



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:58 AM UTC

PDB ID : 1ON4 / pdb_00001on4
Title : Solution structure of soluble domain of Sco1 from Bacillus Subtilis
Authors : Balatri, E.; Banci, L.; Bertini, I.; Cantini, F.; Ciofi-Baffoni, S.; Structural Proteomics in Europe (SPINE)
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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

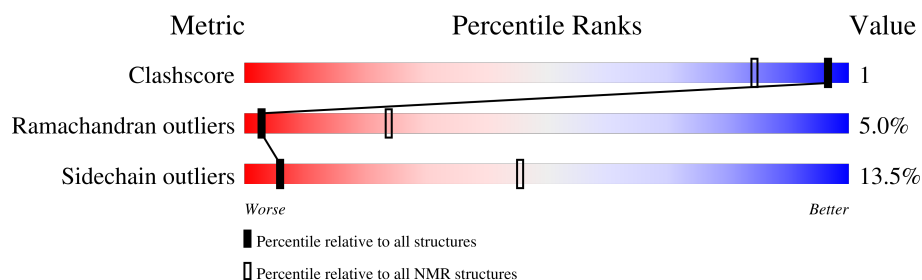
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	68% 11% • 18%

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)	0.79	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:

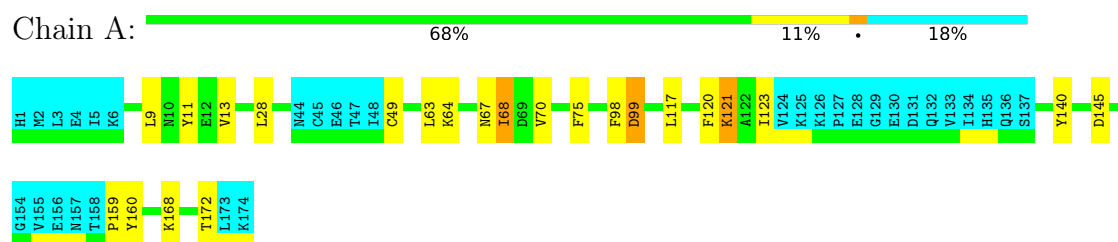
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	cloning artifact	UNP P54178
A	2	MET	-	cloning artifact	UNP P54178
A	3	LEU	-	cloning artifact	UNP P54178
A	4	GLU	-	cloning artifact	UNP P54178
A	66	GLU	GLY	SEE REMARK 999	UNP P54178

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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

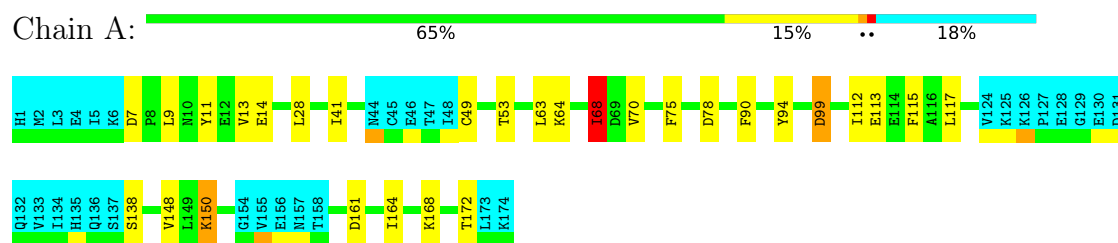


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

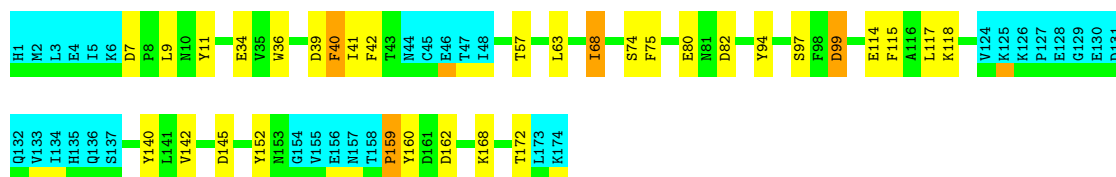
- Molecule 1: Sco1



4.2.2 Score per residue for model 2

- Molecule 1: Sco1

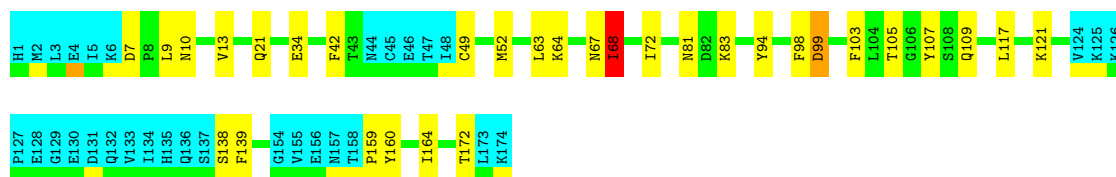




4.2.3 Score per residue for model 3

- Molecule 1: Sco1

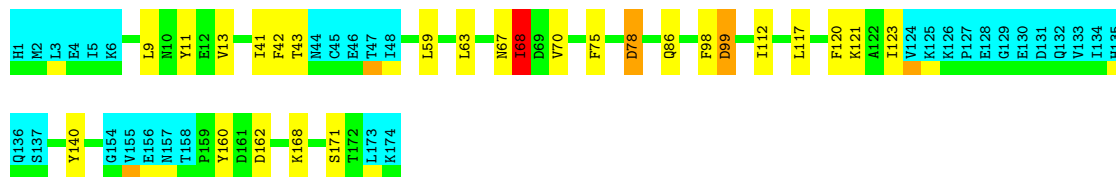
Chain A: 64% 17% 18%



4.2.4 Score per residue for model 4

- Molecule 1: Sco1

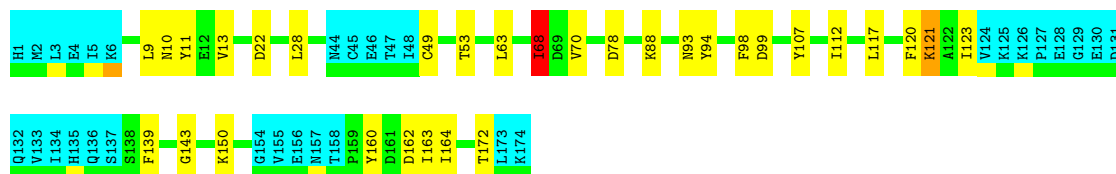
Chain A: 67% 13% 18%



4.2.5 Score per residue for model 5

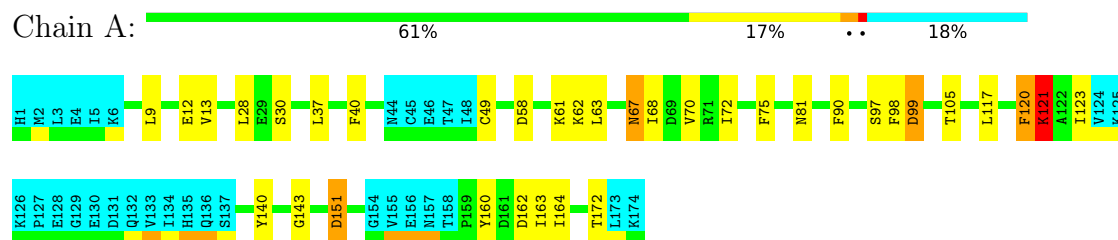
- Molecule 1: Sco1

Chain A: 64% 17% 18%



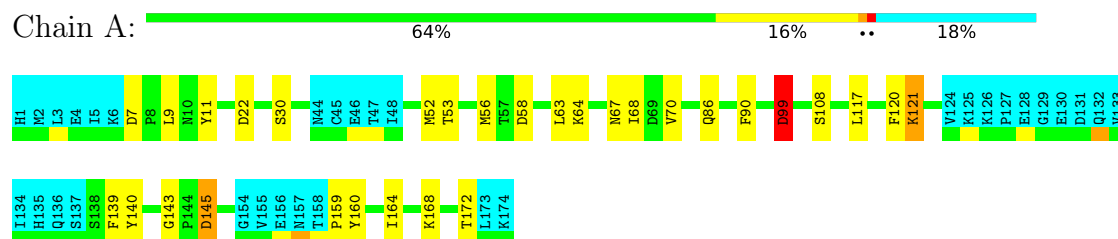
4.2.6 Score per residue for model 6

- Molecule 1: Sco1



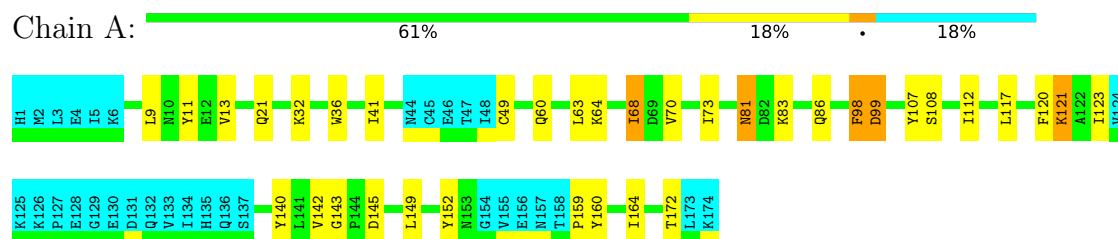
4.2.7 Score per residue for model 7

- Molecule 1: Sco1



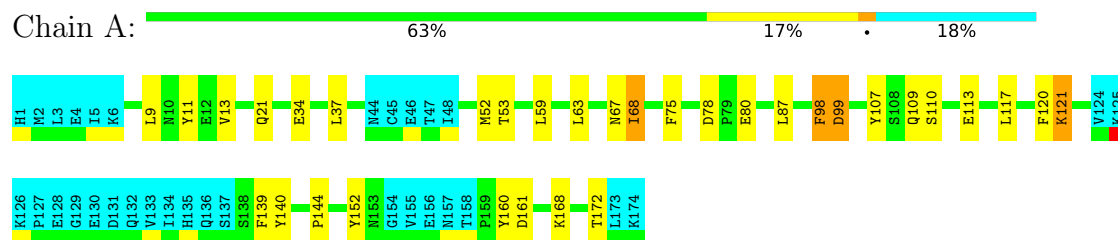
4.2.8 Score per residue for model 8

- Molecule 1: Sco1



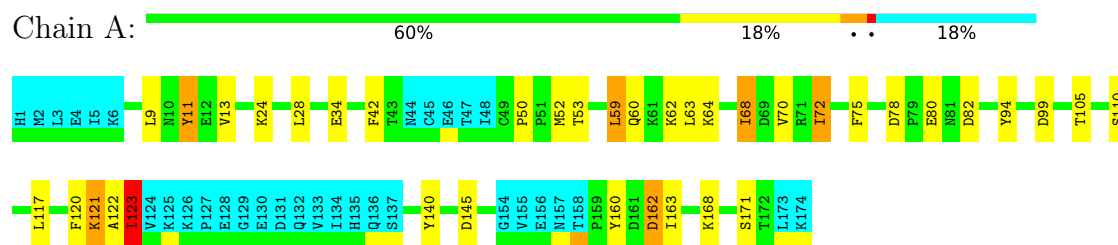
4.2.9 Score per residue for model 9

- Molecule 1: Sco1



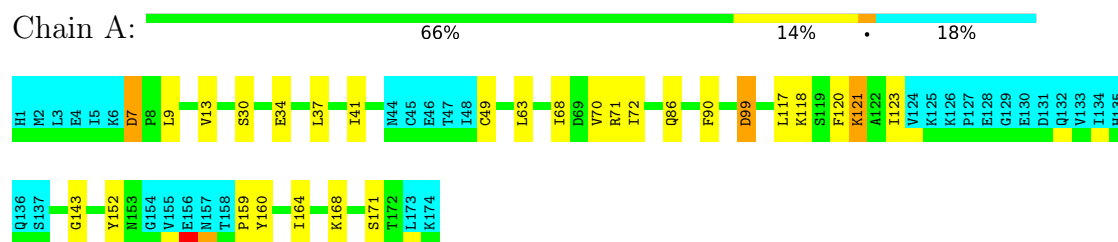
4.2.10 Score per residue for model 10

- Molecule 1: Sco1



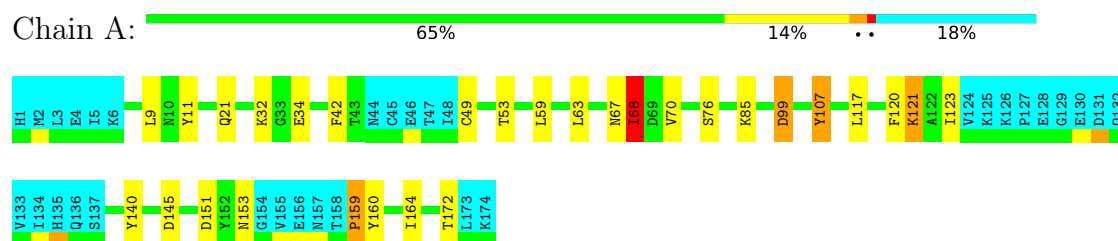
4.2.14 Score per residue for model 14

- Molecule 1: Sco1



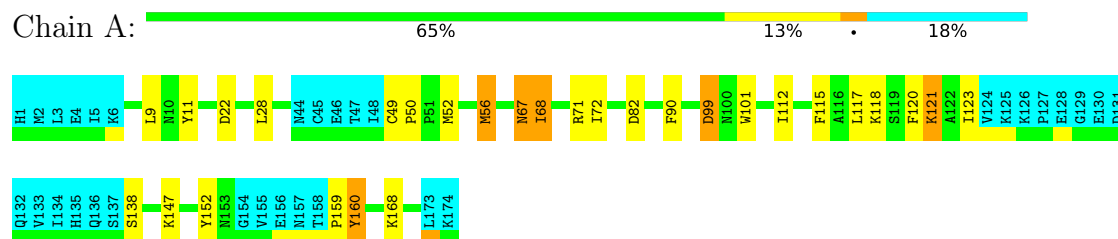
4.2.15 Score per residue for model 15

- Molecule 1: Sco1



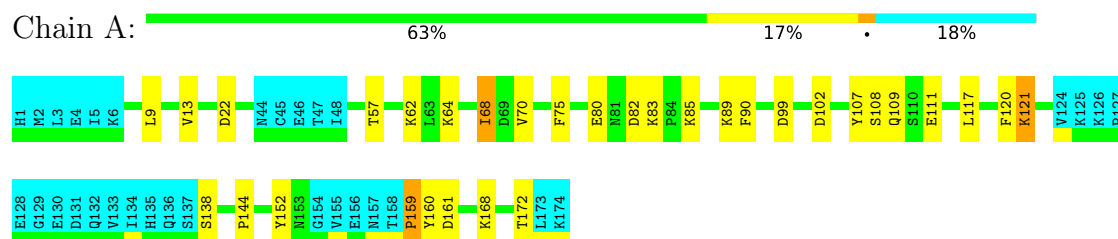
4.2.16 Score per residue for model 16

- Molecule 1: Sco1



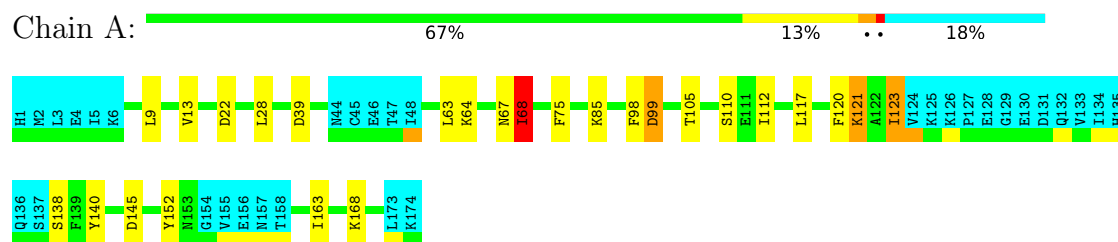
4.2.17 Score per residue for model 17

- Molecule 1: Sco1



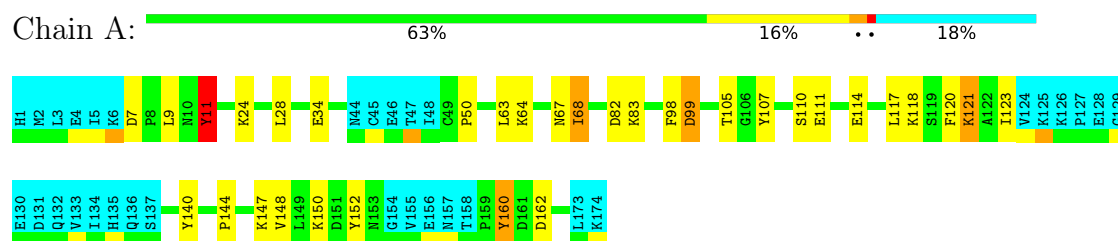
4.2.18 Score per residue for model 18

- Molecule 1: Sco1



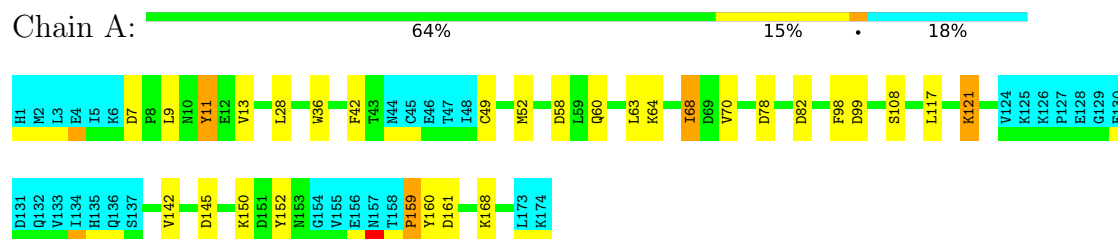
4.2.19 Score per residue for model 19

- Molecule 1: Sco1



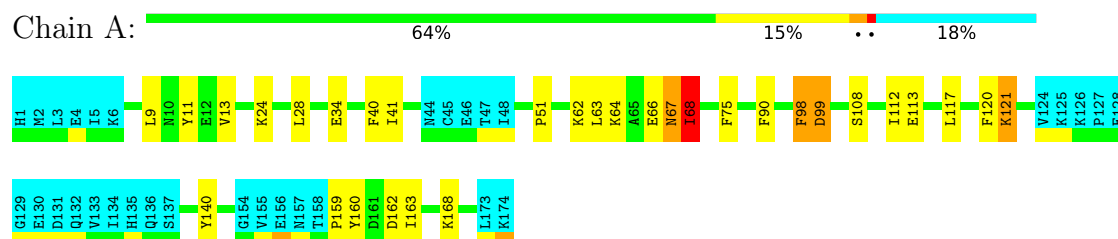
4.2.20 Score per residue for model 20

- Molecule 1: Sco1



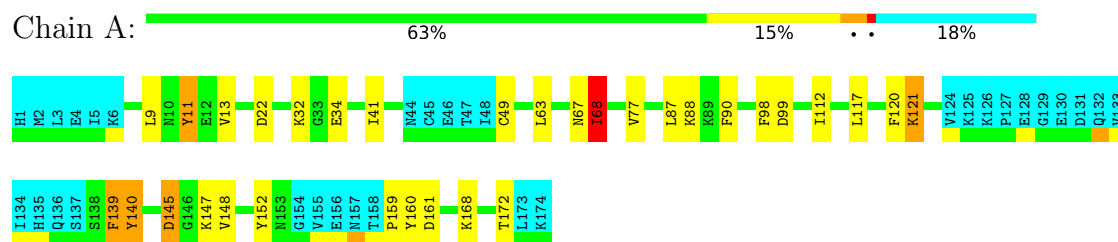
4.2.21 Score per residue for model 21

- Molecule 1: Sco1



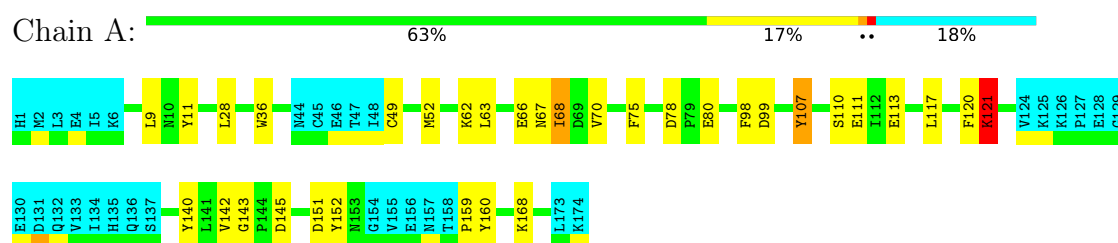
4.2.22 Score per residue for model 22

- Molecule 1: Sco1



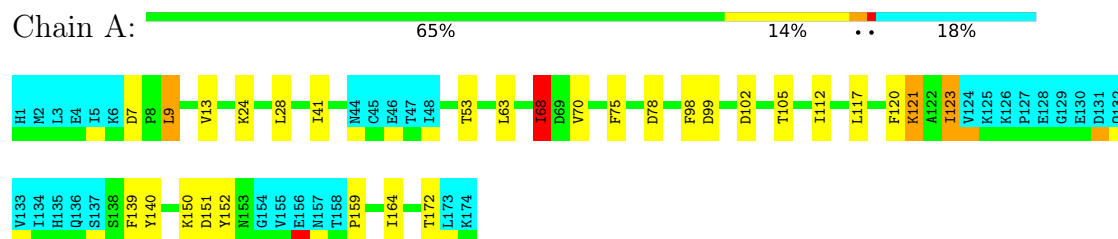
4.2.23 Score per residue for model 23

- Molecule 1: Sco1



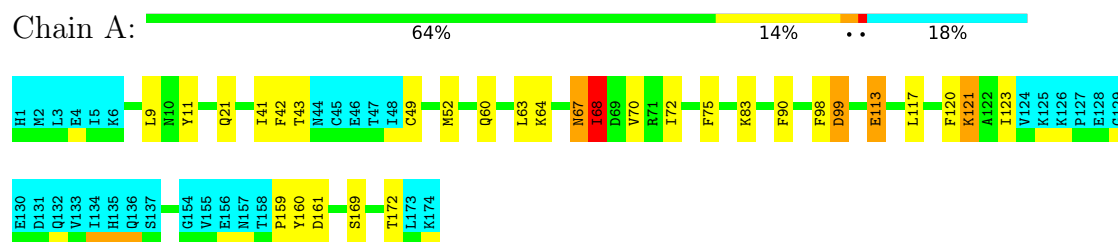
4.2.24 Score per residue for model 24

- Molecule 1: Sco1



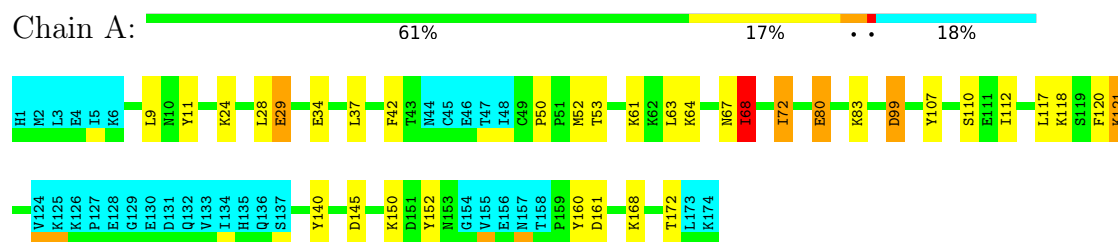
4.2.25 Score per residue for model 25

- Molecule 1: Sco1



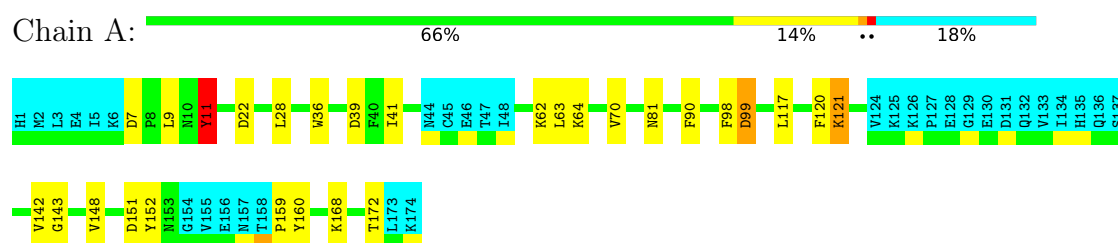
4.2.26 Score per residue for model 26

- Molecule 1: Sco1



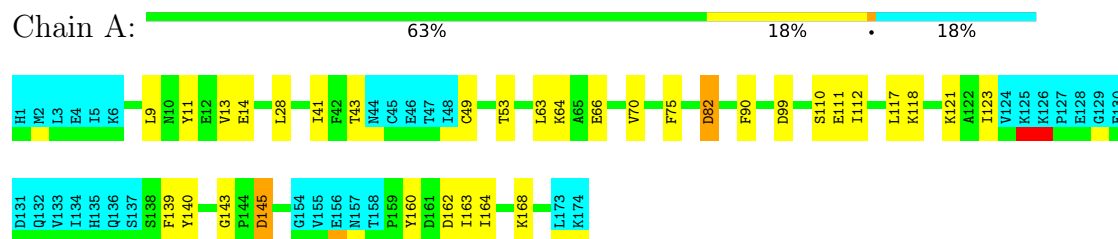
4.2.27 Score per residue for model 27

- Molecule 1: Sco1



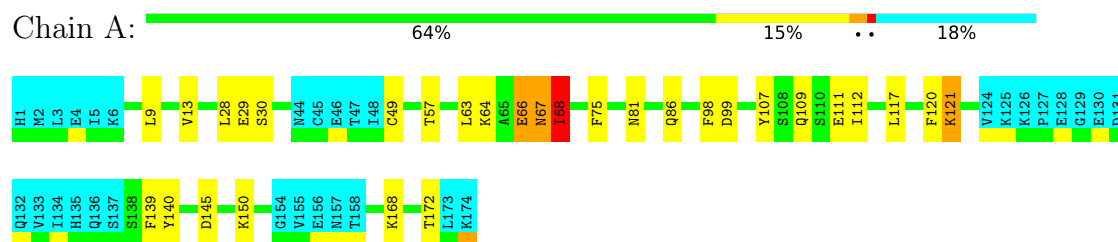
4.2.28 Score per residue for model 28 (medoid)

- Molecule 1: Sco1



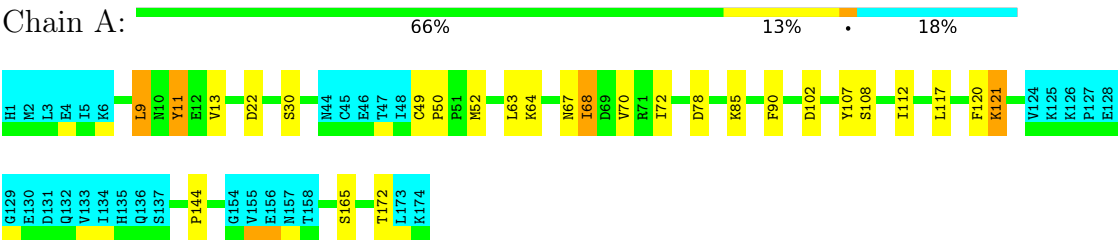
4.2.29 Score per residue for model 29

- 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

No chemical shift data was provided.

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±0.01	0±0/1176 (0.0± 0.0%)	1.31±0.03	4±2/1595 (0.2± 0.1%)
All	All	0.62	0/35280 (0.0%)	1.31	107/47850 (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	0.0±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	151	ASP	CA-CB-CG	8.07	120.67	112.60	15	5
1	A	78	ASP	CA-CB-CG	-7.14	105.46	112.60	4	1
1	A	10	ASN	CA-CB-CG	7.02	119.62	112.60	5	1
1	A	145	ASP	CA-CB-CG	6.23	118.83	112.60	7	3
1	A	161	ASP	CA-CB-CG	6.08	118.68	112.60	17	4
1	A	161	ASP	CA-C-N	6.06	128.65	120.65	17	5
1	A	161	ASP	C-N-CA	6.06	128.65	120.65	17	5
1	A	58	ASP	CA-CB-CG	-5.93	106.67	112.60	11	1
1	A	81	ASN	CA-CB-CG	5.93	118.53	112.60	8	1
1	A	120	PHE	CA-CB-CG	5.86	119.66	113.80	29	1
1	A	159	PRO	CA-C-N	5.84	132.69	121.54	23	11
1	A	159	PRO	C-N-CA	5.84	132.69	121.54	23	11
1	A	72	ILE	CB-CA-C	5.78	117.95	110.96	10	2
1	A	50	PRO	N-CA-CB	5.72	106.39	103.19	12	7
1	A	98	PHE	CA-C-N	5.47	131.99	121.54	22	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	98	PHE	C-N-CA	5.47	131.99	121.54	22	6
1	A	143	GLY	CA-C-N	5.45	124.79	118.85	12	11
1	A	143	GLY	C-N-CA	5.45	124.79	118.85	12	11
1	A	66	GLU	CA-C-N	5.28	128.74	120.82	29	2
1	A	66	GLU	C-N-CA	5.28	128.74	120.82	29	2
1	A	53	THR	CB-CA-C	5.26	117.69	111.22	7	1
1	A	11	TYR	CA-CB-CG	5.22	123.30	113.90	27	1
1	A	83	LYS	CA-C-N	5.16	125.46	119.47	19	1
1	A	83	LYS	C-N-CA	5.16	125.46	119.47	19	1
1	A	9	LEU	CA-C-N	5.09	130.16	122.67	24	1
1	A	9	LEU	C-N-CA	5.09	130.16	122.67	24	1
1	A	162	ASP	CA-C-N	5.09	127.44	120.77	4	1
1	A	162	ASP	C-N-CA	5.09	127.44	120.77	4	1
1	A	120	PHE	CA-C-N	5.06	131.20	121.54	11	1
1	A	120	PHE	C-N-CA	5.06	131.20	121.54	11	1
1	A	80	GLU	N-CA-C	-5.03	104.76	111.24	17	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
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	90	PHE	Sidechain	15
1	A	98	PHE	Sidechain	15
1	A	152	TYR	Sidechain	13
1	A	94	TYR	Sidechain	4
1	A	159	PRO	Peptide	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	66	GLU	Peptide	1
1	A	71	ARG	Sidechain	1
1	A	123	ILE	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	56

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:56:MET:HE2	1:A:101:TRP:CH2	0.53	2.39	16	1
1:A:9:LEU:HD13	1:A:165:SER:CB	0.52	2.35	30	1
1:A:68:ILE:HD12	1:A:68:ILE:H	0.51	1.66	12	12
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
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:109:GLN:CD	1:A:109:GLN:H	0.49	2.16	17	2
1:A:59:LEU:C	1:A:59:LEU:HD13	0.46	2.36	10	1
1:A:75:PHE:HE1	1:A:123:ILE:HD11	0.45	1.72	10	1
1:A:7:ASP:CG	1:A:150:LYS:HZ3	0.45	2.19	19	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:150:LYS:NZ	1:A:161:ASP:CG	0.44	2.76	26	1
1:A:109:GLN:CD	1:A:109:GLN:N	0.44	2.76	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:67:ASN:O	1:A:68:ILE:C	0.42	2.62	29	4
1:A:14:GLU:OE2	1:A:118:LYS:NZ	0.42	2.53	28	1
1:A:7:ASP:OD1	1:A:7:ASP:N	0.41	2.53	2	1
1:A:58:ASP:OD2	1:A:62:LYS:NZ	0.41	2.54	6	1
1:A:9:LEU:HD13	1:A:165:SER:HB3	0.41	1.92	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:GLU:OE1	1:A:118:LYS:NZ	0.40	2.54	19	1
1:A:68:ILE:H	1:A:68:ILE:HD12	0.40	1.75	29	1
1:A:150:LYS:NZ	1:A:161:ASP:OD2	0.40	2.54	1	1
1:A:64:LYS:NZ	1:A:99:ASP:OD1	0.40	2.54	7	1
1:A:122:ALA:HB3	1:A:123:ILE:HD12	0.40	1.92	10	1
1:A:29:GLU:CD	1:A:29:GLU:N	0.40	2.79	26	1
1:A:43:THR:H	1:A:82:ASP:CG	0.40	2.24	28	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%)	3	24
All	All	4260/5220 (82%)	3447 (81%)	598 (14%)	215 (5%)	3	24

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
1	A	68	ILE	27
1	A	121	LYS	23
1	A	49	CYS	18
1	A	172	THR	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	113	GLU	5
1	A	162	ASP	5

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Mol	Chain	Res	Type	Models (Total)
1	A	83	LYS	5
1	A	7	ASP	4
1	A	144	PRO	4
1	A	160	TYR	3
1	A	171	SER	3
1	A	21	GLN	2
1	A	108	SER	1
1	A	145	ASP	1
1	A	51	PRO	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 (86±2%)	17±2 (14±2%)	6	45
All	All	3870/4770 (81%)	3346 (86%)	524 (14%)	6	45

All 81 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	9	LEU	30
1	A	117	LEU	30
1	A	63	LEU	28
1	A	121	LYS	28
1	A	13	VAL	21
1	A	70	VAL	18
1	A	99	ASP	18
1	A	168	LYS	18
1	A	28	LEU	16
1	A	64	LYS	16
1	A	112	ILE	15
1	A	145	ASP	13
1	A	67	ASN	13
1	A	41	ILE	12
1	A	164	ILE	12
1	A	11	TYR	12

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Mol	Chain	Res	Type	Models (Total)
1	A	34	GLU	11
1	A	72	ILE	10
1	A	22	ASP	10
1	A	42	PHE	9
1	A	139	PHE	9
1	A	53	THR	8
1	A	82	ASP	7
1	A	110	SER	7
1	A	138	SER	6
1	A	150	LYS	6
1	A	81	ASN	6
1	A	24	LYS	6
1	A	111	GLU	6
1	A	7	ASP	5
1	A	86	GLN	5
1	A	123	ILE	5
1	A	30	SER	5
1	A	37	LEU	5
1	A	108	SER	5
1	A	102	ASP	5
1	A	39	ASP	4
1	A	57	THR	4
1	A	118	LYS	4
1	A	59	LEU	4
1	A	162	ASP	4
1	A	85	LYS	4
1	A	21	GLN	3
1	A	61	LYS	3
1	A	32	LYS	3
1	A	60	GLN	3
1	A	62	LYS	3
1	A	66	GLU	3
1	A	147	LYS	3
1	A	97	SER	2
1	A	109	GLN	2
1	A	43	THR	2
1	A	88	LYS	2
1	A	151	ASP	2
1	A	56	MET	2
1	A	58	ASP	2
1	A	87	LEU	2
1	A	160	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	107	TYR	2
1	A	29	GLU	2
1	A	14	GLU	1
1	A	40	PHE	1
1	A	74	SER	1
1	A	114	GLU	1
1	A	10	ASN	1
1	A	93	ASN	1
1	A	94	TYR	1
1	A	12	GLU	1
1	A	73	ILE	1
1	A	83	LYS	1
1	A	149	LEU	1
1	A	78	ASP	1
1	A	76	SER	1
1	A	153	ASN	1
1	A	68	ILE	1
1	A	71	ARG	1
1	A	89	LYS	1
1	A	152	TYR	1
1	A	169	SER	1
1	A	52	MET	1
1	A	80	GLU	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 ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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