



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2AFJ / pdb\_00002afj  
Title : SPRY domain-containing SOCS box protein 2 (SSB-2)  
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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](mailto: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>.

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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

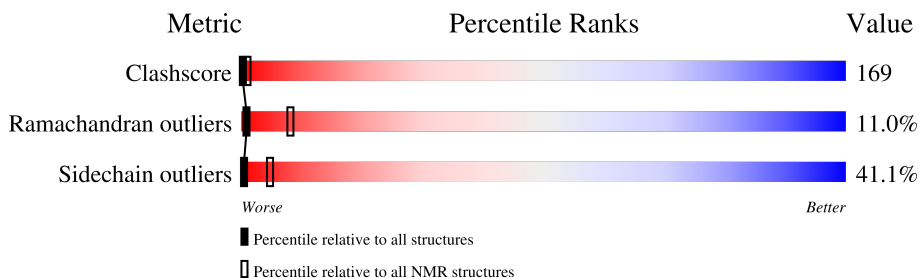
# 1 Overall quality at a glance

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  $\geq 3$ , 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	226	

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:29-A:97, A:105-A:113, A:128-A:135, A:163-A:219 (143)	2.10	14

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. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3458 atoms, of which 1703 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called gene rich cluster, C9 gene.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	226	3458	1096	1703	324	330	5	0

There are 13 discrepancies between the modelled and reference sequences:

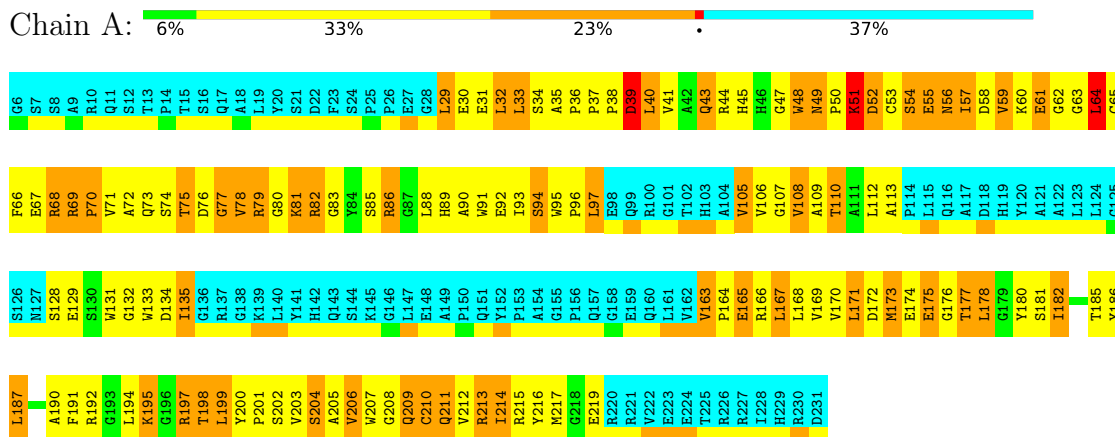
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	-	cloning artifact	UNP O88838
A	7	SER	-	cloning artifact	UNP O88838
A	8	SER	-	cloning artifact	UNP O88838
A	9	ALA	-	cloning artifact	UNP O88838
A	10	ARG	-	cloning artifact	UNP O88838
A	11	GLN	-	cloning artifact	UNP O88838
A	225	THR	-	cloning artifact	UNP O88838
A	226	ARG	-	cloning artifact	UNP O88838
A	227	ARG	-	cloning artifact	UNP O88838
A	228	ILE	-	cloning artifact	UNP O88838
A	229	HIS	-	cloning artifact	UNP O88838
A	230	ARG	-	cloning artifact	UNP O88838
A	231	ASP	-	cloning artifact	UNP O88838

## 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.

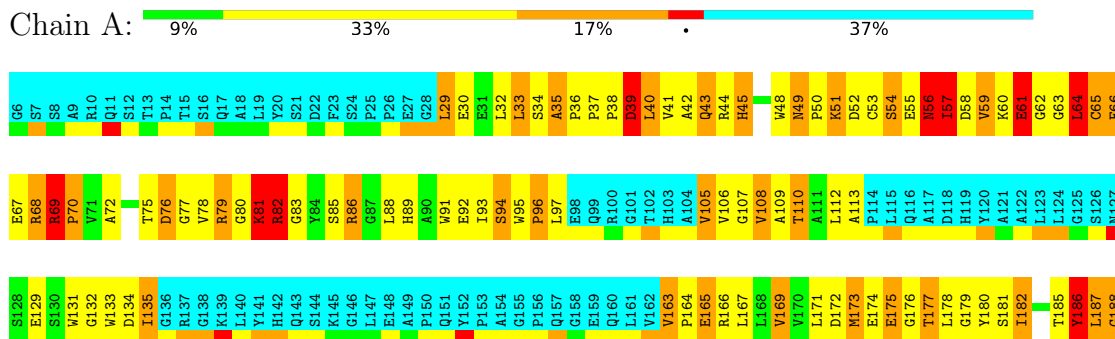
- Molecule 1: gene rich cluster, C9 gene



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

The representative model is number 14. Colouring as in section 4.1 above.

- Molecule 1: gene rich cluster, C9 gene



P189	A190	F191	R192	G193	L194	K195	G196	R197	T198	L199	Y200	P201	S202	V203	S204	A205	V206	W207	G208	Q209	C210	Q211	V212	R213	T214	R215	Y216	W217	G218	E219	R220	R221	V222	E223	E224	T225	R226	R227	T228	H229	R230	D231
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## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing*.

Of the 194 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure solution	1.0.6
X-PLOR	structure solution	2.9.3
X-PLOR	refinement	2.9.3

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	1.47±0.01	0±0/1143 ( 0.0± 0.0%)	1.59±0.01	5±2/1557 ( 0.3± 0.1%)
All	All	1.47	4/22860 ( 0.0%)	1.59	99/31140 ( 0.3%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	75	THR	N-CA	5.59	1.49	1.46	3	3
1	A	51	LYS	C-N	-5.02	1.26	1.33	7	1

5 of 23 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	163	VAL	N-CA-CB	-8.36	104.56	111.67	5	3
1	A	48	TRP	N-CA-CB	-7.33	102.13	110.35	19	4
1	A	57	ILE	N-CA-CB	-7.13	104.21	112.34	15	16
1	A	206	VAL	N-CA-CB	-7.08	104.00	112.07	16	2
1	A	95	TRP	N-CA-CB	-6.91	102.35	111.40	10	2

There are no chirality outliers.

There are no planarity outliers.

### 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	1112	1090	1090	372±24
All	All	22240	21800	21800	7441

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 169.

5 of 3192 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:O	1:A:44:ARG:HB3	1.15	1.39	6	20
1:A:106:VAL:HG22	1:A:203:VAL:HG23	1.13	1.20	18	5
1:A:105:VAL:HG13	1:A:204:SER:O	1.13	1.42	20	4
1:A:108:VAL:HG21	1:A:199:LEU:HD13	1.12	1.21	8	2
1:A:97:LEU:HD22	1:A:97:LEU:O	1.11	1.44	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	143/226 (63%)	106±4 (74±3%)	21±3 (15±2%)	16±2 (11±2%)	<b>1</b> <b>8</b>
All	All	2860/4520 (63%)	2129 (74%)	417 (15%)	314 (11%)	<b>1</b> <b>8</b>

5 of 46 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	61	GLU	20
1	A	64	LEU	20
1	A	39	ASP	18
1	A	70	PRO	16
1	A	77	GLY	15

### 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	116/182 (64%)	68±6 (59±5%)	48±6 (41±5%)	<b>0</b> <b>5</b>
All	All	2320/3640 (64%)	1366 (59%)	954 (41%)	<b>0</b> <b>5</b>

5 of 99 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	33	LEU	20
1	A	40	LEU	20
1	A	51	LYS	20
1	A	182	ILE	20
1	A	197	ARG	20

### 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 oligosaccharides 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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided