

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 5, 2023 – 01:47 AM EDT

PDB ID : 6VBS

Title : The C2 Crystal form of SodCI Superoxide Dismutase at 1.7 A resolution with

6 molecules in the asymmetric unit.

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Deposited on : 2019-12-19

Resolution : 1.70 Å(reported)

This is a wwPDB X-ray 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/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

MolProbity : FAILED

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : FAILED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.70 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14487 atoms, of which 6762 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	A	156	Total	С	Н	N	О	S	0	1	0
1	A	150	2269	716	1126	199	221	7	U	1	
1	В	155	Total	С	Н	N	О	S	0	0	0
1	Ъ	199	2243	708	1115	197	216	7	0		
1	С	156	Total	С	Н	N	О	S	0	0	0
1		100	2263	714	1126	199	217	7			
1	D	159	Total	С	Н	N	О	S	0	1	0
1	D	109	2325	733	1156	203	226	7			
1	Е	156	Total	С	Н	N	О	S	0	1	0
1		150	2275	718	1130	199	220	8	0	1	
1	1 F	152	Total	С	Н	N	О	S	0	1	0
1	I,	102	2231	706	1109	195	213	8		1	

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	LEU	-	expression tag	UNP A0A0D6GQL3
A	159	GLU	-	expression tag	UNP A0A0D6GQL3
A	160	HIS	-	expression tag	UNP A0A0D6GQL3
A	161	HIS	-	expression tag	UNP A0A0D6GQL3
A	162	HIS	-	expression tag	UNP A0A0D6GQL3
A	163	HIS	-	expression tag	UNP A0A0D6GQL3
A	164	HIS	-	expression tag	UNP A0A0D6GQL3
A	165	HIS	-	expression tag	UNP A0A0D6GQL3
В	158	LEU	-	expression tag	UNP A0A0D6GQL3
В	159	GLU	-	expression tag	UNP A0A0D6GQL3
В	160	HIS	-	expression tag	UNP A0A0D6GQL3
В	161	HIS	-	expression tag	UNP A0A0D6GQL3
В	162	HIS	-	expression tag	UNP A0A0D6GQL3
В	163	HIS	-	expression tag	UNP A0A0D6GQL3
В	164	HIS	-	expression tag	UNP A0A0D6GQL3
В	165	HIS		expression tag	UNP A0A0D6GQL3
С	158	LEU	-	expression tag	UNP A0A0D6GQL3

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Chain	Residue	Modelled	Actual	Comment	Reference
С	159	GLU	-	expression tag	UNP A0A0D6GQL3
С	160	HIS	-	expression tag	UNP A0A0D6GQL3
С	161	HIS	-	expression tag	UNP A0A0D6GQL3
С	162	HIS	-	expression tag	UNP A0A0D6GQL3
С	163	HIS	-	expression tag	UNP A0A0D6GQL3
С	164	HIS	-	expression tag	UNP A0A0D6GQL3
С	165	HIS	-	expression tag	UNP A0A0D6GQL3
D	158	LEU	-	expression tag	UNP A0A0D6GQL3
D	159	GLU	-	expression tag	UNP A0A0D6GQL3
D	160	HIS	-	expression tag	UNP A0A0D6GQL3
D	161	HIS	-	expression tag	UNP A0A0D6GQL3
D	162	HIS	-	expression tag	UNP A0A0D6GQL3
D	163	HIS	-	expression tag	UNP A0A0D6GQL3
D	164	HIS	-	expression tag	UNP A0A0D6GQL3
D	165	HIS	-	expression tag	UNP A0A0D6GQL3
Е	158	LEU	-	expression tag	UNP A0A0D6GQL3
Е	159	GLU	-	expression tag	UNP A0A0D6GQL3
Е	160	HIS	-	expression tag	UNP A0A0D6GQL3
Е	161	HIS	-	expression tag	UNP A0A0D6GQL3
Е	162	HIS	-	expression tag	UNP A0A0D6GQL3
Е	163	HIS	-	expression tag	UNP A0A0D6GQL3
Е	164	HIS	-	expression tag	UNP A0A0D6GQL3
Е	165	HIS	-	expression tag	UNP A0A0D6GQL3
F	158	LEU	-	expression tag	UNP A0A0D6GQL3
F	159	GLU	-	expression tag	UNP A0A0D6GQL3
F	160	HIS	-	expression tag	UNP A0A0D6GQL3
F	161	HIS	-	expression tag	UNP A0A0D6GQL3
F	162	HIS	-	expression tag	UNP A0A0D6GQL3
F	163	HIS	-	expression tag	UNP A0A0D6GQL3
F	164	HIS	-	expression tag	UNP A0A0D6GQL3
F	165	HIS	-	expression tag	UNP A0A0D6GQL3

• Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 1 1	0	0
2	В	1	Total Cu 1 1	0	0
2	С	1	Total Cu 1 1	0	0

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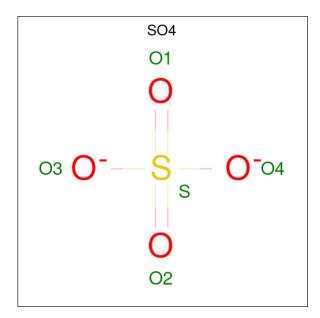
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cu 1 1	0	0
2	E	1	Total Cu 1 1	0	0
2	F	1	Total Cu 1 1	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	В	1	Total Zn 1 1	0	0
3	С	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

 $\bullet$  Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $\mathrm{O_4S}).$ 





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
1	В	1	Total O S	0	0	
4	Ъ	1	5 4 1	U	U	
1	С	1	Total O S	0	0	
4		1	5   4   1		U	
1	С	1	Total O S	0	0	
4		1	5 4 1		U	
1	D	1	Total O S	0	0	
4			5 4 1	U	U	

#### • Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	135	Total O 135 135	0	0
5	В	149	Total O 149 149	0	0
5	С	163	Total O 163 163	0	0
5	D	147	Total O 147 147	0	0
5	Е	131	Total O 131 131	0	0
5	F	124	Total O 124 124	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.



# 3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	152.84Å 69.47Å 95.29Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $116.89^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	35.88 - 1.70	Depositor	
% Data completeness	97.7 (35.88-1.70)	Depositor	
(in resolution range)	, , ,	-	
$R_{merge}$	0.06	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.18  (at  1.52Å)	Xtriage	
Refinement program	PHENIX 1.17	Depositor	
$R, R_{free}$	0.178 , 0.219	Depositor	
Wilson B-factor $(\mathring{A}^2)$	17.3	Xtriage	
Anisotropy	0.024	Xtriage	
L-test for twinning <sup>2</sup>	$ < L > = 0.51, < L^2> = 0.34$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	14487	wwPDB-VP	
Average B, all atoms $(\mathring{A}^2)$	27.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 4 Model quality (i)

# 4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

# 4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

# 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

# 4.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Mol Type Chain Res L		Link	Bond lengths			Bond angles			
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	В	203	-	4,4,4	0.14	0	6,6,6	0.26	0
4	SO4	С	204	-	4,4,4	0.14	0	6,6,6	0.19	0
4	SO4	D	203	-	4,4,4	0.11	0	6,6,6	0.13	0
4	SO4	С	203	-	4,4,4	0.22	0	6,6,6	0.27	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 4.7 Other polymers (i)

There are no such residues in this entry.

# 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 5 Fit of model and data (i)

### 5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

## 5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

