



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:18 PM UTC

PDB ID : 1XYK / pdb_00001xyk
Title : NMR Structure of the canine prion protein
Authors : Lysek, D.A.; Schorn, C.; Esteve-Moya, V.; Herrmann, T.; Wuthrich, K.
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

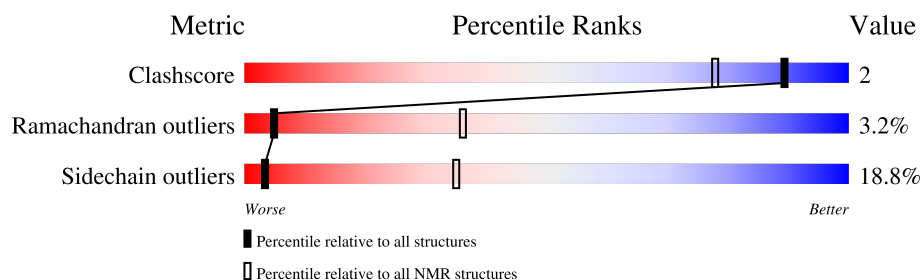
1 Overall quality at a glance

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	75% 17% 8%

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:126-A:227 (102)	1.13	2

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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1773 atoms, of which 858 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called prion protein.

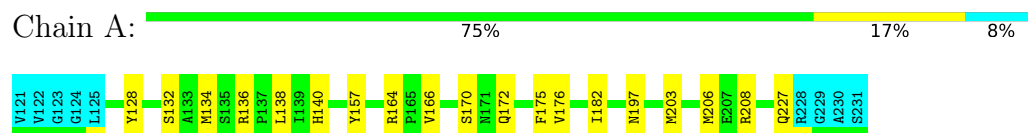
Mol	Chain	Residues	Atoms						Trace
1	A	111	Total	C	H	N	O	S	0
			1773	569	858	158	180	8	

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

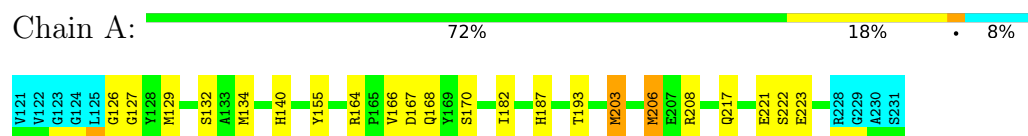


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

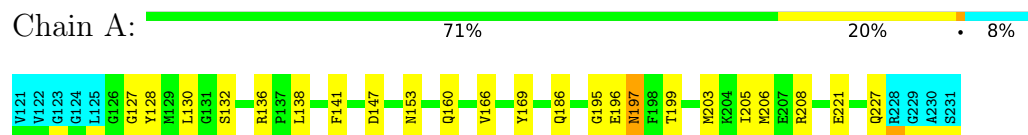
4.2.1 Score per residue for model 1

- Molecule 1: prion protein



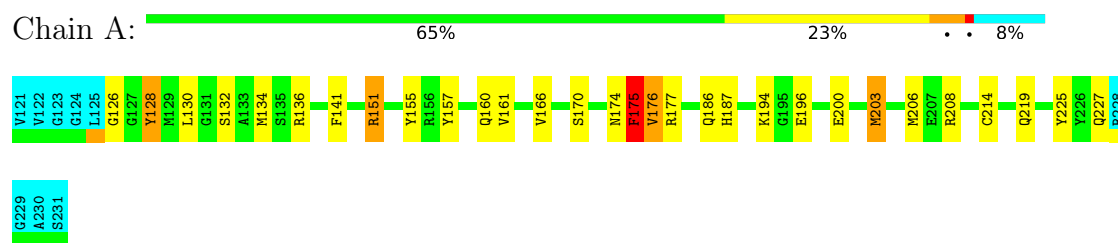
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: prion protein



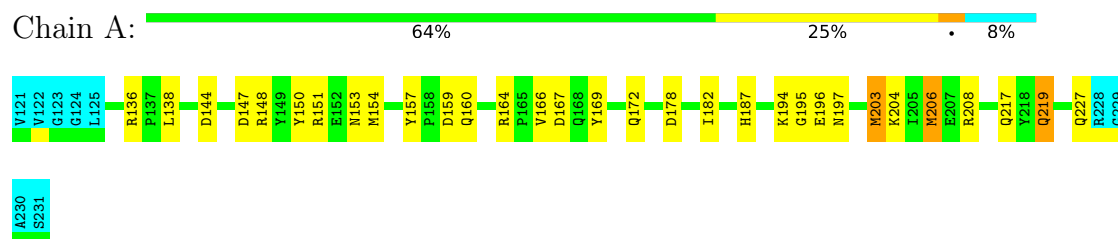
4.2.3 Score per residue for model 3

- Molecule 1: prion protein



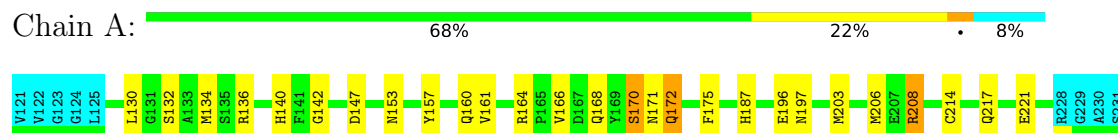
4.2.4 Score per residue for model 4

- Molecule 1: prion protein



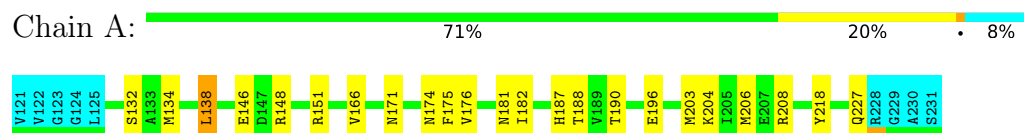
4.2.5 Score per residue for model 5

- Molecule 1: prion protein



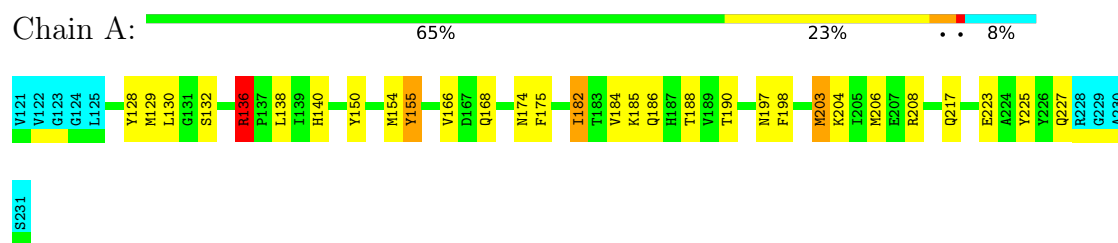
4.2.6 Score per residue for model 6

- Molecule 1: prion protein



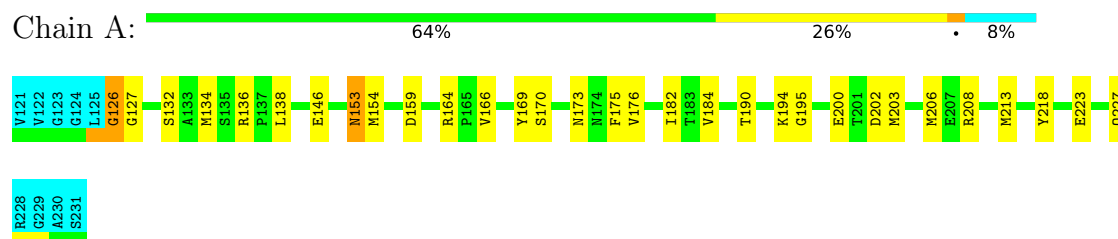
4.2.7 Score per residue for model 7

- Molecule 1: prion protein



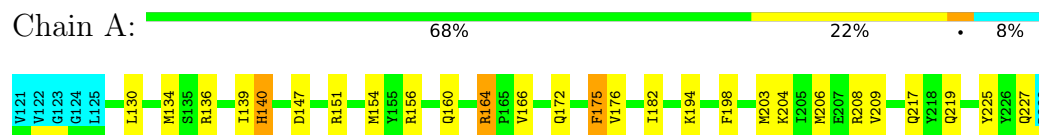
4.2.8 Score per residue for model 8

- Molecule 1: prion protein



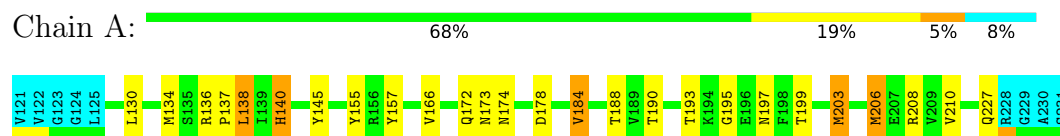
4.2.9 Score per residue for model 9

- Molecule 1: prion protein



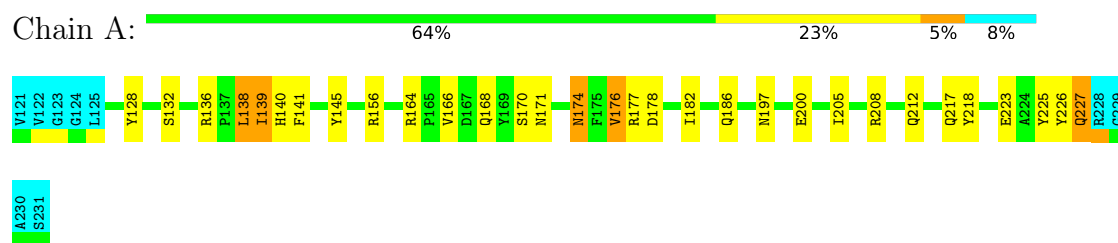
4.2.10 Score per residue for model 10

- Molecule 1: prion protein



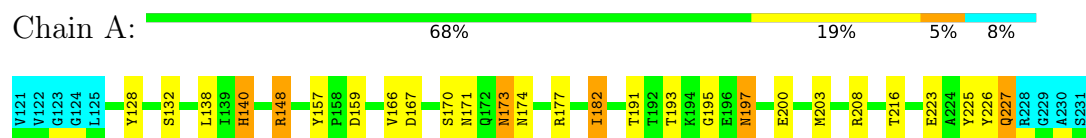
4.2.11 Score per residue for model 11

- Molecule 1: prion protein



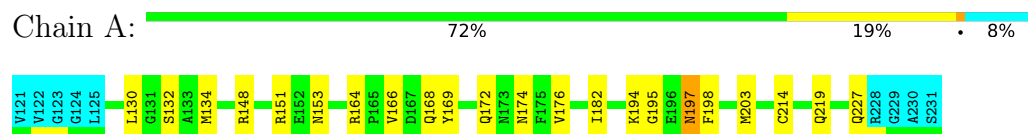
4.2.12 Score per residue for model 12

- Molecule 1: prion protein



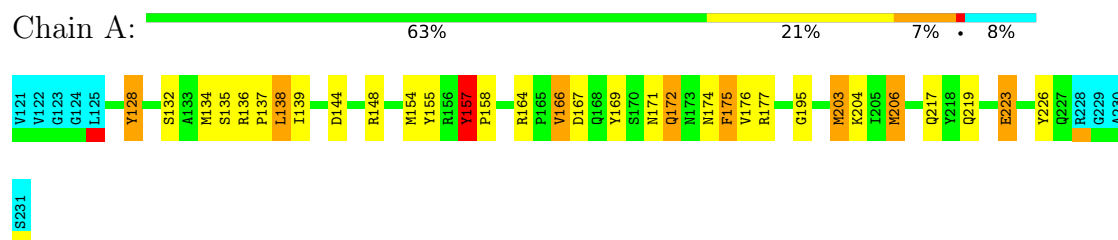
4.2.13 Score per residue for model 13

- Molecule 1: prion protein



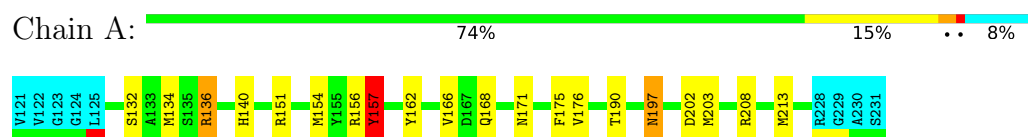
4.2.14 Score per residue for model 14

- Molecule 1: prion protein



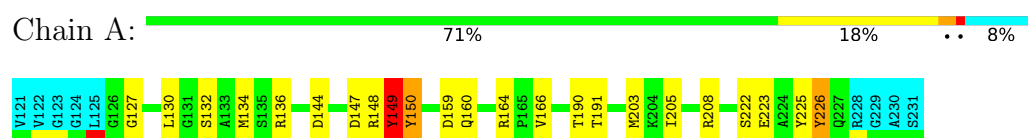
4.2.15 Score per residue for model 15

- Molecule 1: prion protein



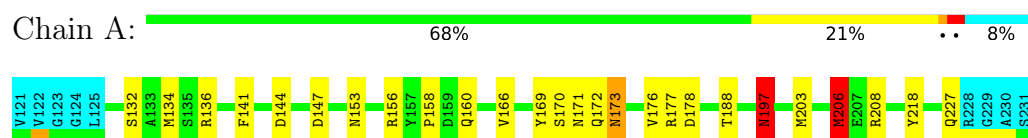
4.2.16 Score per residue for model 16

- Molecule 1: prion protein



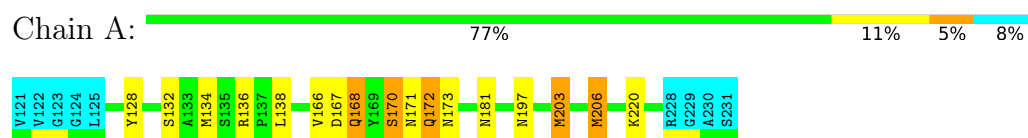
4.2.17 Score per residue for model 17

- Molecule 1: prion protein



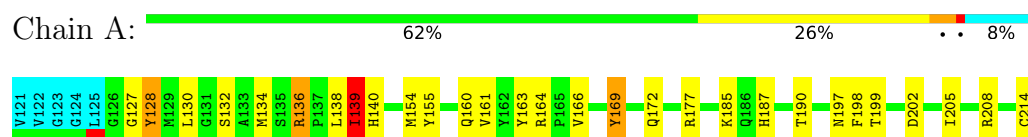
4.2.18 Score per residue for model 18

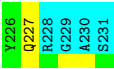
- Molecule 1: prion protein



4.2.19 Score per residue for model 19

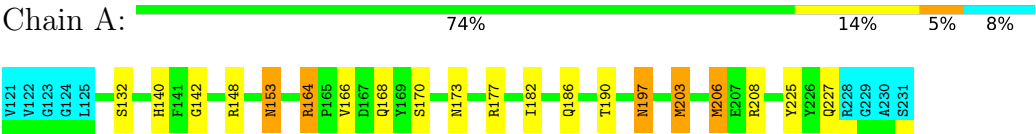
- Molecule 1: prion protein





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 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	6.2
CANDID	refinement	1.0
ATNOS	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	0.70±0.01	0±0/879 (0.0± 0.0%)	1.45±0.04	3±2/1189 (0.3± 0.2%)
All	All	0.70	0/17580 (0.0%)	1.45	63/23780 (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	0.1±0.2	2.2±1.4
All	All	1	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	157	TYR	CB-CA-C	14.31	130.29	109.26	14	4
1	A	153	ASN	CA-CB-CG	8.66	121.26	112.60	20	2
1	A	178	ASP	CA-CB-CG	7.71	120.31	112.60	17	1
1	A	197	ASN	CA-CB-CG	-7.22	105.38	112.60	2	6
1	A	181	ASN	CA-CB-CG	7.12	119.72	112.60	18	2
1	A	172	GLN	CA-C-N	6.91	130.60	121.90	5	1
1	A	172	GLN	C-N-CA	6.91	130.60	121.90	5	1
1	A	226	TYR	CA-C-N	6.42	131.73	122.23	16	1
1	A	226	TYR	C-N-CA	6.42	131.73	122.23	16	1
1	A	138	LEU	CB-CA-C	5.99	119.11	110.79	11	3
1	A	139	ILE	CA-C-N	5.92	130.89	121.66	19	1
1	A	139	ILE	C-N-CA	5.92	130.89	121.66	19	1
1	A	159	ASP	CA-CB-CG	5.89	118.49	112.60	4	3
1	A	176	VAL	CA-C-N	5.78	128.30	120.38	3	2
1	A	176	VAL	C-N-CA	5.78	128.30	120.38	3	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	137	PRO	N-CA-CB	5.67	108.28	103.35	14	2
1	A	140	HIS	CB-CG-CD2	-5.54	124.00	131.20	11	1
1	A	202	ASP	CA-CB-CG	5.45	118.05	112.60	8	2
1	A	175	PHE	CA-C-N	5.42	127.88	120.77	3	1
1	A	175	PHE	C-N-CA	5.42	127.88	120.77	3	1
1	A	141	PHE	CA-CB-CG	5.35	119.15	113.80	3	1
1	A	216	THR	CA-C-N	5.31	127.66	120.38	12	1
1	A	216	THR	C-N-CA	5.31	127.66	120.38	12	1
1	A	225	TYR	CA-C-N	5.31	130.62	121.86	9	3
1	A	225	TYR	C-N-CA	5.31	130.62	121.86	9	3
1	A	141	PHE	N-CA-C	-5.27	105.97	112.72	17	1
1	A	166	VAL	CB-CA-C	5.23	119.87	111.29	14	1
1	A	205	ILE	CA-C-N	5.16	127.15	120.44	19	1
1	A	205	ILE	C-N-CA	5.16	127.15	120.44	19	1
1	A	206	MET	CB-CG-SD	5.11	128.03	112.70	17	1
1	A	140	HIS	CA-CB-CG	5.09	118.89	113.80	10	2
1	A	153	ASN	CA-C-N	5.08	127.80	120.38	13	1
1	A	153	ASN	C-N-CA	5.08	127.80	120.38	13	1
1	A	158	PRO	N-CA-CB	5.08	107.77	103.35	17	1
1	A	173	ASN	CA-CB-CG	-5.07	107.53	112.60	10	1
1	A	184	VAL	CA-CB-CG1	5.07	119.01	110.40	10	1
1	A	210	VAL	CA-C-N	5.05	127.31	120.65	10	1
1	A	210	VAL	C-N-CA	5.05	127.31	120.65	10	1
1	A	157	TYR	CA-C-O	-5.05	115.08	120.23	14	1
1	A	219	GLN	CB-CG-CD	5.00	121.11	112.60	4	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	157	TYR	CA	1

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	208	ARG	Sidechain	7
1	A	164	ARG	Sidechain,Peptide	5
1	A	148	ARG	Sidechain	5
1	A	169	TYR	Sidechain,Peptide	3
1	A	136	ARG	Sidechain	3
1	A	156	ARG	Sidechain	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	142	GLY	Peptide	2
1	A	145	TYR	Sidechain	2
1	A	155	TYR	Sidechain	1
1	A	128	TYR	Sidechain	1
1	A	151	ARG	Sidechain	1
1	A	175	PHE	Sidechain	1
1	A	198	PHE	Sidechain	1
1	A	178	ASP	Peptide	1
1	A	225	TYR	Sidechain	1
1	A	226	TYR	Sidechain	1
1	A	157	TYR	Sidechain	1
1	A	162	TYR	Sidechain	1
1	A	149	TYR	Sidechain	1
1	A	150	TYR	Sidechain	1
1	A	163	TYR	Sidechain	1
1	A	177	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	859	797	799	3±2
All	All	17180	15940	15980	61

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:149:TYR:CE2	1:A:205:ILE:HD13	0.71	2.19	16	1
1:A:203:MET:HE3	1:A:206:MET:HE3	0.71	1.61	4	8
1:A:203:MET:HE3	1:A:206:MET:HE2	0.64	1.70	10	1
1:A:203:MET:SD	1:A:206:MET:HE2	0.64	2.33	17	1
1:A:203:MET:HE2	1:A:206:MET:HG2	0.59	1.73	17	1
1:A:203:MET:CE	1:A:206:MET:HE3	0.57	2.29	9	1
1:A:175:PHE:CD2	1:A:176:VAL:HG13	0.57	2.35	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:ARG:CG	1:A:154:MET:HE2	0.56	2.29	15	1
1:A:161:VAL:HG21	1:A:214:CYS:HA	0.56	1.77	3	3
1:A:203:MET:HE2	1:A:206:MET:CG	0.55	2.32	17	1
1:A:173:ASN:HD22	1:A:173:ASN:C	0.53	2.10	8	3
1:A:184:VAL:CG2	1:A:203:MET:HE1	0.53	2.34	10	1
1:A:138:LEU:HD21	1:A:151:ARG:HE	0.52	1.65	4	1
1:A:128:TYR:CD2	1:A:182:ILE:HG21	0.51	2.40	12	1
1:A:182:ILE:HG22	1:A:186:GLN:HE22	0.50	1.65	11	1
1:A:149:TYR:CE2	1:A:205:ILE:CD1	0.49	2.93	16	1
1:A:203:MET:CE	1:A:206:MET:HE2	0.49	2.38	17	2
1:A:139:ILE:HD13	1:A:209:VAL:HG22	0.48	1.86	9	1
1:A:128:TYR:CE2	1:A:182:ILE:HG13	0.48	2.44	12	1
1:A:149:TYR:CE2	1:A:150:TYR:HB2	0.48	2.44	16	1
1:A:136:ARG:CD	1:A:154:MET:HE3	0.47	2.39	15	1
1:A:172:GLN:CG	1:A:173:ASN:H	0.47	2.23	18	1
1:A:171:ASN:HD21	1:A:223:GLU:HG2	0.46	1.71	14	1
1:A:141:PHE:CZ	1:A:205:ILE:HG23	0.46	2.46	11	2
1:A:175:PHE:CG	1:A:176:VAL:N	0.46	2.83	3	2
1:A:171:ASN:HA	1:A:175:PHE:CE2	0.46	2.46	14	3
1:A:149:TYR:CZ	1:A:150:TYR:HB2	0.46	2.46	16	1
1:A:149:TYR:CG	1:A:150:TYR:N	0.46	2.84	16	1
1:A:149:TYR:CE2	1:A:150:TYR:CG	0.45	3.04	16	1
1:A:128:TYR:CZ	1:A:182:ILE:HG12	0.45	2.47	7	1
1:A:138:LEU:HG	1:A:154:MET:HE3	0.44	1.89	19	1
1:A:136:ARG:HD3	1:A:154:MET:HE2	0.43	1.91	7	1
1:A:203:MET:HA	1:A:203:MET:HE2	0.43	1.91	4	1
1:A:159:ASP:HA	1:A:213:MET:SD	0.42	2.53	8	1
1:A:150:TYR:CD2	1:A:157:TYR:CE2	0.42	3.07	4	1
1:A:151:ARG:HG3	1:A:154:MET:HE2	0.42	1.90	15	1
1:A:139:ILE:N	1:A:139:ILE:HD12	0.41	2.30	11	2
1:A:157:TYR:HB2	1:A:158:PRO:CD	0.41	2.46	14	1
1:A:176:VAL:HG13	1:A:177:ARG:H	0.41	1.75	3	1
1:A:138:LEU:HD23	1:A:154:MET:HE2	0.40	1.91	4	1
1:A:203:MET:HE3	1:A:206:MET:CE	0.40	2.46	20	1
1:A:128:TYR:CE2	1:A:164:ARG:HD2	0.40	2.51	11	1
1:A:138:LEU:O	1:A:138:LEU:HD13	0.40	2.16	14	1
1:A:157:TYR:C	1:A:157:TYR:CD1	0.40	2.99	15	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	102/111 (92%)	86±3 (85±3%)	12±2 (12±2%)	3±2 (3±2%)	5	36
All	All	2040/2220 (92%)	1729 (85%)	246 (12%)	65 (3%)	5	36

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	172	GLN	8
1	A	195	GLY	7
1	A	170	SER	6
1	A	127	GLY	5
1	A	168	GLN	4
1	A	175	PHE	4
1	A	227	GLN	4
1	A	167	ASP	4
1	A	128	TYR	3
1	A	169	TYR	3
1	A	166	VAL	3
1	A	126	GLY	2
1	A	140	HIS	2
1	A	174	ASN	2
1	A	171	ASN	2
1	A	221	GLU	1
1	A	155	TYR	1
1	A	154	MET	1
1	A	176	VAL	1
1	A	149	TYR	1
1	A	197	ASN	1

6.3.2 Protein sidechains [i](#)

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	95/100 (95%)	77±3 (81±3%)	18±3 (19±3%)	3	35
All	All	1900/2000 (95%)	1542 (81%)	358 (19%)	3	35

All 70 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	132	SER	17
1	A	166	VAL	17
1	A	203	MET	15
1	A	134	MET	14
1	A	136	ARG	14
1	A	197	ASN	13
1	A	208	ARG	11
1	A	227	GLN	11
1	A	206	MET	10
1	A	182	ILE	9
1	A	130	LEU	9
1	A	138	LEU	9
1	A	140	HIS	8
1	A	217	GLN	8
1	A	160	GLN	8
1	A	190	THR	8
1	A	223	GLU	7
1	A	174	ASN	7
1	A	164	ARG	7
1	A	187	HIS	6
1	A	147	ASP	6
1	A	153	ASN	6
1	A	196	GLU	5
1	A	155	TYR	5
1	A	194	LYS	5
1	A	219	GLN	5
1	A	204	LYS	5
1	A	168	GLN	5
1	A	170	SER	5
1	A	176	VAL	5
1	A	177	ARG	5
1	A	186	GLN	4
1	A	128	TYR	4
1	A	151	ARG	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	200	GLU	4
1	A	144	ASP	4
1	A	188	THR	4
1	A	218	TYR	4
1	A	225	TYR	4
1	A	193	THR	3
1	A	199	THR	3
1	A	157	TYR	3
1	A	171	ASN	3
1	A	198	PHE	3
1	A	139	ILE	3
1	A	148	ARG	3
1	A	173	ASN	3
1	A	226	TYR	3
1	A	129	MET	2
1	A	221	GLU	2
1	A	222	SER	2
1	A	169	TYR	2
1	A	178	ASP	2
1	A	146	GLU	2
1	A	175	PHE	2
1	A	184	VAL	2
1	A	185	LYS	2
1	A	154	MET	2
1	A	191	THR	2
1	A	172	GLN	2
1	A	167	ASP	1
1	A	150	TYR	1
1	A	212	GLN	1
1	A	214	CYS	1
1	A	135	SER	1
1	A	156	ARG	1
1	A	213	MET	1
1	A	220	LYS	1
1	A	202	ASP	1
1	A	216	THR	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