



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 07:38 PM EDT

PDB ID : 2YXW / pdb_00002yxw
Title : The deletion mutant of Multicopper Oxidase CueO
Authors : Higuchi, Y.; Komori, H.
Deposited on : 2007-04-27
Resolution : 1.50 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 ⓘ 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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

There are 5 unique types of molecules in this entry. The entry contains 7442 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 Blue copper oxidase cueO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3365	2139	591	617	18			
1	B	444	Total	C	N	O	S	0	0	0
			3406	2163	603	622	18			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	GLY	PRO	engineered mutation	UNP P36649
A	?	-	MET	deletion	UNP P36649
A	?	-	LEU	deletion	UNP P36649
A	?	-	ASP	deletion	UNP P36649
A	?	-	MET	deletion	UNP P36649
A	?	-	MET	deletion	UNP P36649
A	?	-	GLY	deletion	UNP P36649
A	?	-	MET	deletion	UNP P36649
A	?	-	GLN	deletion	UNP P36649
A	?	-	MET	deletion	UNP P36649
A	?	-	LEU	deletion	UNP P36649
A	?	-	MET	deletion	UNP P36649
A	?	-	GLU	deletion	UNP P36649
A	?	-	LYS	deletion	UNP P36649
A	?	-	TYR	deletion	UNP P36649
A	?	-	GLY	deletion	UNP P36649
A	?	-	ASP	deletion	UNP P36649
A	?	-	GLN	deletion	UNP P36649
A	?	-	ALA	deletion	UNP P36649
A	?	-	MET	deletion	UNP P36649
A	?	-	ALA	deletion	UNP P36649
A	?	-	GLY	deletion	UNP P36649
A	?	-	MET	deletion	UNP P36649
A	?	-	ASP	deletion	UNP P36649
A	?	-	HIS	deletion	UNP P36649

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P36649
A	?	-	GLN	deletion	UNP P36649
A	?	-	MET	deletion	UNP P36649
A	?	-	MET	deletion	UNP P36649
A	?	-	GLY	deletion	UNP P36649
A	?	-	HIS	deletion	UNP P36649
A	?	-	MET	deletion	UNP P36649
A	?	-	GLY	deletion	UNP P36649
A	?	-	HIS	deletion	UNP P36649
A	?	-	GLY	deletion	UNP P36649
A	?	-	ASN	deletion	UNP P36649
A	?	-	MET	deletion	UNP P36649
A	?	-	ASN	deletion	UNP P36649
A	?	-	HIS	deletion	UNP P36649
A	?	-	MET	deletion	UNP P36649
A	?	-	ASN	deletion	UNP P36649
A	?	-	HIS	deletion	UNP P36649
A	?	-	GLY	deletion	UNP P36649
A	?	-	GLY	deletion	UNP P36649
A	?	-	LYS	deletion	UNP P36649
A	?	-	PHE	deletion	UNP P36649
A	?	-	ASP	deletion	UNP P36649
A	?	-	PHE	deletion	UNP P36649
A	?	-	HIS	deletion	UNP P36649
A	406	GLY	HIS	engineered mutation	UNP P36649
A	517	GLY	-	expression tag	UNP P36649
A	518	HIS	-	expression tag	UNP P36649
A	519	HIS	-	expression tag	UNP P36649
A	520	HIS	-	expression tag	UNP P36649
A	521	HIS	-	expression tag	UNP P36649
A	522	HIS	-	expression tag	UNP P36649
B	357	GLY	PRO	engineered mutation	UNP P36649
B	?	-	MET	deletion	UNP P36649
B	?	-	LEU	deletion	UNP P36649
B	?	-	ASP	deletion	UNP P36649
B	?	-	MET	deletion	UNP P36649
B	?	-	MET	deletion	UNP P36649
B	?	-	GLY	deletion	UNP P36649
B	?	-	MET	deletion	UNP P36649
B	?	-	GLN	deletion	UNP P36649
B	?	-	MET	deletion	UNP P36649
B	?	-	LEU	deletion	UNP P36649

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	MET	deletion	UNP P36649
B	?	-	GLU	deletion	UNP P36649
B	?	-	LYS	deletion	UNP P36649
B	?	-	TYR	deletion	UNP P36649
B	?	-	GLY	deletion	UNP P36649
B	?	-	ASP	deletion	UNP P36649
B	?	-	GLN	deletion	UNP P36649
B	?	-	ALA	deletion	UNP P36649
B	?	-	MET	deletion	UNP P36649
B	?	-	ALA	deletion	UNP P36649
B	?	-	GLY	deletion	UNP P36649
B	?	-	MET	deletion	UNP P36649
B	?	-	ASP	deletion	UNP P36649
B	?	-	HIS	deletion	UNP P36649
B	?	-	SER	deletion	UNP P36649
B	?	-	GLN	deletion	UNP P36649
B	?	-	MET	deletion	UNP P36649
B	?	-	MET	deletion	UNP P36649
B	?	-	GLY	deletion	UNP P36649
B	?	-	HIS	deletion	UNP P36649
B	?	-	MET	deletion	UNP P36649
B	?	-	GLY	deletion	UNP P36649
B	?	-	HIS	deletion	UNP P36649
B	?	-	GLY	deletion	UNP P36649
B	?	-	ASN	deletion	UNP P36649
B	?	-	MET	deletion	UNP P36649
B	?	-	ASN	deletion	UNP P36649
B	?	-	HIS	deletion	UNP P36649
B	?	-	MET	deletion	UNP P36649
B	?	-	ASN	deletion	UNP P36649
B	?	-	HIS	deletion	UNP P36649
B	?	-	GLY	deletion	UNP P36649
B	?	-	GLY	deletion	UNP P36649
B	?	-	LYS	deletion	UNP P36649
B	?	-	PHE	deletion	UNP P36649
B	?	-	ASP	deletion	UNP P36649
B	?	-	PHE	deletion	UNP P36649
B	?	-	HIS	deletion	UNP P36649
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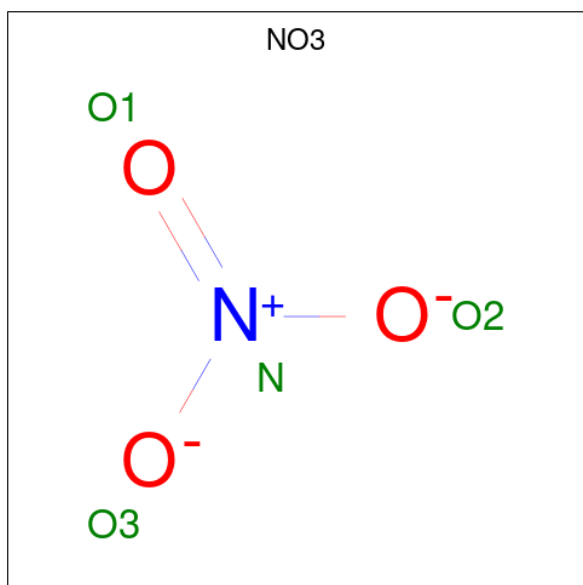
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Chain	Residue	Modelled	Actual	Comment	Reference
B	520	HIS	-	expression tag	UNP P36649
B	521	HIS	-	expression tag	UNP P36649
B	522	HIS	-	expression tag	UNP P36649

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

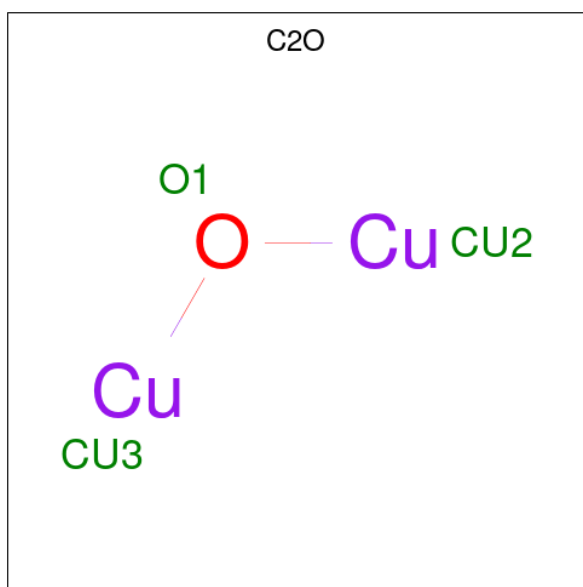
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cu	0	0
			3	3		
2	B	3	Total	Cu	0	0
			3	3		

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is CU-O-CU LINKAGE (CCD ID: C2O) (formula: Cu₂O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Cu	O	0	0
			3	2	1		
4	B	1	Total	Cu	O	0	0
			3	2	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	353	Total	O	0	0
			353	353		
5	B	302	Total	O	0	0
			302	302		

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.33Å 51.57Å 86.70Å 83.77° 90.38° 67.14°	Depositor
Resolution (Å)	25.90 – 1.50	Depositor
% Data completeness (in resolution range)	100.0 (25.90-1.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.07 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.177 , 0.207	Depositor
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.565	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7442	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

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 oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	C2O	B	702	1	0,2,2	-	-	-		
4	C2O	A	702	1	0,2,2	-	-	-		
3	NO3	A	706	-	1,3,3	2.85	1 (100%)	0,3,3	-	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	706	NO3	O1-N	2.85	1.38	1.24

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

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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