



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2AF2 / pdb_00002af2
Title : Solution structure of disulfide reduced and copper depleted Human Superoxide Dismutase
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Deposited on : 2005-07-25

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 i

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
			Total	C	H	N	O	S	
1	A	153	2188	679	1080	203	224	2	0
1	B	153	2185	679	1077	203	224	2	0

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	
			Total	Zn
2	A	1	1	1
2	B	1	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.

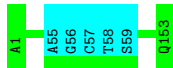
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  99%



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  97%



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

The representative model is number 23. Colouring as in section 4.1 above.

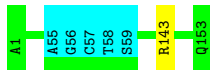
- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain A:  98%



- Molecule 1: Superoxide dismutase [Cu-Zn]

Chain B:  96%



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](#)

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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