wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1ON4
Title	:	Solution structure of soluble domain of Sco1 from Bacillus Subtilis
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This is a wwPDB NMR Structure Validation Summary 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 (i) symbol.

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

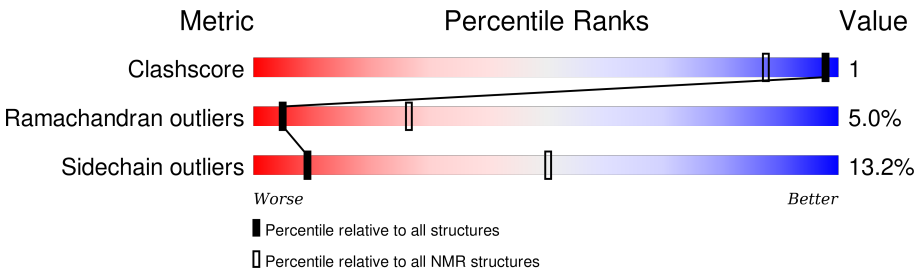
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

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	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	174	72% 7% • 18%

2 Ensemble composition and analysis (i)

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 (i)

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
			Total	C	H	N	O	S	
1	A	174	2765	897	1366	220	277	5	0

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

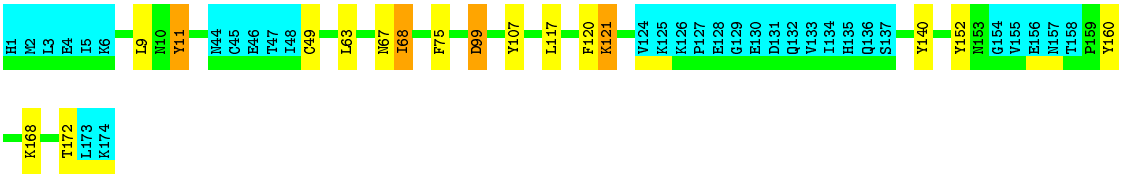
4 Residue-property plots (i)

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

Chain A:

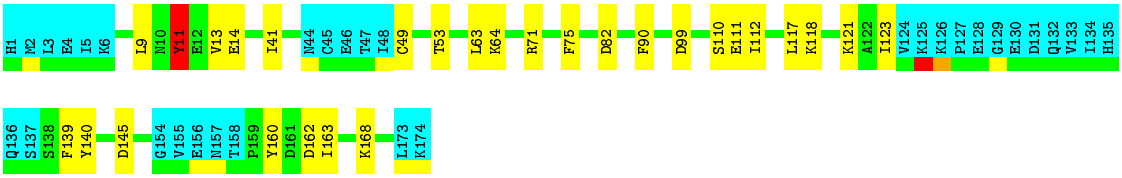


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 28. Colouring as in section 4.1 above.

- Molecule 1: Sco1

Chain A:



5 Refinement protocol and experimental data overview (i)

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.

5 of 6 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(^{o})	Ideal(^{o})	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

There are no chirality outliers.

5 of 19 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

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	140	TYR	Sidechain	18
1	A	11	TYR	Sidechain	17

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	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.

5 of 27 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

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

5 of 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	172	THR	18
1	A	49	CYS	18

6.3.2 Protein sidechains (i)

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%)	9 50
All	All	3870/4770 (81%)	3358 (87%)	512 (13%)	9 50

5 of 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
1	A	11	TYR	30
1	A	9	LEU	30
1	A	63	LEU	27

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 (i)

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 (i)

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 (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	131	2.40 ± 0.11	Should be applied
$^{13}C_{\beta}$	128	2.78 ± 0.17	Should be applied
$^{13}C'$	0	—	—
^{15}N	156	0.93 ± 0.30	Should be applied

7.1.3 Completeness of resonance assignments (i)

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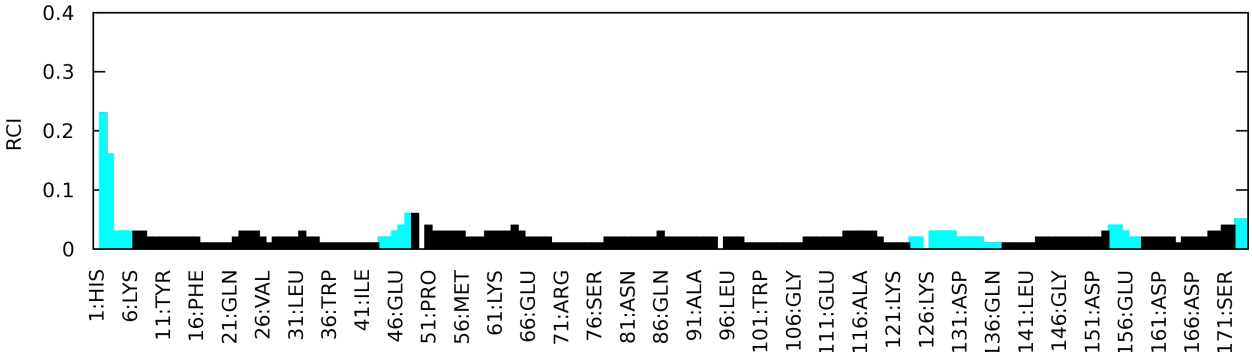
	Total	^{1}H	^{13}C	^{15}N
Aromatic	57/178 (32%)	55/95 (58%)	0/80 (0%)	2/3 (67%)
Overall	1279/1759 (73%)	774/893 (87%)	357/700 (51%)	148/166 (89%)

7.1.4 Statistically unusual chemical shifts (i)

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 (i)

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: