



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 02:30 AM BST

PDB ID : 2MAH
Title : Solution structure of Smoothened
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Deposited on : 2013-07-09

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

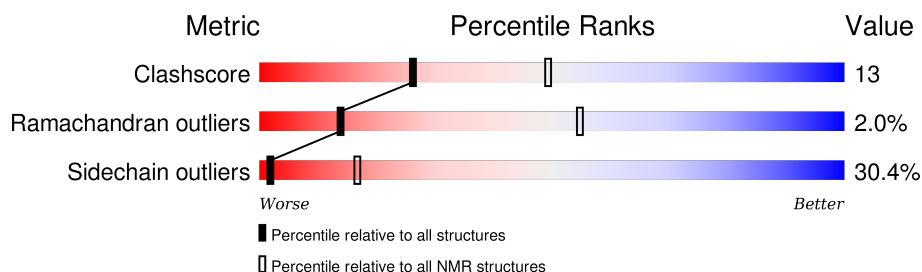
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	128	

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:21-A:137 (117)	0.46	18

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 8 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2061 atoms, of which 1022 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein smoothened.

Mol	Chain	Residues	Atoms						Trace
1	A	128	Total	C	H	N	O	S	0
			2061	667	1022	174	186	12	

There are 10 discrepancies between the modelled and reference sequences:

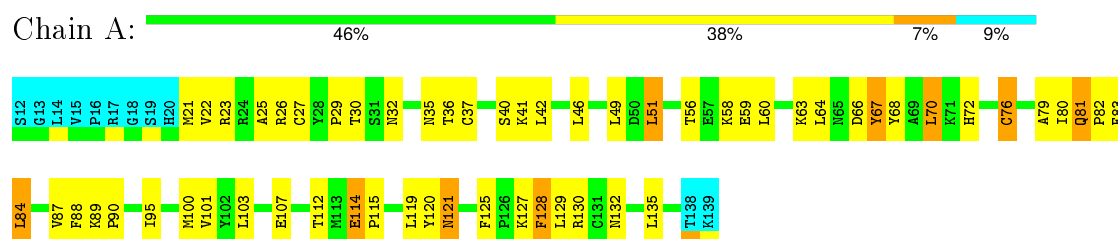
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	-	EXPRESSION TAG	UNP P91682
A	13	GLY	-	EXPRESSION TAG	UNP P91682
A	14	LEU	-	EXPRESSION TAG	UNP P91682
A	15	VAL	-	EXPRESSION TAG	UNP P91682
A	16	PRO	-	EXPRESSION TAG	UNP P91682
A	17	ARG	-	EXPRESSION TAG	UNP P91682
A	18	GLY	-	EXPRESSION TAG	UNP P91682
A	19	SER	-	EXPRESSION TAG	UNP P91682
A	20	HIS	-	EXPRESSION TAG	UNP P91682
A	21	MET	-	EXPRESSION TAG	UNP P91682

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: Protein smoothened

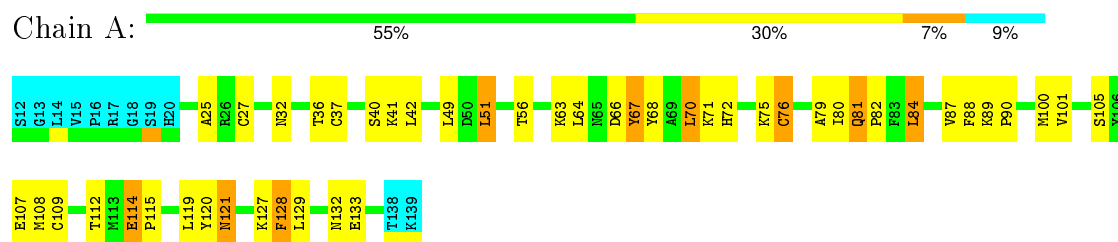


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

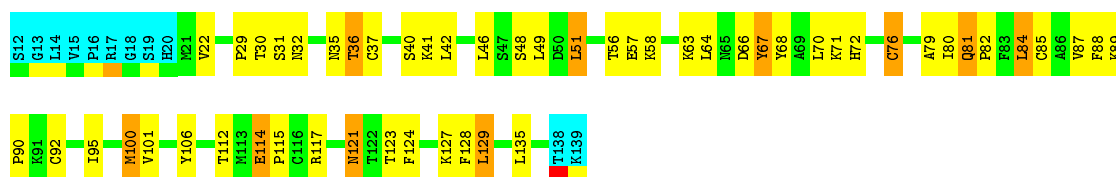
- Molecule 1: Protein smoothened



4.2.2 Score per residue for model 2

- Molecule 1: Protein smoothened

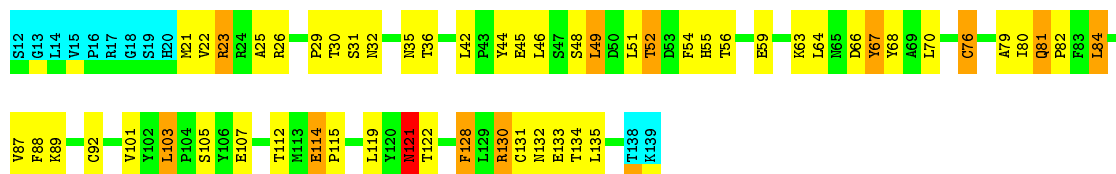




4.2.3 Score per residue for model 3

- Molecule 1: Protein smoothened

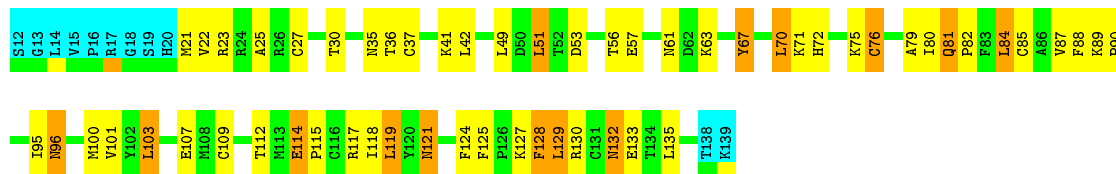
Chain A: 48% 34% 9% 9%



4.2.4 Score per residue for model 4

- Molecule 1: Protein smoothened

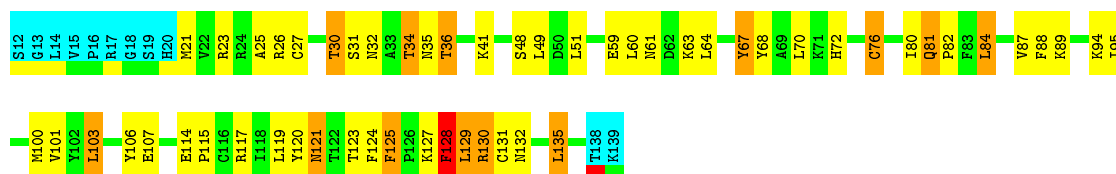
Chain A: 47% 34% 11% 9%



4.2.5 Score per residue for model 5

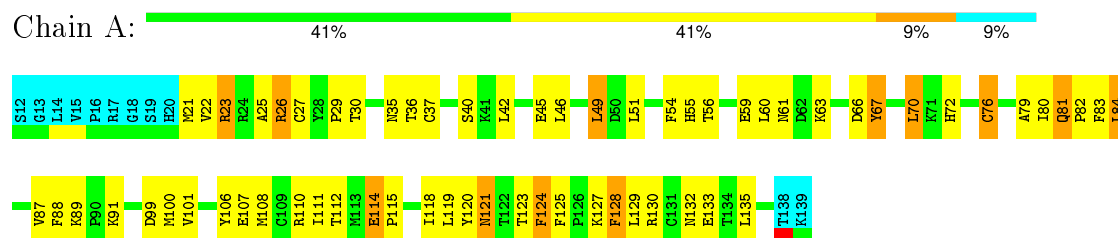
- Molecule 1: Protein smoothened

Chain A: 48% 32% 10% 9%



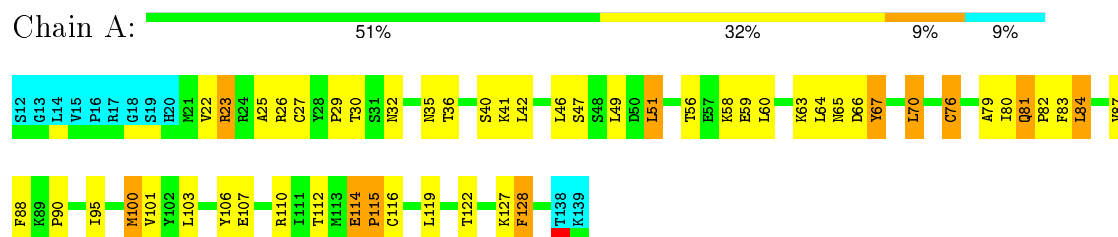
4.2.6 Score per residue for model 6

- Molecule 1: Protein smoothened



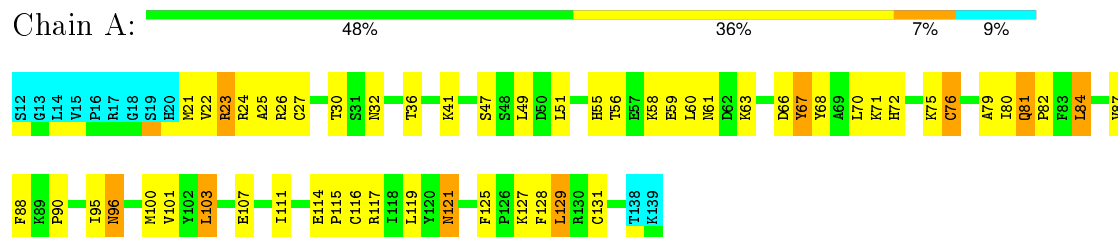
4.2.7 Score per residue for model 7

- Molecule 1: Protein smoothed



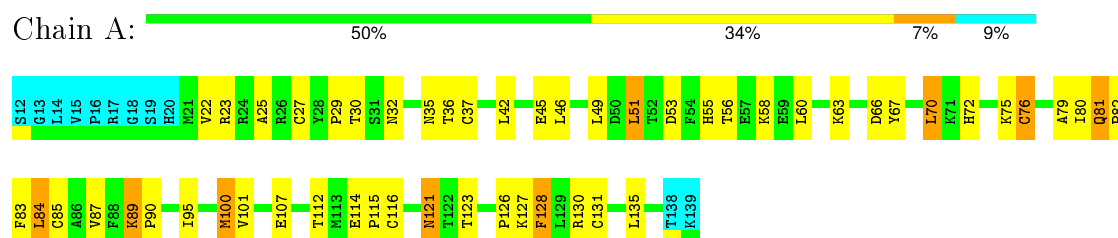
4.2.8 Score per residue for model 8

- Molecule 1: Protein smoothed



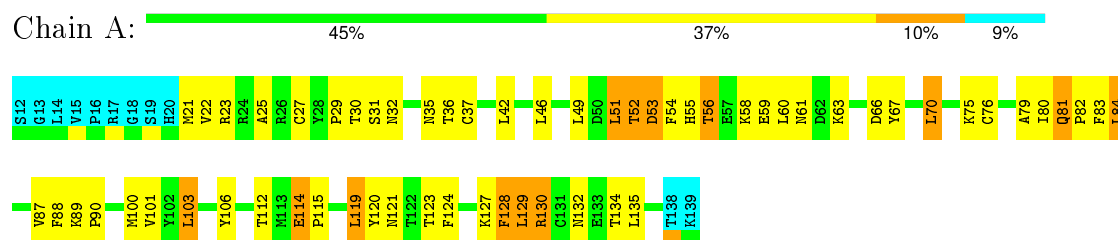
4.2.9 Score per residue for model 9

- Molecule 1: Protein smoothed



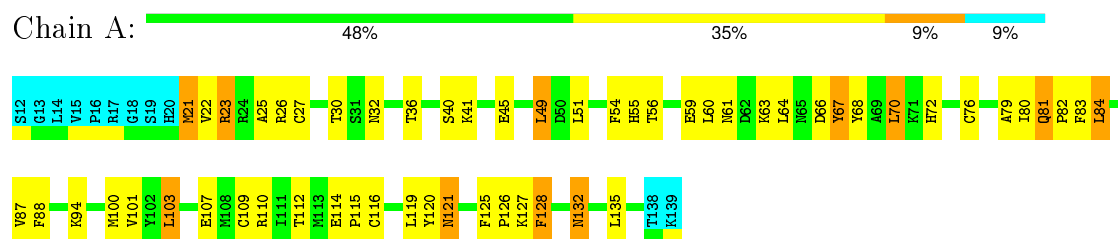
4.2.10 Score per residue for model 10

- Molecule 1: Protein smoothened



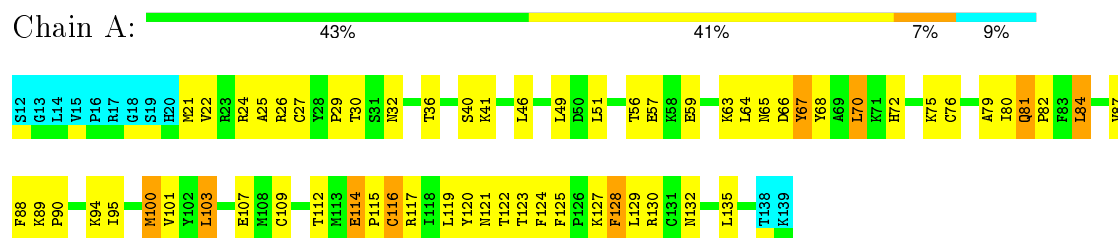
4.2.11 Score per residue for model 11

- Molecule 1: Protein smoothened



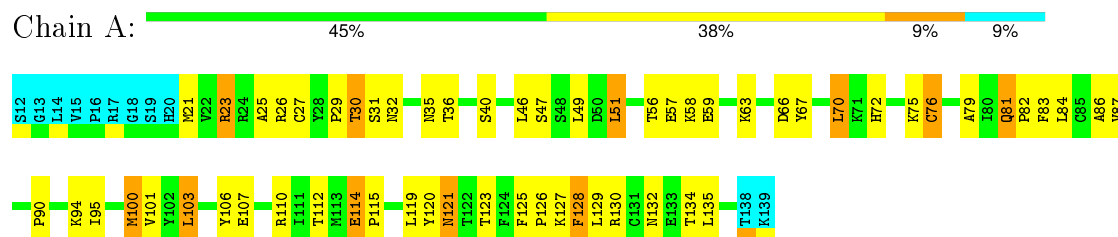
4.2.12 Score per residue for model 12

- Molecule 1: Protein smoothened



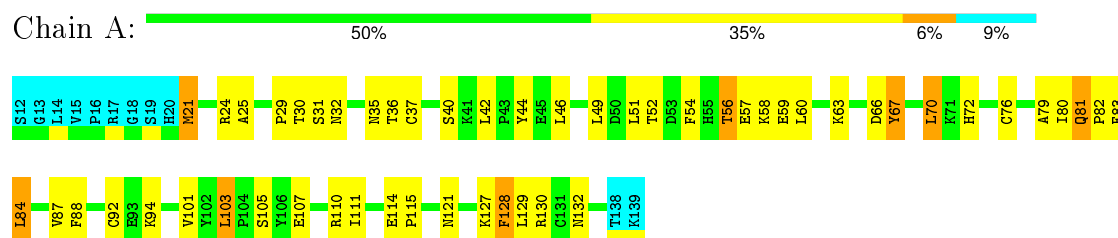
4.2.13 Score per residue for model 13

- Molecule 1: Protein smoothened



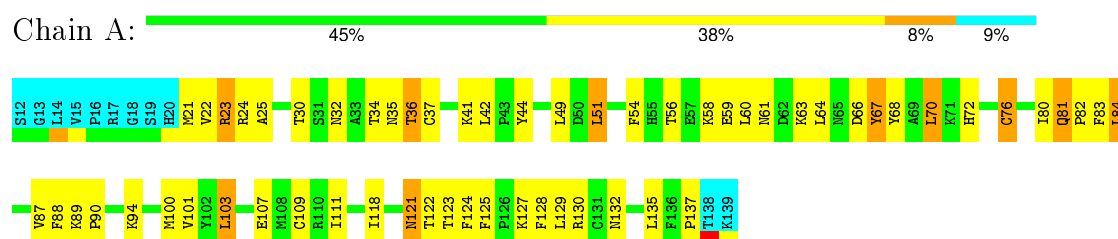
4.2.14 Score per residue for model 14

- Molecule 1: Protein smoothened



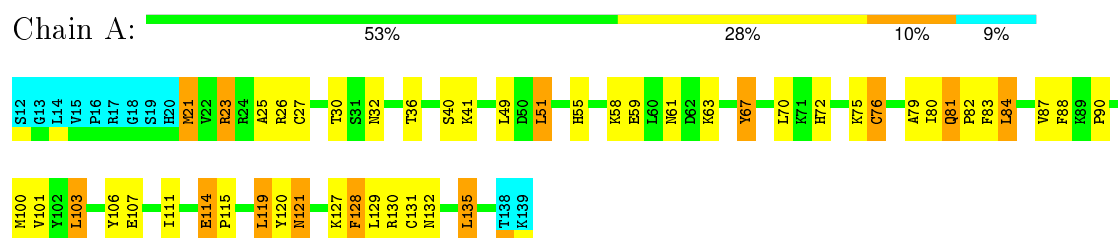
4.2.15 Score per residue for model 15

- Molecule 1: Protein smoothened



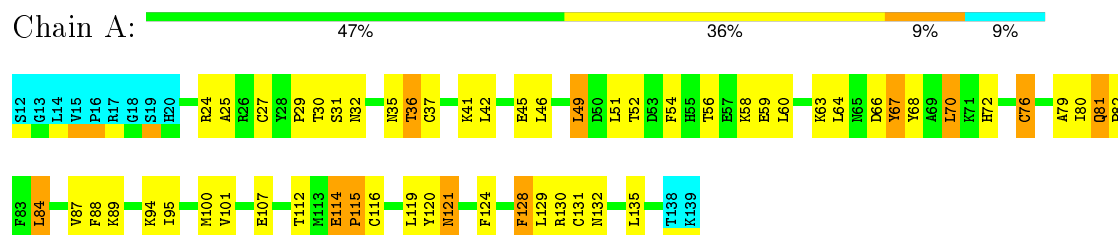
4.2.16 Score per residue for model 16

- Molecule 1: Protein smoothened



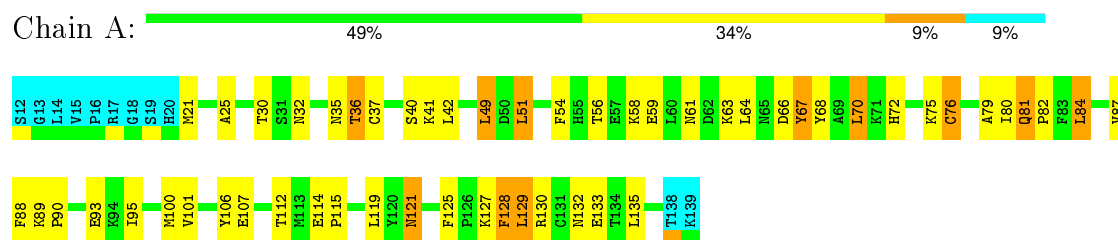
4.2.17 Score per residue for model 17

- Molecule 1: Protein smoothened



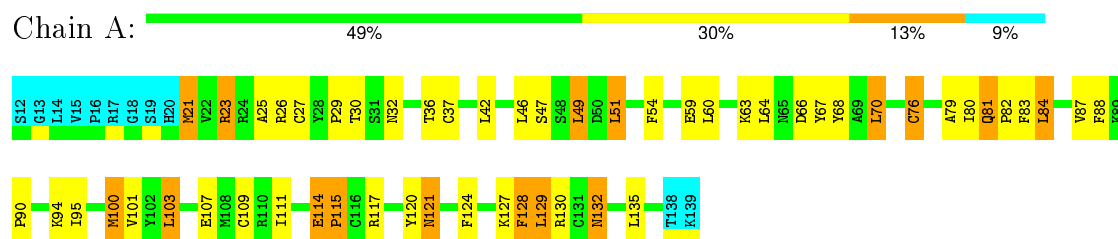
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Protein smoothened



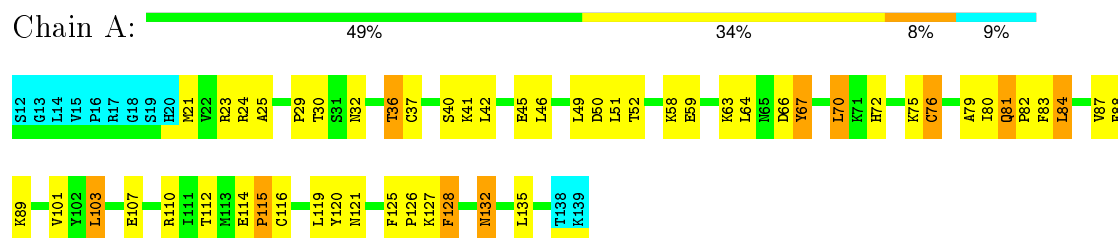
4.2.19 Score per residue for model 19

- Molecule 1: Protein smoothened



4.2.20 Score per residue for model 20

- Molecule 1: Protein smoothened



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 lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2mah_cs.str
Number of chemical shift lists	1
Total number of shifts	1607
Number of shifts mapped to atoms	1607
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	960	939	939	25±3
All	All	19200	18780	18780	505

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:LEU:HD13	1:A:129:LEU:HD11	0.87	1.45	13	2
1:A:83:PHE:O	1:A:87:VAL:HG23	0.79	1.77	9	7
1:A:25:ALA:HB3	1:A:101:VAL:HG13	0.75	1.56	13	19
1:A:51:LEU:HD13	1:A:101:VAL:HG21	0.75	1.58	8	3
1:A:67:TYR:CZ	1:A:84:LEU:HD21	0.71	2.21	17	16
1:A:128:PHE:CE1	1:A:129:LEU:HD23	0.69	2.22	2	4
1:A:25:ALA:HB3	1:A:101:VAL:CG1	0.69	2.16	3	19
1:A:23:ARG:HD2	1:A:25:ALA:HB2	0.66	1.67	15	4
1:A:79:ALA:HB1	1:A:111:ILE:O	0.65	1.91	14	3
1:A:70:LEU:HD13	1:A:128:PHE:CE1	0.64	2.26	1	5
1:A:103:LEU:HD22	1:A:103:LEU:C	0.64	2.12	13	1
1:A:30:THR:HG21	1:A:35:ASN:ND2	0.64	2.07	13	2
1:A:80:ILE:HG23	1:A:84:LEU:HD23	0.64	1.70	6	19
1:A:128:PHE:CE2	1:A:129:LEU:HD23	0.63	2.27	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:HD13	1:A:128:PHE:CE2	0.63	2.28	12	12
1:A:132:ASN:HB3	1:A:135:LEU:HD12	0.62	1.70	16	7
1:A:82:PRO:CG	1:A:111:ILE:HG21	0.62	2.25	15	1
1:A:37:CYS:HB2	1:A:42:LEU:HD21	0.62	1.71	2	9
1:A:21:MET:HA	1:A:103:LEU:HD11	0.61	1.72	12	6
1:A:60:LEU:HD21	1:A:88:PHE:HB3	0.61	1.72	10	9
1:A:21:MET:O	1:A:103:LEU:HD12	0.61	1.96	20	1
1:A:116:CYS:CB	1:A:119:LEU:HD23	0.61	2.26	11	2
1:A:95:ILE:HG22	1:A:96:ASN:ND2	0.61	2.11	8	2
1:A:23:ARG:HG2	1:A:101:VAL:HG22	0.59	1.75	16	5
1:A:116:CYS:HB3	1:A:119:LEU:HD23	0.59	1.75	12	4
1:A:119:LEU:HD21	1:A:124:PHE:CD1	0.58	2.33	12	1
1:A:79:ALA:HB1	1:A:112:THR:HA	0.58	1.76	9	13
1:A:70:LEU:HD22	1:A:128:PHE:CE1	0.58	2.34	9	3
1:A:122:THR:HG23	1:A:129:LEU:HD13	0.57	1.74	15	1
1:A:70:LEU:HD21	1:A:76:CYS:HB3	0.57	1.76	17	14
1:A:49:LEU:HD13	1:A:49:LEU:O	0.57	1.98	17	1
1:A:25:ALA:HB3	1:A:101:VAL:HG11	0.57	1.76	3	2
1:A:49:LEU:O	1:A:49:LEU:HD13	0.56	2.00	3	2
1:A:29:PRO:HA	1:A:46:LEU:HD23	0.56	1.77	12	12
1:A:79:ALA:HB2	1:A:115:PRO:HG3	0.55	1.78	12	10
1:A:132:ASN:HA	1:A:135:LEU:HD12	0.55	1.78	13	2
1:A:119:LEU:HD11	1:A:125:PHE:HB2	0.55	1.78	20	3
1:A:119:LEU:HB3	1:A:129:LEU:HD11	0.55	1.77	1	1
1:A:49:LEU:HD22	1:A:54:PHE:HB2	0.55	1.79	14	2
1:A:119:LEU:HD21	1:A:125:PHE:CD2	0.55	2.36	11	2
1:A:51:LEU:HD23	1:A:90:PRO:HG3	0.54	1.79	12	1
1:A:119:LEU:HD21	1:A:125:PHE:CE2	0.54	2.37	11	1
1:A:30:THR:HG21	1:A:35:ASN:CG	0.54	2.23	5	1
1:A:95:ILE:HD12	1:A:100:MET:HB2	0.54	1.79	17	3
1:A:114:GLU:CB	1:A:115:PRO:CD	0.53	2.87	11	19
1:A:125:PHE:O	1:A:129:LEU:HD12	0.53	2.03	15	1
1:A:23:ARG:NH2	1:A:103:LEU:HD23	0.53	2.18	10	1
1:A:49:LEU:HD11	1:A:56:THR:C	0.53	2.24	10	2
1:A:22:VAL:HG11	1:A:95:ILE:CD1	0.52	2.35	4	5
1:A:103:LEU:HD13	1:A:103:LEU:N	0.52	2.19	16	1
1:A:36:THR:HG23	1:A:41:LYS:HA	0.52	1.80	5	9
1:A:49:LEU:HD11	1:A:54:PHE:HB2	0.52	1.81	17	6
1:A:23:ARG:HG3	1:A:101:VAL:HG22	0.52	1.81	15	1
1:A:76:CYS:O	1:A:79:ALA:HB3	0.52	2.05	6	13
1:A:103:LEU:N	1:A:103:LEU:HD13	0.52	2.20	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:LEU:HD12	1:A:129:LEU:O	0.52	2.04	17	1
1:A:48:SER:CB	1:A:101:VAL:HG11	0.51	2.35	2	1
1:A:132:ASN:CB	1:A:135:LEU:HD21	0.51	2.35	6	1
1:A:81:GLN:CB	1:A:82:PRO:CD	0.51	2.88	9	20
1:A:119:LEU:HA	1:A:122:THR:HG22	0.51	1.81	3	1
1:A:35:ASN:OD1	1:A:42:LEU:HD13	0.51	2.05	3	1
1:A:22:VAL:HG13	1:A:101:VAL:O	0.51	2.06	6	2
1:A:128:PHE:CZ	1:A:129:LEU:HD23	0.50	2.41	5	1
1:A:51:LEU:HD13	1:A:51:LEU:O	0.50	2.06	6	1
1:A:95:ILE:HD13	1:A:100:MET:HE3	0.50	1.83	19	2
1:A:51:LEU:HD13	1:A:90:PRO:CB	0.50	2.36	19	10
1:A:23:ARG:HH22	1:A:103:LEU:HD21	0.49	1.66	7	1
1:A:36:THR:HG23	1:A:41:LYS:CA	0.49	2.37	5	2
1:A:95:ILE:HD12	1:A:100:MET:CB	0.49	2.37	17	2
1:A:54:PHE:CD2	1:A:60:LEU:HD12	0.49	2.43	11	2
1:A:79:ALA:O	1:A:112:THR:HG22	0.49	2.07	6	1
1:A:51:LEU:HD13	1:A:90:PRO:CG	0.49	2.38	2	3
1:A:85:CYS:O	1:A:89:LYS:C	0.48	2.52	9	1
1:A:35:ASN:OD1	1:A:42:LEU:HD23	0.48	2.09	9	9
1:A:95:ILE:HG22	1:A:96:ASN:CG	0.48	2.29	4	2
1:A:37:CYS:HB3	1:A:42:LEU:HD11	0.48	1.85	20	3
1:A:132:ASN:CB	1:A:135:LEU:HD12	0.48	2.37	16	2
1:A:48:SER:HB3	1:A:101:VAL:HG11	0.48	1.84	2	1
1:A:81:GLN:N	1:A:82:PRO:HD2	0.47	2.24	8	19
1:A:83:PHE:CE2	1:A:87:VAL:HG22	0.47	2.44	10	6
1:A:23:ARG:CD	1:A:25:ALA:HB2	0.47	2.36	15	1
1:A:67:TYR:OH	1:A:84:LEU:HD21	0.47	2.10	3	8
1:A:132:ASN:OD1	1:A:135:LEU:HD11	0.47	2.09	10	1
1:A:84:LEU:HD13	1:A:88:PHE:CE1	0.47	2.45	15	4
1:A:128:PHE:CZ	1:A:129:LEU:HD21	0.47	2.45	15	1
1:A:103:LEU:HD22	1:A:103:LEU:O	0.47	2.10	19	3
1:A:121:ASN:HB2	1:A:134:THR:HG21	0.47	1.87	3	1
1:A:70:LEU:HD22	1:A:128:PHE:CE2	0.46	2.45	2	1
1:A:95:ILE:HD13	1:A:100:MET:HB2	0.46	1.87	18	2
1:A:103:LEU:CD2	1:A:103:LEU:C	0.46	2.84	13	1
1:A:122:THR:HG23	1:A:129:LEU:CD1	0.46	2.40	12	1
1:A:87:VAL:HG13	1:A:88:PHE:CG	0.46	2.46	17	13
1:A:84:LEU:HD13	1:A:88:PHE:CD1	0.46	2.46	19	3
1:A:122:THR:HG23	1:A:129:LEU:HD12	0.45	1.87	12	1
1:A:21:MET:H	1:A:103:LEU:HD21	0.45	1.70	15	1
1:A:116:CYS:HB2	1:A:119:LEU:HD23	0.45	1.87	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:LEU:HD11	1:A:125:PHE:CB	0.45	2.42	5	1
1:A:103:LEU:O	1:A:103:LEU:HD12	0.45	2.11	10	3
1:A:51:LEU:HD23	1:A:90:PRO:CB	0.45	2.42	8	1
1:A:51:LEU:HD23	1:A:90:PRO:CG	0.45	2.42	12	1
1:A:21:MET:HA	1:A:103:LEU:HD21	0.45	1.88	14	1
1:A:51:LEU:HD13	1:A:90:PRO:HG3	0.45	1.87	2	2
1:A:119:LEU:HD13	1:A:129:LEU:HD21	0.45	1.88	10	1
1:A:114:GLU:N	1:A:115:PRO:HD2	0.45	2.27	18	8
1:A:118:ILE:HG22	1:A:124:PHE:CD2	0.45	2.47	6	1
1:A:83:PHE:CD1	1:A:86:ALA:HB3	0.44	2.48	13	1
1:A:95:ILE:HD13	1:A:100:MET:HE2	0.44	1.90	13	1
1:A:70:LEU:HD13	1:A:128:PHE:CZ	0.43	2.48	17	4
1:A:119:LEU:HD13	1:A:129:LEU:CD1	0.43	2.43	16	2
1:A:129:LEU:HD22	1:A:131:CYS:SG	0.43	2.53	16	1
1:A:64:LEU:HD22	1:A:88:PHE:CZ	0.43	2.48	20	1
1:A:83:PHE:O	1:A:87:VAL:HG12	0.43	2.14	7	4
1:A:51:LEU:HD22	1:A:90:PRO:HG3	0.43	1.91	2	1
1:A:119:LEU:HD13	1:A:122:THR:CG2	0.43	2.43	3	1
1:A:118:ILE:HG21	1:A:124:PHE:CZ	0.43	2.48	4	1
1:A:21:MET:N	1:A:103:LEU:HD21	0.43	2.28	15	1
1:A:52:THR:HG22	1:A:130:ARG:HD3	0.43	1.90	10	2
1:A:34:THR:HG23	1:A:41:LYS:HE2	0.43	1.91	5	1
1:A:82:PRO:HG3	1:A:111:ILE:HG21	0.43	1.89	15	1
1:A:23:ARG:NH2	1:A:103:LEU:HD21	0.42	2.28	7	1
1:A:49:LEU:HD22	1:A:60:LEU:HD12	0.42	1.91	17	1
1:A:116:CYS:HB3	1:A:119:LEU:HD12	0.42	1.90	7	1
1:A:119:LEU:HD11	1:A:125:PHE:H	0.42	1.74	6	1
1:A:132:ASN:HB2	1:A:135:LEU:HD21	0.42	1.90	6	1
1:A:119:LEU:HD22	1:A:129:LEU:CD1	0.42	2.44	16	1
1:A:103:LEU:CD1	1:A:103:LEU:N	0.42	2.82	13	1
1:A:103:LEU:HD13	1:A:103:LEU:H	0.42	1.71	16	1
1:A:42:LEU:HD22	1:A:44:TYR:CE1	0.42	2.48	3	1
1:A:119:LEU:HD21	1:A:125:PHE:CD1	0.42	2.49	20	1
1:A:121:ASN:C	1:A:121:ASN:ND2	0.42	2.72	15	1
1:A:21:MET:CA	1:A:103:LEU:HD11	0.41	2.45	4	1
1:A:51:LEU:HD23	1:A:90:PRO:HB3	0.41	1.92	8	1
1:A:119:LEU:HD11	1:A:125:PHE:N	0.41	2.30	5	1
1:A:22:VAL:HG12	1:A:100:MET:HB3	0.41	1.91	7	2
1:A:36:THR:HG23	1:A:41:LYS:HG2	0.41	1.91	18	3
1:A:70:LEU:HD13	1:A:128:PHE:CD2	0.41	2.51	2	1
1:A:119:LEU:HG	1:A:129:LEU:HD22	0.41	1.93	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:PHE:CD2	1:A:129:LEU:HD23	0.41	2.51	17	1
1:A:67:TYR:CE1	1:A:84:LEU:HD21	0.41	2.51	16	1
1:A:114:GLU:CB	1:A:115:PRO:HD3	0.41	2.45	11	1
1:A:118:ILE:HG22	1:A:124:PHE:CE2	0.41	2.51	15	1
1:A:64:LEU:HD23	1:A:64:LEU:N	0.40	2.32	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	117/128 (91%)	99±2 (85±2%)	15±2 (13±2%)	2±1 (2±1%)	14	55
All	All	2340/2560 (91%)	1984 (85%)	309 (13%)	47 (2%)	14	55

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	121	ASN	16
1	A	135	LEU	6
1	A	21	MET	4
1	A	126	PRO	4
1	A	130	ARG	4
1	A	115	PRO	4
1	A	123	THR	2
1	A	116	CYS	2
1	A	128	PHE	1
1	A	91	LYS	1
1	A	26	ARG	1
1	A	122	THR	1
1	A	53	ASP	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	109/118 (92%)	76±3 (70±3%)	33±3 (30±3%)	2	17
All	All	2180/2360 (92%)	1517 (70%)	663 (30%)	2	17

All 74 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	67	TYR	20
1	A	63	LYS	20
1	A	84	LEU	20
1	A	81	GLN	20
1	A	49	LEU	18
1	A	76	CYS	18
1	A	107	GLU	18
1	A	32	ASN	18
1	A	127	LYS	18
1	A	30	THR	18
1	A	121	ASN	17
1	A	66	ASP	17
1	A	128	PHE	17
1	A	56	THR	16
1	A	51	LEU	16
1	A	72	HIS	16
1	A	59	GLU	16
1	A	70	LEU	15
1	A	27	CYS	14
1	A	100	MET	14
1	A	36	THR	14
1	A	89	LYS	13
1	A	103	LEU	13
1	A	23	ARG	13
1	A	114	GLU	12
1	A	58	LYS	12
1	A	40	SER	11
1	A	130	ARG	11
1	A	68	TYR	11

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Mol	Chain	Res	Type	Models (Total)
1	A	120	TYR	11
1	A	64	LEU	10
1	A	26	ARG	10
1	A	75	LYS	10
1	A	61	ASN	9
1	A	132	ASN	9
1	A	129	LEU	9
1	A	94	LYS	8
1	A	55	HIS	7
1	A	31	SER	7
1	A	24	ARG	6
1	A	45	GLU	6
1	A	124	PHE	6
1	A	21	MET	6
1	A	110	ARG	6
1	A	123	THR	6
1	A	109	CYS	6
1	A	117	ARG	6
1	A	133	GLU	5
1	A	57	GLU	5
1	A	131	CYS	5
1	A	52	THR	5
1	A	71	LYS	4
1	A	47	SER	4
1	A	119	LEU	4
1	A	105	SER	3
1	A	125	PHE	3
1	A	92	CYS	3
1	A	53	ASP	3
1	A	85	CYS	2
1	A	44	TYR	2
1	A	65	ASN	2
1	A	108	MET	2
1	A	96	ASN	2
1	A	134	THR	2
1	A	48	SER	2
1	A	111	ILE	2
1	A	34	THR	2
1	A	60	LEU	1
1	A	99	ASP	1
1	A	50	ASP	1
1	A	135	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	93	GLU	1
1	A	41	LYS	1
1	A	116	CYS	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

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: 2mah_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1607
Number of shifts mapped to atoms	1607
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	128	0.29 ± 0.24	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	124	0.19 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	109	0.09 ± 0.12	None needed (< 0.5 ppm)
^{15}N	116	1.46 ± 0.43	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1367 atoms were assigned a chemical shift out of a possible 1503. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	549/567 (97%)	224/225 (100%)	218/234 (93%)	107/108 (99%)
Sidechain	683/782 (87%)	430/466 (92%)	245/281 (87%)	8/35 (23%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	135/154 (88%)	75/82 (91%)	59/69 (86%)	1/3 (33%)
Overall	1367/1503 (91%)	729/773 (94%)	522/584 (89%)	116/146 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1474 atoms were assigned a chemical shift out of a possible 1631. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	596/620 (96%)	243/246 (99%)	237/256 (93%)	116/118 (98%)
Sidechain	739/850 (87%)	465/507 (92%)	266/304 (88%)	8/39 (21%)
Aromatic	139/161 (86%)	77/86 (90%)	61/71 (86%)	1/4 (25%)
Overall	1474/1631 (90%)	785/839 (94%)	564/631 (89%)	125/161 (78%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	91	LYS	HB3	-0.07	3.10 – 0.40	-6.8
1	A	91	LYS	HD3	0.35	2.75 – 0.45	-5.4

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

