

# Full wwPDB NMR Structure Validation Report (i)

#### Feb 24, 2022 – 09:20 AM EST

PDB ID : 1YUT

Title: Solution structure of Calcium-S100A13 (minimized mean structure)

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

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)

RCI : v 1n 11 5 13 A (Berjanski et al., 2005)

PANAV : Wang et al. (2010)

ShiftChecker : 2.26

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

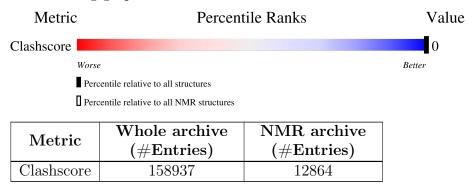
Validation Pipeline (wwPDB-VP) : 2.26

### 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 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.



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	98	100%
1	В	98	100%



## 2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.



## 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3284 atoms, of which 1666 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called S100 calcium-binding protein A13.

Mol	Chain	Residues		Atoms								
1	٨	98	Total	С	Н	N	О	S	0			
1	A	90	1640	512	833	136	157	2	0			
1	D	98	Total	С	Н	N	О	S	0			
	Б	90	1640	512	833	136	157	2	0			

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms
9	٨	9	Total Ca
	A	2	$2 \qquad 2$
9	D	9	Total Ca
	Б	2	2 2



## 4 Residue-property plots (i)

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: S100 calcium-binding protein A13

Cn	ali	1 /	Α:																		1	.00	1%																					
M1 A2	A 43	P5	14	E8	E10	E11	S12 113	E14	T15	V16 V17	T18	T19	F20	T22	F23	A24	R25	426 F27	G28	R29	K30	D31	L33	S34	V35	N36 E37	F38	K39	141	V42	T43	Q45 Q45	L46	P47	1.49	150	K51	D52	G54	355	L56	D57	K59	M60
K61 S62	L63 D64	V65	067 067	D68	E70	L71	K72 F73	N74	E75	Y / 6	R78	L79	180 100	E82	L83	A84	K85	187	10/ R88	K89	K90	K91	L93	K94	195	K96 K97	K98																	
• N	lo	lec	cu	le	1:	S	31(	00	С	al	ci	ur	n-	b	in	di	in	g	р	rc	tε	eir	1 .	A.	13																			
Cha	air	ı I	3:																		1	.00	%																					
M1 A2	F4	P5	T7	E8	E10	E11	S12 T13	E14	T15	V16 V17	T18	T19	F20	T22	F23	A24	R25	U.26	G28	R29	K30	D31	L33	S34	V35	N36 E37	F38	K39	E40 L41	V42	T43	Q45	L46	P47	1.49	L50	K51	D52	G54	355	L56	D57	K59	M60
362	163	765	167	990	170	171	۲72 ۲73	174	375	177	178	.79	180	182	183	184	(85	186	188	683	06)	(91	193	467	195	263	86)																	



### 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: Restrained energy minimization.

Of the 300 calculated structures, 1 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				
Amber	refinement	6				

No chemical shift data was provided.



### 6 Model quality (i)

### 6.1 Standard geometry (i)

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 (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	0	0	0	0
1	В	0	0	0	0
All	All	4	0	0	-

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	0	-	-	-	-
1	В	0	-	-	-	-

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	0	-	-	-	-

There are no Ramachandran outliers.

#### 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	0	-	-	-
1	В	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

#### 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)

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 (i)

No chemical shift data were provided

