



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:46 PM GMT

PDB ID : 3UAD  
Title : Multicopper Oxidase CueO mutant C500SE506Q (data5)  
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Deposited on : 2011-10-21  
Resolution : 1.10 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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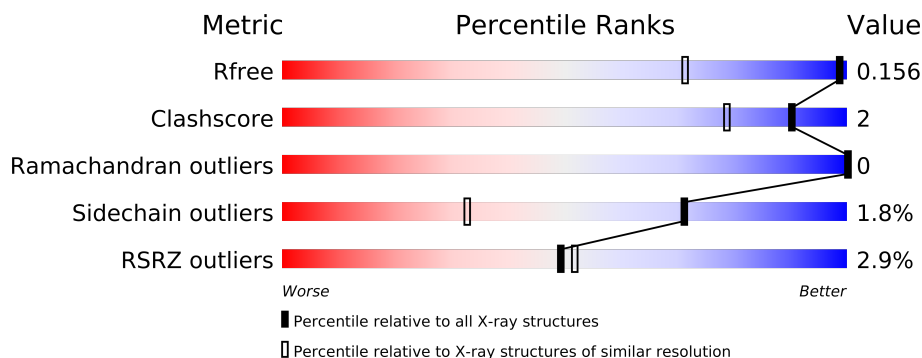
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.10 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))
$R_{free}$	66092	1400 (1.20-1.00)
Clashscore	79885	1559 (1.20-1.00)
Ramachandran outliers	78287	1474 (1.20-1.00)
Sidechain outliers	78261	1472 (1.20-1.00)
RSRZ outliers	66119	1400 (1.20-1.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	489	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	O	A	1006	-	X
4	ACT	A	1007[A]	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4300 atoms, of which 0 are hydrogen and 0 are deuterium.

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	476	Total	C	N	O	S	0	28	0
			3790	2424	650	685	31			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	500	SER	CYS	ENGINEERED MUTATION	UNP P36649
A	506	GLN	GLU	ENGINEERED MUTATION	UNP P36649
A	517	GLY	-	EXPRESSION TAG	UNP P36649

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cu	0	2
			5	5		

- Molecule 3 is OXYGEN ATOM (three-letter code: O) (formula: O).

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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			4	2	2		

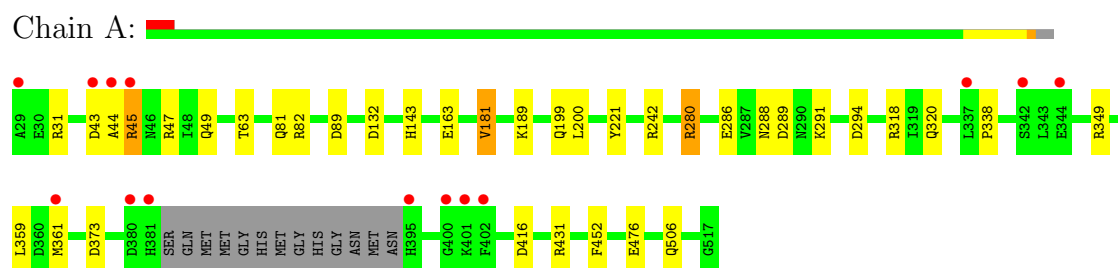
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	493	Total	O	0	6
			498	498		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.48Å 91.19Å 53.31Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	10.00 – 1.10 14.82 – 1.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (10.00-1.10) 99.0 (14.82-1.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 1.10Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.130 , (Not available) 0.128 , 0.156	Depositor DCC
$R_{free}$ test set	9449 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.1	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 60.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 187939 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	4300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.77	0/3966	1.30	36/5382 (0.7%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ARG	NE-CZ-NH1	-14.59	113.00	120.30
1	A	349	ARG	NE-CZ-NH2	-10.84	114.88	120.30
1	A	280	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	132	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	A	221	TYR	CD1-CE1-CZ	-7.58	112.98	119.80
1	A	45	ARG	NE-CZ-NH1	-7.35	116.62	120.30
1	A	431	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	43	ASP	CB-CG-OD2	7.30	124.87	118.30
1	A	181[A]	VAL	CG1-CB-CG2	-7.05	99.62	110.90
1	A	181[B]	VAL	CG1-CB-CG2	-7.05	99.62	110.90
1	A	221	TYR	CG-CD1-CE1	7.02	126.91	121.30
1	A	242	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	A	221	TYR	CB-CG-CD1	6.79	125.08	121.00
1	A	45	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	A	318	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	A	289	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	452	PHE	CB-CG-CD2	-6.42	116.31	120.80
1	A	294	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	63	THR	CA-CB-CG2	-6.17	103.76	112.40
1	A	181[A]	VAL	CA-CB-CG2	6.04	119.95	110.90
1	A	181[B]	VAL	CA-CB-CG2	6.04	119.95	110.90
1	A	47	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	A	82	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	A	452	PHE	CB-CG-CD1	5.75	124.82	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	45	ARG	N-CA-CB	5.25	120.06	110.60
1	A	189	LYS	CA-CB-CG	-5.24	101.88	113.40
1	A	163	GLU	CA-CB-CG	-5.23	101.89	113.40
1	A	44	ALA	O-C-N	5.20	131.03	122.70
1	A	221	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	242	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	476	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	A	373	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	31	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	82	ARG	CG-CD-NE	-5.02	101.26	111.80
1	A	338	PRO	O-C-N	5.01	130.71	122.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3790	0	0	7	0
2	A	5	0	0	0	0
3	A	3	0	0	1	0
4	A	4	0	0	0	0
5	A	498	0	0	5	0
All	All	4300	0	0	8	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (8) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:1005[B]:O:O	3:A:1006:O:O	1.81	0.98
1:A:506:GLN:NE2	5:A:2006[B]:HOH:O	2.48	0.46
1:A:320:GLN:NE2	5:A:2370:HOH:O	2.49	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:200:LEU:N	5:A:2009[B]:HOH:O	2.50	0.43
1:A:81[A]:GLN:NE2	5:A:2309:HOH:O	2.53	0.42
1:A:286:GLU:OE2	1:A:288[A]:ASN:ND2	2.52	0.41
1:A:49[B]:GLN:NE2	1:A:89:ASP:OD2	2.53	0.41
1:A:291[A]:LYS:NZ	5:A:2453:HOH:O	2.55	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	500/489 (102%)	489 (98%)	11 (2%)	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	418/400 (104%)	409 (98%)	9 (2%)	64	22

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	143	HIS
1	A	181[A]	VAL
1	A	181[B]	VAL
1	A	199	GLN

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Mol	Chain	Res	Type
1	A	280	ARG
1	A	359	LEU
1	A	361[A]	MET
1	A	361[B]	MET

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

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is modelled with single atom and 8 are monoatomic - 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.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	476/489 (97%)	-0.16	14 (2%)	49 52	7, 14, 32, 64	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	ALA	9.3
1	A	380	ASP	6.2
1	A	381	HIS	4.2
1	A	395	HIS	3.7
1	A	344	GLU	3.2
1	A	402	PHE	3.1
1	A	401	LYS	3.0
1	A	400	GLY	2.9
1	A	45	ARG	2.9
1	A	43	ASP	2.4
1	A	342	SER	2.3
1	A	44	ALA	2.3
1	A	361[A]	MET	2.2
1	A	337	LEU	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	O	A	1006	1/1	0.16	17.03	14,14,14,14	1
4	ACT	A	1007[A]	1/4	0.15	6.07	14,14,14,14	1
3	O	A	1005[B]	1/1	0.05	0.40	21,21,21,21	1
3	O	A	1005[A]	1/1	0.05	0.40	21,21,21,21	1
2	CU	A	1003[A]	1/1	0.03	-1.85	11,11,11,11	1
2	CU	A	1003[B]	1/1	0.03	-2.16	8,8,8,8	1
2	CU	A	1002[A]	1/1	0.03	-2.27	14,14,14,14	1
2	CU	A	1002[B]	1/1	0.03	-2.66	5,5,5,5	1
2	CU	A	1004	1/1	0.01	-11.05	10,10,10,10	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.