



# wwPDB NMR Structure Validation Summary Report ⓘ

Feb 12, 2017 – 06:53 pm GMT

PDB ID : 1MWN  
Title : Solution NMR structure of S100B bound to the high-affinity target peptide TRTK-12  
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Deposited on : 2002-09-30

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

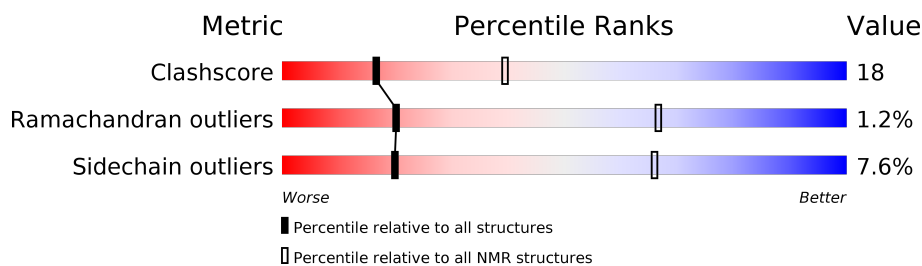
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 82%.

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  $\geq 3$ , 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	92	 67% 26% . . .
1	B	92	 67% 26% . . .
2	X	12	 25% 8% 67%
2	Y	12	 33% 8% 58%

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:1-A:87, B:1-B:87, X:8-X:11, Y:8-Y:12 (183)	0.45	2

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 2 single-model clusters were found.

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

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3330 atoms, of which 1632 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called S-100 protein, beta chain.

Mol	Chain	Residues	Atoms						Trace
1	A	91	Total	C	H	N	O	S	0
			1446	466	703	117	154	6	
1	B	91	Total	C	H	N	O	S	0
			1446	466	703	117	154	6	

- Molecule 2 is a protein called F-actin capping protein alpha-1 subunit.

Mol	Chain	Residues	Atoms					Trace
2	X	12	Total	C	H	N	O	0
			217	66	113	19	19	
2	Y	12	Total	C	H	N	O	0
			217	66	113	19	19	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

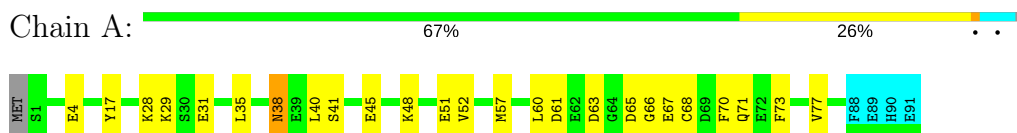
Mol	Chain	Residues	Atoms	
3	B	2	Total	Ca
			2	2
3	A	2	Total	Ca
			2	2

## 4 Residue-property plots [i](#)

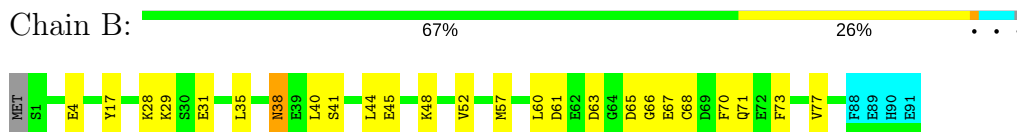
### 4.1 Average score per residue in the NMR ensemble

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: S-100 protein, beta chain



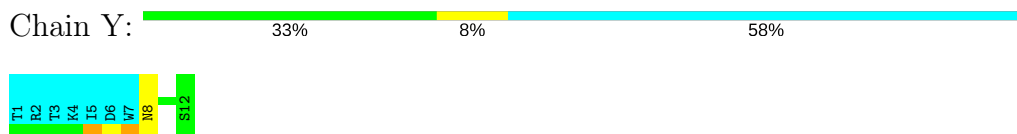
- Molecule 1: S-100 protein, beta chain



- Molecule 2: F-actin capping protein alpha-1 subunit



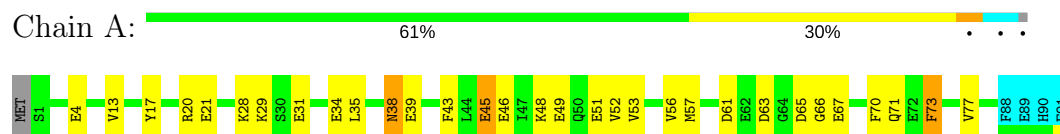
- Molecule 2: F-actin capping protein alpha-1 subunit



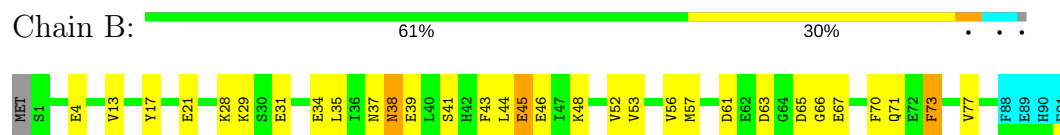
### 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 2. Colouring as in section 4.1 above.

- Molecule 1: S-100 protein, beta chain



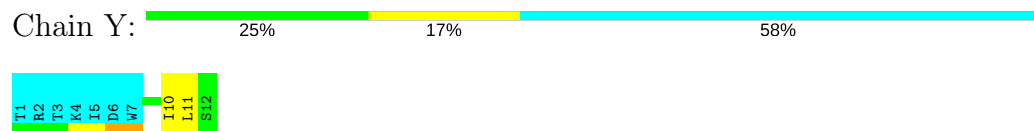
- Molecule 1: S-100 protein, beta chain



- Molecule 2: F-actin capping protein alpha-1 subunit



- Molecule 2: F-actin capping protein alpha-1 subunit



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry, 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
X-PLOR	refinement	3.851

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 5544
Number of chemical shift lists	2
Total number of shifts	2252
Number of shifts mapped to atoms	2252
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
CA

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	703	674	672	26±6
1	B	703	674	672	26±6
2	X	33	41	41	1±1
2	Y	40	46	46	1±1
All	All	29660	28700	28617	1025

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 18.

5 of 416 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:40:LEU:HD22	1:B:40:LEU:N	0.68	2.03	10	4
1:A:40:LEU:N	1:A:40:LEU:HD23	0.68	2.03	16	2
1:A:40:LEU:N	1:A:40:LEU:HD22	0.68	2.03	10	3
1:B:17:TYR:CZ	1:B:35:LEU:HD22	0.68	2.23	2	1
1:B:40:LEU:N	1:B:40:LEU:HD23	0.68	2.03	16	2

## 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	86/92 (93%)	80±1 (93±2%)	5±1 (6±2%)	1±1 (1±1%)	20	66
1	B	86/92 (93%)	80±1 (93±1%)	5±1 (6±2%)	1±1 (1±1%)	20	66
2	X	4/12 (33%)	4±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
2	Y	4/12 (33%)	4±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	3600/4160 (87%)	3364 (93%)	194 (5%)	42 (1%)	20	66

5 of 8 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	41	SER	14
1	B	41	SER	14
1	A	22	GLY	3
1	B	22	GLY	3
1	B	87	PHE	2

### 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	79/84 (94%)	73±1 (93±2%)	6±1 (7±2%)	21	67
1	B	79/84 (94%)	73±1 (93±2%)	6±1 (7±2%)	21	67
2	X	4/12 (33%)	3±1 (85±15%)	1±1 (15±15%)	7	45
2	Y	5/12 (42%)	4±1 (88±12%)	1±1 (12±12%)	10	52
All	All	3340/3840 (87%)	3087 (92%)	253 (8%)	20	66

5 of 52 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	48	LYS	20
1	B	48	LYS	20
1	A	77	VAL	16
1	B	77	VAL	16
1	B	38	ASN	16

### 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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

## 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 82% for the well-defined parts and 77% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 5544

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	2092
Number of shifts mapped to atoms	2092
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	176	$-0.68 \pm 0.12$	Should be applied
$^{13}\text{C}_\beta$	172	$0.37 \pm 0.06$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	174	$-0.59 \pm 0.10$	Should be applied
$^{15}\text{N}$	174	$-0.37 \pm 0.29$	None needed ( $< 0.5$ ppm)

#### 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 80%, i.e. 1812 atoms were assigned a chemical shift out of a possible 2274. 28 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	840/915 (92%)	338/366 (92%)	336/366 (92%)	166/183 (91%)
Sidechain	972/1171 (83%)	606/680 (89%)	356/455 (78%)	10/36 (28%)

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	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Aromatic	0/188 (0%)	0/100 (0%)	0/72 (0%)	0/16 (0%)
Overall	1812/2274 (80%)	944/1146 (82%)	692/893 (77%)	176/235 (75%)

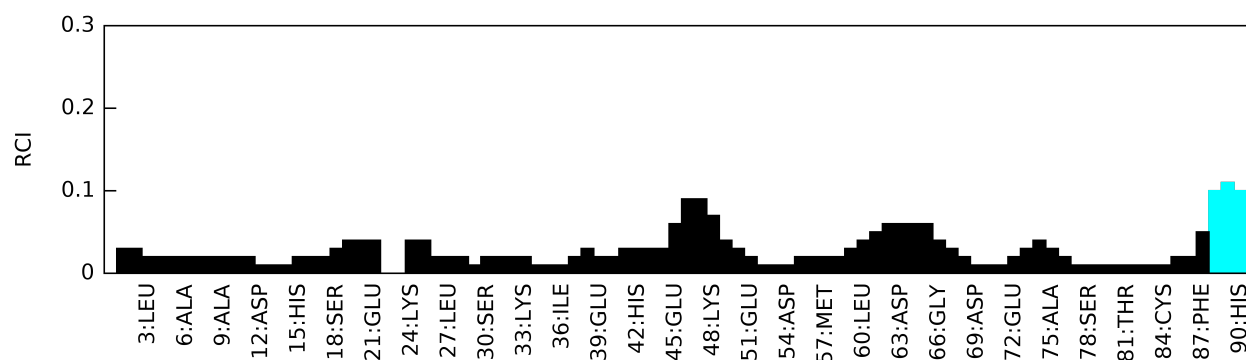
### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

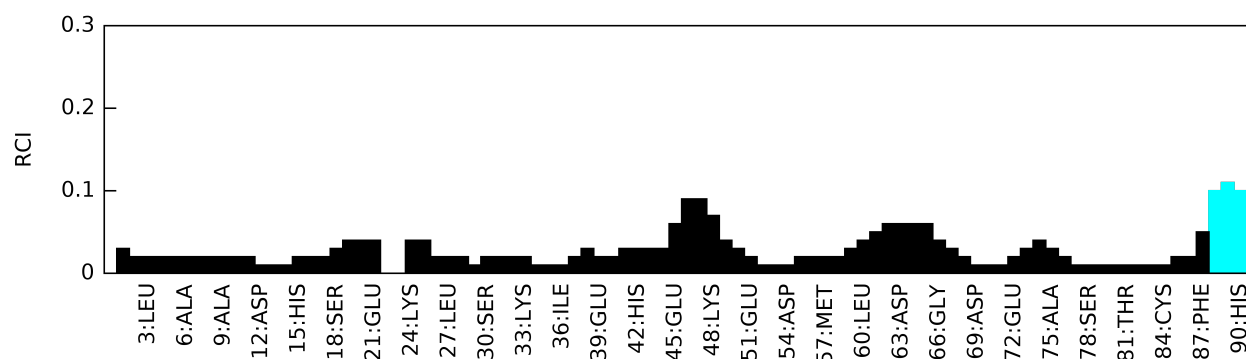
### 7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *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:



Random coil index (RCI) for chain B:



## 7.2 Chemical shift list 2

File name: BMRB entry 5544

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

### 7.2.1 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	160
Number of shifts mapped to atoms	160
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

### 7.2.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

### 7.2.3 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 2%, i.e. 45 atoms were assigned a chemical shift out of a possible 2274. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	18/915 (2%)	18/366 (5%)	0/366 (0%)	0/183 (0%)
Sidechain	27/1171 (2%)	27/680 (4%)	0/455 (0%)	0/36 (0%)
Aromatic	0/188 (0%)	0/100 (0%)	0/72 (0%)	0/16 (0%)
Overall	45/2274 (2%)	45/1146 (4%)	0/893 (0%)	0/235 (0%)

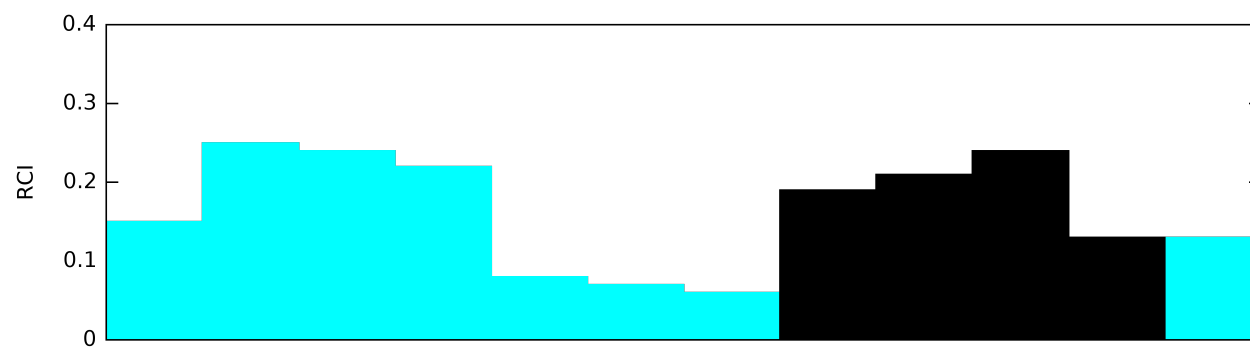
### 7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

### 7.2.5 Random Coil Index (RCI) plots [i](#)

The images below report *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 X:



Random coil index (RCI) for chain Y:

