

# wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1YUT
Title	:	Solution structure of Calcium-S100A13 (minimized mean structure)
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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 https://www.wwpdb.org/validation/2017/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:

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

Clashscore

#### Overall quality at a glance (i) 1

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.

Metri	2	Value		
Clashscore				0
	Worse			Better
	Percentile relative to all str	ructures		
	Percentile relative to all NI	MR structures		
Mada	Whole a	rchive	NMR archive	
Metri	c (#Entr	ries)	(# Entries)	

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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  $\leq 5\%$ 

12864

Mol	Chain	Length	Quality of chain
1	А	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					Trace
1	٨	98	Total	С	Η	Ν	0	S	0
		90	1640	512	833	136	157	2	0
1	В	98	Total	С	Н	Ν	0	S	0
	D	90	1640	512	833	136	157	2	0

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

Mol	Chain	Residues	Atoms
2	А	2	Total Ca 2 2
2	В	2	Total Ca 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

Chain A:	100%	
M 42 42 42 43 43 43 43 14 43 43 43 43 43 44 44 44 44 44 44 44 44	119 721 722 722 722 722 722 722 723 723 723 723	044 045 146 148 148 148 148 148 148 150 053 054 053 055 156 055 156 057 057 057 057 057 057 057 057 057 057
K61 K61 L63 L65 L65 L64 N66 R66 R66 E70 C71 F73 F73 F73 F73 F73 F75 F73 F75 F73 F77 F77 F77	1.79 1810 1810 1821 1832 1833 1834 1835 1835 1836 1836 1836 1836 1836 1836 1836 1932 1932 1932 1955 1956 1956 1957 1957 1958	
• Molecule 1: S100 calci	um-binding protein A13	
Chain B:	100%	
M1 A2 A2 A2 A2 A2 A2 A2 A2 A2 A2 A2 A2 A2	119 712 722 722 723 723 723 723 723 723 723 72	944 945 1465 1448 1448 1448 1455 1455 155 155 155 155 155 155 155 1



# 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	А	0	0	0	0
1	В	0	0	0	0
All	All	4	0	0	-

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score 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	А	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	А	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

