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Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 05:10 PM BST

PDB ID	:	1U3M
Title	:	NMR structure of the chicken prion protein fragment 128-242
Authors	:	Lysek, D.A.; Calzolai, L.; Guntert, P.; Wuthrich, K.
Deposited on	:	2004-07-22

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 (i) symbol.

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

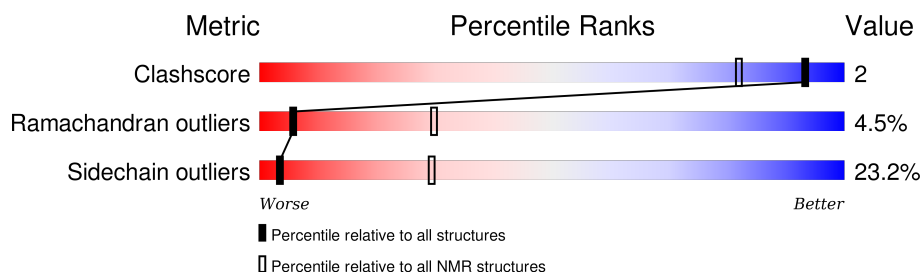|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 is 80%.

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	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		4.5%
Sidechain outliers		23.2%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	117	58% 22% 20%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:135-A:199,　　A:212-A:240 (94)	0.52	8

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 4 clusters and 5 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1819 atoms, of which 884 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called prion-like protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	117	1819	585	884	163	180	7	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	GLY	-	CLONING ARTIFACT	UNP P27177
A	127	SER	-	CLONING ARTIFACT	UNP P27177

4 Residue-property plots (i)

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-like protein
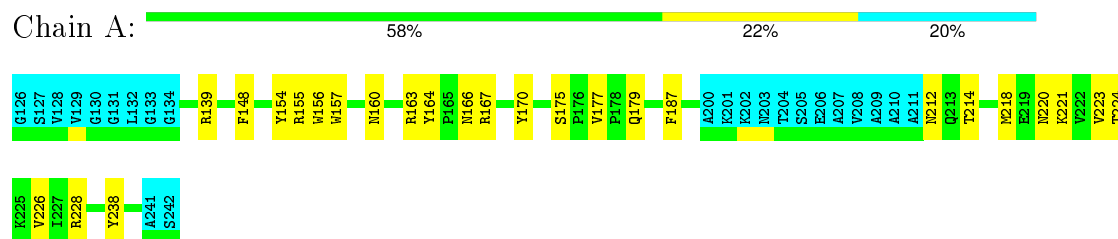
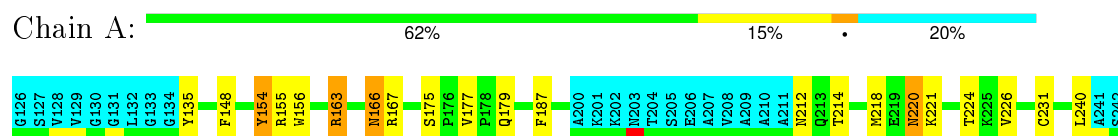

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: prion-like protein

4.2.2 Score per residue for model 2

- Molecule 1: prion-like protein

4.2.3 Score per residue for model 3

• Molecule 1: prion-like protein

4.2.4 Score per residue for model 4
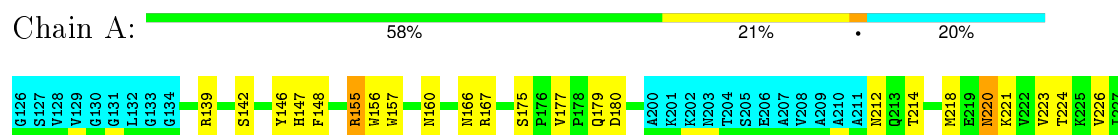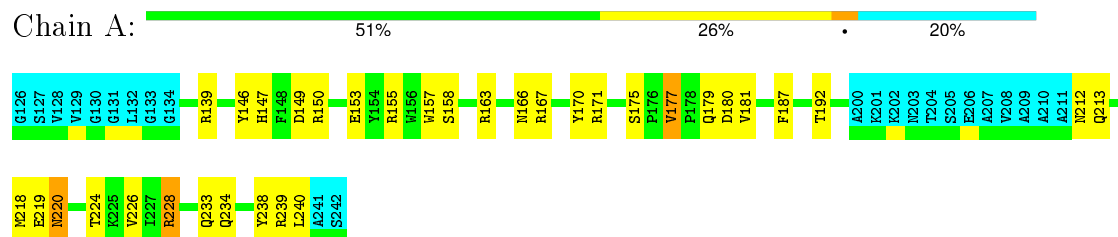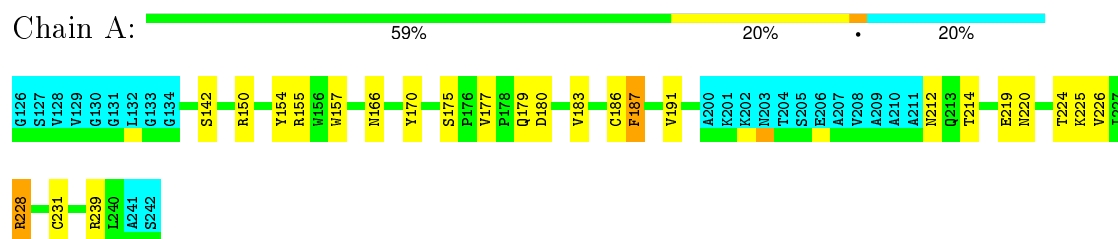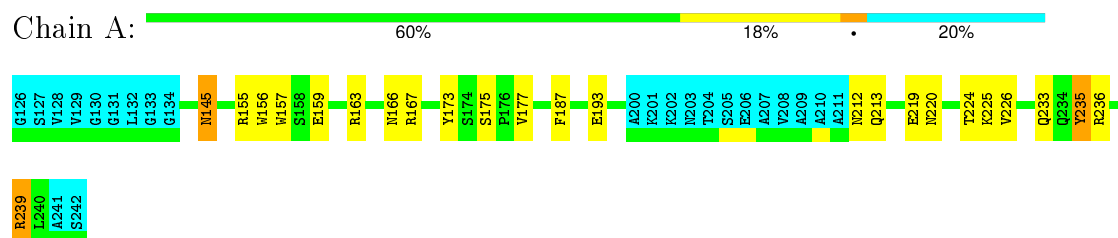
• Molecule 1: prion-like protein
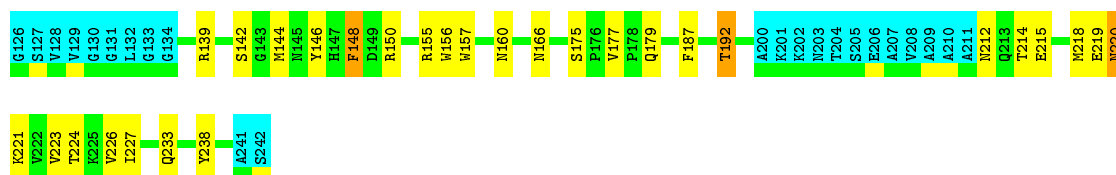

4.2.5 Score per residue for model 5

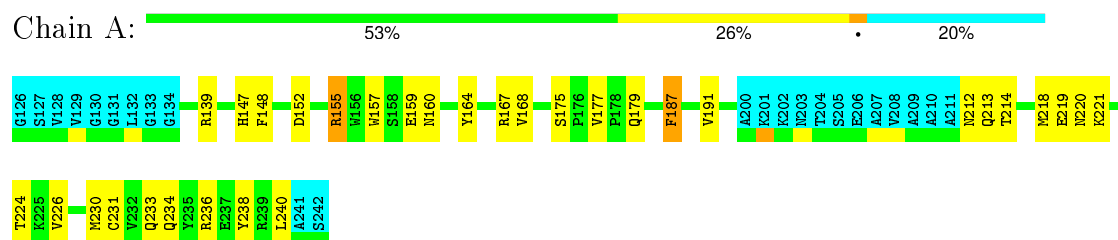• Molecule 1: prion-like protein

4.2.6 Score per residue for model 6

• Molecule 1: prion-like protein

G126 S127 V128 V129 G130 G131 L132 G133 G134 R139 S142 G143 M144 N145 Y146 H147 F148 D149 R150 R155 W156 W157 N160 N166 S175 P176 V177 P178 Q179 F187 T192 A200 K201 K202 N203 T204 S205 E206 A207 V208 A209 A210 A211 N212 Q213 T214 E215 M218 E219 N220

K221 V222 V223 T224 K225 V226 I227 Q233 Y238 A241 S242

4.2.7 Score per residue for model 7

- Molecule 1: prion-like protein

Chain A: 53%   26%   •   20%

G126 S127 V128 V129 G130 G131 L132 G133 G134 R139 H147 F148 D152 R155 W156 W157 S158 E159 N160 Y164 R167 V168 S175 P176 V177 P178 Q179 F187 V191 A200 K201 K202 N203 T204 S205 E206 A207 V208 A209 A210 A211 N212 Q213 T214 M218 E219 N220 K221

T224 K225 V226 M230 C231 V232 Q233 Q234 Y235 R236 E237 Y238 R239 L240 A241 S242

4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: prion-like protein

Chain A: 57%   21%   •   20%

G126 S127 V128 V129 G130 G131 L132 G133 G134 S142 N145 F148 E153 Y154 R155 W156 W157 S158 N166 Y169 Y170 Y173 S174 S175 P176 V177 V183 F187 V191 A200 K201 K202 N203 T204 S205 E206 A207 V208 A209 A210 A211 N212 Q213 T214 E215 V216 N220 K221

V222 V223 V226 Y238 R239 L240 A241 S242

4.2.9 Score per residue for model 9

- Molecule 1: prion-like protein

Chain A: 51%   26%   ••   20%

G126 S127 V128 V129 G130 G131 L132 G133 G134 R139 V140 M141 N145 Y146 R150 Y154 R155 W156 W157 S158 R163 N166 R167 Y170 S174 S175 P176 V177 P178 Q179 V191 A199 A200 K201 K202 N203 T204 S205 E206 A207 V208 A209 A210 A211 T214 M218 E219 N220

V226 I227 R228 E229 M230 C231 V232 Q233 Q234 E237 Y238 R239 L240 A241 S242

4.2.10 Score per residue for model 10

- Molecule 1: prion-like protein

Chain A: 56%   22%   20%

G126 S127 V128 V129 G130 G131 L132 G133 G134 Y135 R139 N145 Y146 H147 F148 D152 E153 Y154 R155 W156 W157 N160 R163 R167 S175 P176 V177 P178 Q179 F187 N188 A200 K201 K202 N203 T204 S205 E206 A207 V208 A209 A210 A211 N212 E215 E219 N220 V223

I227 M230 R236 E237 Y238 A241 S242

4.2.11   Score per residue for model 11

• Molecule 1: prion-like protein

Chain A: 60%   19%   20%

G126 S127 V128 V129 G130 G131 L132 G133 G134 M145 Y154 R155 W156 M160 R163 N166 Y170 S175 P176 V177 P178 Q179 D180 V183 F187 A200 K201 K202 N203 T204 S205 E206 A207 V208 A209 A210 A211 T214 M218 E219 N220 V223 T224 R228 V232

Q233 Q234 Y238 A241 S242

4.2.12   Score per residue for model 12

• Molecule 1: prion-like protein

Chain A: 57%   20%   20%

G126 S127 V128 V129 G130 G131 L132 G133 G134 V140 F148 D152 R155 W156 W157 N160 R163 R167 Y170 R171 S175 P176 V177 P178 Q179 F187 E193 Y194 A200 K201 K202 N203 T204 S205 E206 A207 V208 A209 A210 A211 N212 Q213 T214 M218 E219 N220 K221

T224 R228 C231 Y238 R239 L240 A241 S242

4.2.13   Score per residue for model 13

• Molecule 1: prion-like protein

Chain A: 50%   26%   20%

G126 S127 V128 V129 G130 G131 L132 G133 G134 R139 M144 N145 Y146 H147 F148 Y154 R155 W156 N160 R163 R167 R171 S175 P176 V177 P178 Q179 D180 V183 I189 T190 V191 T192 A200 K201 K202 N203 T204 S205 E206 A207 V208 A209 A210 A211 N212 Q213 T214 E215

M218 E219 N220 K221 V222 V223 V226 I227 R228 Q233 Q234 Y238 R239 L240 A241 S242

4.2.14 Score per residue for model 14

• Molecule 1: prion-like protein

4.2.15 Score per residue for model 15

• Molecule 1: prion-like protein

4.2.16 Score per residue for model 16
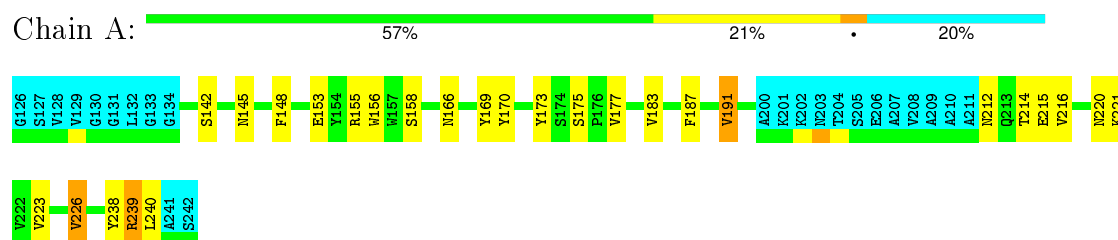
• Molecule 1: prion-like protein

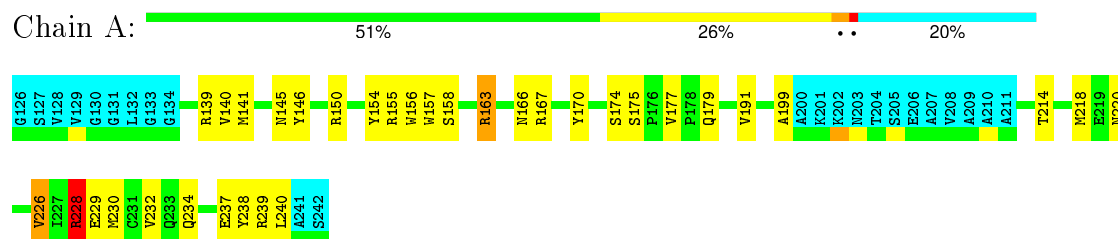### 4.2.17 Score per residue for model 17

• Molecule 1: prion-like protein

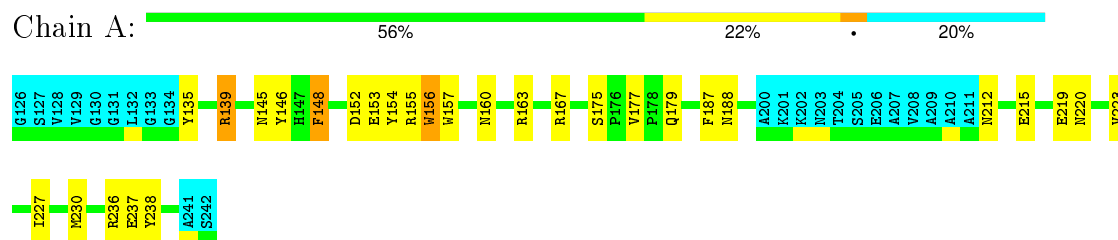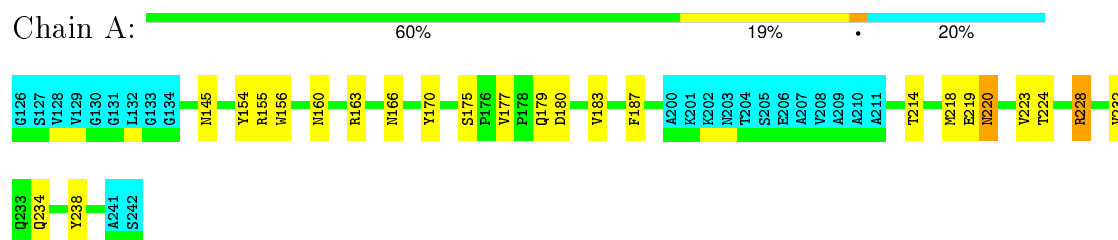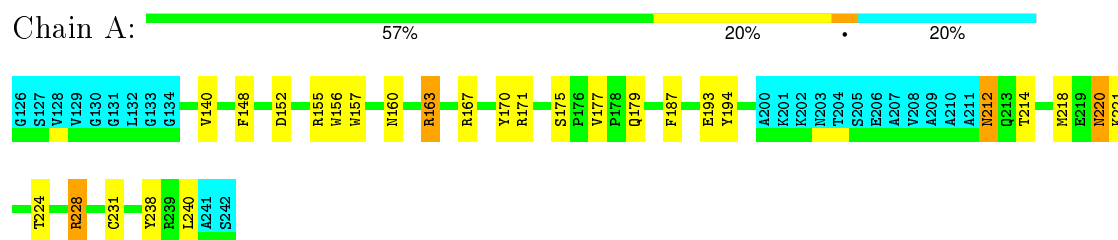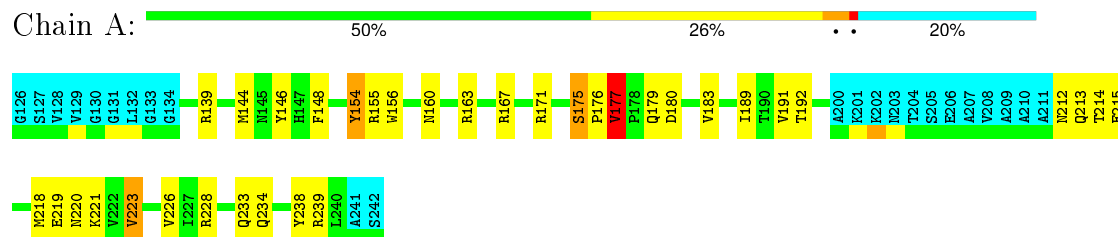### 4.2.18　Score per residue for model 18

• Molecule 1: prion-like protein

4.2.19　Score per residue for model 19

• Molecule 1: prion-like protein

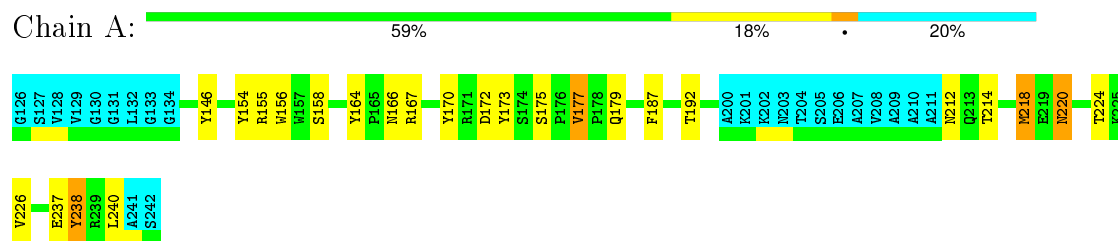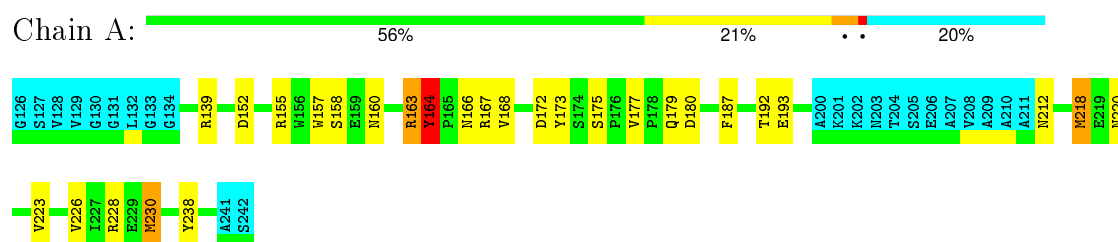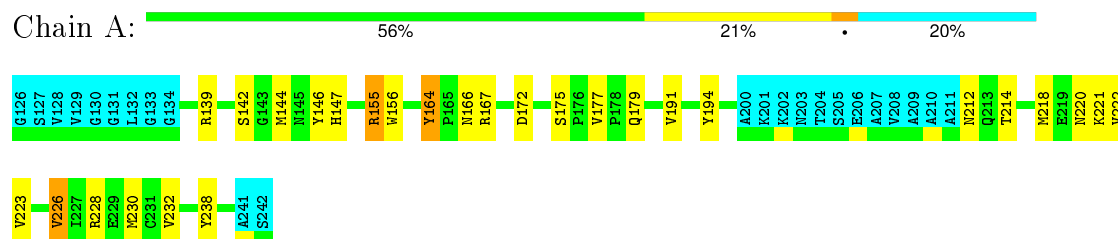### 4.2.20　Score per residue for model 20

• Molecule 1: prion-like protein
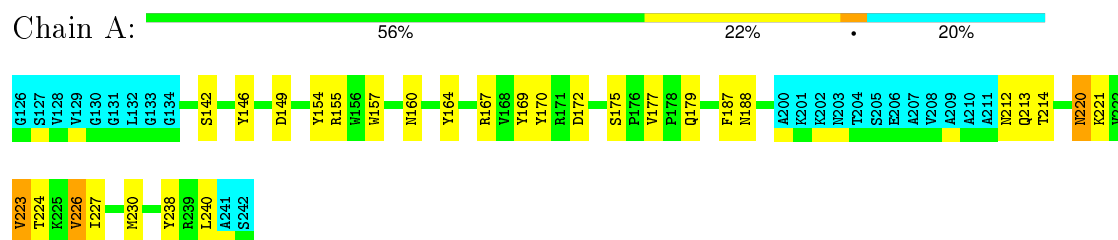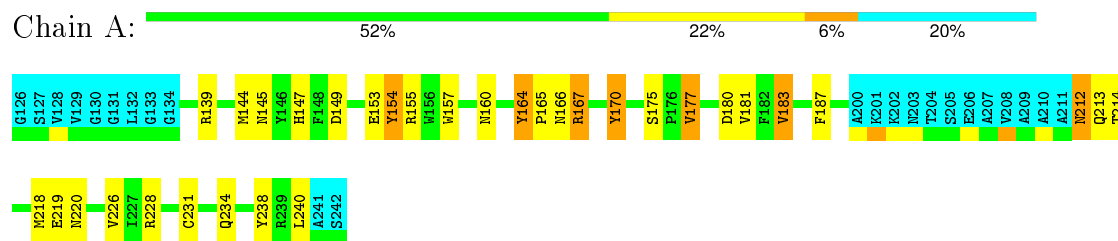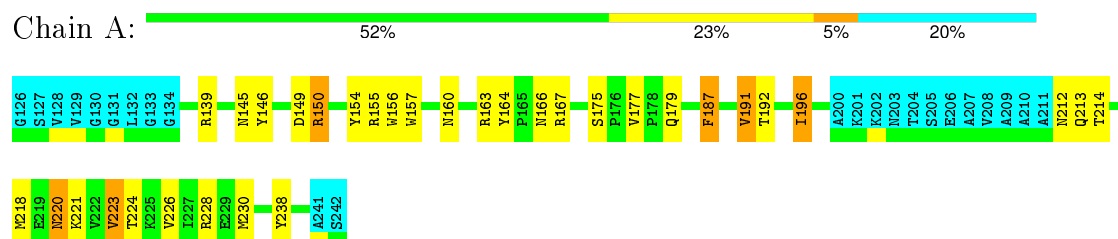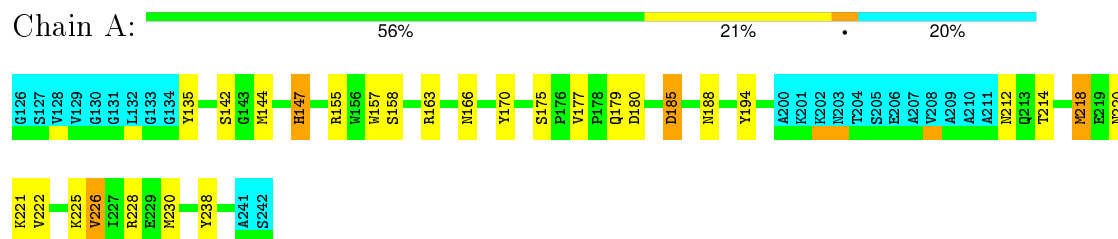
5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
DYANA	structure solution	6.0
DYANA	refinement	6.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 6269
Number of chemical shift lists	1
Total number of shifts	1294
Number of shifts mapped to atoms	1294
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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

6 Model quality (i)

6.1 Standard geometry (i)

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	0.71±0.01	0±0/819 (0.0±0.0%)	1.16±0.05	2±2/1113 (0.2±0.1%)
All	All	0.71	0/16380 (0.0%)	1.16	34/22260 (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	2.1±0.9
All	All	0	43

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(^{o})	Ideal(^{o})	Models Worst	Total
1	A	223	VAL	CA-CB-CG2	8.61	123.81	110.90	19	1
1	A	163	ARG	NE-CZ-NH2	-7.46	116.57	120.30	15	1
1	A	226	VAL	CA-CB-CG2	6.68	120.92	110.90	16	1
1	A	228	ARG	CD-NE-CZ	6.66	132.93	123.60	9	1
1	A	154	TYR	CB-CG-CD2	-6.51	117.09	121.00	18	3
1	A	168	VAL	CG1-CB-CG2	-6.22	100.95	110.90	7	1
1	A	191	VAL	CA-CB-CG2	5.96	119.84	110.90	4	4
1	A	164	TYR	CB-CG-CD2	-5.93	117.44	121.00	15	1
1	A	228	ARG	NE-CZ-NH1	5.77	123.18	120.30	9	1
1	A	185	ASP	CB-CG-OD2	-5.76	113.11	118.30	20	1
1	A	146	TYR	CB-CG-CD2	-5.65	117.61	121.00	13	1
1	A	192	THR	CA-CB-CG2	5.61	120.26	112.40	6	1
1	A	239	ARG	NE-CZ-NH2	-5.57	117.52	120.30	3	3
1	A	177	VAL	CG1-CB-CG2	5.49	119.68	110.90	13	1
1	A	177	VAL	CB-CA-C	5.49	121.83	111.40	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models Worst	Models Total
1	A	187	PHE	CB-CG-CD2	-5.46	116.98	120.80	19	1
1	A	139	ARG	NE-CZ-NH2	-5.20	117.70	120.30	10	1
1	A	238	TYR	CB-CG-CD2	-5.18	117.89	121.00	15	1
1	A	191	VAL	CA-CB-CG1	5.18	118.66	110.90	8	1
1	A	150	ARG	CD-NE-CZ	5.15	130.81	123.60	6	1
1	A	163	ARG	NE-CZ-NH1	5.13	122.87	120.30	20	1
1	A	167	ARG	NE-CZ-NH1	5.13	122.87	120.30	3	1
1	A	226	VAL	CA-CB-CG1	5.12	118.58	110.90	9	3
1	A	139	ARG	NE-CZ-NH1	5.08	122.84	120.30	10	2

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	228	ARG	Sidechain	4
1	A	155	ARG	Sidechain	4
1	A	194	TYR	Sidechain	3
1	A	173	TYR	Sidechain	3
1	A	171	ARG	Sidechain	3
1	A	163	ARG	Sidechain	3
1	A	239	ARG	Sidechain	3
1	A	236	ARG	Sidechain	3
1	A	146	TYR	Sidechain	2
1	A	169	TYR	Sidechain	2
1	A	170	TYR	Sidechain	2
1	A	150	ARG	Sidechain	2
1	A	154	TYR	Sidechain	2
1	A	167	ARG	Sidechain	2
1	A	238	TYR	Sidechain	1
1	A	164	TYR	Sidechain	1
1	A	235	TYR	Sidechain	1
1	A	135	TYR	Sidechain	1
1	A	142	SER	Peptide	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	796	741	741	3±1
All	All	15920	14820	14820	51

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:PHE:CE1	1:A:224:THR:HG23	0.61	2.30	4	3
1:A:187:PHE:CZ	1:A:224:THR:HG22	0.60	2.31	19	1
1:A:226:VAL:HG12	1:A:230:MET:CE	0.56	2.31	17	2
1:A:220:ASN:O	1:A:224:THR:HG23	0.56	2.00	17	9
1:A:177:VAL:HG22	1:A:181:VAL:HG21	0.54	1.78	3	1
1:A:148:PHE:CE2	1:A:156:TRP:CE3	0.53	2.96	2	1
1:A:191:VAL:HG23	1:A:199:ALA:CB	0.52	2.35	9	1
1:A:228:ARG:O	1:A:232:VAL:HG23	0.50	2.06	9	3
1:A:183:VAL:HG23	1:A:231:CYS:HB2	0.49	1.84	18	1
1:A:187:PHE:CE1	1:A:191:VAL:HG11	0.48	2.43	19	1
1:A:226:VAL:HG12	1:A:230:MET:HE2	0.48	1.86	16	1
1:A:187:PHE:CE1	1:A:224:THR:HG22	0.47	2.44	19	1
1:A:164:TYR:CE1	1:A:226:VAL:HG21	0.46	2.45	19	1
1:A:220:ASN:HA	1:A:223:VAL:HG22	0.46	1.86	19	1
1:A:212:ASN:O	1:A:216:VAL:HG13	0.46	2.11	8	1
1:A:177:VAL:HG22	1:A:181:VAL:HG11	0.45	1.87	18	1
1:A:218:MET:HE2	1:A:222:VAL:HG23	0.44	1.90	16	1
1:A:168:VAL:HG21	1:A:230:MET:CB	0.44	2.43	15	1
1:A:140:VAL:HG13	1:A:166:ASN:ND2	0.43	2.28	9	1
1:A:187:PHE:HA	1:A:227:ILE:CG2	0.43	2.43	17	3
1:A:218:MET:CE	1:A:218:MET:HA	0.43	2.43	14	1
1:A:218:MET:O	1:A:222:VAL:HG12	0.43	2.13	20	1
1:A:187:PHE:CZ	1:A:224:THR:HG23	0.43	2.48	7	3
1:A:191:VAL:HG12	1:A:196:ILE:HD12	0.43	1.90	19	1
1:A:218:MET:O	1:A:218:MET:HE2	0.43	2.14	16	1
1:A:218:MET:HA	1:A:218:MET:CE	0.42	2.44	15	1
1:A:173:TYR:CG	1:A:177:VAL:HG11	0.42	2.49	14	1
1:A:183:VAL:HG13	1:A:231:CYS:HB2	0.42	1.90	4	1
1:A:141:MET:SD	1:A:230:MET:HG2	0.41	2.55	9	1
1:A:146:TYR:CD1	1:A:148:PHE:CZ	0.41	3.09	6	1
1:A:183:VAL:HG21	1:A:232:VAL:HG22	0.41	1.92	11	1
1:A:148:PHE:CZ	1:A:156:TRP:CE3	0.41	3.09	10	1
1:A:223:VAL:HA	1:A:226:VAL:HG12	0.41	1.93	13	1
1:A:223:VAL:O	1:A:227:ILE:HD12	0.40	2.16	17	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	94/117 (80%)	81±2 (86±2%)	9±2 (9±2%)	4±1 (5±1%)	6	30
All	All	1880/2340 (80%)	1623 (86%)	172 (9%)	85 (5%)	6	30

All 16 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	175	SER	20
1	A	166	ASN	13
1	A	212	ASN	9
1	A	148	PHE	7
1	A	146	TYR	6
1	A	164	TYR	5
1	A	163	ARG	4
1	A	147	HIS	4
1	A	144	MET	4
1	A	145	ASN	4
1	A	172	ASP	2
1	A	149	ASP	2
1	A	135	TYR	2
1	A	177	VAL	1
1	A	176	PRO	1
1	A	165	PRO	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	87/99 (88%)	67±3 (77±4%)	20±3 (23±4%)	3	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1740/1980 (88%)	1337 (77%)	403 (23%)	3 29

All 60 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	220	ASN	20
1	A	177	VAL	20
1	A	155	ARG	19
1	A	179	GLN	17
1	A	214	THR	16
1	A	238	TYR	15
1	A	157	TRP	14
1	A	226	VAL	14
1	A	218	MET	14
1	A	167	ARG	13
1	A	156	TRP	12
1	A	221	LYS	11
1	A	160	ASN	11
1	A	212	ASN	10
1	A	187	PHE	10
1	A	228	ARG	10
1	A	139	ARG	10
1	A	219	GLU	9
1	A	240	LEU	9
1	A	223	VAL	9
1	A	170	TYR	9
1	A	180	ASP	8
1	A	154	TYR	8
1	A	213	GLN	7
1	A	233	GLN	6
1	A	234	GLN	6
1	A	142	SER	6
1	A	192	THR	6
1	A	163	ARG	6
1	A	158	SER	6
1	A	230	MET	5
1	A	237	GLU	4
1	A	215	GLU	4
1	A	153	GLU	4
1	A	152	ASP	4
1	A	164	TYR	4

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Mol	Chain	Res	Type	Models (Total)
1	A	145	ASN	4
1	A	147	HIS	3
1	A	188	ASN	3
1	A	183	VAL	3
1	A	150	ARG	3
1	A	231	CYS	3
1	A	193	GLU	3
1	A	225	LYS	3
1	A	159	GLU	2
1	A	172	ASP	2
1	A	239	ARG	2
1	A	166	ASN	2
1	A	191	VAL	2
1	A	149	ASP	2
1	A	189	ILE	1
1	A	140	VAL	1
1	A	174	SER	1
1	A	229	GLU	1
1	A	196	ILE	1
1	A	185	ASP	1
1	A	235	TYR	1
1	A	175	SER	1
1	A	186	CYS	1
1	A	144	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 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 (i)

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6269

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1294
Number of shifts mapped to atoms	1294
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	113	0.29 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_\beta$	101	0.68 ± 0.11	Should be applied
$^{13}C'$	0	—	—
^{15}N	110	-1.31 ± 0.30	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 984 atoms were assigned a chemical shift out of a possible 1227. 12 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	358/460 (78%)	180/183 (98%)	90/188 (48%)	88/89 (99%)
Sidechain	526/629 (84%)	336/373 (90%)	168/217 (77%)	22/39 (56%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	100/138 (72%)	64/71 (90%)	34/64 (53%)	2/3 (67%)
Overall	984/1227 (80%)	580/627 (93%)	292/469 (62%)	112/131 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1159 atoms were assigned a chemical shift out of a possible 1434. 15 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	448/575 (78%)	225/229 (98%)	113/234 (48%)	110/112 (98%)
Sidechain	611/721 (85%)	387/425 (91%)	201/254 (79%)	23/42 (55%)
Aromatic	100/138 (72%)	64/71 (90%)	34/64 (53%)	2/3 (67%)
Overall	1159/1434 (81%)	676/725 (93%)	348/552 (63%)	135/157 (86%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	157	TRP	NE1	139.20	139.19 – 119.59	5.0

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A: