



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 14, 2025 – 11:17 am BST

PDB ID : 8R4H / pdb\_00008r4h  
Title : Crystal structure of the copper efflux oxidase (CueO) from Hafnia alvei deleted of the Met-rich domain  
Authors : Leone, P.; Contaldo, U.  
Deposited on : 2023-11-13  
Resolution : 2.94 Å(reported)

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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>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

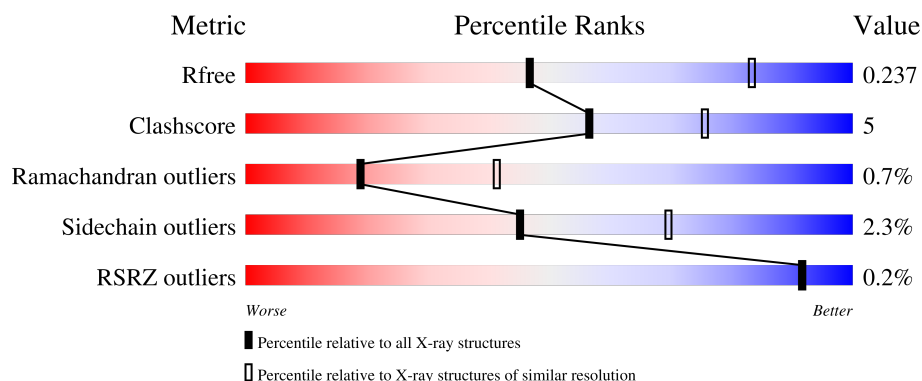
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.94 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))
$R_{free}$	164625	1067 (2.96-2.92)
Clashscore	180529	1122 (2.96-2.92)
Ramachandran outliers	177936	1075 (2.96-2.92)
Sidechain outliers	177891	1075 (2.96-2.92)
RSRZ outliers	164620	1067 (2.96-2.92)

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	452	
1	B	452	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7021 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 Copper efflux oxidase, Multicopper oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3411	2172	596	618	25			
1	B	442	Total	C	N	O	S	0	0	0
			3411	2172	596	618	25			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	358A	GLY	-	linker	UNP A0A377PPH3
A	358B	GLY	-	linker	UNP A0A377PPH3
A	474	THR	ILE	conflict	UNP A0A097R5T5
A	542	SER	-	expression tag	UNP A0A097R5T5
A	543	ALA	-	expression tag	UNP A0A097R5T5
A	544	TRP	-	expression tag	UNP A0A097R5T5
A	545	SER	-	expression tag	UNP A0A097R5T5
A	546	HIS	-	expression tag	UNP A0A097R5T5
A	547	PRO	-	expression tag	UNP A0A097R5T5
A	548	GLN	-	expression tag	UNP A0A097R5T5
A	549	PHE	-	expression tag	UNP A0A097R5T5
A	550	GLU	-	expression tag	UNP A0A097R5T5
A	551	LYS	-	expression tag	UNP A0A097R5T5
B	358A	GLY	-	linker	UNP A0A377PPH3
B	358B	GLY	-	linker	UNP A0A377PPH3
B	474	THR	ILE	conflict	UNP A0A097R5T5
B	542	SER	-	expression tag	UNP A0A097R5T5
B	543	ALA	-	expression tag	UNP A0A097R5T5
B	544	TRP	-	expression tag	UNP A0A097R5T5
B	545	SER	-	expression tag	UNP A0A097R5T5
B	546	HIS	-	expression tag	UNP A0A097R5T5
B	547	PRO	-	expression tag	UNP A0A097R5T5
B	548	GLN	-	expression tag	UNP A0A097R5T5
B	549	PHE	-	expression tag	UNP A0A097R5T5
B	550	GLU	-	expression tag	UNP A0A097R5T5

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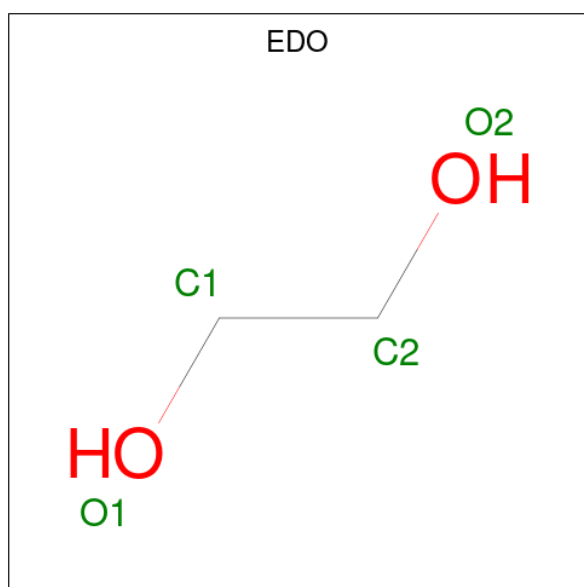
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Chain	Residue	Modelled	Actual	Comment	Reference
B	551	LYS	-	expression tag	UNP A0A097R5T5

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

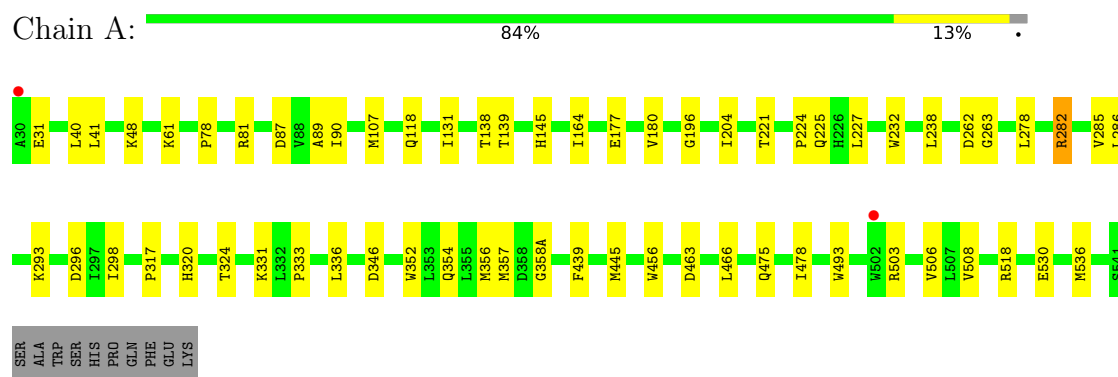
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total 75	O 75	0	0
4	B	68	Total 68	O 68	0	0

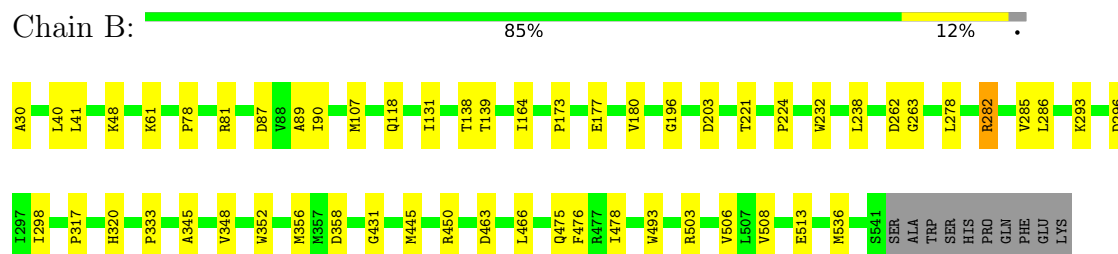
### 3 Residue-property plots

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 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: Copper efflux oxidase,Multicopper oxidase



- Molecule 1: Copper efflux oxidase,Multicopper oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.27Å 169.27Å 90.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.23 – 2.94 30.23 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.23-2.94) 99.6 (30.23-2.94)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.10.4 (26-JUL-2023)	Depositor
R, $R_{free}$	0.198 , 0.245 0.194 , 0.237	Depositor DCC
$R_{free}$ test set	1016 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.8	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7021	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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: EDO, 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	0.34	0/3502	0.56	0/4762
1	B	0.32	0/3502	0.55	0/4762
All	All	0.33	0/7004	0.56	0/9524

There are no bond length outliers.

There are no bond angle outliers.

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	3411	0	3405	34	0
1	B	3411	0	3405	29	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	20	0	30	0	0
3	B	28	0	42	2	0
4	A	75	0	0	2	0
4	B	68	0	0	0	0
All	All	7021	0	6882	62	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 5.



The worst 5 of 62 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:B:352:TRP:HH2	1:B:503:ARG:HH11	1.38	0.72
1:A:138:THR:HG22	1:A:139:THR:N	2.07	0.69
1:A:40:LEU:HD21	1:A:81:ARG:HH11	1.58	0.68
1:B:40:LEU:HD21	1:B:81:ARG:HH11	1.58	0.68
1:B:138:THR:HG22	1:B:139:THR:N	2.07	0.68

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	440/452 (97%)	412 (94%)	23 (5%)	5 (1%)	12	30
1	B	440/452 (97%)	416 (94%)	23 (5%)	1 (0%)	44	66
All	All	880/904 (97%)	828 (94%)	46 (5%)	6 (1%)	19	41

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	ASP
1	A	463	ASP
1	B	463	ASP
1	A	358(A)	GLY
1	A	439	PHE

### 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	363/372 (98%)	355 (98%)	8 (2%)	47	70
1	B	363/372 (98%)	354 (98%)	9 (2%)	42	66
All	All	726/744 (98%)	709 (98%)	17 (2%)	45	69

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	358	ASP
1	B	536	MET
1	A	536	MET
1	B	87	ASP
1	B	118	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	B	354	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	EDO	A	606	-	3,3,3	0.40	0	2,2,2	0.11	0
3	EDO	A	608	-	3,3,3	0.37	0	2,2,2	0.24	0
3	EDO	B	611	-	3,3,3	0.26	0	2,2,2	0.28	0
3	EDO	A	605	-	3,3,3	0.60	0	2,2,2	0.22	0
3	EDO	A	607	-	3,3,3	0.22	0	2,2,2	0.38	0
3	EDO	B	610	-	3,3,3	0.31	0	2,2,2	0.24	0
3	EDO	B	606	-	3,3,3	0.34	0	2,2,2	0.39	0
3	EDO	B	609	-	3,3,3	0.36	0	2,2,2	0.13	0
3	EDO	B	608	-	3,3,3	0.44	0	2,2,2	0.08	0
3	EDO	B	605	-	3,3,3	0.34	0	2,2,2	0.07	0
3	EDO	B	607	-	3,3,3	0.10	0	2,2,2	0.28	0
3	EDO	A	609	-	3,3,3	0.45	0	2,2,2	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	606	-	-	1/1/1/1	-
3	EDO	A	608	-	-	1/1/1/1	-
3	EDO	B	611	-	-	1/1/1/1	-
3	EDO	A	605	-	-	1/1/1/1	-
3	EDO	A	607	-	-	0/1/1/1	-
3	EDO	B	610	-	-	0/1/1/1	-
3	EDO	B	606	-	-	0/1/1/1	-
3	EDO	B	609	-	-	0/1/1/1	-
3	EDO	B	608	-	-	0/1/1/1	-
3	EDO	B	605	-	-	0/1/1/1	-
3	EDO	B	607	-	-	0/1/1/1	-
3	EDO	A	609	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	606	EDO	O1-C1-C2-O2
3	A	609	EDO	O1-C1-C2-O2
3	B	611	EDO	O1-C1-C2-O2
3	A	605	EDO	O1-C1-C2-O2
3	A	608	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	609	EDO	2	0
3	B	605	EDO	1	0

## 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, 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	442/452 (97%)	-0.46	2 (0%) 87 86	51, 70, 91, 102	0
1	B	442/452 (97%)	-0.49	0 100 100	56, 73, 93, 106	0
All	All	884/904 (97%)	-0.48	2 (0%) 92 91	51, 71, 92, 106	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	ALA	3.4
1	A	502	TRP	2.1

### 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	EDO	B	610	4/4	0.46	0.25	90,90,90,90	0
3	EDO	A	609	4/4	0.60	0.22	66,66,66,66	0
3	EDO	B	608	4/4	0.62	0.15	68,68,68,68	0

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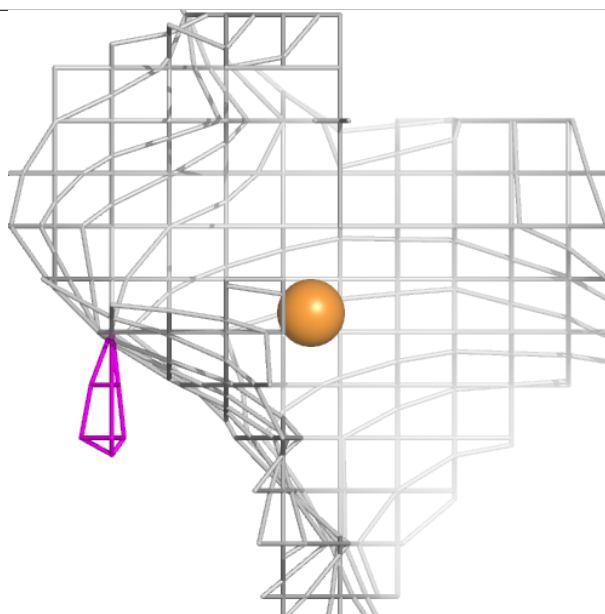
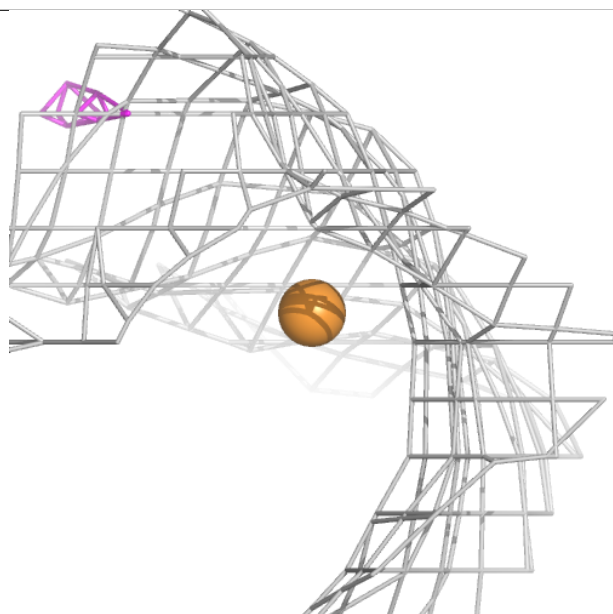
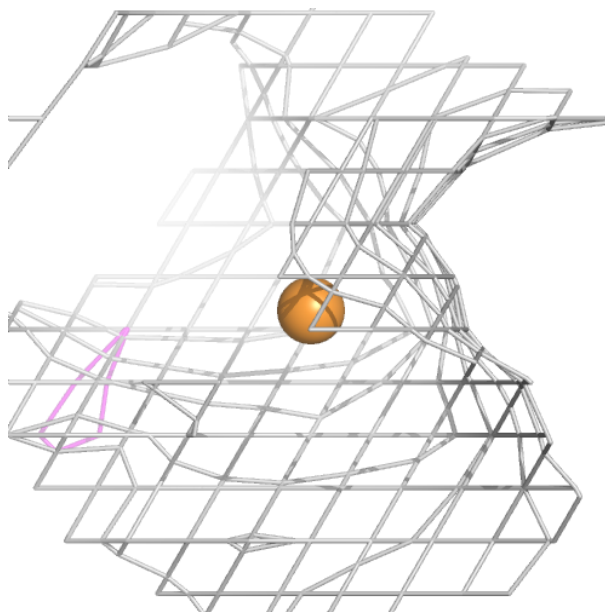
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	606	4/4	0.63	0.19	78,78,78,78	0
3	EDO	B	611	4/4	0.69	0.11	71,72,72,72	0
3	EDO	A	607	4/4	0.74	0.17	79,80,80,80	0
3	EDO	A	605	4/4	0.76	0.13	61,61,61,62	0
3	EDO	B	607	4/4	0.80	0.15	54,54,55,55	0
3	EDO	B	606	4/4	0.80	0.13	58,58,58,58	0
3	EDO	A	608	4/4	0.82	0.14	69,69,70,70	0
3	EDO	B	609	4/4	0.82	0.17	60,61,61,61	0
3	EDO	B	605	4/4	0.92	0.10	64,65,65,65	0
2	CU	B	603	1/1	0.93	0.07	82,82,82,82	1
2	CU	A	602	1/1	0.95	0.04	101,101,101,101	0
2	CU	A	603	1/1	0.96	0.06	101,101,101,101	1
2	CU	B	602	1/1	0.97	0.04	105,105,105,105	0
2	CU	A	601	1/1	0.99	0.05	75,75,75,75	0
2	CU	B	601	1/1	0.99	0.04	87,87,87,87	0
2	CU	B	604	1/1	0.99	0.02	83,83,83,83	0
2	CU	A	604	1/1	1.00	0.02	75,75,75,75	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.

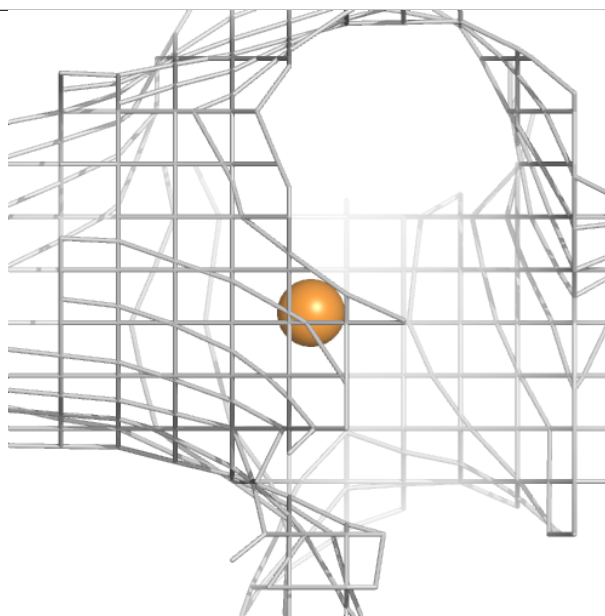
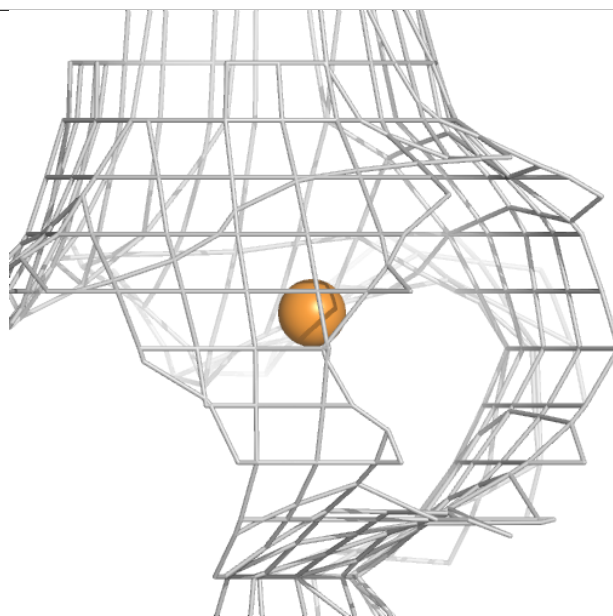
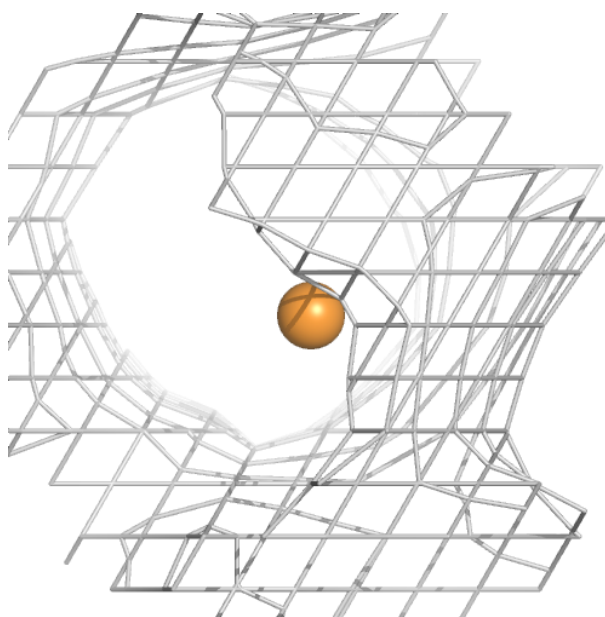
**Electron density around CU B 603:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CU A 602:**

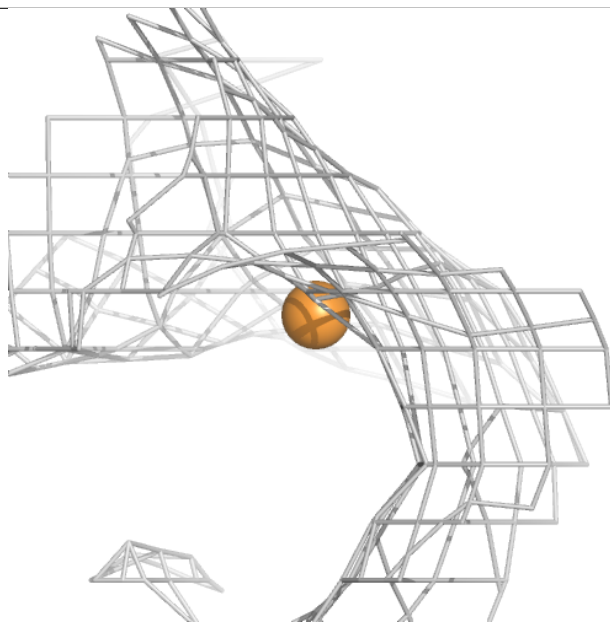
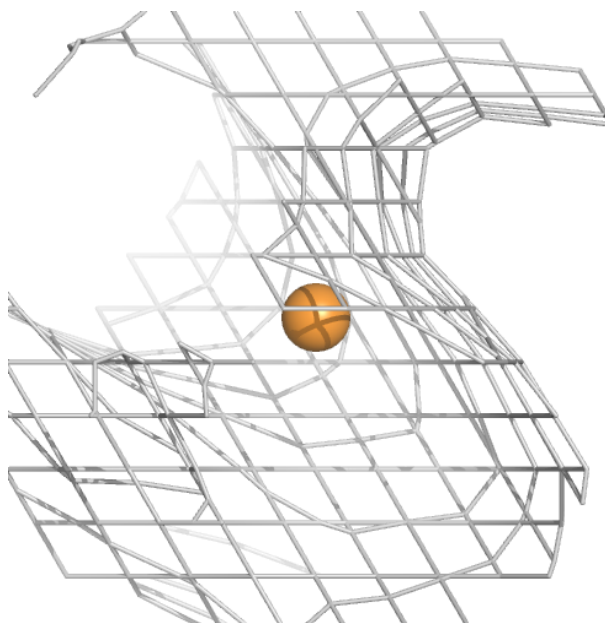
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





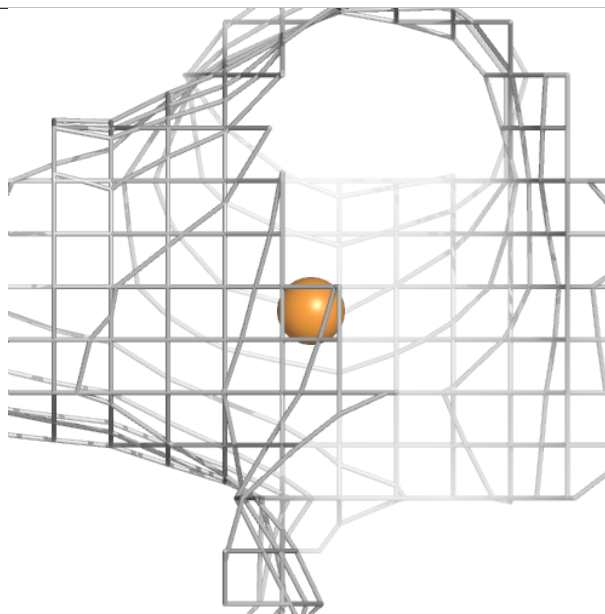
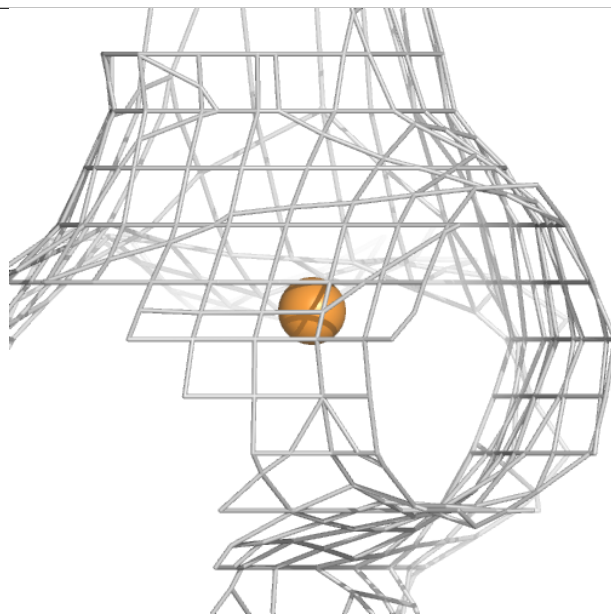
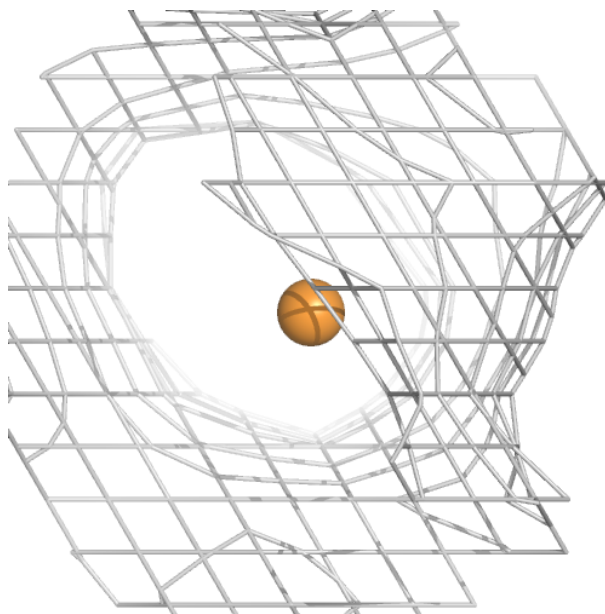
**Electron density around CU A 603:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



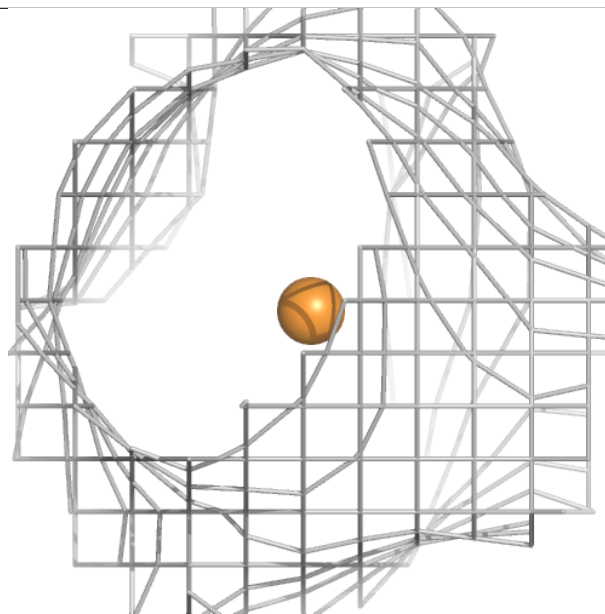
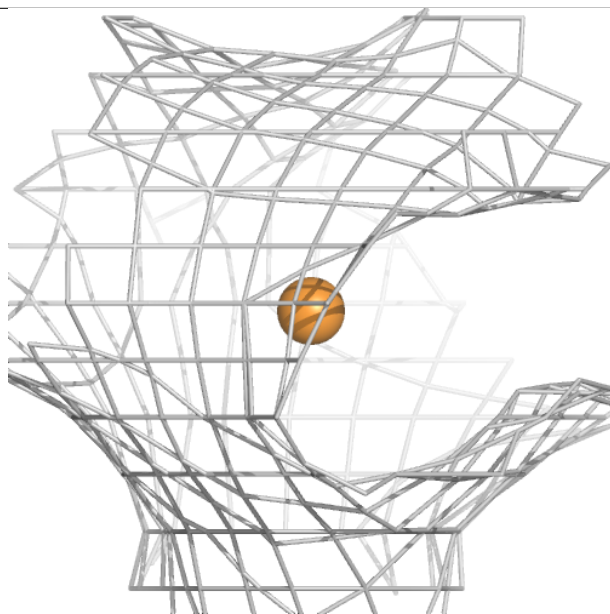
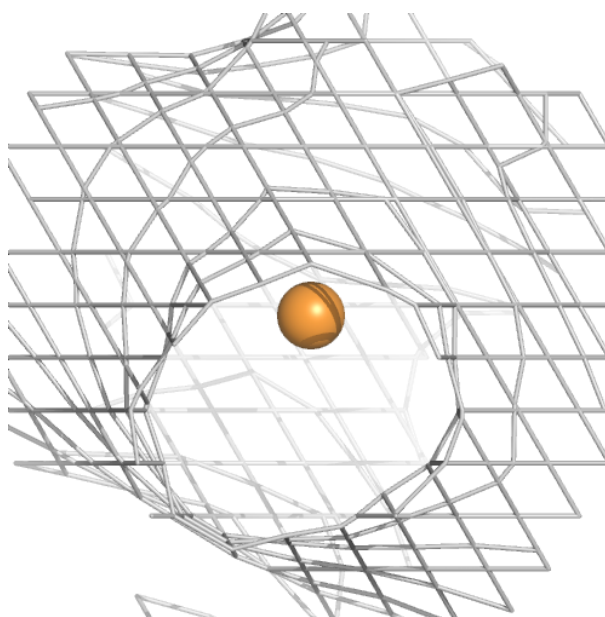
**Electron density around CU B 602:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



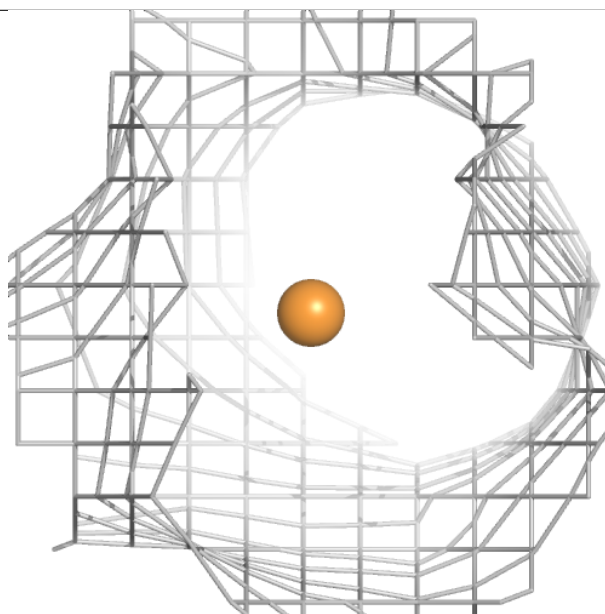
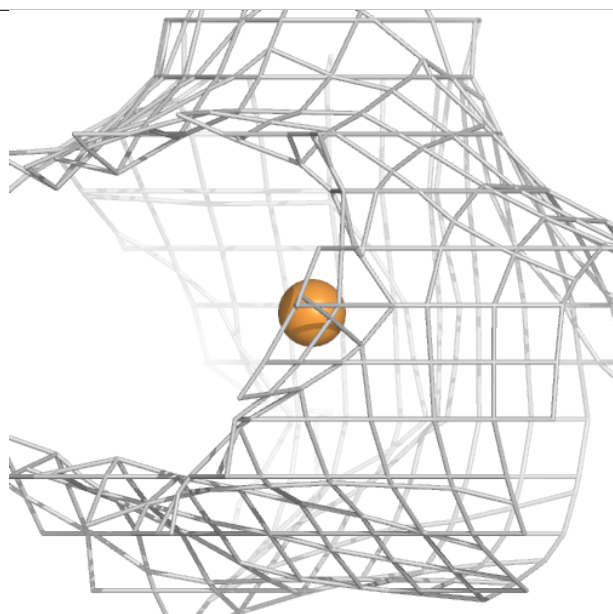
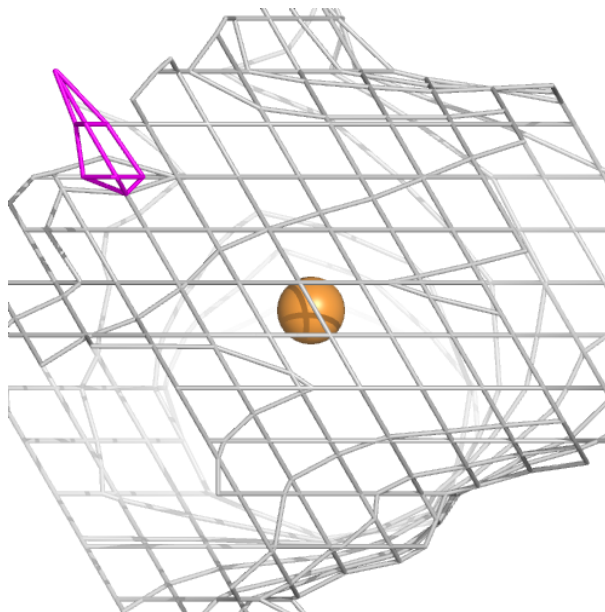
**Electron density around CU A 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



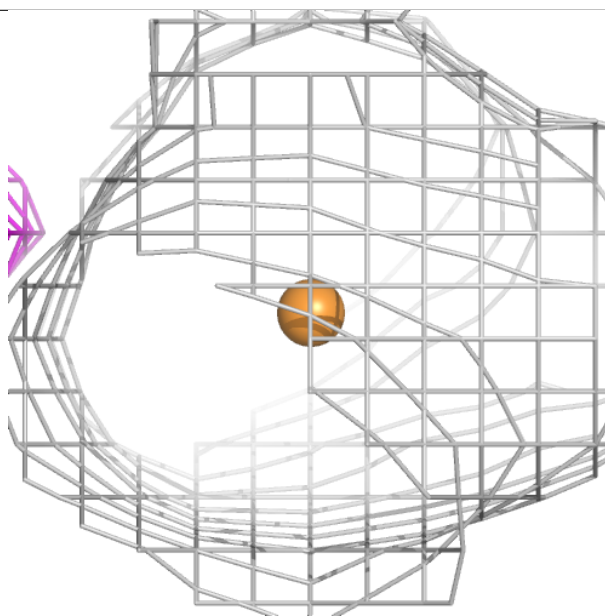
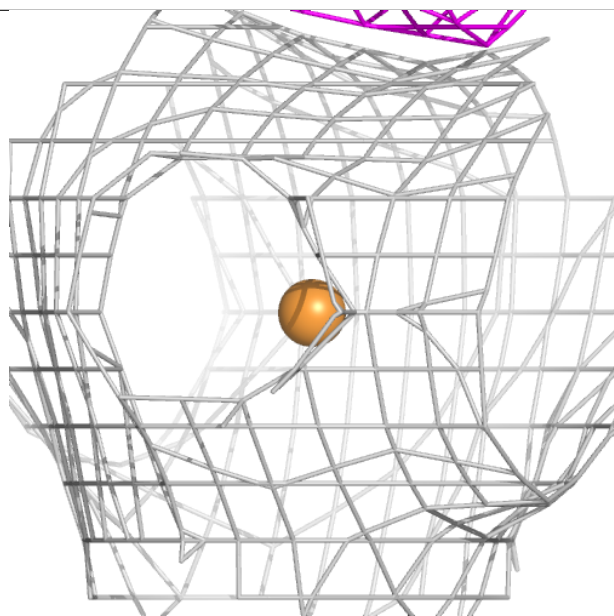
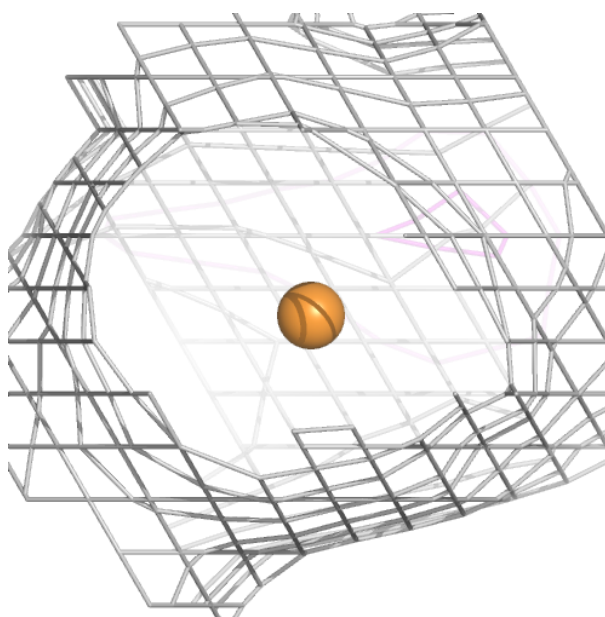
**Electron density around CU B 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CU B 604:**

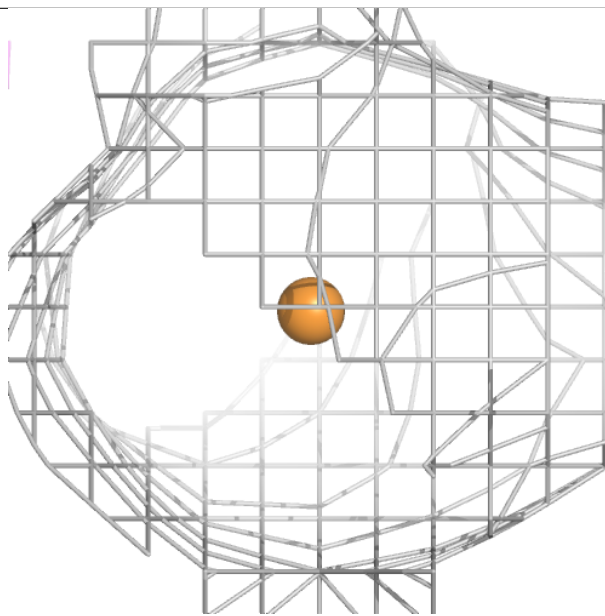
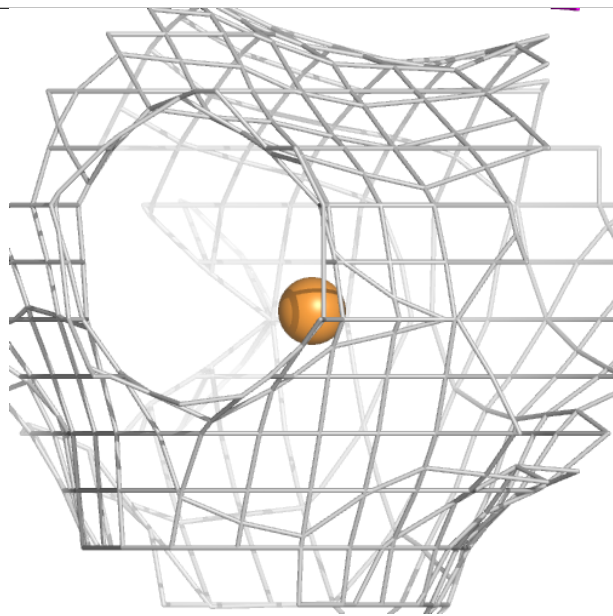
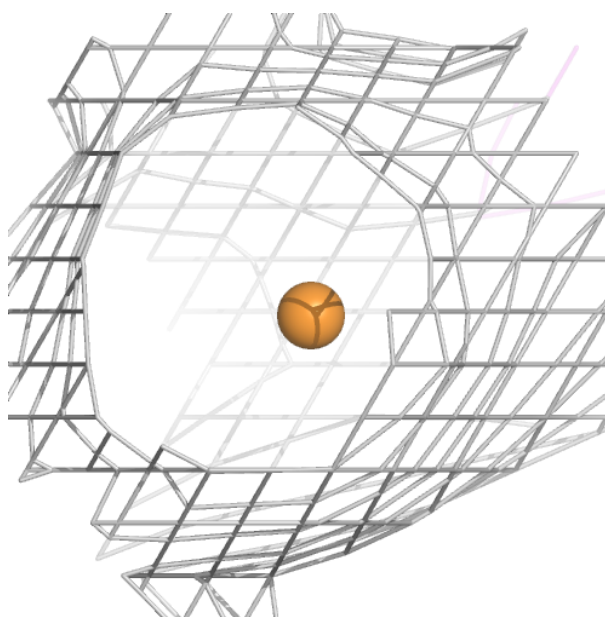
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CU A 604:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.