



Full wwPDB NMR Structure Validation Report ⓘ

Mar 29, 2026 – 11:07 PM UTC

PDB ID : 1XYJ / pdb_00001xyj
Title : NMR Structure of the cat prion protein
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Deposited on : 2004-11-10

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

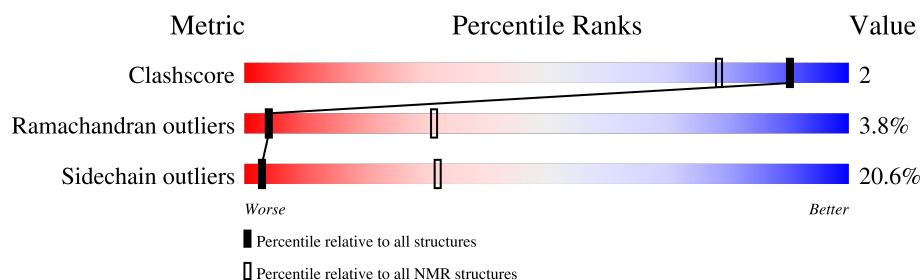
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	111	

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 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:127-A:166, A:175-A:223 (89)	0.88	16

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 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1787 atoms, of which 864 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called prion protein.

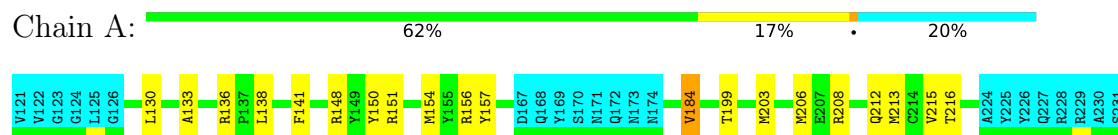
Mol	Chain	Residues	Atoms						Trace
1	A	111	Total	C	H	N	O	S	0
			1787	573	864	163	179	8	

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: prion protein

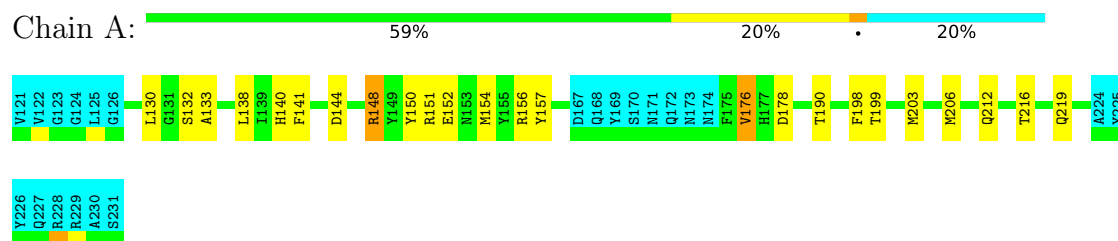


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

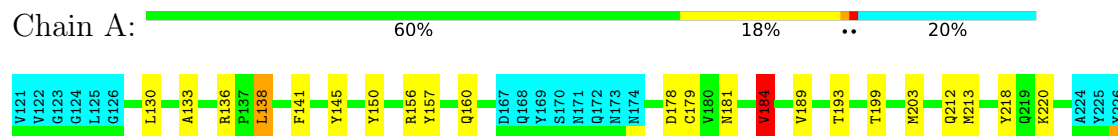
4.2.1 Score per residue for model 1

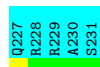
- Molecule 1: prion protein



4.2.2 Score per residue for model 2

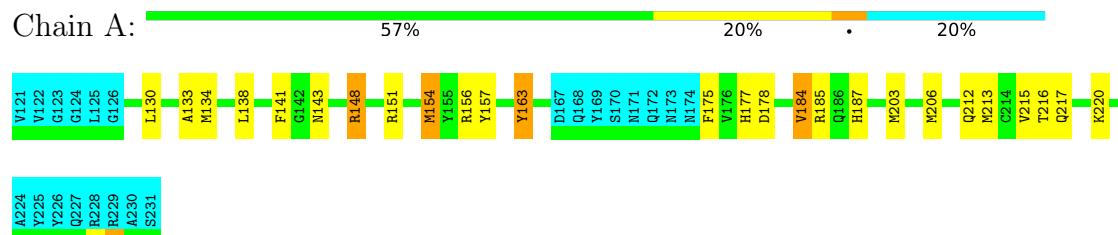
- Molecule 1: prion protein





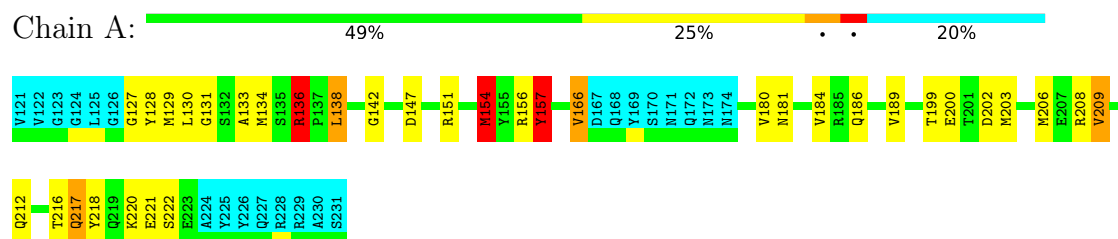
4.2.3 Score per residue for model 3

- Molecule 1: prion protein



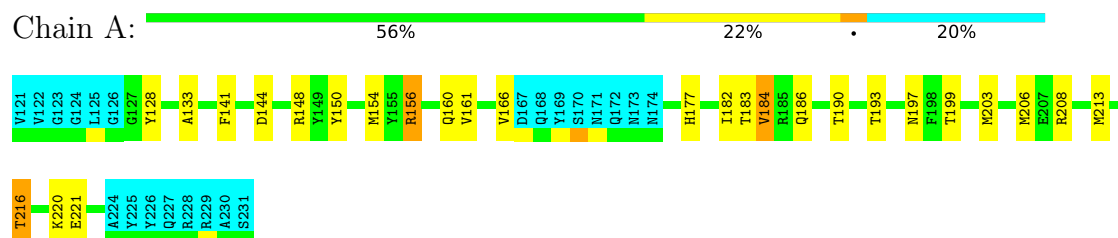
4.2.4 Score per residue for model 4

- Molecule 1: prion protein



4.2.5 Score per residue for model 5

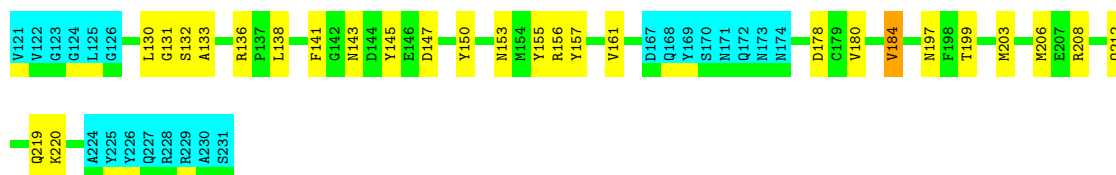
- Molecule 1: prion protein



4.2.6 Score per residue for model 6

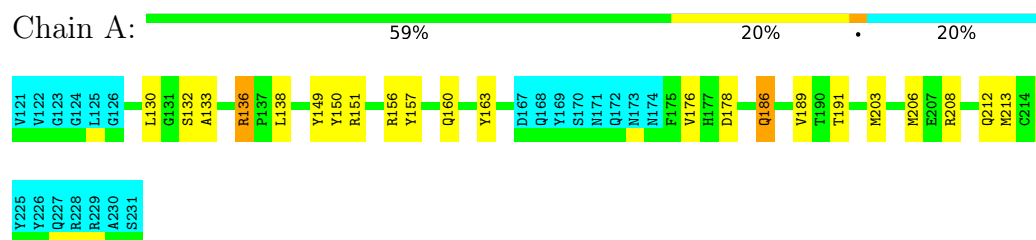
- Molecule 1: prion protein





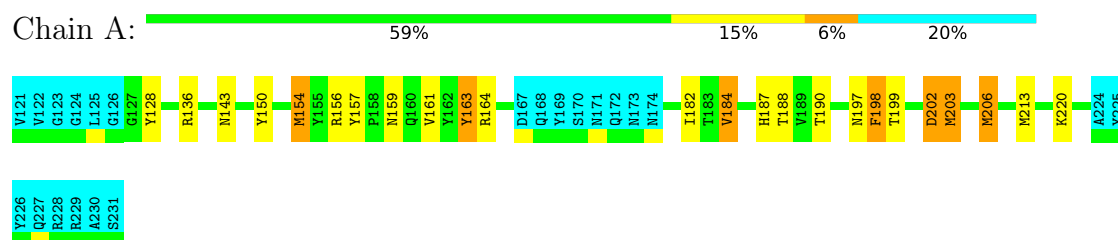
4.2.7 Score per residue for model 7

- Molecule 1: prion protein



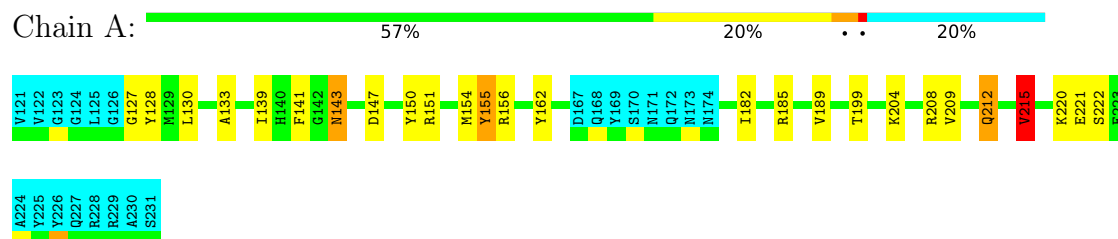
4.2.8 Score per residue for model 8

- Molecule 1: prion protein



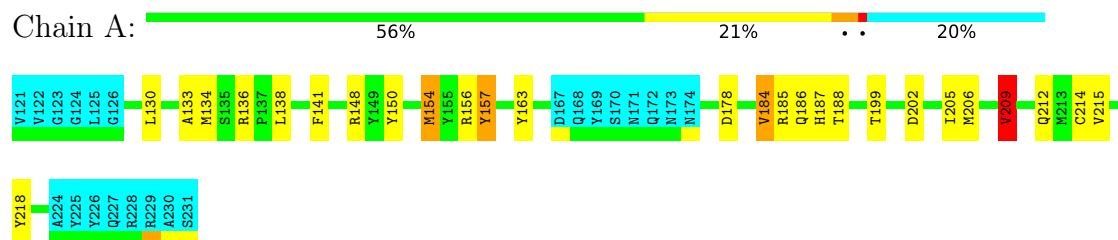
4.2.9 Score per residue for model 9

- Molecule 1: prion protein



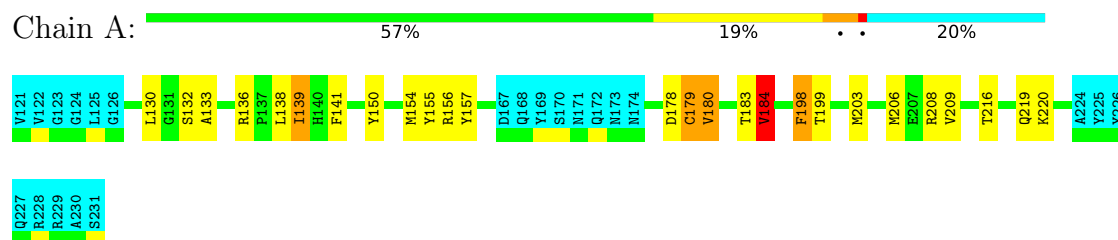
4.2.10 Score per residue for model 10

- Molecule 1: prion protein



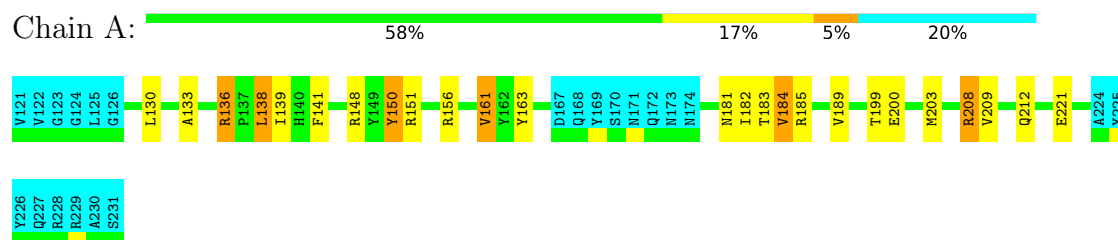
4.2.11 Score per residue for model 11

- Molecule 1: prion protein



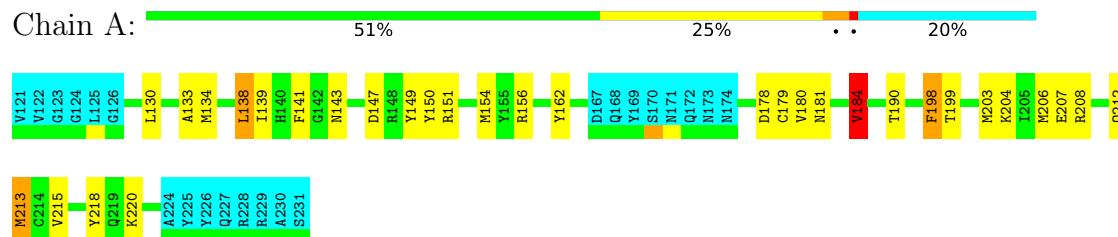
4.2.12 Score per residue for model 12

- Molecule 1: prion protein



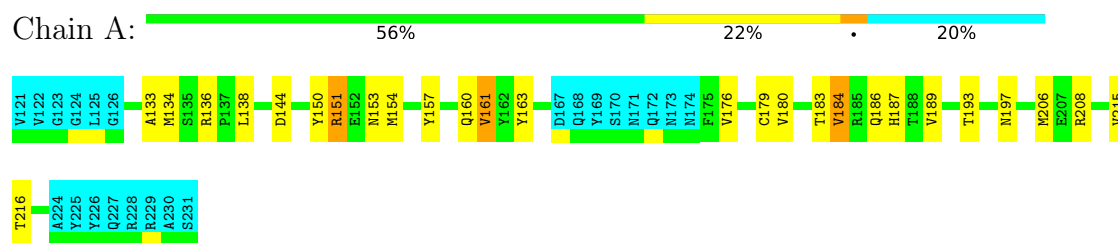
4.2.13 Score per residue for model 13

- Molecule 1: prion protein



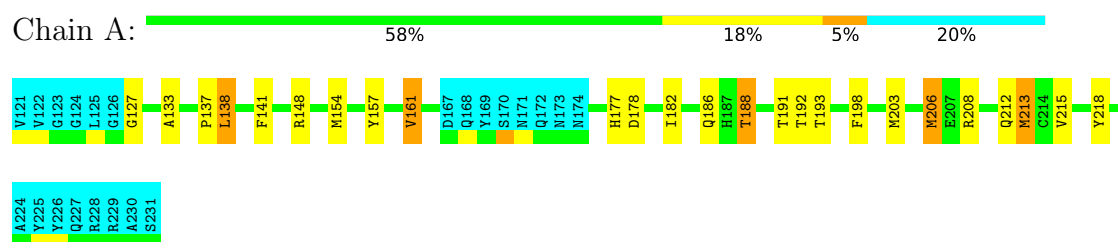
4.2.14 Score per residue for model 14

- Molecule 1: prion protein



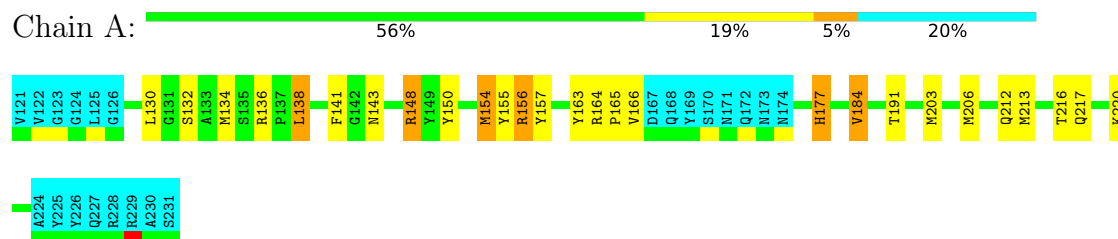
4.2.15 Score per residue for model 15

- Molecule 1: prion protein



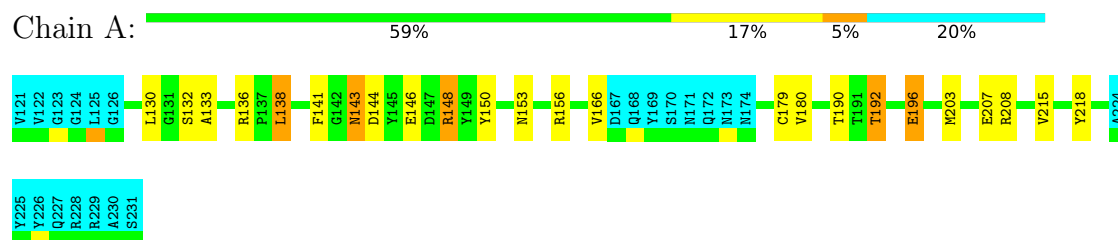
4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: prion protein



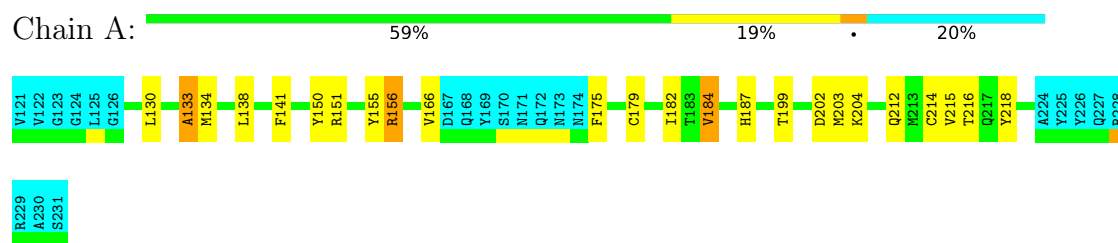
4.2.17 Score per residue for model 17

- Molecule 1: prion protein



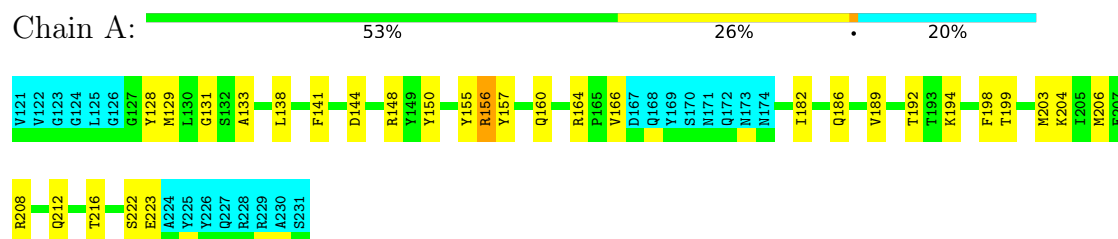
4.2.18 Score per residue for model 18

- Molecule 1: prion protein



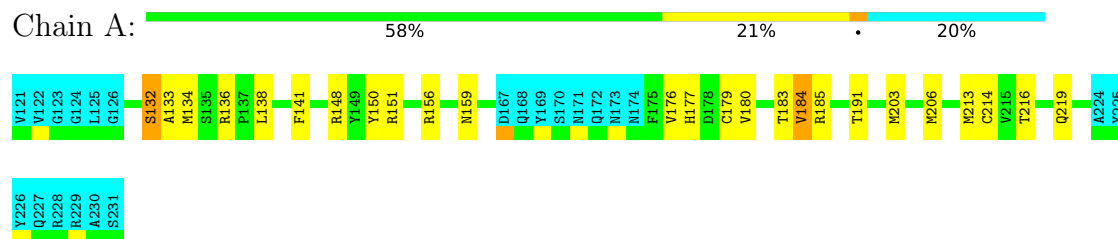
4.2.19 Score per residue for model 19

- Molecule 1: prion protein



4.2.20 Score per residue for model 20

- Molecule 1: prion protein



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *torsion angle dynamics*.

Of the 20 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	6.2
CANDID	refinement	1.0

No chemical shift data was provided.

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	0.72±0.01	0±0/768 (0.0± 0.0%)	1.49±0.04	5±2/1039 (0.5± 0.2%)
All	All	0.72	0/15360 (0.0%)	1.49	101/20780 (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	2.2±1.3
All	All	0	44

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	141	PHE	CA-CB-CG	9.26	123.06	113.80	13	15
1	A	157	TYR	CB-CA-C	8.55	122.22	109.22	7	1
1	A	184	VAL	CA-CB-CG2	7.82	123.69	110.40	18	9
1	A	176	VAL	N-CA-C	-7.59	105.63	111.62	1	1
1	A	180	VAL	CA-CB-CG2	6.92	122.16	110.40	14	5
1	A	148	ARG	CD-NE-CZ	6.61	133.66	124.40	16	1
1	A	209	VAL	CA-CB-CG2	6.52	121.49	110.40	10	2
1	A	222	SER	CA-C-N	6.49	128.88	120.44	9	1
1	A	222	SER	C-N-CA	6.49	128.88	120.44	9	1
1	A	144	ASP	CA-C-N	6.49	129.27	120.38	17	1
1	A	144	ASP	C-N-CA	6.49	129.27	120.38	17	1
1	A	178	ASP	CA-C-N	6.42	133.81	121.54	11	1
1	A	178	ASP	C-N-CA	6.42	133.81	121.54	11	1
1	A	184	VAL	CA-C-N	6.38	131.33	121.19	2	1
1	A	184	VAL	C-N-CA	6.38	131.33	121.19	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	176	VAL	CB-CA-C	6.34	117.12	110.91	7	1
1	A	136	ARG	CB-CA-C	6.11	115.54	111.20	4	2
1	A	180	VAL	N-CA-C	-6.06	104.72	110.42	13	2
1	A	143	ASN	CA-CB-CG	6.06	118.66	112.60	17	2
1	A	132	SER	CA-C-N	5.92	132.86	121.54	6	3
1	A	132	SER	C-N-CA	5.92	132.86	121.54	6	3
1	A	207	GLU	CA-C-N	5.91	128.79	120.28	17	1
1	A	207	GLU	C-N-CA	5.91	128.79	120.28	17	1
1	A	181	ASN	CA-C-N	5.87	128.16	120.60	4	1
1	A	181	ASN	C-N-CA	5.87	128.16	120.60	4	1
1	A	165	PRO	CA-C-N	5.82	132.44	121.97	16	1
1	A	165	PRO	C-N-CA	5.82	132.44	121.97	16	1
1	A	187	HIS	CB-CG-CD2	-5.73	123.76	131.20	10	3
1	A	177	HIS	CA-CB-CG	5.72	119.53	113.80	16	1
1	A	184	VAL	CA-CB-CG1	5.60	119.92	110.40	2	1
1	A	197	ASN	CA-CB-CG	-5.55	107.05	112.60	6	2
1	A	175	PHE	CA-CB-CG	5.55	119.35	113.80	3	1
1	A	221	GLU	CA-C-N	5.45	127.84	120.65	5	1
1	A	221	GLU	C-N-CA	5.45	127.84	120.65	5	1
1	A	198	PHE	CA-CB-CG	5.45	119.25	113.80	19	1
1	A	199	THR	CA-C-N	5.44	127.83	120.38	4	1
1	A	199	THR	C-N-CA	5.44	127.83	120.38	4	1
1	A	145	TYR	CA-C-N	5.41	127.47	120.44	6	1
1	A	145	TYR	C-N-CA	5.41	127.47	120.44	6	1
1	A	215	VAL	N-CA-C	-5.38	105.47	110.53	9	1
1	A	180	VAL	CA-C-N	5.37	127.73	120.38	17	1
1	A	180	VAL	C-N-CA	5.37	127.73	120.38	17	1
1	A	139	ILE	CA-C-N	5.36	127.73	120.38	13	1
1	A	139	ILE	C-N-CA	5.36	127.73	120.38	13	1
1	A	143	ASN	CA-C-N	5.34	128.17	120.38	13	1
1	A	143	ASN	C-N-CA	5.34	128.17	120.38	13	1
1	A	208	ARG	CD-NE-CZ	5.25	131.75	124.40	12	1
1	A	131	GLY	CA-C-N	5.24	128.98	120.60	4	1
1	A	131	GLY	C-N-CA	5.24	128.98	120.60	4	1
1	A	202	ASP	CA-C-N	5.20	127.20	120.44	8	1
1	A	202	ASP	C-N-CA	5.20	127.20	120.44	8	1
1	A	146	GLU	CA-C-N	5.20	128.01	120.79	17	1
1	A	146	GLU	C-N-CA	5.20	128.01	120.79	17	1
1	A	215	VAL	CA-CB-CG1	5.20	119.23	110.40	10	1
1	A	166	VAL	CB-CA-C	5.14	119.72	111.29	4	1
1	A	133	ALA	CA-C-N	5.10	129.84	122.44	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	133	ALA	C-N-CA	5.10	129.84	122.44	18	1
1	A	216	THR	CB-CA-C	5.07	118.83	110.88	5	1
1	A	137	PRO	CA-C-N	5.06	131.21	121.54	15	1
1	A	137	PRO	C-N-CA	5.06	131.21	121.54	15	1
1	A	153	ASN	CA-CB-CG	-5.04	107.56	112.60	14	1
1	A	148	ARG	CA-C-N	5.03	128.36	120.82	3	1
1	A	148	ARG	C-N-CA	5.03	128.36	120.82	3	1
1	A	132	SER	N-CA-C	5.02	118.18	111.75	16	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	7
1	A	151	ARG	Sidechain	5
1	A	163	TYR	Sidechain,Peptide	4
1	A	136	ARG	Sidechain	4
1	A	128	TYR	Sidechain	3
1	A	148	ARG	Sidechain	2
1	A	177	HIS	Peptide	2
1	A	218	TYR	Sidechain	2
1	A	156	ARG	Sidechain	2
1	A	149	TYR	Sidechain	2
1	A	164	ARG	Sidechain	2
1	A	155	TYR	Sidechain	2
1	A	162	TYR	Sidechain	2
1	A	145	TYR	Sidechain	1
1	A	142	GLY	Peptide	1
1	A	150	TYR	Sidechain	1
1	A	196	GLU	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	750	707	709	2±2
All	All	15000	14140	14180	50

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:154:MET:HE3	1:A:157:TYR:CE1	0.67	2.25	3	5
1:A:134:MET:HE1	1:A:216:THR:HG23	0.64	1.69	16	5
1:A:198:PHE:CE2	1:A:206:MET:HE2	0.62	2.30	15	1
1:A:161:VAL:HG12	1:A:183:THR:HG21	0.57	1.76	12	2
1:A:198:PHE:CE1	1:A:206:MET:HE2	0.57	2.34	8	1
1:A:181:ASN:HA	1:A:184:VAL:HG13	0.56	1.76	2	3
1:A:139:ILE:HD11	1:A:209:VAL:HA	0.54	1.79	11	1
1:A:161:VAL:HG11	1:A:213:MET:HG3	0.53	1.79	15	2
1:A:134:MET:HE1	1:A:216:THR:CG2	0.50	2.37	3	2
1:A:166:VAL:HG13	1:A:218:TYR:CE1	0.50	2.42	18	1
1:A:130:LEU:C	1:A:130:LEU:HD12	0.49	2.33	7	1
1:A:139:ILE:HD12	1:A:141:PHE:CE1	0.49	2.42	9	1
1:A:212:GLN:HA	1:A:215:VAL:HG22	0.48	1.84	9	1
1:A:212:GLN:O	1:A:216:THR:HG22	0.48	2.08	18	1
1:A:188:THR:HB	1:A:206:MET:HE1	0.48	1.86	8	2
1:A:198:PHE:CD2	1:A:206:MET:HE2	0.47	2.43	15	1
1:A:139:ILE:HD11	1:A:209:VAL:HG23	0.47	1.87	9	2
1:A:154:MET:HE3	1:A:157:TYR:HE2	0.47	1.69	11	1
1:A:139:ILE:CD1	1:A:209:VAL:HG23	0.46	2.39	12	1
1:A:180:VAL:O	1:A:184:VAL:HG22	0.46	2.11	11	1
1:A:154:MET:HE3	1:A:157:TYR:CZ	0.45	2.46	16	1
1:A:198:PHE:CD1	1:A:206:MET:HE2	0.45	2.46	8	1
1:A:154:MET:HE3	1:A:157:TYR:CE2	0.45	2.45	11	1
1:A:212:GLN:HA	1:A:215:VAL:CG2	0.45	2.42	9	1
1:A:198:PHE:CD2	1:A:206:MET:SD	0.44	3.10	13	1
1:A:192:THR:HG22	1:A:196:GLU:CD	0.44	2.38	17	1
1:A:150:TYR:CG	1:A:205:ILE:HG21	0.43	2.47	10	1
1:A:205:ILE:O	1:A:209:VAL:HG22	0.43	2.13	10	1
1:A:154:MET:HE3	1:A:157:TYR:CD1	0.42	2.48	4	1
1:A:184:VAL:HG11	1:A:203:MET:HE1	0.42	1.89	8	1
1:A:128:TYR:CE2	1:A:182:ILE:HG13	0.41	2.50	8	1
1:A:130:LEU:HD13	1:A:160:GLN:HB3	0.41	1.91	7	1
1:A:184:VAL:HG13	1:A:206:MET:HE3	0.41	1.92	4	1
1:A:134:MET:HE1	1:A:213:MET:O	0.41	2.15	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:MET:HE2	1:A:217:GLN:CG	0.40	2.46	4	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	89/111 (80%)	73±3 (82±4%)	13±3 (14±4%)	3±1 (4±1%)	4	31
All	All	1780/2220 (80%)	1455 (82%)	257 (14%)	68 (4%)	4	31

All 21 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	133	ALA	18
1	A	138	LEU	12
1	A	198	PHE	4
1	A	178	ASP	4
1	A	166	VAL	4
1	A	179	CYS	3
1	A	127	GLY	3
1	A	156	ARG	3
1	A	131	GLY	2
1	A	186	GLN	2
1	A	155	TYR	2
1	A	176	VAL	2
1	A	140	HIS	1
1	A	154	MET	1
1	A	153	ASN	1
1	A	143	ASN	1
1	A	147	ASP	1
1	A	184	VAL	1
1	A	161	VAL	1
1	A	136	ARG	1
1	A	194	LYS	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	84/101 (83%)	67±2 (79±3%)	17±2 (21±3%)	3	32
All	All	1680/2020 (83%)	1334 (79%)	346 (21%)	3	32

All 66 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	156	ARG	17
1	A	203	MET	17
1	A	150	TYR	16
1	A	130	LEU	13
1	A	206	MET	13
1	A	212	GLN	13
1	A	184	VAL	13
1	A	199	THR	12
1	A	138	LEU	12
1	A	208	ARG	12
1	A	148	ARG	10
1	A	154	MET	10
1	A	220	LYS	10
1	A	136	ARG	9
1	A	213	MET	8
1	A	215	VAL	8
1	A	189	VAL	7
1	A	151	ARG	6
1	A	186	GLN	6
1	A	182	ILE	6
1	A	190	THR	5
1	A	218	TYR	5
1	A	143	ASN	5
1	A	163	TYR	5
1	A	185	ARG	5
1	A	179	CYS	5
1	A	144	ASP	4
1	A	178	ASP	4
1	A	216	THR	4

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Mol	Chain	Res	Type	Models (Total)
1	A	219	GLN	4
1	A	160	GLN	4
1	A	193	THR	4
1	A	202	ASP	4
1	A	161	VAL	4
1	A	132	SER	4
1	A	191	THR	4
1	A	204	LYS	4
1	A	217	GLN	3
1	A	147	ASP	3
1	A	221	GLU	3
1	A	177	HIS	3
1	A	155	TYR	3
1	A	214	CYS	3
1	A	183	THR	3
1	A	192	THR	3
1	A	129	MET	2
1	A	200	GLU	2
1	A	209	VAL	2
1	A	222	SER	2
1	A	159	ASN	2
1	A	187	HIS	2
1	A	197	ASN	2
1	A	134	MET	2
1	A	188	THR	2
1	A	152	GLU	1
1	A	176	VAL	1
1	A	157	TYR	1
1	A	166	VAL	1
1	A	139	ILE	1
1	A	198	PHE	1
1	A	207	GLU	1
1	A	153	ASN	1
1	A	175	PHE	1
1	A	128	TYR	1
1	A	164	ARG	1
1	A	223	GLU	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

No chemical shift data were provided