



Full wwPDB NMR Structure Validation Report ⓘ

Dec 19, 2023 – 02:56 AM EST

PDB ID : 2MV8
BMRB ID : 25250
Title : Solution structure of Ovis Aries PrP with mutation delta190-197
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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

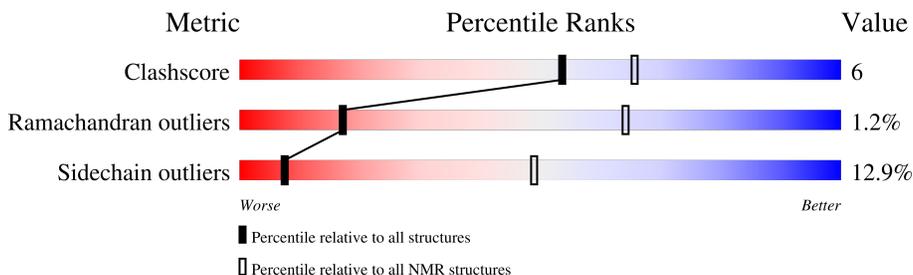
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 87%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	146	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:131-A:189, A:198-A:228 (90)	0.73	6

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 1 single-model cluster was found.

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

3 Entry composition

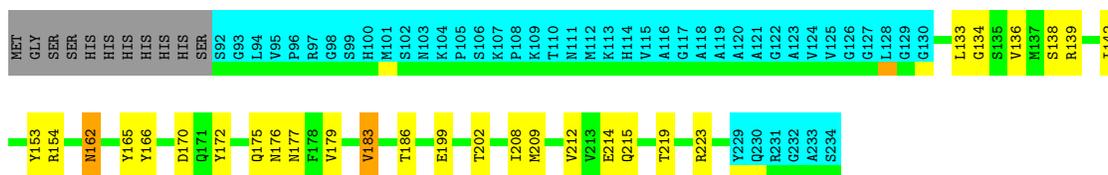
There is only 1 type of molecule in this entry. The entry contains 2105 atoms, of which 1028 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	135	2105	669	1028	195	204	9	0

There are 30 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	?	-	HIS	deletion	UNP Q712V9
A	?	-	THR	deletion	UNP Q712V9
A	?	-	VAL	deletion	UNP Q712V9
A	?	-	THR	deletion	UNP Q712V9
A	?	-	THR	deletion	UNP Q712V9
A	?	-	THR	deletion	UNP Q712V9
A	?	-	THR	deletion	UNP Q712V9
A	?	-	LYS	deletion	UNP Q712V9



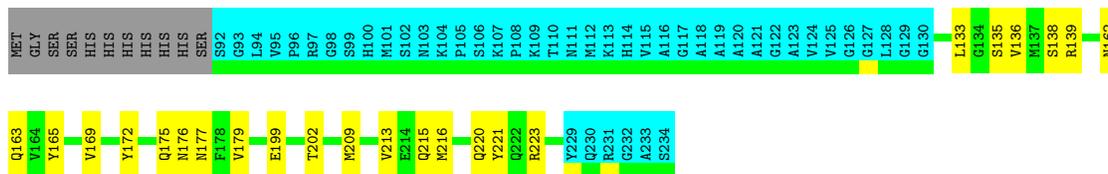
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



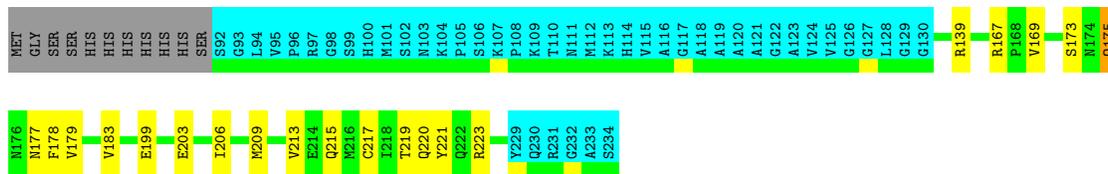
4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



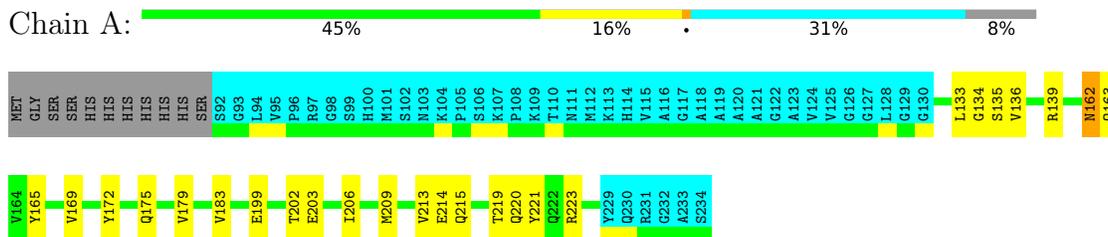
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



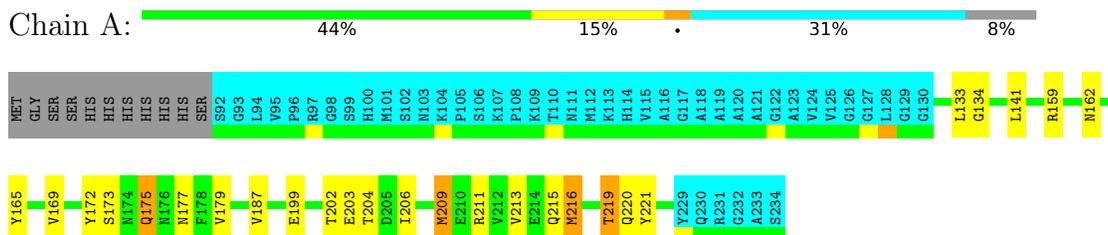
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Major prion protein



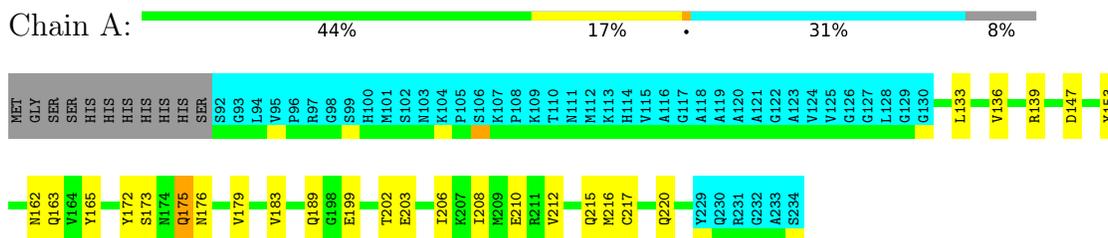
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



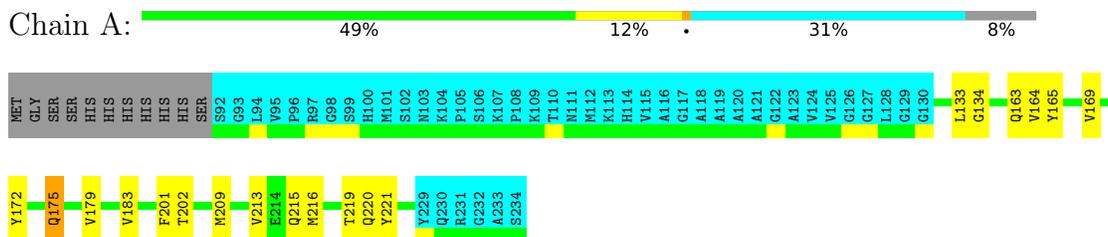
4.2.8 Score per residue for model 8

- 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



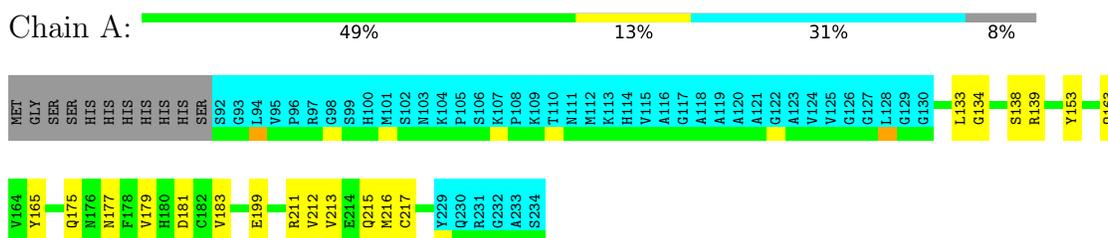
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



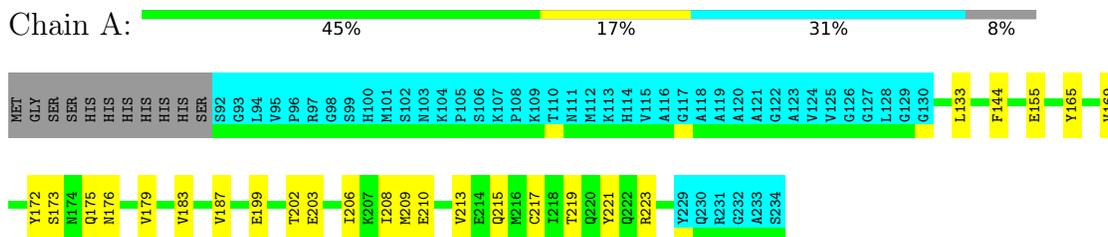
4.2.15 Score per residue for model 15

- 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



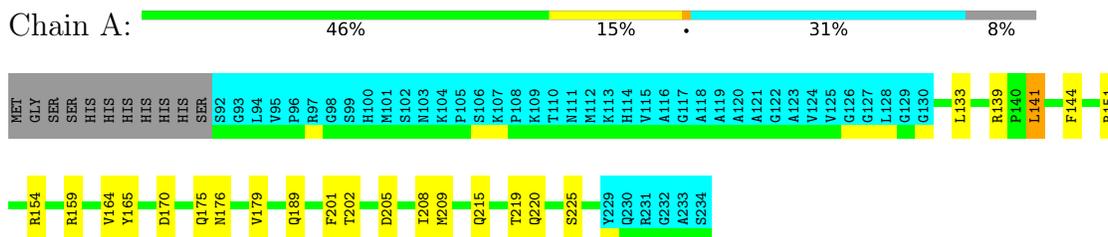
4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



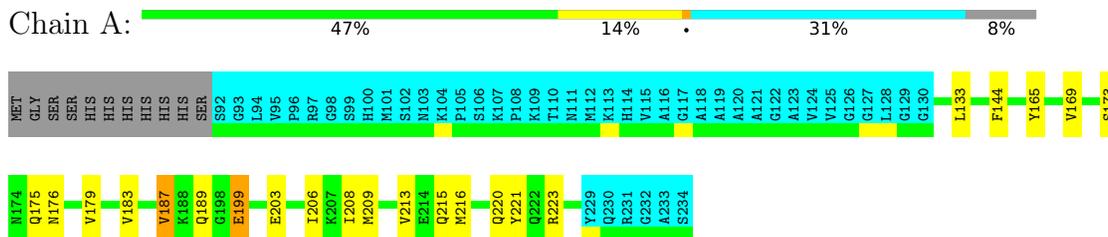
4.2.19 Score per residue for model 19

- 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	structure calculation	3.0
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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1609
Number of shifts mapped to atoms	1590
Number of unparsed shifts	0
Number of shifts with mapping errors	19
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

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	773	716	716	8±2
All	All	15460	14320	14320	164

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:169:VAL:HG21	1:A:221:TYR:CE1	0.69	2.23	9	12
1:A:133:LEU:HD22	1:A:165:TYR:CE2	0.67	2.24	10	13
1:A:169:VAL:HG21	1:A:221:TYR:CD1	0.66	2.26	6	4
1:A:175:GLN:O	1:A:179:VAL:HG23	0.64	1.92	15	19
1:A:133:LEU:HD13	1:A:165:TYR:CE2	0.64	2.28	13	4
1:A:144:PHE:CE1	1:A:208:ILE:HG23	0.63	2.28	16	4
1:A:133:LEU:HD13	1:A:165:TYR:CD2	0.62	2.28	17	4
1:A:169:VAL:HG11	1:A:221:TYR:CD1	0.62	2.29	16	1
1:A:136:VAL:HG13	1:A:162:ASN:HB3	0.62	1.72	8	1
1:A:183:VAL:HG13	1:A:213:VAL:HG11	0.60	1.73	20	1
1:A:133:LEU:HD12	1:A:164:VAL:O	0.60	1.96	13	6
1:A:183:VAL:HG13	1:A:213:VAL:CG1	0.59	2.27	20	1
1:A:136:VAL:HG13	1:A:162:ASN:CB	0.58	2.28	8	2
1:A:133:LEU:HD21	1:A:163:GLN:OE1	0.57	1.99	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:LEU:HD11	1:A:163:GLN:HB3	0.57	1.74	11	6
1:A:203:GLU:HA	1:A:206:ILE:HD12	0.57	1.74	13	9
1:A:208:ILE:O	1:A:212:VAL:HG23	0.56	2.00	2	4
1:A:133:LEU:HD11	1:A:163:GLN:CD	0.56	2.22	8	1
1:A:136:VAL:HG13	1:A:162:ASN:HB2	0.54	1.76	14	7
1:A:133:LEU:HD22	1:A:165:TYR:CZ	0.53	2.38	7	1
1:A:209:MET:O	1:A:213:VAL:HG23	0.52	2.04	16	15
1:A:133:LEU:HD21	1:A:163:GLN:NE2	0.51	2.20	17	2
1:A:136:VAL:HG23	1:A:162:ASN:HB2	0.51	1.81	18	1
1:A:187:VAL:HG12	1:A:199:GLU:OE1	0.51	2.04	7	1
1:A:187:VAL:HG21	1:A:210:GLU:OE2	0.50	2.06	16	1
1:A:202:THR:HG23	1:A:205:ASP:H	0.49	1.67	19	1
1:A:164:VAL:HG12	1:A:186:THR:HG21	0.49	1.83	1	1
1:A:142:ILE:HD11	1:A:212:VAL:HB	0.49	1.83	10	2
1:A:187:VAL:HG22	1:A:199:GLU:HB3	0.49	1.84	20	1
1:A:144:PHE:CZ	1:A:208:ILE:HG23	0.48	2.44	16	3
1:A:133:LEU:HD22	1:A:165:TYR:CE1	0.48	2.43	11	2
1:A:142:ILE:CD1	1:A:212:VAL:HG22	0.47	2.39	2	3
1:A:153:TYR:CE1	1:A:212:VAL:HG21	0.47	2.44	15	6
1:A:169:VAL:HG11	1:A:221:TYR:CE1	0.46	2.45	16	1
1:A:141:LEU:HD12	1:A:141:LEU:O	0.46	2.11	14	2
1:A:133:LEU:HD21	1:A:163:GLN:HE22	0.46	1.70	14	1
1:A:142:ILE:HD11	1:A:212:VAL:HA	0.44	1.89	18	2
1:A:142:ILE:HD12	1:A:212:VAL:HG22	0.44	1.90	2	2
1:A:141:LEU:HD21	1:A:154:ARG:HD2	0.44	1.90	3	1
1:A:216:MET:O	1:A:219:THR:HG22	0.43	2.13	11	2
1:A:183:VAL:HG13	1:A:213:VAL:CB	0.42	2.44	20	1
1:A:187:VAL:HG22	1:A:209:MET:SD	0.42	2.54	10	2
1:A:142:ILE:HD11	1:A:212:VAL:HG22	0.42	1.91	13	1
1:A:133:LEU:HD22	1:A:165:TYR:HE2	0.42	1.73	10	1
1:A:178:PHE:CD1	1:A:178:PHE:C	0.41	2.93	5	1
1:A:183:VAL:HG23	1:A:214:GLU:N	0.41	2.31	2	2
1:A:183:VAL:HG13	1:A:213:VAL:HB	0.41	1.91	15	1
1:A:179:VAL:O	1:A:183:VAL:HG23	0.41	2.15	15	2
1:A:142:ILE:HD11	1:A:212:VAL:CB	0.40	2.46	14	1
1:A:218:ILE:HD12	1:A:219:THR:N	0.40	2.31	18	1

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	90/146 (62%)	84±1 (94±1%)	5±1 (5±2%)	1±1 (1±1%)	17	64
All	All	1800/2920 (62%)	1683 (94%)	96 (5%)	21 (1%)	17	64

All 4 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	134	GLY	9
1	A	172	TYR	8
1	A	201	PHE	3
1	A	174	ASN	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	86/125 (69%)	75±2 (87±3%)	11±2 (13±3%)	7	49
All	All	1720/2500 (69%)	1498 (87%)	222 (13%)	7	49

All 40 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	215	GLN	20
1	A	220	GLN	17
1	A	199	GLU	16
1	A	219	THR	14
1	A	176	ASN	11
1	A	139	ARG	9

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Mol	Chain	Res	Type	Models (Total)
1	A	202	THR	9
1	A	216	MET	9
1	A	138	SER	8
1	A	173	SER	8
1	A	183	VAL	8
1	A	177	ASN	8
1	A	223	ARG	8
1	A	211	ARG	7
1	A	141	LEU	7
1	A	175	GLN	6
1	A	217	CYS	6
1	A	162	ASN	6
1	A	209	MET	6
1	A	167	ARG	4
1	A	159	ARG	4
1	A	135	SER	3
1	A	225	SER	3
1	A	214	GLU	2
1	A	154	ARG	2
1	A	166	TYR	2
1	A	170	ASP	2
1	A	147	ASP	2
1	A	137	MET	2
1	A	181	ASP	2
1	A	207	LYS	2
1	A	172	TYR	1
1	A	186	THR	1
1	A	204	THR	1
1	A	189	GLN	1
1	A	210	GLU	1
1	A	205	ASP	1
1	A	155	GLU	1
1	A	151	ARG	1
1	A	187	VAL	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 monosaccharides 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 87% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_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	1609
Number of shifts mapped to atoms	1590
Number of unparsed shifts	0
Number of shifts with mapping errors	19
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. All 19 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	83	SER	CA	58.05	0.25	1
1	A	83	SER	CB	63.95	0.25	1
1	A	83	SER	C	174.52	0.25	1
1	A	84	SER	N	117.83	0.15	1
1	A	84	SER	H	8.48	0.02	1
1	A	84	SER	CA	58.19	0.25	1
1	A	84	SER	HA	4.41	0.02	1
1	A	84	SER	HB2	3.79	0.02	2
1	A	84	SER	HB3	3.8	0.02	2
1	A	90	HIS	CA	55.62	0.25	1
1	A	90	HIS	CB	29.99	0.25	1
1	A	91	SER	N	118.19	0.15	1
1	A	91	SER	H	8.47	0.02	1
1	A	91	SER	CA	58.1	0.25	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	91	SER	HA	4.46	0.02	1
1	A	91	SER	CB	63.8	0.25	1
1	A	91	SER	HB2	3.83	0.02	2
1	A	91	SER	HB3	3.83	0.02	2
1	A	91	SER	C	174.41	0.25	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	138	-0.02 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	121	0.23 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	124	0.04 ± 0.10	None needed (< 0.5 ppm)
^{15}N	125	0.04 ± 0.13	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 87%, i.e. 1115 atoms were assigned a chemical shift out of a possible 1289. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	421/447 (94%)	170/180 (94%)	170/180 (94%)	81/87 (93%)
Sidechain	589/699 (84%)	400/446 (90%)	174/214 (81%)	15/39 (38%)
Aromatic	105/143 (73%)	55/67 (82%)	50/74 (68%)	0/2 (0%)
Overall	1115/1289 (87%)	625/693 (90%)	394/468 (84%)	96/128 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1589 atoms were assigned a chemical shift out of a possible 1823. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	645/675 (96%)	266/276 (96%)	256/270 (95%)	123/129 (95%)
Sidechain	831/982 (85%)	565/633 (89%)	250/297 (84%)	16/52 (31%)
Aromatic	113/166 (68%)	59/79 (75%)	54/83 (65%)	0/4 (0%)
Overall	1589/1823 (87%)	890/988 (90%)	560/650 (86%)	139/185 (75%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	186	THR	HG1	6.16	0.08 – 2.19	23.8

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

