wwPDB X-ray Structure Validation Summary Report (i)

Oct 14, 2021 – 02:11 PM EDT

PDB ID	:	7RAC
Title	:	Crystal structure of a dodecameric multicopper oxidase from M. hydrothermalis in an orthorhombic lattice
Authors	:	Georgiadis, M.M.; Ogata, C.M.
Deposited on	:	2021-06-30
Resolution	:	2.36 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

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

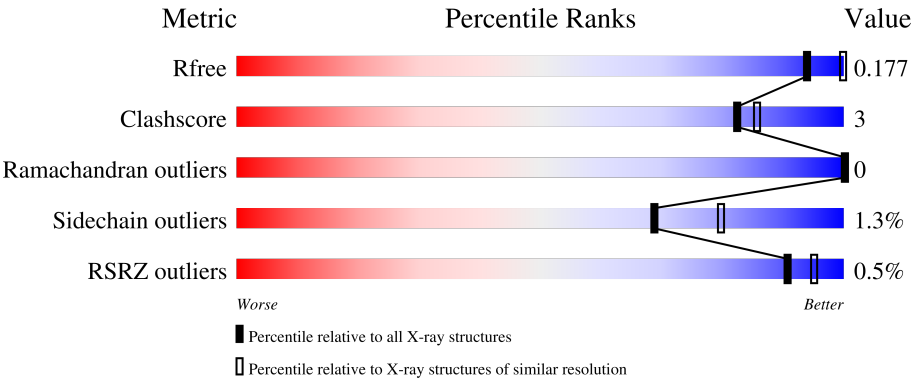
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	348	81% 5% 14%
1	B	348	81% 14%
1	C	348	82% 14%
1	D	348	80% 5% 14%
1	E	348	81% 14%

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Mol	Chain	Length	Quality of chain
1	F	348	80% 5% 14%
1	G	348	82% 14%
1	H	348	80% 6% 14%
1	I	348	% 80% 5% 14%
1	J	348	% 82% 14%
1	K	348	81% 14%
1	L	348	% 81% 5% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 30961 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	2	0
			2431	1569	413	438	11			
1	B	299	Total	C	N	O	S	0	3	0
			2437	1573	413	440	11			
1	C	299	Total	C	N	O	S	0	2	0
			2431	1569	413	438	11			
1	D	299	Total	C	N	O	S	0	2	0
			2431	1569	413	438	11			
1	E	299	Total	C	N	O	S	0	2	0
			2431	1569	413	438	11			
1	F	299	Total	C	N	O	S	0	2	0
			2431	1569	413	438	11			
1	G	299	Total	C	N	O	S	0	2	0
			2431	1569	413	438	11			
1	H	299	Total	C	N	O	S	0	2	0
			2431	1569	413	438	11			
1	I	299	Total	C	N	O	S	0	2	0
			2431	1569	413	438	11			
1	J	299	Total	C	N	O	S	0	2	0
			2431	1569	413	438	11			
1	K	299	Total	C	N	O	S	0	2	0
			2431	1569	413	438	11			
1	L	299	Total	C	N	O	S	0	2	0
			2431	1569	413	438	11			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP F2NNS0
A	13	GLY	-	expression tag	UNP F2NNS0
A	14	SER	-	expression tag	UNP F2NNS0
A	15	SER	-	expression tag	UNP F2NNS0
A	16	HIS	-	expression tag	UNP F2NNS0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	17	HIS	-	expression tag	UNP F2NNS0
A	18	HIS	-	expression tag	UNP F2NNS0
A	19	HIS	-	expression tag	UNP F2NNS0
A	20	HIS	-	expression tag	UNP F2NNS0
A	21	HIS	-	expression tag	UNP F2NNS0
A	22	SER	-	expression tag	UNP F2NNS0
A	23	SER	-	expression tag	UNP F2NNS0
A	24	GLY	-	expression tag	UNP F2NNS0
A	25	LEU	-	expression tag	UNP F2NNS0
A	26	VAL	-	expression tag	UNP F2NNS0
A	27	PRO	-	expression tag	UNP F2NNS0
A	28	ARG	-	expression tag	UNP F2NNS0
A	29	GLY	-	expression tag	UNP F2NNS0
A	30	SER	-	expression tag	UNP F2NNS0
A	31	HIS	-	expression tag	UNP F2NNS0
B	12	MET	-	initiating methionine	UNP F2NNS0
B	13	GLY	-	expression tag	UNP F2NNS0
B	14	SER	-	expression tag	UNP F2NNS0
B	15	SER	-	expression tag	UNP F2NNS0
B	16	HIS	-	expression tag	UNP F2NNS0
B	17	HIS	-	expression tag	UNP F2NNS0
B	18	HIS	-	expression tag	UNP F2NNS0
B	19	HIS	-	expression tag	UNP F2NNS0
B	20	HIS	-	expression tag	UNP F2NNS0
B	21	HIS	-	expression tag	UNP F2NNS0
B	22	SER	-	expression tag	UNP F2NNS0
B	23	SER	-	expression tag	UNP F2NNS0
B	24	GLY	-	expression tag	UNP F2NNS0
B	25	LEU	-	expression tag	UNP F2NNS0
B	26	VAL	-	expression tag	UNP F2NNS0
B	27	PRO	-	expression tag	UNP F2NNS0
B	28	ARG	-	expression tag	UNP F2NNS0
B	29	GLY	-	expression tag	UNP F2NNS0
B	30	SER	-	expression tag	UNP F2NNS0
B	31	HIS	-	expression tag	UNP F2NNS0
C	12	MET	-	initiating methionine	UNP F2NNS0
C	13	GLY	-	expression tag	UNP F2NNS0
C	14	SER	-	expression tag	UNP F2NNS0
C	15	SER	-	expression tag	UNP F2NNS0
C	16	HIS	-	expression tag	UNP F2NNS0
C	17	HIS	-	expression tag	UNP F2NNS0
C	18	HIS	-	expression tag	UNP F2NNS0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	19	HIS	-	expression tag	UNP F2NNS0
C	20	HIS	-	expression tag	UNP F2NNS0
C	21	HIS	-	expression tag	UNP F2NNS0
C	22	SER	-	expression tag	UNP F2NNS0
C	23	SER	-	expression tag	UNP F2NNS0
C	24	GLY	-	expression tag	UNP F2NNS0
C	25	LEU	-	expression tag	UNP F2NNS0
C	26	VAL	-	expression tag	UNP F2NNS0
C	27	PRO	-	expression tag	UNP F2NNS0
C	28	ARG	-	expression tag	UNP F2NNS0
C	29	GLY	-	expression tag	UNP F2NNS0
C	30	SER	-	expression tag	UNP F2NNS0
C	31	HIS	-	expression tag	UNP F2NNS0
D	12	MET	-	initiating methionine	UNP F2NNS0
D	13	GLY	-	expression tag	UNP F2NNS0
D	14	SER	-	expression tag	UNP F2NNS0
D	15	SER	-	expression tag	UNP F2NNS0
D	16	HIS	-	expression tag	UNP F2NNS0
D	17	HIS	-	expression tag	UNP F2NNS0
D	18	HIS	-	expression tag	UNP F2NNS0
D	19	HIS	-	expression tag	UNP F2NNS0
D	20	HIS	-	expression tag	UNP F2NNS0
D	21	HIS	-	expression tag	UNP F2NNS0
D	22	SER	-	expression tag	UNP F2NNS0
D	23	SER	-	expression tag	UNP F2NNS0
D	24	GLY	-	expression tag	UNP F2NNS0
D	25	LEU	-	expression tag	UNP F2NNS0
D	26	VAL	-	expression tag	UNP F2NNS0
D	27	PRO	-	expression tag	UNP F2NNS0
D	28	ARG	-	expression tag	UNP F2NNS0
D	29	GLY	-	expression tag	UNP F2NNS0
D	30	SER	-	expression tag	UNP F2NNS0
D	31	HIS	-	expression tag	UNP F2NNS0
E	12	MET	-	initiating methionine	UNP F2NNS0
E	13	GLY	-	expression tag	UNP F2NNS0
E	14	SER	-	expression tag	UNP F2NNS0
E	15	SER	-	expression tag	UNP F2NNS0
E	16	HIS	-	expression tag	UNP F2NNS0
E	17	HIS	-	expression tag	UNP F2NNS0
E	18	HIS	-	expression tag	UNP F2NNS0
E	19	HIS	-	expression tag	UNP F2NNS0
E	20	HIS	-	expression tag	UNP F2NNS0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	21	HIS	-	expression tag	UNP F2NNS0
E	22	SER	-	expression tag	UNP F2NNS0
E	23	SER	-	expression tag	UNP F2NNS0
E	24	GLY	-	expression tag	UNP F2NNS0
E	25	LEU	-	expression tag	UNP F2NNS0
E	26	VAL	-	expression tag	UNP F2NNS0
E	27	PRO	-	expression tag	UNP F2NNS0
E	28	ARG	-	expression tag	UNP F2NNS0
E	29	GLY	-	expression tag	UNP F2NNS0
E	30	SER	-	expression tag	UNP F2NNS0
E	31	HIS	-	expression tag	UNP F2NNS0
F	12	MET	-	initiating methionine	UNP F2NNS0
F	13	GLY	-	expression tag	UNP F2NNS0
F	14	SER	-	expression tag	UNP F2NNS0
F	15	SER	-	expression tag	UNP F2NNS0
F	16	HIS	-	expression tag	UNP F2NNS0
F	17	HIS	-	expression tag	UNP F2NNS0
F	18	HIS	-	expression tag	UNP F2NNS0
F	19	HIS	-	expression tag	UNP F2NNS0
F	20	HIS	-	expression tag	UNP F2NNS0
F	21	HIS	-	expression tag	UNP F2NNS0
F	22	SER	-	expression tag	UNP F2NNS0
F	23	SER	-	expression tag	UNP F2NNS0
F	24	GLY	-	expression tag	UNP F2NNS0
F	25	LEU	-	expression tag	UNP F2NNS0
F	26	VAL	-	expression tag	UNP F2NNS0
F	27	PRO	-	expression tag	UNP F2NNS0
F	28	ARG	-	expression tag	UNP F2NNS0
F	29	GLY	-	expression tag	UNP F2NNS0
F	30	SER	-	expression tag	UNP F2NNS0
F	31	HIS	-	expression tag	UNP F2NNS0
G	12	MET	-	initiating methionine	UNP F2NNS0
G	13	GLY	-	expression tag	UNP F2NNS0
G	14	SER	-	expression tag	UNP F2NNS0
G	15	SER	-	expression tag	UNP F2NNS0
G	16	HIS	-	expression tag	UNP F2NNS0
G	17	HIS	-	expression tag	UNP F2NNS0
G	18	HIS	-	expression tag	UNP F2NNS0
G	19	HIS	-	expression tag	UNP F2NNS0
G	20	HIS	-	expression tag	UNP F2NNS0
G	21	HIS	-	expression tag	UNP F2NNS0
G	22	SER	-	expression tag	UNP F2NNS0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	23	SER	-	expression tag	UNP F2NNS0
G	24	GLY	-	expression tag	UNP F2NNS0
G	25	LEU	-	expression tag	UNP F2NNS0
G	26	VAL	-	expression tag	UNP F2NNS0
G	27	PRO	-	expression tag	UNP F2NNS0
G	28	ARG	-	expression tag	UNP F2NNS0
G	29	GLY	-	expression tag	UNP F2NNS0
G	30	SER	-	expression tag	UNP F2NNS0
G	31	HIS	-	expression tag	UNP F2NNS0
H	12	MET	-	initiating methionine	UNP F2NNS0
H	13	GLY	-	expression tag	UNP F2NNS0
H	14	SER	-	expression tag	UNP F2NNS0
H	15	SER	-	expression tag	UNP F2NNS0
H	16	HIS	-	expression tag	UNP F2NNS0
H	17	HIS	-	expression tag	UNP F2NNS0
H	18	HIS	-	expression tag	UNP F2NNS0
H	19	HIS	-	expression tag	UNP F2NNS0
H	20	HIS	-	expression tag	UNP F2NNS0
H	21	HIS	-	expression tag	UNP F2NNS0
H	22	SER	-	expression tag	UNP F2NNS0
H	23	SER	-	expression tag	UNP F2NNS0
H	24	GLY	-	expression tag	UNP F2NNS0
H	25	LEU	-	expression tag	UNP F2NNS0
H	26	VAL	-	expression tag	UNP F2NNS0
H	27	PRO	-	expression tag	UNP F2NNS0
H	28	ARG	-	expression tag	UNP F2NNS0
H	29	GLY	-	expression tag	UNP F2NNS0
H	30	SER	-	expression tag	UNP F2NNS0
H	31	HIS	-	expression tag	UNP F2NNS0
I	12	MET	-	initiating methionine	UNP F2NNS0
I	13	GLY	-	expression tag	UNP F2NNS0
I	14	SER	-	expression tag	UNP F2NNS0
I	15	SER	-	expression tag	UNP F2NNS0
I	16	HIS	-	expression tag	UNP F2NNS0
I	17	HIS	-	expression tag	UNP F2NNS0
I	18	HIS	-	expression tag	UNP F2NNS0
I	19	HIS	-	expression tag	UNP F2NNS0
I	20	HIS	-	expression tag	UNP F2NNS0
I	21	HIS	-	expression tag	UNP F2NNS0
I	22	SER	-	expression tag	UNP F2NNS0
I	23	SER	-	expression tag	UNP F2NNS0
I	24	GLY	-	expression tag	UNP F2NNS0

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Chain	Residue	Modelled	Actual	Comment	Reference
I	25	LEU	-	expression tag	UNP F2NNS0
I	26	VAL	-	expression tag	UNP F2NNS0
I	27	PRO	-	expression tag	UNP F2NNS0
I	28	ARG	-	expression tag	UNP F2NNS0
I	29	GLY	-	expression tag	UNP F2NNS0
I	30	SER	-	expression tag	UNP F2NNS0
I	31	HIS	-	expression tag	UNP F2NNS0
J	12	MET	-	initiating methionine	UNP F2NNS0
J	13	GLY	-	expression tag	UNP F2NNS0
J	14	SER	-	expression tag	UNP F2NNS0
J	15	SER	-	expression tag	UNP F2NNS0
J	16	HIS	-	expression tag	UNP F2NNS0
J	17	HIS	-	expression tag	UNP F2NNS0
J	18	HIS	-	expression tag	UNP F2NNS0
J	19	HIS	-	expression tag	UNP F2NNS0
J	20	HIS	-	expression tag	UNP F2NNS0
J	21	HIS	-	expression tag	UNP F2NNS0
J	22	SER	-	expression tag	UNP F2NNS0
J	23	SER	-	expression tag	UNP F2NNS0
J	24	GLY	-	expression tag	UNP F2NNS0
J	25	LEU	-	expression tag	UNP F2NNS0
J	26	VAL	-	expression tag	UNP F2NNS0
J	27	PRO	-	expression tag	UNP F2NNS0
J	28	ARG	-	expression tag	UNP F2NNS0
J	29	GLY	-	expression tag	UNP F2NNS0
J	30	SER	-	expression tag	UNP F2NNS0
J	31	HIS	-	expression tag	UNP F2NNS0
K	12	MET	-	initiating methionine	UNP F2NNS0
K	13	GLY	-	expression tag	UNP F2NNS0
K	14	SER	-	expression tag	UNP F2NNS0
K	15	SER	-	expression tag	UNP F2NNS0
K	16	HIS	-	expression tag	UNP F2NNS0
K	17	HIS	-	expression tag	UNP F2NNS0
K	18	HIS	-	expression tag	UNP F2NNS0
K	19	HIS	-	expression tag	UNP F2NNS0
K	20	HIS	-	expression tag	UNP F2NNS0
K	21	HIS	-	expression tag	UNP F2NNS0
K	22	SER	-	expression tag	UNP F2NNS0
K	23	SER	-	expression tag	UNP F2NNS0
K	24	GLY	-	expression tag	UNP F2NNS0
K	25	LEU	-	expression tag	UNP F2NNS0
K	26	VAL	-	expression tag	UNP F2NNS0

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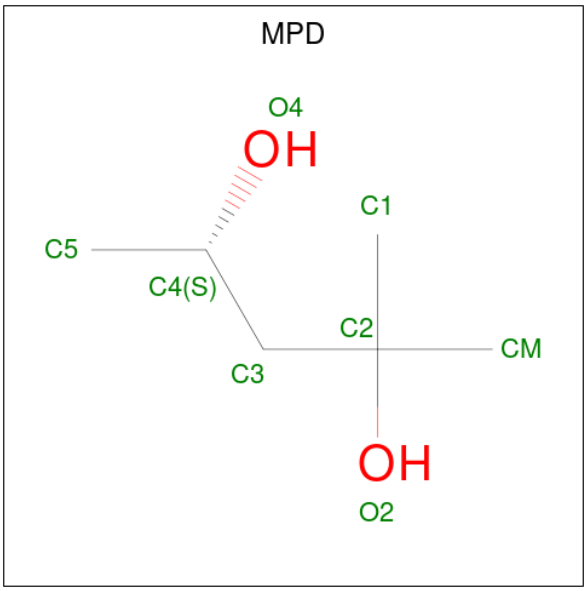
Chain	Residue	Modelled	Actual	Comment	Reference
K	27	PRO	-	expression tag	UNP F2NNS0
K	28	ARG	-	expression tag	UNP F2NNS0
K	29	GLY	-	expression tag	UNP F2NNS0
K	30	SER	-	expression tag	UNP F2NNS0
K	31	HIS	-	expression tag	UNP F2NNS0
L	12	MET	-	initiating methionine	UNP F2NNS0
L	13	GLY	-	expression tag	UNP F2NNS0
L	14	SER	-	expression tag	UNP F2NNS0
L	15	SER	-	expression tag	UNP F2NNS0
L	16	HIS	-	expression tag	UNP F2NNS0
L	17	HIS	-	expression tag	UNP F2NNS0
L	18	HIS	-	expression tag	UNP F2NNS0
L	19	HIS	-	expression tag	UNP F2NNS0
L	20	HIS	-	expression tag	UNP F2NNS0
L	21	HIS	-	expression tag	UNP F2NNS0
L	22	SER	-	expression tag	UNP F2NNS0
L	23	SER	-	expression tag	UNP F2NNS0
L	24	GLY	-	expression tag	UNP F2NNS0
L	25	LEU	-	expression tag	UNP F2NNS0
L	26	VAL	-	expression tag	UNP F2NNS0
L	27	PRO	-	expression tag	UNP F2NNS0
L	28	ARG	-	expression tag	UNP F2NNS0
L	29	GLY	-	expression tag	UNP F2NNS0
L	30	SER	-	expression tag	UNP F2NNS0
L	31	HIS	-	expression tag	UNP F2NNS0

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	D	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	E	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		
2	F	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O 8 6 2	0	0
2	G	1	Total C O 8 6 2	0	0
2	H	1	Total C O 8 6 2	0	0
2	H	1	Total C O 8 6 2	0	0
2	I	1	Total C O 8 6 2	0	0
2	J	1	Total C O 8 6 2	0	0
2	K	1	Total C O 8 6 2	0	0
2	L	1	Total C O 8 6 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cu 2 2	0	0
3	B	2	Total Cu 2 2	0	0
3	C	2	Total Cu 2 2	0	0
3	D	2	Total Cu 2 2	0	0
3	E	2	Total Cu 2 2	0	0
3	F	2	Total Cu 2 2	0	0
3	G	2	Total Cu 2 2	0	0
3	H	2	Total Cu 2 2	0	0
3	I	2	Total Cu 2 2	0	0
3	J	2	Total Cu 2 2	0	0
3	K	2	Total Cu 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	2	Total Cu 2 2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0
4	B	1	Total Ca 1 1	0	0
4	C	2	Total Ca 2 2	0	0
4	D	2	Total Ca 2 2	0	0
4	E	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0
4	G	2	Total Ca 2 2	0	0
4	H	1	Total Ca 1 1	0	0
4	I	1	Total Ca 1 1	0	0
4	J	2	Total Ca 2 2	0	0
4	K	1	Total Ca 1 1	0	0
4	L	1	Total Ca 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	139	Total O 139 139	0	0
5	B	135	Total O 135 135	0	0
5	C	143	Total O 143 143	0	0
5	D	129	Total O 129 129	0	0

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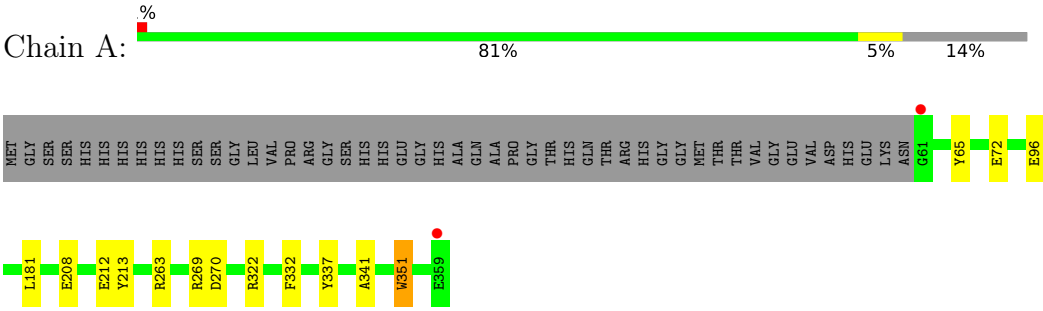
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	132	Total O 132 132	0	0
5	F	141	Total O 141 141	0	0
5	G	143	Total O 143 143	0	0
5	H	107	Total O 107 107	0	0
5	I	133	Total O 133 133	0	0
5	J	131	Total O 131 131	0	0
5	K	132	Total O 132 132	0	0
5	L	101	Total O 101 101	0	0

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.

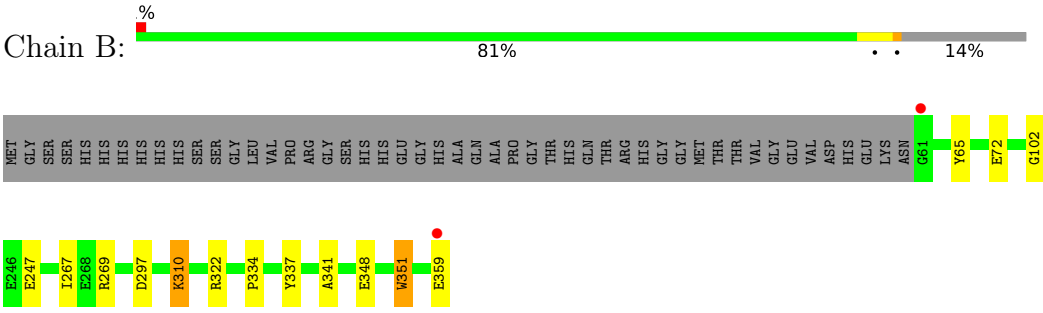
• Molecule 1: multicopper oxidase

Chain A:



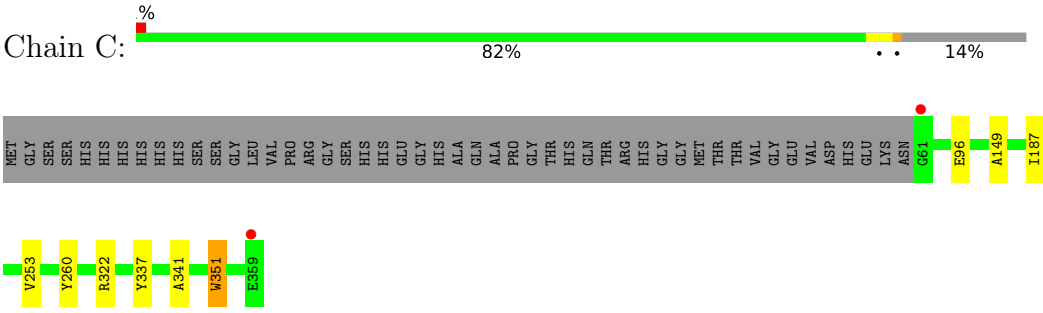
• Molecule 1: multicopper oxidase

Chain B:



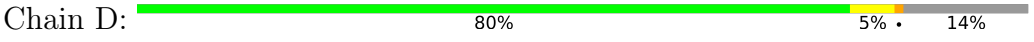
• Molecule 1: multicopper oxidase

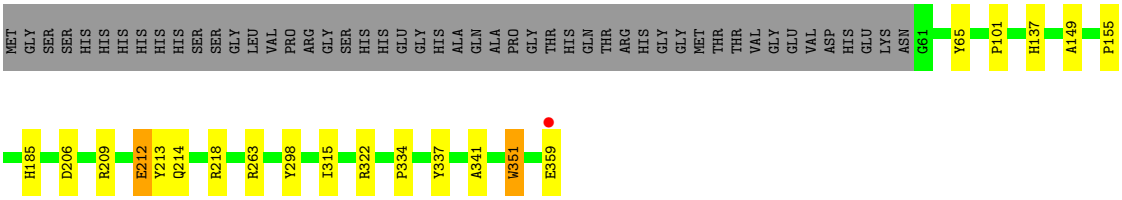
Chain C:



• Molecule 1: multicopper oxidase

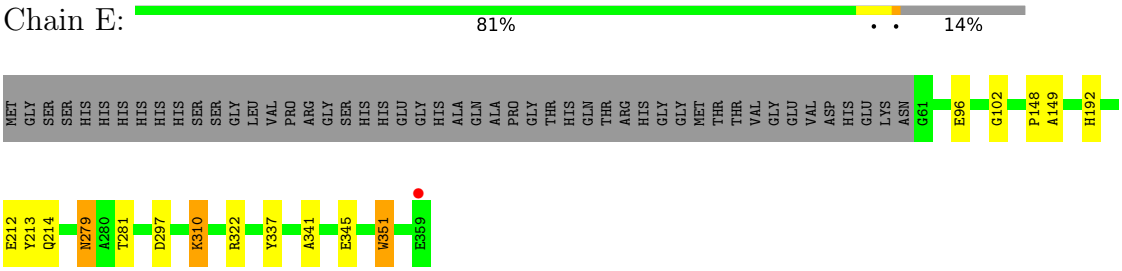
Chain D:





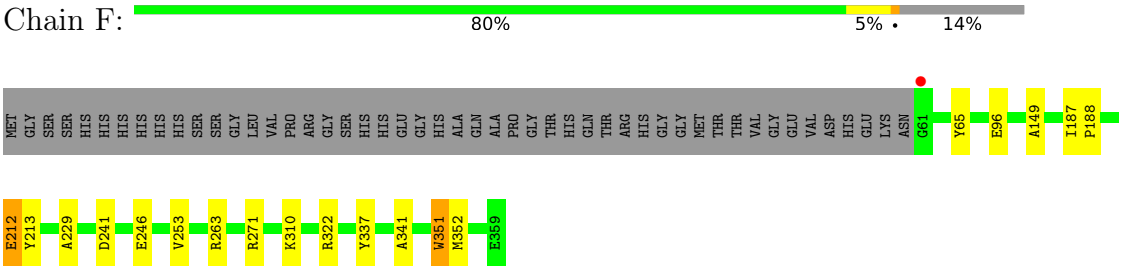
• Molecule 1: multicopper oxidase

Chain E:



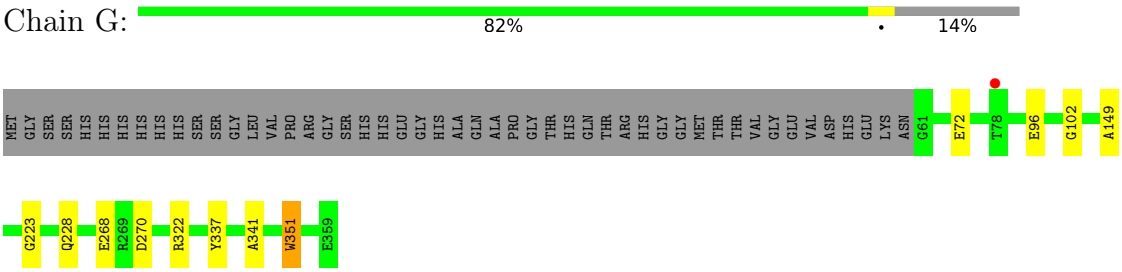
• Molecule 1: multicopper oxidase

Chain F:



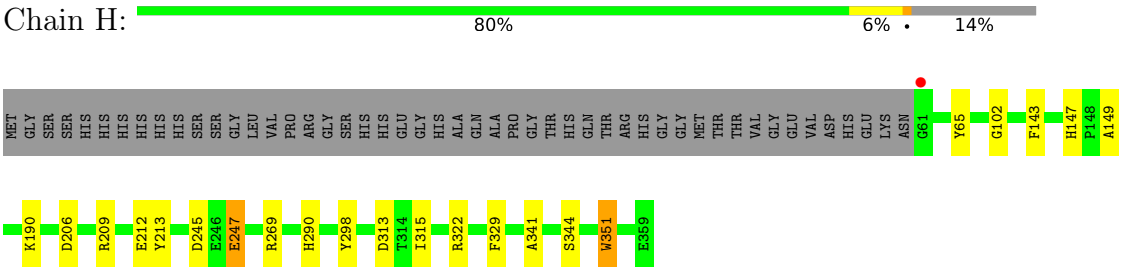
• Molecule 1: multicopper oxidase

Chain G:



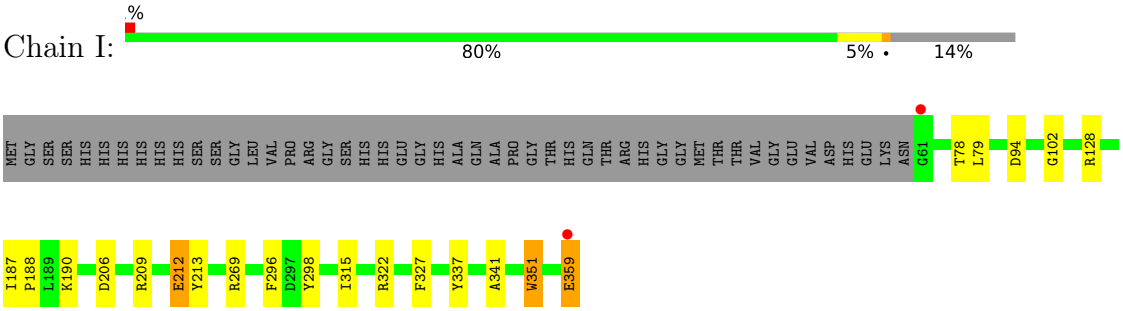
• Molecule 1: multicopper oxidase

Chain H:



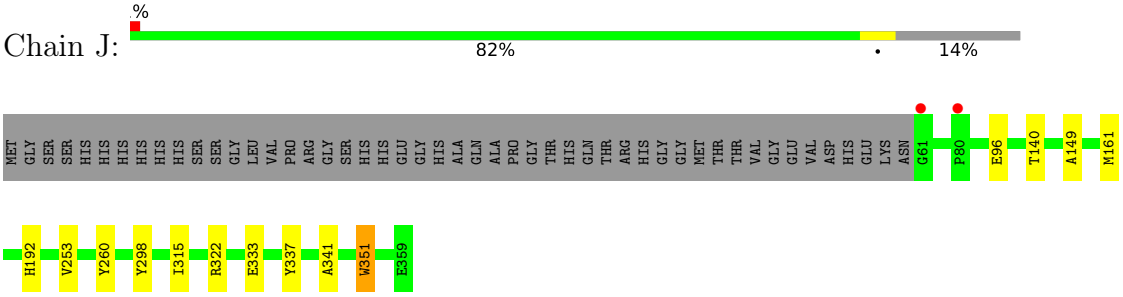
• Molecule 1: multicopper oxidase

Chain I:



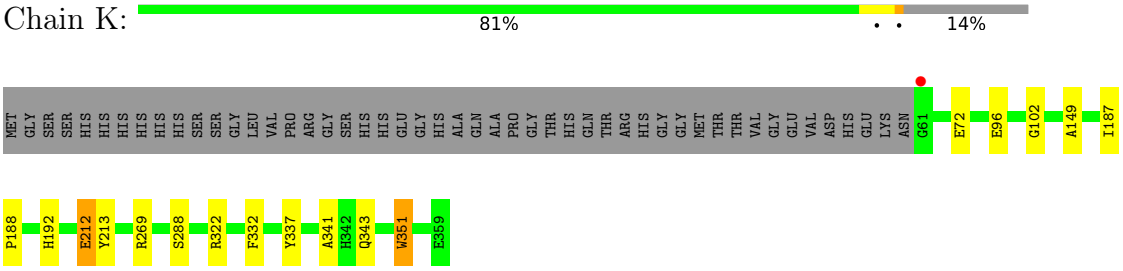
• Molecule 1: multicopper oxidase

Chain J:



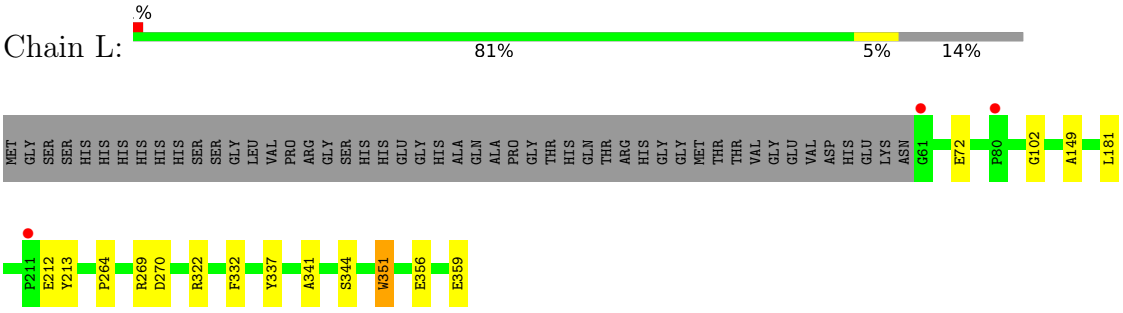
• Molecule 1: multicopper oxidase

Chain K:



• Molecule 1: multicopper oxidase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	169.30Å 176.19Å 176.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.04 – 2.36 61.04 – 2.36	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.04-2.36) 100.0 (61.04-2.36)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.139 , 0.177 0.139 , 0.177	Depositor DCC
R_{free} test set	10721 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -l,-k,-h 0.000 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	30961	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: CA, CU, MPD

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	0.42	0/2526	0.59	0/3445
1	B	0.41	0/2535	0.57	0/3457
1	C	0.44	0/2526	0.58	0/3445
1	D	0.43	0/2526	0.58	0/3445
1	E	0.44	0/2526	0.57	0/3445
1	F	0.42	0/2526	0.58	0/3445
1	G	0.41	0/2526	0.58	0/3445
1	H	0.42	0/2526	0.57	0/3445
1	I	0.42	0/2526	0.58	0/3445
1	J	0.40	0/2526	0.57	0/3445
1	K	0.41	0/2526	0.57	0/3445
1	L	0.41	0/2526	0.57	0/3445
All	All	0.42	0/30321	0.58	0/41352

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	2431	0	2261	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2437	0	2267	16	0
1	C	2431	0	2261	9	0
1	D	2431	0	2261	15	0
1	E	2431	0	2261	14	0
1	F	2431	0	2261	13	0
1	G	2431	0	2261	10	0
1	H	2431	0	2261	16	0
1	I	2431	0	2261	15	0
1	J	2431	0	2261	11	0
1	K	2431	0	2261	15	0
1	L	2431	0	2261	15	0
2	A	24	0	42	1	0
2	B	16	0	28	3	0
2	C	16	0	28	0	0
2	D	16	0	28	1	0
2	E	24	0	42	0	0
2	F	16	0	28	3	0
2	G	16	0	28	1	0
2	H	16	0	28	2	0
2	I	8	0	14	1	0
2	J	8	0	14	1	0
2	K	8	0	14	0	0
2	L	8	0	14	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	2	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	139	0	0	5	0
5	B	135	0	0	2	0
5	C	143	0	0	0	0
5	D	129	0	0	0	0
5	E	132	0	0	2	0
5	F	141	0	0	1	0
5	G	143	0	0	2	0
5	H	107	0	0	1	0
5	I	133	0	0	1	0
5	J	131	0	0	1	0
5	K	132	0	0	2	0
5	L	101	0	0	3	0
All	All	30961	0	27446	144	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 144 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:I:269:ARG:HH11	1:I:359:GLU:HG2	1.61	0.66
1:C:341:ALA:HB2	1:C:351[B]:TRP:CD1	2.31	0.66
1:F:341:ALA:HB2	1:F:351[B]:TRP:CD1	2.31	0.66
1:K:341:ALA:HB2	1:K:351[B]:TRP:CD1	2.30	0.66
1:F:341:ALA:HB2	1:F:351[A]:TRP:CD1	2.32	0.65

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	299/348 (86%)	290 (97%)	9 (3%)	0	100	100
1	B	300/348 (86%)	292 (97%)	8 (3%)	0	100	100
1	C	299/348 (86%)	290 (97%)	9 (3%)	0	100	100
1	D	299/348 (86%)	291 (97%)	8 (3%)	0	100	100
1	E	299/348 (86%)	291 (97%)	8 (3%)	0	100	100
1	F	299/348 (86%)	292 (98%)	7 (2%)	0	100	100
1	G	299/348 (86%)	291 (97%)	8 (3%)	0	100	100
1	H	299/348 (86%)	288 (96%)	11 (4%)	0	100	100
1	I	299/348 (86%)	290 (97%)	9 (3%)	0	100	100
1	J	299/348 (86%)	290 (97%)	9 (3%)	0	100	100
1	K	299/348 (86%)	290 (97%)	9 (3%)	0	100	100
1	L	299/348 (86%)	292 (98%)	7 (2%)	0	100	100
All	All	3589/4176 (86%)	3487 (97%)	102 (3%)	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	254/291 (87%)	249 (98%)	5 (2%)	55	66
1	B	255/291 (88%)	251 (98%)	4 (2%)	62	75
1	C	254/291 (87%)	250 (98%)	4 (2%)	62	75
1	D	254/291 (87%)	250 (98%)	4 (2%)	62	75
1	E	254/291 (87%)	248 (98%)	6 (2%)	49	59
1	F	254/291 (87%)	248 (98%)	6 (2%)	49	59
1	G	254/291 (87%)	251 (99%)	3 (1%)	71	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	254/291 (87%)	250 (98%)	4 (2%)	62 75
1	I	254/291 (87%)	248 (98%)	6 (2%)	49 59
1	J	254/291 (87%)	251 (99%)	3 (1%)	71 82
1	K	254/291 (87%)	250 (98%)	4 (2%)	62 75
1	L	254/291 (87%)	250 (98%)	4 (2%)	62 75
All	All	3049/3492 (87%)	2996 (98%)	53 (2%)	69 72

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	351[B]	TRP
1	H	351[B]	TRP
1	L	181	LEU
1	G	322	ARG
1	H	247	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	279	ASN
1	K	343	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 63 ligands modelled in this entry, 41 are monoatomic - leaving 22 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	MPD	J	401	-	7,7,7	0.25	0	9,10,10	0.44	0
2	MPD	C	401	-	7,7,7	0.41	0	9,10,10	0.62	0
2	MPD	L	401	-	7,7,7	0.28	0	9,10,10	0.71	0
2	MPD	A	402	-	7,7,7	0.37	0	9,10,10	0.52	0
2	MPD	H	402	-	7,7,7	0.29	0	9,10,10	0.47	0
2	MPD	I	401	-	7,7,7	0.30	0	9,10,10	0.64	0
2	MPD	K	401	-	7,7,7	0.26	0	9,10,10	0.32	0
2	MPD	D	401	-	7,7,7	0.29	0	9,10,10	0.52	0
2	MPD	C	402	-	7,7,7	0.36	0	9,10,10	0.78	0
2	MPD	E	402	-	7,7,7	0.23	0	9,10,10	0.32	0
2	MPD	D	402	-	7,7,7	0.47	0	9,10,10	0.54	0
2	MPD	A	401	-	7,7,7	0.27	0	9,10,10	0.32	0
2	MPD	H	401	-	7,7,7	0.23	0	9,10,10	0.70	0
2	MPD	A	403	-	7,7,7	0.34	0	9,10,10	0.74	0
2	MPD	E	401	-	7,7,7	0.27	0	9,10,10	0.56	0
2	MPD	G	402	-	7,7,7	0.29	0	9,10,10	0.51	0
2	MPD	G	401	-	7,7,7	0.31	0	9,10,10	1.05	1 (11%)
2	MPD	E	403	-	7,7,7	0.40	0	9,10,10	0.70	0
2	MPD	B	402	-	7,7,7	0.21	0	9,10,10	0.48	0
2	MPD	B	401	-	7,7,7	0.35	0	9,10,10	0.84	0
2	MPD	F	401	-	7,7,7	0.31	0	9,10,10	0.59	0
2	MPD	F	402	-	7,7,7	0.33	0	9,10,10	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	J	401	-	-	0/5/5/5	-
2	MPD	C	401	-	-	3/5/5/5	-
2	MPD	L	401	-	-	3/5/5/5	-
2	MPD	A	402	-	-	3/5/5/5	-
2	MPD	H	402	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	I	401	-	-	3/5/5/5	-
2	MPD	K	401	-	-	0/5/5/5	-
2	MPD	D	401	-	-	0/5/5/5	-
2	MPD	C	402	-	-	3/5/5/5	-
2	MPD	E	402	-	-	0/5/5/5	-
2	MPD	D	402	-	-	0/5/5/5	-
2	MPD	A	401	-	-	0/5/5/5	-
2	MPD	H	401	-	-	3/5/5/5	-
2	MPD	A	403	-	-	0/5/5/5	-
2	MPD	E	401	-	-	0/5/5/5	-
2	MPD	G	402	-	-	0/5/5/5	-
2	MPD	G	401	-	-	3/5/5/5	-
2	MPD	E	403	-	-	3/5/5/5	-
2	MPD	B	402	-	-	1/5/5/5	-
2	MPD	B	401	-	-	3/5/5/5	-
2	MPD	F	401	-	-	0/5/5/5	-
2	MPD	F	402	-	-	0/5/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	401	MPD	CM-C2-C1	-2.37	105.65	110.57

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	MPD	O2-C2-C3-C4
2	A	402	MPD	CM-C2-C3-C4
2	B	401	MPD	O2-C2-C3-C4
2	B	401	MPD	CM-C2-C3-C4
2	G	401	MPD	O2-C2-C3-C4

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	401	MPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	401	MPD	1	0
2	I	401	MPD	1	0
2	D	402	MPD	1	0
2	H	401	MPD	2	0
2	A	403	MPD	1	0
2	G	401	MPD	1	0
2	B	402	MPD	1	0
2	B	401	MPD	2	0
2	F	401	MPD	2	0
2	F	402	MPD	1	0

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	299/348 (85%)	-0.79	2 (0%)	87	92	13, 18, 33, 62	0
1	B	299/348 (85%)	-0.76	2 (0%)	87	92	13, 18, 35, 63	0
1	C	299/348 (85%)	-0.74	2 (0%)	87	92	13, 19, 35, 61	0
1	D	299/348 (85%)	-0.63	1 (0%)	94	97	14, 20, 36, 60	0
1	E	299/348 (85%)	-0.67	1 (0%)	94	97	12, 20, 36, 64	0
1	F	299/348 (85%)	-0.69	1 (0%)	94	97	12, 19, 34, 57	0
1	G	299/348 (85%)	-0.60	1 (0%)	94	97	13, 20, 36, 53	0
1	H	299/348 (85%)	-0.53	1 (0%)	94	97	14, 21, 39, 61	0
1	I	299/348 (85%)	-0.71	2 (0%)	87	92	13, 20, 36, 65	0
1	J	299/348 (85%)	-0.52	2 (0%)	87	92	15, 20, 35, 67	0
1	K	299/348 (85%)	-0.55	1 (0%)	94	97	14, 20, 38, 62	0
1	L	299/348 (85%)	-0.56	3 (1%)	82	88	14, 21, 40, 57	0
All	All	3588/4176 (85%)	-0.65	19 (0%)	91	95	12, 20, 36, 67	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	359	GLU	3.9
1	A	61	GLY	3.6
1	E	359	GLU	3.5
1	H	61	GLY	3.3
1	J	61	GLY	3.1

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 (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
4	CA	J	405	1/1	0.68	0.13	70,70,70,70	0
2	MPD	E	403	8/8	0.83	0.22	32,41,51,56	0
2	MPD	C	402	8/8	0.85	0.23	35,39,49,50	0
2	MPD	B	402	8/8	0.86	0.22	34,43,45,46	0
2	MPD	D	402	8/8	0.86	0.28	33,46,50,51	0
2	MPD	B	401	8/8	0.88	0.16	30,40,47,49	0
2	MPD	C	401	8/8	0.88	0.21	32,35,39,51	0
2	MPD	D	401	8/8	0.89	0.28	32,38,50,53	0
2	MPD	F	401	8/8	0.89	0.22	32,44,52,53	0
2	MPD	A	402	8/8	0.89	0.30	32,43,53,54	0
2	MPD	A	403	8/8	0.90	0.15	37,40,46,47	0
2	MPD	I	401	8/8	0.91	0.18	32,38,52,54	0
2	MPD	K	401	8/8	0.91	0.36	32,41,53,55	0
2	MPD	F	402	8/8	0.91	0.21	32,48,52,60	0
2	MPD	J	401	8/8	0.92	0.28	32,48,55,56	0
2	MPD	E	402	8/8	0.93	0.22	32,39,48,54	0
2	MPD	G	401	8/8	0.93	0.17	32,40,43,48	0
2	MPD	G	402	8/8	0.93	0.24	32,41,52,53	0
2	MPD	L	401	8/8	0.93	0.22	31,42,51,59	0
2	MPD	H	402	8/8	0.93	0.35	32,43,58,62	0
2	MPD	A	401	8/8	0.94	0.20	32,38,44,46	0
4	CA	G	405	1/1	0.94	0.05	24,24,24,24	1
2	MPD	H	401	8/8	0.94	0.14	32,36,40,49	0
2	MPD	E	401	8/8	0.95	0.19	32,38,51,55	0
4	CA	D	405	1/1	0.96	0.06	35,35,35,35	0
3	CU	G	403	1/1	0.98	0.07	24,24,24,24	1
3	CU	B	403	1/1	0.98	0.03	22,22,22,22	1
3	CU	E	404	1/1	0.98	0.09	20,20,20,20	1
3	CU	F	404	1/1	0.98	0.10	16,16,16,16	1
3	CU	D	404	1/1	0.99	0.11	16,16,16,16	1
3	CU	A	405	1/1	0.99	0.12	11,11,11,11	1
3	CU	F	403	1/1	0.99	0.05	28,28,28,28	1

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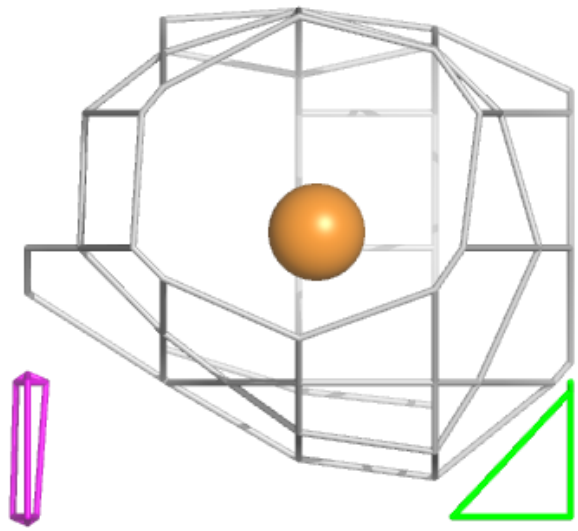
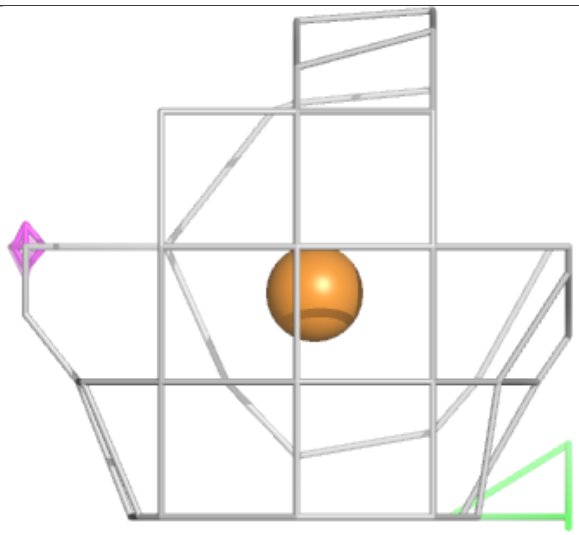
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CU	A	404	1/1	0.99	0.05	22,22,22,22	1
3	CU	B	404	1/1	0.99	0.12	16,16,16,16	1
3	CU	G	404	1/1	0.99	0.11	16,16,16,16	1
3	CU	H	404	1/1	0.99	0.09	22,22,22,22	1
3	CU	I	402	1/1	0.99	0.08	18,18,18,18	1
3	CU	I	403	1/1	0.99	0.06	26,26,26,26	1
3	CU	J	403	1/1	0.99	0.09	15,15,15,15	1
3	CU	K	403	1/1	0.99	0.12	19,19,19,19	1
3	CU	L	402	1/1	0.99	0.09	18,18,18,18	1
3	CU	L	403	1/1	0.99	0.05	21,21,21,21	1
4	CA	A	406	1/1	0.99	0.04	19,19,19,19	1
4	CA	A	407	1/1	0.99	0.08	23,23,23,23	0
4	CA	C	405	1/1	0.99	0.05	29,29,29,29	1
3	CU	C	403	1/1	0.99	0.06	22,22,22,22	1
4	CA	E	406	1/1	0.99	0.10	21,21,21,21	0
4	CA	F	405	1/1	0.99	0.08	22,22,22,22	0
3	CU	C	404	1/1	0.99	0.11	14,14,14,14	1
4	CA	J	404	1/1	0.99	0.10	22,22,22,22	0
3	CU	D	403	1/1	0.99	0.05	23,23,23,23	1
4	CA	K	404	1/1	0.99	0.09	21,21,21,21	0
4	CA	L	404	1/1	0.99	0.10	23,23,23,23	0
3	CU	K	402	1/1	1.00	0.06	21,21,21,21	1
3	CU	E	405	1/1	1.00	0.12	22,22,22,22	1
4	CA	B	405	1/1	1.00	0.08	19,19,19,19	0
4	CA	G	406	1/1	1.00	0.07	22,22,22,22	0
4	CA	H	405	1/1	1.00	0.07	23,23,23,23	0
4	CA	I	404	1/1	1.00	0.10	24,24,24,24	0
3	CU	J	402	1/1	1.00	0.06	21,21,21,21	1
4	CA	C	406	1/1	1.00	0.07	20,20,20,20	0
3	CU	H	403	1/1	1.00	0.05	18,18,18,18	1
4	CA	D	406	1/1	1.00	0.09	23,23,23,23	0

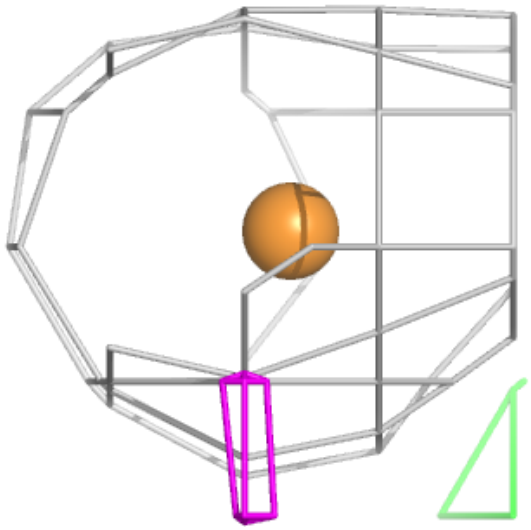
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CU G 403:

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

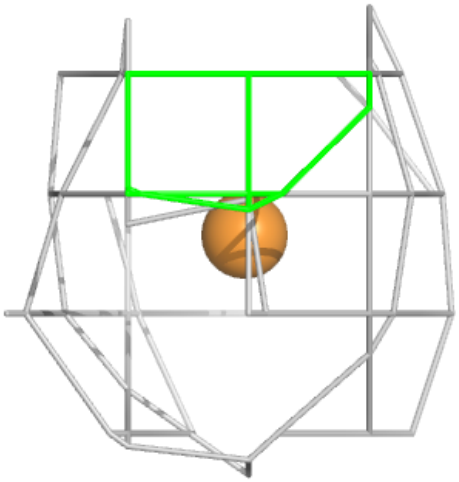


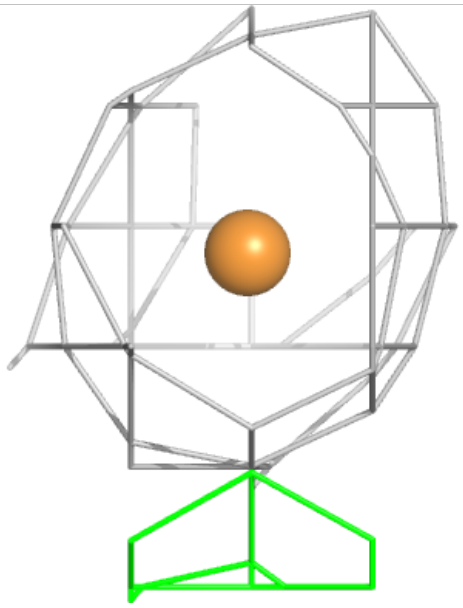


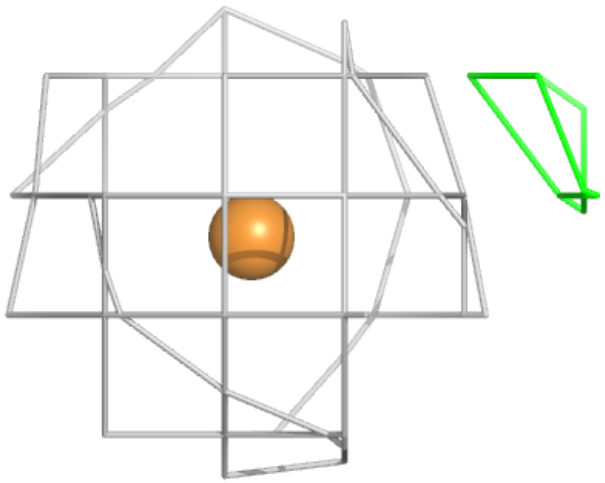


Electron density around CU B 403:

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

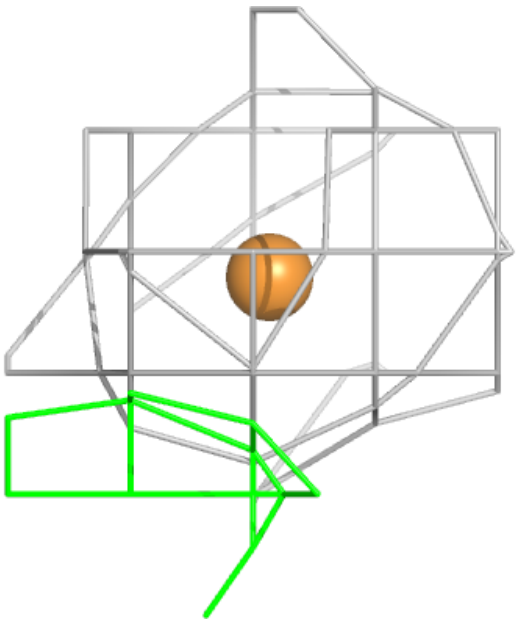


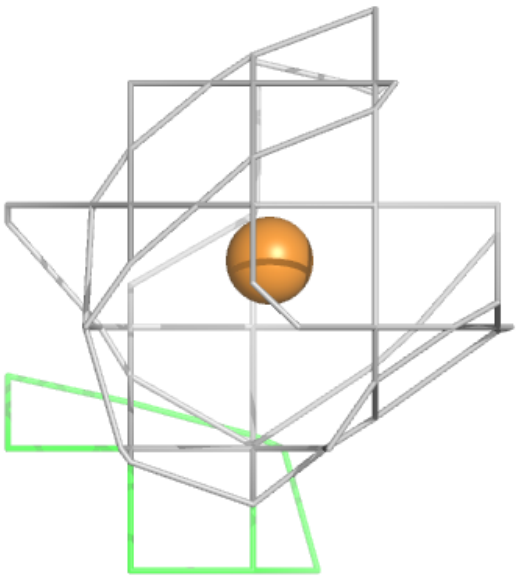


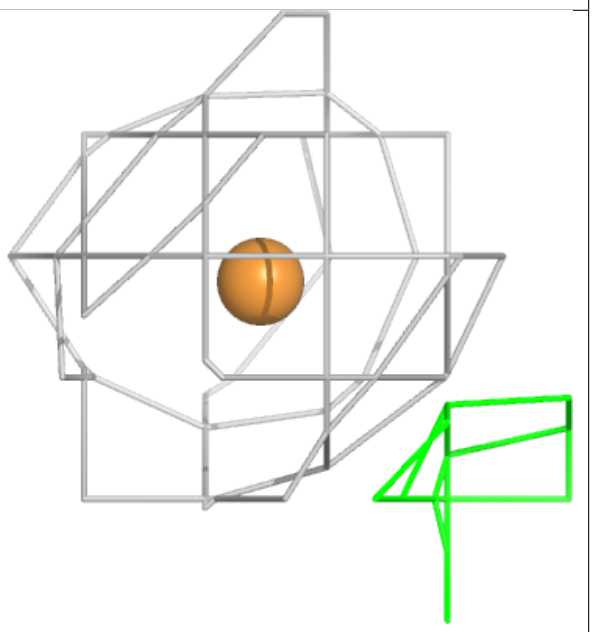


Electron density around CU E 404:

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

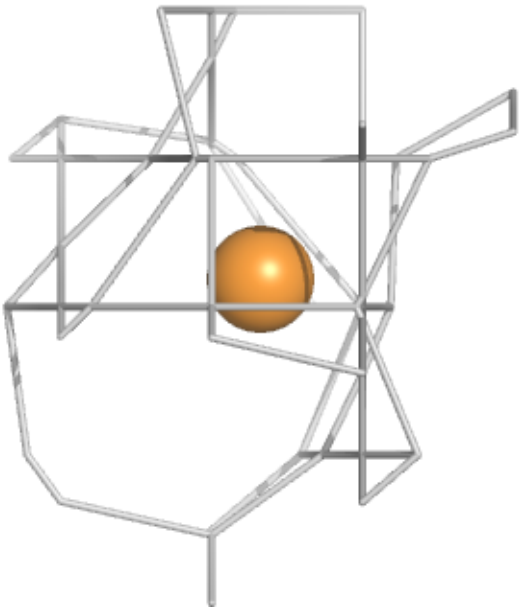


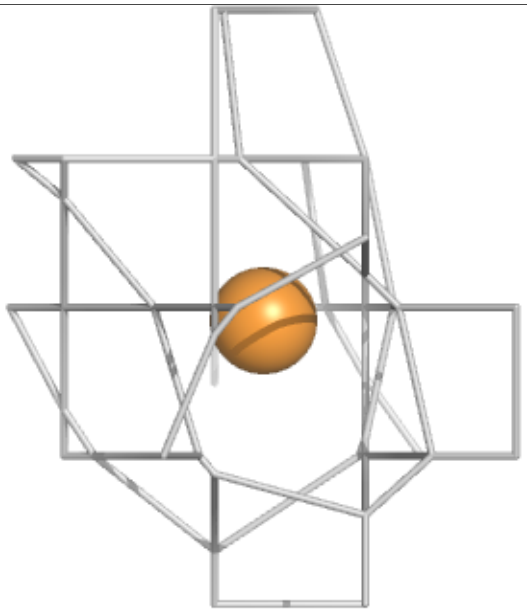


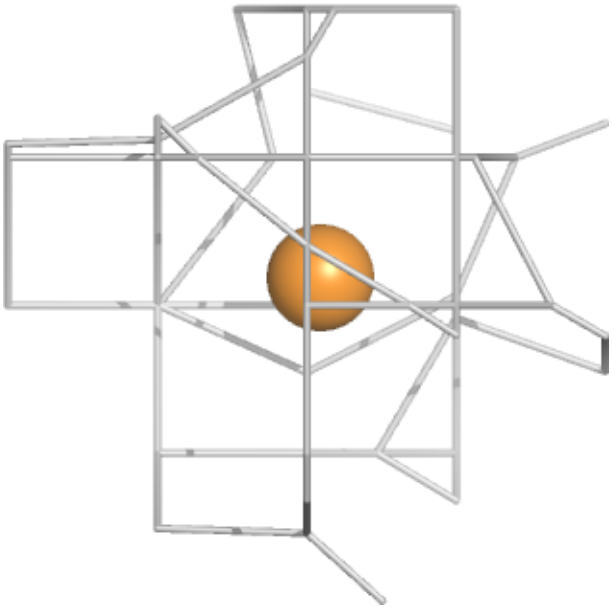


Electron density around CU F 404:

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

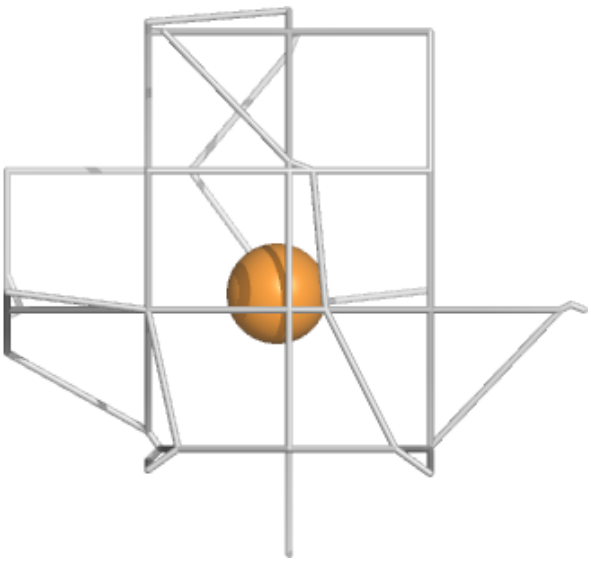


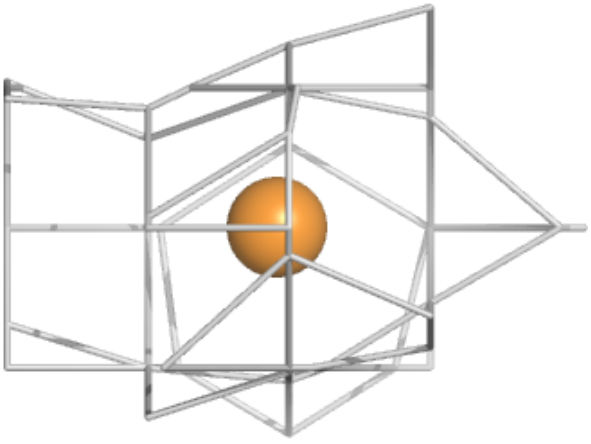


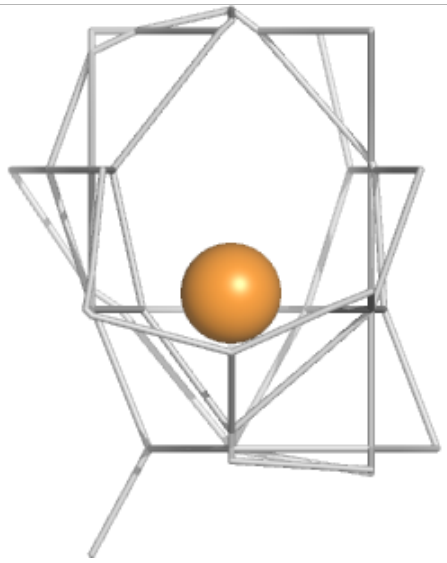


Electron density around CU D 404:

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

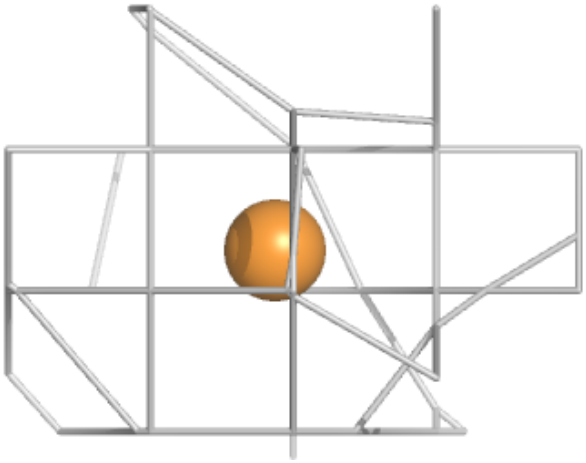


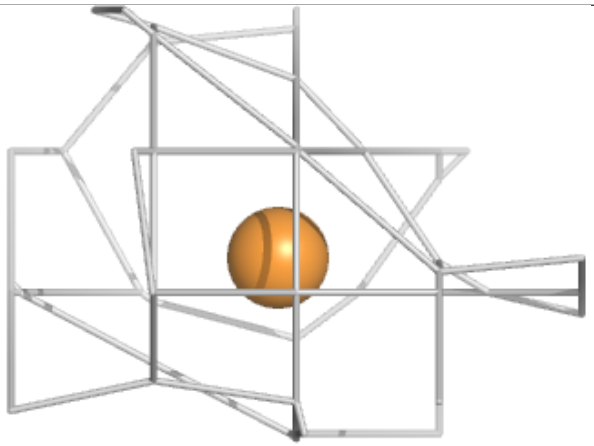


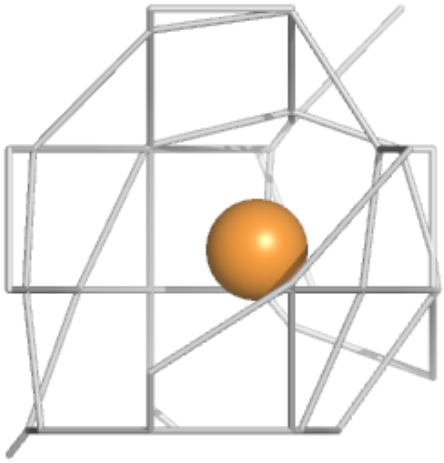


Electron density around CU A 405:

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

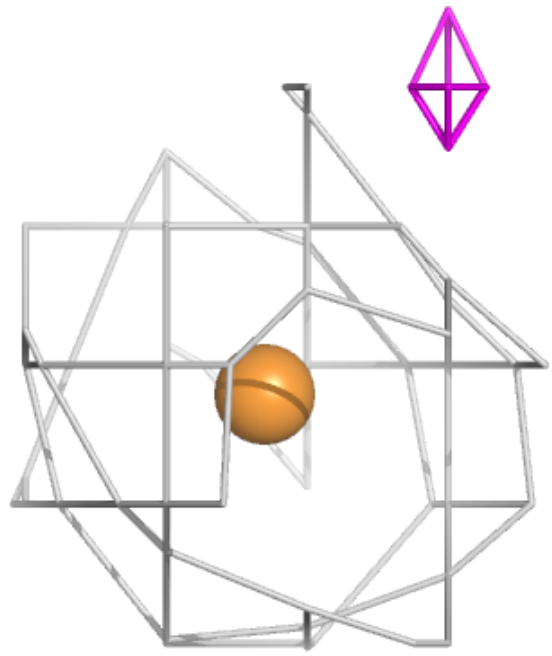


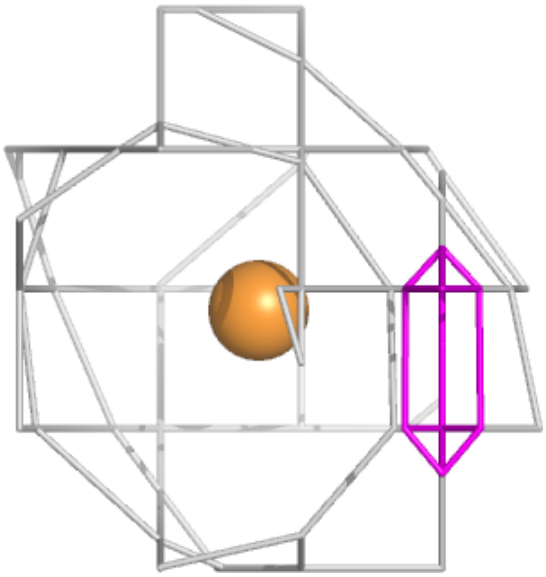


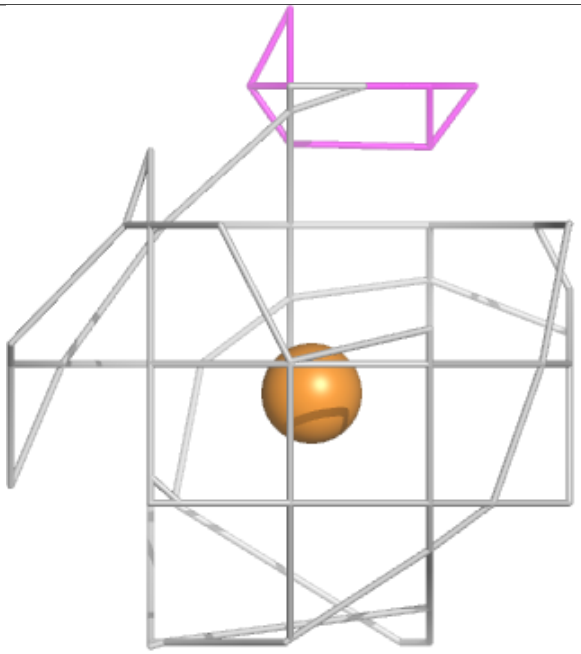


Electron density around CU F 403:

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

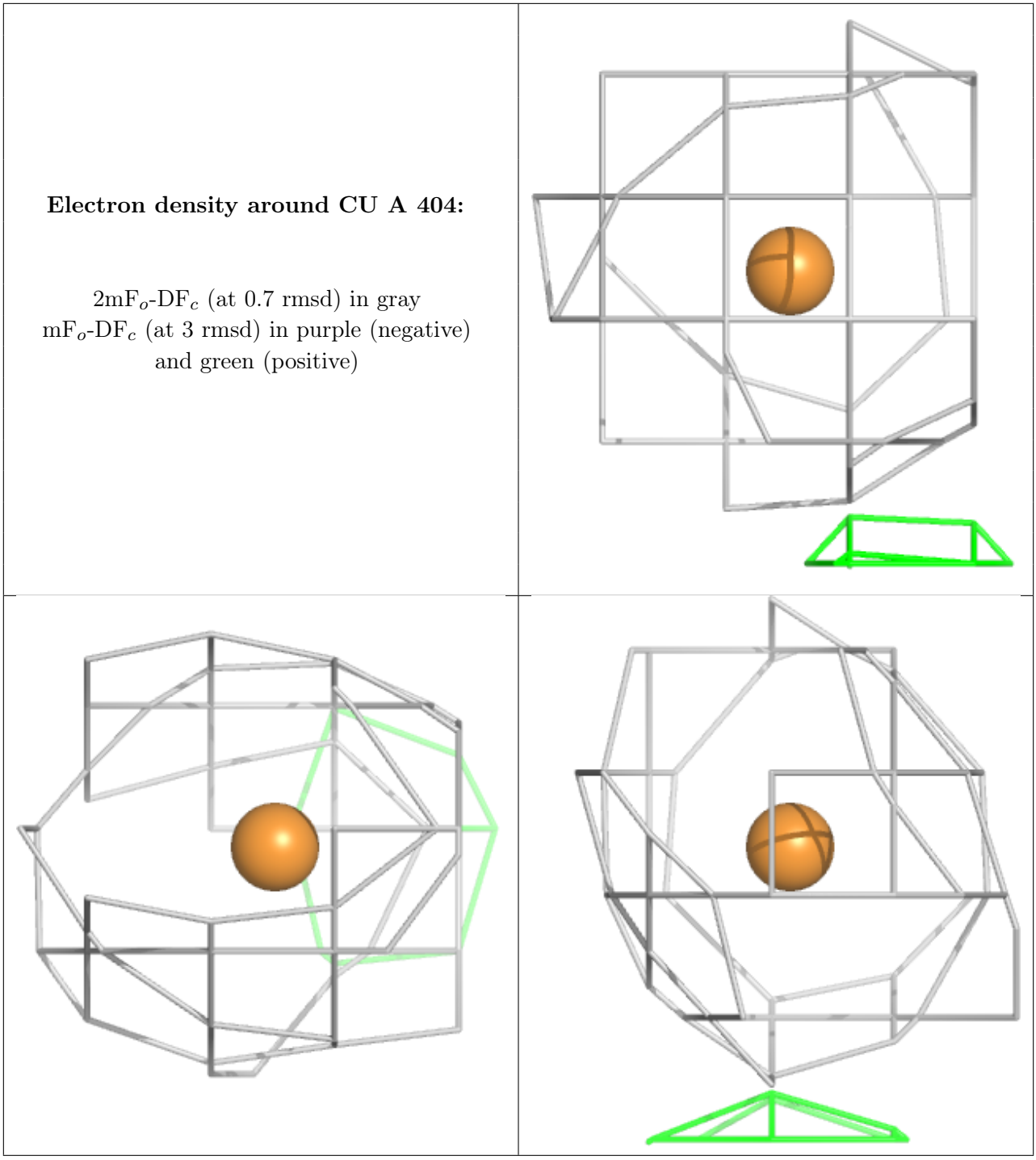






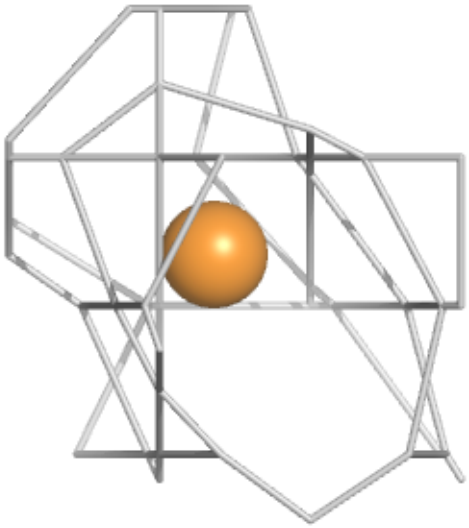
Electron density around CU A 404:

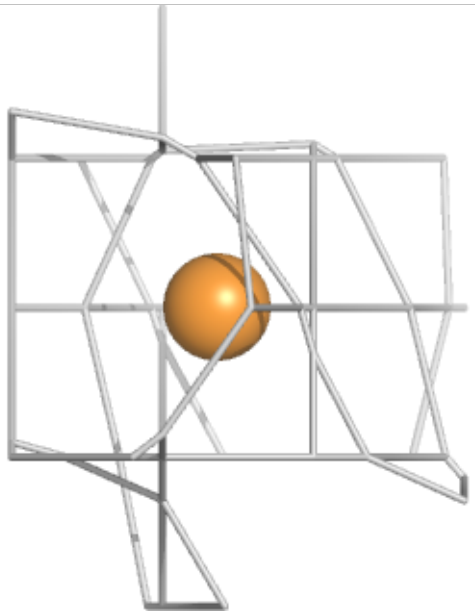
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

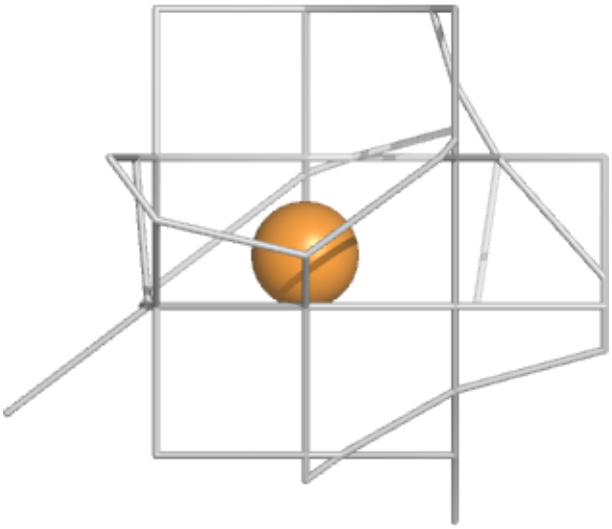


Electron density around CU B 404:

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

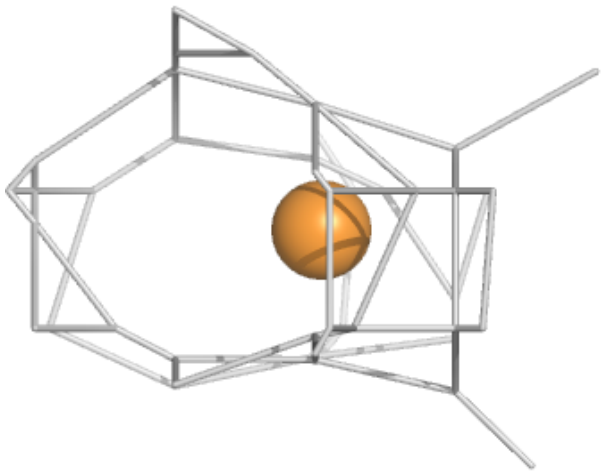


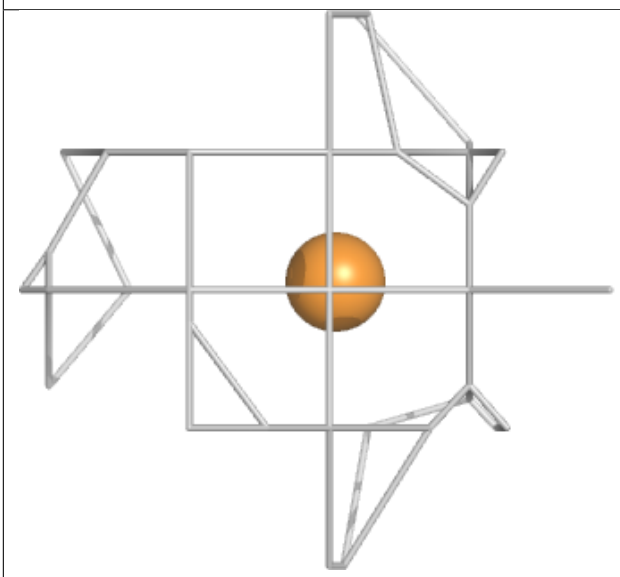


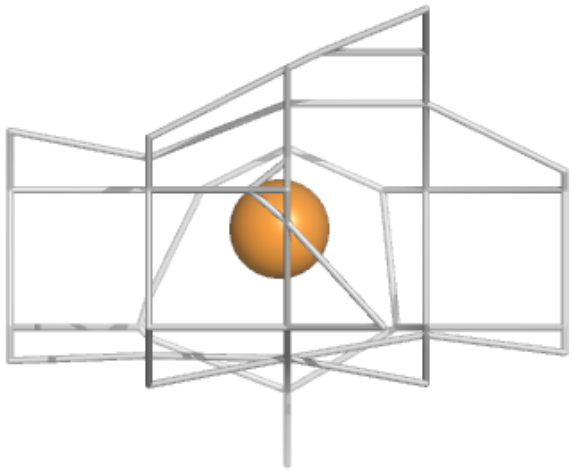


Electron density around CU G 404:

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

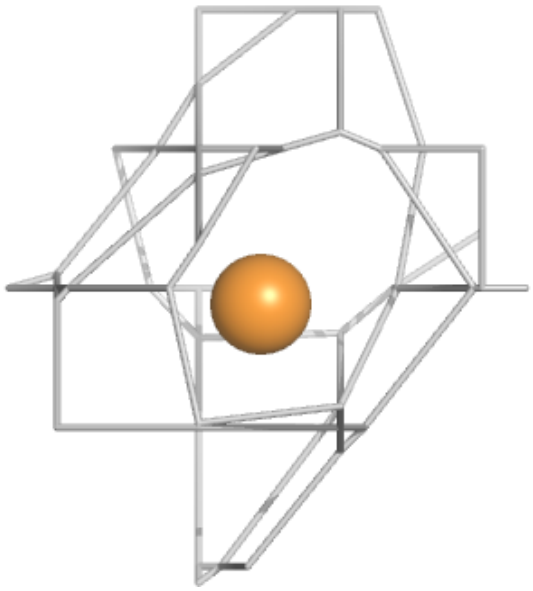


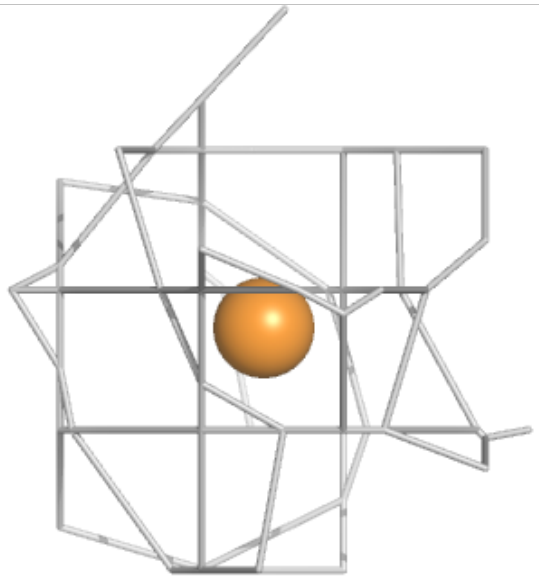


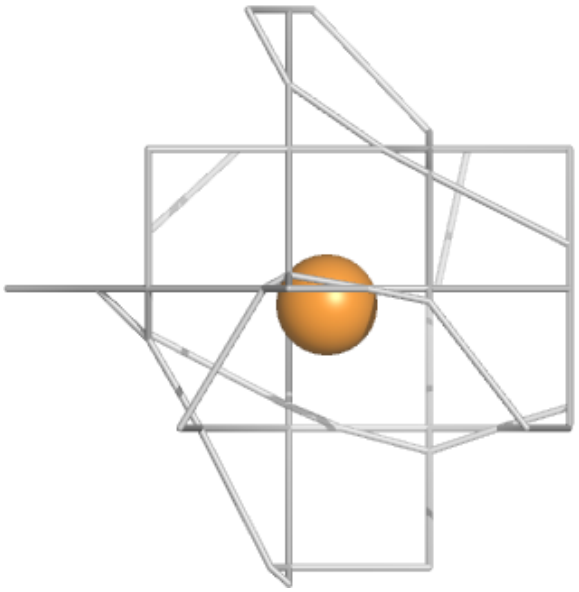


Electron density around CU H 404:

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

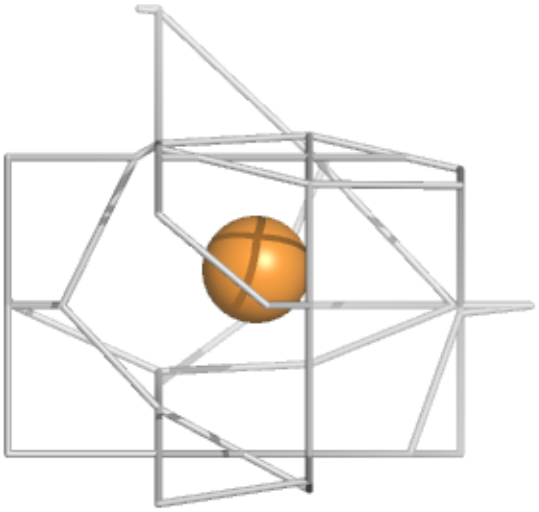


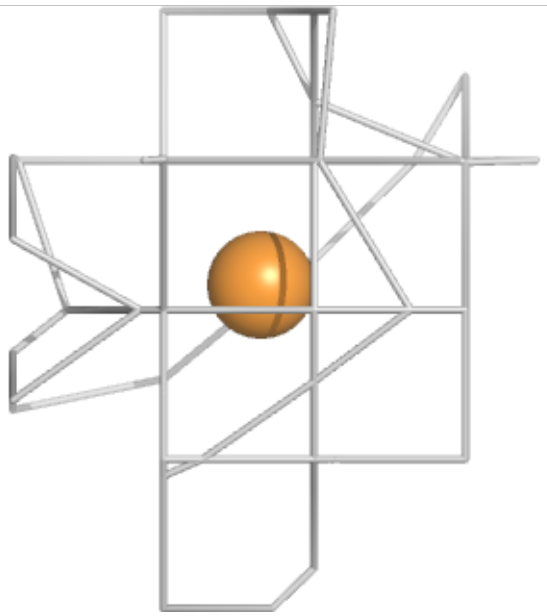


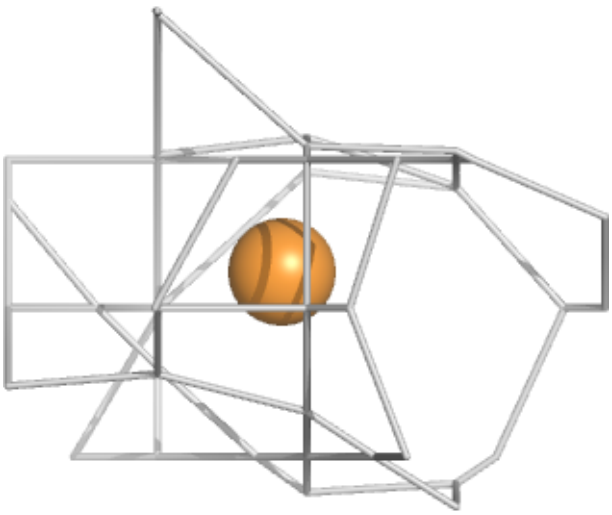


Electron density around CU I 402:

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

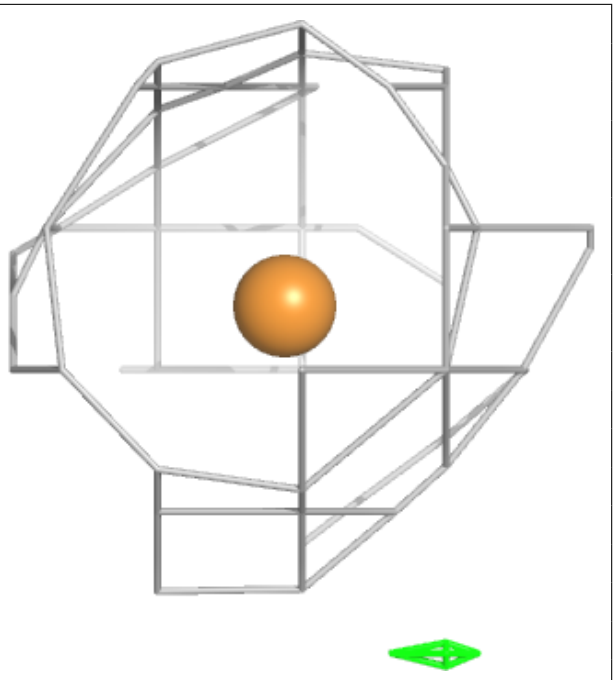


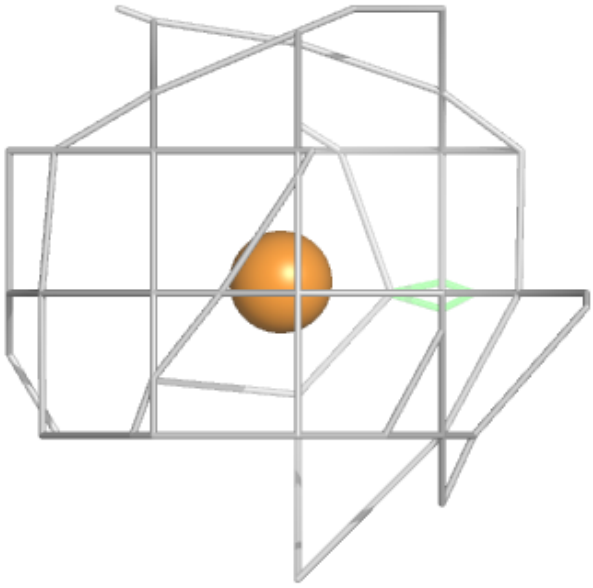


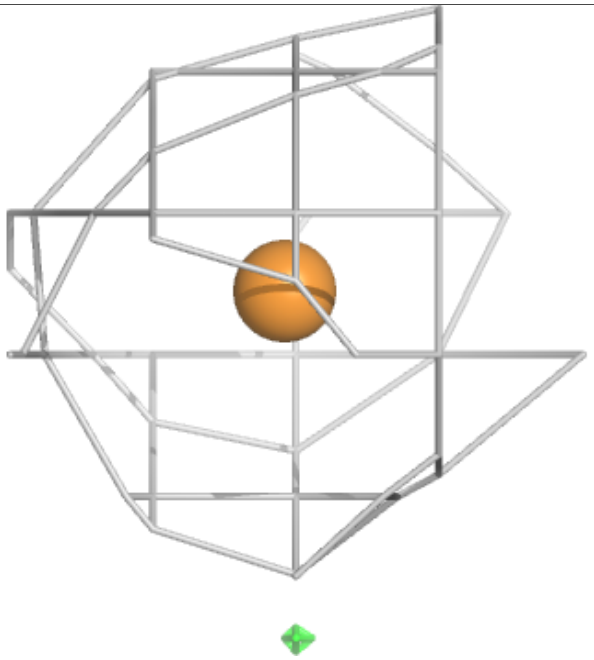


Electron density around CU I 403:

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

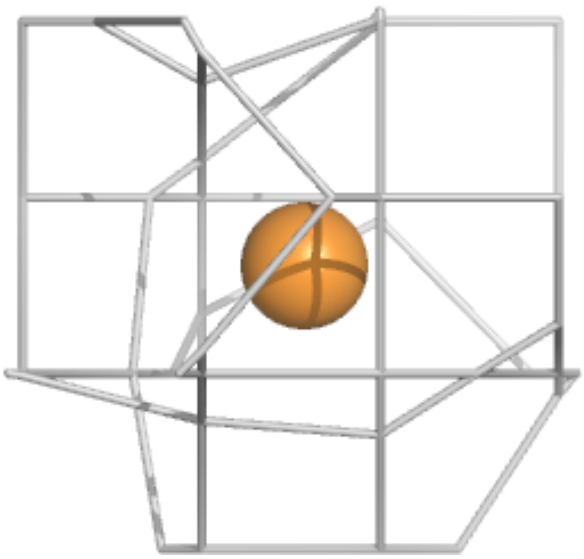


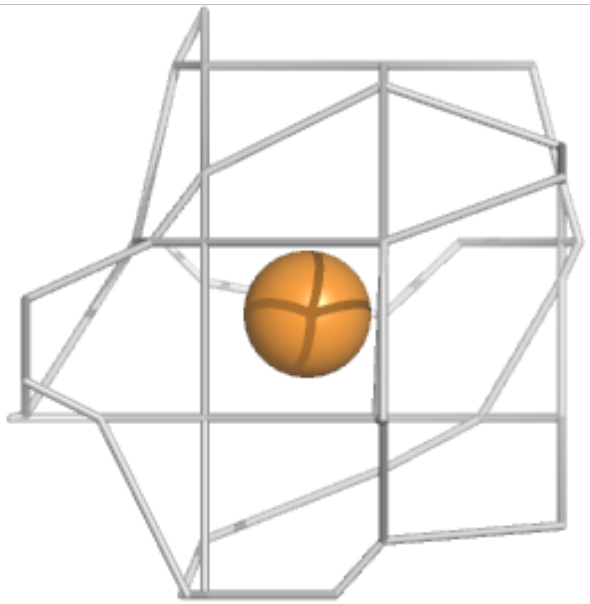


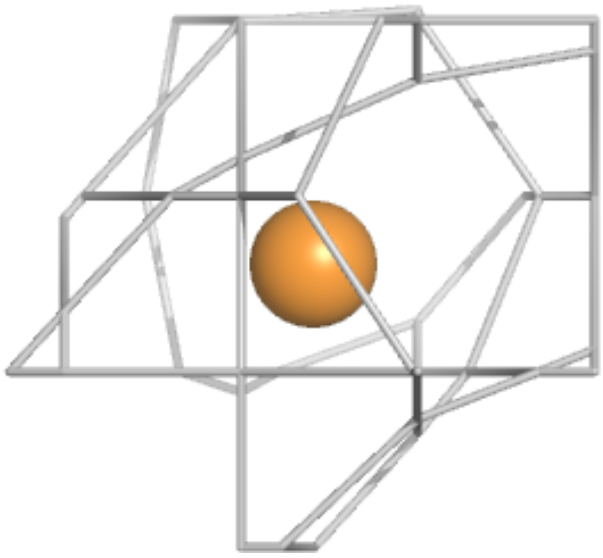


Electron density around CU J 403:

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

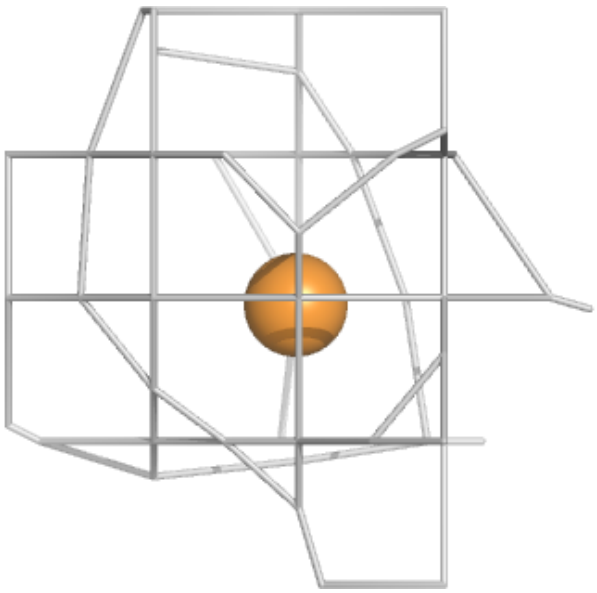


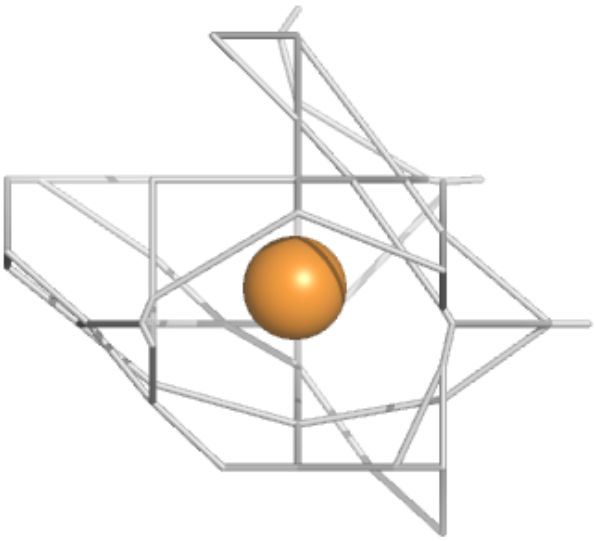


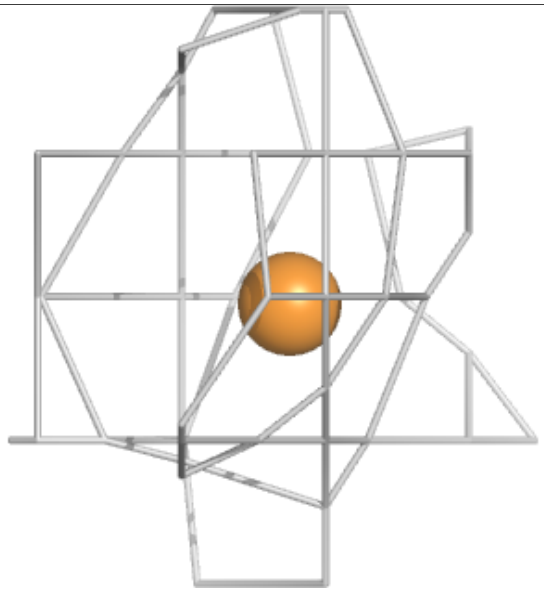


Electron density around CU K 403:

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

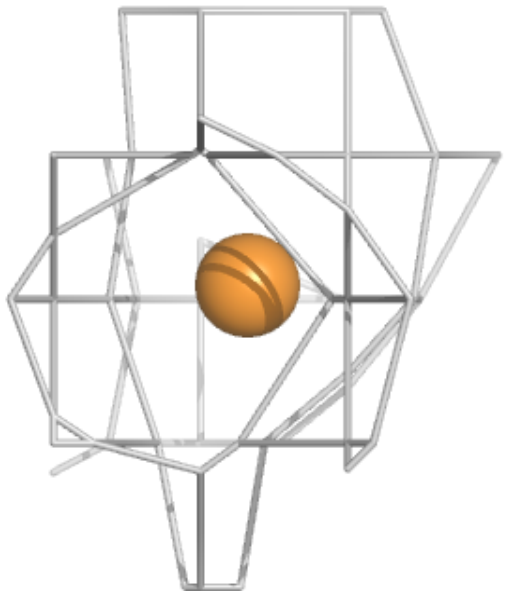


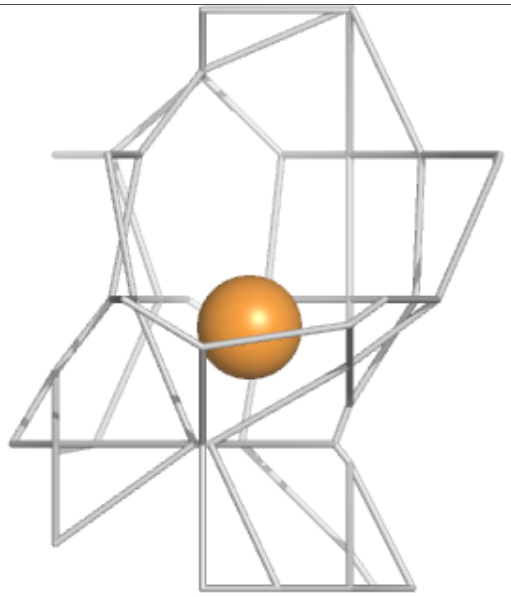


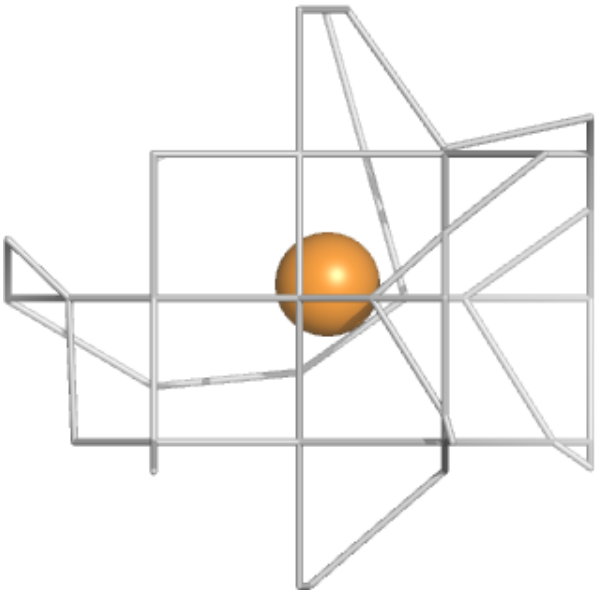


Electron density around CU L 402:

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

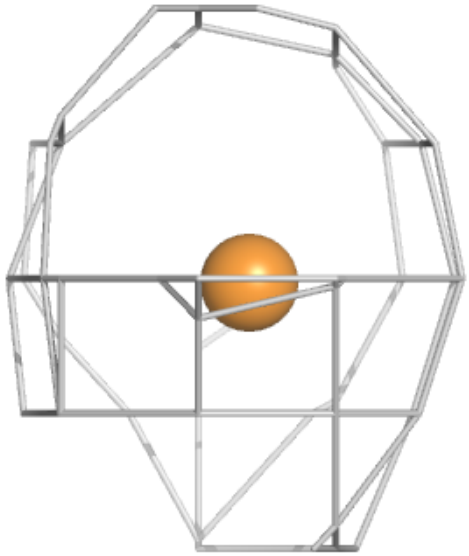


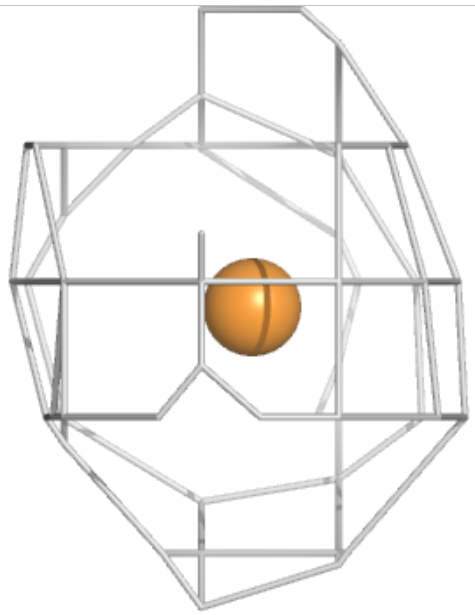


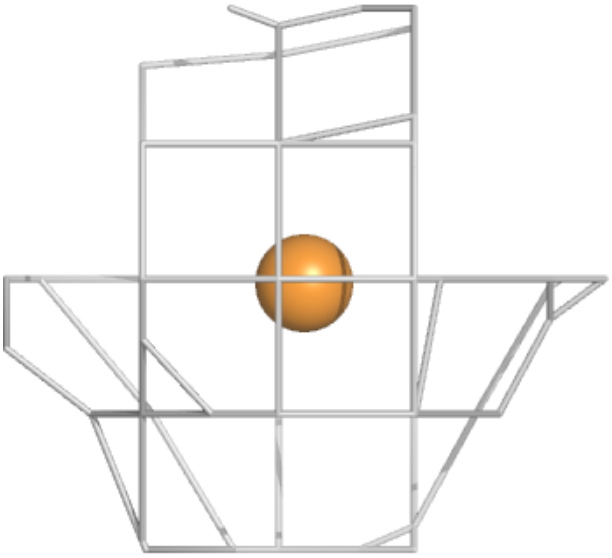


Electron density around CU L 403:

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

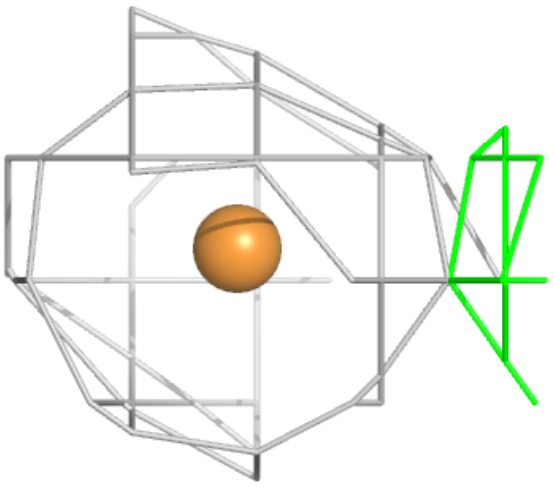


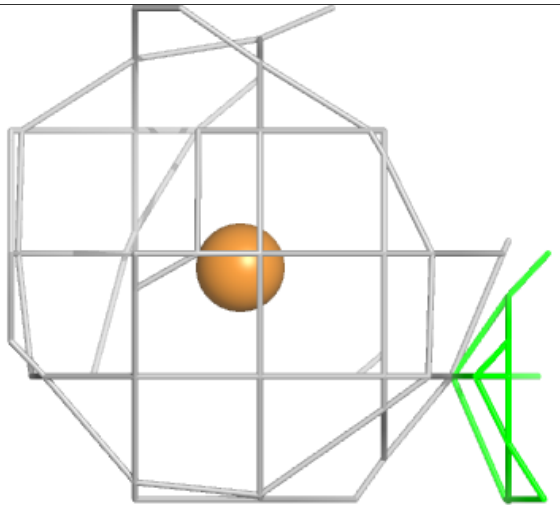


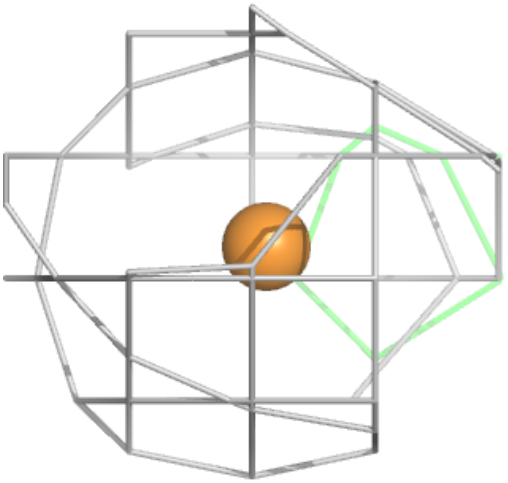


Electron density around CU C 403:

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

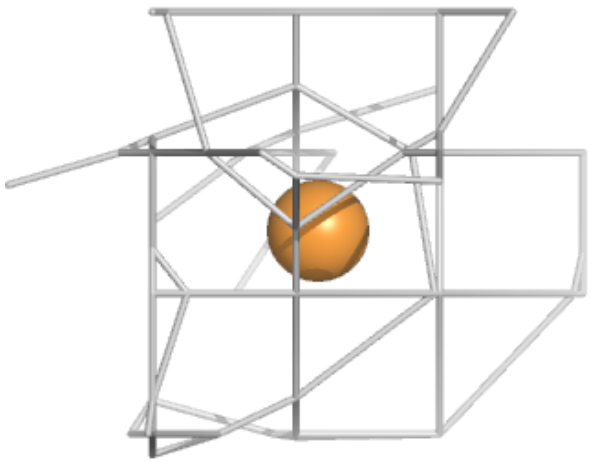


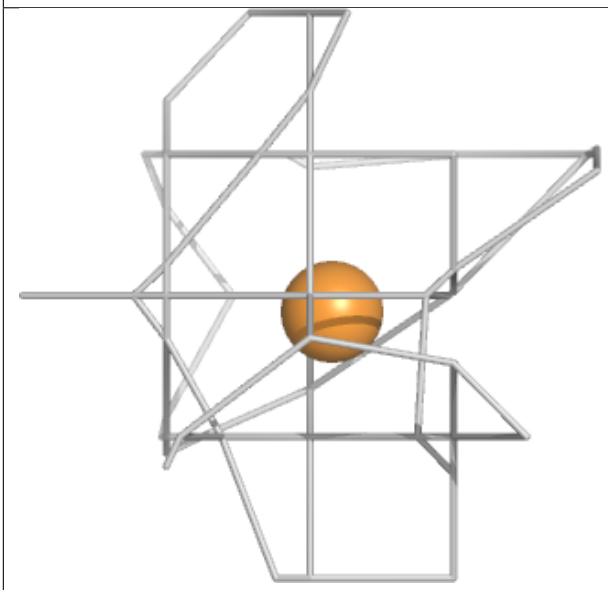


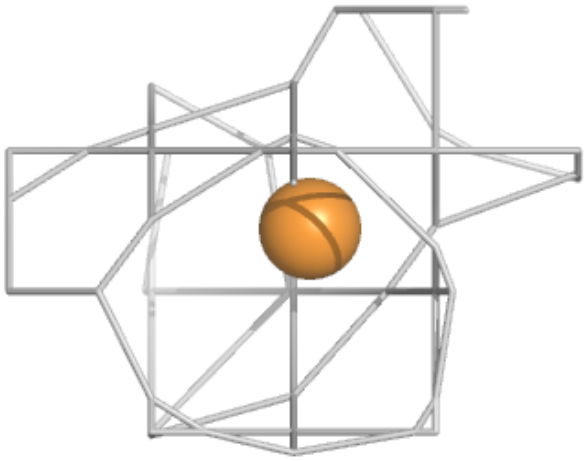


Electron density around CU C 404:

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

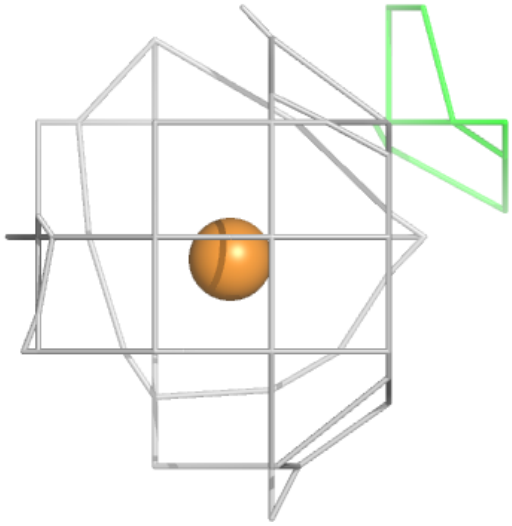


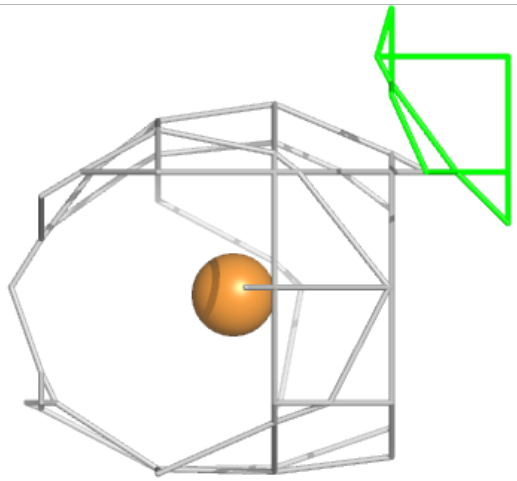


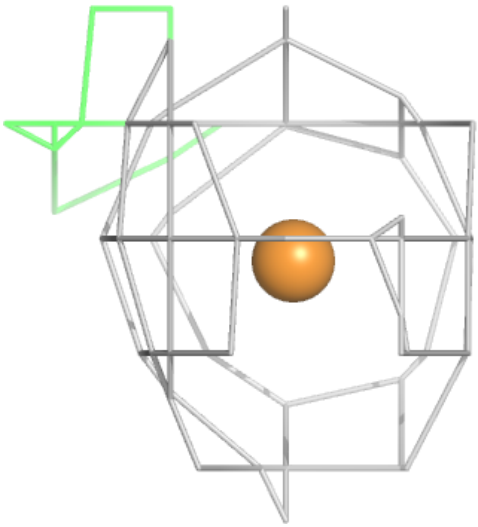


Electron density around CU D 403:

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

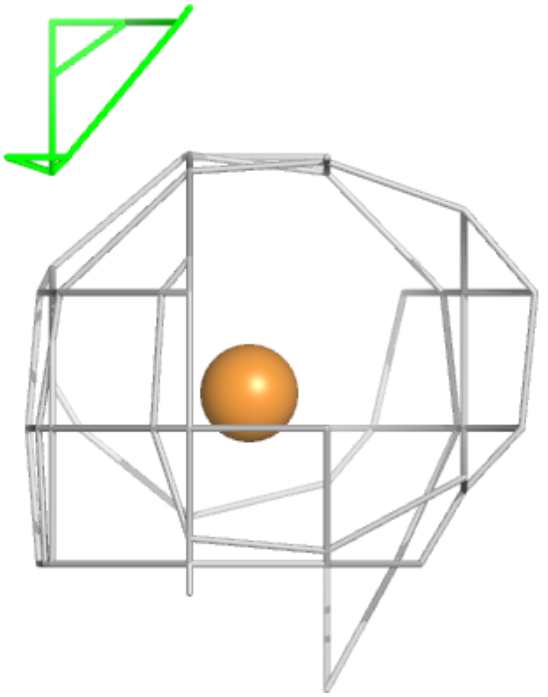


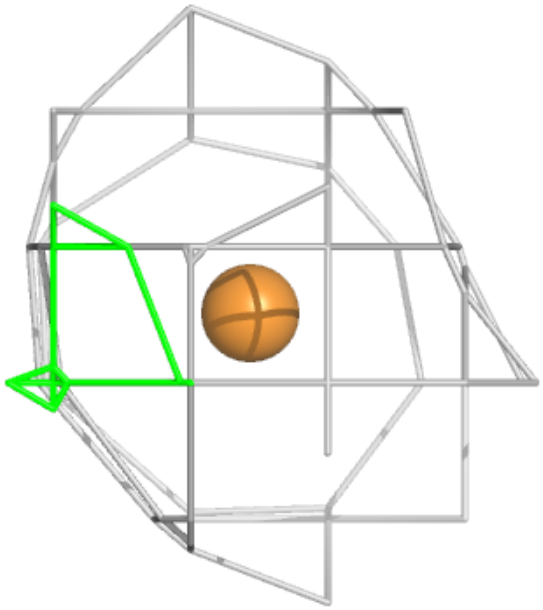


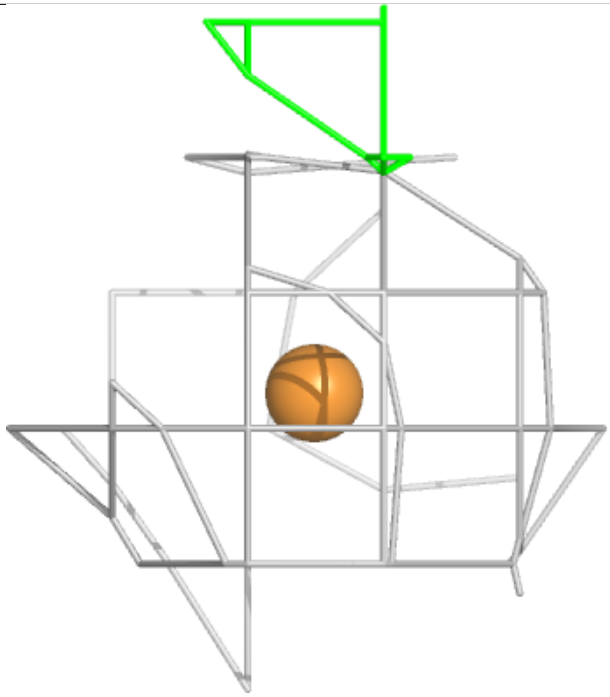


Electron density around CU K 402:

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

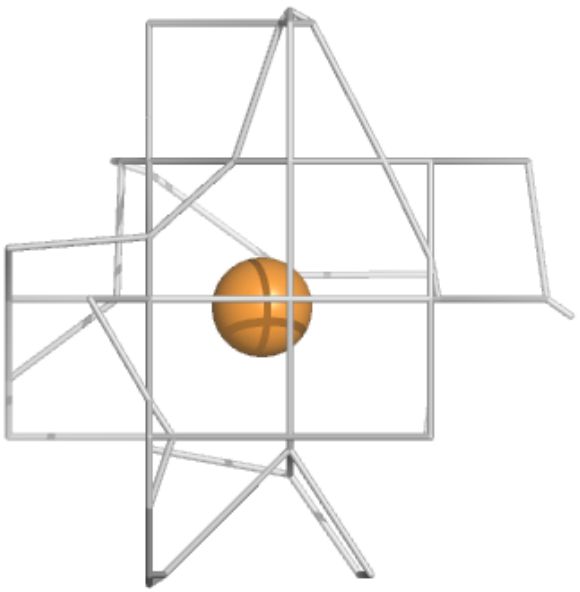


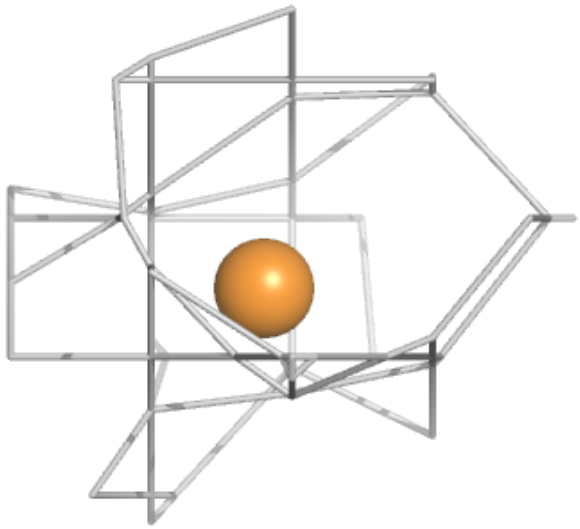


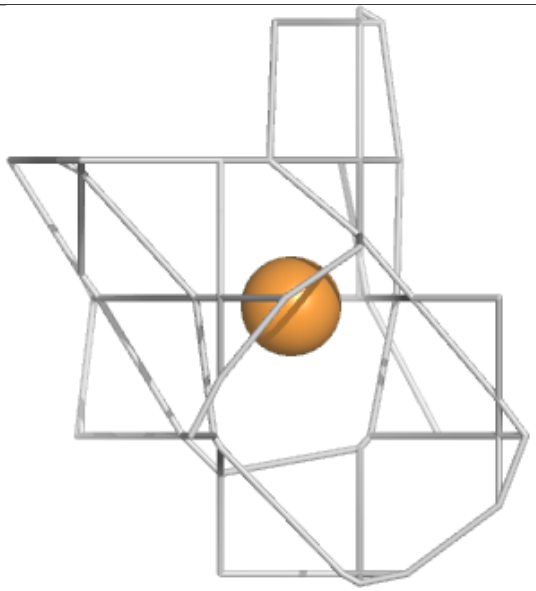


Electron density around CU E 405:

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

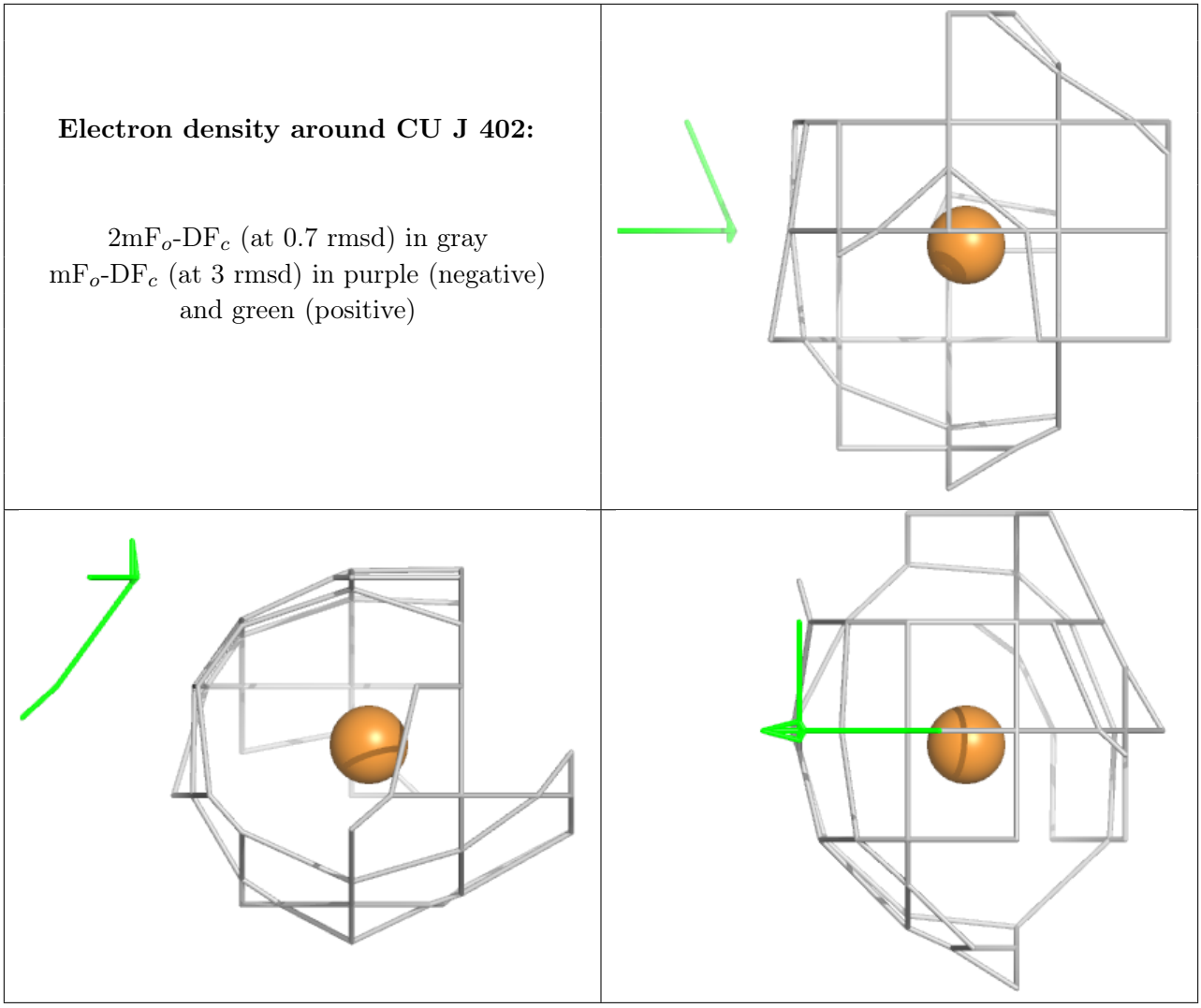






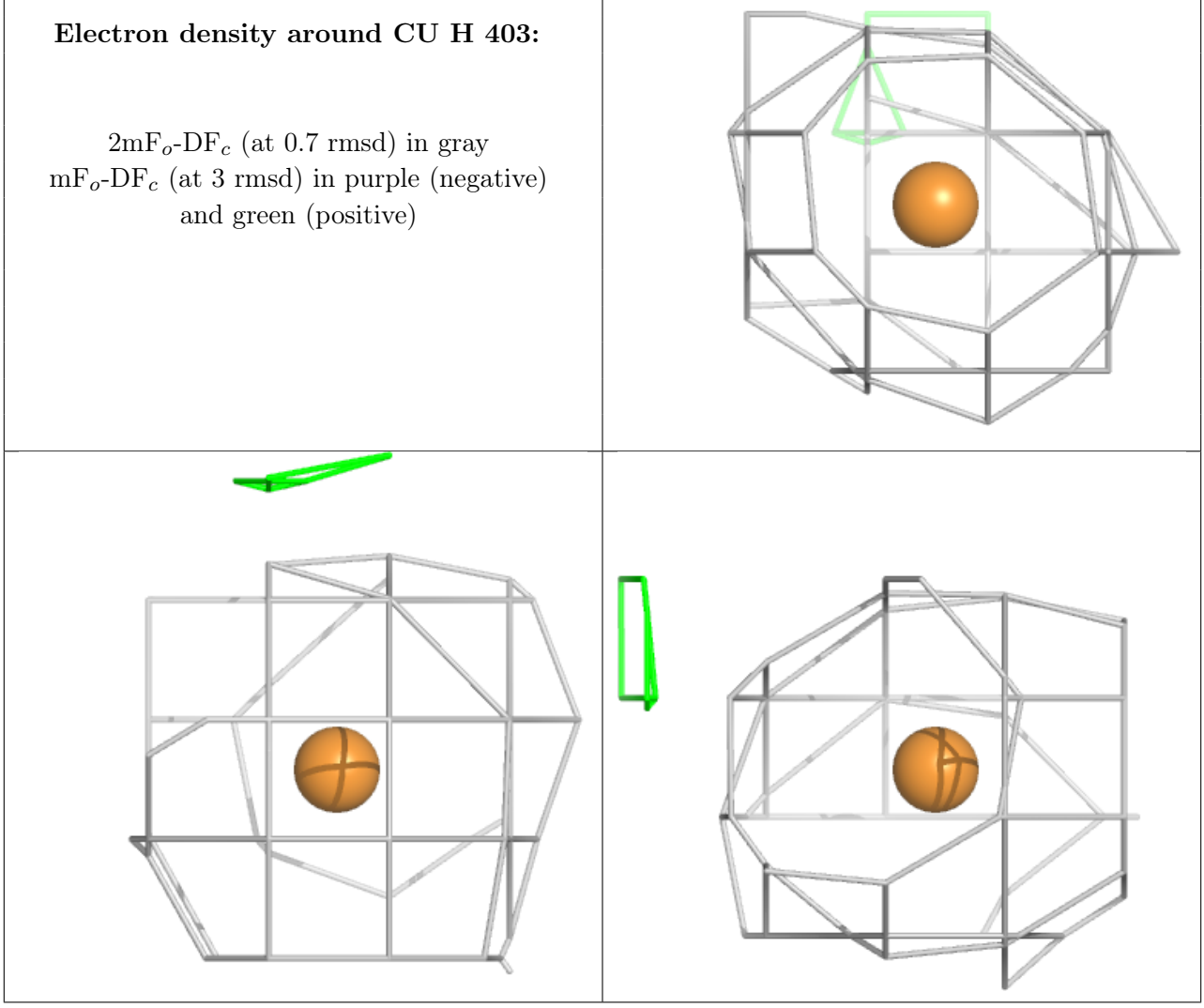
Electron density around CU J 402:

$2mF_o$-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 H 403:

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



6.5 Other polymers (i)

There are no such residues in this entry.