



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 15, 2026 – 10:27 AM UTC

PDB ID : 1QLK / pdb_00001qlk
Title : SOLUTION STRUCTURE OF CA(2+)-LOADED RAT S100B (BETABETA)
NMR, 20 STRUCTURES
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Deposited on : 1997-09-26

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
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.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

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 1 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:88, B:1-B:88 (176)	1.57	1

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2934 atoms, of which 1428 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called S-100 PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	92	Total	C	H	N	O	S	0
			1465	471	714	118	155	7	
1	B	92	Total	C	H	N	O	S	0
			1465	471	714	118	155	7	

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

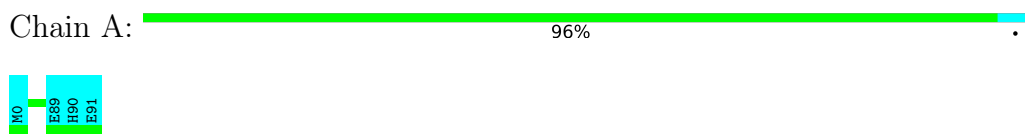
Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2
2	B	2	Total	Ca
			2	2

4 Residue-property plots [i](#)

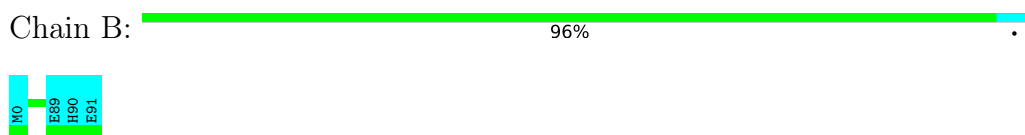
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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: S-100 PROTEIN



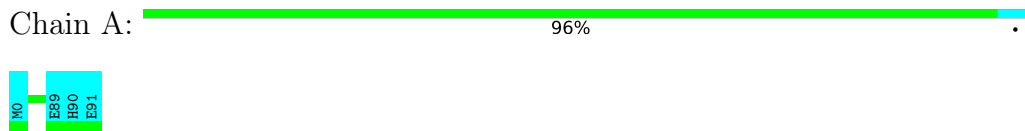
- Molecule 1: S-100 PROTEIN



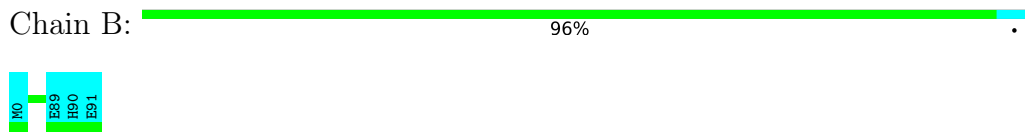
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: S-100 PROTEIN



- Molecule 1: S-100 PROTEIN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SEE MAIN REFERENCE*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *SEE MAIN REFERENCE*.

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

Software name	Classification	Version
X-PLOR	refinement	3.851
X-PLOR V3.851(ONLINE)	structure solution	V3.851(ONLINE)

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

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6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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6.3.2 Protein sidechains [i](#)

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6.3.3 RNA [i](#)

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6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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6.5 Carbohydrates [i](#)

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6.6 Ligand geometry [i](#)

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6.7 Other polymers [i](#)

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6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided