



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:22 AM UTC

PDB ID : 3NSY / pdb_00003nsy
Title : The multi-copper oxidase CueO with six Met to Ser mutations (M358S,M361S,M362S,M364S,M366S,M368S)
Authors : Roberts, S.A.; Montfort, W.R.; Singh, S.K.
Deposited on : 2010-07-02
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

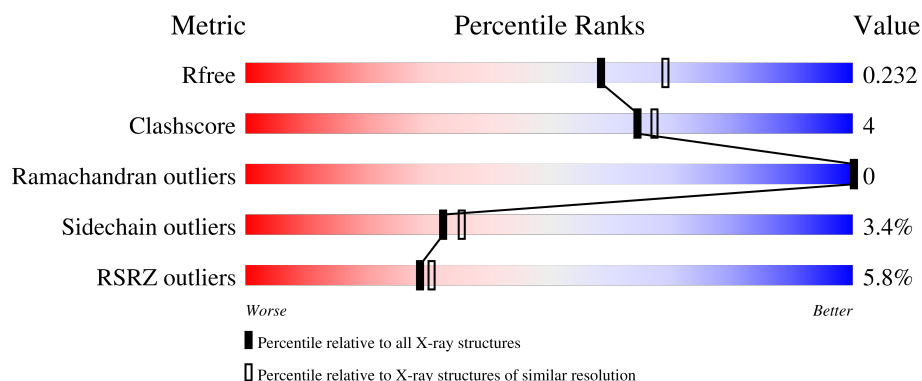
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	511	5% 82% 8% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3895 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
			Total	C	N	O	S			
1	A	465	3583	2272	627	663	21	0	3	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	358	SER	MET	engineered mutation	UNP P36649
A	361	SER	MET	engineered mutation	UNP P36649
A	362	SER	MET	engineered mutation	UNP P36649
A	364	SER	MET	engineered mutation	UNP P36649
A	366	SER	MET	engineered mutation	UNP P36649
A	368	SER	MET	engineered mutation	UNP P36649
A	517	LEU	-	expression tag	UNP P36649
A	518	GLN	-	expression tag	UNP P36649
A	519	GLY	-	expression tag	UNP P36649
A	520	ASP	-	expression tag	UNP P36649
A	521	HIS	-	expression tag	UNP P36649
A	522	GLY	-	expression tag	UNP P36649
A	523	LEU	-	expression tag	UNP P36649
A	524	GLN	-	expression tag	UNP P36649
A	525	GLY	-	expression tag	UNP P36649
A	526	ASP	-	expression tag	UNP P36649
A	527	HIS	-	expression tag	UNP P36649
A	528	GLY	-	expression tag	UNP P36649
A	529	LEU	-	expression tag	UNP P36649
A	530	SER	-	expression tag	UNP P36649
A	531	ALA	-	expression tag	UNP P36649
A	532	TRP	-	expression tag	UNP P36649
A	533	SER	-	expression tag	UNP P36649
A	534	HIS	-	expression tag	UNP P36649
A	535	PRO	-	expression tag	UNP P36649
A	536	GLN	-	expression tag	UNP P36649
A	537	PHE	-	expression tag	UNP P36649

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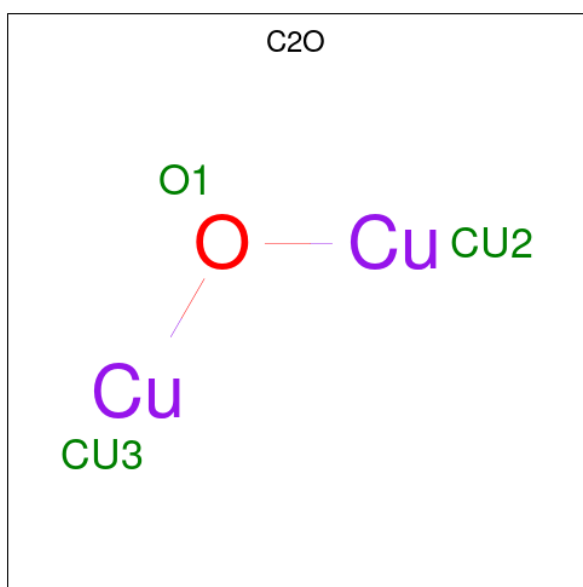
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Chain	Residue	Modelled	Actual	Comment	Reference
A	538	GLU	-	expression tag	UNP P36649
A	539	LYS	-	expression tag	UNP P36649

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Cu 4 4	0	0

- Molecule 3 is CU-O-CU LINKAGE (CCD ID: C2O) (formula: Cu₂O).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	305	Total O 305 305	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.05Å 91.26Å 53.98Å 90.00° 102.34° 90.00°	Depositor
Resolution (Å)	48.00 – 2.10 48.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.00-2.10) 98.5 (48.00-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.45 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.170 , 0.227 0.178 , 0.232	Depositor DCC
R_{free} test set	1402 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3895	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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.

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: C2O, 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	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	0/3682	0.76	1/5004 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	262	GLY	N-CA-C	5.12	117.35	110.43

There are no chirality outliers.

There are no planarity outliers.

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	3583	0	3551	28	0
2	A	4	0	0	0	0
3	A	3	0	0	0	0
4	A	305	0	0	4	0
All	All	3895	0	3551	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 4.

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)
1:A:417:MET:SD	4:A:768:HOH:O	2.43	0.76
1:A:341:PRO:CG	1:A:483:LEU:HD21	2.19	0.72
1:A:106:GLU:H	1:A:133:GLN:HE22	1.40	0.68
1:A:341:PRO:HG2	1:A:483:LEU:HD21	1.80	0.63
1:A:341:PRO:HD2	1:A:483:LEU:HD21	1.82	0.60
1:A:252:ARG:HH12	1:A:288:ASN:HD22	1.50	0.60
1:A:106:GLU:H	1:A:133:GLN:NE2	2.00	0.59
1:A:206:ALA:HB2	1:A:359:LEU:HD22	1.84	0.58
1:A:341:PRO:CD	1:A:483:LEU:HD21	2.34	0.58
1:A:360:ASP:OD2	1:A:379:MET:HE1	2.05	0.56
1:A:341:PRO:HD2	1:A:483:LEU:CD2	2.35	0.56
1:A:355:MET:HG2	1:A:408:ASN:HD22	1.73	0.53
1:A:355:MET:HG2	1:A:408:ASN:ND2	2.23	0.53
1:A:80:LEU:HB3	1:A:131:VAL:HG21	1.92	0.51
1:A:374:GLN:HG2	4:A:670:HOH:O	2.11	0.51
1:A:265:PRO:HD3	1:A:337:LEU:HD22	1.94	0.49
1:A:40:LEU:HD13	1:A:48:ILE:HG23	1.95	0.49
1:A:147:LYS:NZ	4:A:640:HOH:O	2.46	0.49
1:A:170:LEU:HD11	1:A:334:LEU:O	2.13	0.48
1:A:367:LEU:HG	1:A:375:ALA:HB1	1.98	0.46
1:A:350:LYS:C	1:A:351:LEU:HD12	2.41	0.45
1:A:181:VAL:HG22	1:A:233:LEU:HD23	1.99	0.44
1:A:452:PHE:HB3	1:A:484:VAL:HG23	2.00	0.44
1:A:431:ARG:HD2	1:A:481:GLU:OE1	2.18	0.43
1:A:277:MET:HE2	1:A:444:PRO:HG2	2.02	0.42
1:A:105:LEU:HA	1:A:133:GLN:HE22	1.85	0.41
1:A:355:MET:HE2	1:A:360:ASP:OD1	2.21	0.41
1:A:189:LYS:NZ	4:A:573:HOH:O	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	462/511 (90%)	442 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	387/418 (93%)	374 (97%)	13 (3%)	32	35

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

Mol	Chain	Res	Type
1	A	40	LEU
1	A	63	THR
1	A	84	LYS
1	A	143	HIS
1	A	181	VAL
1	A	191	SER
1	A	199	GLN
1	A	228	ARG
1	A	284	LEU
1	A	343	LEU
1	A	359	LEU
1	A	360	ASP
1	A	470	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	186	GLN
1	A	288	ASN
1	A	408	ASN
1	A	428	GLN

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Mol	Chain	Res	Type
1	A	487	ASN
1	A	518	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
3	C2O	A	602	1	0,2,2	-	-	-		

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	465/511 (90%)	0.39	27 (5%)	29 30	26, 40, 59, 77	3 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	ILE	5.2
1	A	378	GLY	5.0
1	A	521	HIS	4.0
1	A	379	MET	4.0
1	A	520	ASP	3.8
1	A	522	GLY	3.8
1	A	519	GLY	3.7
1	A	323	ALA	3.4
1	A	350	LYS	3.2
1	A	332	ASP	3.1
1	A	376	MET	3.1
1	A	517	LEU	2.8
1	A	171[A]	MET	2.8
1	A	130	ASN	2.6
1	A	132	ASP	2.5
1	A	340	LEU	2.5
1	A	341	PRO	2.4
1	A	418	ASN	2.3
1	A	440	MET	2.3
1	A	356	ASP	2.3
1	A	330	LEU	2.2
1	A	361	SER	2.2
1	A	413	GLN	2.1
1	A	428	GLN	2.1
1	A	289	ASP	2.1
1	A	322	ILE	2.1
1	A	336	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CU	A	606	1/1	0.91	0.12	45,45,45,45	1
2	CU	A	605	1/1	0.99	0.03	32,32,32,32	1
2	CU	A	601	1/1	0.99	0.04	45,45,45,45	1
3	C2O	A	602	3/3	0.99	0.05	27,27,35,39	0
2	CU	A	604	1/1	1.00	0.05	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.