

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

Sep 22, 2022 – 04:31 am BST

PDB ID : 7NXX

Title: Structure of Superoxide Dismutase 1 (SOD1) in complex with nanobody 2

(Nb2).

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Deposited on : 2021-03-19

Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray 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/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 (1)) were used in the production of this report:

 $\begin{array}{ccc} \text{MolProbity} & : & 4.02\text{b-}467 \\ \text{Xtriage (Phenix)} & : & 1.13 \end{array}$ 

EDS : 2.30

buster-report : 1.1.7 (2018)

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

Refmac : 5.8.0267

CCP4 : 7.1.010 (Gargrove)

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

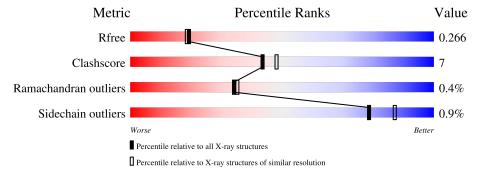
Validation Pipeline (wwPDB-VP) : 2.30

## 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.19 Å.

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	Similar resolution
Metric	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Mol	Chain	Length	Quality of chain				
1	A	153	88%	11%	<del>-</del>		
2	В	136	88%	11%	<u>.</u>		



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2145 atoms, of which 0 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].

$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	153	Total 1109	C 679	N 203	O 223	S 4	0	1	0

• Molecule 2 is a protein called nanobody 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	136	Total 1034	C 638	N 187	O 202	S 7	0	0	0

• Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 1 1	0	1

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total Zi	1	0	1



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Superoxide dismutase [Cu-Zn]





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	115.83Å 115.83Å 83.79Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.91 - 2.19	Depositor
Resolution (A)	57.91 - 2.19	EDS
% Data completeness	67.1 (57.91-2.19)	Depositor
(in resolution range)	67.1 (57.91-2.19)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.32 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
D D.	0.202 , 0.245	Depositor
$R, R_{free}$	0.234 , $0.266$	DCC
$R_{free}$ test set	1008  reflections  (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$  <  L  > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	2145	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.07% 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.

## 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CU

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| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain		nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.40	0/1127	0.64	1/1520 (0.1%)	
2	В	2.08	$2/1060 \ (0.2\%)$	1.03	3/1438 (0.2%)	
All	All	1.47	$2/2187 \ (0.1\%)$	0.85	4/2958 (0.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	В	0	3

#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
2	В	40	GLY	CA-C	53.70	2.37	1.51
2	В	40	GLY	N-CA	-38.74	0.88	1.46

#### All (4) bond angle outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
2	В	39	MET	C-N-CA	-26.11	67.47	122.30
2	В	40	GLY	CA-C-O	-11.13	100.57	120.60
2	В	40	GLY	N-CA-C	-10.76	86.19	113.10
1	A	79	ARG	NE-CZ-NH1	-6.86	116.87	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:



$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type	Group
2	В	39	MET	Peptide
2	В	40	GLY	Peptide, Mainchain

### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1109	0	1076	17	0
2	В	1034	0	973	12	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
All	All	2145	0	2049	28	0

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 7.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
2:B:40:GLY:CA	2:B:40:GLY:C	2.37	0.93	
1:A:74:PRO:HA	1:A:79:ARG:HE	1.51	0.75	
1:A:73:GLY:HA3	1:A:126:LEU:HD23	1.69	0.74	
2:B:1:MET:HA	2:B:28:GLY:HA2	1.70	0.73	
1:A:79:ARG:HH12	1:A:103:VAL:HB	1.57	0.68	
2:B:40:GLY:C	2:B:40:GLY:N	2.47	0.67	
1:A:79:ARG:HH12	1:A:103:VAL:CB	2.18	0.57	
1:A:11:ASP:HB3	2:B:32:ARG:HH22	1.71	0.54	
1:A:69:ARG:HG3	1:A:70:LYS:H	1.73	0.53	
2:B:60:GLY:O	2:B:79:LYS:NZ	2.39	0.53	
2:B:43:ARG:HG3	2:B:53:VAL:HG21	1.92	0.52	
2:B:39:MET:HG2	2:B:84:VAL:HG21	1.92	0.52	
1:A:69:ARG:HE	1:A:78:GLU:HG3	1.75	0.51	
1:A:79:ARG:HG2	1:A:80:HIS:O	2.11	0.51	
2:B:55:THR:HB	2:B:114:LEU:HD13	1.94	0.50	
1:A:31:VAL:HG22	1:A:99:ILE:HB	1.95	0.49	
2:B:32:ARG:HD2	2:B:34:TYR:OH	2.15	0.47	
2:B:56:ILE:HG13	2:B:63:THR:HG22	1.97	0.47	

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASP:OD1	1:A:138:GLY:HA3	2.14	0.47
1:A:69:ARG:HG3	1:A:70:LYS:N	2.31	0.45
1:A:124:ASP:O	1:A:126:LEU:HD12	2.17	0.45
2:B:53:VAL:HG13	2:B:69:VAL:HG11	1.98	0.45
1:A:74:PRO:HA	1:A:79:ARG:NE	2.26	0.43
2:B:39:MET:HG3	2:B:40:GLY:HA2	2.00	0.43
1:A:31:VAL:CG2	1:A:99:ILE:HB	2.50	0.41
1:A:127:GLY:HA2	1:A:134:SER:O	2.19	0.41
1:A:79:ARG:HH11	1:A:79:ARG:HD3	1.68	0.41
1:A:45:PHE:O	1:A:84:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles (i)

#### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	Per	centiles
1	A	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
2	В	134/136~(98%)	128 (96%)	5 (4%)	1 (1%)	22	20
All	All	$285/289 \ (99\%)$	278 (98%)	6 (2%)	1 (0%)	34	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	2	ALA

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.



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	Percenti	$\mathbf{les}$
1	A	118/118 (100%)	116 (98%)	2 (2%)	60 72	2
2	В	106/106 (100%)	106 (100%)	0	100 10	00
All	All	224/224 (100%)	222 (99%)	2 (1%)	78 87	7

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	69	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

# 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates (i)

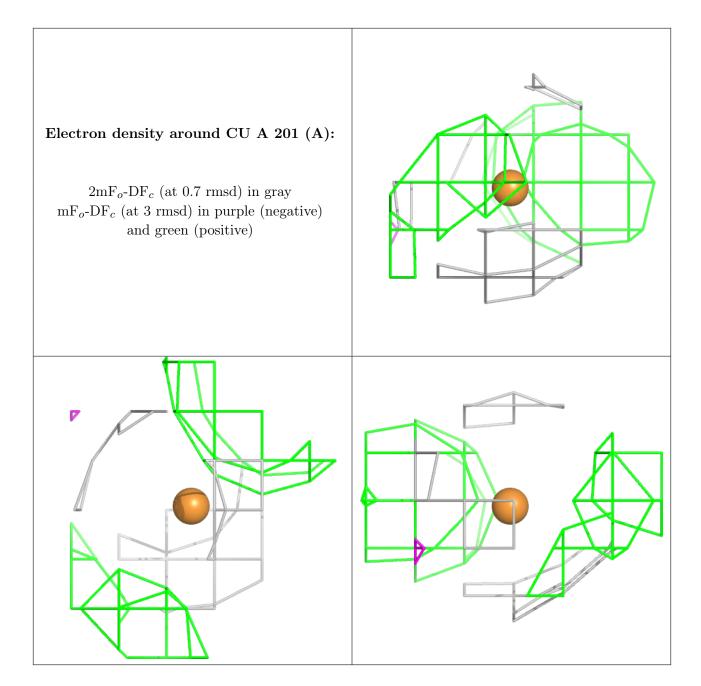
Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands (i)

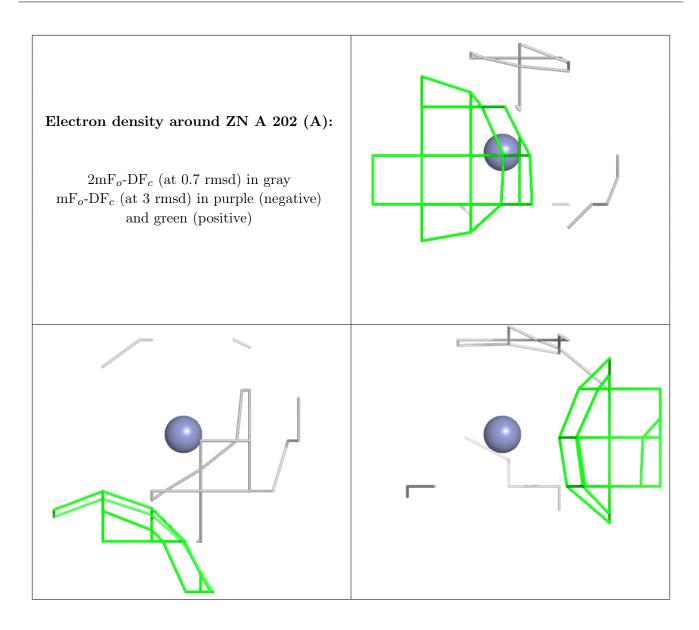
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









## 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

