Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2022 – 09:13 pm GMT

PDB ID	:	7PFR
Title	:	Crystal Structure of Two-Domain Laccase mutant M199A from Streptomyces griseoflavus
Authors	:	Gabdulkhakov, A.; Tishchenko, S.; Kolyadenko, I.
Deposited on	:	2021-08-12
Resolution	:	1.75 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 following versions of software and data (see references ⓘ) were used in the production of this report:

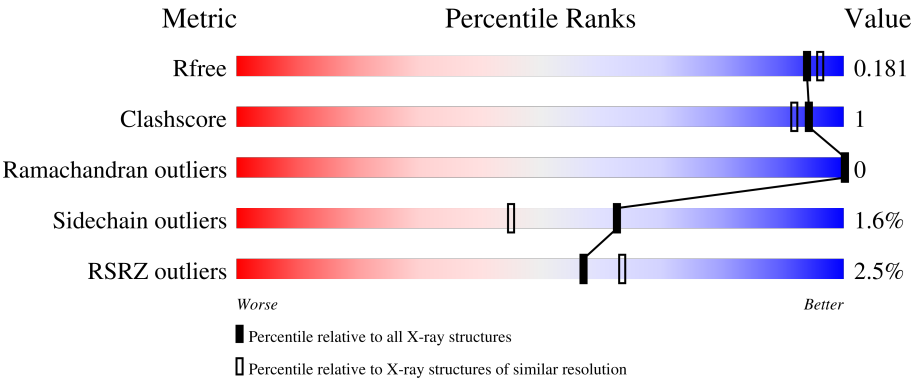
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	283	2% 93% 5%
1	B	283	3% 93% 5%
1	C	283	94%
1	D	283	2% 93% 5%
1	E	283	2% 95%

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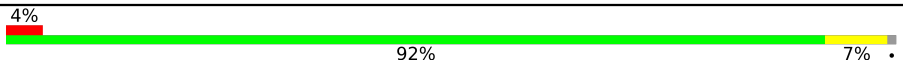
Mol	Chain	Length	Quality of chain
1	F	283	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14045 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 Two-domain laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	5	0
			2168	1351	397	408	12			
1	B	278	Total	C	N	O	S	0	10	0
			2207	1373	405	416	13			
1	C	277	Total	C	N	O	S	0	7	0
			2180	1358	400	409	13			
1	D	278	Total	C	N	O	S	0	6	0
			2182	1360	399	410	13			
1	E	278	Total	C	N	O	S	0	5	0
			2169	1352	398	407	12			
1	F	279	Total	C	N	O	S	0	4	0
			2176	1354	398	413	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ALA	MET	engineered mutation	UNP A0A0M4FJ81
B	199	ALA	MET	engineered mutation	UNP A0A0M4FJ81
C	199	ALA	MET	engineered mutation	UNP A0A0M4FJ81
D	199	ALA	MET	engineered mutation	UNP A0A0M4FJ81
E	199	ALA	MET	engineered mutation	UNP A0A0M4FJ81
F	199	ALA	MET	engineered mutation	UNP A0A0M4FJ81

- 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	A	4	Total	Cu	0	0
			4	4		
2	B	4	Total	Cu	0	0
			4	4		
2	C	4	Total	Cu	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	3	Total Cu 3 3	0	0
2	E	5	Total Cu 5 5	0	0
2	F	4	Total Cu 4 4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0

- Molecule 4 is water.

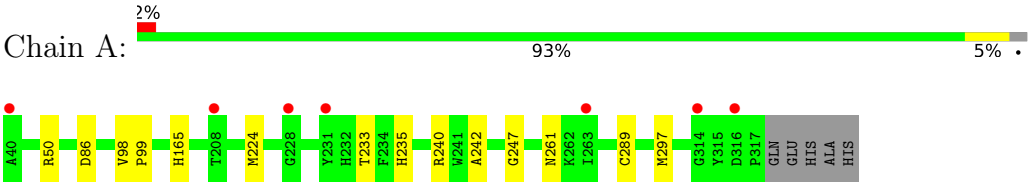
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	180	Total O 180 180	0	0
4	B	141	Total O 141 141	0	0
4	C	148	Total O 148 148	0	0
4	D	152	Total O 152 152	0	0
4	E	139	Total O 139 139	0	0
4	F	177	Total O 177 177	0	0

3 Residue-property plots (i)

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.

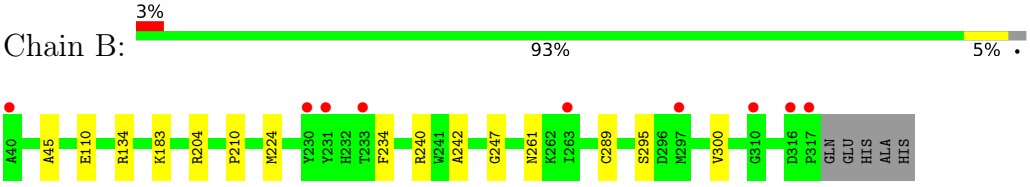
• Molecule 1: Two-domain laccase

Chain A:



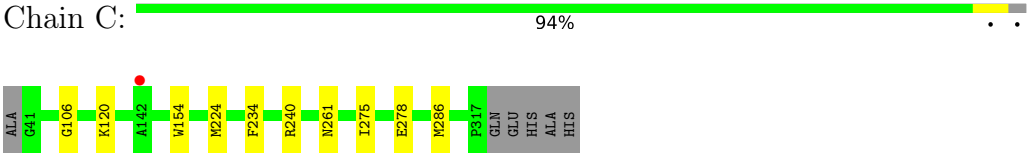
• Molecule 1: Two-domain laccase

Chain B:



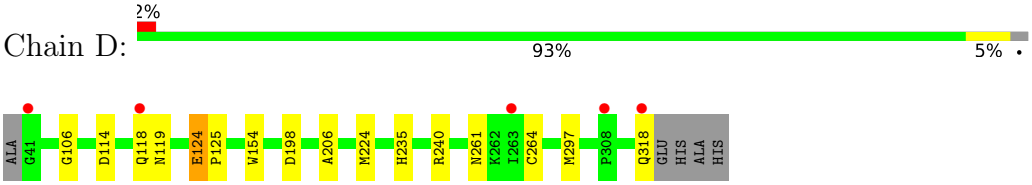
• Molecule 1: Two-domain laccase

Chain C:



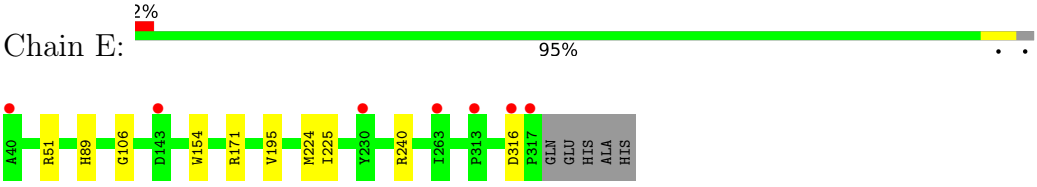
• Molecule 1: Two-domain laccase

Chain D:



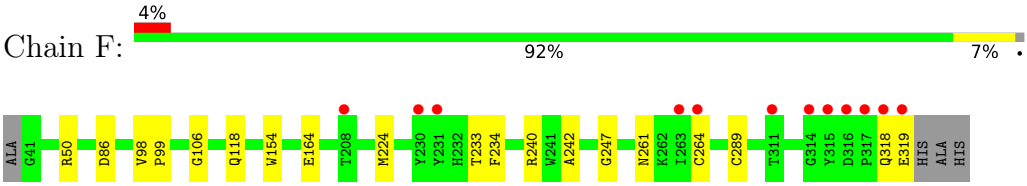
• Molecule 1: Two-domain laccase

Chain E:



• Molecule 1: Two-domain laccase

Chain F:


4%
92%
7%
ALA
G41
R50
D86
V98
P99
G106
Q118
W154
E164
T208
M224
Y230
Y231
H232
T233
F234
R240
W241
A242
G247
N261
K262
I263
C264
C289
T311
G314
Y315
D316
P317
Q318
E319
HIS
ALA
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.98Å 94.12Å 119.73Å 90.00° 91.16° 90.00°	Depositor
Resolution (Å)	47.24 – 1.75 47.24 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.24-1.75) 99.8 (47.24-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0230, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.131 , 0.169 0.141 , 0.181	Depositor DCC
R_{free} test set	5013 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	14045	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NA, CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.34	0/2230	0.59	0/3029
1	B	0.33	0/2269	0.60	0/3080
1	C	0.34	0/2242	0.59	0/3043
1	D	0.33	0/2244	0.60	0/3047
1	E	0.33	0/2231	0.59	0/3031
1	F	0.34	0/2238	0.60	0/3040
All	All	0.34	0/13454	0.59	0/18270

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2168	0	2038	8	0
1	B	2207	0	2071	7	0
1	C	2180	0	2053	4	0
1	D	2182	0	2051	6	0
1	E	2169	0	2040	4	0
1	F	2176	0	2036	8	0
2	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
2	E	5	0	0	0	0
2	F	4	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	180	0	0	0	0
4	B	141	0	0	1	0
4	C	148	0	0	0	0
4	D	152	0	0	0	0
4	E	139	0	0	0	0
4	F	177	0	0	0	0
All	All	14045	0	12289	33	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 1.

All (33) 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:F:118:GLN:NE2	1:F:164:GLU:OE1	2.31	0.60
1:A:297:MET:HE1	1:D:198:ASP:HB3	1.86	0.57
1:A:99:PRO:HD2	1:F:98:VAL:HG12	1.90	0.52
1:D:114:ASP:OD2	1:D:119:ASN:ND2	2.43	0.51
1:E:51:ARG:HG2	1:E:89:HIS:HB2	1.93	0.51
4:B:501:HOH:O	1:C:286:MET:HG3	2.12	0.49
1:F:242:ALA:O	1:F:247:GLY:HA2	2.13	0.49
1:E:171[B]:ARG:HH11	1:E:171[B]:ARG:HG2	1.77	0.49
1:D:206:ALA:HB1	1:D:297[A]:MET:O	2.14	0.48
1:A:50:ARG:NH2	1:A:86:ASP:OD2	2.47	0.48
1:D:106:GLY:HA3	1:D:154:TRP:CD2	2.49	0.48
1:B:242:ALA:O	1:B:247:GLY:HA2	2.14	0.47
1:A:98:VAL:HG12	1:F:99:PRO:HD2	1.98	0.45
1:D:124:GLU:HG3	1:D:125:PRO:HD2	1.98	0.45
1:E:106:GLY:HA3	1:E:154:TRP:CD2	2.53	0.44
1:F:234:PHE:O	1:F:261:ASN:HA	2.17	0.44
1:B:45:ALA:HB2	1:B:183:LYS:HD2	2.00	0.43
1:C:275:ILE:HB	1:C:278:GLU:HB2	1.99	0.43
1:E:195:VAL:HA	1:E:225:ILE:O	2.19	0.43
1:F:50:ARG:NH2	1:F:86:ASP:OD2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:THR:O	1:F:289:CYS:HA	2.18	0.43
1:C:106:GLY:HA3	1:C:154:TRP:CD2	2.54	0.43
1:B:110:GLU:HG3	1:B:134[B]:ARG:HH22	1.84	0.43
1:A:233:THR:O	1:A:289:CYS:HA	2.19	0.43
1:A:165:HIS:CE1	1:B:300[B]:VAL:HG11	2.54	0.42
1:A:235:HIS:HB2	1:A:261:ASN:OD1	2.19	0.42
1:A:242:ALA:O	1:A:247:GLY:HA2	2.19	0.42
1:B:234:PHE:O	1:B:261:ASN:HA	2.20	0.42
1:D:235:HIS:HB2	1:D:261:ASN:OD1	2.20	0.41
1:C:234:PHE:O	1:C:261:ASN:HA	2.21	0.41
1:B:204:ARG:HD2	1:B:210:PRO:HD3	2.03	0.40
1:B:289:CYS:O	1:B:295:SER:HB3	2.21	0.40
1:F:106:GLY:HA3	1:F:154:TRP:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/283 (99%)	278 (99%)	3 (1%)	0	100	100
1	B	286/283 (101%)	281 (98%)	5 (2%)	0	100	100
1	C	282/283 (100%)	276 (98%)	6 (2%)	0	100	100
1	D	282/283 (100%)	277 (98%)	5 (2%)	0	100	100
1	E	281/283 (99%)	277 (99%)	4 (1%)	0	100	100
1	F	281/283 (99%)	278 (99%)	3 (1%)	0	100	100
All	All	1693/1698 (100%)	1667 (98%)	26 (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	A	223/222 (100%)	221 (99%)	2 (1%)	78	67
1	B	227/222 (102%)	225 (99%)	2 (1%)	78	67
1	C	225/222 (101%)	221 (98%)	4 (2%)	59	40
1	D	225/222 (101%)	219 (97%)	6 (3%)	44	22
1	E	223/222 (100%)	220 (99%)	3 (1%)	69	54
1	F	224/222 (101%)	219 (98%)	5 (2%)	52	29
All	All	1347/1332 (101%)	1325 (98%)	22 (2%)	62	45

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	MET
1	A	240	ARG
1	B	224	MET
1	B	240	ARG
1	C	120[A]	LYS
1	C	120[B]	LYS
1	C	224	MET
1	C	240	ARG
1	D	118	GLN
1	D	124	GLU
1	D	224	MET
1	D	240	ARG
1	D	264	CYS
1	D	318	GLN
1	E	224	MET
1	E	240	ARG
1	E	316	ASP
1	F	224	MET
1	F	240	ARG
1	F	264	CYS
1	F	318	GLN
1	F	319	GLU

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

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 26 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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	278/283 (98%)	-0.20	7 (2%)	57	63	20, 28, 44, 73	0
1	B	278/283 (98%)	-0.06	9 (3%)	47	54	22, 31, 49, 98	1 (0%)
1	C	277/283 (97%)	-0.24	1 (0%)	92	94	23, 30, 47, 62	1 (0%)
1	D	278/283 (98%)	-0.15	5 (1%)	68	76	20, 31, 49, 71	0
1	E	278/283 (98%)	-0.12	7 (2%)	57	63	22, 31, 52, 87	2 (0%)
1	F	279/283 (98%)	-0.10	12 (4%)	35	41	20, 29, 49, 93	2 (0%)
All	All	1668/1698 (98%)	-0.15	41 (2%)	57	63	20, 30, 48, 98	6 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	PRO	8.9
1	F	319	GLU	6.9
1	F	316	ASP	5.4
1	F	318	GLN	4.8
1	A	40	ALA	4.7
1	E	40	ALA	4.7
1	E	316	ASP	4.6
1	B	40	ALA	4.0
1	D	318	GLN	3.4
1	E	317	PRO	3.4
1	A	316	ASP	3.3
1	E	313	PRO	3.1
1	B	316	ASP	2.8
1	A	231	TYR	2.8
1	B	263	ILE	2.8
1	A	314	GLY	2.7
1	C	142	ALA	2.6
1	F	230	TYR	2.6
1	F	317	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	41	GLY	2.6
1	F	314	GLY	2.6
1	B	230	TYR	2.6
1	F	231	TYR	2.5
1	A	208	THR	2.5
1	F	263	ILE	2.5
1	F	264	CYS	2.4
1	B	310	GLY	2.4
1	E	230	TYR	2.4
1	B	297[A]	MET	2.3
1	A	263	ILE	2.3
1	D	263	ILE	2.3
1	F	208	THR	2.3
1	B	231	TYR	2.3
1	A	228	GLY	2.2
1	E	143	ASP	2.1
1	D	118	GLN	2.1
1	E	263	ILE	2.1
1	F	315	TYR	2.1
1	B	233	THR	2.0
1	F	311	THR	2.0
1	D	308	PRO	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^{th} 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
2	CU	F	402	1/1	0.96	0.21	24,24,24,24	1

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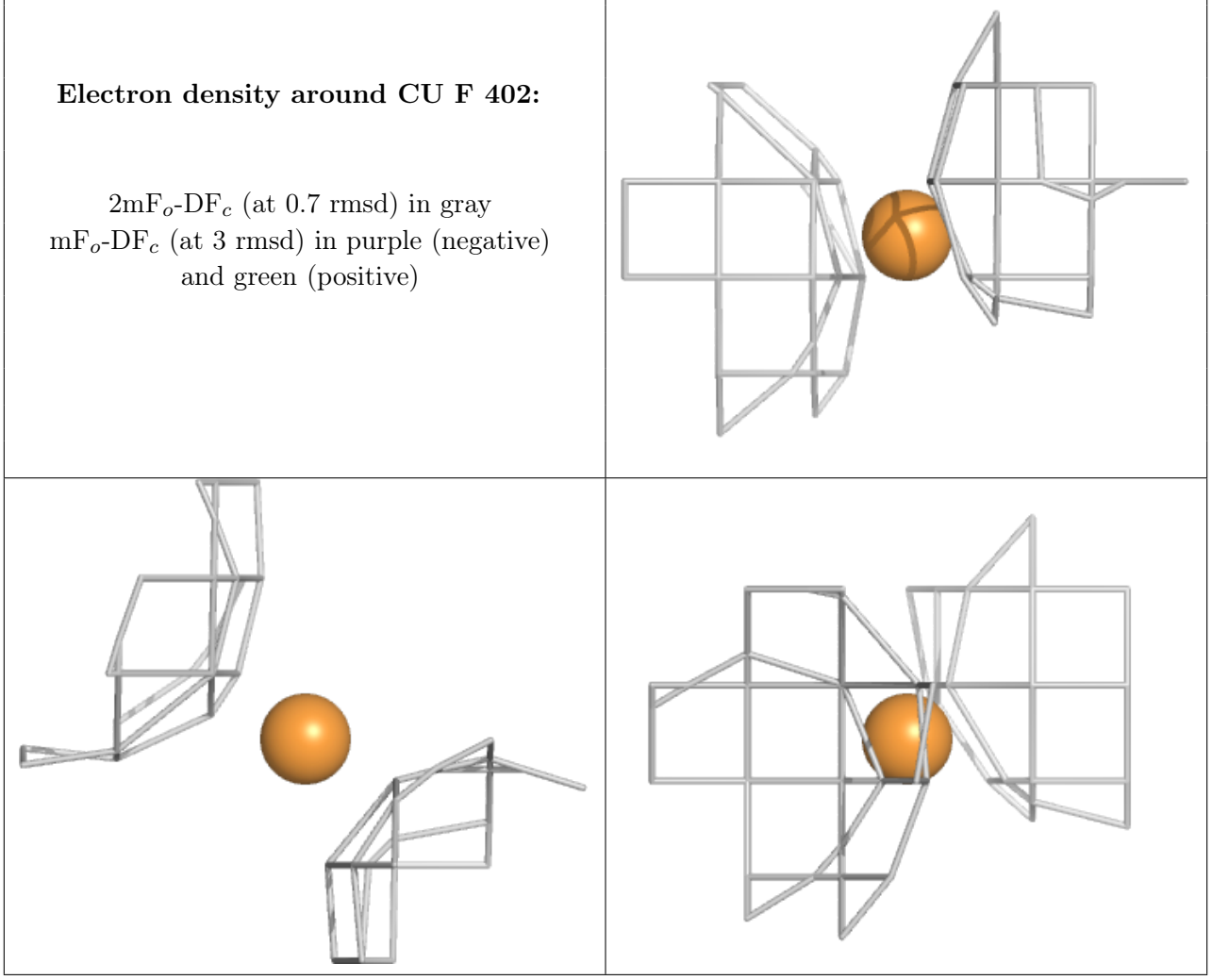
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	D	404	1/1	0.97	0.06	48,48,48,48	0
2	CU	E	403	1/1	0.98	0.15	37,37,37,37	1
2	CU	E	405	1/1	0.98	0.21	39,39,39,39	1
2	CU	B	403	1/1	0.98	0.23	59,59,59,59	1
2	CU	C	404	1/1	0.98	0.17	51,51,51,51	1
2	CU	E	402	1/1	0.99	0.04	39,39,39,39	1
2	CU	A	403	1/1	0.99	0.23	38,38,38,38	1
2	CU	E	404	1/1	0.99	0.09	34,34,34,34	1
2	CU	C	403	1/1	0.99	0.05	36,36,36,36	1
2	CU	A	404	1/1	0.99	0.17	46,46,46,46	1
3	NA	A	405	1/1	0.99	0.06	44,44,44,44	0
2	CU	D	403	1/1	0.99	0.04	37,37,37,37	1
2	CU	D	402	1/1	1.00	0.06	27,27,27,27	1
2	CU	B	402	1/1	1.00	0.06	30,30,30,30	1
2	CU	E	401	1/1	1.00	0.09	28,28,28,28	1
2	CU	A	401	1/1	1.00	0.08	28,28,28,28	0
2	CU	B	404	1/1	1.00	0.06	33,33,33,33	1
2	CU	C	401	1/1	1.00	0.06	40,40,40,40	1
2	CU	C	402	1/1	1.00	0.07	29,29,29,29	0
2	CU	F	401	1/1	1.00	0.06	41,41,41,41	1
2	CU	A	402	1/1	1.00	0.04	34,34,34,34	1
2	CU	F	403	1/1	1.00	0.07	29,29,29,29	0
2	CU	F	404	1/1	1.00	0.04	36,36,36,36	1
2	CU	B	401	1/1	1.00	0.09	26,26,26,26	0
2	CU	D	401	1/1	1.00	0.07	25,25,25,25	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.

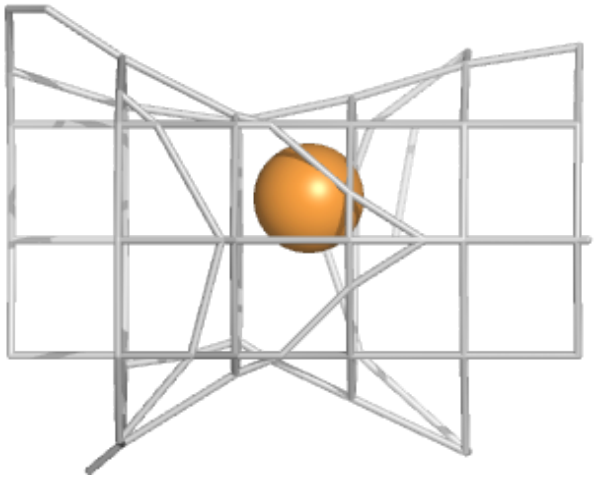
Electron density around CU F 402:

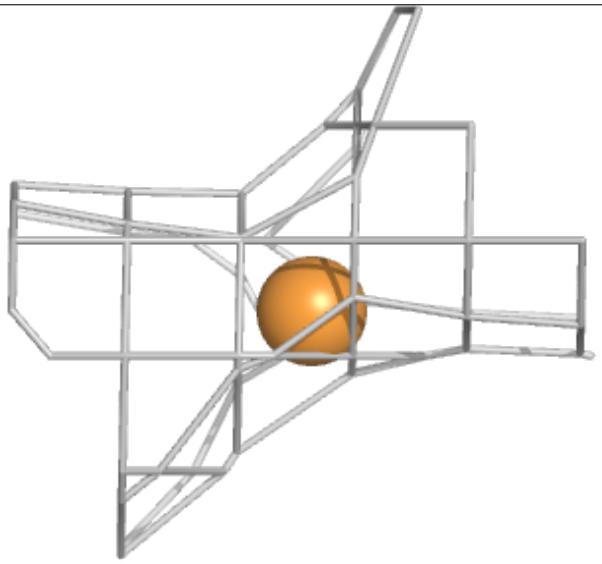
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

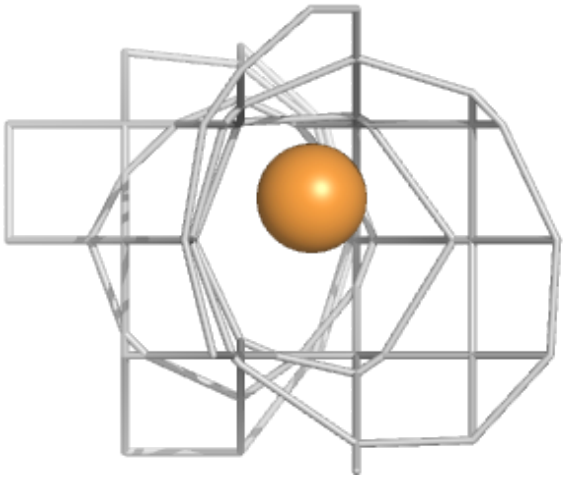


Electron density around CU E 403:

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

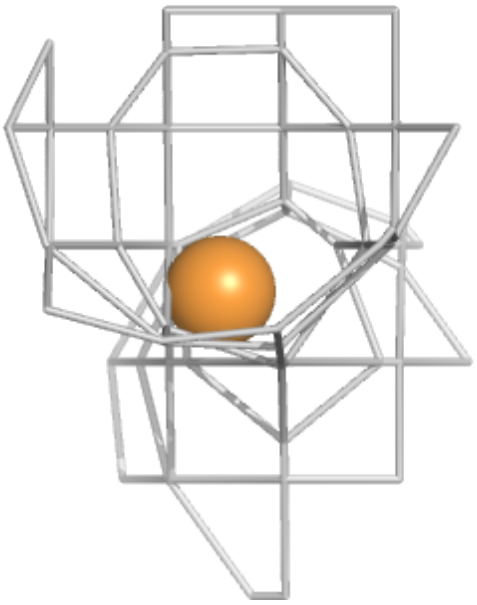


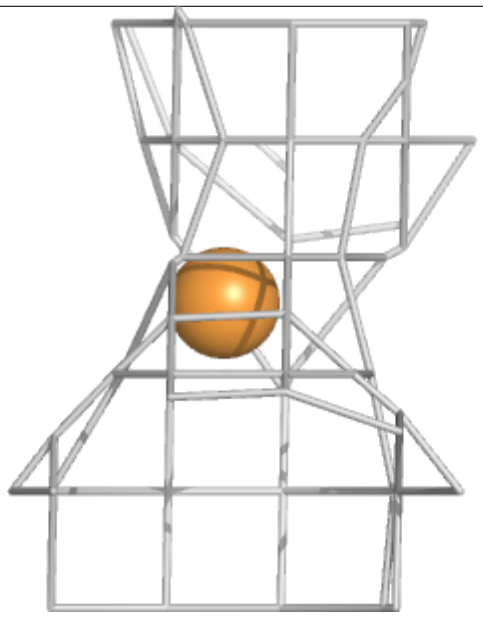


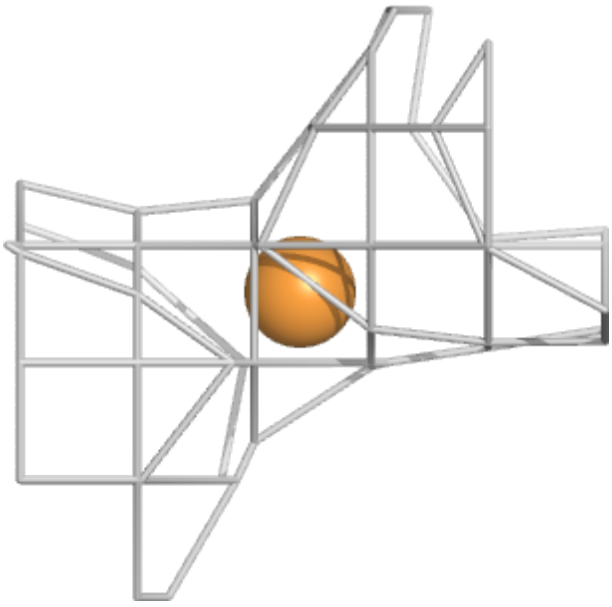


Electron density around CU E 405:

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

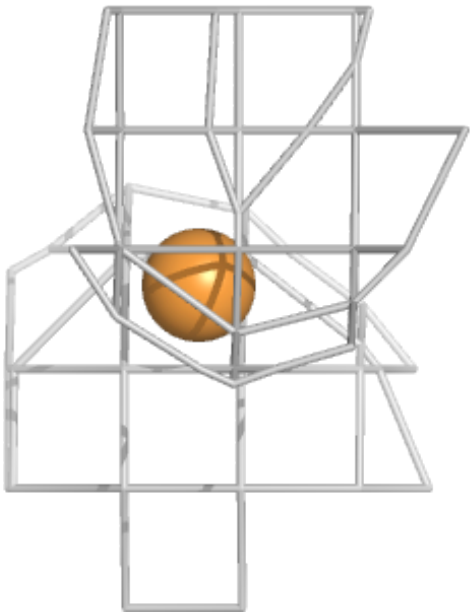


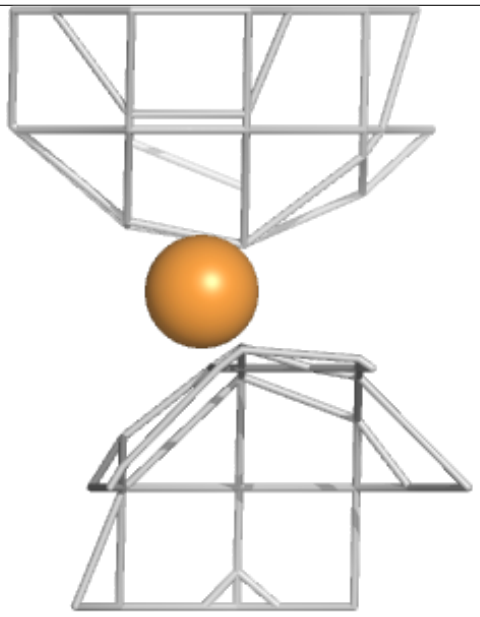


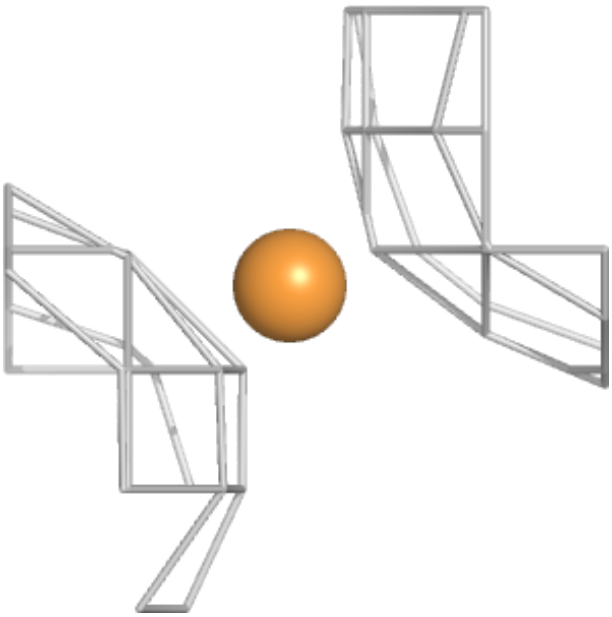


Electron density around CU B 403:

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

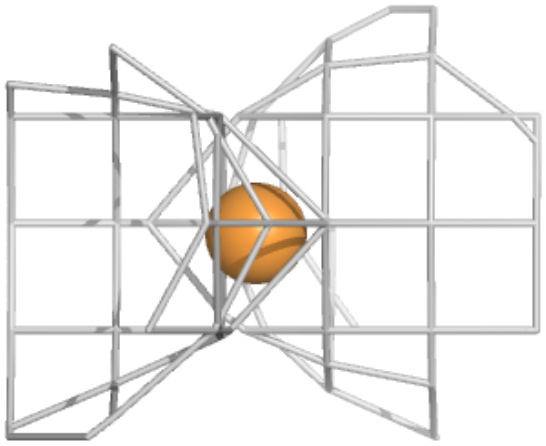


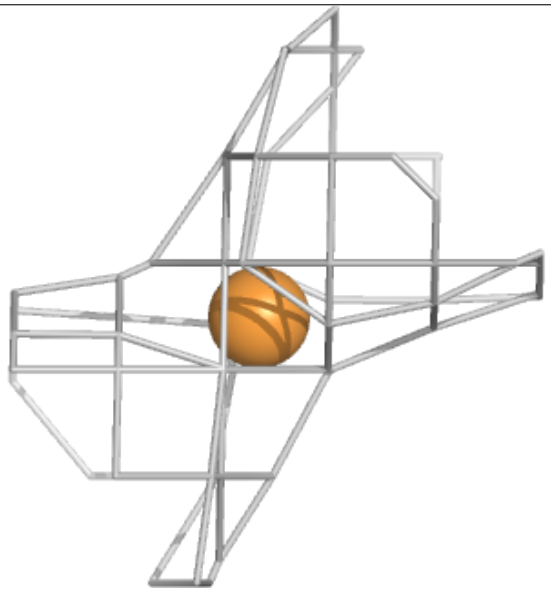


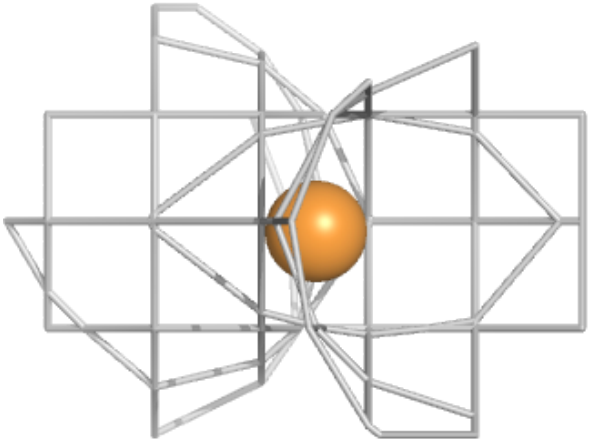


Electron density around CU C 404:

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

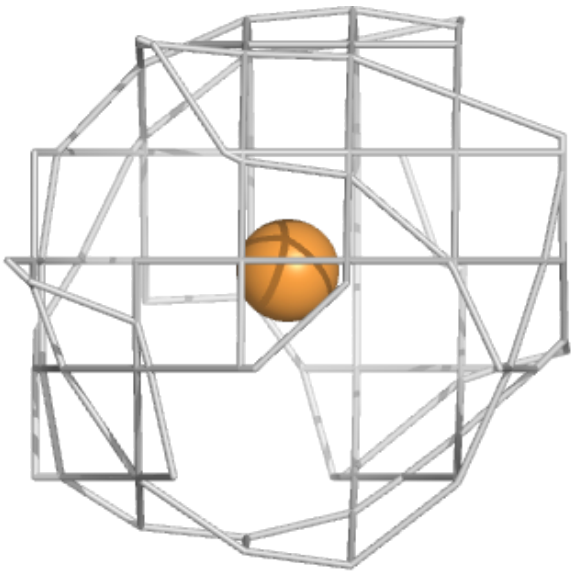


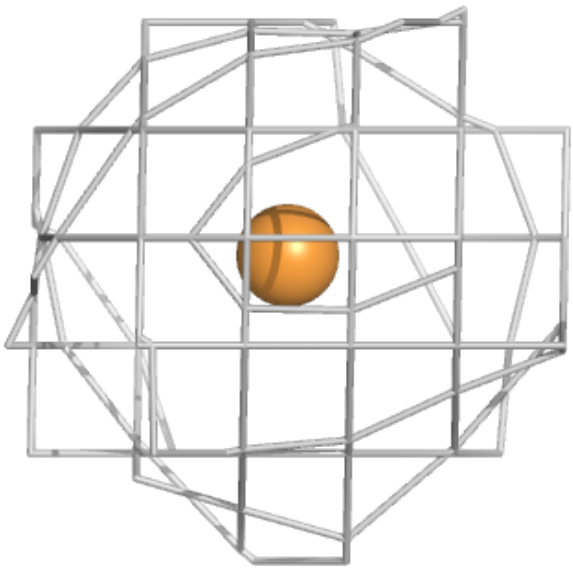


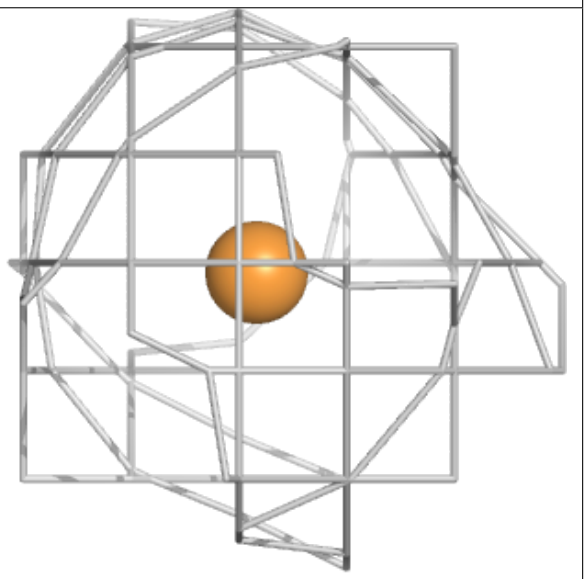


Electron density around CU E 402:

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

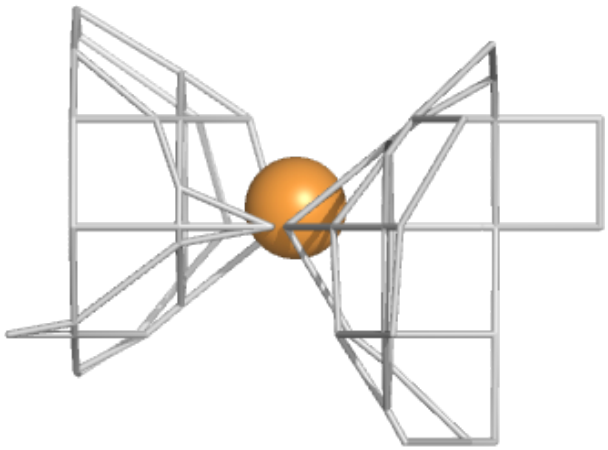


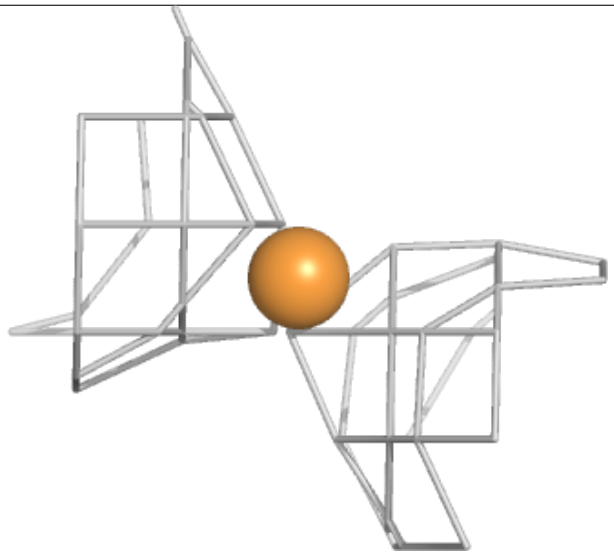


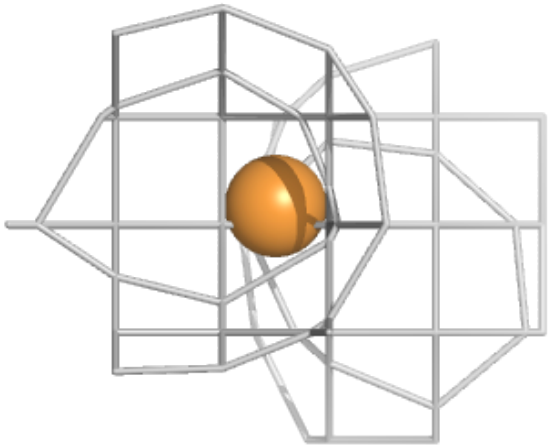


Electron density around CU A 403:

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

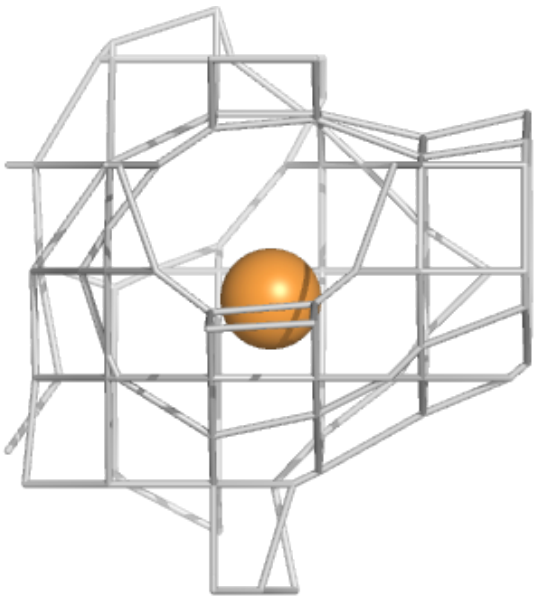


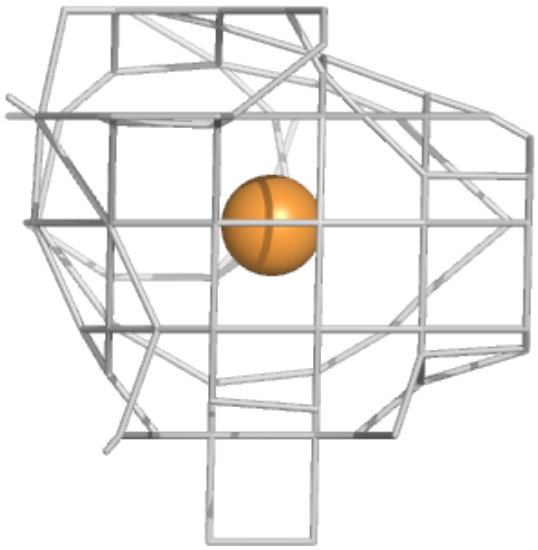


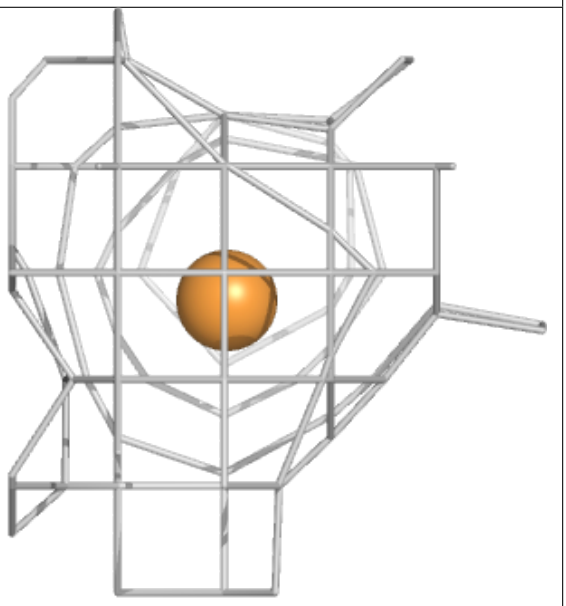


Electron density around CU E 404:

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

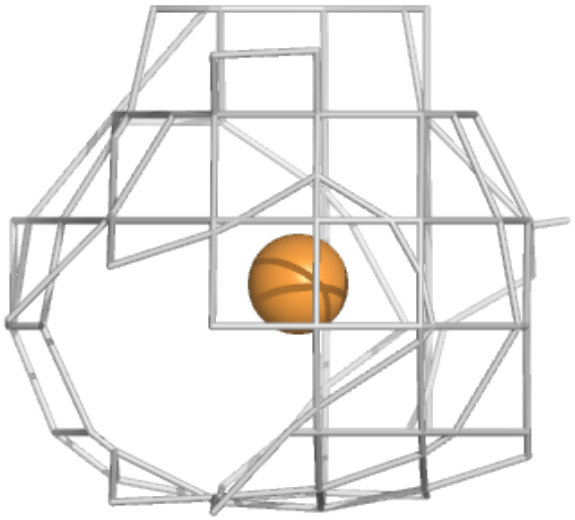


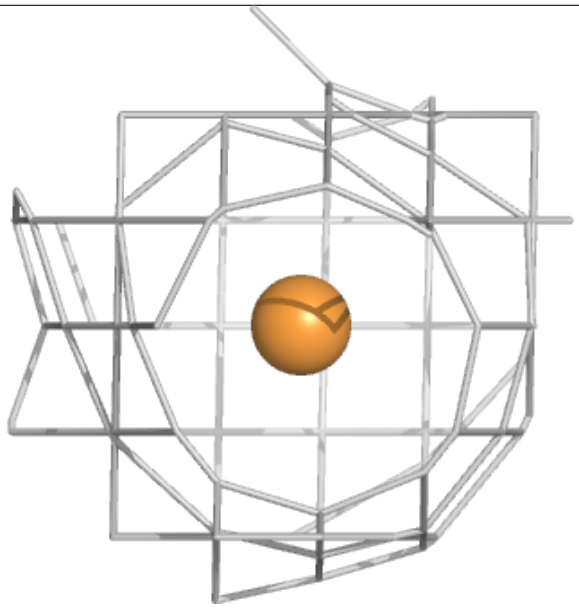


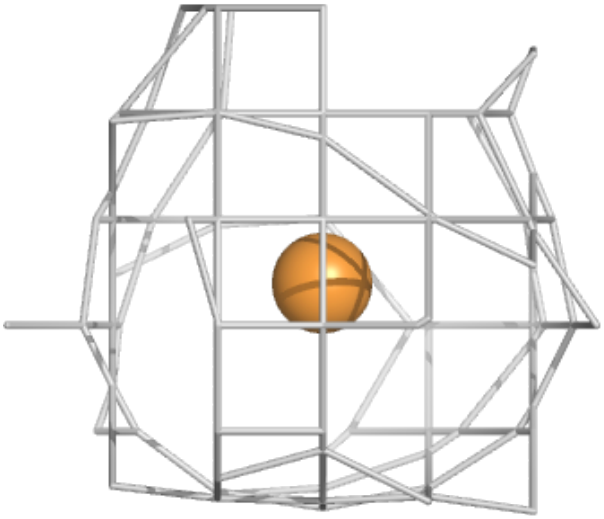


Electron density around CU C 403:

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

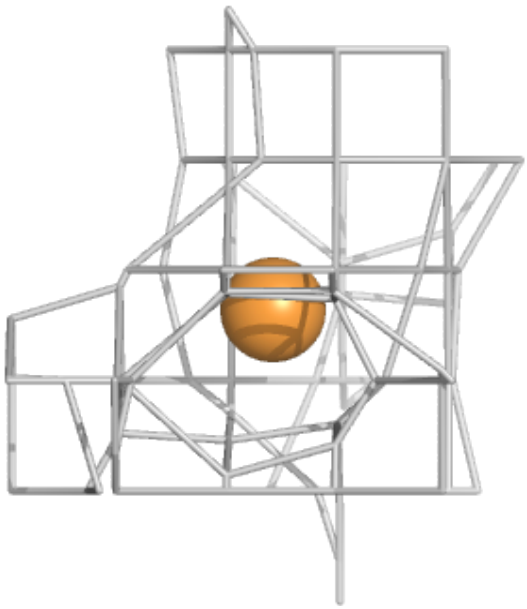


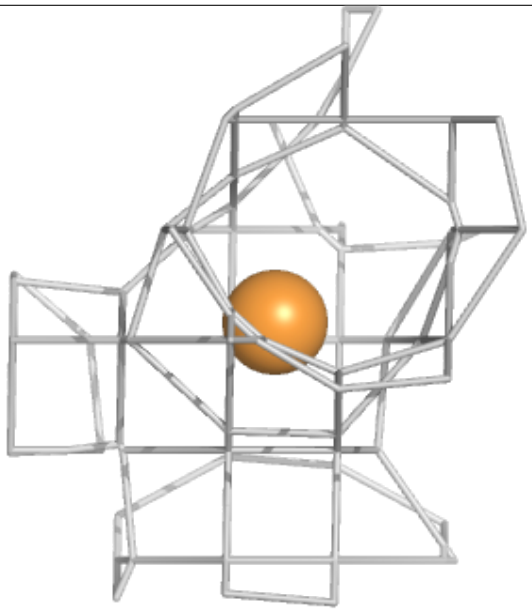


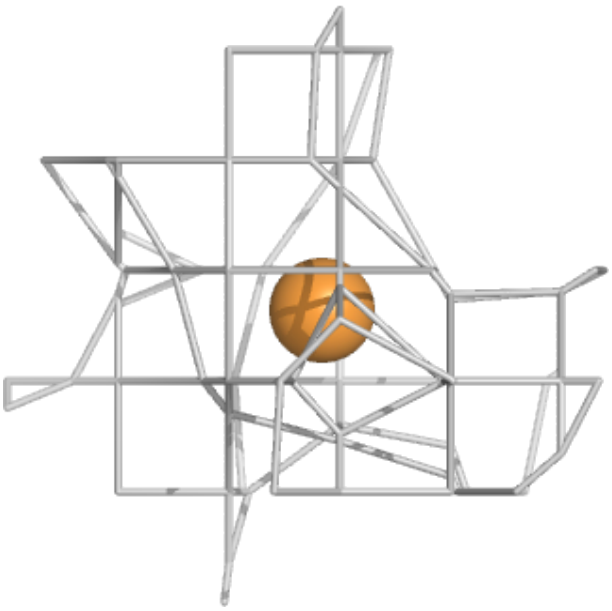


Electron density around CU A 404:

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

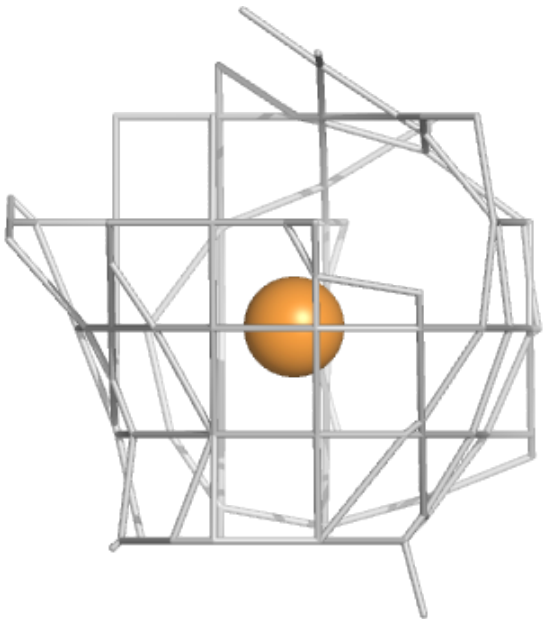


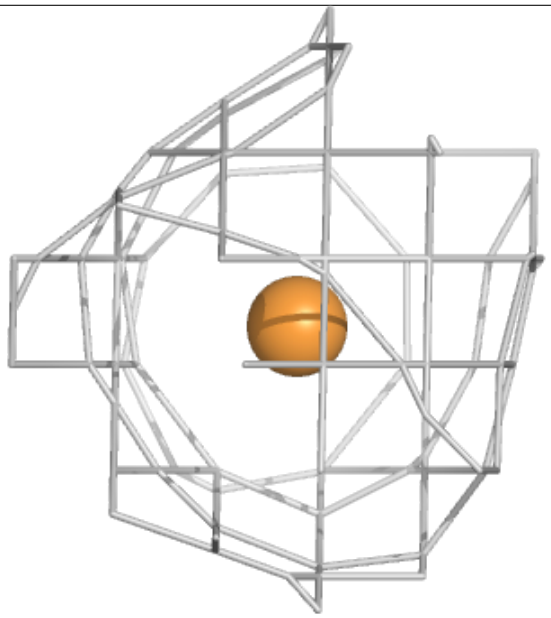


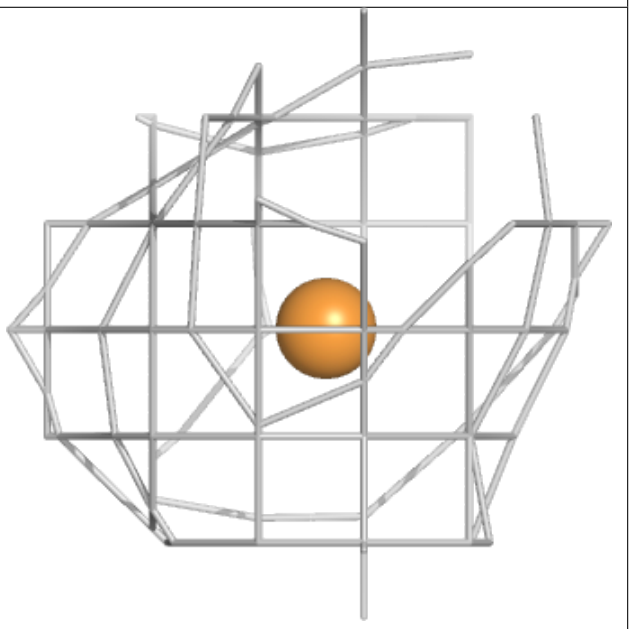


Electron density around CU D 403:

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

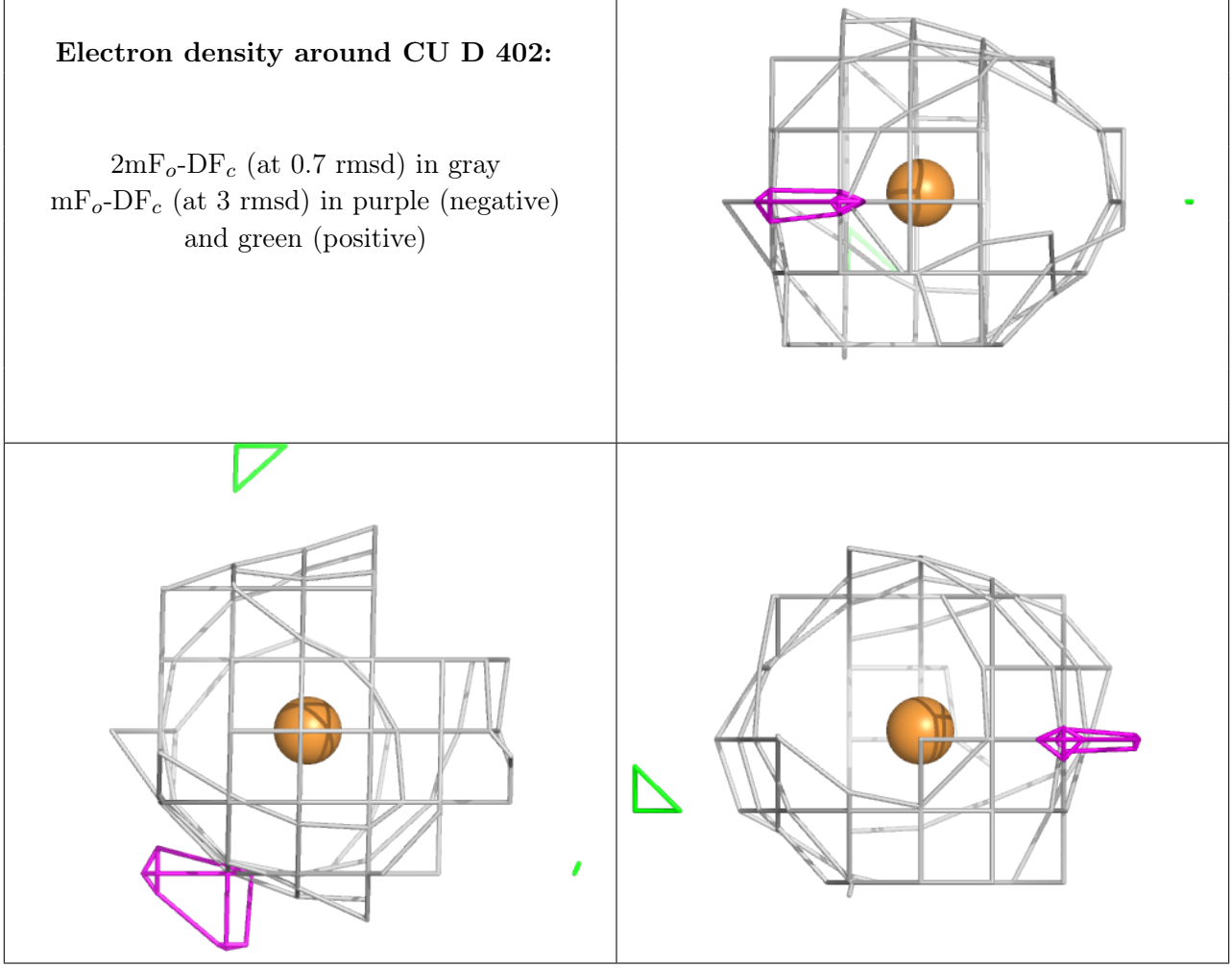






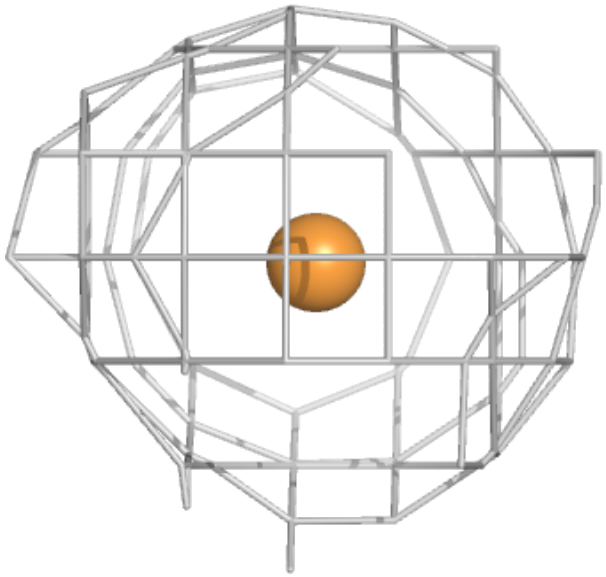
Electron density around CU D 402:

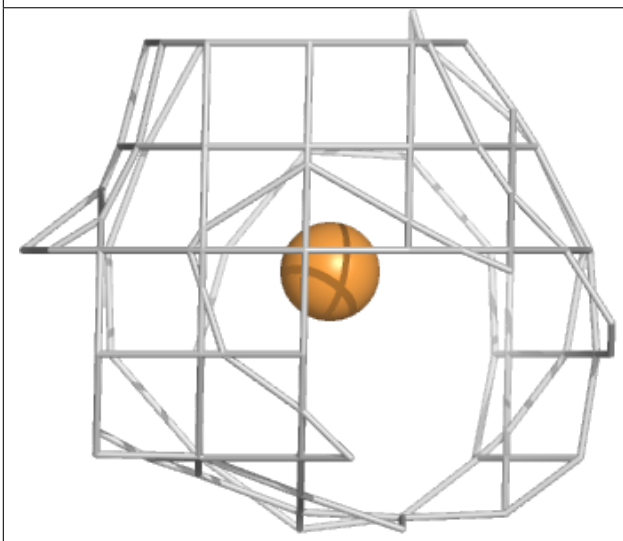
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

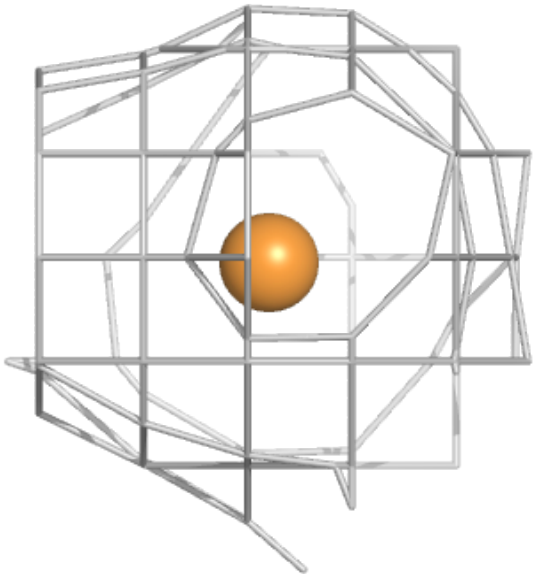


Electron density around CU B 402:

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

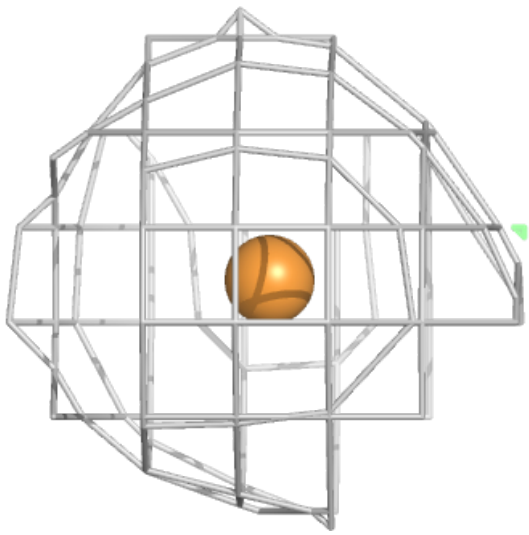


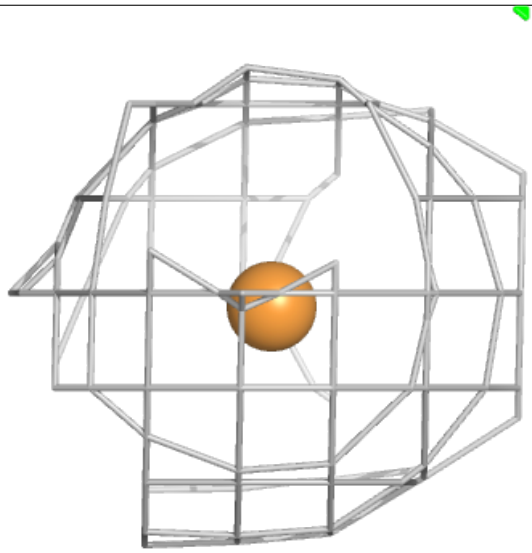


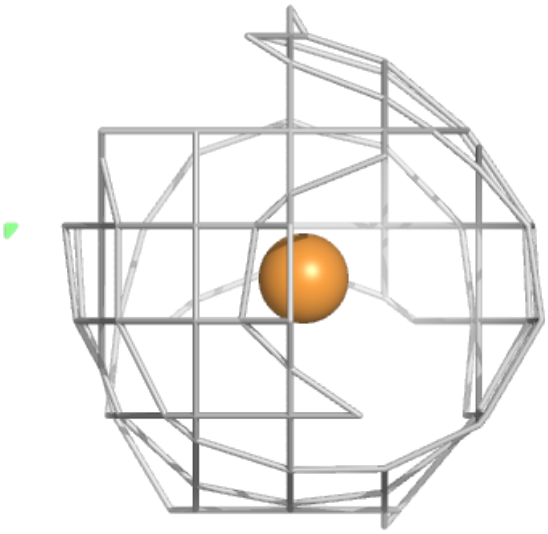


Electron density around CU E 401:

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

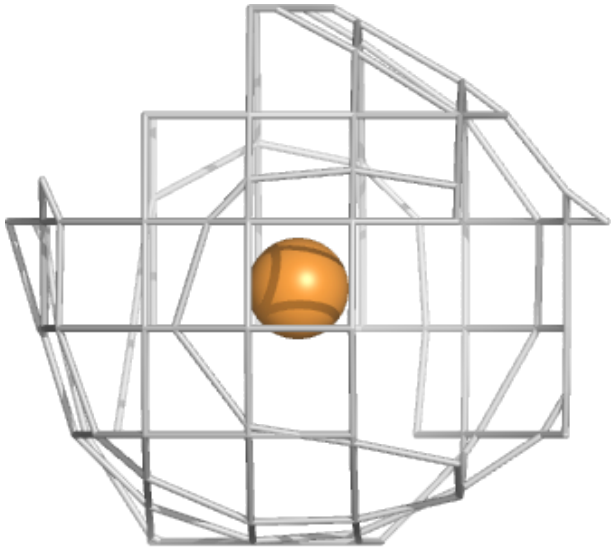


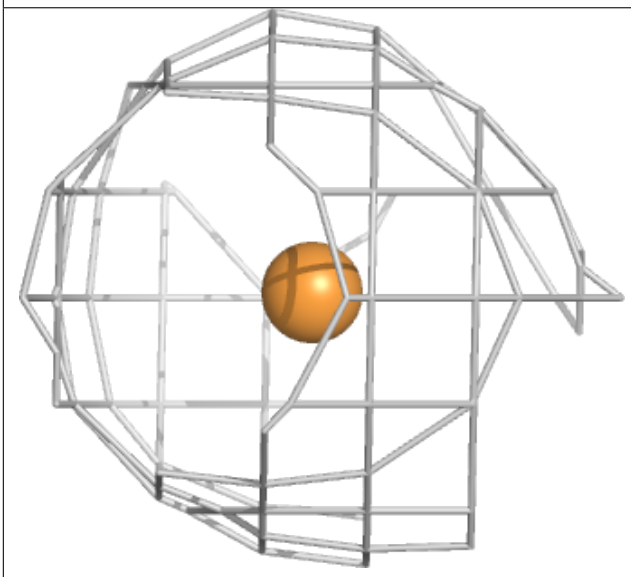


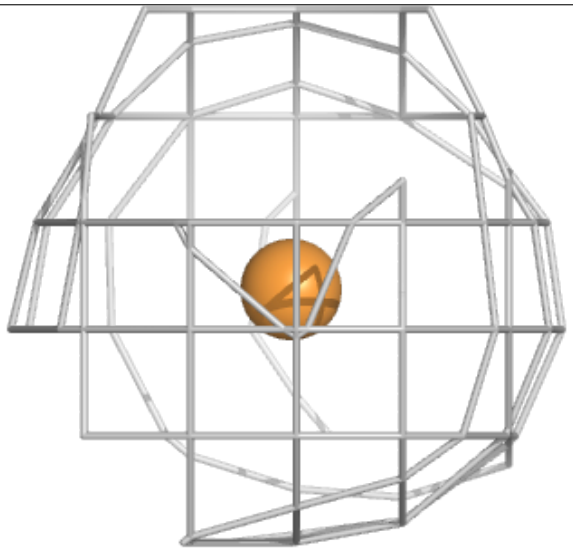


Electron density around CU A 401:

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

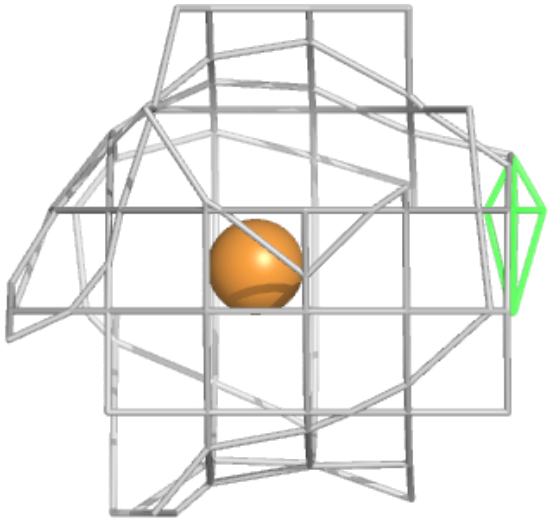


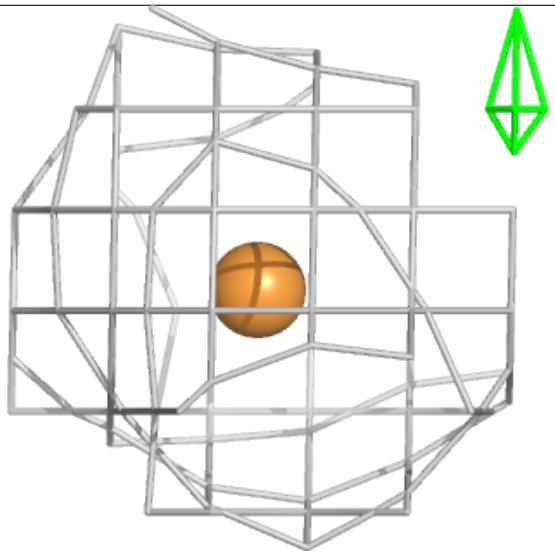


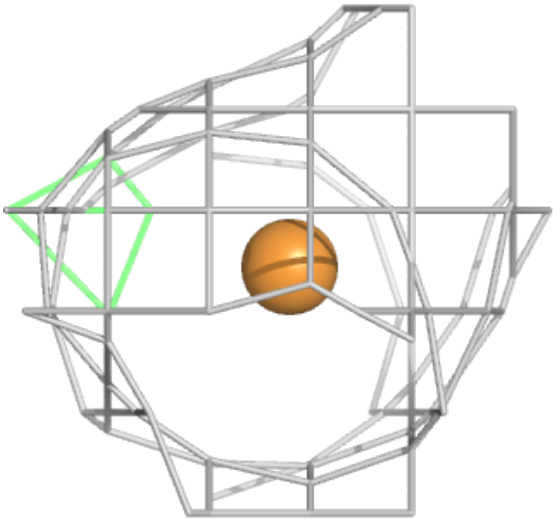


Electron density around CU B 404:

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

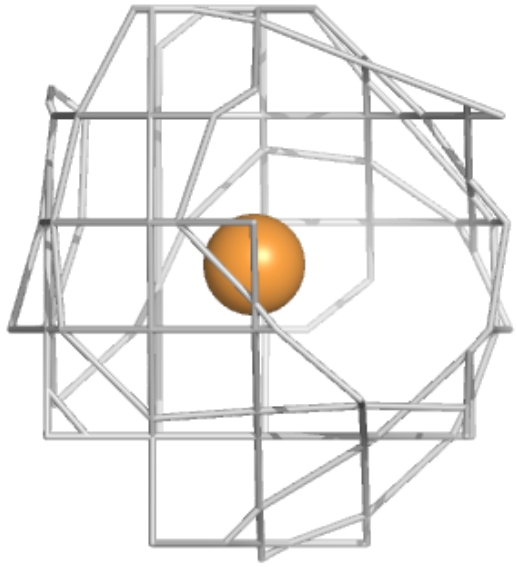


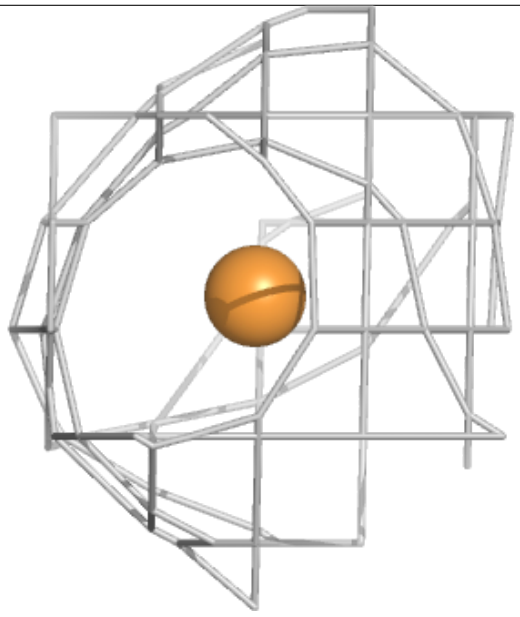


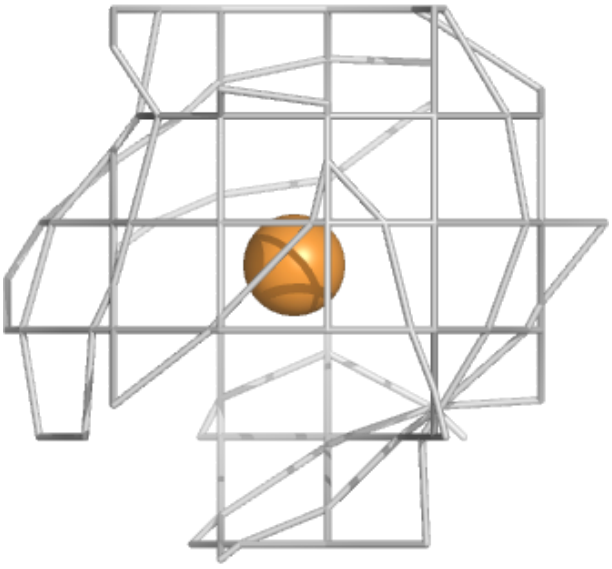


Electron density around CU C 401:

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

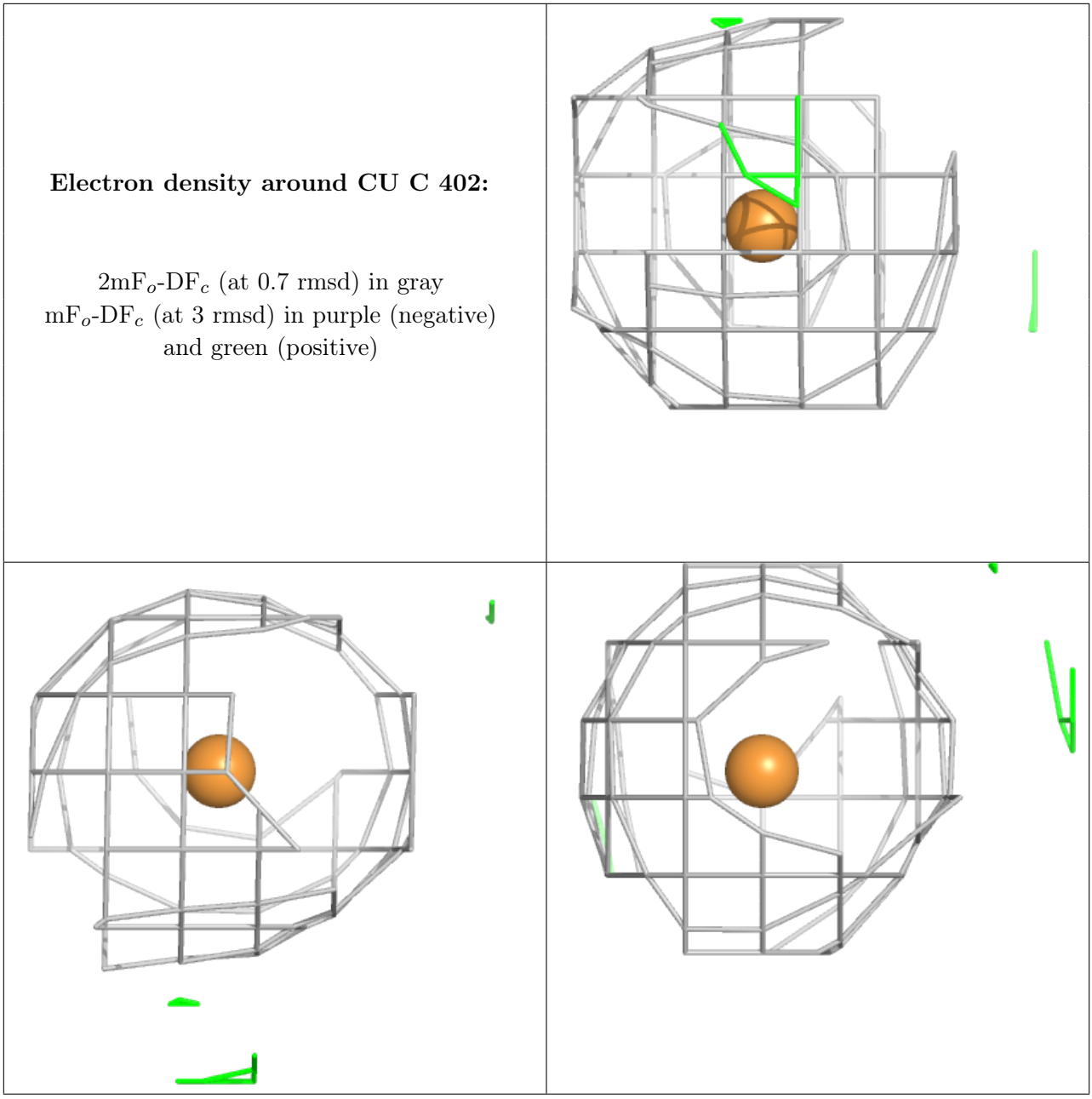






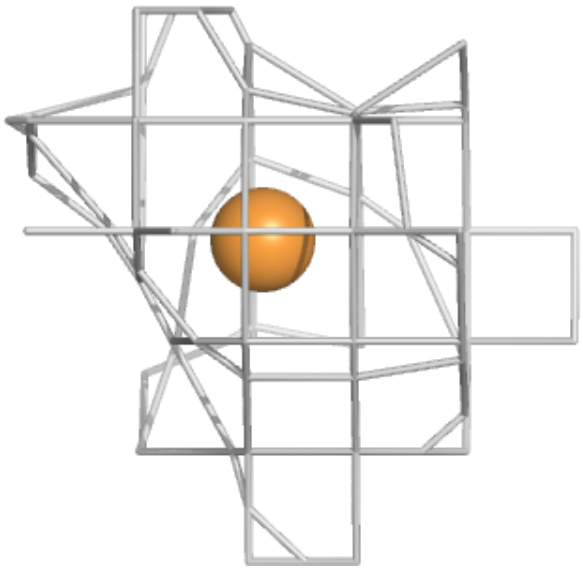
Electron density around CU C 402:

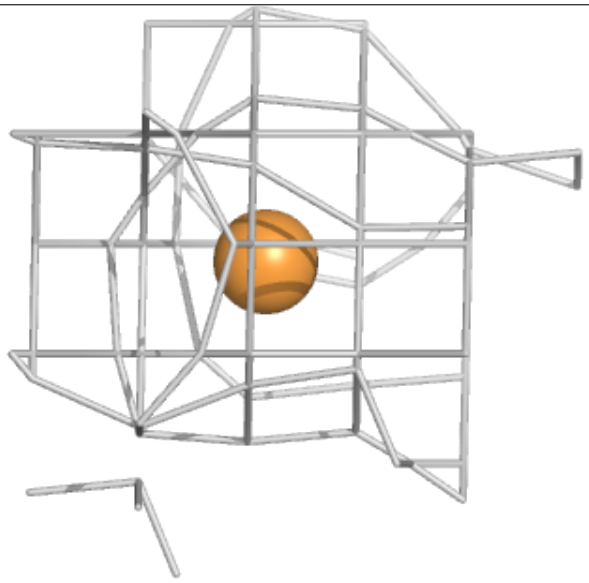
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

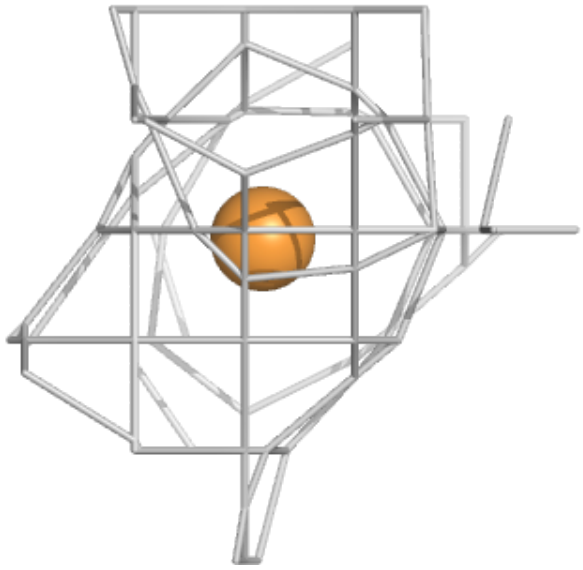


Electron density around CU F 401:

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

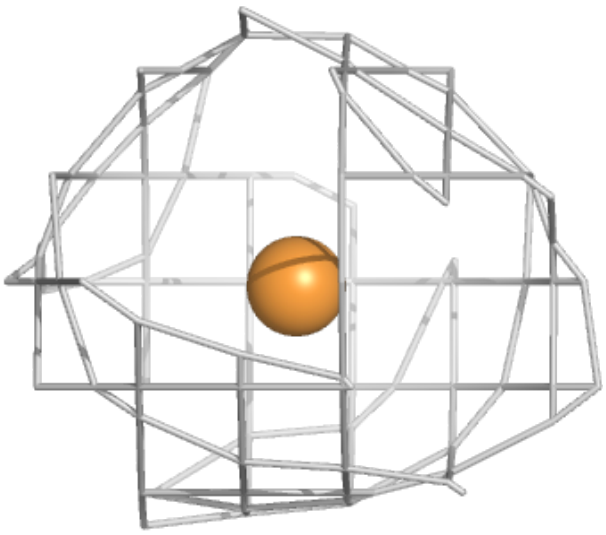


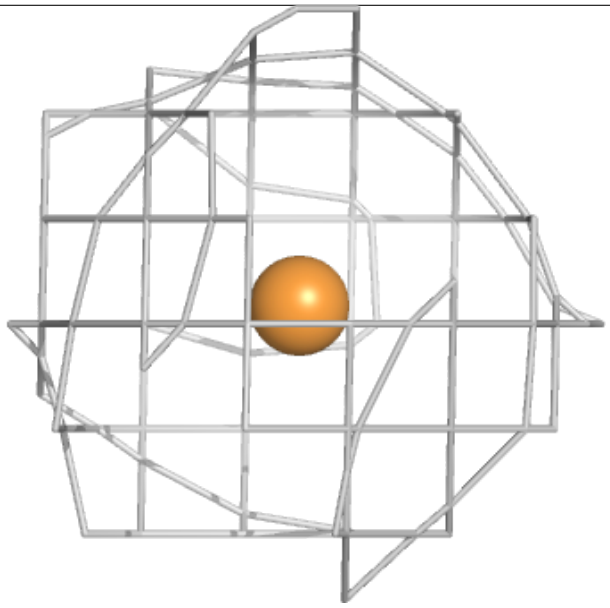


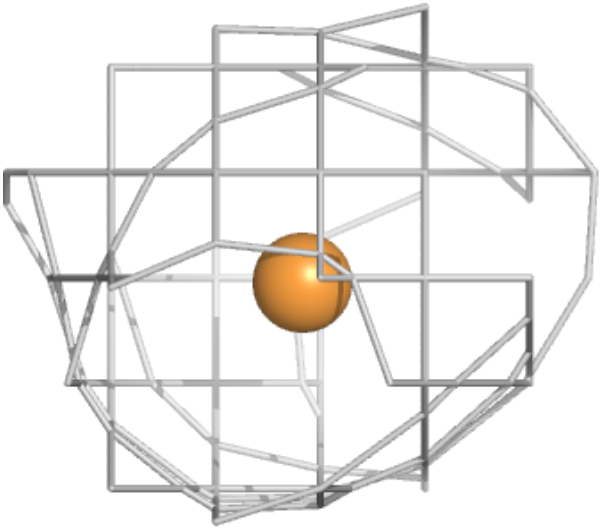


Electron density around CU A 402:

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

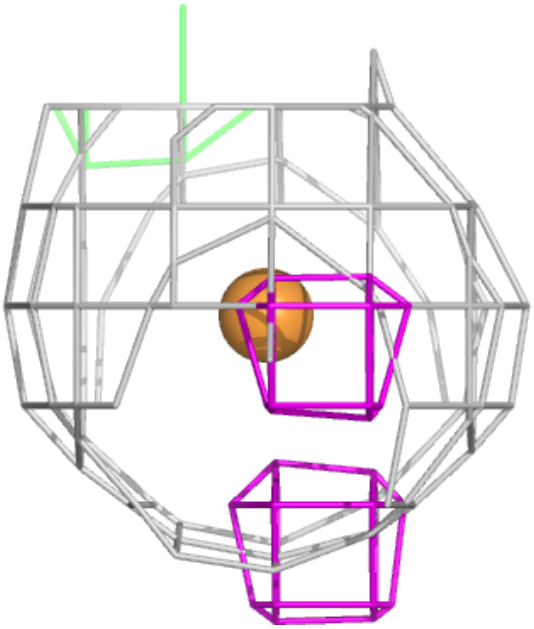


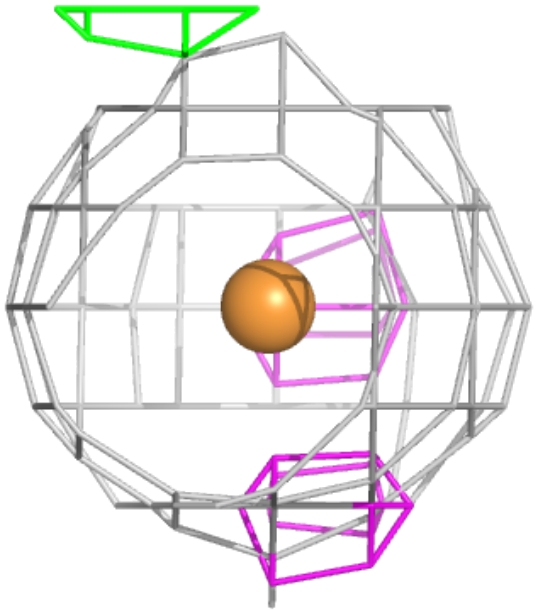


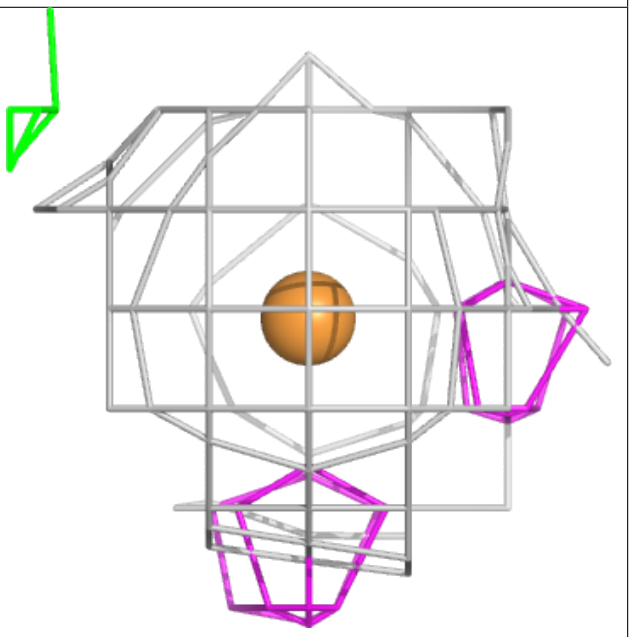


Electron density around CU F 403:

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

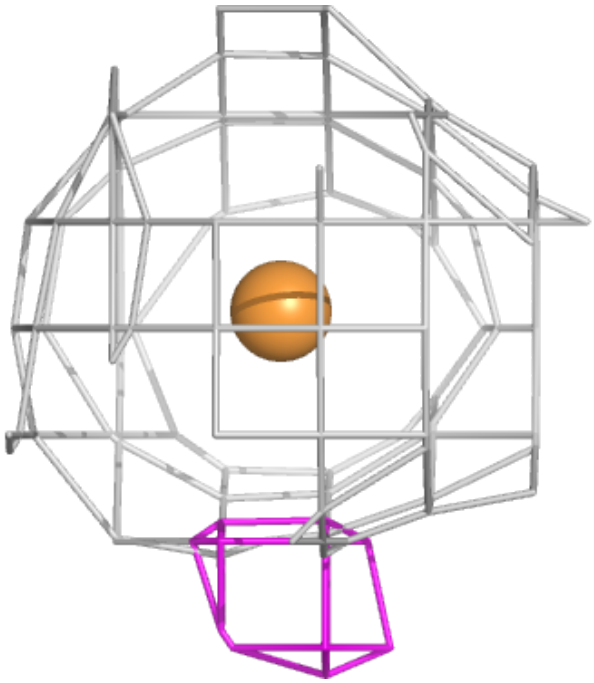


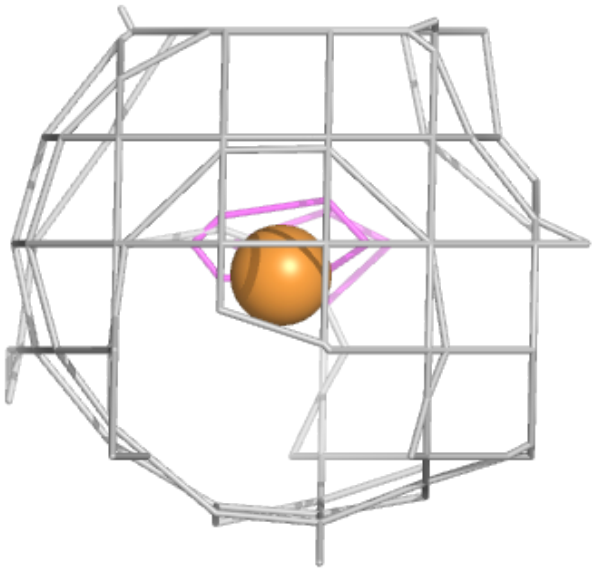


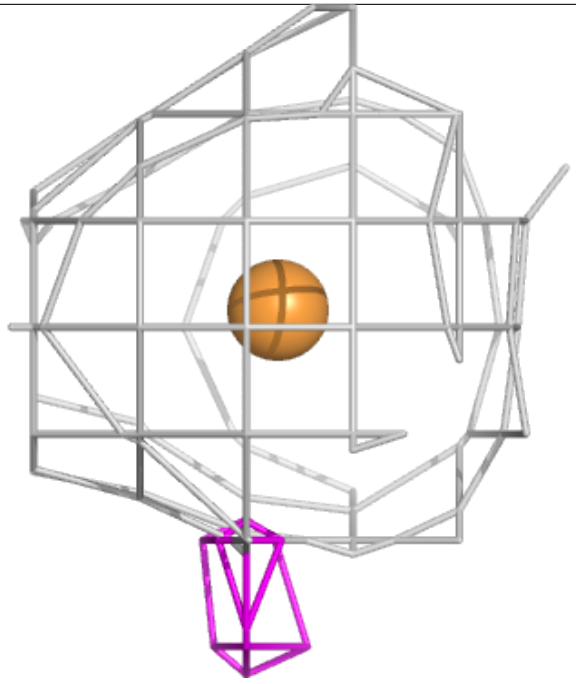


Electron density around CU F 404:

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

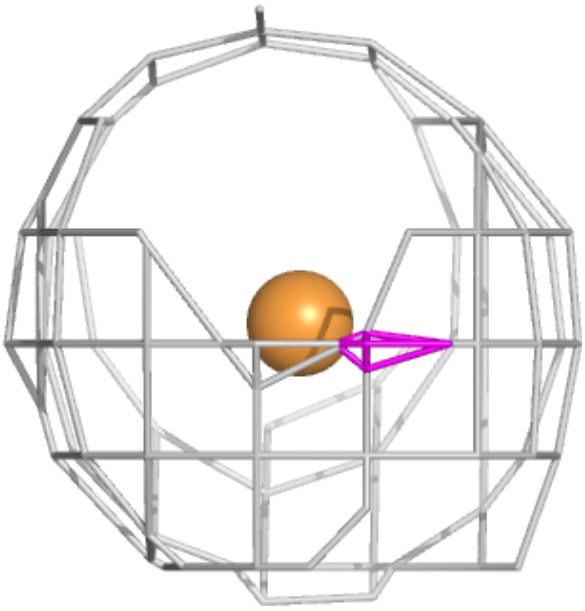


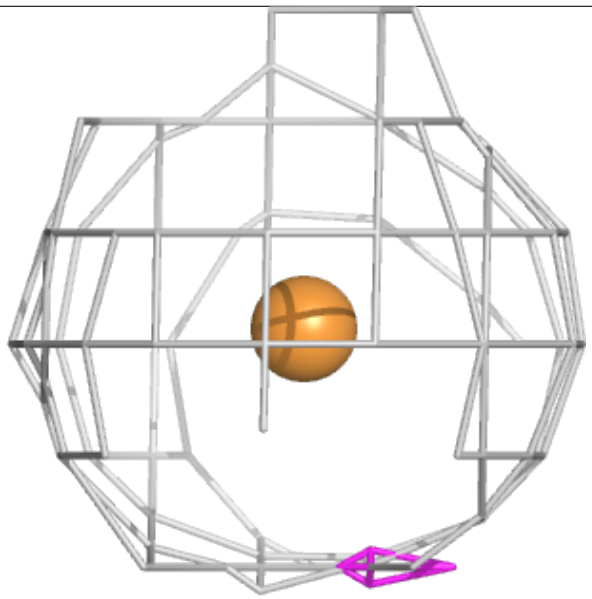


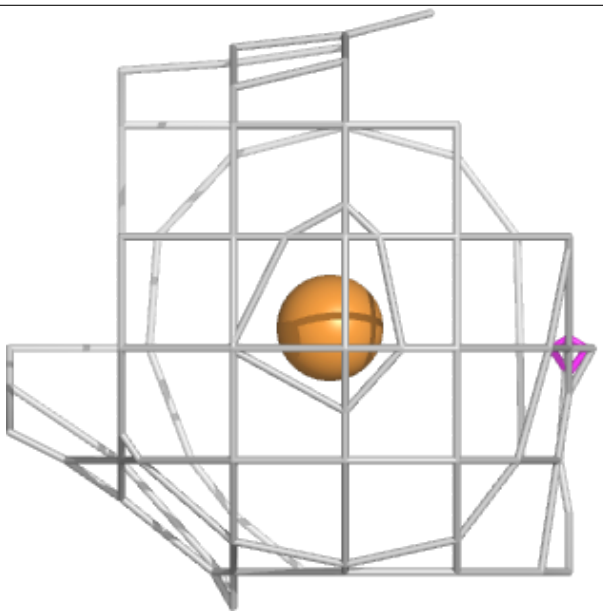


Electron density around CU B 401:

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

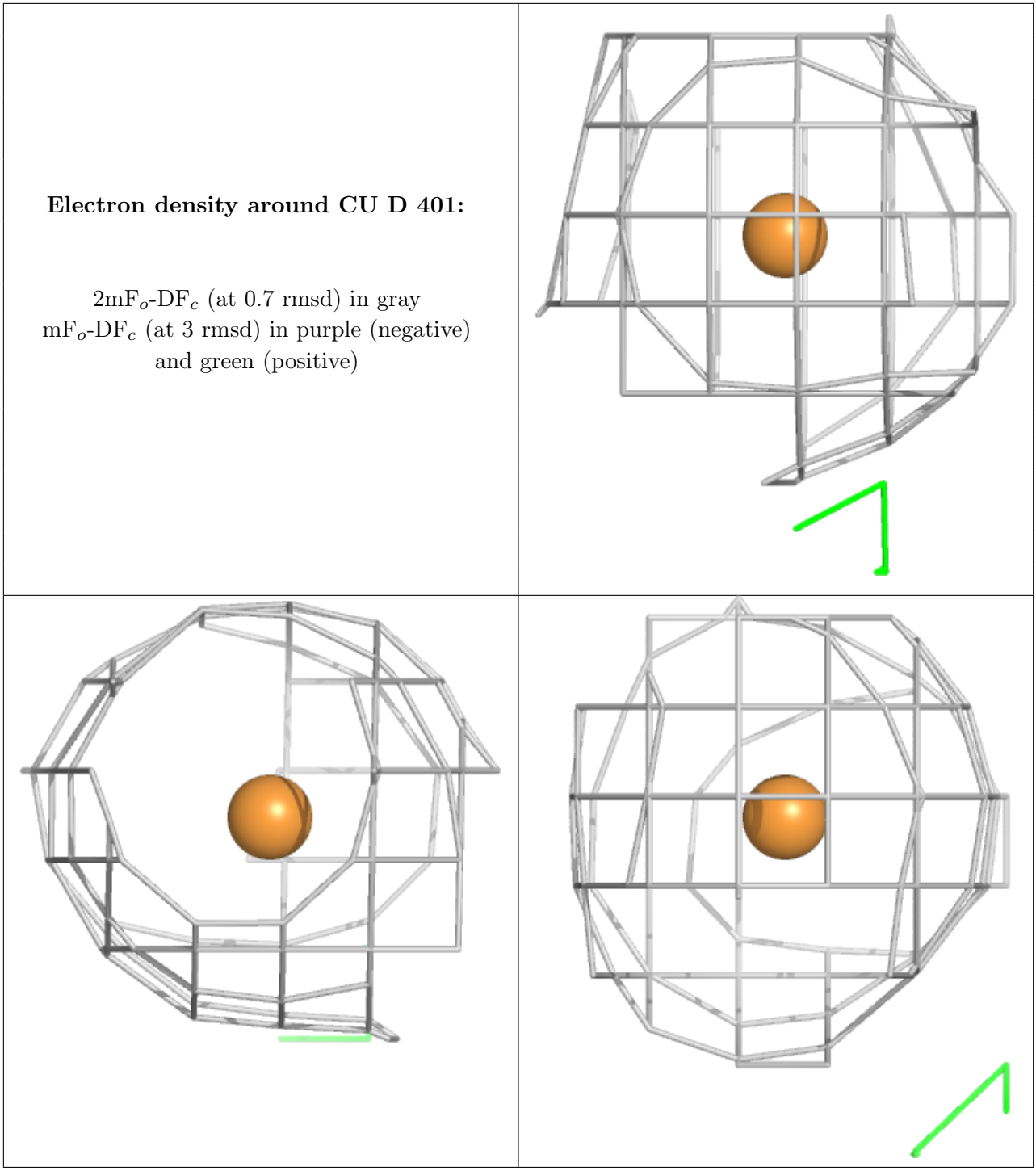






Electron density around CU D 401:

$2mF_o$-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

There are no such residues in this entry.