



Full wwPDB NMR Structure Validation Report ⓘ

Apr 15, 2026 – 11:24 AM UTC

PDB ID : 2AF2 / pdb_00002af2
Title : Solution structure of disulfide reduced and copper depleted Human Superoxide Dismutase
Authors : Banci, L.; Bertini, I.; Cantini, F.; D'Amelio, N.; Gaggelli, E.; Structural Proteomics in Europe (SPINE)
Deposited on : 2005-07-25

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 30 models. Model 23 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:153, B:1-B:54, B:60-B:153 (300)	1.95	23

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 2 single-model clusters were found.

Cluster number	Models
1	5, 7, 9, 12, 15, 19, 23, 24, 25, 26, 27, 28
2	4, 8, 16, 18, 22, 29
3	6, 10, 13, 14, 20, 30
4	1, 11, 17, 21
Single-model clusters	2; 3

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4375 atoms, of which 2157 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms						Trace
1	A	153	Total	C	H	N	O	S	0
			2188	679	1080	203	224	2	
1	B	153	Total	C	H	N	O	S	0
			2185	679	1077	203	224	2	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	CYS	engineered mutation	UNP P00441
A	111	SER	CYS	engineered mutation	UNP P00441
B	6	ALA	CYS	engineered mutation	UNP P00441
B	111	SER	CYS	engineered mutation	UNP P00441

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

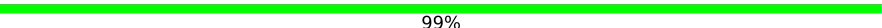
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1
2	B	1	Total	Zn
			1	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

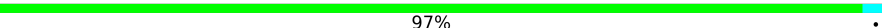
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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.

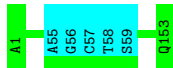
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99%



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  97%

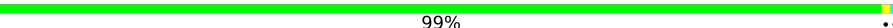


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

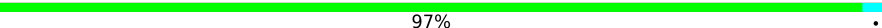
4.2.1 Score per residue for model 1

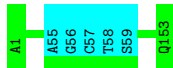
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99%



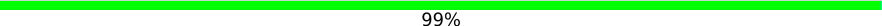
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  97%



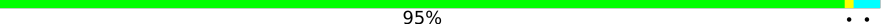
4.2.2 Score per residue for model 2

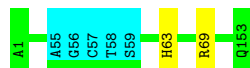
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% .



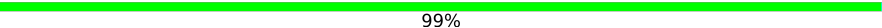
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  95% ..



4.2.3 Score per residue for model 3

- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% .



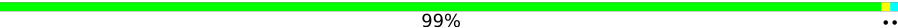
- Molecule 1: Superoxide dismutase [Cu-Zn]

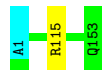
Chain B:  95% ..



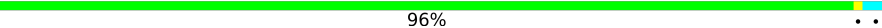
4.2.4 Score per residue for model 4

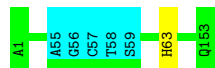
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% ..



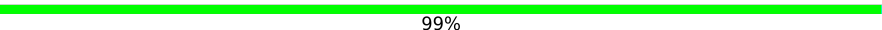
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  96% ..



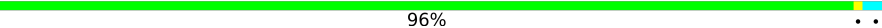
4.2.5 Score per residue for model 5

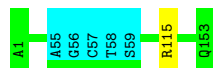
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% .



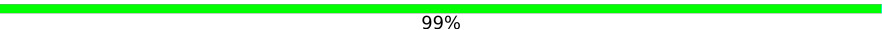
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  96% ..



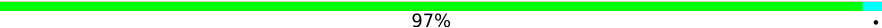
4.2.6 Score per residue for model 6

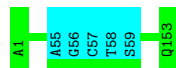
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% .



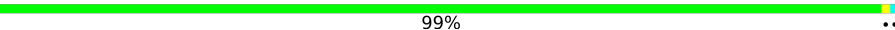
- Molecule 1: Superoxide dismutase [Cu-Zn]

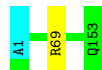
Chain B:  97% .



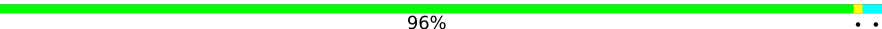
4.2.7 Score per residue for model 7

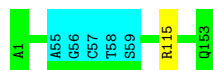
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% ..



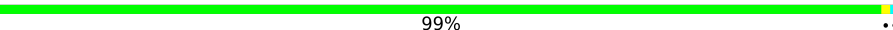
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  96% ..



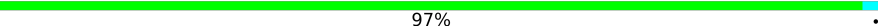
4.2.8 Score per residue for model 8

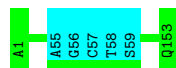
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% ..



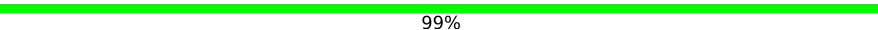
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  97% .



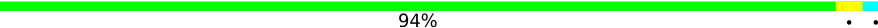
4.2.9 Score per residue for model 9

- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% .



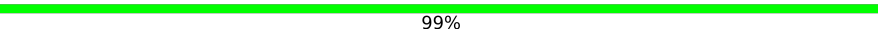
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  94% . .



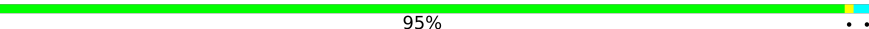
4.2.10 Score per residue for model 10

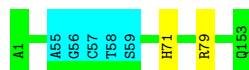
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% .



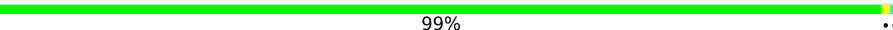
- Molecule 1: Superoxide dismutase [Cu-Zn]

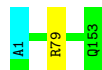
Chain B:  95% . .



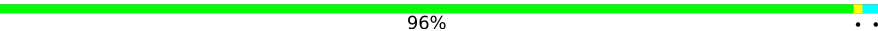
4.2.11 Score per residue for model 11

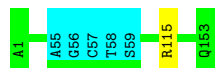
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% ..



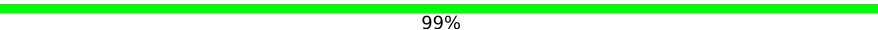
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  96% ..



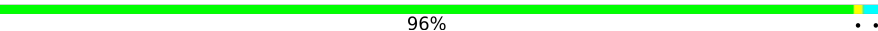
4.2.12 Score per residue for model 12

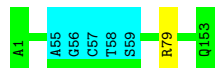
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% .



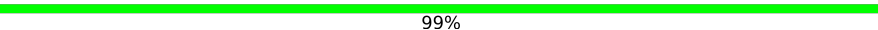
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  96% ..



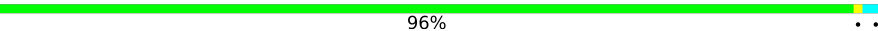
4.2.13 Score per residue for model 13

- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% .



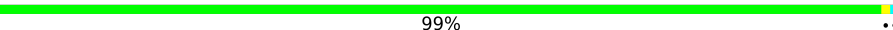
- Molecule 1: Superoxide dismutase [Cu-Zn]

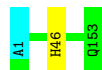
Chain B:  96% ..



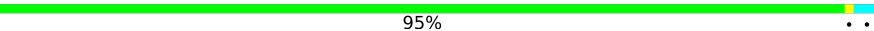
4.2.14 Score per residue for model 14

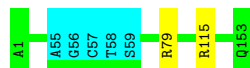
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% ..



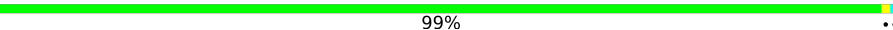
- Molecule 1: Superoxide dismutase [Cu-Zn]

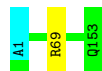
Chain B:  95% ..



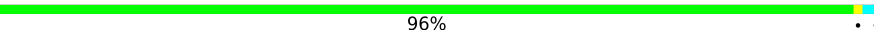
4.2.15 Score per residue for model 15

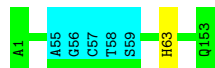
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% ..



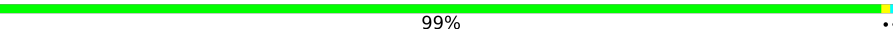
- Molecule 1: Superoxide dismutase [Cu-Zn]

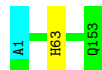
Chain B:  96% ..



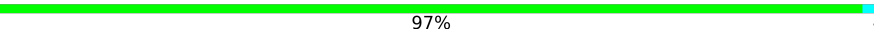
4.2.16 Score per residue for model 16

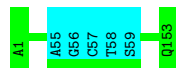
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% ..



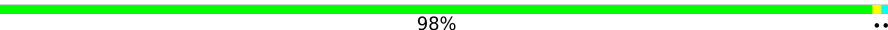
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  97% .



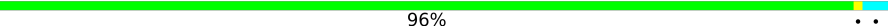
4.2.17 Score per residue for model 17

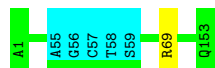
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  98% ..



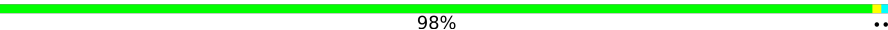
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  96% ..



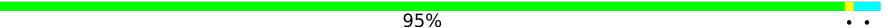
4.2.18 Score per residue for model 18

- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  98% ..



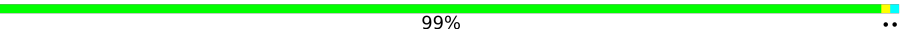
- Molecule 1: Superoxide dismutase [Cu-Zn]

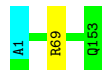
Chain B:  95% ..



4.2.19 Score per residue for model 19

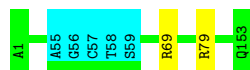
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% ..



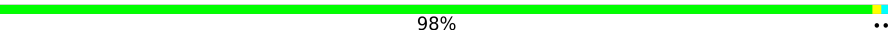
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  95% ..



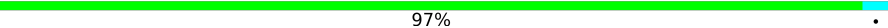
4.2.20 Score per residue for model 20

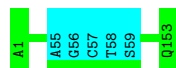
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  98% ..



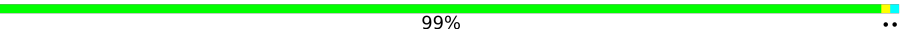
- Molecule 1: Superoxide dismutase [Cu-Zn]

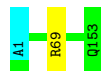
Chain B:  97% .



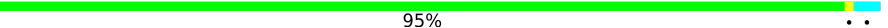
4.2.21 Score per residue for model 21

- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% ..



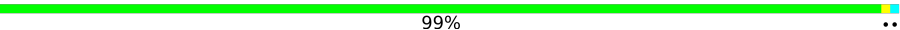
- Molecule 1: Superoxide dismutase [Cu-Zn]

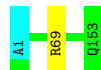
Chain B:  95% ..



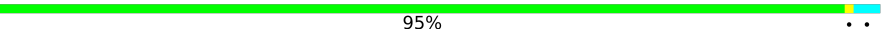
4.2.22 Score per residue for model 22

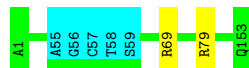
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% ..



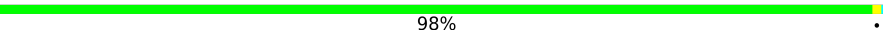
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  95% ..



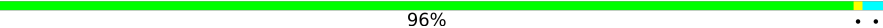
4.2.23 Score per residue for model 23 (medoid)

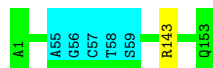
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  98% ..



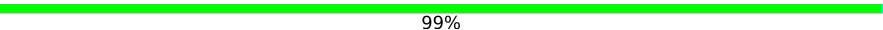
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  96% ..



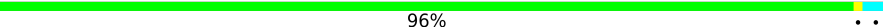
4.2.24 Score per residue for model 24

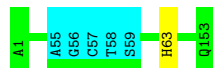
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% .



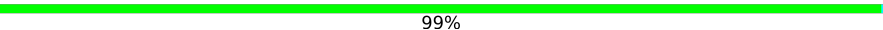
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  96% ..



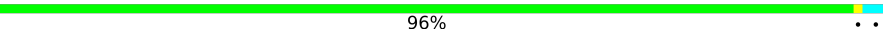
4.2.25 Score per residue for model 25

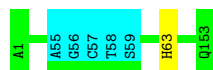
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% .



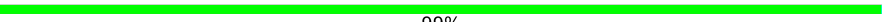
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  96% ..



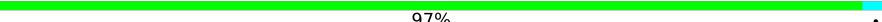
4.2.26 Score per residue for model 26

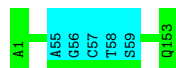
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% .



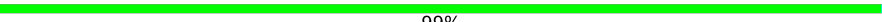
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  97% .



4.2.27 Score per residue for model 27

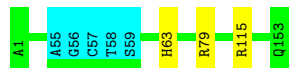
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% .



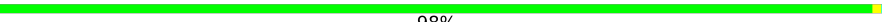
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  95% . .



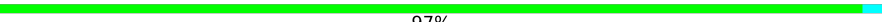
4.2.28 Score per residue for model 28

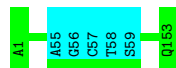
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  98% ..



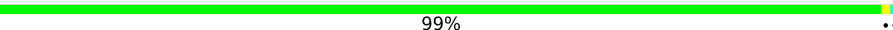
- Molecule 1: Superoxide dismutase [Cu-Zn]

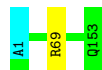
Chain B:  97% .



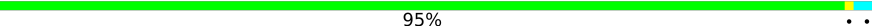
4.2.29 Score per residue for model 29

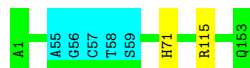
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% ..



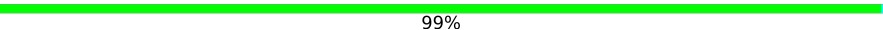
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  95% ..



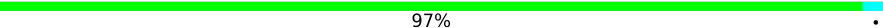
4.2.30 Score per residue for model 30

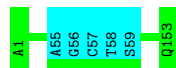
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99% .



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  97% .



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing, restrained energy minimization*.

Of the 600 calculated structures, 30 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
CYANA	structure solution	1.03
Amber	refinement	8

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