WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2025 – 03:10 pm GMT

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)

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

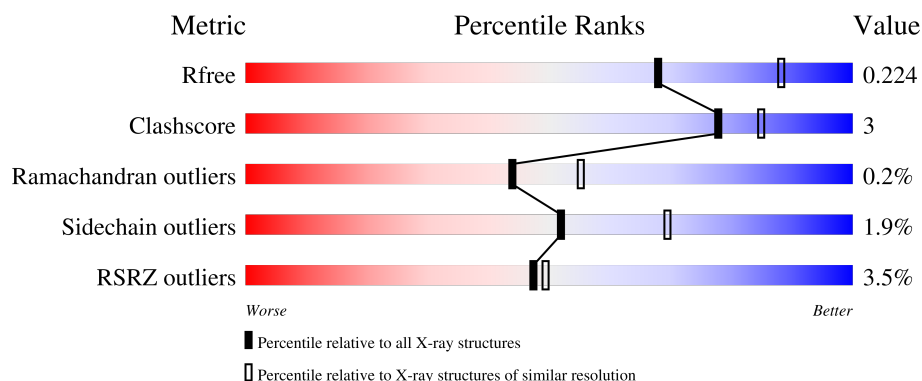|		
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	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:
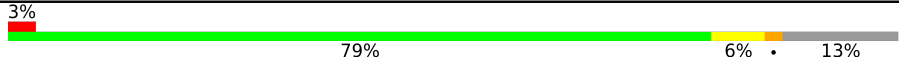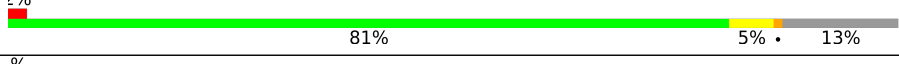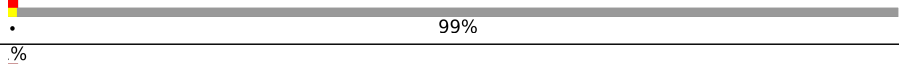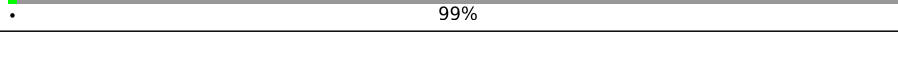*X-RAY DIFFRACTION*

The reported resolution of this entry is 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (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 <=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	3% 79% 6% · 13%
1	B	532	2% 81% 5% · 13%
1	C	532	.% · 99%
1	E	532	.% · 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 45	C 27	N 13	O 5		0	0	0
1	A	461	Total 3629	C 2319	N 619	O 679	S 12	0	1	0
1	B	462	Total 3628	C 2319	N 618	O 679	S 12	0	0	0
1	E	4	Total 30	C 18	N 8	O 4		0	0	0

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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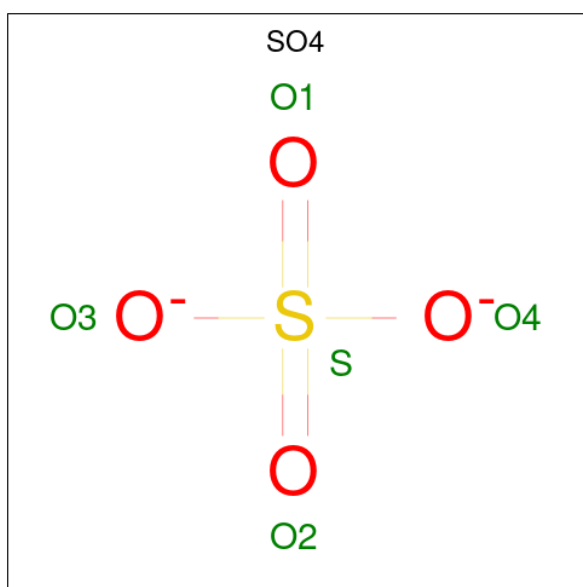
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP A0AB73HHR8
B	-14	HIS	-	expression tag	UNP A0AB73HHR8
B	-13	HIS	-	expression tag	UNP A0AB73HHR8
B	-12	SER	-	expression tag	UNP A0AB73HHR8
B	-11	SER	-	expression tag	UNP A0AB73HHR8
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: O_4S) (labeled as "Ligand of Interest" by depositor).

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

- 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 11	Cu 11	0	0
3	B	10	Total 10	Cu 10	0	0
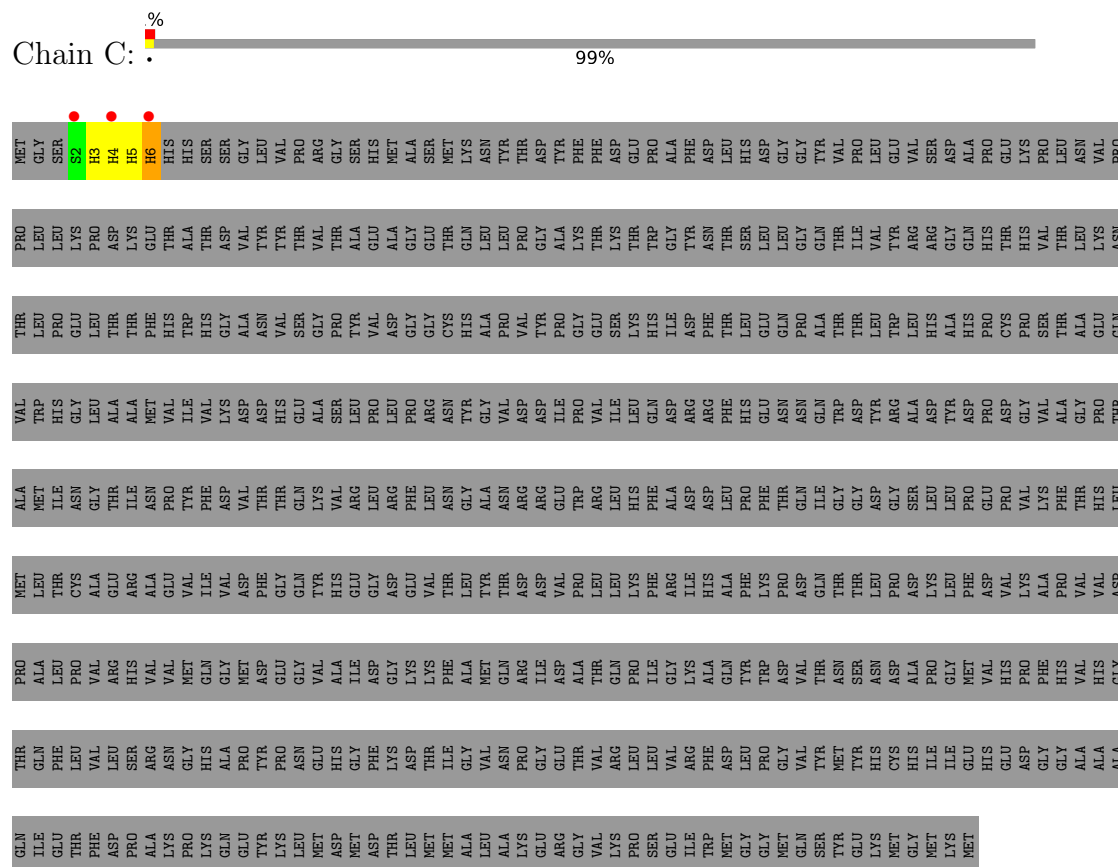
- Molecule 4 is water.

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
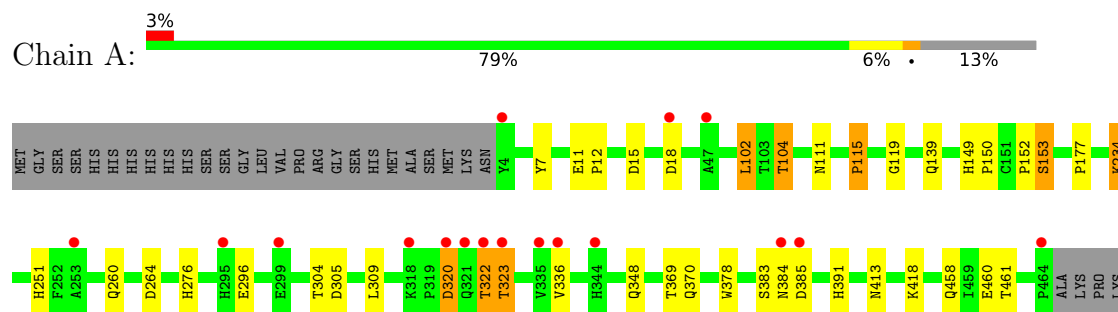
3 Residue-property plots ⓘ

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: Multicopper oxidase domain-containing protein
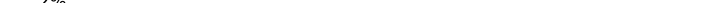
Chain C:

• Molecule 1: Multicopper oxidase domain-containing protein

Chain A:

GLN GLU TYR LYS MET LEU MET ASP ASP THR LEU MET MET ALA LEU ALA LYS GLU ARG GLY VAL 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 B:

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER MET LYS N3 Y7 D18 T46 L102 T103 T104 N111 P115 G119 Q139 A148 P152 S153 M165 A174 R180 P188 W248

H251 Q260 D264 H276 L277 M278 D305 D306 Q321 V336 M350 Q364 Q370 W378 N384 D385 N413 K418 P464 ALA LYS PRO LYS GLN GLU TYR LYS LEU MET ASP MET ASP THR LEU MET ALA LEU ALA LYS GLU ARG GLY VAL 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 H5 H6 HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER MET LYS ASN TYR THR ASP TYR PHE PHE ASP GLU PRO ALA PHE ASP LEU HIS ASP GLY TYR VAL PRO LEU GLU VAL SER ASP ALA PRO GLU LYS PRO LEU ASN VAL PRO

PRO LEU LEU LYS PRO ASP LYS GLU THR ALA THR ASP VAL TYR THR THR VAL THR ALA GLU ALA GLY GLU THR GLN LEU LEU PRO GLY ALA LYS THR TRP GLY TYR ASN GLY SER LEU LEU GLY PRO ALA THR ILE VAL TYR ARG ARG GLY GLN HIS THR HIS VAL THR LEU LYS ASN

THR LEU PRO GLU LEU THR THR PHE HIS TRP HIS GLY ALA ASN VAL SER GLY PRO TYR VAL ASP GLY GLY CYS HIS ALA PRO VAL TYR PRO GLY GLU SER LYS ILE ASP PHE LEU GLU GLN PRO ALA THR THR LEU TRP LEU HIS ALA HIS PRO CYS PRO SER THR ALA GLU GLN

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

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

MET LEU THR CYS ALA GLU ARG ALA GLU VAL ILE VAL ASP PHE GLY GLN TYR HIS ASP ASP VAL THR LEU TYR THR ASP ASP VAL LEU PHE ASP ALA PHE LYS PRO ASP GLN THR LEU PRO ASP LYS LEU PHE ASP VAL LYS ALA PRO VAL VAL ASP

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

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

GLN ILE GLU THR PHE ASP PRO ALA LYS PRO LYS GLN GLU TYR LYS LEU MET ASP MET ASP THR LEU MET ALA LEU ALA LYS GLU ARG GLY VAL LYS PRO SER GLU ILE TRP MET GLY GLY MET GLN SER TYR GLU LYS MET GLY MET LYS MET

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< |L| > = 0.49, < L^2 > = 0.33$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	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(^{o})	Ideal(^{o})
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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	44	55
1	B	460/532 (86%)	445 (97%)	14 (3%)	1 (0%)	44	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%)	44	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 ⓘ

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%)	48	66
1	B	384/452 (85%)	379 (99%)	5 (1%)	65	79
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%)	52	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	0.33	0	6,6,6	0.16	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 then 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.

Ligand SO4 C 601
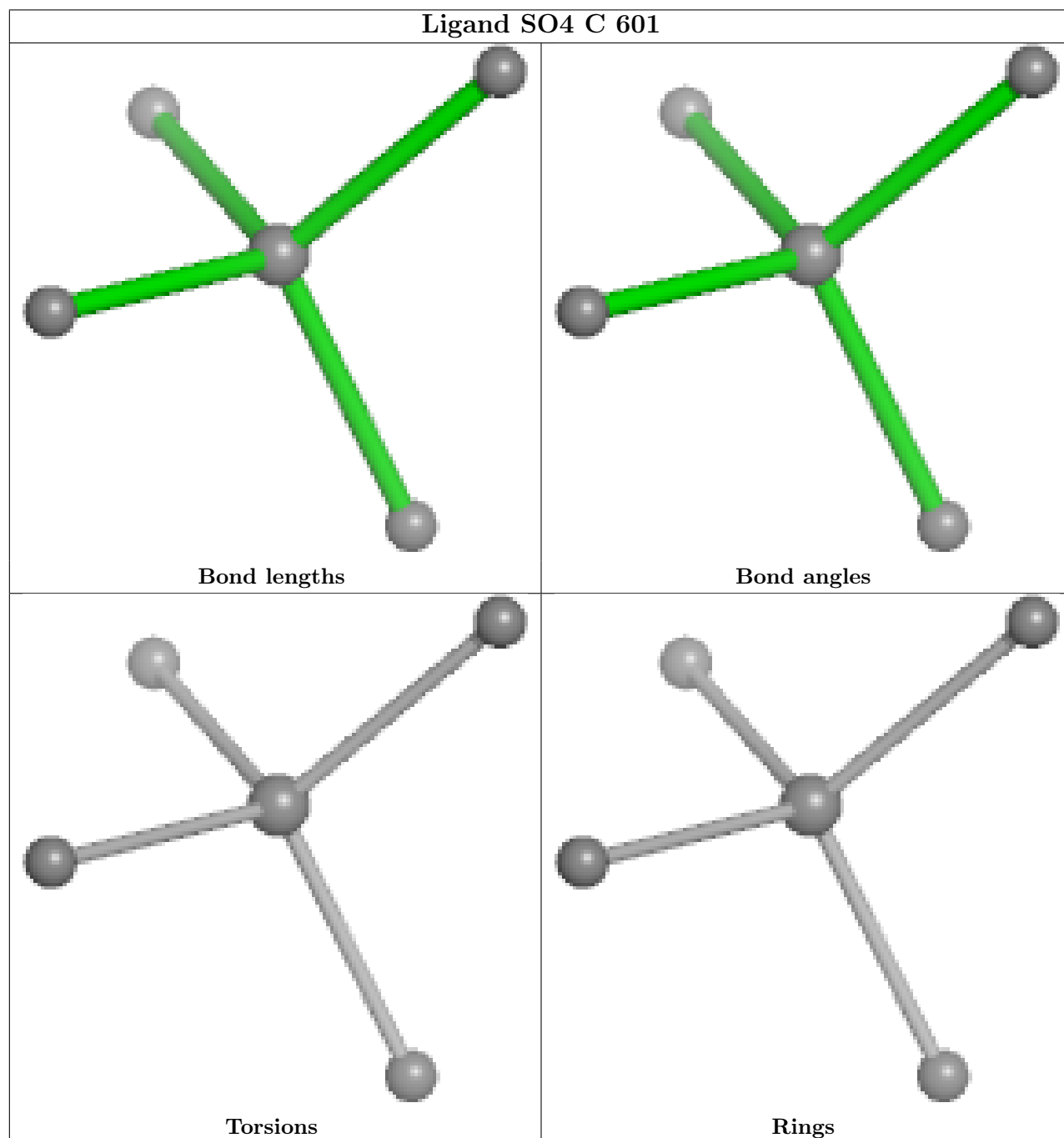
5.7 Other polymers (i)

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, 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(Å²)	Q<0.9
1	A	461/532 (86%)	0.00	17 (3%)	45	47	21, 43, 65, 113	1 (0%)
1	B	462/532 (86%)	-0.03	9 (1%)	66	67	33, 44, 66, 87	0
1	C	5/532 (0%)	2.94	3 (60%)	0	0	54, 60, 74, 75	0
1	E	4/532 (0%)	6.19	4 (100%)	0	0	100, 108, 110, 111	0
All	All	932/2128 (43%)	0.03	33 (3%)	47	49	21, 44, 68, 113	1 (0%)

All (33) 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	7.2
1	B	3	ASN	6.4
1	A	322	THR	6.2
1	A	323	THR	6.0
1	A	321	GLN	5.5
1	E	6	HIS	5.4
1	B	385	ASP	4.3
1	E	5	HIS	4.2
1	A	464	PRO	3.8
1	B	464	PRO	3.7
1	A	4	TYR	3.5
1	A	47	ALA	3.2
1	A	335	VAL	3.2
1	B	384	ASN	3.1
1	B	18	ASP	3.0
1	A	253	ALA	3.0
1	C	4	HIS	2.9
1	A	295	HIS	2.9
1	C	6	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	384	ASN	2.7
1	A	318	LYS	2.6
1	A	344[A]	HIS	2.5
1	A	18	ASP	2.4
1	B	46	THR	2.3
1	B	153	SER	2.3
1	A	385	ASP	2.3
1	A	320	ASP	2.2
1	B	350	MET	2.2
1	B	364	GLN	2.1
1	A	299	GLU	2.0
1	A	336	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
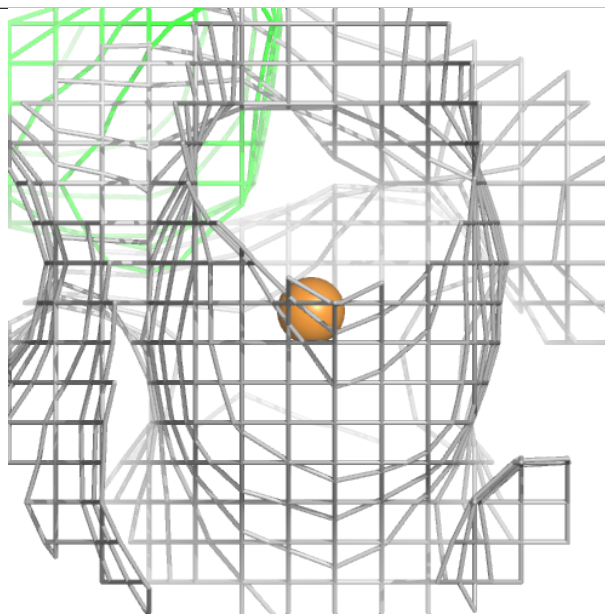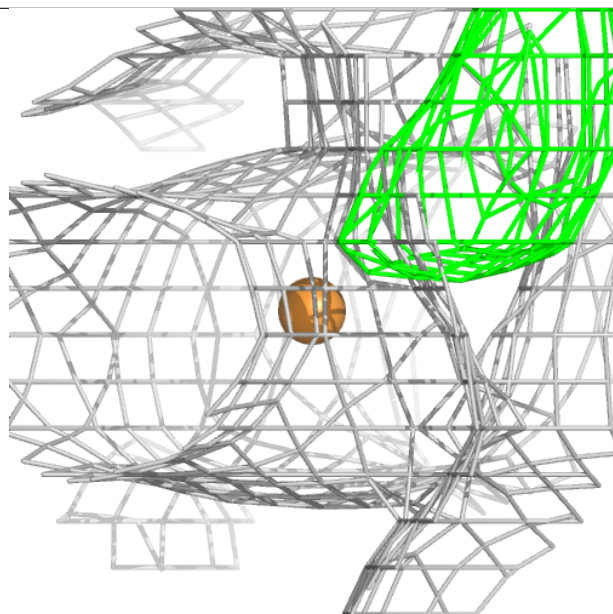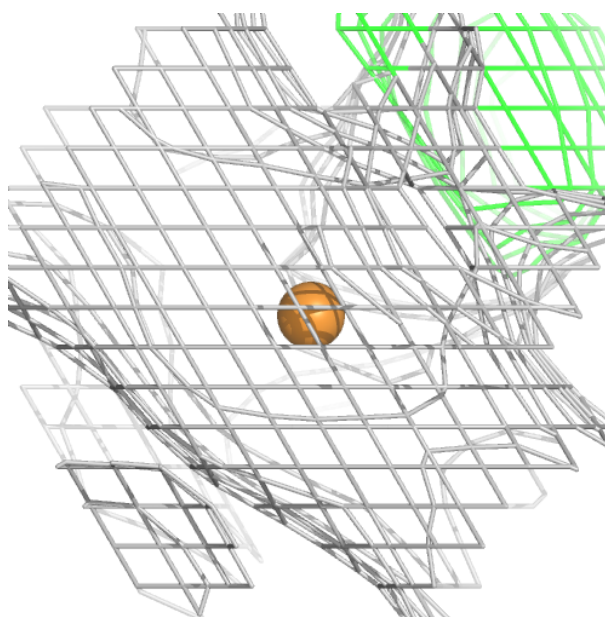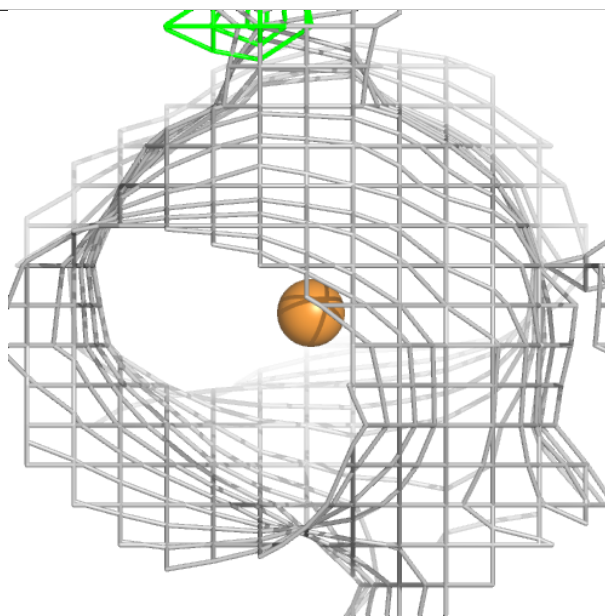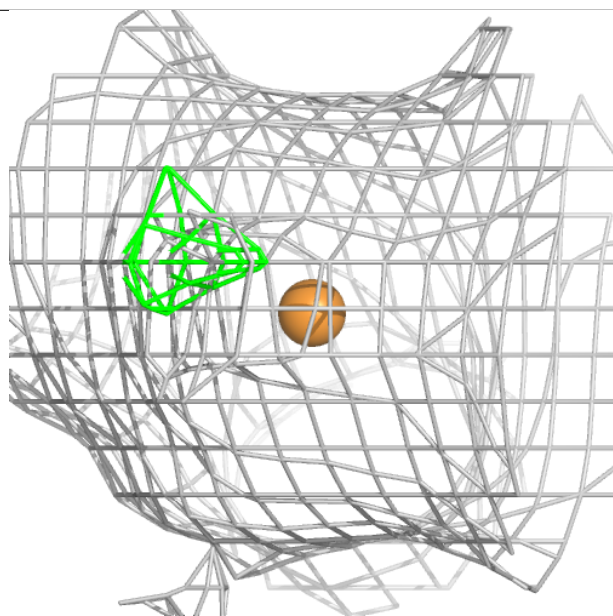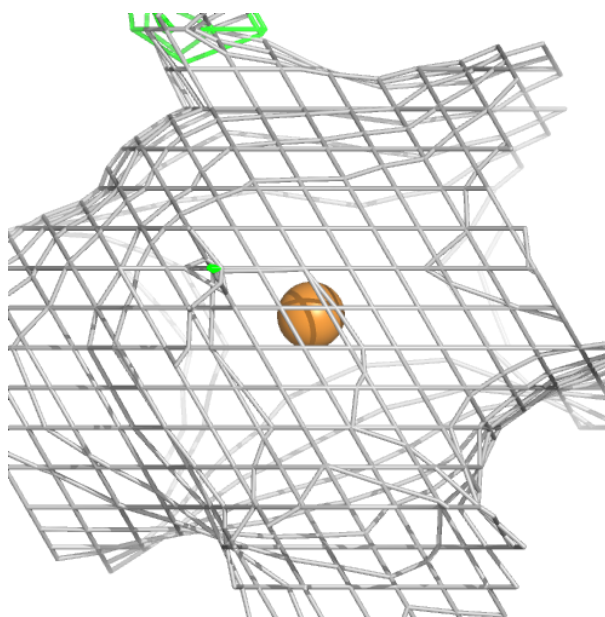$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
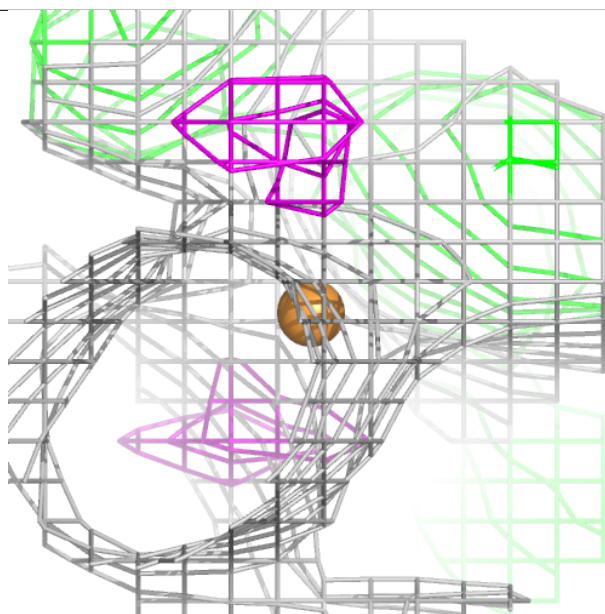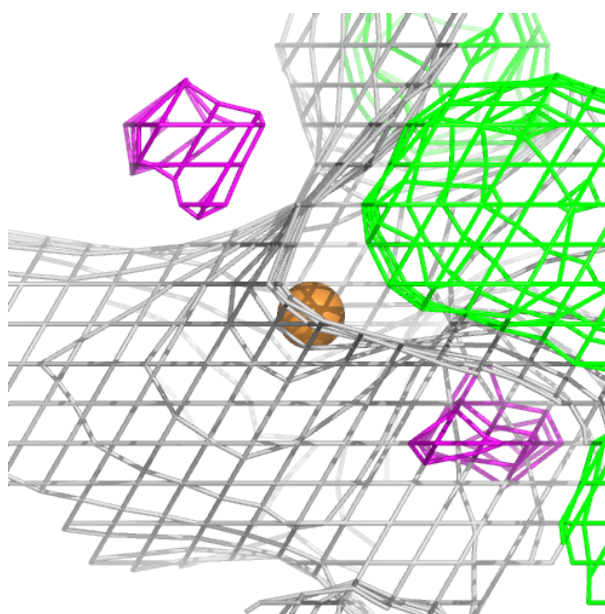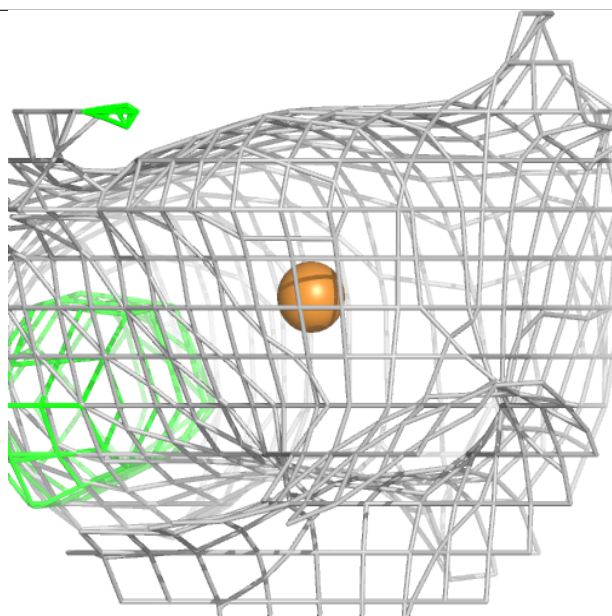
Electron density around CU A 611:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
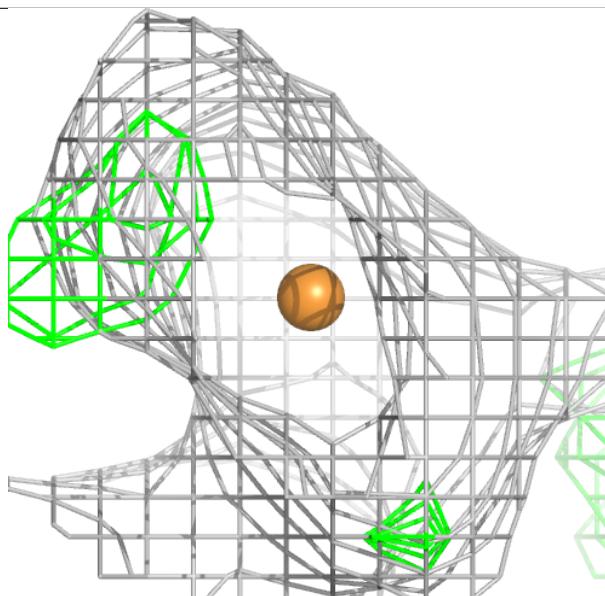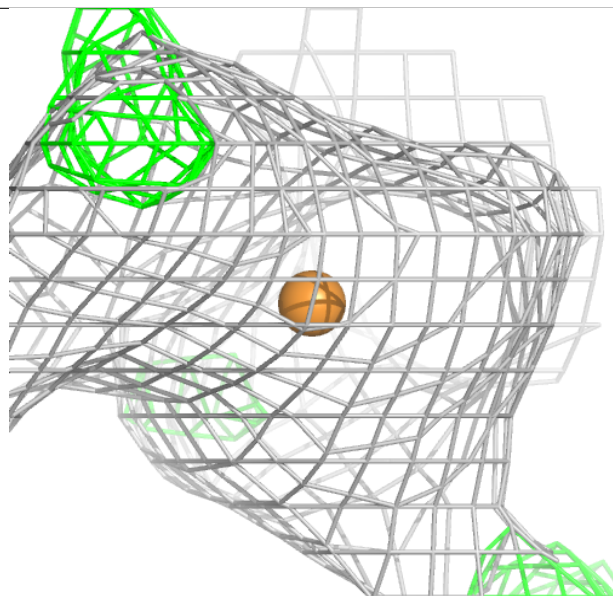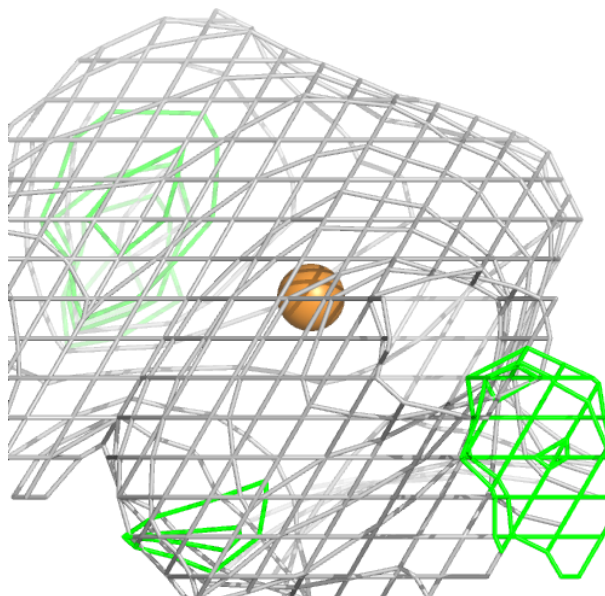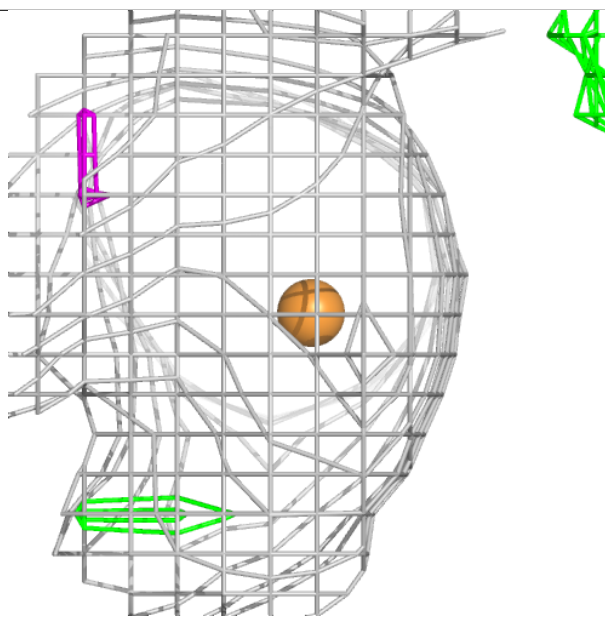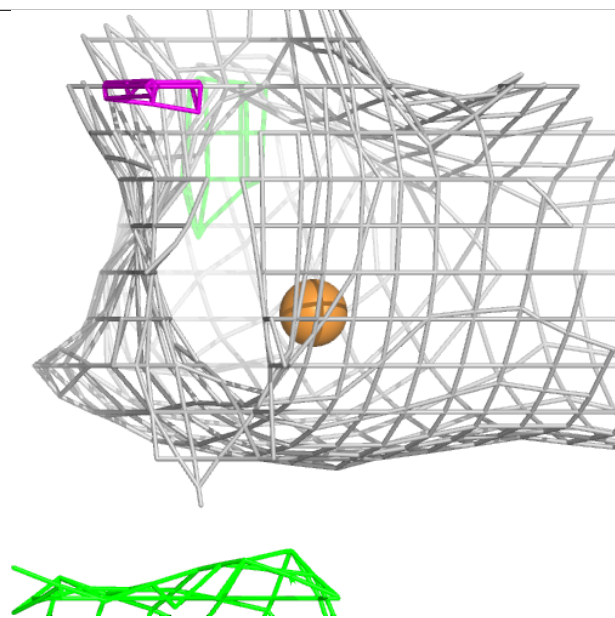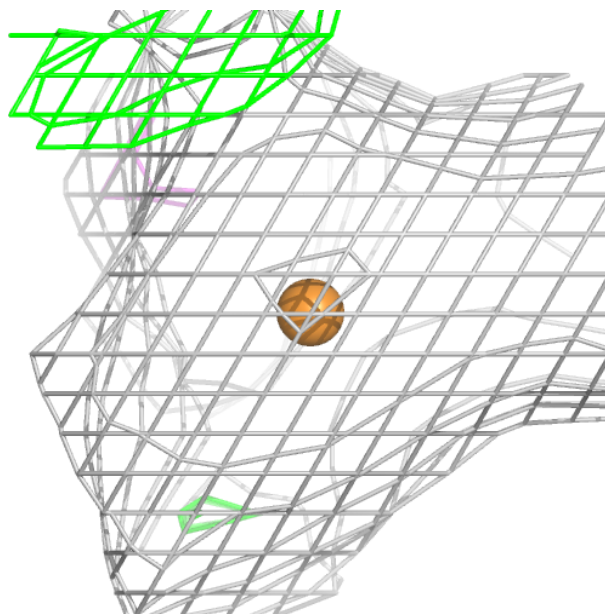
Electron density around CU B 609:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
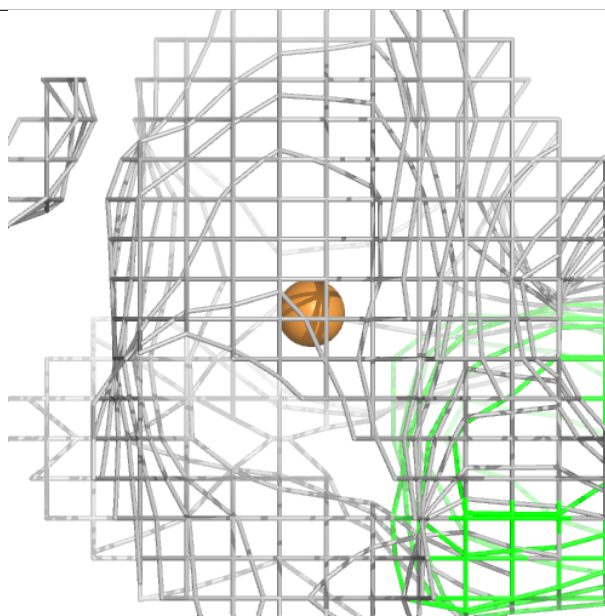$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
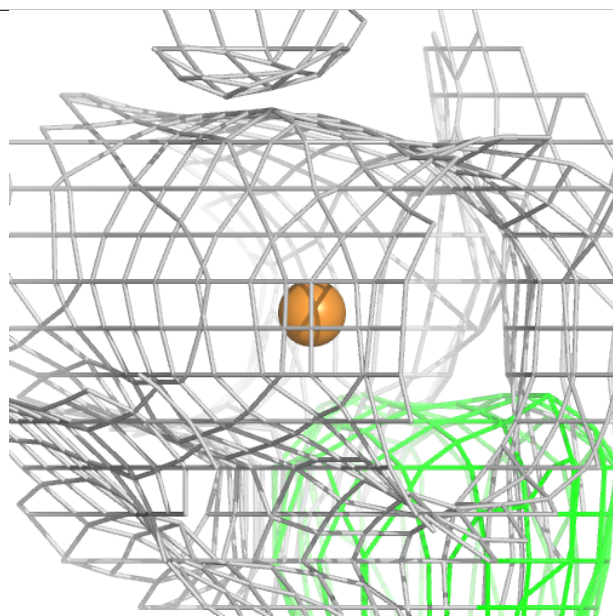and green (positive)
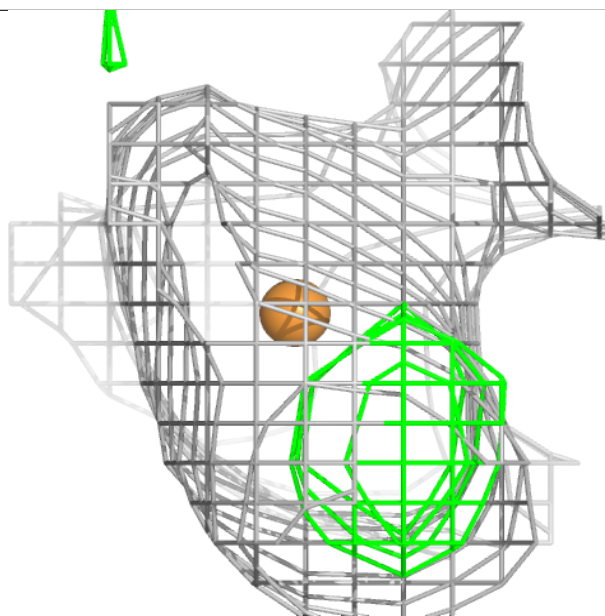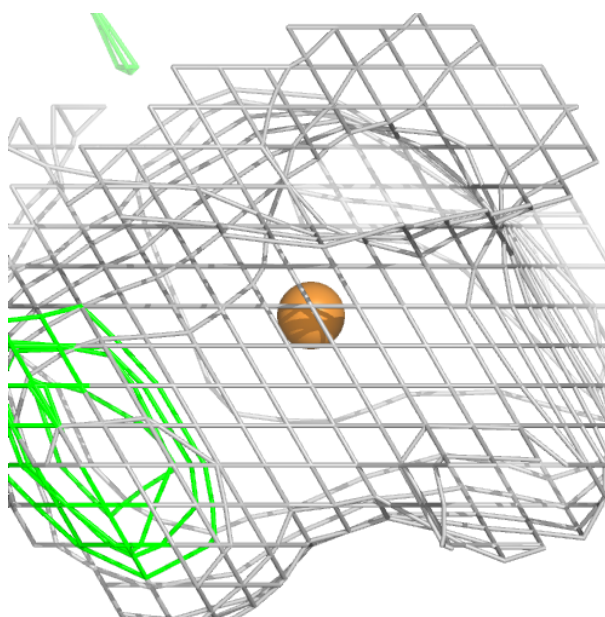
Electron density around CU A 607:

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

Electron density around CU B 608:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
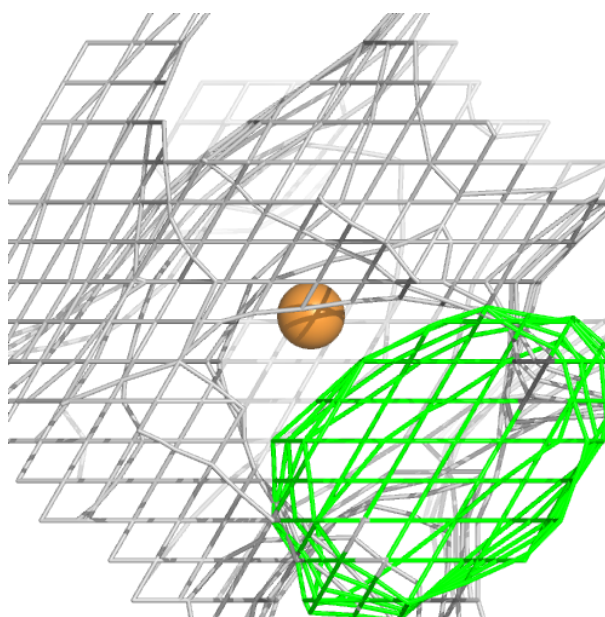$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
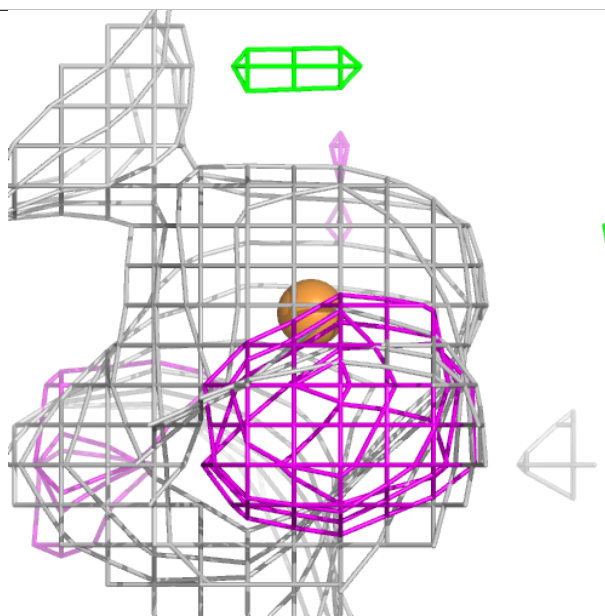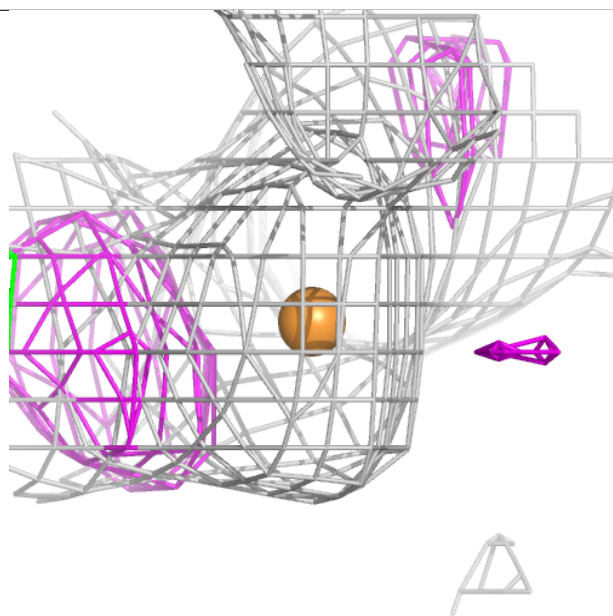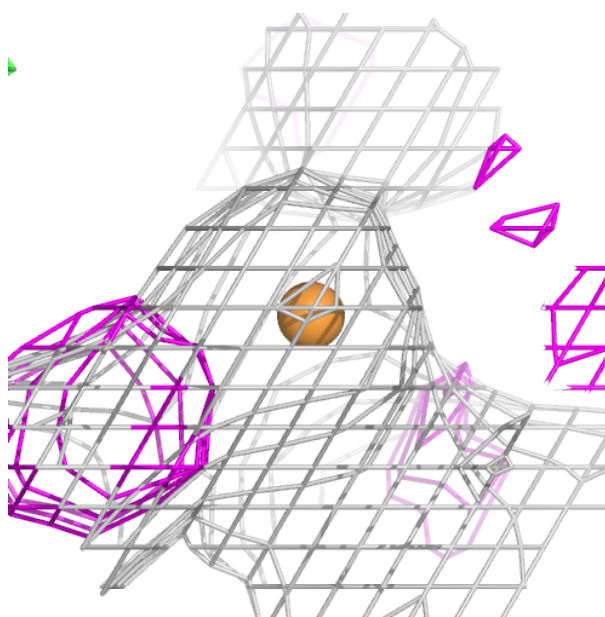
Electron density around CU A 610:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
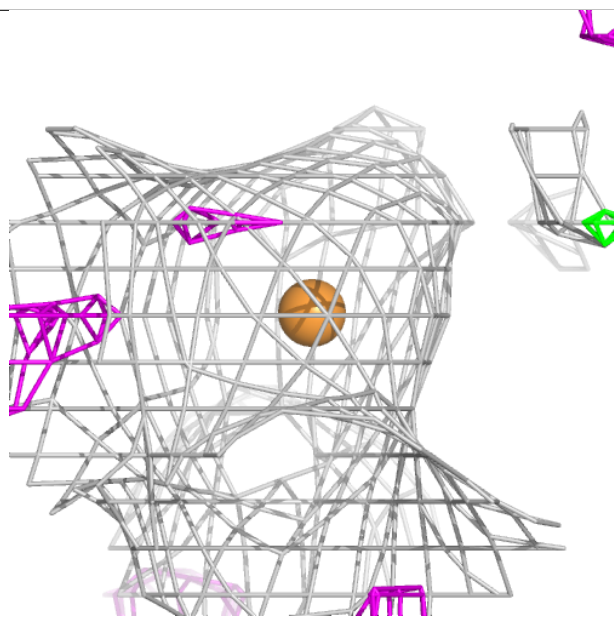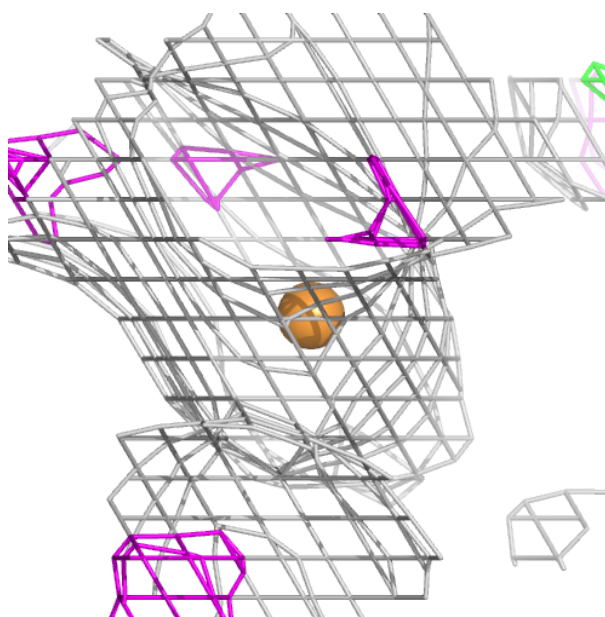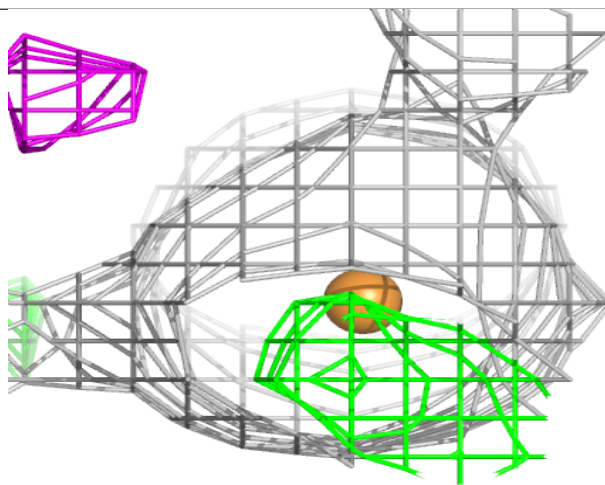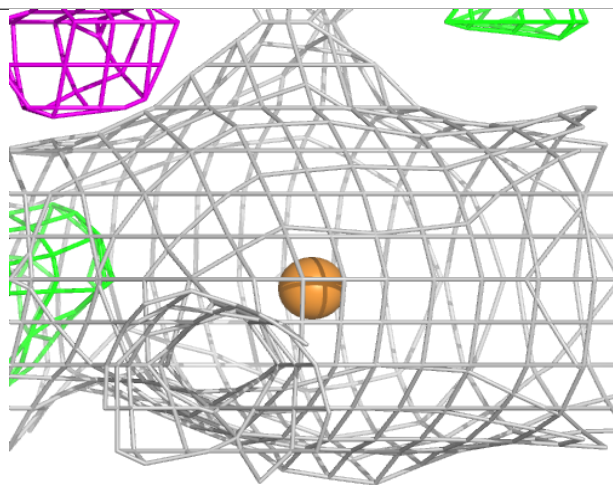
Electron density around CU B 607:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
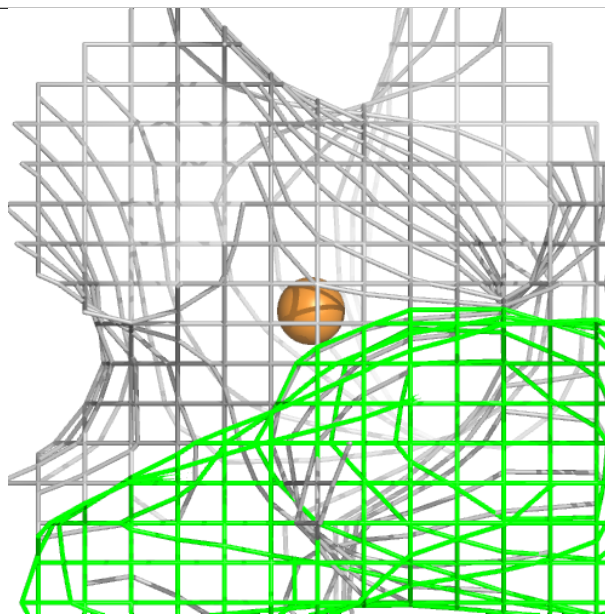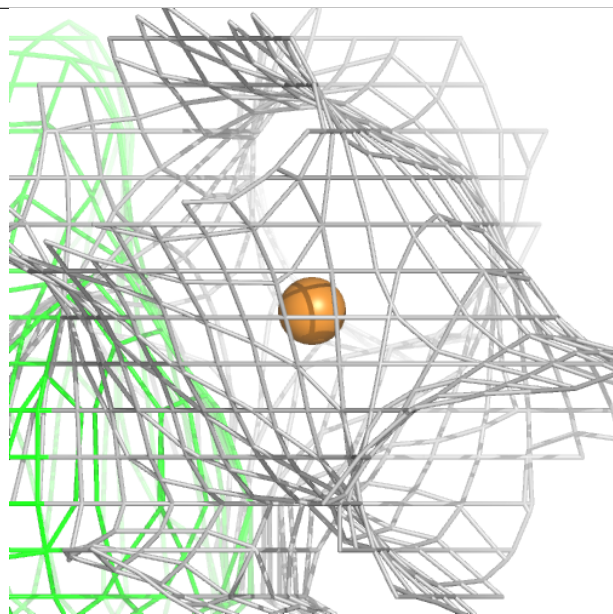$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
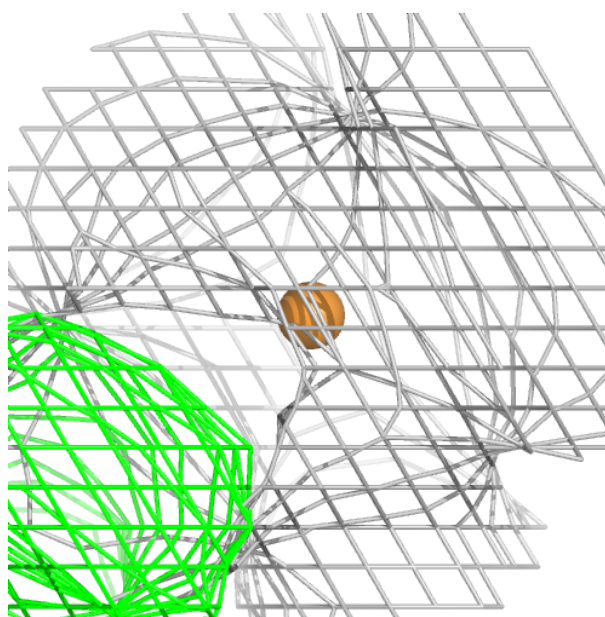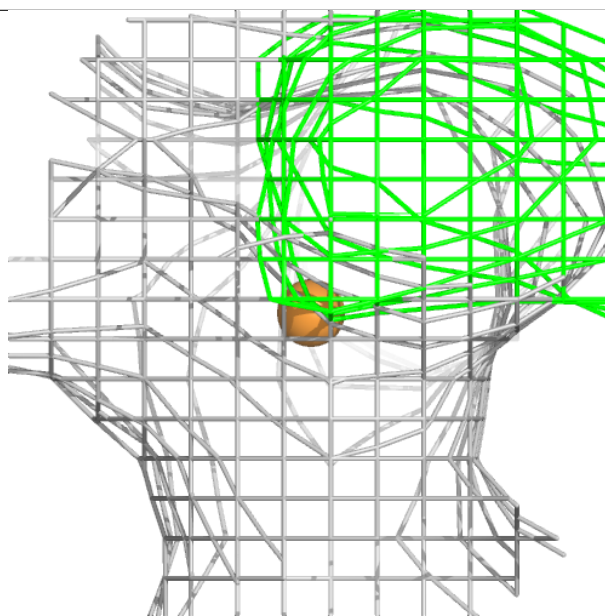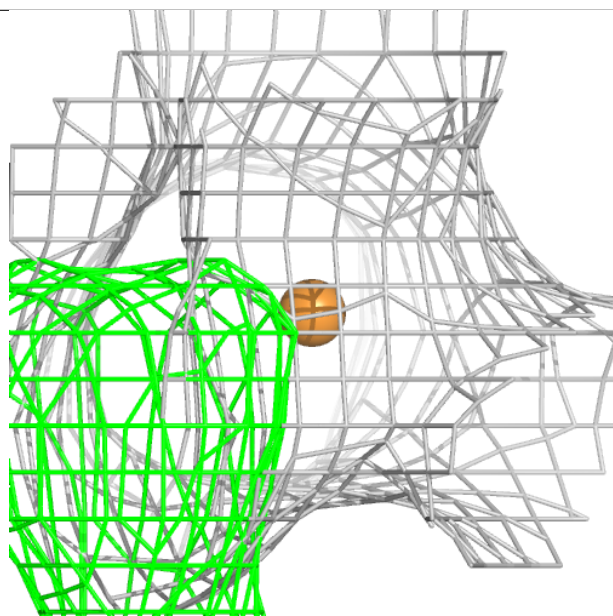and green (positive)
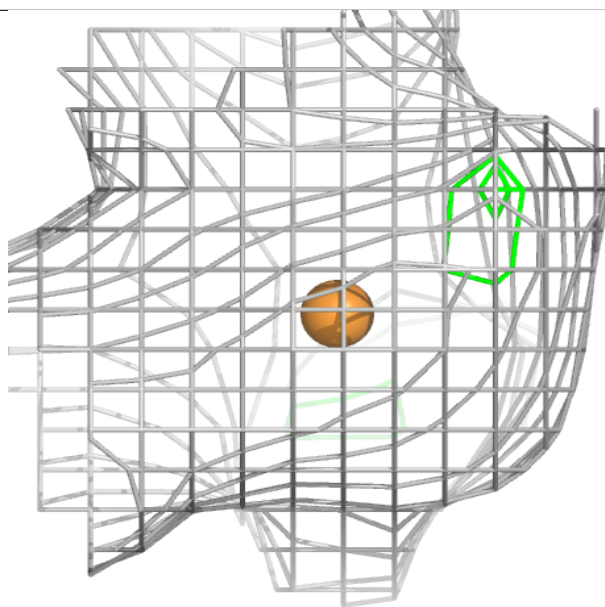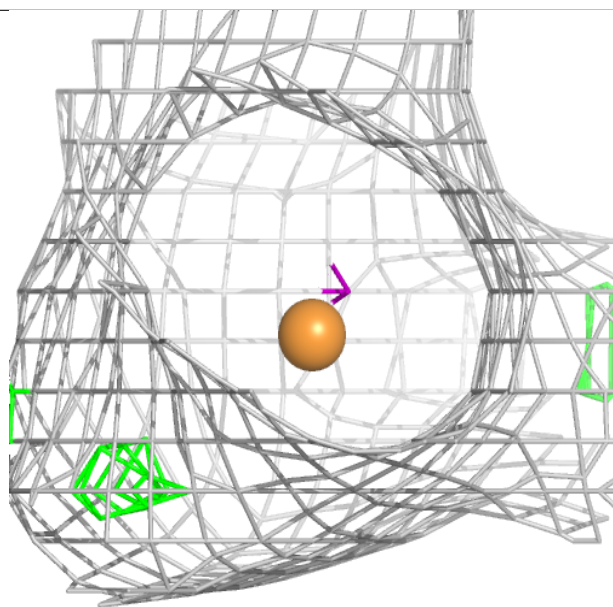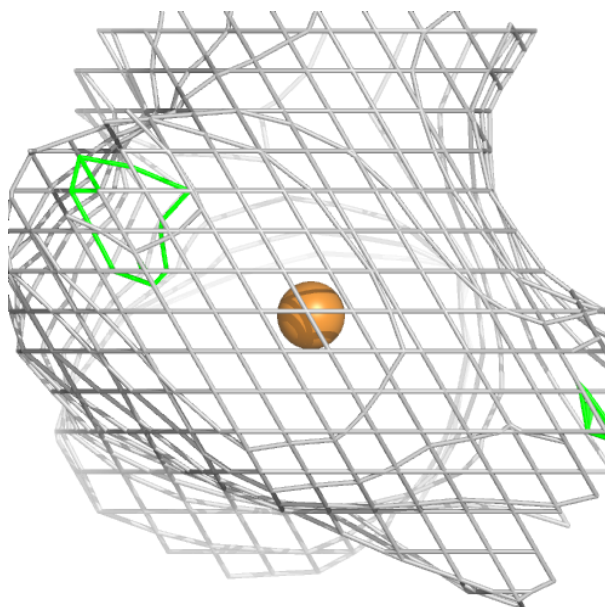
Electron density around CU A 609:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
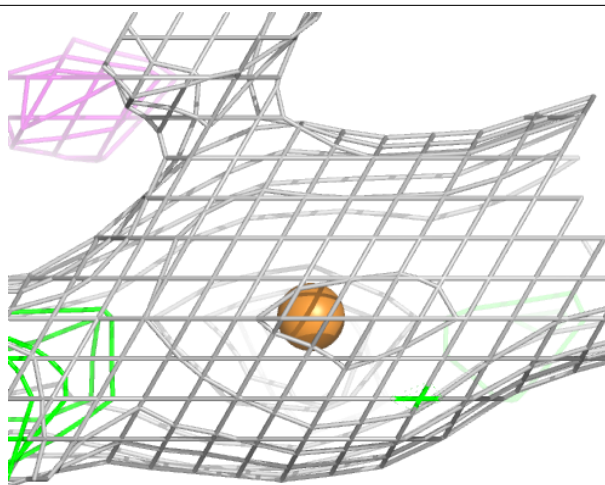
Electron density around CU A 606:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
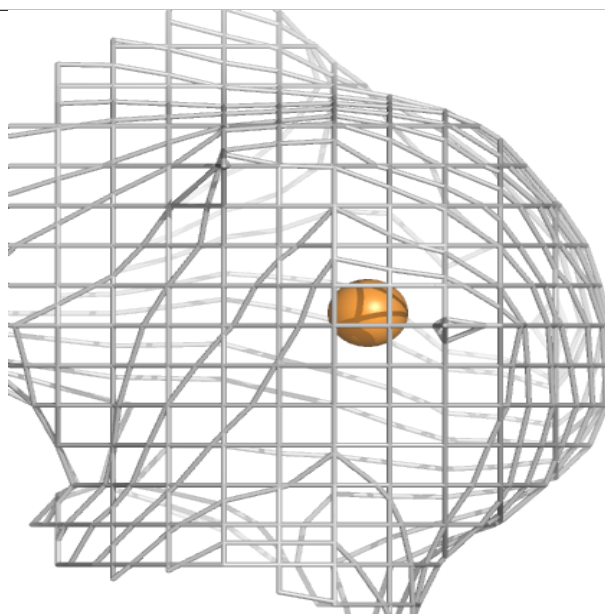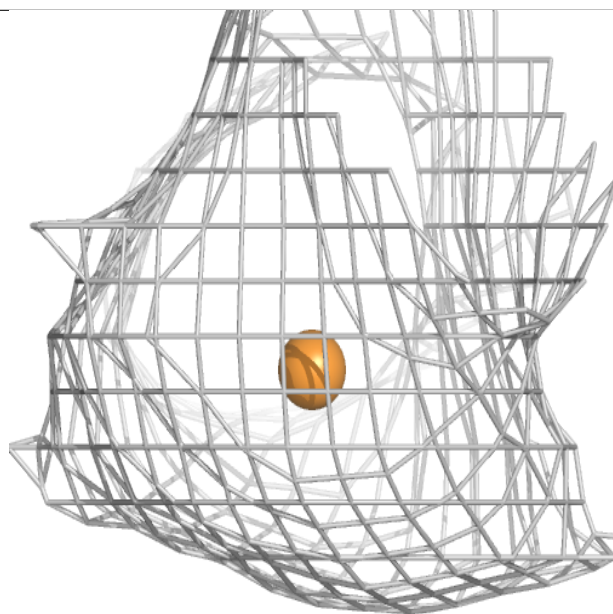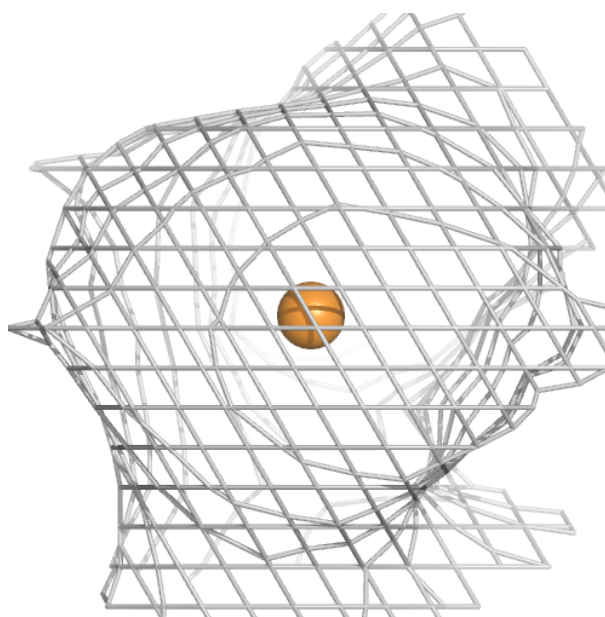
Electron density around CU B 606:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
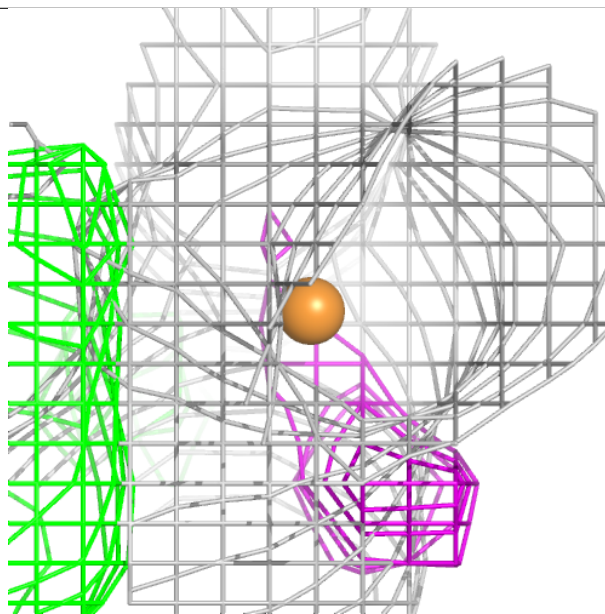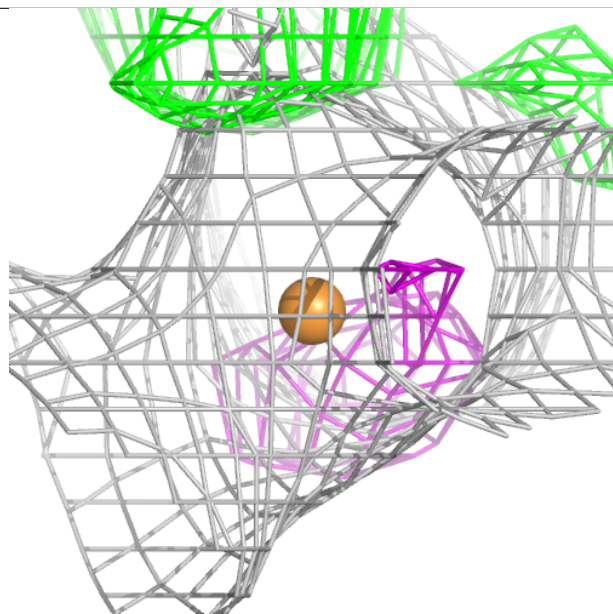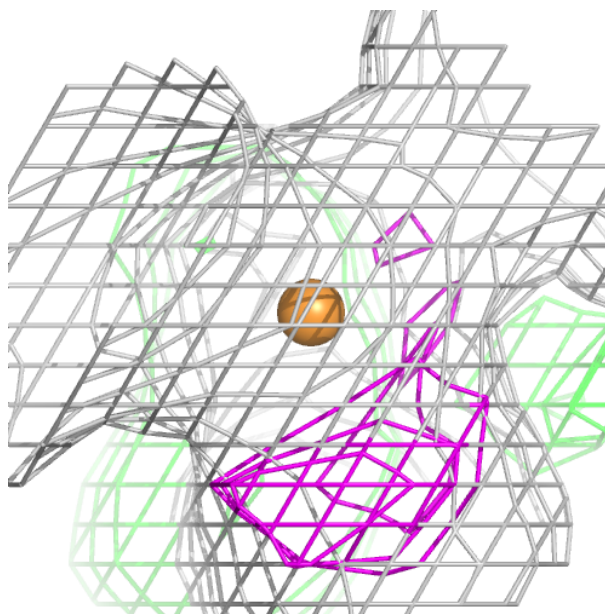
Electron density around CU A 605:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
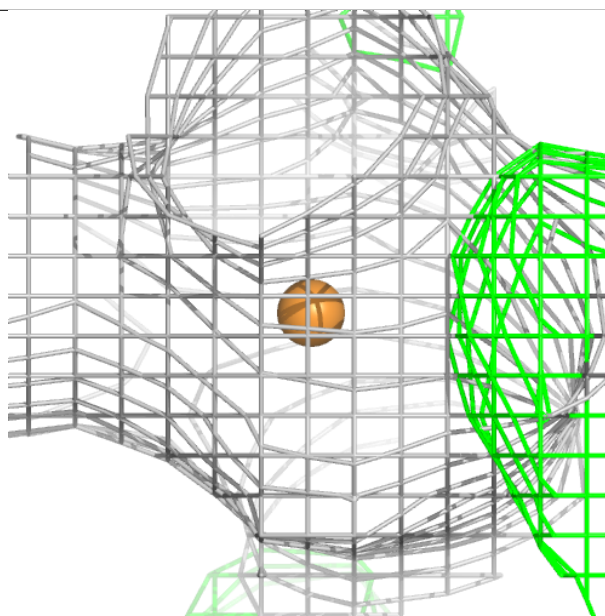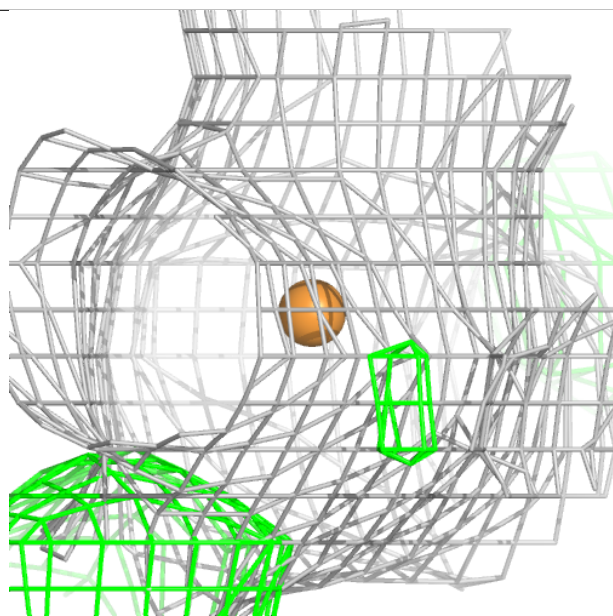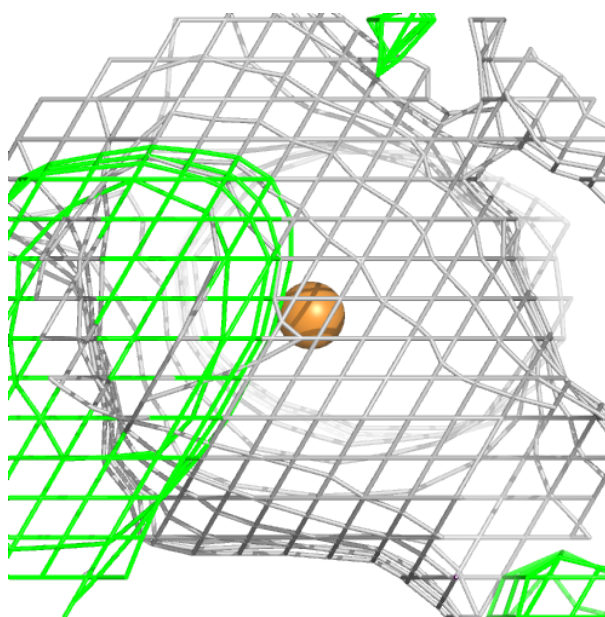
Electron density around CU A 608:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
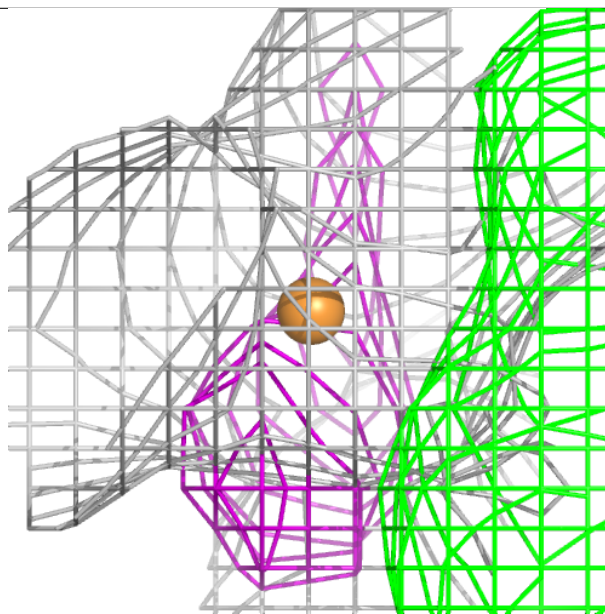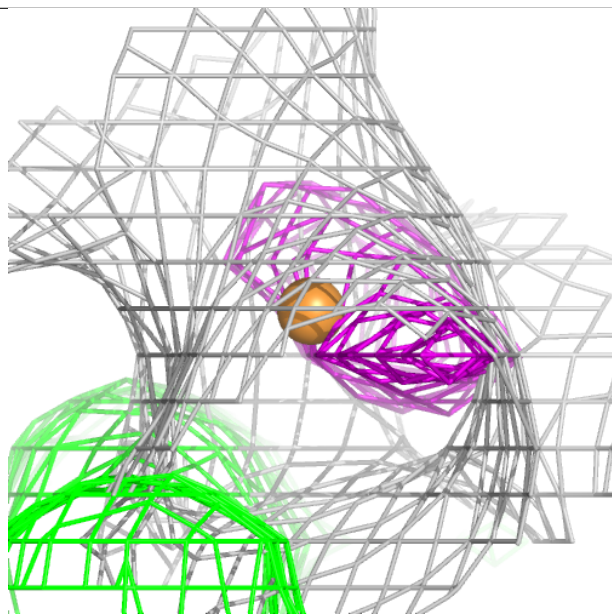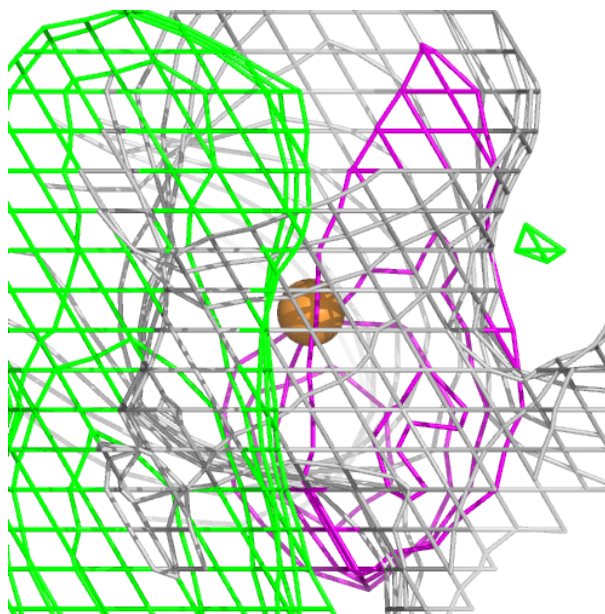
Electron density around CU B 605:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
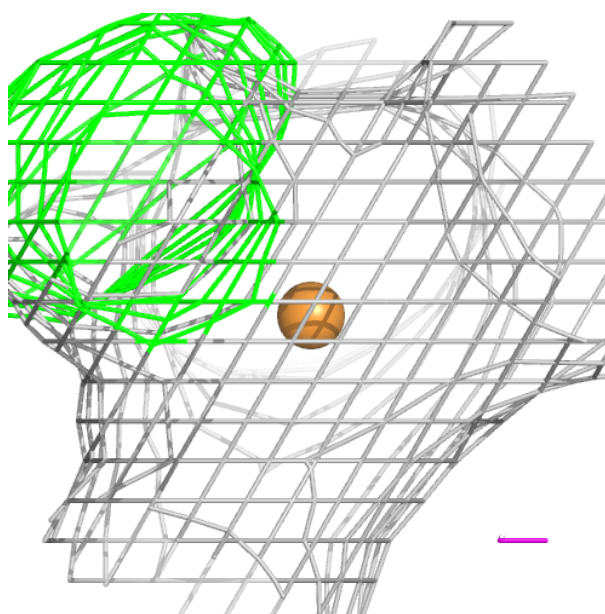$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
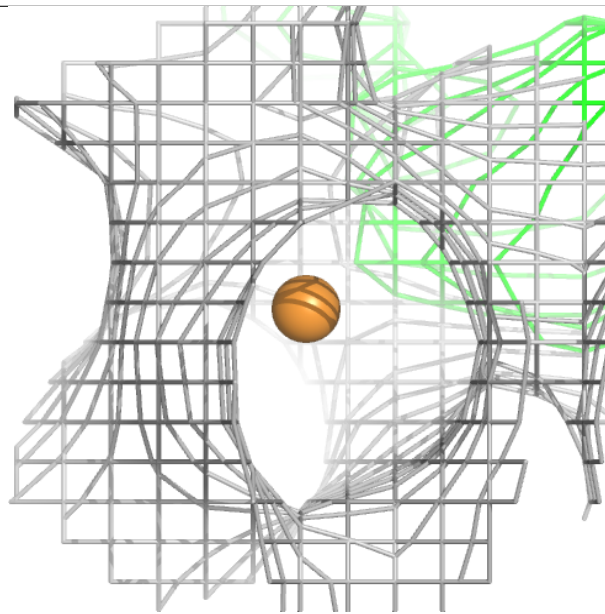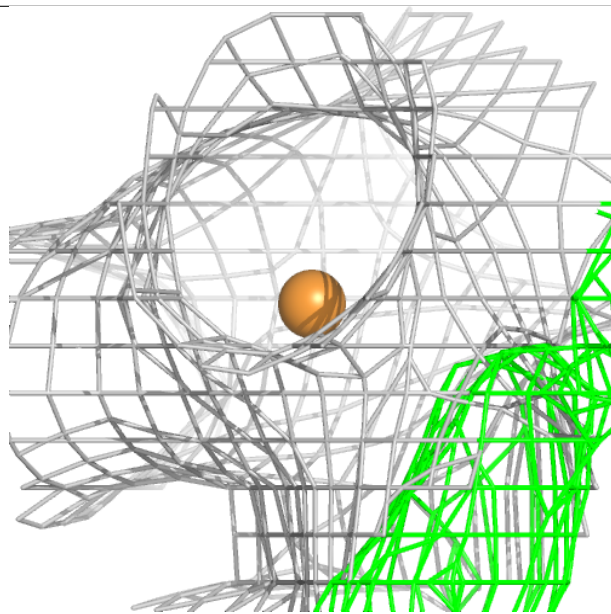and green (positive)
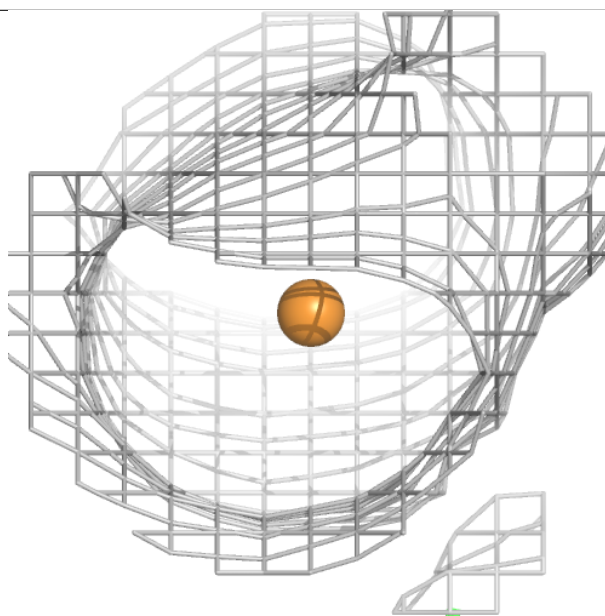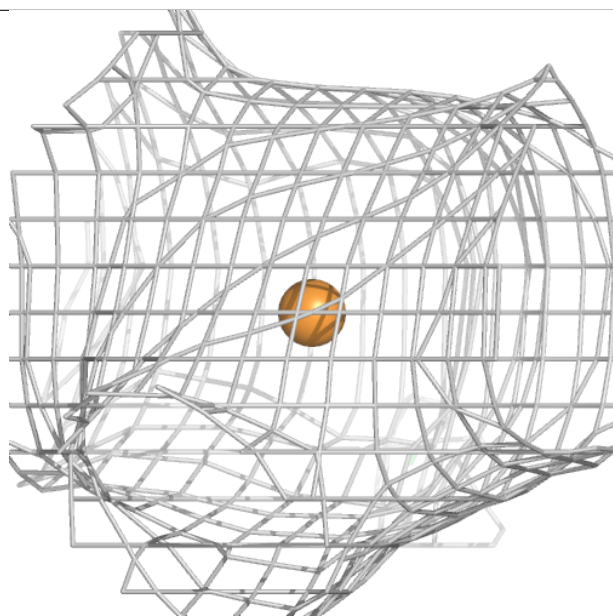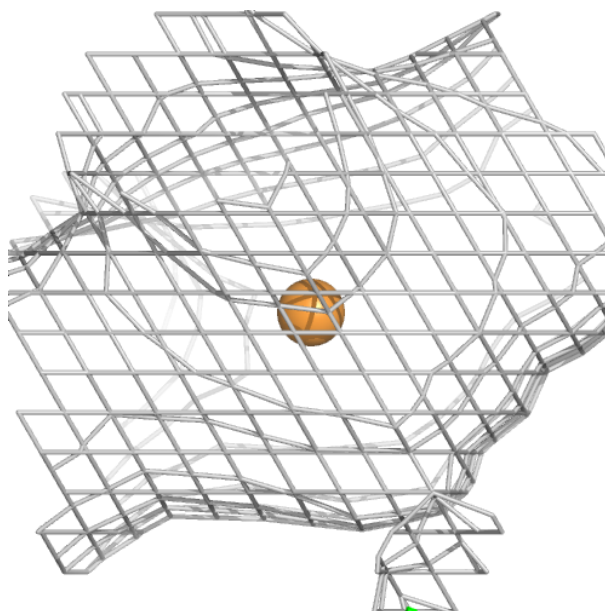
Electron density around SO4 C 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
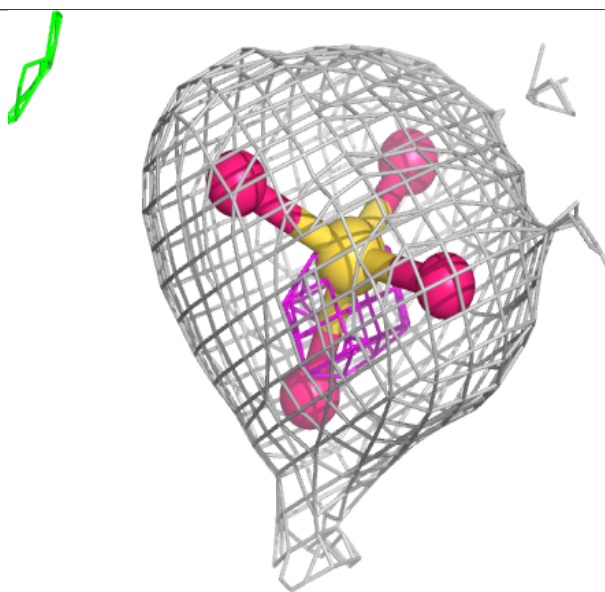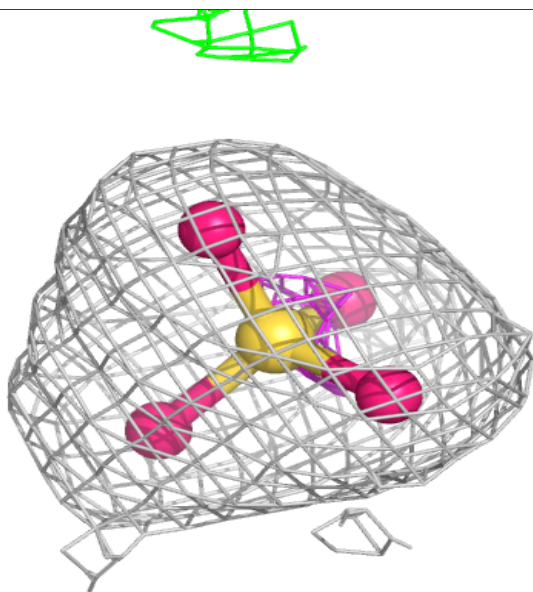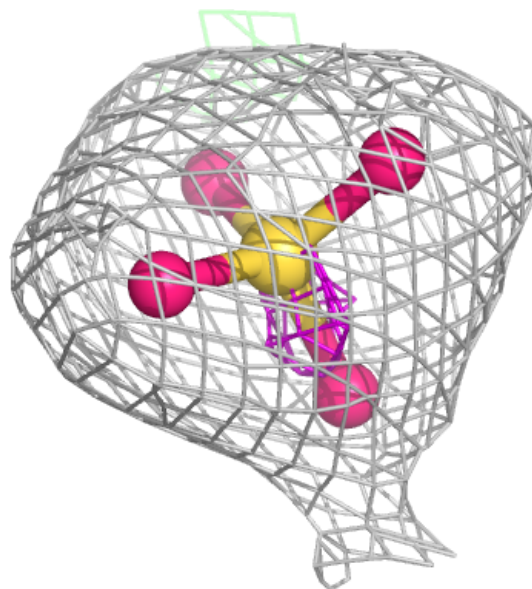
Electron density around CU B 603:

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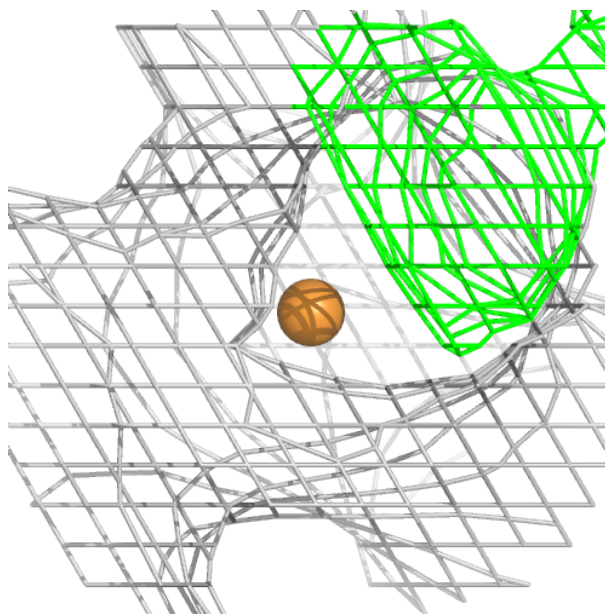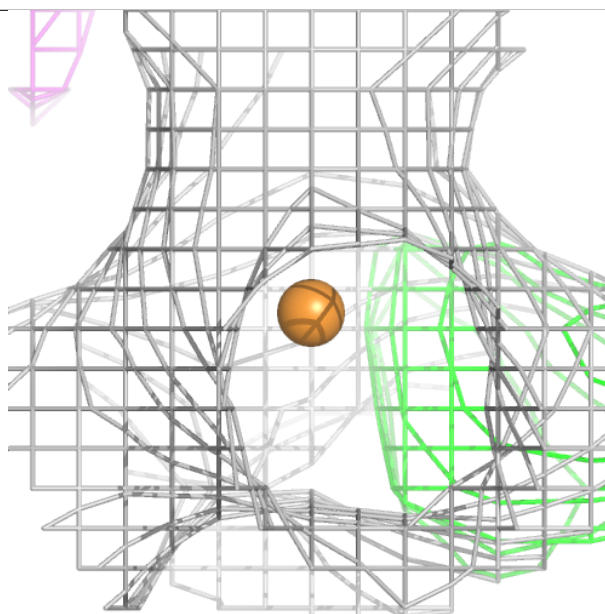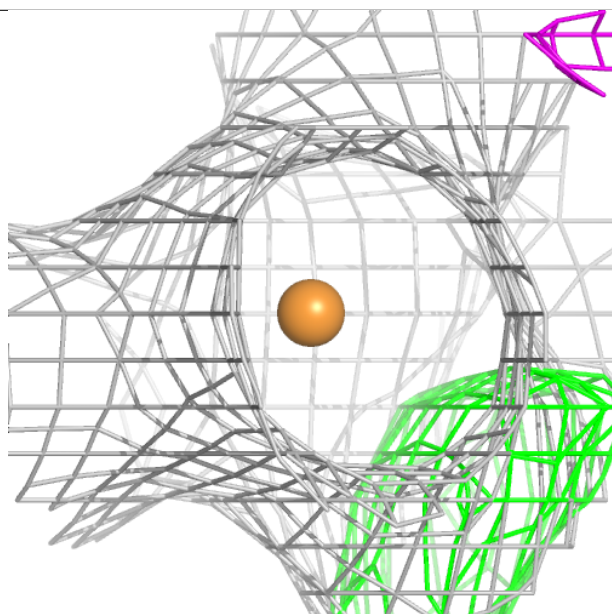mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around CU A 602:

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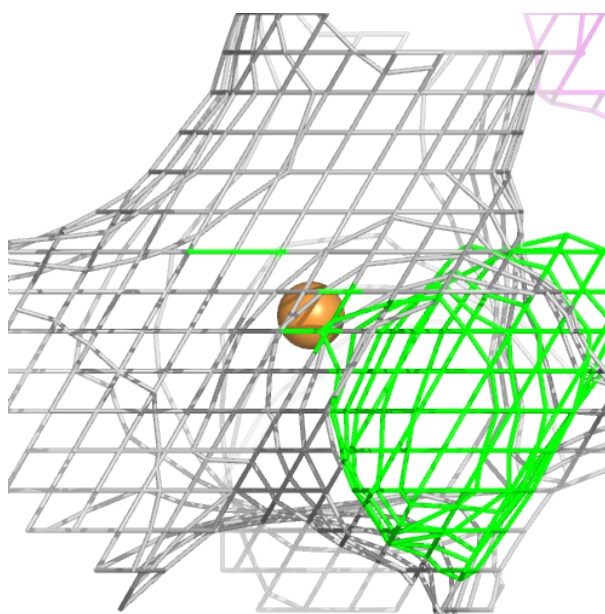and green (positive)

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:

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

Electron density around CU B 602:

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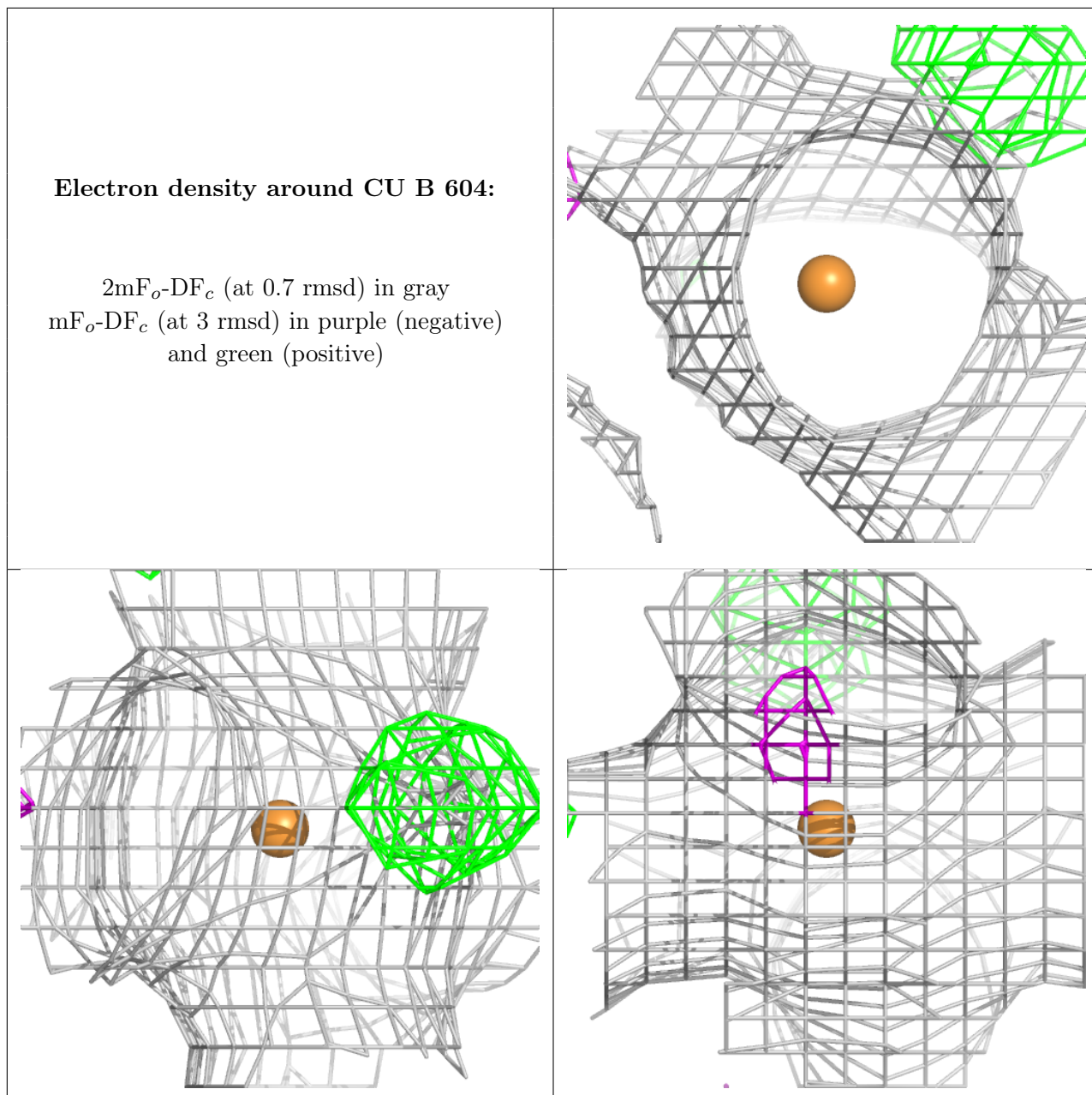$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

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.