



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 10:28 AM UTC

PDB ID : 1QLK / pdb_00001qlk
Title : SOLUTION STRUCTURE OF CA(2+)-LOADED RAT S100B (BETABETA)
NMR, 20 STRUCTURES
Authors : Drohat, A.C.; Baldisseri, D.M.; Rustandi, R.R.; Weber, D.J.
Deposited on : 1997-09-26

This is a Full wwPDB NMR Structure Validation 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

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).

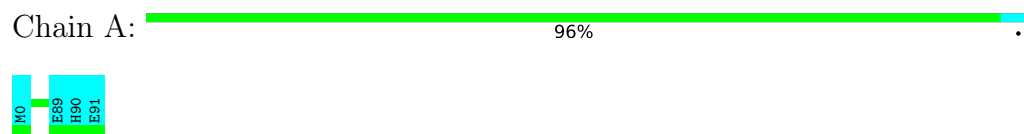
Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2
2	B	2	Total	Ca
			2	2

4 Residue-property plots

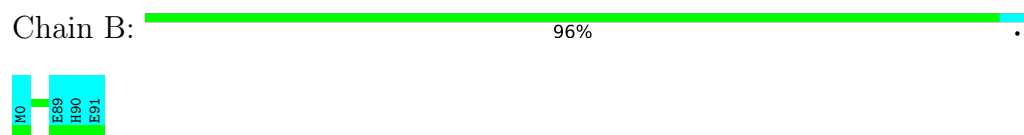
4.1 Average score per residue in the NMR ensemble

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

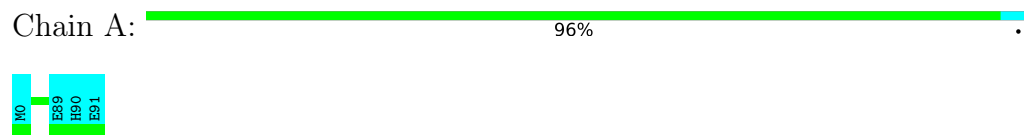


4.2 Scores per residue for each member of the ensemble

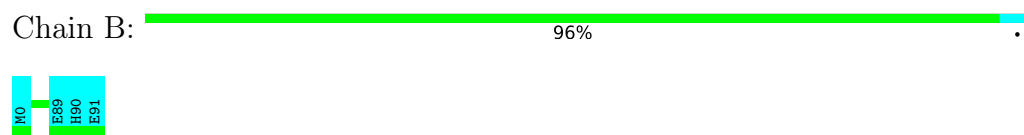
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: S-100 PROTEIN

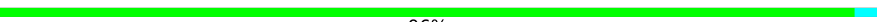


- Molecule 1: S-100 PROTEIN



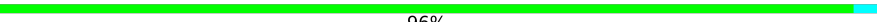
4.2.2 Score per residue for model 2

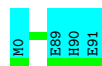
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



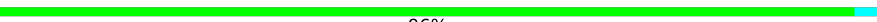
- Molecule 1: S-100 PROTEIN

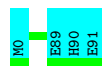
Chain B:  96% .



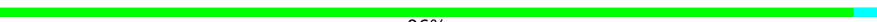
4.2.3 Score per residue for model 3

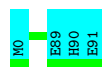
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



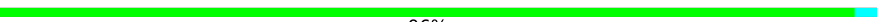
- Molecule 1: S-100 PROTEIN

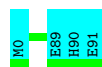
Chain B:  96% .



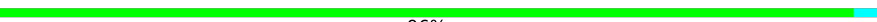
4.2.4 Score per residue for model 4

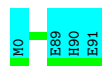
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



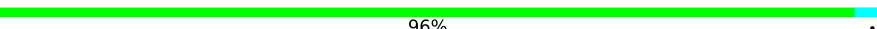
- Molecule 1: S-100 PROTEIN

Chain B:  96% .



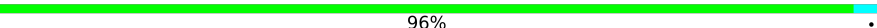
4.2.5 Score per residue for model 5

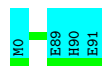
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



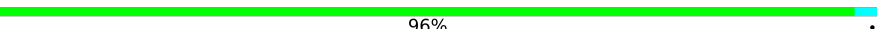
- Molecule 1: S-100 PROTEIN

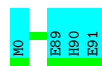
Chain B:  96% .



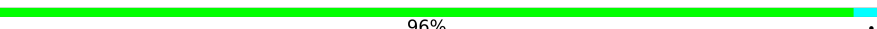
4.2.6 Score per residue for model 6

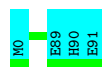
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



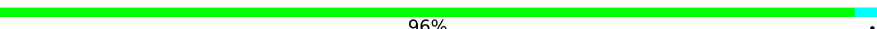
- Molecule 1: S-100 PROTEIN

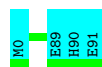
Chain B:  96% .



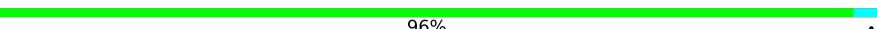
4.2.7 Score per residue for model 7

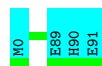
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



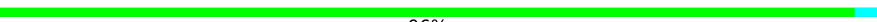
- Molecule 1: S-100 PROTEIN

Chain B:  96% .



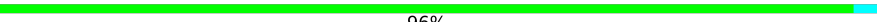
4.2.8 Score per residue for model 8

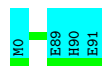
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



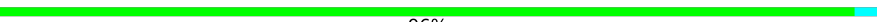
- Molecule 1: S-100 PROTEIN

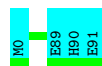
Chain B:  96% .



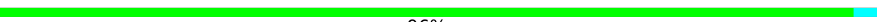
4.2.9 Score per residue for model 9

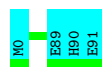
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



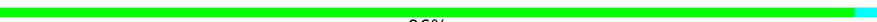
- Molecule 1: S-100 PROTEIN

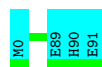
Chain B:  96% .



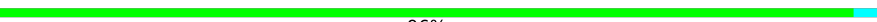
4.2.10 Score per residue for model 10

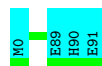
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



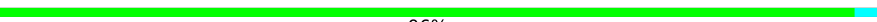
- Molecule 1: S-100 PROTEIN

Chain B:  96% .



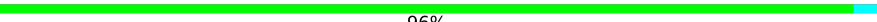
4.2.11 Score per residue for model 11

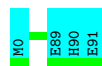
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



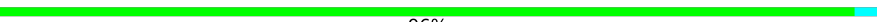
- Molecule 1: S-100 PROTEIN

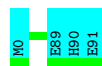
Chain B:  96% .



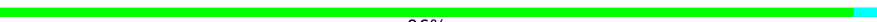
4.2.12 Score per residue for model 12

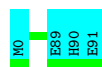
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



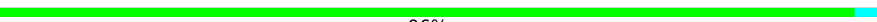
- Molecule 1: S-100 PROTEIN

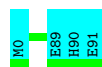
Chain B:  96% .



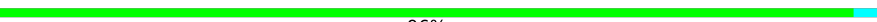
4.2.13 Score per residue for model 13

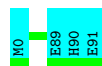
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



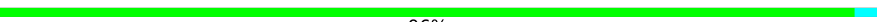
- Molecule 1: S-100 PROTEIN

Chain B:  96% .



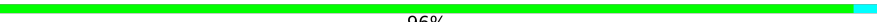
4.2.14 Score per residue for model 14

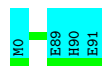
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



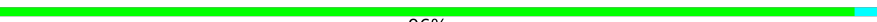
- Molecule 1: S-100 PROTEIN

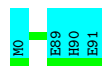
Chain B:  96% .



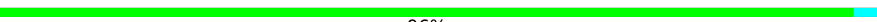
4.2.15 Score per residue for model 15

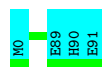
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



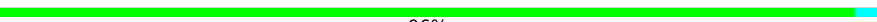
- Molecule 1: S-100 PROTEIN

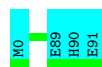
Chain B:  96% .



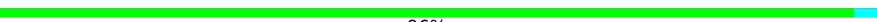
4.2.16 Score per residue for model 16

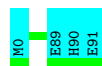
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



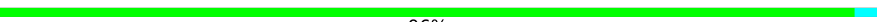
- Molecule 1: S-100 PROTEIN

Chain B:  96% .



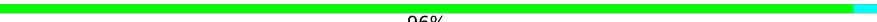
4.2.17 Score per residue for model 17

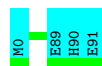
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



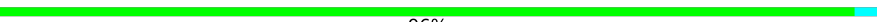
- Molecule 1: S-100 PROTEIN

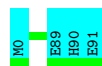
Chain B:  96% .



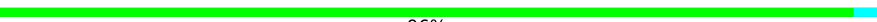
4.2.18 Score per residue for model 18

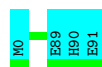
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



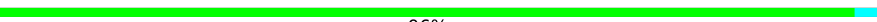
- Molecule 1: S-100 PROTEIN

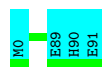
Chain B:  96% .



4.2.19 Score per residue for model 19

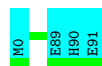
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



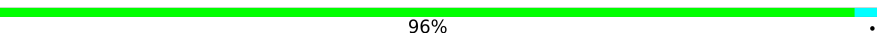
- Molecule 1: S-100 PROTEIN

Chain B:  96% .



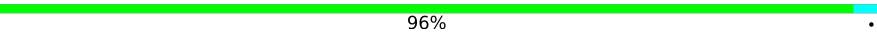
4.2.20 Score per residue for model 20

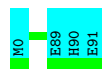
- Molecule 1: S-100 PROTEIN

Chain A:  96% .



- Molecule 1: S-100 PROTEIN

Chain B:  96% .



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](#)

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

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

6.3.2 Protein sidechains [i](#)

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

6.3.3 RNA [i](#)

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

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

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

6.5 Carbohydrates [i](#)

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

6.6 Ligand geometry [i](#)

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

6.7 Other polymers [i](#)

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

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided