



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 06:48 PM JST

PDB ID : 8Z59
Title : The X-Ray crystal structure of multicopper oxidase from Sulfurimonas sp.
Authors : Wang, Y.; Qian, H.
Deposited on : 2024-04-18
Resolution : 2.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

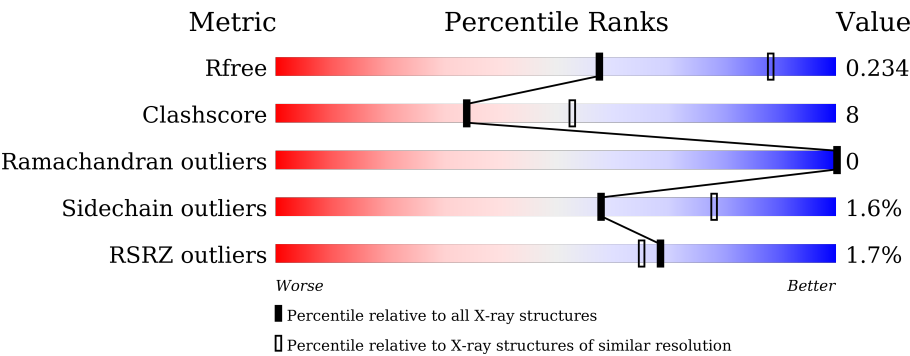
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div><div></div><div>73%13%13%</div></div>
1	B	514	<div><div>%</div><div>69%17%13%</div></div>
1	C	514	<div><div>%</div><div>72%15%13%</div></div>
1	D	514	<div><div>3%</div><div>66%20%13%</div></div>
1	E	514	<div><div>%</div><div>69%17%13%</div></div>
1	F	514	<div><div>2%</div><div>67%19%13%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	514	<div><div>2%</div><div><div></div><div>71%</div><div>16%</div><div>13%</div></div></div>
1	H	514	<div><div>3%</div><div><div></div><div>71%</div><div>15%</div><div>13%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29103 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 Bilirubin oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3584	2296	606	667	15			
1	B	445	Total	C	N	O	S	0	0	0
			3575	2291	605	664	15			
1	C	445	Total	C	N	O	S	0	0	0
			3575	2291	605	664	15			
1	D	446	Total	C	N	O	S	0	0	0
			3584	2296	606	667	15			
1	E	445	Total	C	N	O	S	0	0	0
			3575	2291	605	664	15			
1	F	445	Total	C	N	O	S	0	0	0
			3575	2291	605	664	15			
1	G	445	Total	C	N	O	S	0	0	0
			3575	2291	605	664	15			
1	H	446	Total	C	N	O	S	0	0	0
			3584	2296	606	667	15			

There are 272 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP A0A2K2VPI4
A	-17	GLY	-	expression tag	UNP A0A2K2VPI4
A	-16	SER	-	expression tag	UNP A0A2K2VPI4
A	-15	SER	-	expression tag	UNP A0A2K2VPI4
A	-14	HIS	-	expression tag	UNP A0A2K2VPI4
A	-13	HIS	-	expression tag	UNP A0A2K2VPI4
A	-12	HIS	-	expression tag	UNP A0A2K2VPI4
A	-11	HIS	-	expression tag	UNP A0A2K2VPI4
A	-10	HIS	-	expression tag	UNP A0A2K2VPI4
A	-9	HIS	-	expression tag	UNP A0A2K2VPI4
A	-8	SER	-	expression tag	UNP A0A2K2VPI4
A	-7	SER	-	expression tag	UNP A0A2K2VPI4
A	-6	GLY	-	expression tag	UNP A0A2K2VPI4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP A0A2K2VPI4
A	-4	VAL	-	expression tag	UNP A0A2K2VPI4
A	-3	PRO	-	expression tag	UNP A0A2K2VPI4
A	-2	ARG	-	expression tag	UNP A0A2K2VPI4
A	-1	GLY	-	expression tag	UNP A0A2K2VPI4
A	0	SER	-	expression tag	UNP A0A2K2VPI4
A	1	HIS	-	expression tag	UNP A0A2K2VPI4
A	2	MET	-	expression tag	UNP A0A2K2VPI4
A	3	ALA	-	expression tag	UNP A0A2K2VPI4
A	4	SER	-	expression tag	UNP A0A2K2VPI4
A	5	MET	-	expression tag	UNP A0A2K2VPI4
A	6	THR	-	expression tag	UNP A0A2K2VPI4
A	7	GLY	-	expression tag	UNP A0A2K2VPI4
A	8	GLY	-	expression tag	UNP A0A2K2VPI4
A	9	GLN	-	expression tag	UNP A0A2K2VPI4
A	10	GLN	-	expression tag	UNP A0A2K2VPI4
A	11	MET	-	expression tag	UNP A0A2K2VPI4
A	12	GLY	-	expression tag	UNP A0A2K2VPI4
A	13	ARG	-	expression tag	UNP A0A2K2VPI4
A	14	GLY	-	expression tag	UNP A0A2K2VPI4
A	15	SER	-	expression tag	UNP A0A2K2VPI4
B	-18	MET	-	initiating methionine	UNP A0A2K2VPI4
B	-17	GLY	-	expression tag	UNP A0A2K2VPI4
B	-16	SER	-	expression tag	UNP A0A2K2VPI4
B	-15	SER	-	expression tag	UNP A0A2K2VPI4
B	-14	HIS	-	expression tag	UNP A0A2K2VPI4
B	-13	HIS	-	expression tag	UNP A0A2K2VPI4
B	-12	HIS	-	expression tag	UNP A0A2K2VPI4
B	-11	HIS	-	expression tag	UNP A0A2K2VPI4
B	-10	HIS	-	expression tag	UNP A0A2K2VPI4
B	-9	HIS	-	expression tag	UNP A0A2K2VPI4
B	-8	SER	-	expression tag	UNP A0A2K2VPI4
B	-7	SER	-	expression tag	UNP A0A2K2VPI4
B	-6	GLY	-	expression tag	UNP A0A2K2VPI4
B	-5	LEU	-	expression tag	UNP A0A2K2VPI4
B	-4	VAL	-	expression tag	UNP A0A2K2VPI4
B	-3	PRO	-	expression tag	UNP A0A2K2VPI4
B	-2	ARG	-	expression tag	UNP A0A2K2VPI4
B	-1	GLY	-	expression tag	UNP A0A2K2VPI4
B	0	SER	-	expression tag	UNP A0A2K2VPI4
B	1	HIS	-	expression tag	UNP A0A2K2VPI4
B	2	MET	-	expression tag	UNP A0A2K2VPI4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	ALA	-	expression tag	UNP A0A2K2VPI4
B	4	SER	-	expression tag	UNP A0A2K2VPI4
B	5	MET	-	expression tag	UNP A0A2K2VPI4
B	6	THR	-	expression tag	UNP A0A2K2VPI4
B	7	GLY	-	expression tag	UNP A0A2K2VPI4
B	8	GLY	-	expression tag	UNP A0A2K2VPI4
B	9	GLN	-	expression tag	UNP A0A2K2VPI4
B	10	GLN	-	expression tag	UNP A0A2K2VPI4
B	11	MET	-	expression tag	UNP A0A2K2VPI4
B	12	GLY	-	expression tag	UNP A0A2K2VPI4
B	13	ARG	-	expression tag	UNP A0A2K2VPI4
B	14	GLY	-	expression tag	UNP A0A2K2VPI4
B	15	SER	-	expression tag	UNP A0A2K2VPI4
C	-18	MET	-	initiating methionine	UNP A0A2K2VPI4
C	-17	GLY	-	expression tag	UNP A0A2K2VPI4
C	-16	SER	-	expression tag	UNP A0A2K2VPI4
C	-15	SER	-	expression tag	UNP A0A2K2VPI4
C	-14	HIS	-	expression tag	UNP A0A2K2VPI4
C	-13	HIS	-	expression tag	UNP A0A2K2VPI4
C	-12	HIS	-	expression tag	UNP A0A2K2VPI4
C	-11	HIS	-	expression tag	UNP A0A2K2VPI4
C	-10	HIS	-	expression tag	UNP A0A2K2VPI4
C	-9	HIS	-	expression tag	UNP A0A2K2VPI4
C	-8	SER	-	expression tag	UNP A0A2K2VPI4
C	-7	SER	-	expression tag	UNP A0A2K2VPI4
C	-6	GLY	-	expression tag	UNP A0A2K2VPI4
C	-5	LEU	-	expression tag	UNP A0A2K2VPI4
C	-4	VAL	-	expression tag	UNP A0A2K2VPI4
C	-3	PRO	-	expression tag	UNP A0A2K2VPI4
C	-2	ARG	-	expression tag	UNP A0A2K2VPI4
C	-1	GLY	-	expression tag	UNP A0A2K2VPI4
C	0	SER	-	expression tag	UNP A0A2K2VPI4
C	1	HIS	-	expression tag	UNP A0A2K2VPI4
C	2	MET	-	expression tag	UNP A0A2K2VPI4
C	3	ALA	-	expression tag	UNP A0A2K2VPI4
C	4	SER	-	expression tag	UNP A0A2K2VPI4
C	5	MET	-	expression tag	UNP A0A2K2VPI4
C	6	THR	-	expression tag	UNP A0A2K2VPI4
C	7	GLY	-	expression tag	UNP A0A2K2VPI4
C	8	GLY	-	expression tag	UNP A0A2K2VPI4
C	9	GLN	-	expression tag	UNP A0A2K2VPI4
C	10	GLN	-	expression tag	UNP A0A2K2VPI4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	11	MET	-	expression tag	UNP A0A2K2VPI4
C	12	GLY	-	expression tag	UNP A0A2K2VPI4
C	13	ARG	-	expression tag	UNP A0A2K2VPI4
C	14	GLY	-	expression tag	UNP A0A2K2VPI4
C	15	SER	-	expression tag	UNP A0A2K2VPI4
D	-18	MET	-	initiating methionine	UNP A0A2K2VPI4
D	-17	GLY	-	expression tag	UNP A0A2K2VPI4
D	-16	SER	-	expression tag	UNP A0A2K2VPI4
D	-15	SER	-	expression tag	UNP A0A2K2VPI4
D	-14	HIS	-	expression tag	UNP A0A2K2VPI4
D	-13	HIS	-	expression tag	UNP A0A2K2VPI4
D	-12	HIS	-	expression tag	UNP A0A2K2VPI4
D	-11	HIS	-	expression tag	UNP A0A2K2VPI4
D	-10	HIS	-	expression tag	UNP A0A2K2VPI4
D	-9	HIS	-	expression tag	UNP A0A2K2VPI4
D	-8	SER	-	expression tag	UNP A0A2K2VPI4
D	-7	SER	-	expression tag	UNP A0A2K2VPI4
D	-6	GLY	-	expression tag	UNP A0A2K2VPI4
D	-5	LEU	-	expression tag	UNP A0A2K2VPI4
D	-4	VAL	-	expression tag	UNP A0A2K2VPI4
D	-3	PRO	-	expression tag	UNP A0A2K2VPI4
D	-2	ARG	-	expression tag	UNP A0A2K2VPI4
D	-1	GLY	-	expression tag	UNP A0A2K2VPI4
D	0	SER	-	expression tag	UNP A0A2K2VPI4
D	1	HIS	-	expression tag	UNP A0A2K2VPI4
D	2	MET	-	expression tag	UNP A0A2K2VPI4
D	3	ALA	-	expression tag	UNP A0A2K2VPI4
D	4	SER	-	expression tag	UNP A0A2K2VPI4
D	5	MET	-	expression tag	UNP A0A2K2VPI4
D	6	THR	-	expression tag	UNP A0A2K2VPI4
D	7	GLY	-	expression tag	UNP A0A2K2VPI4
D	8	GLY	-	expression tag	UNP A0A2K2VPI4
D	9	GLN	-	expression tag	UNP A0A2K2VPI4
D	10	GLN	-	expression tag	UNP A0A2K2VPI4
D	11	MET	-	expression tag	UNP A0A2K2VPI4
D	12	GLY	-	expression tag	UNP A0A2K2VPI4
D	13	ARG	-	expression tag	UNP A0A2K2VPI4
D	14	GLY	-	expression tag	UNP A0A2K2VPI4
D	15	SER	-	expression tag	UNP A0A2K2VPI4
E	-18	MET	-	initiating methionine	UNP A0A2K2VPI4
E	-17	GLY	-	expression tag	UNP A0A2K2VPI4
E	-16	SER	-	expression tag	UNP A0A2K2VPI4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	SER	-	expression tag	UNP A0A2K2VPI4
E	-14	HIS	-	expression tag	UNP A0A2K2VPI4
E	-13	HIS	-	expression tag	UNP A0A2K2VPI4
E	-12	HIS	-	expression tag	UNP A0A2K2VPI4
E	-11	HIS	-	expression tag	UNP A0A2K2VPI4
E	-10	HIS	-	expression tag	UNP A0A2K2VPI4
E	-9	HIS	-	expression tag	UNP A0A2K2VPI4
E	-8	SER	-	expression tag	UNP A0A2K2VPI4
E	-7	SER	-	expression tag	UNP A0A2K2VPI4
E	-6	GLY	-	expression tag	UNP A0A2K2VPI4
E	-5	LEU	-	expression tag	UNP A0A2K2VPI4
E	-4	VAL	-	expression tag	UNP A0A2K2VPI4
E	-3	PRO	-	expression tag	UNP A0A2K2VPI4
E	-2	ARG	-	expression tag	UNP A0A2K2VPI4
E	-1	GLY	-	expression tag	UNP A0A2K2VPI4
E	0	SER	-	expression tag	UNP A0A2K2VPI4
E	1	HIS	-	expression tag	UNP A0A2K2VPI4
E	2	MET	-	expression tag	UNP A0A2K2VPI4
E	3	ALA	-	expression tag	UNP A0A2K2VPI4
E	4	SER	-	expression tag	UNP A0A2K2VPI4
E	5	MET	-	expression tag	UNP A0A2K2VPI4
E	6	THR	-	expression tag	UNP A0A2K2VPI4
E	7	GLY	-	expression tag	UNP A0A2K2VPI4
E	8	GLY	-	expression tag	UNP A0A2K2VPI4
E	9	GLN	-	expression tag	UNP A0A2K2VPI4
E	10	GLN	-	expression tag	UNP A0A2K2VPI4
E	11	MET	-	expression tag	UNP A0A2K2VPI4
E	12	GLY	-	expression tag	UNP A0A2K2VPI4
E	13	ARG	-	expression tag	UNP A0A2K2VPI4
E	14	GLY	-	expression tag	UNP A0A2K2VPI4
E	15	SER	-	expression tag	UNP A0A2K2VPI4
F	-18	MET	-	initiating methionine	UNP A0A2K2VPI4
F	-17	GLY	-	expression tag	UNP A0A2K2VPI4
F	-16	SER	-	expression tag	UNP A0A2K2VPI4
F	-15	SER	-	expression tag	UNP A0A2K2VPI4
F	-14	HIS	-	expression tag	UNP A0A2K2VPI4
F	-13	HIS	-	expression tag	UNP A0A2K2VPI4
F	-12	HIS	-	expression tag	UNP A0A2K2VPI4
F	-11	HIS	-	expression tag	UNP A0A2K2VPI4
F	-10	HIS	-	expression tag	UNP A0A2K2VPI4
F	-9	HIS	-	expression tag	UNP A0A2K2VPI4
F	-8	SER	-	expression tag	UNP A0A2K2VPI4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	SER	-	expression tag	UNP A0A2K2VPI4
F	-6	GLY	-	expression tag	UNP A0A2K2VPI4
F	-5	LEU	-	expression tag	UNP A0A2K2VPI4
F	-4	VAL	-	expression tag	UNP A0A2K2VPI4
F	-3	PRO	-	expression tag	UNP A0A2K2VPI4
F	-2	ARG	-	expression tag	UNP A0A2K2VPI4
F	-1	GLY	-	expression tag	UNP A0A2K2VPI4
F	0	SER	-	expression tag	UNP A0A2K2VPI4
F	1	HIS	-	expression tag	UNP A0A2K2VPI4
F	2	MET	-	expression tag	UNP A0A2K2VPI4
F	3	ALA	-	expression tag	UNP A0A2K2VPI4
F	4	SER	-	expression tag	UNP A0A2K2VPI4
F	5	MET	-	expression tag	UNP A0A2K2VPI4
F	6	THR	-	expression tag	UNP A0A2K2VPI4
F	7	GLY	-	expression tag	UNP A0A2K2VPI4
F	8	GLY	-	expression tag	UNP A0A2K2VPI4
F	9	GLN	-	expression tag	UNP A0A2K2VPI4
F	10	GLN	-	expression tag	UNP A0A2K2VPI4
F	11	MET	-	expression tag	UNP A0A2K2VPI4
F	12	GLY	-	expression tag	UNP A0A2K2VPI4
F	13	ARG	-	expression tag	UNP A0A2K2VPI4
F	14	GLY	-	expression tag	UNP A0A2K2VPI4
F	15	SER	-	expression tag	UNP A0A2K2VPI4
G	-18	MET	-	initiating methionine	UNP A0A2K2VPI4
G	-17	GLY	-	expression tag	UNP A0A2K2VPI4
G	-16	SER	-	expression tag	UNP A0A2K2VPI4
G	-15	SER	-	expression tag	UNP A0A2K2VPI4
G	-14	HIS	-	expression tag	UNP A0A2K2VPI4
G	-13	HIS	-	expression tag	UNP A0A2K2VPI4
G	-12	HIS	-	expression tag	UNP A0A2K2VPI4
G	-11	HIS	-	expression tag	UNP A0A2K2VPI4
G	-10	HIS	-	expression tag	UNP A0A2K2VPI4
G	-9	HIS	-	expression tag	UNP A0A2K2VPI4
G	-8	SER	-	expression tag	UNP A0A2K2VPI4
G	-7	SER	-	expression tag	UNP A0A2K2VPI4
G	-6	GLY	-	expression tag	UNP A0A2K2VPI4
G	-5	LEU	-	expression tag	UNP A0A2K2VPI4
G	-4	VAL	-	expression tag	UNP A0A2K2VPI4
G	-3	PRO	-	expression tag	UNP A0A2K2VPI4
G	-2	ARG	-	expression tag	UNP A0A2K2VPI4
G	-1	GLY	-	expression tag	UNP A0A2K2VPI4
G	0	SER	-	expression tag	UNP A0A2K2VPI4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	HIS	-	expression tag	UNP A0A2K2VPI4
G	2	MET	-	expression tag	UNP A0A2K2VPI4
G	3	ALA	-	expression tag	UNP A0A2K2VPI4
G	4	SER	-	expression tag	UNP A0A2K2VPI4
G	5	MET	-	expression tag	UNP A0A2K2VPI4
G	6	THR	-	expression tag	UNP A0A2K2VPI4
G	7	GLY	-	expression tag	UNP A0A2K2VPI4
G	8	GLY	-	expression tag	UNP A0A2K2VPI4
G	9	GLN	-	expression tag	UNP A0A2K2VPI4
G	10	GLN	-	expression tag	UNP A0A2K2VPI4
G	11	MET	-	expression tag	UNP A0A2K2VPI4
G	12	GLY	-	expression tag	UNP A0A2K2VPI4
G	13	ARG	-	expression tag	UNP A0A2K2VPI4
G	14	GLY	-	expression tag	UNP A0A2K2VPI4
G	15	SER	-	expression tag	UNP A0A2K2VPI4
H	-18	MET	-	initiating methionine	UNP A0A2K2VPI4
H	-17	GLY	-	expression tag	UNP A0A2K2VPI4
H	-16	SER	-	expression tag	UNP A0A2K2VPI4
H	-15	SER	-	expression tag	UNP A0A2K2VPI4
H	-14	HIS	-	expression tag	UNP A0A2K2VPI4
H	-13	HIS	-	expression tag	UNP A0A2K2VPI4
H	-12	HIS	-	expression tag	UNP A0A2K2VPI4
H	-11	HIS	-	expression tag	UNP A0A2K2VPI4
H	-10	HIS	-	expression tag	UNP A0A2K2VPI4
H	-9	HIS	-	expression tag	UNP A0A2K2VPI4
H	-8	SER	-	expression tag	UNP A0A2K2VPI4
H	-7	SER	-	expression tag	UNP A0A2K2VPI4
H	-6	GLY	-	expression tag	UNP A0A2K2VPI4
H	-5	LEU	-	expression tag	UNP A0A2K2VPI4
H	-4	VAL	-	expression tag	UNP A0A2K2VPI4
H	-3	PRO	-	expression tag	UNP A0A2K2VPI4
H	-2	ARG	-	expression tag	UNP A0A2K2VPI4
H	-1	GLY	-	expression tag	UNP A0A2K2VPI4
H	0	SER	-	expression tag	UNP A0A2K2VPI4
H	1	HIS	-	expression tag	UNP A0A2K2VPI4
H	2	MET	-	expression tag	UNP A0A2K2VPI4
H	3	ALA	-	expression tag	UNP A0A2K2VPI4
H	4	SER	-	expression tag	UNP A0A2K2VPI4
H	5	MET	-	expression tag	UNP A0A2K2VPI4
H	6	THR	-	expression tag	UNP A0A2K2VPI4
H	7	GLY	-	expression tag	UNP A0A2K2VPI4
H	8	GLY	-	expression tag	UNP A0A2K2VPI4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	9	GLN	-	expression tag	UNP A0A2K2VPI4
H	10	GLN	-	expression tag	UNP A0A2K2VPI4
H	11	MET	-	expression tag	UNP A0A2K2VPI4
H	12	GLY	-	expression tag	UNP A0A2K2VPI4
H	13	ARG	-	expression tag	UNP A0A2K2VPI4
H	14	GLY	-	expression tag	UNP A0A2K2VPI4
H	15	SER	-	expression tag	UNP A0A2K2VPI4

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Cu 4 4	0	0
2	B	4	Total Cu 4 4	0	0
2	C	4	Total Cu 4 4	0	0
2	D	4	Total Cu 4 4	0	0
2	E	4	Total Cu 4 4	0	0
2	F	4	Total Cu 4 4	0	0
2	G	4	Total Cu 4 4	0	0
2	H	4	Total Cu 4 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	68	Total O 68 68	0	0
3	B	59	Total O 59 59	0	0
3	C	90	Total O 90 90	0	0
3	D	61	Total O 61 61	0	0
3	E	52	Total O 52 52	0	0

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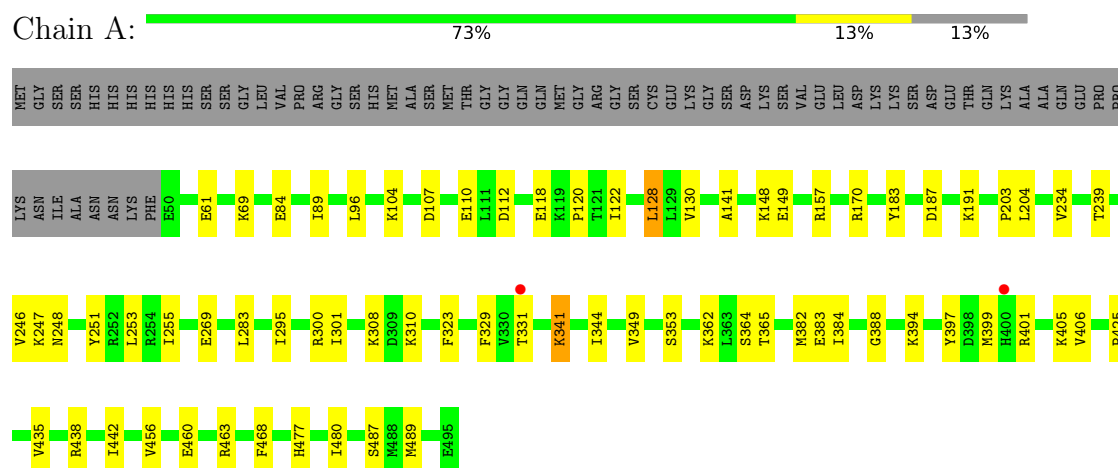
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	45	Total 45	O 45	0	0
3	G	42	Total 42	O 42	0	0
3	H	27	Total 27	O 27	0	0

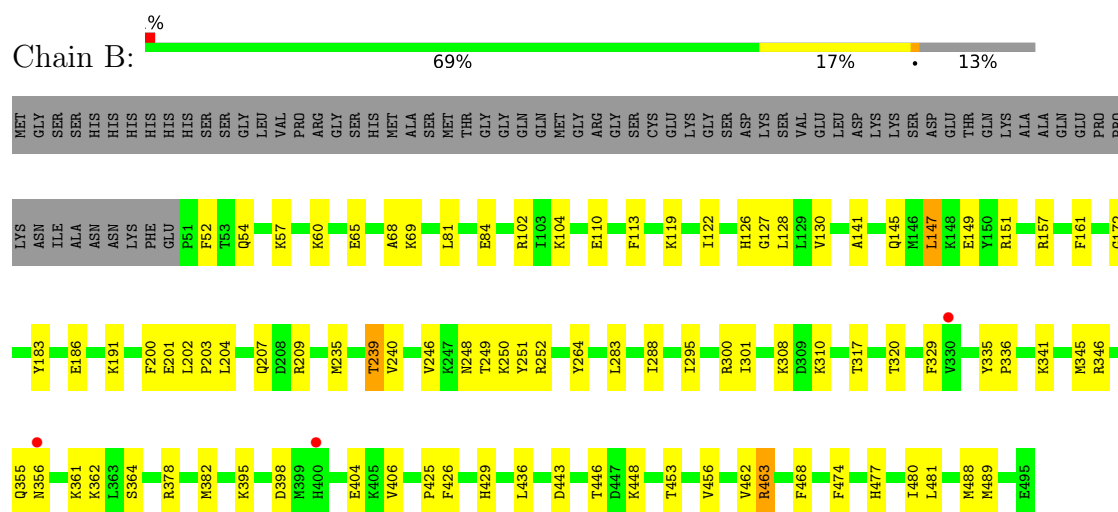
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

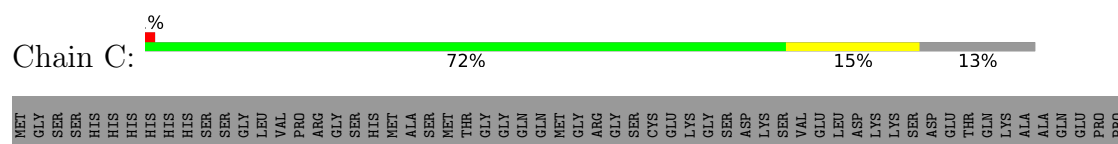
• Molecule 1: Bilirubin oxidase

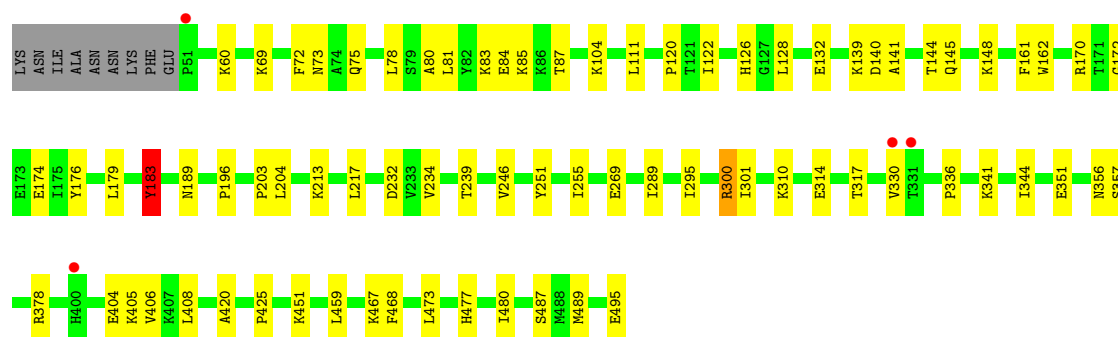


• Molecule 1: Bilirubin oxidase

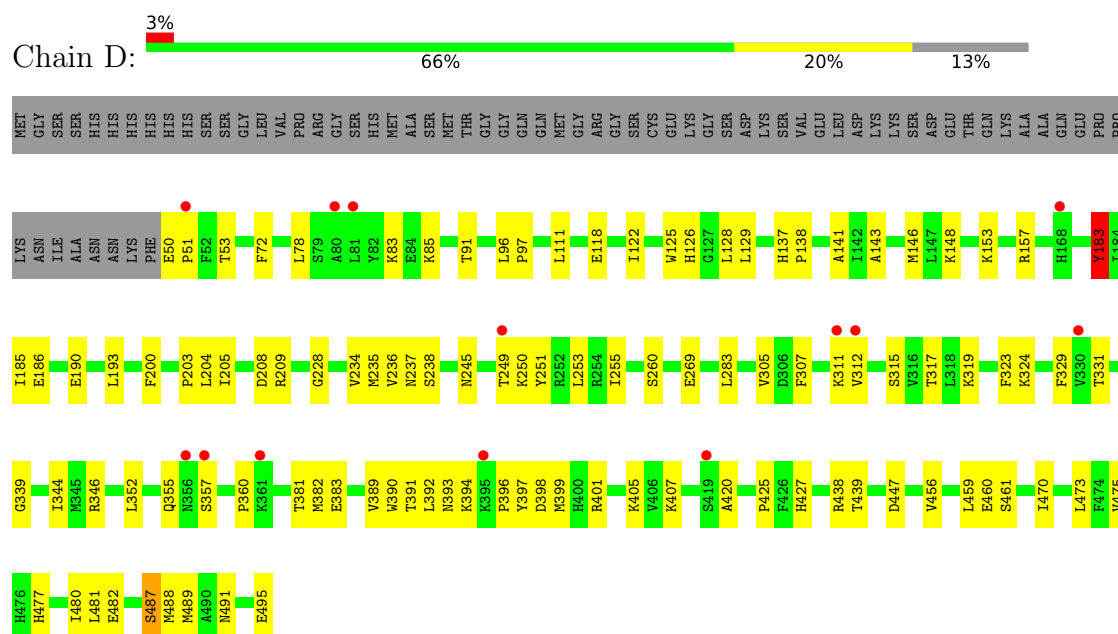


• Molecule 1: Bilirubin oxidase

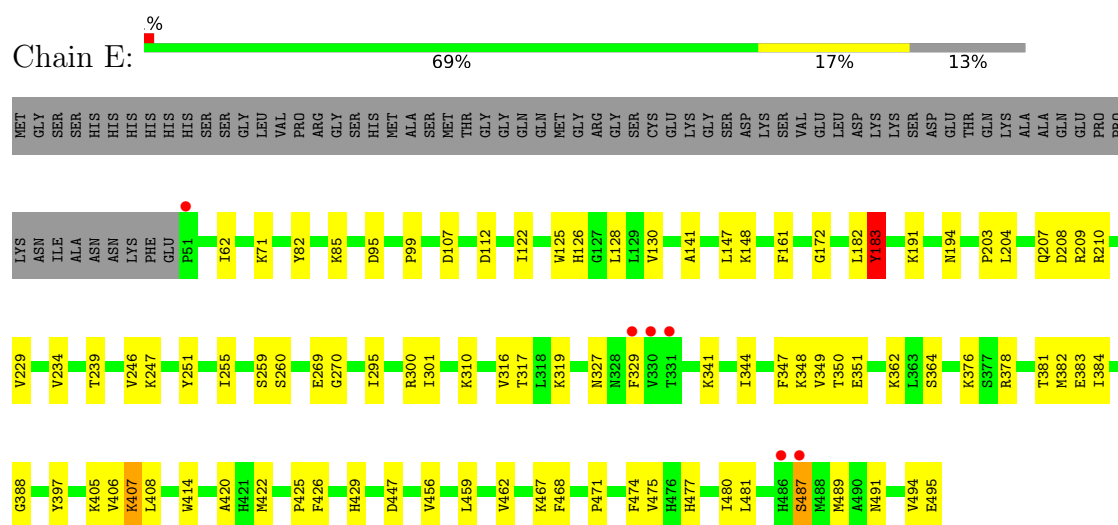




• Molecule 1: Bilirubin oxidase

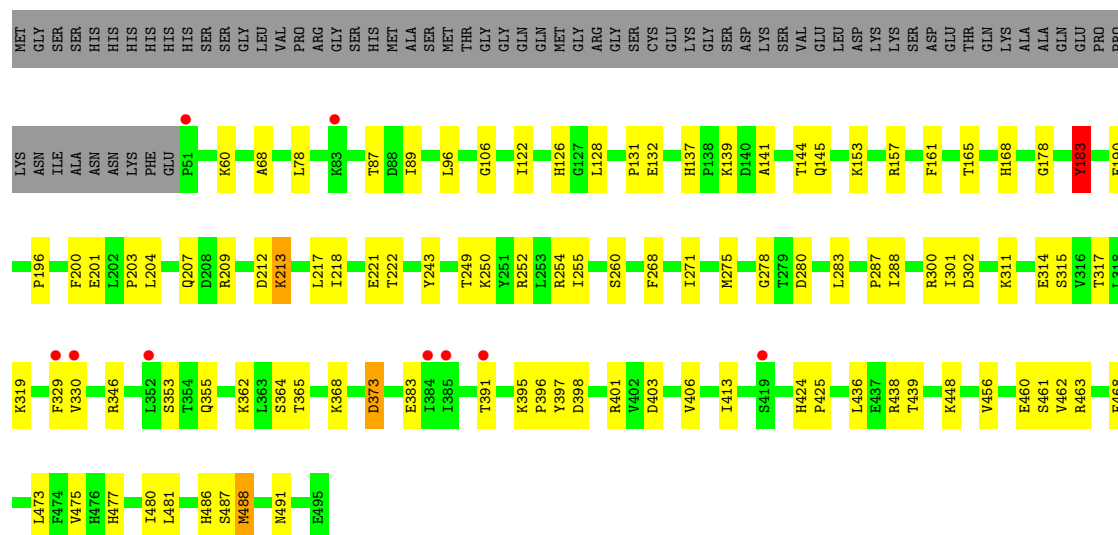


• Molecule 1: Bilirubin oxidase

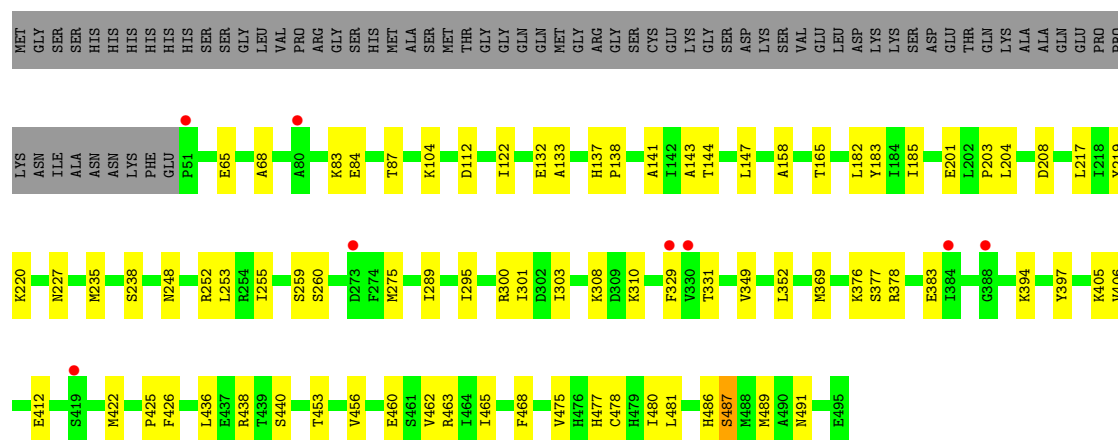


• Molecule 1: Bilirubin oxidase

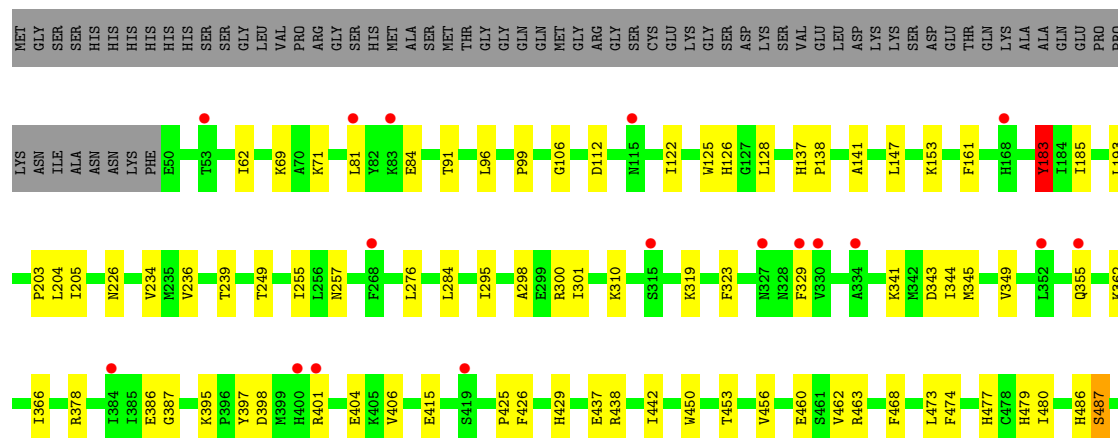




• Molecule 1: Bilirubin oxidase



• Molecule 1: Bilirubin oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.64Å 103.39Å 131.91Å 104.86° 103.96° 98.35°	Depositor
Resolution (Å)	39.52 – 2.58 39.52 – 2.58	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.52-2.58) 96.0 (39.52-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.191 , 0.240 0.195 , 0.234	Depositor DCC
R_{free} test set	129826 reflections (1.57%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29103	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.62	3/3667 (0.1%)	0.76	4/4955 (0.1%)
1	B	0.64	1/3658 (0.0%)	0.79	5/4942 (0.1%)
1	C	0.61	0/3658	0.77	3/4942 (0.1%)
1	D	0.58	0/3667	0.78	3/4955 (0.1%)
1	E	0.59	0/3658	0.77	5/4942 (0.1%)
1	F	0.59	0/3658	0.78	4/4942 (0.1%)
1	G	0.61	0/3658	0.76	3/4942 (0.1%)
1	H	0.57	0/3667	0.74	3/4955 (0.1%)
All	All	0.60	4/29291 (0.0%)	0.77	30/39575 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	H	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	LYS	CD-CE	6.18	1.66	1.51
1	B	463	ARG	CB-CG	-5.60	1.37	1.52
1	A	118	GLU	CD-OE1	5.09	1.31	1.25
1	A	269	GLU	CG-CD	5.06	1.59	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	TYR	CB-CG-CD2	-10.60	114.64	121.00
1	B	463	ARG	NE-CZ-NH1	-9.93	115.34	120.30
1	F	183	TYR	CB-CG-CD2	-9.76	115.14	121.00
1	D	183	TYR	CB-CG-CD2	-9.22	115.47	121.00
1	E	183	TYR	CB-CG-CD2	-8.54	115.88	121.00
1	H	183	TYR	CB-CG-CD2	-8.10	116.14	121.00
1	D	118	GLU	CA-CB-CG	7.86	130.68	113.40
1	B	463	ARG	CD-NE-CZ	7.79	134.51	123.60
1	G	463	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	A	487	SER	N-CA-C	6.99	129.87	111.00
1	E	487	SER	N-CA-C	6.41	128.31	111.00
1	F	488	MET	CG-SD-CE	6.36	110.38	100.20
1	G	436	LEU	CB-CG-CD2	-6.22	100.43	111.00
1	F	373	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	C	487	SER	N-CA-C	6.04	127.30	111.00
1	D	487	SER	N-CA-C	6.03	127.29	111.00
1	H	226	ASN	CB-CG-OD1	-5.80	110.00	121.60
1	C	183	TYR	CA-CB-CG	5.79	124.40	113.40
1	F	78	LEU	CA-CB-CG	5.76	128.54	115.30
1	E	407	LYS	CA-CB-CG	-5.61	101.06	113.40
1	A	118	GLU	N-CA-CB	-5.58	100.55	110.60
1	G	487	SER	N-CA-C	5.55	125.97	111.00
1	A	128	LEU	CB-CG-CD2	-5.51	101.62	111.00
1	H	487	SER	N-CA-C	5.50	125.84	111.00
1	E	407	LYS	CD-CE-NZ	-5.43	99.22	111.70
1	B	361	LYS	CB-CG-CD	-5.30	97.81	111.60
1	E	183	TYR	CA-CB-CG	5.30	123.47	113.40
1	B	147	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	A	341	LYS	CB-CG-CD	-5.11	98.32	111.60
1	B	398	ASP	N-CA-C	-5.07	97.30	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	183	TYR	Sidechain
1	D	183	TYR	Sidechain
1	E	183	TYR	Sidechain
1	F	183	TYR	Sidechain
1	H	183	TYR	Sidechain

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	3584	0	3591	36	0
1	B	3575	0	3586	59	0
1	C	3575	0	3586	48	0
1	D	3584	0	3591	73	0
1	E	3575	0	3586	57	0
1	F	3575	0	3586	67	0
1	G	3575	0	3586	46	0
1	H	3584	0	3591	54	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
3	A	68	0	0	4	0
3	B	59	0	0	4	0
3	C	90	0	0	11	0
3	D	61	0	0	5	0
3	E	52	0	0	7	0
3	F	45	0	0	11	0
3	G	42	0	0	2	0
3	H	27	0	0	1	0
All	All	29103	0	28703	432	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 8.

All (432) 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:E:348:LYS:NZ	3:E:702:HOH:O	1.97	0.96
1:A:107:ASP:OD2	3:A:701:HOH:O	1.83	0.95
1:D:245:ASN:OD1	3:D:701:HOH:O	1.83	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ILE:O	3:D:702:HOH:O	1.85	0.93
1:F:401:ARG:NH1	1:F:403:ASP:OD1	2.00	0.93
1:A:61:GLU:OE2	3:A:702:HOH:O	1.91	0.89
1:B:60:LYS:NZ	3:B:701:HOH:O	2.06	0.87
1:C:351:GLU:OE2	3:C:701:HOH:O	1.93	0.86
1:F:196:PRO:O	3:F:701:HOH:O	1.91	0.86
1:G:405:LYS:HD2	1:G:406:VAL:N	1.91	0.85
1:B:477:HIS:HB3	1:B:489:MET:HG3	1.59	0.84
1:E:107:ASP:OD2	3:E:701:HOH:O	1.97	0.83
1:B:191:LYS:NZ	3:B:702:HOH:O	2.13	0.80
1:C:310:LYS:NZ	3:C:706:HOH:O	2.14	0.80
1:B:207:GLN:OE1	1:B:209:ARG:NH2	2.16	0.79
1:H:319:LYS:HZ1	1:H:341:LYS:HG2	1.48	0.78
1:C:310:LYS:O	3:C:702:HOH:O	2.00	0.78
1:C:405:LYS:NZ	1:C:495:GLU:OE1	2.18	0.77
1:F:398:ASP:HB3	1:F:401:ARG:HG2	1.67	0.76
1:F:221:GLU:HG2	1:F:222:THR:HG23	1.66	0.76
1:E:247:LYS:HG2	1:E:351:GLU:HB2	1.68	0.75
1:H:319:LYS:NZ	1:H:341:LYS:HG2	2.03	0.73
1:H:249:THR:HG21	1:H:355:GLN:HB3	1.70	0.71
1:F:486:HIS:HB3	3:F:704:HOH:O	1.90	0.70
1:F:424:HIS:CE1	1:F:488:MET:HE1	2.26	0.70
1:E:407:LYS:HG3	1:E:408:LEU:N	2.06	0.69
1:C:330:VAL:O	3:C:703:HOH:O	2.09	0.69
1:C:196:PRO:O	3:C:704:HOH:O	2.10	0.69
1:E:191:LYS:NZ	3:E:706:HOH:O	2.25	0.69
1:E:316:VAL:HG22	1:E:347:PHE:HB2	1.74	0.69
1:C:140:ASP:OD2	3:C:705:HOH:O	2.12	0.67
1:D:383:GLU:N	1:D:383:GLU:OE1	2.27	0.67
1:B:102:ARG:NH1	1:B:186:GLU:OE1	2.28	0.67
1:E:447:ASP:O	3:E:703:HOH:O	2.12	0.67
1:A:362:LYS:HE3	1:A:364:SER:O	1.95	0.67
1:E:269:GLU:HG3	1:E:317:THR:HB	1.77	0.66
1:D:203:PRO:O	1:D:204:LEU:HD23	1.95	0.66
1:G:405:LYS:HD2	1:G:406:VAL:H	1.60	0.66
1:G:438:ARG:HB2	1:G:460:GLU:OE1	1.96	0.66
1:D:405:LYS:HD2	1:D:495:GLU:OE2	1.95	0.66
1:A:365:THR:HG21	1:B:119:LYS:HE3	1.77	0.65
1:E:319:LYS:HD2	1:E:341:LYS:NZ	2.11	0.65
1:G:397:TYR:H	1:G:487:SER:HB3	1.62	0.64
1:F:122:ILE:HB	1:F:141:ALA:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:LYS:NZ	1:E:495:GLU:OE2	2.30	0.64
1:C:174:GLU:HB3	1:C:179:LEU:HD12	1.78	0.64
1:D:425:PRO:HD2	1:D:480:ILE:HG12	1.79	0.64
1:B:68:ALA:HB3	1:H:69:LYS:HB3	1.80	0.63
1:B:69:LYS:HG3	1:B:110:GLU:HB3	1.80	0.63
1:E:381:THR:OG1	1:E:383:GLU:OE2	2.12	0.63
1:C:122:ILE:HD11	1:C:148:LYS:HD3	1.80	0.63
1:E:327:ASN:ND2	1:E:329:PHE:H	1.97	0.63
1:F:368:LYS:NZ	3:F:706:HOH:O	2.26	0.63
1:C:189:ASN:ND2	3:C:711:HOH:O	2.32	0.63
1:B:406:VAL:HG11	1:B:468:PHE:CD2	2.35	0.62
1:H:397:TYR:H	1:H:487:SER:HB3	1.64	0.62
1:H:395:LYS:HB3	1:H:401:ARG:NH2	2.15	0.62
1:G:275:MET:HG2	1:G:289:ILE:HD13	1.81	0.62
1:E:420:ALA:HA	1:E:459:LEU:HD22	1.81	0.61
1:G:477:HIS:HB3	1:G:489:MET:HG3	1.81	0.61
1:E:207:GLN:NE2	3:E:708:HOH:O	2.34	0.61
1:E:362:LYS:HE3	1:E:364:SER:O	2.00	0.61
1:D:447:ASP:O	3:D:704:HOH:O	2.16	0.60
1:G:112:ASP:HB3	1:G:147:LEU:HD11	1.83	0.60
1:A:425:PRO:HD2	1:A:480:ILE:HG12	1.83	0.60
1:D:382:MET:HE1	1:D:456:VAL:HB	1.84	0.60
1:F:397:TYR:H	1:F:487:SER:HB2	1.66	0.60
1:A:382:MET:HE1	1:A:456:VAL:HB	1.85	0.59
1:C:144:THR:O	1:C:145:GLN:HB2	2.01	0.59
1:D:324:LYS:CG	1:D:339:GLY:HA3	2.32	0.59
1:D:249:THR:HG22	1:D:250:LYS:H	1.68	0.59
1:E:122:ILE:HD11	1:E:148:LYS:HD3	1.85	0.59
1:F:200:PHE:CZ	1:F:355:GLN:HG3	2.37	0.58
1:F:207:GLN:HG3	3:F:715:HOH:O	2.04	0.58
1:G:122:ILE:HB	1:G:141:ALA:HA	1.86	0.58
1:B:317:THR:OG1	1:B:346:ARG:NH1	2.37	0.58
1:A:104:LYS:HE2	1:A:107:ASP:OD2	2.04	0.58
1:D:383:GLU:OE2	1:D:394:LYS:HG3	2.03	0.58
1:C:269:GLU:HG2	1:C:317:THR:HB	1.84	0.58
1:H:386:GLU:HG3	1:H:387:GLY:H	1.68	0.58
1:F:413:ILE:HG21	1:F:463:ARG:HD2	1.85	0.58
1:E:319:LYS:HD2	1:E:341:LYS:HZ2	1.69	0.58
1:F:353:SER:OG	1:F:355:GLN:HG2	2.04	0.58
1:C:234:VAL:HG11	1:C:344:ILE:HG12	1.85	0.57
1:D:50:GLU:HG2	1:D:53:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:HIS:HB3	1:E:489:MET:HG3	1.87	0.57
1:F:396:PRO:O	1:F:401:ARG:NH2	2.36	0.57
1:H:415:GLU:HG3	1:H:463:ARG:HB3	1.86	0.57
1:G:87:THR:HG21	1:G:217:LEU:H	1.70	0.57
1:D:249:THR:HG22	1:D:250:LYS:N	2.19	0.57
1:F:203:PRO:O	1:F:204:LEU:HD23	2.05	0.57
1:A:69:LYS:HG3	1:A:110:GLU:HB3	1.86	0.57
1:H:362:LYS:HG2	3:H:703:HOH:O	2.04	0.57
1:A:253:LEU:HB3	1:A:255:ILE:HD11	1.85	0.56
1:H:398:ASP:HB3	1:H:401:ARG:HD3	1.87	0.56
1:H:323:PHE:HZ	1:H:442:ILE:HD13	1.69	0.56
1:E:122:ILE:HB	1:E:141:ALA:HA	1.86	0.56
1:E:327:ASN:HD21	1:E:329:PHE:HB2	1.69	0.56
1:G:378:ARG:HH21	1:G:412:GLU:CD	2.07	0.56
1:H:203:PRO:O	1:H:204:LEU:HD23	2.05	0.56
1:H:395:LYS:HB3	1:H:401:ARG:HH22	1.70	0.56
1:H:438:ARG:HB3	1:H:460:GLU:OE1	2.06	0.56
1:E:456:VAL:HG13	1:E:462:VAL:HG23	1.88	0.56
1:F:395:LYS:HB3	1:F:401:ARG:NH2	2.21	0.56
1:D:324:LYS:HG2	1:D:339:GLY:HA3	1.86	0.56
1:A:255:ILE:HB	1:A:301:ILE:HG13	1.87	0.56
1:D:249:THR:H	1:D:307:PHE:HB2	1.69	0.56
1:D:407:LYS:NZ	3:D:703:HOH:O	1.97	0.56
1:C:425:PRO:HD2	1:C:480:ILE:HG12	1.88	0.55
1:F:475:VAL:HG23	1:F:477:HIS:HD2	1.71	0.55
1:B:54:GLN:HG2	1:B:239:THR:HG22	1.87	0.55
1:B:425:PRO:HD2	1:B:480:ILE:HG12	1.86	0.55
1:C:120:PRO:O	1:C:170:ARG:NH2	2.39	0.55
1:F:280:ASP:HB2	1:F:300:ARG:CZ	2.36	0.55
1:B:320:THR:O	1:B:341:LYS:HA	2.07	0.55
1:E:467:LYS:NZ	3:E:704:HOH:O	2.21	0.55
1:A:401:ARG:HG3	1:F:145:GLN:HG2	1.87	0.55
1:G:295:ILE:HD12	1:G:301:ILE:HG12	1.89	0.55
1:H:378:ARG:NH1	1:H:404:GLU:HB3	2.22	0.54
1:D:186:GLU:OE2	3:D:705:HOH:O	2.18	0.54
1:D:250:LYS:NZ	1:D:357:SER:O	2.30	0.54
1:D:312:VAL:HG23	1:D:352:LEU:CD1	2.38	0.54
1:F:201:GLU:OE1	1:F:254:ARG:HD2	2.08	0.54
1:G:203:PRO:O	1:G:204:LEU:HD23	2.08	0.54
1:C:295:ILE:HD12	1:C:301:ILE:HG12	1.90	0.54
1:A:435:VAL:O	3:A:704:HOH:O	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:406:VAL:HG11	1:F:468:PHE:CD1	2.44	0.53
1:G:378:ARG:NH2	1:G:412:GLU:OE1	2.41	0.53
1:F:425:PRO:HD2	1:F:480:ILE:HG12	1.89	0.53
1:F:486:HIS:O	3:F:704:HOH:O	2.18	0.53
1:A:203:PRO:O	1:A:204:LEU:HD23	2.09	0.53
1:A:438:ARG:HB3	1:A:460:GLU:OE1	2.08	0.53
1:D:475:VAL:HG23	1:D:477:HIS:HD2	1.73	0.53
1:G:406:VAL:HG11	1:G:468:PHE:CD1	2.44	0.53
1:E:406:VAL:HG11	1:E:468:PHE:CE1	2.44	0.53
1:E:270:GLY:O	1:E:310:LYS:NZ	2.30	0.53
1:H:126:HIS:CE1	1:H:298:ALA:HB1	2.44	0.53
1:B:127:GLY:HA3	1:B:161:PHE:HD2	1.73	0.53
1:C:232:ASP:HB3	1:C:336:PRO:HD2	1.91	0.53
1:C:80:ALA:HA	1:C:85:LYS:O	2.09	0.53
1:D:249:THR:HG21	1:D:355:GLN:HG2	1.91	0.53
1:H:91:THR:HG22	1:H:96:LEU:HG	1.91	0.53
1:H:122:ILE:HB	1:H:141:ALA:HA	1.91	0.52
1:A:295:ILE:HD12	1:A:301:ILE:HG12	1.89	0.52
1:D:381:THR:HG22	1:D:393:ASN:OD1	2.08	0.52
1:F:168:HIS:N	3:F:702:HOH:O	2.05	0.52
1:G:425:PRO:HD2	1:G:480:ILE:HG12	1.91	0.52
1:B:157:ARG:NH2	1:B:283:LEU:O	2.43	0.52
1:G:255:ILE:HB	1:G:301:ILE:HG13	1.91	0.52
1:G:425:PRO:HD2	1:G:478:CYS:SG	2.50	0.52
1:D:473:LEU:HD11	1:D:491:ASN:HB3	1.92	0.52
1:H:128:LEU:HD21	1:H:183:TYR:OH	2.09	0.52
1:H:425:PRO:HD2	1:H:480:ILE:HG13	1.91	0.52
1:D:122:ILE:HB	1:D:141:ALA:HA	1.91	0.52
1:D:190:GLU:HG3	1:D:283:LEU:HD11	1.91	0.52
1:D:389:VAL:HG12	1:D:391:THR:HG23	1.92	0.51
1:C:104:LYS:NZ	3:C:718:HOH:O	2.43	0.51
1:D:383:GLU:OE2	1:D:394:LYS:N	2.43	0.51
1:A:122:ILE:HB	1:A:141:ALA:HA	1.93	0.51
1:D:315:SER:CB	1:D:346:ARG:HD3	2.41	0.51
1:A:477:HIS:HB3	1:A:489:MET:HG3	1.93	0.51
1:F:137:HIS:ND1	1:F:139:LYS:HG2	2.25	0.51
1:E:208:ASP:O	1:E:209:ARG:HD3	2.11	0.51
1:F:212:ASP:HB3	1:F:218:ILE:HD11	1.93	0.51
1:D:438:ARG:HB3	1:D:460:GLU:OE1	2.10	0.50
1:H:456:VAL:HG13	1:H:462:VAL:HG23	1.93	0.50
1:H:477:HIS:HE1	1:H:479:HIS:CD2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LEU:HB3	1:B:130:VAL:HG13	1.94	0.50
1:F:456:VAL:HG13	1:F:462:VAL:HG23	1.93	0.50
1:G:158:ALA:HA	1:G:185:ILE:HG22	1.93	0.50
1:A:89:ILE:HD12	1:A:96:LEU:HG	1.93	0.50
1:A:463:ARG:NH1	3:A:715:HOH:O	2.44	0.50
1:B:65:GLU:OE1	1:B:104:LYS:HE2	2.12	0.50
1:F:89:ILE:HD12	1:F:96:LEU:HG	1.93	0.50
1:D:125:TRP:HB3	1:D:128:LEU:HD13	1.93	0.49
1:B:443:ASP:N	3:B:704:HOH:O	2.26	0.49
1:D:72:PHE:HB2	1:D:111:LEU:HD21	1.94	0.49
1:E:384:ILE:HD11	1:E:388:GLY:HA2	1.93	0.49
1:G:456:VAL:HG13	1:G:462:VAL:HG23	1.94	0.49
1:H:426:PHE:O	1:H:453:THR:HA	2.12	0.49
1:B:200:PHE:HA	1:B:251:TYR:CD1	2.47	0.49
1:F:260:SER:HA	1:F:481:LEU:HD12	1.93	0.49
1:H:398:ASP:H	1:H:401:ARG:NH1	2.10	0.49
1:H:234:VAL:HG11	1:H:344:ILE:HD13	1.95	0.49
1:C:203:PRO:O	1:C:204:LEU:HD23	2.12	0.49
1:H:429:HIS:HB2	1:H:474:PHE:HB3	1.92	0.49
1:B:126:HIS:O	1:B:161:PHE:HB3	2.12	0.49
1:F:106:GLY:O	1:F:153:LYS:NZ	2.41	0.49
1:F:362:LYS:HE2	1:F:364:SER:O	2.12	0.49
1:G:208:ASP:OD1	1:G:259:SER:HB3	2.12	0.49
1:F:268:PHE:HB2	1:F:271:ILE:HG12	1.94	0.49
1:C:132:GLU:OE1	3:C:707:HOH:O	2.20	0.49
1:D:143:ALA:O	1:D:146:MET:HB2	2.12	0.48
1:F:317:THR:OG1	1:F:346:ARG:HG3	2.13	0.48
1:F:319:LYS:NZ	3:F:705:HOH:O	2.26	0.48
1:F:278:GLY:HA3	1:F:302:ASP:HB3	1.95	0.48
1:F:406:VAL:HG11	1:F:468:PHE:CE1	2.49	0.48
1:H:112:ASP:HB3	1:H:147:LEU:HD11	1.95	0.48
1:H:236:VAL:HG21	1:H:345:MET:HE3	1.95	0.48
1:A:234:VAL:HG11	1:A:344:ILE:HG12	1.94	0.48
1:A:323:PHE:HZ	1:A:442:ILE:HD13	1.76	0.48
1:B:378:ARG:NH1	1:B:404:GLU:HB3	2.28	0.48
1:A:187:ASP:O	1:A:191:LYS:HG3	2.13	0.48
1:B:145:GLN:HG2	1:B:145:GLN:O	2.13	0.48
1:C:378:ARG:NH1	1:C:404:GLU:OE2	2.46	0.48
1:H:125:TRP:HB3	1:H:128:LEU:HD13	1.95	0.48
1:C:78:LEU:HA	1:C:87:THR:O	2.13	0.48
1:E:234:VAL:HG11	1:E:344:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:SER:HA	1:D:481:LEU:HD12	1.96	0.48
1:E:295:ILE:HD12	1:E:301:ILE:HG12	1.95	0.48
1:F:395:LYS:HB3	1:F:401:ARG:HH22	1.79	0.48
1:B:149:GLU:OE1	1:C:467:LYS:NZ	2.40	0.48
1:E:125:TRP:HB3	1:E:128:LEU:HD13	1.94	0.48
1:F:190:GLU:OE1	1:F:252:ARG:NH2	2.42	0.48
1:D:253:LEU:HB3	1:D:255:ILE:HD11	1.96	0.47
1:A:120:PRO:O	1:A:170:ARG:NH2	2.47	0.47
1:C:255:ILE:HB	1:C:301:ILE:HG13	1.96	0.47
1:E:429:HIS:HB2	1:E:474:PHE:HB3	1.96	0.47
1:B:362:LYS:HE2	1:B:364:SER:O	2.13	0.47
1:E:471:PRO:HA	1:E:494:VAL:HB	1.97	0.47
1:G:376:LYS:HG2	1:G:377:SER:N	2.29	0.47
1:F:311:LYS:HB2	1:F:314:GLU:HG3	1.97	0.47
1:G:369:MET:HB2	1:G:465:ILE:HG21	1.97	0.47
1:D:91:THR:HG22	1:D:96:LEU:HG	1.95	0.47
1:E:425:PRO:HD2	1:E:480:ILE:HG12	1.96	0.47
1:G:137:HIS:HE2	1:G:491:ASN:ND2	2.12	0.47
1:H:319:LYS:HB2	1:H:343:ASP:HA	1.96	0.47
1:A:397:TYR:CZ	1:A:399:MET:HA	2.50	0.47
1:B:161:PHE:HZ	3:B:721:HOH:O	1.98	0.47
1:E:203:PRO:O	1:E:204:LEU:HD23	2.15	0.47
1:F:157:ARG:NH2	1:F:283:LEU:O	2.48	0.47
1:H:437:GLU:OE2	1:H:463:ARG:HD3	2.15	0.47
1:F:131:PRO:HA	3:F:703:HOH:O	2.16	0.46
1:G:376:LYS:HD2	1:G:378:ARG:NH2	2.29	0.46
1:H:204:LEU:HD12	1:H:255:ILE:CD1	2.45	0.46
1:A:112:ASP:OD1	1:A:149:GLU:HG2	2.16	0.46
1:B:310:LYS:HA	1:B:310:LYS:HD3	1.71	0.46
1:A:122:ILE:HD11	1:A:148:LYS:HD3	1.96	0.46
1:D:398:ASP:HB3	1:D:401:ARG:HB3	1.97	0.46
1:E:247:LYS:HG2	1:E:351:GLU:CB	2.41	0.46
1:B:436:LEU:HB2	1:B:463:ARG:O	2.15	0.46
1:E:350:THR:HG23	1:E:351:GLU:HG2	1.98	0.46
1:F:132:GLU:N	3:F:703:HOH:O	2.14	0.46
1:G:227:ASN:O	1:G:422:MET:HE1	2.15	0.46
1:H:366:ILE:HG23	1:H:450:TRP:NE1	2.29	0.46
1:E:208:ASP:OD1	1:E:259:SER:HB3	2.16	0.46
1:D:228:GLY:HA2	1:D:482:GLU:OE2	2.15	0.46
1:H:137:HIS:ND1	1:H:138:PRO:HD2	2.30	0.46
1:G:144:THR:N	3:G:702:HOH:O	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LEU:HB3	1:D:470:ILE:HD11	1.98	0.46
1:D:97:PRO:HG3	1:D:237:ASN:O	2.16	0.46
1:D:157:ARG:NH2	1:D:283:LEU:O	2.48	0.46
1:E:112:ASP:HB3	1:E:147:LEU:HD11	1.97	0.46
1:F:128:LEU:HD21	1:F:183:TYR:OH	2.16	0.46
1:B:122:ILE:HB	1:B:141:ALA:HA	1.98	0.45
1:D:235:MET:HE3	1:D:238:SER:HA	1.97	0.45
1:E:210:ARG:CZ	1:E:229:VAL:HG13	2.46	0.45
1:B:456:VAL:HG13	1:B:462:VAL:HG23	1.98	0.45
1:C:162:TRP:CD1	1:C:300:ARG:HD2	2.51	0.45
1:F:439:THR:HG23	1:F:461:SER:O	2.17	0.45
1:B:249:THR:OG1	1:B:250:LYS:N	2.49	0.45
1:B:355:GLN:HG3	1:B:356:ASN:N	2.31	0.45
1:B:382:MET:HB3	1:B:488:MET:CE	2.46	0.45
1:D:315:SER:HB2	1:D:346:ARG:HD3	1.98	0.45
1:A:383:GLU:OE2	1:A:394:LYS:N	2.41	0.45
1:C:87:THR:HG21	1:C:217:LEU:H	1.82	0.45
1:C:139:LYS:HE2	1:C:473:LEU:HD23	1.99	0.45
1:C:406:VAL:HG11	1:C:468:PHE:CG	2.51	0.45
1:C:451:LYS:HE2	3:C:755:HOH:O	2.15	0.45
1:D:193:LEU:HB3	1:D:360:PRO:HG2	1.97	0.45
1:D:397:TYR:CZ	1:D:399:MET:HA	2.51	0.45
1:D:425:PRO:CD	1:D:480:ILE:HG12	2.47	0.45
1:B:65:GLU:HA	1:H:71:LYS:HE2	1.98	0.45
1:F:362:LYS:NZ	1:F:365:THR:HG22	2.32	0.45
1:H:257:ASN:HB2	1:H:295:ILE:HG12	1.98	0.45
1:B:248:ASN:O	1:B:308:LYS:HA	2.17	0.45
1:D:269:GLU:HB2	1:D:319:LYS:HE3	1.98	0.45
1:D:153:LYS:HE2	1:E:376:LYS:HD2	1.98	0.45
1:D:324:LYS:HG3	1:D:339:GLY:HA3	1.98	0.45
1:D:439:THR:HG23	1:D:461:SER:O	2.17	0.45
1:H:310:LYS:HB2	1:H:349:VAL:HG21	1.99	0.45
1:G:394:LYS:HE2	1:G:394:LYS:HB2	1.72	0.44
1:D:205:ILE:O	1:D:236:VAL:HA	2.17	0.44
1:F:213:LYS:HD2	1:F:213:LYS:O	2.17	0.44
1:F:436:LEU:HD23	1:F:436:LEU:HA	1.71	0.44
1:G:260:SER:HA	1:G:481:LEU:HD12	2.00	0.44
1:B:246:VAL:HB	1:B:251:TYR:CE2	2.52	0.44
1:B:264:TYR:HB2	1:B:295:ILE:HG23	2.00	0.44
1:C:60:LYS:HE3	1:C:60:LYS:HB2	1.89	0.44
1:G:132:GLU:HG3	1:G:133:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:426:PHE:O	1:G:453:THR:HA	2.18	0.44
1:H:128:LEU:HD21	1:H:183:TYR:CZ	2.53	0.44
1:A:157:ARG:NH2	1:A:283:LEU:O	2.51	0.44
1:B:203:PRO:O	1:B:204:LEU:HD23	2.18	0.44
1:B:295:ILE:HD12	1:B:301:ILE:HG12	2.00	0.44
1:C:69:LYS:HB3	1:G:68:ALA:HB3	1.99	0.44
1:C:72:PHE:HB2	1:C:111:LEU:HD21	2.00	0.44
1:H:255:ILE:HB	1:H:301:ILE:HG13	2.00	0.44
1:B:406:VAL:HG11	1:B:468:PHE:CE2	2.51	0.44
1:A:341:LYS:HB2	1:A:341:LYS:HE3	1.61	0.44
1:B:346:ARG:HG3	1:B:346:ARG:HH11	1.83	0.44
1:D:122:ILE:HD11	1:D:148:LYS:HD3	2.00	0.44
1:H:62:ILE:HG13	1:H:99:PRO:HB2	2.00	0.44
1:H:406:VAL:HG11	1:H:468:PHE:CE1	2.53	0.43
1:B:52:PHE:HE1	1:B:345:MET:HA	1.83	0.43
1:G:248:ASN:OD1	1:G:352:LEU:HA	2.18	0.43
1:G:310:LYS:HB3	1:G:349:VAL:HG21	1.99	0.43
1:E:246:VAL:HB	1:E:251:TYR:CE2	2.53	0.43
1:G:65:GLU:OE1	1:G:104:LYS:HE2	2.18	0.43
1:E:397:TYR:H	1:E:487:SER:HB3	1.82	0.43
1:H:69:LYS:HD3	1:H:112:ASP:OD2	2.18	0.43
1:D:200:PHE:HA	1:D:251:TYR:CD1	2.53	0.43
1:D:50:GLU:HA	1:D:51:PRO:HD3	1.88	0.43
1:D:250:LYS:HA	1:D:305:VAL:O	2.19	0.43
1:F:87:THR:HG21	1:F:217:LEU:H	1.84	0.43
1:F:207:GLN:OE1	1:F:209:ARG:NH2	2.52	0.43
1:B:127:GLY:HA3	1:B:161:PHE:CD2	2.52	0.43
1:D:391:THR:HG22	1:D:396:PRO:HA	2.00	0.43
1:A:310:LYS:HB3	1:A:349:VAL:HG21	1.99	0.43
1:C:122:ILE:HB	1:C:141:ALA:HA	2.01	0.43
1:C:406:VAL:HG11	1:C:468:PHE:CD1	2.54	0.43
1:E:126:HIS:O	1:E:161:PHE:HB3	2.19	0.43
1:C:408:LEU:N	1:C:495:GLU:O	2.38	0.43
1:D:420:ALA:HB2	1:D:459:LEU:HD21	2.00	0.43
1:E:378:ARG:HD2	1:E:414:TRP:CE2	2.54	0.43
1:A:128:LEU:HB3	1:A:130:VAL:HG13	2.01	0.43
1:B:113:PHE:O	1:B:147:LEU:HA	2.19	0.43
1:D:50:GLU:CG	1:D:53:THR:HG21	2.48	0.43
1:E:172:GLY:HA2	1:E:481:LEU:HD13	2.01	0.43
1:F:413:ILE:CG2	1:F:463:ARG:HD2	2.47	0.43
1:F:438:ARG:HB3	1:F:460:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LYS:HD2	1:B:362:LYS:HA	1.76	0.42
1:G:132:GLU:CG	1:G:133:ALA:N	2.81	0.42
1:C:341:LYS:HB3	1:C:341:LYS:HE2	1.82	0.42
1:D:126:HIS:CE1	1:D:427:HIS:CE1	3.07	0.42
1:D:311:LYS:HB2	1:D:311:LYS:HE3	1.82	0.42
1:D:382:MET:HG2	1:D:392:LEU:CD1	2.48	0.42
1:E:71:LYS:HD2	1:F:68:ALA:HB2	2.01	0.42
1:C:477:HIS:HB3	1:C:489:MET:HA	2.01	0.42
1:D:475:VAL:HG23	1:D:477:HIS:CD2	2.53	0.42
1:D:208:ASP:O	1:D:209:ARG:HG2	2.20	0.42
1:F:315:SER:OG	1:F:346:ARG:HD3	2.20	0.42
1:H:401:ARG:HG2	1:H:401:ARG:HH11	1.85	0.42
1:F:275:MET:CG	1:F:287:PRO:HB3	2.50	0.42
1:G:122:ILE:O	1:G:165:THR:HA	2.19	0.42
1:G:219:TYR:CG	1:G:220:LYS:N	2.87	0.42
1:H:161:PHE:CE2	1:H:185:ILE:HD12	2.54	0.42
1:E:128:LEU:HD21	1:E:183:TYR:OH	2.19	0.42
1:C:420:ALA:HB2	1:C:459:LEU:HD21	2.01	0.42
1:G:83:LYS:HB3	1:G:84:GLU:H	1.56	0.42
1:G:201:GLU:HA	1:G:252:ARG:O	2.20	0.42
1:C:172:GLY:O	1:C:176:TYR:HB2	2.20	0.42
1:C:289:ILE:HD12	1:C:289:ILE:HG23	1.82	0.42
1:F:207:GLN:NE2	3:F:715:HOH:O	2.53	0.42
1:F:278:GLY:CA	1:F:302:ASP:HB3	2.50	0.42
1:B:128:LEU:HD21	1:B:183:TYR:CZ	2.55	0.42
1:B:157:ARG:HH21	1:B:283:LEU:N	2.18	0.42
1:C:128:LEU:HD21	1:C:183:TYR:OH	2.19	0.42
1:D:317:THR:OG1	1:D:346:ARG:HG3	2.20	0.42
1:E:62:ILE:HG13	1:E:99:PRO:HB2	2.01	0.42
1:E:128:LEU:HB3	1:E:130:VAL:HG13	2.01	0.42
1:E:310:LYS:CB	1:E:349:VAL:HG21	2.50	0.42
1:H:406:VAL:HG11	1:H:468:PHE:CD1	2.55	0.42
1:F:255:ILE:HB	1:F:301:ILE:HG12	2.01	0.41
1:H:106:GLY:O	1:H:153:LYS:HE3	2.20	0.41
1:D:128:LEU:HD21	1:D:183:TYR:OH	2.19	0.41
1:D:323:PHE:H	1:D:339:GLY:HA2	1.85	0.41
1:E:207:GLN:HA	1:E:259:SER:OG	2.20	0.41
1:F:144:THR:O	1:F:145:GLN:HB3	2.21	0.41
1:G:440:SER:HB3	1:G:460:GLU:HG3	2.01	0.41
1:A:247:LYS:HB3	1:A:353:SER:HB2	2.02	0.41
1:F:128:LEU:HD21	1:F:183:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ILE:HD11	1:B:448:LYS:HD2	2.03	0.41
1:C:73:ASN:O	1:C:75:GLN:HG2	2.21	0.41
1:D:234:VAL:HG11	1:D:344:ILE:HG12	2.02	0.41
1:D:249:THR:HG23	1:D:355:GLN:HB3	2.02	0.41
1:E:382:MET:HE3	1:E:426:PHE:HB2	2.03	0.41
1:B:149:GLU:HG2	1:B:151:ARG:NH2	2.36	0.41
1:D:83:LYS:HD3	1:D:83:LYS:HA	1.84	0.41
1:F:126:HIS:O	1:F:161:PHE:HB3	2.20	0.41
1:B:235:MET:HG2	1:B:240:VAL:HG22	2.02	0.41
1:B:426:PHE:O	1:B:453:THR:HA	2.21	0.41
1:D:477:HIS:HB3	1:D:489:MET:HA	2.02	0.41
1:E:194:ASN:O	3:E:705:HOH:O	2.22	0.41
1:F:178:GLY:HA2	3:F:720:HOH:O	2.20	0.41
1:B:341:LYS:H	1:B:341:LYS:HG2	1.48	0.41
1:C:83:LYS:HB3	1:C:84:GLU:H	1.56	0.41
1:H:473:LEU:HD12	1:H:473:LEU:HA	1.92	0.41
1:B:57:LYS:HE3	1:B:239:THR:HG23	2.02	0.41
1:B:172:GLY:HA2	1:B:481:LEU:HB3	2.03	0.41
1:D:137:HIS:ND1	1:D:138:PRO:HD2	2.36	0.41
1:F:122:ILE:O	1:F:165:THR:HA	2.20	0.41
1:G:137:HIS:ND1	1:G:138:PRO:HD2	2.36	0.41
1:H:205:ILE:O	1:H:236:VAL:HA	2.21	0.41
1:B:104:LYS:HE3	1:B:104:LYS:HB2	1.78	0.41
1:C:246:VAL:HB	1:C:251:TYR:CE2	2.56	0.41
1:F:473:LEU:HD11	1:F:491:ASN:HB3	2.03	0.41
1:G:248:ASN:O	1:G:308:LYS:HA	2.21	0.41
1:H:204:LEU:HD12	1:H:255:ILE:HD12	2.03	0.41
1:H:319:LYS:HE2	1:H:343:ASP:OD1	2.21	0.41
1:D:126:HIS:NE2	1:D:427:HIS:CE1	2.89	0.40
1:D:397:TYR:H	1:D:487:SER:HB3	1.86	0.40
1:E:204:LEU:HD12	1:E:255:ILE:CD1	2.51	0.40
1:G:143:ALA:HA	3:G:702:HOH:O	2.21	0.40
1:G:475:VAL:HG12	1:G:491:ASN:ND2	2.36	0.40
1:H:276:LEU:HG	1:H:284:LEU:HD11	2.03	0.40
1:B:429:HIS:HB2	1:B:474:PHE:HB3	2.03	0.40
1:C:126:HIS:O	1:C:161:PHE:HB3	2.21	0.40
1:E:475:VAL:HG12	1:E:491:ASN:OD1	2.20	0.40
1:F:60:LYS:HA	1:F:60:LYS:HD3	1.80	0.40
1:G:253:LEU:HD12	1:G:303:ILE:HD11	2.02	0.40
1:H:249:THR:HB	1:H:355:GLN:OE1	2.22	0.40
1:A:246:VAL:HB	1:A:251:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ILE:HD11	1:A:388:GLY:HA2	2.02	0.40
1:A:406:VAL:HG11	1:A:468:PHE:CD1	2.55	0.40
1:B:201:GLU:HA	1:B:252:ARG:O	2.21	0.40
1:B:335:TYR:HA	1:B:336:PRO:HD3	1.95	0.40
1:C:314:GLU:HB3	3:C:706:HOH:O	2.22	0.40
1:E:182:LEU:HD23	1:E:182:LEU:HA	1.75	0.40
1:A:248:ASN:O	1:A:308:LYS:HA	2.21	0.40
1:B:201:GLU:O	1:B:202:LEU:HD23	2.22	0.40
1:C:213:LYS:HE2	1:C:213:LYS:HB2	1.84	0.40
1:D:390:TRP:HB3	1:D:488:MET:SD	2.62	0.40
1:E:269:GLU:CG	1:E:317:THR:HB	2.50	0.40
1:E:319:LYS:HD2	1:E:341:LYS:HZ1	1.85	0.40
1:F:243:TYR:HA	1:F:346:ARG:O	2.21	0.40
1:B:395:LYS:HE2	1:B:395:LYS:HB2	1.81	0.40
1:F:249:THR:HG23	1:F:250:LYS:N	2.37	0.40
1:F:288:ILE:HD11	1:F:448:LYS:HD2	2.03	0.40
1:G:235:MET:HE3	1:G:238:SER:HA	2.04	0.40
1:H:295:ILE:HD12	1:H:301:ILE:HG12	2.04	0.40
1:H:298:ALA:HB2	1:H:479:HIS:ND1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/514 (86%)	427 (96%)	17 (4%)	0	100	100
1	B	443/514 (86%)	419 (95%)	24 (5%)	0	100	100
1	C	443/514 (86%)	427 (96%)	16 (4%)	0	100	100
1	D	444/514 (86%)	431 (97%)	13 (3%)	0	100	100
1	E	443/514 (86%)	425 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	443/514 (86%)	420 (95%)	23 (5%)	0	100	100
1	G	443/514 (86%)	421 (95%)	22 (5%)	0	100	100
1	H	444/514 (86%)	429 (97%)	15 (3%)	0	100	100
All	All	3547/4112 (86%)	3399 (96%)	148 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/452 (88%)	390 (98%)	6 (2%)	60	80
1	B	395/452 (87%)	389 (98%)	6 (2%)	60	80
1	C	395/452 (87%)	389 (98%)	6 (2%)	60	80
1	D	396/452 (88%)	391 (99%)	5 (1%)	65	83
1	E	395/452 (87%)	388 (98%)	7 (2%)	54	75
1	F	395/452 (87%)	388 (98%)	7 (2%)	54	75
1	G	395/452 (87%)	388 (98%)	7 (2%)	54	75
1	H	396/452 (88%)	388 (98%)	8 (2%)	50	73
All	All	3163/3616 (88%)	3111 (98%)	52 (2%)	58	78

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	GLU
1	A	183	TYR
1	A	239	THR
1	A	300	ARG
1	A	329	PHE
1	A	331	THR
1	B	81	LEU
1	B	84	GLU

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Mol	Chain	Res	Type
1	B	239	THR
1	B	300	ARG
1	B	329	PHE
1	B	446	THR
1	C	81	LEU
1	C	183	TYR
1	C	239	THR
1	C	300	ARG
1	C	356	ASN
1	C	357	SER
1	D	78	LEU
1	D	85	LYS
1	D	183	TYR
1	D	329	PHE
1	D	331	THR
1	E	82	TYR
1	E	85	LYS
1	E	95	ASP
1	E	239	THR
1	E	260	SER
1	E	300	ARG
1	E	422	MET
1	F	183	TYR
1	F	213	LYS
1	F	329	PHE
1	F	330	VAL
1	F	373	ASP
1	F	383	GLU
1	F	391	THR
1	G	182	LEU
1	G	183	TYR
1	G	300	ARG
1	G	329	PHE
1	G	331	THR
1	G	383	GLU
1	G	486	HIS
1	H	81	LEU
1	H	84	GLU
1	H	183	TYR
1	H	193	LEU
1	H	239	THR
1	H	300	ARG

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Mol	Chain	Res	Type
1	H	329	PHE
1	H	486	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	486	HIS
1	E	66	HIS
1	E	207	GLN
1	E	226	ASN
1	E	327	ASN
1	F	355	GLN
1	G	491	ASN
1	H	54	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	446/514 (86%)	-0.18	2 (0%) 89 87	26, 42, 69, 96	0
1	B	445/514 (86%)	-0.06	3 (0%) 84 82	27, 45, 67, 102	0
1	C	445/514 (86%)	-0.12	4 (0%) 81 78	25, 42, 64, 96	0
1	D	446/514 (86%)	0.15	13 (2%) 54 49	30, 48, 72, 108	0
1	E	445/514 (86%)	0.09	6 (1%) 74 71	31, 48, 75, 109	0
1	F	445/514 (86%)	0.15	9 (2%) 64 61	32, 50, 72, 105	0
1	G	445/514 (86%)	0.25	8 (1%) 67 64	31, 55, 77, 105	0
1	H	446/514 (86%)	0.53	17 (3%) 44 40	39, 62, 86, 114	0
All	All	3563/4112 (86%)	0.10	62 (1%) 69 65	25, 48, 75, 114	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	330	VAL	4.4
1	G	329	PHE	4.2
1	E	330	VAL	4.0
1	C	330	VAL	4.0
1	H	330	VAL	3.9
1	F	330	VAL	3.8
1	B	356	ASN	3.4
1	E	51	PRO	3.2
1	F	51	PRO	3.2
1	D	357	SER	3.1
1	D	51	PRO	3.1
1	E	331	THR	3.1
1	D	361	LYS	3.0
1	B	400	HIS	3.0
1	D	419	SER	3.0
1	D	356	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	391	THR	2.9
1	B	330	VAL	2.9
1	D	330	VAL	2.9
1	H	53	THR	2.9
1	G	51	PRO	2.8
1	H	355	GLN	2.8
1	F	419	SER	2.7
1	D	395	LYS	2.6
1	D	80	ALA	2.6
1	H	329	PHE	2.5
1	C	51	PRO	2.4
1	G	419	SER	2.4
1	H	315	SER	2.4
1	G	388	GLY	2.4
1	H	115	ASN	2.4
1	H	268	PHE	2.4
1	E	486	HIS	2.4
1	H	419	SER	2.4
1	C	400	HIS	2.3
1	C	331	THR	2.3
1	H	327	ASN	2.3
1	D	249	THR	2.3
1	E	329	PHE	2.3
1	H	384	ILE	2.3
1	G	80	ALA	2.3
1	F	384	ILE	2.2
1	D	311	LYS	2.2
1	D	312	VAL	2.2
1	H	400	HIS	2.2
1	D	81	LEU	2.1
1	F	385	ILE	2.1
1	H	334	ALA	2.1
1	A	331	THR	2.1
1	F	329	PHE	2.1
1	F	83	LYS	2.1
1	G	273	ASP	2.1
1	H	352	LEU	2.1
1	H	168	HIS	2.1
1	H	81	LEU	2.1
1	A	400	HIS	2.1
1	D	168	HIS	2.1
1	F	352	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	487	SER	2.0
1	G	384	ILE	2.0
1	H	83	LYS	2.0
1	H	401	ARG	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
2	CU	H	603	1/1	0.88	0.11	64,64,64,64	1
2	CU	G	601	1/1	0.93	0.09	79,79,79,79	1
2	CU	A	601	1/1	0.93	0.09	51,51,51,51	1
2	CU	G	603	1/1	0.95	0.06	55,55,55,55	1
2	CU	E	601	1/1	0.96	0.07	59,59,59,59	1
2	CU	E	602	1/1	0.97	0.04	39,39,39,39	1
2	CU	F	601	1/1	0.97	0.05	57,57,57,57	1
2	CU	C	603	1/1	0.97	0.07	38,38,38,38	1
2	CU	D	601	1/1	0.97	0.05	56,56,56,56	1
2	CU	B	603	1/1	0.97	0.06	41,41,41,41	1
2	CU	E	603	1/1	0.98	0.10	47,47,47,47	1
2	CU	E	604	1/1	0.98	0.05	63,63,63,63	0
2	CU	A	603	1/1	0.98	0.04	38,38,38,38	1
2	CU	F	602	1/1	0.98	0.05	51,51,51,51	1
2	CU	F	603	1/1	0.98	0.05	49,49,49,49	1
2	CU	D	603	1/1	0.98	0.04	43,43,43,43	1
2	CU	C	601	1/1	0.98	0.04	52,52,52,52	1
2	CU	H	601	1/1	0.98	0.08	71,71,71,71	1
2	CU	H	602	1/1	0.98	0.03	44,44,44,44	1

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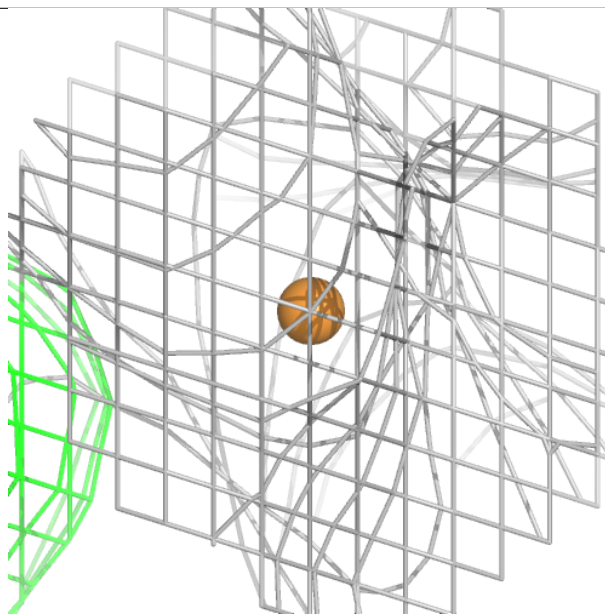
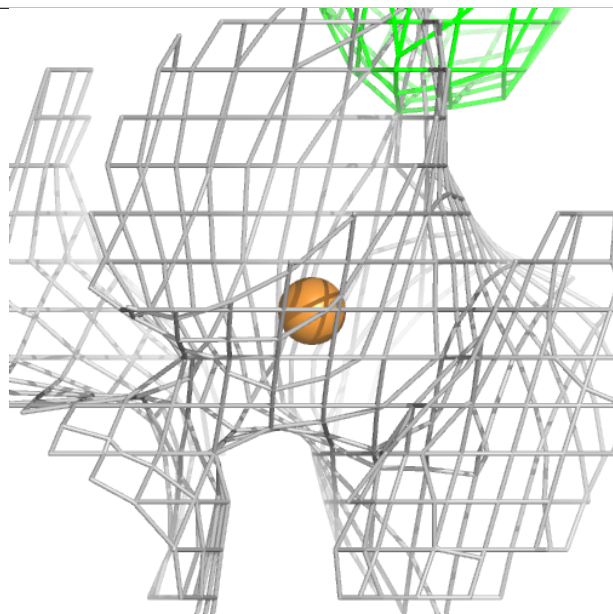
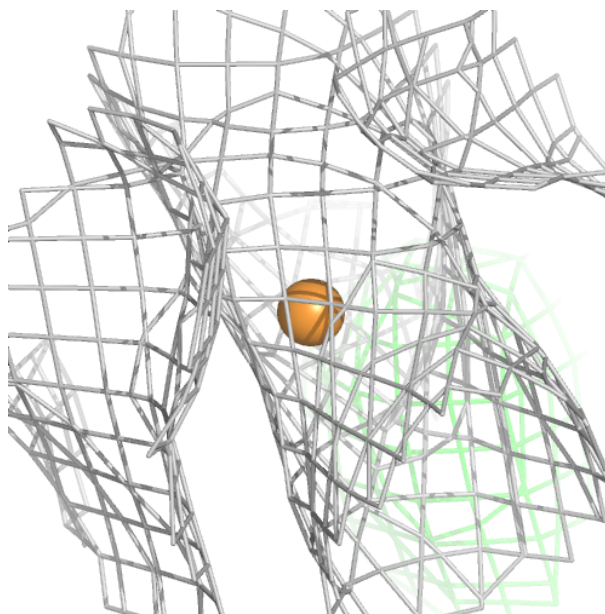
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CU	B	601	1/1	0.98	0.05	56,56,56,56	1
2	CU	H	604	1/1	0.98	0.04	66,66,66,66	1
2	CU	D	604	1/1	0.99	0.03	63,63,63,63	1
2	CU	F	604	1/1	0.99	0.03	63,63,63,63	0
2	CU	C	602	1/1	0.99	0.03	36,36,36,36	1
2	CU	G	602	1/1	0.99	0.03	47,47,47,47	1
2	CU	B	602	1/1	0.99	0.02	34,34,34,34	1
2	CU	G	604	1/1	0.99	0.04	63,63,63,63	0
2	CU	C	604	1/1	0.99	0.06	63,63,63,63	0
2	CU	A	604	1/1	0.99	0.09	63,63,63,63	0
2	CU	D	602	1/1	0.99	0.04	44,44,44,44	1
2	CU	A	602	1/1	0.99	0.03	32,32,32,32	1
2	CU	B	604	1/1	1.00	0.07	63,63,63,63	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.

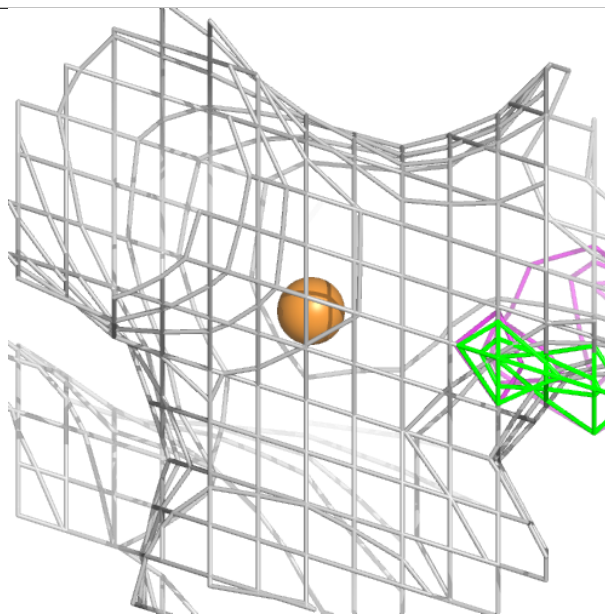
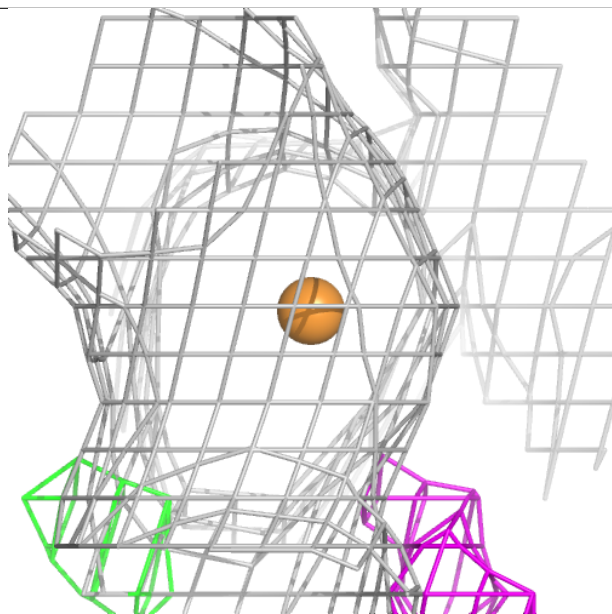
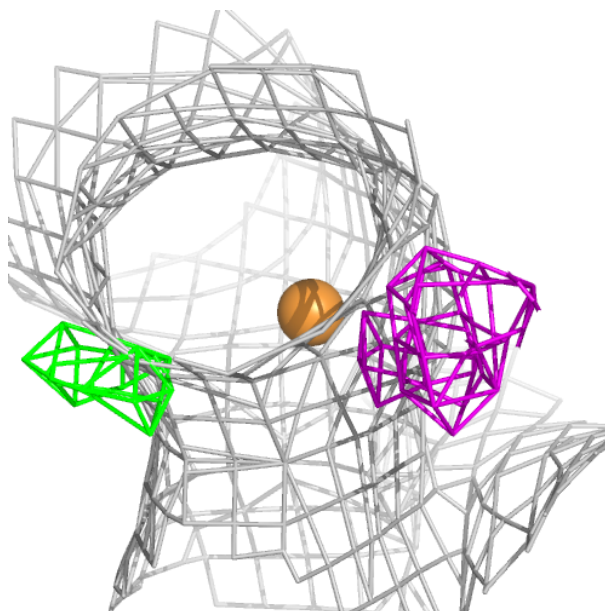
Electron density around CU H 603:

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



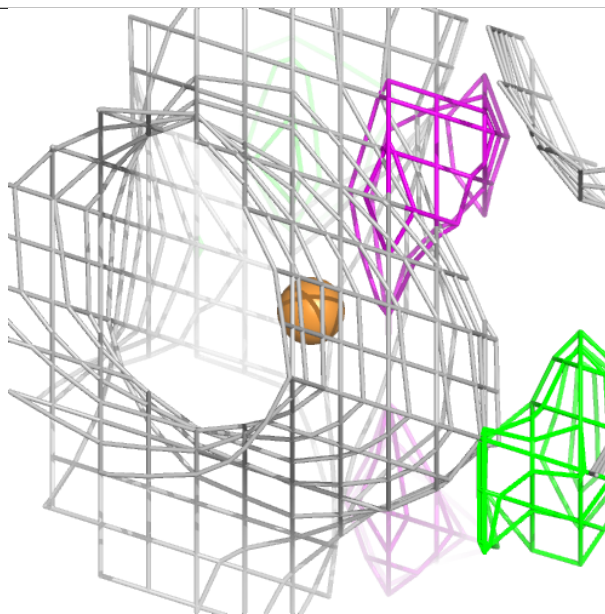
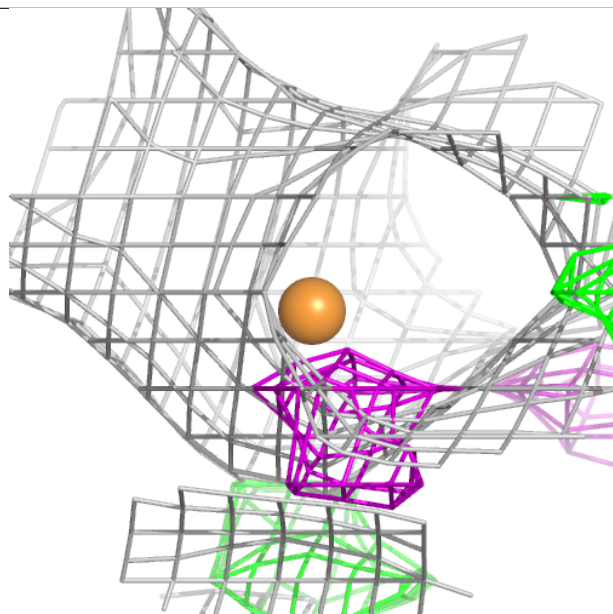
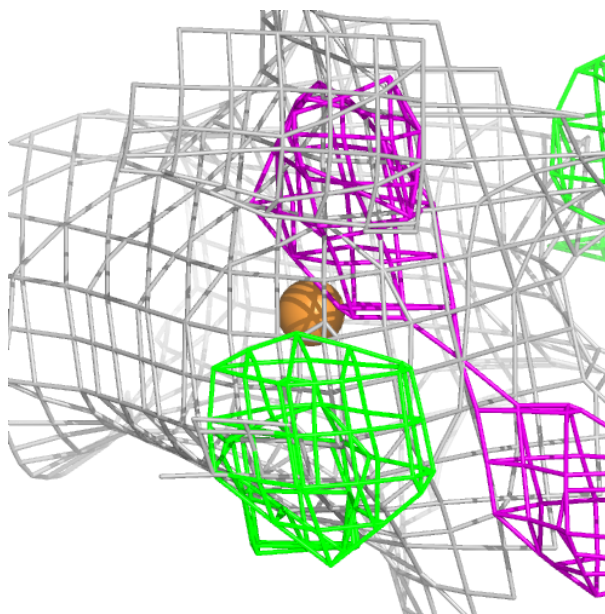
Electron density around CU G 601:

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



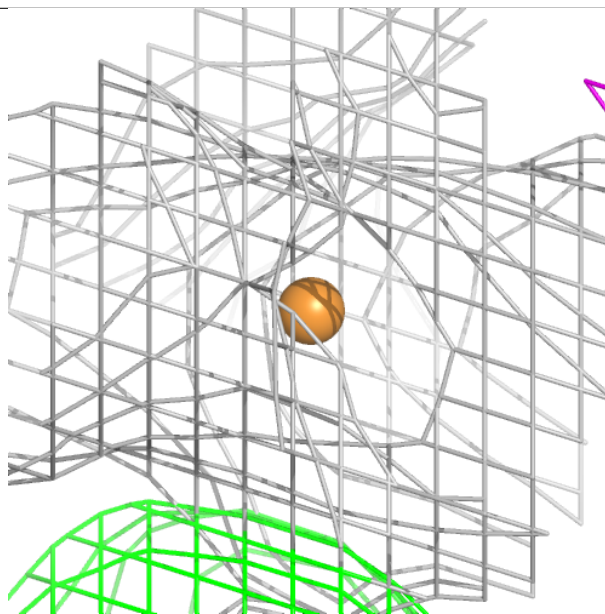
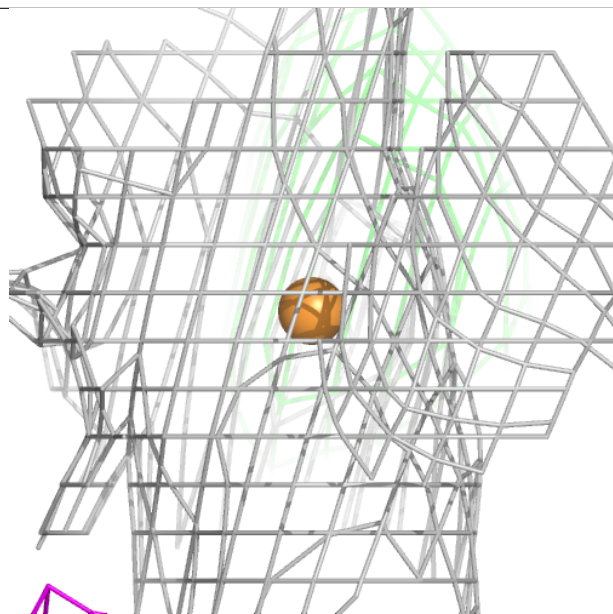
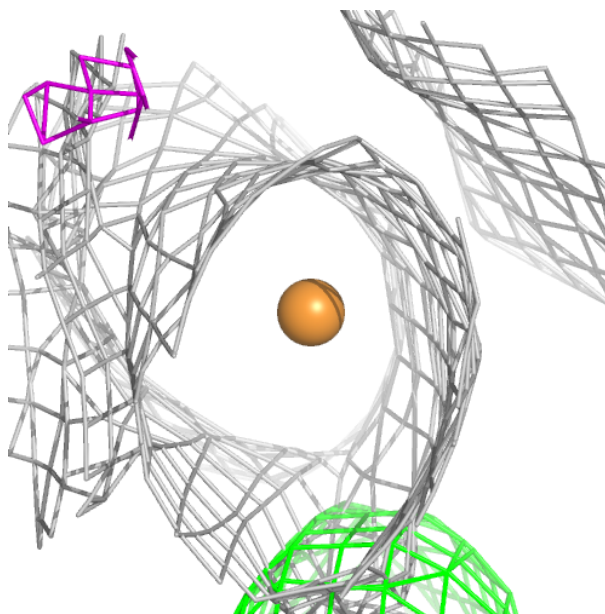
Electron density around CU A 601:

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



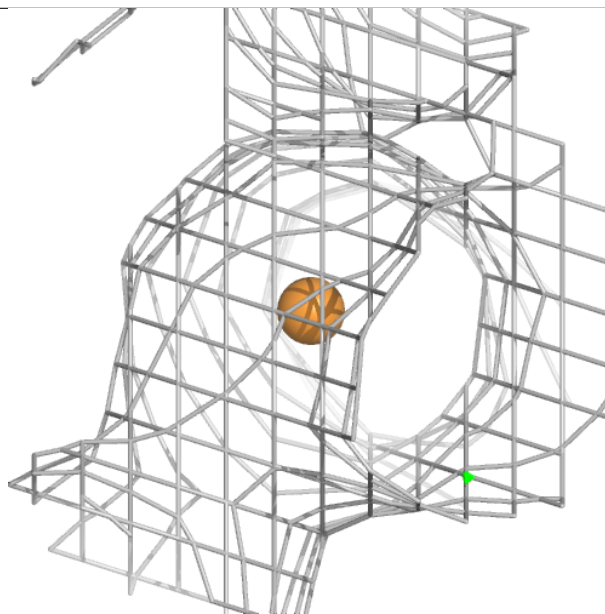
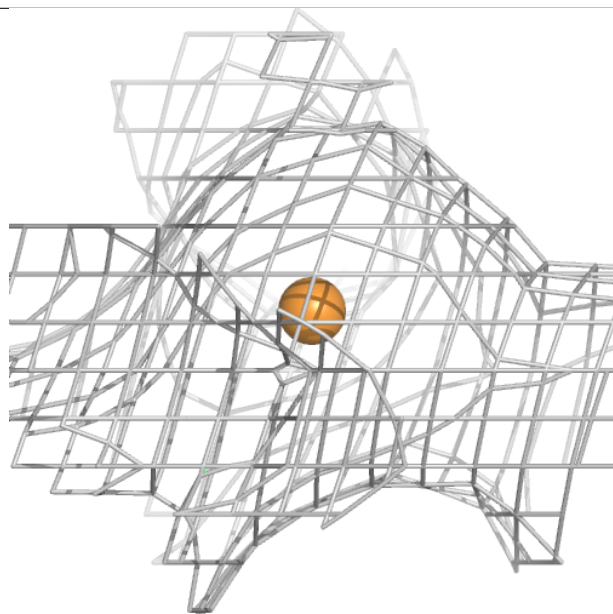
Electron density around CU G 603:

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



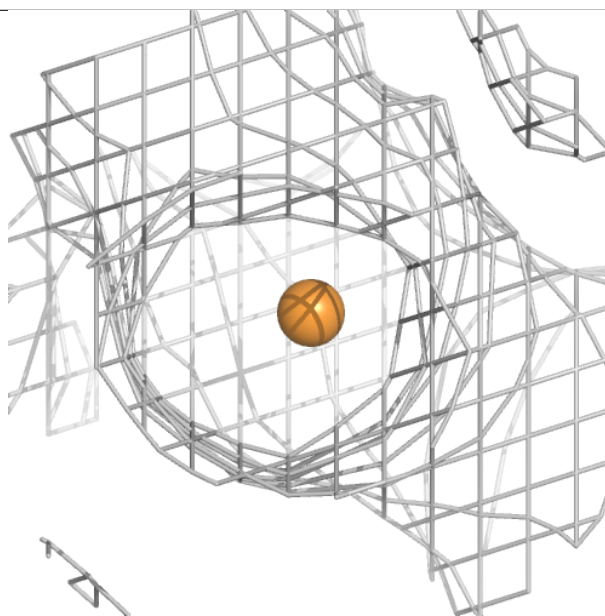
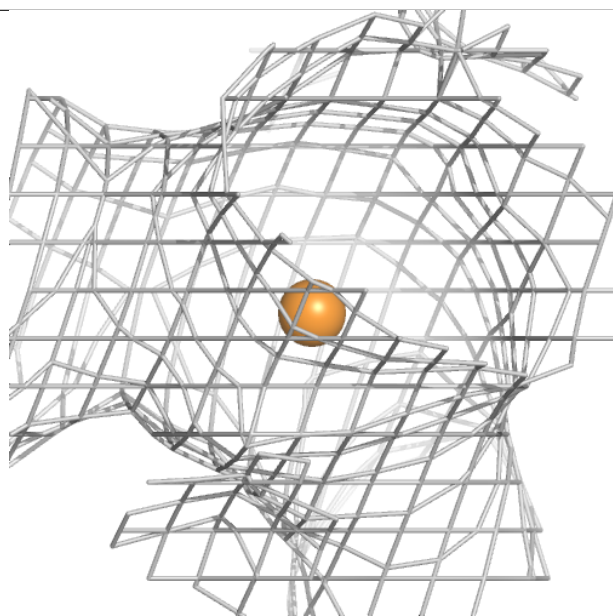
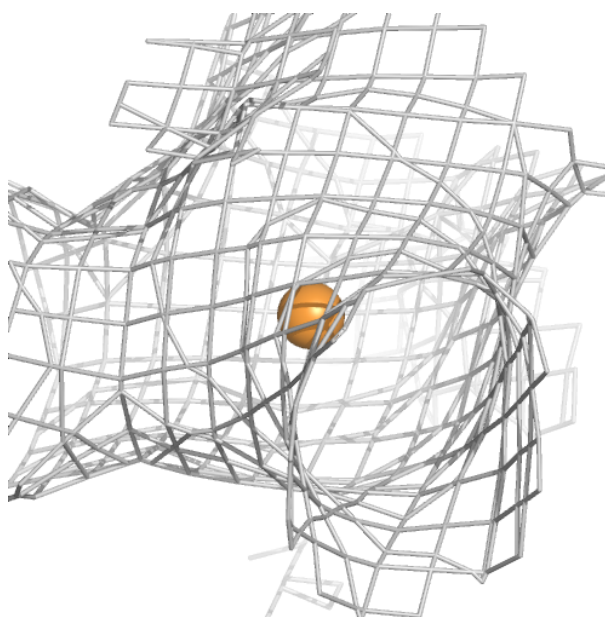
Electron density around CU E 601:

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



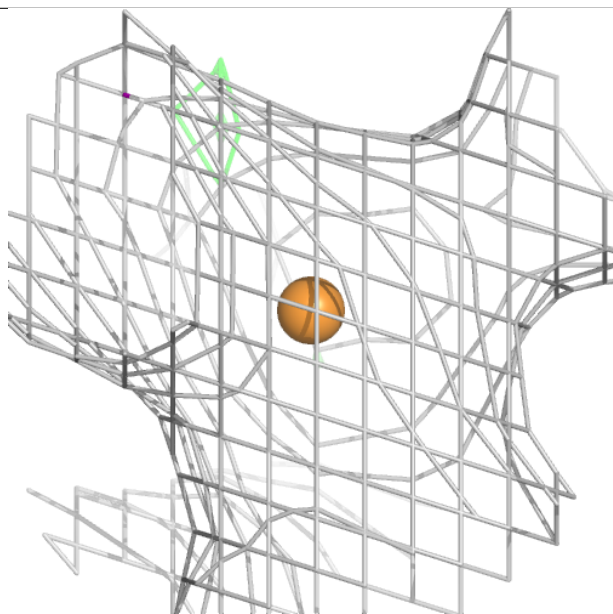
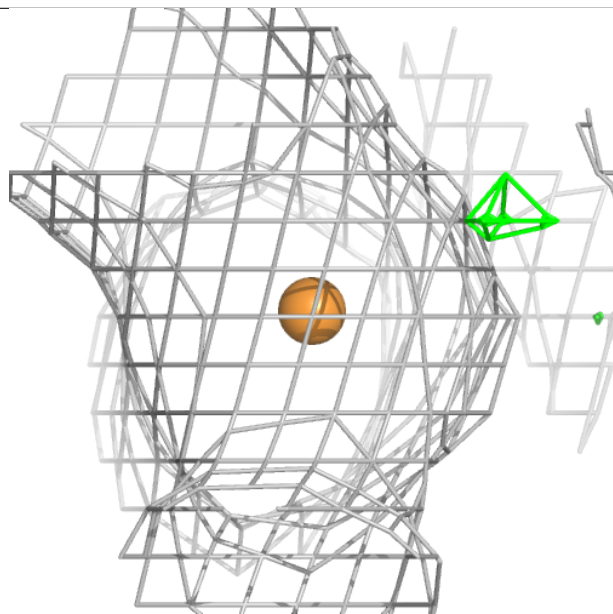
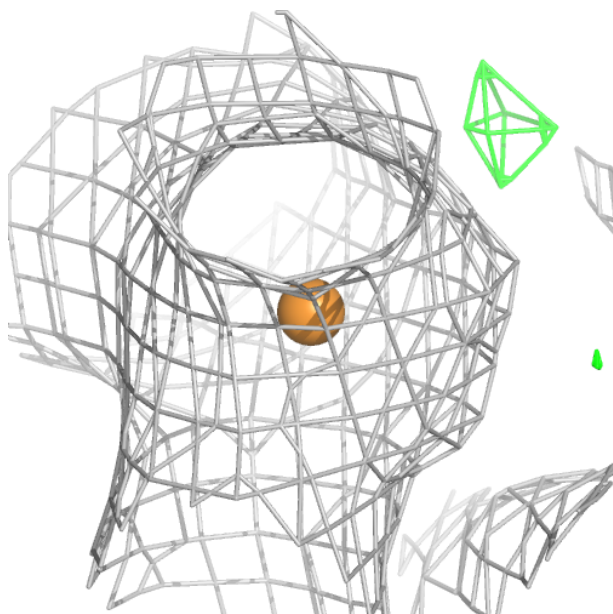
Electron density around CU E 602:

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



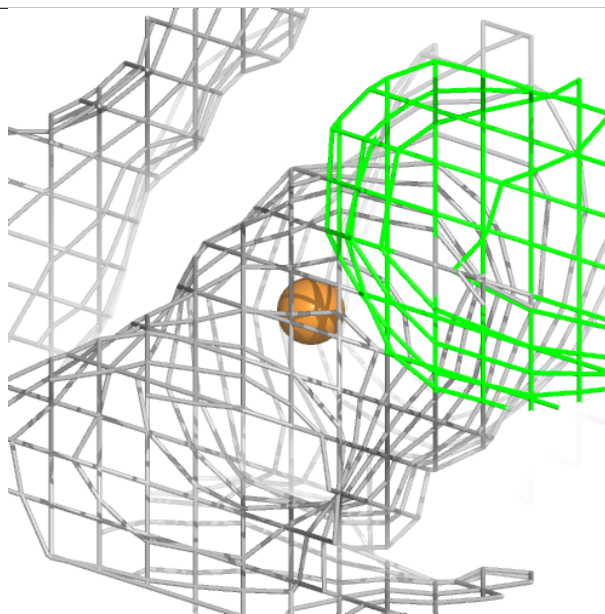
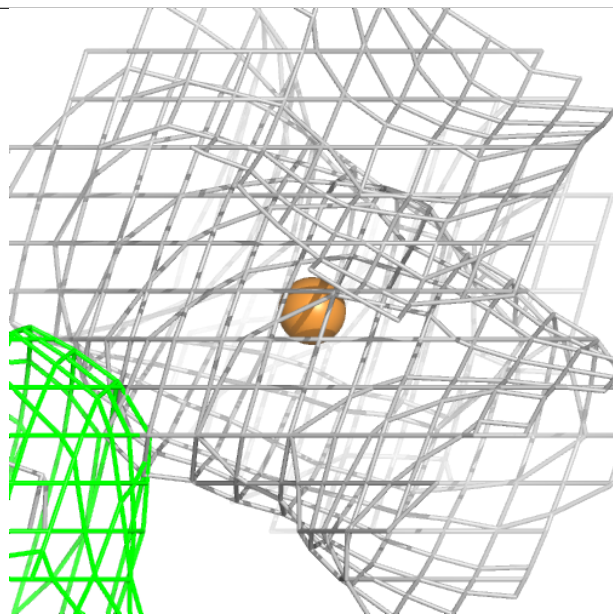
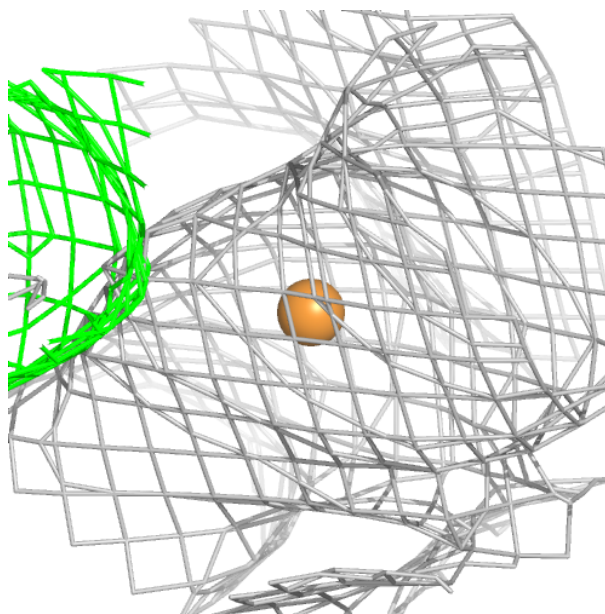
Electron density around CU F 601:

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



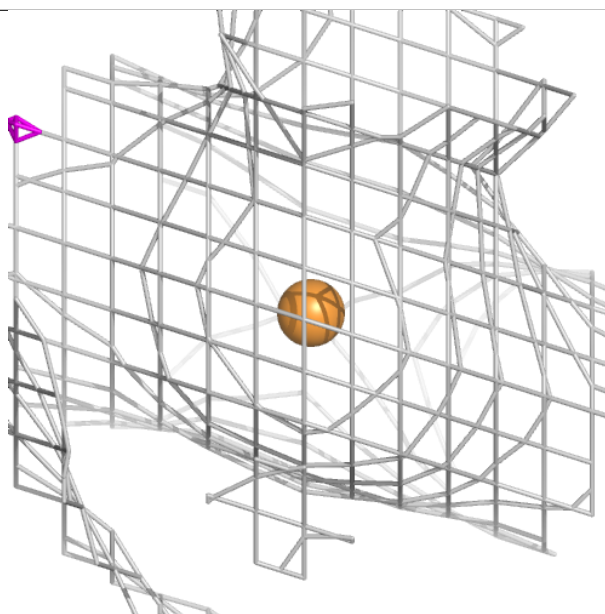
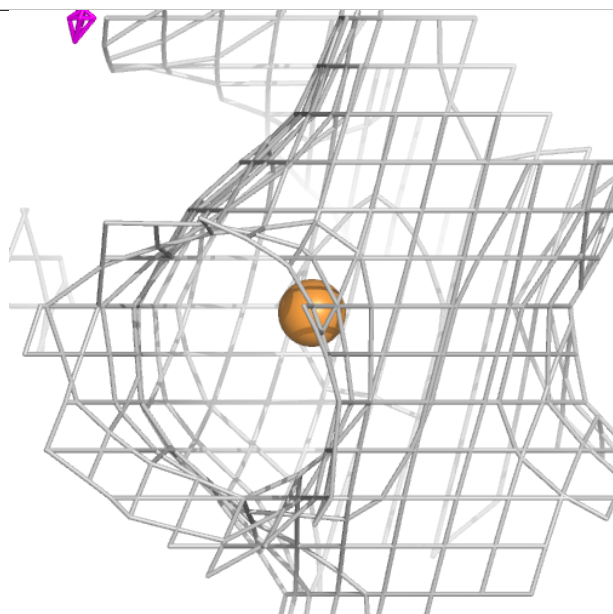
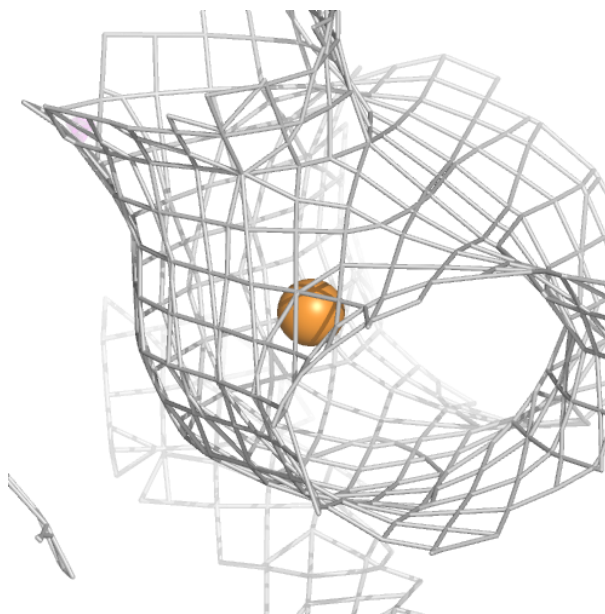
Electron density around CU C 603:

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



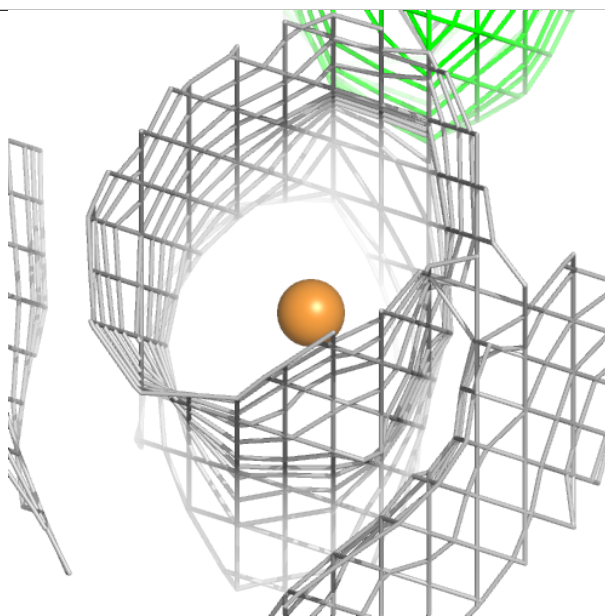
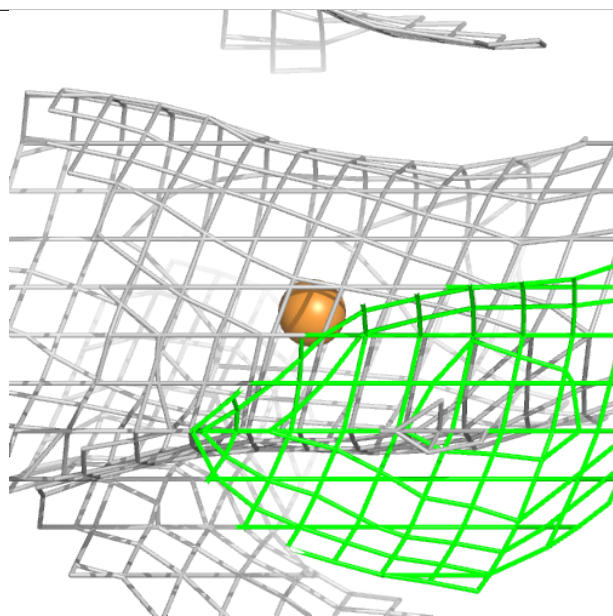
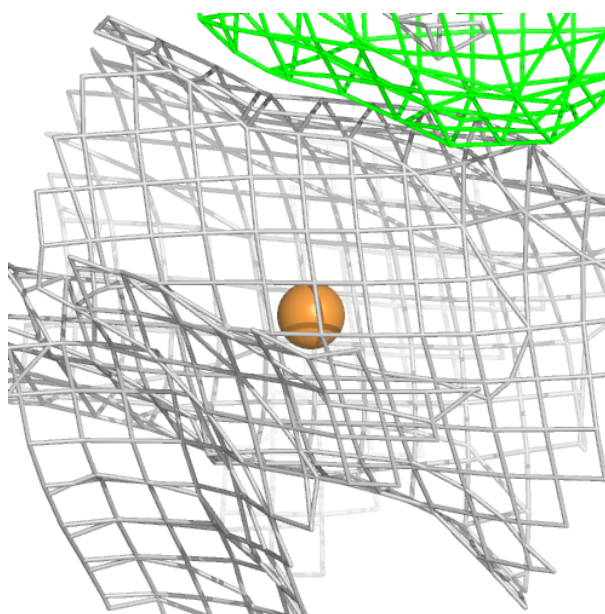
Electron density around CU D 601:

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



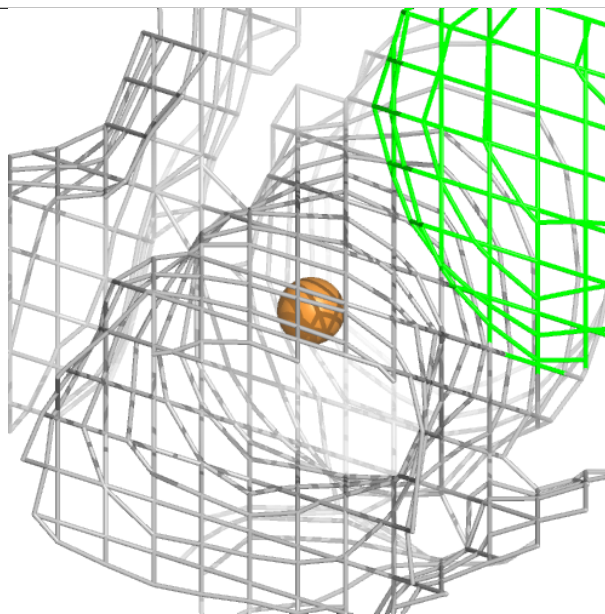
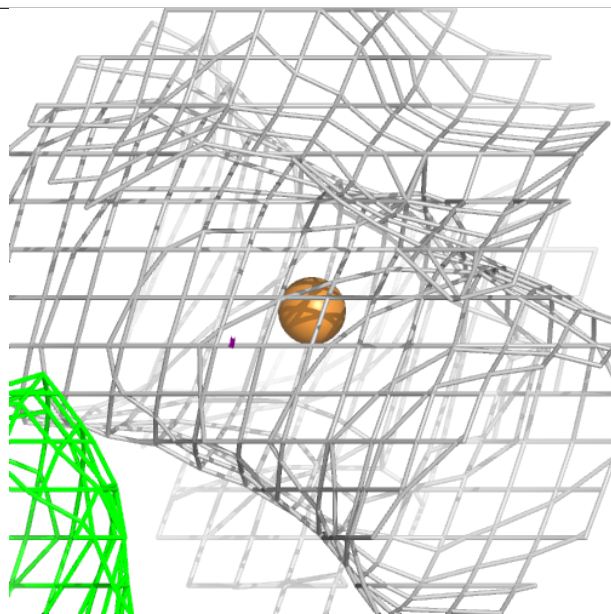
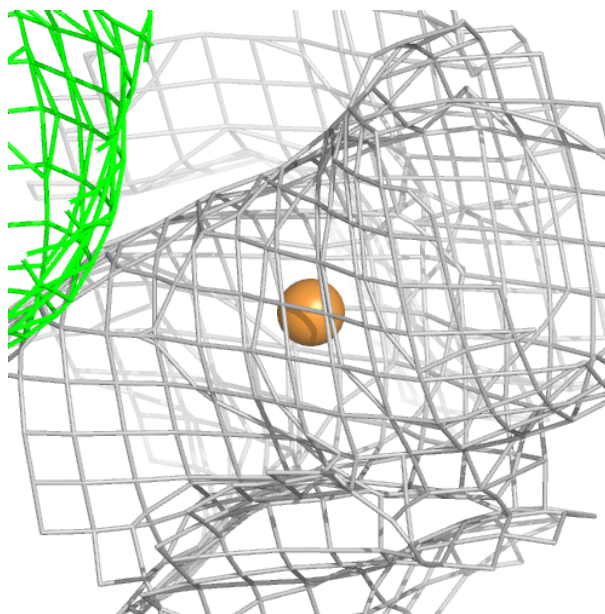
Electron density around CU B 603:

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



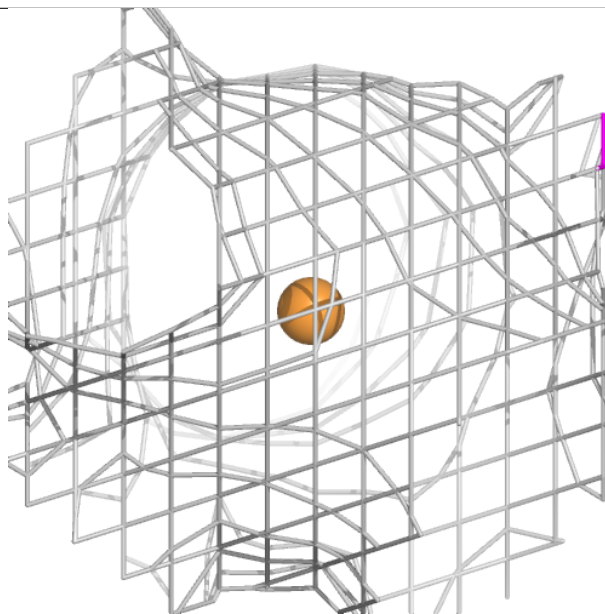
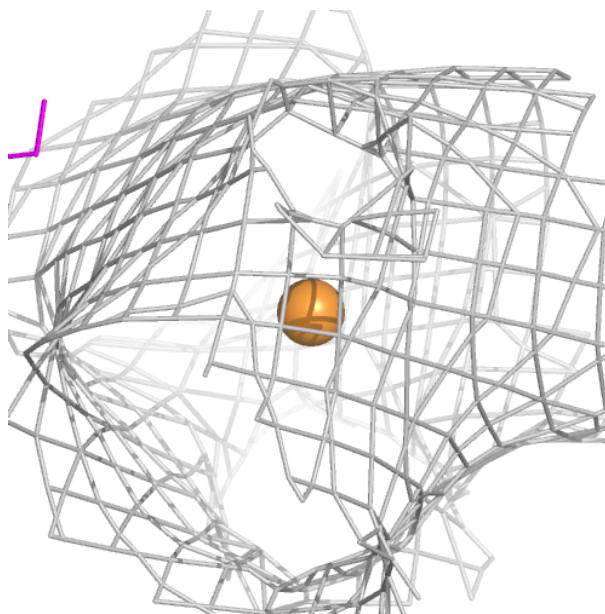
Electron density around CU E 603:

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



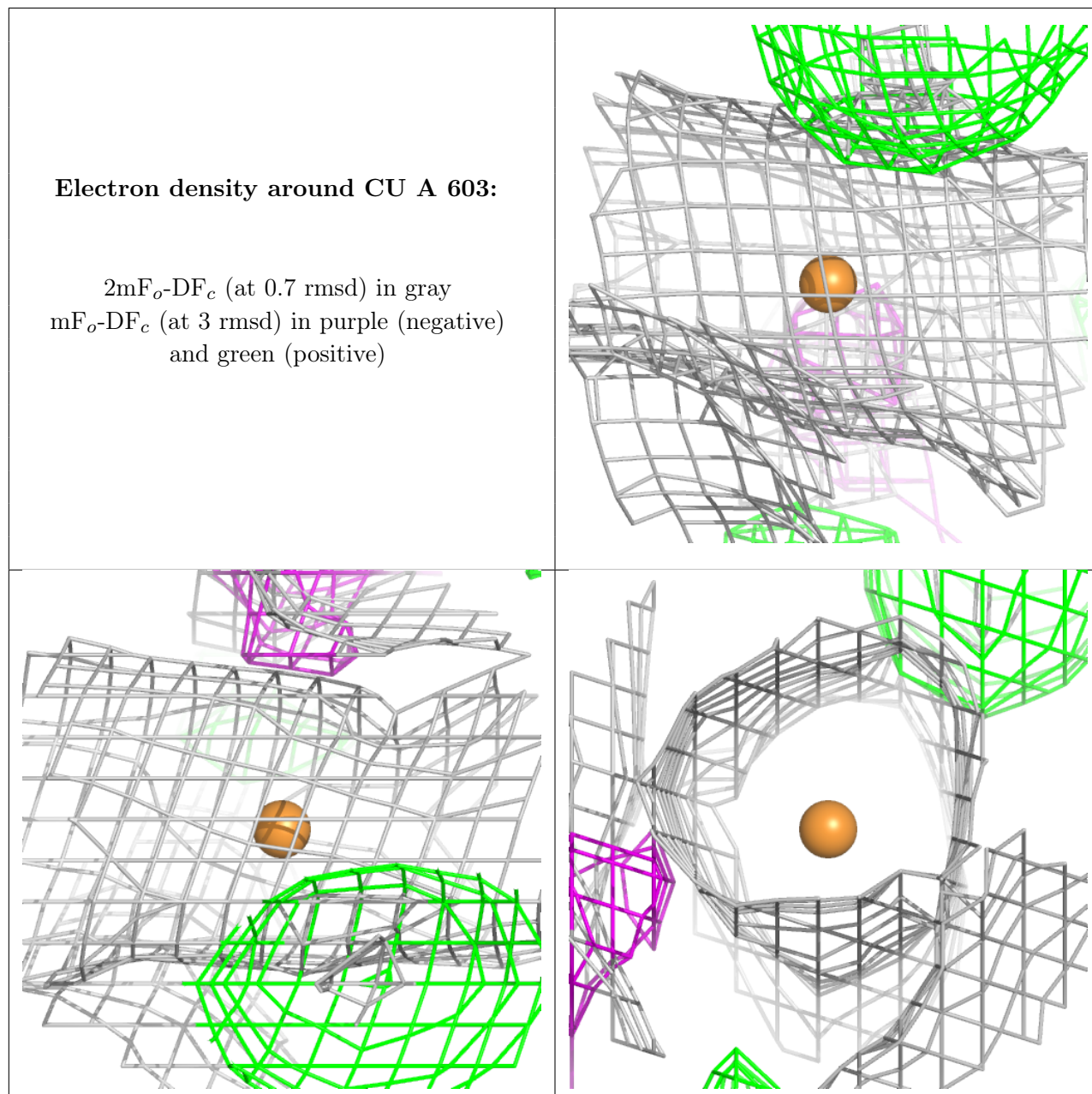
Electron density around CU E 604:

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



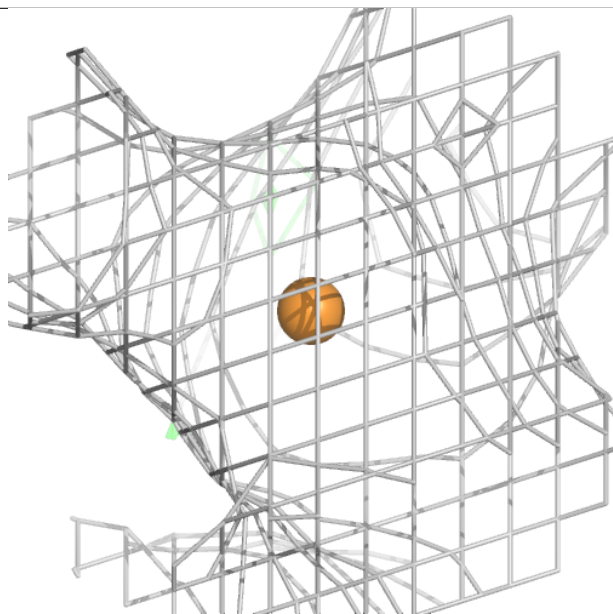
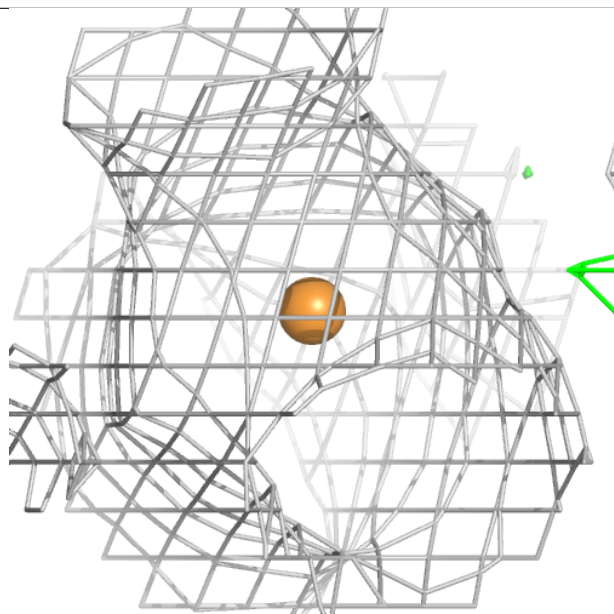
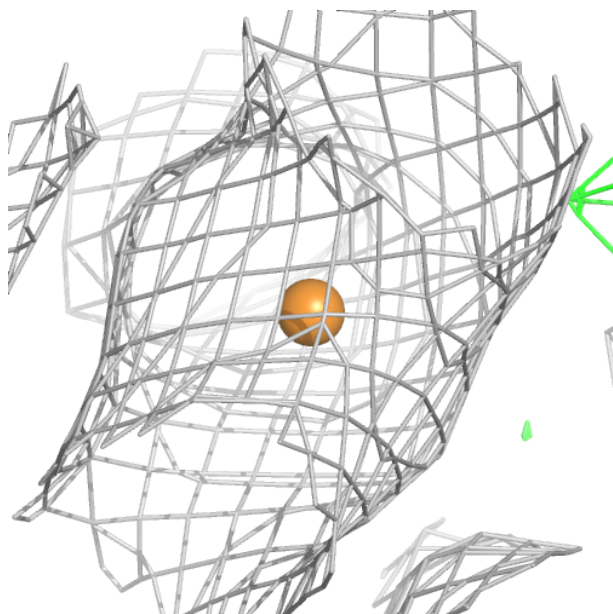
Electron density around CU A 603:

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



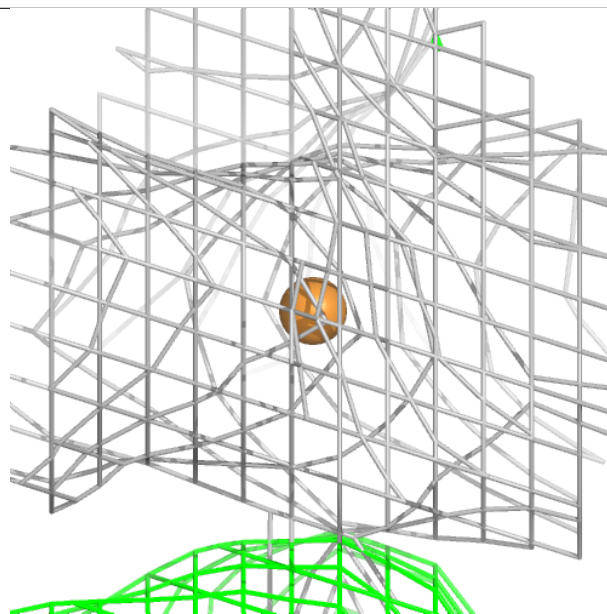
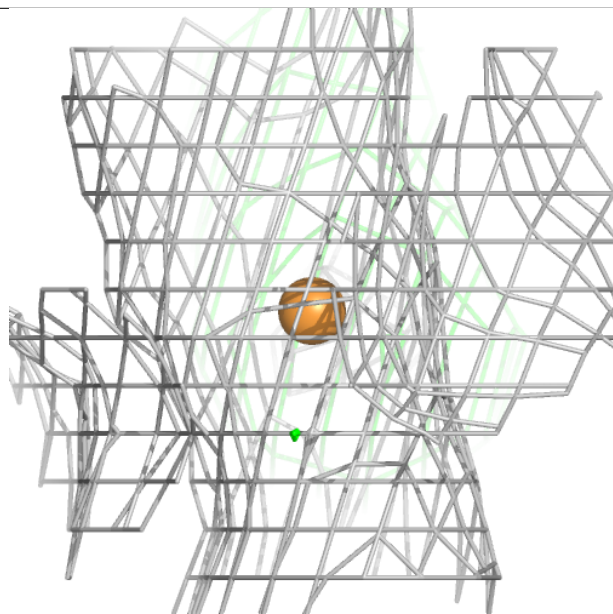
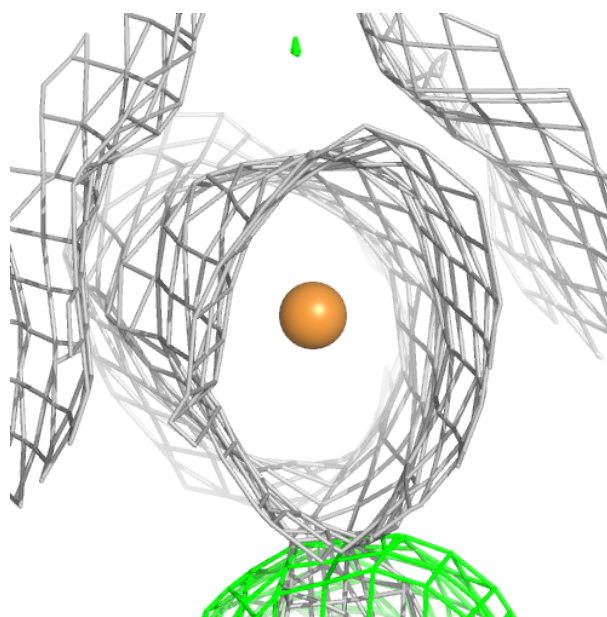
Electron density around CU F 602:

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



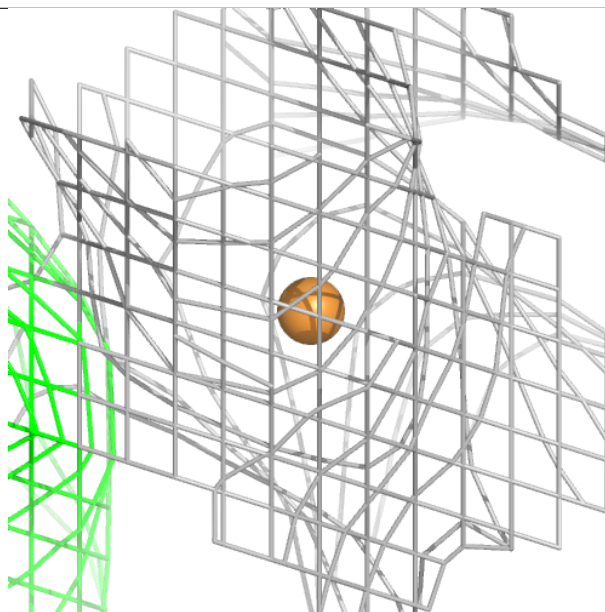
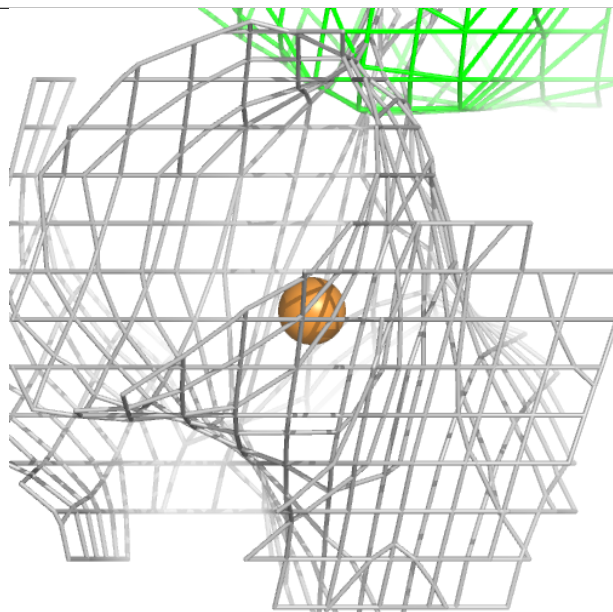
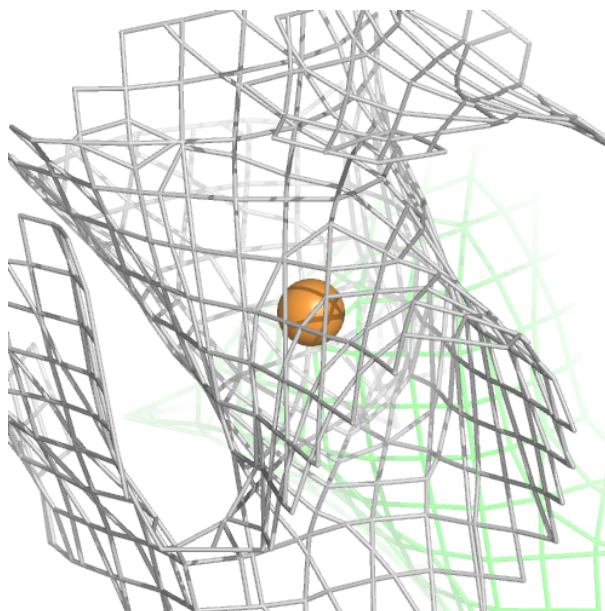
Electron density around CU F 603:

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



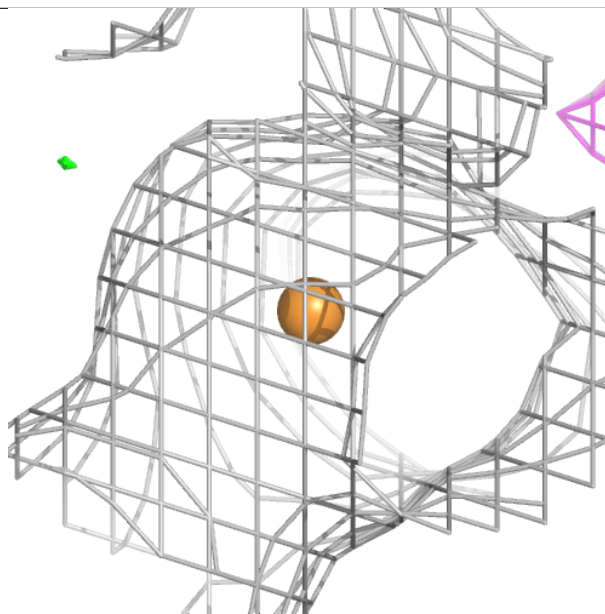
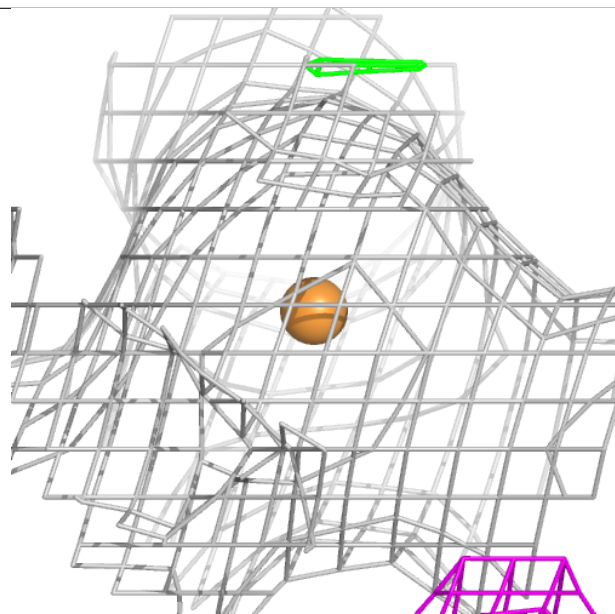
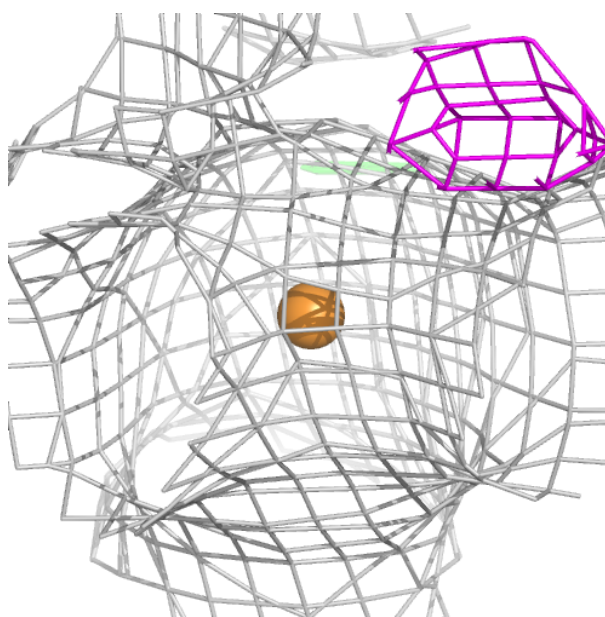
Electron density around CU D 603:

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



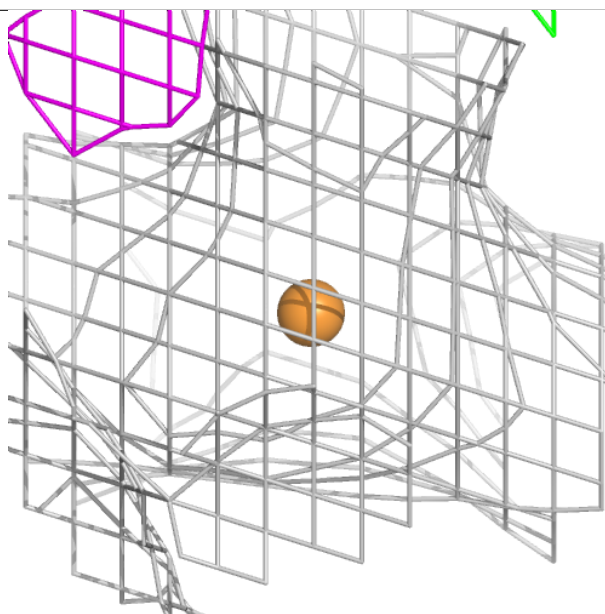
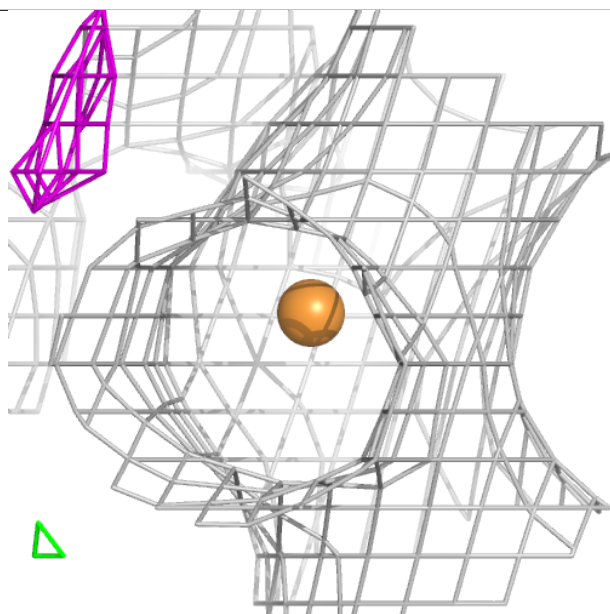
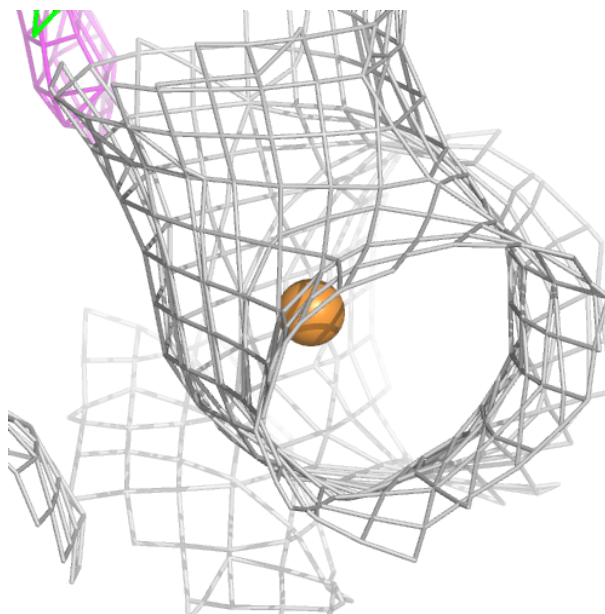
Electron density around CU C 601:

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



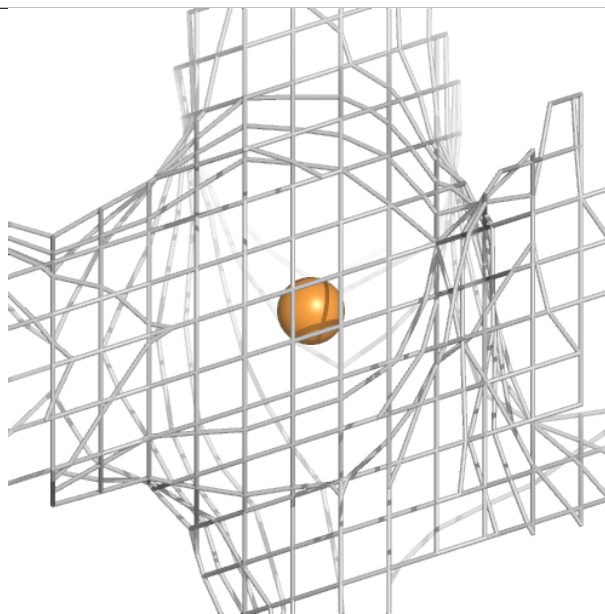
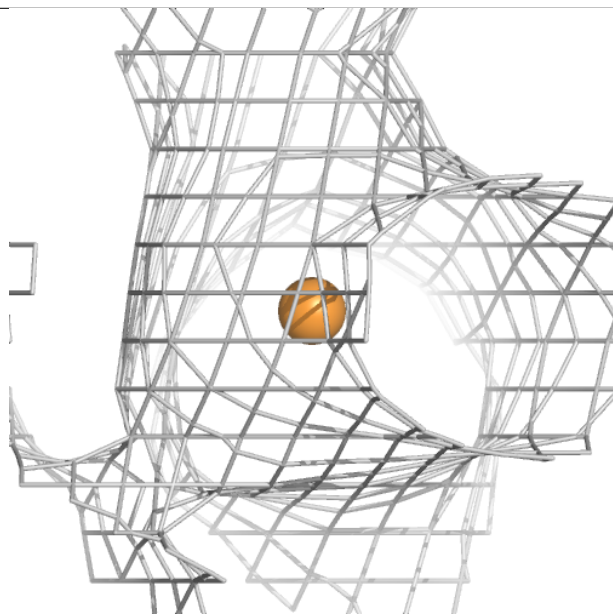
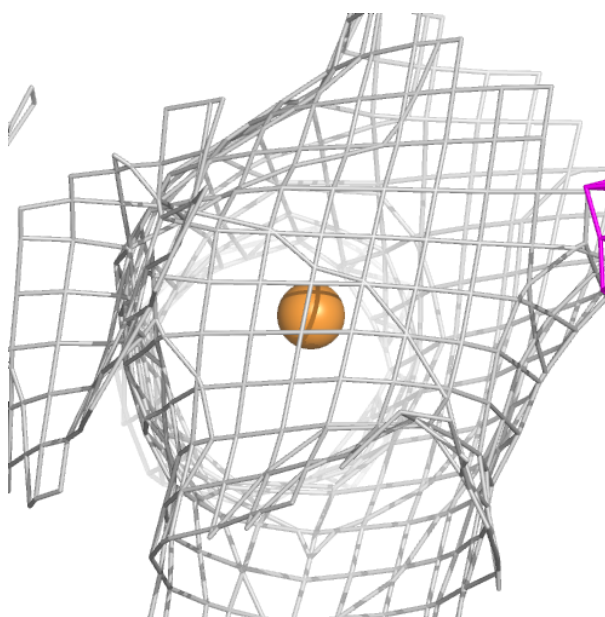
Electron density around CU H 601:

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



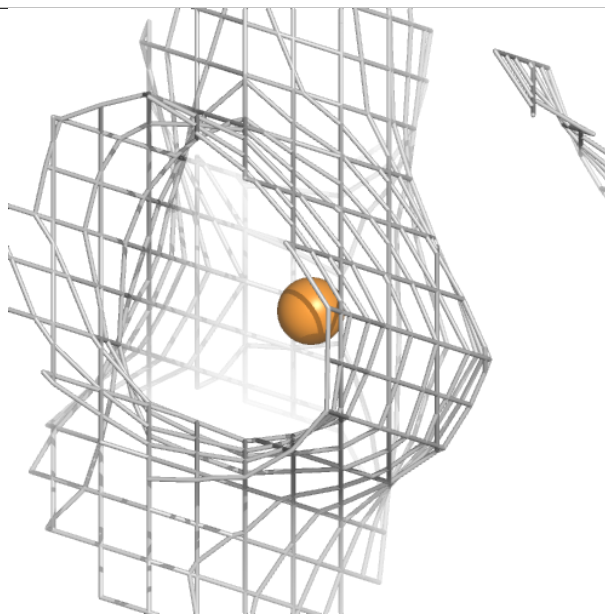
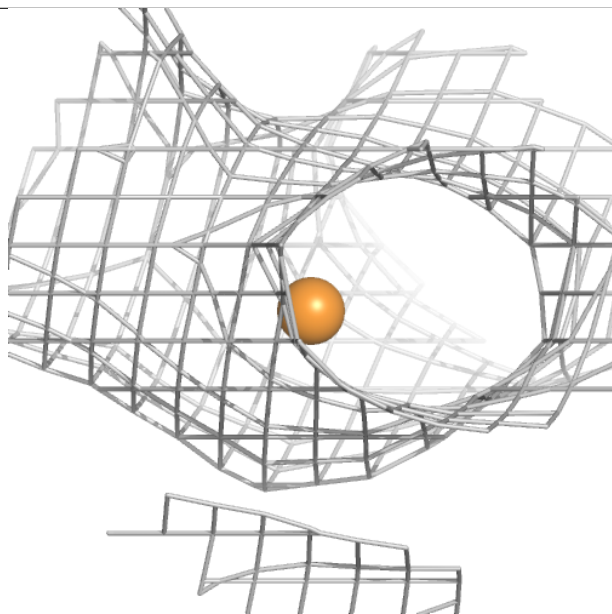
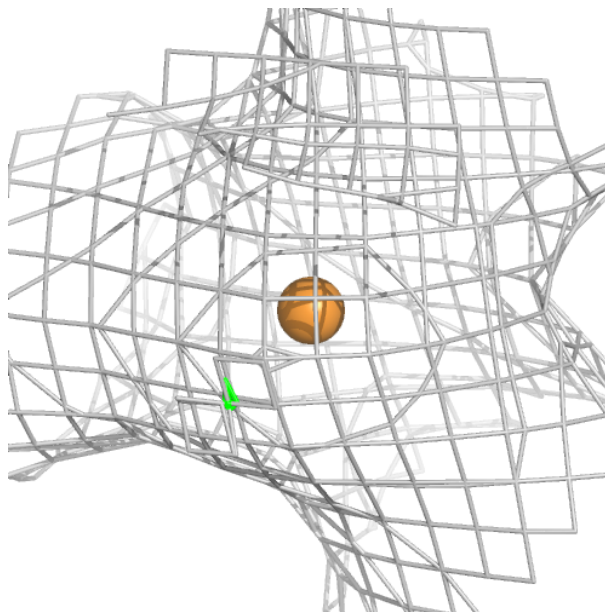
Electron density around CU H 602:

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



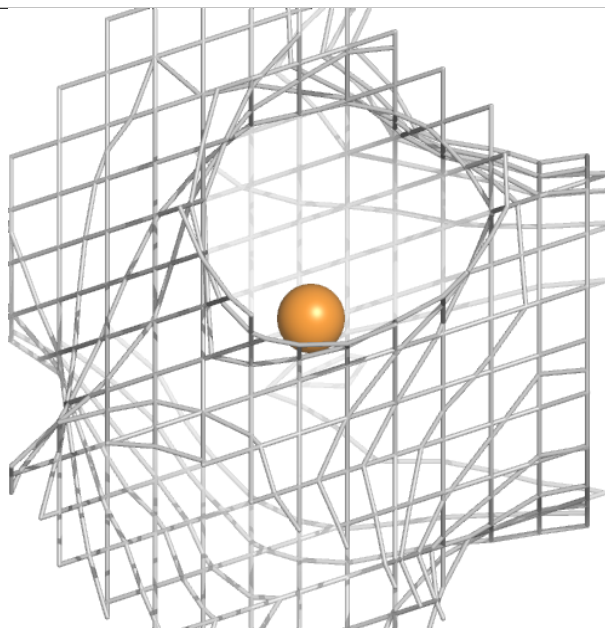
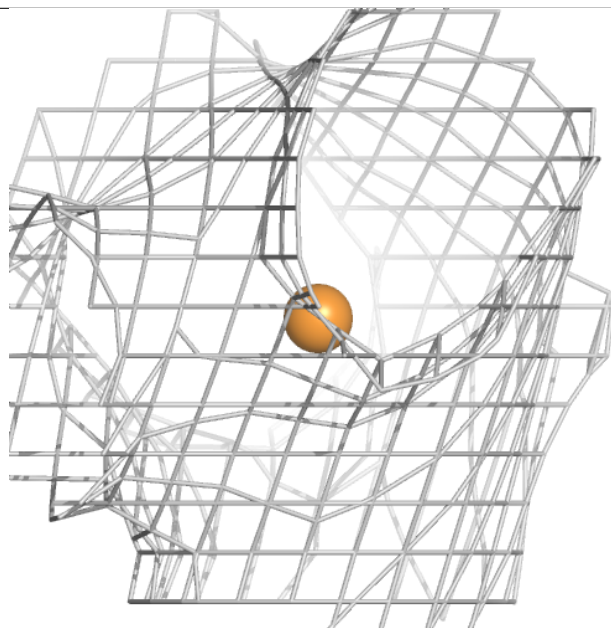
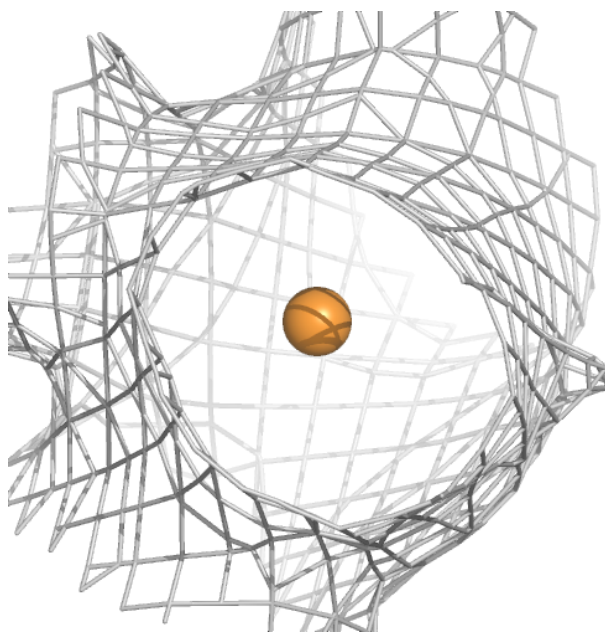
Electron density around CU B 601:

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



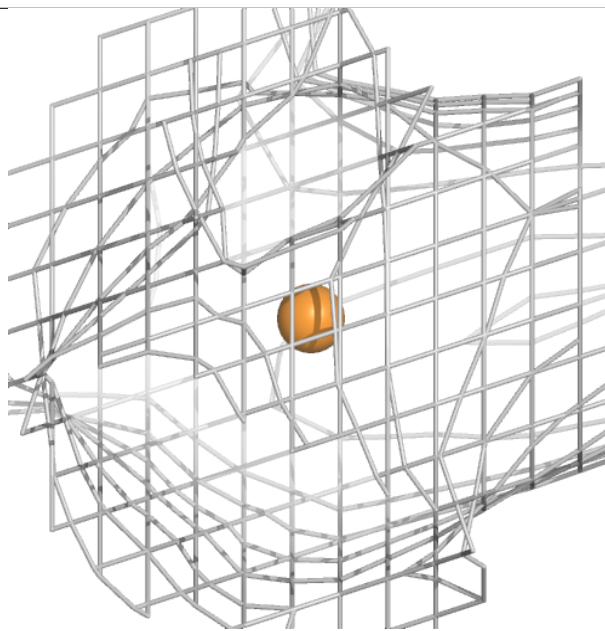
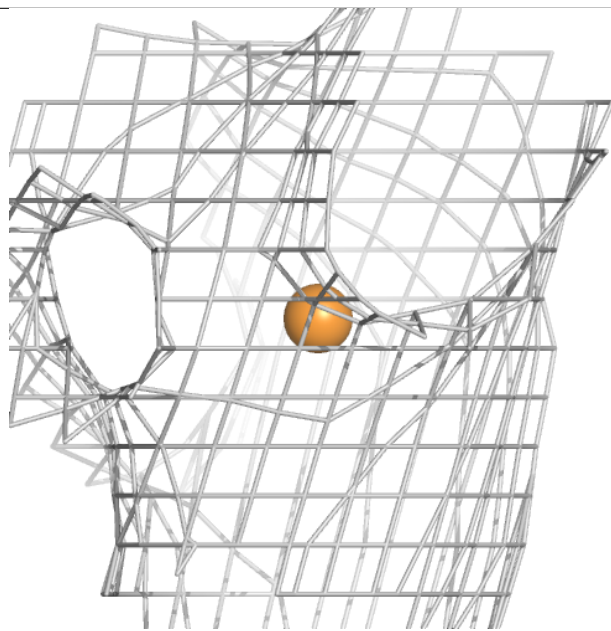
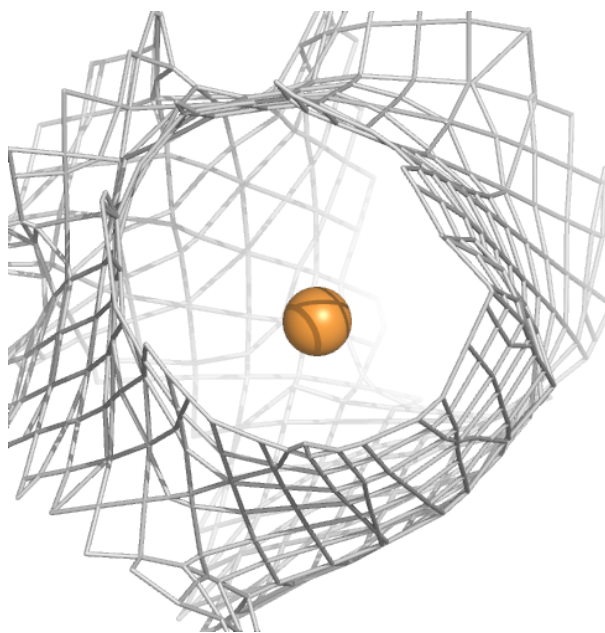
Electron density around CU H 604:

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



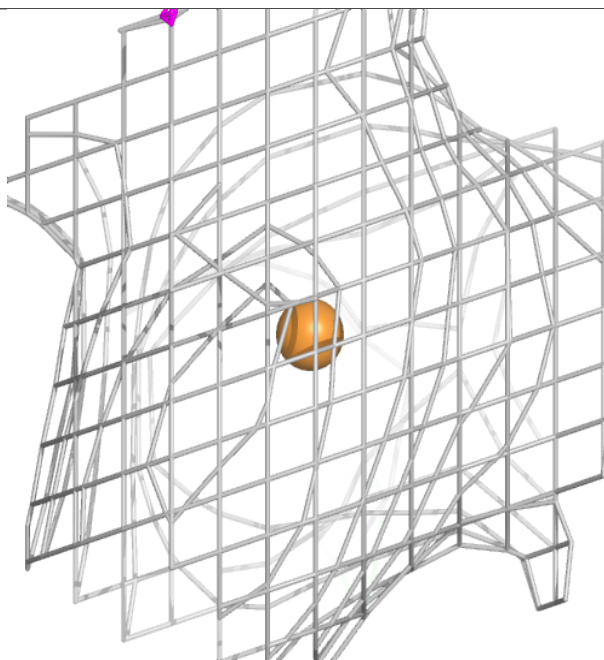
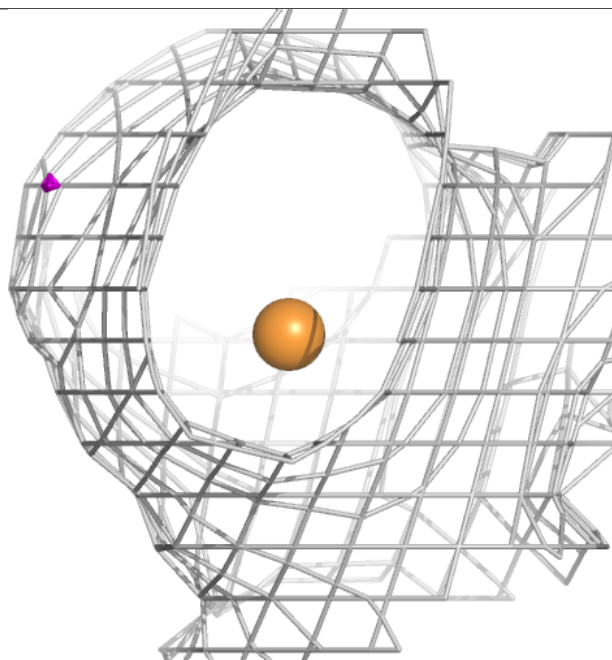
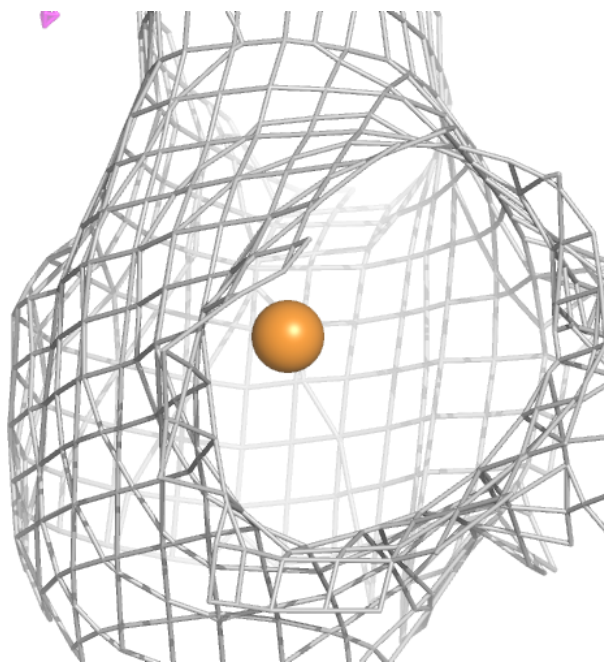
Electron density around CU D 604:

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



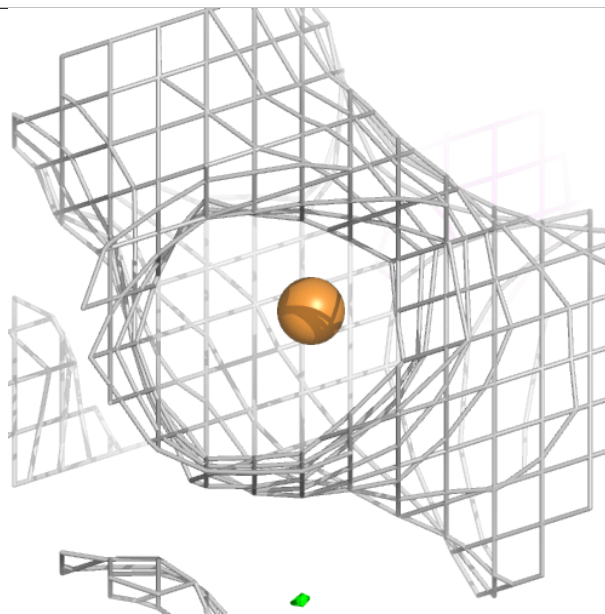
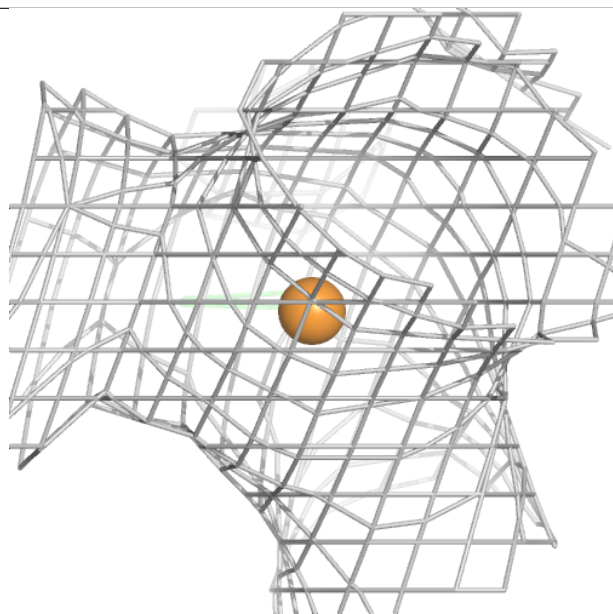
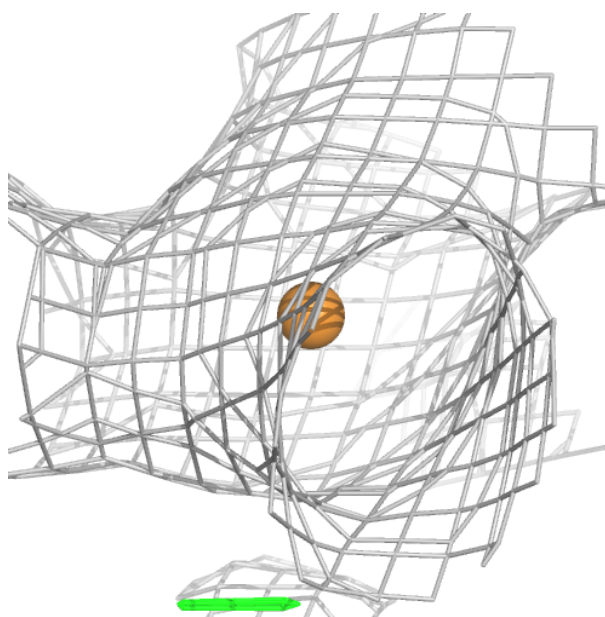
Electron density around CU F 604:

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



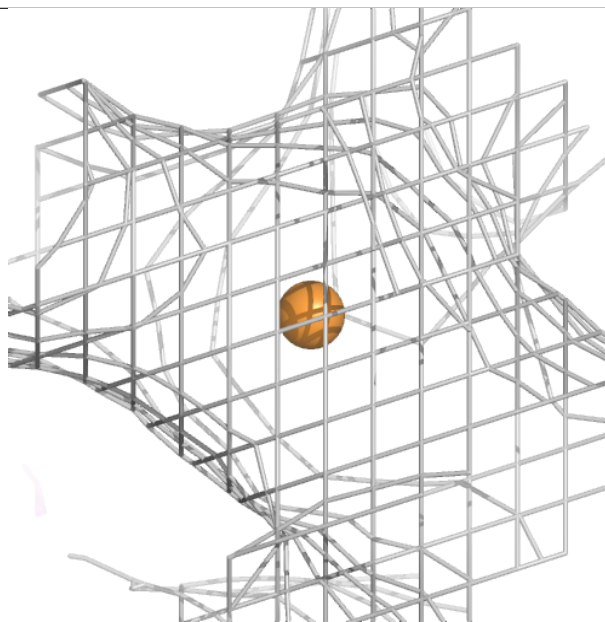
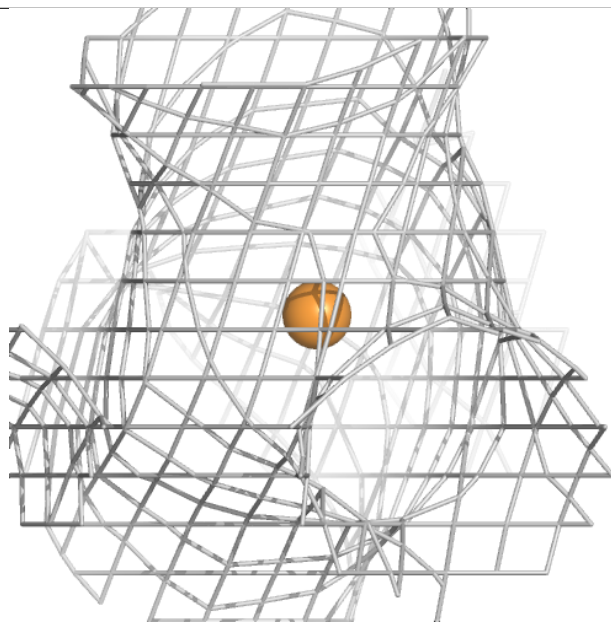
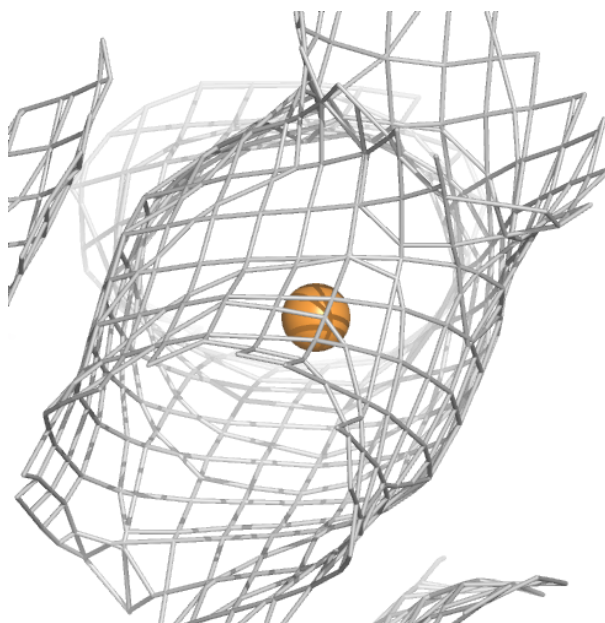
Electron density around CU C 602:

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



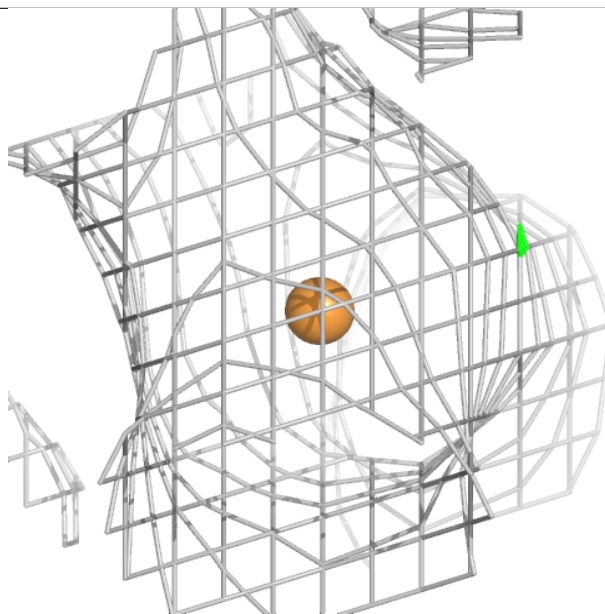
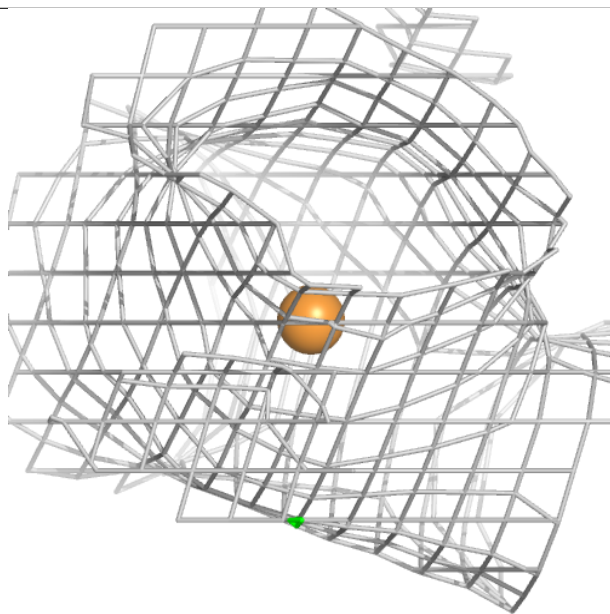
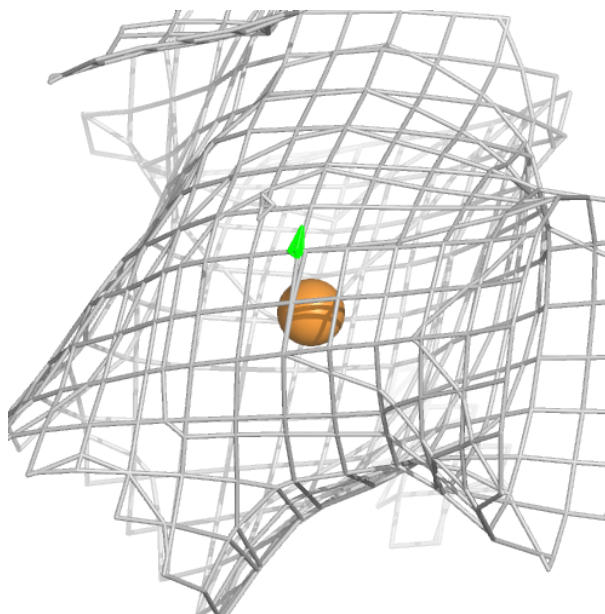
Electron density around CU G 602:

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



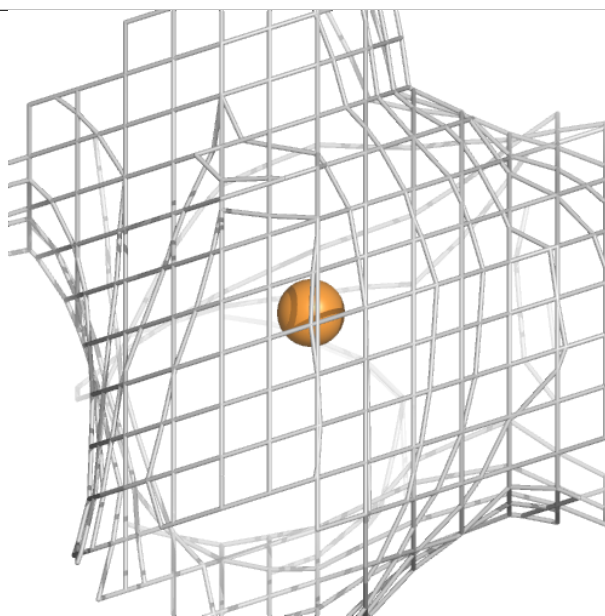
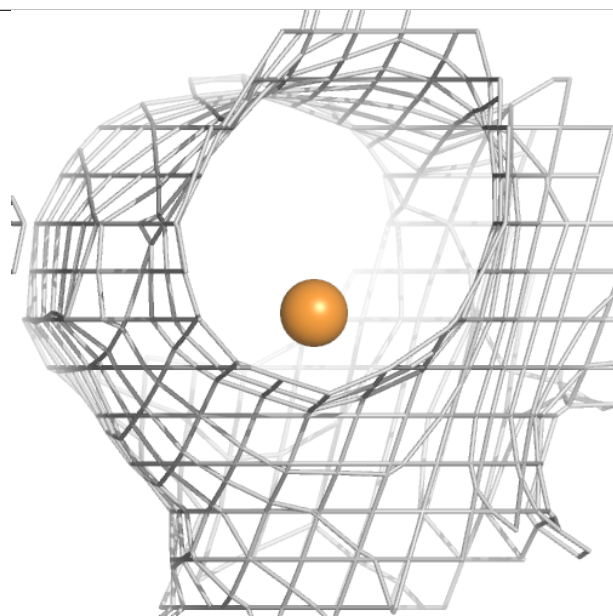
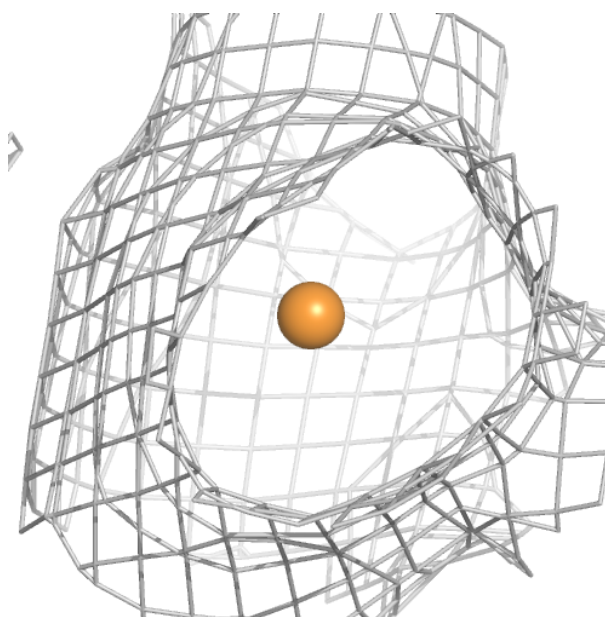
Electron density around CU B 602:

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



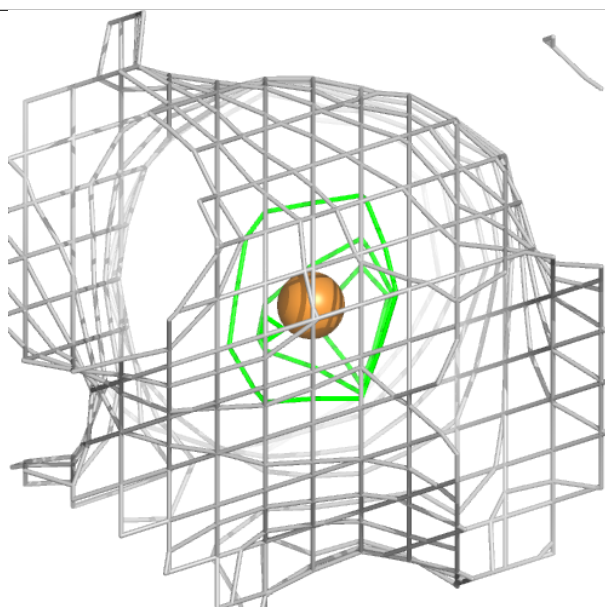
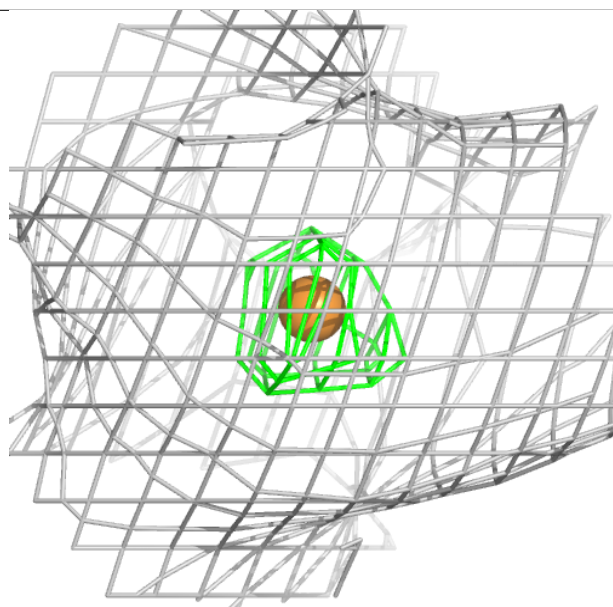
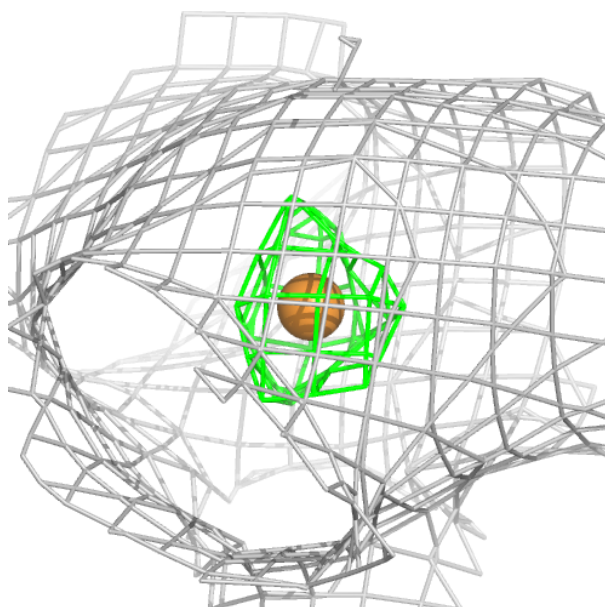
Electron density around CU G 604:

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



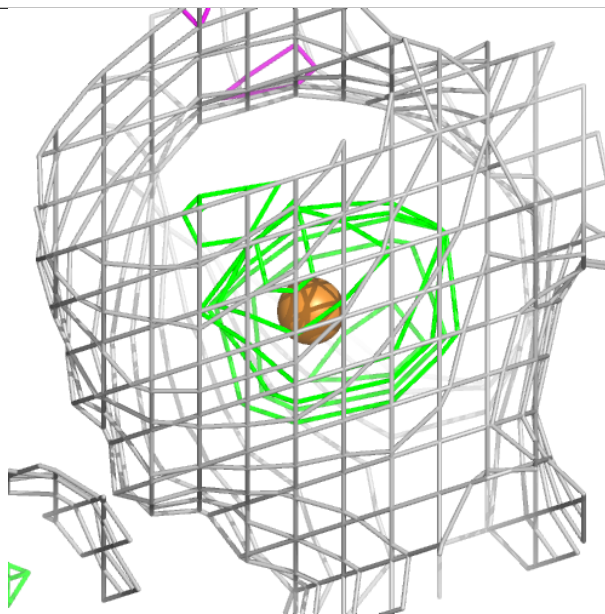
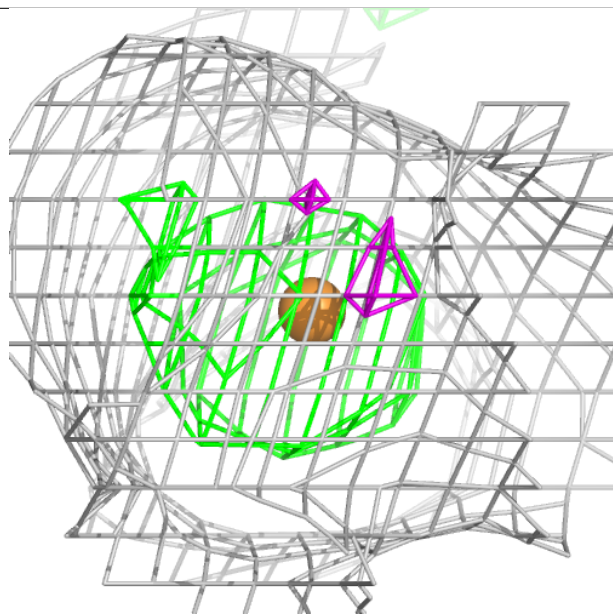
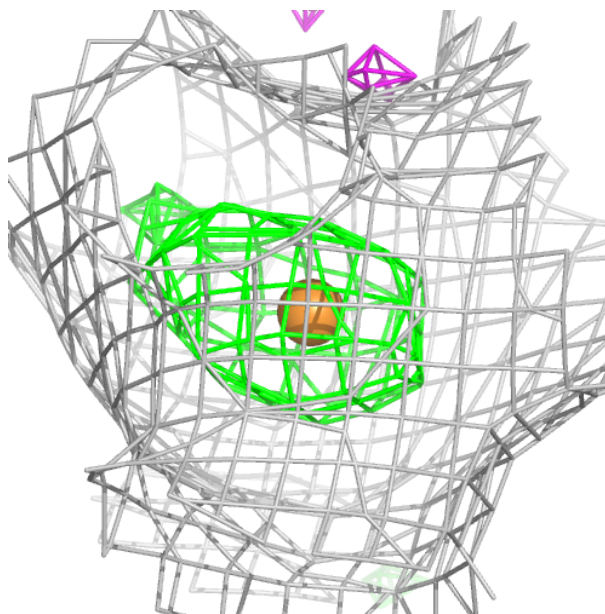
Electron density around CU C 604:

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



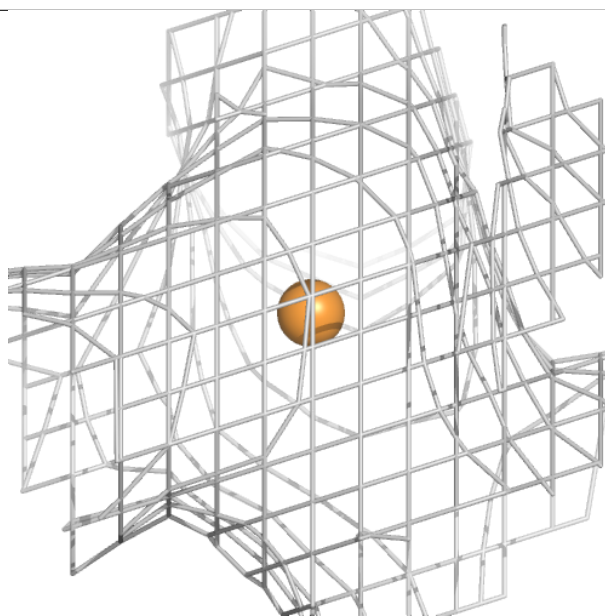
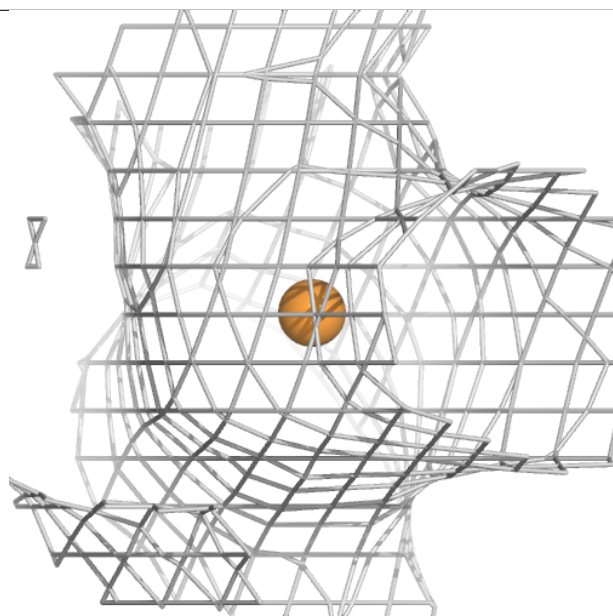
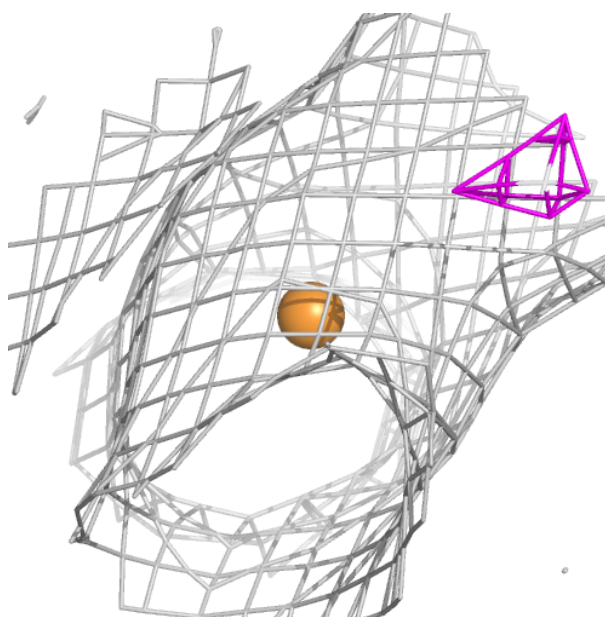
Electron density around CU A 604:

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



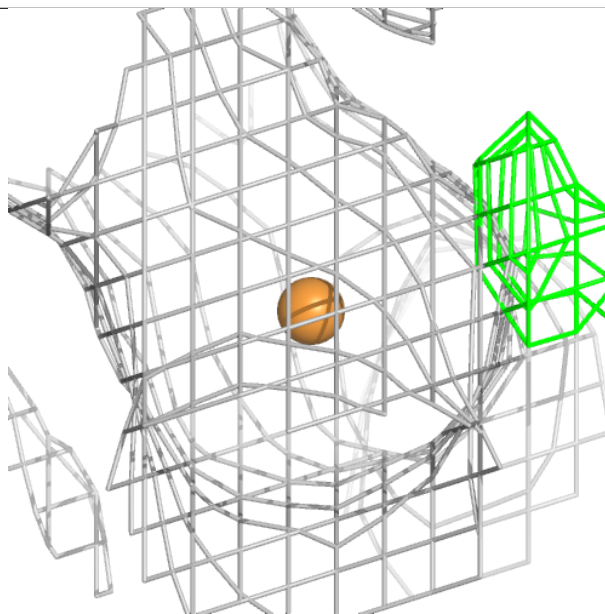
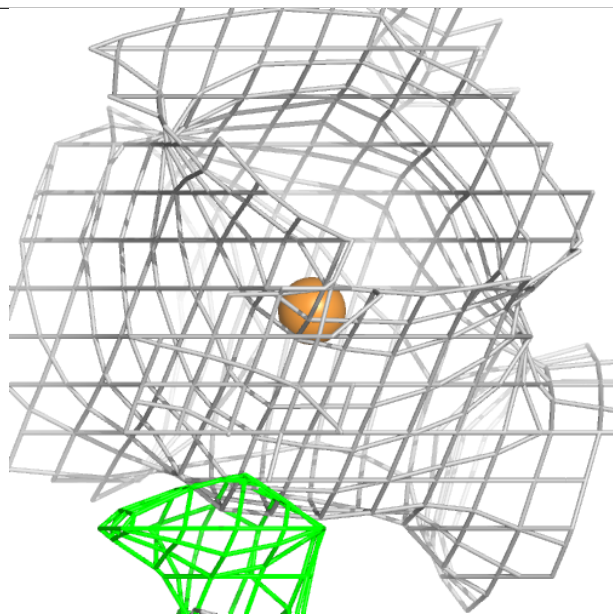
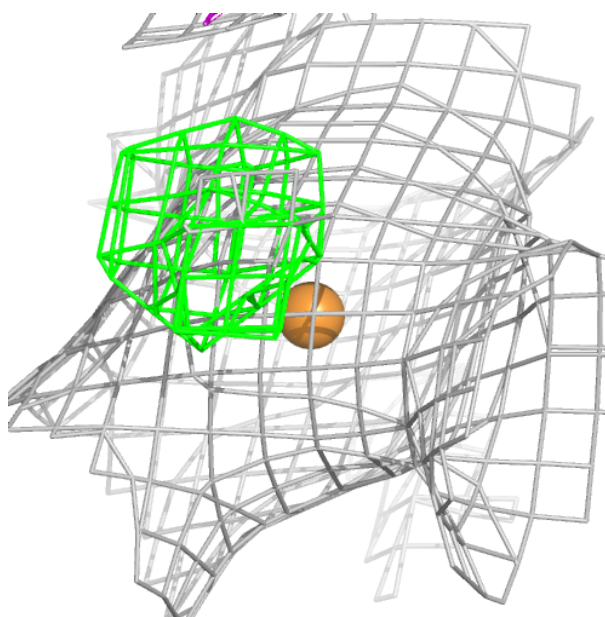
Electron density around CU D 602:

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



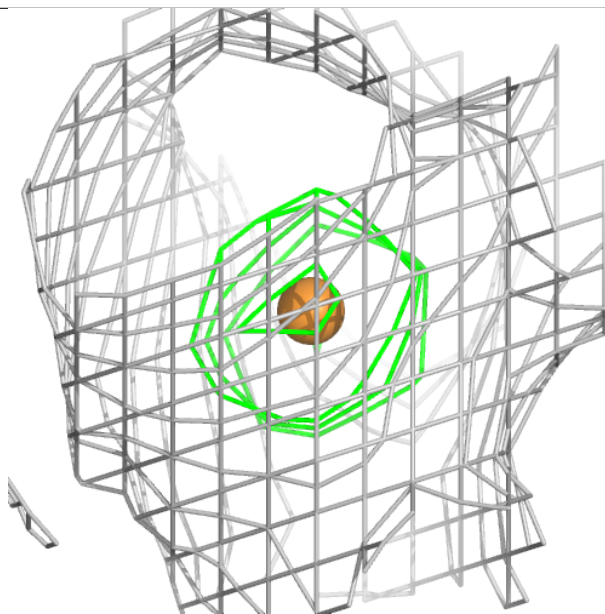
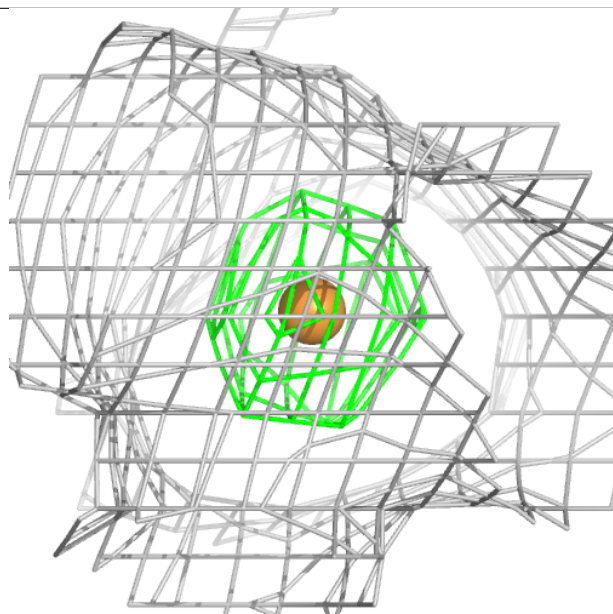
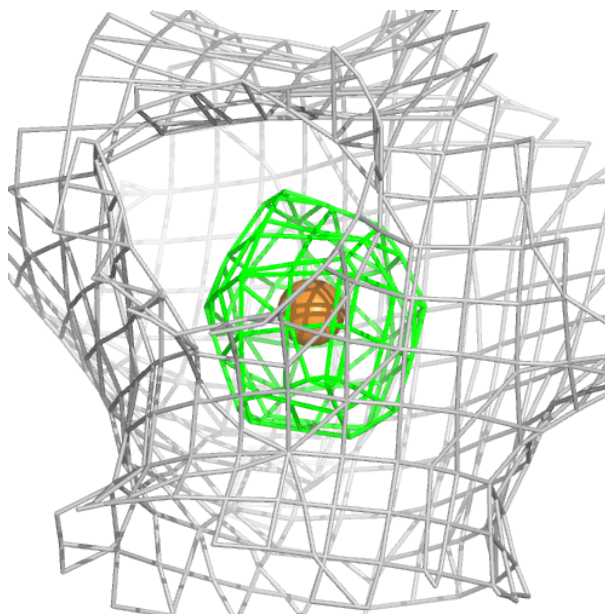
Electron density around CU A 602:

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



Electron density around CU B 604:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.