



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2025 – 03:06 pm GMT

PDB ID : 9RC8 / pdb\_00009rc8  
Title : Laccase (multicopper oxidase) from *Pediococcus pentosaceus* 4618 deletion  
482-509 co-crystallized with Copper Chloride  
Authors : Paredes, F.; Casino, P.  
Deposited on : 2025-05-27  
Resolution : 3.20 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.

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 : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

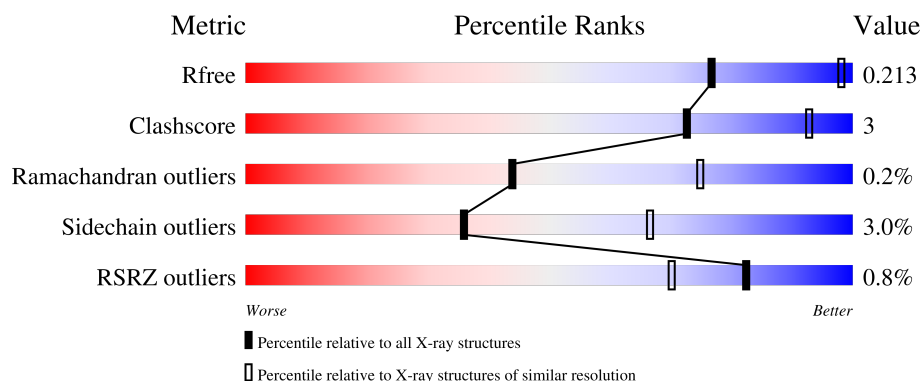
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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	503	 83% 8% • 8%
1	C	503	 81% 10% • 8%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7377 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 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3637	2321	620	682	14			
1	C	462	Total	C	N	O	S	0	0	0
			3651	2332	622	683	14			

- 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	0	0
			4	4		
2	C	4	Total	Cu	0	0
			4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total	O	0	0
			65	65		
3	C	16	Total	O	0	0
			16	16		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.36Å 124.36Å 182.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	107.70 – 3.20 107.70 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (107.70-3.20) 100.0 (107.70-3.20)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.159 , 0.210 0.168 , 0.213	Depositor DCC
$R_{free}$ test set	1359 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.9	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7377	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: 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	0.51	0/3753	0.94	6/5138 (0.1%)
1	C	0.51	0/3767	0.96	4/5155 (0.1%)
All	All	0.51	0/7520	0.95	10/10293 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	THR	CA-CB-OG1	-8.95	96.17	109.60
1	C	275	THR	CA-CB-OG1	-8.16	97.36	109.60
1	C	6	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	28	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	185	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	170	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	6	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	298	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	104	THR	CA-CB-OG1	-5.16	101.86	109.60
1	A	170	ASP	CA-CB-CG	5.02	117.62	112.60

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	3637	0	3421	17	0
1	C	3651	0	3462	27	0
2	A	4	0	0	0	0
2	C	4	0	0	0	0
3	A	65	0	0	1	0
3	C	16	0	0	0	0
All	All	7377	0	6883	44	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 3.

All (44) 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:386:ALA:HB3	1:A:387:PRO:HD3	1.73	0.71
1:A:7:TYR:CE1	1:A:276:HIS:HB3	2.28	0.69
1:C:7:TYR:CE1	1:C:276:HIS:HB3	2.28	0.69
1:C:63:LEU:HD13	1:C:219:MET:HE1	1.77	0.66
1:C:275:THR:HG22	1:C:276:HIS:CD2	2.31	0.66
1:A:451:GLU:HG3	1:A:456:MET:HE3	1.79	0.64
1:C:451:GLU:HG3	1:C:456:MET:HE3	1.79	0.63
1:C:336:VAL:HG21	1:C:377:TYR:CE1	2.37	0.60
1:A:275:THR:HG22	1:A:276:HIS:CD2	2.41	0.56
1:C:251:HIS:HE1	1:C:305:ASP:O	1.90	0.55
1:C:336:VAL:HG21	1:C:377:TYR:CZ	2.41	0.55
1:C:148:ALA:O	1:C:154:THR:HG23	2.08	0.54
1:C:384:ASN:HD21	1:C:391:HIS:HE2	1.54	0.54
1:C:16:LEU:C	1:C:16:LEU:HD12	2.33	0.53
1:C:260:GLN:HE22	1:C:413:ASN:HD22	1.59	0.51
1:A:251:HIS:HE1	1:A:305:ASP:O	1.93	0.51
1:A:149:HIS:N	1:A:150:PRO:CD	2.75	0.49
1:C:386:ALA:HB3	1:C:387:PRO:CD	2.44	0.47
1:C:275:THR:HG22	1:C:276:HIS:NE2	2.29	0.47
1:C:149:HIS:N	1:C:150:PRO:CD	2.79	0.46
1:C:396:HIS:HB2	1:C:441:TYR:HB3	1.97	0.45
1:C:11:GLU:N	1:C:12:PRO:CD	2.80	0.44
1:C:204:TYR:CE1	1:C:213:VAL:HG21	2.52	0.44
1:C:393:PHE:O	1:C:420:THR:HA	2.17	0.44
1:C:386:ALA:HB3	1:C:387:PRO:HD3	1.98	0.44
1:A:32:LYS:HE3	3:A:636:HOH:O	2.18	0.44
1:A:102:LEU:C	1:A:102:LEU:HD12	2.43	0.43
1:A:56:ALA:HB1	1:A:99:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:HB3	1:A:68:LYS:HB3	2.00	0.43
1:C:194:ARG:C	1:C:215:GLY:HA3	2.44	0.43
1:A:260:GLN:HE22	1:A:413:ASN:HD22	1.65	0.43
1:A:191:LEU:HD23	1:A:220:ILE:HD12	2.01	0.42
1:A:36:VAL:HG11	1:A:183:GLY:HA2	2.02	0.42
1:A:148:ALA:O	1:A:154:THR:HG23	2.20	0.41
1:A:156:GLU:HG3	1:A:204:TYR:CD2	2.56	0.41
1:C:281:CYS:O	1:C:282:ALA:HB3	2.20	0.41
1:A:85:TYR:CE1	1:A:91:THR:HG21	2.55	0.41
1:C:16:LEU:HA	1:C:21:TYR:CD1	2.56	0.41
1:C:264:ASP:HB2	1:C:418:LYS:HA	2.03	0.41
1:C:318:LYS:HA	1:C:319:PRO:HD3	1.96	0.41
1:C:236:ARG:HA	1:C:287:VAL:O	2.21	0.41
1:C:16:LEU:HA	1:C:21:TYR:CG	2.56	0.40
1:C:364:GLN:H	1:C:364:GLN:HE21	1.69	0.40
1:A:264:ASP:N	1:A:264:ASP:OD1	2.53	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	460/503 (92%)	432 (94%)	27 (6%)	1 (0%)	44	75
1	C	460/503 (92%)	440 (96%)	19 (4%)	1 (0%)	44	75
All	All	920/1006 (92%)	872 (95%)	46 (5%)	2 (0%)	44	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	387	PRO
1	C	387	PRO



### 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	386/431 (90%)	374 (97%)	12 (3%)	35	66
1	C	391/431 (91%)	380 (97%)	11 (3%)	38	68
All	All	777/862 (90%)	754 (97%)	23 (3%)	36	66

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	96	LYS
1	A	102	LEU
1	A	104	THR
1	A	134	ASP
1	A	199	ASN
1	A	264	ASP
1	A	301	THR
1	A	321	GLN
1	A	322	THR
1	A	369	THR
1	A	442	MET
1	C	102	LEU
1	C	104	THR
1	C	216	PRO
1	C	264	ASP
1	C	273	LYS
1	C	321	GLN
1	C	327	LYS
1	C	336	VAL
1	C	364	GLN
1	C	369	THR
1	C	442	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	251	HIS
1	A	260	GLN
1	A	344	HIS
1	A	370	GLN
1	A	384	ASN
1	A	458	GLN
1	C	62	GLN
1	C	81	GLN
1	C	92	HIS
1	C	160	HIS
1	C	199	ASN
1	C	251	HIS
1	C	260	GLN
1	C	321	GLN
1	C	344	HIS
1	C	364	GLN
1	C	370	GLN
1	C	384	ASN
1	C	458	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 8 ligands modelled in this entry, 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.

No monomer is involved in short contacts.

## 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 [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	462/503 (91%)	-0.49	5 (1%) 77 63	39, 57, 81, 121	0
1	C	462/503 (91%)	-0.53	2 (0%) 89 81	41, 56, 77, 101	0
All	All	924/1006 (91%)	-0.51	7 (0%) 82 70	39, 56, 79, 121	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASN	4.0
1	C	3	ASN	3.8
1	A	386	ALA	3.6
1	A	323	THR	2.8
1	C	386	ALA	2.3
1	A	351	ASP	2.2
1	A	337	ASP	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](#)

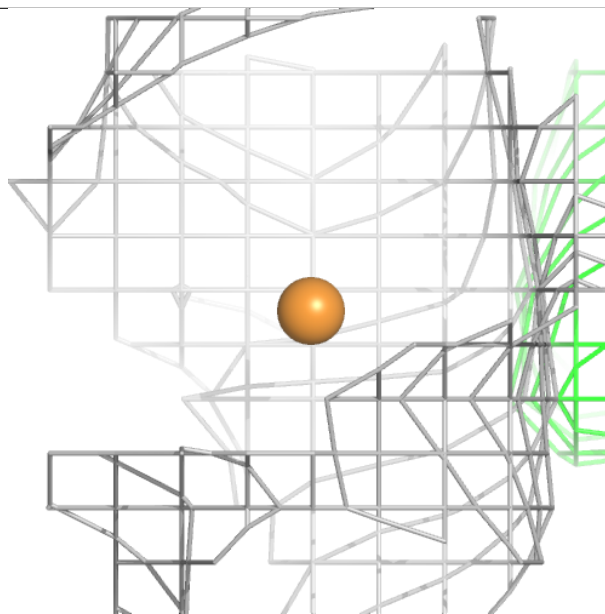
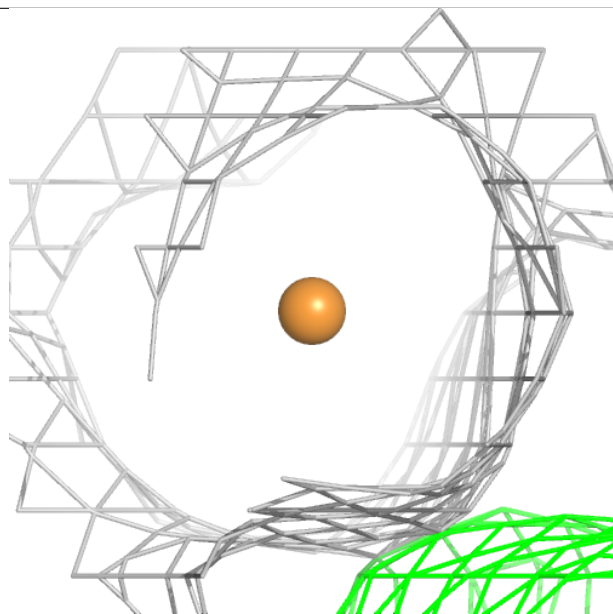
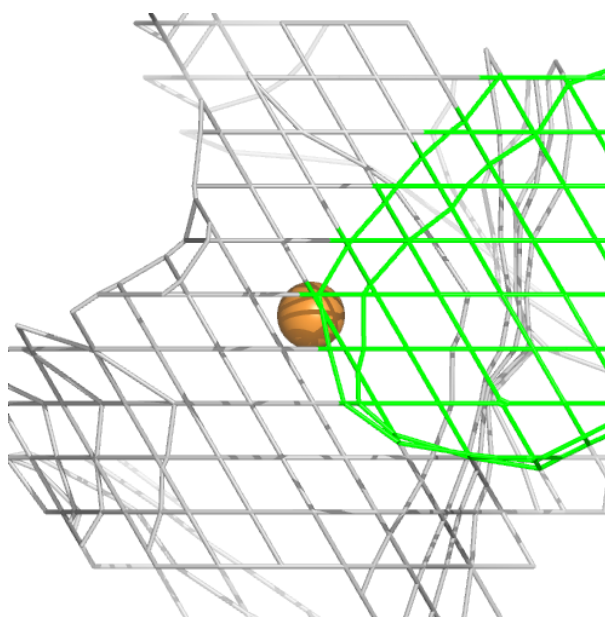
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CU	A	503	1/1	0.99	0.04	74,74,74,74	0
2	CU	A	504	1/1	0.99	0.05	88,88,88,88	0
2	CU	C	503	1/1	0.99	0.04	78,78,78,78	0
2	CU	C	504	1/1	0.99	0.06	91,91,91,91	0
2	CU	C	501	1/1	1.00	0.03	59,59,59,59	0
2	CU	C	502	1/1	1.00	0.02	60,60,60,60	0
2	CU	A	501	1/1	1.00	0.02	61,61,61,61	0
2	CU	A	502	1/1	1.00	0.02	60,60,60,60	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.

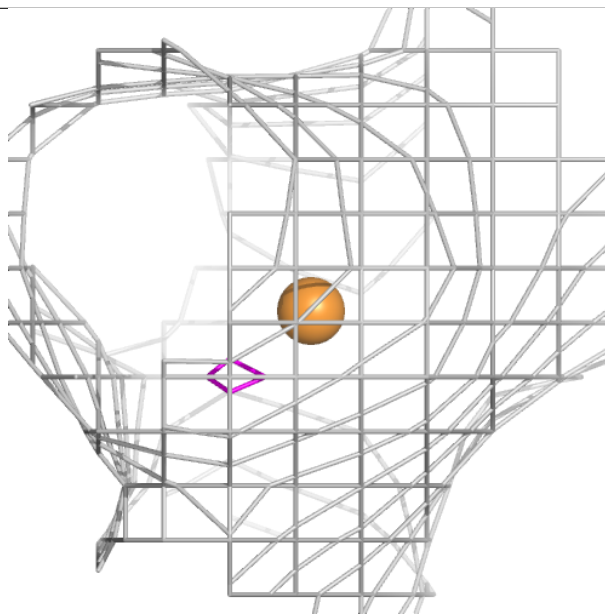
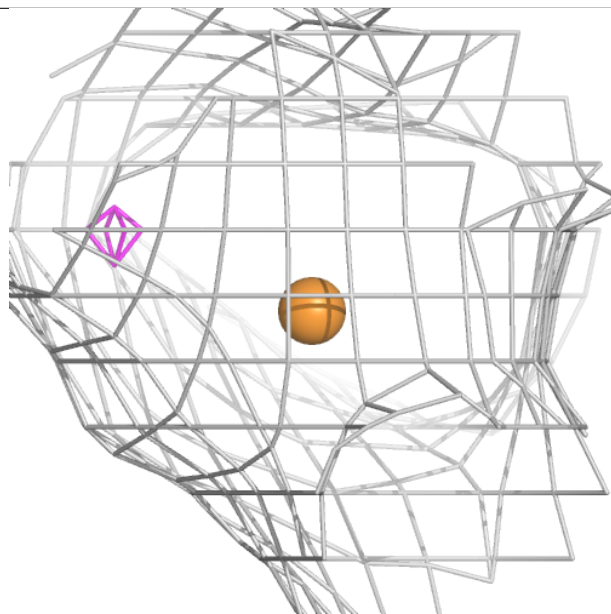
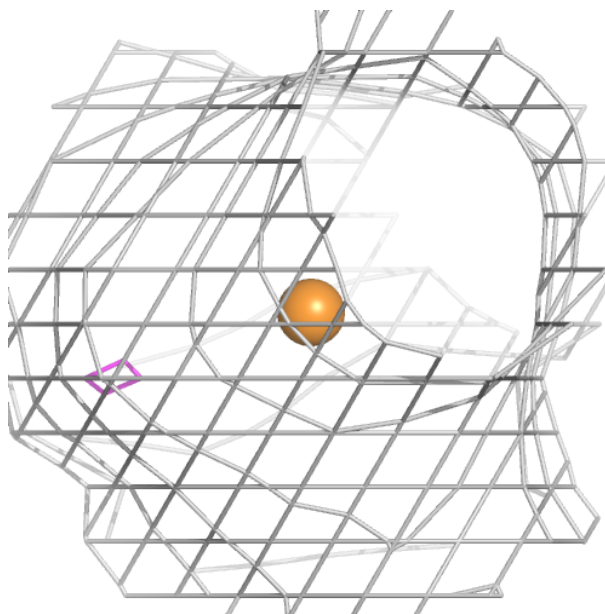
**Electron density around CU A 503:**

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



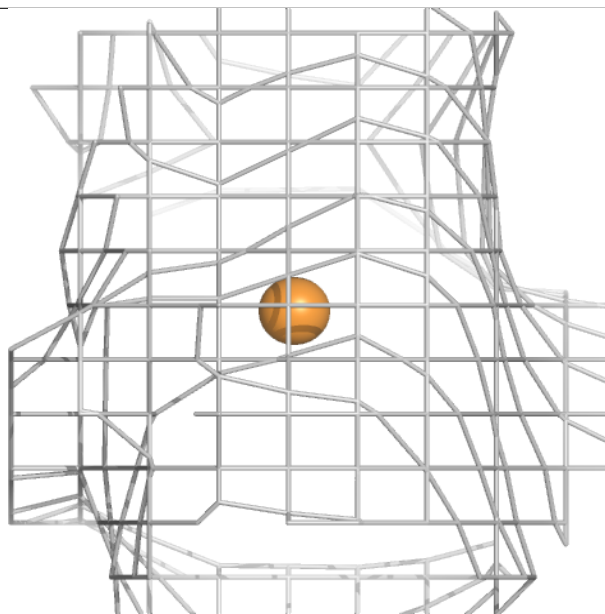
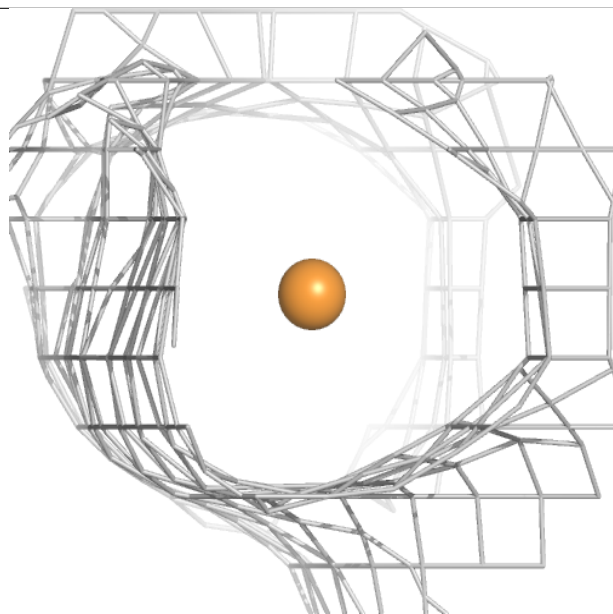
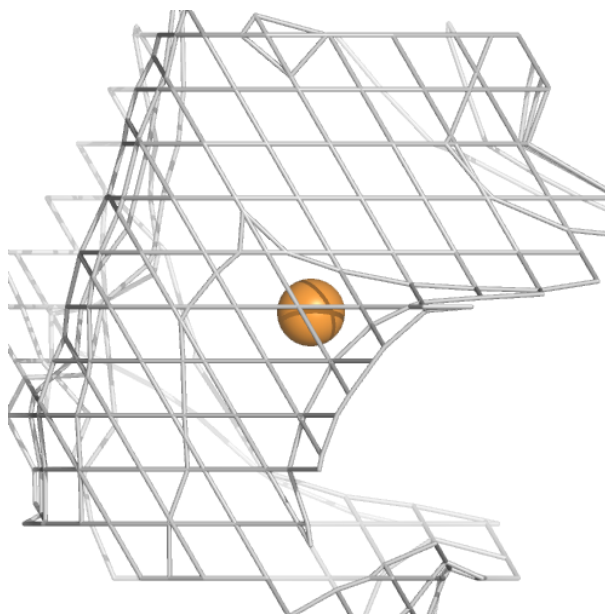
**Electron density around CU A 504:**

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



**Electron density around CU C 503:**

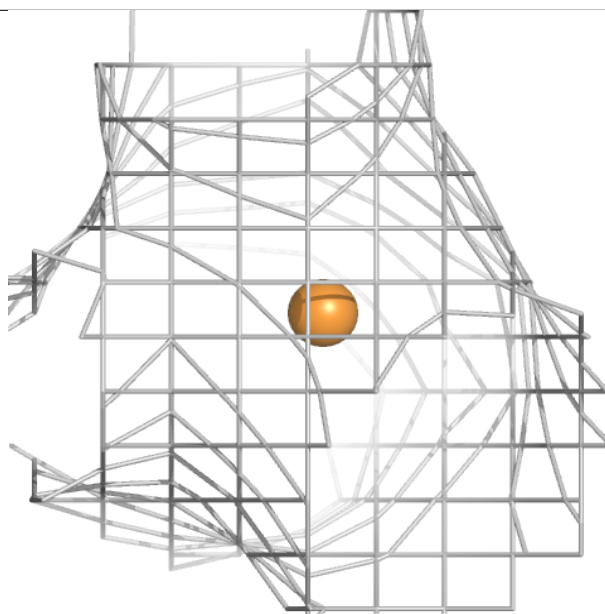
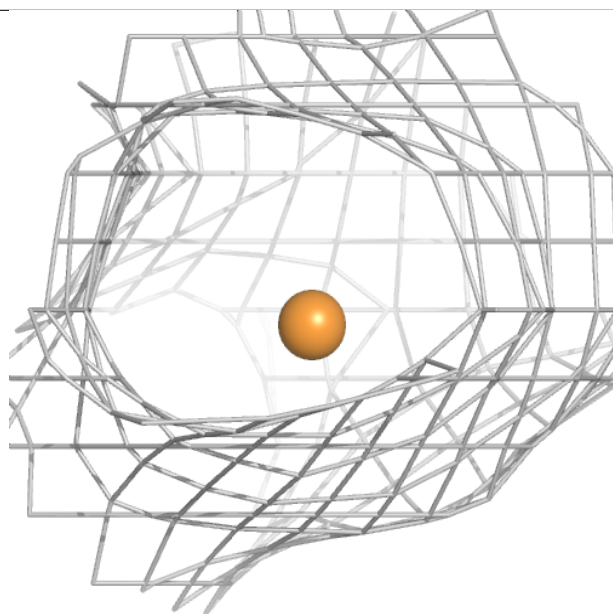
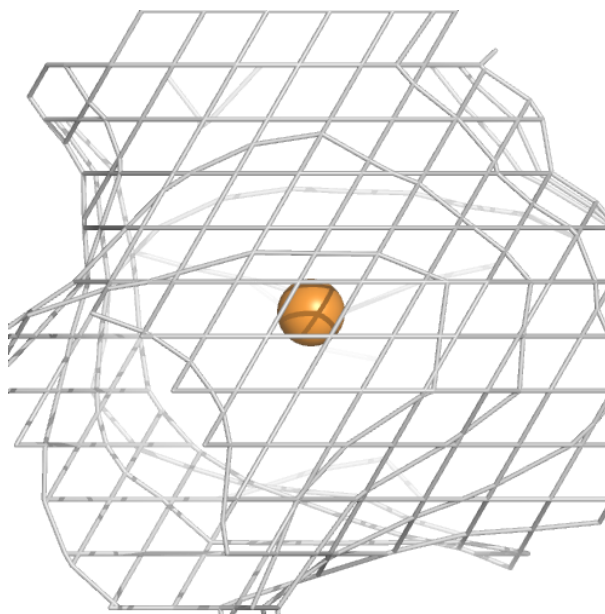
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





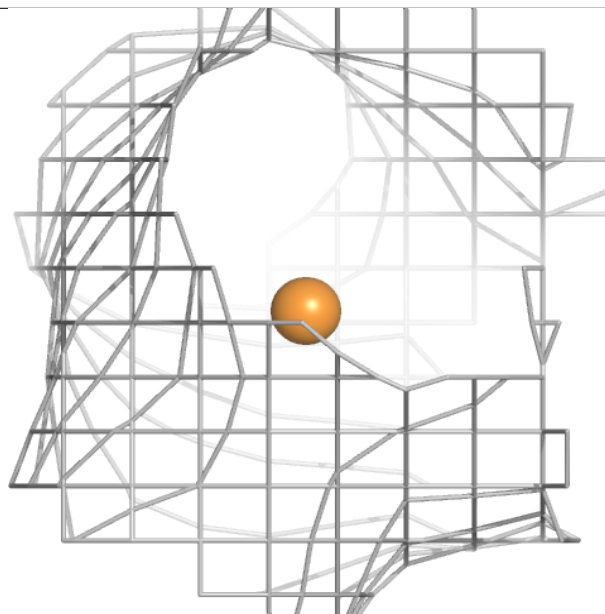
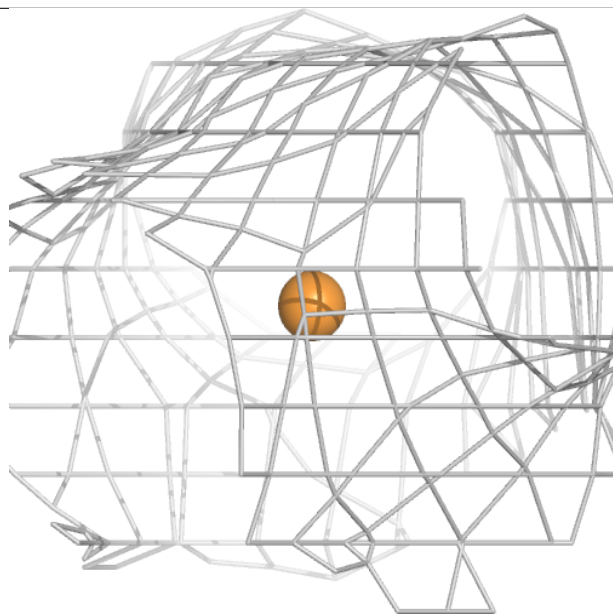
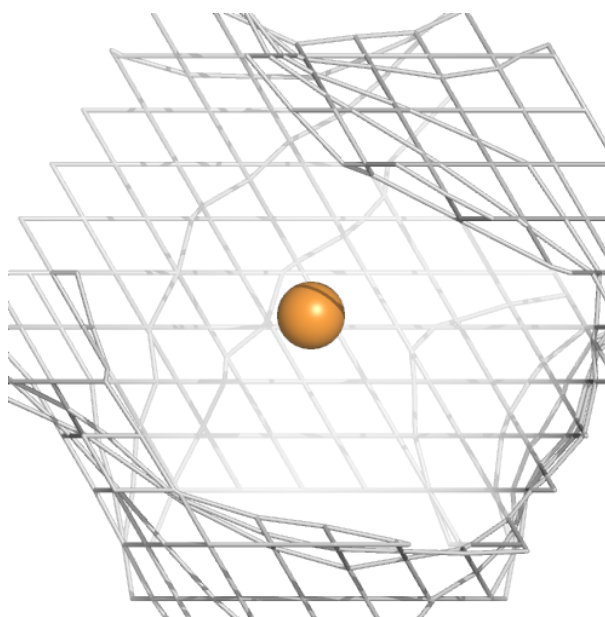
**Electron density around CU C 504:**

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



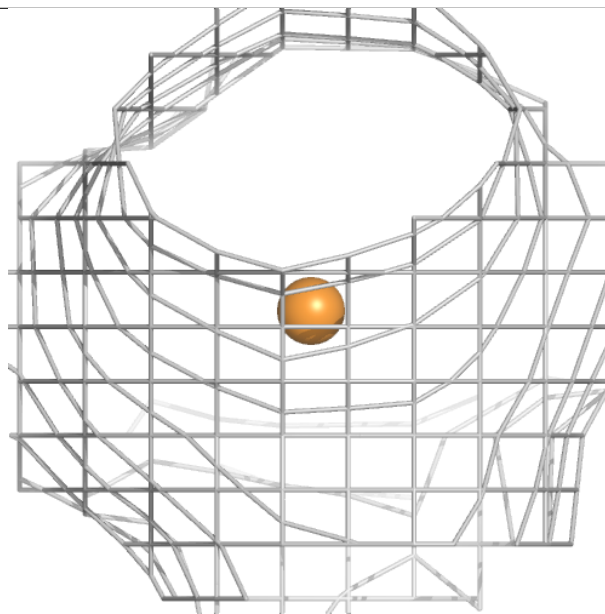
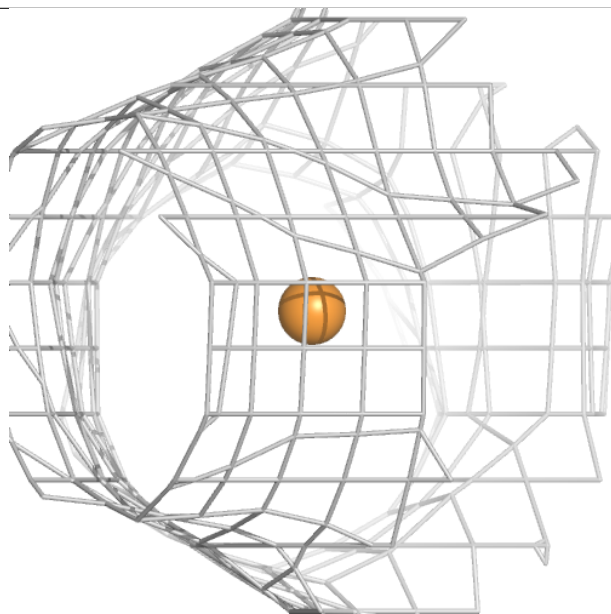
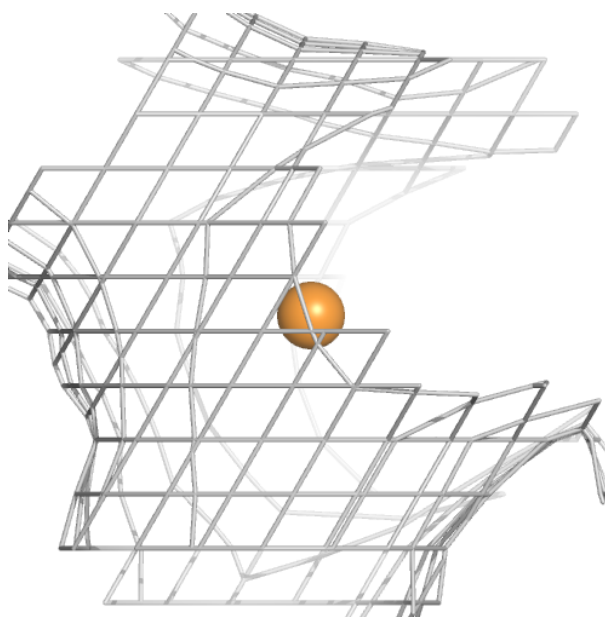
**Electron density around CU C 501:**

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



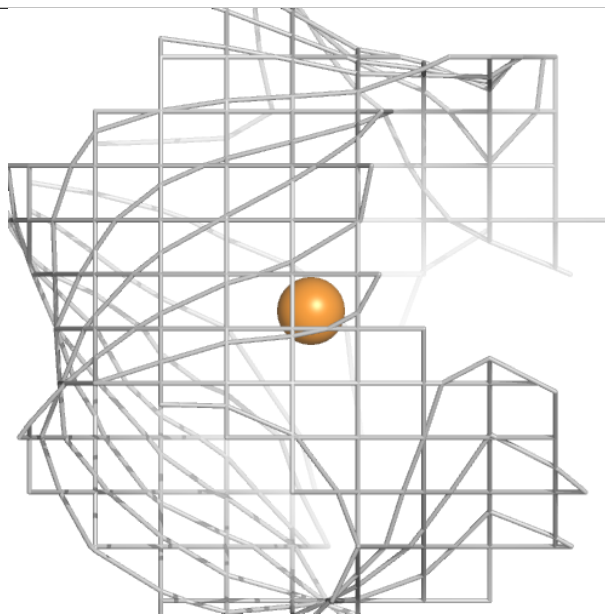
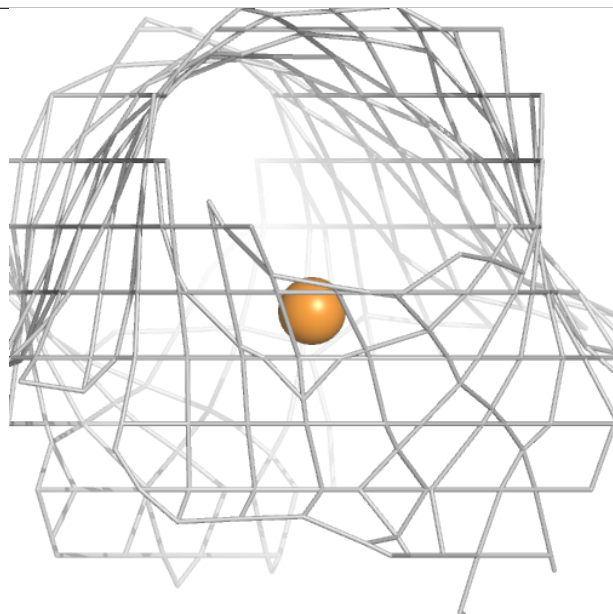
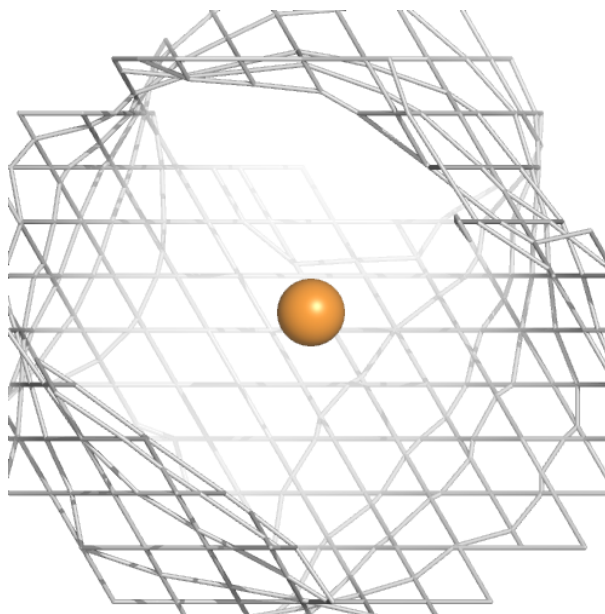
**Electron density around CU C 502:**

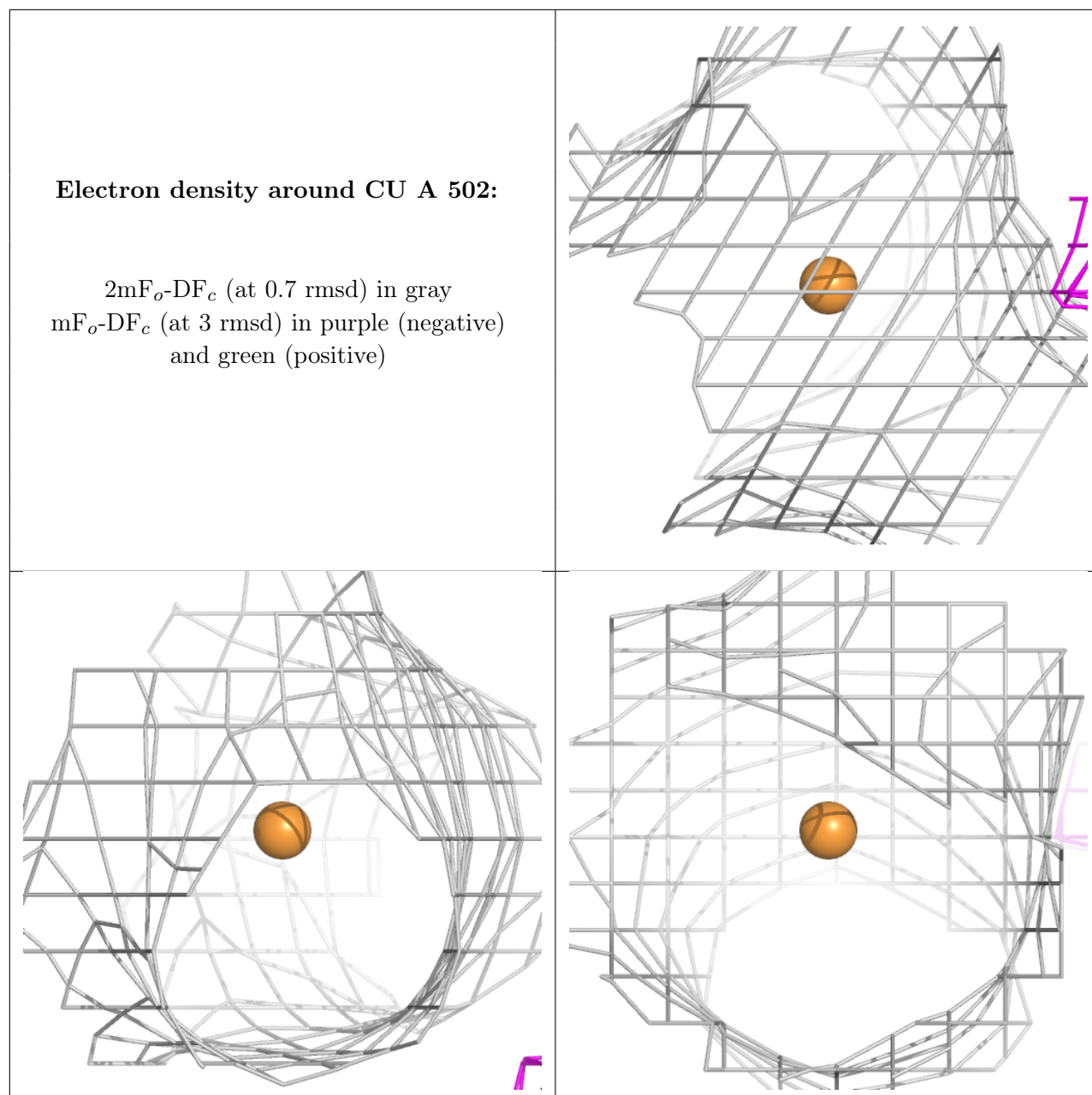
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CU A 501:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.