



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 11:42 AM UTC

PDB ID : 2JPT / pdb_00002jpt
Title : Structural changes induced in apo-s100a1 protein by the disulphide formation between its CYS85 residue and b-mercaptoethanol
Authors : Zhukov, I.; Ejchart, A.; Bierzynski, A.
Deposited on : 2007-05-23

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
Mogul	:	2022.3.0, CSD as543be (2022)
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 10 models. 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:2-A:21, A:28-A:87, B:2-B:21, B:28-B:87 (160)	0.56	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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2872 atoms, of which 1404 are hydrogens and 0 are deuteriums.

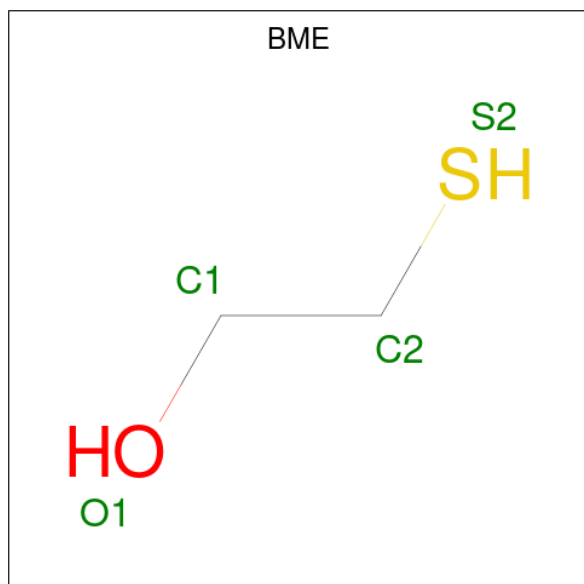
- Molecule 1 is a protein called Protein S100-A1.

Mol	Chain	Residues	Atoms						Trace
1	A	93	Total	C	H	N	O	S	0
			1427	459	697	114	154	3	
1	B	93	Total	C	H	N	O	S	0
			1427	459	697	114	154	3	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	ASP	ASN	engineered mutation	UNP P02639
B	64	ASP	ASN	engineered mutation	UNP P02639

- Molecule 2 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



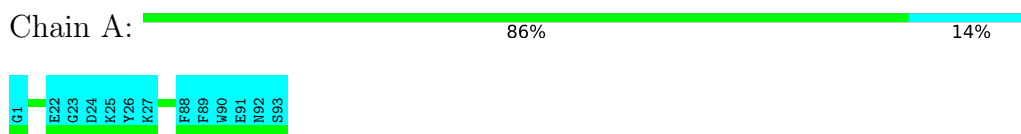
Mol	Chain	Residues	Atoms				
2	A	1	Total	C	H	O	S
			9	2	5	1	1
2	B	1	Total	C	H	O	S
			9	2	5	1	1

4 Residue-property plots

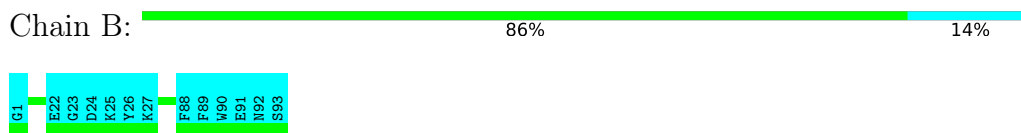
4.1 Average score per residue in the NMR ensemble

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: Protein S100-A1



- Molecule 1: Protein S100-A1

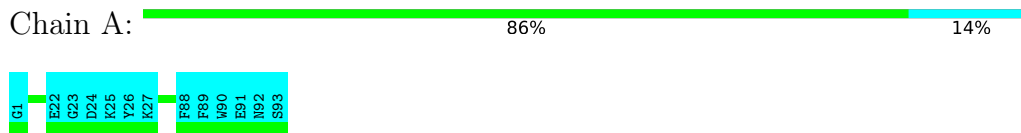


4.2 Scores per residue for each member of the ensemble

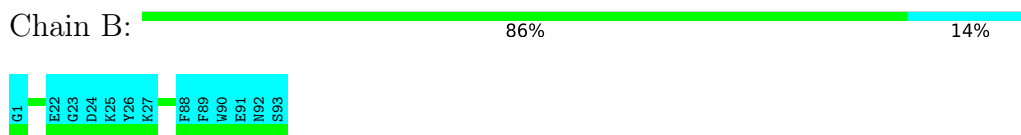
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Protein S100-A1



- Molecule 1: Protein S100-A1



4.2.2 Score per residue for model 2

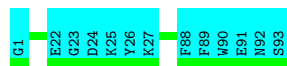
- Molecule 1: Protein S100-A1

Chain A:  86% 14%



- Molecule 1: Protein S100-A1

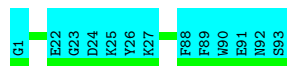
Chain B:  86% 14%



4.2.3 Score per residue for model 3

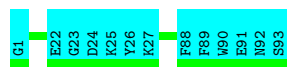
- Molecule 1: Protein S100-A1

Chain A:  86% 14%



- Molecule 1: Protein S100-A1

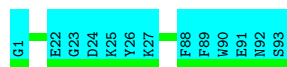
Chain B:  86% 14%



4.2.4 Score per residue for model 4

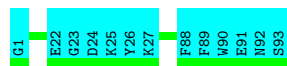
- Molecule 1: Protein S100-A1

Chain A:  86% 14%



- Molecule 1: Protein S100-A1

Chain B:  86% 14%



4.2.5 Score per residue for model 5

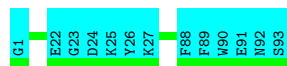
- Molecule 1: Protein S100-A1

Chain A:  86% 14%



- Molecule 1: Protein S100-A1

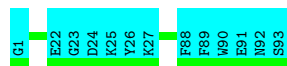
Chain B:  86% 14%



4.2.6 Score per residue for model 6

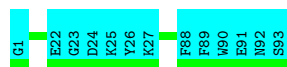
- Molecule 1: Protein S100-A1

Chain A:  86% 14%



- Molecule 1: Protein S100-A1

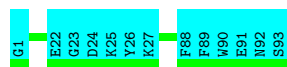
Chain B:  86% 14%



4.2.7 Score per residue for model 7

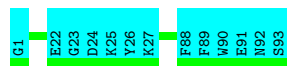
- Molecule 1: Protein S100-A1

Chain A:  86% 14%



- Molecule 1: Protein S100-A1

Chain B:  86% 14%



4.2.8 Score per residue for model 8

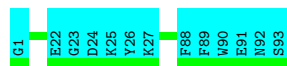
- Molecule 1: Protein S100-A1

Chain A:  86% 14%



- Molecule 1: Protein S100-A1

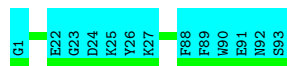
Chain B:  86% 14%



4.2.9 Score per residue for model 9

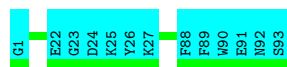
- Molecule 1: Protein S100-A1

Chain A:  86% 14%



- Molecule 1: Protein S100-A1

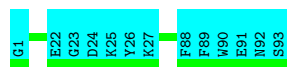
Chain B:  86% 14%



4.2.10 Score per residue for model 10

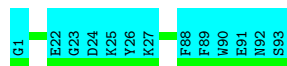
- Molecule 1: Protein S100-A1

Chain A:  86% 14%



- Molecule 1: Protein S100-A1

Chain B:  86% 14%



5 Refinement protocol and experimental data overview

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
NMRPipe	structure solution	
NMRPipe	refinement	

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