



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 08:44 pm GMT

PDB ID : 1XYJ  
Title : NMR Structure of the cat prion protein  
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Deposited on : 2004-11-10

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

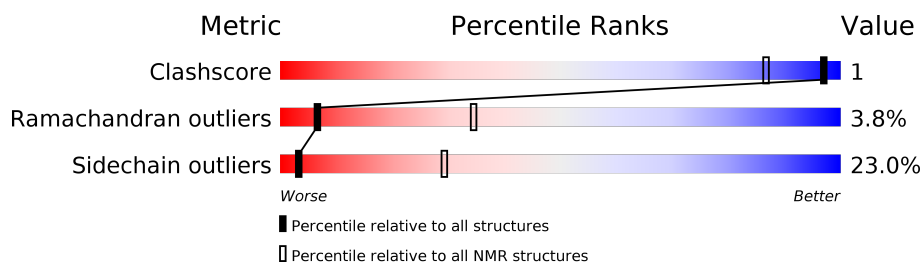
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 79%.

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  $\geq 3$ , 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>63% 17% 20%</div>

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 16 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:127-A:166, A:175-A:223 (89)	0.51	16

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 2 single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1787 atoms, of which 864 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called prion protein.

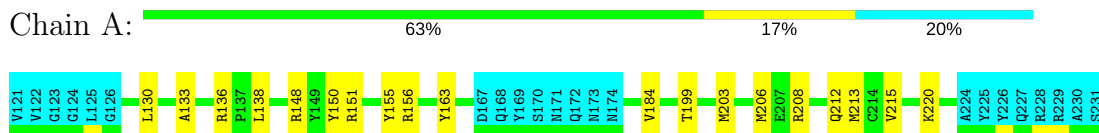
Mol	Chain	Residues	Atoms						Trace
1	A	111	Total	C	H	N	O	S	0
			1787	573	864	163	179	8	

## 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: prion protein

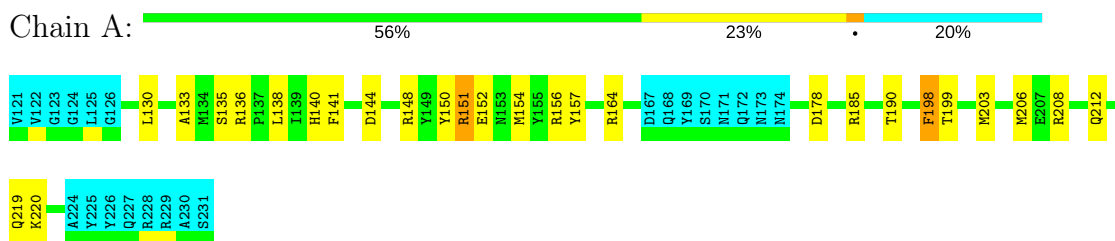


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

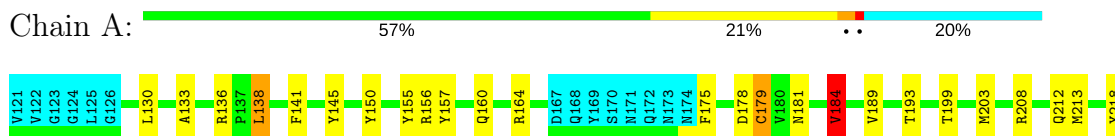
#### 4.2.1 Score per residue for model 1

- Molecule 1: prion protein



#### 4.2.2 Score per residue for model 2

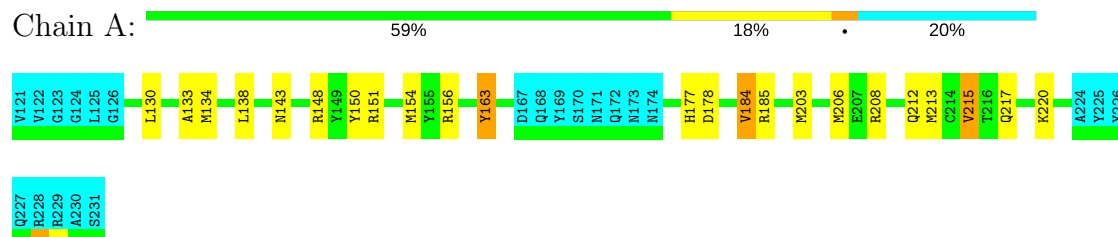
- Molecule 1: prion protein





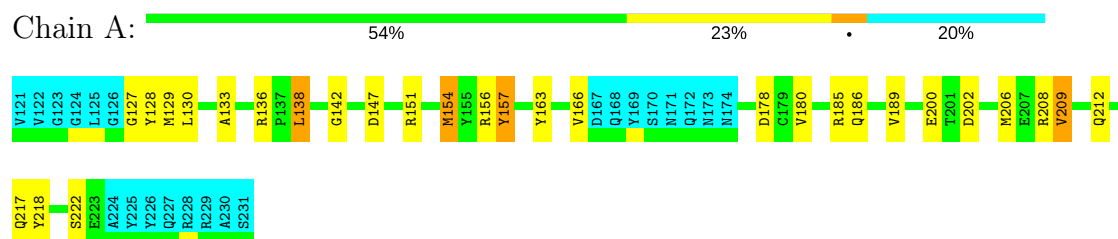
### 4.2.3 Score per residue for model 3

- Molecule 1: prion protein



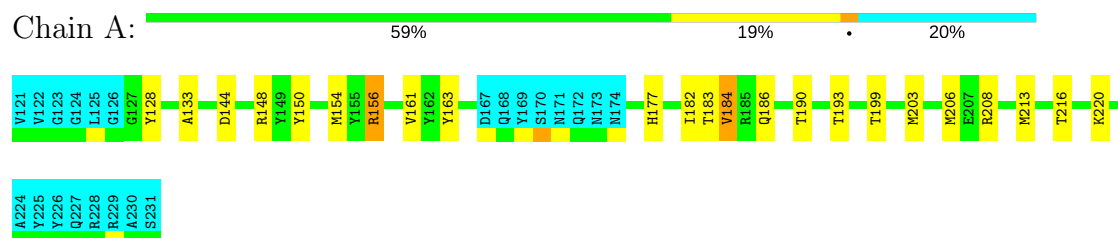
### 4.2.4 Score per residue for model 4

- Molecule 1: prion protein



### 4.2.5 Score per residue for model 5

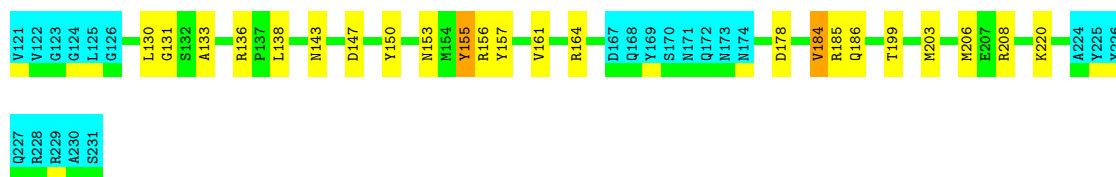
- Molecule 1: prion protein



### 4.2.6 Score per residue for model 6

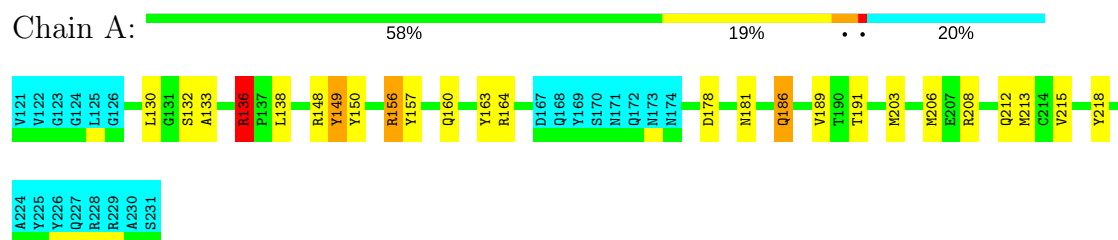
- Molecule 1: prion protein





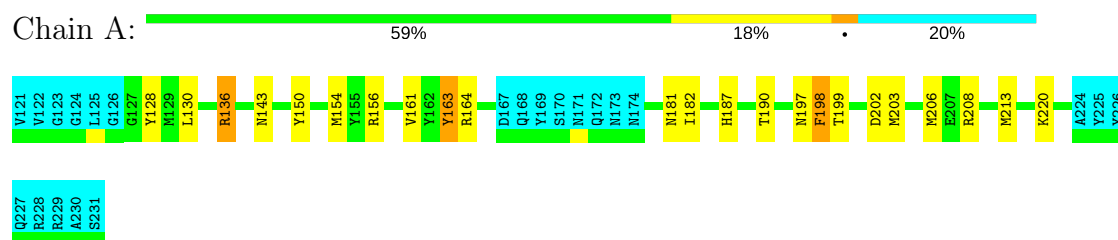
#### 4.2.7 Score per residue for model 7

- Molecule 1: prion protein



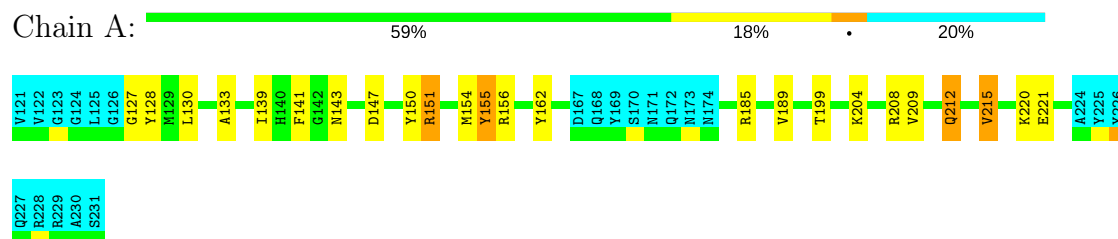
#### 4.2.8 Score per residue for model 8

- Molecule 1: prion protein



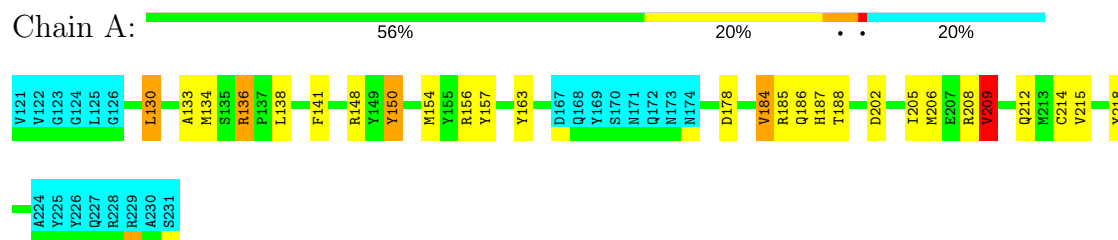
#### 4.2.9 Score per residue for model 9

- Molecule 1: prion protein



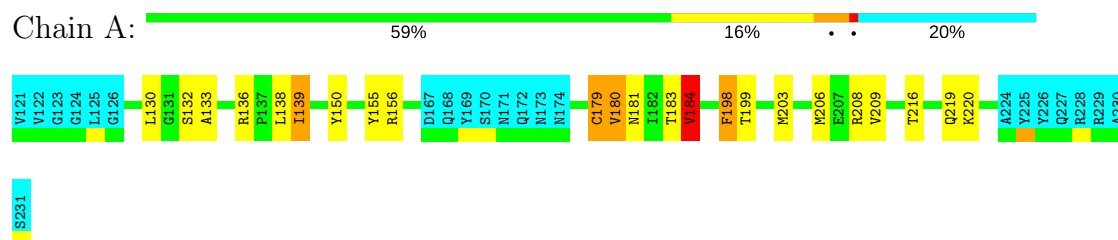
#### 4.2.10 Score per residue for model 10

- Molecule 1: prion protein



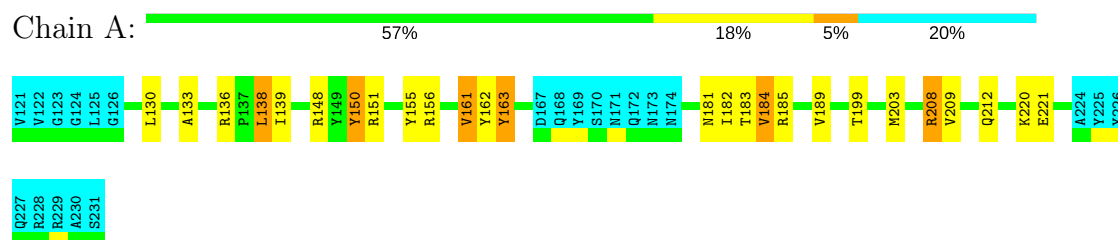
#### 4.2.11 Score per residue for model 11

- Molecule 1: prion protein



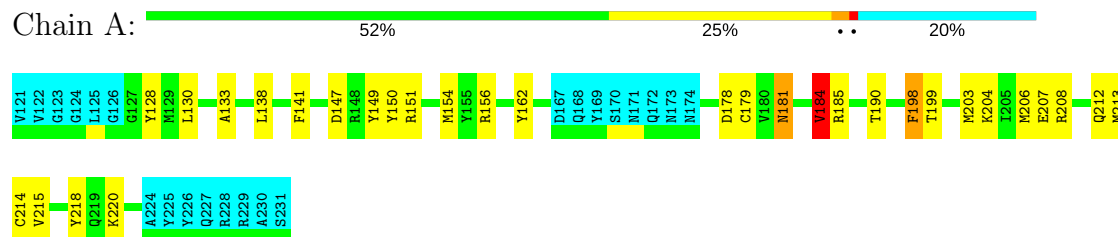
#### 4.2.12 Score per residue for model 12

- Molecule 1: prion protein



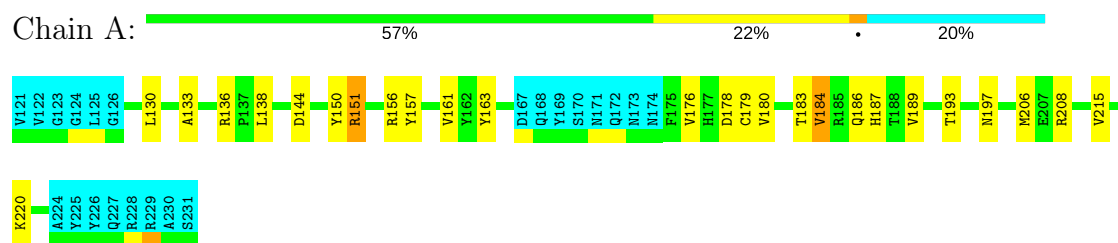
#### 4.2.13 Score per residue for model 13

- Molecule 1: prion protein



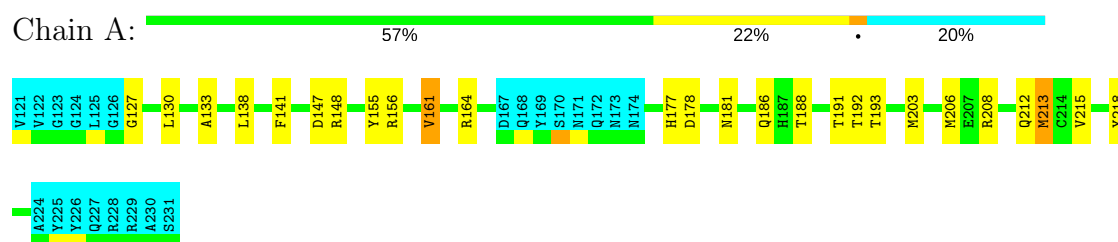
#### 4.2.14 Score per residue for model 14

- Molecule 1: prion protein



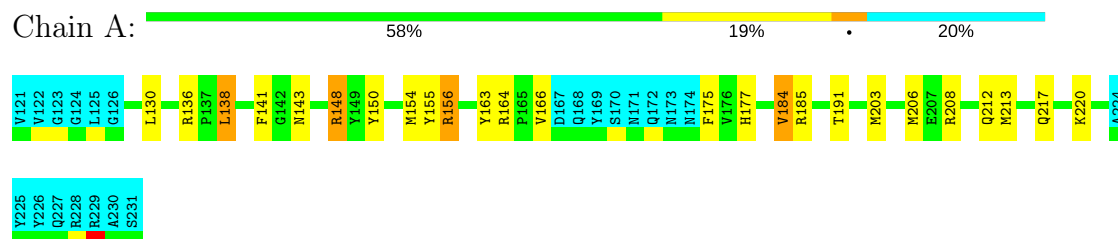
#### 4.2.15 Score per residue for model 15

- Molecule 1: prion protein



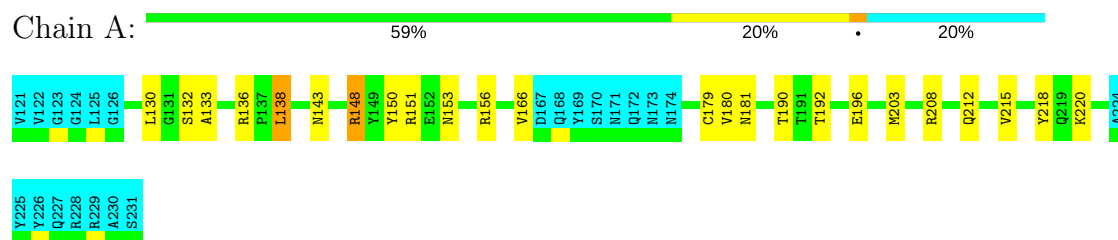
#### 4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: prion protein



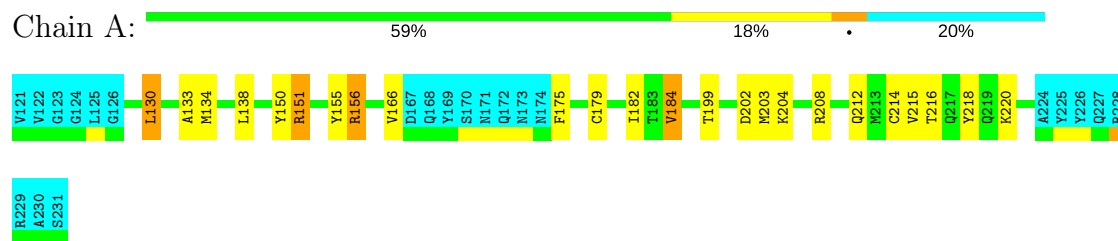
#### 4.2.17 Score per residue for model 17

- Molecule 1: prion protein



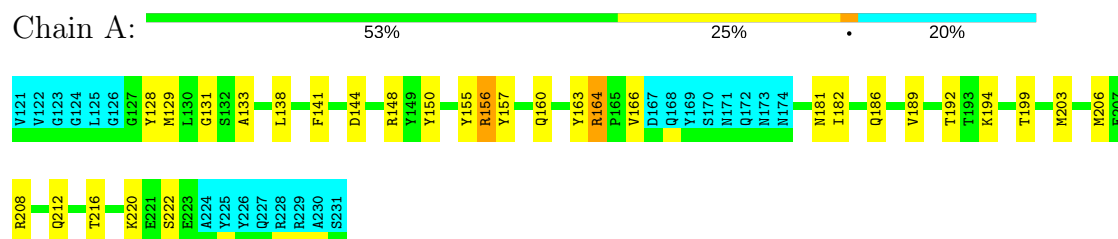
### 4.2.18 Score per residue for model 18

- Molecule 1: prion protein



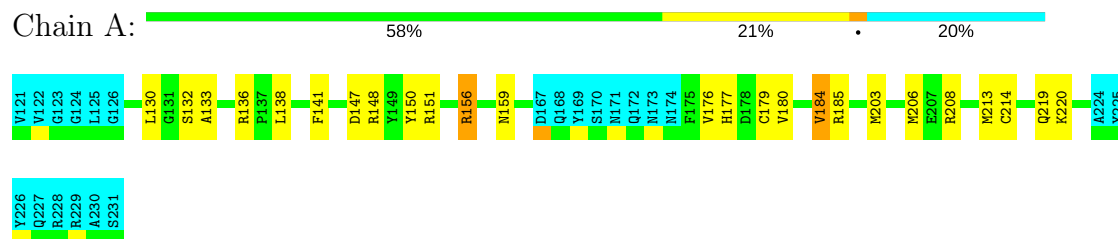
### 4.2.19 Score per residue for model 19

- Molecule 1: prion protein



### 4.2.20 Score per residue for model 20

- Molecule 1: prion protein



## 5 Refinement protocol and experimental data overview

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

Of the 20 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 6377
Number of chemical shift lists	1
Total number of shifts	1230
Number of shifts mapped to atoms	1220
Number of unparsed shifts	0
Number of shifts with mapping errors	10
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

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±0/768 (0.0±0.0%)	1.15±0.03	3±1/1039 (0.2±0.1%)
All	All	0.68	0/15360 (0.0%)	1.15	50/20780 (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	2.2±1.3
All	All	0	44

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	157	TYR	CB-CG-CD1	-9.11	115.54	121.00	7	1
1	A	184	VAL	CA-CB-CG2	8.52	123.69	110.90	18	9
1	A	180	VAL	CA-CB-CG2	7.51	122.16	110.90	14	5
1	A	148	ARG	CD-NE-CZ	7.18	133.66	123.60	16	1
1	A	209	VAL	CA-CB-CG2	7.06	121.49	110.90	10	2
1	A	185	ARG	NE-CZ-NH2	-6.82	116.89	120.30	1	1
1	A	151	ARG	NE-CZ-NH2	-6.47	117.06	120.30	1	3
1	A	164	ARG	NE-CZ-NH2	-6.41	117.09	120.30	1	4
1	A	141	PHE	CB-CG-CD2	-6.20	116.46	120.80	10	8
1	A	156	ARG	NE-CZ-NH2	-6.12	117.24	120.30	7	1
1	A	184	VAL	CA-CB-CG1	6.01	119.92	110.90	2	1
1	A	136	ARG	NE-CZ-NH2	-5.98	117.31	120.30	7	1
1	A	208	ARG	NE-CZ-NH2	-5.96	117.32	120.30	12	1
1	A	130	LEU	CB-CG-CD1	-5.95	100.88	111.00	18	1
1	A	157	TYR	CB-CA-C	5.91	122.22	110.40	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	208	ARG	CD-NE-CZ	5.82	131.75	123.60	12	1
1	A	148	ARG	NE-CZ-NH1	5.68	123.14	120.30	16	1
1	A	215	VAL	CA-CB-CG1	5.56	119.23	110.90	10	2
1	A	151	ARG	NE-CZ-NH1	5.47	123.03	120.30	18	1
1	A	164	ARG	NE-CZ-NH1	5.46	123.03	120.30	2	1
1	A	155	TYR	CB-CG-CD2	-5.25	117.85	121.00	6	1
1	A	163	TYR	CB-CG-CD2	-5.20	117.88	121.00	12	1
1	A	148	ARG	NE-CZ-NH2	-5.11	117.75	120.30	16	1
1	A	130	LEU	CB-CA-C	5.02	119.74	110.20	10	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	157	TYR	Sidechain	7
1	A	151	ARG	Sidechain	5
1	A	136	ARG	Sidechain	4
1	A	163	TYR	Sidechain,Peptide	4
1	A	128	TYR	Sidechain	3
1	A	162	TYR	Sidechain	2
1	A	148	ARG	Sidechain	2
1	A	149	TYR	Sidechain	2
1	A	218	TYR	Sidechain	2
1	A	164	ARG	Sidechain	2
1	A	156	ARG	Sidechain	2
1	A	177	HIS	Peptide	2
1	A	155	TYR	Sidechain	2
1	A	142	GLY	Peptide	1
1	A	196	GLU	Peptide	1
1	A	145	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	750	707	709	1±1
All	All	15000	14140	14180	23

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:161:VAL:HG12	1:A:183:THR:HG21	0.57	1.76	12	2
1:A:181:ASN:HA	1:A:184:VAL:HG13	0.56	1.76	2	3
1:A:139:ILE:HD11	1:A:209:VAL:HA	0.54	1.79	11	1
1:A:161:VAL:HG11	1:A:213:MET:HG3	0.53	1.79	15	2
1:A:166:VAL:HG13	1:A:218:TYR:CE1	0.50	2.42	18	1
1:A:139:ILE:HD12	1:A:141:PHE:CE1	0.49	2.42	9	1
1:A:212:GLN:HA	1:A:215:VAL:HG22	0.48	1.84	9	1
1:A:212:GLN:O	1:A:216:THR:HG22	0.48	2.08	18	1
1:A:139:ILE:HD11	1:A:209:VAL:HG23	0.47	1.87	9	2
1:A:139:ILE:CD1	1:A:209:VAL:HG23	0.46	2.39	12	1
1:A:180:VAL:O	1:A:184:VAL:HG22	0.46	2.11	11	1
1:A:212:GLN:HA	1:A:215:VAL:CG2	0.45	2.42	9	1
1:A:198:PHE:CD2	1:A:206:MET:SD	0.44	3.10	13	1
1:A:150:TYR:CG	1:A:205:ILE:HG21	0.43	2.47	10	1
1:A:205:ILE:O	1:A:209:VAL:HG22	0.43	2.13	10	1
1:A:130:LEU:C	1:A:130:LEU:HD12	0.43	2.33	7	1
1:A:128:TYR:CE2	1:A:182:ILE:HG13	0.41	2.50	8	1
1:A:130:LEU:HD13	1:A:160:GLN:HB3	0.41	1.91	7	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	89/111 (80%)	73±3 (82±4%)	13±3 (14±4%)	3±1 (4±1%)	7	34
All	All	1780/2220 (80%)	1455 (82%)	257 (14%)	68 (4%)	7	34

All 21 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	133	ALA	18
1	A	138	LEU	12
1	A	198	PHE	4
1	A	166	VAL	4
1	A	178	ASP	4
1	A	156	ARG	3
1	A	127	GLY	3
1	A	179	CYS	3
1	A	155	TYR	2
1	A	131	GLY	2
1	A	176	VAL	2
1	A	186	GLN	2
1	A	153	ASN	1
1	A	147	ASP	1
1	A	140	HIS	1
1	A	143	ASN	1
1	A	136	ARG	1
1	A	154	MET	1
1	A	161	VAL	1
1	A	184	VAL	1
1	A	194	LYS	1

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/101 (83%)	65±2 (77±2%)	19±2 (23±2%)	3	29
All	All	1680/2020 (83%)	1294 (77%)	386 (23%)	3	29

All 67 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	156	ARG	20
1	A	208	ARG	20
1	A	150	TYR	18
1	A	130	LEU	17

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Mol	Chain	Res	Type	Models (Total)
1	A	203	MET	16
1	A	220	LYS	16
1	A	206	MET	14
1	A	212	GLN	13
1	A	184	VAL	12
1	A	199	THR	11
1	A	136	ARG	11
1	A	138	LEU	10
1	A	148	ARG	10
1	A	185	ARG	9
1	A	154	MET	9
1	A	213	MET	8
1	A	215	VAL	8
1	A	163	TYR	8
1	A	181	ASN	7
1	A	189	VAL	7
1	A	186	GLN	7
1	A	178	ASP	6
1	A	179	CYS	6
1	A	155	TYR	6
1	A	151	ARG	6
1	A	147	ASP	5
1	A	143	ASN	5
1	A	218	TYR	5
1	A	190	THR	5
1	A	144	ASP	4
1	A	214	CYS	4
1	A	182	ILE	4
1	A	132	SER	4
1	A	202	ASP	4
1	A	193	THR	4
1	A	134	MET	3
1	A	192	THR	3
1	A	187	HIS	3
1	A	219	GLN	3
1	A	204	LYS	3
1	A	198	PHE	3
1	A	191	THR	3
1	A	161	VAL	3
1	A	177	HIS	3
1	A	175	PHE	3
1	A	216	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	164	ARG	3
1	A	217	GLN	3
1	A	222	SER	2
1	A	221	GLU	2
1	A	183	THR	2
1	A	128	TYR	2
1	A	209	VAL	2
1	A	197	ASN	2
1	A	160	GLN	2
1	A	188	THR	2
1	A	129	MET	2
1	A	157	TYR	1
1	A	159	ASN	1
1	A	162	TYR	1
1	A	149	TYR	1
1	A	135	SER	1
1	A	139	ILE	1
1	A	153	ASN	1
1	A	207	GLU	1
1	A	152	GLU	1
1	A	200	GLU	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 79% for the well-defined parts and 77% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 6377

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	1230
Number of shifts mapped to atoms	1220
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	3.91	0.005	1
A	2	SER	CA	57.9	0.1	1
A	1	GLY	CA	43.1	0.1	1
A	2	SER	N	115.8	0.1	1
A	2	SER	CB	63.9	0.1	1
A	2	SER	HB3	3.84	0.005	1
A	2	SER	H	8.67	0.005	1
A	2	SER	HB2	3.84	0.005	1
A	2	SER	HA	4.59	0.005	1
A	1	GLY	HA3	3.91	0.005	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
$^{13}\text{C}_\alpha$	106	$-0.23 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	96	$0.24 \pm 0.21$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	104	$-0.04 \pm 0.15$	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 79%, i.e. 912 atoms were assigned a chemical shift out of a possible 1153. 11 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	345/439 (79%)	173/175 (99%)	87/178 (49%)	85/86 (99%)
Sidechain	483/594 (81%)	303/350 (87%)	165/210 (79%)	15/34 (44%)
Aromatic	84/120 (70%)	55/63 (87%)	29/54 (54%)	0/3 (0%)
Overall	912/1153 (79%)	531/588 (90%)	281/442 (64%)	100/123 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1089 atoms were assigned a chemical shift out of a possible 1418. 14 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	418/549 (76%)	211/219 (96%)	104/222 (47%)	103/108 (95%)
Sidechain	569/725 (78%)	358/427 (84%)	189/252 (75%)	22/46 (48%)
Aromatic	102/144 (71%)	67/75 (89%)	35/66 (53%)	0/3 (0%)
Overall	1089/1418 (77%)	636/721 (88%)	328/540 (61%)	125/157 (80%)

### 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:

