



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:44 PM BST

PDB ID : 1QM1
Title : HUMAN PRION PROTEIN FRAGMENT 90-230
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Deposited on : 1999-09-20

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

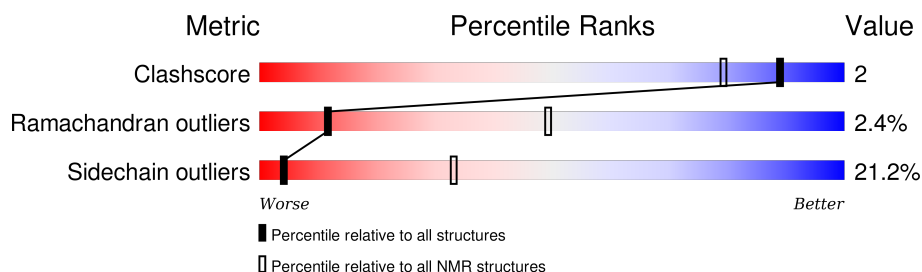
1 Overall quality at a glance

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	143	

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 19 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:129-A:166, A:172-A:228 (95)	0.45	11

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1688 atoms, of which 811 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PRION PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	104	Total	C	H	N	O	S	0
			1688	544	811	153	171	9	

There are 2 discrepancies between the modelled and reference sequences:

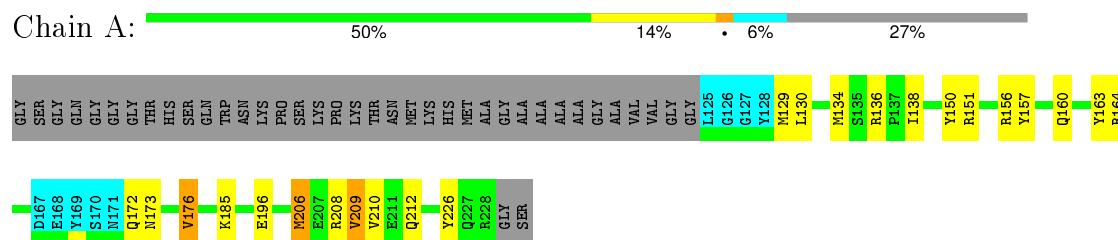
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLY	-	CLONING ARTIFACT	UNP P04156
A	89	SER	-	CLONING ARTIFACT	UNP P04156

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: PRION PROTEIN

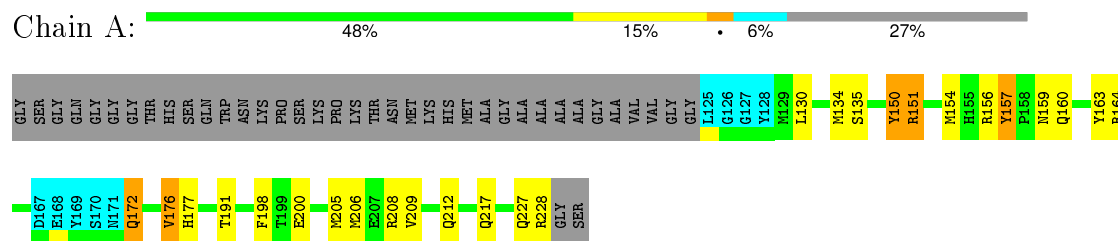


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

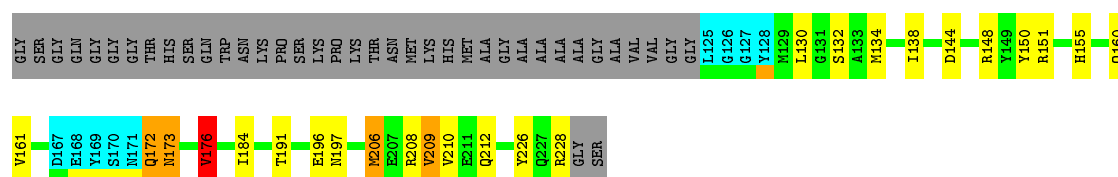
- Molecule 1: PRION PROTEIN



4.2.2 Score per residue for model 2

- Molecule 1: PRION PROTEIN

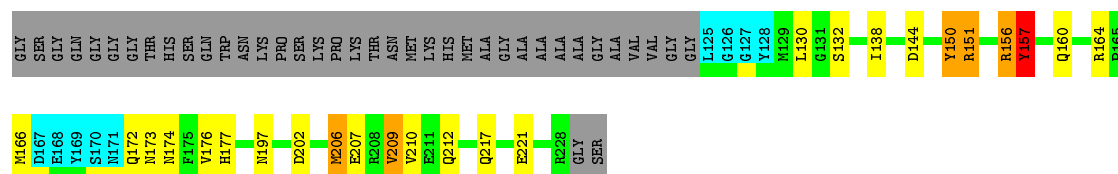




4.2.3 Score per residue for model 3

- Molecule 1: PRION PROTEIN

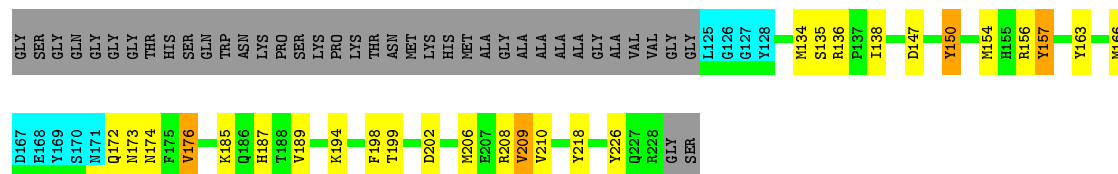
Chain A: 49% 13% 6% 27%



4.2.4 Score per residue for model 4

- Molecule 1: PRION PROTEIN

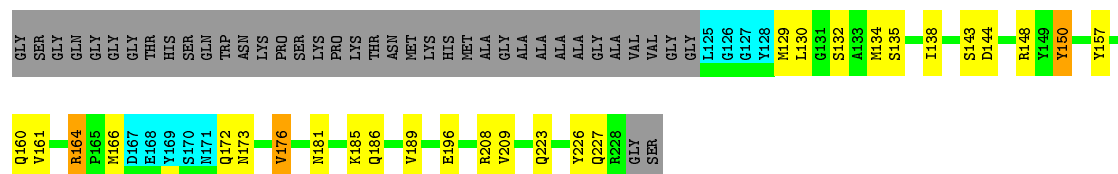
Chain A: 47% 17% 6% 27%



4.2.5 Score per residue for model 5

- Molecule 1: PRION PROTEIN

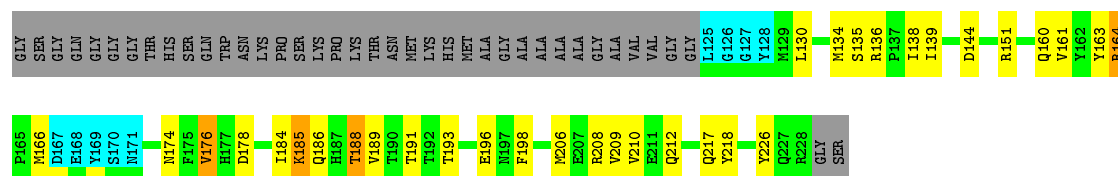
Chain A: 47% 17% 6% 27%



4.2.6 Score per residue for model 6

- Molecule 1: PRION PROTEIN

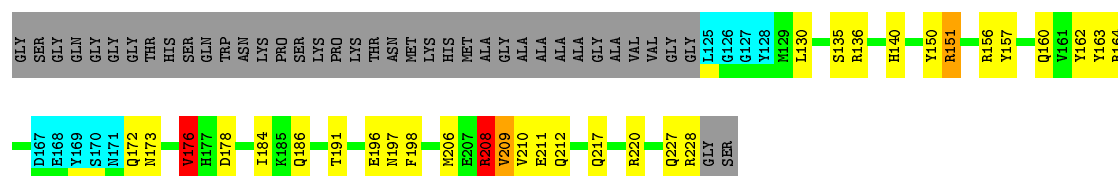
Chain A: 43% 20% 6% 27%



4.2.7 Score per residue for model 7

- Molecule 1: PRION PROTEIN

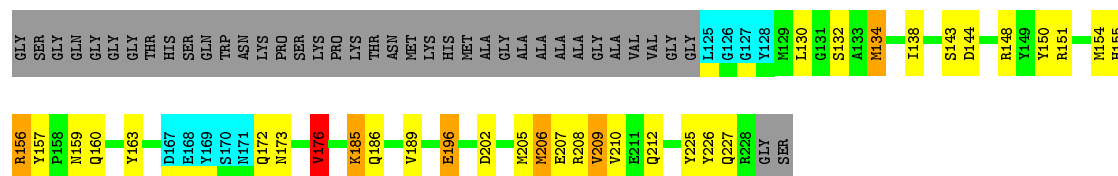
Chain A: 44% 20% 6% 27%



4.2.8 Score per residue for model 8

- Molecule 1: PRION PROTEIN

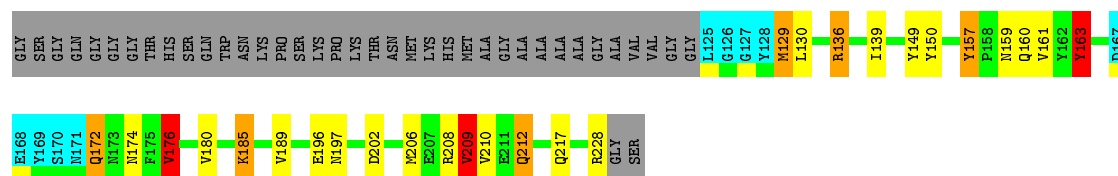
Chain A: 43% 19% 6% 27%



4.2.9 Score per residue for model 9

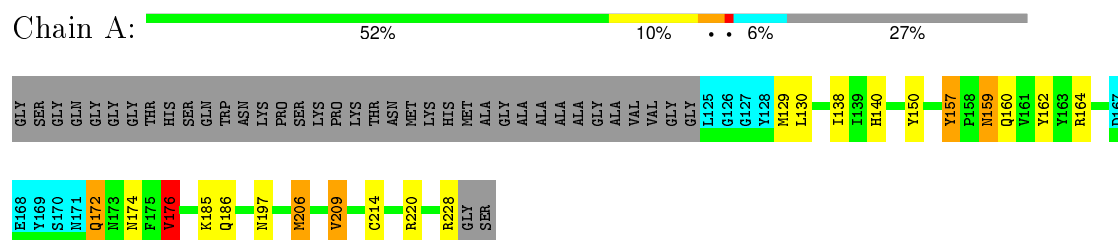
- Molecule 1: PRION PROTEIN

Chain A: 48% 13% 6% 27%



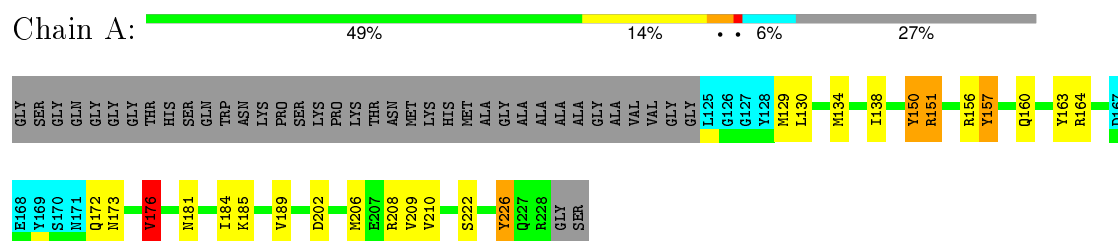
4.2.10 Score per residue for model 10

- Molecule 1: PRION PROTEIN



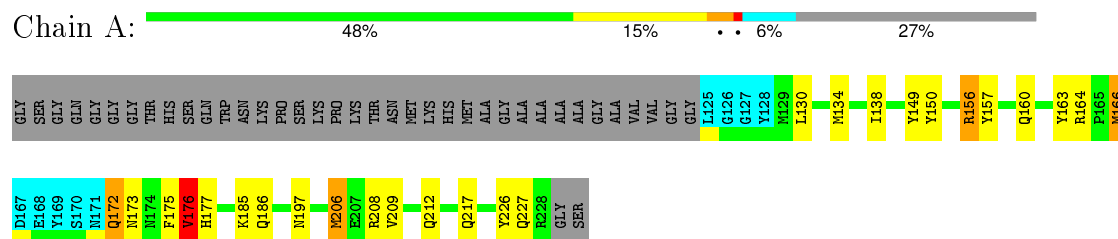
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: PRION PROTEIN



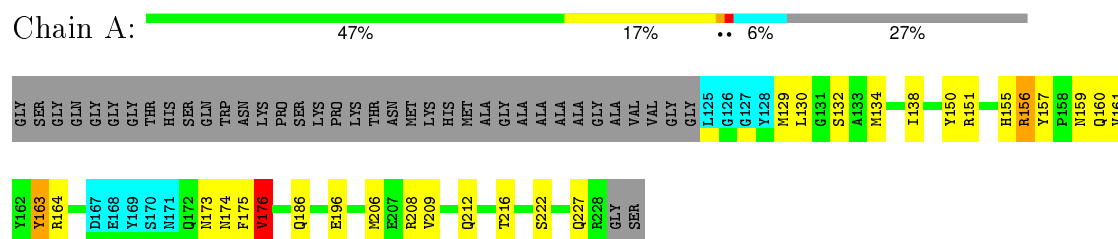
4.2.12 Score per residue for model 12

- Molecule 1: PRION PROTEIN



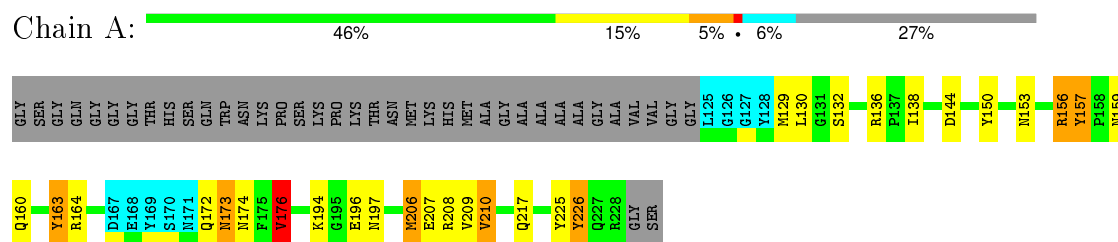
4.2.13 Score per residue for model 13

- Molecule 1: PRION PROTEIN



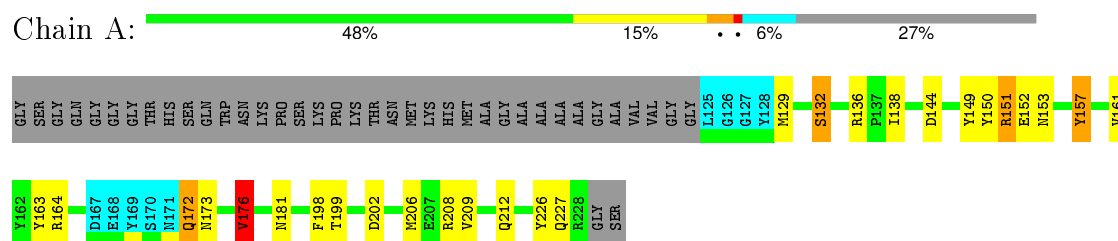
4.2.14 Score per residue for model 14

• Molecule 1: PRION PROTEIN



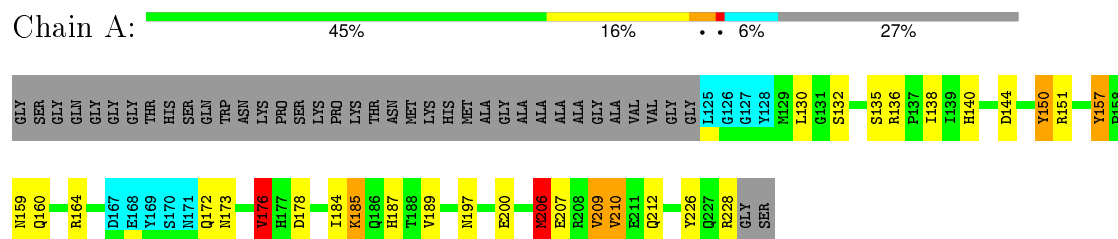
4.2.15 Score per residue for model 15

• Molecule 1: PRION PROTEIN



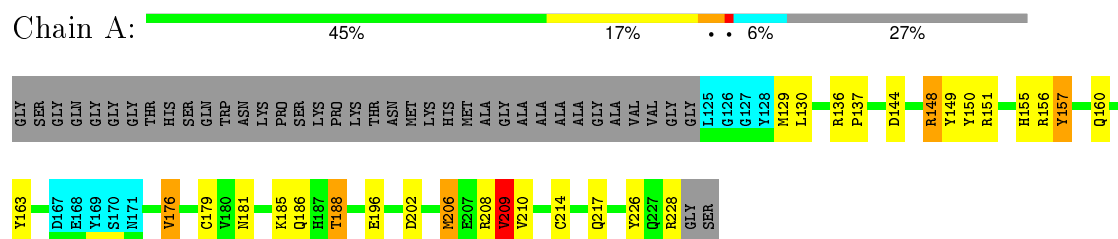
4.2.16 Score per residue for model 16

• Molecule 1: PRION PROTEIN



4.2.17 Score per residue for model 17

• Molecule 1: PRION PROTEIN



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: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
OPALP	refinement	
DYANA	structure solution	

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 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	0.68±0.01	0±0/824 (0.0±0.0%)	1.15±0.04	4±1/1111 (0.4±0.1%)
All	All	0.68	0/16480 (0.0%)	1.15	78/22220 (0.4%)

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±1.5
All	All	0	45

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	164	ARG	CD-NE-CZ	7.74	134.43	123.60	5	1
1	A	176	VAL	CG1-CB-CG2	-7.27	99.26	110.90	8	18
1	A	148	ARG	NE-CZ-NH2	-7.21	116.70	120.30	19	3
1	A	156	ARG	NE-CZ-NH2	-7.00	116.80	120.30	13	2
1	A	164	ARG	NE-CZ-NH1	6.89	123.74	120.30	5	1
1	A	176	VAL	CA-CB-CG2	6.88	121.21	110.90	20	5
1	A	188	THR	CA-CB-CG2	6.82	121.95	112.40	17	2
1	A	151	ARG	NE-CZ-NH2	-6.74	116.93	120.30	3	3
1	A	206	MET	CA-CB-CG	6.41	124.19	113.30	12	4
1	A	209	VAL	CG1-CB-CG2	-6.16	101.05	110.90	8	10
1	A	134	MET	CG-SD-CE	-6.04	90.54	100.20	20	3
1	A	209	VAL	CA-CB-CG1	5.96	119.83	110.90	7	1
1	A	208	ARG	NE-CZ-NH1	5.92	123.26	120.30	7	1
1	A	208	ARG	NE-CZ-NH2	-5.87	117.37	120.30	7	2
1	A	163	TYR	CB-CG-CD2	-5.79	117.52	121.00	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	164	ARG	NE-CZ-NH2	-5.77	117.42	120.30	20	1
1	A	210	VAL	CA-CB-CG2	5.58	119.28	110.90	19	5
1	A	151	ARG	CD-NE-CZ	5.57	131.40	123.60	15	1
1	A	148	ARG	NE-CZ-NH1	5.48	123.04	120.30	19	1
1	A	227	GLN	C-N-CA	5.44	135.31	121.70	15	1
1	A	210	VAL	CG1-CB-CG2	-5.36	102.32	110.90	9	1
1	A	129	MET	CB-CA-C	5.23	120.86	110.40	9	1
1	A	205	MET	CG-SD-CE	-5.18	91.91	100.20	1	2
1	A	161	VAL	CG1-CB-CG2	-5.18	102.61	110.90	15	1
1	A	156	ARG	CD-NE-CZ	5.13	130.78	123.60	12	1
1	A	138	ILE	CG1-CB-CG2	-5.05	100.29	111.40	19	1
1	A	156	ARG	CB-CG-CD	5.04	124.70	111.60	12	1
1	A	209	VAL	CA-CB-CG2	5.03	118.44	110.90	5	1
1	A	156	ARG	NE-CZ-NH1	5.03	122.81	120.30	8	1
1	A	220	ARG	NE-CZ-NH1	5.01	122.81	120.30	7	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	150	TYR	Sidechain	6
1	A	151	ARG	Sidechain	5
1	A	136	ARG	Sidechain	5
1	A	163	TYR	Sidechain	4
1	A	226	TYR	Sidechain	4
1	A	208	ARG	Sidechain	3
1	A	164	ARG	Sidechain	3
1	A	148	ARG	Sidechain	2
1	A	157	TYR	Sidechain	2
1	A	156	ARG	Sidechain	2
1	A	228	ARG	Sidechain	2
1	A	198	PHE	Sidechain	2
1	A	218	TYR	Sidechain	2
1	A	225	TYR	Sidechain	1
1	A	220	ARG	Sidechain	1
1	A	162	TYR	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	806	755	758	4±2
All	All	16120	15100	15160	72

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:130:LEU:HD11	1:A:160:GLN:HB3	0.93	1.41	18	18
1:A:185:LYS:O	1:A:189:VAL:HG23	0.58	1.98	11	7
1:A:173:ASN:HA	1:A:176:VAL:HG23	0.57	1.75	14	10
1:A:191:THR:HG22	1:A:196:GLU:HB3	0.52	1.82	6	3
1:A:206:MET:O	1:A:210:VAL:HG23	0.51	2.05	19	8
1:A:184:ILE:CG1	1:A:210:VAL:HG21	0.49	2.37	11	5
1:A:130:LEU:HD12	1:A:161:VAL:O	0.48	2.08	13	5
1:A:176:VAL:HG12	1:A:214:CYS:HB2	0.48	1.86	10	1
1:A:136:ARG:HH12	1:A:209:VAL:CG2	0.48	2.22	9	1
1:A:191:THR:HG21	1:A:198:PHE:CE2	0.47	2.45	1	2
1:A:191:THR:HG21	1:A:198:PHE:CZ	0.46	2.46	7	2
1:A:130:LEU:HD13	1:A:162:TYR:CD1	0.45	2.47	19	1
1:A:176:VAL:O	1:A:180:VAL:HG23	0.44	2.11	9	1
1:A:130:LEU:HD13	1:A:162:TYR:CE1	0.44	2.47	10	1
1:A:156:ARG:CG	1:A:157:TYR:H	0.43	2.27	3	1
1:A:172:GLN:CD	1:A:172:GLN:H	0.42	2.18	10	1
1:A:139:ILE:HD11	1:A:212:GLN:HG3	0.42	1.90	6	2
1:A:136:ARG:HH12	1:A:209:VAL:HG21	0.41	1.75	9	1
1:A:137:PRO:HG2	1:A:209:VAL:HG23	0.40	1.93	17	1
1:A:150:TYR:CD1	1:A:157:TYR:CD2	0.40	3.09	11	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	94/143 (66%)	85±2 (90±2%)	7±2 (7±2%)	2±1 (2±1%)	12	49
All	All	1880/2860 (66%)	1695 (90%)	140 (7%)	45 (2%)	12	49

All 10 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	138	ILE	16
1	A	172	GLN	10
1	A	157	TYR	8
1	A	166	MET	4
1	A	196	GLU	2
1	A	132	SER	1
1	A	159	ASN	1
1	A	136	ARG	1
1	A	198	PHE	1
1	A	135	SER	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	90/120 (75%)	71±3 (79±4%)	19±3 (21±4%)	4	33
All	All	1800/2400 (75%)	1419 (79%)	381 (21%)	4	33

All 63 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	176	VAL	19
1	A	209	VAL	18
1	A	150	TYR	18
1	A	206	MET	18
1	A	157	TYR	15
1	A	208	ARG	13

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Mol	Chain	Res	Type	Models (Total)
1	A	164	ARG	13
1	A	172	GLN	12
1	A	212	GLN	12
1	A	156	ARG	11
1	A	226	TYR	11
1	A	144	ASP	10
1	A	163	TYR	10
1	A	202	ASP	10
1	A	186	GLN	10
1	A	217	GLN	10
1	A	129	MET	10
1	A	197	ASN	9
1	A	151	ARG	9
1	A	185	LYS	8
1	A	132	SER	8
1	A	134	MET	8
1	A	227	GLN	7
1	A	174	ASN	7
1	A	159	ASN	7
1	A	196	GLU	6
1	A	207	GLU	6
1	A	135	SER	6
1	A	228	ARG	6
1	A	136	ARG	5
1	A	173	ASN	5
1	A	149	TYR	5
1	A	181	ASN	4
1	A	178	ASP	4
1	A	155	HIS	4
1	A	143	SER	3
1	A	140	HIS	3
1	A	194	LYS	3
1	A	154	MET	3
1	A	177	HIS	3
1	A	187	HIS	3
1	A	166	MET	2
1	A	188	THR	2
1	A	175	PHE	2
1	A	200	GLU	2
1	A	199	THR	2
1	A	222	SER	2
1	A	153	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	211	GLU	1
1	A	223	GLN	1
1	A	147	ASP	1
1	A	216	THR	1
1	A	221	GLU	1
1	A	179	CYS	1
1	A	191	THR	1
1	A	192	THR	1
1	A	138	ILE	1
1	A	214	CYS	1
1	A	193	THR	1
1	A	190	THR	1
1	A	152	GLU	1
1	A	148	ARG	1
1	A	225	TYR	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