



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 08:04 PM EDT

PDB ID : 1BZO  
Title : THREE-DIMENSIONAL STRUCTURE OF PROKARYOTIC CU,ZN SUPEROXIDE DISMUTASE FROM P.LEIOGNATHI, SOLVED BY X-RAY CRYSTALLOGRAPHY.  
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Deposited on : 1998-11-02  
Resolution : 2.10 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

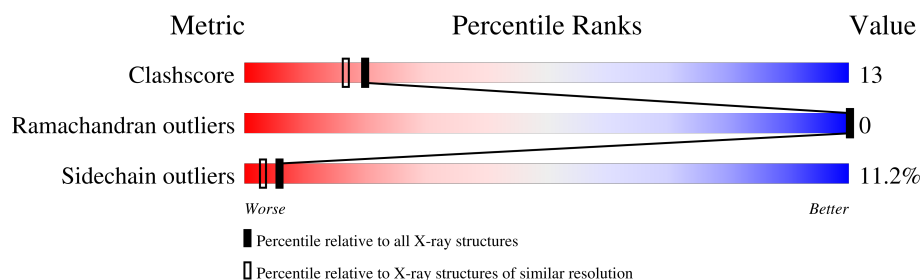
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	151	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1215 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 PROTEIN (SUPEROXIDE DISMUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	48	0	0
			1109	693	200	210	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ILE	THR	SEE REMARK 999	UNP P00446

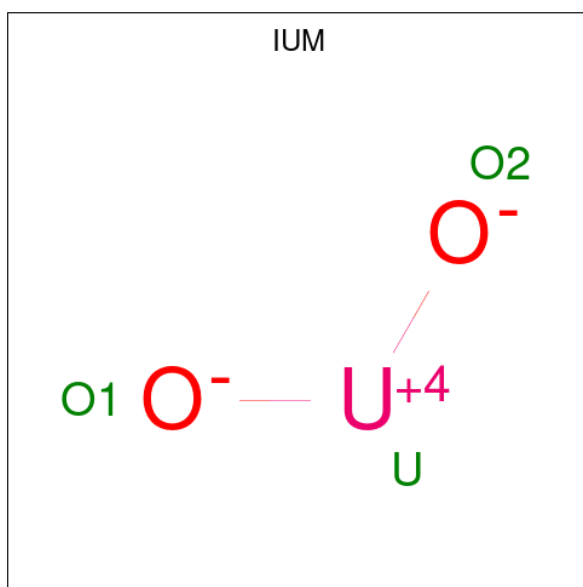
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 4 is URANYL (VI) ION (three-letter code: IUM) (formula: O<sub>2</sub>U).



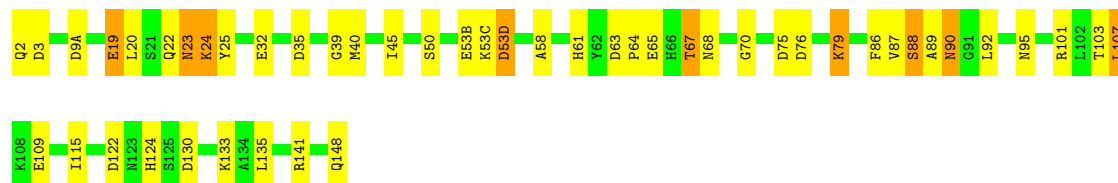
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total U 1 1	0	0
4	A	1	Total U 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	102	Total O 102 102	0	0



- Molecule 1: PROTEIN (SUPEROXIDE DISMUTASE)



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.89Å 86.89Å 99.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.70 – 2.10 24.66 – 2.11	Depositor EDS
% Data completeness (in resolution range)	96.0 (24.70-2.10) 100.0 (24.66-2.11)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.99 (at 2.11Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.180 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 119.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	1215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.11	3/1135 (0.3%)	1.51	19/1538 (1.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53(B)	GLU	CD-OE2	6.27	1.32	1.25
1	A	65	GLU	CD-OE2	6.04	1.32	1.25
1	A	19	GLU	CD-OE2	5.27	1.31	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ARG	NE-CZ-NH1	14.20	127.40	120.30
1	A	141	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	A	101	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	141	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	A	3	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	A	75	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	75	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	A	3	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	53(D)	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	67	THR	CA-CB-CG2	-6.37	103.48	112.40
1	A	63	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	A	9(A)	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	76	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	130	ASP	CB-CG-OD1	5.47	123.23	118.30
1	A	35	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	A	76	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	23	ASN	N-CA-CB	5.27	120.09	110.60
1	A	89	ALA	N-CA-CB	-5.09	102.98	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 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	1082	26	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	102	0	0	1	3
All	All	1215	0	1082	26	3

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.

All (26) 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)
1:A:40:MET:HE1	1:A:86:PHE:HB2	1.43	1.00
1:A:45:ILE:HD13	1:A:115:ILE:HD13	1.57	0.86
1:A:24:LYS:HD3	1:A:25:TYR:CZ	2.12	0.85
1:A:50:SER:O	1:A:58:ALA:HB2	1.86	0.75
1:A:40:MET:CE	1:A:86:PHE:HB2	2.22	0.65
1:A:67:THR:O	1:A:68:ASN:HB3	2.01	0.60
1:A:39:GLY:O	1:A:87:VAL:N	2.33	0.55
1:A:88:SER:HB2	1:A:90:ASN:ND2	2.22	0.55
1:A:64:PRO:HD2	1:A:79:LYS:HB2	1.88	0.55
1:A:45:ILE:HD13	1:A:115:ILE:CD1	2.34	0.55
1:A:40:MET:HE2	1:A:86:PHE:HD1	1.73	0.53
1:A:32:GLU:HA	1:A:32:GLU:OE1	2.09	0.53
1:A:95:ASN:HB2	5:A:594:HOH:O	2.08	0.53
1:A:45:ILE:CD1	1:A:115:ILE:HD13	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:HIS:CE1	1:A:135:LEU:HD22	2.44	0.51
1:A:24:LYS:HD3	1:A:25:TYR:CE2	2.48	0.49
1:A:45:ILE:CD1	1:A:115:ILE:CD1	2.92	0.48
1:A:20:LEU:HB3	1:A:107:LEU:HD21	1.97	0.46
1:A:40:MET:HE2	1:A:86:PHE:CD1	2.51	0.45
1:A:24:LYS:O	1:A:24:LYS:HG2	2.17	0.44
1:A:61:HIS:CE1	1:A:135:LEU:CD2	3.01	0.43
1:A:67:THR:O	1:A:68:ASN:CB	2.66	0.43
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.82	0.43
1:A:22:GLN:NE2	1:A:107:LEU:H	2.18	0.42
1:A:70:GLY:O	1:A:124:HIS:HD2	2.02	0.42
1:A:103:THR:O	1:A:109:GLU:HG2	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:596:HOH:O	5:A:596:HOH:O[4_555]	0.67	1.53
5:A:508:HOH:O	5:A:508:HOH:O[12_555]	1.83	0.37
5:A:542:HOH:O	5:A:542:HOH:O[18_655]	2.08	0.12

## 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	Percentiles	
1	A	149/151 (99%)	146 (98%)	3 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 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 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	Percentiles
1	A	116/116 (100%)	103 (89%)	13 (11%)	<b>6</b> <b>3</b>

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	19	GLU
1	A	23	ASN
1	A	24	LYS
1	A	53(C)	LYS
1	A	53(D)	ASP
1	A	79	LYS
1	A	88	SER
1	A	90	ASN
1	A	92	LEU
1	A	107	LEU
1	A	133	LYS
1	A	148	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	90	ASN
1	A	124	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 4 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - 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.

### 6.5 Other polymers [i](#)

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