



wwPDB NMR Structure Validation Summary Report ⓘ

May 28, 2020 – 11:21 pm BST

PDB ID : 2LU5
Title : Structure and chemical shifts of Cu(I),Zn(II) superoxide dismutase by solid-state NMR
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Deposited on : 2012-06-08

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

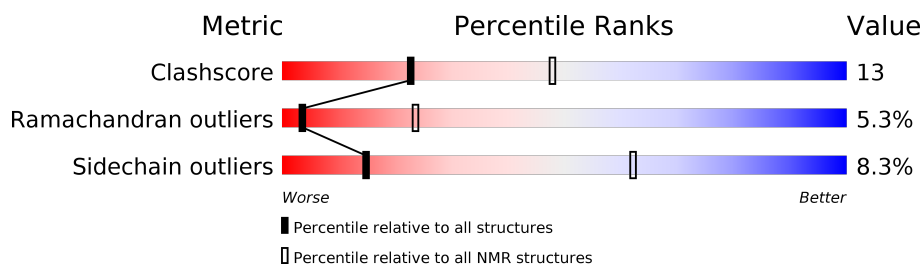
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 30%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	153	<div>62% 36% .</div>

2 Ensemble composition and analysis

This entry contains 19 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest target function*.

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:80, A:84-A:153 (150)	1.18	14

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 and 12 single-model clusters were found.

Cluster number	Models
1	5, 10, 17
2	4, 14
3	1, 16
Single-model clusters	2; 3; 6; 7; 8; 9; 11; 12; 13; 15; 18; 19

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2195 atoms, of which 1085 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
			2194	679	1085	203	225	2	

There are 2 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

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Cu
			1	1

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 80 calculated structures, 19 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	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	517
Number of shifts mapped to atoms	517
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	30%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1090	1069	1061	27±5
All	All	20729	20311	20157	512

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

5 of 384 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:THR:HB	1:A:146:CYS:SG	0.77	2.19	6	3
1:A:60:ALA:HB2	1:A:116:THR:HB	0.76	1.57	7	1
1:A:87:VAL:HB	1:A:95:ALA:HB1	0.75	1.58	9	4
1:A:57:CYS:SG	1:A:143:ARG:HA	0.73	2.22	19	3
1:A:67:LEU:O	1:A:78:GLU:HA	0.71	1.86	10	1

5.2 Torsion angles [i](#)

5.2.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/153 (97%)	113±4 (76±3%)	27±5 (19±3%)	8±3 (5±2%)	3	23
All	All	2812/2907 (97%)	2141 (76%)	522 (19%)	149 (5%)	3	23

5 of 42 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	26	ASN	10
1	A	129	GLY	6
1	A	80	HIS	6
1	A	79	ARG	6
1	A	52	ASP	6

5.2.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/117 (98%)	105±2 (92±2%)	10±2 (8±2%)	15	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2185/2223 (98%)	2004 (92%)	181 (8%)	15 62

5 of 72 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	49	GLU	7
1	A	115	ARG	7
1	A	30	LYS	6
1	A	78	GLU	6
1	A	22	GLN	5

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 30% for the well-defined parts and 30% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

6.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	517
Number of shifts mapped to atoms	517
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	125	3.23 ± 0.22	Should be applied
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	120	3.47 ± 0.26	Should be applied
^{15}N	136	1.06 ± 0.59	None needed (imprecise)

6.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 30%, i.e. 508 atoms were assigned a chemical shift out of a possible 1673. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	508/740 (69%)	134/295 (45%)	240/300 (80%)	134/145 (92%)
Sidechain	0/821 (0%)	0/476 (0%)	0/312 (0%)	0/33 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/112 (0%)	0/58 (0%)	0/37 (0%)	0/17 (0%)
Overall	508/1673 (30%)	134/829 (16%)	240/649 (37%)	134/195 (69%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

6.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

