



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:55 PM UTC

PDB ID : 1N68 / pdb_00001n68
Title : Copper bound to the Multicopper Oxidase CueO
Authors : Roberts, S.A.; Wildner, G.F.; Grass, G.; Weichsel, A.; Ambrus, A.; Rensing, C.; Montfort, W.R.
Deposited on : 2002-11-08
Resolution : 1.70 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

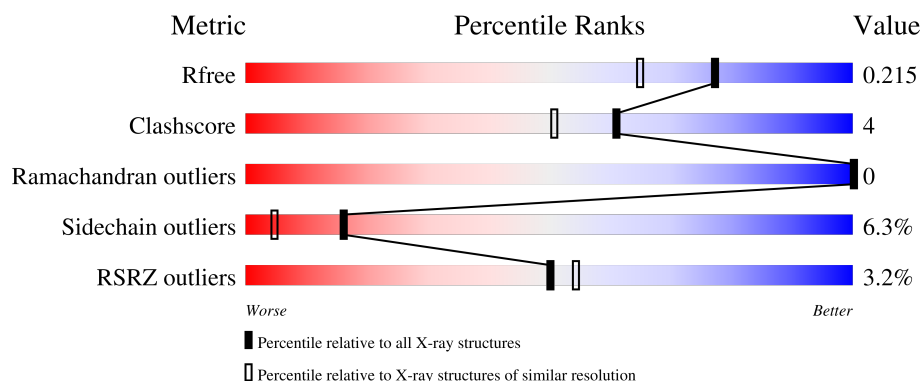
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

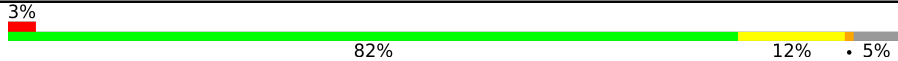
The reported resolution of this entry is 1.70 Å.

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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	488	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4027 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.

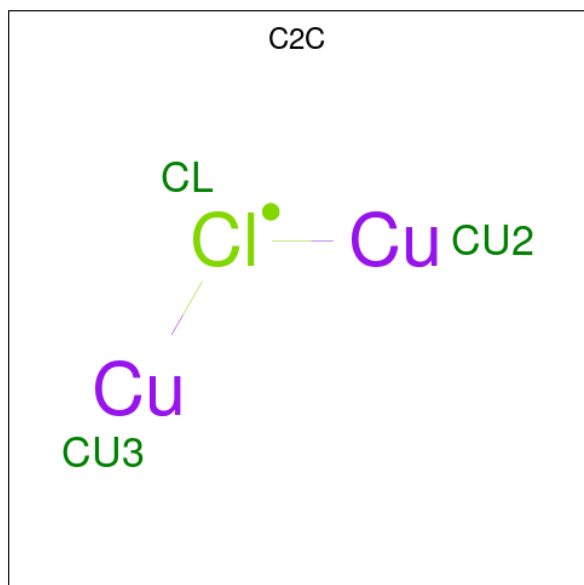
- Molecule 1 is a protein called Blue copper oxidase cueO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	2	0
			3568	2265	621	656	26			

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

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

- Molecule 3 is CU-CL-CU LINKAGE (CCD ID: C2C) (formula: ClCu₂).

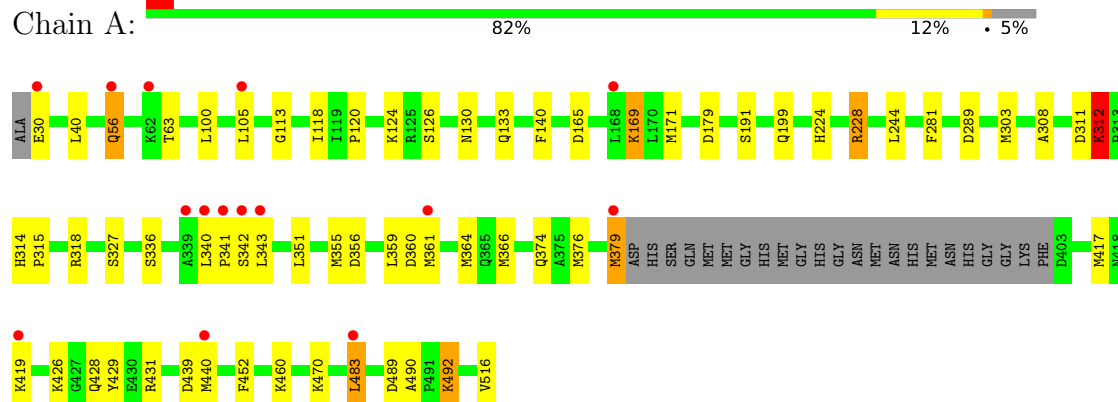


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Cl	Cu	0	0
			3	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	452	Total 452	O 452	0	0

- Molecule 1: Blue copper oxidase cueO



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.00Å 90.94Å 53.81Å 90.00° 102.35° 90.00°	Depositor
Resolution (Å)	26.30 – 1.70 26.30 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (26.30-1.70) 99.7 (26.30-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 1.70Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.165 , 0.222 0.173 , 0.215	Depositor DCC
R_{free} test set	2604 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4027	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C2C, 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	0.54	1/3668 (0.0%)	1.31	15/4981 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	VAL	C-OXT	8.93	1.41	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	ARG	CD-NE-CZ	7.12	134.36	124.40
1	A	228	ARG	CD-NE-CZ	6.65	133.71	124.40
1	A	179	ASP	CA-CB-CG	6.50	119.09	112.60
1	A	312	LYS	CA-C-O	-6.42	114.45	120.94
1	A	120	PRO	O-C-N	6.28	124.10	121.15
1	A	490	ALA	O-C-N	6.07	128.31	121.32
1	A	140	PHE	CA-CB-CG	5.79	119.59	113.80
1	A	452	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	224	HIS	CA-CB-CG	-5.62	108.18	113.80
1	A	244	LEU	O-C-N	-5.62	115.25	122.94
1	A	281	PHE	CA-C-O	-5.59	114.57	121.06
1	A	244	LEU	CA-C-N	5.39	131.74	121.87
1	A	244	LEU	C-N-CA	5.39	131.74	121.87
1	A	356	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	312	LYS	O-C-N	5.06	125.62	121.32

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	3568	0	3538	30	0
2	A	4	0	0	0	0
3	A	3	0	0	0	0
4	A	452	0	0	7	0
All	All	4027	0	3538	30	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 (30) 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:376:MET:O	1:A:379:MET:HB2	1.82	0.79
1:A:374:GLN:HG2	4:A:2189:HOH:O	1.91	0.70
1:A:303:MET:SD	1:A:364:MET:HE3	2.34	0.67
1:A:228:ARG:HD3	1:A:289:ASP:OD1	1.96	0.66
1:A:105:LEU:HD13	1:A:133:GLN:NE2	2.11	0.65
1:A:312:LYS:HD2	4:A:2338:HOH:O	1.96	0.64
1:A:355:MET:HE2	1:A:360:ASP:OD1	1.99	0.62
1:A:63:THR:HG22	4:A:2247:HOH:O	2.01	0.61
1:A:439:ASP:O	1:A:440:MET:HE2	2.04	0.58
1:A:105:LEU:HD13	1:A:133:GLN:HE22	1.68	0.57
1:A:308:ALA:HA	1:A:311:ASP:OD1	2.05	0.57
1:A:314:HIS:HD2	1:A:315:PRO:O	1.92	0.53
1:A:130:ASN:HB3	4:A:2336:HOH:O	2.10	0.52
1:A:429:TYR:HE1	4:A:2214:HOH:O	1.93	0.51
1:A:426:LYS:HD2	1:A:489:ASP:OD1	2.11	0.51
1:A:314:HIS:HE1	4:A:2211:HOH:O	1.94	0.49
1:A:439:ASP:C	1:A:440:MET:HE2	2.38	0.49
1:A:419:LYS:O	1:A:419:LYS:HG2	2.13	0.48
1:A:303:MET:HE2	1:A:376:MET:HE1	1.96	0.48
1:A:492:LYS:HB3	1:A:492:LYS:HE3	1.65	0.46
1:A:361:MET:HA	1:A:361:MET:HE2	1.97	0.46
1:A:100:LEU:O	1:A:113:GLY:HA3	2.15	0.46
1:A:165:ASP:OD1	1:A:165:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:PRO:CG	1:A:483:LEU:HD21	2.47	0.44
1:A:124:LYS:HE3	1:A:126:SER:OG	2.18	0.43
1:A:56:GLN:HG2	1:A:63:THR:CG2	2.50	0.42
1:A:56:GLN:HG2	4:A:2247:HOH:O	2.20	0.42
1:A:341:PRO:HG2	1:A:483:LEU:HD11	2.03	0.41
1:A:165:ASP:O	1:A:169:LYS:HE3	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	Percentiles	
1	A	462/488 (95%)	447 (97%)	15 (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	Rotameric	Outliers	Percentiles	
1	A	384/400 (96%)	360 (94%)	24 (6%)	16	5

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	40	LEU
1	A	56	GLN
1	A	118	ILE
1	A	169	LYS
1	A	171	MET
1	A	191	SER
1	A	199	GLN
1	A	312	LYS
1	A	318	ARG
1	A	327	SER
1	A	336	SER
1	A	340	LEU
1	A	342	SER
1	A	343	LEU
1	A	359	LEU
1	A	366	MET
1	A	379	MET
1	A	417	MET
1	A	428	GLN
1	A	460	LYS
1	A	470	LYS
1	A	483	LEU
1	A	492	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	186	GLN
1	A	314	HIS
1	A	408	ASN
1	A	413	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C2C	A	702	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 [i](#)

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

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	464/488 (95%)	0.00	15 (3%)	50 54	10, 18, 39, 73	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	MET	3.4
1	A	440	MET	3.0
1	A	342	SER	2.8
1	A	339	ALA	2.7
1	A	341	PRO	2.6
1	A	30	GLU	2.6
1	A	343	LEU	2.5
1	A	361	MET	2.5
1	A	483	LEU	2.4
1	A	56	GLN	2.4
1	A	340	LEU	2.4
1	A	62	LYS	2.3
1	A	419	LYS	2.1
1	A	105	LEU	2.0
1	A	168	LEU	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

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(Å ²)	Q<0.9
2	CU	A	705	1/1	0.94	0.09	30,30,30,30	1
2	CU	A	704	1/1	0.98	0.09	38,38,38,38	0
2	CU	A	703	1/1	0.99	0.05	24,24,24,24	0
3	C2C	A	702	3/3	0.99	0.06	21,21,21,23	0
2	CU	A	701	1/1	1.00	0.07	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.