



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 12:35 PM UTC

PDB ID : 2KFO / pdb_00002kfo
BMRB ID : 16185
Title : Mouse Prion Protein (121-231) with Mutation V166A
Authors : Christen, B.; Hornemann, S.; Damberger, F.F.; Wuthrich, K.
Deposited on : 2009-02-24

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:

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

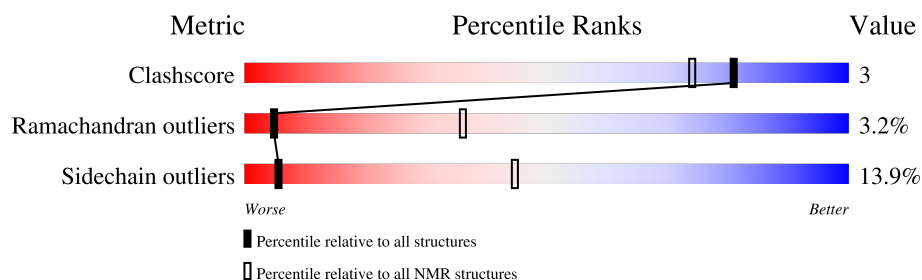
1 Overall quality at a glance

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	 81% 11% • 7%

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 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:120-A:225 (106)	0.50	13

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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1803 atoms, of which 868 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	114	Total	C	H	N	O	S	0
			1803	578	868	165	183	9	

There are 3 discrepancies between the modelled and reference sequences:

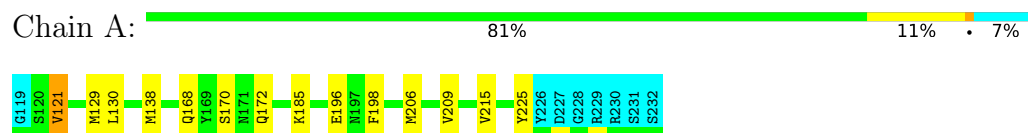
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	expression tag	UNP P04925
A	120	SER	-	expression tag	UNP P04925
A	166	ALA	VAL	engineered mutation	UNP P04925

4 Residue-property plots [i](#)

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

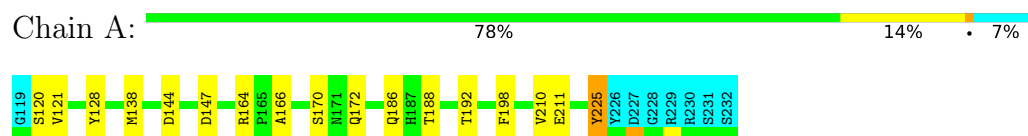


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

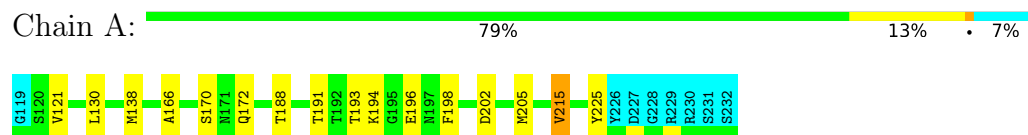
4.2.1 Score per residue for model 1

- Molecule 1: Major prion protein



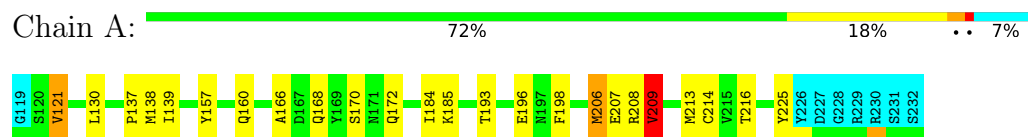
4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein



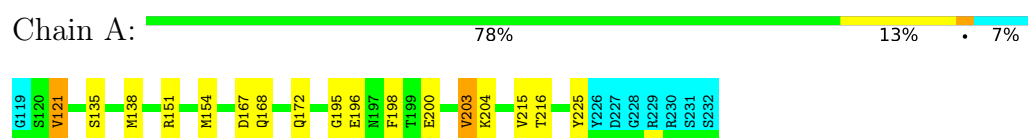
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



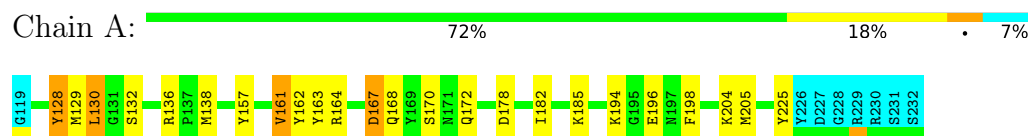
4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



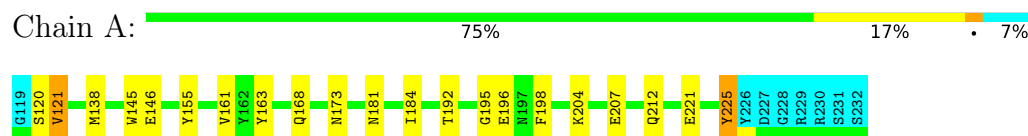
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



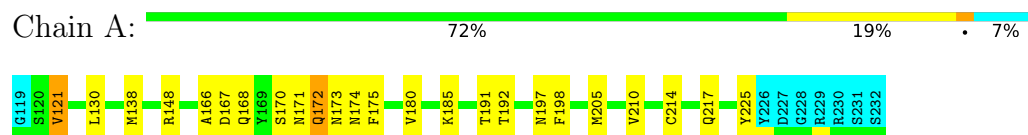
4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



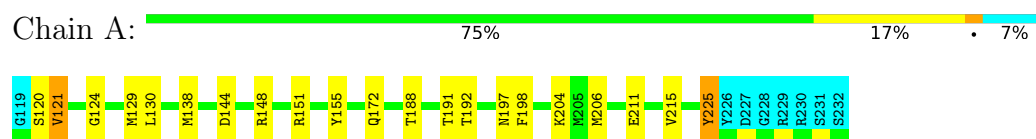
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



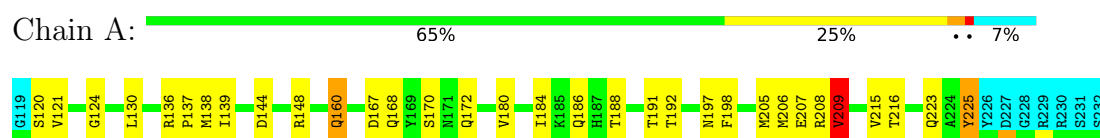
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



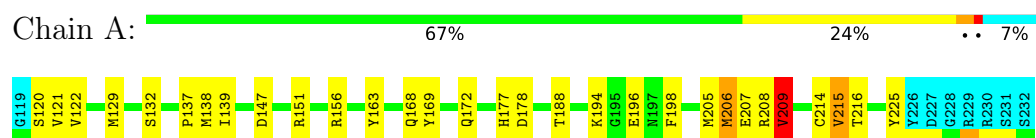
4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



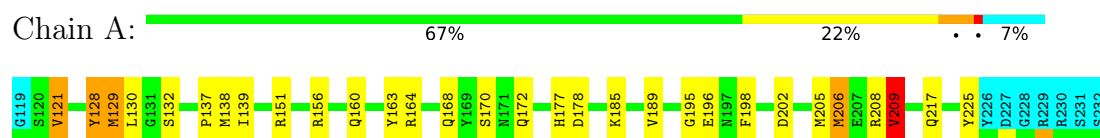
4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



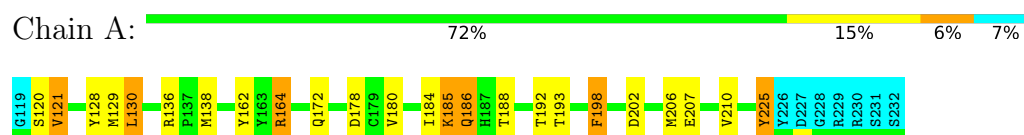
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



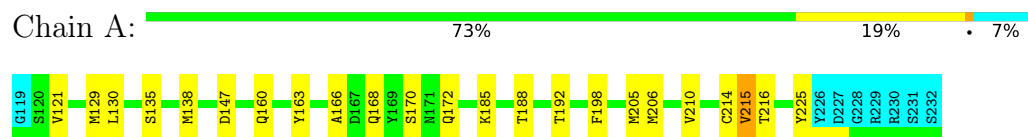
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



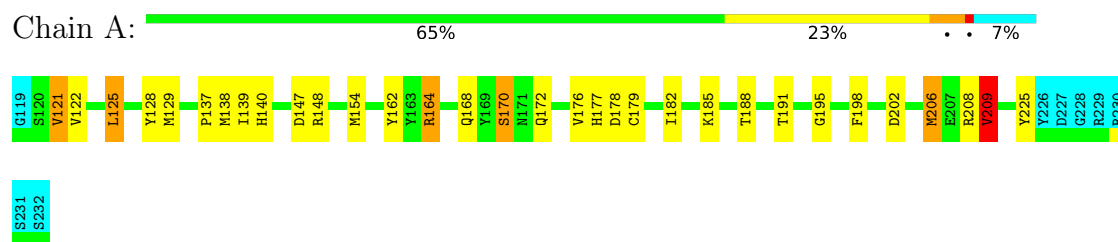
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Major prion protein



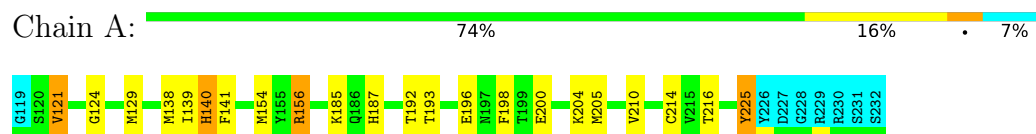
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



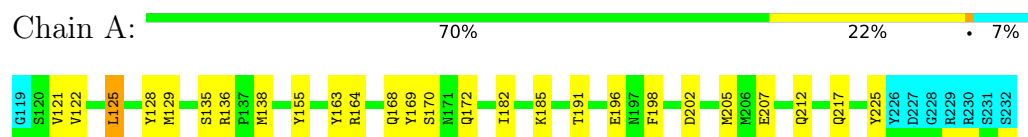
4.2.15 Score per residue for model 15

- 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

Chain A: 66% 25% 7%



4.2.19 Score per residue for model 19

- Molecule 1: Major prion protein

Chain A: 72% 18% 7%



4.2.20 Score per residue for model 20

- Molecule 1: Major prion protein

Chain A: 73% 19% 7%



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
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	924
Number of shifts mapped to atoms	924
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	0.71±0.02	0±0/894 (0.0± 0.0%)	1.50±0.03	5±2/1210 (0.4± 0.2%)
All	All	0.71	0/17880 (0.0%)	1.50	93/24200 (0.4%)

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	1.6±1.0
All	All	0	32

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	209	VAL	CA-CB-CG1	8.78	125.33	110.40	3	5
1	A	206	MET	CA-C-N	6.96	129.49	120.44	10	5
1	A	206	MET	C-N-CA	6.96	129.49	120.44	10	5
1	A	188	THR	CA-C-N	6.76	129.22	122.66	1	10
1	A	188	THR	C-N-CA	6.76	129.22	122.66	1	10
1	A	161	VAL	CA-CB-CG1	6.46	121.38	110.40	5	1
1	A	139	ILE	CA-C-N	6.41	130.81	121.26	15	1
1	A	139	ILE	C-N-CA	6.41	130.81	121.26	15	1
1	A	181	ASN	CA-C-N	6.29	128.49	120.56	6	2
1	A	181	ASN	C-N-CA	6.29	128.49	120.56	6	2
1	A	174	ASN	CA-C-N	6.19	128.48	120.44	7	1
1	A	174	ASN	C-N-CA	6.19	128.48	120.44	7	1
1	A	203	VAL	CA-CB-CG2	6.16	120.88	110.40	4	1
1	A	175	PHE	CA-C-N	6.16	128.89	120.46	7	1
1	A	175	PHE	C-N-CA	6.16	128.89	120.46	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	166	ALA	CA-C-N	6.15	130.53	120.63	1	6
1	A	166	ALA	C-N-CA	6.15	130.53	120.63	1	6
1	A	215	VAL	CA-CB-CG1	6.10	120.78	110.40	2	3
1	A	189	VAL	N-CA-C	-5.97	107.06	111.90	11	1
1	A	203	VAL	CG1-CB-CG2	5.92	123.83	110.80	4	1
1	A	177	HIS	CB-CG-CD2	-5.67	123.83	131.20	11	3
1	A	209	VAL	CA-CB-CG2	5.67	120.03	110.40	18	2
1	A	140	HIS	CA-C-N	5.63	132.30	121.54	15	1
1	A	140	HIS	C-N-CA	5.63	132.30	121.54	15	1
1	A	217	GLN	OE1-CD-NE2	-5.63	116.97	122.60	11	2
1	A	173	ASN	CA-CB-CG	5.50	118.10	112.60	6	1
1	A	140	HIS	CB-CG-CD2	-5.50	124.05	131.20	15	2
1	A	197	ASN	CA-CB-CG	-5.48	107.12	112.60	7	1
1	A	187	HIS	CA-CB-CG	-5.44	108.36	113.80	15	1
1	A	193	THR	CB-CA-C	5.43	116.50	109.28	2	1
1	A	136	ARG	CA-C-N	5.37	126.56	119.84	12	1
1	A	136	ARG	C-N-CA	5.37	126.56	119.84	12	1
1	A	147	ASP	CA-CB-CG	5.35	117.95	112.60	1	1
1	A	120	SER	CA-C-N	5.31	131.52	121.97	1	1
1	A	120	SER	C-N-CA	5.31	131.52	121.97	1	1
1	A	171	ASN	OD1-CG-ND2	-5.31	117.29	122.60	7	1
1	A	159	ASN	CA-CB-CG	5.28	117.88	112.60	20	1
1	A	210	VAL	CA-C-O	-5.21	115.65	121.17	7	1
1	A	195	GLY	CA-C-N	5.20	129.75	122.05	17	1
1	A	195	GLY	C-N-CA	5.20	129.75	122.05	17	1
1	A	223	GLN	N-CA-CB	-5.18	102.99	110.56	9	1
1	A	140	HIS	CA-CB-CG	5.14	118.94	113.80	15	1
1	A	184	ILE	CA-C-N	5.10	129.30	121.19	6	1
1	A	184	ILE	C-N-CA	5.10	129.30	121.19	6	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	151	ARG	Sidechain	5
1	A	157	TYR	Sidechain	4
1	A	148	ARG	Sidechain	4
1	A	128	TYR	Sidechain	3
1	A	155	TYR	Sidechain	3
1	A	156	ARG	Sidechain	3

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	169	TYR	Sidechain	3
1	A	163	TYR	Sidechain	2
1	A	164	ARG	Sidechain	2
1	A	136	ARG	Sidechain	1
1	A	162	TYR	Sidechain	1
1	A	218	TYR	Sidechain	1

6.2 Too-close contacts [i](#)

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	873	813	813	4±3
All	All	17460	16260	16260	87

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:VAL:HB	1:A:125:LEU:HD11	0.64	1.69	16	1
1:A:139:ILE:HD13	1:A:208:ARG:HB2	0.58	1.75	9	7
1:A:137:PRO:HD2	1:A:209:VAL:HG23	0.58	1.74	9	7
1:A:206:MET:HA	1:A:209:VAL:CG1	0.56	2.30	18	7
1:A:125:LEU:HD12	1:A:125:LEU:N	0.56	2.14	16	2
1:A:130:LEU:HD11	1:A:160:GLN:NE2	0.56	2.16	20	2
1:A:180:VAL:O	1:A:184:ILE:HD12	0.54	2.02	9	1
1:A:137:PRO:CD	1:A:209:VAL:HG23	0.51	2.36	14	3
1:A:125:LEU:HD12	1:A:125:LEU:H	0.51	1.64	16	2
1:A:122:VAL:HG21	1:A:162:TYR:CE1	0.51	2.40	14	1
1:A:139:ILE:HD11	1:A:209:VAL:HB	0.50	1.82	10	5
1:A:198:PHE:HB3	1:A:206:MET:HE1	0.49	1.84	17	1
1:A:209:VAL:HG22	1:A:213:MET:HE2	0.48	1.84	19	3
1:A:129:MET:HE3	1:A:163:TYR:CE2	0.48	2.43	10	2
1:A:128:TYR:CD2	1:A:182:ILE:HG13	0.48	2.42	16	2
1:A:128:TYR:CE2	1:A:164:ARG:HG3	0.47	2.44	20	5
1:A:225:TYR:C	1:A:225:TYR:CD1	0.46	2.93	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:200:GLU:HA	1:A:203:VAL:CG2	0.46	2.41	4	1
1:A:121:VAL:HG13	1:A:129:MET:HA	0.46	1.88	14	1
1:A:191:THR:HG21	1:A:197:ASN:HA	0.45	1.88	9	2
1:A:176:VAL:HA	1:A:179:CYS:SG	0.45	2.52	14	1
1:A:145:TRP:CE2	1:A:146:GLU:HG3	0.45	2.47	6	3
1:A:130:LEU:HD11	1:A:160:GLN:HE21	0.44	1.73	9	1
1:A:185:LYS:HG3	1:A:186:GLN:N	0.44	2.28	12	1
1:A:138:MET:HE1	1:A:154:MET:HE1	0.43	1.90	18	1
1:A:129:MET:CE	1:A:163:TYR:CE2	0.43	3.02	5	2
1:A:184:ILE:HD11	1:A:207:GLU:HA	0.43	1.89	9	3
1:A:128:TYR:CE2	1:A:182:ILE:HG13	0.43	2.49	16	2
1:A:130:LEU:HD23	1:A:162:TYR:CE1	0.43	2.49	20	2
1:A:180:VAL:HA	1:A:210:VAL:HG23	0.43	1.89	12	1
1:A:128:TYR:CZ	1:A:182:ILE:HD11	0.42	2.49	14	1
1:A:128:TYR:CE1	1:A:164:ARG:HG3	0.42	2.49	11	1
1:A:129:MET:HE3	1:A:163:TYR:CD2	0.42	2.49	13	1
1:A:225:TYR:CD1	1:A:225:TYR:C	0.42	2.98	12	4
1:A:172:GLN:O	1:A:173:ASN:C	0.42	2.62	7	1
1:A:139:ILE:CD1	1:A:209:VAL:HB	0.42	2.45	10	1
1:A:198:PHE:CG	1:A:206:MET:HE1	0.40	2.51	12	1
1:A:130:LEU:HG	1:A:162:TYR:CE1	0.40	2.52	5	1
1:A:200:GLU:HA	1:A:203:VAL:CB	0.40	2.46	4	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	106/114 (93%)	89±2 (84±2%)	13±2 (13±2%)	3±1 (3±1%)	5	36
All	All	2120/2280 (93%)	1786 (84%)	267 (13%)	67 (3%)	5	36

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	198	PHE	20
1	A	121	VAL	19
1	A	170	SER	7
1	A	195	GLY	5
1	A	194	LYS	3
1	A	124	GLY	3
1	A	132	SER	3
1	A	120	SER	2
1	A	136	ARG	1
1	A	167	ASP	1
1	A	191	THR	1
1	A	141	PHE	1
1	A	171	ASN	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	96/102 (94%)	83±2 (86±2%)	13±2 (14±2%)	5	45
All	All	1920/2040 (94%)	1654 (86%)	266 (14%)	5	45

All 48 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	138	MET	20
1	A	225	TYR	19
1	A	172	GLN	16
1	A	196	GLU	12
1	A	185	LYS	12
1	A	121	VAL	11
1	A	168	GLN	11
1	A	192	THR	10
1	A	130	LEU	10
1	A	205	MET	10
1	A	215	VAL	8
1	A	216	THR	8
1	A	202	ASP	7

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Mol	Chain	Res	Type	Models (Total)
1	A	209	VAL	7
1	A	170	SER	7
1	A	129	MET	7
1	A	214	CYS	6
1	A	178	ASP	6
1	A	186	GLN	5
1	A	193	THR	5
1	A	167	ASP	5
1	A	204	LYS	5
1	A	207	GLU	5
1	A	144	ASP	4
1	A	135	SER	4
1	A	154	MET	4
1	A	120	SER	4
1	A	210	VAL	3
1	A	191	THR	3
1	A	160	GLN	3
1	A	206	MET	3
1	A	147	ASP	3
1	A	125	LEU	3
1	A	211	GLU	2
1	A	194	LYS	2
1	A	132	SER	2
1	A	161	VAL	2
1	A	212	GLN	2
1	A	221	GLU	1
1	A	180	VAL	1
1	A	217	GLN	1
1	A	122	VAL	1
1	A	164	ARG	1
1	A	140	HIS	1
1	A	156	ARG	1
1	A	200	GLU	1
1	A	136	ARG	1
1	A	173	ASN	1

6.3.3 RNA ⓘ

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 oligosaccharides 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 60% for the well-defined parts and 60% 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	924
Number of shifts mapped to atoms	924
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
$^{13}\text{C}_\alpha$	114	-0.47 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	105	0.34 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	110	0.01 ± 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 60%, i.e. 875 atoms were assigned a chemical shift out of a possible 1449. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	312/531 (59%)	103/216 (48%)	106/212 (50%)	103/103 (100%)
Sidechain	509/765 (67%)	285/491 (58%)	202/236 (86%)	22/38 (58%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	54/153 (35%)	14/73 (19%)	39/76 (51%)	1/4 (25%)
Overall	875/1449 (60%)	402/780 (52%)	347/524 (66%)	126/145 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 60%, i.e. 923 atoms were assigned a chemical shift out of a possible 1549. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	334/573 (58%)	110/234 (47%)	114/228 (50%)	110/111 (99%)
Sidechain	533/814 (65%)	297/521 (57%)	212/249 (85%)	24/44 (55%)
Aromatic	56/162 (35%)	14/77 (18%)	41/81 (51%)	1/4 (25%)
Overall	923/1549 (60%)	421/832 (51%)	367/558 (66%)	135/159 (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	6.38	0.08 – 2.19	24.9

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:

