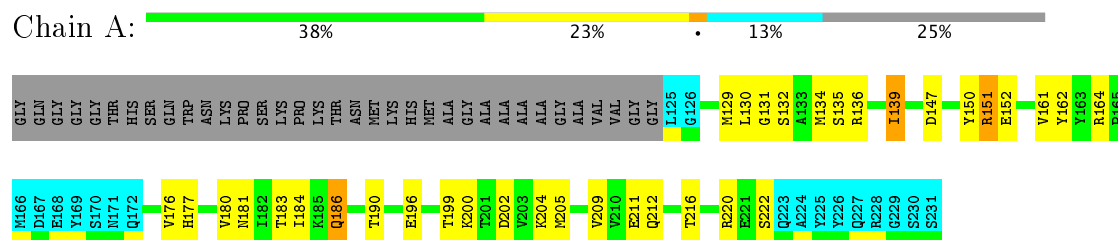
4.2.5 Score per residue for model 5

- Molecule 1: PRION PROTEIN



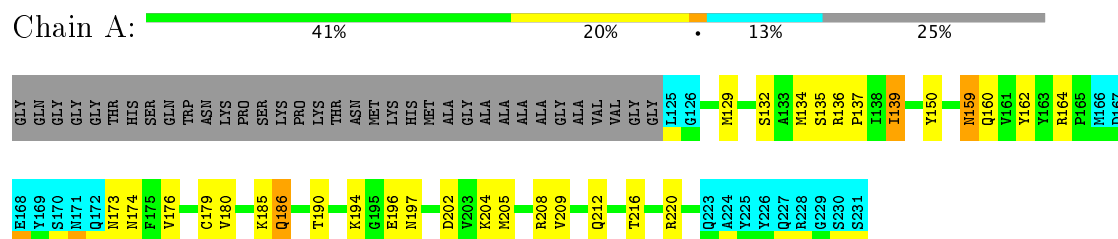
4.2.6 Score per residue for model 6

- Molecule 1: PRION PROTEIN



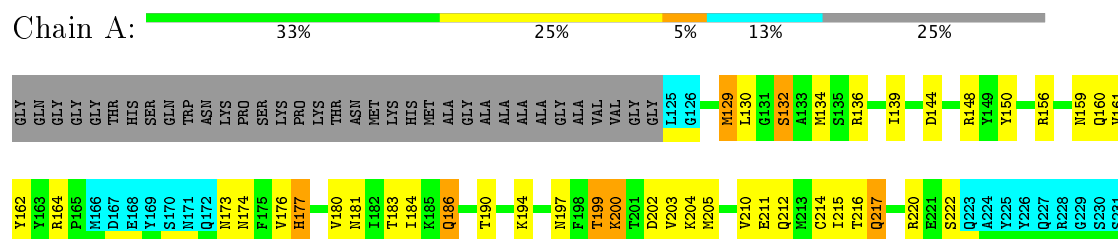
4.2.7 Score per residue for model 7

- Molecule 1: PRION PROTEIN



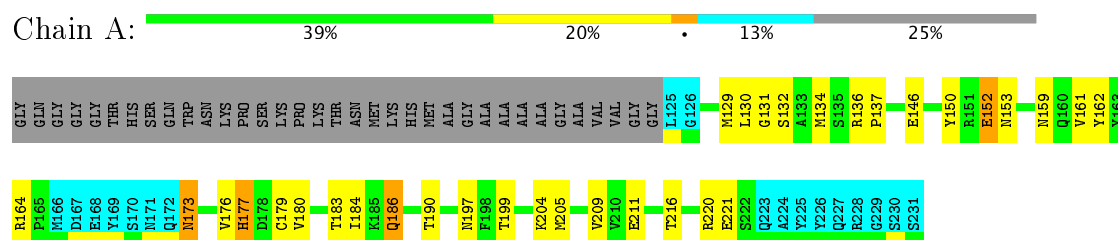
4.2.8 Score per residue for model 8

- Molecule 1: PRION PROTEIN



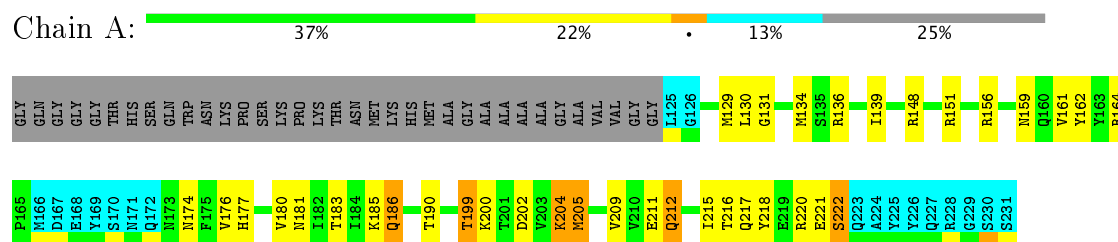
4.2.9 Score per residue for model 9

- Molecule 1: PRION PROTEIN



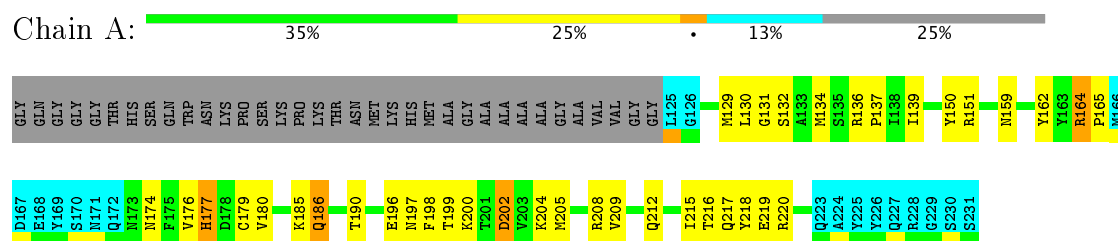
4.2.10 Score per residue for model 10

- Molecule 1: PRION PROTEIN



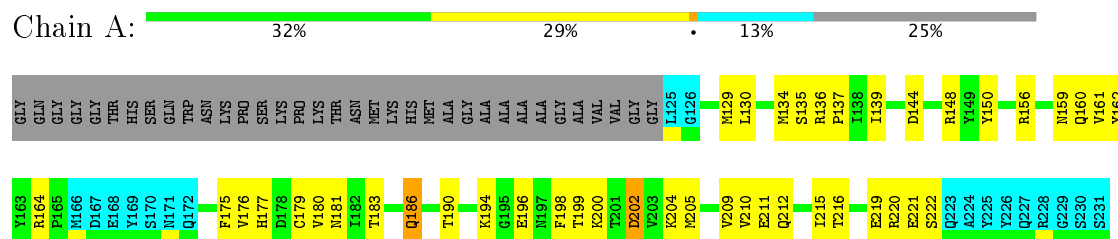
4.2.11 Score per residue for model 11

- Molecule 1: PRION PROTEIN



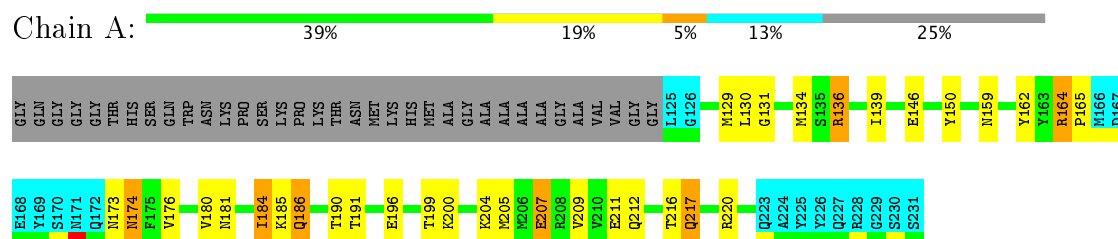
4.2.12 Score per residue for model 12

- Molecule 1: PRION PROTEIN



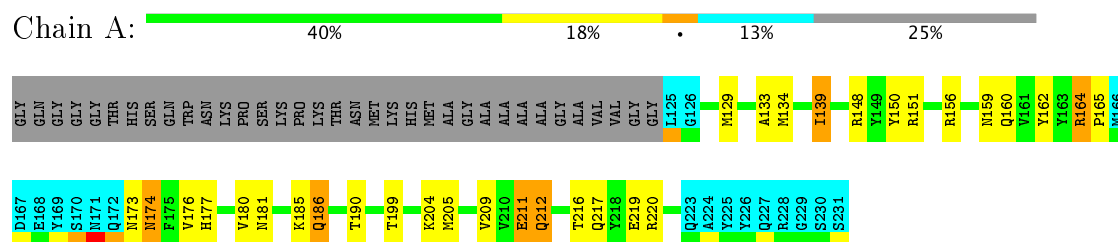
4.2.13 Score per residue for model 13

- Molecule 1: PRION PROTEIN



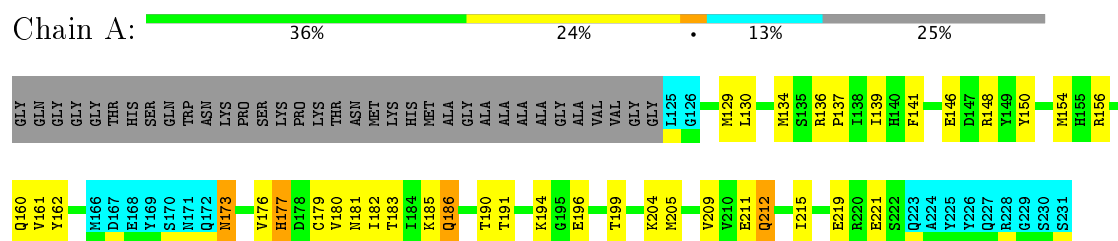
4.2.14 Score per residue for model 14

- Molecule 1: PRION PROTEIN



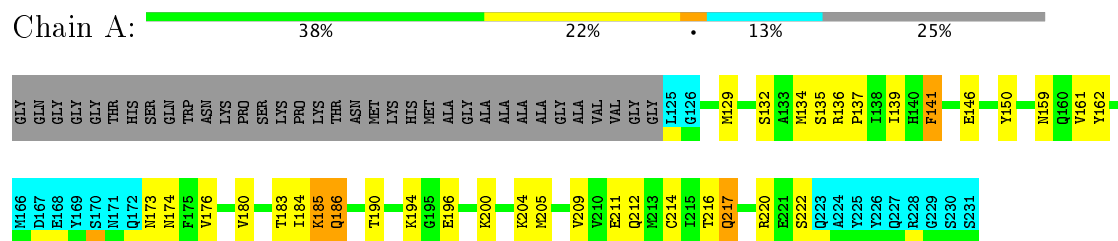
4.2.15 Score per residue for model 15

- Molecule 1: PRION PROTEIN



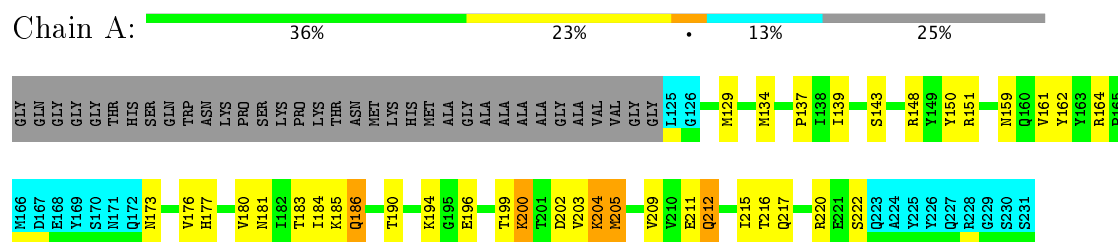
4.2.16 Score per residue for model 16

- Molecule 1: PRION PROTEIN



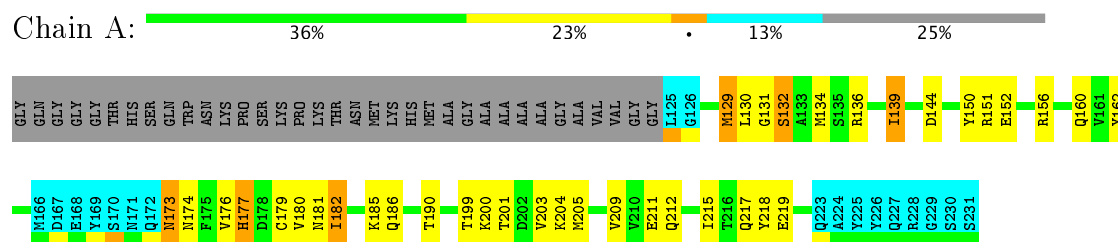
4.2.17 Score per residue for model 17

- Molecule 1: PRION PROTEIN



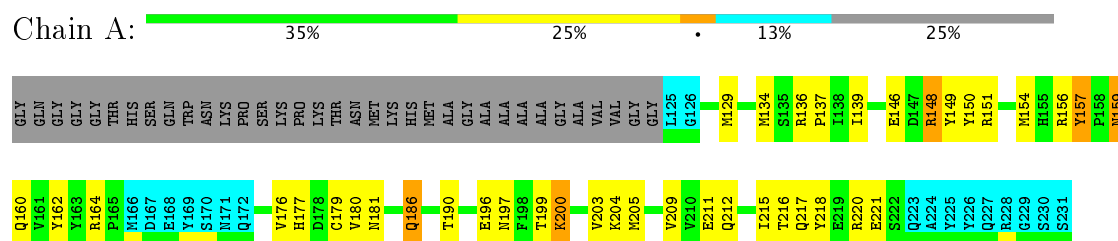
4.2.18 Score per residue for model 18

- Molecule 1: PRION PROTEIN



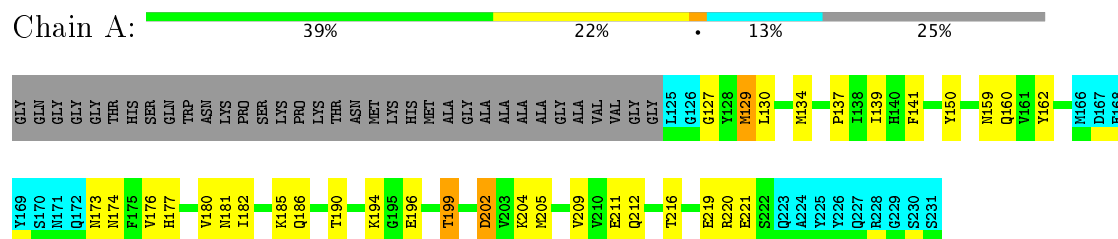
4.2.19 Score per residue for model 19

- Molecule 1: PRION PROTEIN



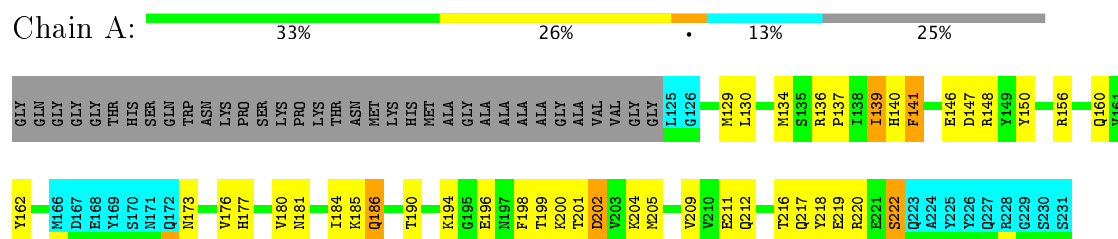
4.2.20 Score per residue for model 20

- Molecule 1: PRION PROTEIN



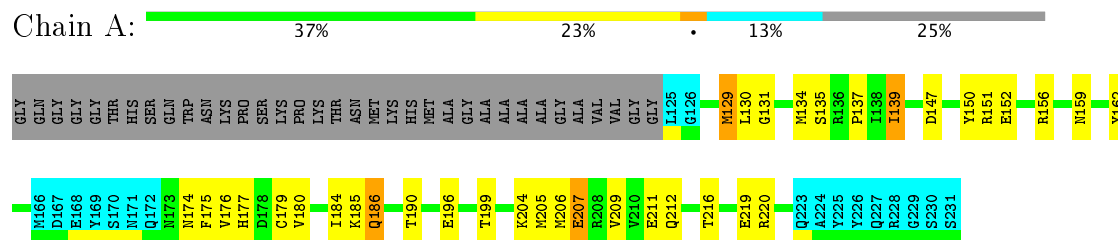
4.2.21 Score per residue for model 21

- Molecule 1: PRION PROTEIN



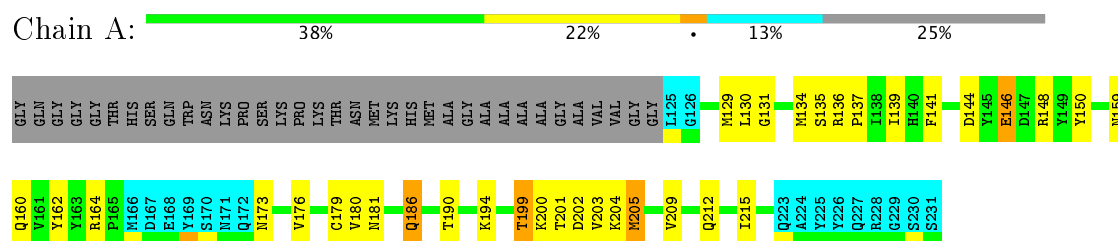
4.2.22 Score per residue for model 22

- Molecule 1: PRION PROTEIN



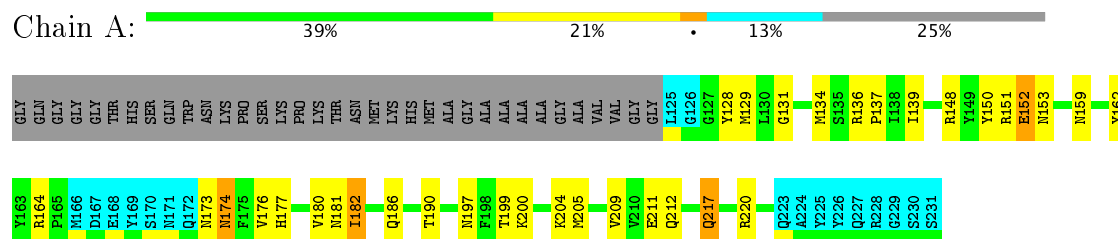
4.2.23 Score per residue for model 23

- Molecule 1: PRION PROTEIN



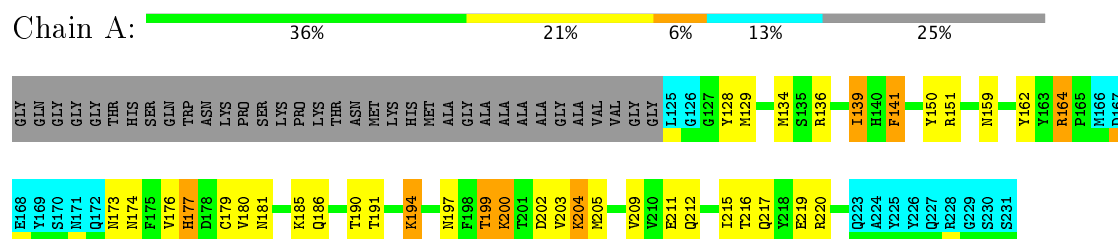
4.2.24 Score per residue for model 24

- Molecule 1: PRION PROTEIN



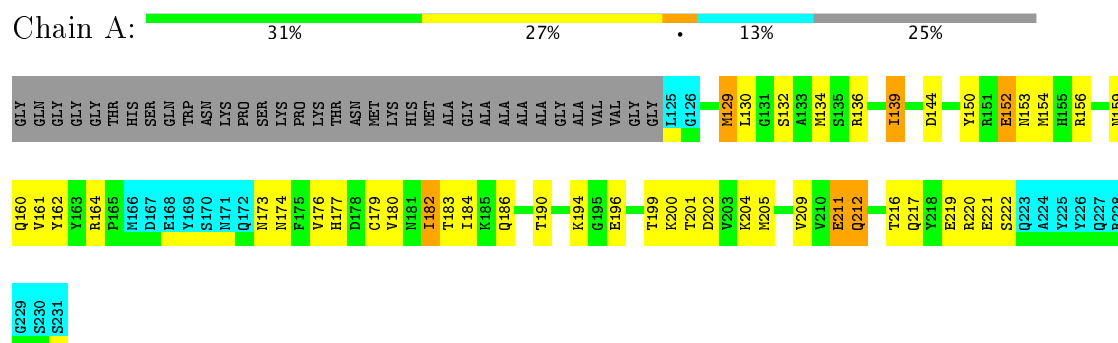
4.2.25 Score per residue for model 25

- Molecule 1: PRION PROTEIN



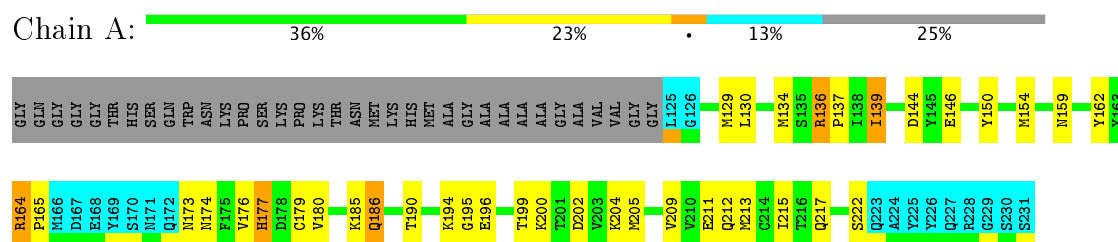
4.2.26 Score per residue for model 26

- Molecule 1: PRION PROTEIN



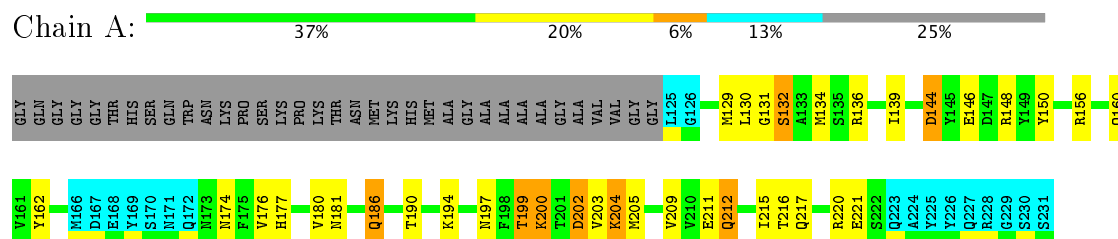
4.2.27 Score per residue for model 27

- Molecule 1: PRION PROTEIN



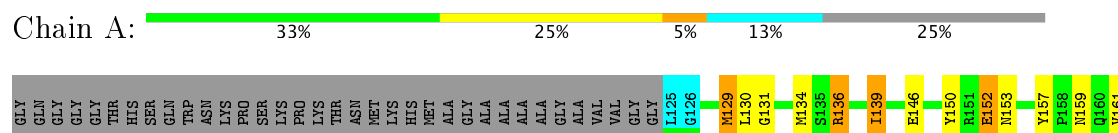
4.2.28 Score per residue for model 28

- Molecule 1: PRION PROTEIN



4.2.29 Score per residue for model 29

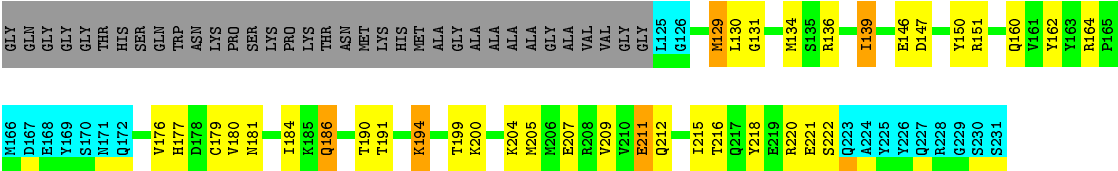
- Molecule 1: PRION PROTEIN





4.2.30 Score per residue for model 30

- Molecule 1: PRION PROTEIN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 60 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	0.9
CNS	structure solution	0.9
CNS	refinement	0.9

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

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	747	712	708	13±2
All	All	22410	21360	21240	403

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:216:THR:HG22	1:A:220:ARG:HD2	0.77	1.57	16	1
1:A:204:LYS:HG3	1:A:205:MET:N	0.68	2.04	25	3
1:A:137:PRO:HD2	1:A:209:VAL:HG13	0.67	1.66	16	15
1:A:161:VAL:HG12	1:A:183:THR:HG21	0.62	1.71	16	13
1:A:214:CYS:HA	1:A:217:GLN:NE2	0.62	2.10	16	2
1:A:176:VAL:HG11	1:A:215:ILE:HG13	0.60	1.72	8	2
1:A:184:ILE:HD13	1:A:207:GLU:OE2	0.59	1.97	13	2
1:A:176:VAL:O	1:A:180:VAL:HG23	0.59	1.98	11	30
1:A:161:VAL:HG21	1:A:217:GLN:HE22	0.58	1.58	16	2
1:A:186:GLN:O	1:A:190:THR:HG22	0.57	1.99	6	30
1:A:130:LEU:HD23	1:A:131:GLY:N	0.57	2.15	5	15
1:A:130:LEU:HD21	1:A:160:GLN:HB3	0.55	1.77	23	11
1:A:212:GLN:HA	1:A:215:ILE:HD12	0.55	1.78	19	10
1:A:139:ILE:HG13	1:A:209:VAL:HG22	0.55	1.77	30	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:GLU:HG3	1:A:153:ASN:HD22	0.54	1.63	29	3
1:A:136:ARG:HD2	1:A:154:MET:HB3	0.54	1.79	3	4
1:A:184:ILE:HD13	1:A:207:GLU:CD	0.54	2.23	22	2
1:A:139:ILE:HD12	1:A:208:ARG:HB3	0.53	1.79	7	1
1:A:191:THR:HA	1:A:194:LYS:HD3	0.53	1.79	30	1
1:A:150:TYR:HB2	1:A:205:MET:SD	0.53	2.43	23	29
1:A:200:LYS:O	1:A:203:VAL:HG22	0.51	2.05	25	7
1:A:129:MET:O	1:A:162:TYR:HA	0.51	2.06	29	30
1:A:146:GLU:HA	1:A:146:GLU:OE1	0.50	2.06	23	2
1:A:215:ILE:HG22	1:A:219:GLU:OE1	0.50	2.06	15	3
1:A:152:GLU:HG3	1:A:153:ASN:ND2	0.50	2.21	29	3
1:A:154:MET:HA	1:A:157:TYR:HB2	0.50	1.83	19	1
1:A:159:ASN:HD22	1:A:160:GLN:HG3	0.50	1.65	19	2
1:A:182:ILE:HG23	1:A:186:GLN:OE1	0.50	2.06	24	4
1:A:217:GLN:HA	1:A:220:ARG:HD3	0.50	1.83	16	1
1:A:185:LYS:HE3	1:A:186:GLN:HE22	0.49	1.66	11	2
1:A:136:ARG:NH2	1:A:209:VAL:HG11	0.49	2.21	13	1
1:A:182:ILE:HD12	1:A:186:GLN:OE1	0.49	2.08	18	3
1:A:216:THR:O	1:A:220:ARG:HG3	0.49	2.07	21	23
1:A:136:ARG:NH2	1:A:157:TYR:HB3	0.49	2.23	29	1
1:A:217:GLN:HA	1:A:220:ARG:HB2	0.49	1.84	16	1
1:A:205:MET:O	1:A:209:VAL:HG23	0.48	2.08	30	12
1:A:211:GLU:HG3	1:A:212:GLN:N	0.48	2.24	14	1
1:A:164:ARG:HD2	1:A:165:PRO:HD2	0.47	1.85	27	2
1:A:129:MET:HE2	1:A:129:MET:HA	0.47	1.86	27	1
1:A:199:THR:N	1:A:202:ASP:HB2	0.46	2.25	28	7
1:A:152:GLU:HG2	1:A:153:ASN:HD22	0.46	1.70	9	1
1:A:173:ASN:O	1:A:177:HIS:HB3	0.46	2.11	29	2
1:A:164:ARG:HG2	1:A:165:PRO:HD2	0.46	1.88	14	3
1:A:184:ILE:HG12	1:A:206:MET:HB3	0.46	1.87	22	1
1:A:217:GLN:HA	1:A:220:ARG:HD2	0.46	1.88	8	3
1:A:132:SER:HA	1:A:160:GLN:HE21	0.46	1.71	4	4
1:A:129:MET:HA	1:A:129:MET:CE	0.45	2.41	20	6
1:A:217:GLN:HA	1:A:220:ARG:HG3	0.45	1.88	24	1
1:A:129:MET:CE	1:A:129:MET:HA	0.45	2.41	27	5
1:A:147:ASP:O	1:A:151:ARG:HG2	0.45	2.12	22	3
1:A:204:LYS:HD2	1:A:205:MET:SD	0.45	2.52	10	1
1:A:198:PHE:HD1	1:A:202:ASP:HB3	0.45	1.72	11	3
1:A:173:ASN:O	1:A:177:HIS:HB2	0.45	2.12	1	7
1:A:213:MET:O	1:A:217:GLN:HG2	0.45	2.11	27	1
1:A:148:ARG:O	1:A:152:GLU:HB3	0.44	2.13	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:THR:HA	1:A:194:LYS:HB2	0.44	1.88	25	1
1:A:136:ARG:HH21	1:A:157:TYR:HB3	0.44	1.71	29	1
1:A:217:GLN:HA	1:A:220:ARG:CD	0.44	2.43	16	1
1:A:133:ALA:N	1:A:160:GLN:HG2	0.44	2.27	14	1
1:A:146:GLU:OE1	1:A:146:GLU:HA	0.44	2.13	21	1
1:A:128:TYR:CD2	1:A:164:ARG:HG3	0.44	2.48	24	2
1:A:191:THR:O	1:A:196:GLU:HB2	0.43	2.13	15	2
1:A:201:THR:O	1:A:205:MET:HG3	0.43	2.13	21	5
1:A:139:ILE:HG21	1:A:208:ARG:HB3	0.43	1.89	7	1
1:A:161:VAL:HG12	1:A:210:VAL:HG13	0.43	1.90	12	2
1:A:132:SER:HA	1:A:160:GLN:NE2	0.43	2.27	18	1
1:A:161:VAL:HG21	1:A:217:GLN:NE2	0.43	2.26	16	1
1:A:139:ILE:HD11	1:A:209:VAL:HA	0.43	1.91	10	2
1:A:144:ASP:O	1:A:148:ARG:HG2	0.43	2.14	28	1
1:A:140:HIS:HA	1:A:147:ASP:OD1	0.43	2.13	21	1
1:A:180:VAL:HG12	1:A:207:GLU:OE2	0.43	2.13	22	1
1:A:131:GLY:HA3	1:A:217:GLN:OE1	0.42	2.15	13	2
1:A:141:PHE:CE1	1:A:205:MET:HA	0.42	2.49	25	1
1:A:218:TYR:O	1:A:222:SER:HB3	0.42	2.14	21	2
1:A:152:GLU:HG2	1:A:153:ASN:ND2	0.42	2.29	9	1
1:A:148:ARG:HG3	1:A:149:TYR:N	0.42	2.28	19	1
1:A:135:SER:O	1:A:137:PRO:HD3	0.42	2.15	7	5
1:A:139:ILE:HB	1:A:141:PHE:CZ	0.42	2.50	16	2
1:A:137:PRO:HD2	1:A:209:VAL:CG1	0.42	2.42	16	1
1:A:184:ILE:CG1	1:A:206:MET:HB3	0.42	2.45	22	1
1:A:207:GLU:O	1:A:211:GLU:HB3	0.42	2.15	30	1
1:A:211:GLU:HG2	1:A:212:GLN:N	0.41	2.30	26	2
1:A:215:ILE:O	1:A:218:TYR:HB3	0.41	2.15	5	6
1:A:174:ASN:HA	1:A:177:HIS:CD2	0.41	2.50	11	1
1:A:181:ASN:ND2	1:A:182:ILE:N	0.41	2.69	15	1
1:A:162:TYR:N	1:A:162:TYR:CD1	0.41	2.89	20	1
1:A:185:LYS:HG2	1:A:185:LYS:O	0.41	2.15	14	1
1:A:163:TYR:HB2	1:A:175:PHE:CZ	0.41	2.51	29	1
1:A:192:THR:HG23	1:A:197:ASN:HA	0.41	1.91	5	1
1:A:185:LYS:HE3	1:A:186:GLN:NE2	0.41	2.31	11	1
1:A:146:GLU:OE2	1:A:205:MET:HE3	0.41	2.15	19	1
1:A:162:TYR:CD1	1:A:162:TYR:N	0.40	2.89	26	2
1:A:185:LYS:HE2	1:A:186:GLN:NE2	0.40	2.32	16	1
1:A:182:ILE:O	1:A:186:GLN:HB2	0.40	2.17	29	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	89/142 (63%)	80±1 (90±1%)	8±1 (9±1%)	1±1 (1±1%)	30	75
All	All	2670/4260 (63%)	2414 (90%)	236 (9%)	20 (1%)	30	75

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	132	SER	10
1	A	141	PHE	7
1	A	195	GLY	2
1	A	127	GLY	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	84/120 (70%)	65±3 (77±3%)	19±3 (23±3%)	3	30
All	All	2520/3600 (70%)	1952 (77%)	568 (23%)	3	30

All 41 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	134	MET	30
1	A	204	LYS	29
1	A	211	GLU	27
1	A	199	THR	26
1	A	186	GLN	25
1	A	177	HIS	25

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Mol	Chain	Res	Type	Models (Total)
1	A	139	ILE	23
1	A	212	GLN	23
1	A	136	ARG	22
1	A	159	ASN	22
1	A	200	LYS	21
1	A	181	ASN	21
1	A	164	ARG	19
1	A	194	LYS	18
1	A	196	GLU	17
1	A	179	CYS	16
1	A	173	ASN	15
1	A	185	LYS	15
1	A	174	ASN	14
1	A	217	GLN	13
1	A	156	ARG	13
1	A	222	SER	12
1	A	184	ILE	12
1	A	202	ASP	12
1	A	151	ARG	11
1	A	219	GLU	11
1	A	197	ASN	10
1	A	144	ASP	10
1	A	148	ARG	9
1	A	146	GLU	9
1	A	221	GLU	9
1	A	129	MET	8
1	A	152	GLU	7
1	A	205	MET	3
1	A	182	ILE	3
1	A	135	SER	2
1	A	207	GLU	2
1	A	208	ARG	1
1	A	130	LEU	1
1	A	143	SER	1
1	A	157	TYR	1

6.3.3 RNA ⓘ

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 carbohydrates 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