

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

#### Nov 1, 2021 – 08:41 PM EDT

PDB ID	:	2YXW
Title	:	The deletion mutant of Multicopper Oxidase CueO
Authors	:	Higuchi, Y.; Komori, H.
Deposited on		
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

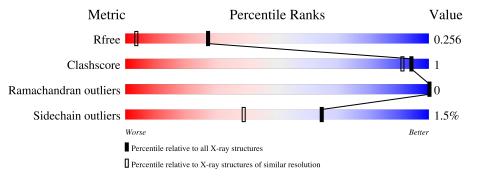
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)

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	А	446	94% •••						
1	В	446	95% •						



# 2 Entry composition (i)

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	Λ	440	Total	С	Ν	0	$\mathbf{S}$	0	0	0
		440	3365	2139	591	617	18			
1	В	444	Total	С	Ν	0	S	0	0	0
1	I B		3406	2163	603	622	18	0	0	0

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

There are 112 discrepancies between the modelled and reference sequences:



	Continued from previous page							
Chain	Residue	Modelled	Actual	Comment	Reference			
А	?	-	SER	deletion	UNP P36649			
А	?	-	GLN	deletion	UNP P36649			
А	?	-	MET	deletion	UNP P36649			
А	?	-	MET	deletion	UNP P36649			
А	?	-	GLY	deletion	UNP P36649			
А	?	-	HIS	deletion	UNP P36649			
А	?	-	MET	deletion	UNP P36649			
А	?	-	GLY	deletion	UNP P36649			
А	?	-	HIS	deletion	UNP P36649			
А	?	-	GLY	deletion	UNP P36649			
А	?	-	ASN	deletion	UNP P36649			
А	?	-	MET	deletion	UNP P36649			
А	?	-	ASN	deletion	UNP P36649			
А	?	-	HIS	deletion	UNP P36649			
А	?	-	MET	deletion	UNP P36649			
А	?	-	ASN	deletion	UNP P36649			
А	?	-	HIS	deletion	UNP P36649			
А	?	-	GLY	deletion	UNP P36649			
А	?	_	GLY	deletion	UNP P36649			
А	?	-	LYS	deletion	UNP P36649			
А	?	_	PHE	deletion	UNP P36649			
А	?	-	ASP	deletion	UNP P36649			
А	?	_	PHE	deletion	UNP P36649			
А	?	-	HIS	deletion	UNP P36649			
А	406	GLY	HIS	engineered mutation	UNP P36649			
А	517	GLY	-	expression tag	UNP P36649			
А	518	HIS	-	expression tag	UNP P36649			
А	519	HIS	-	expression tag	UNP P36649			
А	520	HIS	_	expression tag	UNP P36649			
А	521	HIS	-	expression tag	UNP P36649			
А	522	HIS	-	expression tag	UNP P36649			
В	357	GLY	PRO	engineered mutation	UNP P36649			
В	?	_	MET	deletion	UNP P36649			
В	?	-	LEU	deletion	UNP P36649			
В	?	-	ASP	deletion	UNP P36649			
В	?	-	MET	deletion	UNP P36649			
В	?	-	MET	deletion	UNP P36649			
В	?	-	GLY	deletion	UNP P36649			
В	?	_	MET	deletion	UNP P36649			
В	?	-	GLN	deletion	UNP P36649			
В	?	-	MET	deletion	UNP P36649			
D	•							

Continued from previous page...



Continued from previous page							
Chain	Residue	Modelled	Actual	Comment	Reference		
В	?	-	MET	deletion	UNP P36649		
В	?	-	GLU	deletion	UNP P36649		
В	?	-	LYS	deletion	UNP P36649		
В	?	-	TYR	deletion	UNP P36649		
В	?	-	GLY	deletion	UNP P36649		
В	?	-	ASP	deletion	UNP P36649		
В	?	-	GLN	deletion	UNP P36649		
В	?	-	ALA	deletion	UNP P36649		
В	?	-	MET	deletion	UNP P36649		
В	?	-	ALA	deletion	UNP P36649		
В	?	-	GLY	deletion	UNP P36649		
В	?	-	MET	deletion	UNP P36649		
В	?	-	ASP	deletion	UNP P36649		
В	?	-	HIS	deletion	UNP P36649		
В	?	-	SER	deletion	UNP P36649		
В	?	-	GLN	deletion	UNP P36649		
В	?	-	MET	deletion	UNP P36649		
В	?	-	MET	deletion	UNP P36649		
В	?	-	GLY	deletion	UNP P36649		
В	?	-	HIS	deletion	UNP P36649		
В	?	-	MET	deletion	UNP P36649		
В	?	-	GLY	deletion	UNP P36649		
В	?	-	HIS	deletion	UNP P36649		
В	?	-	GLY	deletion	UNP P36649		
В	?	-	ASN	deletion	UNP P36649		
В	?	-	MET	deletion	UNP P36649		
В	?	-	ASN	deletion	UNP P36649		
В	?	-	HIS	deletion	UNP P36649		
В	?	-	MET	deletion	UNP P36649		
В	?	-	ASN	deletion	UNP P36649		
В	?	-	HIS	deletion	UNP P36649		
В	?	-	GLY	deletion	UNP P36649		
В	?	-	GLY	deletion	UNP P36649		
В	?	-	LYS	deletion	UNP P36649		
В	?	-	PHE	deletion	UNP P36649		
В	?	-	ASP	deletion	UNP P36649		
В	?	-	PHE	deletion	UNP P36649		
В	?	-	HIS	deletion	UNP P36649		
В	406	GLY	HIS	engineered mutation	UNP P36649		
В	517	GLY	-	expression tag	UNP P36649		
В	518	HIS	-	expression tag	UNP P36649		
В	519	HIS	-	expression tag	UNP P36649		

Continued from previous page...



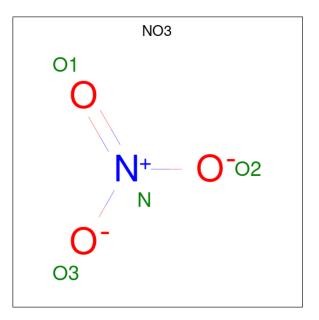
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
В	520	HIS	-	expression tag	UNP P36649
В	521	HIS	-	expression tag	UNP P36649
В	522	HIS	-	expression tag	UNP P36649

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	3	Total Cu 3 3	0	0
2	В	3	Total Cu 3 3	0	0

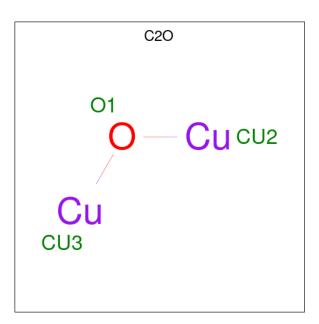
• Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



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

• Molecule 4 is CU-O-CU LINKAGE (three-letter code: C2O) (formula: Cu<sub>2</sub>O).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	А	1	Total 3	Cu 2	0 1	0	0
4	В	1	Total 3	Cu 2	0 1	0	0

• Molecule 5 is water.

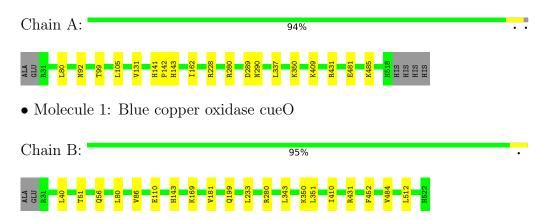
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	353	Total O 353 353	0	0
5	В	302	Total O 302 302	0	0



# 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: Blue copper oxidase cueO





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	50.33Å 51.57Å 86.70Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$83.77^{\circ}$ $90.38^{\circ}$ $67.14^{\circ}$	Depositor
Resolution (Å)	25.90 - 1.50	Depositor
Resolution (A)	25.94 - 1.50	EDS
% Data completeness	$100.0\ (25.90-1.50)$	Depositor
(in resolution range)	$95.1\ (25.94\text{-}1.50)$	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$6.07 (at 1.50 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D.	0.177 , $0.207$	Depositor
$R, R_{free}$	0.232 , $0.256$	DCC
$R_{free}$ test set	6112 reflections $(5.05%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	17.3	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.39, 45.1	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
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.

<sup>&</sup>lt;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.



<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: NO3, CU, C2O  $\,$ 

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	Bo	nd lengths	Bond angles	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.55	1/3450~(0.0%)	0.69	0/4696
1	В	0.44	0/3495	0.63	0/4756
All	All	0.50	1/6945~(0.0%)	0.66	0/9452

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
1	А	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	А	92	ASN	CG-ND2	6.63	1.49	1.32

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	290	ASN	Peptide

### 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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3365	0	3352	10	0
1	В	3406	0	3380	8	0
2	А	3	0	0	0	0
2	В	3	0	0	0	0
3	А	4	0	0	0	0
4	А	3	0	0	0	0
4	В	3	0	0	0	0
5	А	353	0	0	2	0
5	В	302	0	0	1	0
All	All	7442	0	6732	18	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 1.

All (18) 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:431:ARG:HD2	1:A:481:GLU:OE2	2.04	0.58
1:B:181:VAL:HG13	1:B:233:LEU:HD23	1.87	0.57
1:B:343:LEU:HG	1:B:431:ARG:HD2	1.87	0.56
1:A:485:LYS:HE3	5:A:992:HOH:O	2.08	0.53
1:A:228:ARG:HD2	1:A:289:ASP:OD2	2.11	0.51
1:A:337:LEU:HD13	5:A:1014:HOH:O	2.11	0.50
1:A:141:HIS:HB2	1:A:142:PRO:HD2	1.93	0.50
1:A:228:ARG:HG2	1:A:289:ASP:HA	1.95	0.49
1:A:105:LEU:CD2	1:A:162:ILE:HD11	2.45	0.47
1:A:431:ARG:CD	1:A:481:GLU:OE2	2.64	0.46
1:A:80:LEU:HD13	1:A:131:VAL:HG21	1.98	0.45
1:B:350:LYS:C	1:B:351:LEU:HD12	2.38	0.44
1:B:80:LEU:CD2	1:B:86:VAL:HG21	2.48	0.43
1:B:452:PHE:HB3	1:B:484:VAL:HG12	2.01	0.42
1:B:181:VAL:CG1	1:B:233:LEU:HD23	2.49	0.42
1:B:51:THR:HG23	5:B:839:HOH:O	2.19	0.42
1:B:410:ILE:HG21	1:B:512:LEU:HD23	2.03	0.41
1:A:99:THR:O	1:A:142:PRO:HA	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	Perce	ntiles
1	А	438/446~(98%)	421 (96%)	17~(4%)	0	100	100
1	В	442/446~(99%)	429~(97%)	13 (3%)	0	100	100
All	All	880/892~(99%)	850 (97%)	30~(3%)	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	Analysed Rotameric Outliers		Percentiles		
1	А	360/365~(99%)	356~(99%)	4 (1%)	73 53		
1	В	364/365~(100%)	357~(98%)	7(2%)	57 27		
All	All	724/730~(99%)	713~(98%)	11 (2%)	65 39		

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	143	HIS
1	А	280	ARG
1	А	350	LYS
1	А	409	LYS
1	В	40	LEU
1	В	56	GLN
1	В	110	GLU
1	В	143	HIS



Continued from previous page...

Mol	Chain	Res	Type
1	В	169	LYS
1	В	199	GLN
1	В	280	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 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 Tuno		Chain	Res	Link	Bond lengths			Bond angles		
Moi Type	Counts				RMSZ	# Z  > 2	Counts	RMSZ	# Z >2	
4	C2O	В	702	1	0,2,2	-	-	-		
3	NO3	А	706	-	1,3,3	3.09	1 (100%)	0,3,3	-	-
4	C2O	А	702	1	0,2,2	-	-	-		

All (1) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	706	NO3	O1-N	3.09	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.

## 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.

