



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 07:25 AM UTC

PDB ID : 1U3M / pdb_00001u3m
Title : NMR structure of the chicken prion protein fragment 128-242
Authors : Lysek, D.A.; Calzolari, L.; Guntert, P.; Wuthrich, K.
Deposited on : 2004-07-22

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

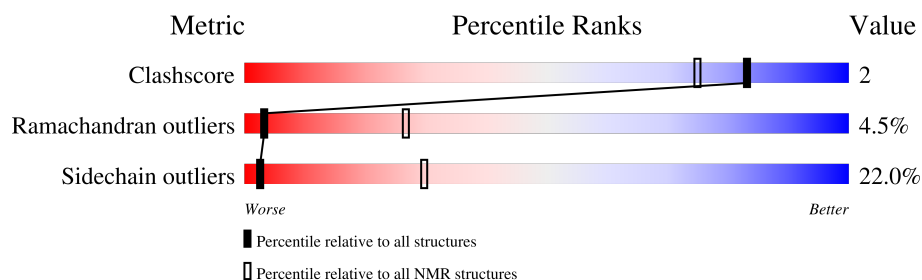
1 Overall quality at a glance

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	117	62% 18% • 20%

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:135-A:199, A:212-A:240 (94)	0.90	8

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 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1819 atoms, of which 884 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called prion-like protein.

Mol	Chain	Residues	Atoms						Trace
1	A	117	Total	C	H	N	O	S	0
			1819	585	884	163	180	7	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	GLY	-	cloning artifact	UNP P27177
A	127	SER	-	cloning artifact	UNP P27177

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-like protein

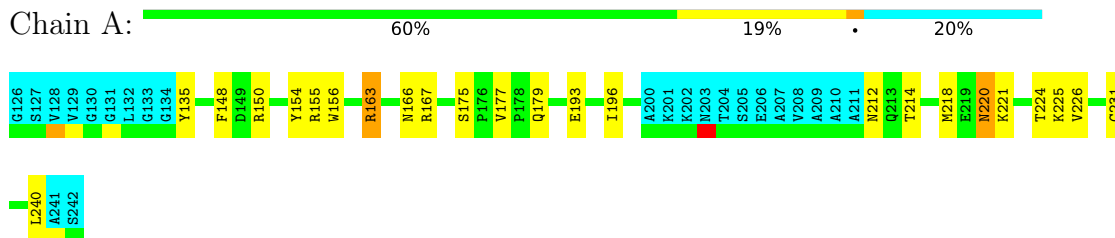


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

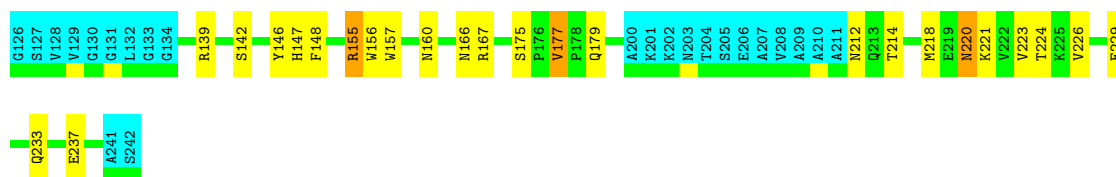
- Molecule 1: prion-like protein



4.2.2 Score per residue for model 2

- Molecule 1: prion-like protein





4.2.3 Score per residue for model 3

- Molecule 1: prion-like protein

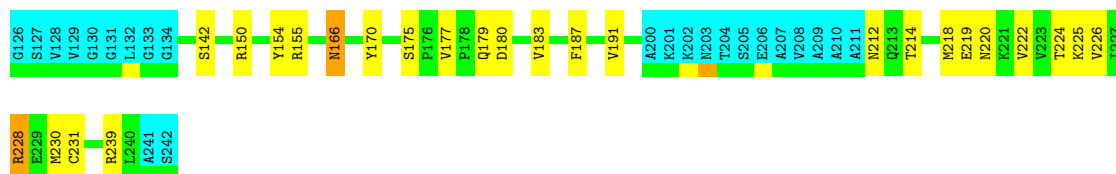
Chain A: 54% 24% 20%



4.2.4 Score per residue for model 4

- Molecule 1: prion-like protein

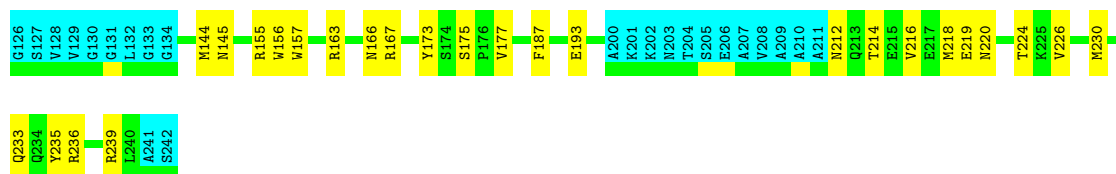
Chain A: 58% 21% 20%



4.2.5 Score per residue for model 5

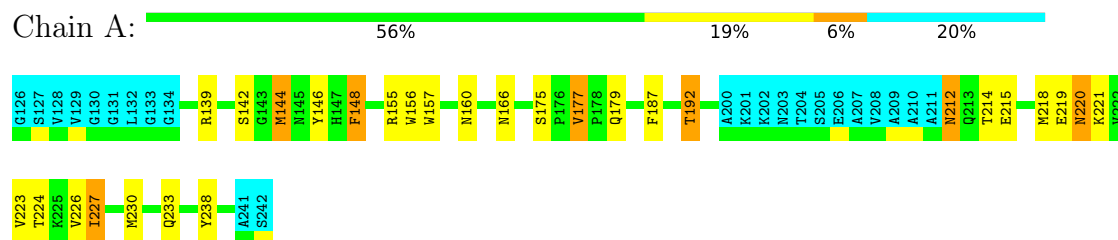
- Molecule 1: prion-like protein

Chain A: 58% 22% 20%



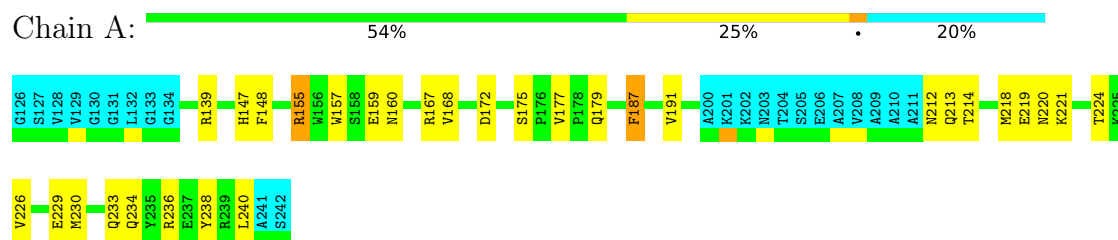
4.2.6 Score per residue for model 6

- Molecule 1: prion-like protein



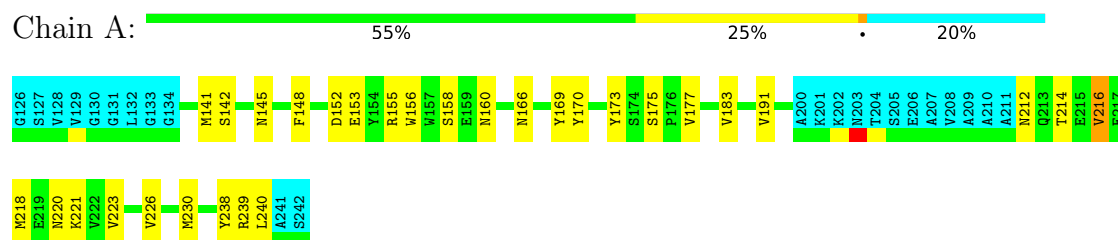
4.2.7 Score per residue for model 7

- Molecule 1: prion-like protein



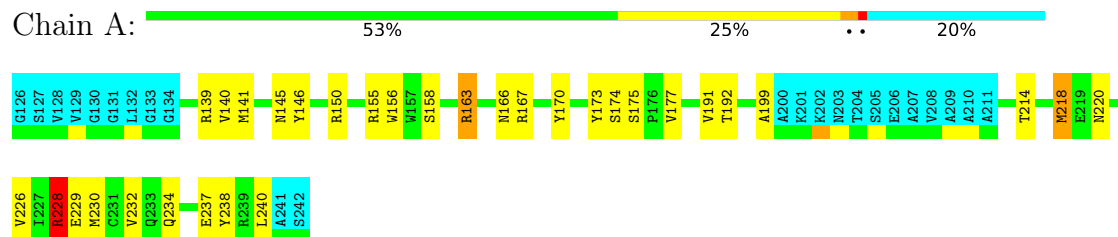
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: prion-like protein



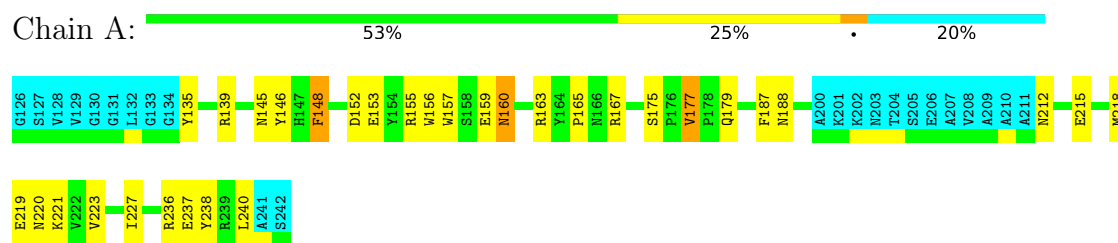
4.2.9 Score per residue for model 9

- Molecule 1: prion-like protein



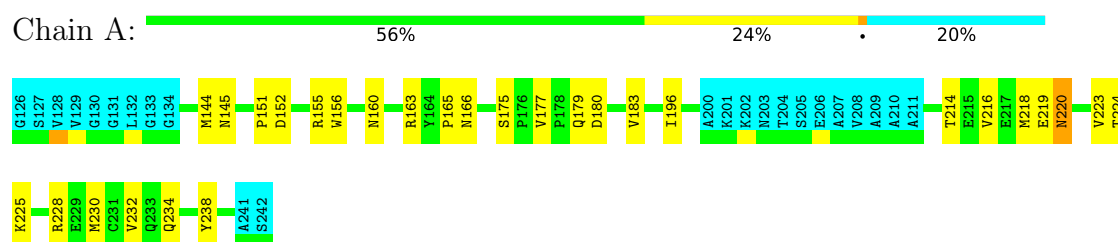
4.2.10 Score per residue for model 10

- Molecule 1: prion-like protein



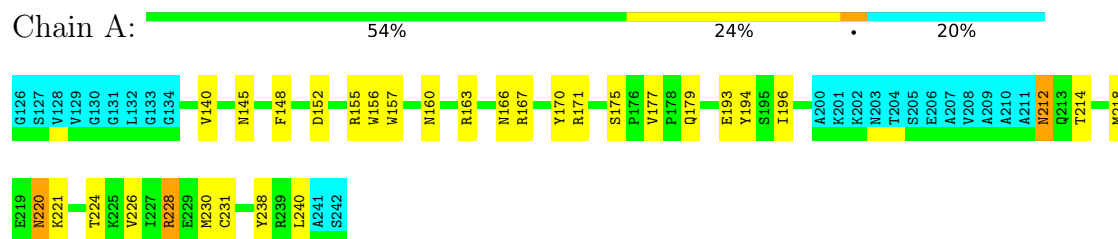
4.2.11 Score per residue for model 11

- Molecule 1: prion-like protein



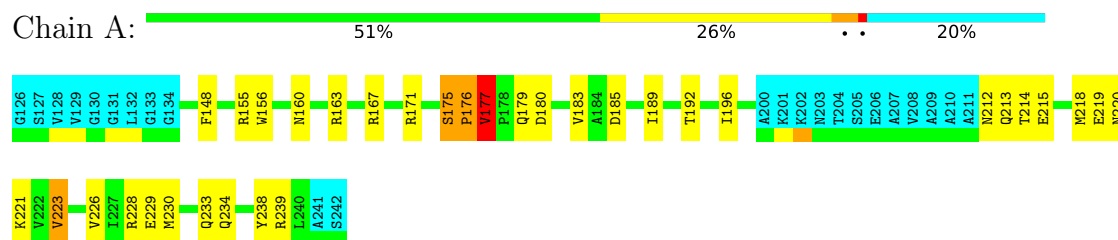
4.2.12 Score per residue for model 12

- Molecule 1: prion-like protein



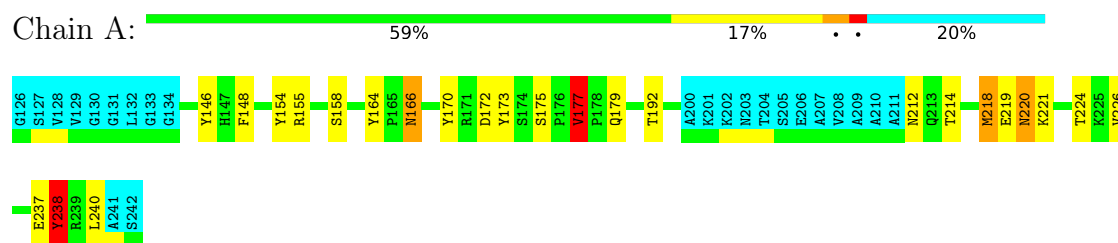
4.2.13 Score per residue for model 13

- Molecule 1: prion-like protein



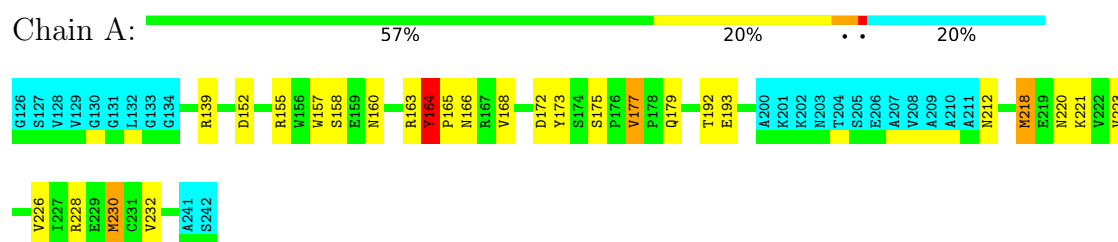
4.2.14 Score per residue for model 14

- Molecule 1: prion-like protein



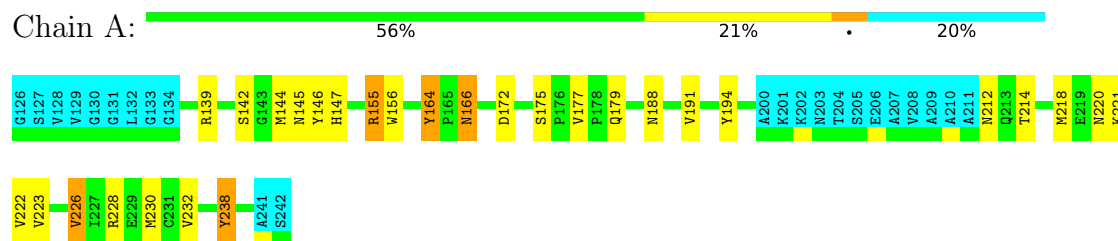
4.2.15 Score per residue for model 15

- Molecule 1: prion-like protein



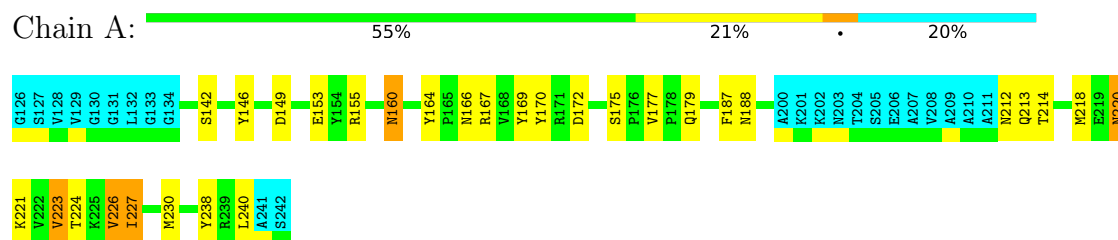
4.2.16 Score per residue for model 16

- Molecule 1: prion-like protein



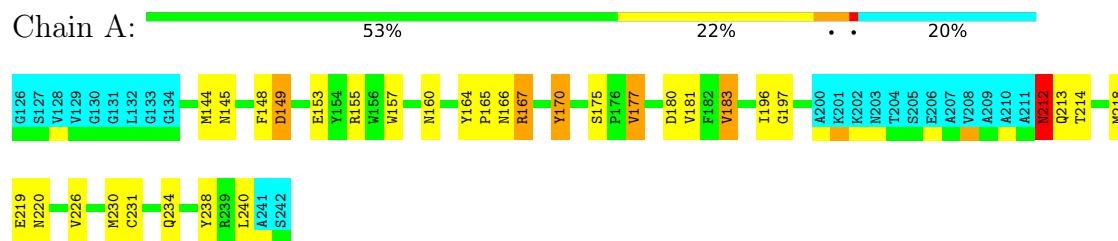
4.2.17 Score per residue for model 17

- Molecule 1: prion-like protein



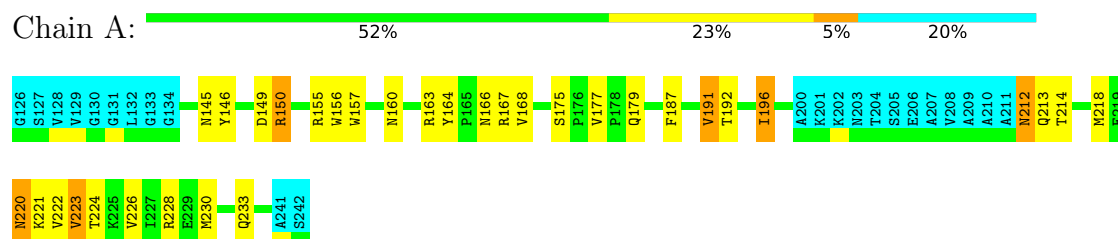
4.2.18 Score per residue for model 18

- Molecule 1: prion-like protein



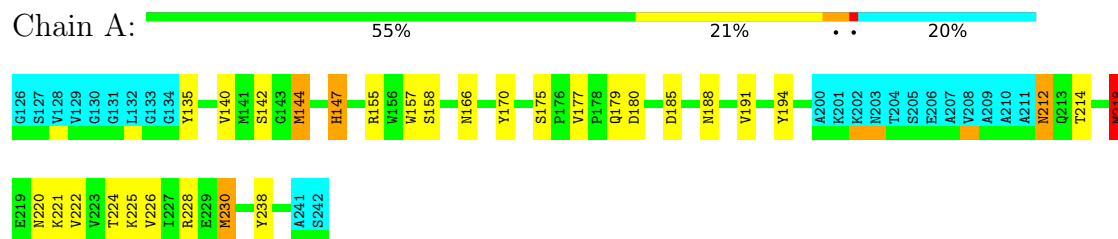
4.2.19 Score per residue for model 19

- Molecule 1: prion-like protein



4.2.20 Score per residue for model 20

- Molecule 1: prion-like 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: *structures with the least restraint violations*.

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

Software name	Classification	Version
DYANA	structure solution	6.0
DYANA	refinement	6.0

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	0.71±0.02	0±0/819 (0.0± 0.0%)	1.50±0.04	3±2/1113 (0.3± 0.2%)
All	All	0.71	0/16380 (0.0%)	1.50	65/22260 (0.3%)

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	2.1±0.9
All	All	0	43

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	177	VAL	CB-CA-C	8.71	117.86	109.33	2	6
1	A	160	ASN	CA-CB-CG	8.47	121.08	112.60	17	2
1	A	223	VAL	CA-CB-CG2	7.89	123.81	110.40	19	1
1	A	212	ASN	CA-CB-CG	-7.25	105.35	112.60	6	4
1	A	225	LYS	CA-C-O	-6.81	113.69	120.70	11	2
1	A	226	VAL	CA-CB-CG2	6.19	120.92	110.40	16	1
1	A	228	ARG	CD-NE-CZ	6.09	132.93	124.40	9	1
1	A	148	PHE	CA-CB-CG	5.90	119.70	113.80	14	1
1	A	218	MET	CA-C-N	5.87	128.95	120.38	20	1
1	A	218	MET	C-N-CA	5.87	128.95	120.38	20	1
1	A	188	ASN	CA-CB-CG	5.85	118.45	112.60	16	1
1	A	149	ASP	CA-C-N	5.81	130.16	120.86	18	1
1	A	149	ASP	C-N-CA	5.81	130.16	120.86	18	1
1	A	165	PRO	CA-C-N	5.77	132.56	121.54	15	2
1	A	165	PRO	C-N-CA	5.77	132.56	121.54	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	166	ASN	CA-CB-CG	5.74	118.34	112.60	16	3
1	A	192	THR	CA-CB-CG2	5.74	120.26	110.50	6	1
1	A	160	ASN	CA-C-N	5.74	128.76	120.38	8	1
1	A	160	ASN	C-N-CA	5.74	128.76	120.38	8	1
1	A	176	PRO	CA-C-N	5.57	132.43	122.13	13	1
1	A	176	PRO	C-N-CA	5.57	132.43	122.13	13	1
1	A	191	VAL	CA-CB-CG2	5.55	119.84	110.40	4	2
1	A	152	ASP	CA-CB-CG	5.46	118.06	112.60	8	2
1	A	151	PRO	CA-C-N	5.42	127.55	120.28	11	1
1	A	151	PRO	C-N-CA	5.42	127.55	120.28	11	1
1	A	197	GLY	CA-C-N	5.38	126.57	119.84	18	1
1	A	197	GLY	C-N-CA	5.38	126.57	119.84	18	1
1	A	150	ARG	CA-C-N	5.29	124.62	118.85	1	1
1	A	150	ARG	C-N-CA	5.29	124.62	118.85	1	1
1	A	191	VAL	CA-C-N	5.28	127.36	120.28	7	1
1	A	191	VAL	C-N-CA	5.28	127.36	120.28	7	1
1	A	159	GLU	CA-C-N	5.25	127.84	120.28	10	1
1	A	159	GLU	C-N-CA	5.25	127.84	120.28	10	1
1	A	219	GLU	CA-C-N	5.20	127.19	120.44	5	1
1	A	219	GLU	C-N-CA	5.20	127.19	120.44	5	1
1	A	238	TYR	CA-C-N	5.18	127.17	120.44	16	1
1	A	238	TYR	C-N-CA	5.18	127.17	120.44	16	1
1	A	232	VAL	CA-C-N	5.17	127.21	120.28	15	1
1	A	232	VAL	C-N-CA	5.17	127.21	120.28	15	1
1	A	172	ASP	CA-CB-CG	5.15	117.75	112.60	7	1
1	A	173	TYR	CA-C-N	5.12	127.45	120.54	9	1
1	A	173	TYR	C-N-CA	5.12	127.45	120.54	9	1
1	A	153	GLU	CB-CG-CD	5.11	121.30	112.60	17	1
1	A	148	PHE	CA-C-N	5.11	131.29	121.54	18	1
1	A	148	PHE	C-N-CA	5.11	131.29	121.54	18	1
1	A	185	ASP	CA-C-N	5.10	127.43	120.54	13	1
1	A	185	ASP	C-N-CA	5.10	127.43	120.54	13	1
1	A	240	LEU	CA-C-N	5.04	131.18	121.54	10	1
1	A	240	LEU	C-N-CA	5.04	131.18	121.54	10	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	ARG	Sidechain	4

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	228	ARG	Sidechain	4
1	A	163	ARG	Sidechain	3
1	A	171	ARG	Sidechain	3
1	A	173	TYR	Sidechain	3
1	A	236	ARG	Sidechain	3
1	A	239	ARG	Sidechain	3
1	A	194	TYR	Sidechain	3
1	A	154	TYR	Sidechain	2
1	A	167	ARG	Sidechain	2
1	A	169	TYR	Sidechain	2
1	A	146	TYR	Sidechain	2
1	A	150	ARG	Sidechain	2
1	A	170	TYR	Sidechain	2
1	A	135	TYR	Sidechain	1
1	A	235	TYR	Sidechain	1
1	A	238	TYR	Sidechain	1
1	A	164	TYR	Sidechain	1
1	A	142	SER	Peptide	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	796	741	741	4±2
All	All	15920	14820	14820	73

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:226:VAL:HG12	1:A:230:MET:HE1	0.89	1.43	17	2
1:A:226:VAL:HG22	1:A:230:MET:HE1	0.65	1.68	12	1
1:A:187:PHE:CE1	1:A:224:THR:HG23	0.61	2.30	4	3
1:A:218:MET:HE3	1:A:218:MET:HA	0.61	1.72	5	8
1:A:187:PHE:CZ	1:A:224:THR:HG22	0.60	2.31	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:226:VAL:CG1	1:A:230:MET:HE1	0.57	2.28	16	1
1:A:218:MET:HE2	1:A:222:VAL:HG23	0.56	1.77	16	2
1:A:220:ASN:O	1:A:224:THR:HG23	0.56	2.00	17	9
1:A:165:PRO:O	1:A:230:MET:HE1	0.55	2.02	11	1
1:A:177:VAL:HG22	1:A:181:VAL:HG21	0.54	1.78	3	1
1:A:148:PHE:CE2	1:A:156:TRP:CE3	0.53	2.96	2	1
1:A:191:VAL:HG23	1:A:199:ALA:CB	0.52	2.35	9	1
1:A:144:MET:HE1	1:A:230:MET:SD	0.50	2.46	20	2
1:A:228:ARG:O	1:A:232:VAL:HG23	0.50	2.06	9	3
1:A:183:VAL:HG23	1:A:231:CYS:HB2	0.49	1.84	18	1
1:A:187:PHE:CE1	1:A:191:VAL:HG11	0.48	2.43	19	1
1:A:144:MET:HE1	1:A:230:MET:HG3	0.48	1.85	11	1
1:A:187:PHE:CE1	1:A:224:THR:HG22	0.47	2.44	19	1
1:A:166:ASN:C	1:A:230:MET:HE3	0.47	2.35	9	2
1:A:144:MET:HE1	1:A:230:MET:HG2	0.46	1.87	5	1
1:A:164:TYR:CE1	1:A:226:VAL:HG21	0.46	2.45	19	1
1:A:141:MET:HE3	1:A:230:MET:HB3	0.46	1.86	8	1
1:A:220:ASN:HA	1:A:223:VAL:HG22	0.46	1.86	19	1
1:A:212:ASN:O	1:A:216:VAL:HG13	0.46	2.11	8	1
1:A:177:VAL:HG22	1:A:181:VAL:HG11	0.45	1.87	18	1
1:A:166:ASN:O	1:A:230:MET:HE3	0.45	2.12	9	1
1:A:238:TYR:CD1	1:A:238:TYR:C	0.45	2.94	14	1
1:A:168:VAL:HG21	1:A:230:MET:CB	0.44	2.43	15	1
1:A:226:VAL:HG12	1:A:230:MET:CE	0.44	2.40	16	1
1:A:187:PHE:HA	1:A:227:ILE:CG2	0.43	2.43	17	3
1:A:140:VAL:HG13	1:A:166:ASN:ND2	0.43	2.28	9	1
1:A:218:MET:HA	1:A:218:MET:CE	0.43	2.43	14	2
1:A:187:PHE:CZ	1:A:224:THR:HG23	0.43	2.48	7	3
1:A:218:MET:O	1:A:222:VAL:HG12	0.43	2.13	20	1
1:A:191:VAL:HG12	1:A:196:ILE:HD12	0.43	1.90	19	1
1:A:166:ASN:C	1:A:230:MET:SD	0.43	3.02	4	1
1:A:144:MET:HE1	1:A:230:MET:CG	0.42	2.44	11	1
1:A:173:TYR:CG	1:A:177:VAL:HG11	0.42	2.49	14	1
1:A:183:VAL:HG13	1:A:231:CYS:HB2	0.42	1.90	4	1
1:A:141:MET:SD	1:A:230:MET:HG2	0.41	2.55	9	1
1:A:146:TYR:CD1	1:A:148:PHE:CZ	0.41	3.09	6	1
1:A:183:VAL:HG21	1:A:232:VAL:HG22	0.41	1.92	11	1
1:A:148:PHE:CZ	1:A:156:TRP:CE3	0.41	3.09	10	1
1:A:223:VAL:HA	1:A:226:VAL:HG12	0.41	1.93	13	1
1:A:223:VAL:O	1:A:227:ILE:HD12	0.40	2.16	17	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	94/117 (80%)	81±2 (86±2%)	9±2 (9±2%)	4±1 (5±1%)	3	27
All	All	1880/2340 (80%)	1623 (86%)	172 (9%)	85 (5%)	3	27

All 16 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	175	SER	20
1	A	166	ASN	13
1	A	212	ASN	9
1	A	148	PHE	7
1	A	146	TYR	6
1	A	164	TYR	5
1	A	147	HIS	4
1	A	145	ASN	4
1	A	144	MET	4
1	A	163	ARG	4
1	A	135	TYR	2
1	A	172	ASP	2
1	A	149	ASP	2
1	A	176	PRO	1
1	A	177	VAL	1
1	A	165	PRO	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	87/99 (88%)	68±4 (78±4%)	19±4 (22±4%)	2	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1740/1980 (88%)	1358 (78%)	382 (22%)	2 30

All 62 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	177	VAL	20
1	A	220	ASN	20
1	A	155	ARG	19
1	A	214	THR	17
1	A	179	GLN	16
1	A	218	MET	14
1	A	221	LYS	14
1	A	226	VAL	14
1	A	238	TYR	14
1	A	157	TRP	11
1	A	160	ASN	11
1	A	156	TRP	10
1	A	167	ARG	10
1	A	240	LEU	9
1	A	212	ASN	9
1	A	223	VAL	9
1	A	219	GLU	9
1	A	139	ARG	8
1	A	170	TYR	8
1	A	196	ILE	7
1	A	233	GLN	7
1	A	192	THR	7
1	A	142	SER	6
1	A	158	SER	6
1	A	180	ASP	6
1	A	213	GLN	6
1	A	234	GLN	6
1	A	228	ARG	6
1	A	230	MET	6
1	A	163	ARG	5
1	A	145	ASN	5
1	A	193	GLU	4
1	A	229	GLU	4
1	A	237	GLU	4
1	A	153	GLU	4
1	A	150	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	216	VAL	3
1	A	215	GLU	3
1	A	183	VAL	3
1	A	191	VAL	3
1	A	152	ASP	3
1	A	188	ASN	3
1	A	231	CYS	2
1	A	149	ASP	2
1	A	166	ASN	2
1	A	225	LYS	2
1	A	227	ILE	2
1	A	147	HIS	2
1	A	168	VAL	2
1	A	140	VAL	2
1	A	164	TYR	2
1	A	172	ASP	2
1	A	239	ARG	1
1	A	159	GLU	1
1	A	187	PHE	1
1	A	174	SER	1
1	A	175	SER	1
1	A	189	ILE	1
1	A	154	TYR	1
1	A	222	VAL	1
1	A	185	ASP	1
1	A	224	THR	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