



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 07:50 AM UTC

PDB ID : 2KFM / pdb_00002kfm
BMRB ID : 16184
Title : Mouse Prion Protein (121-231) with Mutations Y225A and Y226A
Authors : Christen, B.; Hornemann, S.; Damberger, F.F.; Wuthrich, K.
Deposited on : 2009-02-24

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We welcome your comments at validation@mail.wwpdb.org

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<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:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

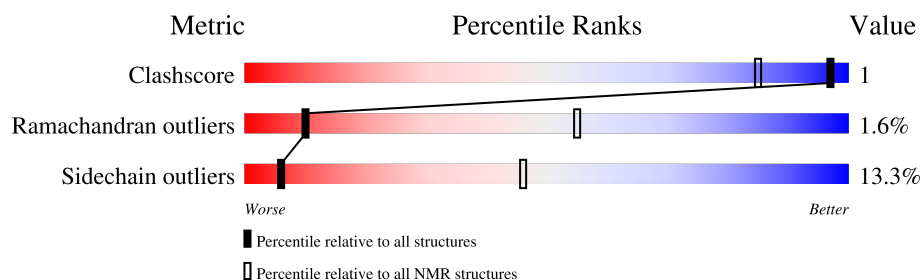
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 60%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	114	

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 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:122-A:223 (102)	0.58	10

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1780 atoms, of which 861 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	113	Total	C	H	N	O	S	0
			1780	566	861	164	180	9	

There are 4 discrepancies between the modelled and reference sequences:

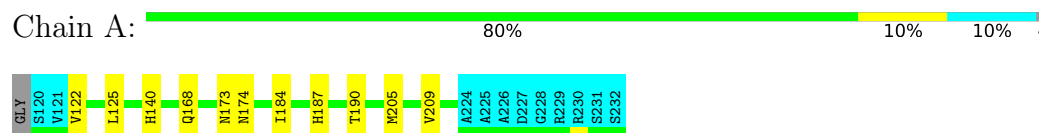
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	expression tag	UNP P04925
A	120	SER	-	expression tag	UNP P04925
A	225	ALA	TYR	engineered mutation	UNP P04925
A	226	ALA	TYR	engineered mutation	UNP P04925

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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

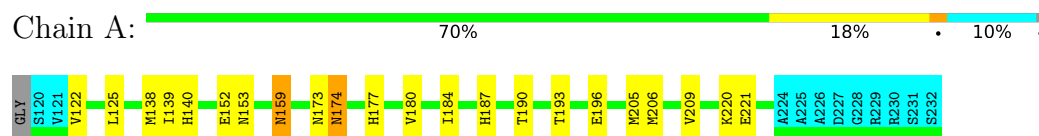


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

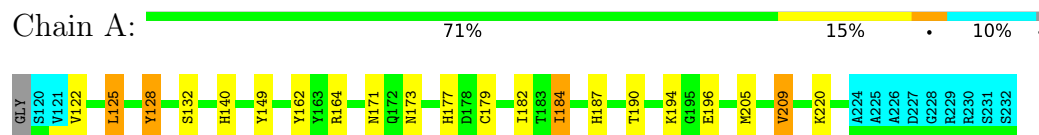
4.2.1 Score per residue for model 1

- Molecule 1: Major prion protein



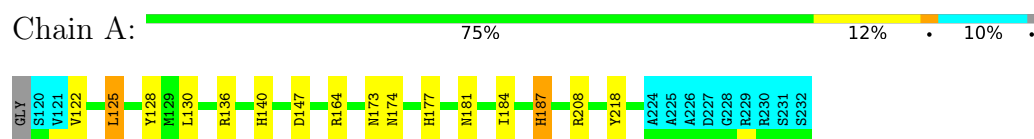
4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein



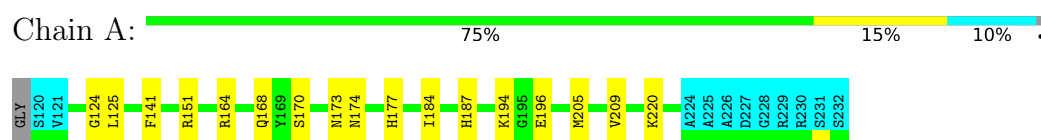
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



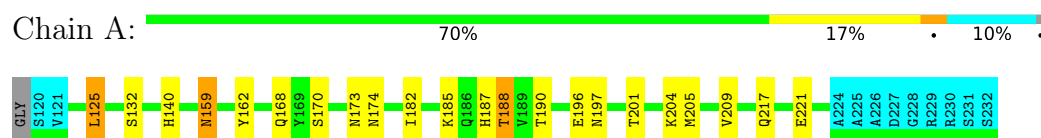
4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



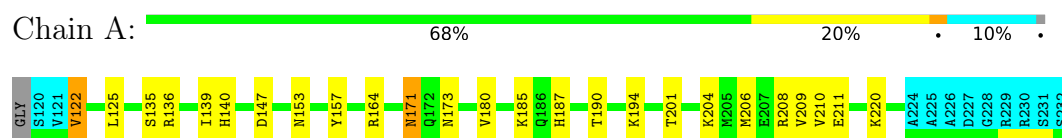
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



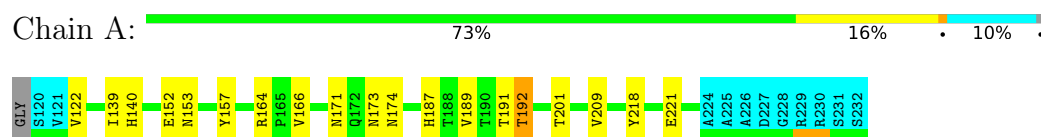
4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



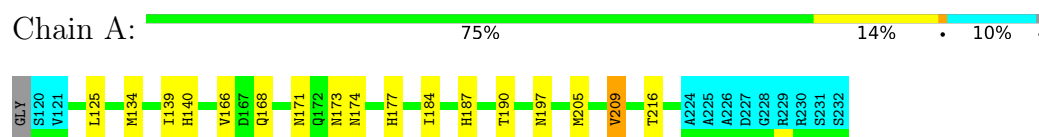
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



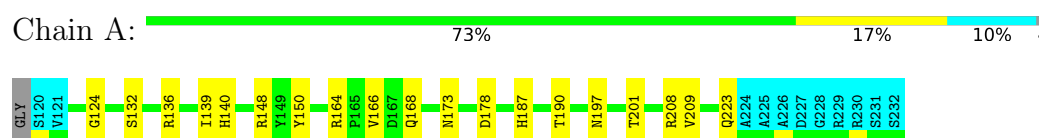
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



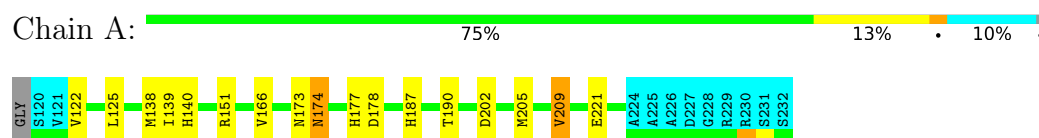
4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



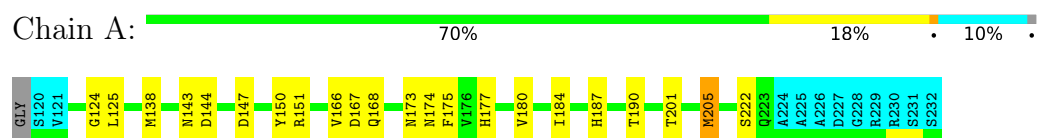
4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Major prion protein



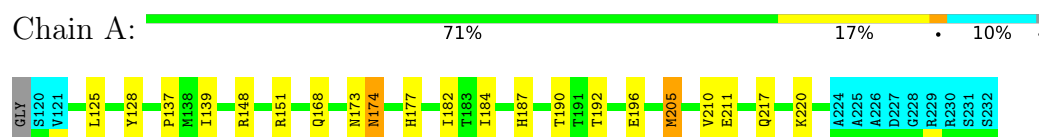
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



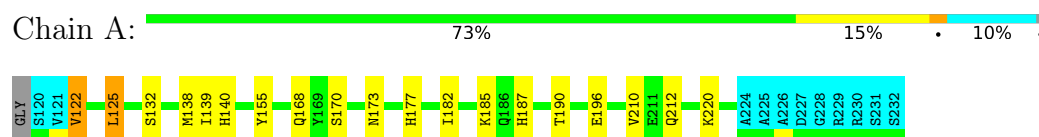
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



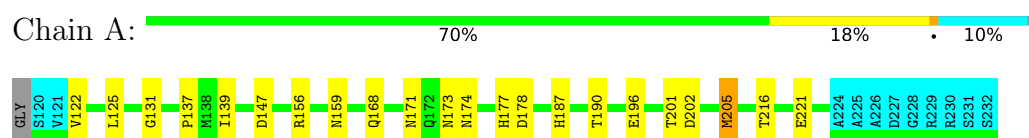
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



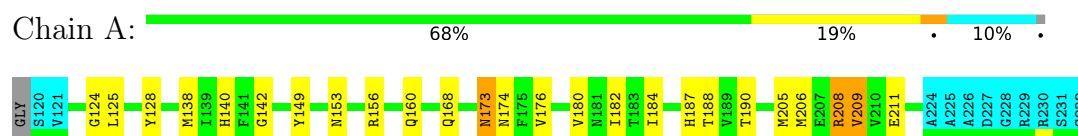
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



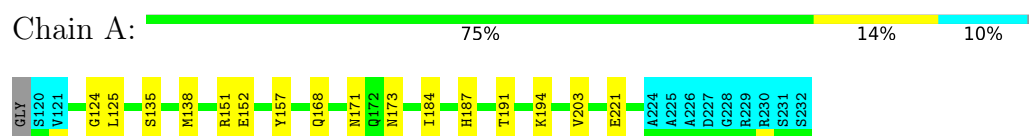
4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



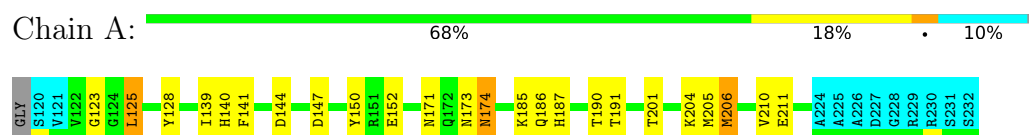
4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein



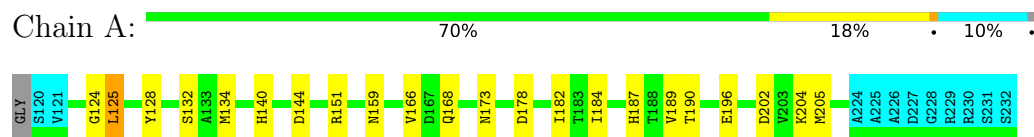
4.2.17 Score per residue for model 17

- Molecule 1: Major prion protein



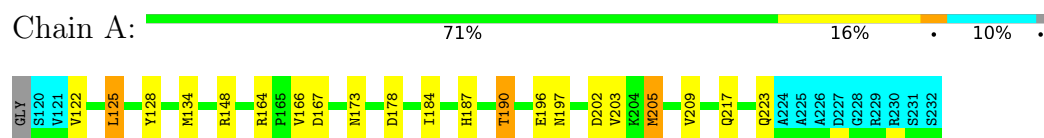
4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



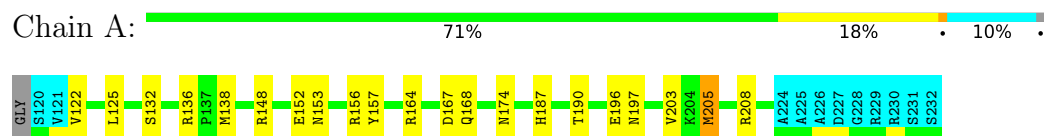
4.2.19 Score per residue for model 19

- 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 80 calculated structures, 20 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DYANA	structure solution	1.0.3
OPALp	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	911
Number of shifts mapped to atoms	911
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	60%

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	0.67±0.01	0±0/865 (0.0± 0.0%)	1.50±0.03	5±2/1170 (0.5± 0.1%)
All	All	0.67	0/17300 (0.0%)	1.50	107/23400 (0.5%)

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	1.4±1.2
All	All	0	28

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	140	HIS	CA-CB-CG	9.54	123.34	113.80	18	11
1	A	174	ASN	CA-CB-CG	7.93	120.53	112.60	1	8
1	A	177	HIS	CA-CB-CG	7.80	121.60	113.80	11	10
1	A	187	HIS	CB-CG-CD2	-7.80	121.06	131.20	8	20
1	A	205	MET	CA-C-N	6.49	128.98	120.28	14	6
1	A	205	MET	C-N-CA	6.49	128.98	120.28	14	6
1	A	211	GLU	CA-CB-CG	6.32	126.75	114.10	12	1
1	A	159	ASN	CA-CB-CG	6.28	118.88	112.60	1	2
1	A	122	VAL	CA-CB-CG1	6.28	121.08	110.40	13	2
1	A	188	THR	CB-CA-C	5.96	120.19	110.95	15	1
1	A	185	LYS	CB-CA-C	5.92	118.52	109.34	5	1
1	A	122	VAL	CB-CA-C	5.92	120.99	111.29	20	1
1	A	197	ASN	CA-CB-CG	-5.90	106.70	112.60	9	1
1	A	211	GLU	CA-C-N	5.69	128.22	120.54	17	1
1	A	211	GLU	C-N-CA	5.69	128.22	120.54	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	173	ASN	CA-CB-CG	5.62	118.22	112.60	15	1
1	A	218	TYR	N-CA-C	-5.62	104.79	111.03	3	2
1	A	171	ASN	CA-CB-CG	5.58	118.18	112.60	6	1
1	A	188	THR	N-CA-C	-5.57	104.85	111.03	15	2
1	A	178	ASP	CA-C-N	5.52	127.94	120.65	9	1
1	A	178	ASP	C-N-CA	5.52	127.94	120.65	9	1
1	A	191	THR	CB-CA-C	5.43	118.14	109.02	16	1
1	A	166	VAL	CA-C-N	5.42	131.89	121.54	19	1
1	A	166	VAL	C-N-CA	5.42	131.89	121.54	19	1
1	A	132	SER	CA-C-N	5.37	128.97	121.02	13	1
1	A	132	SER	C-N-CA	5.37	128.97	121.02	13	1
1	A	143	ASN	CA-CB-CG	5.33	117.93	112.60	11	1
1	A	209	VAL	CA-CB-CG1	5.32	119.45	110.40	2	1
1	A	153	ASN	CA-C-N	5.30	127.64	120.38	20	1
1	A	153	ASN	C-N-CA	5.30	127.64	120.38	20	1
1	A	189	VAL	CB-CA-C	5.27	115.74	111.05	18	1
1	A	209	VAL	CA-CB-CG2	5.23	119.29	110.40	5	2
1	A	210	VAL	CA-C-O	-5.21	115.26	121.05	12	1
1	A	177	HIS	CA-C-N	5.19	127.50	120.44	4	1
1	A	177	HIS	C-N-CA	5.19	127.50	120.44	4	1
1	A	206	MET	N-CA-C	-5.17	105.54	111.07	17	1
1	A	209	VAL	CB-CA-C	5.16	118.48	111.88	10	2
1	A	142	GLY	CA-C-N	5.13	127.99	120.71	15	1
1	A	142	GLY	C-N-CA	5.13	127.99	120.71	15	1
1	A	217	GLN	OE1-CD-NE2	-5.09	117.51	122.60	19	1
1	A	140	HIS	CA-C-N	5.03	131.15	121.54	17	1
1	A	140	HIS	C-N-CA	5.03	131.15	121.54	17	1
1	A	221	GLU	CA-C-N	5.02	127.25	120.38	10	1
1	A	221	GLU	C-N-CA	5.02	127.25	120.38	10	1
1	A	192	THR	CA-C-N	5.00	128.60	120.60	7	1
1	A	192	THR	C-N-CA	5.00	128.60	120.60	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	157	TYR	Sidechain	4
1	A	136	ARG	Sidechain	3
1	A	208	ARG	Sidechain	3
1	A	148	ARG	Sidechain	3

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	150	TYR	Sidechain	3
1	A	156	ARG	Sidechain	3
1	A	149	TYR	Sidechain	2
1	A	162	TYR	Sidechain	2
1	A	151	ARG	Sidechain	2
1	A	128	TYR	Sidechain	1
1	A	170	SER	Peptide	1
1	A	190	THR	Peptide	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	845	789	789	1±1
All	All	16900	15780	15780	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:180:VAL:HG13	1:A:210:VAL:CG2	0.54	2.32	6	1
1:A:125:LEU:HD11	1:A:182:ILE:HD12	0.53	1.81	5	3
1:A:208:ARG:HA	1:A:211:GLU:HG2	0.52	1.81	15	1
1:A:186:GLN:O	1:A:190:THR:HG22	0.49	2.07	17	1
1:A:128:TYR:CE2	1:A:182:ILE:HG13	0.47	2.44	2	4
1:A:125:LEU:HD23	1:A:128:TYR:CG	0.47	2.44	3	3
1:A:206:MET:HA	1:A:209:VAL:HG12	0.46	1.87	15	1
1:A:180:VAL:HG12	1:A:184:ILE:HD12	0.46	1.88	11	2
1:A:184:ILE:O	1:A:184:ILE:HG22	0.46	2.10	19	1
1:A:139:ILE:HD11	1:A:212:GLN:NE2	0.43	2.29	13	1
1:A:125:LEU:HD21	1:A:182:ILE:CG2	0.41	2.44	12	1
1:A:206:MET:O	1:A:210:VAL:HG23	0.41	2.15	17	1
1:A:176:VAL:O	1:A:180:VAL:HG23	0.41	2.16	15	1
1:A:125:LEU:HD12	1:A:128:TYR:CD1	0.41	2.50	18	1
1:A:175:PHE:CD1	1:A:175:PHE:C	0.40	2.99	11	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	102/114 (89%)	88±2 (86±2%)	13±2 (12±2%)	2±1 (2±1%)	10	55
All	All	2040/2280 (89%)	1755 (86%)	252 (12%)	33 (2%)	10	55

All 13 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	122	VAL	8
1	A	124	GLY	6
1	A	168	GLN	4
1	A	167	ASP	3
1	A	141	PHE	2
1	A	137	PRO	2
1	A	132	SER	2
1	A	184	ILE	1
1	A	189	VAL	1
1	A	192	THR	1
1	A	170	SER	1
1	A	131	GLY	1
1	A	123	GLY	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	94/101 (93%)	82±2 (87±3%)	12±2 (13±3%)	6	46
All	All	1880/2020 (93%)	1630 (87%)	250 (13%)	6	46

All 56 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	173	ASN	19
1	A	125	LEU	17
1	A	190	THR	15
1	A	205	MET	13
1	A	196	GLU	10
1	A	139	ILE	9
1	A	174	ASN	9
1	A	209	VAL	9
1	A	164	ARG	8
1	A	184	ILE	8
1	A	168	GLN	8
1	A	138	MET	7
1	A	171	ASN	7
1	A	201	THR	7
1	A	220	LYS	6
1	A	166	VAL	6
1	A	152	GLU	5
1	A	221	GLU	5
1	A	147	ASP	5
1	A	153	ASN	4
1	A	159	ASN	4
1	A	194	LYS	4
1	A	151	ARG	4
1	A	197	ASN	4
1	A	204	LYS	4
1	A	178	ASP	4
1	A	202	ASP	4
1	A	132	SER	3
1	A	185	LYS	3
1	A	134	MET	3
1	A	144	ASP	3
1	A	203	VAL	3
1	A	206	MET	2
1	A	217	GLN	2
1	A	135	SER	2
1	A	191	THR	2
1	A	216	THR	2
1	A	208	ARG	2
1	A	193	THR	1
1	A	179	CYS	1
1	A	130	LEU	1
1	A	181	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	187	HIS	1
1	A	170	SER	1
1	A	188	THR	1
1	A	122	VAL	1
1	A	211	GLU	1
1	A	192	THR	1
1	A	136	ARG	1
1	A	223	GLN	1
1	A	140	HIS	1
1	A	222	SER	1
1	A	155	TYR	1
1	A	210	VAL	1
1	A	160	GLN	1
1	A	148	ARG	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 oligosaccharides 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 60% for the well-defined parts and 59% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

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	911
Number of shifts mapped to atoms	911
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	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
$^{13}\text{C}_\alpha$	113	-0.39 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	105	0.43 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	110	-0.06 ± 0.15	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 60%, i.e. 847 atoms were assigned a chemical shift out of a possible 1406. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	300/511 (59%)	99/208 (48%)	102/204 (50%)	99/99 (100%)
Sidechain	495/751 (66%)	275/481 (57%)	198/232 (85%)	22/38 (58%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	52/144 (36%)	14/69 (20%)	37/71 (52%)	1/4 (25%)
Overall	847/1406 (60%)	388/758 (51%)	337/507 (66%)	122/141 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 59%, i.e. 910 atoms were assigned a chemical shift out of a possible 1533. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	332/567 (59%)	109/231 (47%)	113/226 (50%)	110/110 (100%)
Sidechain	526/822 (64%)	288/527 (55%)	214/251 (85%)	24/44 (55%)
Aromatic	52/144 (36%)	14/69 (20%)	37/71 (52%)	1/4 (25%)
Overall	910/1533 (59%)	411/827 (50%)	364/548 (66%)	135/158 (85%)

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	183	THR	HG1	6.41	0.08 – 2.19	25.0

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:

