Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2L93
BMRB ID	:	17435
Title	:	Solution structure of the C-terminal domain of Salmonella H-NS
Authors	:	Li, Y.
Deposited on	:	2011-01-29

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 (i) 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 (i)) were used in the production of this report:

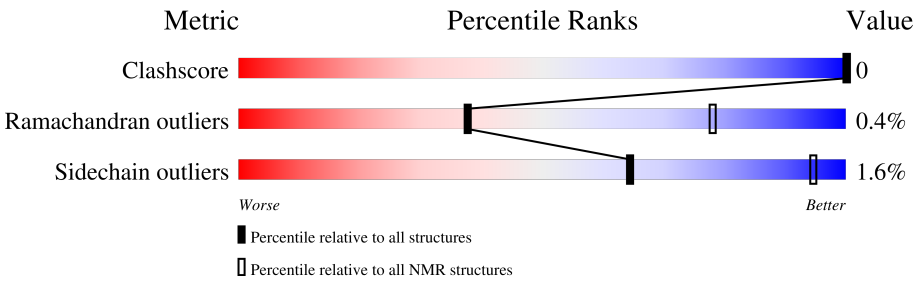
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 87%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	55	76% 13% 11%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 19 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:95-A:136 (42)	0.69	19

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 5 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 779 atoms, of which 389 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-binding protein H-NS.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	49	779	245	389	66	78	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	LEU	-	expression tag	UNP P0A1S2
A	139	GLU	-	expression tag	UNP P0A1S2
A	140	HIS	-	expression tag	UNP P0A1S2
A	141	HIS	-	expression tag	UNP P0A1S2
A	142	HIS	-	expression tag	UNP P0A1S2
A	143	HIS	-	expression tag	UNP P0A1S2
A	144	HIS	-	expression tag	UNP P0A1S2
A	145	HIS	-	expression tag	UNP P0A1S2

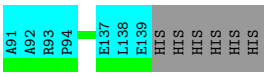
4 Residue-property plots (i)

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: DNA-binding protein H-NS

Chain A: 76% 13% 11%



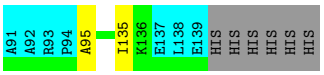
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: DNA-binding protein H-NS

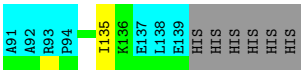
Chain A: 73% • 13% 11%



4.2.2 Score per residue for model 2

• Molecule 1: DNA-binding protein H-NS

Chain A: 75% • 13% 11%



4.2.3 Score per residue for model 3

• Molecule 1: DNA-binding protein H-NS

Chain A: 76% 13% 11%

A91 A92 R93 P94 E137 L138 E139 HIS HIS HIS HIS HIS HIS

4.2.4 Score per residue for model 4

• Molecule 1: DNA-binding protein H-NS

Chain A: 75% • 13% 11%

A91 A92 R93 P94 I135 K136 E137 L138 E139 HIS HIS HIS HIS HIS HIS

4.2.5 Score per residue for model 5

• Molecule 1: DNA-binding protein H-NS

Chain A: 75% • 13% 11%

A91 A92 R93 P94 R114 E137 L138 E139 HIS HIS HIS HIS HIS HIS

4.2.6 Score per residue for model 6

• Molecule 1: DNA-binding protein H-NS

Chain A: 75% • 13% 11%

A91 A92 R93 P94 I135 K136 E137 L138 E139 HIS HIS HIS HIS HIS HIS

4.2.7 Score per residue for model 7

• Molecule 1: DNA-binding protein H-NS

Chain A: 75% • 13% 11%

A91 A92 R93 P94 K120 E137 L138 E139 HIS HIS HIS HIS HIS HIS

4.2.8 Score per residue for model 8

- Molecule 1: DNA-binding protein H-NS

Chain A: 75% • 13% 11%

A91 A92 R93 P94 I135 K136 E137 L138 E139 HIS HIS HIS HIS HIS

4.2.9 Score per residue for model 9

- Molecule 1: DNA-binding protein H-NS

Chain A: 76% 13% 11%

A91 A92 R93 P94 E137 L138 E139 HIS HIS HIS HIS HIS HIS

4.2.10 Score per residue for model 10

- Molecule 1: DNA-binding protein H-NS

Chain A: 75% • 13% 11%

A91 A92 R93 P94 E105 E137 L138 E139 HIS HIS HIS HIS HIS HIS

4.2.11 Score per residue for model 11

- Molecule 1: DNA-binding protein H-NS

Chain A: 75% • 13% 11%

A91 A92 R93 P94 I135 K136 E137 L138 E139 HIS HIS HIS HIS HIS HIS

4.2.12 Score per residue for model 12

- Molecule 1: DNA-binding protein H-NS

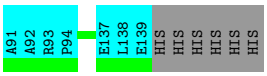
Chain A: 75% • 13% 11%

A91 A92 R93 P94 I135 K136 E137 L138 E139 HIS HIS HIS HIS HIS HIS

4.2.13 Score per residue for model 13

• Molecule 1: DNA-binding protein H-NS

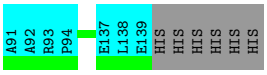
Chain A: 76% 13% 11%



4.2.14 Score per residue for model 14

• Molecule 1: DNA-binding protein H-NS

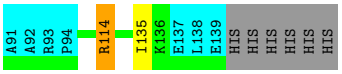
Chain A: 76% 13% 11%



4.2.15 Score per residue for model 15

• Molecule 1: DNA-binding protein H-NS

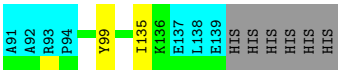
Chain A: 73% • • 13% 11%



4.2.16 Score per residue for model 16

• Molecule 1: DNA-binding protein H-NS

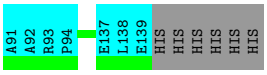
Chain A: 73% • 13% 11%



4.2.17 Score per residue for model 17

• Molecule 1: DNA-binding protein H-NS

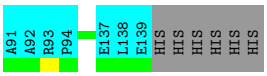
Chain A: 76% 13% 11%



4.2.18 Score per residue for model 18

- Molecule 1: DNA-binding protein H-NS

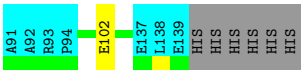
Chain A:



4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: DNA-binding protein H-NS

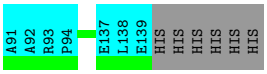
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: DNA-binding protein H-NS

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 200 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
Amber	geometry optimization	
Amber	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	574
Number of shifts mapped to atoms	574
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

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	0.74±0.01	0±0/342 (0.0± 0.0%)	0.94±0.02	0±0/459 (0.0± 0.1%)
All	All	0.74	0/6840 (0.0%)	0.95	2/9180 (0.0%)

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	0.1±0.2
All	All	0	1

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	114	ARG	NE-CZ-NH1	5.34	122.97	120.30	5	2

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	99	TYR	Sidechain	1

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
All	All	6720	6680	6680	-

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 -.

There are no clashes.

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	42/55 (76%)	39±1 (93±3%)	3±1 (7±2%)	0±0 (0±1%)	38	78
All	All	840/1100 (76%)	781 (93%)	56 (7%)	3 (0%)	38	78

All 3 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	95	ALA	1
1	A	105	GLU	1
1	A	102	GLU	1

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	35/46 (76%)	34±1 (98±2%)	1±1 (2±2%)	64	94
All	All	700/920 (76%)	689 (98%)	11 (2%)	64	94

All 3 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	135	ILE	9
1	A	120	LYS	1
1	A	114	ARG	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 monosaccharides 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 87% for the well-defined parts and 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	574
Number of shifts mapped to atoms	574
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	49	-0.01 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	45	-0.11 ± 0.21	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	46	-1.00 ± 0.32	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 87%, i.e. 498 atoms were assigned a chemical shift out of a possible 570. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	168/212 (79%)	86/87 (99%)	42/84 (50%)	40/41 (98%)
Sidechain	292/318 (92%)	198/203 (98%)	90/102 (88%)	4/13 (31%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	38/40 (95%)	19/19 (100%)	18/20 (90%)	1/1 (100%)
Overall	498/570 (87%)	303/309 (98%)	150/206 (73%)	45/55 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 574 atoms were assigned a chemical shift out of a possible 665. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	193/245 (79%)	98/100 (98%)	49/98 (50%)	46/47 (98%)
Sidechain	343/380 (90%)	233/243 (96%)	106/121 (88%)	4/16 (25%)
Aromatic	38/40 (95%)	19/19 (100%)	18/20 (90%)	1/1 (100%)
Overall	574/665 (86%)	350/362 (97%)	173/239 (72%)	51/64 (80%)

7.1.4 Statistically unusual chemical shifts (i)

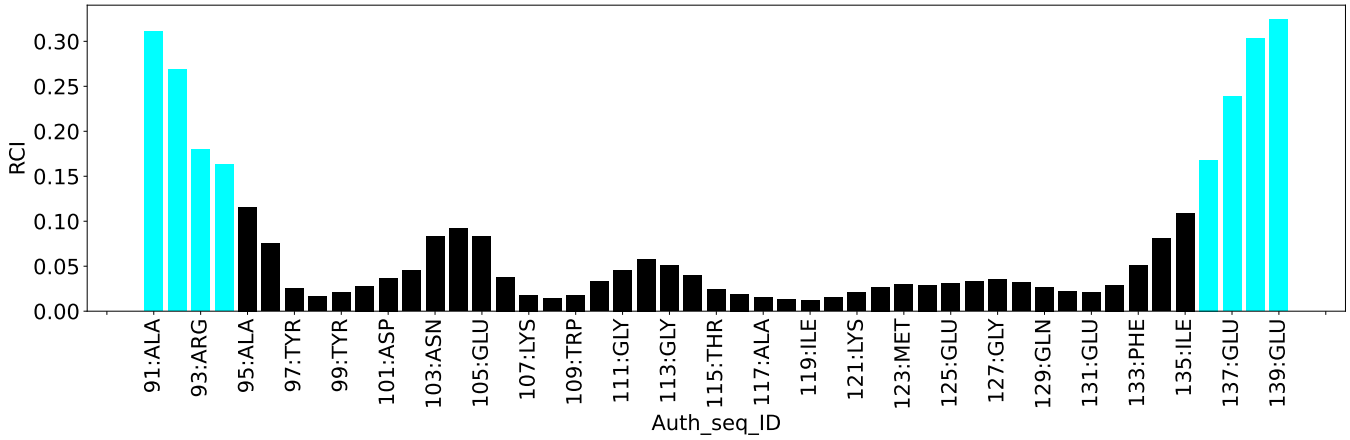
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	111	GLY	HA2	0.97	2.15 – 5.77	-8.3
1	A	116	PRO	HD3	1.49	1.76 – 5.48	-5.7
1	A	116	PRO	HD2	1.74	1.93 – 5.38	-5.5

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.00
0.05
0.10
0.15
0.20
0.25
0.30
91:ALA
93:ARG
95:ALA
97:TYR
99:TYR
101:ASP
103:ASN
105:GLU
107:LYS
109:TRP
111:GLY
113:GLY
115:THR
117:ALA
119:ILE
121:LYS
123:MET
125:GLU
127:GLY
129:GLN
131:GLU
133:PHE
135:ILE
137:GLU
139:GLU
Auth_seq_ID