Full wwPDB NMR Structure Validation Report (i)

Sep 29, 2024 – 02:38 AM EDT

PDB ID	:	1FO7
Title	:	HUMAN PRION PROTEIN MUTANT E200K FRAGMENT 90-231
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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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

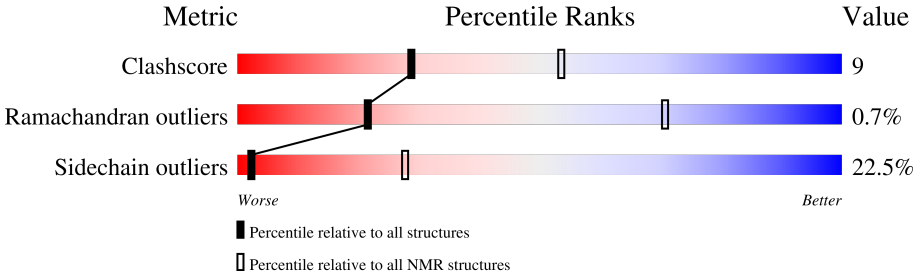
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	142	38% 24% • 13% 25%

2 Ensemble composition and analysis (i)

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)	0.32	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
			Total	C	H	N	O	S	
1	A	107	1731	553	837	157	175	9	0

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 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

Chain A: 38% 24% • 13% 25%

GLY GLN GLY GLY GLY THR HIS SER GLN TRP ASN LYS PRO SER LYS PRO LYS THR ASN MET LYS HIS MET ALA GLY ALA ALA ALA ALA GLY ALA VAL VAL GLY GLY L125 G126 M129 L130 G131 M134 S135 R136 P137 I138 I139 Y150 N159 Y162 Y163 R164 P165 M166 D167 E168

Y169 S170 N171 Q172 N173 N174 F175 V176 H177 D178 C179 V180 N181 K185 Q186 T190 K194 G195 E196 T199 K200 T201 D202 V203 K204 M205 V209 V210 E211 Q212 I215 T216 Q217 R220 Q223 A224 Y225 Y226 Q227 R228 G229 S230 S231

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: 37% 23% • 13% 25%

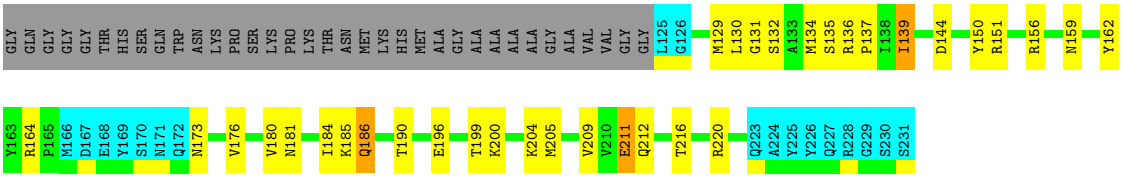
GLY GLN GLY GLY GLY THR HIS SER GLN TRP ASN LYS PRO SER LYS PRO LYS THR ASN MET LYS HIS MET ALA GLY ALA ALA ALA ALA GLY ALA VAL VAL GLY GLY L125 G126 M129 L130 G131 M134 S135 R136 I139 Y150 R151 N159 Q160 V161 Y162 Y163 R164 P165 M166 D167

E168 Y169 S170 N171 Q172 N173 V176 H177 D178 C179 V180 T183 I184 K185 Q186 T190 K194 G195 E196 T199 K200 T201 D202 V203 K204 M205 V209 V210 E211 Q212 I215 T216 Q217 Y218 E219 R220 Q223 A224 Y225 Y226 Q227 R228 G229 S230 S231

4.2.2 Score per residue for model 2

• Molecule 1: PRION PROTEIN

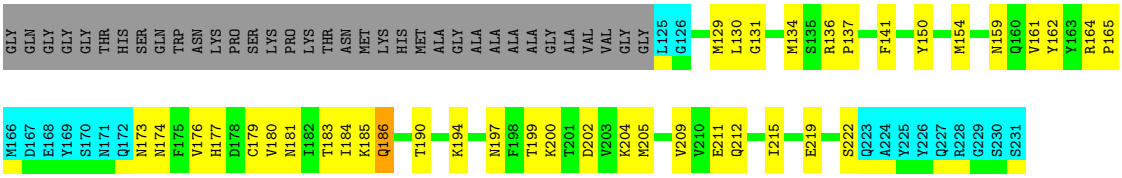
Chain A: 39% 22% • 13% 25%



4.2.3 Score per residue for model 3

- Molecule 1: PRION PROTEIN

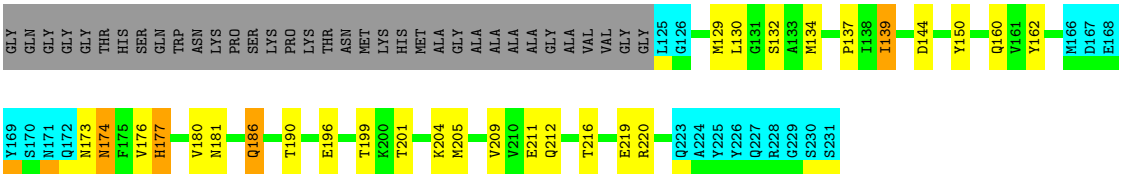
Chain A: 35% 27% • 13% 25%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: PRION PROTEIN

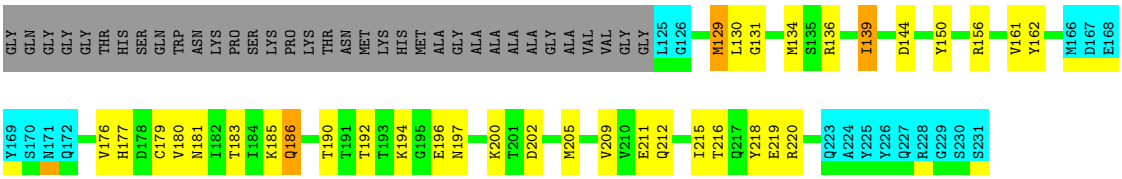
Chain A: 42% 18% • 13% 25%



4.2.5 Score per residue for model 5

- Molecule 1: PRION PROTEIN

Chain A: 38% 23% • 13% 25%



4.2.6 Score per residue for model 6

- Molecule 1: PRION PROTEIN

Chain A: 38% 23% • 13% 25%

GLY GLN GLY GLY GLY THR HIS SER GLN TRP ASN LYS PRO SER LYS PRO LYS THR ASN MET LYS HIS MET ALA GLY ALA ALA ALA ALA GLY ALA VAL VAL GLY GLY L125 G126 M129 L130 G131 S132 A133 M134 S135 R136 I139 D147 Y150 R151 E152 V161 Y162 Y163 R164 P165

M166 D167 E168 Y169 S170 N171 Q172 V176 H177 V180 N181 I182 T183 I184 K185 Q186 T190 E196 T199 K200 T201 D202 V203 K204 M205 V209 V210 E211 Q212 T216 R220 E221 S222 Q223 A224 Y225 Y226 Q227 R228 G229 S230 S231

4.2.7 Score per residue for model 7

- Molecule 1: PRION PROTEIN

Chain A: 41% 20% • 13% 25%

GLY GLN GLY GLY GLY THR HIS SER GLN TRP ASN LYS PRO SER LYS PRO LYS THR ASN MET LYS HIS MET ALA GLY ALA ALA ALA ALA GLY ALA VAL VAL GLY GLY L125 G126 M129 S132 A133 M134 S135 R136 P137 I138 I139 Y150 N159 Q160 V161 Y162 Y163 R164 P165 M166 D167

E168 Y169 S170 N171 Q172 N173 N174 F175 V176 C179 V180 K185 Q186 T190 K194 G195 E196 N197 D202 V203 K204 M205 R208 V209 Q212 T216 R220 Q223 A224 Y225 Y226 Q227 R228 G229 S230 S231

4.2.8 Score per residue for model 8

- Molecule 1: PRION PROTEIN

Chain A: 33% 25% 5% 13% 25%

GLY GLN GLY GLY GLY THR HIS SER GLN TRP ASN LYS PRO SER LYS PRO LYS THR ASN MET LYS HIS MET ALA GLY ALA ALA ALA ALA GLY ALA VAL VAL GLY GLY L125 G126 M129 L130 G131 S132 A133 M134 S135 R136 I139 D144 R148 Y149 Y150 R156 N159 Q160 V161

Y162 Y163 R164 P165 M166 D167 E168 Y169 S170 N171 Q172 N173 N174 F175 V176 H177 V180 N181 I182 T183 I184 K185 Q186 T190 K194 N197 F198 T199 K200 T201 D202 V203 K204 M205 V210 E211 Q212 M213 C214 I215 T216 Q217 R220 E221 S222 Q223 A224 Y225 Y226 Q227 R228 G229 S230 S231

4.2.9 Score per residue for model 9

- Molecule 1: PRION PROTEIN

Chain A: 39% 20% • 13% 25%

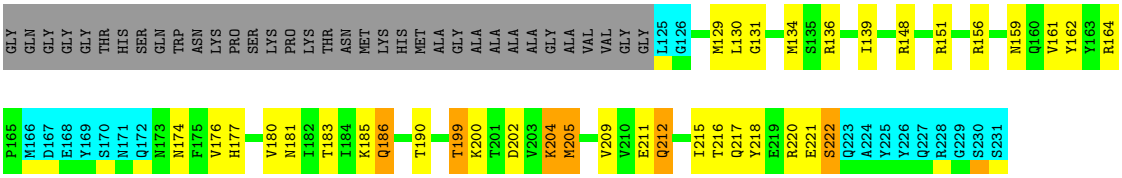
GLY GLN GLY GLY GLY THR HIS SER GLN TRP ASN LYS PRO SER LYS PRO LYS THR ASN MET LYS HIS MET ALA GLY ALA ALA ALA ALA GLY ALA VAL VAL GLY GLY L125 G126 M129 L130 G131 S132 A133 M134 S135 R136 P137 E146 Y150 R151 E152 N153 N159 Q160 V161 Y162 Y163

R164 P165 M166 D167 E168 Y169 S170 N171 Q172 N173 V176 H177 D178 C179 V180 T183 I184 K185 Q186 T190 N197 F198 T199 K204 M205 V209 V210 E211 T216 R220 E221 S222 Q223 A224 Y225 Y226 Q227 R228 G229 S230 S231

4.2.10 Score per residue for model 10

- Molecule 1: PRION PROTEIN

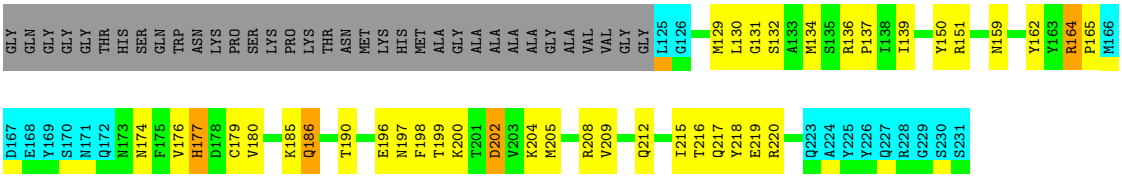
Chain A: 37% 22% • 13% 25%



4.2.11 Score per residue for model 11

- Molecule 1: PRION PROTEIN

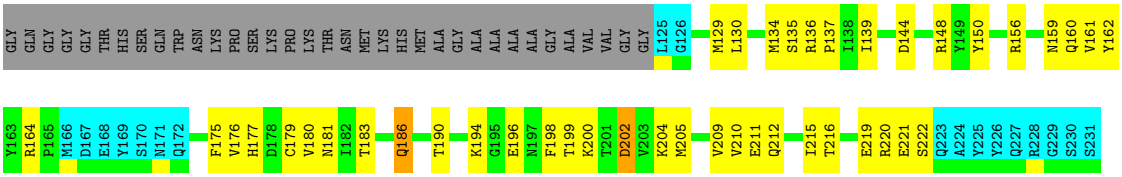
Chain A: 35% 25% • 13% 25%



4.2.12 Score per residue for model 12

- Molecule 1: PRION PROTEIN

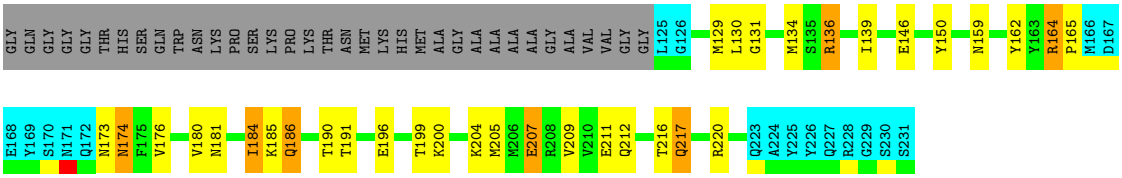
Chain A: 32% 29% • 13% 25%



4.2.13 Score per residue for model 13

- Molecule 1: PRION PROTEIN

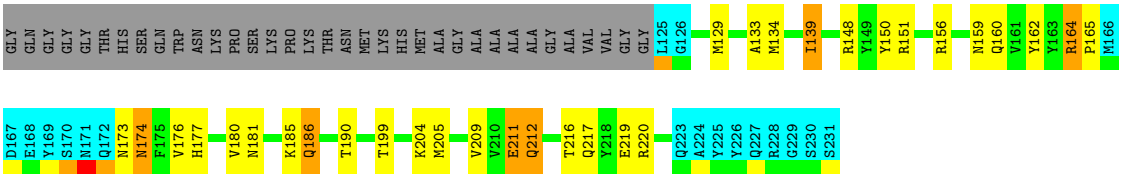
Chain A: 39% 19% 5% 13% 25%



4.2.14 Score per residue for model 14

- Molecule 1: PRION PROTEIN

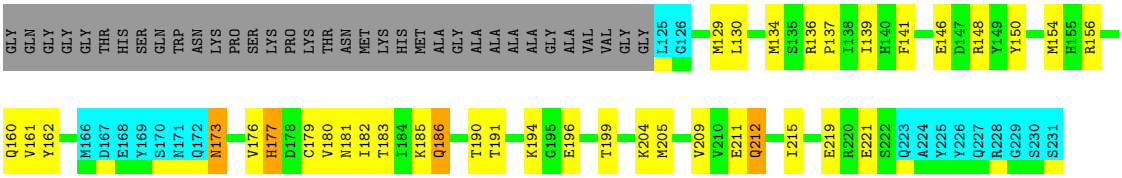
Chain A: 40% 18% • 13% 25%



4.2.15 Score per residue for model 15

- Molecule 1: PRION PROTEIN

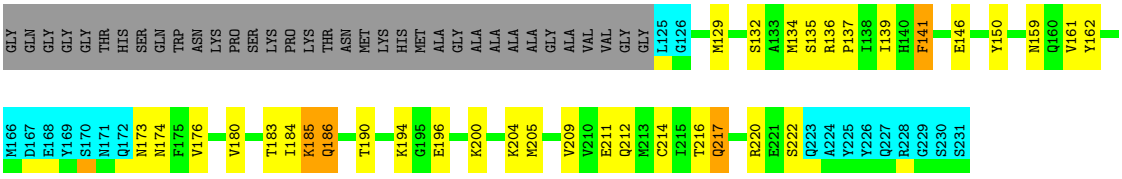
Chain A: 36% 24% • 13% 25%



4.2.16 Score per residue for model 16

- Molecule 1: PRION PROTEIN

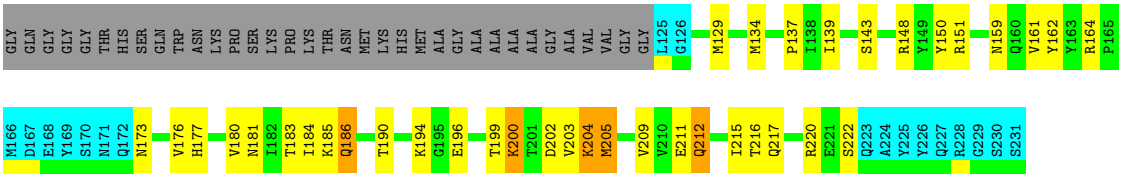
Chain A: 38% 22% • 13% 25%



4.2.17 Score per residue for model 17

- Molecule 1: PRION PROTEIN

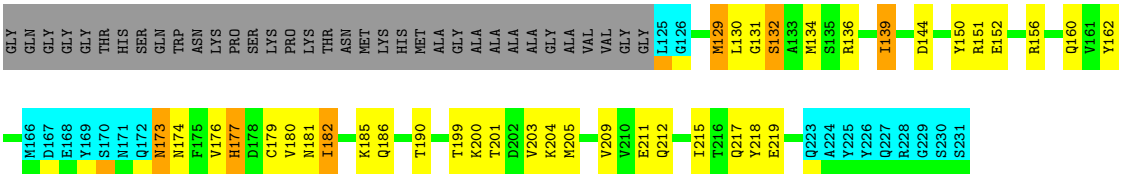
Chain A: 36% 23% • 13% 25%



4.2.18 Score per residue for model 18

- Molecule 1: PRION PROTEIN

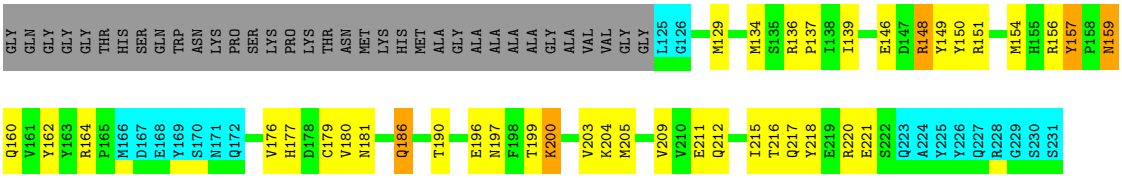
Chain A: 36% 23% • 13% 25%



4.2.19 Score per residue for model 19

- Molecule 1: PRION PROTEIN

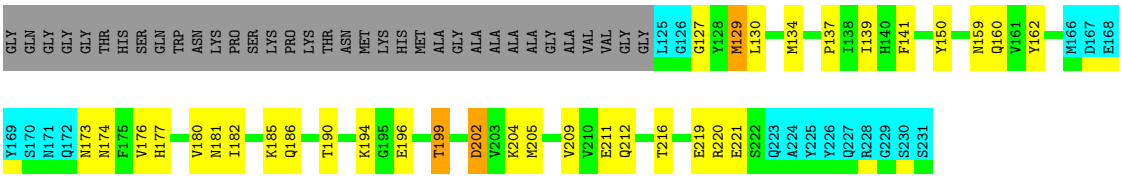
Chain A: 35% 25% • 13% 25%



4.2.20 Score per residue for model 20

- Molecule 1: PRION PROTEIN

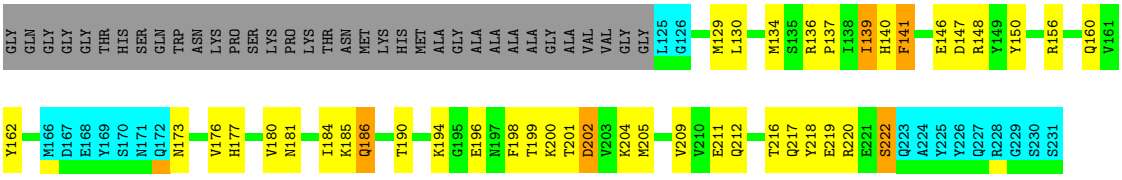
Chain A: 39% 22% • 13% 25%



4.2.21 Score per residue for model 21

- Molecule 1: PRION PROTEIN

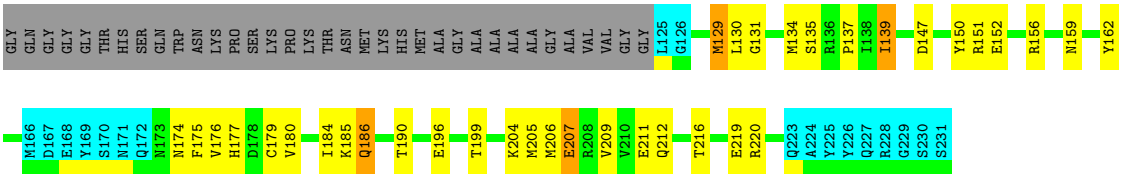
Chain A: 33% 26% • 13% 25%



4.2.22 Score per residue for model 22

- Molecule 1: PRION PROTEIN

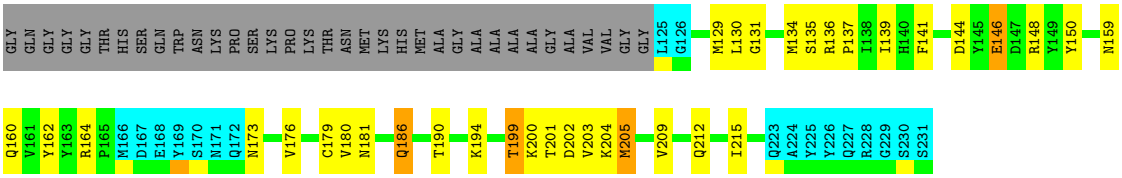
Chain A: 37% 23% • 13% 25%



4.2.23 Score per residue for model 23

- Molecule 1: PRION PROTEIN

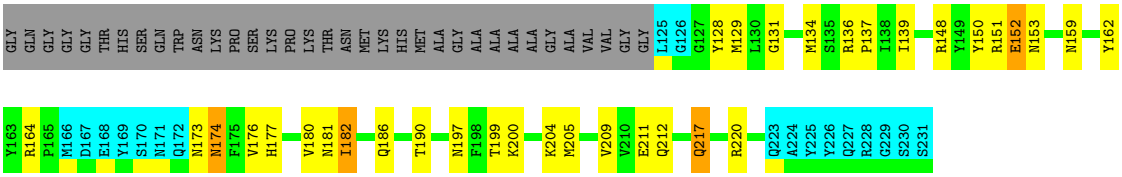
Chain A: 38% 22% • 13% 25%



4.2.24 Score per residue for model 24

- Molecule 1: PRION PROTEIN

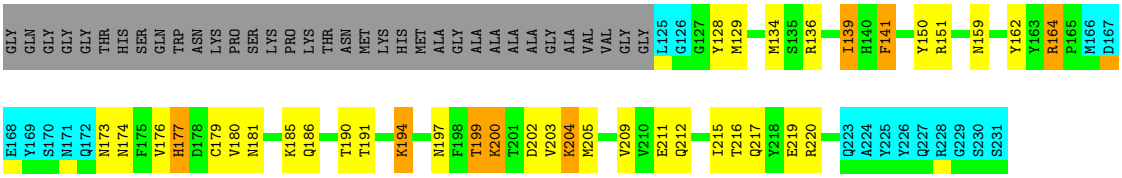
Chain A: 39% 21% • 13% 25%



4.2.25 Score per residue for model 25

- Molecule 1: PRION PROTEIN

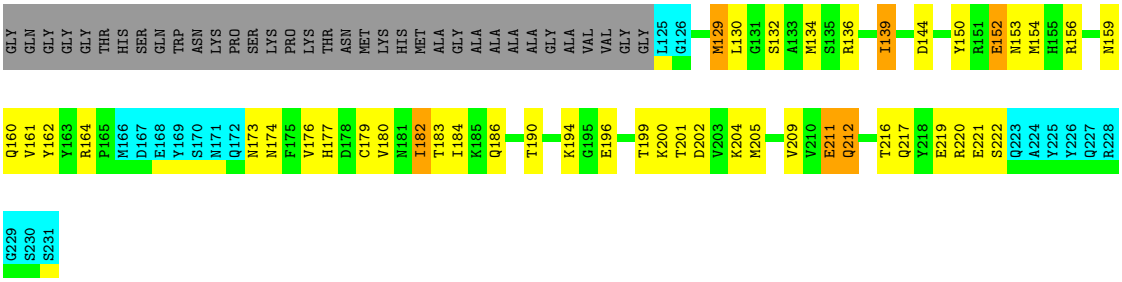
Chain A: 36% 21% 6% 13% 25%



4.2.26 Score per residue for model 26

- Molecule 1: PRION PROTEIN

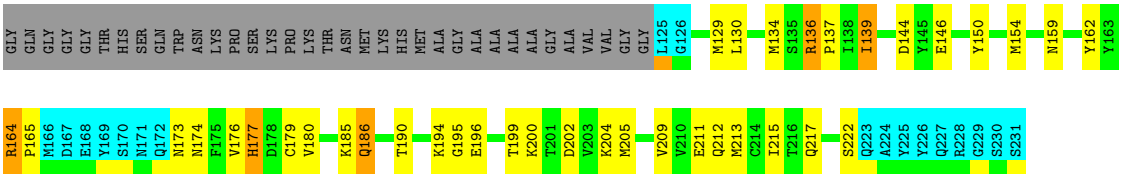
Chain A: 31% 27% • 13% 25%



4.2.27 Score per residue for model 27

- Molecule 1: PRION PROTEIN

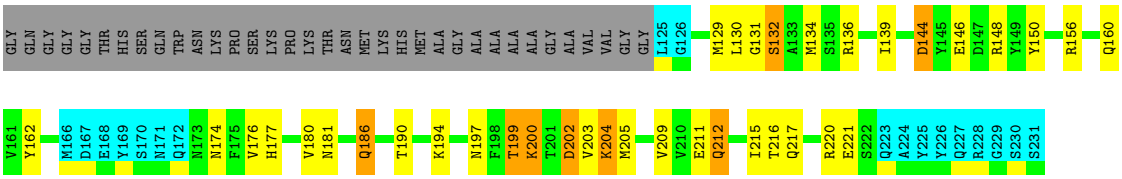
Chain A: 36% 23% • 13% 25%



4.2.28 Score per residue for model 28

- Molecule 1: PRION PROTEIN

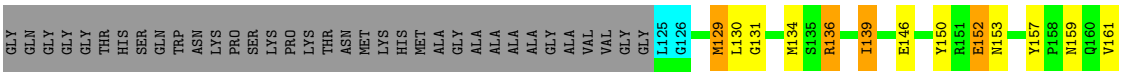
Chain A: 37% 20% 6% 13% 25%



4.2.29 Score per residue for model 29

- Molecule 1: PRION PROTEIN

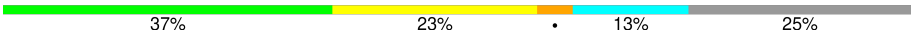
Chain A: 33% 25% 5% 13% 25%

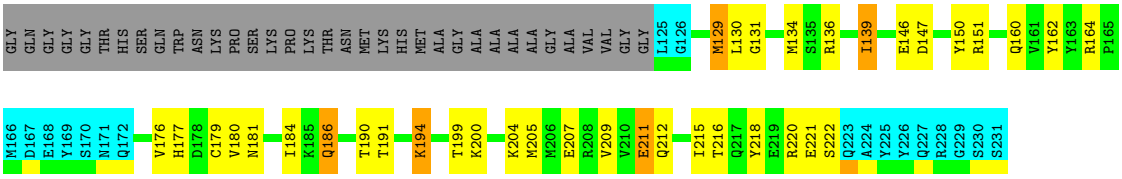


4.2.30 Score per residue for model 30

- Molecule 1: PRION PROTEIN

Chain A:





5 Refinement protocol and experimental data overview (i)

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.

6 Model quality (i)

6.1 Standard geometry (i)

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 (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	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:HA	1:A:129:MET:HE2	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:CE	1:A:129:MET:HA	0.45	2.41	20	10
1:A:217:GLN:HA	1:A:220:ARG:HG3	0.45	1.88	24	1
1:A:147:ASP:O	1:A:151:ARG:HG2	0.45	2.12	22	3
1:A:129:MET:HA	1:A:129:MET:CE	0.45	2.41	27	1
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: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:CD1	1:A:162:TYR:N	0.41	2.89	20	2
1:A:185:LYS:O	1:A:185:LYS:HG2	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:N	1:A:162:TYR:CD1	0.40	2.89	14	1
1:A:146:GLU:OE1	1:A:146:GLU:HA	0.40	2.17	19	1
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 (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	89/142 (63%)	80±1 (90±1%)	8±1 (9±1%)	1±1 (1±1%)	21 71
All	All	2670/4260 (63%)	2414 (90%)	236 (9%)	20 (1%)	21 71

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 (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	84/120 (70%)	65±3 (77±3%)	19±3 (23±3%)	2 28
All	All	2520/3600 (70%)	1952 (77%)	568 (23%)	2 28

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	177	HIS	25
1	A	186	GLN	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	185	LYS	15
1	A	173	ASN	15
1	A	174	ASN	14
1	A	156	ARG	13
1	A	217	GLN	13
1	A	202	ASP	12
1	A	184	ILE	12
1	A	222	SER	12
1	A	151	ARG	11
1	A	219	GLU	11
1	A	144	ASP	10
1	A	197	ASN	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	143	SER	1
1	A	157	TYR	1
1	A	130	LEU	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 (i)

No chemical shift data were provided