



wwPDB X-ray Structure Validation Summary Report ⓘ

May 30, 2023 – 04:30 pm BST

PDB ID : 8P3M
Title : The structure of thiocyanate dehydrogenase mutant form with Lys 281 replaced by Ala from *Thioalkalivibrio paradoxus*
Authors : Varfolomeeva, L.A.; Polyakov, K.M.; Komolov, A.S.; Rakitina, T.V.; Dergousova, N.I.; Dorovatovskii, P.V.; Boyko, K.M.; Tikhonova, T.V.; Popov, V.O.
Deposited on : 2023-05-18
Resolution : 2.07 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.33
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) : 2.33

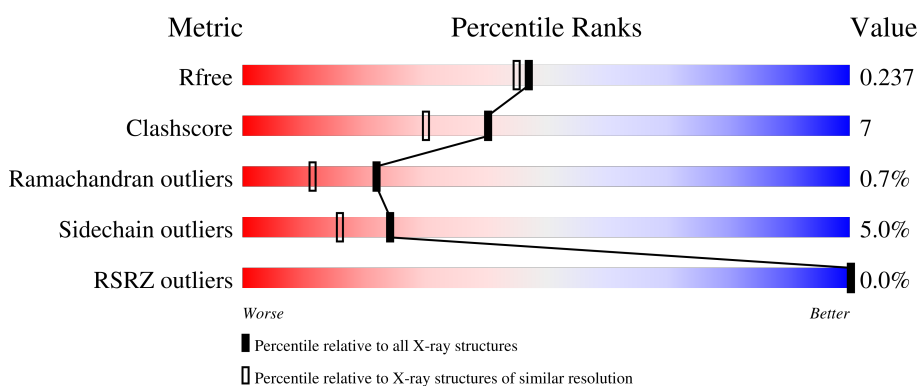
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	494	
1	5	494	
1	8	494	
1	A	494	
1	D	494	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	494	 75% 16% • 5%
1	J	494	 78% 13% •• 5%
1	M	494	 76% 16% • 5%
1	P	494	 73% 18% • 5%
1	S	494	 73% 19% • 5%
1	V	494	 69% 23% •• 5%
1	Y	494	 76% 16% •• 5%
1	e	494	 86% 7% • 5%
1	h	494	 86% 7% • 5%
1	k	494	 84% 10% 5%
1	x	494	 83% 10% • 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 60462 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 Twin-arginine translocation signal domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	467	Total 3636	C 2319	N 607	O 692	S 18	0	1	0
1	D	467	Total 3628	C 2316	N 606	O 688	S 18	0	0	0
1	G	467	Total 3636	C 2320	N 607	O 690	S 19	0	2	0
1	J	467	Total 3620	C 2312	N 602	O 688	S 18	0	0	0
1	M	467	Total 3627	C 2315	N 606	O 688	S 18	0	0	0
1	P	467	Total 3626	C 2313	N 603	O 692	S 18	0	0	0
1	S	467	Total 3614	C 2309	N 605	O 682	S 18	0	0	0
1	V	467	Total 3621	C 2309	N 604	O 690	S 18	0	0	0
1	Y	467	Total 3617	C 2310	N 604	O 685	S 18	0	1	0
1	2	467	Total 3627	C 2315	N 604	O 690	S 18	0	0	0
1	5	467	Total 3617	C 2309	N 606	O 684	S 18	0	1	0
1	8	467	Total 3617	C 2308	N 603	O 688	S 18	0	0	0
1	x	467	Total 3608	C 2304	N 600	O 686	S 18	0	0	0
1	e	467	Total 3608	C 2304	N 598	O 688	S 18	0	1	0
1	h	467	Total 3602	C 2302	N 596	O 686	S 18	0	0	0
1	k	467	Total 3611	C 2304	N 603	O 686	S 18	0	1	0

There are 448 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	MET	-	initiating methionine	UNP W0DP94
A	56	SER	-	expression tag	UNP W0DP94
A	57	TYR	-	expression tag	UNP W0DP94
A	58	TYR	-	expression tag	UNP W0DP94
A	59	HIS	-	expression tag	UNP W0DP94
A	60	HIS	-	expression tag	UNP W0DP94
A	61	HIS	-	expression tag	UNP W0DP94
A	62	HIS	-	expression tag	UNP W0DP94
A	63	HIS	-	expression tag	UNP W0DP94
A	64	HIS	-	expression tag	UNP W0DP94
A	65	ASP	-	expression tag	UNP W0DP94
A	66	TYR	-	expression tag	UNP W0DP94
A	67	ASP	-	expression tag	UNP W0DP94
A	68	ILE	-	expression tag	UNP W0DP94
A	69	PRO	-	expression tag	UNP W0DP94
A	70	THR	-	expression tag	UNP W0DP94
A	71	THR	-	expression tag	UNP W0DP94
A	72	GLU	-	expression tag	UNP W0DP94
A	73	ASN	-	expression tag	UNP W0DP94
A	74	LEU	-	expression tag	UNP W0DP94
A	75	TYR	-	expression tag	UNP W0DP94
A	76	PHE	-	expression tag	UNP W0DP94
A	77	GLN	-	expression tag	UNP W0DP94
A	78	GLY	-	expression tag	UNP W0DP94
A	79	ALA	-	expression tag	UNP W0DP94
A	80	MET	-	expression tag	UNP W0DP94
A	81	GLY	-	expression tag	UNP W0DP94
A	281	ALA	LYS	engineered mutation	UNP W0DP94
D	55	MET	-	initiating methionine	UNP W0DP94
D	56	SER	-	expression tag	UNP W0DP94
D	57	TYR	-	expression tag	UNP W0DP94
D	58	TYR	-	expression tag	UNP W0DP94
D	59	HIS	-	expression tag	UNP W0DP94
D	60	HIS	-	expression tag	UNP W0DP94
D	61	HIS	-	expression tag	UNP W0DP94
D	62	HIS	-	expression tag	UNP W0DP94
D	63	HIS	-	expression tag	UNP W0DP94
D	64	HIS	-	expression tag	UNP W0DP94
D	65	ASP	-	expression tag	UNP W0DP94
D	66	TYR	-	expression tag	UNP W0DP94
D	67	ASP	-	expression tag	UNP W0DP94
D	68	ILE	-	expression tag	UNP W0DP94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	69	PRO	-	expression tag	UNP W0DP94
D	70	THR	-	expression tag	UNP W0DP94
D	71	THR	-	expression tag	UNP W0DP94
D	72	GLU	-	expression tag	UNP W0DP94
D	73	ASN	-	expression tag	UNP W0DP94
D	74	LEU	-	expression tag	UNP W0DP94
D	75	TYR	-	expression tag	UNP W0DP94
D	76	PHE	-	expression tag	UNP W0DP94
D	77	GLN	-	expression tag	UNP W0DP94
D	78	GLY	-	expression tag	UNP W0DP94
D	79	ALA	-	expression tag	UNP W0DP94
D	80	MET	-	expression tag	UNP W0DP94
D	81	GLY	-	expression tag	UNP W0DP94
D	281	ALA	LYS	engineered mutation	UNP W0DP94
G	55	MET	-	initiating methionine	UNP W0DP94
G	56	SER	-	expression tag	UNP W0DP94
G	57	TYR	-	expression tag	UNP W0DP94
G	58	TYR	-	expression tag	UNP W0DP94
G	59	HIS	-	expression tag	UNP W0DP94
G	60	HIS	-	expression tag	UNP W0DP94
G	61	HIS	-	expression tag	UNP W0DP94
G	62	HIS	-	expression tag	UNP W0DP94
G	63	HIS	-	expression tag	UNP W0DP94
G	64	HIS	-	expression tag	UNP W0DP94
G	65	ASP	-	expression tag	UNP W0DP94
G	66	TYR	-	expression tag	UNP W0DP94
G	67	ASP	-	expression tag	UNP W0DP94
G	68	ILE	-	expression tag	UNP W0DP94
G	69	PRO	-	expression tag	UNP W0DP94
G	70	THR	-	expression tag	UNP W0DP94
G	71	THR	-	expression tag	UNP W0DP94
G	72	GLU	-	expression tag	UNP W0DP94
G	73	ASN	-	expression tag	UNP W0DP94
G	74	LEU	-	expression tag	UNP W0DP94
G	75	TYR	-	expression tag	UNP W0DP94
G	76	PHE	-	expression tag	UNP W0DP94
G	77	GLN	-	expression tag	UNP W0DP94
G	78	GLY	-	expression tag	UNP W0DP94
G	79	ALA	-	expression tag	UNP W0DP94
G	80	MET	-	expression tag	UNP W0DP94
G	81	GLY	-	expression tag	UNP W0DP94
G	281	ALA	LYS	engineered mutation	UNP W0DP94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	55	MET	-	initiating methionine	UNP W0DP94
J	56	SER	-	expression tag	UNP W0DP94
J	57	TYR	-	expression tag	UNP W0DP94
J	58	TYR	-	expression tag	UNP W0DP94
J	59	HIS	-	expression tag	UNP W0DP94
J	60	HIS	-	expression tag	UNP W0DP94
J	61	HIS	-	expression tag	UNP W0DP94
J	62	HIS	-	expression tag	UNP W0DP94
J	63	HIS	-	expression tag	UNP W0DP94
J	64	HIS	-	expression tag	UNP W0DP94
J	65	ASP	-	expression tag	UNP W0DP94
J	66	TYR	-	expression tag	UNP W0DP94
J	67	ASP	-	expression tag	UNP W0DP94
J	68	ILE	-	expression tag	UNP W0DP94
J	69	PRO	-	expression tag	UNP W0DP94
J	70	THR	-	expression tag	UNP W0DP94
J	71	THR	-	expression tag	UNP W0DP94
J	72	GLU	-	expression tag	UNP W0DP94
J	73	ASN	-	expression tag	UNP W0DP94
J	74	LEU	-	expression tag	UNP W0DP94
J	75	TYR	-	expression tag	UNP W0DP94
J	76	PHE	-	expression tag	UNP W0DP94
J	77	GLN	-	expression tag	UNP W0DP94
J	78	GLY	-	expression tag	UNP W0DP94
J	79	ALA	-	expression tag	UNP W0DP94
J	80	MET	-	expression tag	UNP W0DP94
J	81	GLY	-	expression tag	UNP W0DP94
J	281	ALA	LYS	engineered mutation	UNP W0DP94
M	55	MET	-	initiating methionine	UNP W0DP94
M	56	SER	-	expression tag	UNP W0DP94
M	57	TYR	-	expression tag	UNP W0DP94
M	58	TYR	-	expression tag	UNP W0DP94
M	59	HIS	-	expression tag	UNP W0DP94
M	60	HIS	-	expression tag	UNP W0DP94
M	61	HIS	-	expression tag	UNP W0DP94
M	62	HIS	-	expression tag	UNP W0DP94
M	63	HIS	-	expression tag	UNP W0DP94
M	64	HIS	-	expression tag	UNP W0DP94
M	65	ASP	-	expression tag	UNP W0DP94
M	66	TYR	-	expression tag	UNP W0DP94
M	67	ASP	-	expression tag	UNP W0DP94
M	68	ILE	-	expression tag	UNP W0DP94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	69	PRO	-	expression tag	UNP W0DP94
M	70	THR	-	expression tag	UNP W0DP94
M	71	THR	-	expression tag	UNP W0DP94
M	72	GLU	-	expression tag	UNP W0DP94
M	73	ASN	-	expression tag	UNP W0DP94
M	74	LEU	-	expression tag	UNP W0DP94
M	75	TYR	-	expression tag	UNP W0DP94
M	76	PHE	-	expression tag	UNP W0DP94
M	77	GLN	-	expression tag	UNP W0DP94
M	78	GLY	-	expression tag	UNP W0DP94
M	79	ALA	-	expression tag	UNP W0DP94
M	80	MET	-	expression tag	UNP W0DP94
M	81	GLY	-	expression tag	UNP W0DP94
M	281	ALA	LYS	engineered mutation	UNP W0DP94
P	55	MET	-	initiating methionine	UNP W0DP94
P	56	SER	-	expression tag	UNP W0DP94
P	57	TYR	-	expression tag	UNP W0DP94
P	58	TYR	-	expression tag	UNP W0DP94
P	59	HIS	-	expression tag	UNP W0DP94
P	60	HIS	-	expression tag	UNP W0DP94
P	61	HIS	-	expression tag	UNP W0DP94
P	62	HIS	-	expression tag	UNP W0DP94
P	63	HIS	-	expression tag	UNP W0DP94
P	64	HIS	-	expression tag	UNP W0DP94
P	65	ASP	-	expression tag	UNP W0DP94
P	66	TYR	-	expression tag	UNP W0DP94
P	67	ASP	-	expression tag	UNP W0DP94
P	68	ILE	-	expression tag	UNP W0DP94
P	69	PRO	-	expression tag	UNP W0DP94
P	70	THR	-	expression tag	UNP W0DP94
P	71	THR	-	expression tag	UNP W0DP94
P	72	GLU	-	expression tag	UNP W0DP94
P	73	ASN	-	expression tag	UNP W0DP94
P	74	LEU	-	expression tag	UNP W0DP94
P	75	TYR	-	expression tag	UNP W0DP94
P	76	PHE	-	expression tag	UNP W0DP94
P	77	GLN	-	expression tag	UNP W0DP94
P	78	GLY	-	expression tag	UNP W0DP94
P	79	ALA	-	expression tag	UNP W0DP94
P	80	MET	-	expression tag	UNP W0DP94
P	81	GLY	-	expression tag	UNP W0DP94
P	281	ALA	LYS	engineered mutation	UNP W0DP94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
S	55	MET	-	initiating methionine	UNP W0DP94
S	56	SER	-	expression tag	UNP W0DP94
S	57	TYR	-	expression tag	UNP W0DP94
S	58	TYR	-	expression tag	UNP W0DP94
S	59	HIS	-	expression tag	UNP W0DP94
S	60	HIS	-	expression tag	UNP W0DP94
S	61	HIS	-	expression tag	UNP W0DP94
S	62	HIS	-	expression tag	UNP W0DP94
S	63	HIS	-	expression tag	UNP W0DP94
S	64	HIS	-	expression tag	UNP W0DP94
S	65	ASP	-	expression tag	UNP W0DP94
S	66	TYR	-	expression tag	UNP W0DP94
S	67	ASP	-	expression tag	UNP W0DP94
S	68	ILE	-	expression tag	UNP W0DP94
S	69	PRO	-	expression tag	UNP W0DP94
S	70	THR	-	expression tag	UNP W0DP94
S	71	THR	-	expression tag	UNP W0DP94
S	72	GLU	-	expression tag	UNP W0DP94
S	73	ASN	-	expression tag	UNP W0DP94
S	74	LEU	-	expression tag	UNP W0DP94
S	75	TYR	-	expression tag	UNP W0DP94
S	76	PHE	-	expression tag	UNP W0DP94
S	77	GLN	-	expression tag	UNP W0DP94
S	78	GLY	-	expression tag	UNP W0DP94
S	79	ALA	-	expression tag	UNP W0DP94
S	80	MET	-	expression tag	UNP W0DP94
S	81	GLY	-	expression tag	UNP W0DP94
S	281	ALA	LYS	engineered mutation	UNP W0DP94
V	55	MET	-	initiating methionine	UNP W0DP94
V	56	SER	-	expression tag	UNP W0DP94
V	57	TYR	-	expression tag	UNP W0DP94
V	58	TYR	-	expression tag	UNP W0DP94
V	59	HIS	-	expression tag	UNP W0DP94
V	60	HIS	-	expression tag	UNP W0DP94
V	61	HIS	-	expression tag	UNP W0DP94
V	62	HIS	-	expression tag	UNP W0DP94
V	63	HIS	-	expression tag	UNP W0DP94
V	64	HIS	-	expression tag	UNP W0DP94
V	65	ASP	-	expression tag	UNP W0DP94
V	66	TYR	-	expression tag	UNP W0DP94
V	67	ASP	-	expression tag	UNP W0DP94
V	68	ILE	-	expression tag	UNP W0DP94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
V	69	PRO	-	expression tag	UNP W0DP94
V	70	THR	-	expression tag	UNP W0DP94
V	71	THR	-	expression tag	UNP W0DP94
V	72	GLU	-	expression tag	UNP W0DP94
V	73	ASN	-	expression tag	UNP W0DP94
V	74	LEU	-	expression tag	UNP W0DP94
V	75	TYR	-	expression tag	UNP W0DP94
V	76	PHE	-	expression tag	UNP W0DP94
V	77	GLN	-	expression tag	UNP W0DP94
V	78	GLY	-	expression tag	UNP W0DP94
V	79	ALA	-	expression tag	UNP W0DP94
V	80	MET	-	expression tag	UNP W0DP94
V	81	GLY	-	expression tag	UNP W0DP94
V	281	ALA	LYS	engineered mutation	UNP W0DP94
Y	55	MET	-	initiating methionine	UNP W0DP94
Y	56	SER	-	expression tag	UNP W0DP94
Y	57	TYR	-	expression tag	UNP W0DP94
Y	58	TYR	-	expression tag	UNP W0DP94
Y	59	HIS	-	expression tag	UNP W0DP94
Y	60	HIS	-	expression tag	UNP W0DP94
Y	61	HIS	-	expression tag	UNP W0DP94
Y	62	HIS	-	expression tag	UNP W0DP94
Y	63	HIS	-	expression tag	UNP W0DP94
Y	64	HIS	-	expression tag	UNP W0DP94
Y	65	ASP	-	expression tag	UNP W0DP94
Y	66	TYR	-	expression tag	UNP W0DP94
Y	67	ASP	-	expression tag	UNP W0DP94
Y	68	ILE	-	expression tag	UNP W0DP94
Y	69	PRO	-	expression tag	UNP W0DP94
Y	70	THR	-	expression tag	UNP W0DP94
Y	71	THR	-	expression tag	UNP W0DP94
Y	72	GLU	-	expression tag	UNP W0DP94
Y	73	ASN	-	expression tag	UNP W0DP94
Y	74	LEU	-	expression tag	UNP W0DP94
Y	75	TYR	-	expression tag	UNP W0DP94
Y	76	PHE	-	expression tag	UNP W0DP94
Y	77	GLN	-	expression tag	UNP W0DP94
Y	78	GLY	-	expression tag	UNP W0DP94
Y	79	ALA	-	expression tag	UNP W0DP94
Y	80	MET	-	expression tag	UNP W0DP94
Y	81	GLY	-	expression tag	UNP W0DP94
Y	281	ALA	LYS	engineered mutation	UNP W0DP94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
2	55	MET	-	initiating methionine	UNP W0DP94
2	56	SER	-	expression tag	UNP W0DP94
2	57	TYR	-	expression tag	UNP W0DP94
2	58	TYR	-	expression tag	UNP W0DP94
2	59	HIS	-	expression tag	UNP W0DP94
2	60	HIS	-	expression tag	UNP W0DP94
2	61	HIS	-	expression tag	UNP W0DP94
2	62	HIS	-	expression tag	UNP W0DP94
2	63	HIS	-	expression tag	UNP W0DP94
2	64	HIS	-	expression tag	UNP W0DP94
2	65	ASP	-	expression tag	UNP W0DP94
2	66	TYR	-	expression tag	UNP W0DP94
2	67	ASP	-	expression tag	UNP W0DP94
2	68	ILE	-	expression tag	UNP W0DP94
2	69	PRO	-	expression tag	UNP W0DP94
2	70	THR	-	expression tag	UNP W0DP94
2	71	THR	-	expression tag	UNP W0DP94
2	72	GLU	-	expression tag	UNP W0DP94
2	73	ASN	-	expression tag	UNP W0DP94
2	74	LEU	-	expression tag	UNP W0DP94
2	75	TYR	-	expression tag	UNP W0DP94
2	76	PHE	-	expression tag	UNP W0DP94
2	77	GLN	-	expression tag	UNP W0DP94
2	78	GLY	-	expression tag	UNP W0DP94
2	79	ALA	-	expression tag	UNP W0DP94
2	80	MET	-	expression tag	UNP W0DP94
2	81	GLY	-	expression tag	UNP W0DP94
2	281	ALA	LYS	engineered mutation	UNP W0DP94
5	55	MET	-	initiating methionine	UNP W0DP94
5	56	SER	-	expression tag	UNP W0DP94
5	57	TYR	-	expression tag	UNP W0DP94
5	58	TYR	-	expression tag	UNP W0DP94
5	59	HIS	-	expression tag	UNP W0DP94
5	60	HIS	-	expression tag	UNP W0DP94
5	61	HIS	-	expression tag	UNP W0DP94
5	62	HIS	-	expression tag	UNP W0DP94
5	63	HIS	-	expression tag	UNP W0DP94
5	64	HIS	-	expression tag	UNP W0DP94
5	65	ASP	-	expression tag	UNP W0DP94
5	66	TYR	-	expression tag	UNP W0DP94
5	67	ASP	-	expression tag	UNP W0DP94
5	68	ILE	-	expression tag	UNP W0DP94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
5	69	PRO	-	expression tag	UNP W0DP94
5	70	THR	-	expression tag	UNP W0DP94
5	71	THR	-	expression tag	UNP W0DP94
5	72	GLU	-	expression tag	UNP W0DP94
5	73	ASN	-	expression tag	UNP W0DP94
5	74	LEU	-	expression tag	UNP W0DP94
5	75	TYR	-	expression tag	UNP W0DP94
5	76	PHE	-	expression tag	UNP W0DP94
5	77	GLN	-	expression tag	UNP W0DP94
5	78	GLY	-	expression tag	UNP W0DP94
5	79	ALA	-	expression tag	UNP W0DP94
5	80	MET	-	expression tag	UNP W0DP94
5	81	GLY	-	expression tag	UNP W0DP94
5	281	ALA	LYS	engineered mutation	UNP W0DP94
8	55	MET	-	initiating methionine	UNP W0DP94
8	56	SER	-	expression tag	UNP W0DP94
8	57	TYR	-	expression tag	UNP W0DP94
8	58	TYR	-	expression tag	UNP W0DP94
8	59	HIS	-	expression tag	UNP W0DP94
8	60	HIS	-	expression tag	UNP W0DP94
8	61	HIS	-	expression tag	UNP W0DP94
8	62	HIS	-	expression tag	UNP W0DP94
8	63	HIS	-	expression tag	UNP W0DP94
8	64	HIS	-	expression tag	UNP W0DP94
8	65	ASP	-	expression tag	UNP W0DP94
8	66	TYR	-	expression tag	UNP W0DP94
8	67	ASP	-	expression tag	UNP W0DP94
8	68	ILE	-	expression tag	UNP W0DP94
8	69	PRO	-	expression tag	UNP W0DP94
8	70	THR	-	expression tag	UNP W0DP94
8	71	THR	-	expression tag	UNP W0DP94
8	72	GLU	-	expression tag	UNP W0DP94
8	73	ASN	-	expression tag	UNP W0DP94
8	74	LEU	-	expression tag	UNP W0DP94
8	75	TYR	-	expression tag	UNP W0DP94
8	76	PHE	-	expression tag	UNP W0DP94
8	77	GLN	-	expression tag	UNP W0DP94
8	78	GLY	-	expression tag	UNP W0DP94
8	79	ALA	-	expression tag	UNP W0DP94
8	80	MET	-	expression tag	UNP W0DP94
8	81	GLY	-	expression tag	UNP W0DP94
8	281	ALA	LYS	engineered mutation	UNP W0DP94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
x	55	MET	-	initiating methionine	UNP W0DP94
x	56	SER	-	expression tag	UNP W0DP94
x	57	TYR	-	expression tag	UNP W0DP94
x	58	TYR	-	expression tag	UNP W0DP94
x	59	HIS	-	expression tag	UNP W0DP94
x	60	HIS	-	expression tag	UNP W0DP94
x	61	HIS	-	expression tag	UNP W0DP94
x	62	HIS	-	expression tag	UNP W0DP94
x	63	HIS	-	expression tag	UNP W0DP94
x	64	HIS	-	expression tag	UNP W0DP94
x	65	ASP	-	expression tag	UNP W0DP94
x	66	TYR	-	expression tag	UNP W0DP94
x	67	ASP	-	expression tag	UNP W0DP94
x	68	ILE	-	expression tag	UNP W0DP94
x	69	PRO	-	expression tag	UNP W0DP94
x	70	THR	-	expression tag	UNP W0DP94
x	71	THR	-	expression tag	UNP W0DP94
x	72	GLU	-	expression tag	UNP W0DP94
x	73	ASN	-	expression tag	UNP W0DP94
x	74	LEU	-	expression tag	UNP W0DP94
x	75	TYR	-	expression tag	UNP W0DP94
x	76	PHE	-	expression tag	UNP W0DP94
x	77	GLN	-	expression tag	UNP W0DP94
x	78	GLY	-	expression tag	UNP W0DP94
x	79	ALA	-	expression tag	UNP W0DP94
x	80	MET	-	expression tag	UNP W0DP94
x	81	GLY	-	expression tag	UNP W0DP94
x	281	ALA	LYS	engineered mutation	UNP W0DP94
e	55	MET	-	initiating methionine	UNP W0DP94
e	56	SER	-	expression tag	UNP W0DP94
e	57	TYR	-	expression tag	UNP W0DP94
e	58	TYR	-	expression tag	UNP W0DP94
e	59	HIS	-	expression tag	UNP W0DP94
e	60	HIS	-	expression tag	UNP W0DP94
e	61	HIS	-	expression tag	UNP W0DP94
e	62	HIS	-	expression tag	UNP W0DP94
e	63	HIS	-	expression tag	UNP W0DP94
e	64	HIS	-	expression tag	UNP W0DP94
e	65	ASP	-	expression tag	UNP W0DP94
e	66	TYR	-	expression tag	UNP W0DP94
e	67	ASP	-	expression tag	UNP W0DP94
e	68	ILE	-	expression tag	UNP W0DP94

Continued on next page...

Continued from previous page...

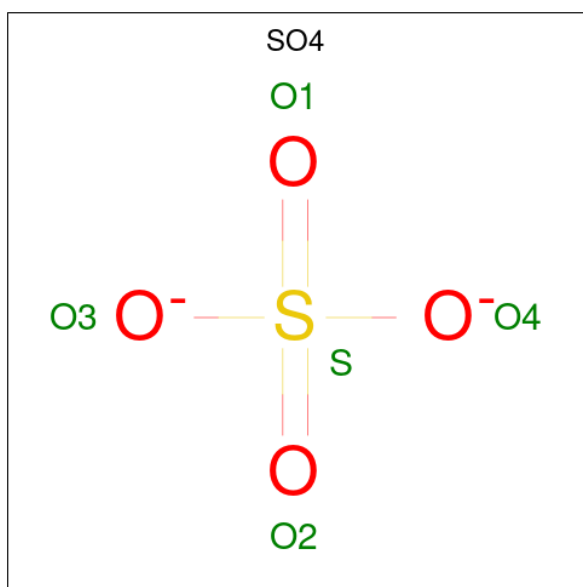
Chain	Residue	Modelled	Actual	Comment	Reference
e	69	PRO	-	expression tag	UNP W0DP94
e	70	THR	-	expression tag	UNP W0DP94
e	71	THR	-	expression tag	UNP W0DP94
e	72	GLU	-	expression tag	UNP W0DP94
e	73	ASN	-	expression tag	UNP W0DP94
e	74	LEU	-	expression tag	UNP W0DP94
e	75	TYR	-	expression tag	UNP W0DP94
e	76	PHE	-	expression tag	UNP W0DP94
e	77	GLN	-	expression tag	UNP W0DP94
e	78	GLY	-	expression tag	UNP W0DP94
e	79	ALA	-	expression tag	UNP W0DP94
e	80	MET	-	expression tag	UNP W0DP94
e	81	GLY	-	expression tag	UNP W0DP94
e	281	ALA	LYS	engineered mutation	UNP W0DP94
h	55	MET	-	initiating methionine	UNP W0DP94
h	56	SER	-	expression tag	UNP W0DP94
h	57	TYR	-	expression tag	UNP W0DP94
h	58	TYR	-	expression tag	UNP W0DP94
h	59	HIS	-	expression tag	UNP W0DP94
h	60	HIS	-	expression tag	UNP W0DP94
h	61	HIS	-	expression tag	UNP W0DP94
h	62	HIS	-	expression tag	UNP W0DP94
h	63	HIS	-	expression tag	UNP W0DP94
h	64	HIS	-	expression tag	UNP W0DP94
h	65	ASP	-	expression tag	UNP W0DP94
h	66	TYR	-	expression tag	UNP W0DP94
h	67	ASP	-	expression tag	UNP W0DP94
h	68	ILE	-	expression tag	UNP W0DP94
h	69	PRO	-	expression tag	UNP W0DP94
h	70	THR	-	expression tag	UNP W0DP94
h	71	THR	-	expression tag	UNP W0DP94
h	72	GLU	-	expression tag	UNP W0DP94
h	73	ASN	-	expression tag	UNP W0DP94
h	74	LEU	-	expression tag	UNP W0DP94
h	75	TYR	-	expression tag	UNP W0DP94
h	76	PHE	-	expression tag	UNP W0DP94
h	77	GLN	-	expression tag	UNP W0DP94
h	78	GLY	-	expression tag	UNP W0DP94
h	79	ALA	-	expression tag	UNP W0DP94
h	80	MET	-	expression tag	UNP W0DP94
h	81	GLY	-	expression tag	UNP W0DP94
h	281	ALA	LYS	engineered mutation	UNP W0DP94

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
k	55	MET	-	initiating methionine	UNP W0DP94
k	56	SER	-	expression tag	UNP W0DP94
k	57	TYR	-	expression tag	UNP W0DP94
k	58	TYR	-	expression tag	UNP W0DP94
k	59	HIS	-	expression tag	UNP W0DP94
k	60	HIS	-	expression tag	UNP W0DP94
k	61	HIS	-	expression tag	UNP W0DP94
k	62	HIS	-	expression tag	UNP W0DP94
k	63	HIS	-	expression tag	UNP W0DP94
k	64	HIS	-	expression tag	UNP W0DP94
k	65	ASP	-	expression tag	UNP W0DP94
k	66	TYR	-	expression tag	UNP W0DP94
k	67	ASP	-	expression tag	UNP W0DP94
k	68	ILE	-	expression tag	UNP W0DP94
k	69	PRO	-	expression tag	UNP W0DP94
k	70	THR	-	expression tag	UNP W0DP94
k	71	THR	-	expression tag	UNP W0DP94
k	72	GLU	-	expression tag	UNP W0DP94
k	73	ASN	-	expression tag	UNP W0DP94
k	74	LEU	-	expression tag	UNP W0DP94
k	75	TYR	-	expression tag	UNP W0DP94
k	76	PHE	-	expression tag	UNP W0DP94
k	77	GLN	-	expression tag	UNP W0DP94
k	78	GLY	-	expression tag	UNP W0DP94
k	79	ALA	-	expression tag	UNP W0DP94
k	80	MET	-	expression tag	UNP W0DP94
k	81	GLY	-	expression tag	UNP W0DP94
k	281	ALA	LYS	engineered mutation	UNP W0DP94

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



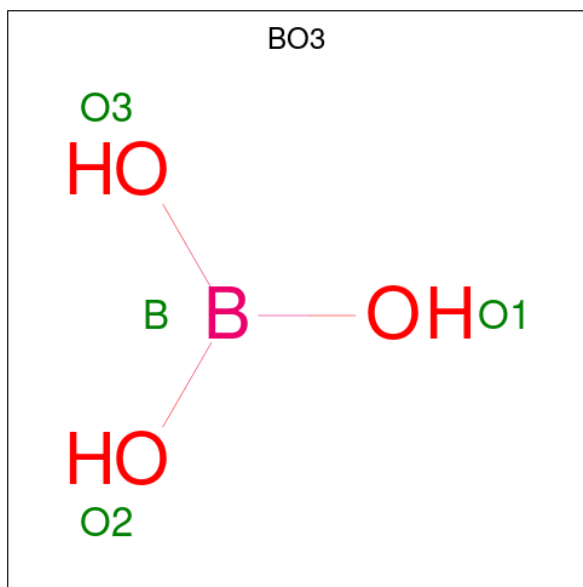
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	S	1	Total O S 5 4 1	0	0
2	V	1	Total O S 5 4 1	0	0
2	Y	1	Total O S 5 4 1	0	0
2	2	1	Total O S 5 4 1	0	0
2	5	1	Total O S 5 4 1	0	0
2	8	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	x	1	Total	O	S	0	0
			5	4	1		
2	h	1	Total	O	S	0	0
			5	4	1		
2	k	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is BORIC ACID (three-letter code: BO3) (formula: BH_3O_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	B	O	0	0
			4	1	3		
3	D	1	Total	B	O	0	0
			4	1	3		

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cu	0	0
			2	2		
4	D	2	Total	Cu	0	0
			2	2		
4	G	2	Total	Cu	0	0
			2	2		
4	J	2	Total	Cu	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	2	Total Cu 2 2	0	0
4	P	2	Total Cu 2 2	0	0
4	S	2	Total Cu 2 2	0	0
4	V	2	Total Cu 2 2	0	0
4	Y	2	Total Cu 2 2	0	0
4	2	2	Total Cu 2 2	0	0
4	5	2	Total Cu 2 2	0	0
4	8	2	Total Cu 2 2	0	0
4	x	2	Total Cu 2 2	0	0
4	e	2	Total Cu 2 2	0	0
4	h	2	Total Cu 2 2	0	0
4	k	2	Total Cu 2 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	1	Total Na 1 1	0	0
5	V	1	Total Na 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	193	Total O 193 193	0	0
6	D	198	Total O 198 198	0	0
6	G	199	Total O 199 199	0	0

Continued on next page...


Continued from previous page...

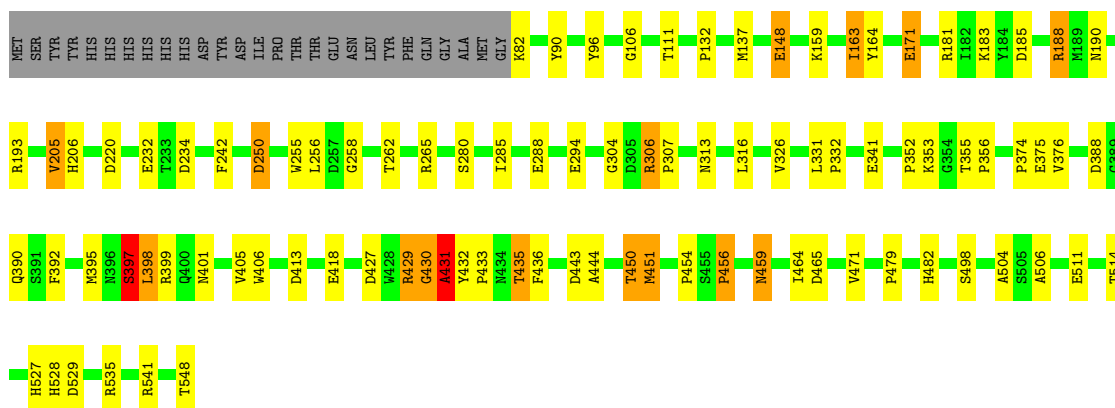
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	219	Total 219	O 219	0	0
6	M	140	Total 140	O 140	0	0
6	P	154	Total 154	O 154	0	0
6	S	145	Total 145	O 145	0	0
6	V	145	Total 145	O 145	0	0
6	Y	173	Total 173	O 173	0	0
6	2	143	Total 143	O 143	0	0
6	5	187	Total 187	O 187	0	0
6	8	137	Total 137	O 137	0	0
6	x	104	Total 104	O 104	0	0
6	e	94	Total 94	O 94	0	0
6	h	89	Total 89	O 89	0	0
6	k	100	Total 100	O 100	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.

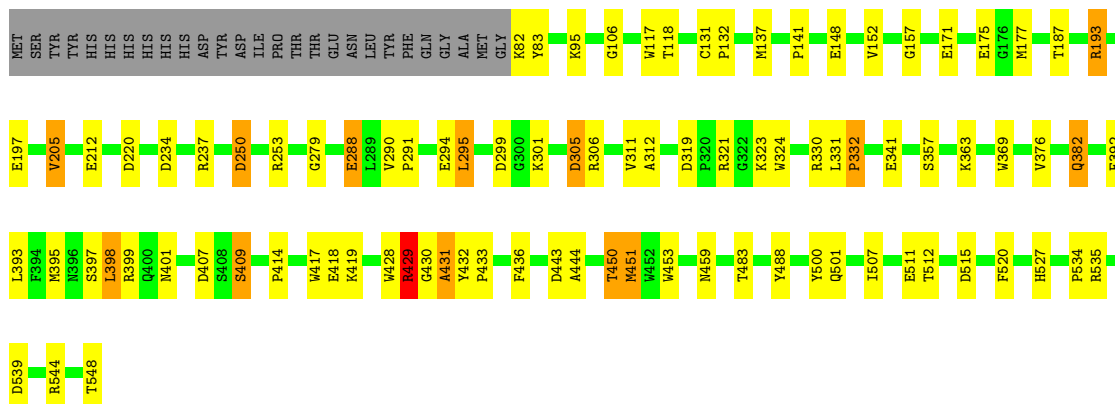
- Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain A: 



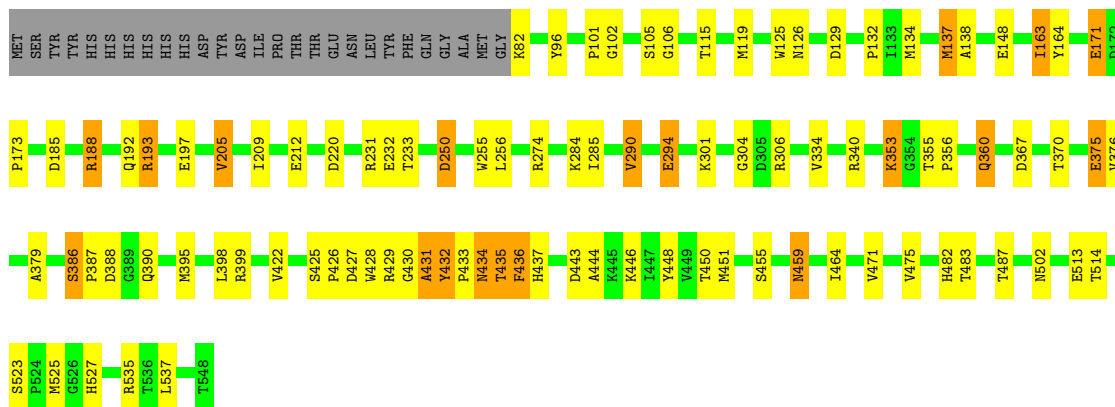
- Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain D: 



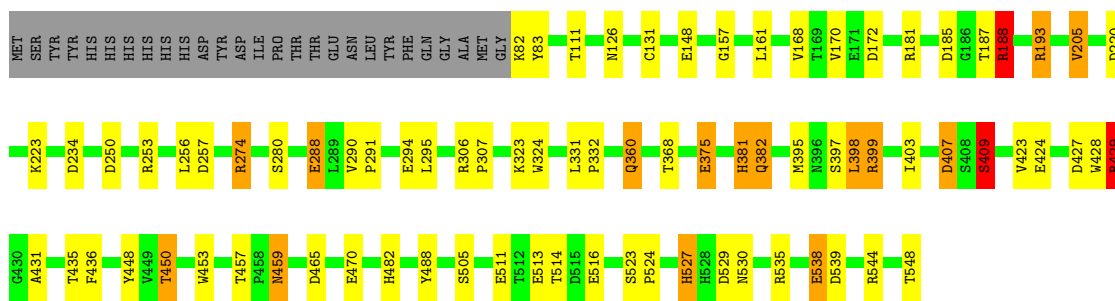
- Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain G: 



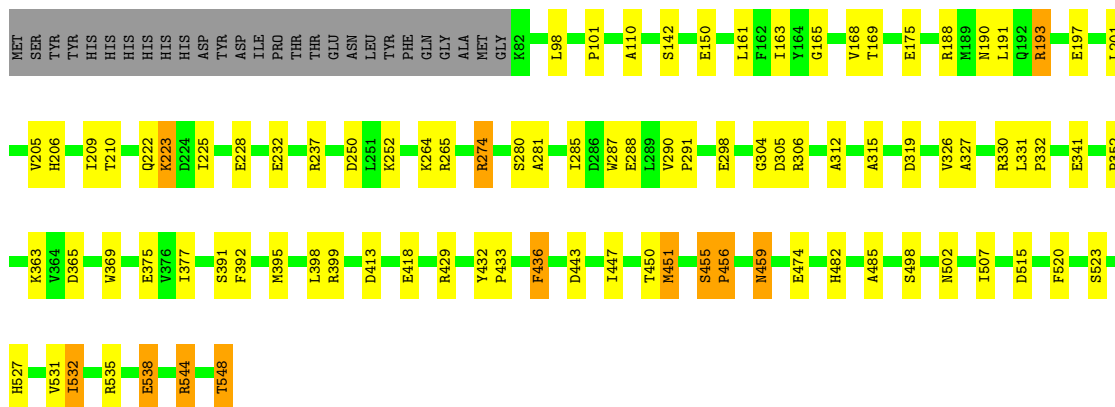
- Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain J: 78% 13% 5%



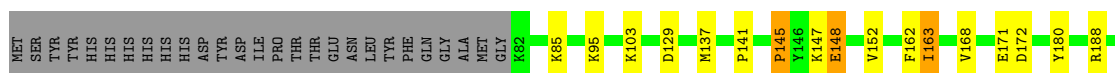
- Molecule 1: Twin-arginine translocation signal domain-containing protein

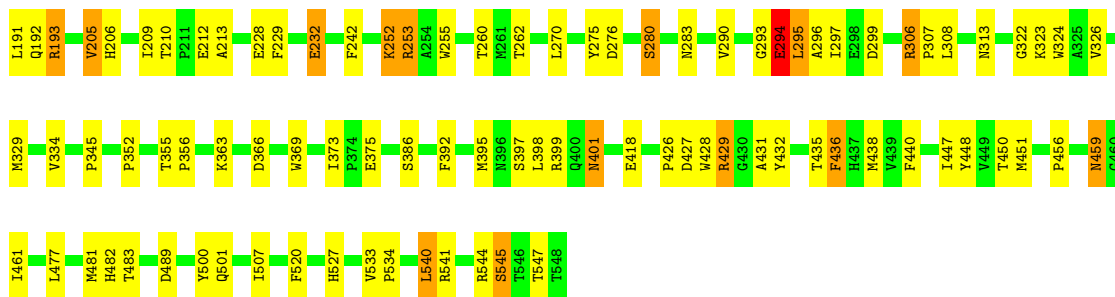
Chain M: 76% 16% 5%



- Molecule 1: Twin-arginine translocation signal domain-containing protein

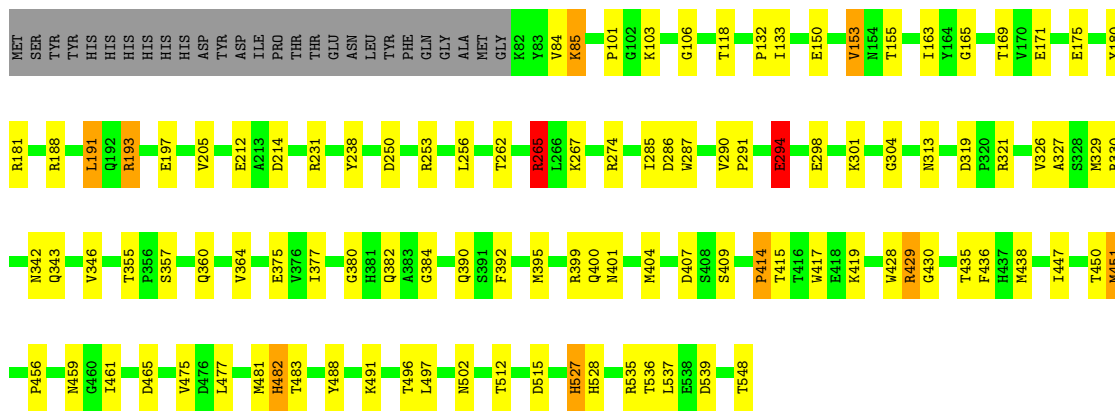
Chain P: 73% 18% 5%





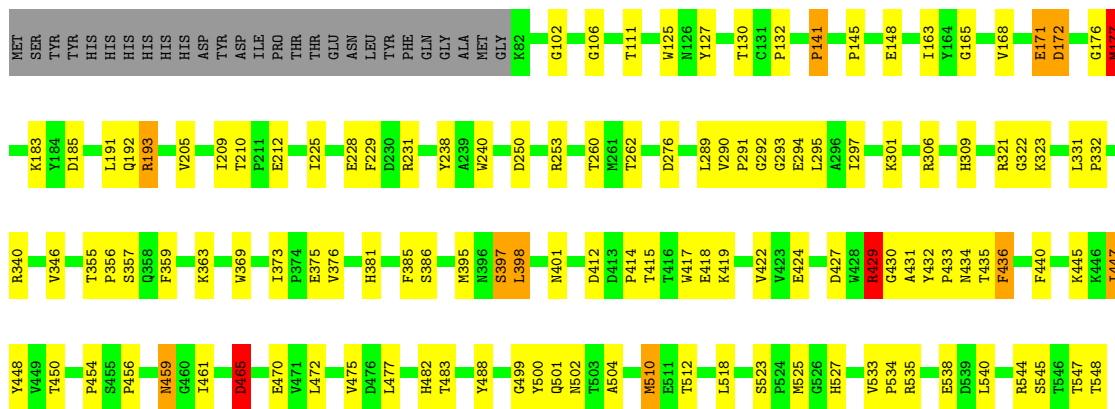
• Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain S: 73% 19% 5%



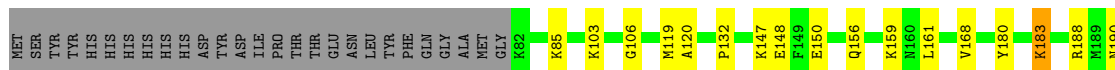
• Molecule 1: Twin-arginine translocation signal domain-containing protein

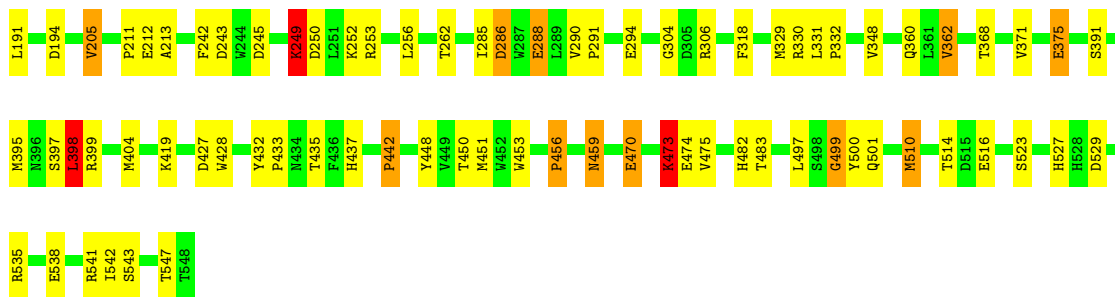
Chain V: 69% 23% 5%



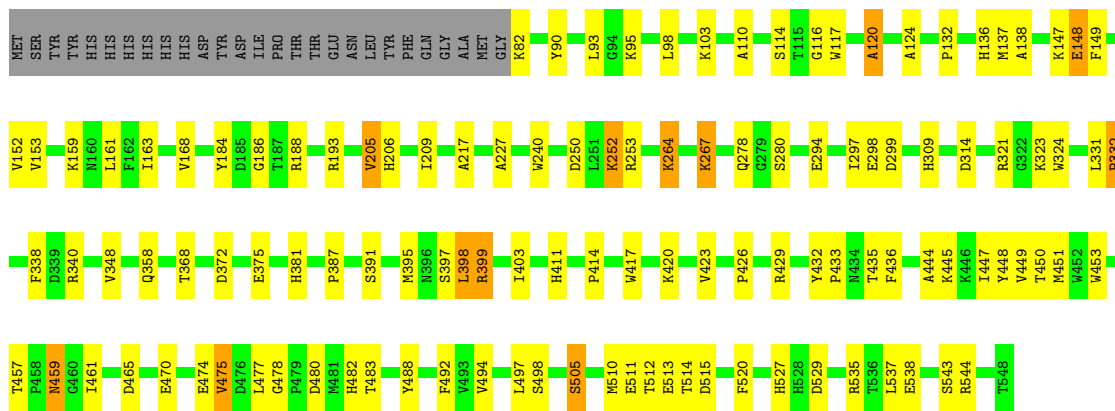
• Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain Y: 76% 16% 5%

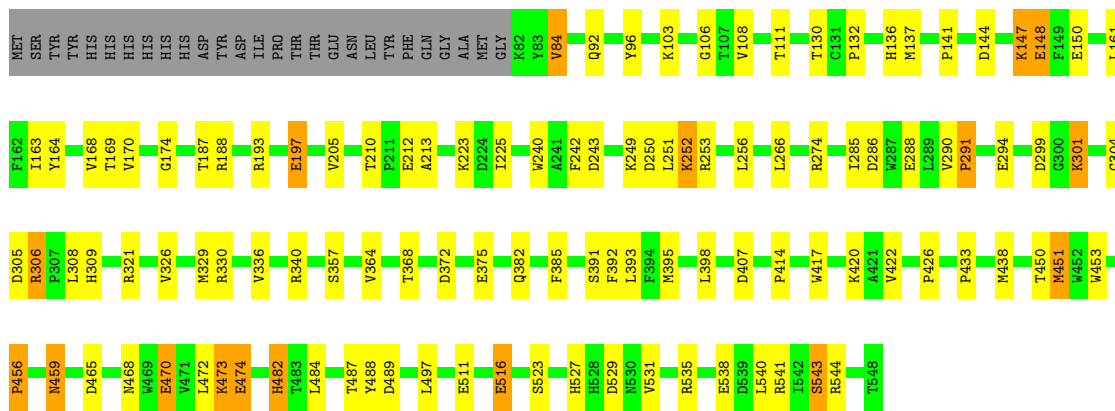




• Molecule 1: Twin-arginine translocation signal domain-containing protein

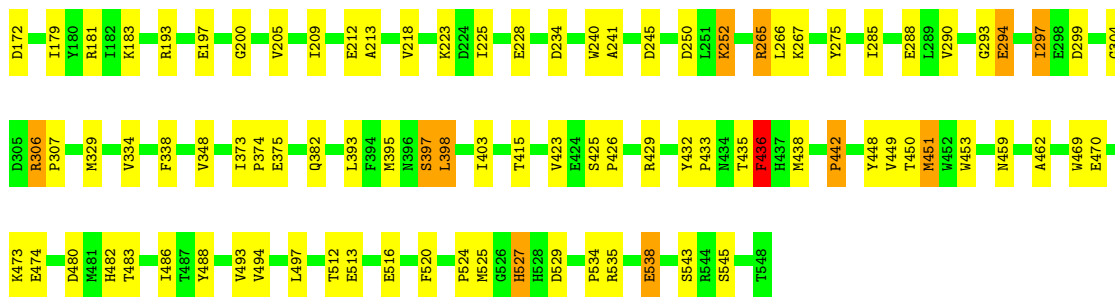


• Molecule 1: Twin-arginine translocation signal domain-containing protein



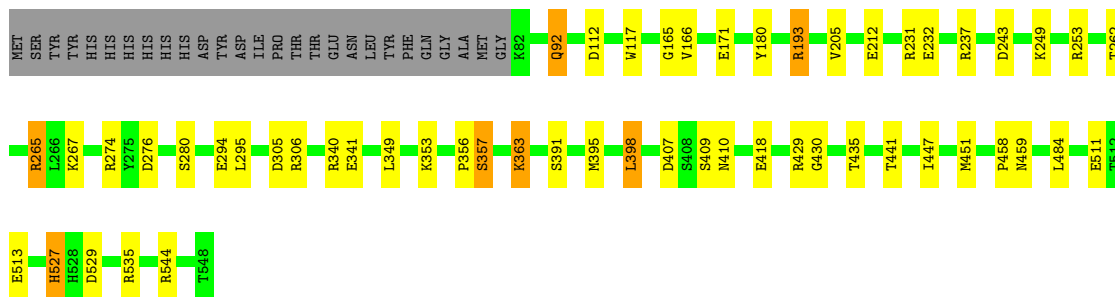
• Molecule 1: Twin-arginine translocation signal domain-containing protein





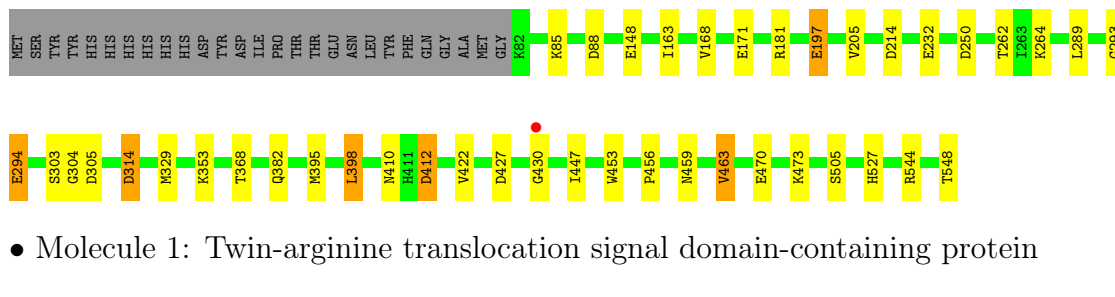
• Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain x:



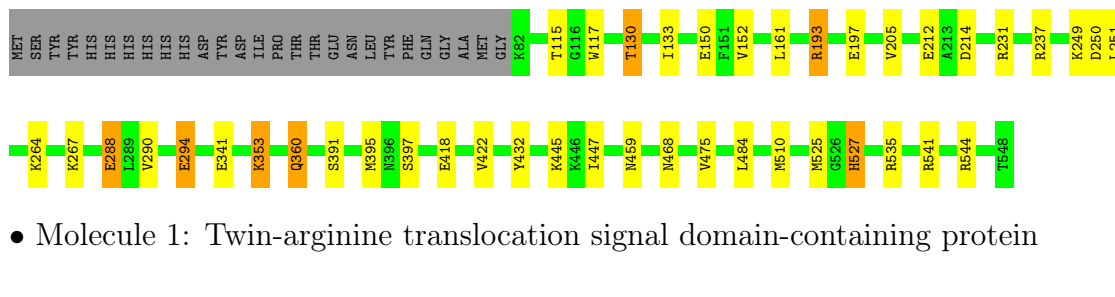
• Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain e:



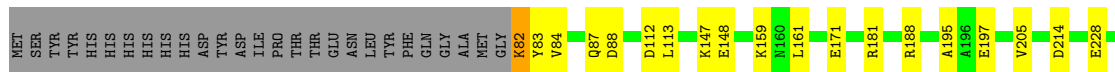
• Molecule 1: Twin-arginine translocation signal domain-containing protein

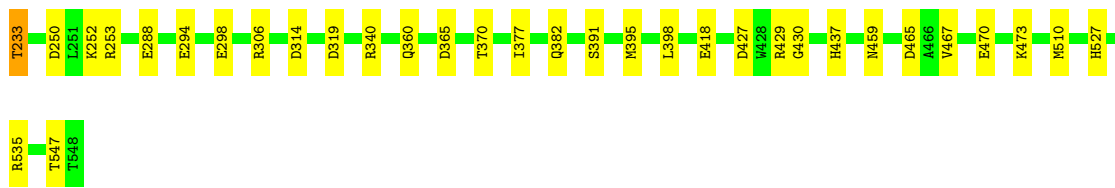
Chain h:



• Molecule 1: Twin-arginine translocation signal domain-containing protein

Chain k:





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.15Å 142.42Å 294.40Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	49.12 – 2.07 49.07 – 2.07	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.12-2.07) 98.5 (49.07-2.07)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.07Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.179 , 0.234 0.185 , 0.237	Depositor DCC
R_{free} test set	24463 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtrriage
Anisotropy	0.214	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.456 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	60462	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CU, NA, BO3

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	2	0.84	3/3730 (0.1%)	1.41	28/5094 (0.5%)
1	5	0.91	8/3727 (0.2%)	1.49	42/5090 (0.8%)
1	8	0.85	3/3720 (0.1%)	1.43	29/5083 (0.6%)
1	A	0.98	9/3743 (0.2%)	1.50	36/5111 (0.7%)
1	D	0.95	5/3731 (0.1%)	1.45	23/5094 (0.5%)
1	G	0.96	6/3749 (0.2%)	1.51	46/5118 (0.9%)
1	J	0.97	6/3723 (0.2%)	1.47	32/5085 (0.6%)
1	M	0.94	14/3730 (0.4%)	1.40	28/5093 (0.5%)
1	P	0.90	4/3729 (0.1%)	1.44	23/5094 (0.5%)
1	S	0.90	6/3717 (0.2%)	1.46	37/5077 (0.7%)
1	V	0.92	8/3724 (0.2%)	1.43	37/5087 (0.7%)
1	Y	0.90	7/3726 (0.2%)	1.43	26/5089 (0.5%)
1	e	0.84	1/3719 (0.0%)	1.35	19/5083 (0.4%)
1	h	0.90	7/3705 (0.2%)	1.36	31/5065 (0.6%)
1	k	0.82	5/3721 (0.1%)	1.39	31/5085 (0.6%)
1	x	0.86	1/3711 (0.0%)	1.38	31/5072 (0.6%)
All	All	0.90	93/59605 (0.2%)	1.43	499/81420 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	3
1	5	0	1
1	V	0	2
1	Y	0	1
1	e	0	3
1	h	0	1
1	k	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	x	0	1
All	All	0	14

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	h	288	GLU	CD-OE1	12.68	1.39	1.25
1	M	175	GLU	CD-OE2	-10.92	1.13	1.25
1	V	538	GLU	CD-OE1	10.78	1.37	1.25
1	Y	538	GLU	CD-OE1	9.57	1.36	1.25
1	Y	538	GLU	CD-OE2	8.98	1.35	1.25

The worst 5 of 499 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	k	365	ASP	CB-CA-C	-13.43	83.54	110.40
1	Y	330	ARG	NE-CZ-NH1	-12.83	113.89	120.30
1	x	231	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	A	188	ARG	NE-CZ-NH1	12.38	126.49	120.30
1	G	274	ARG	NE-CZ-NH1	12.29	126.44	120.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	117	TRP	Peptide
1	2	497	LEU	Peptide
1	V	322	GLY	Mainchain
1	V	429	ARG	Peptide
1	Y	497	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	3627	0	3482	56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	3617	0	3474	39	0
1	8	3617	0	3463	54	0
1	A	3636	0	3491	41	0
1	D	3628	0	3494	48	0
1	G	3636	0	3496	42	0
1	J	3620	0	3476	47	0
1	M	3627	0	3492	36	0
1	P	3626	0	3473	60	0
1	S	3614	0	3475	41	0
1	V	3621	0	3467	55	0
1	Y	3617	0	3475	39	0
1	e	3608	0	3435	0	0
1	h	3602	0	3436	0	0
1	k	3611	0	3449	0	0
1	x	3608	0	3450	0	0
2	2	5	0	0	0	0
2	5	5	0	0	0	0
2	8	5	0	0	0	0
2	A	10	0	0	1	0
2	D	5	0	0	0	0
2	G	5	0	0	0	0
2	J	5	0	0	0	0
2	M	5	0	0	0	0
2	P	10	0	0	0	0
2	S	5	0	0	0	0
2	V	5	0	0	0	0
2	Y	5	0	0	0	0
2	h	5	0	0	0	0
2	k	5	0	0	0	0
2	x	5	0	0	0	0
3	A	4	0	3	0	0
3	D	4	0	3	0	0
4	2	2	0	0	0	0
4	5	2	0	0	0	0
4	8	2	0	0	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
4	G	2	0	0	0	0
4	J	2	0	0	0	0
4	M	2	0	0	0	0
4	P	2	0	0	0	0
4	S	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	2	0	0	0	0
4	Y	2	0	0	0	0
4	e	2	0	0	0	0
4	h	2	0	0	0	0
4	k	2	0	0	0	0
4	x	2	0	0	0	0
5	P	1	0	0	0	0
5	V	1	0	0	0	0
6	2	143	0	0	3	0
6	5	187	0	0	1	0
6	8	137	0	0	3	0
6	A	193	0	0	3	0
6	D	198	0	0	2	0
6	G	199	0	0	0	0
6	J	219	0	0	3	0
6	M	140	0	0	2	0
6	P	154	0	0	3	0
6	S	145	0	0	2	0
6	V	145	0	0	2	0
6	Y	173	0	0	1	0
6	e	94	0	0	0	0
6	h	89	0	0	0	0
6	k	100	0	0	0	0
6	x	104	0	0	0	0
All	All	60462	0	55534	547	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 7.

The worst 5 of 547 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:D:197:GLU:OE2	1:5:197:GLU:OE2	1.59	1.19
1:8:148:GLU:OE1	1:8:183:LYS:HE3	1.42	1.18
1:P:429:ARG:HG3	1:P:429:ARG:HH11	1.01	1.17
1:J:450:THR:HG21	1:J:482:HIS:O	1.58	1.03
1:2:397:SER:O	1:2:398:LEU:CB	2.00	1.02

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	2	465/494 (94%)	435 (94%)	27 (6%)	3 (1%)	25	15
1	5	466/494 (94%)	439 (94%)	23 (5%)	4 (1%)	17	8
1	8	465/494 (94%)	430 (92%)	32 (7%)	3 (1%)	25	15
1	A	466/494 (94%)	432 (93%)	30 (6%)	4 (1%)	17	8
1	D	465/494 (94%)	437 (94%)	26 (6%)	2 (0%)	34	25
1	G	467/494 (94%)	438 (94%)	27 (6%)	2 (0%)	34	25
1	J	465/494 (94%)	435 (94%)	26 (6%)	4 (1%)	17	8
1	M	465/494 (94%)	436 (94%)	27 (6%)	2 (0%)	34	25
1	P	465/494 (94%)	431 (93%)	31 (7%)	3 (1%)	25	15
1	S	465/494 (94%)	431 (93%)	33 (7%)	1 (0%)	47	39
1	V	465/494 (94%)	432 (93%)	29 (6%)	4 (1%)	17	8
1	Y	466/494 (94%)	432 (93%)	30 (6%)	4 (1%)	17	8
1	e	466/494 (94%)	426 (91%)	36 (8%)	4 (1%)	17	8
1	h	465/494 (94%)	427 (92%)	37 (8%)	1 (0%)	47	39
1	k	466/494 (94%)	423 (91%)	40 (9%)	3 (1%)	25	15
1	x	465/494 (94%)	425 (91%)	30 (6%)	10 (2%)	6	1
All	All	7447/7904 (94%)	6909 (93%)	484 (6%)	54 (1%)	22	11

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	398	LEU
1	2	398	LEU
1	8	398	LEU
1	x	171	GLU
1	A	205	VAL

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	2	387/415 (93%)	363 (94%)	24 (6%)	18	10
1	5	386/415 (93%)	364 (94%)	22 (6%)	20	12
1	8	385/415 (93%)	369 (96%)	16 (4%)	30	23
1	A	389/415 (94%)	373 (96%)	16 (4%)	30	23
1	D	388/415 (94%)	374 (96%)	14 (4%)	35	28
1	G	389/415 (94%)	380 (98%)	9 (2%)	50	45
1	J	386/415 (93%)	373 (97%)	13 (3%)	37	30
1	M	388/415 (94%)	371 (96%)	17 (4%)	28	21
1	P	387/415 (93%)	369 (95%)	18 (5%)	26	18
1	S	384/415 (92%)	361 (94%)	23 (6%)	19	11
1	V	386/415 (93%)	365 (95%)	21 (5%)	22	14
1	Y	386/415 (93%)	367 (95%)	19 (5%)	25	17
1	e	383/415 (92%)	355 (93%)	28 (7%)	14	6
1	h	381/415 (92%)	358 (94%)	23 (6%)	19	11
1	k	384/415 (92%)	362 (94%)	22 (6%)	20	12
1	x	383/415 (92%)	358 (94%)	25 (6%)	17	9
All	All	6172/6640 (93%)	5862 (95%)	310 (5%)	24	16

5 of 310 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	x	458	PRO
1	h	510	MET
1	e	148	GLU
1	e	463	VAL
1	k	395	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	8	343	GLN
1	x	309	HIS
1	k	459	ASN
1	e	434	ASN
1	k	390	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 53 ligands modelled in this entry, 34 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	x	601	-	4,4,4	0.67	0	6,6,6	0.45	0
2	SO4	D	601	-	4,4,4	1.08	0	6,6,6	0.76	0
2	SO4	A	705	-	4,4,4	1.44	1 (25%)	6,6,6	0.61	0
2	SO4	P	702	-	4,4,4	0.51	0	6,6,6	0.13	0
2	SO4	M	701	-	4,4,4	0.83	0	6,6,6	0.30	0
2	SO4	8	701	-	4,4,4	0.73	0	6,6,6	0.25	0
2	SO4	5	601	-	4,4,4	0.92	0	6,6,6	0.38	0
2	SO4	S	601	-	4,4,4	0.66	0	6,6,6	0.52	0
2	SO4	G	701	-	4,4,4	1.56	1 (25%)	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	P	701	-	4,4,4	0.98	0	6,6,6	0.63	0
2	SO4	2	701	-	4,4,4	0.86	0	6,6,6	0.72	0
2	SO4	A	701	-	4,4,4	0.74	0	6,6,6	0.29	0
2	SO4	J	601	-	4,4,4	1.18	0	6,6,6	0.42	0
2	SO4	k	701	-	4,4,4	0.80	0	6,6,6	0.24	0
2	SO4	V	601	-	4,4,4	0.80	0	6,6,6	0.67	0
2	SO4	h	601	-	4,4,4	0.69	0	6,6,6	0.22	0
3	BO3	A	702	-	3,3,3	0.42	0	3,3,3	1.06	0
2	SO4	Y	601	-	4,4,4	1.15	0	6,6,6	0.31	0
3	BO3	D	602	-	3,3,3	0.35	0	3,3,3	1.70	1 (33%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	SO4	O2-S	-2.14	1.34	1.46
2	A	705	SO4	O1-S	-2.12	1.34	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	BO3	O3-B-O1	-2.31	111.89	119.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	2	467/494 (94%)	-0.90	0 100 100	19, 30, 43, 73	0
1	5	467/494 (94%)	-0.95	0 100 100	17, 26, 40, 61	3 (0%)
1	8	467/494 (94%)	-0.90	0 100 100	19, 30, 43, 71	1 (0%)
1	A	467/494 (94%)	-0.95	0 100 100	16, 25, 38, 99	3 (0%)
1	D	467/494 (94%)	-0.97	0 100 100	16, 24, 38, 62	2 (0%)
1	G	467/494 (94%)	-0.93	0 100 100	16, 25, 38, 59	0
1	J	467/494 (94%)	-0.96	0 100 100	16, 24, 38, 61	1 (0%)
1	M	467/494 (94%)	-0.94	0 100 100	20, 28, 41, 55	0
1	P	467/494 (94%)	-0.91	0 100 100	17, 28, 44, 79	1 (0%)
1	S	467/494 (94%)	-0.93	0 100 100	19, 28, 41, 67	0
1	V	467/494 (94%)	-0.92	0 100 100	18, 28, 43, 75	0
1	Y	467/494 (94%)	-0.93	0 100 100	16, 26, 41, 68	1 (0%)
1	e	467/494 (94%)	-0.82	1 (0%) 95 95	23, 35, 50, 78	1 (0%)
1	h	467/494 (94%)	-0.78	0 100 100	22, 34, 49, 70	0
1	k	467/494 (94%)	-0.77	0 100 100	24, 36, 51, 80	0
1	x	467/494 (94%)	-0.85	0 100 100	21, 33, 48, 75	1 (0%)
All	All	7472/7904 (94%)	-0.90	1 (0%) 100 100	16, 29, 45, 99	14 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	e	430	GLY	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BO3	D	602	4/4	0.95	0.06	33,34,39,42	0
3	BO3	A	702	4/4	0.96	0.05	41,41,43,49	0
2	SO4	k	701	5/5	0.96	0.11	25,27,34,34	5
2	SO4	P	702	5/5	0.97	0.08	29,29,31,39	5
2	SO4	A	701	5/5	0.97	0.13	20,23,29,33	5
2	SO4	2	701	5/5	0.98	0.10	22,27,31,36	5
2	SO4	Y	601	5/5	0.98	0.18	19,23,26,28	5
4	CU	V	603	1/1	0.98	0.05	41,41,41,41	0
5	NA	P	705	1/1	0.98	0.14	27,27,27,27	1
5	NA	V	604	1/1	0.98	0.19	24,24,24,24	1
2	SO4	D	601	5/5	0.99	0.10	29,33,39,41	5
2	SO4	G	701	5/5	0.99	0.14	17,18,20,22	5
2	SO4	5	601	5/5	0.99	0.14	19,20,22,23	5
2	SO4	x	601	5/5	0.99	0.07	29,30,34,36	5
2	SO4	h	601	5/5	0.99	0.07	36,36,38,38	5
2	SO4	J	601	5/5	0.99	0.11	30,31,35,38	5
2	SO4	M	701	5/5	0.99	0.10	30,33,34,34	5
2	SO4	P	701	5/5	0.99	0.09	26,26,28,33	5
4	CU	A	704	1/1	0.99	0.07	37,37,37,37	0
4	CU	D	603	1/1	0.99	0.08	27,27,27,27	0
4	CU	D	604	1/1	0.99	0.08	34,34,34,34	0
4	CU	G	703	1/1	0.99	0.08	35,35,35,35	0
4	CU	J	602	1/1	0.99	0.07	28,28,28,28	0
4	CU	J	603	1/1	0.99	0.09	35,35,35,35	0
4	CU	M	703	1/1	0.99	0.06	39,39,39,39	0
4	CU	P	704	1/1	0.99	0.07	39,39,39,39	0
4	CU	S	603	1/1	0.99	0.06	38,38,38,38	0
2	SO4	A	705	5/5	0.99	0.14	18,19,22,24	5
4	CU	Y	602	1/1	0.99	0.08	31,31,31,31	0
4	CU	Y	603	1/1	0.99	0.08	37,37,37,37	0
4	CU	2	703	1/1	0.99	0.08	38,38,38,38	0
4	CU	8	702	1/1	0.99	0.05	35,35,35,35	0

Continued on next page...

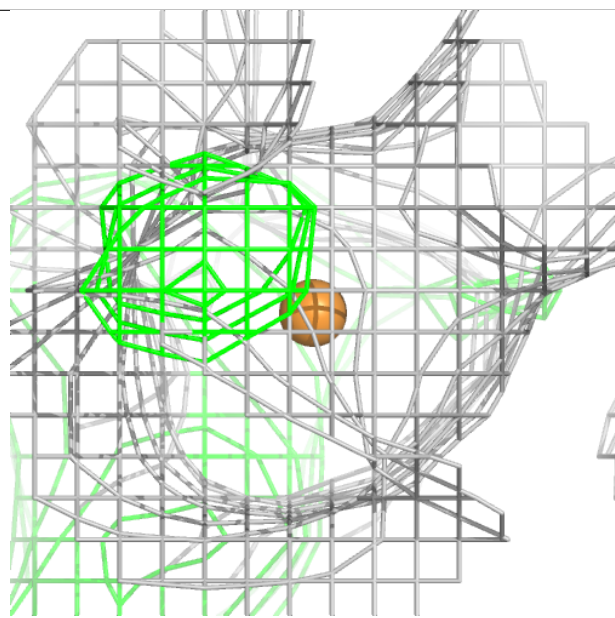
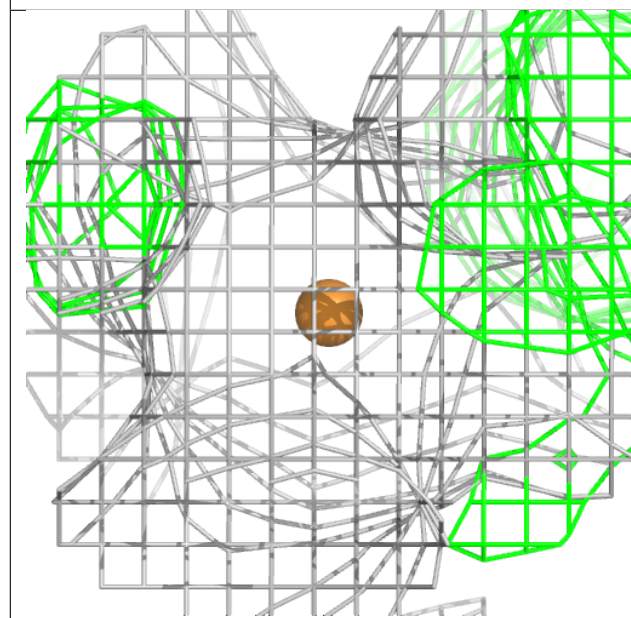
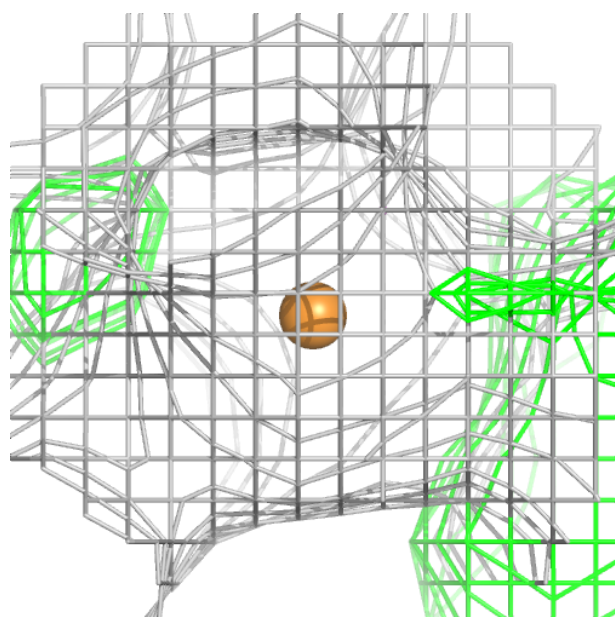
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CU	k	703	1/1	0.99	0.05	43,43,43,43	0
2	SO4	S	601	5/5	0.99	0.13	27,28,31,31	5
2	SO4	V	601	5/5	0.99	0.10	27,27,31,31	5
4	CU	A	703	1/1	1.00	0.07	32,32,32,32	0
4	CU	P	703	1/1	1.00	0.10	32,32,32,32	0
4	CU	2	702	1/1	1.00	0.08	33,33,33,33	0
2	SO4	8	701	5/5	1.00	0.09	25,28,31,35	5
4	CU	5	602	1/1	1.00	0.06	33,33,33,33	0
4	CU	5	603	1/1	1.00	0.06	38,38,38,38	0
4	CU	S	602	1/1	1.00	0.06	33,33,33,33	0
4	CU	8	703	1/1	1.00	0.08	39,39,39,39	0
4	CU	x	602	1/1	1.00	0.07	36,36,36,36	0
4	CU	x	603	1/1	1.00	0.07	42,42,42,42	0
4	CU	e	601	1/1	1.00	0.06	38,38,38,38	0
4	CU	e	602	1/1	1.00	0.06	41,41,41,41	0
4	CU	h	602	1/1	1.00	0.06	37,37,37,37	0
4	CU	h	603	1/1	1.00	0.05	42,42,42,42	0
4	CU	k	702	1/1	1.00	0.05	40,40,40,40	0
4	CU	G	702	1/1	1.00	0.08	29,29,29,29	0
4	CU	V	602	1/1	1.00	0.06	35,35,35,35	0
4	CU	M	702	1/1	1.00	0.07	31,31,31,31	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.

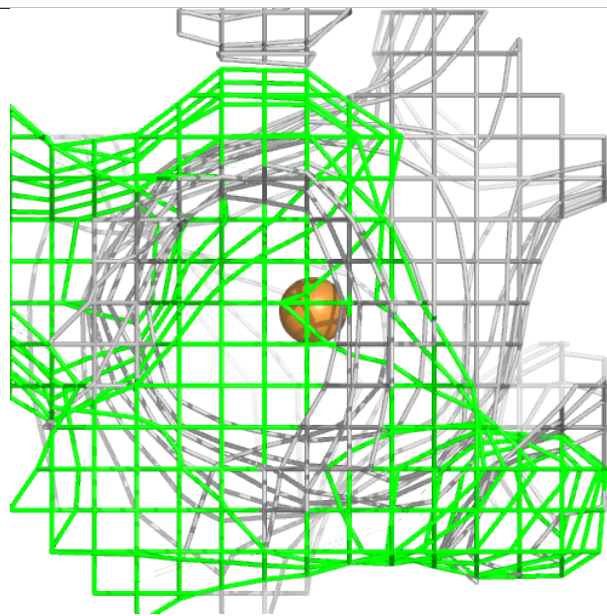
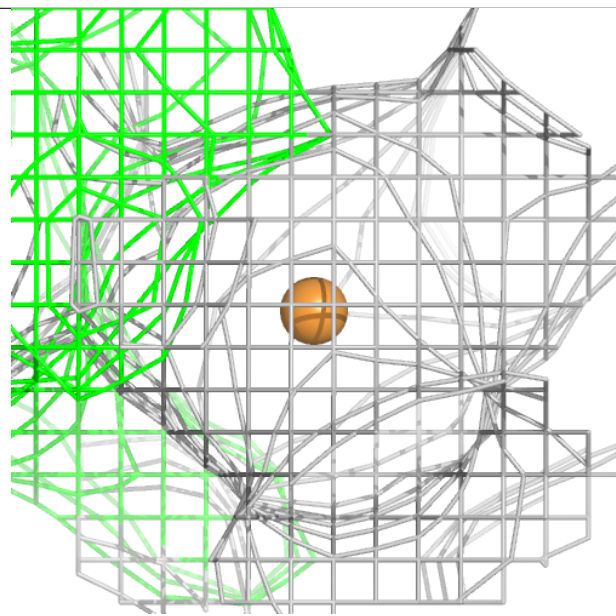
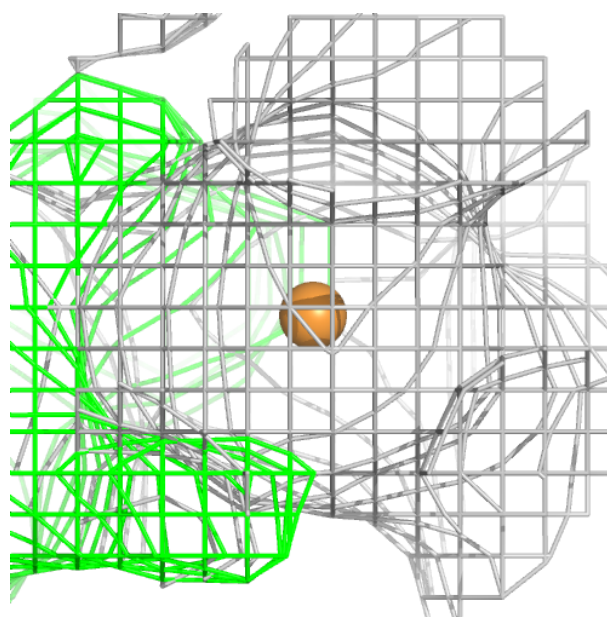
Electron density around CU V 603:

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



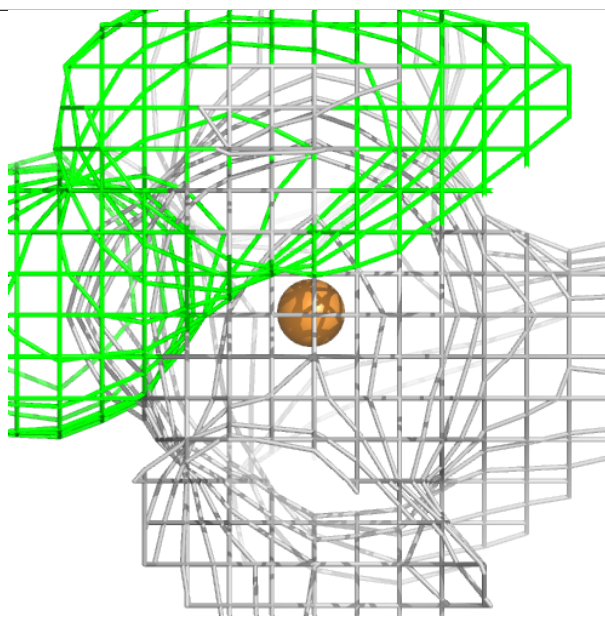
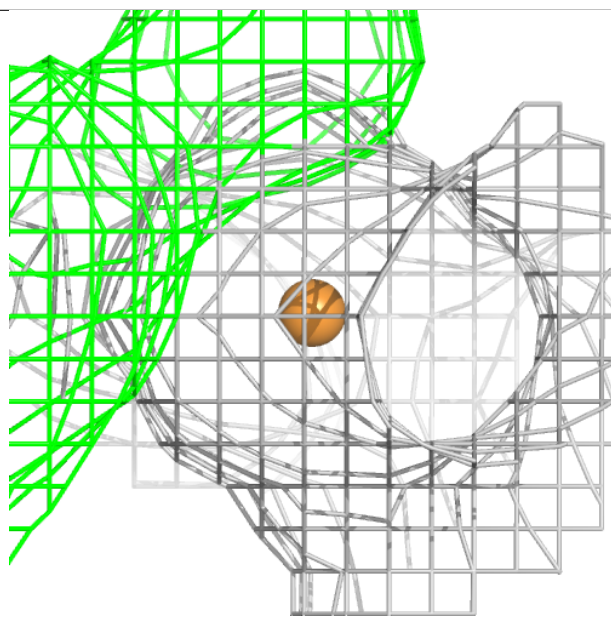
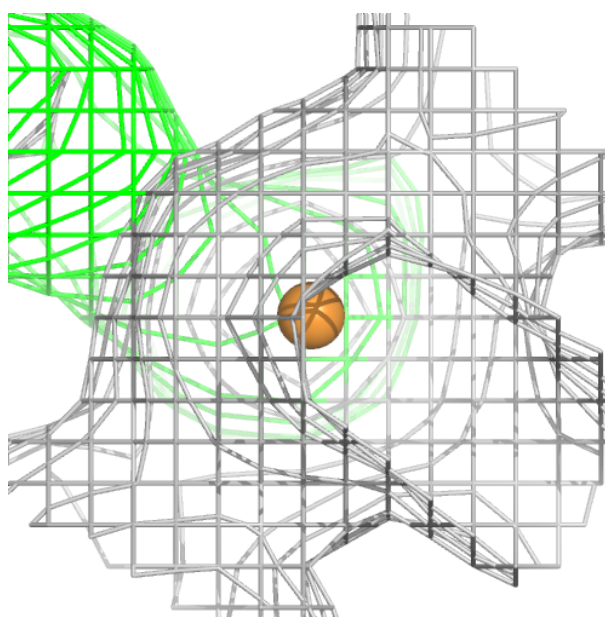
Electron density around CU A 704:

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



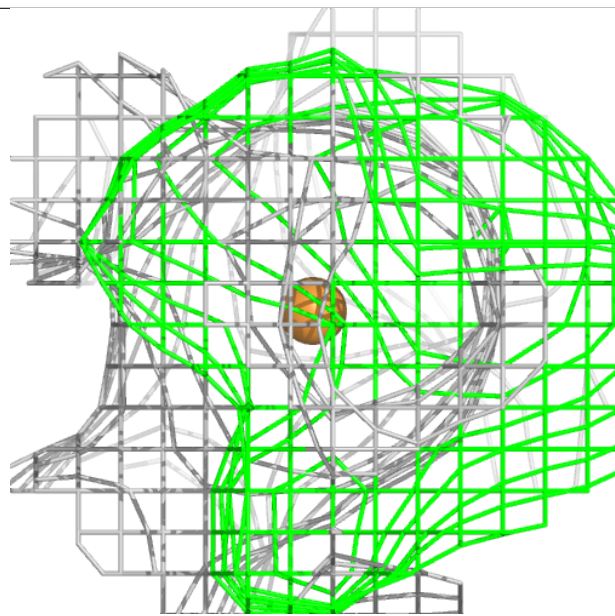
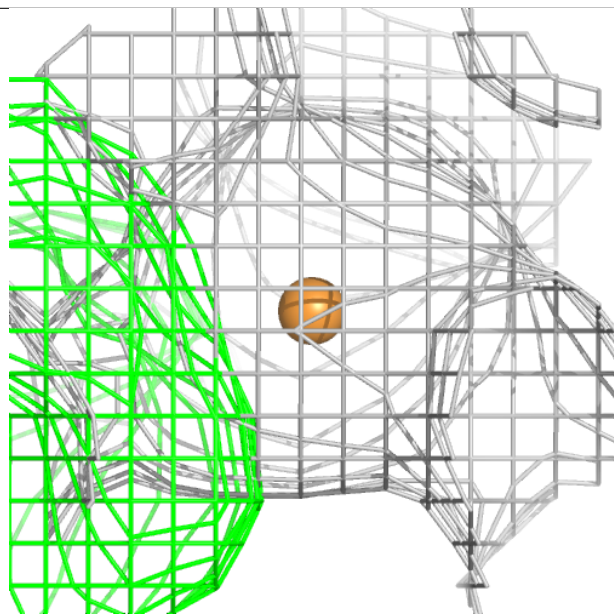
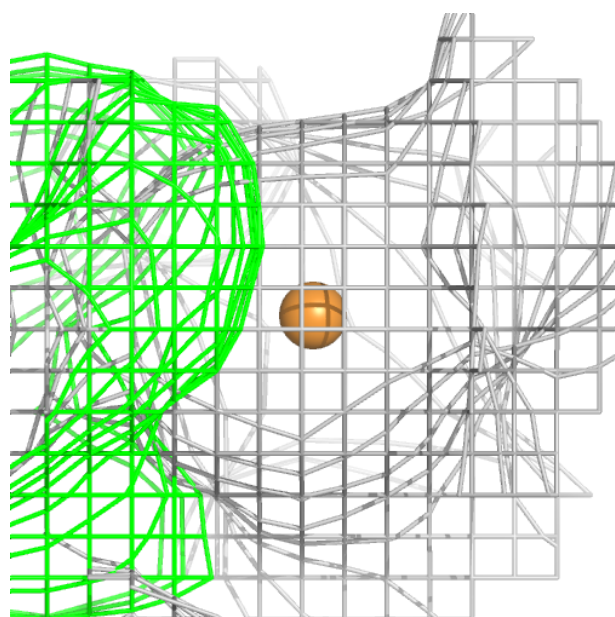
Electron density around CU D 603:

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



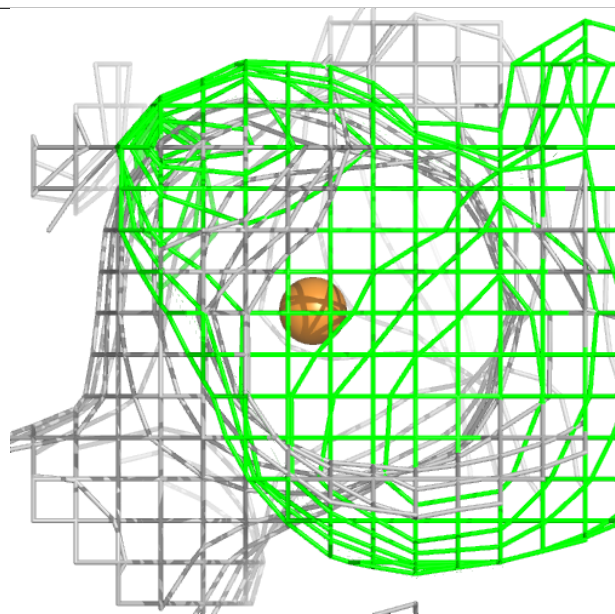
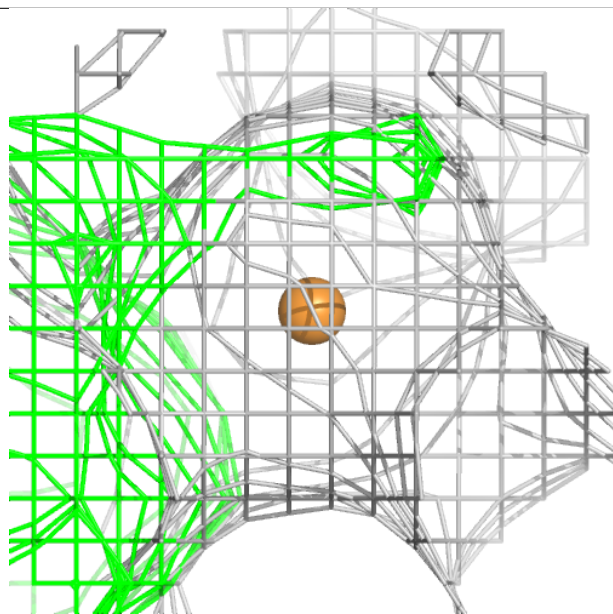
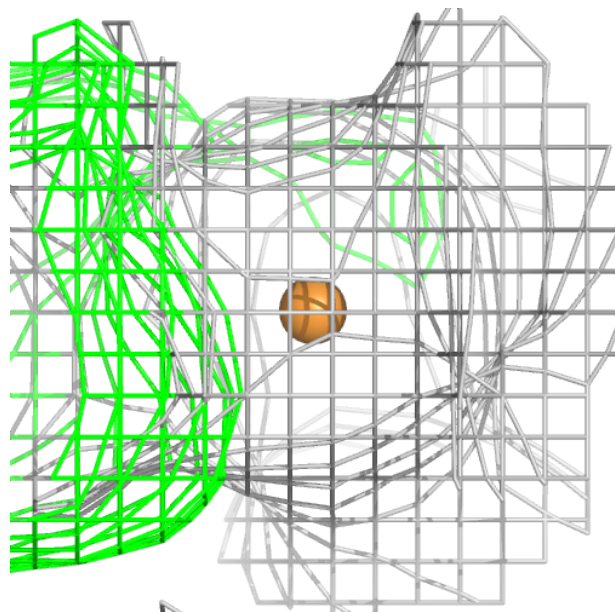
Electron density around CU D 604:

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



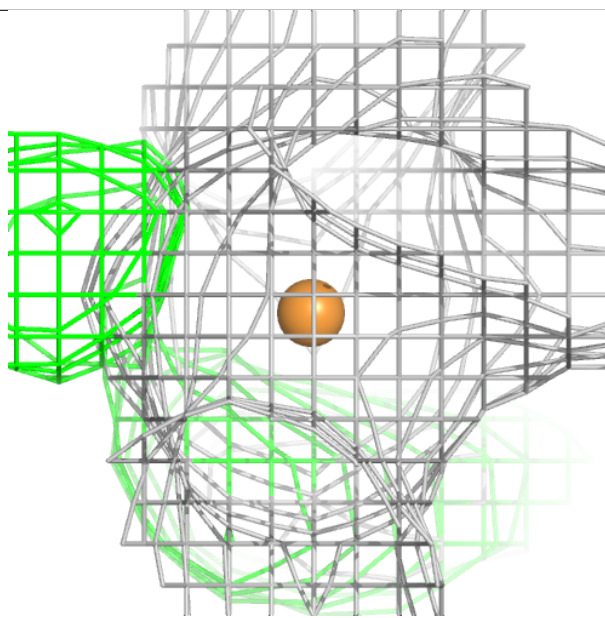
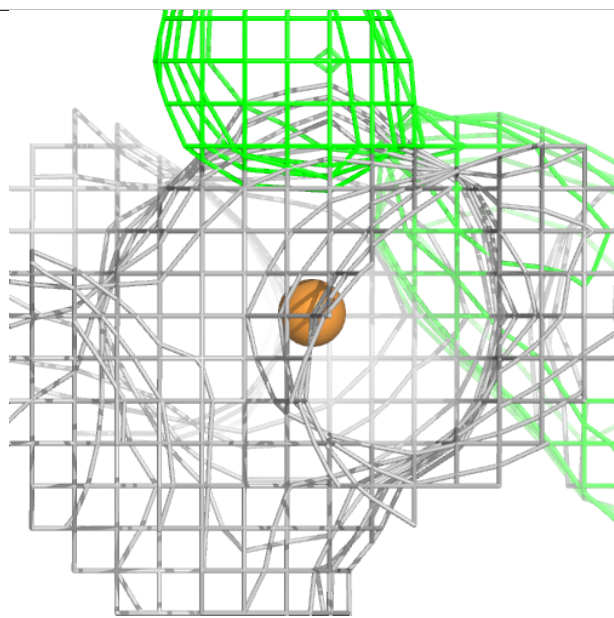
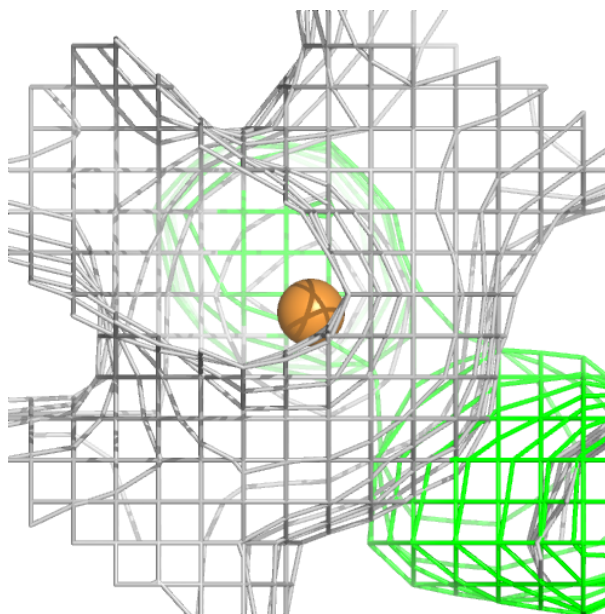
Electron density around CU G 703:

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



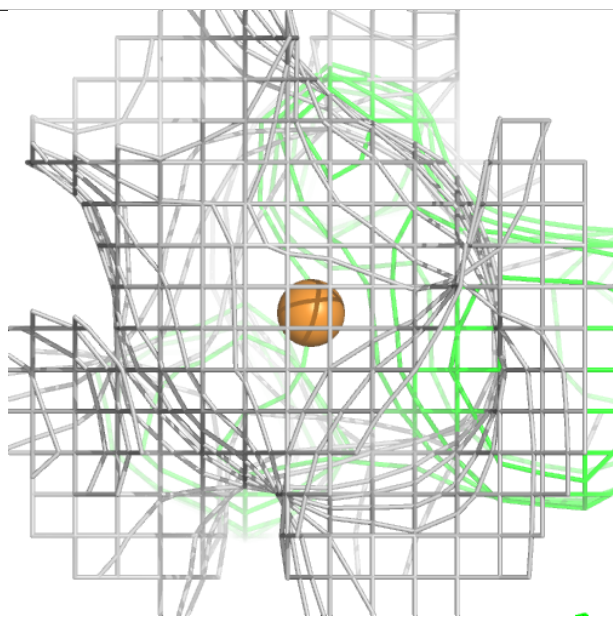
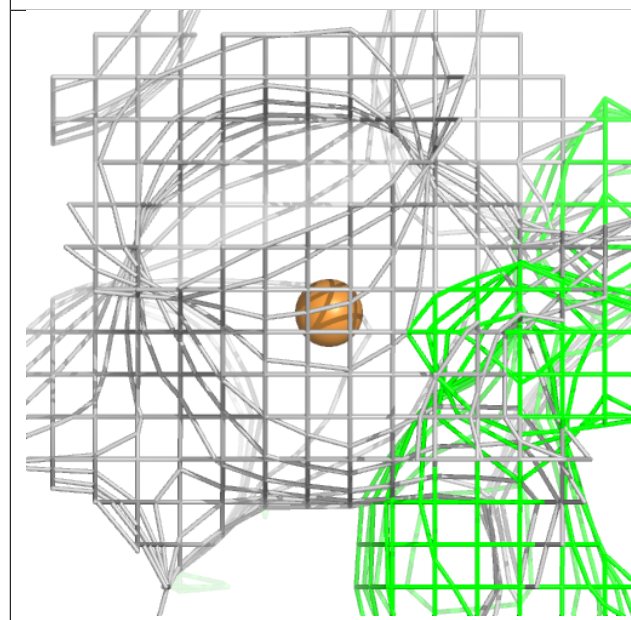
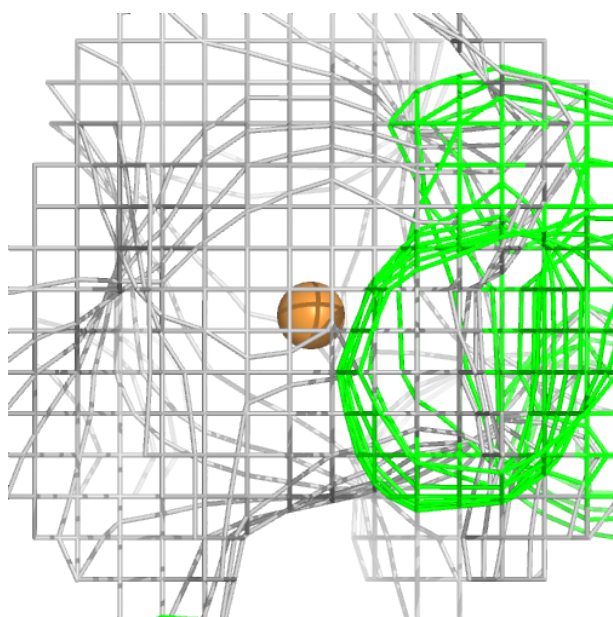
Electron density around CU J 602:

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



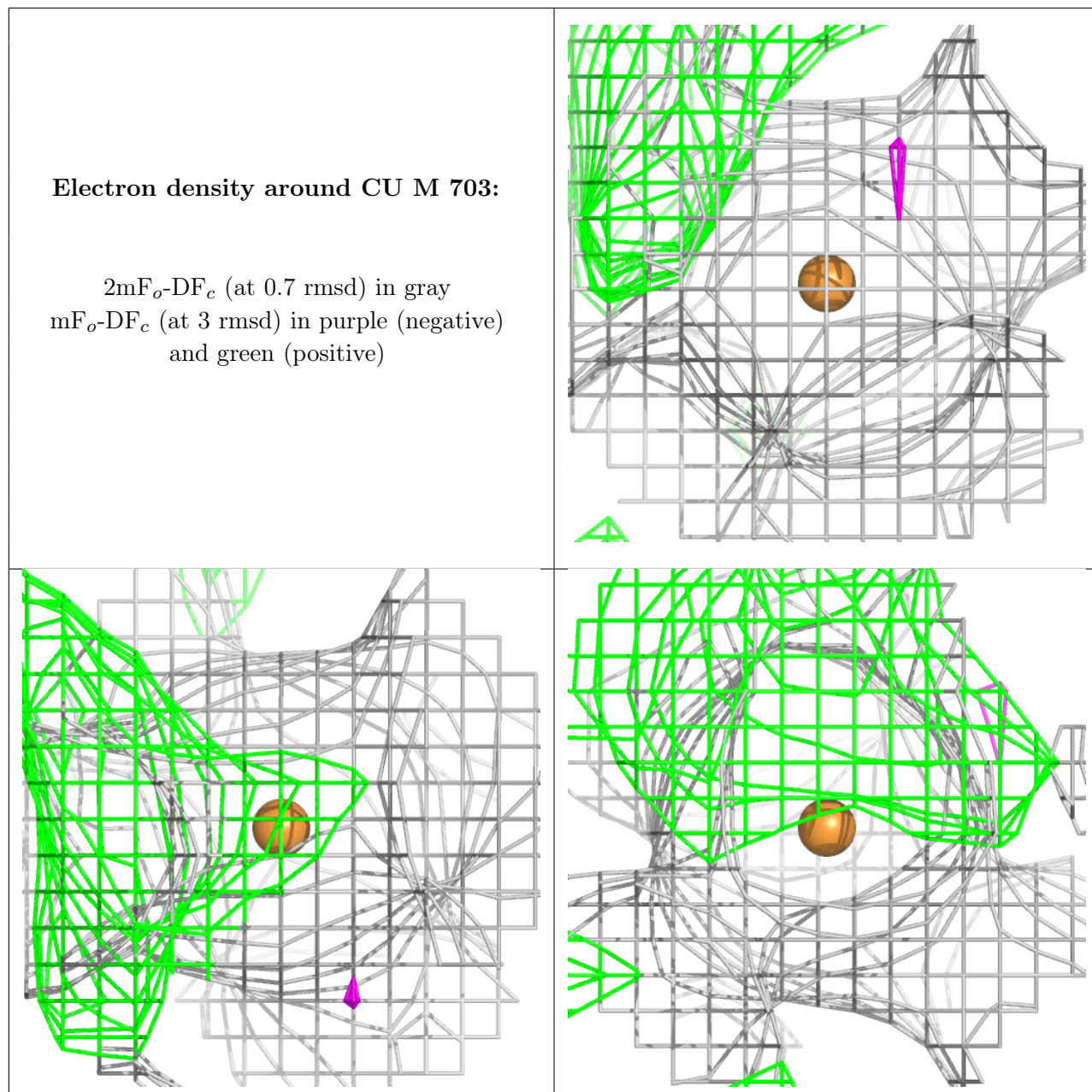
Electron density around CU J 603:

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



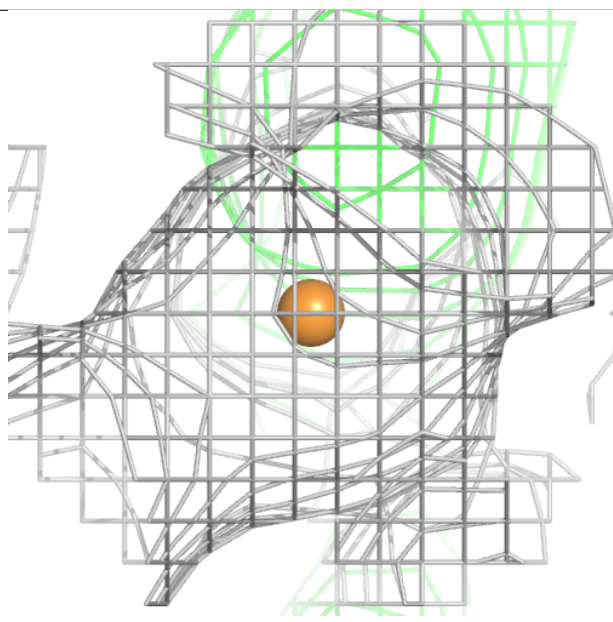
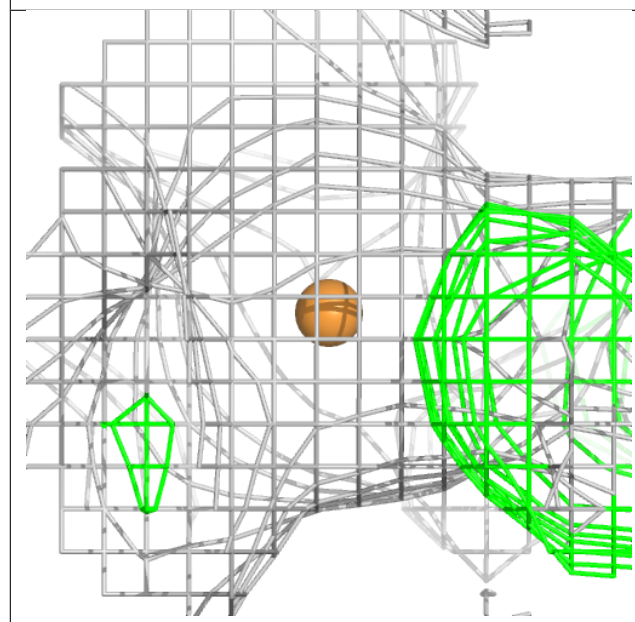
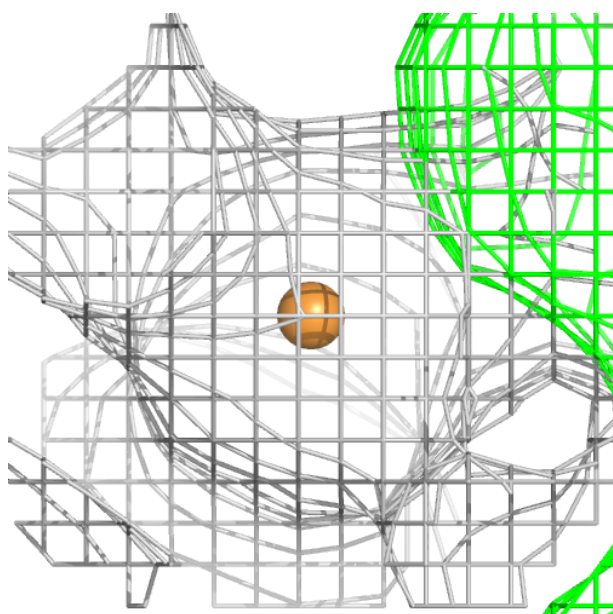
Electron density around CU M 703:

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



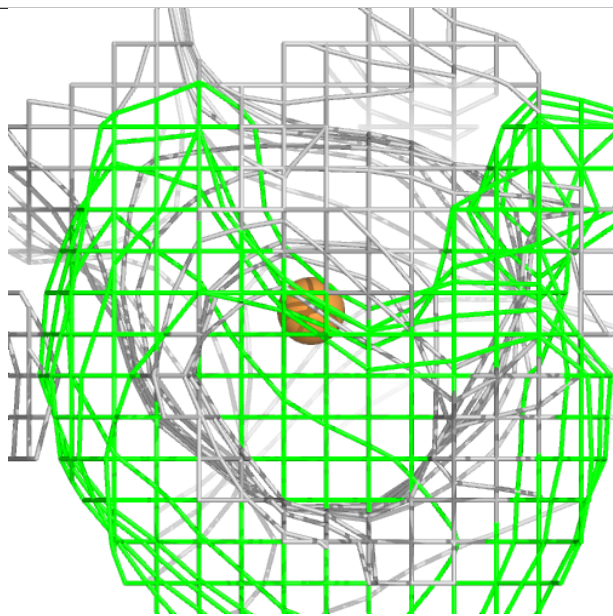
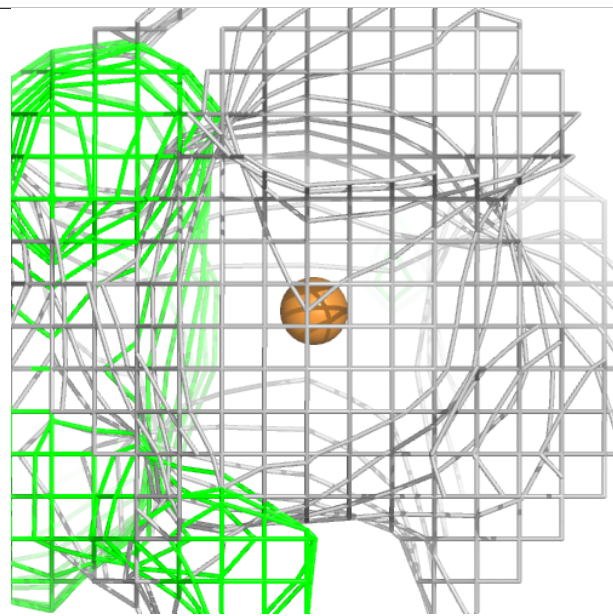
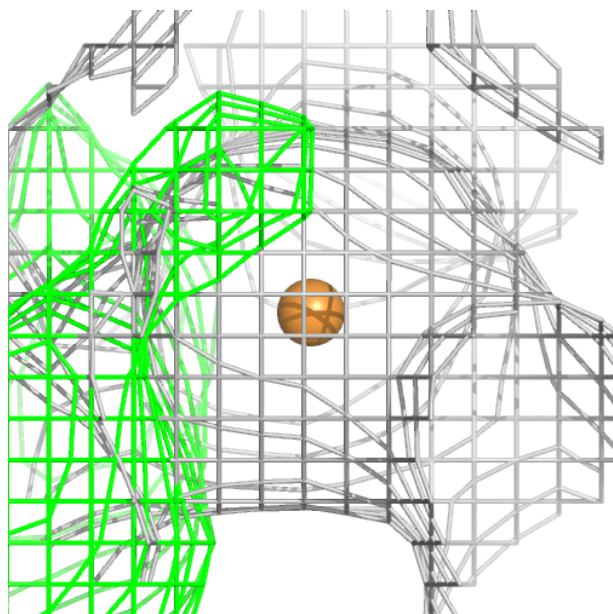
Electron density around CU P 704:

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



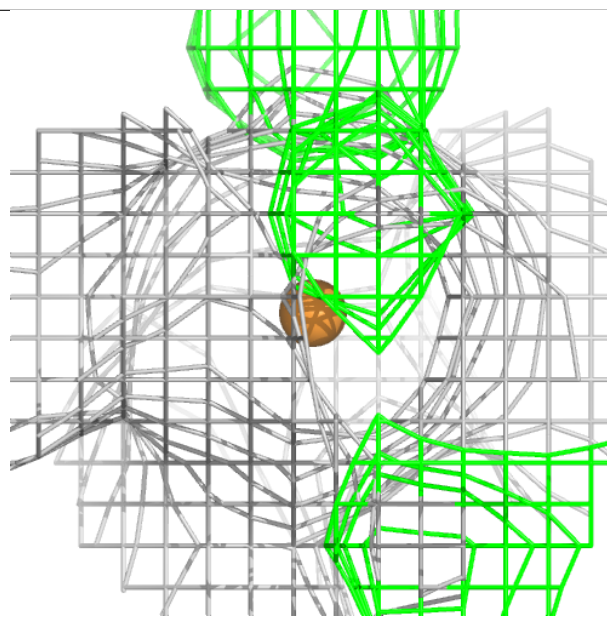
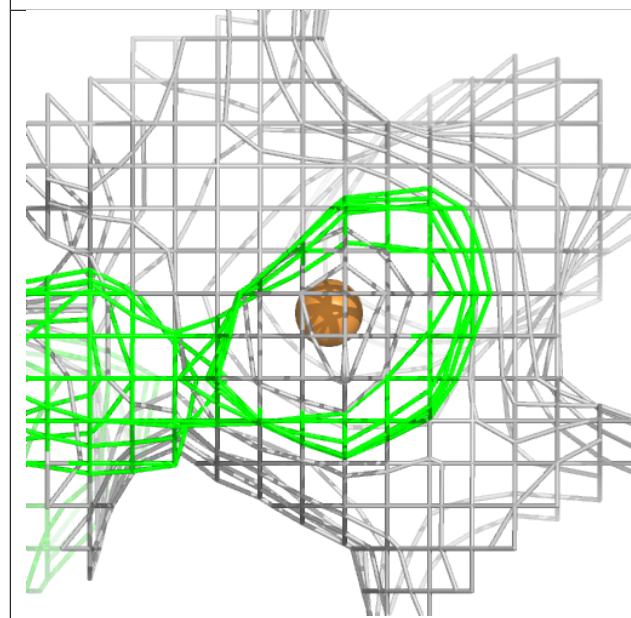
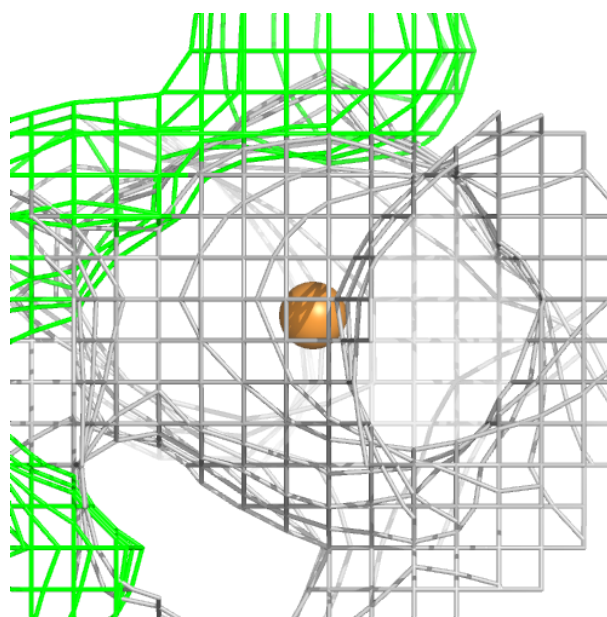
Electron density around CU S 603:

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



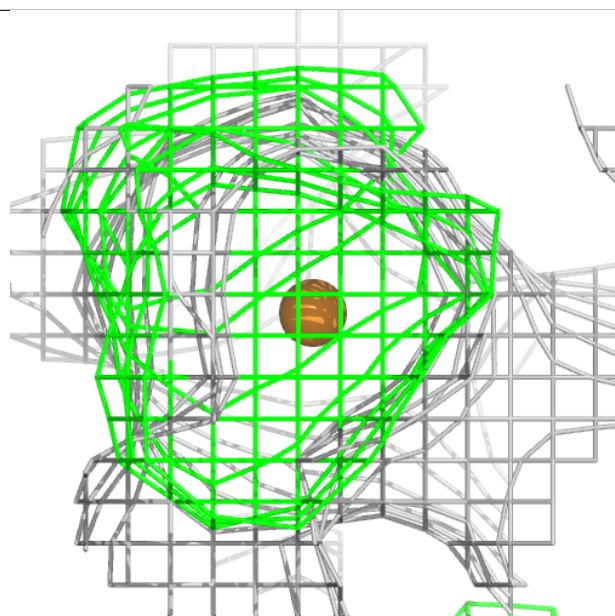
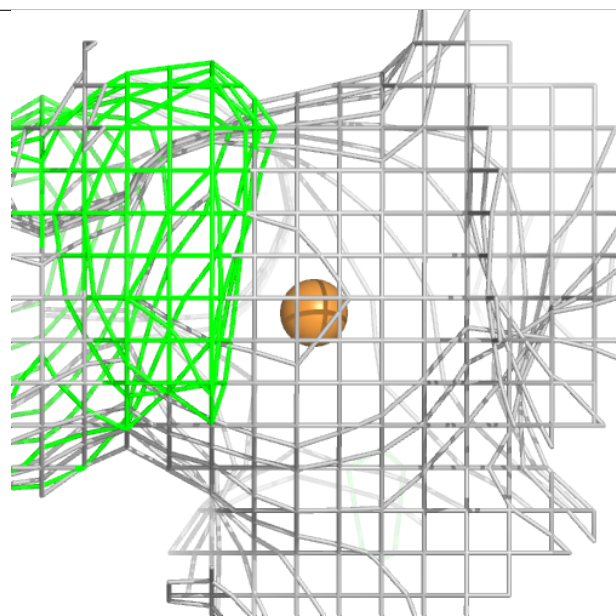
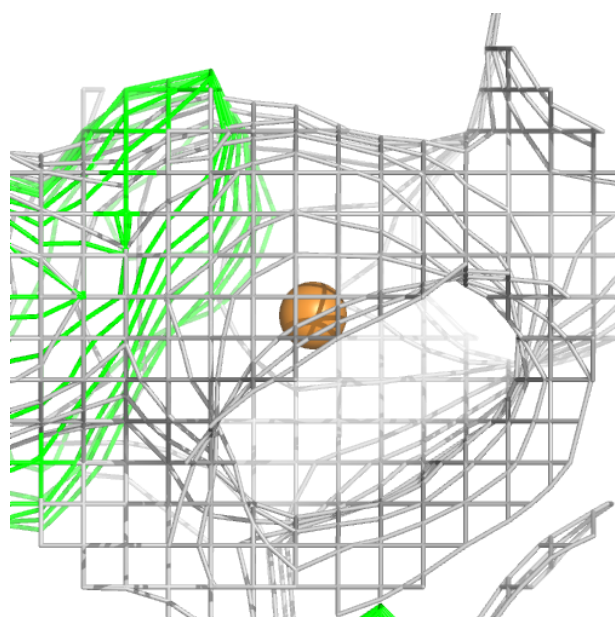
Electron density around CU Y 602:

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



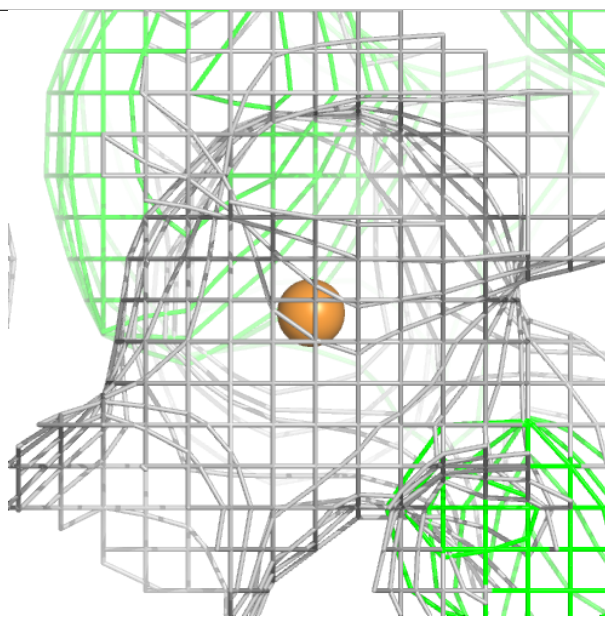
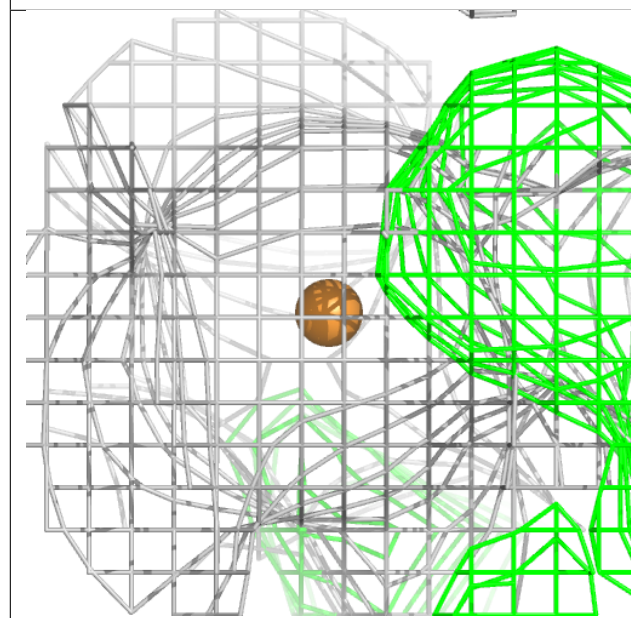
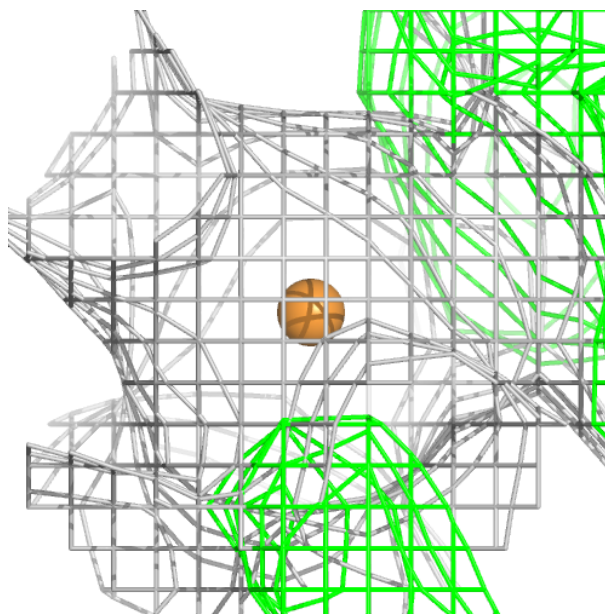
Electron density around CU Y 603:

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



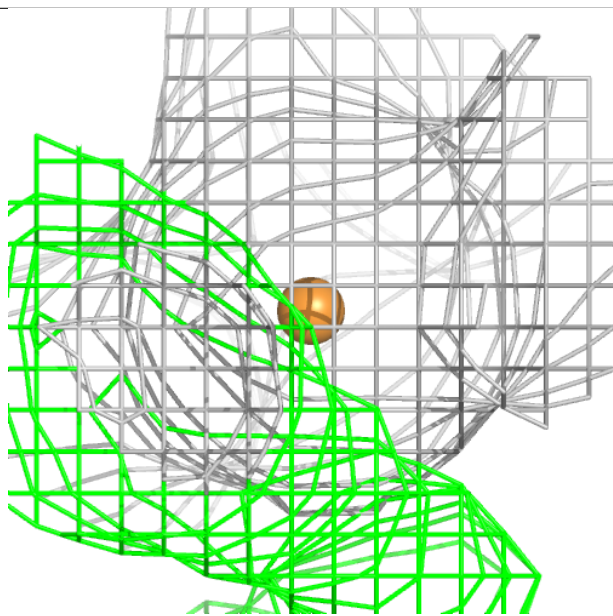
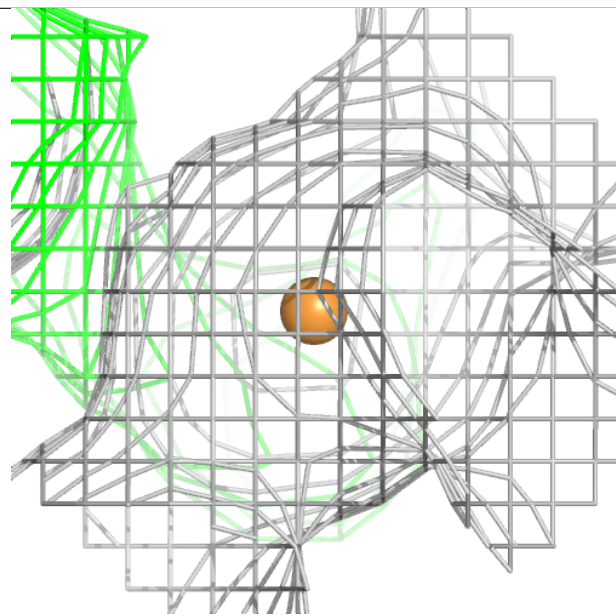
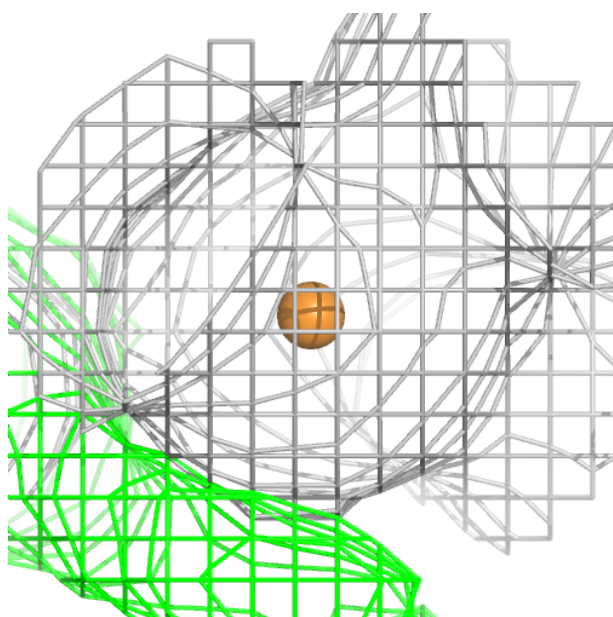
Electron density around CU 2 703:

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



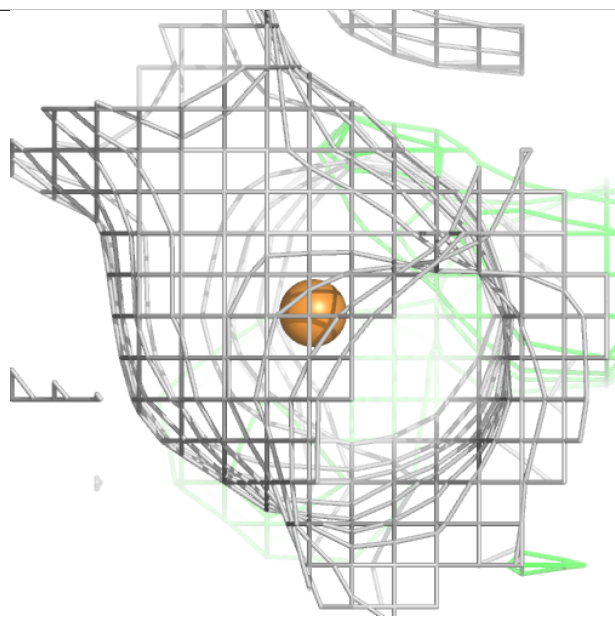
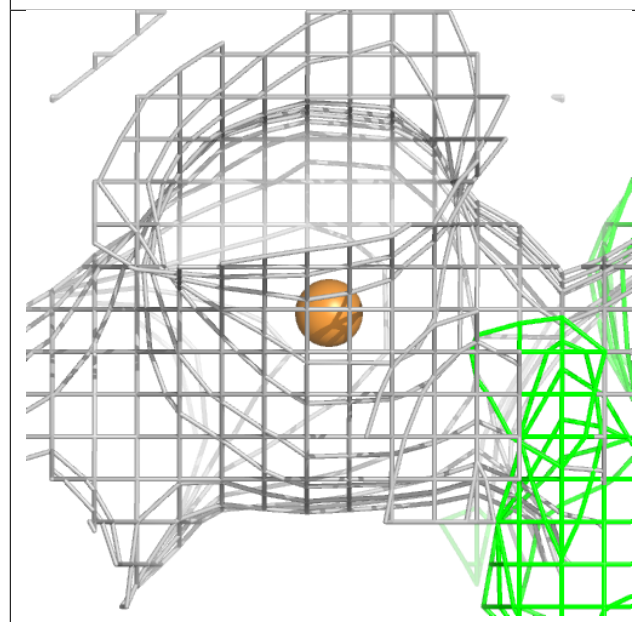
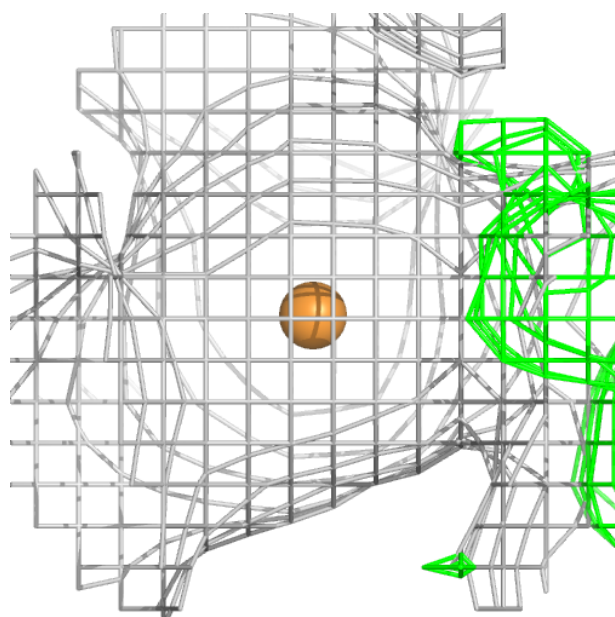
Electron density around CU 8 702:

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



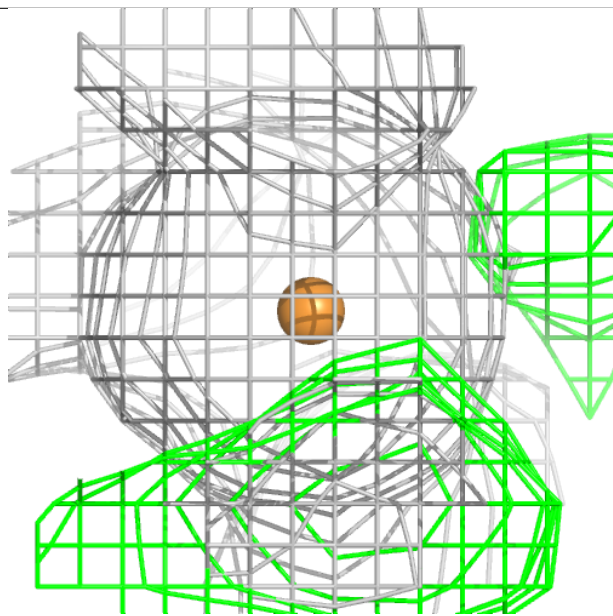
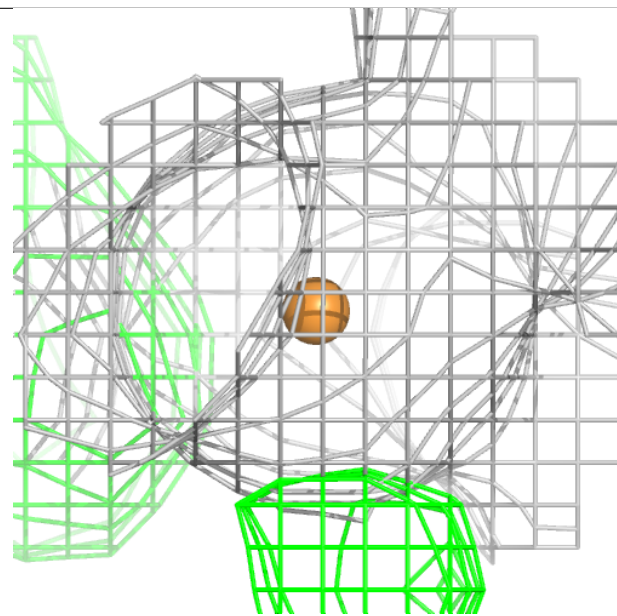
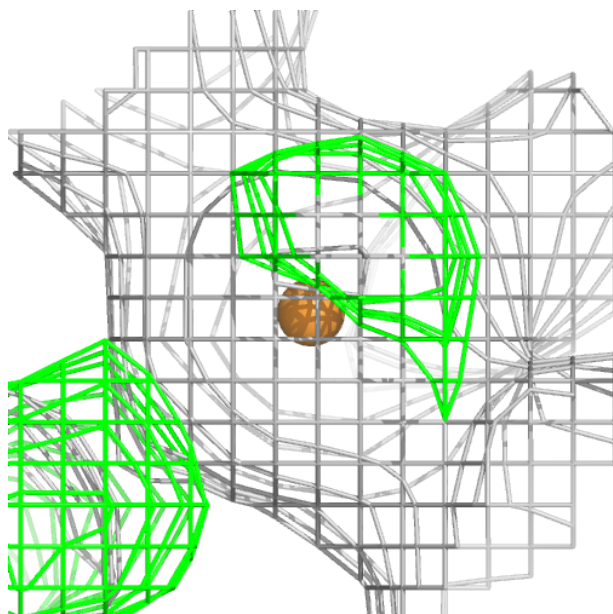
Electron density around CU k 703:

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



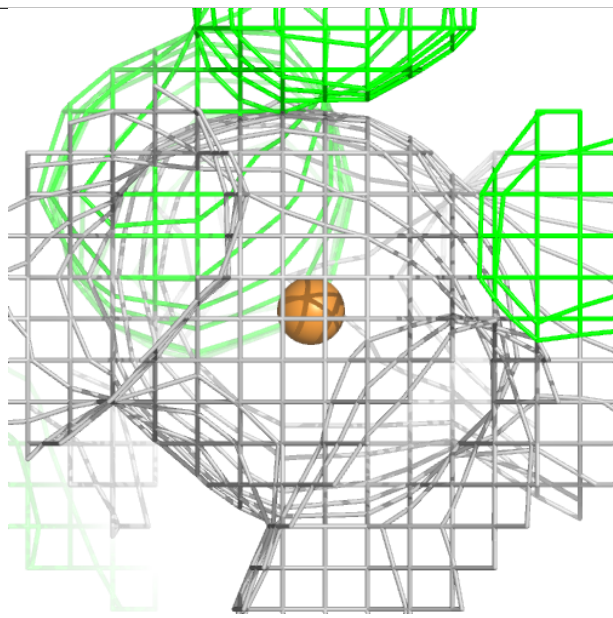
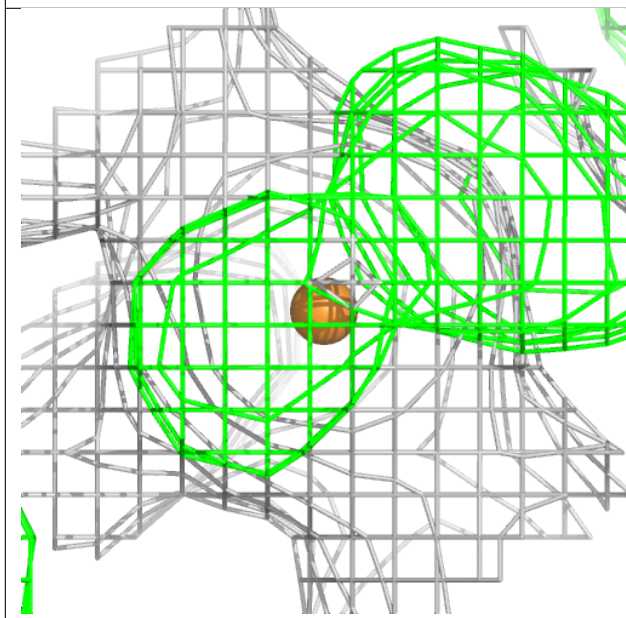
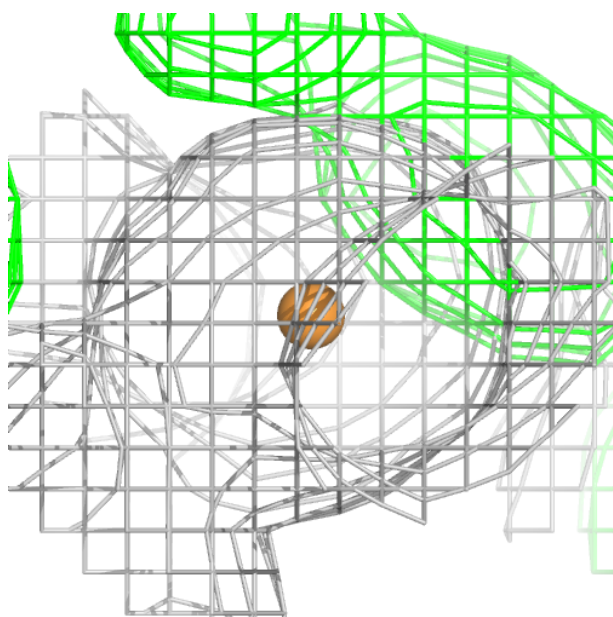
Electron density around CU A 703:

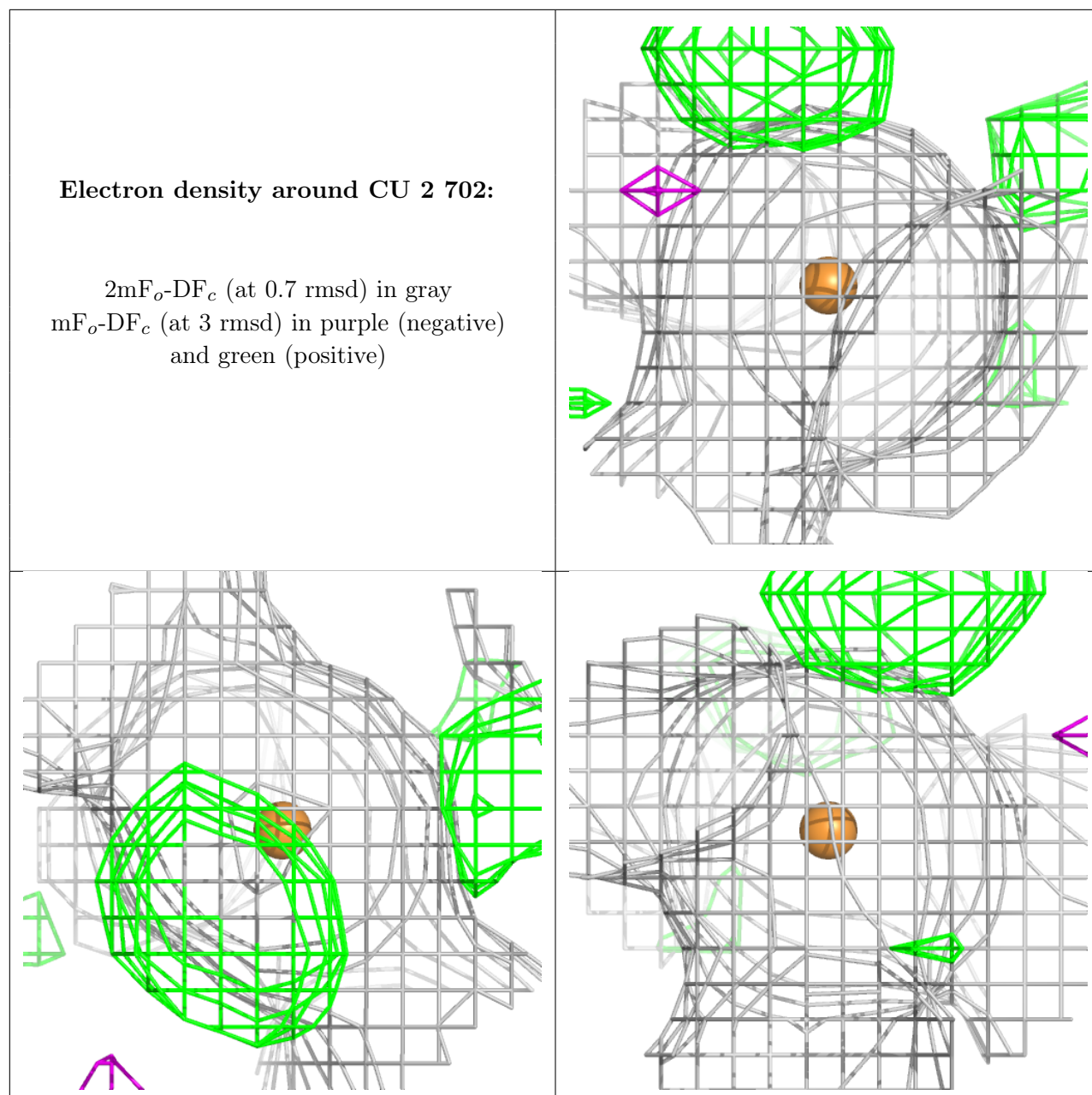
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CU P 703:

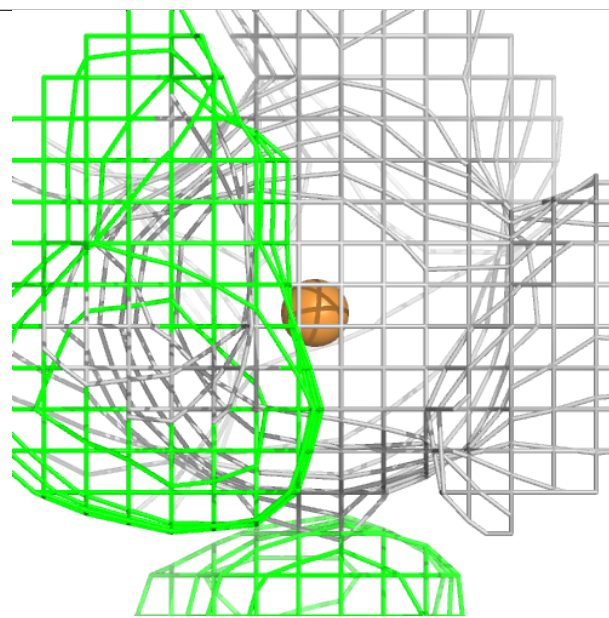
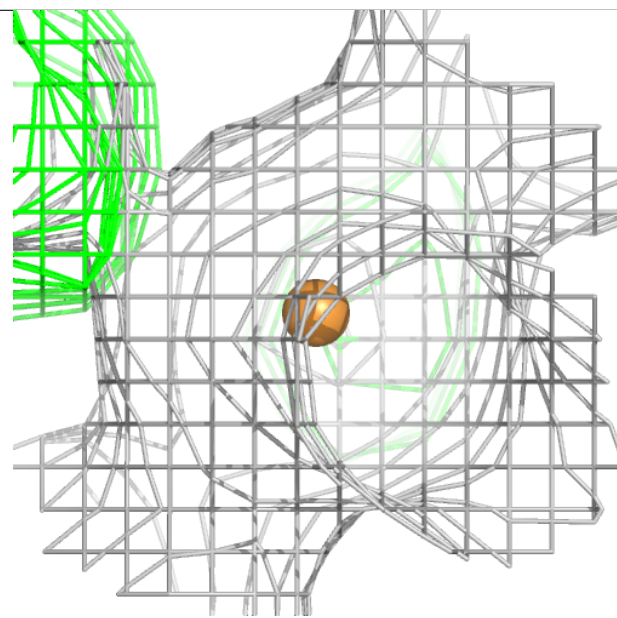
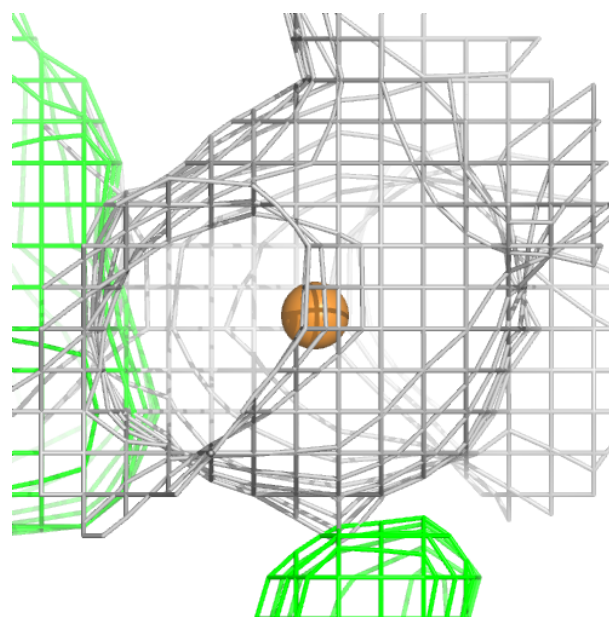
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





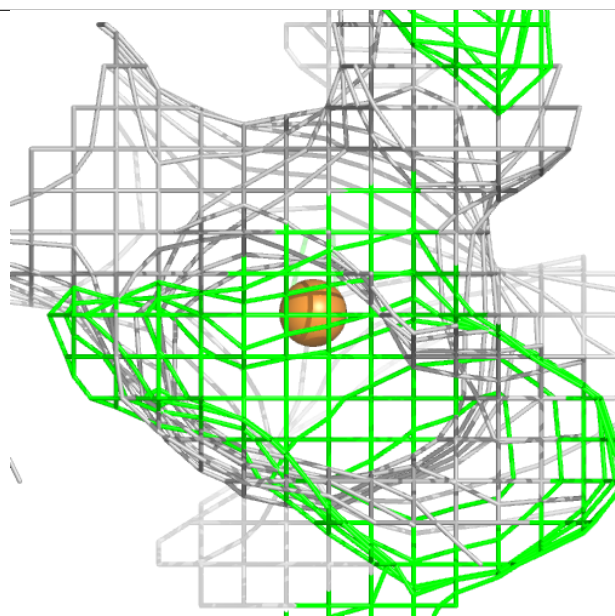
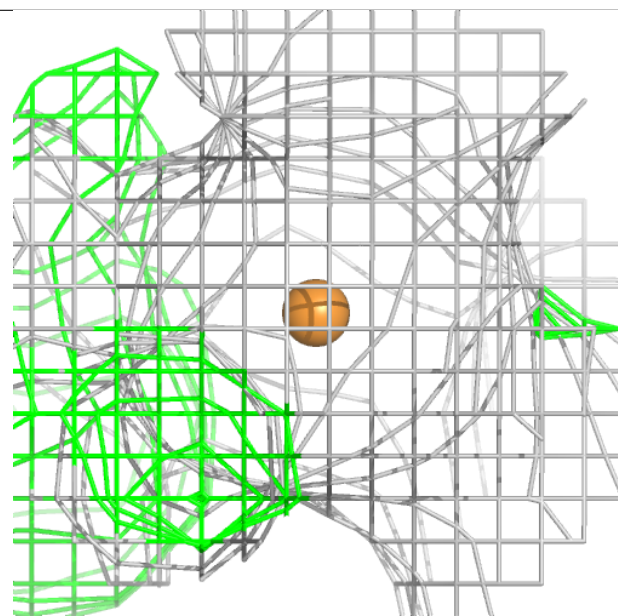
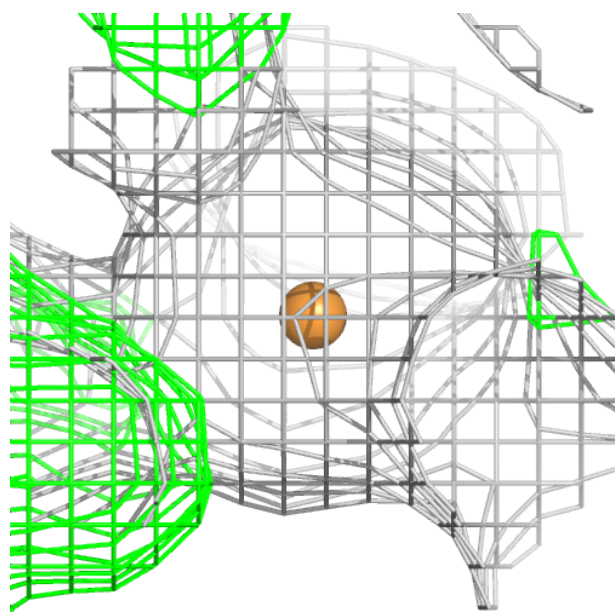
Electron density around CU 5 602:

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



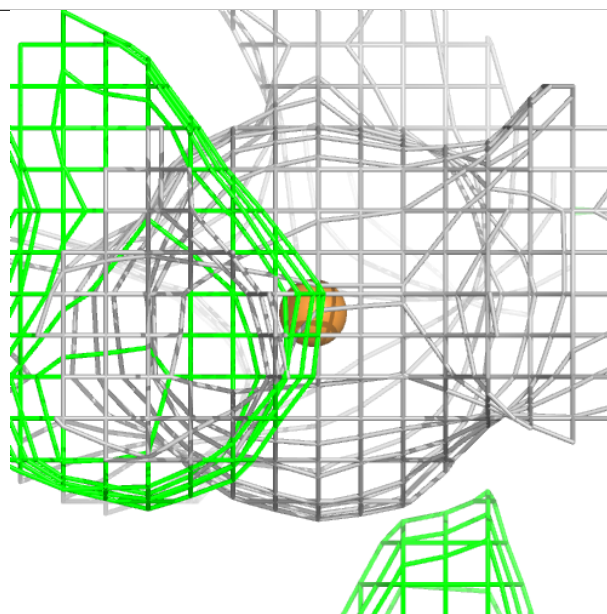
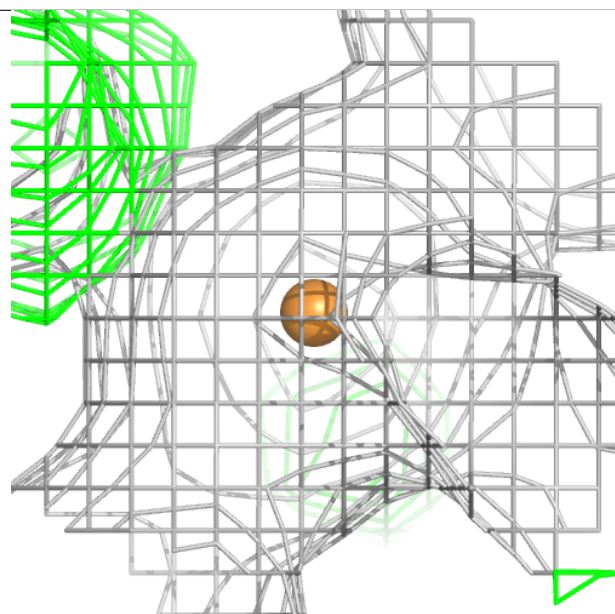
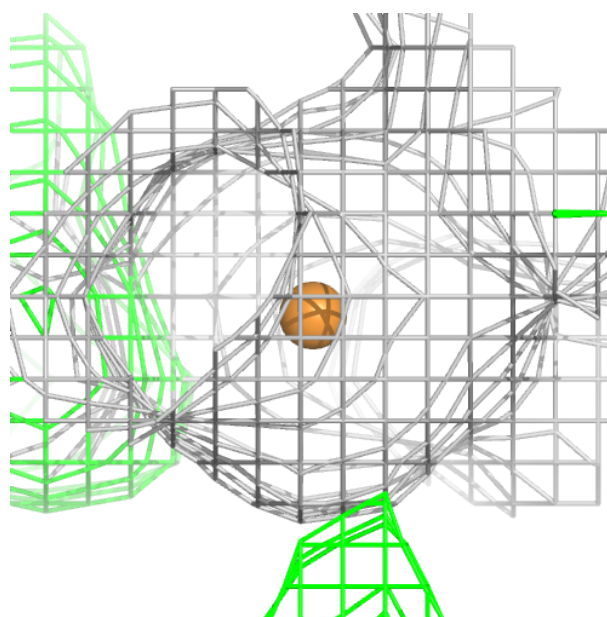
Electron density around CU 5 603:

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



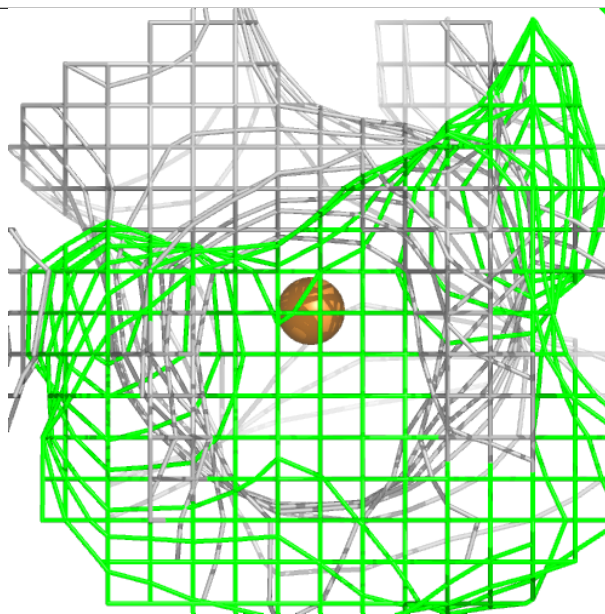
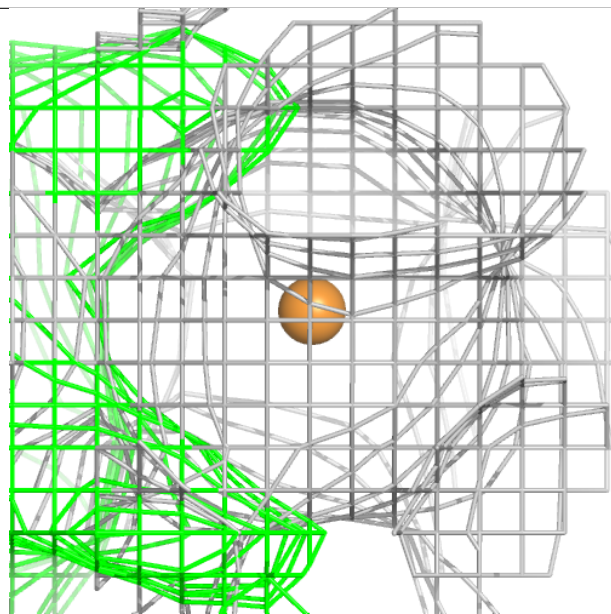
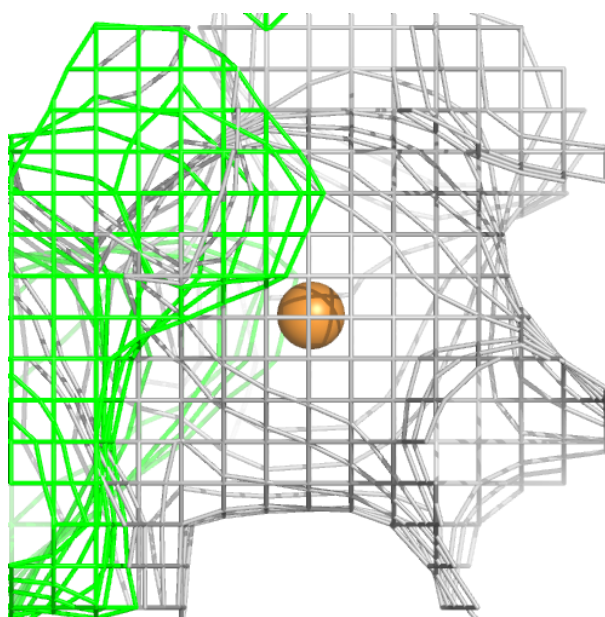
Electron density around CU S 602:

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



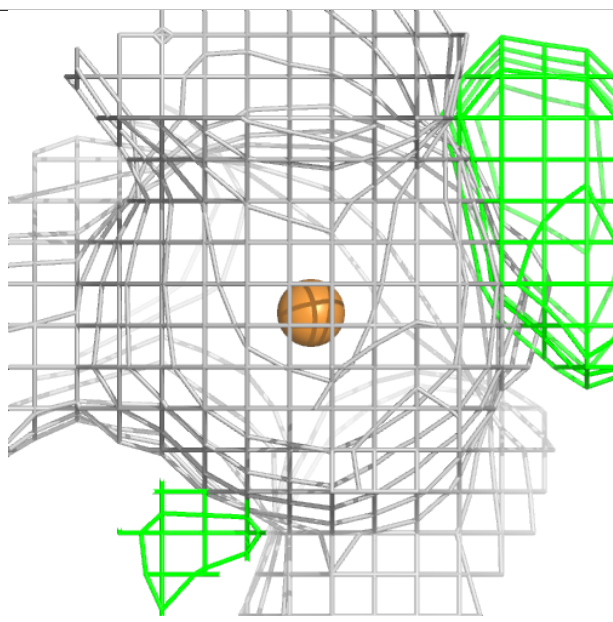
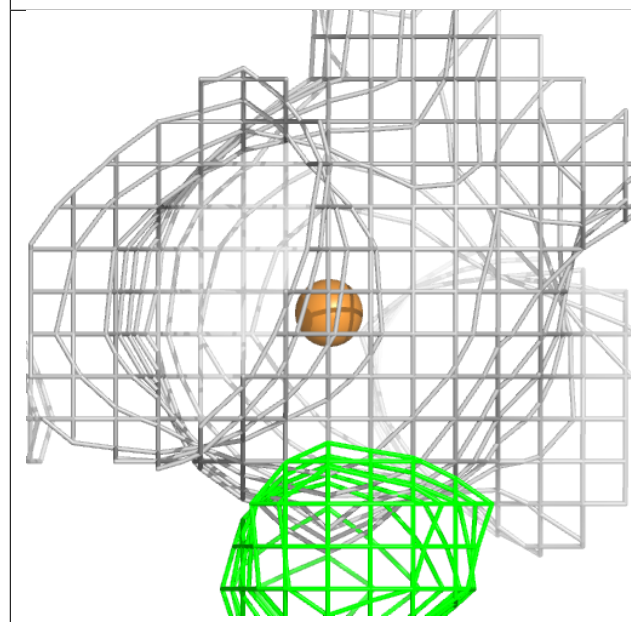
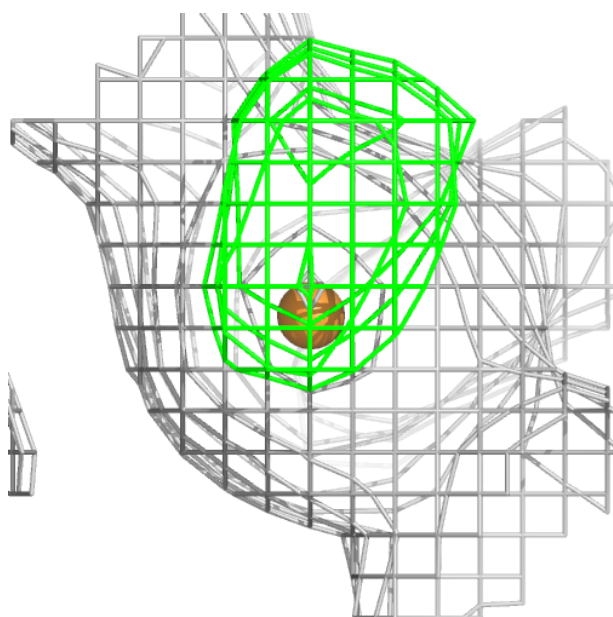
Electron density around CU 8 703:

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



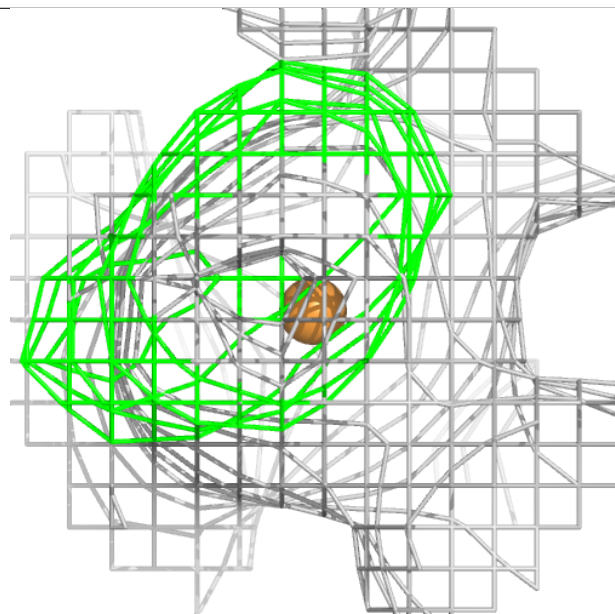
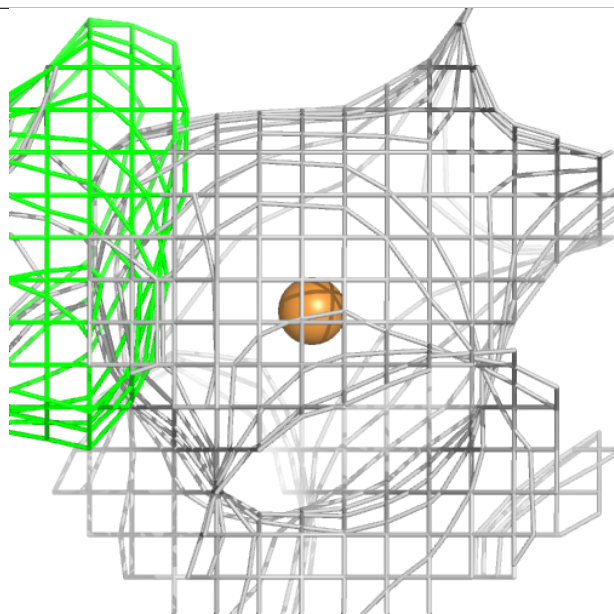
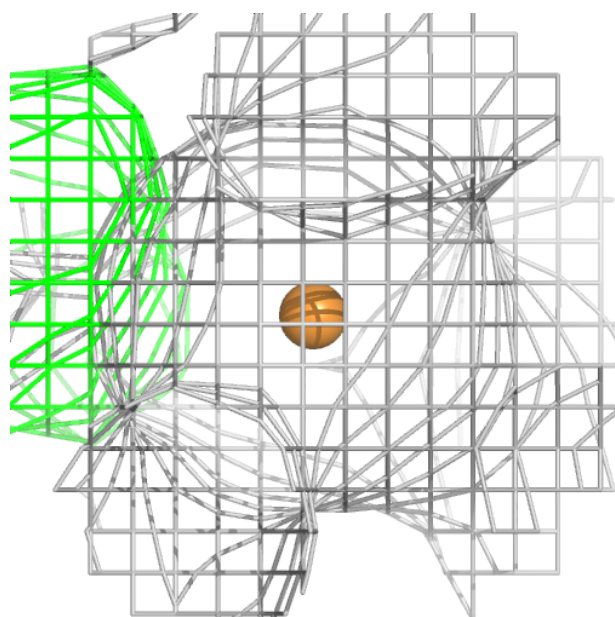
Electron density around CU x 602:

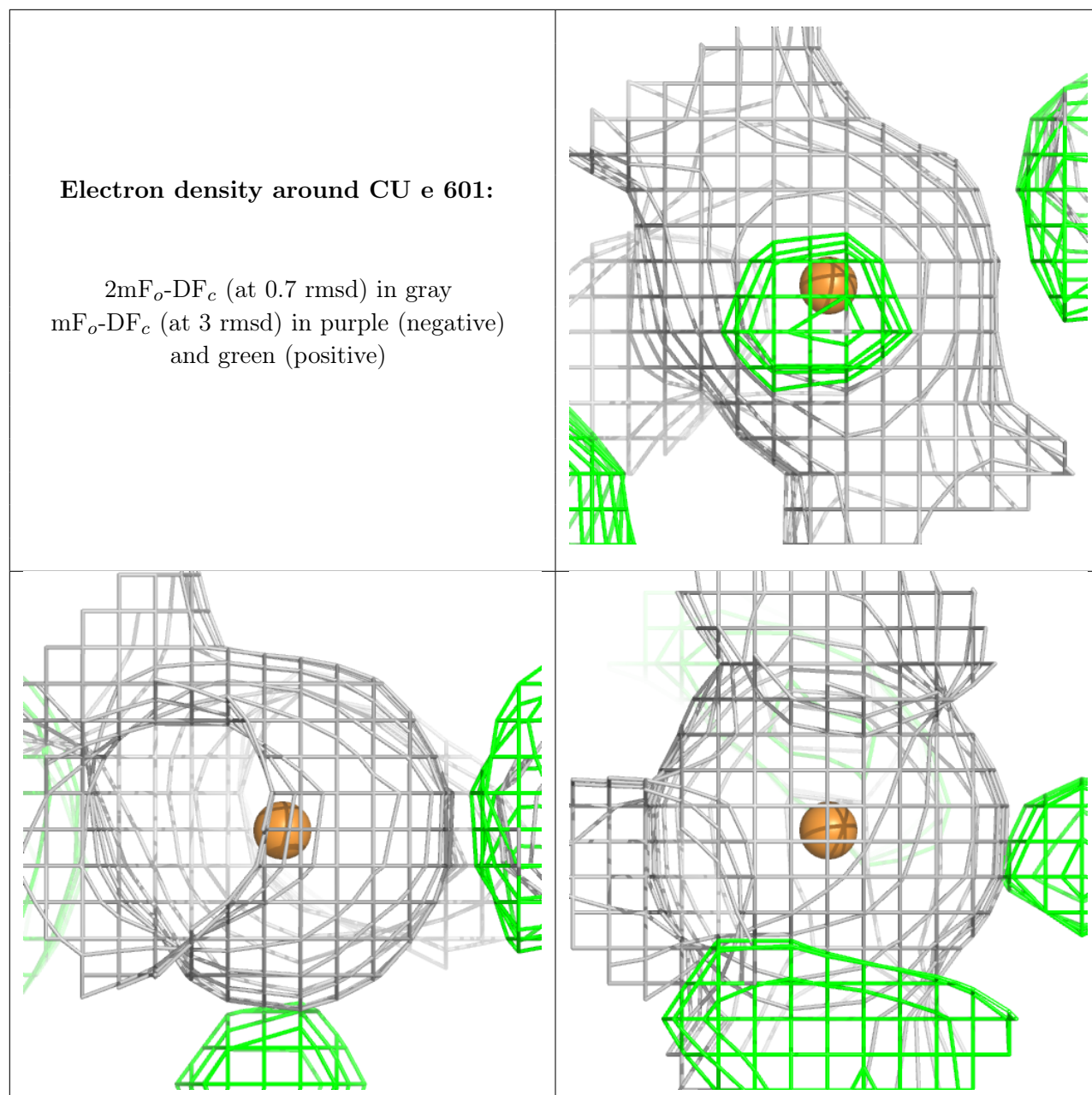
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

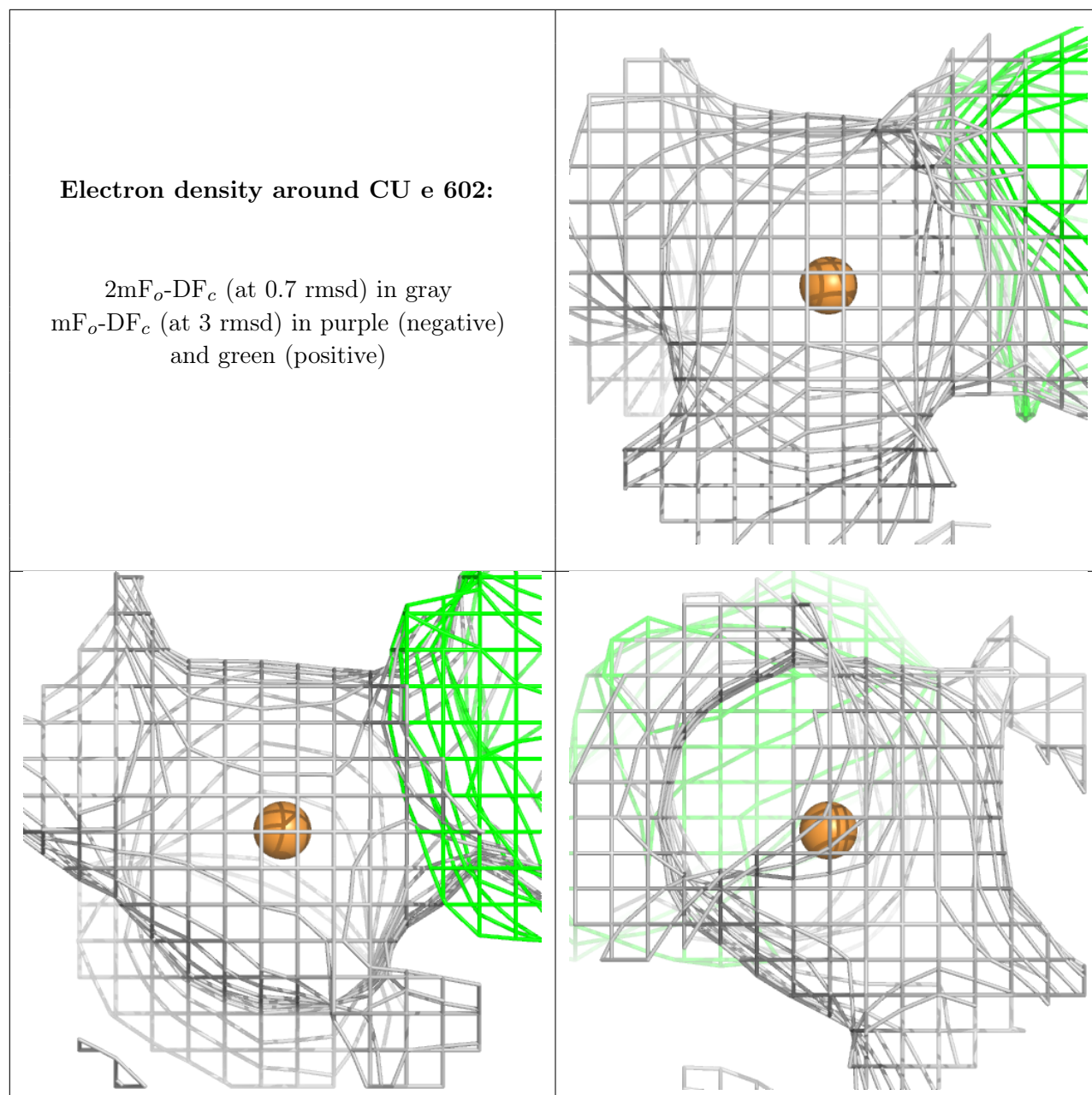


Electron density around CU x 603:

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

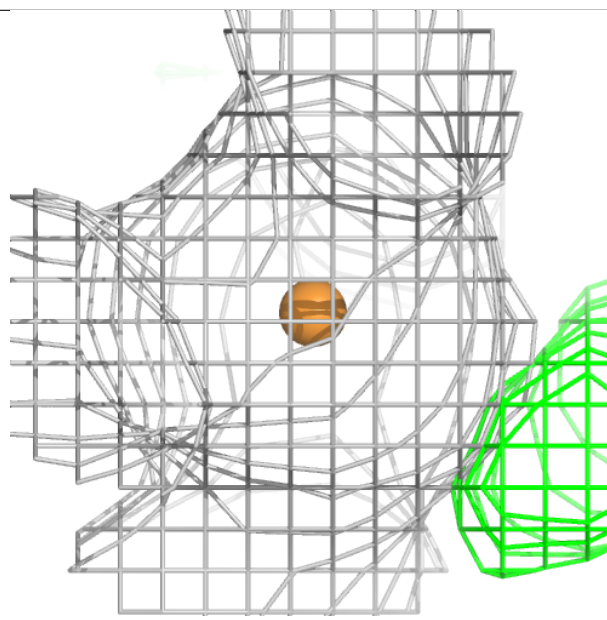
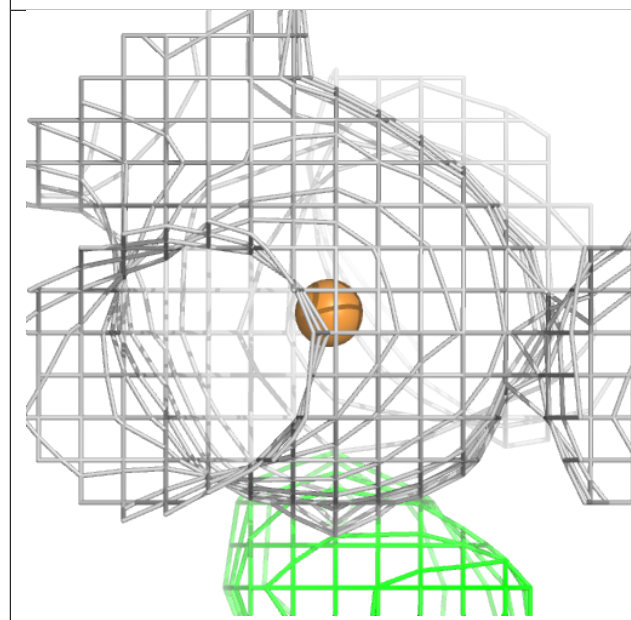
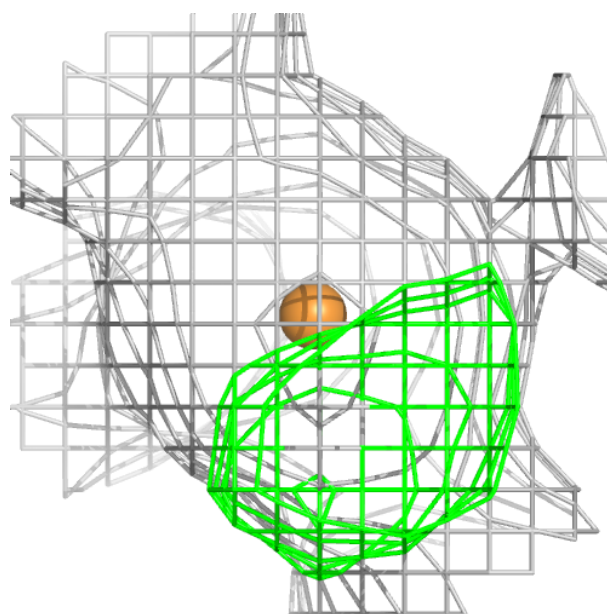






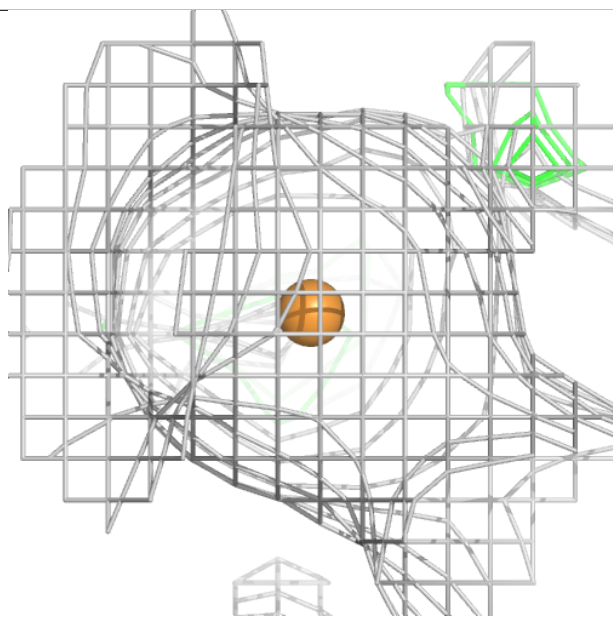
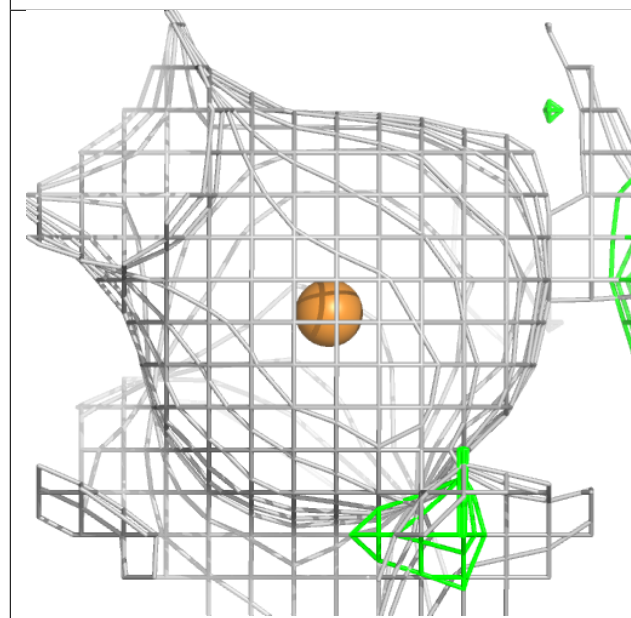
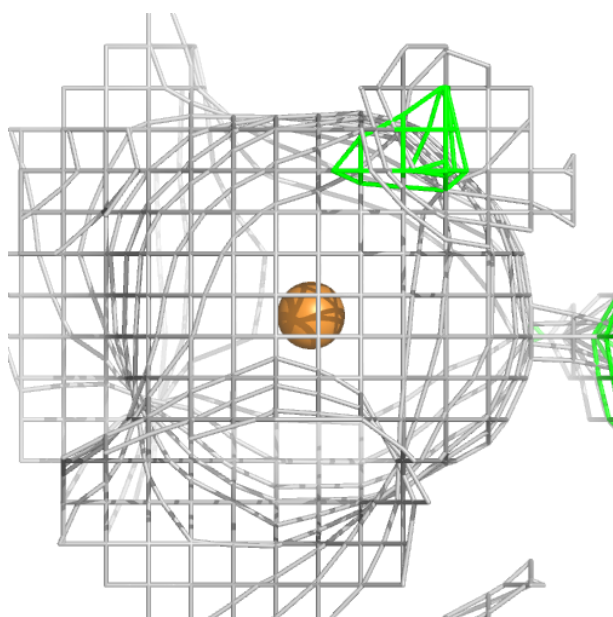
Electron density around CU h 602:

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



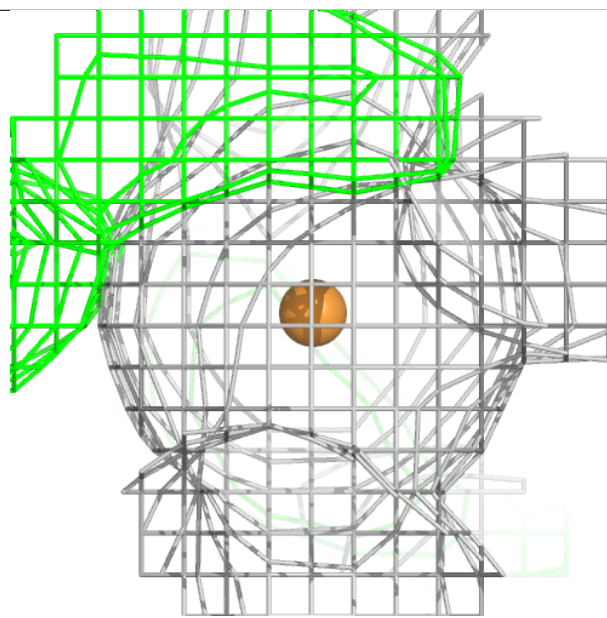
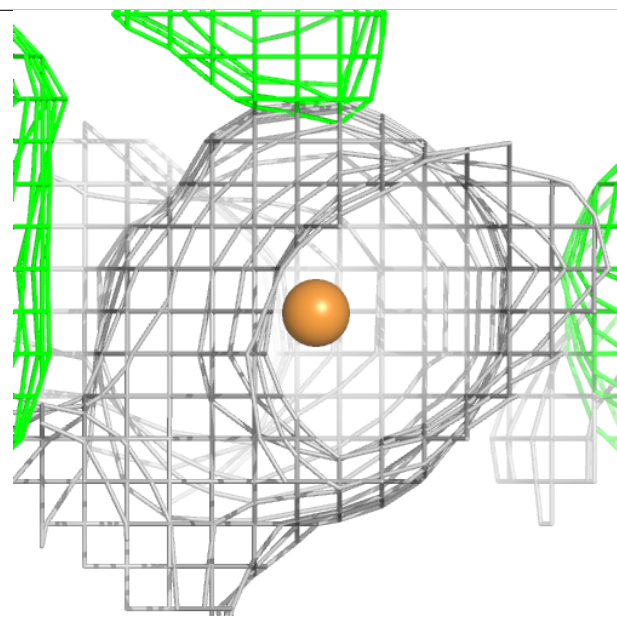
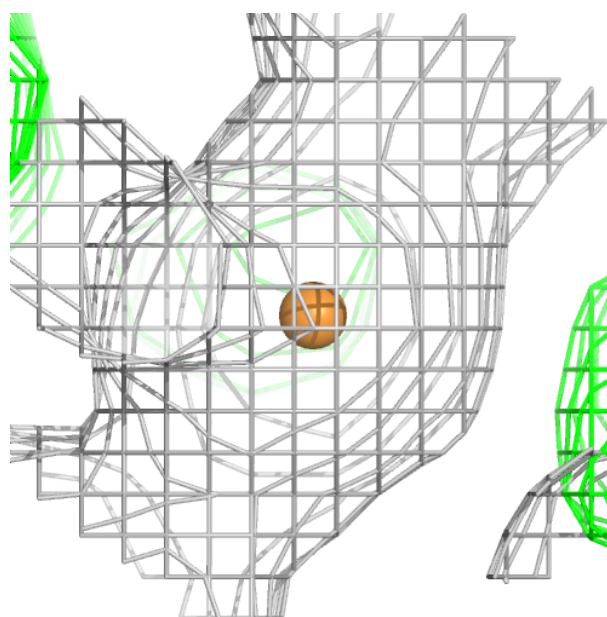
Electron density around CU h 603:

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



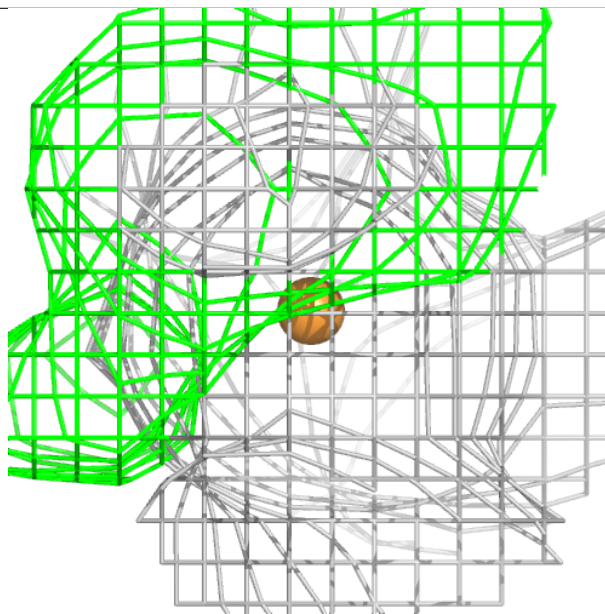
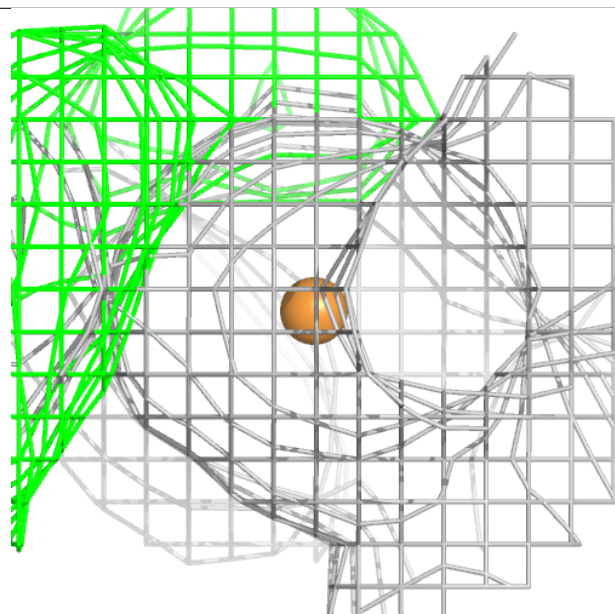
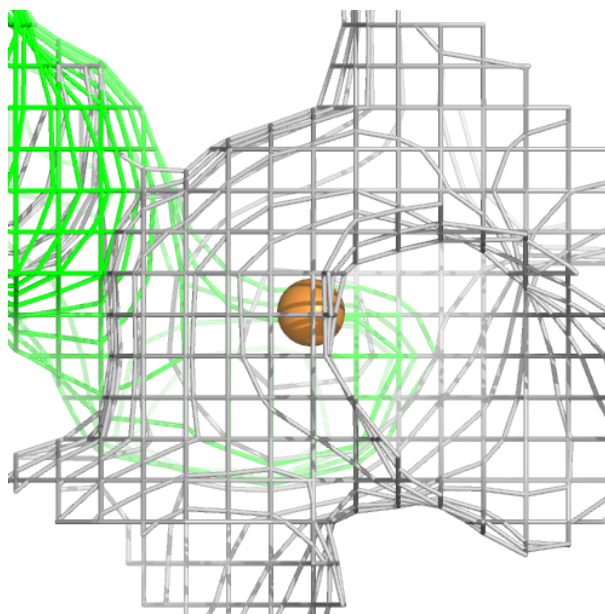
Electron density around CU k 702:

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



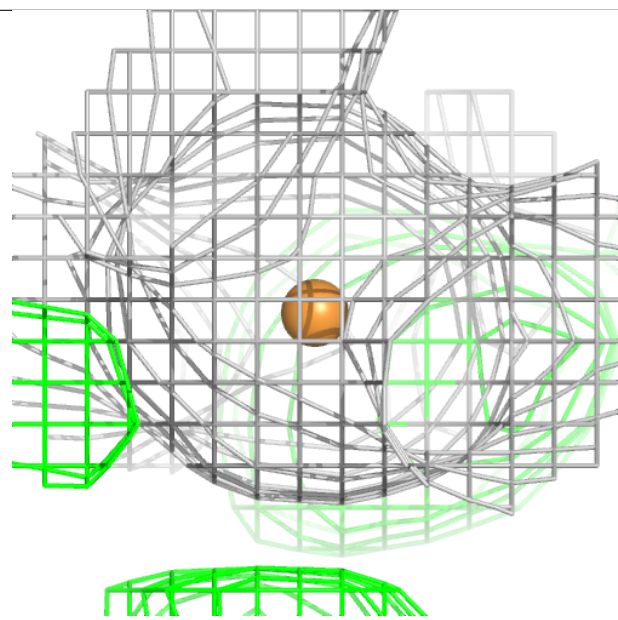
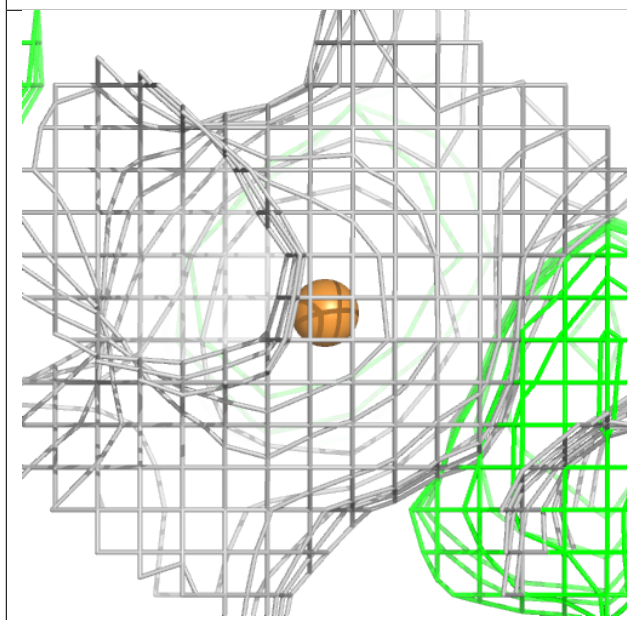
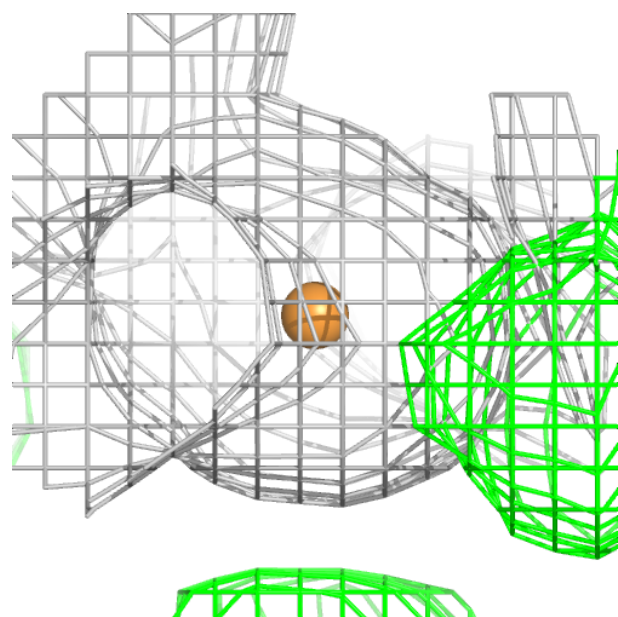
Electron density around CU G 702:

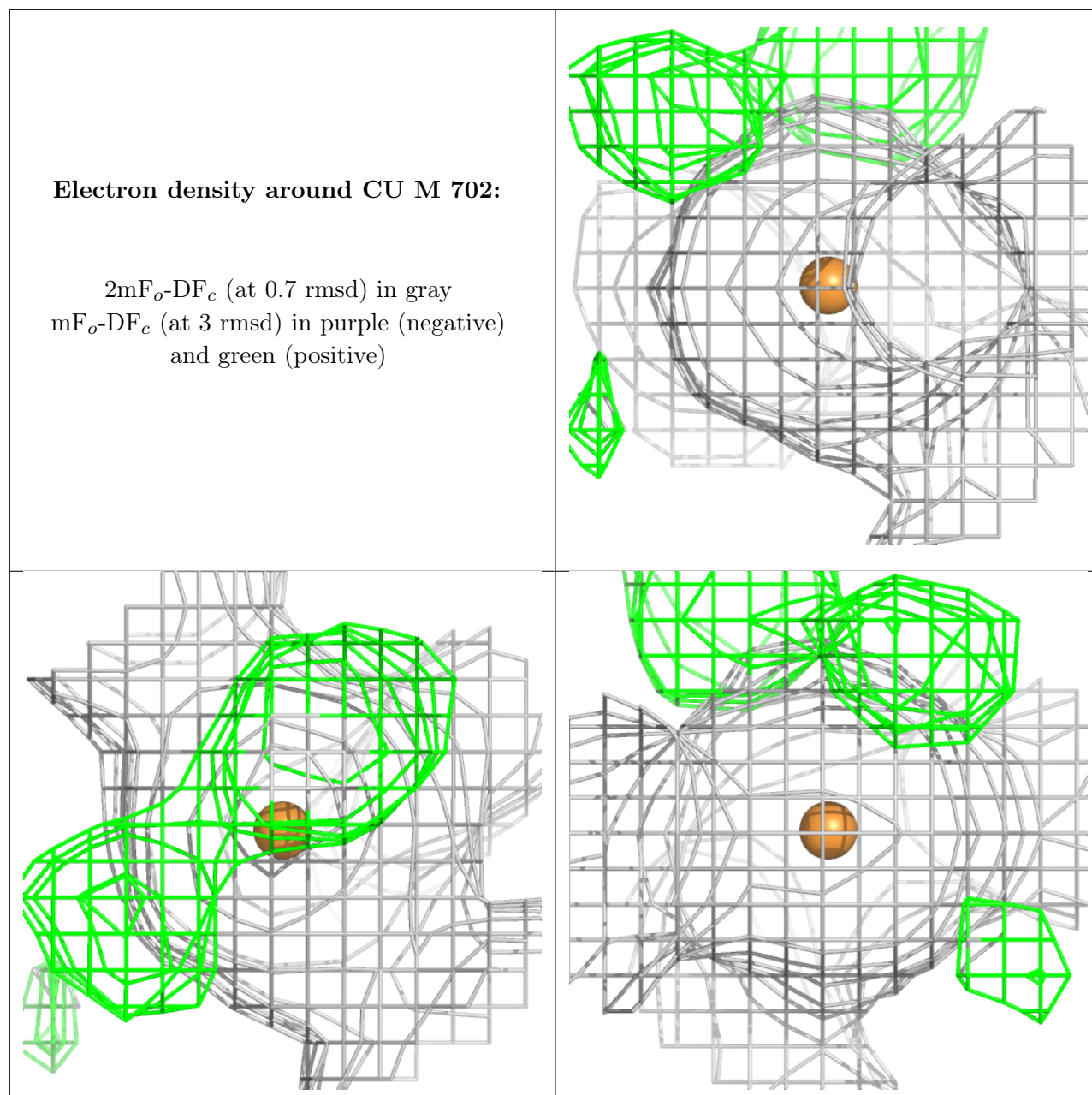
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CU V 602:

$2mF_o-DF_c$ (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.