



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:14 PM UTC

PDB ID : 1Y2S / pdb_00001y2s
Title : Ovine Prion Protein Variant R168
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Deposited on : 2004-11-23

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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

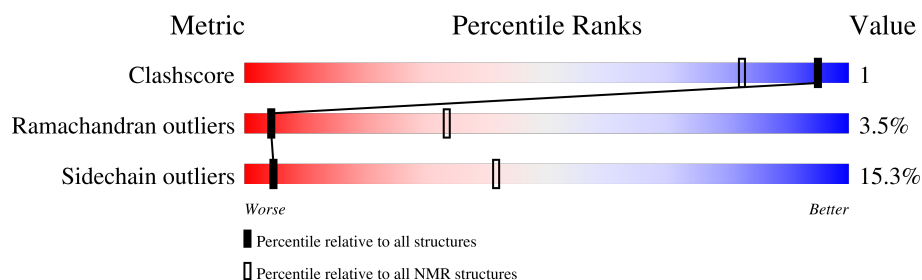
1 Overall quality at a glance

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	113	

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:164, A:173-A:220 (85)	0.88	12

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1802 atoms, of which 873 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
			1802	577	873	165	180	7	

There are 2 discrepancies between the modelled and reference sequences:

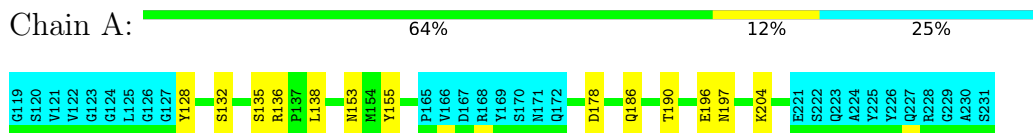
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	cloning artifact	UNP P23907
A	120	SER	-	cloning artifact	UNP P23907

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

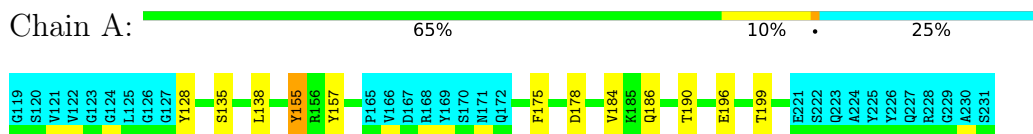


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Major prion protein



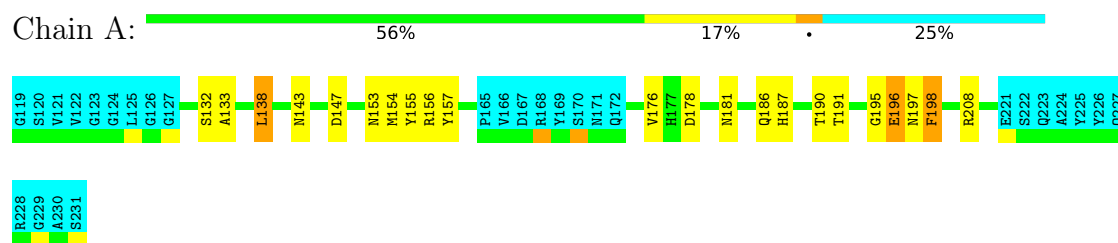
4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein



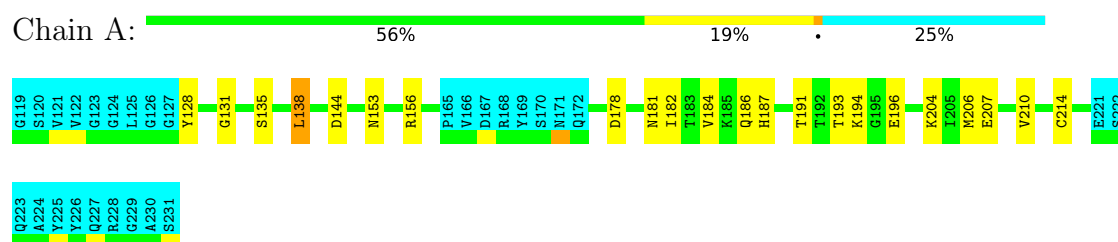
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



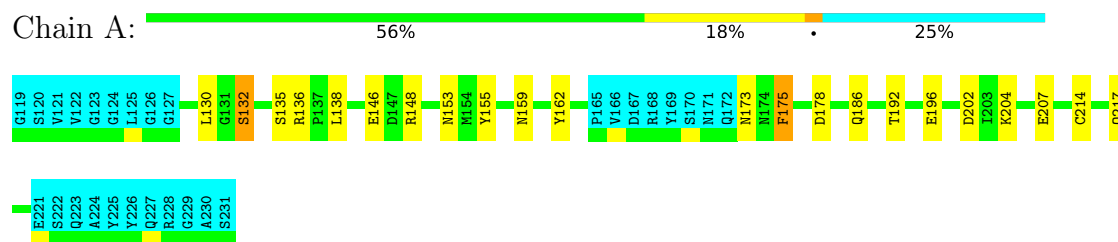
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



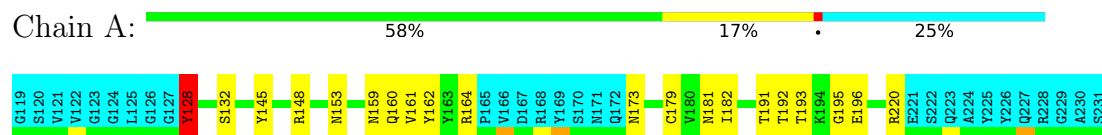
4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



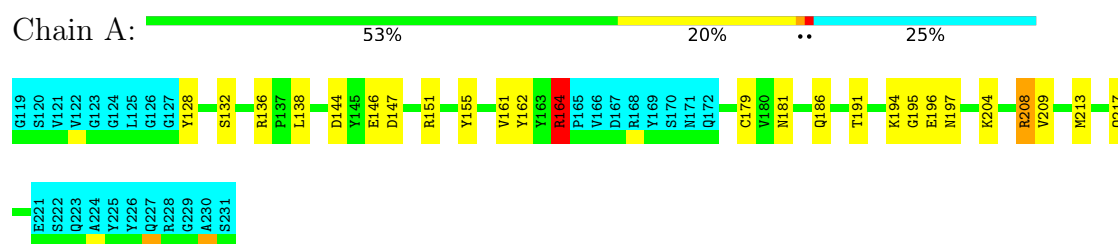
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



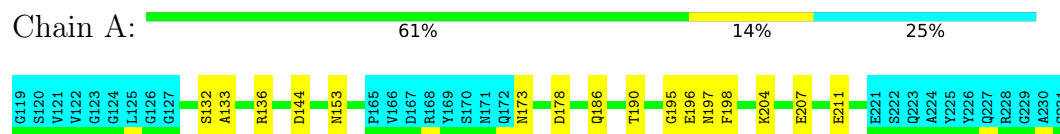
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



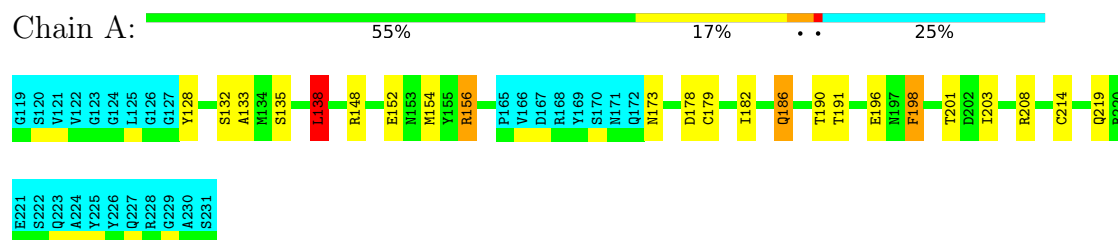
4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



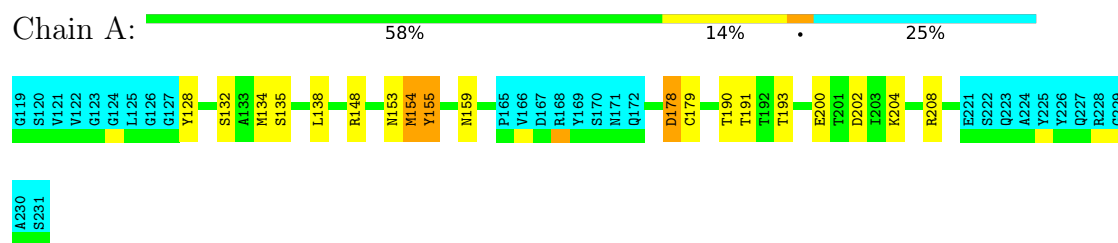
4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



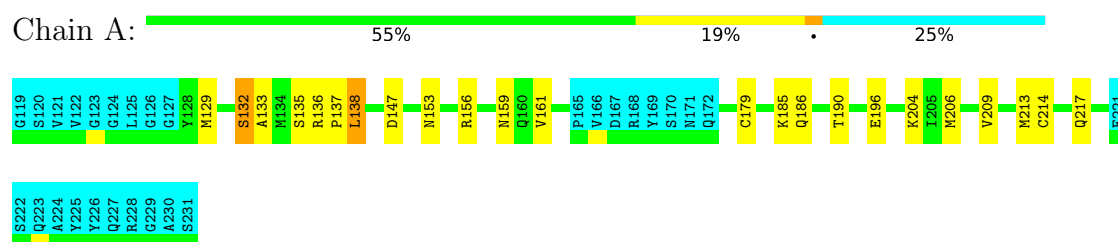
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



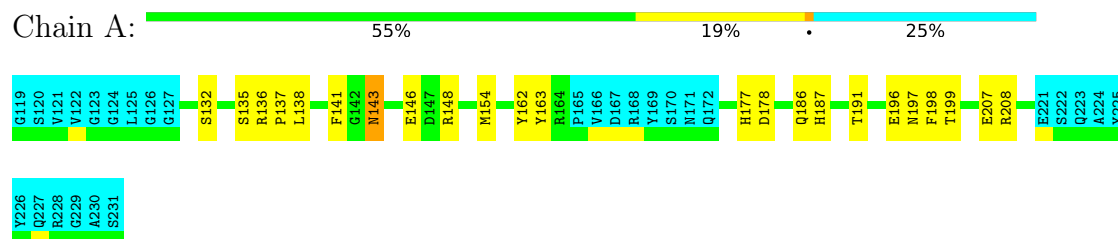
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Major prion protein



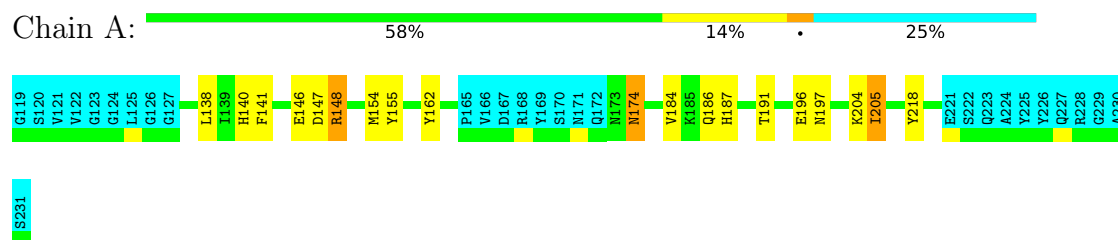
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



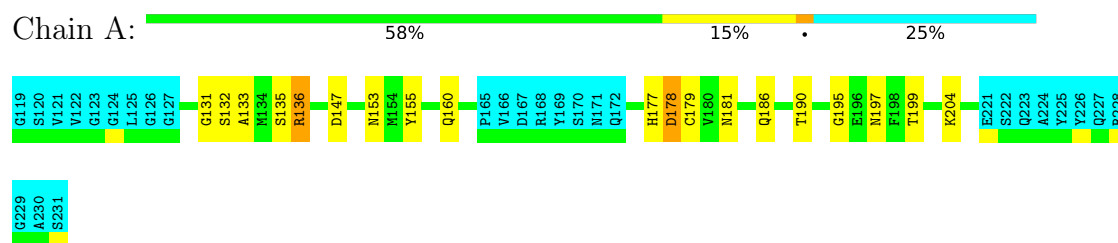
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



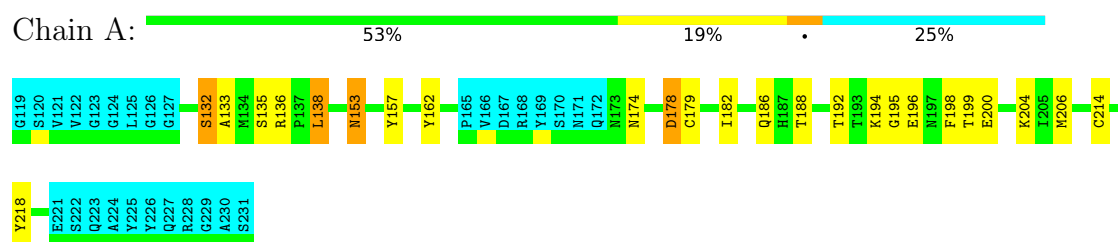
4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



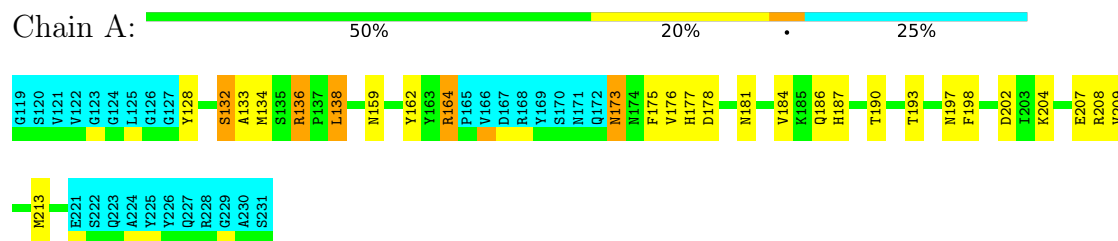
4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein



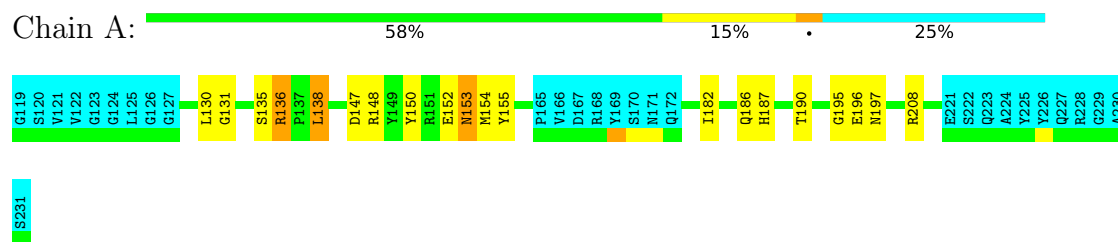
4.2.17 Score per residue for model 17

- Molecule 1: Major prion protein



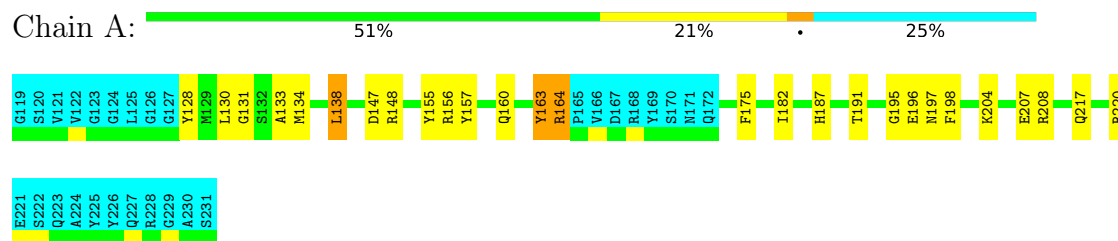
4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



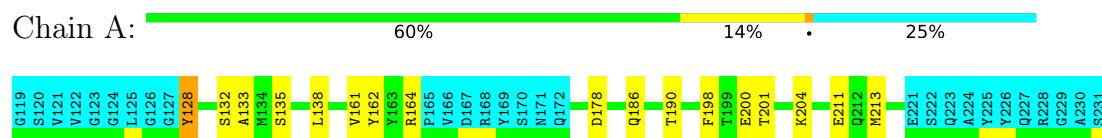
4.2.19 Score per residue for model 19

- 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
DYANA	structure solution	
OPALp	refinement	

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	0.71±0.01	0±0/742 (0.0± 0.0%)	1.46±0.05	5±3/1005 (0.5± 0.3%)
All	All	0.71	0/14840 (0.0%)	1.47	93/20100 (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	2.4±1.6
All	All	0	47

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	178	ASP	CA-CB-CG	9.19	121.79	112.60	15	3
1	A	153	ASN	CA-C-N	8.44	132.52	120.79	18	10
1	A	153	ASN	C-N-CA	8.44	132.52	120.79	18	10
1	A	153	ASN	CA-CB-CG	7.71	120.31	112.60	16	3
1	A	178	ASP	CA-C-N	7.70	131.10	120.63	16	1
1	A	178	ASP	C-N-CA	7.70	131.10	120.63	16	1
1	A	175	PHE	CA-CB-CG	7.14	120.94	113.80	17	3
1	A	132	SER	CA-C-N	6.94	134.80	121.54	12	5
1	A	132	SER	C-N-CA	6.94	134.80	121.54	12	5
1	A	179	CYS	CA-C-N	6.84	129.73	120.77	2	3
1	A	179	CYS	C-N-CA	6.84	129.73	120.77	2	3
1	A	174	ASN	CA-CB-CG	6.41	119.00	112.60	14	1
1	A	184	VAL	CA-CB-CG1	6.21	120.96	110.40	1	5
1	A	141	PHE	CA-CB-CG	6.14	119.94	113.80	13	1
1	A	191	THR	CB-CA-C	6.10	120.35	110.96	3	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	214	CYS	CA-C-N	5.98	128.96	120.53	16	1
1	A	214	CYS	C-N-CA	5.98	128.96	120.53	16	1
1	A	217	GLN	CA-C-N	5.75	128.23	120.65	8	1
1	A	217	GLN	C-N-CA	5.75	128.23	120.65	8	1
1	A	181	ASN	CA-CB-CG	-5.67	106.93	112.60	7	1
1	A	151	ARG	CD-NE-CZ	5.57	132.19	124.40	5	1
1	A	195	GLY	CA-C-N	5.50	132.03	121.54	7	4
1	A	195	GLY	C-N-CA	5.50	132.03	121.54	7	4
1	A	202	ASP	CA-CB-CG	-5.46	107.14	112.60	11	1
1	A	205	ILE	N-CA-C	-5.43	105.43	110.53	14	1
1	A	193	THR	N-CA-CB	-5.42	103.69	110.90	11	1
1	A	131	GLY	CA-C-N	5.38	131.81	121.54	18	3
1	A	131	GLY	C-N-CA	5.38	131.81	121.54	18	3
1	A	137	PRO	CA-C-N	5.24	131.54	121.54	12	1
1	A	137	PRO	C-N-CA	5.24	131.54	121.54	12	1
1	A	177	HIS	CB-CG-CD2	-5.22	124.42	131.20	15	1
1	A	137	PRO	N-CA-CB	5.16	105.86	102.25	13	1
1	A	187	HIS	CB-CG-CD2	-5.15	124.51	131.20	3	1
1	A	147	ASP	CA-C-N	5.12	127.59	120.63	14	1
1	A	147	ASP	C-N-CA	5.12	127.59	120.63	14	1
1	A	198	PHE	CA-CB-CG	-5.10	108.70	113.80	9	1
1	A	186	GLN	CA-CB-CG	5.04	124.17	114.10	10	1
1	A	197	ASN	CA-CB-CG	5.00	117.60	112.60	19	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	155	TYR	Sidechain	7
1	A	162	TYR	Sidechain	6
1	A	128	TYR	Sidechain	5
1	A	157	TYR	Sidechain	5
1	A	208	ARG	Sidechain	5
1	A	156	ARG	Sidechain	4
1	A	220	ARG	Sidechain	2
1	A	164	ARG	Sidechain	2
1	A	163	TYR	Sidechain,Peptide	2
1	A	148	ARG	Sidechain	2
1	A	218	TYR	Sidechain	2
1	A	149	TYR	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	132	SER	Peptide	1
1	A	151	ARG	Sidechain	1
1	A	195	GLY	Peptide	1
1	A	136	ARG	Sidechain	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	725	687	687	2±1
All	All	14500	13740	13740	30

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:138:LEU:HD23	1:A:154:MET:HE1	0.72	1.62	10	1
1:A:138:LEU:HD21	1:A:154:MET:HE1	0.70	1.62	11	1
1:A:138:LEU:HD21	1:A:154:MET:CE	0.65	2.21	11	1
1:A:132:SER:OG	1:A:134:MET:HE3	0.59	1.97	17	1
1:A:209:VAL:HG12	1:A:213:MET:HE2	0.56	1.77	8	3
1:A:161:VAL:HG13	1:A:213:MET:HE2	0.51	1.81	20	1
1:A:161:VAL:HG13	1:A:213:MET:HE3	0.50	1.84	8	2
1:A:206:MET:O	1:A:210:VAL:HG23	0.49	2.06	5	2
1:A:138:LEU:HA	1:A:150:TYR:CE2	0.45	2.47	18	1
1:A:198:PHE:CE2	1:A:203:ILE:HD11	0.45	2.47	10	1
1:A:188:THR:O	1:A:192:THR:HG23	0.45	2.11	16	1
1:A:179:CYS:SG	1:A:214:CYS:CB	0.45	3.05	10	2
1:A:138:LEU:HD23	1:A:154:MET:CE	0.45	2.42	5	1
1:A:128:TYR:CE2	1:A:162:TYR:CD2	0.44	3.05	20	1
1:A:141:PHE:CZ	1:A:205:ILE:HG23	0.43	2.48	14	1
1:A:143:ASN:CG	1:A:146:GLU:HB2	0.43	2.39	13	1
1:A:187:HIS:CE1	1:A:198:PHE:CZ	0.42	3.07	13	1
1:A:128:TYR:CE2	1:A:162:TYR:CE2	0.42	3.08	7	1
1:A:187:HIS:O	1:A:191:THR:HG23	0.42	2.14	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:209:VAL:CG1	1:A:213:MET:HE2	0.42	2.45	17	1
1:A:130:LEU:HD22	1:A:160:GLN:CG	0.42	2.45	19	1
1:A:173:ASN:HD22	1:A:173:ASN:C	0.41	2.23	17	1
1:A:179:CYS:CB	1:A:214:CYS:SG	0.41	3.06	12	1
1:A:131:GLY:HA2	1:A:163:TYR:CE1	0.41	2.51	19	1
1:A:128:TYR:CE2	1:A:182:ILE:HG21	0.40	2.51	5	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	85/113 (75%)	75±2 (88±2%)	7±2 (8±2%)	3±1 (4±2%)	4	33
All	All	1700/2260 (75%)	1504 (88%)	136 (8%)	60 (4%)	4	33

All 12 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	196	GLU	16
1	A	138	LEU	10
1	A	133	ALA	9
1	A	136	ARG	7
1	A	195	GLY	4
1	A	132	SER	4
1	A	164	ARG	4
1	A	128	TYR	2
1	A	198	PHE	1
1	A	192	THR	1
1	A	135	SER	1
1	A	152	GLU	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	81/101 (80%)	69±2 (85±3%)	12±2 (15±3%)	5 41
All	All	1620/2020 (80%)	1372 (85%)	248 (15%)	5 41

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	186	GLN	16
1	A	204	LYS	14
1	A	190	THR	12
1	A	138	LEU	12
1	A	135	SER	11
1	A	178	ASP	11
1	A	197	ASN	10
1	A	132	SER	8
1	A	148	ARG	8
1	A	182	ILE	7
1	A	207	GLU	7
1	A	147	ASP	6
1	A	198	PHE	6
1	A	173	ASN	6
1	A	199	THR	5
1	A	154	MET	5
1	A	181	ASN	5
1	A	208	ARG	5
1	A	159	ASN	5
1	A	155	TYR	4
1	A	175	PHE	4
1	A	187	HIS	4
1	A	193	THR	4
1	A	146	GLU	4
1	A	136	ARG	4
1	A	143	ASN	3
1	A	156	ARG	3
1	A	144	ASP	3
1	A	194	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	217	GLN	3
1	A	128	TYR	3
1	A	179	CYS	3
1	A	164	ARG	3
1	A	191	THR	3
1	A	200	GLU	3
1	A	192	THR	2
1	A	176	VAL	2
1	A	214	CYS	2
1	A	161	VAL	2
1	A	130	LEU	2
1	A	202	ASP	2
1	A	160	GLN	2
1	A	211	GLU	2
1	A	201	THR	2
1	A	134	MET	2
1	A	206	MET	2
1	A	177	HIS	2
1	A	174	ASN	2
1	A	153	ASN	2
1	A	139	ILE	1
1	A	196	GLU	1
1	A	145	TYR	1
1	A	152	GLU	1
1	A	129	MET	1
1	A	185	LYS	1
1	A	140	HIS	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

No chemical shift data were provided