



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 04:59 am GMT

PDB ID : 6YZD  
Title : Crystal structure of the M295A variant of Ssl1  
Authors : Mielenbrink, S.; Olbrich, A.; Urlacher, V.; Span, I.  
Deposited on : 2020-05-06  
Resolution : 1.41 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)

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<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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

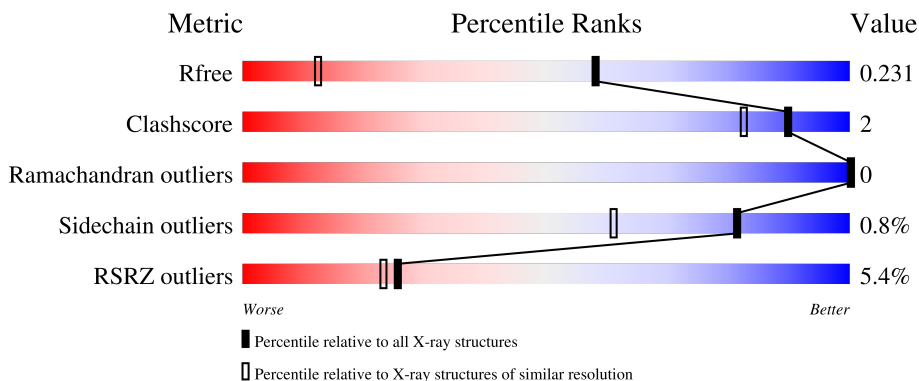
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.41 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	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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	AAA	325	 4% 79% 17%
1	BBB	325	 6% 78% 17%
1	CCC	325	 4% 78% 17%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12574 atoms, of which 6001 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 oxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	270	4087	1307	1994	383	394	9	106	0	0
1	BBB	270	4107	1312	2006	386	394	9	106	1	0
1	CCC	271	4101	1312	2001	384	395	9	105	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	initiating methionine	UNP B5HSR1
AAA	2	HIS	-	expression tag	UNP B5HSR1
AAA	3	HIS	-	expression tag	UNP B5HSR1
AAA	4	HIS	-	expression tag	UNP B5HSR1
AAA	5	HIS	-	expression tag	UNP B5HSR1
AAA	6	HIS	-	expression tag	UNP B5HSR1
AAA	7	HIS	-	expression tag	UNP B5HSR1
AAA	295	ALA	MET	engineered mutation	UNP B5HSR1
BBB	1	MET	-	initiating methionine	UNP B5HSR1
BBB	2	HIS	-	expression tag	UNP B5HSR1
BBB	3	HIS	-	expression tag	UNP B5HSR1
BBB	4	HIS	-	expression tag	UNP B5HSR1
BBB	5	HIS	-	expression tag	UNP B5HSR1
BBB	6	HIS	-	expression tag	UNP B5HSR1
BBB	7	HIS	-	expression tag	UNP B5HSR1
BBB	295	ALA	MET	engineered mutation	UNP B5HSR1
CCC	1	MET	-	initiating methionine	UNP B5HSR1
CCC	2	HIS	-	expression tag	UNP B5HSR1
CCC	3	HIS	-	expression tag	UNP B5HSR1
CCC	4	HIS	-	expression tag	UNP B5HSR1
CCC	5	HIS	-	expression tag	UNP B5HSR1
CCC	6	HIS	-	expression tag	UNP B5HSR1
CCC	7	HIS	-	expression tag	UNP B5HSR1

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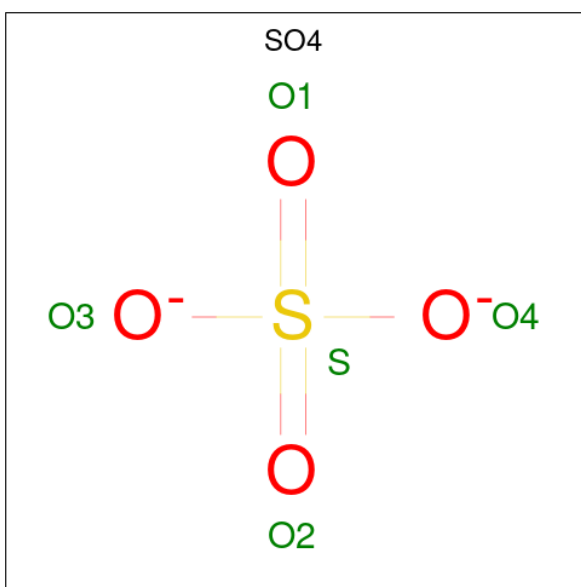
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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	295	ALA	MET	engineered mutation	UNP B5HSR1

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	5	Total Cu 5 5	0	0
2	BBB	5	Total Cu 5 5	0	0
2	CCC	4	Total Cu 4 4	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total O S 5 4 1	0	0
3	CCC	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	103	Total O 103 103	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	BBB	75	Total	O	0	0
			75	75		
4	CCC	77	Total	O	0	0
			77	77		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.44Å 104.10Å 163.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.36 – 1.41 30.36 – 1.41	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.36-1.41) 99.9 (30.36-1.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 1.41Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.200 , 0.225 0.207 , 0.231	Depositor DCC
$R_{free}$ test set	8343 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.1	Xtrriage
Anisotropy	0.237	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 35.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12574	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	AAA	0.73	0/2151	0.91	2/2919 (0.1%)
1	BBB	0.74	0/2162	0.88	1/2933 (0.0%)
1	CCC	0.74	0/2159	0.90	1/2931 (0.0%)
All	All	0.74	0/6472	0.90	4/8783 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	177	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	AAA	200	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	AAA	178	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	CCC	241	ARG	NE-CZ-NH2	-5.23	117.68	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	AAA	2093	1994	1974	6	0
1	BBB	2101	2006	1987	7	0
1	CCC	2100	2001	1981	10	0
2	AAA	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	5	0	0	0	0
2	CCC	4	0	0	0	0
3	AAA	5	0	0	0	0
3	CCC	5	0	0	0	0
4	AAA	103	0	0	0	0
4	BBB	75	0	0	0	0
4	CCC	77	0	0	0	0
All	All	6573	6001	5942	22	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 2.

All (22) 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:CCC:59:GLN:HE22	1:CCC:199:ASN:HB3	1.44	0.82
1:AAA:59:GLN:HE22	1:AAA:199:ASN:HB3	1.55	0.71
1:CCC:44:GLU:OE1	1:CCC:46:ARG:NH2	2.30	0.64
1:AAA:53:GLU:HG2	1:AAA:91:THR:OG1	2.02	0.60
1:BBB:53:GLU:OE2	1:BBB:66:LYS:HA	2.04	0.58
1:AAA:59:GLN:NE2	1:AAA:199:ASN:HD22	2.04	0.55
1:CCC:59:GLN:NE2	1:CCC:199:ASN:HD22	2.08	0.52
1:CCC:53:GLU:OE2	1:CCC:66:LYS:HA	2.15	0.47
1:BBB:75:LEU:HA	1:BBB:173:PRO:HG2	1.97	0.46
1:CCC:102:GLY:HA3	1:CCC:150:TRP:CD2	2.51	0.46
1:CCC:53:GLU:OE2	1:CCC:67:GLY:N	2.39	0.45
1:AAA:102:GLY:HA3	1:AAA:150:TRP:CD2	2.51	0.45
1:CCC:229:THR:O	1:CCC:285:CYS:HA	2.17	0.45
1:AAA:238:ALA:O	1:AAA:243:GLY:HA2	2.17	0.45
1:BBB:47[B]:ARG:HG3	1:BBB:85:HIS:HB2	1.99	0.44
1:BBB:231:HIS:CE1	1:CCC:101:HIS:CE1	3.05	0.44
1:BBB:102:GLY:HA3	1:BBB:150:TRP:CD2	2.52	0.44
1:BBB:238:ALA:O	1:BBB:243:GLY:HA2	2.18	0.44
1:CCC:46:ARG:NH1	1:CCC:82:ASP:OD2	2.51	0.44
1:CCC:55:LEU:HD21	1:CCC:69:ALA:HB3	2.03	0.41
1:AAA:230:PHE:O	1:AAA:257:ASN:HA	2.21	0.41
1:BBB:188:HIS:HB3	1:BBB:208:PHE:CE1	2.56	0.41

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	AAA	268/325 (82%)	264 (98%)	4 (2%)	0	100	100
1	BBB	269/325 (83%)	263 (98%)	6 (2%)	0	100	100
1	CCC	269/325 (83%)	264 (98%)	5 (2%)	0	100	100
All	All	806/975 (83%)	791 (98%)	15 (2%)	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	AAA	216/255 (85%)	214 (99%)	2 (1%)	78	56
1	BBB	217/255 (85%)	216 (100%)	1 (0%)	88	73
1	CCC	217/255 (85%)	215 (99%)	2 (1%)	78	56
All	All	650/765 (85%)	645 (99%)	5 (1%)	81	61

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	220	MET
1	AAA	236	ARG
1	BBB	220	MET
1	CCC	220	MET
1	CCC	236	ARG

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

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 14 are monoatomic - leaving 2 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	SO4	CCC	405	-	4,4,4	0.32	0	6,6,6	0.21	0
3	SO4	AAA	406	-	4,4,4	0.19	0	6,6,6	0.30	0

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

### 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	AAA	270/325 (83%)	-0.14	12 (4%) 34 34	13, 19, 32, 65	14 (5%)
1	BBB	270/325 (83%)	0.18	18 (6%) 17 15	14, 23, 46, 77	14 (5%)
1	CCC	271/325 (83%)	0.16	14 (5%) 27 25	14, 22, 43, 57	14 (5%)
All	All	811/975 (83%)	0.07	44 (5%) 25 23	13, 21, 43, 77	42 (5%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	43	GLY	6.0
1	BBB	204	SER	5.8
1	AAA	312	GLU	5.5
1	BBB	203	HIS	5.2
1	CCC	43	GLY	5.0
1	CCC	58	GLY	4.7
1	BBB	307	THR	4.6
1	CCC	203	HIS	4.6
1	CCC	45	VAL	4.6
1	BBB	312	GLU	4.5
1	BBB	304	THR	4.5
1	AAA	43	GLY	4.5
1	CCC	56	ALA	4.4
1	CCC	57	ASP	4.2
1	CCC	204	SER	3.8
1	AAA	311	TYR	3.7
1	CCC	46	ARG	3.7
1	BBB	305	ASP	3.6
1	CCC	138	SER	3.5
1	BBB	309	PRO	3.4
1	BBB	308	ILE	3.3
1	BBB	202	ALA	3.1
1	AAA	205	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	AAA	203	HIS	2.8
1	CCC	313	PRO	2.7
1	AAA	100	VAL	2.7
1	AAA	204	SER	2.6
1	BBB	116	LYS	2.6
1	CCC	68	ARG	2.5
1	BBB	311	TYR	2.5
1	CCC	44	GLU	2.5
1	CCC	47	ARG	2.4
1	AAA	182	VAL	2.4
1	BBB	45	VAL	2.4
1	BBB	201	PRO	2.4
1	BBB	205	GLY	2.3
1	BBB	44	GLU	2.3
1	BBB	306	GLY	2.2
1	AAA	310	GLY	2.2
1	AAA	47	ARG	2.2
1	CCC	201	PRO	2.2
1	AAA	68	ARG	2.1
1	AAA	304	THR	2.1
1	BBB	303	LYS	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.

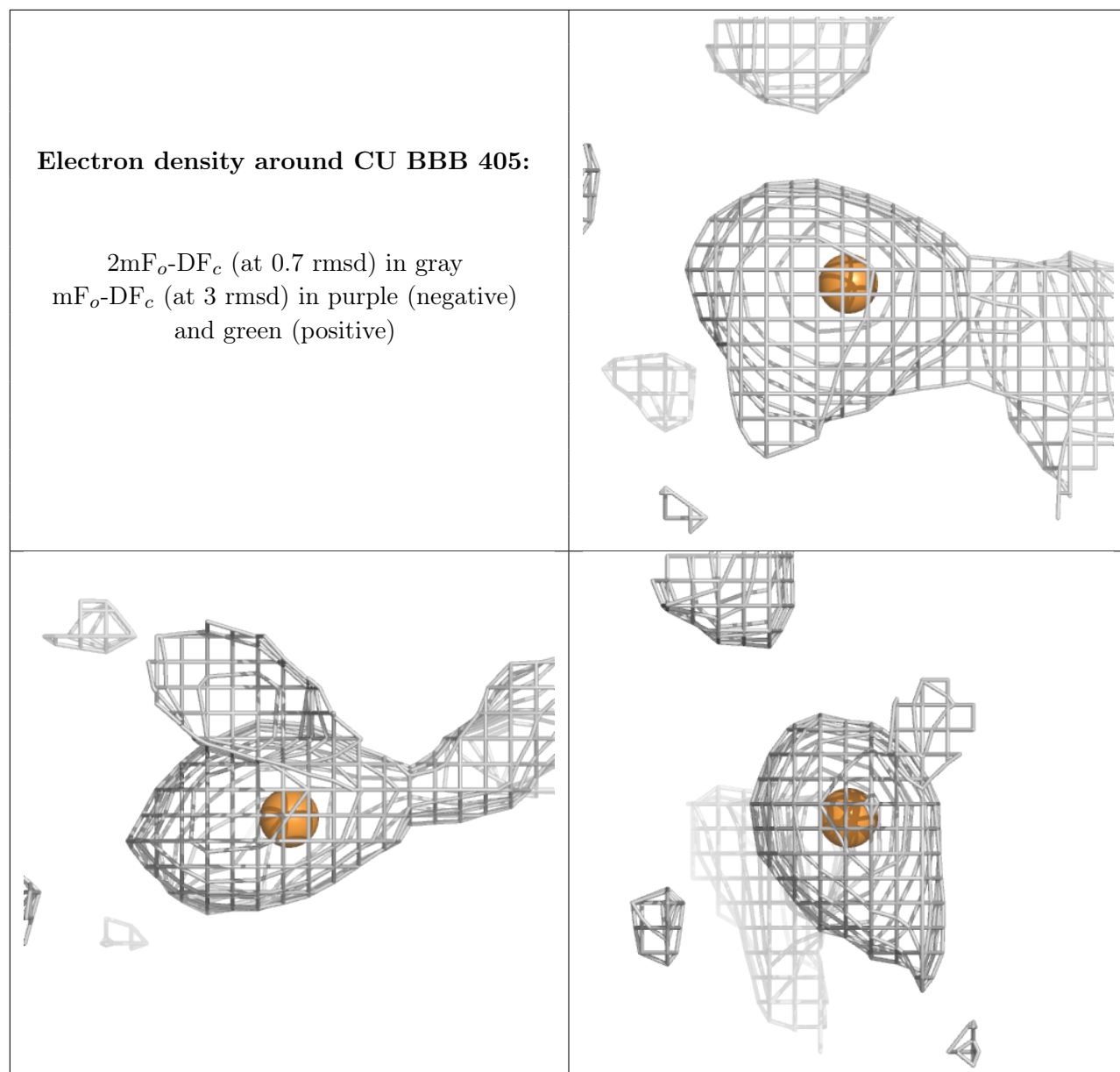
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CU	BBB	405	1/1	0.90	0.45	92,92,92,92	0
2	CU	AAA	405	1/1	0.93	0.23	60,60,60,60	0

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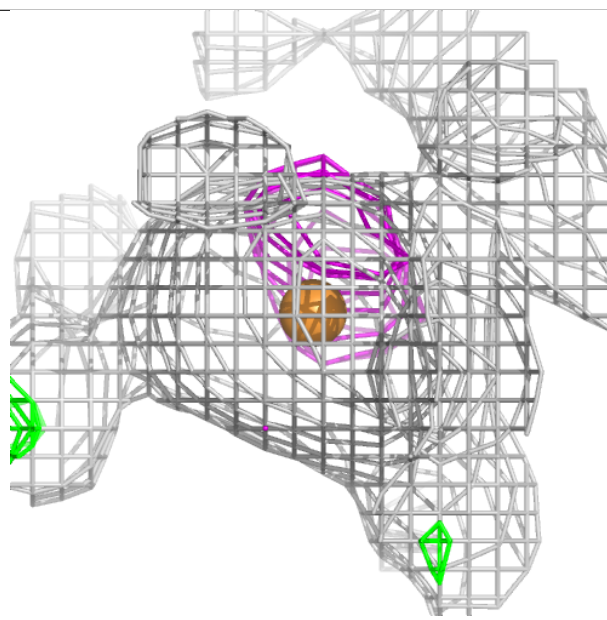
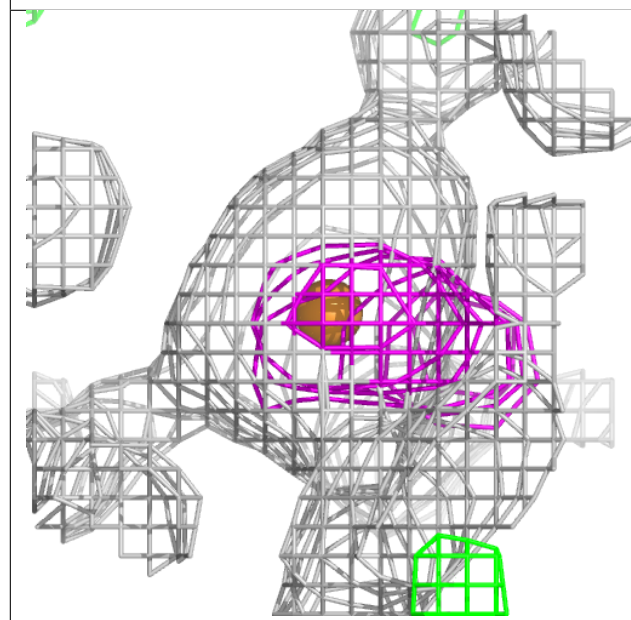
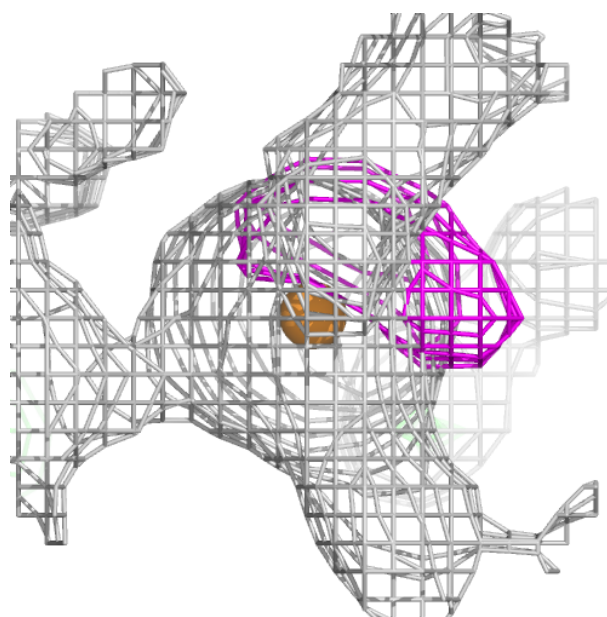
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	AAA	406	5/5	0.95	0.18	28,30,37,38	0
2	CU	BBB	402	1/1	0.96	0.06	22,22,22,22	0
2	CU	AAA	404	1/1	0.97	0.07	22,22,22,22	0
3	SO4	CCC	405	5/5	0.97	0.19	41,44,46,57	0
2	CU	AAA	403	1/1	0.98	0.11	30,30,30,30	0
2	CU	CCC	402	1/1	0.98	0.04	24,24,24,24	0
2	CU	AAA	402	1/1	0.98	0.05	22,22,22,22	0
2	CU	BBB	403	1/1	0.98	0.05	27,27,27,27	0
2	CU	BBB	401	1/1	0.99	0.03	23,23,23,23	0
2	CU	CCC	403	1/1	0.99	0.05	21,21,21,21	0
2	CU	CCC	404	1/1	0.99	0.09	28,28,28,28	0
2	CU	BBB	404	1/1	0.99	0.10	34,34,34,34	0
2	CU	AAA	401	1/1	0.99	0.03	19,19,19,19	0
2	CU	CCC	401	1/1	1.00	0.04	20,20,20,20	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.



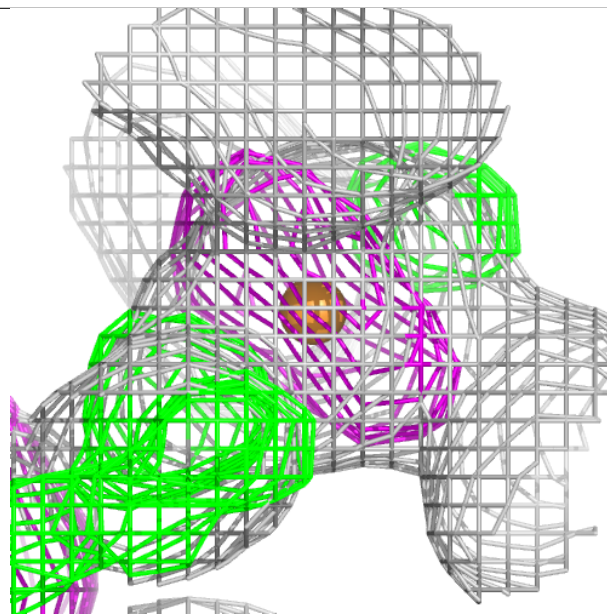
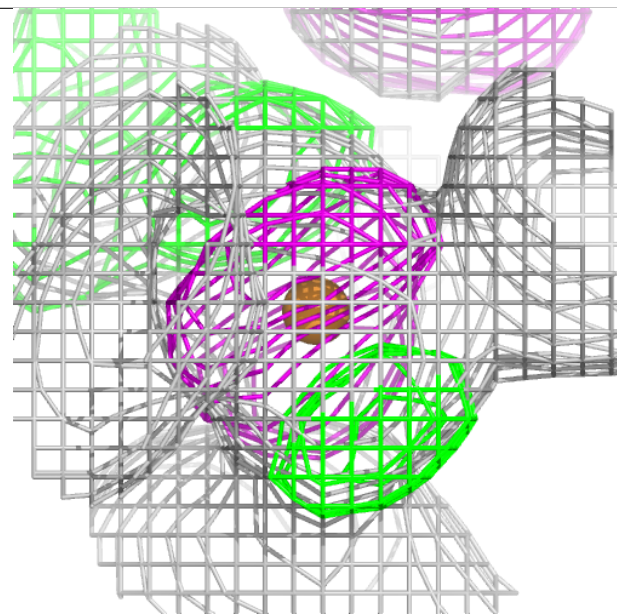
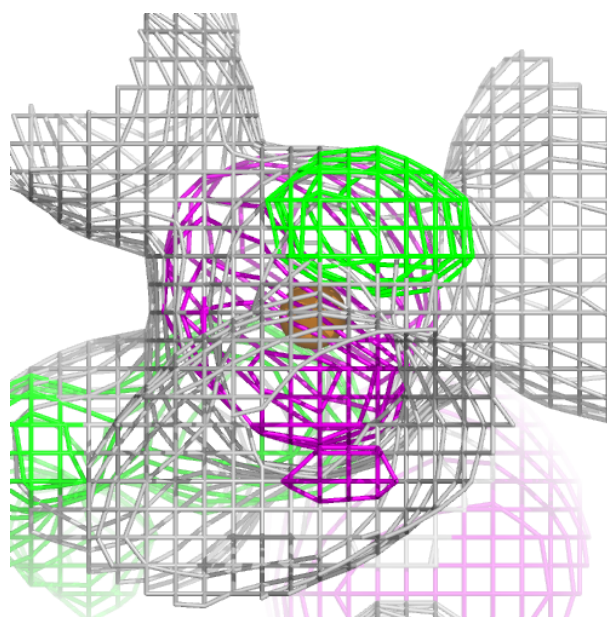
**Electron density around CU AAA 405:**

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



**Electron density around CU BBB 402:**

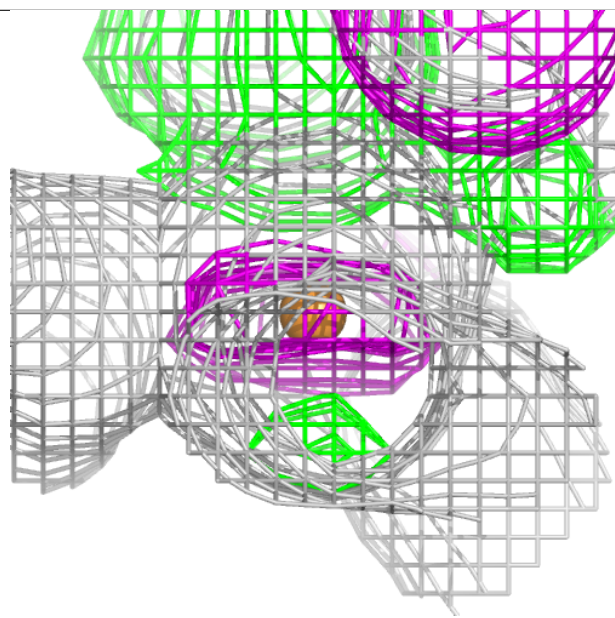
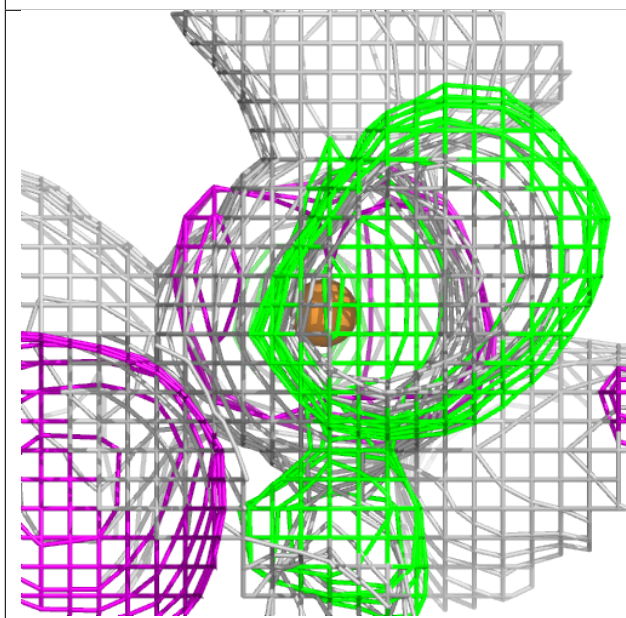
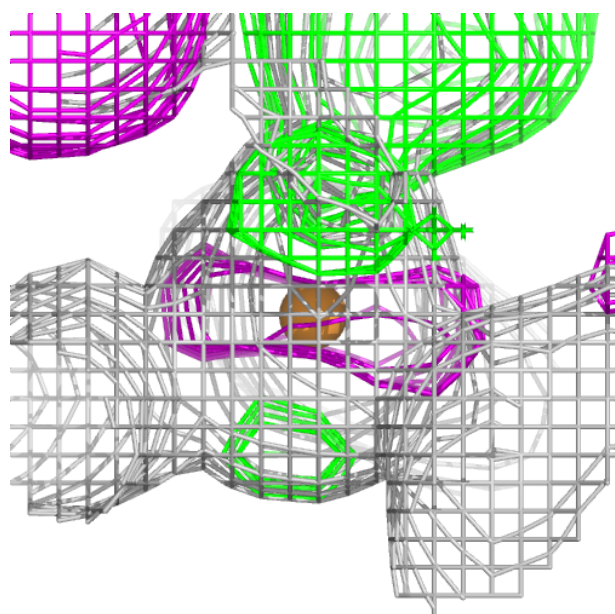
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





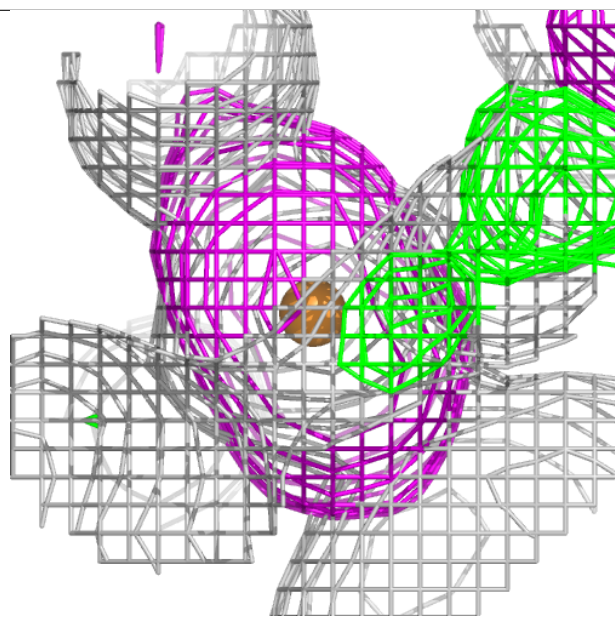
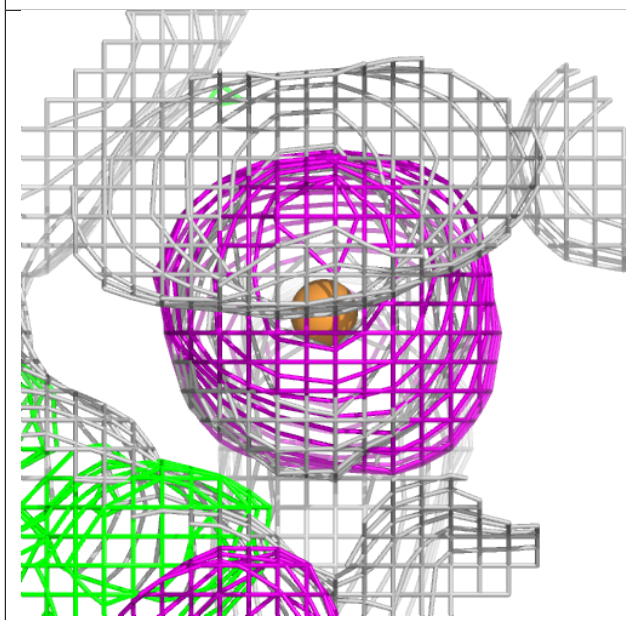
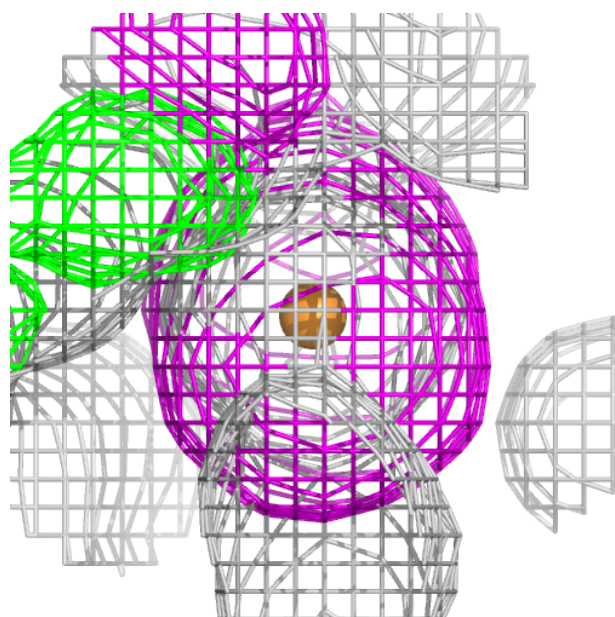
**Electron density around CU AAA 404:**

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



**Electron density around CU AAA 403:**

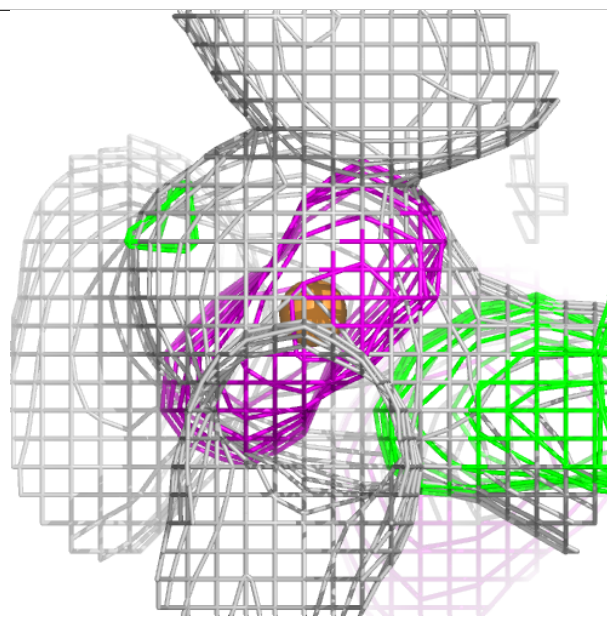
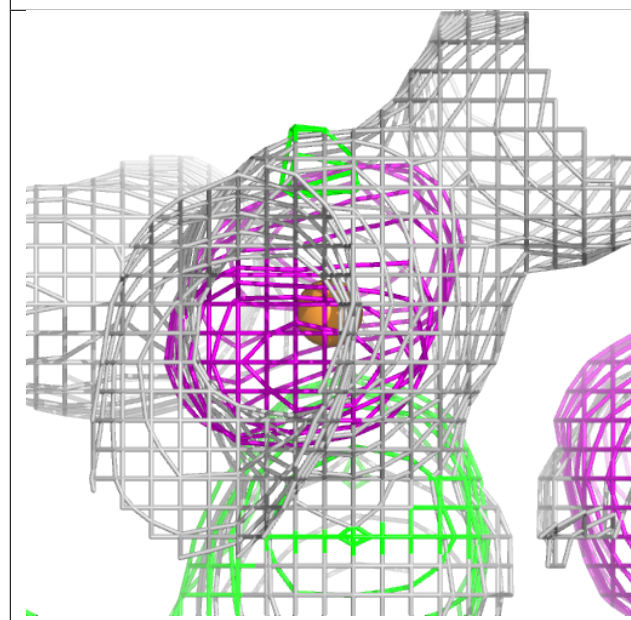
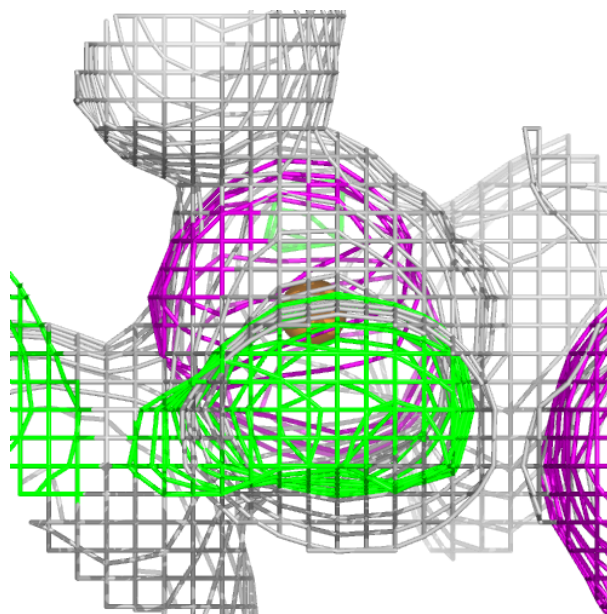
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





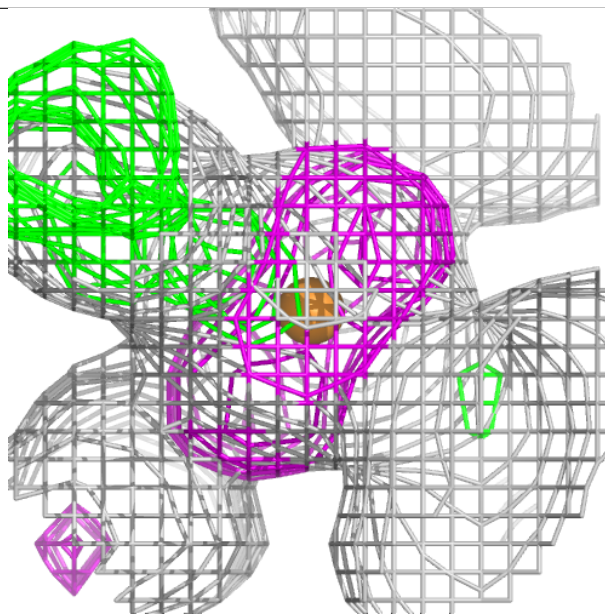
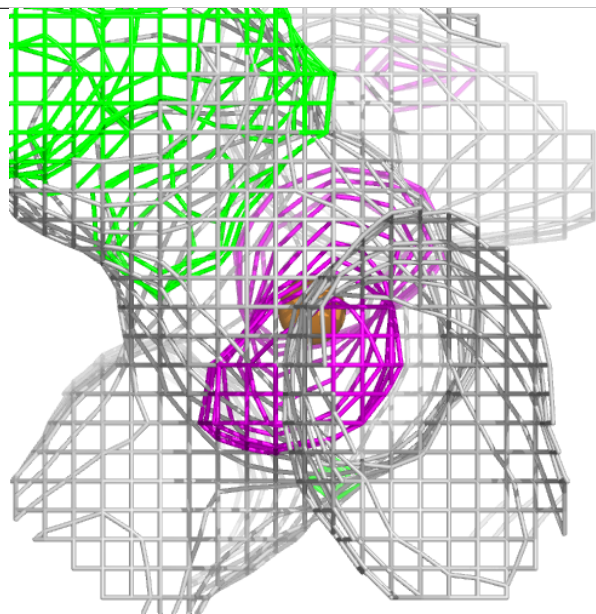
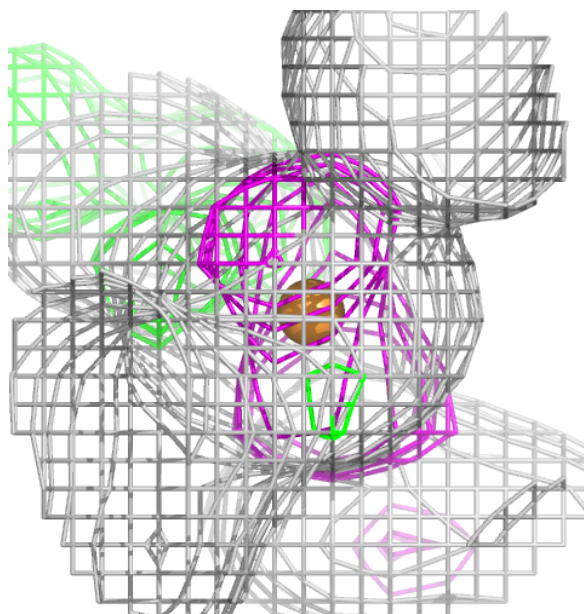
**Electron density around CU CCC 402:**

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



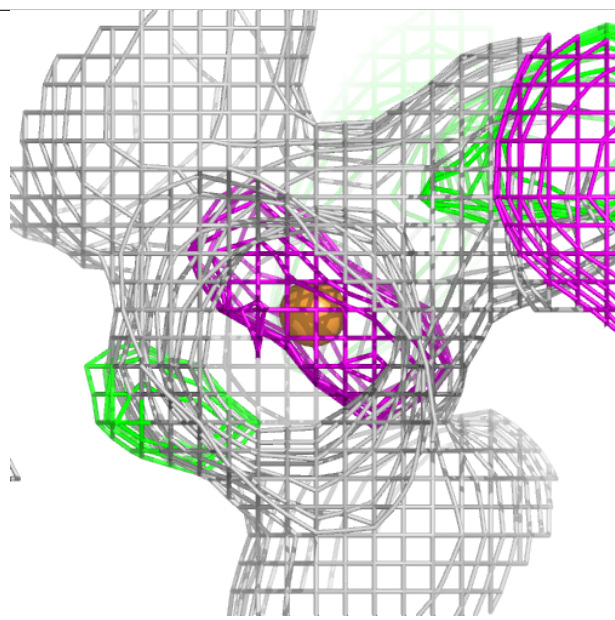
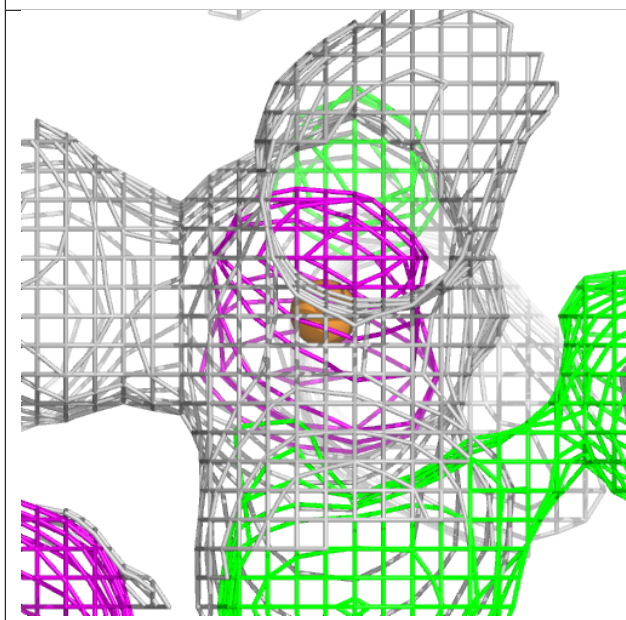
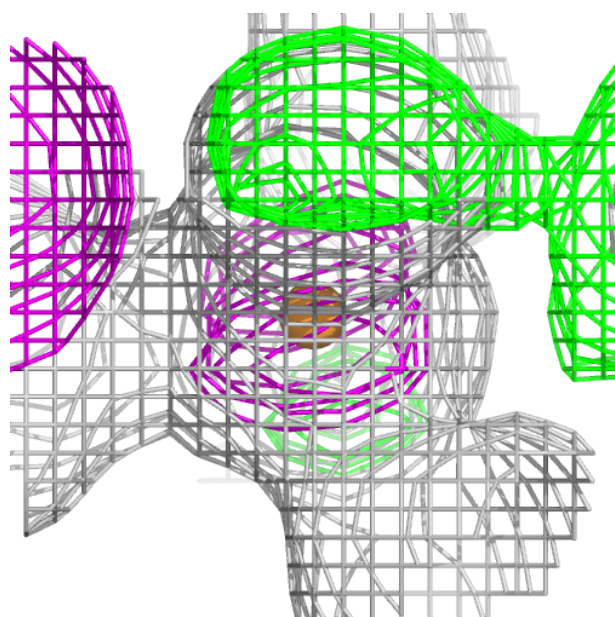
**Electron density around CU AAA 402:**

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



**Electron density around CU BBB 403:**

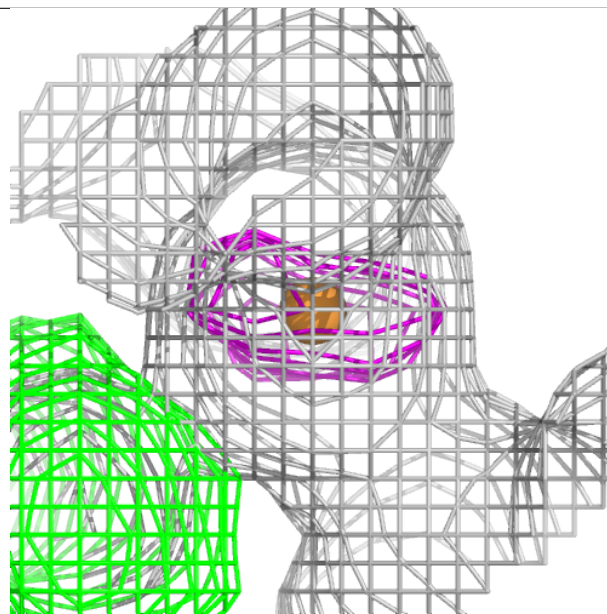
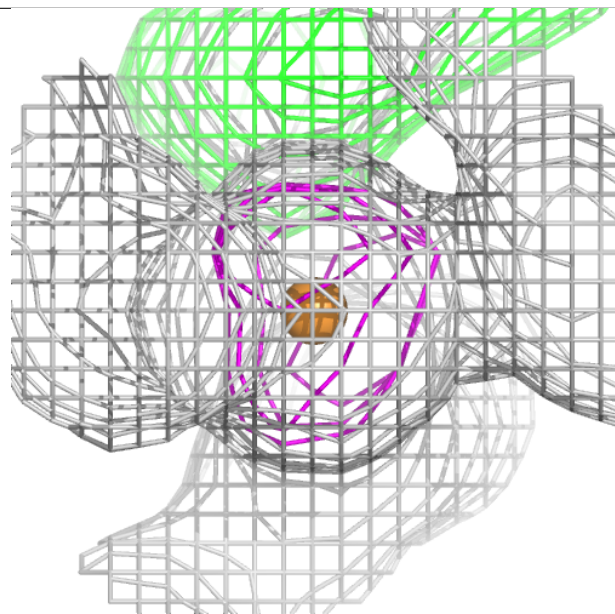
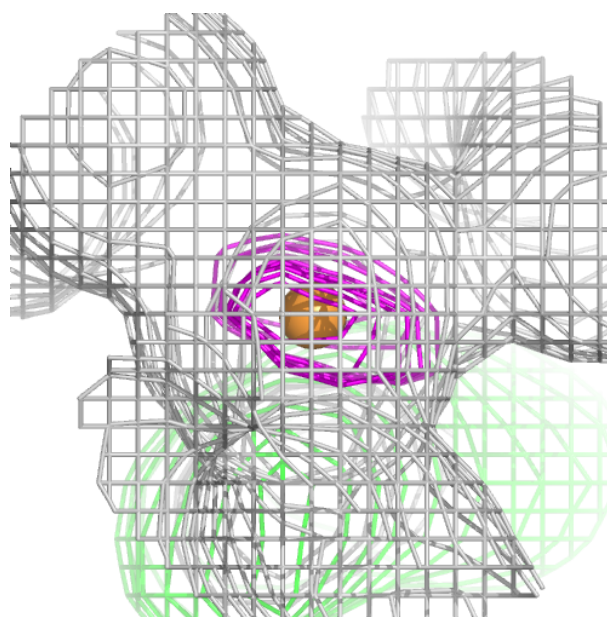
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





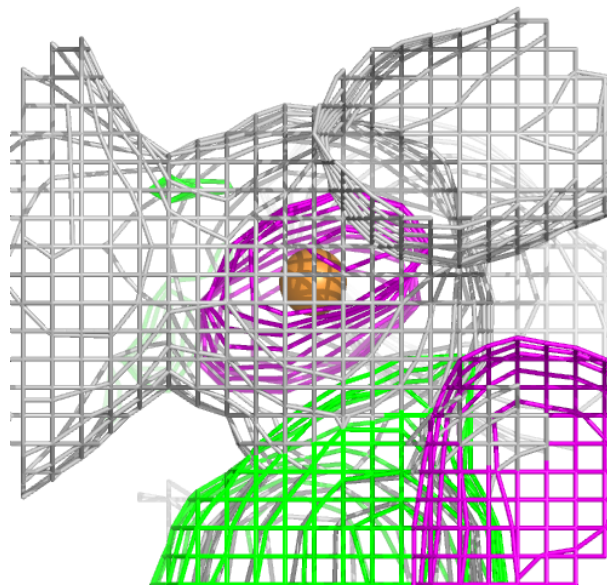
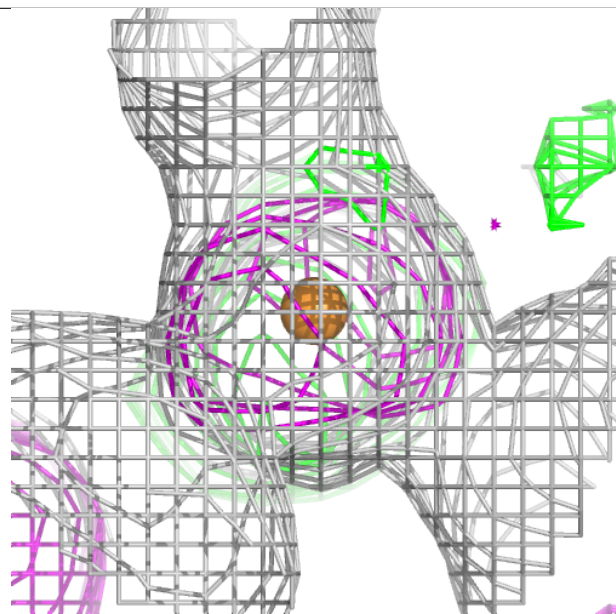
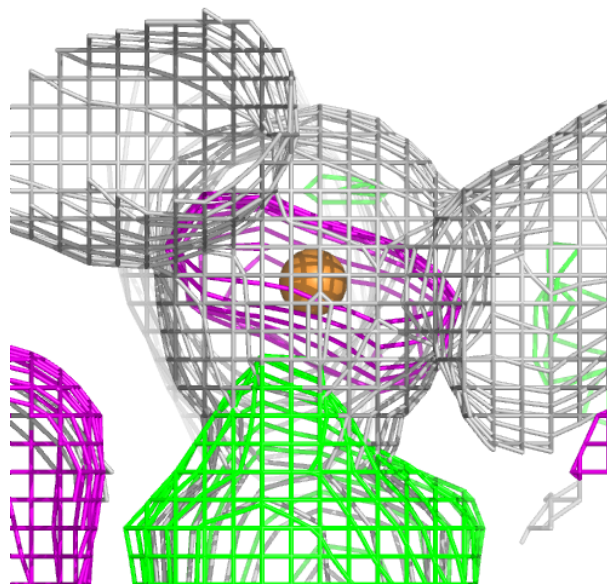
**Electron density around CU BBB 401:**

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



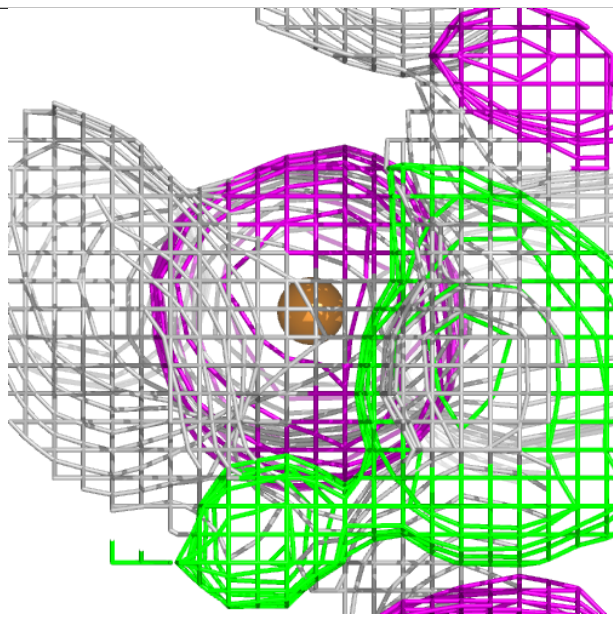
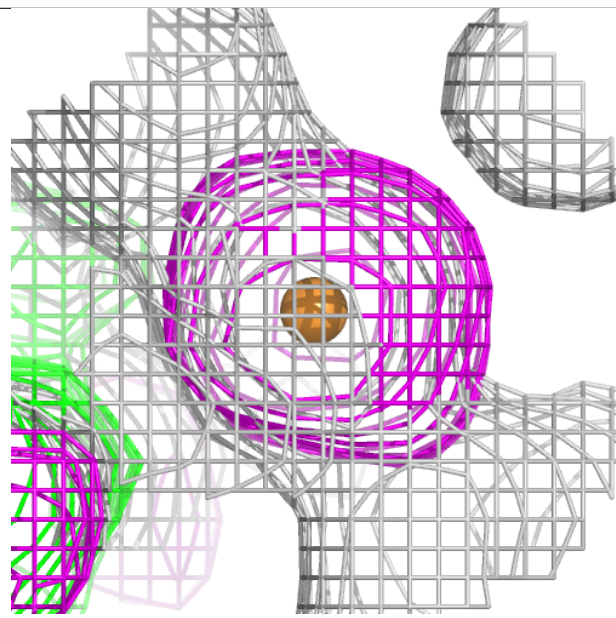
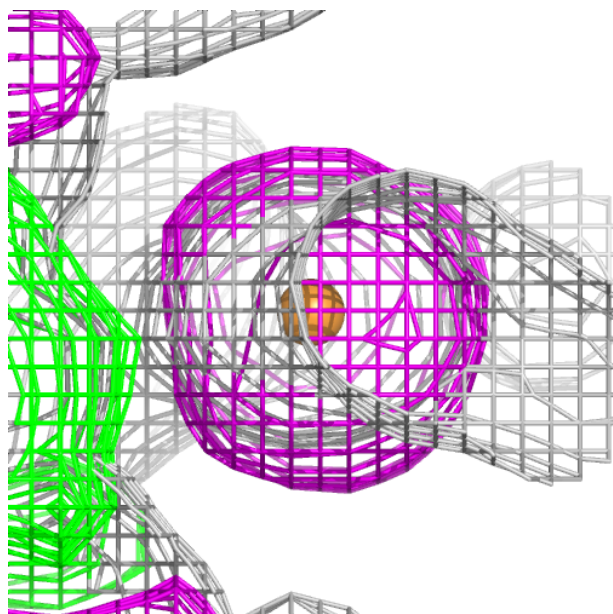
**Electron density around CU CCC 403:**

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



**Electron density around CU CCC 404:**

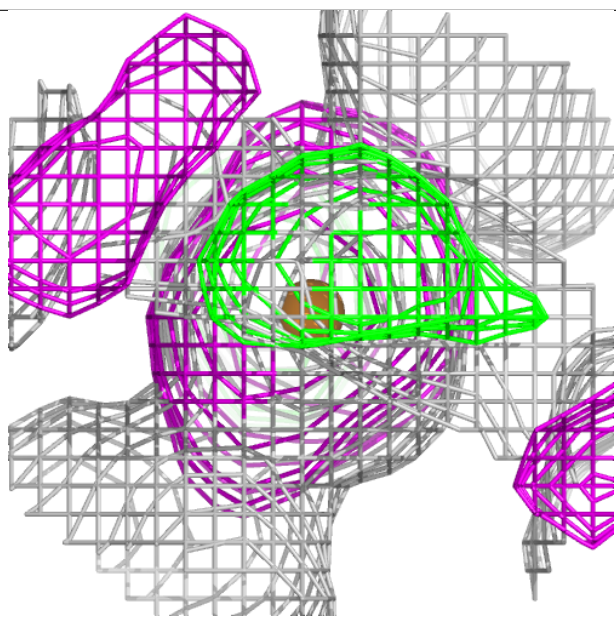
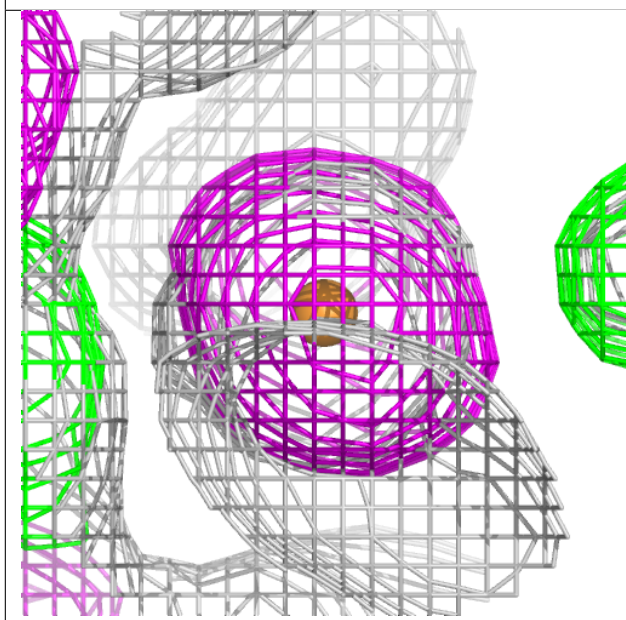
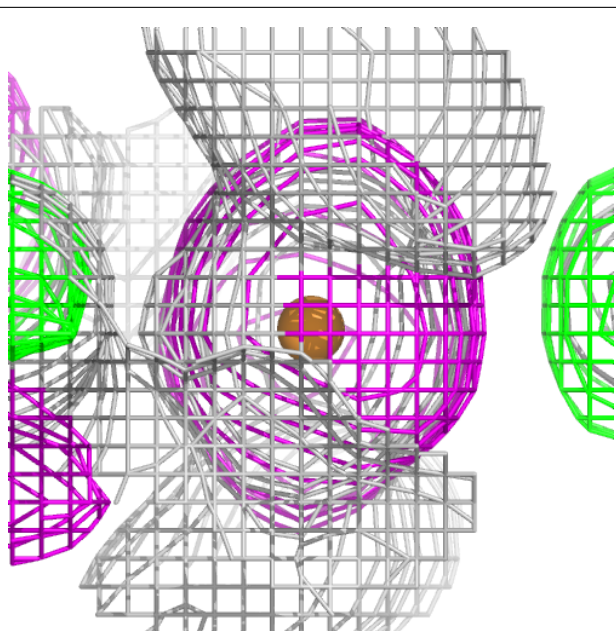
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





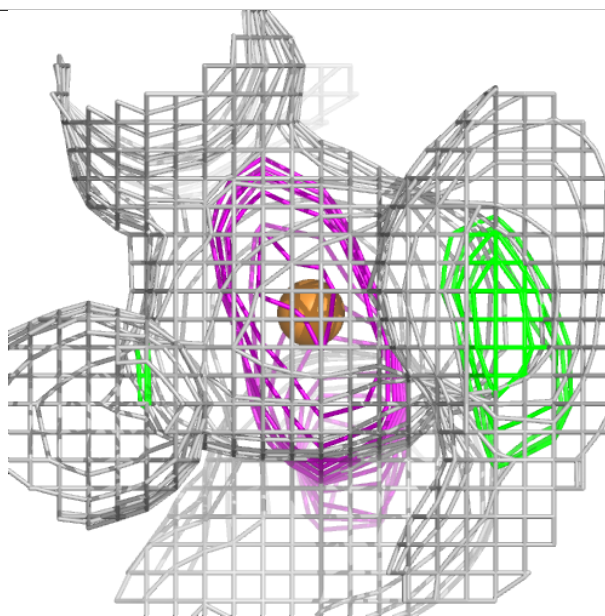
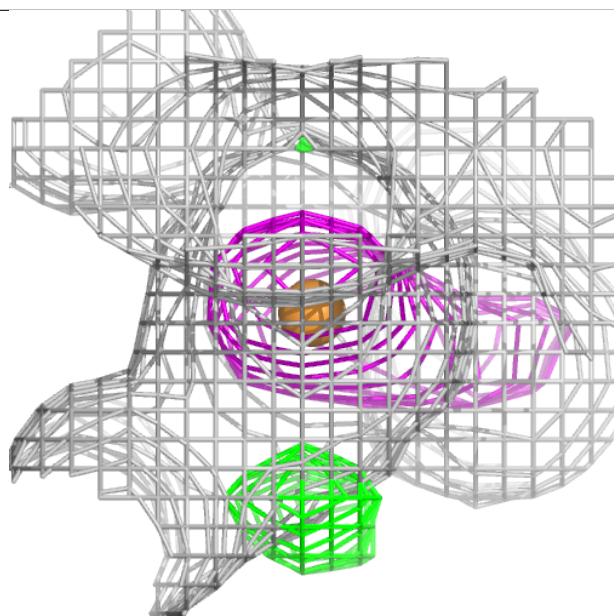
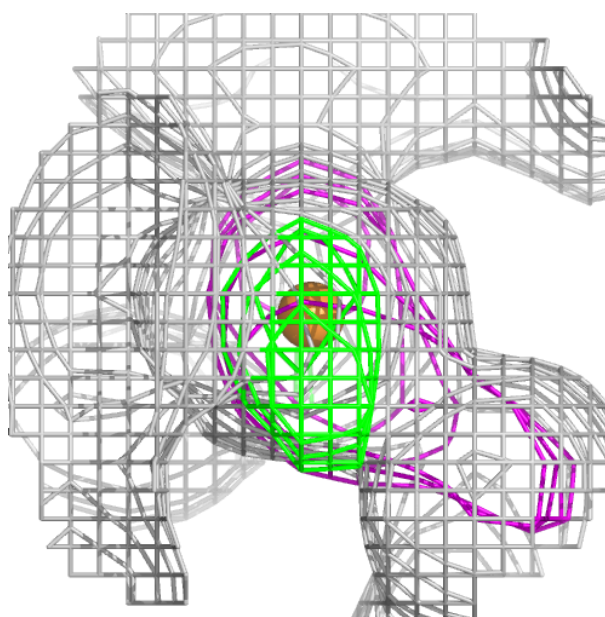
**Electron density around CU BBB 404:**

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

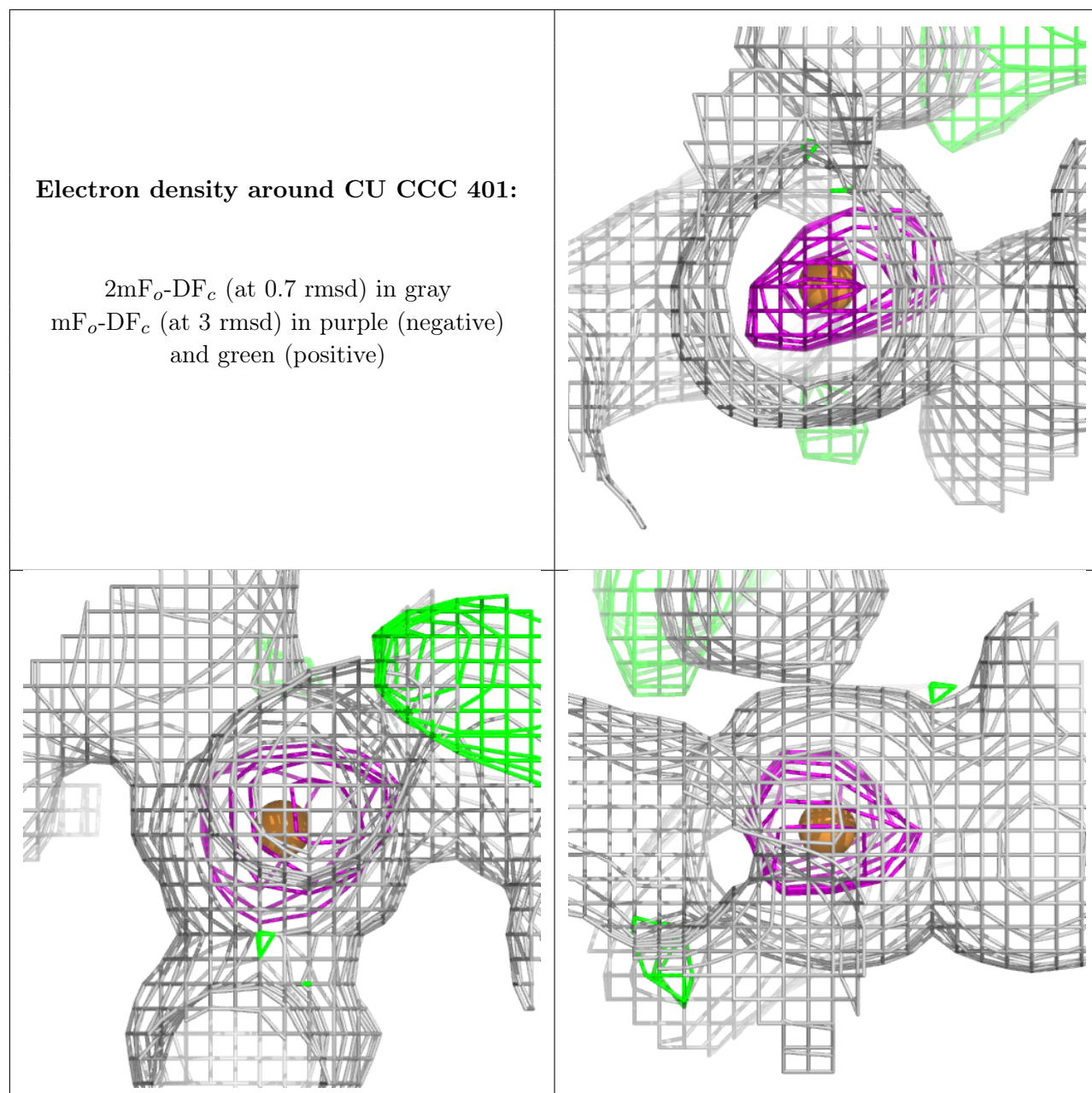


**Electron density around CU AAA 401:**

$2mF_o-DF_c$  (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.