



Full wwPDB NMR Structure Validation Report ⓘ

Jul 18, 2016 – 04:12 PM EDT

PDB ID : 2MV9
Title : Solution structure of Ovis Aries PrP with mutation delta193-196
Authors : Munoz, C.; Egalon, A.; Beringue, V.; Rezaei, H.; Dron, M.; Sizun, C.
Deposited on : 2014-09-25

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-20027790
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

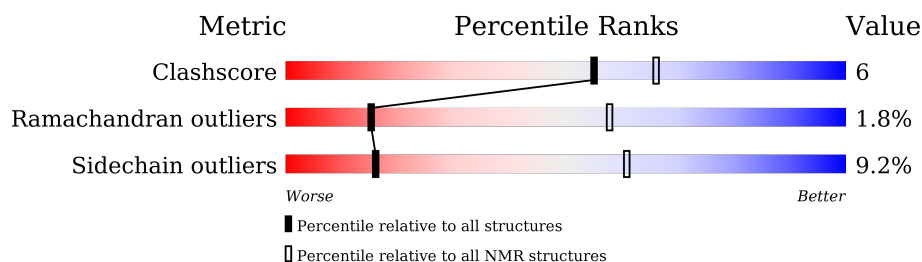
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 56%.

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	150	

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:192, A:197-A:229 (98)	0.53	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 5 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2174 atoms, of which 1064 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	139	Total	C	H	N	O	S	0
			2174	690	1064	202	209	9	

There are 26 discrepancies between the modelled and reference sequences:

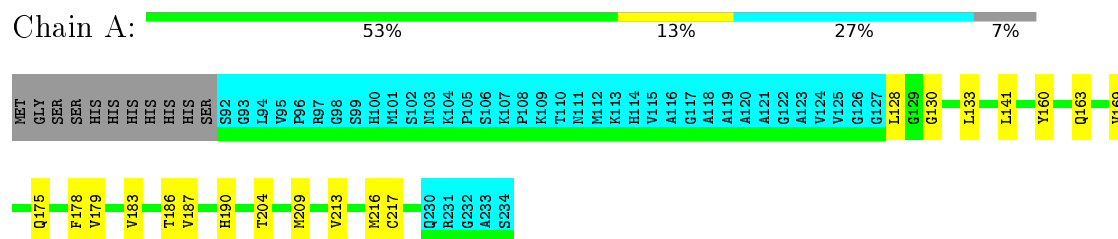
Chain	Residue	Modelled	Actual	Comment	Reference
A	81	MET	-	EXPRESSION TAG	UNP Q712V9
A	82	GLY	-	EXPRESSION TAG	UNP Q712V9
A	83	SER	-	EXPRESSION TAG	UNP Q712V9
A	84	SER	-	EXPRESSION TAG	UNP Q712V9
A	85	HIS	-	EXPRESSION TAG	UNP Q712V9
A	86	HIS	-	EXPRESSION TAG	UNP Q712V9
A	87	HIS	-	EXPRESSION TAG	UNP Q712V9
A	88	HIS	-	EXPRESSION TAG	UNP Q712V9
A	89	HIS	-	EXPRESSION TAG	UNP Q712V9
A	90	HIS	-	EXPRESSION TAG	UNP Q712V9
A	91	SER	-	EXPRESSION TAG	UNP Q712V9
A	92	SER	-	EXPRESSION TAG	UNP Q712V9
A	93	GLY	-	EXPRESSION TAG	UNP Q712V9
A	94	LEU	-	EXPRESSION TAG	UNP Q712V9
A	95	VAL	-	EXPRESSION TAG	UNP Q712V9
A	96	PRO	-	EXPRESSION TAG	UNP Q712V9
A	97	ARG	-	EXPRESSION TAG	UNP Q712V9
A	98	GLY	-	EXPRESSION TAG	UNP Q712V9
A	99	SER	-	EXPRESSION TAG	UNP Q712V9
A	100	HIS	-	EXPRESSION TAG	UNP Q712V9
A	101	MET	-	EXPRESSION TAG	UNP Q712V9
A	102	SER	-	EXPRESSION TAG	UNP Q712V9
A	?	-	THR	DELETION	UNP Q712V9
A	?	-	THR	DELETION	UNP Q712V9
A	?	-	THR	DELETION	UNP Q712V9
A	?	-	THR	DELETION	UNP Q712V9

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: Major prion protein

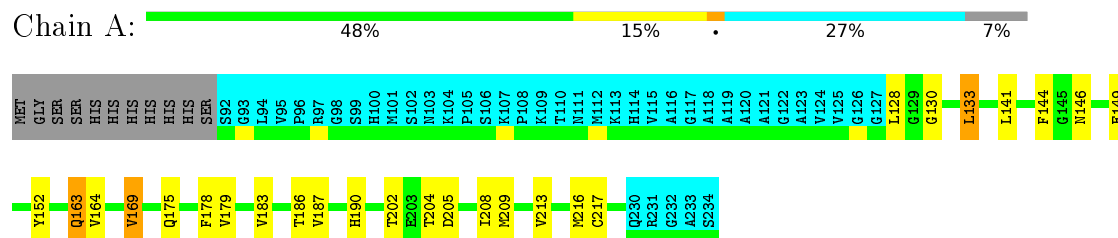


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

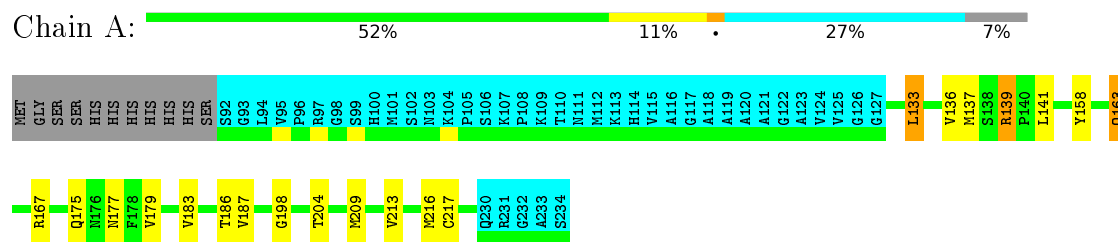
- Molecule 1: Major prion protein



4.2.2 Score per residue for model 2

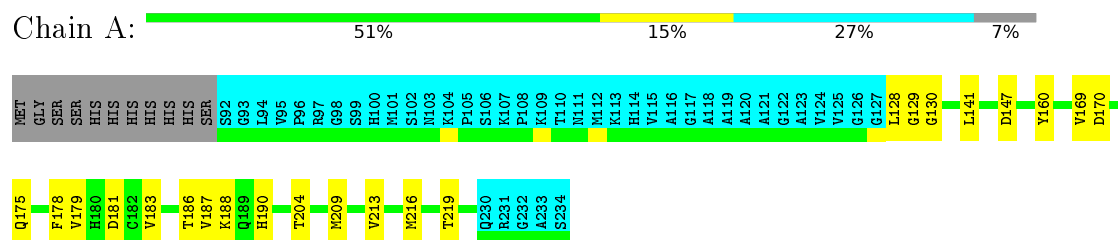
- Molecule 1: Major prion protein





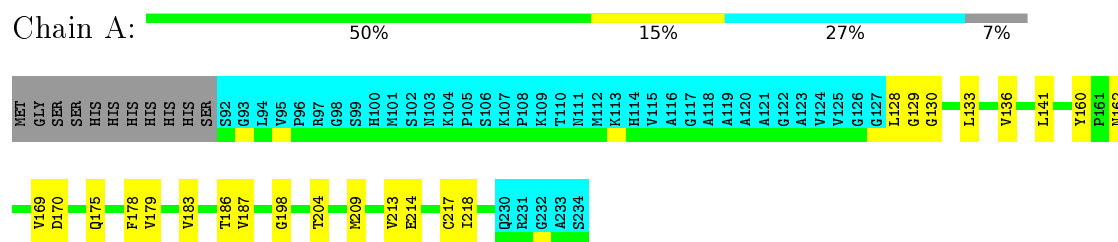
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



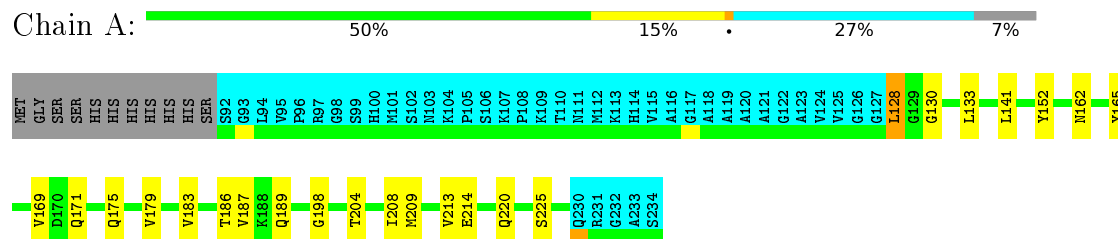
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



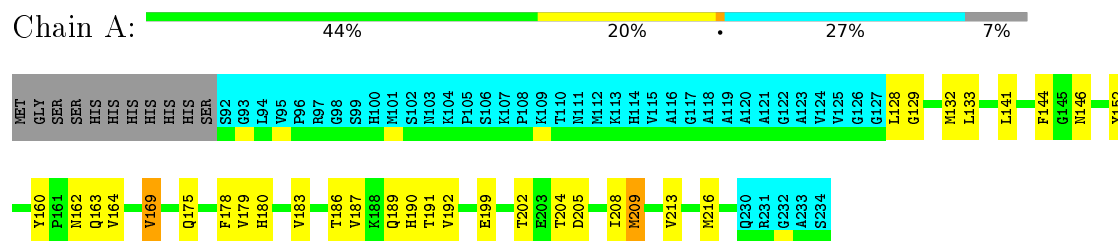
4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



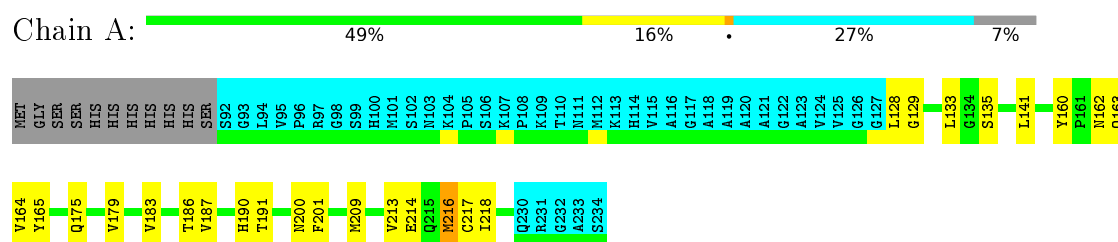
4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



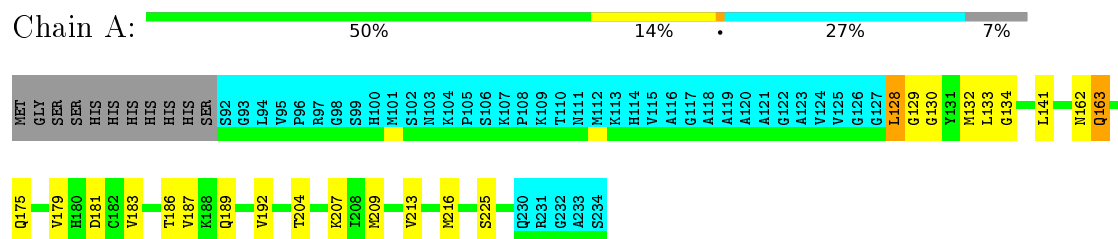
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



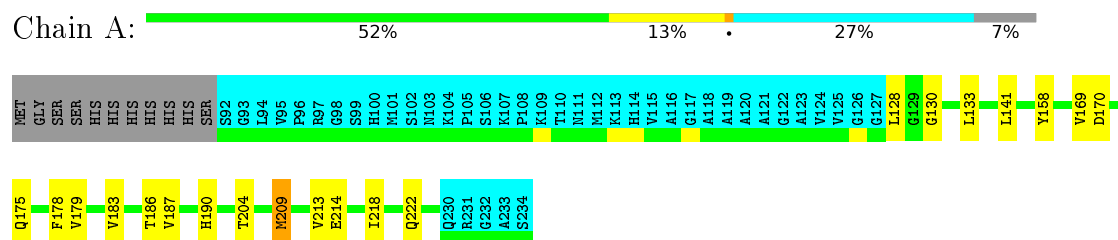
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



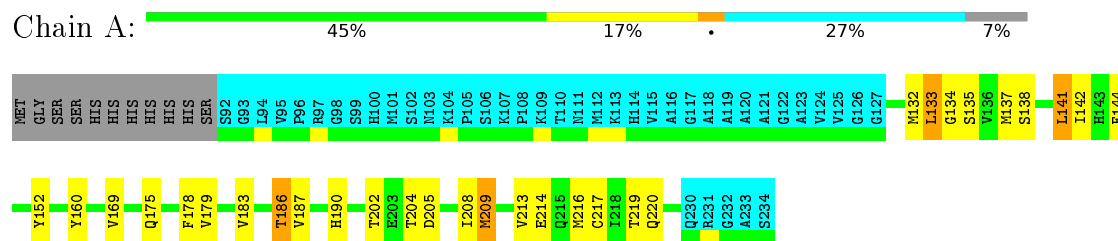
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



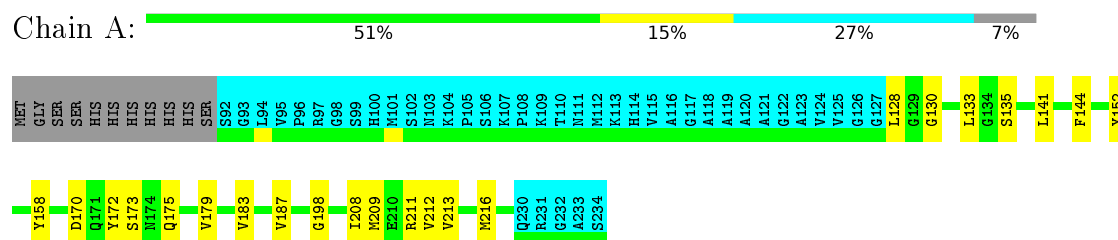
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



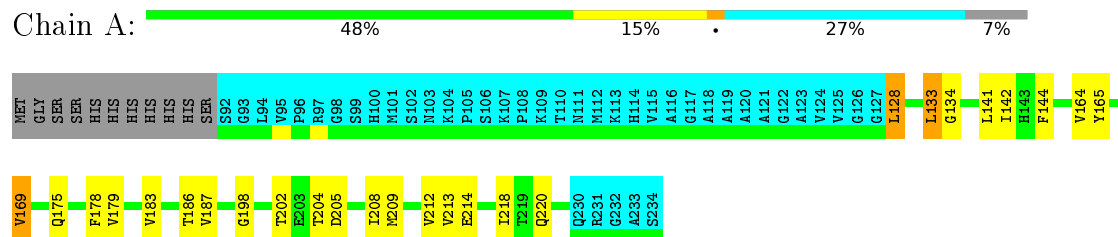
4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



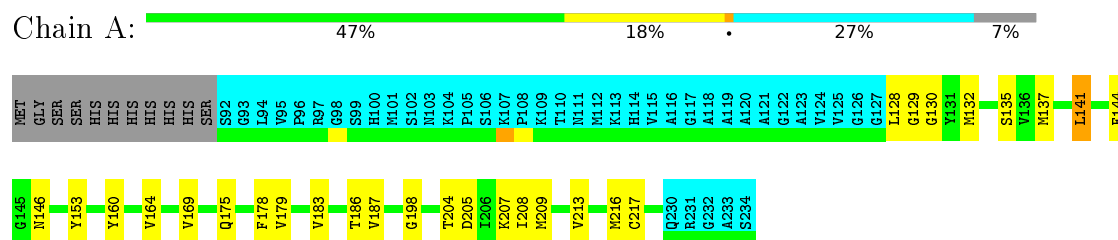
4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein



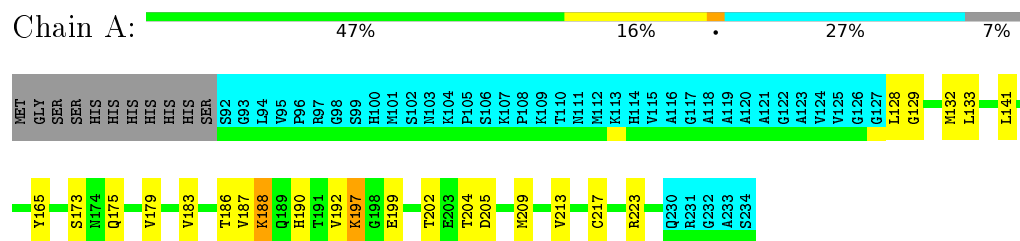
4.2.17 Score per residue for model 17

- Molecule 1: Major prion protein



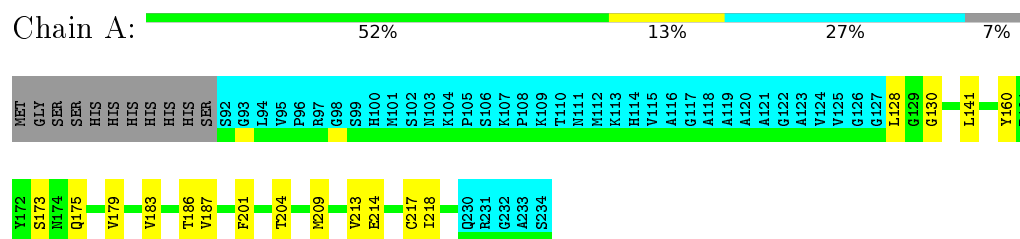
4.2.18 Score per residue for model 18

- 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
CYANA	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)	2mv9_cs.cif
Number of chemical shift lists	1
Total number of shifts	1072
Number of shifts mapped to atoms	1072
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	56%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	834	778	778	10±3
All	All	16680	15560	15560	209

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:VAL:O	1:A:187:VAL:HG23	0.63	1.93	15	16
1:A:209:MET:O	1:A:213:VAL:HG23	0.62	1.94	16	20
1:A:169:VAL:HG12	1:A:178:PHE:CE2	0.62	2.29	13	11
1:A:186:THR:CG2	1:A:213:VAL:HG13	0.60	2.26	19	3
1:A:183:VAL:HG13	1:A:213:VAL:CG1	0.60	2.27	16	2
1:A:183:VAL:HG11	1:A:214:GLU:OE2	0.60	1.95	9	2
1:A:179:VAL:HG13	1:A:217:CYS:HB3	0.60	1.73	17	10
1:A:186:THR:HG21	1:A:213:VAL:HG13	0.59	1.74	10	12
1:A:191:THR:HG22	1:A:199:GLU:O	0.58	1.97	2	2
1:A:188:LYS:O	1:A:192:VAL:HG23	0.58	1.99	18	1
1:A:141:LEU:HD11	1:A:153:TYR:OH	0.58	1.99	17	1
1:A:164:VAL:HG23	1:A:186:THR:OG1	0.57	1.99	16	2
1:A:128:LEU:HD13	1:A:165:TYR:CE2	0.56	2.35	16	2
1:A:202:THR:HG22	1:A:205:ASP:OD2	0.56	2.00	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:LEU:HD12	1:A:129:GLY:N	0.56	2.15	11	7
1:A:212:VAL:HG22	1:A:216:MET:CE	0.56	2.31	15	1
1:A:144:PHE:CE1	1:A:208:ILE:HG23	0.56	2.35	16	3
1:A:152:TYR:CD1	1:A:208:ILE:HD12	0.56	2.35	15	5
1:A:175:GLN:O	1:A:179:VAL:HG23	0.54	2.01	10	19
1:A:186:THR:HG22	1:A:190:HIS:CD2	0.54	2.38	14	1
1:A:164:VAL:HG11	1:A:216:MET:CG	0.54	2.32	2	2
1:A:133:LEU:HD13	1:A:134:GLY:N	0.53	2.18	14	4
1:A:164:VAL:HG21	1:A:216:MET:HG3	0.53	1.81	17	3
1:A:169:VAL:HG12	1:A:178:PHE:CE1	0.53	2.38	14	1
1:A:153:TYR:CE1	1:A:212:VAL:HG21	0.53	2.38	5	1
1:A:189:GLN:O	1:A:192:VAL:HG12	0.53	2.03	12	4
1:A:144:PHE:CZ	1:A:208:ILE:HG23	0.52	2.39	5	5
1:A:133:LEU:HD23	1:A:134:GLY:N	0.51	2.20	12	1
1:A:146:ASN:ND2	1:A:149:GLU:H	0.51	2.04	1	2
1:A:136:VAL:HG23	1:A:139:ARG:HG2	0.50	1.83	6	1
1:A:133:LEU:HD11	1:A:163:GLN:CG	0.50	2.36	6	1
1:A:144:PHE:CE2	1:A:208:ILE:HG23	0.50	2.41	1	2
1:A:133:LEU:HD21	1:A:163:GLN:CD	0.49	2.27	6	1
1:A:202:THR:HG23	1:A:205:ASP:H	0.49	1.67	10	7
1:A:169:VAL:HG21	1:A:225:SER:HA	0.49	1.85	9	1
1:A:133:LEU:HD12	1:A:163:GLN:HG2	0.48	1.84	2	1
1:A:183:VAL:O	1:A:187:VAL:HG13	0.48	2.08	17	3
1:A:186:THR:HG21	1:A:216:MET:CE	0.48	2.38	12	1
1:A:169:VAL:HG11	1:A:221:TYR:CD1	0.48	2.43	3	2
1:A:212:VAL:HG22	1:A:216:MET:HE2	0.48	1.84	15	1
1:A:164:VAL:HG11	1:A:216:MET:HG3	0.48	1.86	3	3
1:A:179:VAL:HG13	1:A:217:CYS:CB	0.47	2.40	5	3
1:A:128:LEU:HD13	1:A:165:TYR:CD2	0.47	2.45	5	1
1:A:133:LEU:HD11	1:A:163:GLN:NE2	0.46	2.25	12	1
1:A:142:ILE:HD13	1:A:144:PHE:CZ	0.46	2.46	14	1
1:A:133:LEU:HD11	1:A:163:GLN:HG3	0.46	1.87	6	1
1:A:183:VAL:HG13	1:A:213:VAL:HG12	0.46	1.88	4	2
1:A:133:LEU:HD11	1:A:165:TYR:CE1	0.45	2.46	11	1
1:A:133:LEU:HD12	1:A:163:GLN:CG	0.45	2.41	2	1
1:A:186:THR:HG21	1:A:216:MET:HE1	0.45	1.89	12	1
1:A:141:LEU:HA	1:A:219:THR:HG21	0.45	1.87	14	1
1:A:142:ILE:HD12	1:A:212:VAL:HA	0.44	1.89	4	3
1:A:183:VAL:HG13	1:A:213:VAL:HG11	0.44	1.89	16	1
1:A:164:VAL:HG11	1:A:216:MET:CE	0.44	2.42	10	1
1:A:183:VAL:O	1:A:187:VAL:HG22	0.44	2.13	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:PHE:HE1	1:A:208:ILE:HG23	0.43	1.74	16	1
1:A:133:LEU:HD21	1:A:163:GLN:NE2	0.43	2.28	6	1
1:A:133:LEU:HD21	1:A:163:GLN:OE1	0.42	2.14	10	1
1:A:133:LEU:HD12	1:A:163:GLN:NE2	0.42	2.29	11	1
1:A:214:GLU:O	1:A:218:ILE:HD12	0.42	2.15	16	6
1:A:183:VAL:O	1:A:187:VAL:HG12	0.41	2.15	19	1
1:A:169:VAL:HG13	1:A:224:GLU:HB3	0.41	1.92	20	2
1:A:133:LEU:HD13	1:A:165:TYR:CD2	0.41	2.49	18	1
1:A:133:LEU:HD11	1:A:163:GLN:CD	0.41	2.36	4	1
1:A:136:VAL:HG23	1:A:139:ARG:HD3	0.41	1.91	6	1
1:A:190:HIS:CE1	1:A:213:VAL:HG22	0.40	2.51	20	1
1:A:164:VAL:HG21	1:A:216:MET:CG	0.40	2.46	17	1
1:A:187:VAL:O	1:A:191:THR:HG23	0.40	2.17	11	1
1:A:164:VAL:HG11	1:A:216:MET:HG2	0.40	1.93	1	1
1:A:133:LEU:HD21	1:A:163:GLN:HE21	0.40	1.76	1	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	98/150 (65%)	88±2 (90±2%)	8±2 (8±2%)	2±1 (2±1%)	15	58
All	All	1960/3000 (65%)	1760 (90%)	165 (8%)	35 (2%)	15	58

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	130	GLY	11
1	A	198	GLY	8
1	A	169	VAL	6
1	A	173	SER	3
1	A	134	GLY	2
1	A	197	LYS	1
1	A	136	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	132	MET	1
1	A	129	GLY	1
1	A	135	SER	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	92/129 (71%)	84±3 (91±3%)	8±3 (9±3%)	16	61
All	All	1840/2580 (71%)	1671 (91%)	169 (9%)	16	61

All 44 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	141	LEU	20
1	A	204	THR	17
1	A	133	LEU	12
1	A	160	TYR	11
1	A	128	LEU	9
1	A	190	HIS	9
1	A	162	ASN	7
1	A	132	MET	5
1	A	170	ASP	5
1	A	135	SER	4
1	A	216	MET	4
1	A	163	GLN	4
1	A	137	MET	3
1	A	197	LYS	3
1	A	171	GLN	3
1	A	220	GLN	3
1	A	158	TYR	3
1	A	225	SER	3
1	A	146	ASN	3
1	A	209	MET	3
1	A	207	LYS	3
1	A	173	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	A	167	ARG	3
1	A	181	ASP	2
1	A	201	PHE	2
1	A	138	SER	2
1	A	205	ASP	2
1	A	214	GLU	2
1	A	188	LYS	2
1	A	139	ARG	2
1	A	186	THR	2
1	A	219	THR	1
1	A	189	GLN	1
1	A	200	ASN	1
1	A	149	GLU	1
1	A	211	ARG	1
1	A	147	ASP	1
1	A	172	TYR	1
1	A	222	GLN	1
1	A	177	ASN	1
1	A	223	ARG	1
1	A	199	GLU	1
1	A	154	ARG	1
1	A	180	HIS	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 56% for the well-defined parts and 54% for the entire structure.

7.1 Chemical shift list 1

File name: 2mv9_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	1072
Number of shifts mapped to atoms	1072
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
$^{13}\text{C}_\alpha$	138	-0.21 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	0	—	—
^{15}N	130	0.03 ± 0.20	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 56%, i.e. 719 atoms were assigned a chemical shift out of a possible 1285. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	368/484 (76%)	183/193 (95%)	94/196 (48%)	91/95 (96%)
Sidechain	294/657 (45%)	279/388 (72%)	0/229 (0%)	15/40 (38%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	57/144 (40%)	57/75 (76%)	0/66 (0%)	0/3 (0%)
Overall	719/1285 (56%)	519/656 (79%)	94/491 (19%)	106/138 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 54%, i.e. 937 atoms were assigned a chemical shift out of a possible 1725. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	526/683 (77%)	262/272 (96%)	135/278 (49%)	129/133 (97%)
Sidechain	354/884 (40%)	338/524 (65%)	0/307 (0%)	16/53 (30%)
Aromatic	57/158 (36%)	57/83 (69%)	0/70 (0%)	0/5 (0%)
Overall	937/1725 (54%)	657/879 (75%)	135/655 (21%)	145/191 (76%)

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:

