



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:23 PM BST

PDB ID : 1XYU
Title : Solution structure of the sheep prion protein with polymorphism H168
Authors : Calzolari, L.; Lysek, D.A.; Guntert, P.; Wuthrich, K.
Deposited on : 2004-11-11

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
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

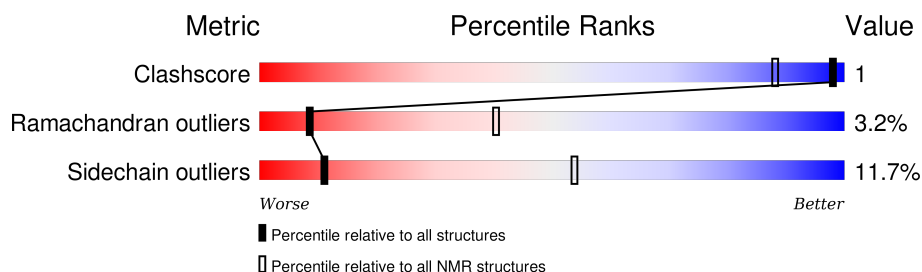
1 Overall quality at a glance

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	111	<div> <div></div> <div>70%</div> <div>12%</div> <div>18%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:128-A:189, A:198-A:226 (91)	0.35	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 8 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1777 atoms, of which 859 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms							Trace
1	A	111	Total	C	H	N	O	S		0
			1777	572	859	162	177	7		

There is a discrepancy between the modelled and reference sequences:

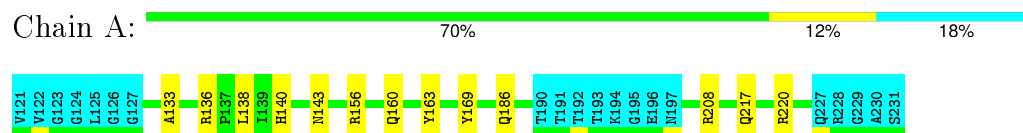
Chain	Residue	Modelled	Actual	Comment	Reference
A	168	HIS	ARG	SEE REMARK 999	UNP P23907

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

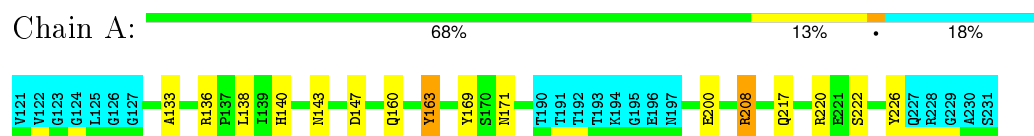


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

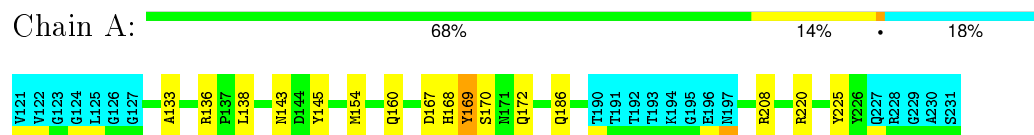
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Major prion protein



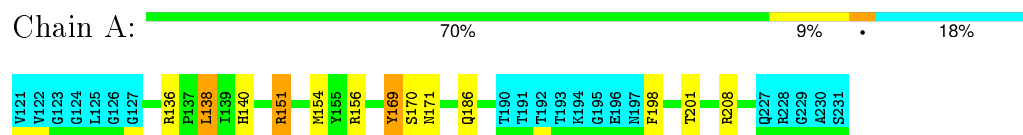
4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein



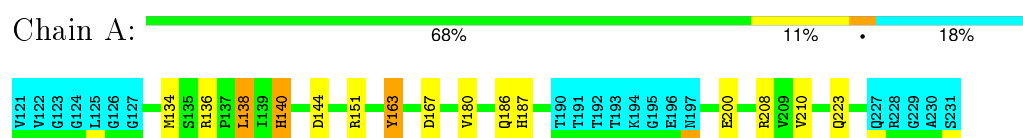
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



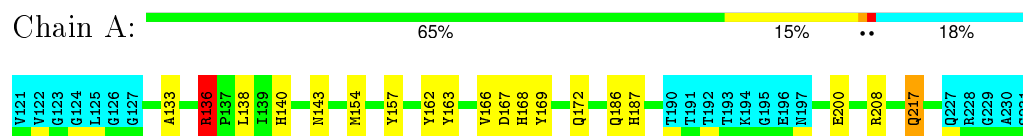
4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



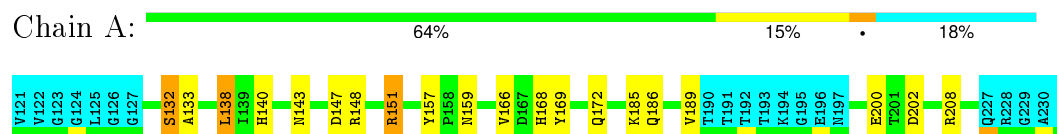
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



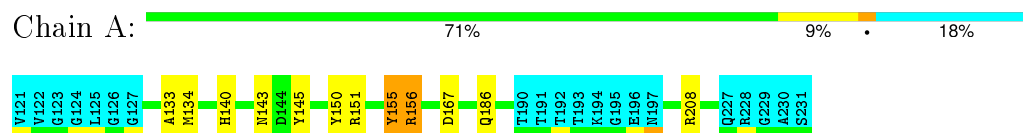
4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



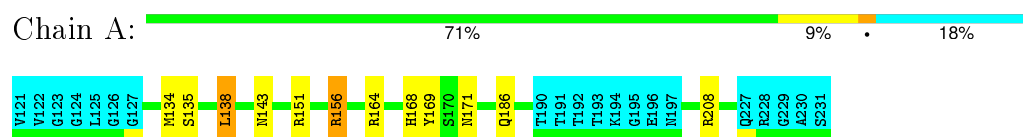
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



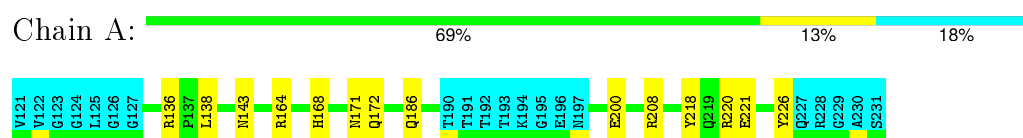
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



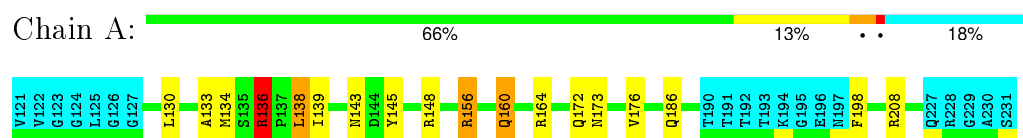
4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



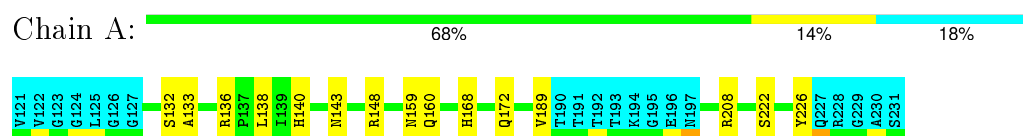
4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



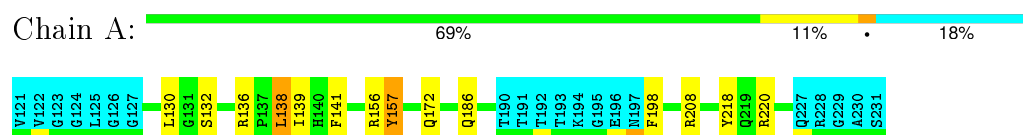
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



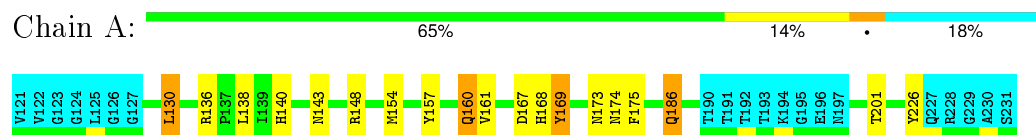
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



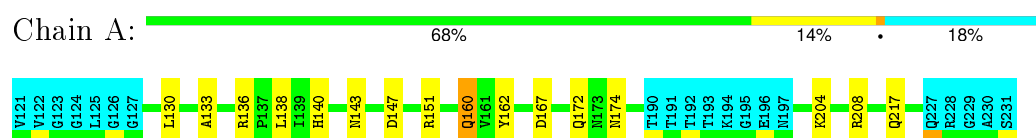
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



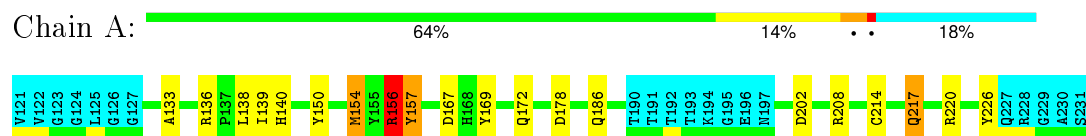
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



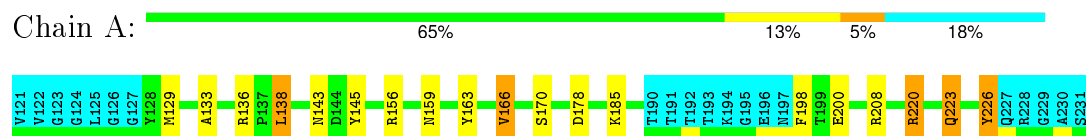
4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



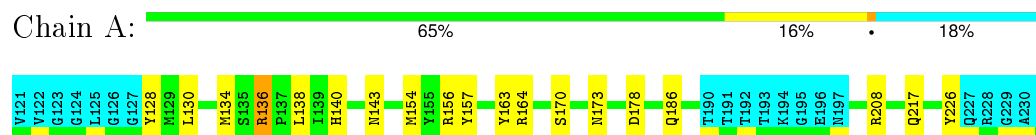
4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein



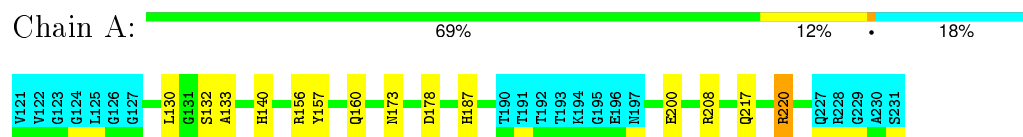
4.2.17 Score per residue for model 17

- Molecule 1: Major prion protein



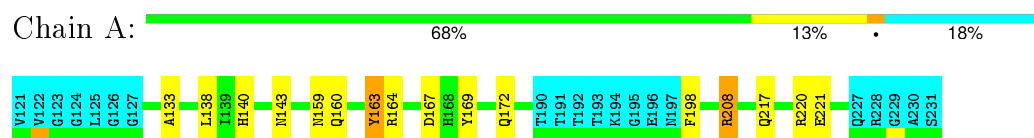
4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



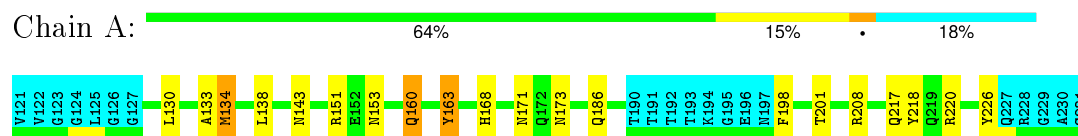
4.2.19 Score per residue for model 19

- 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 100 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	6.2
CANDID	refinement	1.0

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 6381
Number of chemical shift lists	1
Total number of shifts	1291
Number of shifts mapped to atoms	1281
Number of unparsed shifts	0
Number of shifts with mapping errors	10
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	0.70±0.01	0±0/809 (0.0±0.0%)	1.08±0.03	2±2/1097 (0.2±0.2%)
All	All	0.70	0/16180 (0.0%)	1.08	45/21940 (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±1.2
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(°)	Ideal(°)	Models	
								Worst	Total
1	A	208	ARG	NE-CZ-NH2	-7.52	116.54	120.30	19	4
1	A	136	ARG	NE-CZ-NH1	7.41	124.00	120.30	17	5
1	A	157	TYR	CB-CG-CD2	-7.02	116.79	121.00	15	6
1	A	148	ARG	CD-NE-CZ	6.70	132.97	123.60	13	1
1	A	136	ARG	CD-NE-CZ	6.45	132.62	123.60	10	4
1	A	220	ARG	NE-CZ-NH2	-6.21	117.19	120.30	19	2
1	A	226	TYR	CB-CG-CD1	-6.20	117.28	121.00	15	2
1	A	148	ARG	NE-CZ-NH2	-6.18	117.21	120.30	13	2
1	A	148	ARG	NE-CZ-NH1	5.83	123.21	120.30	13	1
1	A	166	VAL	CG1-CB-CG2	-5.80	101.62	110.90	6	2
1	A	136	ARG	NE-CZ-NH2	-5.79	117.41	120.30	1	3
1	A	156	ARG	NE-CZ-NH2	-5.60	117.50	120.30	10	1
1	A	156	ARG	NE-CZ-NH1	5.60	123.10	120.30	15	1
1	A	163	TYR	CB-CG-CD2	-5.49	117.70	121.00	1	3
1	A	140	HIS	CA-CB-CG	5.44	122.85	113.60	4	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	166	VAL	CA-CB-CG1	5.43	119.04	110.90	16	1
1	A	226	TYR	CB-CG-CD2	-5.37	117.78	121.00	11	2
1	A	161	VAL	CA-CB-CG2	5.19	118.69	110.90	13	1
1	A	218	TYR	CB-CG-CD2	-5.17	117.90	121.00	20	1
1	A	132	SER	C-N-CA	5.15	134.57	121.70	11	1
1	A	155	TYR	CB-CG-CD2	-5.01	118.00	121.00	7	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	151	ARG	Sidechain	6
1	A	156	ARG	Sidechain	6
1	A	220	ARG	Sidechain	5
1	A	164	ARG	Sidechain	4
1	A	157	TYR	Sidechain	3
1	A	145	TYR	Sidechain	3
1	A	148	ARG	Sidechain	2
1	A	218	TYR	Sidechain	2
1	A	162	TYR	Sidechain	2
1	A	136	ARG	Sidechain	2
1	A	163	TYR	Sidechain	2
1	A	134	MET	Peptide	1
1	A	140	HIS	Peptide	1
1	A	153	ASN	Peptide	1
1	A	225	TYR	Sidechain	1
1	A	226	TYR	Peptide	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	787	728	728	1±1
All	All	15740	14560	14560	19

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:180:VAL:HG22	1:A:210:VAL:HG23	0.58	1.74	4	1
1:A:130:LEU:HD11	1:A:160:GLN:NE2	0.55	2.15	14	4
1:A:172:GLN:HE21	1:A:176:VAL:HG21	0.52	1.64	10	1
1:A:133:ALA:HB1	1:A:159:ASN:HD22	0.49	1.68	16	1
1:A:139:ILE:HG21	1:A:141:PHE:CZ	0.48	2.43	12	1
1:A:169:TYR:CE1	1:A:175:PHE:CZ	0.42	3.08	13	1
1:A:130:LEU:HD11	1:A:160:GLN:HE22	0.42	1.74	18	1
1:A:223:GLN:HA	1:A:226:TYR:CD2	0.42	2.49	16	1
1:A:185:LYS:O	1:A:189:VAL:HG23	0.42	2.14	6	1
1:A:214:CYS:HA	1:A:217:GLN:CG	0.41	2.45	15	1
1:A:150:TYR:CE1	1:A:154:MET:HB3	0.41	2.50	15	1
1:A:169:TYR:CZ	1:A:175:PHE:CE1	0.41	3.08	13	1
1:A:172:GLN:HE21	1:A:176:VAL:CG2	0.41	2.29	10	1
1:A:136:ARG:CG	1:A:136:ARG:HH11	0.40	2.29	10	1
1:A:169:TYR:CE1	1:A:175:PHE:CE1	0.40	3.09	13	1
1:A:163:TYR:CD1	1:A:217:GLN:HG2	0.40	2.51	5	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	91/111 (82%)	80±3 (87±3%)	9±2 (9±2%)	3±1 (3±1%)	8	40
All	All	1820/2220 (82%)	1592 (87%)	170 (9%)	58 (3%)	8	40

All 10 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	143	ASN	15
1	A	133	ALA	12
1	A	138	LEU	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	198	PHE	6
1	A	170	SER	4
1	A	167	ASP	4
1	A	147	ASP	3
1	A	132	SER	2
1	A	169	TYR	2
1	A	171	ASN	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	87/100 (87%)	77±2 (88±2%)	10±2 (12±2%)	11	54
All	All	1740/2000 (87%)	1537 (88%)	203 (12%)	11	54

All 43 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	208	ARG	17
1	A	138	LEU	16
1	A	186	GLN	14
1	A	140	HIS	12
1	A	136	ARG	9
1	A	172	GLN	9
1	A	169	TYR	9
1	A	160	GLN	8
1	A	217	GLN	8
1	A	168	HIS	8
1	A	200	GLU	7
1	A	156	ARG	6
1	A	134	MET	6
1	A	154	MET	6
1	A	173	ASN	5
1	A	163	TYR	5
1	A	171	ASN	4
1	A	167	ASP	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	178	ASP	4
1	A	220	ARG	4
1	A	226	TYR	3
1	A	159	ASN	3
1	A	187	HIS	3
1	A	201	THR	3
1	A	151	ARG	3
1	A	130	LEU	3
1	A	132	SER	2
1	A	174	ASN	2
1	A	202	ASP	2
1	A	222	SER	2
1	A	139	ILE	2
1	A	221	GLU	2
1	A	223	GLN	2
1	A	144	ASP	1
1	A	204	LYS	1
1	A	189	VAL	1
1	A	135	SER	1
1	A	164	ARG	1
1	A	145	TYR	1
1	A	129	MET	1
1	A	166	VAL	1
1	A	155	TYR	1
1	A	185	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

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 6381

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	1291
Number of shifts mapped to atoms	1281
Number of unparsed shifts	0
Number of shifts with mapping errors	10
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 10 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1	GLY	HA2	3.88	0.01	1
A	2	SER	CA	57.8	0.1	1
A	1	GLY	CA	43.3	0.1	1
A	2	SER	N	115.6	0.1	1
A	2	SER	CB	63.9	0.1	1
A	2	SER	HB3	3.81	0.01	1
A	2	SER	H	8.64	0.01	1
A	2	SER	HB2	3.81	0.01	1
A	2	SER	HA	4.57	0.01	1
A	1	GLY	HA3	3.88	0.01	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	112	-0.24 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	104	0.46 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	106	0.35 ± 0.19	None needed (< 0.5 ppm)

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 82%, i.e. 993 atoms were assigned a chemical shift out of a possible 1210. 10 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	350/449 (78%)	175/179 (98%)	90/182 (49%)	85/88 (97%)
Sidechain	544/610 (89%)	348/361 (96%)	175/212 (83%)	21/37 (57%)
Aromatic	99/151 (66%)	66/79 (84%)	33/68 (49%)	0/4 (0%)
Overall	993/1210 (82%)	589/619 (95%)	298/462 (65%)	106/129 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1153 atoms were assigned a chemical shift out of a possible 1407. 13 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	430/549 (78%)	215/219 (98%)	110/222 (50%)	105/108 (97%)
Sidechain	624/707 (88%)	397/416 (95%)	203/248 (82%)	24/43 (56%)
Aromatic	99/151 (66%)	66/79 (84%)	33/68 (49%)	0/4 (0%)
Overall	1153/1407 (82%)	678/714 (95%)	346/538 (64%)	129/155 (83%)

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:

