



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1Y16
Title : mouse prion protein with mutations S170N and N174T
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Deposited on : 2004-11-17

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

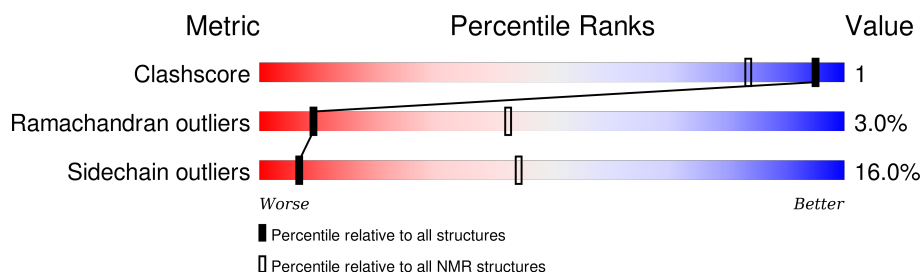
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	112	<div> <div></div> <div>78%</div> <div>16%</div> <div>6%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 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:125-A:229 (105)	0.41	14

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 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1794 atoms, of which 866 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	112	Total	C	H	N	O	S	0
			1794	576	866	163	180	9	

There are 2 discrepancies between the modelled and reference sequences:

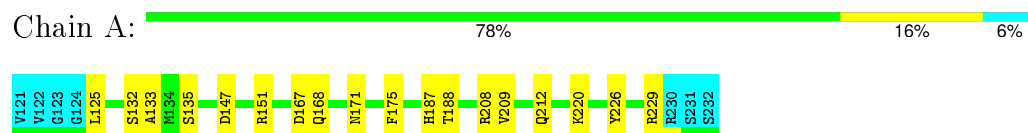
Chain	Residue	Modelled	Actual	Comment	Reference
A	170	ASN	SER	ENGINEERED	UNP P04925
A	174	THR	ASN	ENGINEERED	UNP P04925

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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

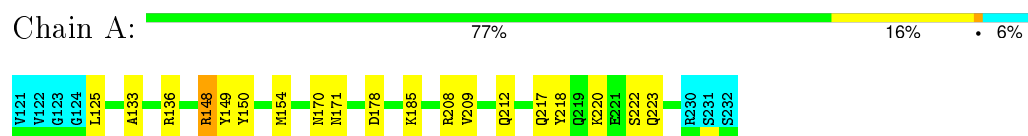


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

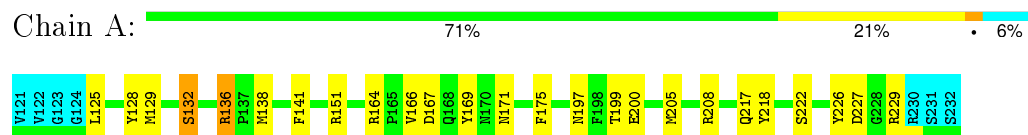
4.2.1 Score per residue for model 1

- Molecule 1: Major prion protein



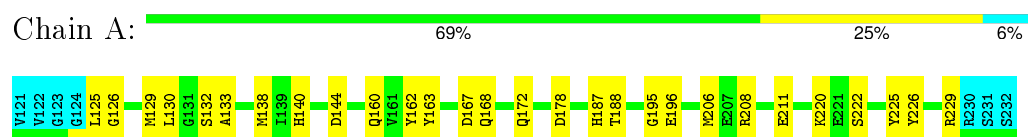
4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein



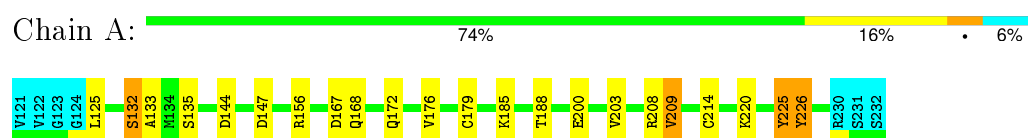
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



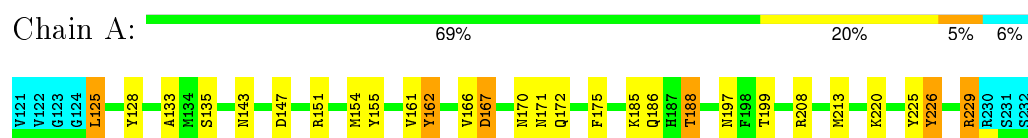
4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



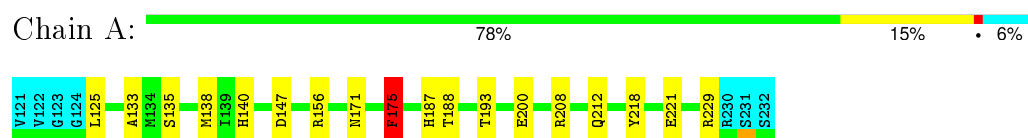
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



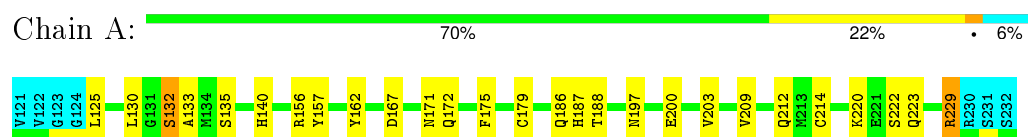
4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



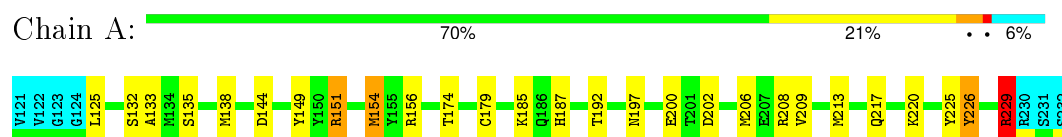
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



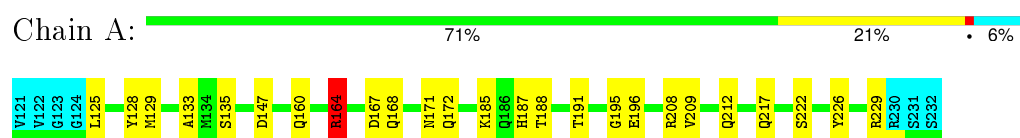
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



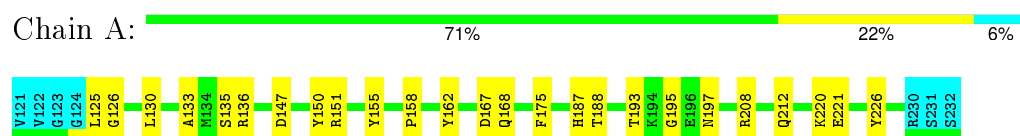
4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



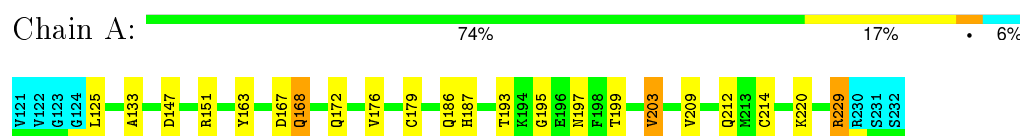
4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



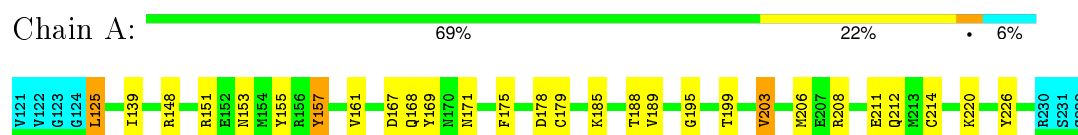
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



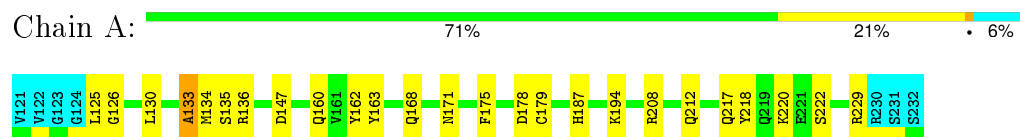
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



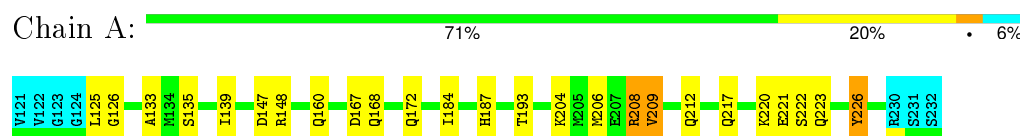
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



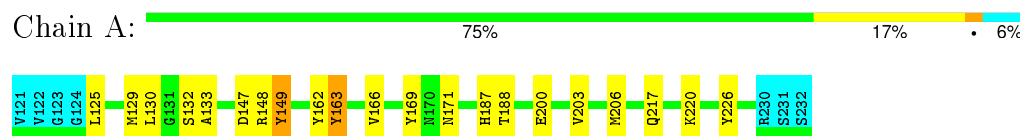
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Major prion protein



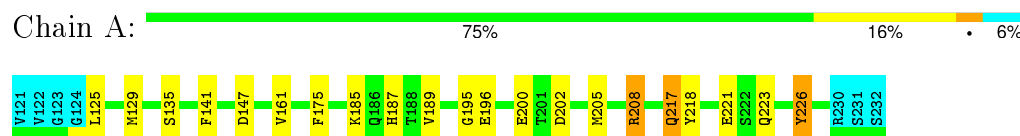
4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



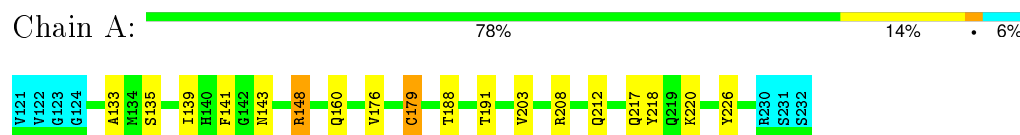
4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein



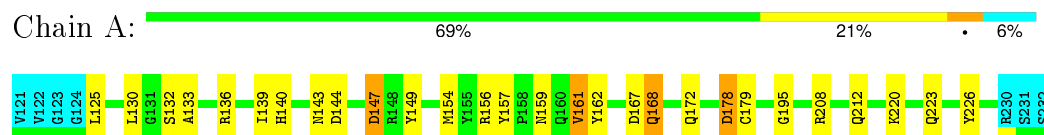
4.2.17 Score per residue for model 17

- Molecule 1: Major prion protein



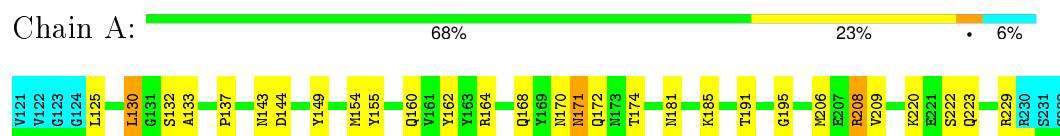
4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



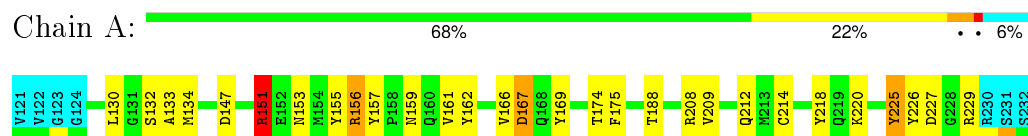
4.2.19 Score per residue for model 19

- 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	6.2
CANDID	refinement	1.0

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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	0.68±0.01	0±0/905 (0.0±0.0%)	1.15±0.04	3±2/1225 (0.2±0.2%)
All	All	0.68	0/18100 (0.0%)	1.15	56/24500 (0.2%)

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	2.3±1.3
All	All	1	46

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	151	ARG	NE-CZ-NH1	7.77	124.18	120.30	20	1
1	A	151	ARG	CD-NE-CZ	7.41	133.97	123.60	20	1
1	A	203	VAL	CA-CB-CG2	7.00	121.39	110.90	11	4
1	A	164	ARG	NE-CZ-NH2	-6.95	116.83	120.30	9	1
1	A	226	TYR	CB-CG-CD1	-6.93	116.84	121.00	5	3
1	A	151	ARG	NE-CZ-NH2	-6.87	116.87	120.30	20	2
1	A	157	TYR	CB-CG-CD2	-6.76	116.94	121.00	12	1
1	A	226	TYR	CB-CG-CD2	-6.58	117.05	121.00	2	4
1	A	208	ARG	NE-CZ-NH1	6.15	123.38	120.30	16	1
1	A	148	ARG	NE-CZ-NH2	-6.04	117.28	120.30	15	2
1	A	148	ARG	NE-CZ-NH1	5.97	123.28	120.30	1	1
1	A	229	ARG	CD-NE-CZ	5.95	131.93	123.60	7	1
1	A	128	TYR	CB-CG-CD1	-5.92	117.45	121.00	5	1
1	A	229	ARG	NE-CZ-NH1	5.91	123.25	120.30	11	2
1	A	225	TYR	CB-CG-CD2	-5.87	117.48	121.00	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	192	THR	CA-CB-CG2	5.81	120.54	112.40	8	1
1	A	132	SER	C-N-CA	5.72	136.01	121.70	18	1
1	A	175	PHE	CB-CG-CD2	-5.68	116.82	120.80	6	1
1	A	156	ARG	NE-CZ-NH2	5.58	123.09	120.30	6	3
1	A	209	VAL	CA-CB-CG1	5.55	119.23	110.90	4	1
1	A	136	ARG	NE-CZ-NH2	-5.50	117.55	120.30	2	2
1	A	208	ARG	NE-CZ-NH2	-5.47	117.56	120.30	16	1
1	A	191	THR	CA-CB-CG2	5.42	119.99	112.40	17	2
1	A	178	ASP	CB-CG-OD1	5.38	123.15	118.30	18	2
1	A	149	TYR	CB-CG-CD1	-5.30	117.82	121.00	15	2
1	A	189	VAL	CA-CB-CG1	5.28	118.82	110.90	16	2
1	A	156	ARG	NE-CZ-NH1	5.28	122.94	120.30	18	1
1	A	132	SER	N-CA-CB	-5.19	102.71	110.50	4	1
1	A	229	ARG	NE-CZ-NH2	-5.18	117.71	120.30	11	2
1	A	147	ASP	CB-CG-OD1	5.15	122.93	118.30	18	1
1	A	179	CYS	CA-CB-SG	5.15	123.26	114.00	8	2
1	A	161	VAL	CA-CB-CG1	5.11	118.56	110.90	18	1
1	A	164	ARG	NE-CZ-NH1	5.10	122.85	120.30	19	1
1	A	174	THR	CA-CB-CG2	-5.06	105.31	112.40	8	1
1	A	169	TYR	CB-CG-CD1	-5.01	117.99	121.00	12	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	151	ARG	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	6
1	A	229	ARG	Sidechain	6
1	A	149	TYR	Sidechain	4
1	A	157	TYR	Sidechain	4
1	A	226	TYR	Sidechain	4
1	A	156	ARG	Sidechain	3
1	A	163	TYR	Sidechain	3
1	A	151	ARG	Sidechain	2
1	A	150	TYR	Sidechain	2
1	A	169	TYR	Sidechain	2
1	A	196	GLU	Peptide	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	155	TYR	Sidechain	1
1	A	218	TYR	Sidechain	1
1	A	164	ARG	Sidechain	1
1	A	225	TYR	Sidechain	1
1	A	148	ARG	Sidechain	1
1	A	137	PRO	Peptide	1
1	A	162	TYR	Sidechain	1
1	A	175	PHE	Sidechain	1
1	A	171	ASN	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	883	819	819	2±2
All	All	17660	16380	16380	46

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:184:ILE:HG23	1:A:187:HIS:CE1	0.79	2.12	14	1
1:A:130:LEU:HD23	1:A:162:TYR:CD1	0.59	2.32	10	2
1:A:185:LYS:HA	1:A:188:THR:HG22	0.56	1.76	5	2
1:A:199:THR:O	1:A:203:VAL:HG13	0.52	2.04	12	2
1:A:130:LEU:HD13	1:A:162:TYR:CD1	0.50	2.41	15	1
1:A:130:LEU:HD23	1:A:162:TYR:CG	0.48	2.42	10	4
1:A:129:MET:HG3	1:A:163:TYR:CE1	0.48	2.44	3	2
1:A:130:LEU:HD23	1:A:162:TYR:CE1	0.48	2.44	3	1
1:A:225:TYR:HA	1:A:229:ARG:HG2	0.47	1.86	8	1
1:A:184:ILE:HG23	1:A:187:HIS:HE1	0.46	1.66	14	1
1:A:187:HIS:CE1	1:A:206:MET:CE	0.45	2.99	14	1
1:A:130:LEU:HG	1:A:162:TYR:CE1	0.45	2.47	19	1
1:A:158:PRO:HG3	1:A:187:HIS:CE1	0.45	2.46	10	1
1:A:218:TYR:CE1	1:A:222:SER:HB2	0.45	2.47	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:VAL:HG13	1:A:214:CYS:HB3	0.44	1.88	4	2
1:A:128:TYR:CE1	1:A:164:ARG:HD2	0.44	2.48	2	1
1:A:133:ALA:HA	1:A:160:GLN:CG	0.44	2.43	13	1
1:A:167:ASP:HB3	1:A:225:TYR:CE2	0.44	2.48	5	1
1:A:171:ASN:HD21	1:A:174:THR:HB	0.43	1.73	19	1
1:A:217:GLN:HE22	1:A:221:GLU:HG3	0.43	1.74	16	1
1:A:130:LEU:HD13	1:A:160:GLN:NE2	0.43	2.29	19	2
1:A:191:THR:HG22	1:A:196:GLU:HB3	0.43	1.91	9	1
1:A:162:TYR:CE1	1:A:186:GLN:HG3	0.42	2.48	5	1
1:A:141:PHE:CZ	1:A:205:MET:SD	0.42	3.13	16	2
1:A:187:HIS:CE1	1:A:206:MET:HE1	0.42	2.50	14	1
1:A:187:HIS:NE2	1:A:206:MET:CE	0.42	2.83	14	1
1:A:176:VAL:HA	1:A:179:CYS:SG	0.42	2.55	17	1
1:A:130:LEU:HD13	1:A:162:TYR:CG	0.41	2.50	15	1
1:A:169:TYR:CG	1:A:175:PHE:HB2	0.41	2.50	2	1
1:A:128:TYR:CE2	1:A:164:ARG:HD3	0.41	2.51	9	1
1:A:139:ILE:HD11	1:A:209:VAL:HA	0.40	1.92	14	1
1:A:130:LEU:HD23	1:A:162:TYR:CD2	0.40	2.51	13	1
1:A:130:LEU:HD13	1:A:162:TYR:CE2	0.40	2.51	7	1
1:A:184:ILE:HA	1:A:187:HIS:NE2	0.40	2.31	14	1
1:A:200:GLU:HA	1:A:203:VAL:HG22	0.40	1.93	7	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	105/112 (94%)	89±3 (85±2%)	13±2 (12±2%)	3±1 (3±1%)	9	42
All	All	2100/2240 (94%)	1784 (85%)	254 (12%)	62 (3%)	9	42

All 14 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	17

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Mol	Chain	Res	Type	Models (Total)
1	A	167	ASP	11
1	A	195	GLY	8
1	A	168	GLN	6
1	A	132	SER	5
1	A	126	GLY	4
1	A	193	THR	3
1	A	125	LEU	2
1	A	154	MET	1
1	A	229	ARG	1
1	A	151	ARG	1
1	A	134	MET	1
1	A	141	PHE	1
1	A	170	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	97/102 (95%)	81±3 (84±3%)	16±3 (16±3%)	7	44
All	All	1940/2040 (95%)	1629 (84%)	311 (16%)	7	44

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	125	LEU	18
1	A	220	LYS	16
1	A	208	ARG	13
1	A	147	ASP	12
1	A	212	GLN	12
1	A	135	SER	11
1	A	188	THR	10
1	A	217	GLN	9
1	A	187	HIS	9
1	A	172	GLN	9
1	A	209	VAL	9
1	A	171	ASN	9

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Mol	Chain	Res	Type	Models (Total)
1	A	175	PHE	8
1	A	226	TYR	8
1	A	200	GLU	6
1	A	223	GLN	6
1	A	222	SER	6
1	A	179	CYS	6
1	A	197	ASN	6
1	A	168	GLN	6
1	A	185	LYS	6
1	A	206	MET	5
1	A	154	MET	5
1	A	151	ARG	5
1	A	132	SER	5
1	A	229	ARG	5
1	A	161	VAL	5
1	A	144	ASP	5
1	A	140	HIS	4
1	A	218	TYR	4
1	A	136	ARG	4
1	A	178	ASP	4
1	A	138	MET	4
1	A	166	VAL	4
1	A	155	TYR	4
1	A	143	ASN	4
1	A	148	ARG	3
1	A	129	MET	3
1	A	221	GLU	3
1	A	139	ILE	3
1	A	214	CYS	3
1	A	160	GLN	3
1	A	199	THR	2
1	A	153	ASN	2
1	A	213	MET	2
1	A	167	ASP	2
1	A	159	ASN	2
1	A	211	GLU	2
1	A	186	GLN	2
1	A	225	TYR	2
1	A	170	ASN	2
1	A	202	ASP	2
1	A	227	ASP	2
1	A	204	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	203	VAL	1
1	A	196	GLU	1
1	A	181	ASN	1
1	A	194	LYS	1
1	A	174	THR	1
1	A	130	LEU	1
1	A	134	MET	1
1	A	193	THR	1

6.3.3 RNA [i](#)

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 carbohydrates 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