



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:39 AM UTC

PDB ID : 9RCK / pdb_00009rck
Title : Laccase (multicopper oxidase) from *Pediococcus pentosaceus* 4618 mutant
M455A-M456A soaked with Copper 2 minutes
Authors : Paredes, F.; Casino, P.
Deposited on : 2025-05-29
Resolution : 2.30 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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

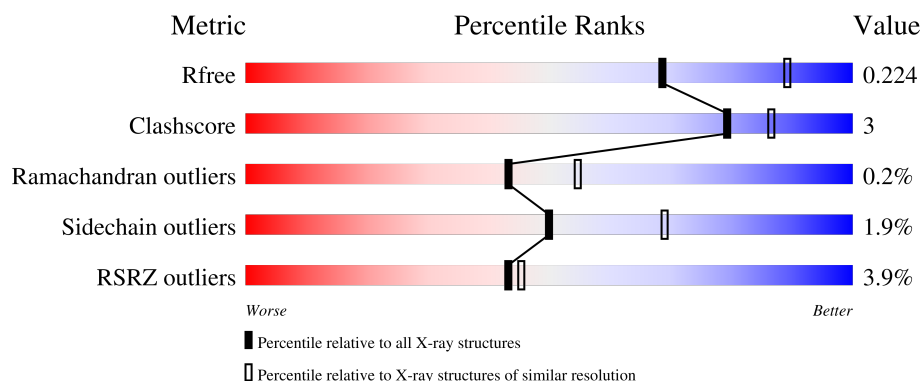
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 ≥ 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	532	4% 79% 6% 13%
1	B	532	2% 81% 5% 13%
1	C	532	0% 99%
1	E	532	0% 99%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7594 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	C	5	Total	C	N	O		0	0	0
			45	27	13	5				
1	A	461	Total	C	N	O	S	0	1	0
			3629	2319	619	679	12			
1	B	462	Total	C	N	O	S	0	0	0
			3628	2319	618	679	12			
1	E	4	Total	C	N	O		0	0	0
			30	18	8	4				

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	initiating methionine	UNP A0AB73HHR8
C	0	GLY	-	expression tag	UNP A0AB73HHR8
C	1	SER	-	expression tag	UNP A0AB73HHR8
C	2	SER	-	expression tag	UNP A0AB73HHR8
C	3	HIS	-	expression tag	UNP A0AB73HHR8
C	4	HIS	-	expression tag	UNP A0AB73HHR8
C	5	HIS	-	expression tag	UNP A0AB73HHR8
C	6	HIS	-	expression tag	UNP A0AB73HHR8
C	7	HIS	-	expression tag	UNP A0AB73HHR8
C	8	HIS	-	expression tag	UNP A0AB73HHR8
C	9	SER	-	expression tag	UNP A0AB73HHR8
C	10	SER	-	expression tag	UNP A0AB73HHR8
C	11	GLY	-	expression tag	UNP A0AB73HHR8
C	12	LEU	-	expression tag	UNP A0AB73HHR8
C	13	VAL	-	expression tag	UNP A0AB73HHR8
C	14	PRO	-	expression tag	UNP A0AB73HHR8
C	15	ARG	-	expression tag	UNP A0AB73HHR8
C	16	GLY	-	expression tag	UNP A0AB73HHR8
C	17	SER	-	expression tag	UNP A0AB73HHR8
C	18	HIS	-	expression tag	UNP A0AB73HHR8
C	19	MET	-	expression tag	UNP A0AB73HHR8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	ALA	-	expression tag	UNP A0AB73HHR8
C	21	SER	-	expression tag	UNP A0AB73HHR8
C	33	PRO	GLN	variant	UNP A0AB73HHR8
C	262	ASN	ASP	variant	UNP A0AB73HHR8
C	274	ALA	SER	variant	UNP A0AB73HHR8
C	476	ALA	MET	engineered mutation	UNP A0AB73HHR8
C	477	ALA	MET	engineered mutation	UNP A0AB73HHR8
A	-22	MET	-	initiating methionine	UNP A0AB73HHR8
A	-21	GLY	-	expression tag	UNP A0AB73HHR8
A	-20	SER	-	expression tag	UNP A0AB73HHR8
A	-19	SER	-	expression tag	UNP A0AB73HHR8
A	-18	HIS	-	expression tag	UNP A0AB73HHR8
A	-17	HIS	-	expression tag	UNP A0AB73HHR8
A	-16	HIS	-	expression tag	UNP A0AB73HHR8
A	-15	HIS	-	expression tag	UNP A0AB73HHR8
A	-14	HIS	-	expression tag	UNP A0AB73HHR8
A	-13	HIS	-	expression tag	UNP A0AB73HHR8
A	-12	SER	-	expression tag	UNP A0AB73HHR8
A	-11	SER	-	expression tag	UNP A0AB73HHR8
A	-10	GLY	-	expression tag	UNP A0AB73HHR8
A	-9	LEU	-	expression tag	UNP A0AB73HHR8
A	-8	VAL	-	expression tag	UNP A0AB73HHR8
A	-7	PRO	-	expression tag	UNP A0AB73HHR8
A	-6	ARG	-	expression tag	UNP A0AB73HHR8
A	-5	GLY	-	expression tag	UNP A0AB73HHR8
A	-4	SER	-	expression tag	UNP A0AB73HHR8
A	-3	HIS	-	expression tag	UNP A0AB73HHR8
A	-2	MET	-	expression tag	UNP A0AB73HHR8
A	-1	ALA	-	expression tag	UNP A0AB73HHR8
A	0	SER	-	expression tag	UNP A0AB73HHR8
A	12	PRO	GLN	variant	UNP A0AB73HHR8
A	241	ASN	ASP	variant	UNP A0AB73HHR8
A	253	ALA	SER	variant	UNP A0AB73HHR8
A	455	ALA	MET	engineered mutation	UNP A0AB73HHR8
A	456	ALA	MET	engineered mutation	UNP A0AB73HHR8
B	-22	MET	-	initiating methionine	UNP A0AB73HHR8
B	-21	GLY	-	expression tag	UNP A0AB73HHR8
B	-20	SER	-	expression tag	UNP A0AB73HHR8
B	-19	SER	-	expression tag	UNP A0AB73HHR8
B	-18	HIS	-	expression tag	UNP A0AB73HHR8
B	-17	HIS	-	expression tag	UNP A0AB73HHR8
B	-16	HIS	-	expression tag	UNP A0AB73HHR8

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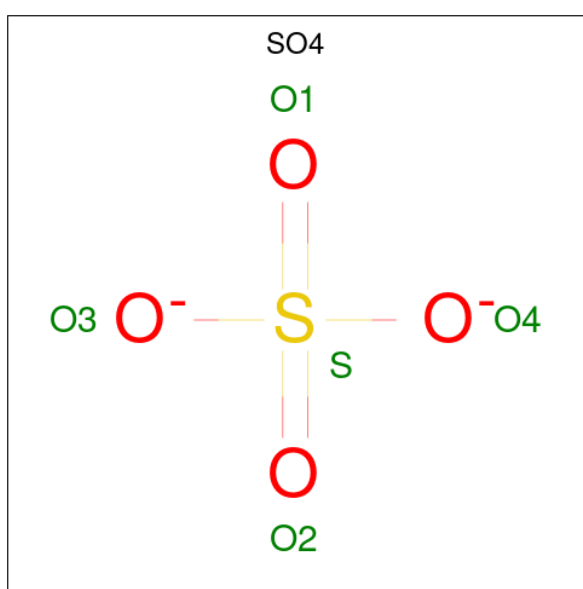
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP A0AB73HHR8
B	-14	HIS	-	expression tag	UNP A0AB73HHR8
B	-13	HIS	-	expression tag	UNP A0AB73HHR8
B	-12	SER	-	expression tag	UNP A0AB73HHR8
B	-11	SER	-	expression tag	UNP A0AB73HHR8
B	-10	GLY	-	expression tag	UNP A0AB73HHR8
B	-9	LEU	-	expression tag	UNP A0AB73HHR8
B	-8	VAL	-	expression tag	UNP A0AB73HHR8
B	-7	PRO	-	expression tag	UNP A0AB73HHR8
B	-6	ARG	-	expression tag	UNP A0AB73HHR8
B	-5	GLY	-	expression tag	UNP A0AB73HHR8
B	-4	SER	-	expression tag	UNP A0AB73HHR8
B	-3	HIS	-	expression tag	UNP A0AB73HHR8
B	-2	MET	-	expression tag	UNP A0AB73HHR8
B	-1	ALA	-	expression tag	UNP A0AB73HHR8
B	0	SER	-	expression tag	UNP A0AB73HHR8
B	12	PRO	GLN	variant	UNP A0AB73HHR8
B	241	ASN	ASP	variant	UNP A0AB73HHR8
B	253	ALA	SER	variant	UNP A0AB73HHR8
B	455	ALA	MET	engineered mutation	UNP A0AB73HHR8
B	456	ALA	MET	engineered mutation	UNP A0AB73HHR8
E	1	MET	-	initiating methionine	UNP A0AB73HHR8
E	2	GLY	-	expression tag	UNP A0AB73HHR8
E	3	SER	-	expression tag	UNP A0AB73HHR8
E	4	SER	-	expression tag	UNP A0AB73HHR8
E	5	HIS	-	expression tag	UNP A0AB73HHR8
E	6	HIS	-	expression tag	UNP A0AB73HHR8
E	7	HIS	-	expression tag	UNP A0AB73HHR8
E	8	HIS	-	expression tag	UNP A0AB73HHR8
E	9	HIS	-	expression tag	UNP A0AB73HHR8
E	10	HIS	-	expression tag	UNP A0AB73HHR8
E	11	SER	-	expression tag	UNP A0AB73HHR8
E	12	SER	-	expression tag	UNP A0AB73HHR8
E	13	GLY	-	expression tag	UNP A0AB73HHR8
E	14	LEU	-	expression tag	UNP A0AB73HHR8
E	15	VAL	-	expression tag	UNP A0AB73HHR8
E	16	PRO	-	expression tag	UNP A0AB73HHR8
E	17	ARG	-	expression tag	UNP A0AB73HHR8
E	18	GLY	-	expression tag	UNP A0AB73HHR8
E	19	SER	-	expression tag	UNP A0AB73HHR8
E	20	HIS	-	expression tag	UNP A0AB73HHR8
E	21	MET	-	expression tag	UNP A0AB73HHR8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	22	ALA	-	expression tag	UNP A0AB73HHR8
E	23	SER	-	expression tag	UNP A0AB73HHR8
E	35	PRO	GLN	variant	UNP A0AB73HHR8
E	264	ASN	ASP	variant	UNP A0AB73HHR8
E	276	ALA	SER	variant	UNP A0AB73HHR8
E	478	ALA	MET	engineered mutation	UNP A0AB73HHR8
E	479	ALA	MET	engineered mutation	UNP A0AB73HHR8

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	Cu	0	0
			11	11		
3	B	10	Total	Cu	0	0
			10	10		

- Molecule 4 is water.

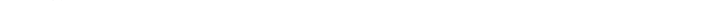
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	O 1	0	0
4	A	123	Total 123	O 123	0	0
4	B	111	Total 111	O 111	0	0
4	E	1	Total 1	O 1	0	0

- Molecule 1: Multicopper oxidase domain-containing protein



LYS	PRO	LYS	GLN	GLU	TYR	LYS	LEU	ASP	MET	ASP	THR	LEU	MET	MET	ALA	LEU	ALA	LYS	GLU	ARG	GLY	VAL	LYS	PRO	SER	GLU	ILE	TRP	GLY	GLY	MET	MET	GLN	SER	TYR	GLU	LYS	MET	GLY	MET	LYS	MET
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- Molecule 1: Multicopper oxidase domain-containing protein

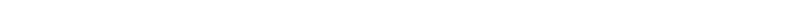
Chain B:  2% 81% 5% 13%

MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	HIS	MET	ALA	MET	MET	LYS	N3	Y7	D18	T46	L102	T103	T104	M111	P115	G119	Q139	A148	P152	S153	M165	A174	R180	P188	W248
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H251	Q260	D264	H276	L277	M278	D305	D306	Q321	K327	V336	M350	Q364	Q370	W378	N384	D385	M413	K418	P464	ALA	LYS	PRO	LYS	GLN	GLU	THR	LYS	LEU	MET	ASP	ASP	THR	MET	ALA	LEU	ALA	LYS	GLU	ARG	GLY	VAL
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LYS PRO SER GLU ILE TRP MET GLY GLY MET GLN SER TYR GLU LYS MET GLY MET LYS MET

- Molecule 1: Multicopper oxidase domain-containing protein

Chain E: 

MET GLY S3 S4 S5 H6 HIS HIS HIS HIS HIS SER SER GLY LEU VAL VAL ARG GLY SER HIS SER MET MET MET LYS ASN TYR THR ASP TYR PHE ASP ASP GLU GLU PRO PRO ALA PHE ASP LEU LEU HIS ASP GLY GLY TYR VAL VAL LEU VAL SER ASP ALA PRO GLU LYS PRO PRO LEU ASN VAL VAL PRO

[illegible]

THR	LEU	PRO	LEU	GLU	LEU	THR	THR	PHE	HIS	HIS	TRP	GLY	ALA	ASN	VAL	GLY	GLY	PRO	TYR	VAL	ASP	GLY	GLY	CYS	HIS	ALA	ALA	PRO	PRO	TYR	VAL	THR	PRO	GLY	GLU	GLU	SER	LYS	HIS	ILE	ASP	PHE	THR	THR	LEU	LEU	GLN	PRO	ALA	ALA	THR	THR	LEU	TRP	LEU	CYS	PRO	SER	THR	ALA	ALA	GLU	TYR
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VAL	TRP	HIS	HIS	LEU	ALA	ALA	MET	VAL	ILE	VAL	LYS	ASP	ASP	HIS	HIS	ALA	ALA	SER	LEU	PRO	PRO	LEU	LEU	PRO	PRO	ARG	ASN	TYR	GLY	VAL	ASP	ASP	ILE	ILE	PRO	VAL	VAL	ILE	LEU	LEU	GLN	ASN	ASP	ASP	ARG	ARG	PHE	ASP	HIS	HIS	GLU	ASN	ASN	ASN	GLN	TRP	ASP	ASP	TYR	TYR	ASP	PRO	PRO	ASP	ASP	GLY	VAL	VAL	ALA	ALA	GLY	GLY	PRO	PRO	THR
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[illegible]

MET	LEU	THR	THR	CYS	ALA	GLU	ARG	ALA	ALA	VAL	GLU	VAL	ILE	ASP	VAL	PHE	GLY	GLN	TYR	HIS	GLY	GLU	ASP	GLU	VAL	THR	LEU	THR	THR	ASP	ASP	PRO	LEU	LYS	PHE	ARG	ILE	HIS	ALA	PHE	LYS	PRO	ASP	GLN	THR	THR	LEU	PRO	ASP	LYS	LEU	PHE	ASP	VAL	LYS	VAL	VAL	VAL	ASP
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PRO	ALA	LEU	PRO	VAL	ARG	HIS	VAL	VAL	MET	GLN	GLY	MET	ASP	GLU	VAL	ALA	ILE	ASP	GLY	LYS	PHE	ALA	MET	GLN	ARG	ILE	ASP	ALA	THR	GLN	PRO	ILE	GLY	LYS	ALA	GLN	TRP	TYR	ASP	VAL	THR	ASN	SER	ASN	ASP	ALA	GLY	PRO	HIS	PRO	PHE	HIS	VAL	VAL	HIS	STY
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[illegible][illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.11Å 123.11Å 179.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.29 – 2.30 52.29 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (52.29-2.30) 100.0 (52.29-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.188 , 0.217 0.196 , 0.224	Depositor DCC
R_{free} test set	3446 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7594	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, SO4

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	0.49	0/3746	0.95	8/5133 (0.2%)
1	B	0.50	0/3744	0.87	0/5129
1	C	0.66	0/48	1.85	2/64 (3.1%)
1	E	0.57	0/31	1.40	0/41
All	All	0.49	0/7569	0.92	10/10367 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	323	THR	N-CA-C	-16.06	82.53	108.55
1	A	322	THR	CB-CA-C	-15.53	81.91	109.86
1	A	320	ASP	CB-CA-C	-6.77	98.06	109.50
1	A	385	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	18	ASP	CA-CB-CG	6.05	118.65	112.60
1	C	6	HIS	CA-CB-CG	-5.54	108.26	113.80
1	A	320	ASP	N-CA-C	5.35	118.78	110.17
1	C	5	HIS	CA-CB-CG	-5.16	108.64	113.80
1	A	15	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	115	PRO	N-CA-CB	-5.01	97.09	102.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	5	HIS	Peptide

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	3629	0	3415	22	1
1	B	3628	0	3422	16	1
1	C	45	0	29	1	0
1	E	30	0	17	0	0
2	C	5	0	0	1	0
3	A	11	0	0	0	0
3	B	10	0	0	0	0
4	A	123	0	0	1	0
4	B	111	0	0	1	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	7594	0	6883	39	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 3.

All (39) 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:260:GLN:HE22	1:B:413:ASN:HD22	1.32	0.77
1:A:322:THR:HG22	1:A:323:THR:N	2.05	0.70
1:A:260:GLN:HE22	1:A:413:ASN:HD22	1.41	0.68
1:A:104:THR:CG2	1:A:119:GLY:O	2.45	0.65
1:A:384:ASN:ND2	1:A:391:HIS:HE2	1.96	0.64
1:B:104:THR:CG2	1:B:119:GLY:O	2.49	0.60
1:A:152:PRO:O	1:A:153:SER:CB	2.49	0.60
1:A:104:THR:HG23	1:A:119:GLY:O	2.02	0.59
1:A:251:HIS:HE1	1:A:305:ASP:O	1.87	0.57
1:A:177:PRO:O	1:A:322:THR:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:THR:HG23	1:B:119:GLY:O	2.06	0.56
1:B:152:PRO:O	1:B:153:SER:CB	2.54	0.56
1:A:153:SER:HA	4:A:723:HOH:O	2.05	0.55
1:A:102:LEU:C	1:A:102:LEU:HD12	2.32	0.53
1:B:370:GLN:HE22	1:B:378:TRP:HE1	1.57	0.53
1:B:264:ASP:HB2	1:B:418:LYS:HA	1.91	0.52
1:B:111:ASN:H	1:B:139:GLN:HE22	1.56	0.52
1:A:370:GLN:HE22	1:A:378:TRP:HE1	1.56	0.52
1:B:251:HIS:HE1	1:B:305:ASP:O	1.98	0.45
1:B:111:ASN:H	1:B:139:GLN:NE2	2.14	0.45
1:A:304:THR:HB	1:A:309:LEU:HD11	1.98	0.45
1:A:264:ASP:HB2	1:A:418:LYS:HA	1.98	0.45
1:B:165:MET:SD	1:B:188:PRO:HB3	2.57	0.44
1:B:306:ASP:HB2	4:B:758:HOH:O	2.17	0.44
1:B:7:TYR:CE1	1:B:276:HIS:HB3	2.53	0.43
1:B:102:LEU:C	1:B:102:LEU:HD12	2.43	0.43
1:A:7:TYR:CE1	1:A:276:HIS:HB3	2.54	0.42
1:A:111:ASN:H	1:A:139:GLN:HE22	1.66	0.42
1:B:104:THR:O	1:B:148:ALA:HA	2.20	0.42
1:A:149:HIS:N	1:A:150:PRO:CD	2.83	0.42
1:B:248:TRP:O	1:B:278:MET:HA	2.20	0.42
1:A:370:GLN:O	1:A:461:THR:HA	2.20	0.41
1:A:11:GLU:N	1:A:12:PRO:CD	2.83	0.41
1:B:174:ALA:HA	1:B:180:ARG:NH2	2.35	0.41
1:A:234:LYS:HG3	1:A:320:ASP:CG	2.46	0.41
1:A:251:HIS:CE1	1:A:305:ASP:O	2.70	0.41
1:C:6:HIS:HA	2:C:601:SO4:O2	2.21	0.41
1:A:111:ASN:H	1:A:139:GLN:NE2	2.20	0.40
1:A:369:THR:HA	1:A:460:GLU:O	2.22	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)
1:A:383:SER:O	1:B:385:ASP:OD1[6_444]	2.17	0.03

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	460/532 (86%)	445 (97%)	14 (3%)	1 (0%)	43	55
1	B	460/532 (86%)	445 (97%)	14 (3%)	1 (0%)	43	55
1	C	3/532 (1%)	3 (100%)	0	0	100	100
1	E	2/532 (0%)	2 (100%)	0	0	100	100
All	All	925/2128 (44%)	895 (97%)	28 (3%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	153	SER
1	A	153	SER

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	384/452 (85%)	376 (98%)	8 (2%)	47	66
1	B	384/452 (85%)	379 (99%)	5 (1%)	61	77
1	C	4/452 (1%)	2 (50%)	2 (50%)	0	0
1	E	2/452 (0%)	2 (100%)	0	100	100
All	All	774/1808 (43%)	759 (98%)	15 (2%)	50	69

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3	HIS
1	C	4	HIS
1	A	102	LEU
1	A	104	THR
1	A	115	PRO
1	A	234	LYS
1	A	296	GLU
1	A	336	VAL
1	A	348	GLN
1	A	458	GLN
1	B	102	LEU
1	B	104	THR
1	B	115	PRO
1	B	321	GLN
1	B	336	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	111	ASN
1	A	139	GLN
1	A	199	ASN
1	A	251	HIS
1	A	260	GLN
1	A	370	GLN
1	A	384	ASN
1	A	458	GLN
1	B	62	GLN
1	B	139	GLN
1	B	197	HIS
1	B	251	HIS
1	B	260	GLN
1	B	295	HIS
1	B	321	GLN
1	B	344	HIS
1	B	370	GLN
1	B	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 22 ligands modelled in this entry, 21 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	SO4	C	601	-	4,4,4	0.30	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

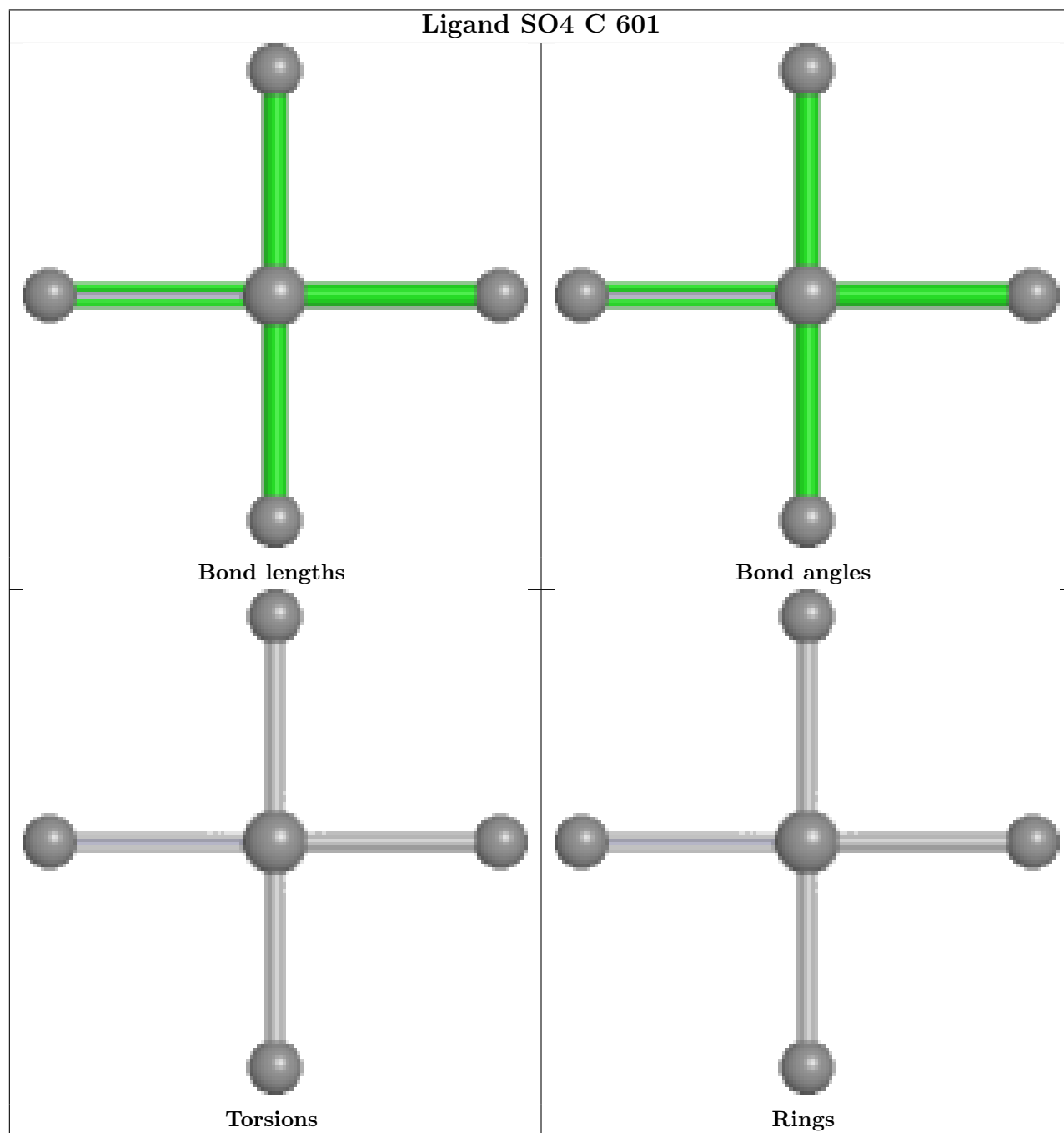
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	SO4	1	0

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	461/532 (86%)	0.10	19 (4%) 41 43	21, 43, 65, 113	1 (0%)
1	B	462/532 (86%)	0.07	10 (2%) 62 64	33, 44, 66, 87	0
1	C	5/532 (0%)	3.03	3 (60%) 0 0	54, 60, 74, 75	0
1	E	4/532 (0%)	6.26	4 (100%) 0 0	100, 108, 110, 111	0
All	All	932/2128 (43%)	0.13	36 (3%) 43 45	21, 44, 68, 113	1 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	4	SER	8.0
1	C	2	SER	7.6
1	E	3	SER	7.3
1	B	3	ASN	6.4
1	A	322	THR	6.3
1	A	323	THR	6.1
1	A	321	GLN	5.5
1	E	6	HIS	5.4
1	B	385	ASP	4.4
1	E	5	HIS	4.3
1	A	464	PRO	3.9
1	B	464	PRO	3.8
1	A	4	TYR	3.7
1	A	47	ALA	3.4
1	A	335	VAL	3.3
1	B	384	ASN	3.2
1	B	18	ASP	3.1
1	A	253	ALA	3.1
1	C	4	HIS	3.0
1	A	295	HIS	2.9
1	C	6	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	384	ASN	2.8
1	A	344[A]	HIS	2.6
1	A	318	LYS	2.6
1	A	18	ASP	2.5
1	B	46	THR	2.4
1	B	153	SER	2.4
1	A	385	ASP	2.3
1	A	320	ASP	2.3
1	B	350	MET	2.3
1	B	364	GLN	2.2
1	A	336	VAL	2.2
1	A	299	GLU	2.1
1	A	339	ALA	2.1
1	A	46	THR	2.0
1	B	327	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 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, 95th 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 ²)	Q<0.9
3	CU	B	610	1/1	0.64	0.18	106,106,106,106	0
3	CU	A	611	1/1	0.77	0.13	98,98,98,98	0
3	CU	B	609	1/1	0.84	0.11	95,95,95,95	0
3	CU	A	607	1/1	0.90	0.08	93,93,93,93	0
3	CU	B	608	1/1	0.90	0.19	103,103,103,103	0
3	CU	A	610	1/1	0.92	0.14	101,101,101,101	0
3	CU	B	607	1/1	0.93	0.08	90,90,90,90	0
3	CU	A	609	1/1	0.94	0.07	83,83,83,83	0

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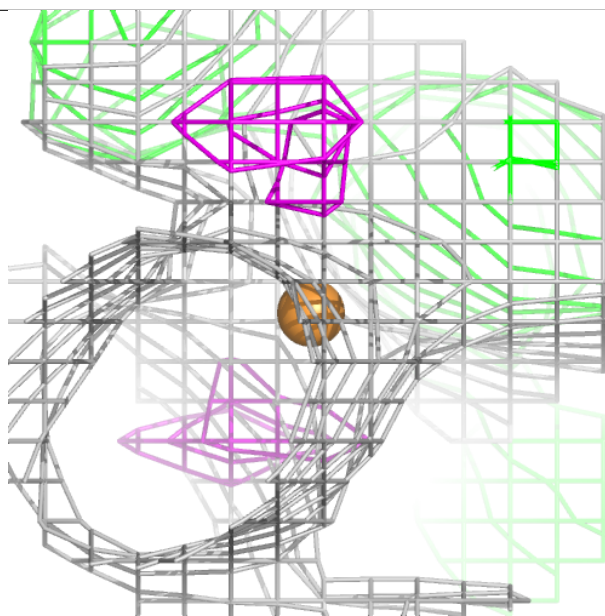
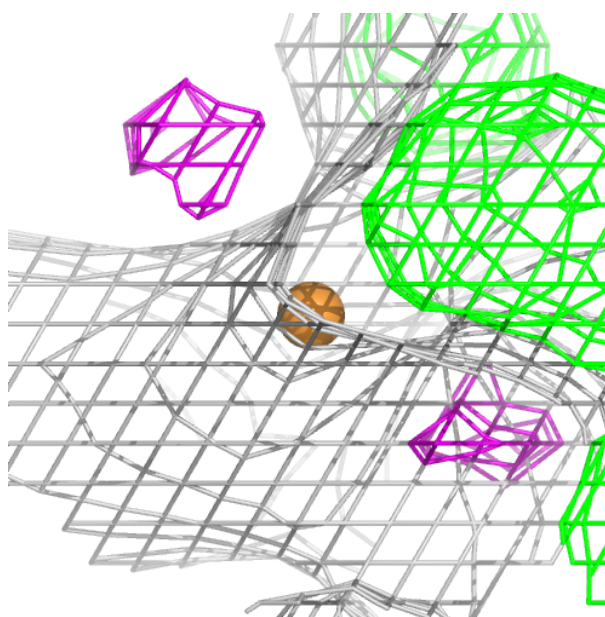
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CU	A	606	1/1	0.96	0.05	85,85,85,85	0
3	CU	B	606	1/1	0.96	0.12	68,68,68,68	0
3	CU	A	605	1/1	0.96	0.06	74,74,74,74	0
3	CU	A	608	1/1	0.97	0.11	63,63,63,63	0
3	CU	B	605	1/1	0.98	0.04	63,63,63,63	0
2	SO4	C	601	5/5	0.98	0.09	42,48,50,54	0
3	CU	B	603	1/1	0.99	0.03	45,45,45,45	0
3	CU	A	604	1/1	0.99	0.03	65,65,65,65	0
3	CU	A	601	1/1	0.99	0.03	45,45,45,45	0
3	CU	A	602	1/1	0.99	0.02	38,38,38,38	0
3	CU	A	603	1/1	0.99	0.03	46,46,46,46	0
3	CU	B	601	1/1	0.99	0.02	38,38,38,38	0
3	CU	B	602	1/1	0.99	0.03	46,46,46,46	0
3	CU	B	604	1/1	1.00	0.05	50,50,50,50	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.

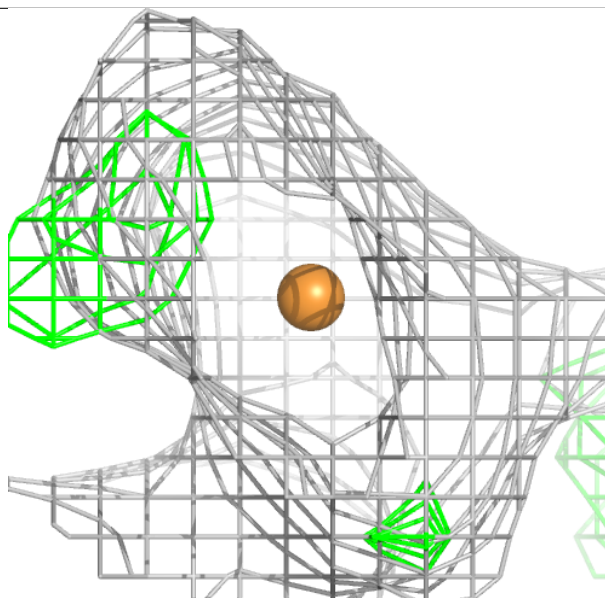
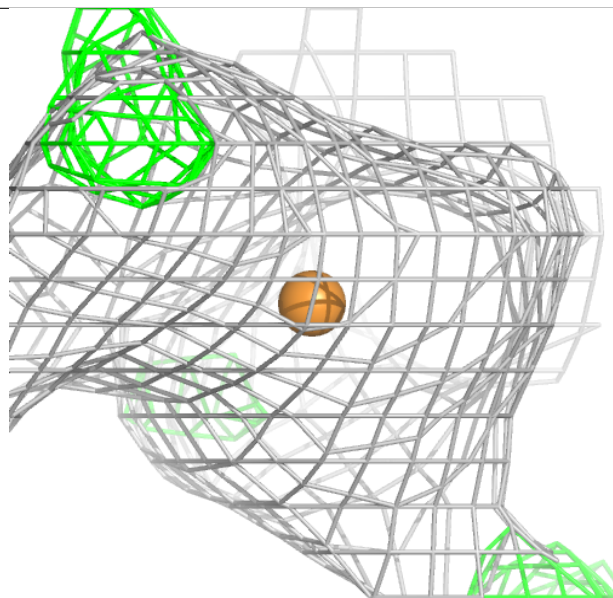
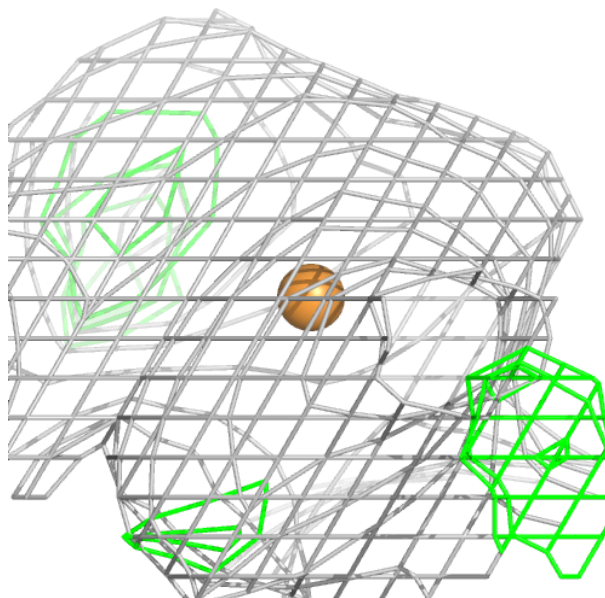
Electron density around CU B 610:

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



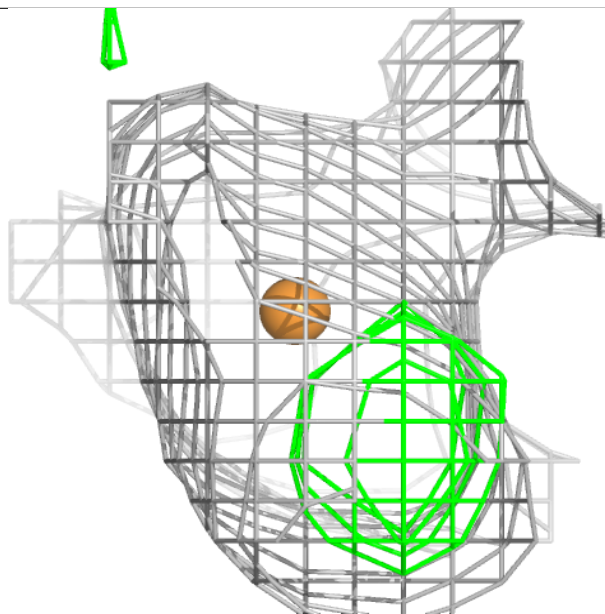
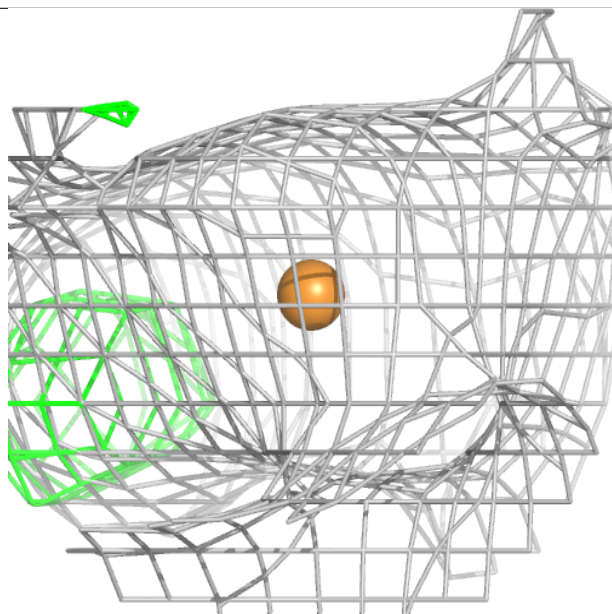
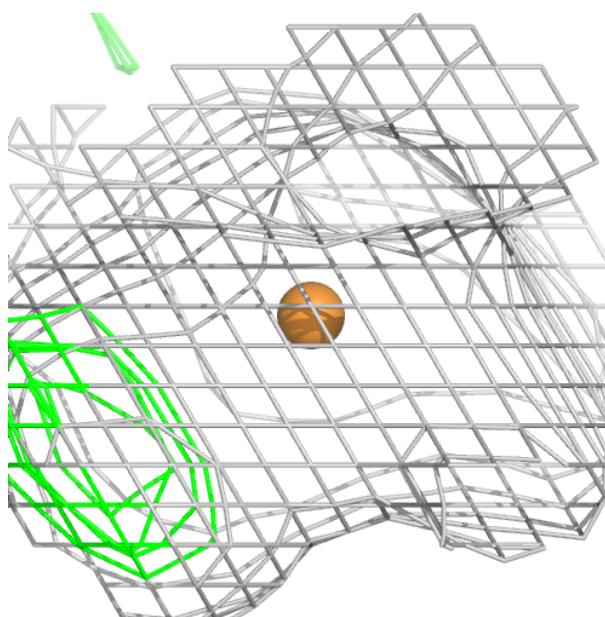
Electron density around CU A 611:

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



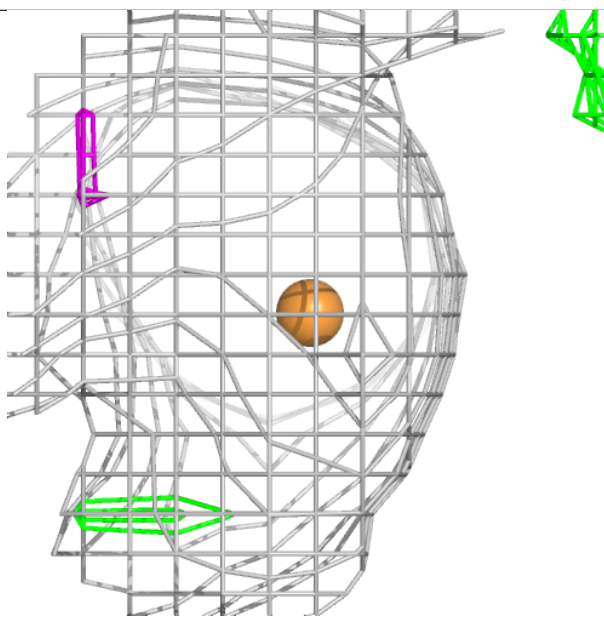
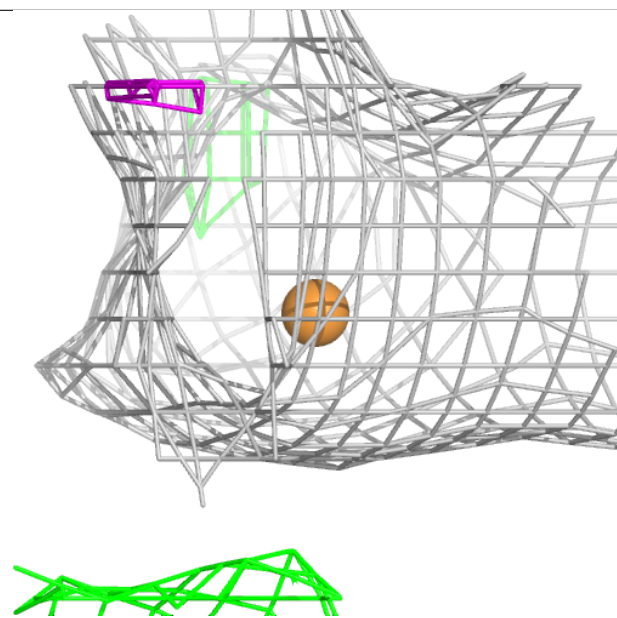
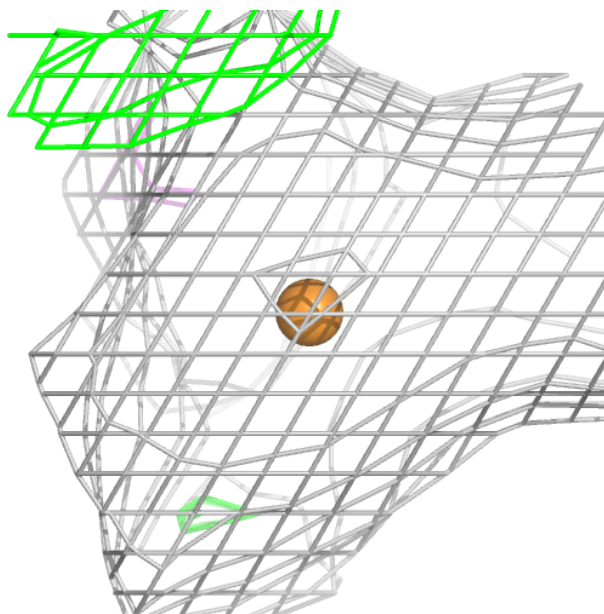
Electron density around CU B 609:

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and green (positive)



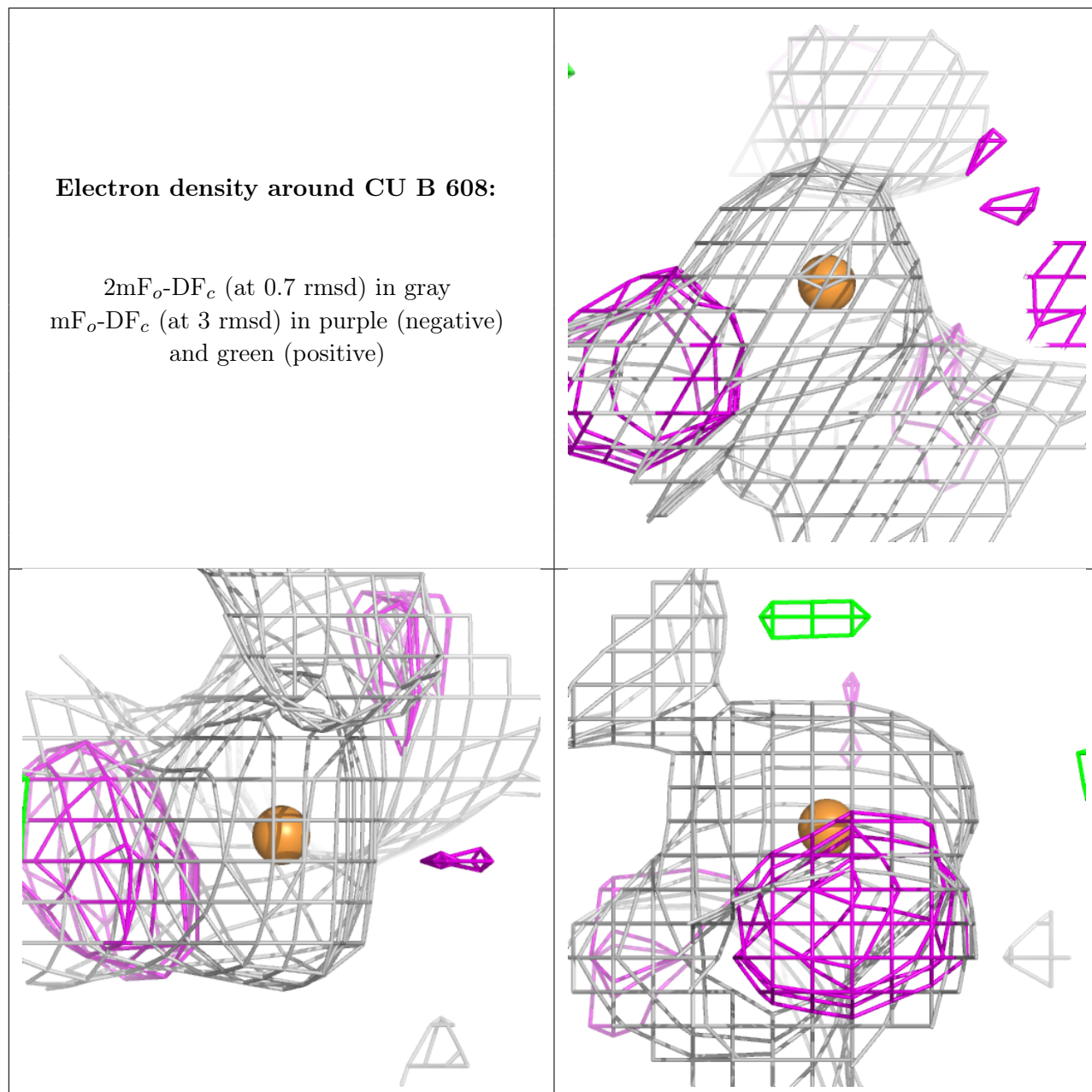
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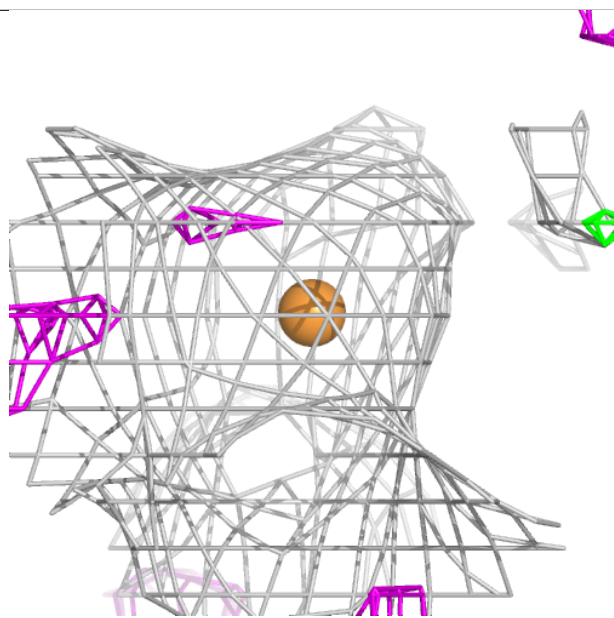
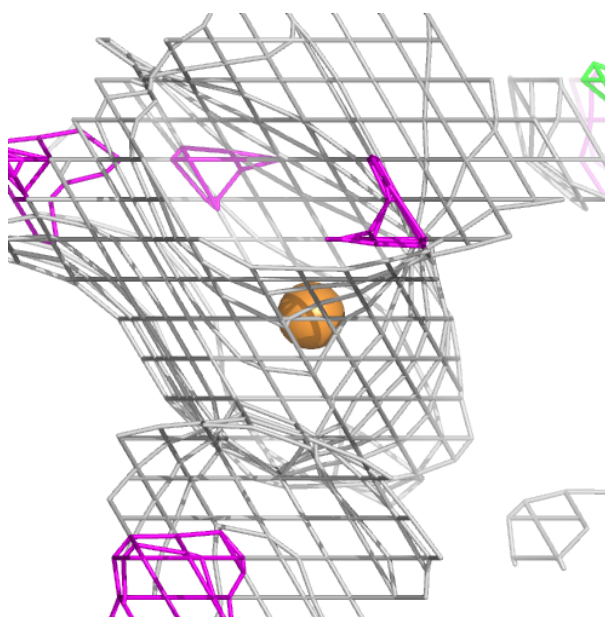
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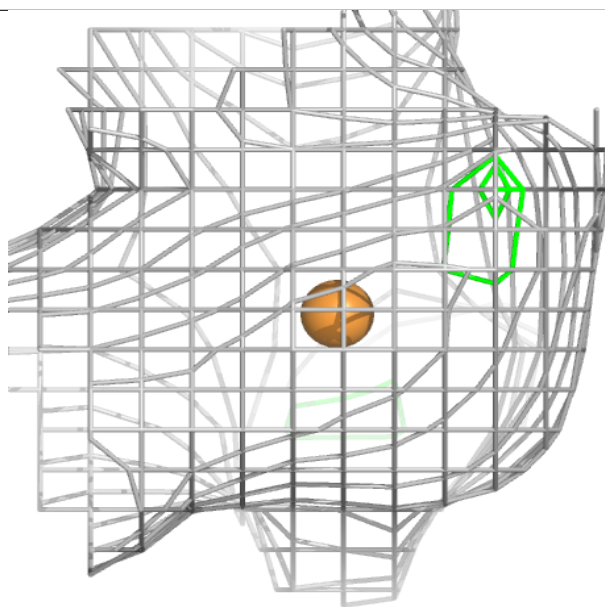
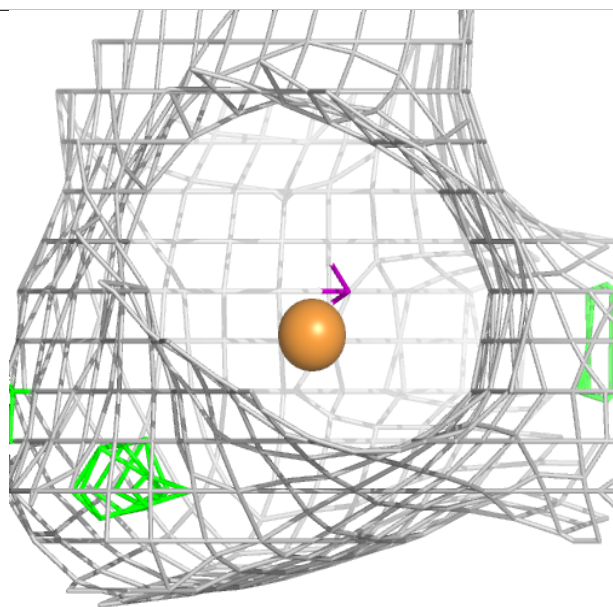
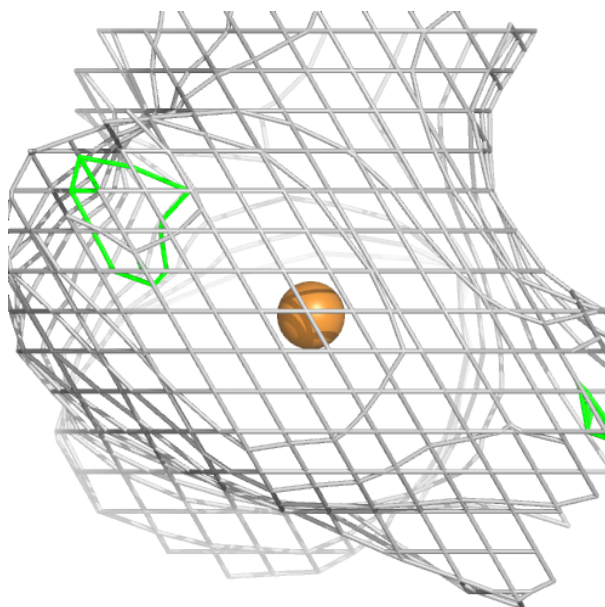
Electron density around CU A 610:

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and green (positive)



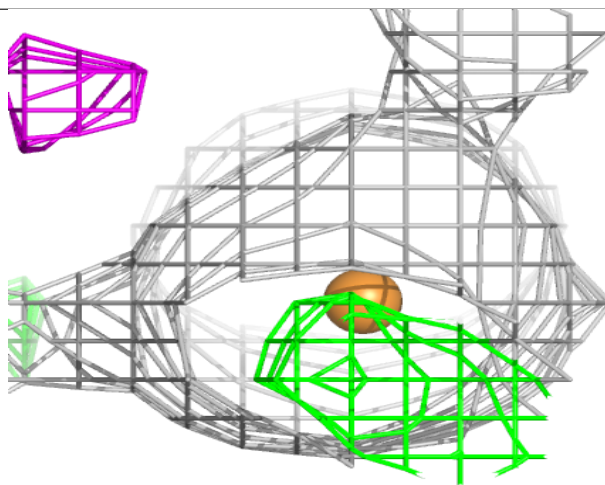
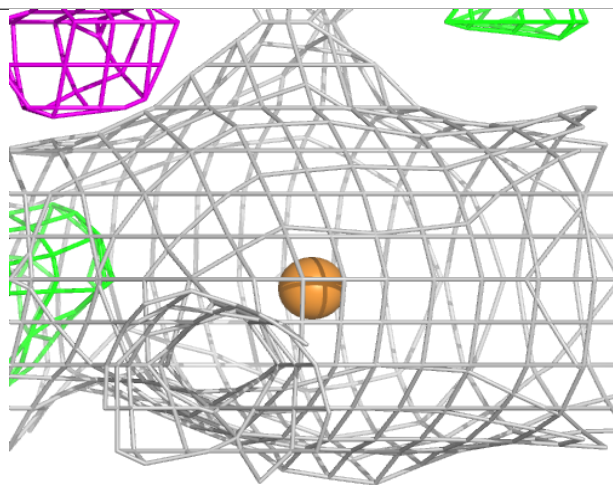
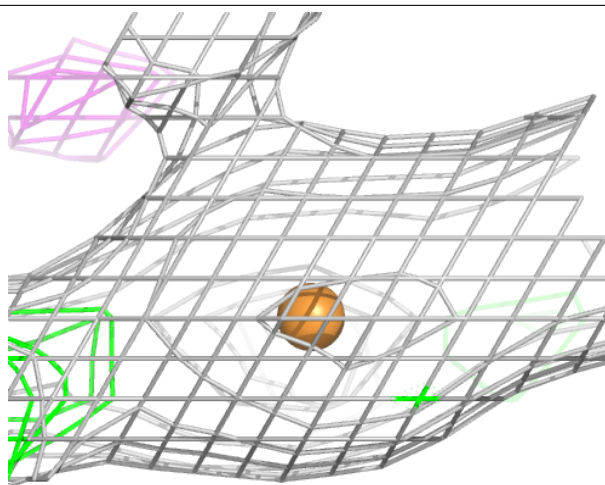
Electron density around CU B 607:

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and green (positive)



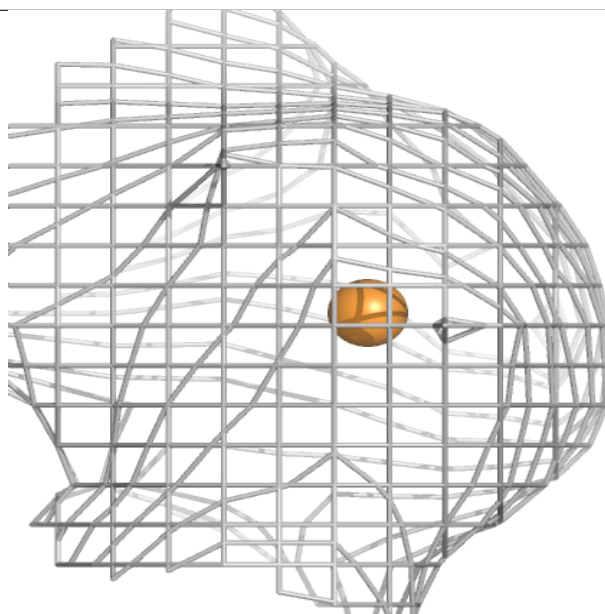
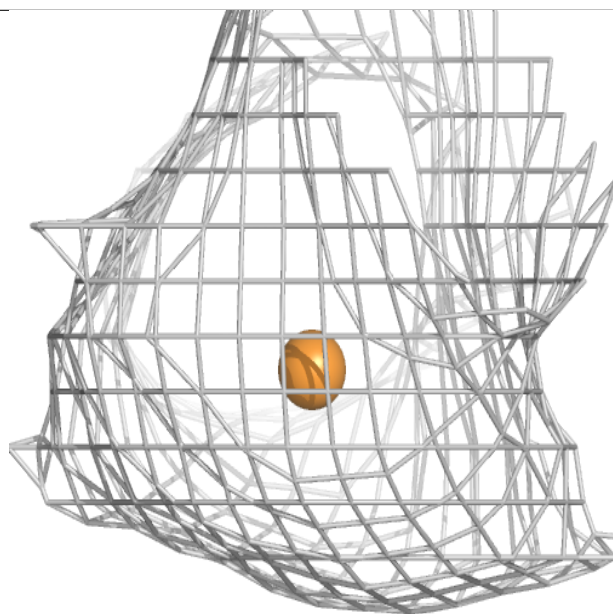
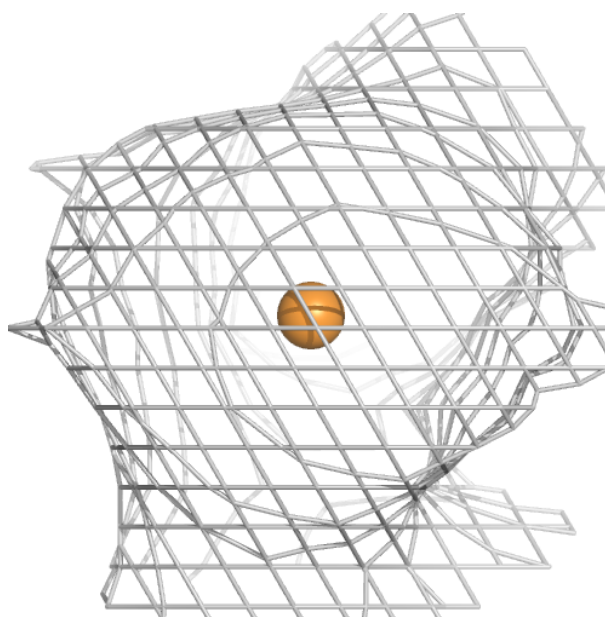
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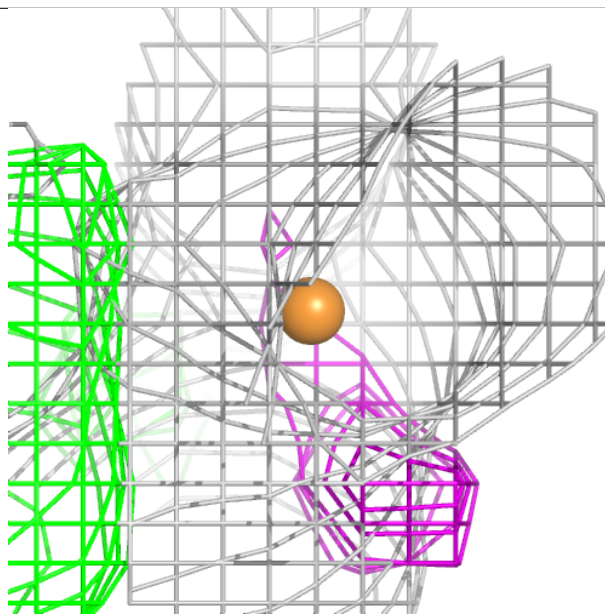
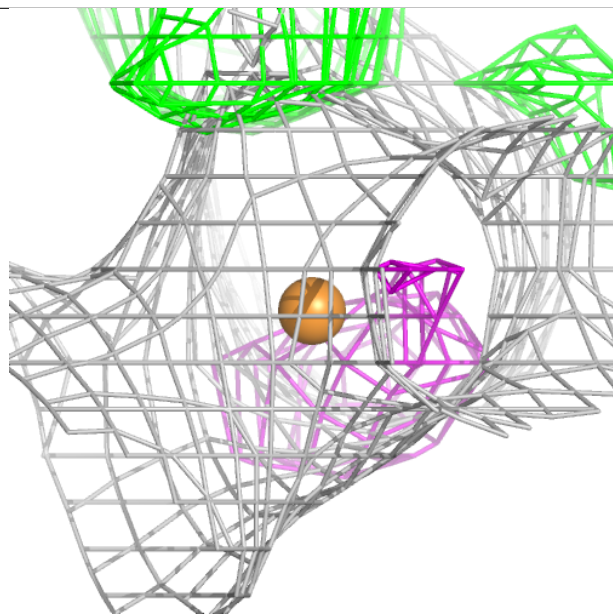
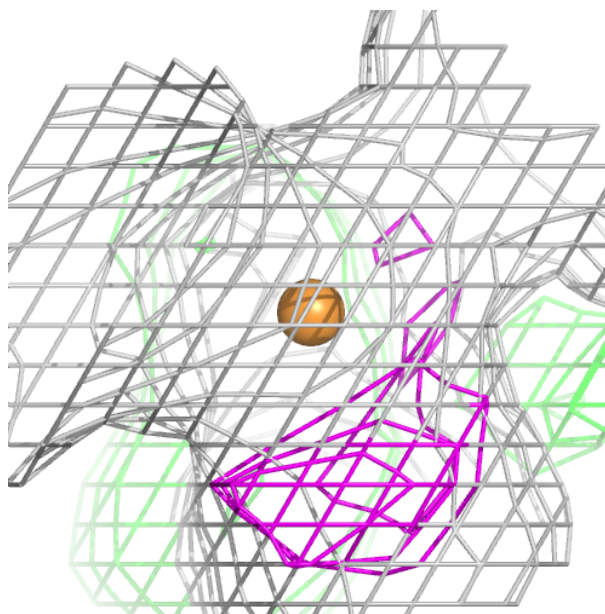
Electron density around CU A 606:

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and green (positive)



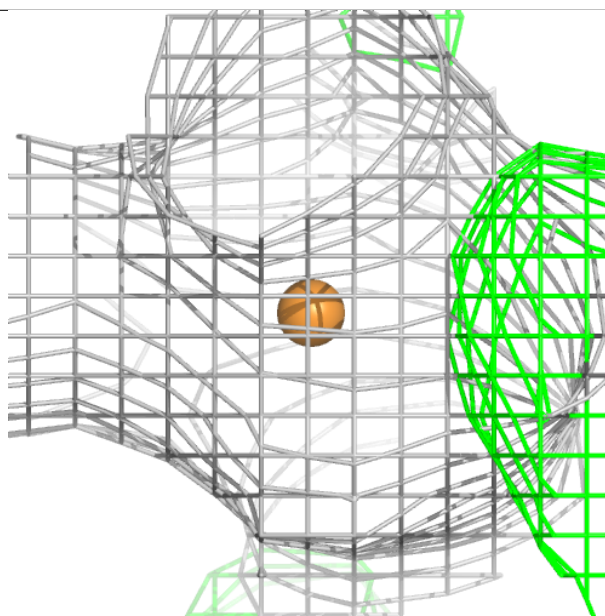
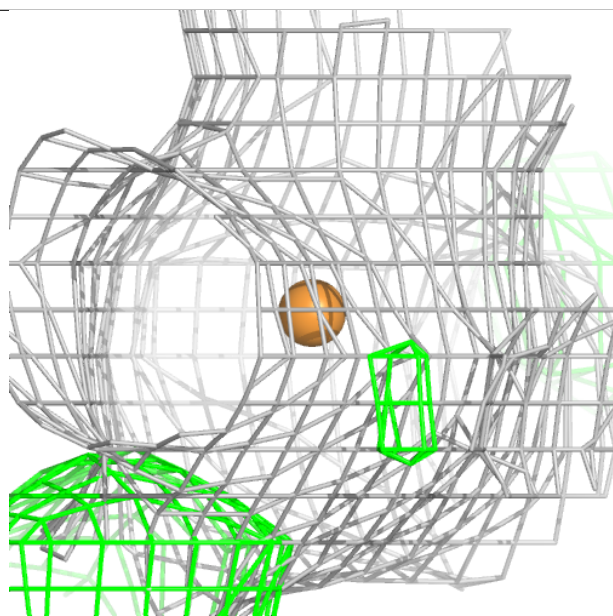
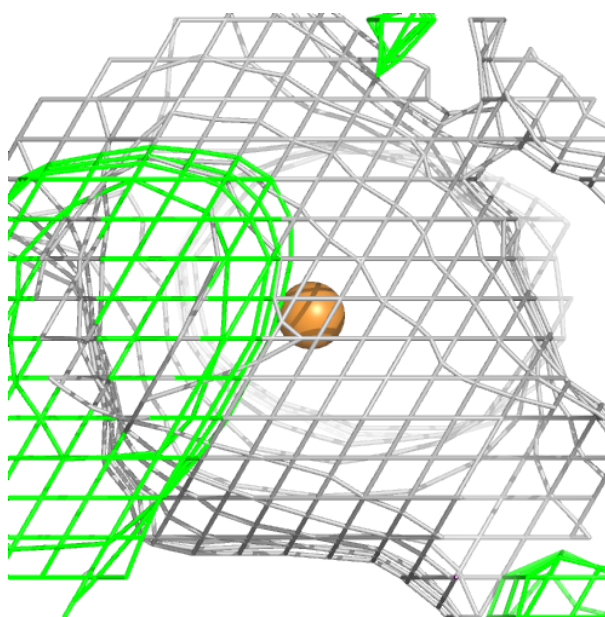
Electron density around CU B 606:

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



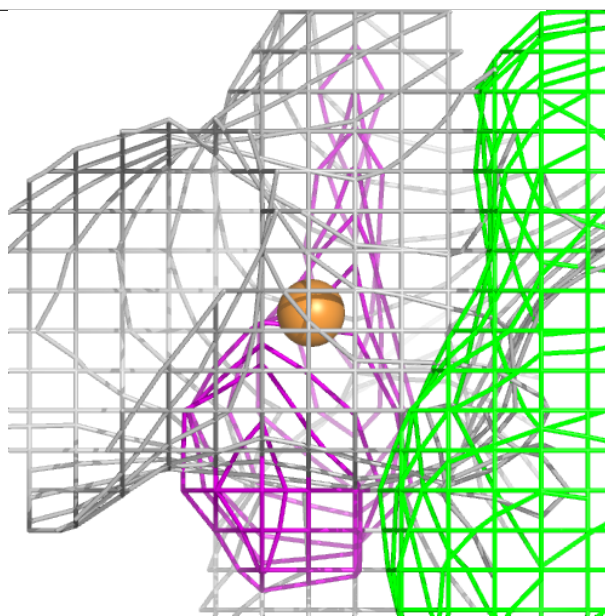
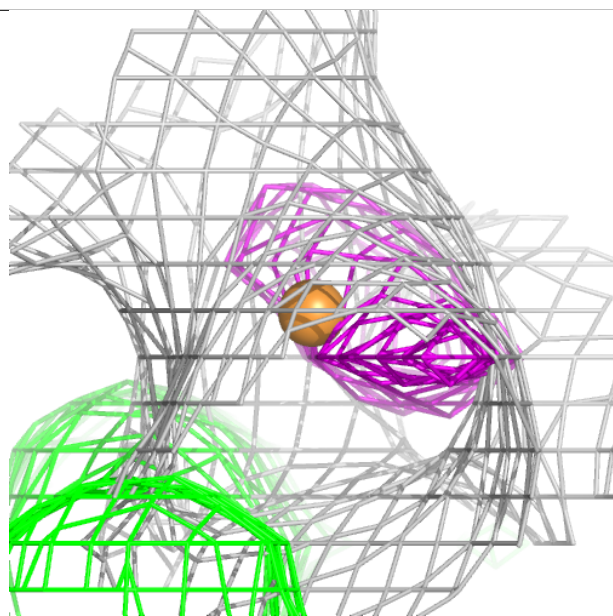
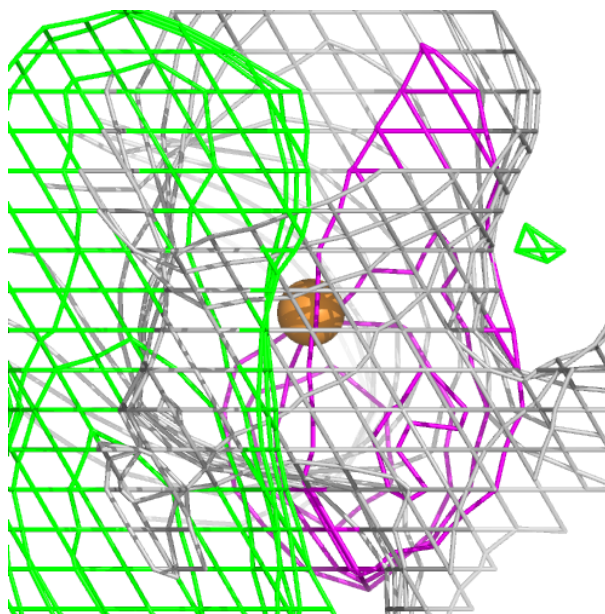
Electron density around CU A 605:

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



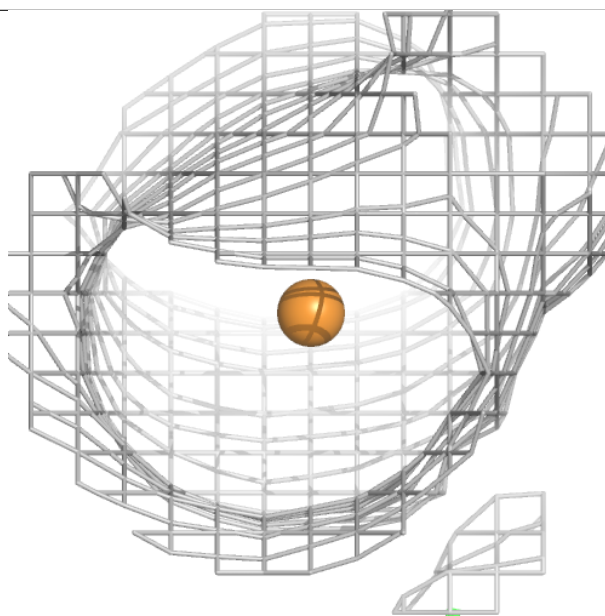
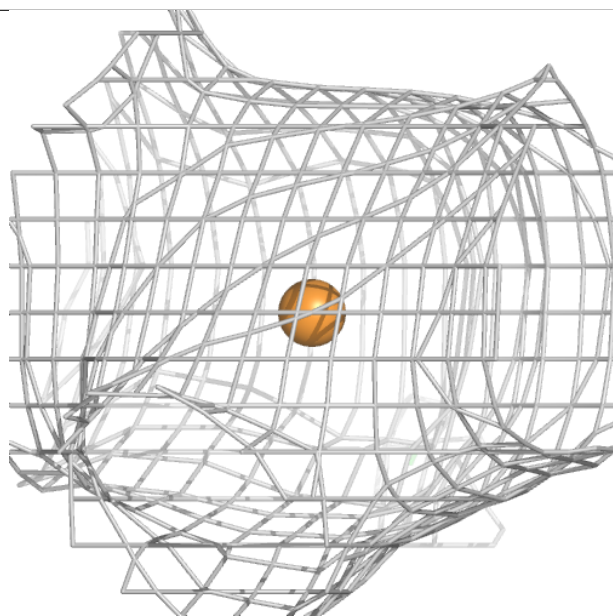
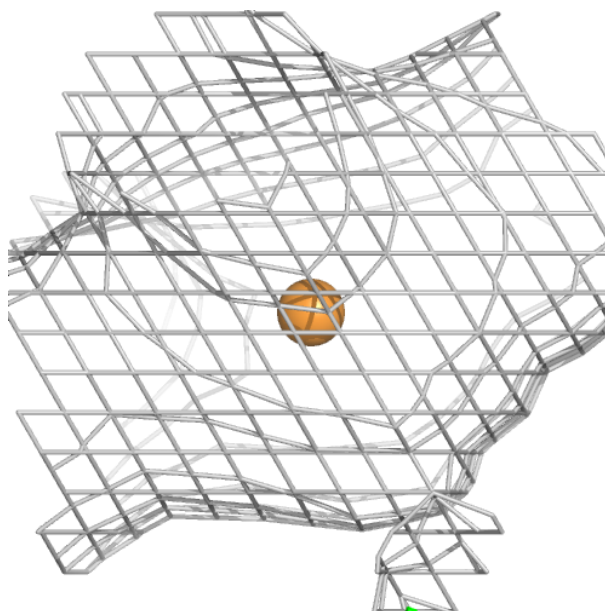
Electron density around CU A 608:

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



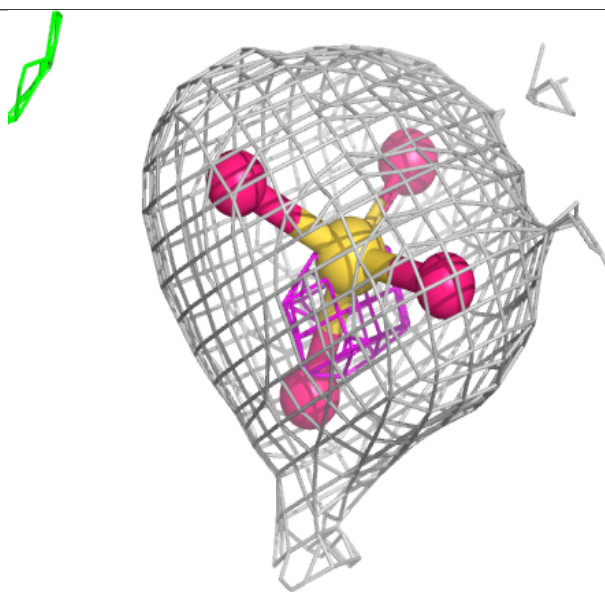
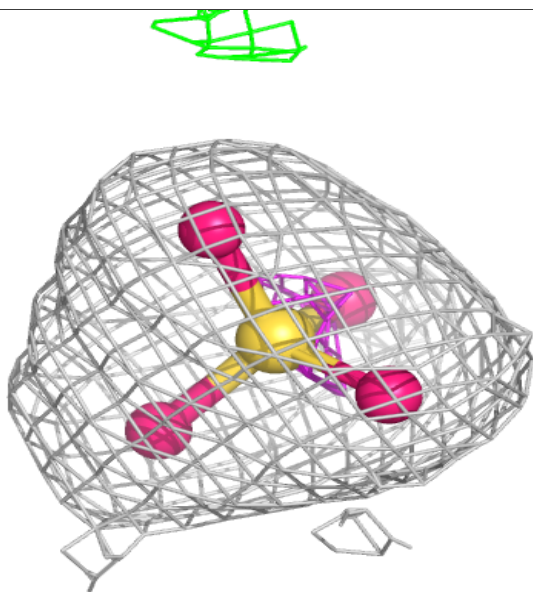
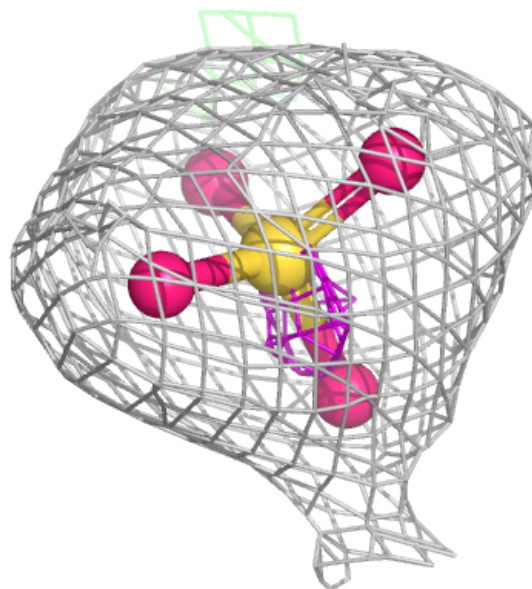
Electron density around CU B 605:

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



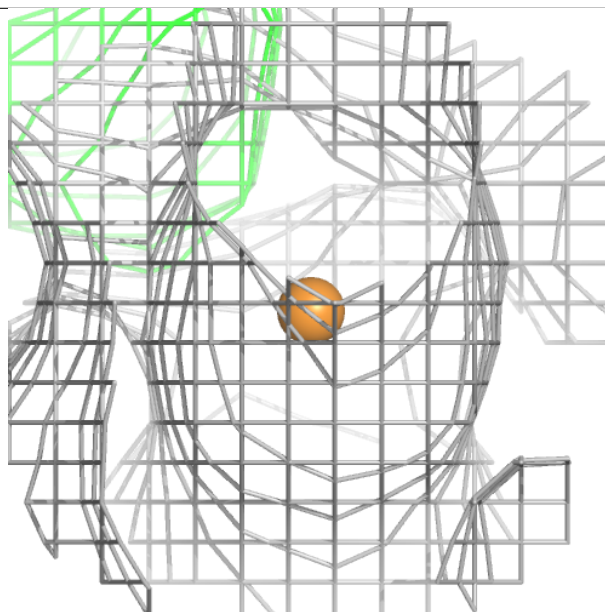
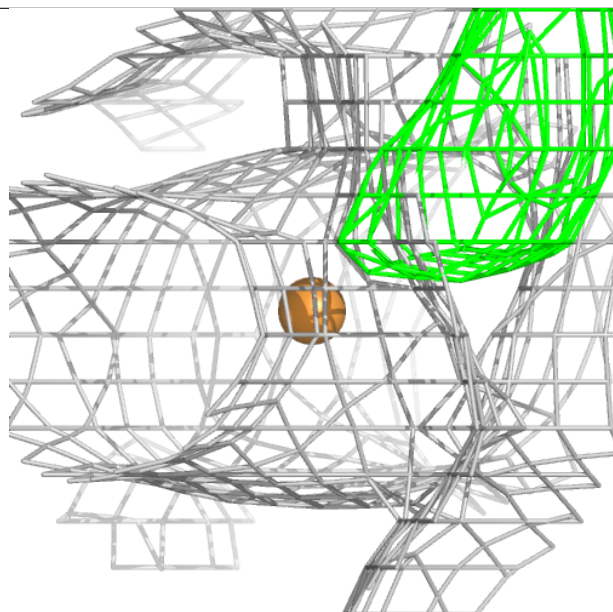
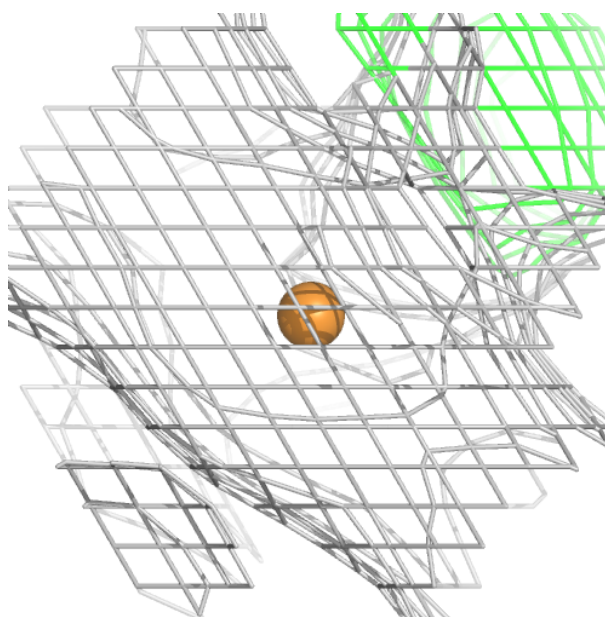
Electron density around SO4 C 601:

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



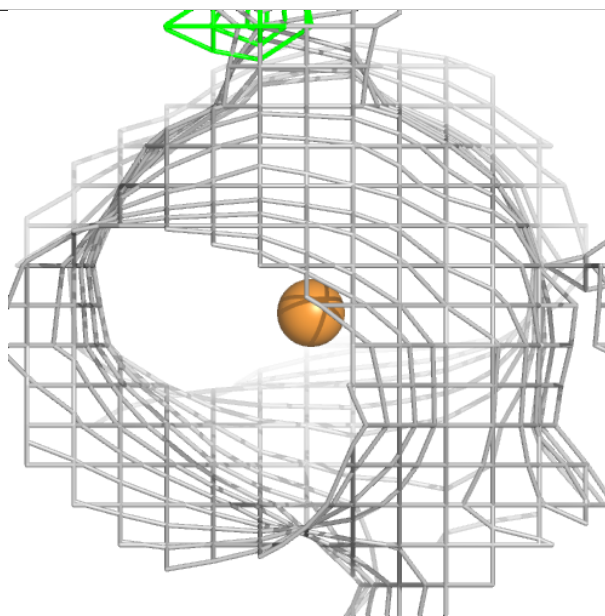
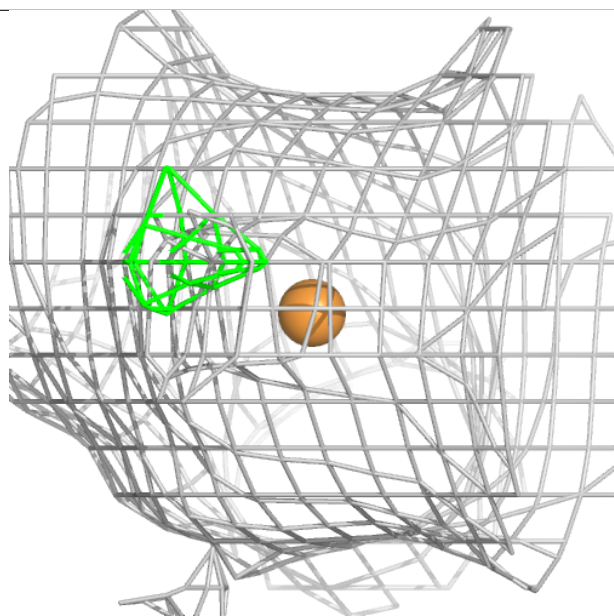
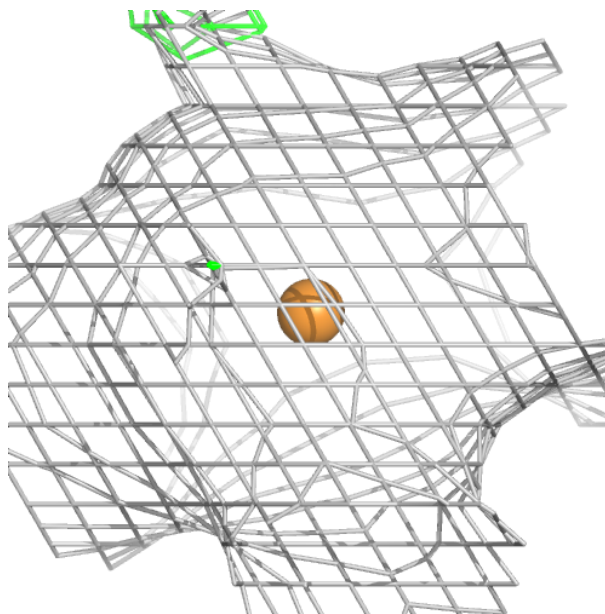
Electron density around CU B 603:

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



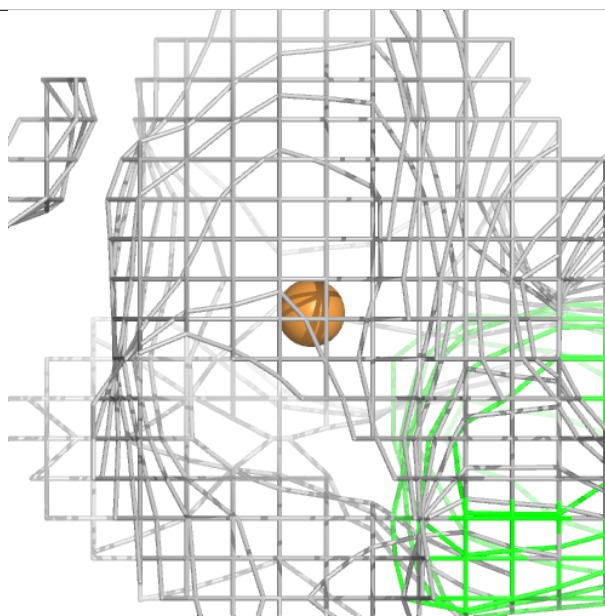
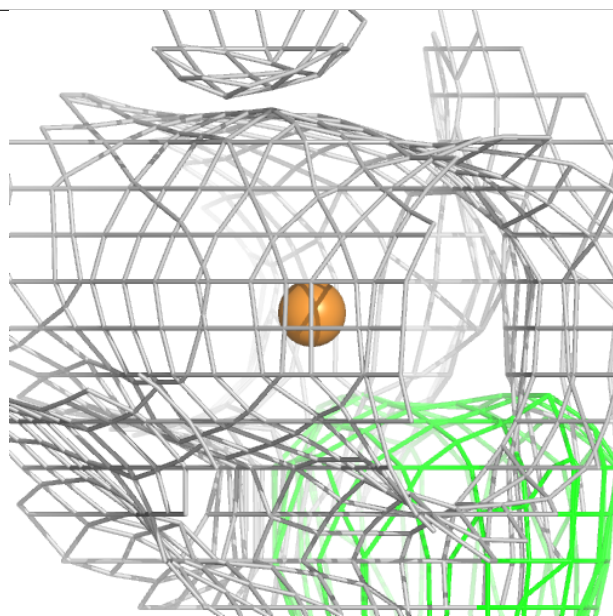
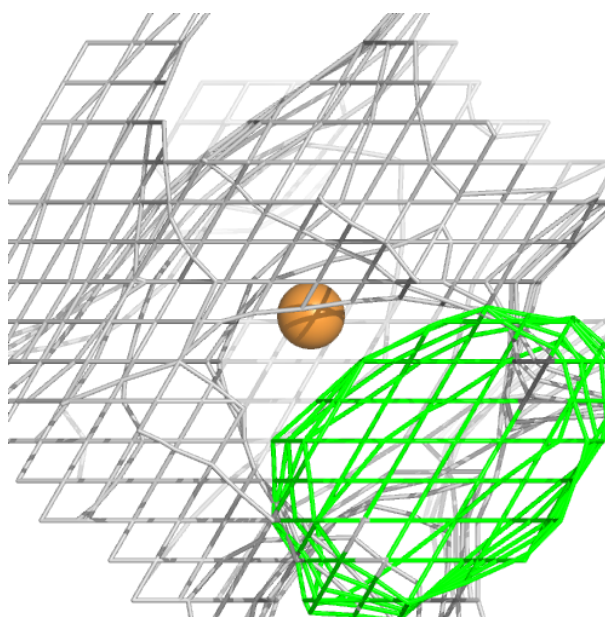
Electron density around CU A 604:

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



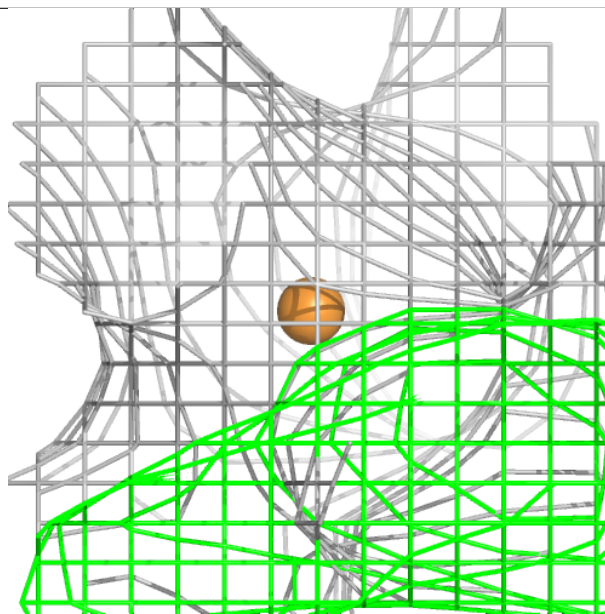
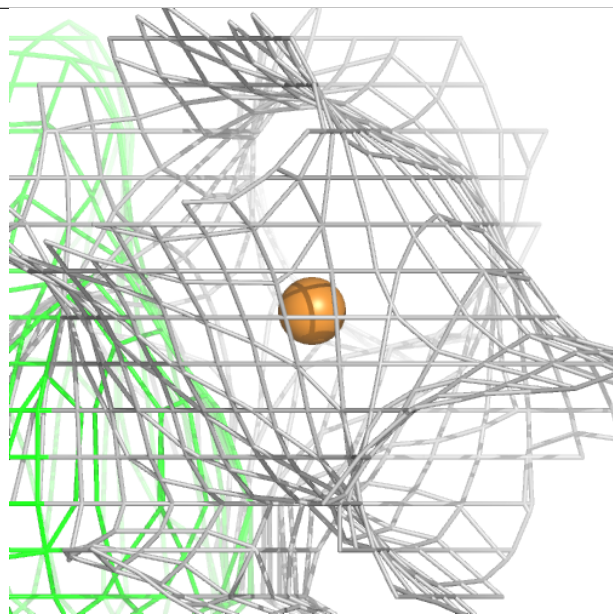
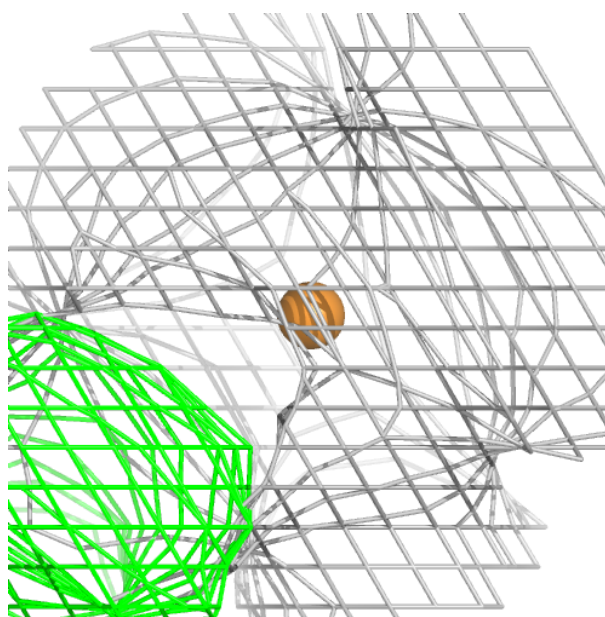
Electron density around CU A 601:

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



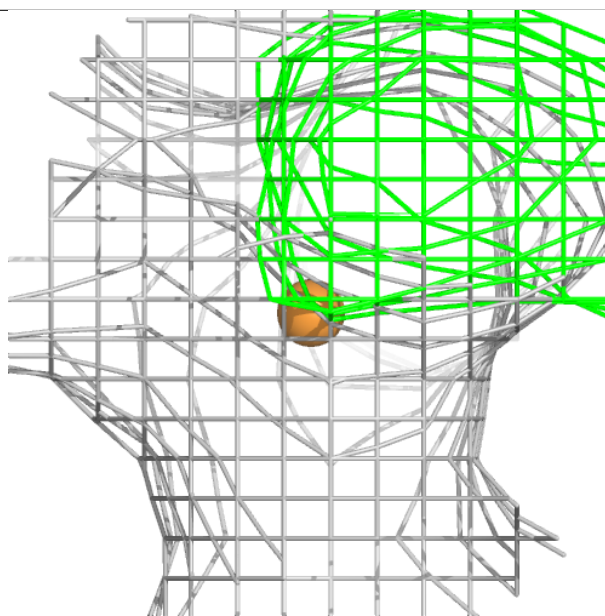
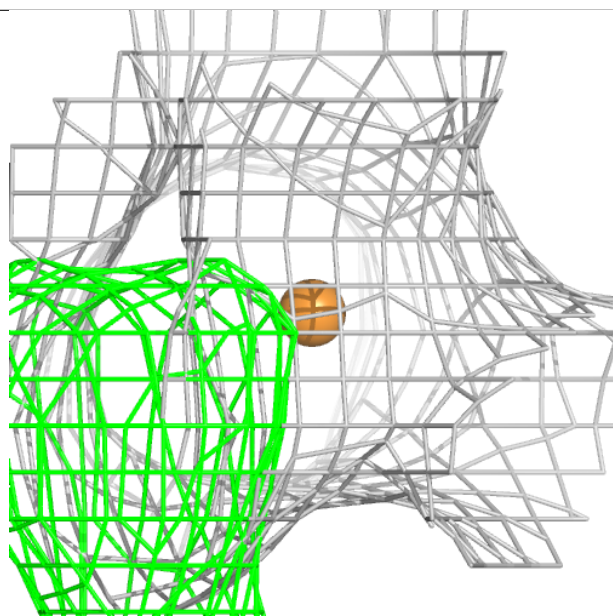
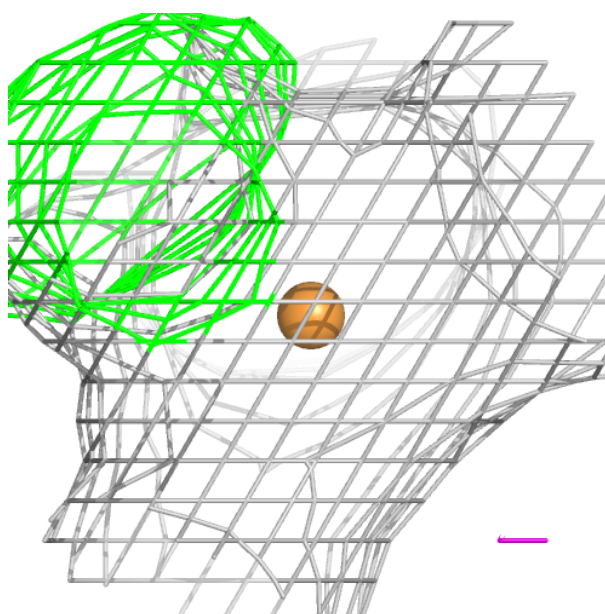
Electron density around CU A 602:

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



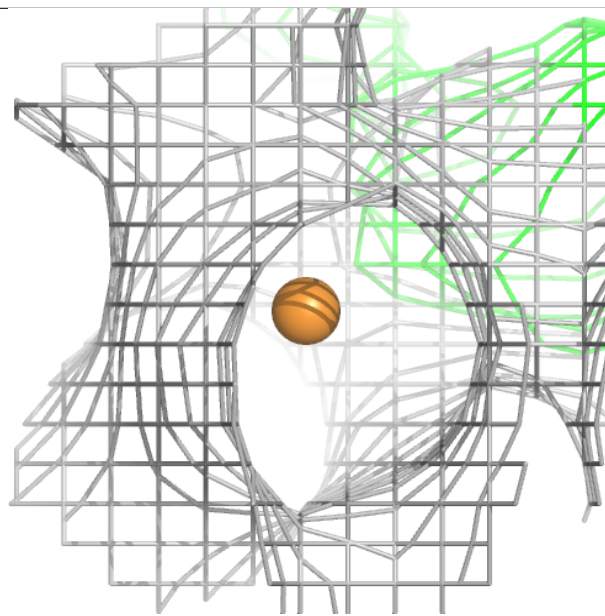
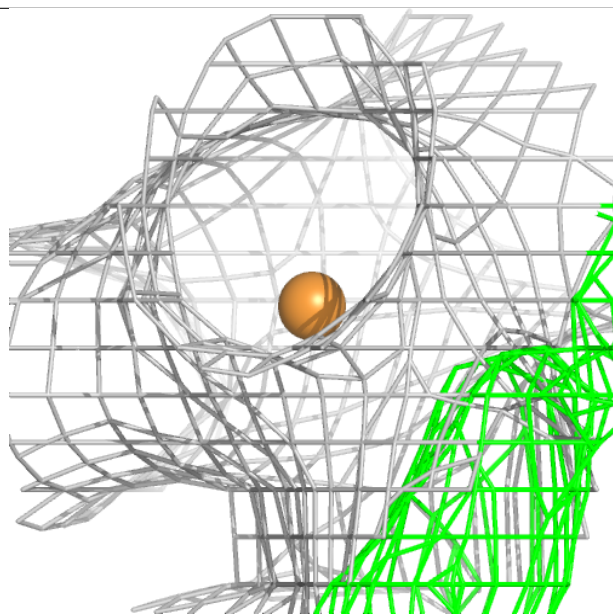
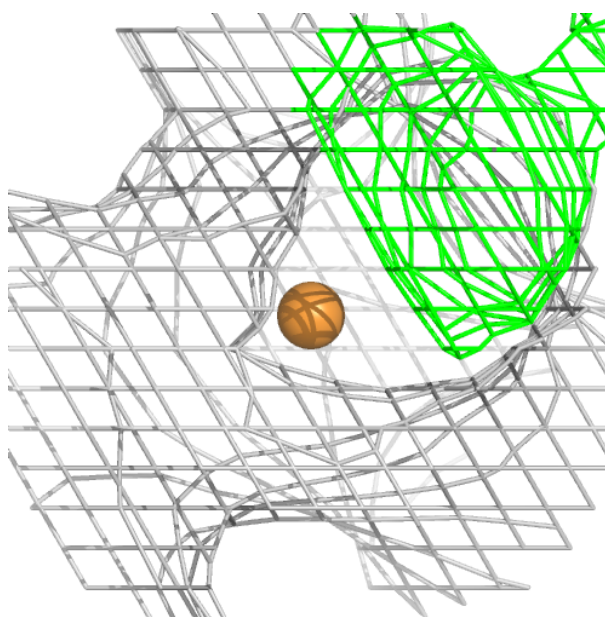
Electron density around CU A 603:

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



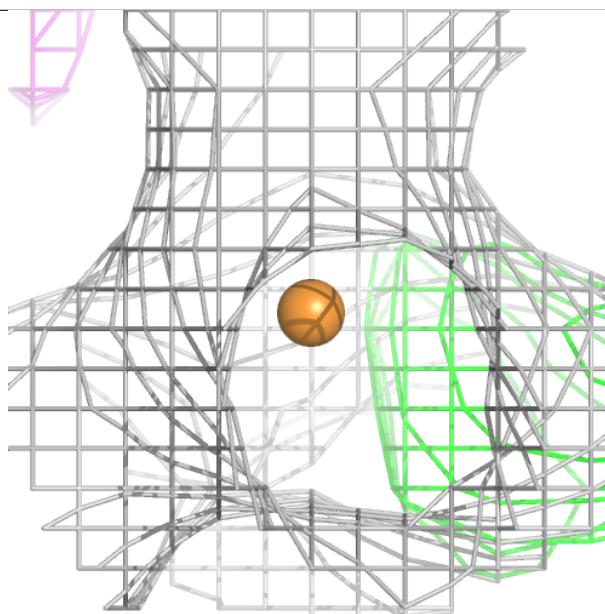
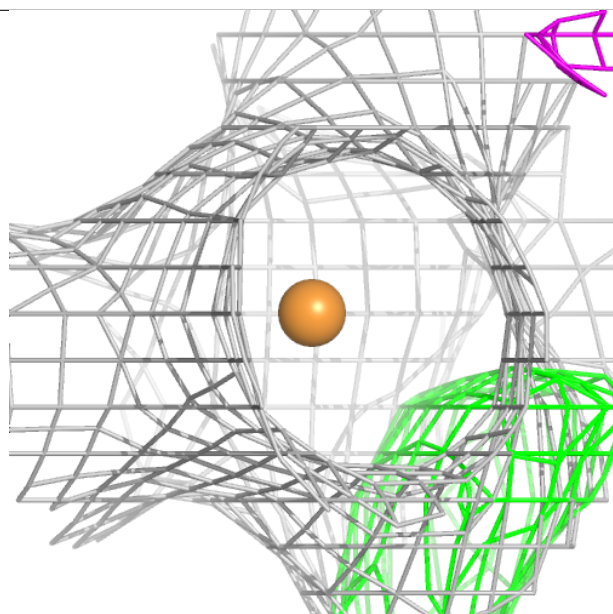
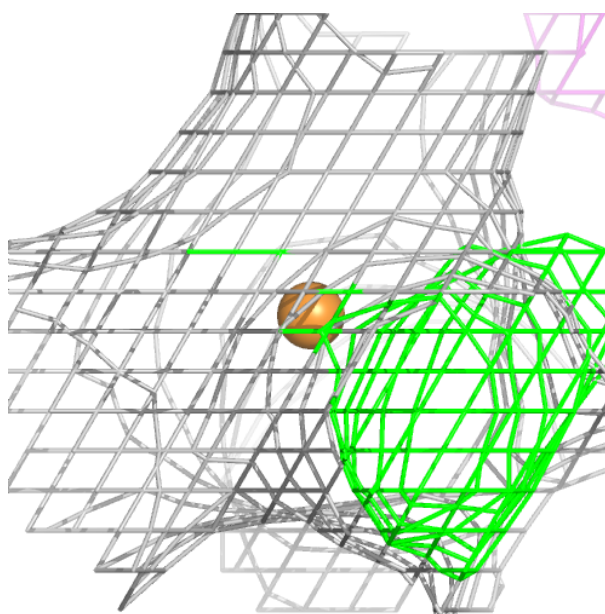
Electron density around CU B 601:

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



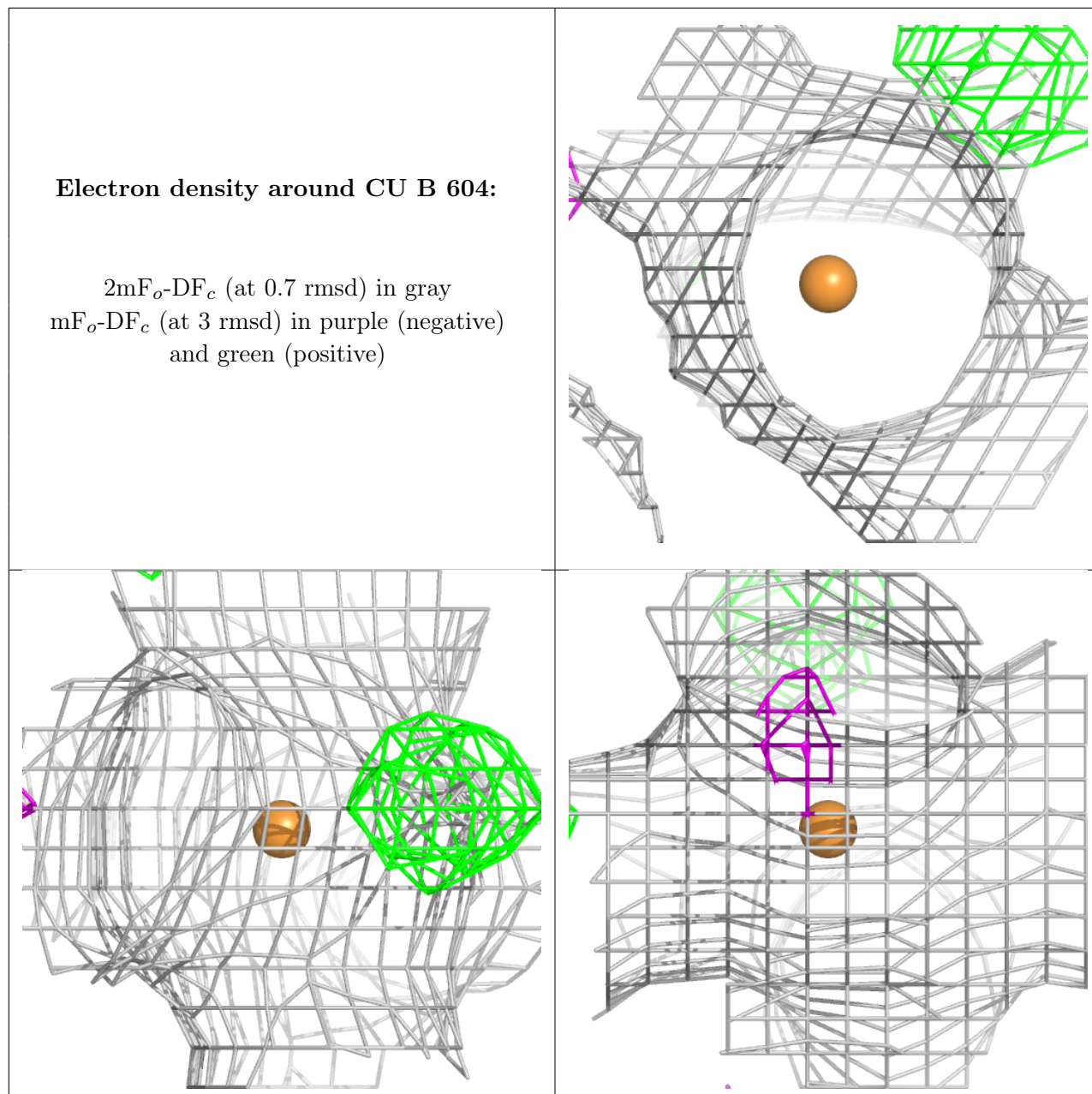
Electron density around CU B 602:

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



Electron density around CU 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.