



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:17 pm GMT

PDB ID : 1ON4
Title : Solution structure of soluble domain of Sco1 from Bacillus Subtilis
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Deposited on : 2003-02-27

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

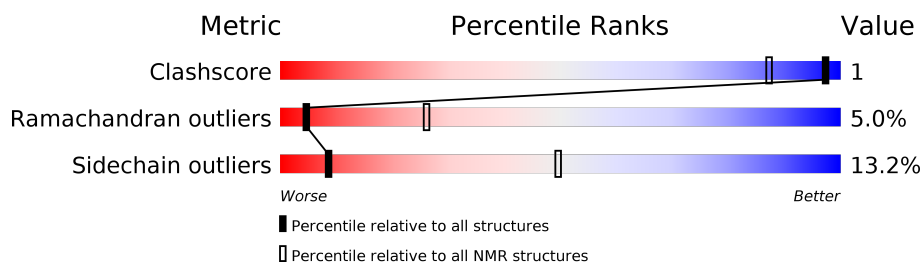
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment is 73%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	174	

2 Ensemble composition and analysis

This entry contains 30 models. Model 28 is the overall representative, medoid model (most similar to other models).

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:7-A:43, A:49-A:123, A:138-A:153, A:159-A:172 (142)	0.46	28

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 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 4, 7, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 20, 21, 22, 25, 26, 27, 28, 29
2	8, 23, 24
3	6, 30
4	5, 19
Single-model clusters	2

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2765 atoms, of which 1366 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sco1.

Mol	Chain	Residues	Atoms						Trace
1	A	174	Total	C	H	N	O	S	0
			2765	897	1366	220	277	5	

There are 5 discrepancies between the modelled and reference sequences:

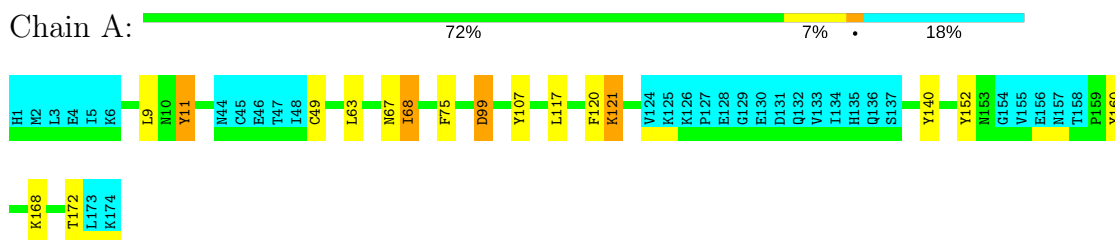
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	CLONING ARTIFACT	UNP P54178
A	2	MET	-	CLONING ARTIFACT	UNP P54178
A	3	LEU	-	CLONING ARTIFACT	UNP P54178
A	4	GLU	-	CLONING ARTIFACT	UNP P54178
A	66	GLU	GLY	SEE REMARK 999	UNP P54178

4 Residue-property plots [i](#)

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: Sco1

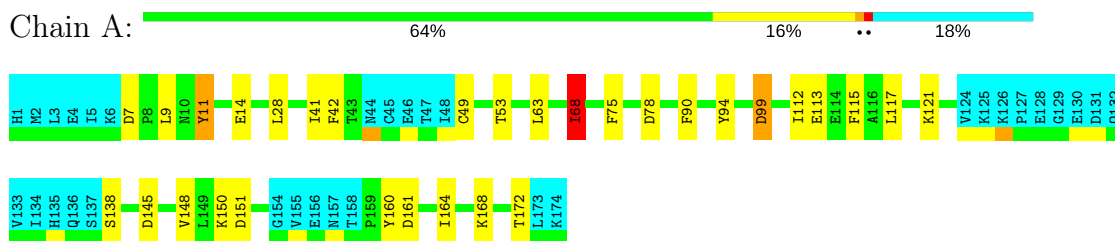


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

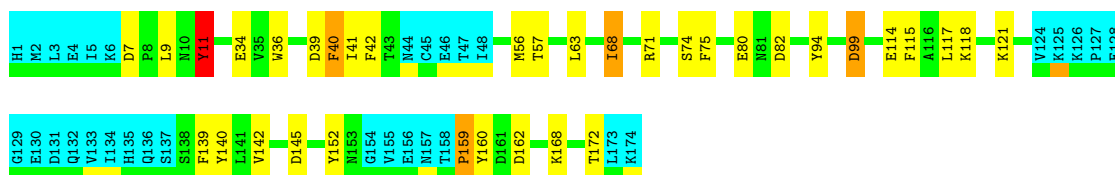
- Molecule 1: Sco1



4.2.2 Score per residue for model 2

- Molecule 1: Sco1

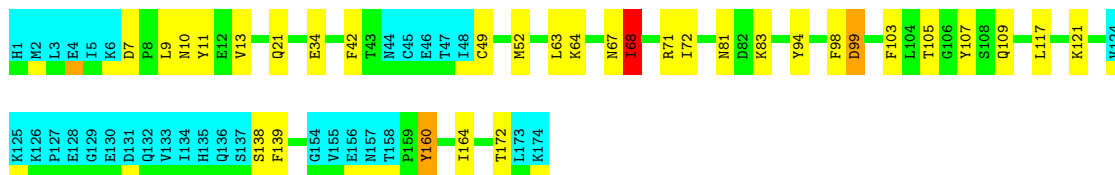




4.2.3 Score per residue for model 3

- Molecule 1: Sco1

Chain A: 63% 17% 18%



4.2.4 Score per residue for model 4

- Molecule 1: Sco1

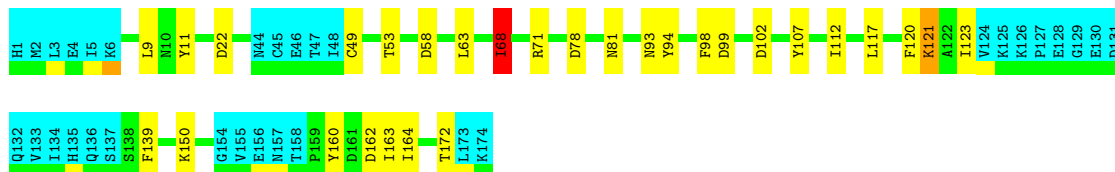
Chain A: 68% 11% 18%



4.2.5 Score per residue for model 5

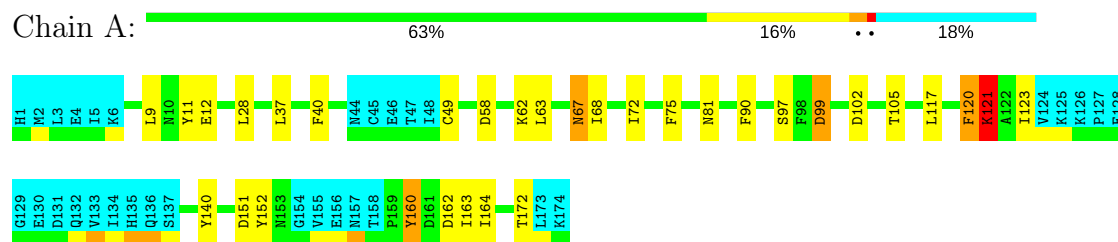
- Molecule 1: Sco1

Chain A: 65% 16% 18%



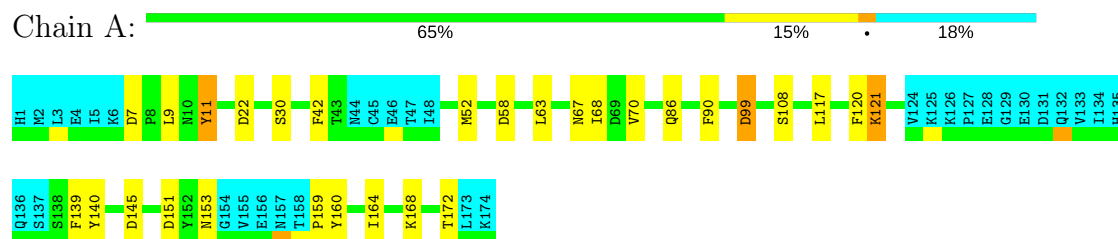
4.2.6 Score per residue for model 6

- Molecule 1: Sco1



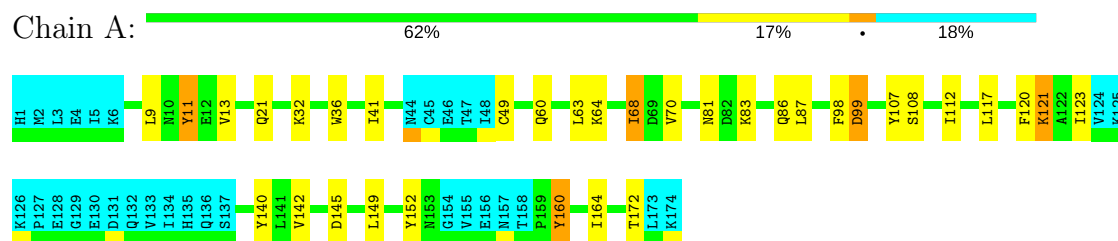
4.2.7 Score per residue for model 7

- Molecule 1: Sco1



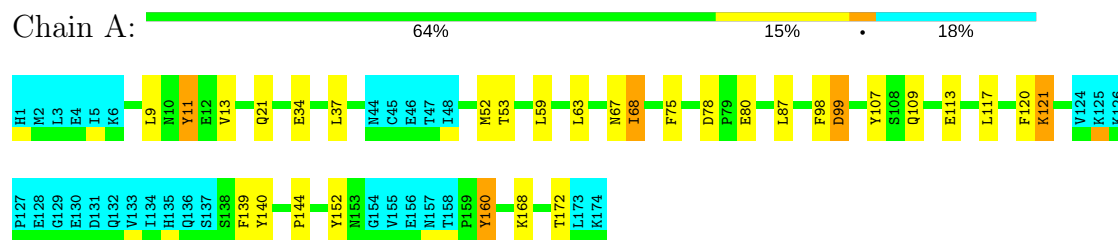
4.2.8 Score per residue for model 8

- Molecule 1: Sco1



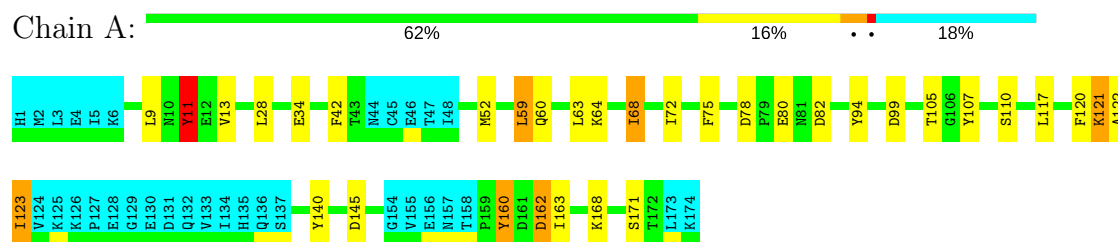
4.2.9 Score per residue for model 9

- Molecule 1: Sco1



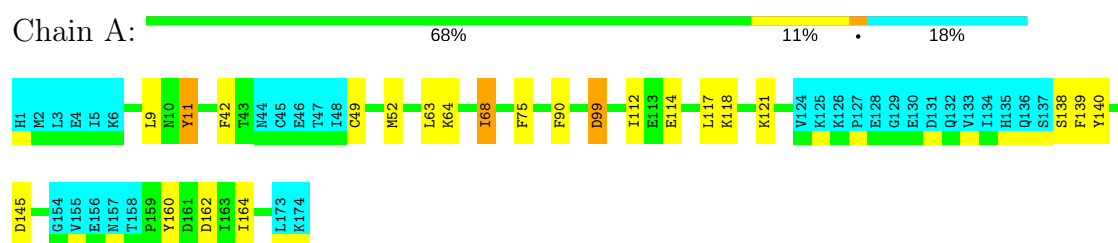
4.2.10 Score per residue for model 10

- Molecule 1: Sco1



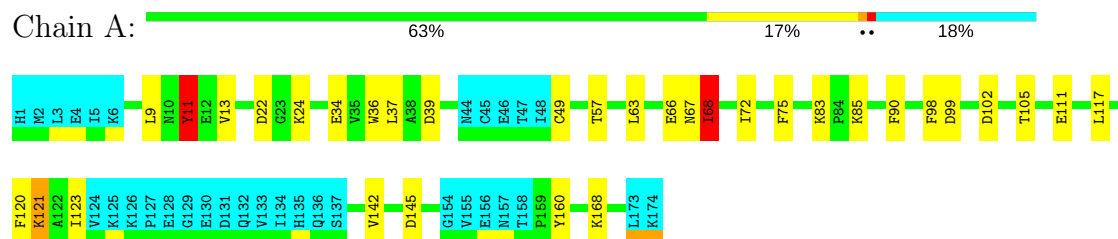
4.2.11 Score per residue for model 11

- Molecule 1: Sco1



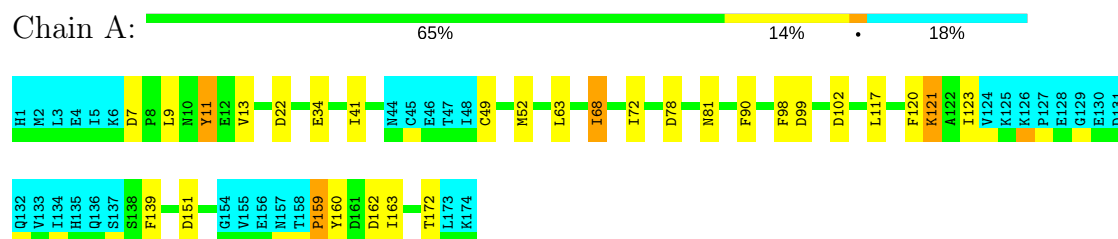
4.2.12 Score per residue for model 12

- Molecule 1: Sco1



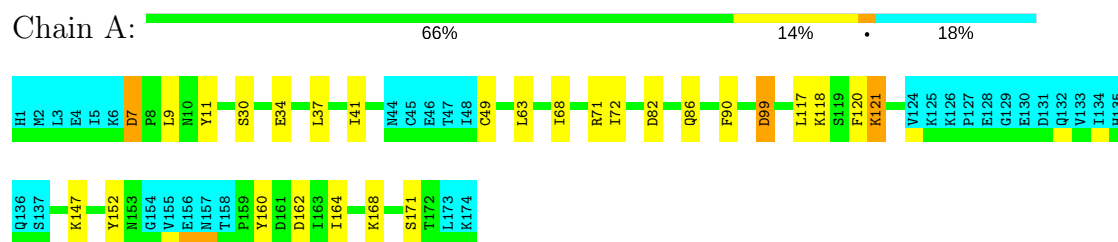
4.2.13 Score per residue for model 13

- Molecule 1: Sco1



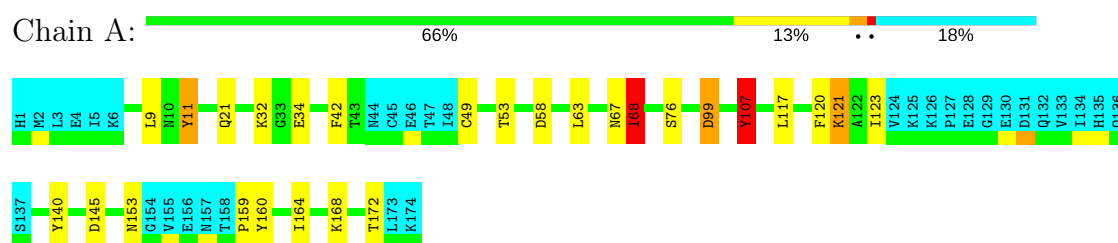
4.2.14 Score per residue for model 14

- Molecule 1: Sco1



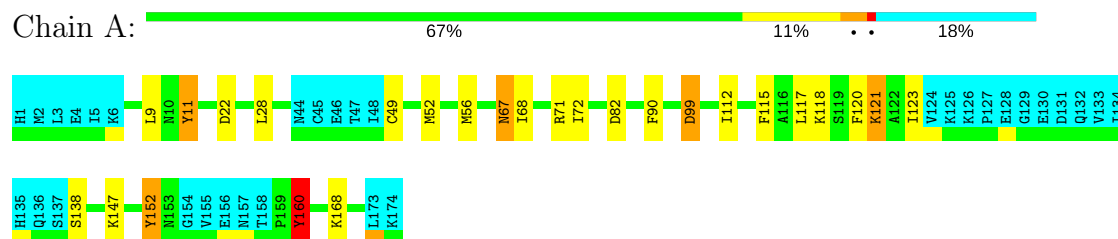
4.2.15 Score per residue for model 15

- Molecule 1: Sco1



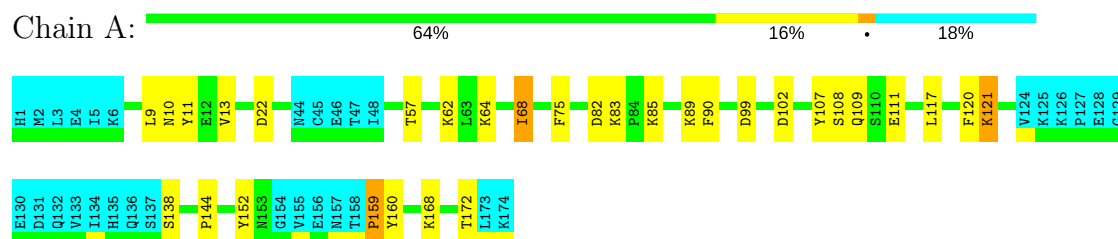
4.2.16 Score per residue for model 16

- Molecule 1: Sco1



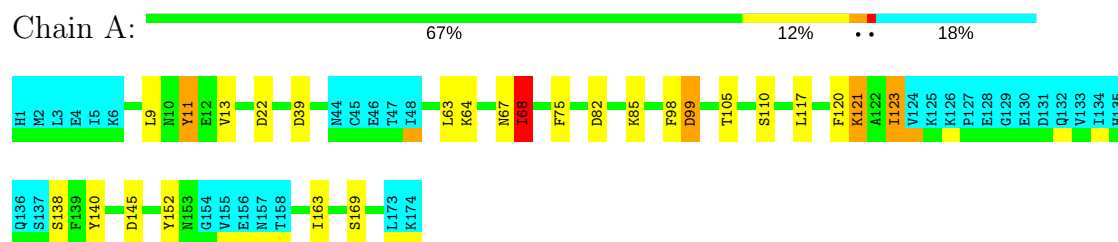
4.2.17 Score per residue for model 17

- Molecule 1: Sco1



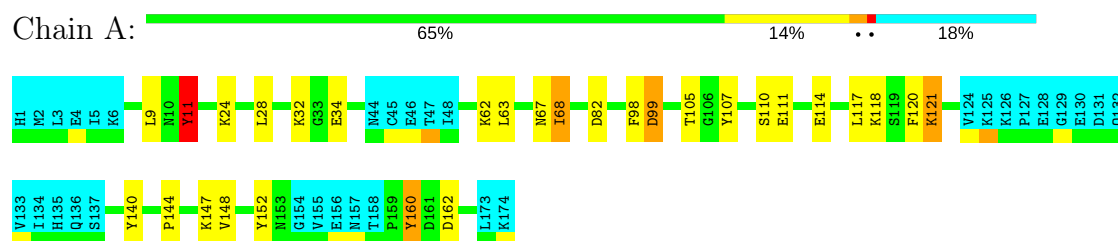
4.2.18 Score per residue for model 18

- Molecule 1: Sco1



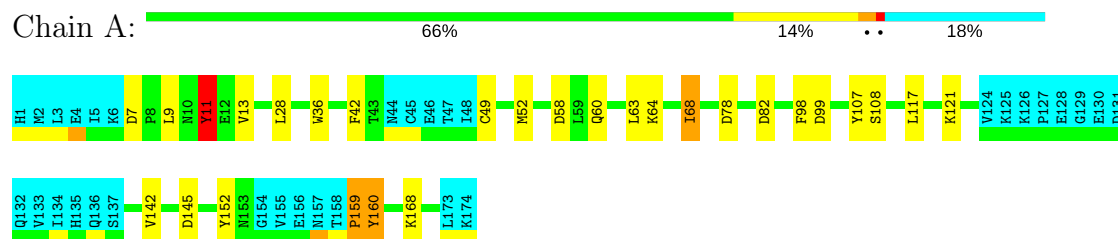
4.2.19 Score per residue for model 19

- Molecule 1: Sco1



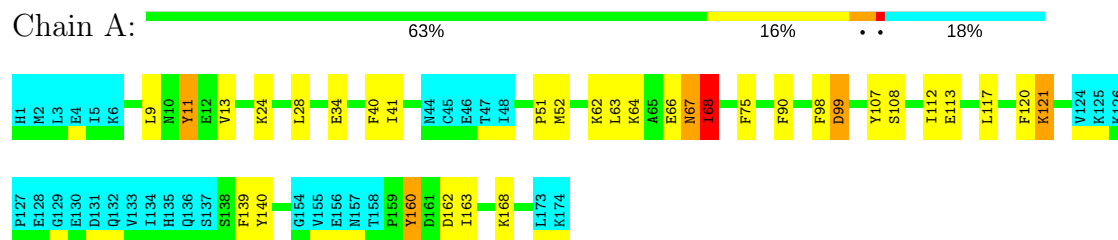
4.2.20 Score per residue for model 20

- Molecule 1: Sco1



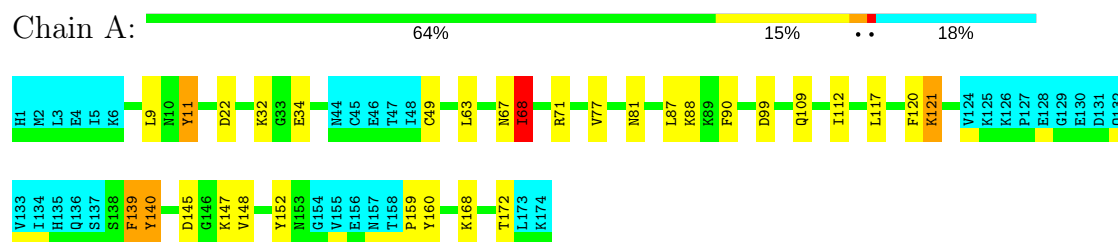
4.2.21 Score per residue for model 21

- Molecule 1: Sco1



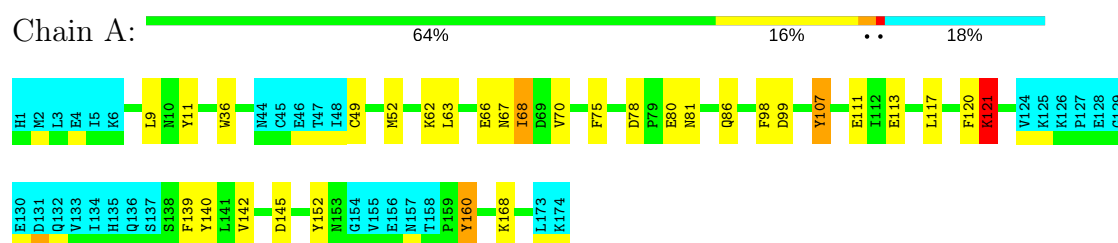
4.2.22 Score per residue for model 22

- Molecule 1: Sco1



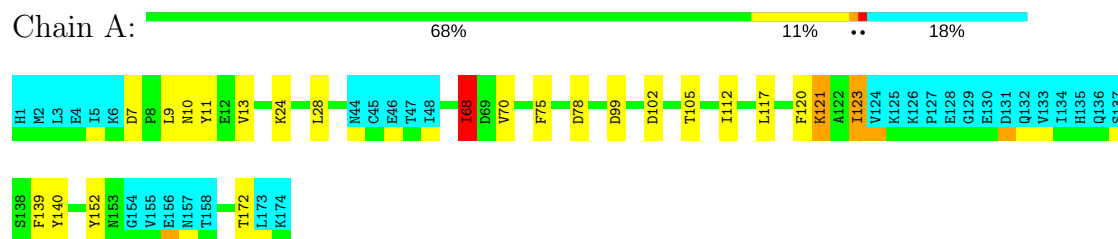
4.2.23 Score per residue for model 23

- Molecule 1: Sco1



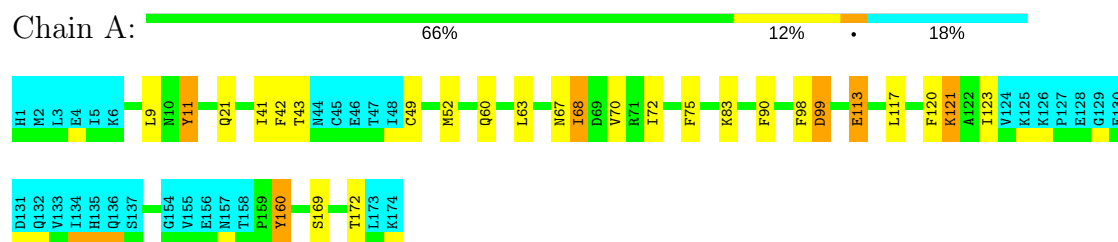
4.2.24 Score per residue for model 24

- Molecule 1: Sco1



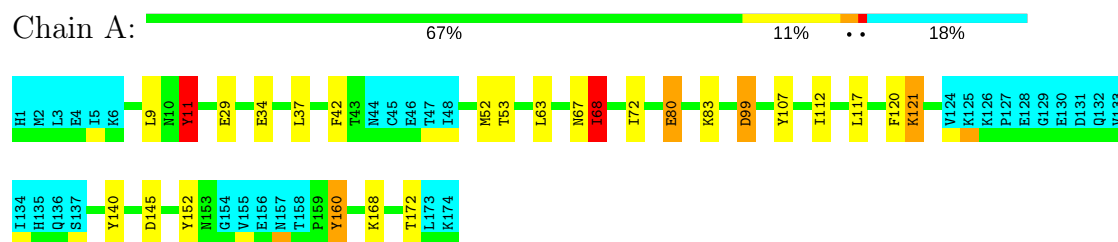
4.2.25 Score per residue for model 25

- Molecule 1: Sco1



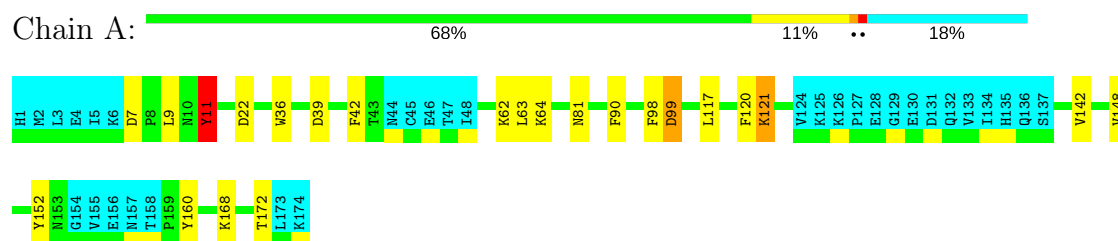
4.2.26 Score per residue for model 26

- Molecule 1: Sco1



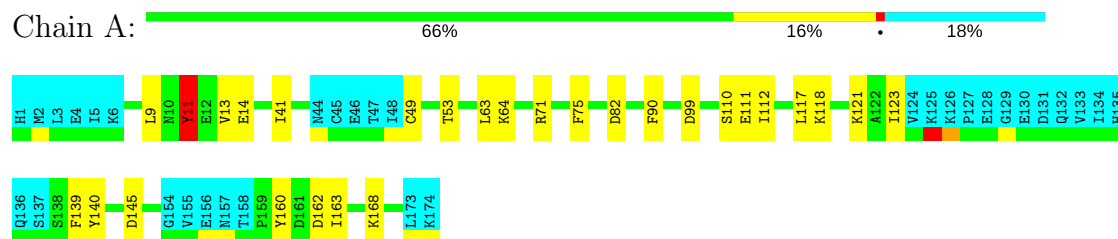
4.2.27 Score per residue for model 27

- Molecule 1: Sco1



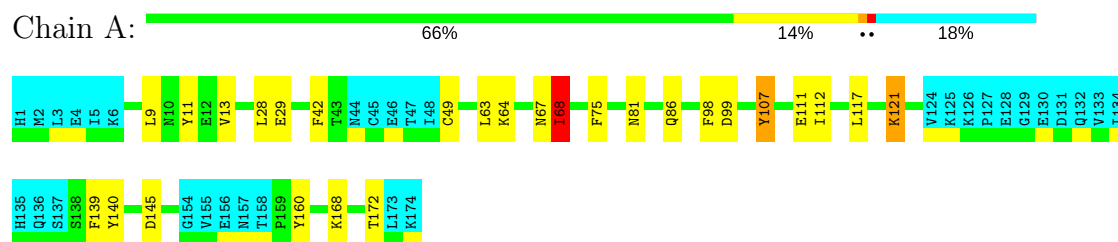
4.2.28 Score per residue for model 28 (medoid)

- Molecule 1: Sco1



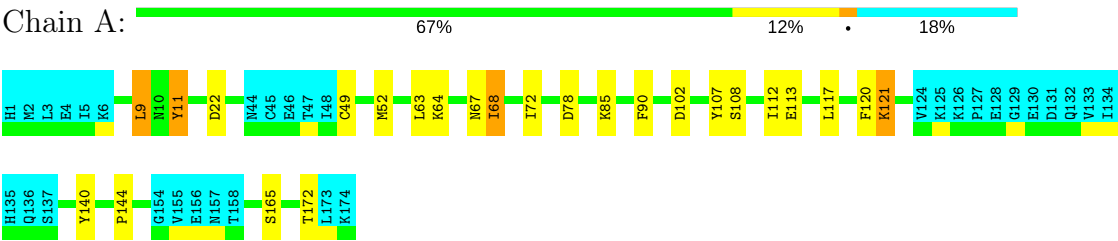
4.2.29 Score per residue for model 29

- Molecule 1: Sco1



4.2.30 Score per residue for model 30

● Molecule 1: Sco1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics coupled to simulated annealing followed by restrained energy minimization*.

Of the 300 calculated structures, 30 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	1.5
CYANA	structure solution	1.0
AMBER	refinement	5

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)	BMRB entry 5742
Number of chemical shift lists	1
Total number of shifts	1669
Number of shifts mapped to atoms	1669
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	73%

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	0.62±0.00	0±0/1176 (0.0±0.0%)	1.01±0.02	1±1/1595 (0.1±0.0%)
All	All	0.62	0/35280 (0.0%)	1.01	30/47850 (0.1%)

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	6.2±1.4
All	All	0	185

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	160	TYR	CB-CG-CD2	-9.14	115.52	121.00	10	10
1	A	11	TYR	CB-CG-CD2	-8.56	115.86	121.00	12	10
1	A	71	ARG	NE-CZ-NH2	-6.87	116.86	120.30	3	5
1	A	160	TYR	CB-CG-CD1	-5.91	117.45	121.00	9	3
1	A	107	TYR	CB-CG-CD2	-5.48	117.71	121.00	15	1
1	A	11	TYR	CA-CB-CG	5.21	123.30	113.40	27	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	68	ILE	Peptide	24
1	A	120	PHE	Peptide,Sidechain	23

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	160	TYR	Sidechain,Peptide	22
1	A	140	TYR	Sidechain	18
1	A	11	TYR	Sidechain	17
1	A	75	PHE	Sidechain	15
1	A	98	PHE	Sidechain	15
1	A	90	PHE	Sidechain	15
1	A	152	TYR	Sidechain	13
1	A	159	PRO	Peptide	4
1	A	94	TYR	Sidechain	4
1	A	115	PHE	Sidechain	3
1	A	40	PHE	Sidechain	3
1	A	139	PHE	Sidechain	2
1	A	103	PHE	Sidechain	1
1	A	71	ARG	Sidechain	1
1	A	123	ILE	Peptide	1
1	A	66	GLU	Peptide	1
1	A	107	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	1145	1108	1108	2±1
All	All	34350	33240	33240	45

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:11:TYR:CB	1:A:148:VAL:HG22	0.60	2.26	1	1
1:A:11:TYR:HB2	1:A:148:VAL:HG22	0.55	1.79	1	1
1:A:9:LEU:HD13	1:A:165:SER:CB	0.52	2.35	30	1
1:A:68:ILE:H	1:A:68:ILE:HD12	0.51	1.66	12	9
1:A:162:ASP:OD1	1:A:163:ILE:HD12	0.51	2.05	6	1
1:A:75:PHE:CE1	1:A:123:ILE:HD11	0.50	2.41	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:TYR:HB3	1:A:148:VAL:CG2	0.50	2.37	27	2
1:A:36:TRP:CZ2	1:A:142:VAL:HG11	0.49	2.42	23	6
1:A:68:ILE:HD12	1:A:68:ILE:H	0.45	1.71	5	4
1:A:75:PHE:HE1	1:A:123:ILE:HD11	0.45	1.72	10	1
1:A:120:PHE:O	1:A:121:LYS:HD2	0.45	2.12	6	1
1:A:114:GLU:OE2	1:A:118:LYS:NZ	0.44	2.48	11	1
1:A:109:GLN:CD	1:A:109:GLN:H	0.44	2.16	17	1
1:A:140:TYR:CD2	1:A:148:VAL:HG11	0.44	2.47	22	1
1:A:62:LYS:NZ	1:A:66:GLU:OE2	0.43	2.50	21	2
1:A:59:LEU:HD13	1:A:60:GLN:N	0.42	2.28	10	1
1:A:122:ALA:CB	1:A:123:ILE:HD12	0.42	2.45	10	1
1:A:11:TYR:HB3	1:A:148:VAL:HG22	0.42	1.91	27	1
1:A:11:TYR:CG	1:A:168:LYS:NZ	0.42	2.88	12	1
1:A:14:GLU:OE2	1:A:118:LYS:NZ	0.42	2.53	28	1
1:A:7:ASP:N	1:A:7:ASP:OD1	0.41	2.53	2	1
1:A:9:LEU:HD13	1:A:165:SER:HB3	0.41	1.92	30	1
1:A:58:ASP:OD2	1:A:62:LYS:NZ	0.41	2.54	6	1
1:A:59:LEU:HD13	1:A:59:LEU:C	0.41	2.36	10	1
1:A:114:GLU:OE1	1:A:118:LYS:NZ	0.40	2.54	19	1
1:A:150:LYS:NZ	1:A:161:ASP:OD2	0.40	2.54	1	1
1:A:122:ALA:HB3	1:A:123:ILE:HD12	0.40	1.92	10	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	142/174 (82%)	115±3 (81±2%)	20±3 (14±2%)	7±2 (5±1%)	5	26
All	All	4260/5220 (82%)	3447 (81%)	598 (14%)	215 (5%)	5	26

All 24 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	99	ASP	29

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Mol	Chain	Res	Type	Models (Total)
1	A	68	ILE	27
1	A	121	LYS	23
1	A	172	THR	18
1	A	49	CYS	18
1	A	52	MET	11
1	A	107	TYR	10
1	A	123	ILE	10
1	A	78	ASP	9
1	A	159	PRO	7
1	A	105	THR	7
1	A	163	ILE	6
1	A	67	ASN	6
1	A	83	LYS	5
1	A	162	ASP	5
1	A	113	GLU	5
1	A	144	PRO	4
1	A	7	ASP	4
1	A	160	TYR	3
1	A	171	SER	3
1	A	21	GLN	2
1	A	108	SER	1
1	A	51	PRO	1
1	A	145	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	129/159 (81%)	112±2 (87±2%)	17±2 (13±2%)	8	49
All	All	3870/4770 (81%)	3358 (87%)	512 (13%)	8	49

All 78 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	121	LYS	30
1	A	117	LEU	30

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Mol	Chain	Res	Type	Models (Total)
1	A	11	TYR	30
1	A	9	LEU	30
1	A	63	LEU	27
1	A	99	ASP	18
1	A	168	LYS	18
1	A	13	VAL	14
1	A	145	ASP	14
1	A	67	ASN	14
1	A	42	PHE	13
1	A	34	GLU	12
1	A	112	ILE	12
1	A	139	PHE	12
1	A	64	LYS	12
1	A	82	ASP	10
1	A	22	ASP	10
1	A	72	ILE	10
1	A	28	LEU	9
1	A	41	ILE	9
1	A	164	ILE	9
1	A	81	ASN	9
1	A	102	ASP	7
1	A	138	SER	6
1	A	107	TYR	6
1	A	53	THR	6
1	A	86	GLN	6
1	A	111	GLU	6
1	A	162	ASP	5
1	A	70	VAL	5
1	A	108	SER	5
1	A	37	LEU	5
1	A	7	ASP	5
1	A	147	LYS	4
1	A	85	LYS	4
1	A	32	LYS	4
1	A	58	ASP	4
1	A	151	ASP	4
1	A	110	SER	4
1	A	39	ASP	4
1	A	24	LYS	4
1	A	160	TYR	3
1	A	57	THR	3
1	A	118	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	59	LEU	3
1	A	109	GLN	3
1	A	10	ASN	3
1	A	60	GLN	3
1	A	62	LYS	3
1	A	87	LEU	3
1	A	152	TYR	3
1	A	21	GLN	3
1	A	43	THR	2
1	A	169	SER	2
1	A	56	MET	2
1	A	30	SER	2
1	A	29	GLU	2
1	A	153	ASN	2
1	A	52	MET	2
1	A	12	GLU	1
1	A	80	GLU	1
1	A	123	ILE	1
1	A	149	LEU	1
1	A	94	TYR	1
1	A	140	TYR	1
1	A	71	ARG	1
1	A	83	LYS	1
1	A	76	SER	1
1	A	89	LYS	1
1	A	74	SER	1
1	A	14	GLU	1
1	A	97	SER	1
1	A	88	LYS	1
1	A	40	PHE	1
1	A	78	ASP	1
1	A	93	ASN	1
1	A	114	GLU	1
1	A	150	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 73% for the well-defined parts and 69% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5742

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	1669
Number of shifts mapped to atoms	1669
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	131	2.40 ± 0.11	Should be applied
$^{13}\text{C}_\beta$	128	2.78 ± 0.17	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	156	0.93 ± 0.30	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 73%, i.e. 1279 atoms were assigned a chemical shift out of a possible 1759. 18 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	522/692 (75%)	271/275 (99%)	119/284 (42%)	132/133 (99%)
Sidechain	700/889 (79%)	448/523 (86%)	238/336 (71%)	14/30 (47%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	57/178 (32%)	55/95 (58%)	0/80 (0%)	2/3 (67%)
Overall	1279/1759 (73%)	774/893 (87%)	357/700 (51%)	148/166 (89%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 1478 atoms were assigned a chemical shift out of a possible 2156. 19 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	608/850 (72%)	322/338 (95%)	131/348 (38%)	155/164 (95%)
Sidechain	811/1114 (73%)	533/654 (81%)	260/422 (62%)	18/38 (47%)
Aromatic	59/192 (31%)	57/103 (55%)	0/84 (0%)	2/5 (40%)
Overall	1478/2156 (69%)	912/1095 (83%)	391/854 (46%)	175/207 (85%)

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	71	ARG	NE	123.68	92.63 – 76.73	24.5
1	A	142	VAL	HB	-0.20	3.59 – 0.39	-6.8
1	A	21	GLN	CG	26.28	39.38 – 28.18	-6.7
1	A	163	ILE	HG13	-1.37	3.26 – -0.84	-6.3
1	A	105	THR	CG2	15.34	27.15 – 15.95	-5.5
1	A	16	PHE	HB3	0.84	4.85 – 1.05	-5.5
1	A	72	ILE	HD12	-0.77	2.13 – -0.77	-5.0
1	A	72	ILE	HD13	-0.77	2.13 – -0.77	-5.0
1	A	72	ILE	HD11	-0.77	2.13 – -0.77	-5.0

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:

