



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 01:58 AM BST

PDB ID : 2LV1
Title : Solution-state NMR structure of prion protein mutant V210I at neutral pH
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Deposited on : 2012-06-26

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

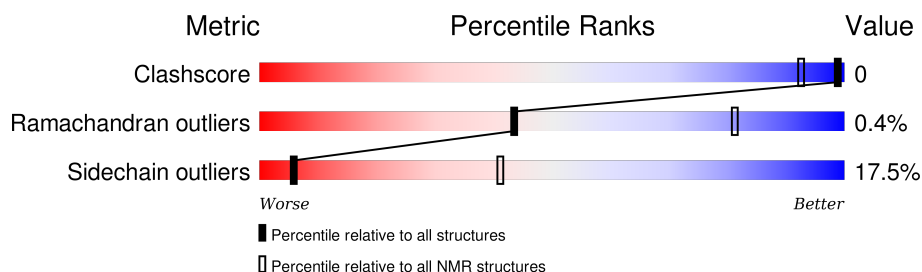
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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	147	<div> <div>48%</div> <div>10%</div> <div>43%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:128-A:163, A:173-A:220 (84)	0.18	11

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 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2254 atoms, of which 1091 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	147	Total	C	H	N	O	S	0
			2254	715	1091	209	227	12	

There are 6 discrepancies between the modelled and reference sequences:

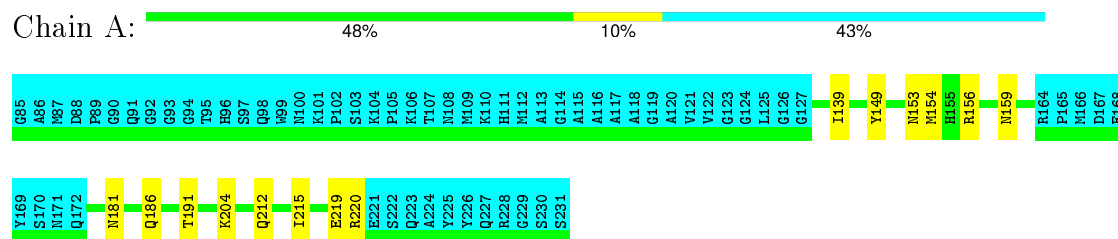
Chain	Residue	Modelled	Actual	Comment	Reference
A	85	GLY	-	EXPRESSION TAG	UNP P04156
A	86	ALA	-	EXPRESSION TAG	UNP P04156
A	87	MET	-	EXPRESSION TAG	UNP P04156
A	88	ASP	-	EXPRESSION TAG	UNP P04156
A	89	PRO	-	EXPRESSION TAG	UNP P04156
A	210	ILE	VAL	ENGINEERED MUTATION	UNP P04156

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

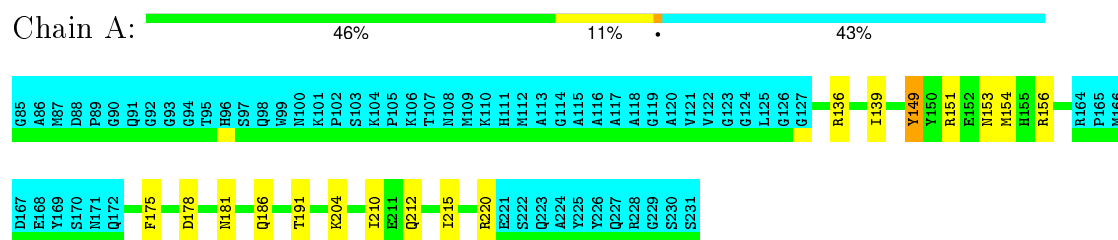


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

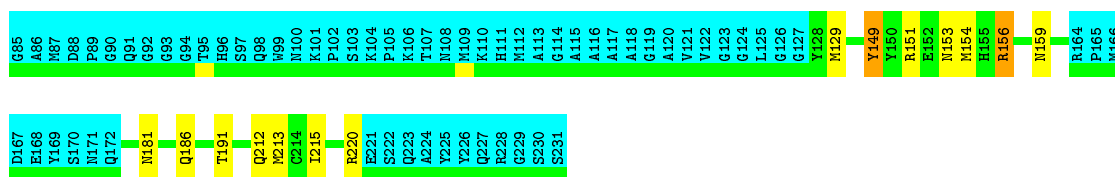
- Molecule 1: Major prion protein



4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein

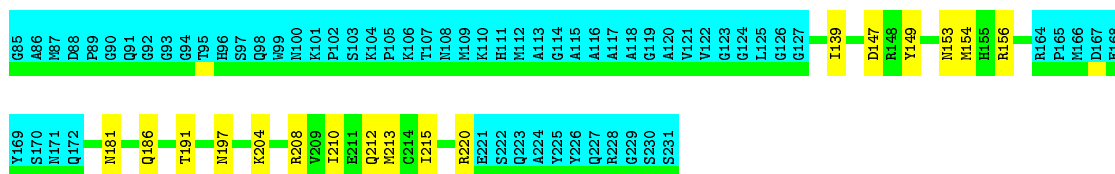




4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein

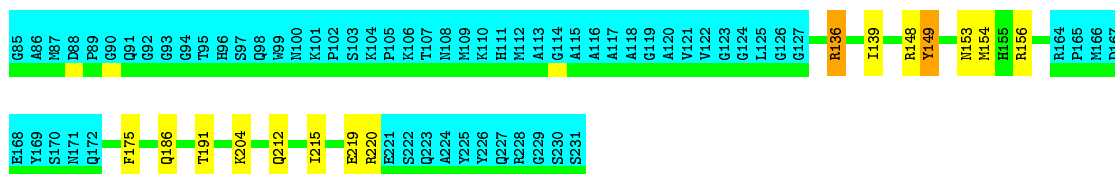
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein

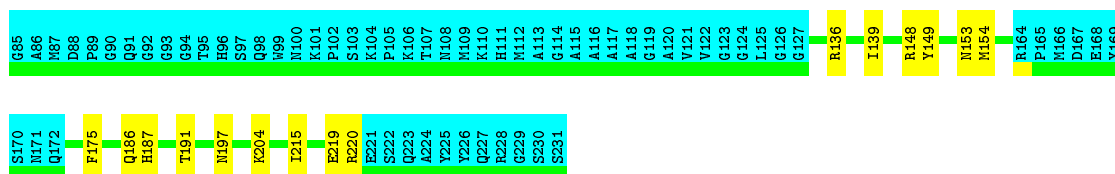
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein

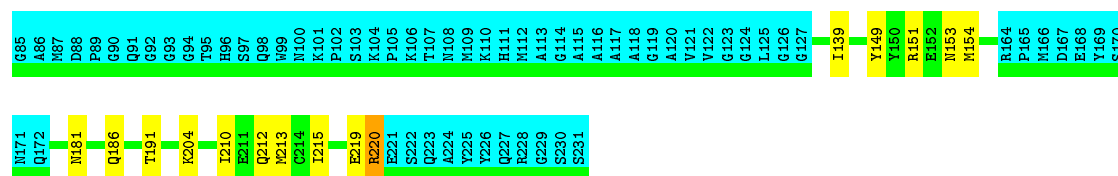
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein

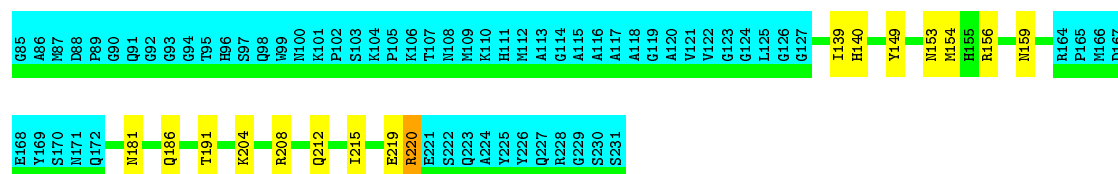
Chain A: 



4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein

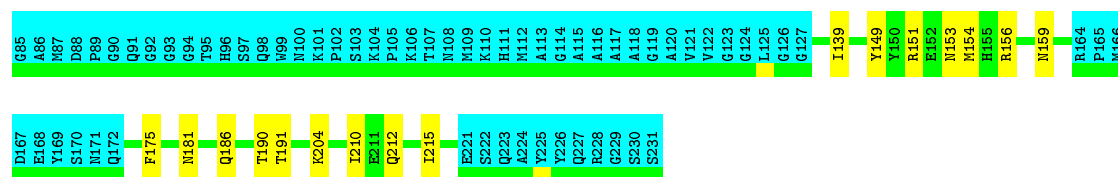
Chain A: 



4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein

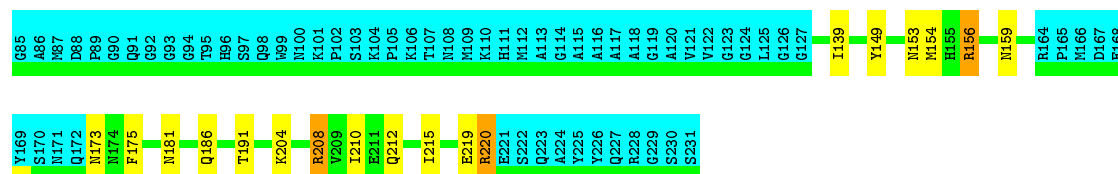
Chain A: 



4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein

Chain A: 



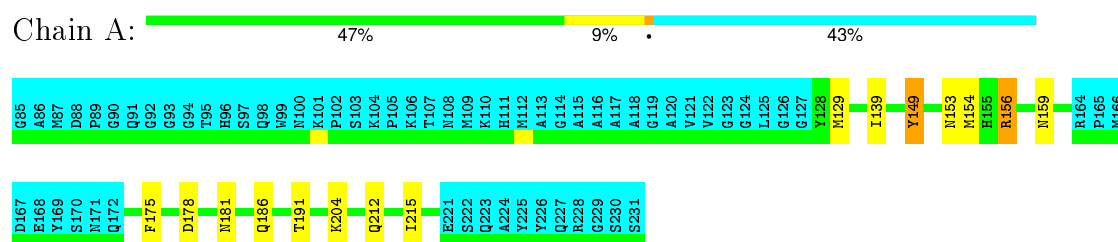
4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Major prion protein



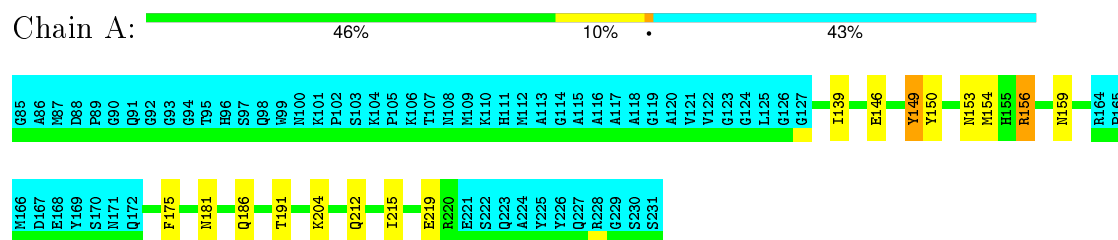
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



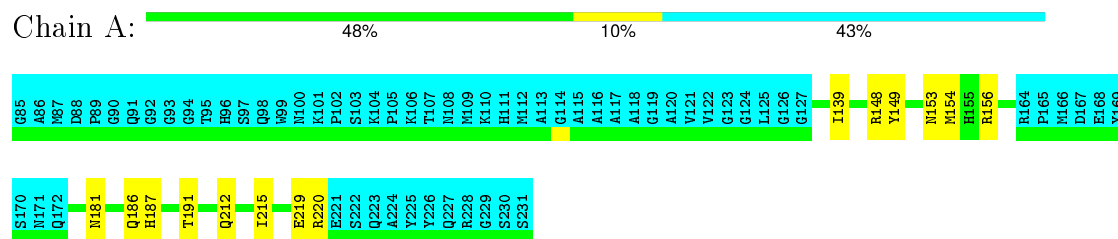
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



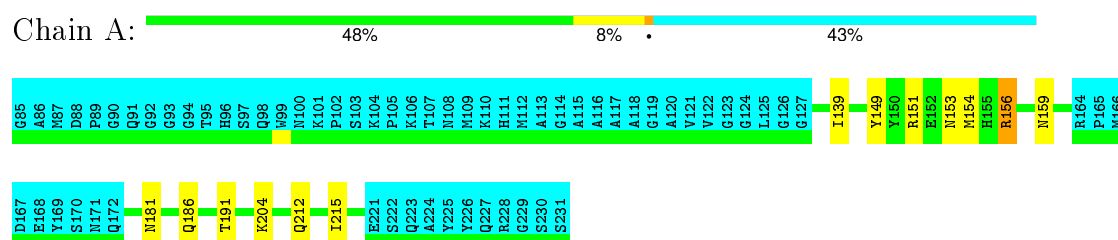
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



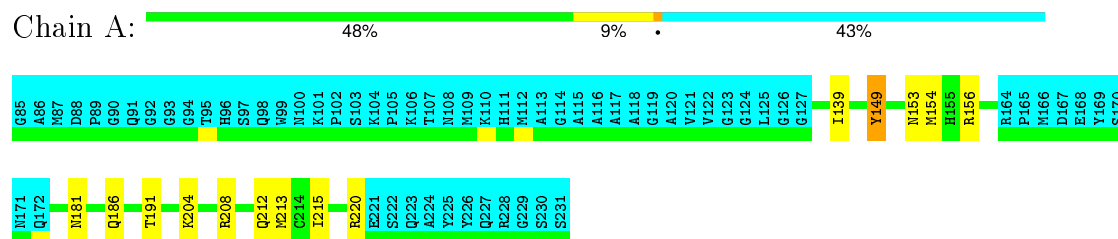
4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



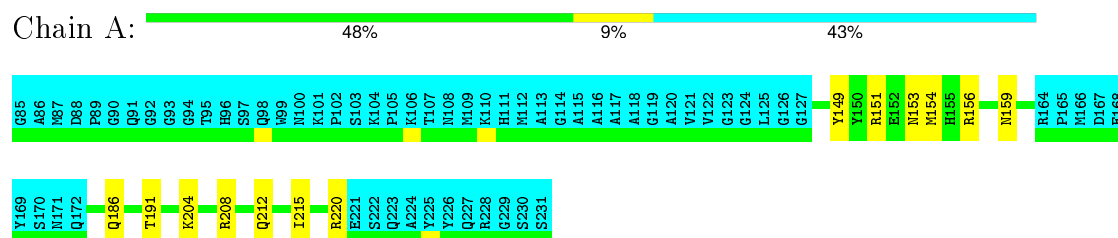
4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein



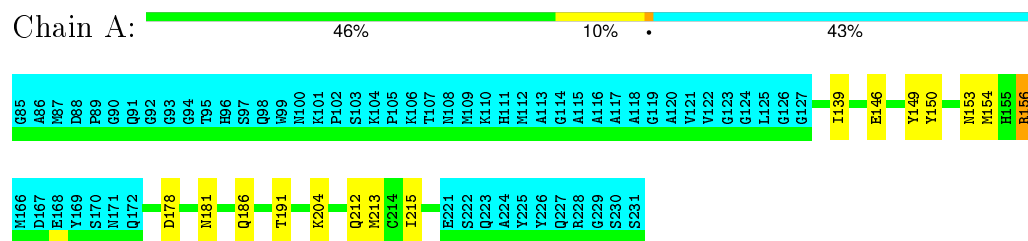
4.2.17 Score per residue for model 17

- Molecule 1: Major prion protein



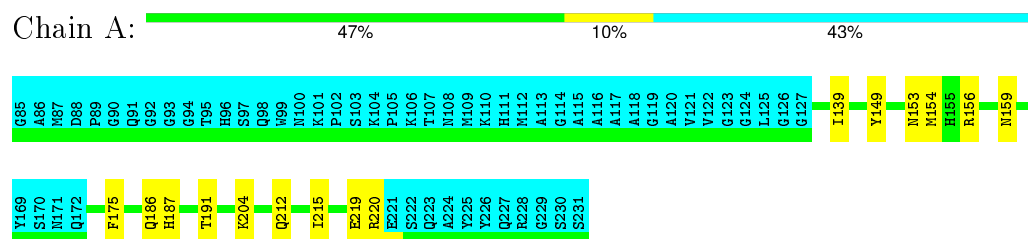
4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



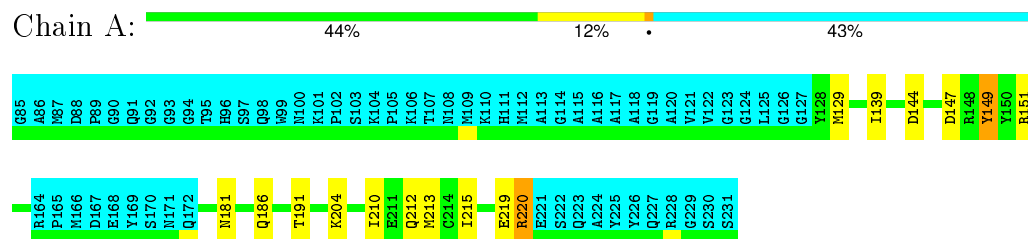
4.2.19 Score per residue for model 19

- 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: *molecular dynamics, simulated annealing*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	3.0
YASARA	geometry optimization	
YASARA	refinement	
CYANA	refinement	3.0

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)	2lv1_cs.str
Number of chemical shift lists	1
Total number of shifts	1507
Number of shifts mapped to atoms	1507
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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

6 Model quality

6.1 Standard geometry

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	0.75±0.02	0±0/728 (0.0±0.0%)	0.76±0.02	2±1/984 (0.2±0.1%)
All	All	0.75	0/14560 (0.0%)	0.76	37/19680 (0.2%)

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	220	ARG	NE-CZ-NH1	6.53	123.56	120.30	9	7
1	A	208	ARG	NE-CZ-NH1	6.19	123.39	120.30	7	6
1	A	151	ARG	NE-CZ-NH1	5.99	123.30	120.30	20	8
1	A	156	ARG	NE-CZ-NH1	5.93	123.27	120.30	3	11
1	A	148	ARG	NE-CZ-NH1	5.68	123.14	120.30	4	3
1	A	136	ARG	NE-CZ-NH1	5.52	123.06	120.30	4	2

There are no chirality outliers.

There are no planarity outliers.

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	711	669	669	0±0
All	All	14220	13380	13380	3

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:GLN:HA	1:A:217:GLN:HE21	0.47	1.69	12	1
1:A:146:GLU:HA	1:A:150:TYR:HB3	0.42	1.91	13	2

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	84/147 (57%)	81±1 (96±1%)	3±1 (3±1%)	0±0 (0±1%)	43	81
All	All	1680/2940 (57%)	1620 (96%)	53 (3%)	7 (0%)	43	81

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	149	TYR	7

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	80/123 (65%)	66±2 (82±2%)	14±2 (18±2%)	6	41
All	All	1600/2460 (65%)	1320 (82%)	280 (18%)	6	41

All 29 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	153	ASN	20
1	A	149	TYR	20

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Mol	Chain	Res	Type	Models (Total)
1	A	186	GLN	20
1	A	191	THR	20
1	A	154	MET	20
1	A	215	ILE	20
1	A	212	GLN	19
1	A	204	LYS	18
1	A	139	ILE	17
1	A	181	ASN	16
1	A	220	ARG	12
1	A	156	ARG	12
1	A	219	GLU	11
1	A	159	ASN	11
1	A	175	PHE	9
1	A	213	MET	6
1	A	210	ILE	6
1	A	187	HIS	4
1	A	136	ARG	3
1	A	129	MET	3
1	A	178	ASP	3
1	A	147	ASP	2
1	A	197	ASN	2
1	A	140	HIS	1
1	A	173	ASN	1
1	A	144	ASP	1
1	A	208	ARG	1
1	A	190	THR	1
1	A	217	GLN	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 81% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: 2lv1_cs.str

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	1507
Number of shifts mapped to atoms	1507
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
$^{13}\text{C}_\alpha$	136	-0.17 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	126	0.11 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	118	-0.11 ± 0.13	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 81%, i.e. 881 atoms were assigned a chemical shift out of a possible 1092. 7 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	326/416 (78%)	163/166 (98%)	82/168 (49%)	81/82 (99%)
Sidechain	458/557 (82%)	287/328 (88%)	161/198 (81%)	10/31 (32%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	97/119 (82%)	50/63 (79%)	47/52 (90%)	0/4 (0%)
Overall	881/1092 (81%)	500/557 (90%)	290/418 (69%)	91/117 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1344 atoms were assigned a chemical shift out of a possible 1779. 10 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	508/723 (70%)	254/288 (88%)	136/294 (46%)	118/141 (84%)
Sidechain	711/887 (80%)	448/527 (85%)	250/311 (80%)	13/49 (27%)
Aromatic	125/169 (74%)	64/89 (72%)	60/73 (82%)	1/7 (14%)
Overall	1344/1779 (76%)	766/904 (85%)	446/678 (66%)	132/197 (67%)

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:

