



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1UWO
Title : CALCIUM FORM OF HUMAN S100B, NMR, 20 STRUCTURES
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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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

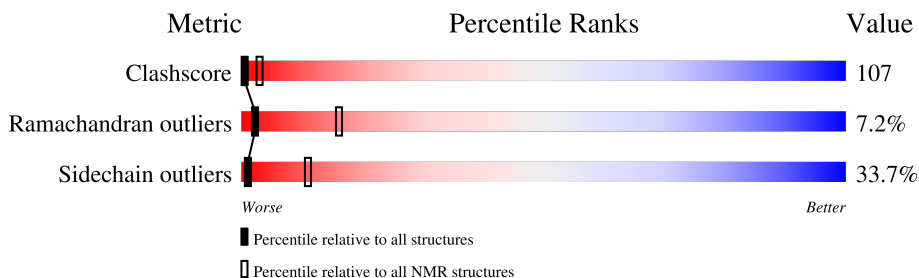
1 Overall quality at a glance

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	91	5% 66% 19% 10%
1	B	91	5% 66% 19% 10%

2 Ensemble composition and analysis

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 18 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:41, A:47-A:87, B:1-B:41, B:47-B:87 (164)	0.67	18

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 4 clusters and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2876 atoms, of which 1394 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called S100B.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	91	1438	465	697	118	152	6	0
1	B	91	1438	465	697	118	152	6	0

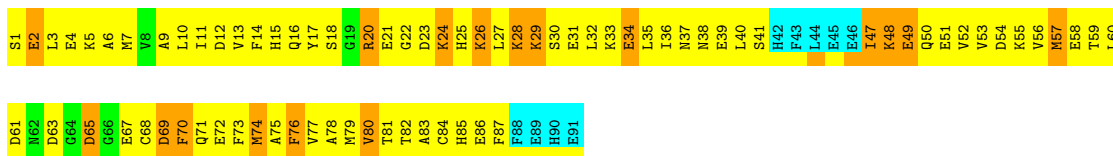
4 Residue-property plots [i](#)

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.

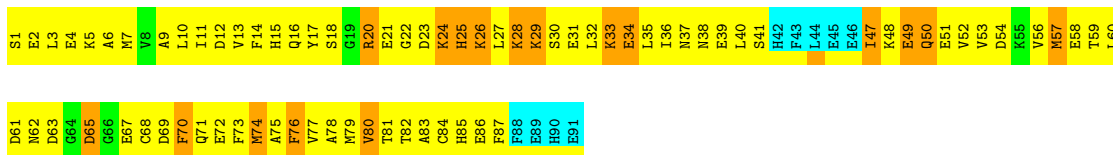
- Molecule 1: S100B

Chain A: 5% 66% 19% 10%



- Molecule 1: S100B

Chain B: 5% 66% 19% 10%

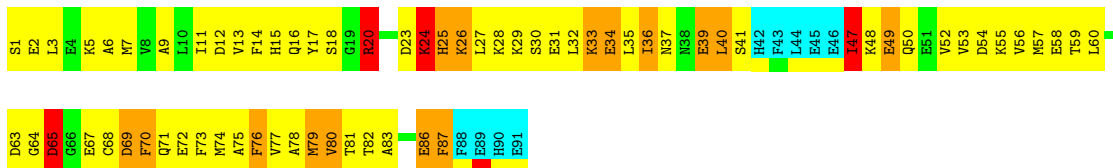


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

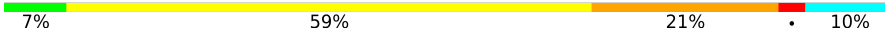
The representative model is number 18. Colouring as in section 4.1 above.

- Molecule 1: S100B

Chain A: 14% 55% 16% 10%



- Molecule 1: S100B

Chain B:  7% 59% 21% 10%

S1 E2 L3 E4 K5 A6 W7 W8 A9 L10 I11 D12 V13 F14 H15 Q16 Y17 S18 R20 E21 G22 D23 K24 H25 K26 L27 K28 K29 S30 E31 L32 K33 E34 L35 I36 N37 M38 E39 L40 H42 F43 L44 S45 E46 I47 K48 E49 Q50 E51 V52 V53 D54 K55 K56 M57 E58 L60

D61 M62 D63 G64 K65 G66 E67 C68 D69 F70 Q71 E72 F73 M74 A75 F76 Y77 A78 M79 R80 T81 T82 A83 C84 H85 E86 F87 F88 E89 H90 S91

5 Refinement protocol and experimental data overview

The models were refined using the following method: *HYBRID DISTANCE GEOMETRY AND SIMULATED ANNEALING*.

Of the 30 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATIONS*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

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	0.9±0.2
1	B	0.0±0.0	1.0±0.0
All	All	0	39

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	20	ARG	Sidechain	20
1	A	20	ARG	Sidechain	19

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	654	633	633	155±16
1	B	654	633	633	159±12
All	All	26160	25314	25320	5522

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 107.

5 of 2396 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:32:LEU:HD22	1:B:60:LEU:HD12	1.15	1.15	19	3
1:A:75:ALA:HB2	1:B:75:ALA:HB2	1.13	1.16	9	11
1:B:36:ILE:HD12	1:B:53:VAL:HG22	1.09	1.23	11	3
1:A:47:ILE:HD12	1:A:53:VAL:HG23	1.06	1.24	10	3
1:B:17:TYR:CE2	1:B:35:LEU:HD23	1.06	1.86	3	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	81/91 (89%)	58±3 (71±4%)	17±3 (22±3%)	6±2 (7±2%)	2	16
1	B	81/91 (89%)	55±4 (68±4%)	20±3 (25±4%)	6±1 (7±2%)	2	16
All	All	3240/3640 (89%)	2257 (70%)	749 (23%)	234 (7%)	2	16

5 of 39 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	65	ASP	20
1	B	65	ASP	20
1	A	29	LYS	16
1	B	29	LYS	13
1	B	47	ILE	12

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	73/82 (89%)	49±3 (68±4%)	24±3 (32±4%)	1	12
1	B	73/82 (89%)	48±4 (65±5%)	26±4 (35±5%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2920/3280 (89%)	1936 (66%)	984 (34%)	1 11

5 of 135 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	B	80	VAL	20
1	A	34	GLU	19
1	A	80	VAL	19
1	B	70	PHE	19
1	A	70	PHE	18

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

No chemical shift data were provided