



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:12 PM BST

PDB ID : 1Y7K
Title : NMR structure family of Human Agouti Signalling Protein (80-132: Q115Y, S124Y)
Authors : McNulty, J.C.; Jackson, P.J.; Thompson, D.A.; Chai, B.; Gantz, I.; Barsh, G.S.; Dawson, P.E.; Millhauser, G.L.
Deposited on : 2004-12-08

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

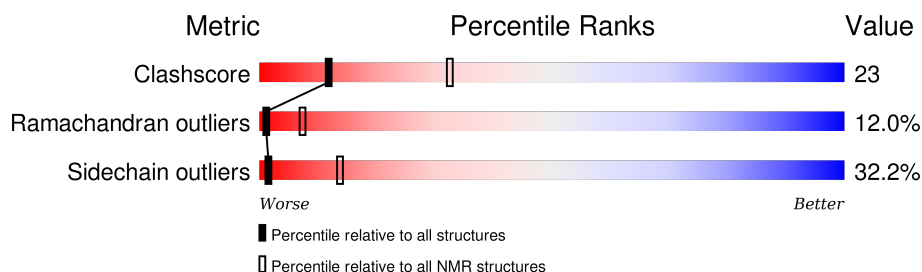
1 Overall quality at a glance

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	53	<div> <div></div> <div>23%</div> <div>45%</div> <div>8%</div> <div>25%</div> </div>

2 Ensemble composition and analysis ⓘ

This entry contains 21 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:93-A:132 (40)	0.64	7

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 575 atoms, of which 277 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Agouti Signaling Protein.

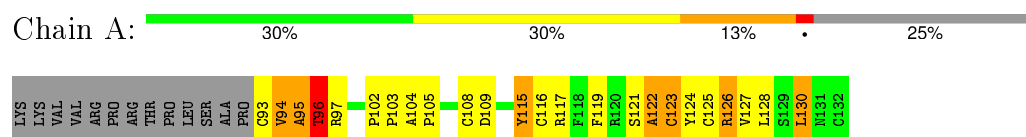
Mol	Chain	Residues	Atoms						Trace
1	A	40	Total	C	H	N	O	S	0
			575	181	277	55	52	10	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	TYR	GLN	ENGINEERED	UNP P42127
A	124	TYR	SER	ENGINEERED	UNP P42127

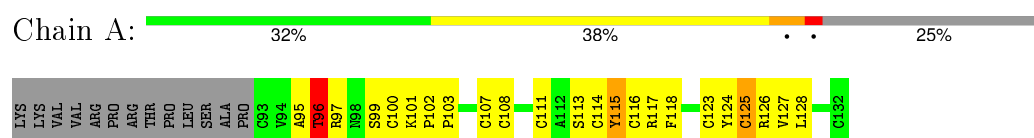
4.2.3 Score per residue for model 3

- Molecule 1: Agouti Signaling Protein



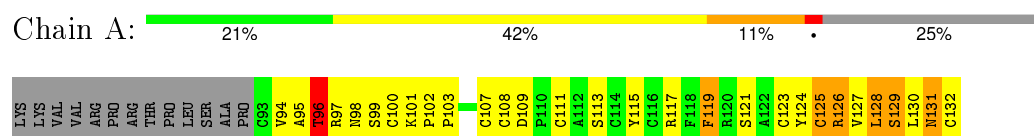
4.2.4 Score per residue for model 4

- Molecule 1: Agouti Signaling Protein



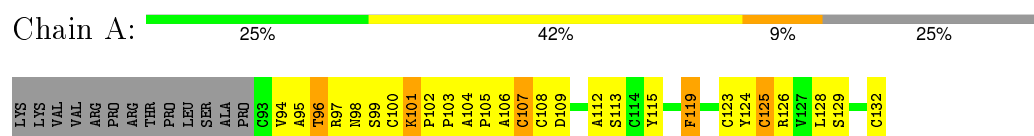
4.2.5 Score per residue for model 5

- Molecule 1: Agouti Signaling Protein



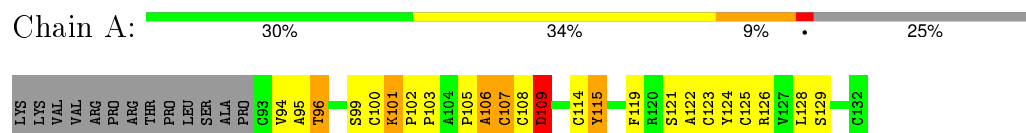
4.2.6 Score per residue for model 6

- Molecule 1: Agouti Signaling Protein



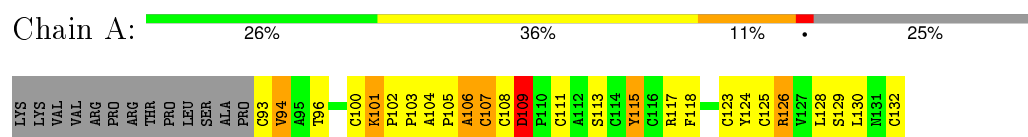
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Agouti Signaling Protein



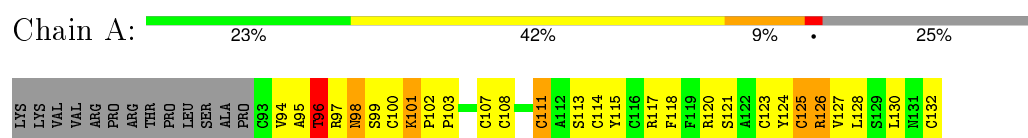
4.2.8 Score per residue for model 8

- Molecule 1: Agouti Signaling Protein



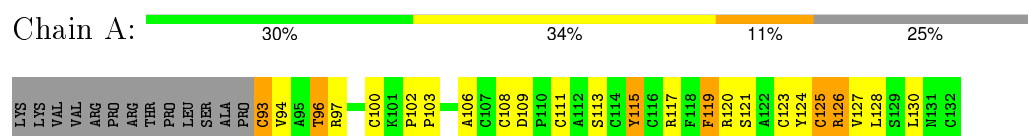
4.2.9 Score per residue for model 9

- Molecule 1: Agouti Signaling Protein



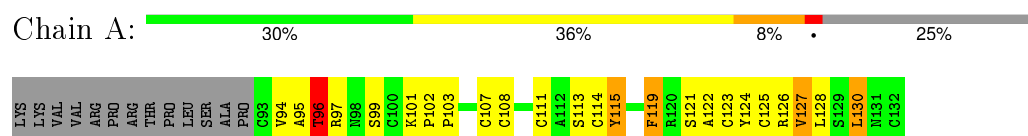
4.2.10 Score per residue for model 10

- Molecule 1: Agouti Signaling Protein



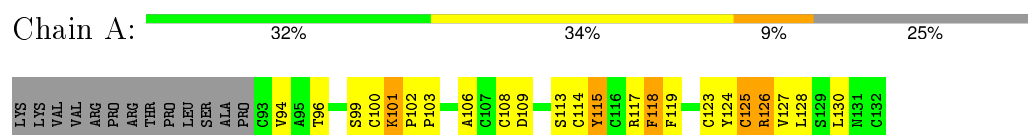
4.2.11 Score per residue for model 11

- Molecule 1: Agouti Signaling Protein



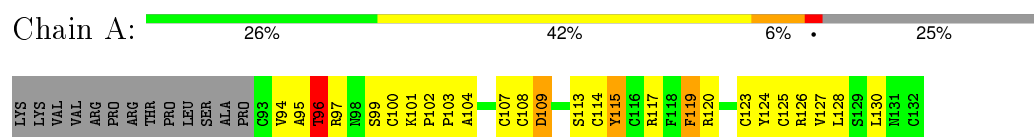
4.2.12 Score per residue for model 12

- Molecule 1: Agouti Signaling Protein



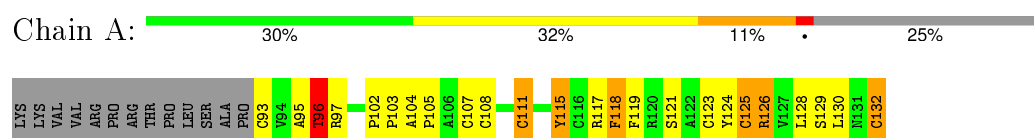
4.2.13 Score per residue for model 13

- Molecule 1: Agouti Signaling Protein



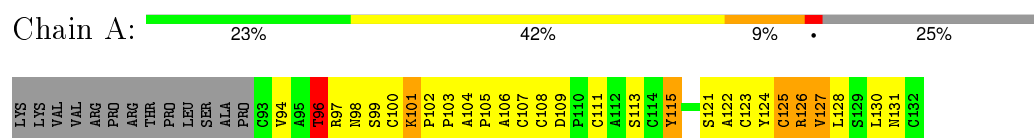
4.2.14 Score per residue for model 14

- Molecule 1: Agouti Signaling Protein



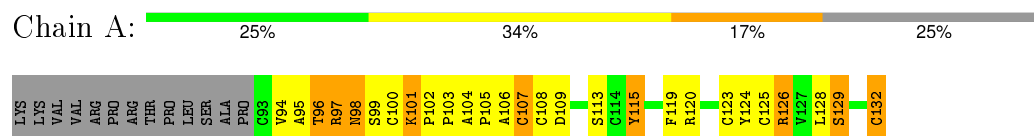
4.2.15 Score per residue for model 15

- Molecule 1: Agouti Signaling Protein



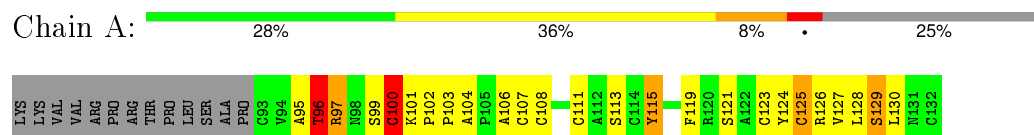
4.2.16 Score per residue for model 16

- Molecule 1: Agouti Signaling Protein



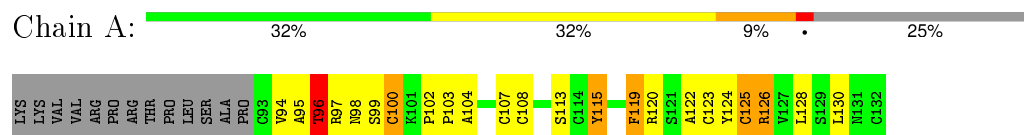
4.2.17 Score per residue for model 17

- Molecule 1: Agouti Signaling Protein



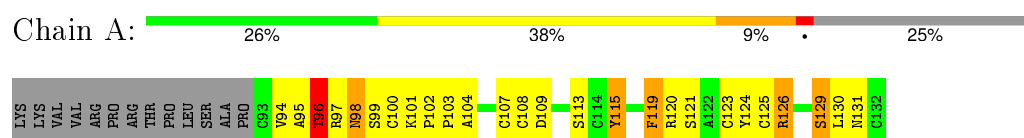
4.2.18 Score per residue for model 18

- Molecule 1: Agouti Signaling Protein



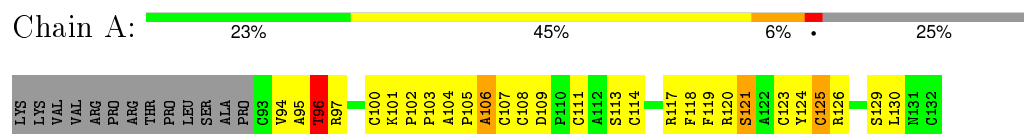
4.2.19 Score per residue for model 19

- Molecule 1: Agouti Signaling Protein



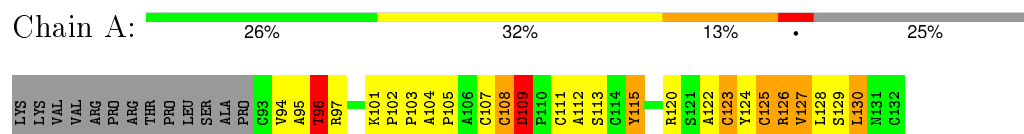
4.2.20 Score per residue for model 20

- Molecule 1: Agouti Signaling Protein



4.2.21 Score per residue for model 21

- Molecule 1: Agouti Signaling Protein



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing / torsion angle dynamics*.

Of the 1000 calculated structures, 21 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
CYANA	structure solution	1.0.6
CYANA	refinement	1.0.6

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	0.73±0.11	0±0/305 (0.0±0.0%)	0.89±0.17	0±1/412 (0.1±0.4%)
All	All	0.74	0/6385 (0.0%)	0.91	7/8652 (0.1%)

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	126	ARG	NE-CZ-NH1	9.72	125.16	120.30	1	1
1	A	120	ARG	NE-CZ-NH1	8.84	124.72	120.30	1	1
1	A	120	ARG	NE-CZ-NH2	-7.16	116.72	120.30	1	1
1	A	117	ARG	NE-CZ-NH1	7.04	123.82	120.30	1	1
1	A	97	ARG	NE-CZ-NH1	6.78	123.69	120.30	1	1
1	A	106	ALA	CB-CA-C	6.38	119.67	110.10	1	1
1	A	117	ARG	NE-CZ-NH2	-5.67	117.47	120.30	1	1

There are no chirality outliers.

There are no planarity outliers.

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	297	277	276	13±5
All	All	6238	5817	5796	274

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 23.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:TYR:CD1	1:A:128:LEU:HD21	1.03	1.87	12	2
1:A:115:TYR:CZ	1:A:128:LEU:HD21	1.01	1.90	16	2
1:A:115:TYR:CE1	1:A:128:LEU:HD21	0.94	1.97	13	6
1:A:115:TYR:CD1	1:A:128:LEU:HD11	0.91	2.00	16	1
1:A:115:TYR:CE1	1:A:128:LEU:HD11	0.89	2.02	17	9
1:A:111:CYS:O	1:A:127:VAL:HG23	0.84	1.73	9	7
1:A:127:VAL:C	1:A:128:LEU:HD22	0.80	1.97	3	6
1:A:115:TYR:CZ	1:A:128:LEU:HD11	0.78	2.13	12	5
1:A:94:VAL:HG13	1:A:99:SER:O	0.76	1.80	15	4
1:A:115:TYR:CE2	1:A:128:LEU:HD11	0.72	2.18	5	1
1:A:128:LEU:N	1:A:128:LEU:HD22	0.72	1.99	5	4
1:A:126:ARG:NH1	1:A:128:LEU:HD13	0.66	2.05	3	2
1:A:105:PRO:O	1:A:106:ALA:HB3	0.63	1.93	15	4
1:A:94:VAL:HG11	1:A:125:CYS:SG	0.63	2.34	11	6
1:A:123:CYS:O	1:A:124:TYR:CD1	0.62	2.53	17	20
1:A:115:TYR:OH	1:A:128:LEU:HD21	0.62	1.93	16	1
1:A:115:TYR:CD1	1:A:128:LEU:CD2	0.62	2.75	12	1
1:A:101:LYS:O	1:A:104:ALA:HB2	0.61	1.96	8	1
1:A:97:ARG:O	1:A:124:TYR:CD1	0.60	2.55	6	14
1:A:97:ARG:C	1:A:124:TYR:CG	0.55	2.80	19	7
1:A:128:LEU:HD22	1:A:128:LEU:N	0.54	2.16	3	2
1:A:128:LEU:N	1:A:128:LEU:CD2	0.54	2.70	5	1
1:A:118:PHE:O	1:A:119:PHE:CB	0.54	2.55	20	3
1:A:94:VAL:HG12	1:A:95:ALA:N	0.54	2.18	3	1
1:A:126:ARG:NH1	1:A:128:LEU:CD1	0.54	2.71	10	2
1:A:97:ARG:O	1:A:124:TYR:CG	0.53	2.60	13	6
1:A:115:TYR:CG	1:A:128:LEU:HD21	0.53	2.38	12	1
1:A:105:PRO:O	1:A:106:ALA:CB	0.52	2.58	16	3
1:A:101:LYS:CD	1:A:101:LYS:O	0.51	2.59	16	1
1:A:115:TYR:CD2	1:A:126:ARG:HG2	0.51	2.41	17	1
1:A:100:CYS:O	1:A:104:ALA:HB2	0.51	2.05	20	1
1:A:94:VAL:HG21	1:A:100:CYS:HA	0.50	1.82	15	3
1:A:94:VAL:CG1	1:A:125:CYS:SG	0.50	2.99	19	6
1:A:94:VAL:CG1	1:A:98:ASN:O	0.50	2.60	9	5
1:A:106:ALA:O	1:A:107:CYS:CB	0.49	2.60	15	1
1:A:115:TYR:CE1	1:A:128:LEU:CD2	0.49	2.94	12	1
1:A:115:TYR:CD2	1:A:126:ARG:HB3	0.49	2.43	5	3
1:A:102:PRO:HA	1:A:104:ALA:N	0.48	2.23	20	7
1:A:102:PRO:HA	1:A:103:PRO:C	0.48	2.29	17	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:TYR:CG	1:A:126:ARG:HB3	0.48	2.44	17	4
1:A:94:VAL:HG12	1:A:125:CYS:SG	0.48	2.48	10	2
1:A:94:VAL:HG23	1:A:107:CYS:HA	0.47	1.86	2	2
1:A:94:VAL:CG1	1:A:99:SER:O	0.47	2.59	15	2
1:A:101:LYS:CG	1:A:101:LYS:O	0.47	2.61	16	3
1:A:117:ARG:C	1:A:118:PHE:CD1	0.47	2.88	8	1
1:A:100:CYS:O	1:A:101:LYS:CG	0.47	2.62	13	2
1:A:94:VAL:HG12	1:A:125:CYS:HB2	0.47	1.87	20	1
1:A:99:SER:O	1:A:101:LYS:N	0.46	2.48	6	8
1:A:111:CYS:O	1:A:127:VAL:CG2	0.46	2.62	21	1
1:A:115:TYR:CD1	1:A:126:ARG:HB3	0.46	2.46	3	2
1:A:129:SER:O	1:A:131:ASN:N	0.46	2.49	2	3
1:A:115:TYR:CE1	1:A:128:LEU:CD1	0.46	2.96	12	3
1:A:115:TYR:OH	1:A:128:LEU:HD11	0.45	2.10	12	2
1:A:103:PRO:O	1:A:104:ALA:HB3	0.45	2.11	3	3
1:A:98:ASN:OD1	1:A:99:SER:N	0.45	2.49	6	1
1:A:111:CYS:SG	1:A:129:SER:CB	0.45	3.05	17	1
1:A:115:TYR:CE2	1:A:128:LEU:HD21	0.45	2.47	6	1
1:A:127:VAL:O	1:A:128:LEU:HD13	0.45	2.12	3	1
1:A:115:TYR:CB	1:A:126:ARG:CB	0.45	2.94	18	5
1:A:115:TYR:HE1	1:A:128:LEU:HD11	0.44	1.69	15	1
1:A:93:CYS:SG	1:A:94:VAL:N	0.44	2.90	10	1
1:A:94:VAL:HG13	1:A:100:CYS:O	0.43	2.13	6	1
1:A:101:LYS:O	1:A:104:ALA:CB	0.43	2.66	8	1
1:A:115:TYR:HB2	1:A:126:ARG:CB	0.43	2.44	15	5
1:A:117:ARG:HB3	1:A:118:PHE:CE1	0.43	2.49	4	1
1:A:126:ARG:CZ	1:A:128:LEU:CD1	0.43	2.97	5	1
1:A:97:ARG:O	1:A:124:TYR:CD2	0.43	2.72	13	1
1:A:101:LYS:O	1:A:104:ALA:CA	0.43	2.67	8	1
1:A:126:ARG:CD	1:A:127:VAL:O	0.43	2.67	21	1
1:A:106:ALA:O	1:A:107:CYS:O	0.42	2.38	8	3
1:A:96:THR:O	1:A:125:CYS:O	0.42	2.37	11	14
1:A:94:VAL:O	1:A:108:CYS:CB	0.42	2.67	21	1
1:A:126:ARG:NH1	1:A:127:VAL:O	0.42	2.50	5	1
1:A:129:SER:HB3	1:A:132:CYS:CB	0.42	2.45	16	1
1:A:115:TYR:CB	1:A:126:ARG:HB2	0.41	2.45	15	2
1:A:106:ALA:O	1:A:109:ASP:O	0.41	2.39	8	1
1:A:129:SER:CB	1:A:132:CYS:HB3	0.41	2.45	16	1
1:A:115:TYR:HE2	1:A:128:LEU:HD21	0.41	1.76	6	1
1:A:117:ARG:HB2	1:A:122:ALA:HB3	0.41	1.92	3	1
1:A:99:SER:O	1:A:100:CYS:C	0.41	2.58	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:SER:O	1:A:100:CYS:O	0.41	2.39	17	1
1:A:116:CYS:O	1:A:117:ARG:C	0.41	2.60	4	1
1:A:94:VAL:O	1:A:108:CYS:SG	0.41	2.79	20	1
1:A:107:CYS:SG	1:A:112:ALA:O	0.41	2.79	6	1
1:A:117:ARG:O	1:A:118:PHE:CG	0.40	2.74	8	1
1:A:105:PRO:O	1:A:106:ALA:O	0.40	2.39	7	1
1:A:107:CYS:O	1:A:109:ASP:N	0.40	2.49	7	1
1:A:109:ASP:HB3	1:A:112:ALA:CB	0.40	2.46	21	1
1:A:111:CYS:SG	1:A:132:CYS:C	0.40	3.00	14	1
1:A:128:LEU:CD2	1:A:128:LEU:N	0.40	2.83	3	1
1:A:94:VAL:HG12	1:A:95:ALA:H	0.40	1.76	3	1
1:A:101:LYS:CG	1:A:102:PRO:HD2	0.40	2.46	21	1
1:A:118:PHE:CB	1:A:121:SER:HB2	0.40	2.46	20	1
1:A:94:VAL:HG12	1:A:98:ASN:O	0.40	2.16	19	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	38/53 (72%)	26±2 (69±6%)	7±1 (19±4%)	5±2 (12±5%)		
All	All	798/1113 (72%)	551 (69%)	151 (19%)	96 (12%)		

All 13 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	96	THR	17
1	A	95	ALA	16
1	A	107	CYS	13
1	A	119	PHE	13
1	A	100	CYS	10
1	A	122	ALA	6
1	A	106	ALA	6
1	A	105	PRO	5

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Mol	Chain	Res	Type	Models (Total)
1	A	109	ASP	4
1	A	130	LEU	3
1	A	104	ALA	1
1	A	129	SER	1
1	A	94	VAL	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	35/47 (74%)	24±3 (68±9%)	11±3 (32±9%)	1	14
All	All	735/987 (74%)	498 (68%)	237 (32%)	1	14

All 29 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	96	THR	20
1	A	108	CYS	19
1	A	126	ARG	19
1	A	113	SER	17
1	A	130	LEU	15
1	A	115	TYR	15
1	A	125	CYS	13
1	A	109	ASP	13
1	A	121	SER	11
1	A	101	LYS	10
1	A	129	SER	10
1	A	117	ARG	8
1	A	114	CYS	8
1	A	120	ARG	8
1	A	132	CYS	7
1	A	119	PHE	7
1	A	97	ARG	5
1	A	127	VAL	5
1	A	111	CYS	5
1	A	93	CYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	98	ASN	4
1	A	128	LEU	3
1	A	118	PHE	3
1	A	131	ASN	2
1	A	123	CYS	2
1	A	107	CYS	1
1	A	100	CYS	1
1	A	116	CYS	1
1	A	94	VAL	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