



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 11:39 pm GMT

PDB ID : 2L40
Title : Mouse prion protein (121-231) containing the substitution Y169A
Authors : Christen, B.; Damberger, F.F.; Perez, D.R.; Hornemann, S.; Wuthrich, K.
Deposited on : 2010-09-28

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 : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

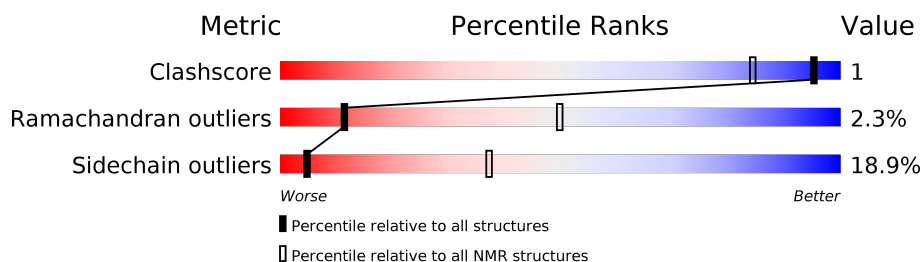
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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	114	<div>74% 14% • 11%</div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:125-A:226 (102)	0.37	3

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 and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1798 atoms, of which 868 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	114	Total	C	H	N	O	S	0
			1798	574	868	165	182	9	

There are 3 discrepancies between the modelled and reference sequences:

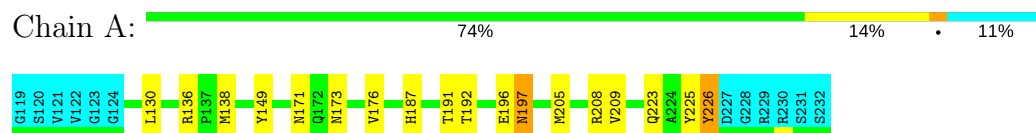
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	EXPRESSION TAG	UNP Q4FJQ7
A	120	SER	-	EXPRESSION TAG	UNP Q4FJQ7
A	169	ALA	TYR	ENGINEERED MUTATION	UNP Q4FJQ7

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: Major prion protein

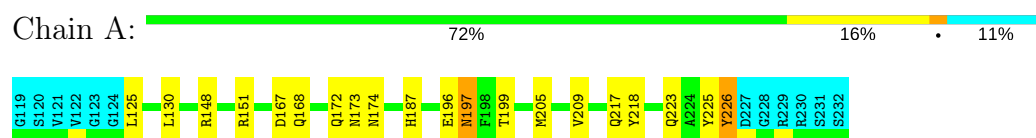


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

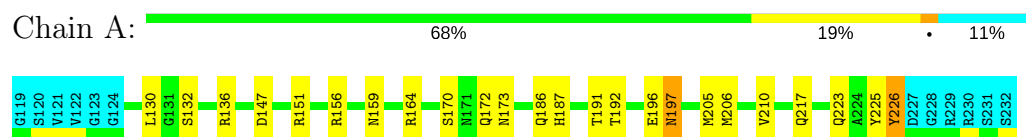
4.2.1 Score per residue for model 1

- Molecule 1: Major prion protein



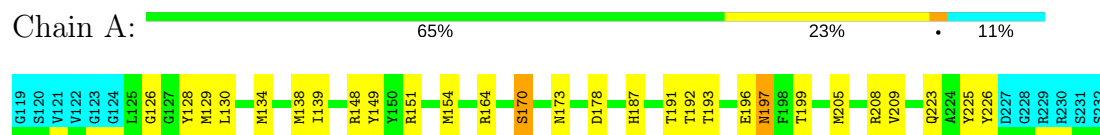
4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein



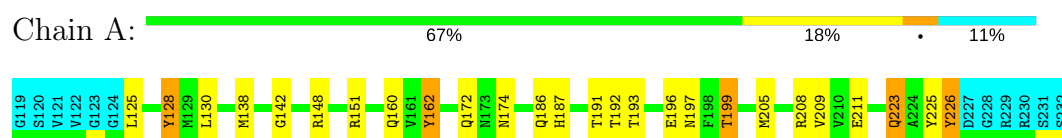
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Major prion protein



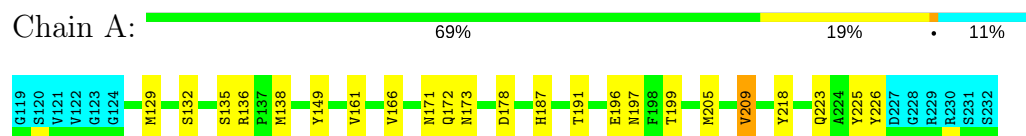
4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



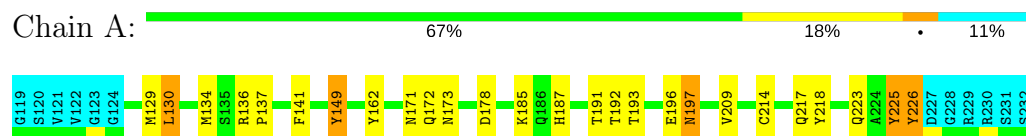
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



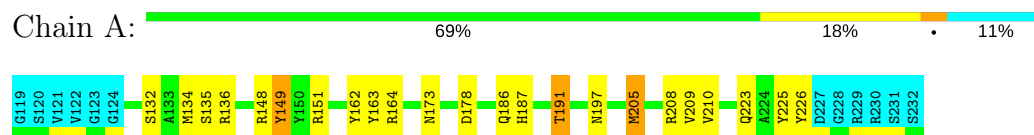
4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



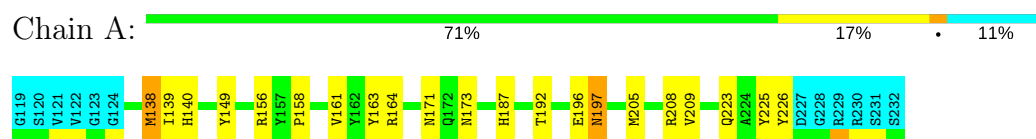
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



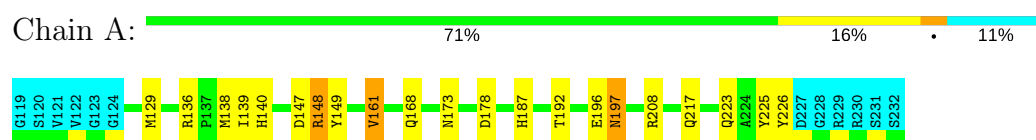
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



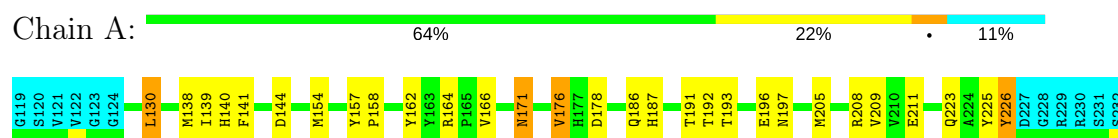
4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



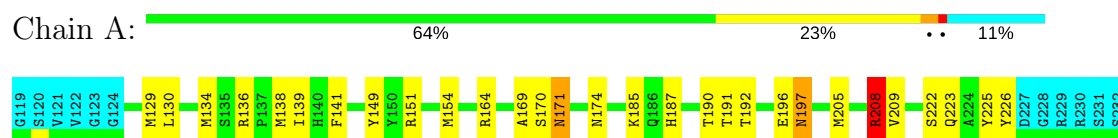
4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



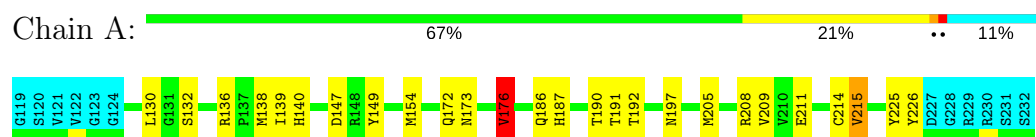
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



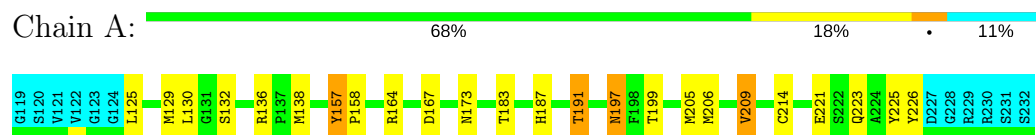
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



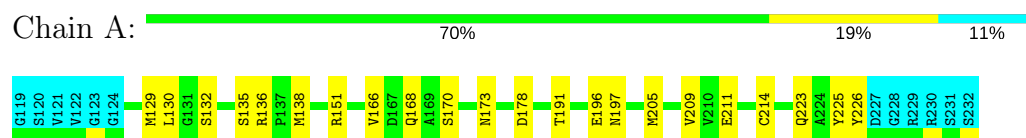
4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



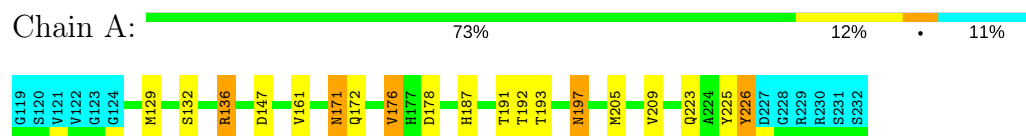
4.2.19 Score per residue for model 19

- Molecule 1: Major prion protein



4.2.20 Score per residue for model 20

- Molecule 1: Major prion protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS*.

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *TARGET FUNCTION*.

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

Software name	Classification	Version
DYANA	structure solution	1.0.3
OPALP	refinement	

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 17213
Number of chemical shift lists	1
Total number of shifts	1292
Number of shifts mapped to atoms	1292
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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	0.68±0.01	0±0/873 (0.0±0.0%)	1.13±0.03	2±1/1182 (0.2±0.1%)
All	All	0.68	0/17460 (0.0%)	1.13	36/23640 (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	2.3±1.3
All	All	0	46

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	209	VAL	CA-CB-CG2	10.44	126.56	110.90	18	1
1	A	149	TYR	CB-CG-CD2	-7.06	116.76	121.00	7	2
1	A	157	TYR	CB-CG-CD2	-6.64	117.02	121.00	10	6
1	A	208	ARG	NE-CZ-NH2	-6.58	117.01	120.30	7	1
1	A	164	ARG	NE-CZ-NH2	-6.58	117.01	120.30	17	2
1	A	176	VAL	CA-CB-CG2	6.45	120.58	110.90	12	2
1	A	199	THR	CA-CB-CG2	-6.31	103.57	112.40	4	1
1	A	151	ARG	NE-CZ-NH2	-6.17	117.22	120.30	1	1
1	A	226	TYR	CB-CG-CD2	-5.97	117.42	121.00	20	2
1	A	164	ARG	NE-CZ-NH1	5.82	123.21	120.30	3	1
1	A	161	VAL	CA-CB-CG1	5.81	119.61	110.90	9	2
1	A	167	ASP	C-N-CA	5.74	136.04	121.70	14	2
1	A	148	ARG	NE-CZ-NH2	-5.68	117.46	120.30	13	1
1	A	226	TYR	CB-CA-C	5.59	121.58	110.40	13	1
1	A	226	TYR	CB-CG-CD1	-5.44	117.74	121.00	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	215	VAL	CG1-CB-CG2	5.43	119.59	110.90	12	1
1	A	226	TYR	CD1-CG-CD2	5.36	123.79	117.90	16	1
1	A	140	HIS	C-N-CA	5.36	135.09	121.70	10	1
1	A	209	VAL	CG1-CB-CG2	5.30	119.38	110.90	18	1
1	A	176	VAL	CG1-CB-CG2	-5.28	102.44	110.90	10	1
1	A	169	ALA	CB-CA-C	5.24	117.96	110.10	11	1
1	A	205	MET	CG-SD-CE	-5.20	91.87	100.20	7	1
1	A	215	VAL	CA-CB-CG1	5.13	118.60	110.90	17	1
1	A	209	VAL	CA-CB-CG1	5.11	118.56	110.90	5	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	136	ARG	Sidechain	5
1	A	226	TYR	Sidechain	4
1	A	164	ARG	Sidechain	4
1	A	218	TYR	Sidechain	3
1	A	148	ARG	Sidechain	3
1	A	128	TYR	Sidechain	3
1	A	140	HIS	Sidechain	3
1	A	163	TYR	Sidechain	2
1	A	208	ARG	Sidechain	2
1	A	149	TYR	Sidechain	2
1	A	151	ARG	Sidechain	2
1	A	162	TYR	Sidechain	2
1	A	186	GLN	Peptide	2
1	A	171	ASN	Peptide	2
1	A	141	PHE	Sidechain	1
1	A	156	ARG	Sidechain	1
1	A	157	TYR	Sidechain	1
1	A	190	THR	Peptide	1
1	A	142	GLY	Peptide	1
1	A	225	TYR	Sidechain	1
1	A	150	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	852	793	793	2±2
All	All	17040	15860	15860	38

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:139:ILE:HD13	1:A:208:ARG:HB3	0.61	1.72	13	6
1:A:206:MET:HA	1:A:209:VAL:HG22	0.61	1.72	18	1
1:A:172:GLN:O	1:A:176:VAL:HG22	0.58	1.98	16	3
1:A:130:LEU:HD13	1:A:162:TYR:CZ	0.57	2.35	14	1
1:A:125:LEU:HD12	1:A:128:TYR:HB2	0.57	1.75	4	1
1:A:139:ILE:HG21	1:A:208:ARG:NH1	0.56	2.16	11	1
1:A:183:THR:HG22	1:A:187:HIS:CE1	0.53	2.38	18	1
1:A:145:TRP:CH2	1:A:201:THR:HG23	0.52	2.39	17	1
1:A:208:ARG:HB2	1:A:208:ARG:CZ	0.52	2.35	11	1
1:A:211:GLU:O	1:A:215:VAL:HG13	0.50	2.05	12	1
1:A:130:LEU:HD23	1:A:162:TYR:CD1	0.50	2.42	4	1
1:A:223:GLN:HA	1:A:226:TYR:CD2	0.48	2.44	17	2
1:A:125:LEU:HA	1:A:128:TYR:CD1	0.47	2.45	4	1
1:A:141:PHE:CZ	1:A:208:ARG:NH1	0.46	2.83	11	1
1:A:141:PHE:CE2	1:A:208:ARG:NH1	0.46	2.84	11	1
1:A:158:PRO:CG	1:A:187:HIS:CE1	0.45	2.99	10	3
1:A:139:ILE:HD13	1:A:208:ARG:HB2	0.45	1.88	9	1
1:A:171:ASN:HD22	1:A:174:ASN:ND2	0.43	2.11	11	1
1:A:171:ASN:ND2	1:A:174:ASN:HD21	0.43	2.11	15	1
1:A:130:LEU:HG	1:A:162:TYR:CE1	0.43	2.49	17	3
1:A:170:SER:HA	1:A:174:ASN:HD21	0.43	1.73	13	1
1:A:130:LEU:HD21	1:A:160:GLN:HB3	0.43	1.91	4	1
1:A:125:LEU:HD12	1:A:128:TYR:CB	0.42	2.44	4	1
1:A:141:PHE:CZ	1:A:208:ARG:CZ	0.42	3.03	11	1
1:A:225:TYR:CD2	1:A:226:TYR:HB3	0.41	2.50	6	1
1:A:138:MET:HA	1:A:138:MET:CE	0.41	2.46	8	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	102/114 (89%)	88±2 (87±2%)	11±3 (11±2%)	2±1 (2±1%)	11	50
All	All	2040/2280 (89%)	1766 (87%)	227 (11%)	47 (2%)	11	50

All 9 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	197	ASN	18
1	A	191	THR	8
1	A	186	GLN	6
1	A	168	GLN	4
1	A	170	SER	3
1	A	166	VAL	3
1	A	171	ASN	2
1	A	141	PHE	2
1	A	154	MET	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	94/102 (92%)	76±2 (81±2%)	18±2 (19±2%)	5	37
All	All	1880/2040 (92%)	1525 (81%)	355 (19%)	5	37

All 55 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	226	TYR	20

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Mol	Chain	Res	Type	Models (Total)
1	A	225	TYR	20
1	A	223	GLN	19
1	A	205	MET	18
1	A	209	VAL	17
1	A	187	HIS	16
1	A	173	ASN	16
1	A	192	THR	15
1	A	138	MET	14
1	A	191	THR	13
1	A	197	ASN	13
1	A	136	ARG	11
1	A	196	GLU	11
1	A	129	MET	10
1	A	130	LEU	10
1	A	132	SER	9
1	A	178	ASP	8
1	A	149	TYR	8
1	A	172	GLN	7
1	A	217	GLN	7
1	A	193	THR	6
1	A	171	ASN	5
1	A	161	VAL	5
1	A	199	THR	5
1	A	134	MET	5
1	A	147	ASP	5
1	A	214	CYS	5
1	A	211	GLU	4
1	A	148	ARG	4
1	A	151	ARG	4
1	A	174	ASN	4
1	A	176	VAL	4
1	A	208	ARG	3
1	A	135	SER	3
1	A	159	ASN	3
1	A	154	MET	3
1	A	144	ASP	2
1	A	164	ARG	2
1	A	185	LYS	2
1	A	170	SER	2
1	A	143	ASN	2
1	A	210	VAL	2
1	A	215	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	206	MET	1
1	A	152	GLU	1
1	A	125	LEU	1
1	A	222	SER	1
1	A	216	THR	1
1	A	167	ASP	1
1	A	202	ASP	1
1	A	204	LYS	1
1	A	156	ARG	1
1	A	221	GLU	1
1	A	137	PRO	1
1	A	190	THR	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

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 17213

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	1292
Number of shifts mapped to atoms	1292
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	114	0.09 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	105	0.67 ± 0.17	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	110	-0.04 ± 0.19	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1068 atoms were assigned a chemical shift out of a possible 1302. 11 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	397/504 (79%)	196/201 (98%)	102/204 (50%)	99/99 (100%)
Sidechain	567/658 (86%)	356/388 (92%)	189/232 (81%)	22/38 (58%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	104/140 (74%)	66/73 (90%)	37/63 (59%)	1/4 (25%)
Overall	1068/1302 (82%)	618/662 (93%)	328/499 (66%)	122/141 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1160 atoms were assigned a chemical shift out of a possible 1423. 13 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	443/564 (79%)	219/225 (97%)	114/228 (50%)	110/111 (99%)
Sidechain	613/719 (85%)	384/424 (91%)	205/251 (82%)	24/44 (55%)
Aromatic	104/140 (74%)	66/73 (90%)	37/63 (59%)	1/4 (25%)
Overall	1160/1423 (82%)	669/722 (93%)	356/542 (66%)	135/159 (85%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

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:

