



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2021 – 06:03 PM EST

PDB ID : 6VOW  
Title : Crystal structure of multi-copper oxidase from Pseudomonas Thermotolerans  
Authors : Coler, E.A.; Soares, A.S.; Collins, R.E.  
Deposited on : 2020-01-31  
Resolution : 1.92 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.16  
buster-report : 1.1.7 (2018)  
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) : 2.16

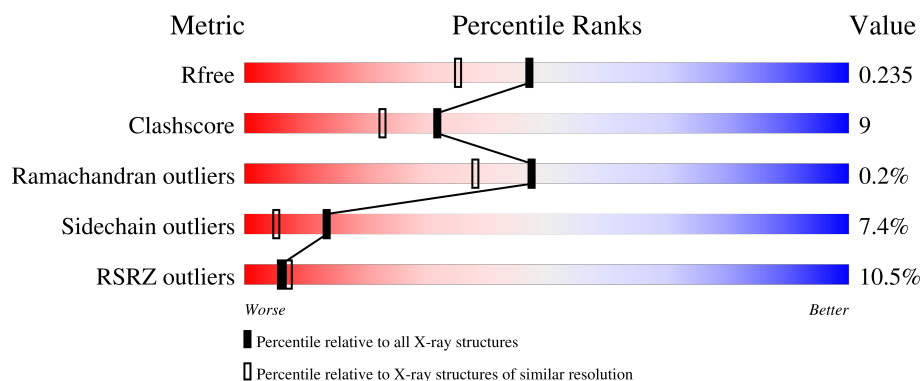
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
$R_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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  $\geq 3$ , 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	456	

## 2 Entry composition [i](#)

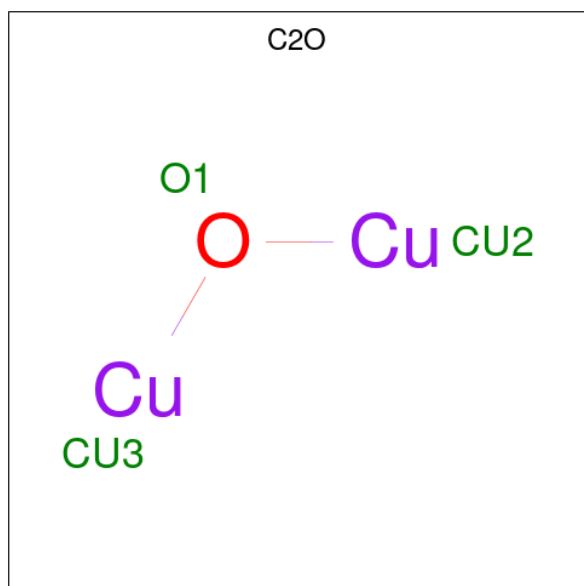
There are 4 unique types of molecules in this entry. The entry contains 3419 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 multicopper oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	4	0
			3276	2094	587	584	11			

- Molecule 2 is CU-O-CU LINKAGE (three-letter code: C2O) (formula:  $\text{Cu}_2\text{O}$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	136	Total 138	O 138	0	10



- Molecule 1: multicopper oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.11Å 68.84Å 49.52Å 90.00° 93.05° 90.00°	Depositor
Resolution (Å)	30.00 – 1.92 28.58 – 1.92	Depositor EDS
% Data completeness (in resolution range)	89.9 (30.00-1.92) 90.0 (28.58-1.92)	Depositor EDS
$R_{merge}$	0.42	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.163 , 0.232 0.171 , 0.235	Depositor DCC
$R_{free}$ test set	1590 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.4	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.0	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	0.97	EDS
Total number of atoms	3419	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<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.

## 5 Model quality

### 5.1 Standard geometry

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	1.23	7/3372 (0.2%)	1.17	13/4600 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	VAL	C-N	25.09	1.91	1.34
1	A	78	SER	CB-OG	8.74	1.53	1.42
1	A	322	TRP	CB-CG	8.06	1.64	1.50
1	A	297	GLU	CG-CD	6.70	1.61	1.51
1	A	56	GLU	CD-OE2	-5.79	1.19	1.25
1	A	402	TRP	CB-CG	-5.71	1.40	1.50
1	A	323	ASP	CB-CG	5.20	1.62	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	246	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	240	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	A	39	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	240	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	A	323	ASP	CB-CG-OD2	6.56	124.21	118.30
1	A	173	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	372	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	408	VAL	N-CA-C	-5.31	96.66	111.00
1	A	325	ASN	CB-CA-C	5.21	120.82	110.40
1	A	173	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	91	VAL	CB-CA-C	-5.15	101.61	111.40
1	A	6	ASP	CB-CG-OD2	5.15	122.94	118.30

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	3276	0	3212	58	0
2	A	3	0	0	0	0
3	A	2	0	0	0	0
4	A	138	0	0	16	1
All	All	3419	0	3212	58	1

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 9.

All (58) 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:422:VAL:C	1:A:423:ALA:N	1.91	1.21
1:A:132:HIS:CD2	1:A:184:GLN:HG2	2.17	0.79
1:A:163:THR:O	1:A:196:THR:HG21	1.88	0.73
1:A:202:ASN:HD21	1:A:251:ARG:HE	1.37	0.72
1:A:361:GLY:HA2	4:A:706[A]:HOH:O	1.90	0.72
1:A:47[B]:ARG:NH2	4:A:603:HOH:O	2.23	0.70
1:A:156[B]:ARG:HH11	1:A:156[B]:ARG:HG2	1.55	0.70
1:A:316:GLN:HG3	4:A:606:HOH:O	1.91	0.69
1:A:361:GLY:N	4:A:602[B]:HOH:O	2.22	0.69
1:A:156[B]:ARG:NH1	1:A:156[B]:ARG:HG2	2.08	0.67
1:A:179:GLU:HB3	1:A:263:VAL:HG21	1.78	0.65
1:A:316:GLN:CG	4:A:606:HOH:O	2.44	0.65
1:A:208:ALA:HB1	1:A:237:LEU:HD11	1.81	0.62
1:A:73:GLY:HA2	1:A:79:GLN:HE21	1.64	0.61
1:A:411:HIS:CD2	4:A:606:HOH:O	2.56	0.58
1:A:133:GLU:CD	1:A:189:ARG:HE	2.09	0.56
1:A:139[B]:LYS:HE3	4:A:663:HOH:O	2.06	0.56
1:A:50:PHE:O	1:A:87:TYR:HA	2.09	0.52
1:A:160:ARG:HD3	1:A:161:GLU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HG3	4:A:729:HOH:O	2.09	0.52
1:A:156[B]:ARG:HH11	1:A:156[B]:ARG:CG	2.22	0.51
1:A:157:GLU:HA	1:A:160:ARG:HG3	1.92	0.51
1:A:296:PHE:CE1	1:A:357:ILE:HD12	2.45	0.51
1:A:242:PRO:HD3	1:A:248:LEU:HD21	1.94	0.49
1:A:175:ASN:HA	1:A:257:LEU:O	2.13	0.49
1:A:322:TRP:CE3	1:A:322:TRP:O	2.66	0.49
1:A:369:SER:OG	1:A:388:GLU:OE2	2.13	0.48
1:A:134:LEU:HD22	1:A:180:LEU:HD21	1.95	0.47
1:A:14:VAL:HG22	4:A:716:HOH:O	2.14	0.47
1:A:33:ALA:HA	1:A:34:PRO:C	2.35	0.46
1:A:202:ASN:ND2	1:A:251:ARG:HE	2.11	0.46
1:A:131:ARG:HB2	1:A:132:HIS:CD2	2.51	0.46
1:A:242:PRO:HG3	1:A:248:LEU:HD21	1.99	0.45
1:A:352:GLN:HA	1:A:352:GLN:NE2	2.32	0.45
1:A:47[A]:ARG:NH2	4:A:618:HOH:O	2.50	0.45
1:A:316:GLN:NE2	4:A:606:HOH:O	2.35	0.45
1:A:328:SER:OG	4:A:601:HOH:O	2.21	0.44
1:A:190:LEU:O	1:A:234:ARG:HA	2.17	0.44
1:A:39:ARG:HD2	1:A:121:VAL:HB	1.98	0.44
1:A:196:THR:HG22	4:A:652:HOH:O	2.18	0.44
1:A:345:PHE:CE1	1:A:394:LEU:HD21	2.53	0.44
1:A:123:GLU:CD	4:A:645:HOH:O	2.56	0.43
1:A:63:HIS:CE1	1:A:358:HIS:CE1	3.07	0.43
1:A:73:GLY:HA2	1:A:79:GLN:NE2	2.32	0.43
1:A:319:GLY:CA	4:A:669:HOH:O	2.68	0.42
1:A:67:LEU:HD12	4:A:706[A]:HOH:O	2.18	0.42
1:A:50:PHE:CD1	1:A:60:ILE:HD11	2.55	0.42
1:A:201:LEU:O	1:A:226:GLU:HA	2.20	0.42
1:A:32:GLN:HG3	1:A:34:PRO:O	2.20	0.42
1:A:216:HIS:HA	1:A:217:PRO:HD3	1.91	0.41
1:A:37:GLU:OE2	1:A:135:SER:OG	2.30	0.41
1:A:140:THR:HG21	1:A:197:VAL:HG21	2.03	0.41
1:A:135:SER:O	1:A:136:LEU:HD12	2.20	0.41
1:A:9:LEU:HD11	1:A:29:TYR:HB3	2.03	0.41
1:A:133:GLU:HA	1:A:187:ARG:O	2.21	0.40
1:A:163:THR:OG1	1:A:410:ASP:OD2	2.28	0.40
1:A:285:ASP:H	1:A:342:HIS:HD2	1.67	0.40
1:A:291:THR:C	1:A:292:LEU:HD12	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:618:HOH:O	4:A:700:HOH:O[2_656]	2.05	0.15

## 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	410/456 (90%)	393 (96%)	16 (4%)	1 (0%)	47 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	PRO

### 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	343/373 (92%)	315 (92%)	28 (8%)	11 4

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36[A]	VAL
1	A	36[B]	VAL
1	A	67	LEU
1	A	91	VAL
1	A	131	ARG

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Mol	Chain	Res	Type
1	A	153	MET
1	A	156[A]	ARG
1	A	156[B]	ARG
1	A	156[C]	ARG
1	A	160	ARG
1	A	184	GLN
1	A	196	THR
1	A	203	LEU
1	A	225	LYS
1	A	234	ARG
1	A	248	LEU
1	A	271	ASP
1	A	288	ILE
1	A	293	SER
1	A	297	GLU
1	A	313	LYS
1	A	317	ILE
1	A	322	TRP
1	A	325	ASN
1	A	327	ILE
1	A	362	MET
1	A	371	ARG
1	A	392	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	79	GLN
1	A	111	GLN
1	A	202	ASN
1	A	342	HIS
1	A	352	GLN

### 5.3.3 RNA ⓘ

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 3 ligands modelled in this entry, 2 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	$\# Z  > 2$
2	C2O	A	501	1	0,2,2	0.00	-	-		

There are no bond length outliers.

There are no bond angle outliers.

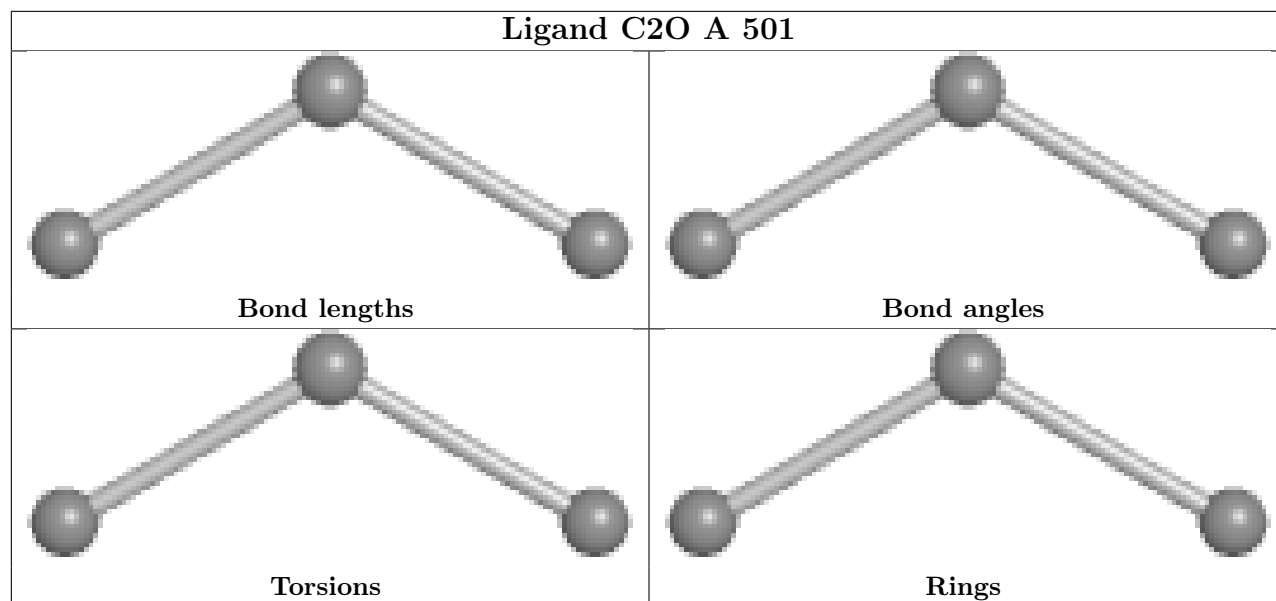
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	422:VAL	C	423:ALA	N	1.91

## 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	409/456 (89%)	0.40	43 (10%) <b>6</b> <b>7</b>	35, 50, 78, 103	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	TRP	6.4
1	A	266	VAL	4.3
1	A	312	TYR	4.2
1	A	64	GLY	4.1
1	A	263	VAL	4.0
1	A	320	GLN	3.9
1	A	160	ARG	3.8
1	A	63	HIS	3.3
1	A	232	GLY	3.3
1	A	359	LEU	3.2
1	A	358	HIS	3.2
1	A	423	ALA	3.0
1	A	406	CYS	3.0
1	A	101	TRP	3.0
1	A	65	ILE	2.9
1	A	314	TYR	2.9
1	A	156[A]	ARG	2.9
1	A	282	ALA	2.9
1	A	322	TRP	2.8
1	A	330	ALA	2.7
1	A	271	ASP	2.7
1	A	373	GLU	2.7
1	A	285	ASP	2.6
1	A	405	HIS	2.6
1	A	412	MET	2.5
1	A	155	PRO	2.5
1	A	233	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	234	ARG	2.4
1	A	100	PHE	2.4
1	A	361	GLY	2.3
1	A	161	GLU	2.3
1	A	10	ILE	2.2
1	A	229	LEU	2.2
1	A	381	THR	2.2
1	A	336	THR	2.2
1	A	338	LYS	2.2
1	A	326	ASP	2.2
1	A	357	ILE	2.1
1	A	235	ILE	2.1
1	A	244	ALA	2.1
1	A	324	ILE	2.1
1	A	360	HIS	2.0
1	A	290	GLU	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](#)

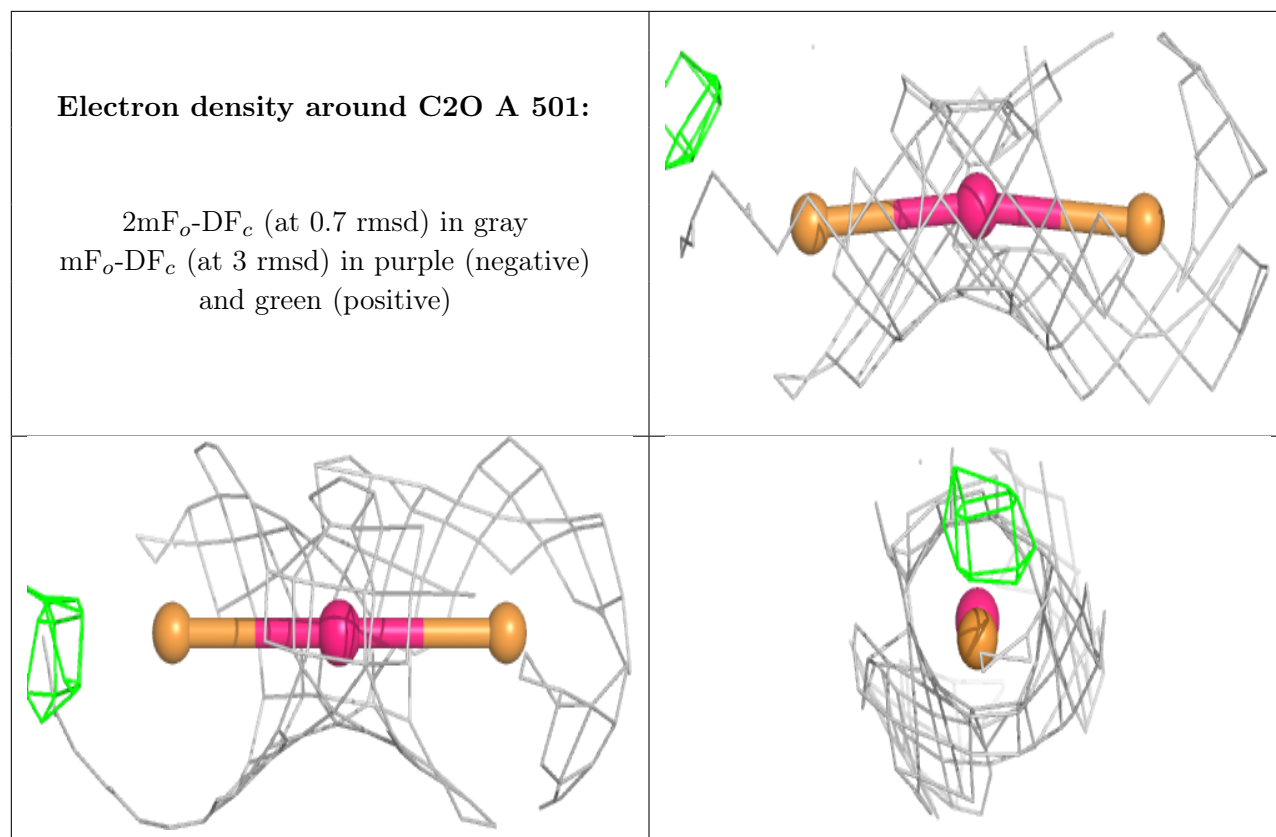
There are no monosaccharides in this entry.

## 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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CU	A	503	1/1	0.99	0.09	51,51,51,51	0
2	C2O	A	501	3/3	1.00	0.15	42,42,46,49	0
3	CU	A	502	1/1	1.00	0.14	48,48,48,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.