



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:05 PM UTC

PDB ID : 8Z59 / pdb_00008z59
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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

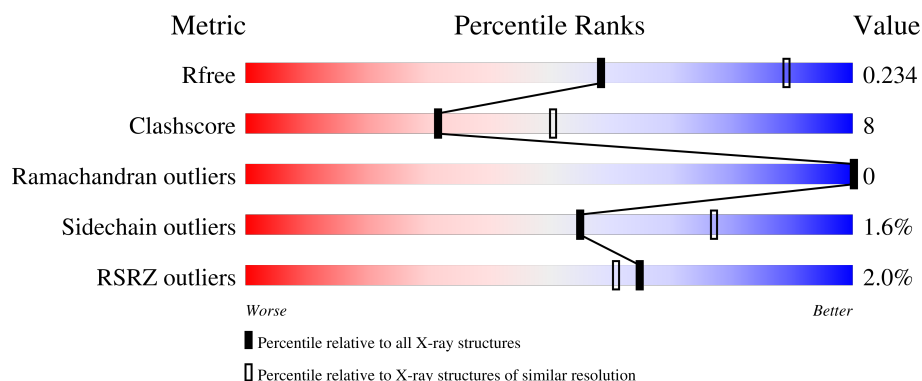
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (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	70% 17% 13%
1	B	514	65% 21% 13%
1	C	514	69% 17% 13%
1	D	514	3% 62% 24% 13%
1	E	514	67% 18% 13%

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Mol	Chain	Length	Quality of chain
1	F	514	2% 64% 21% • 13%
1	G	514	2% 69% 17% • 13%
1	H	514	4% 68% 18% • 13%

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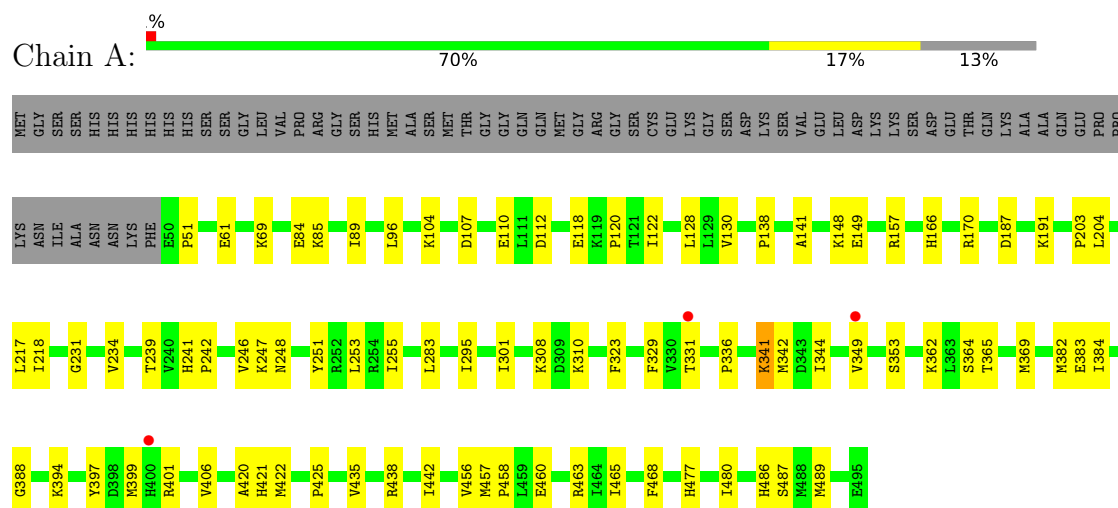
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	45	Total 45	O 45	0	0
3	G	42	Total 42	O 42	0	0
3	H	27	Total 27	O 27	0	0

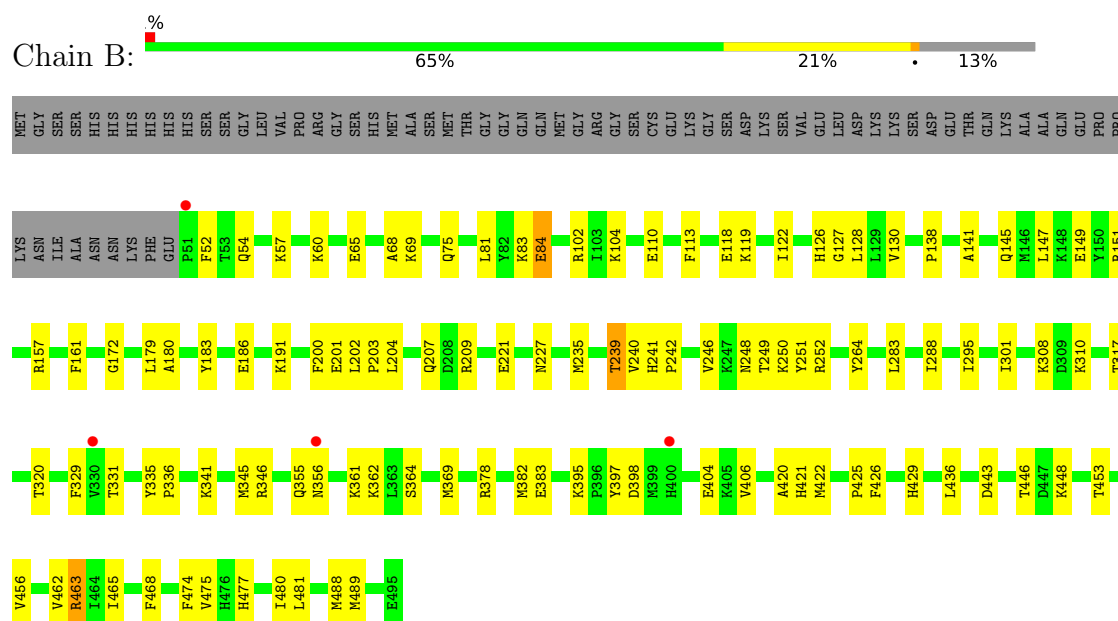
3 Residue-property plots [i](#)

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: Bilirubin oxidase

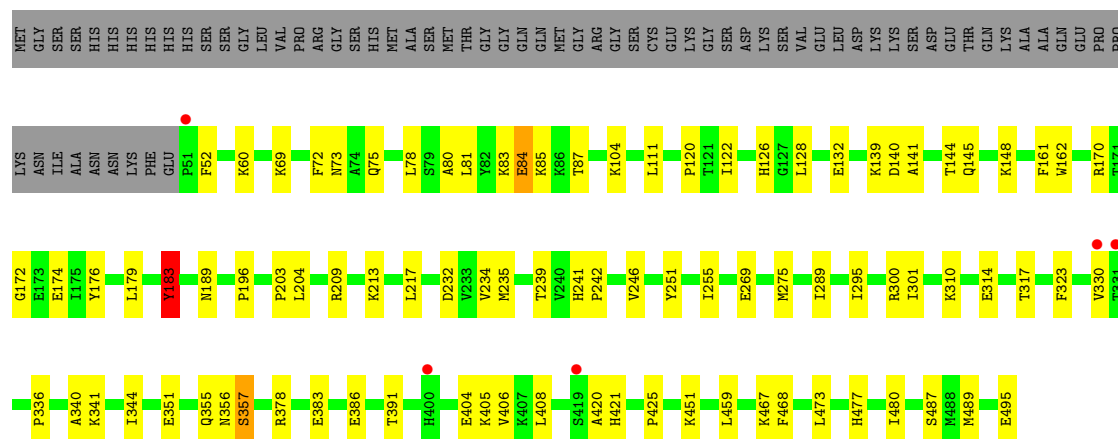


• Molecule 1: Bilirubin oxidase

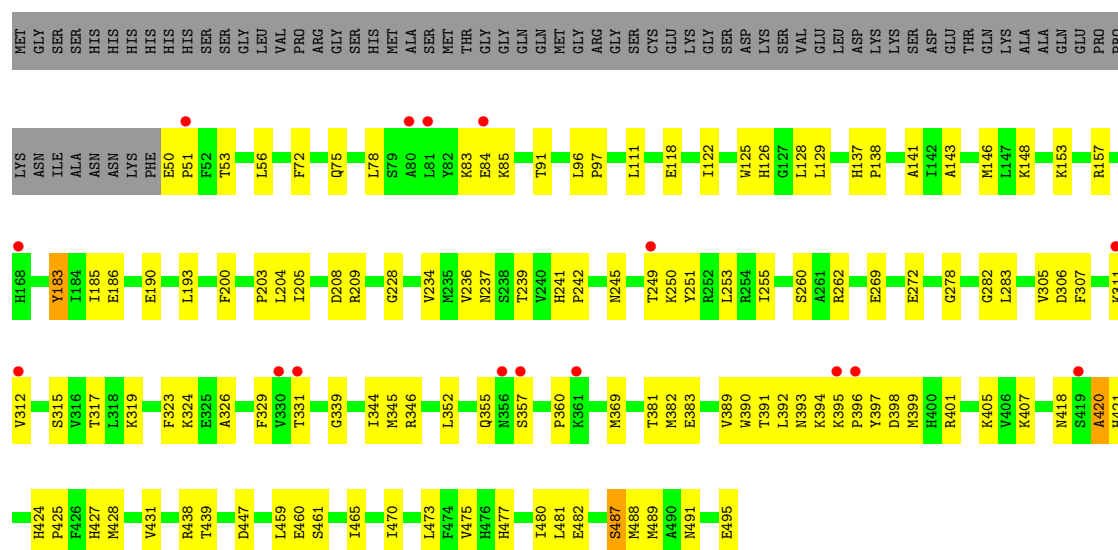


• Molecule 1: Bilirubin oxidase

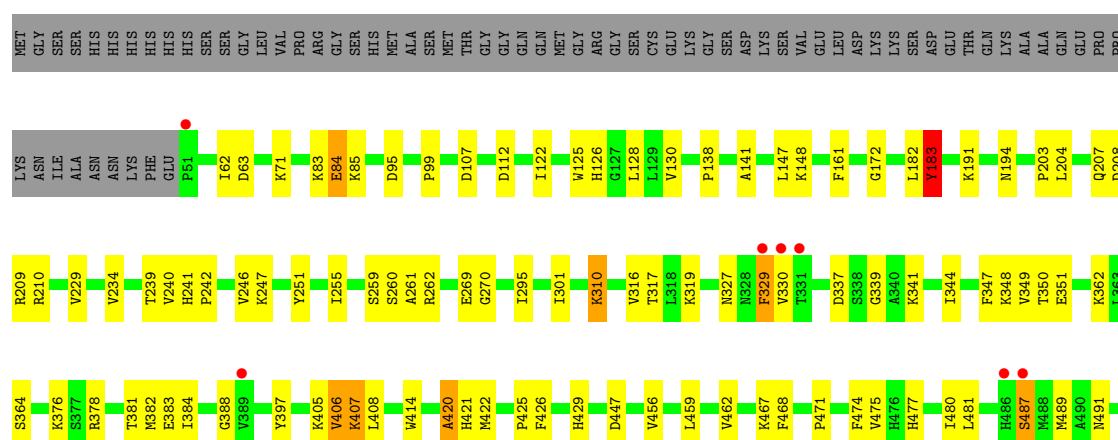




• Molecule 1: Bilirubin oxidase

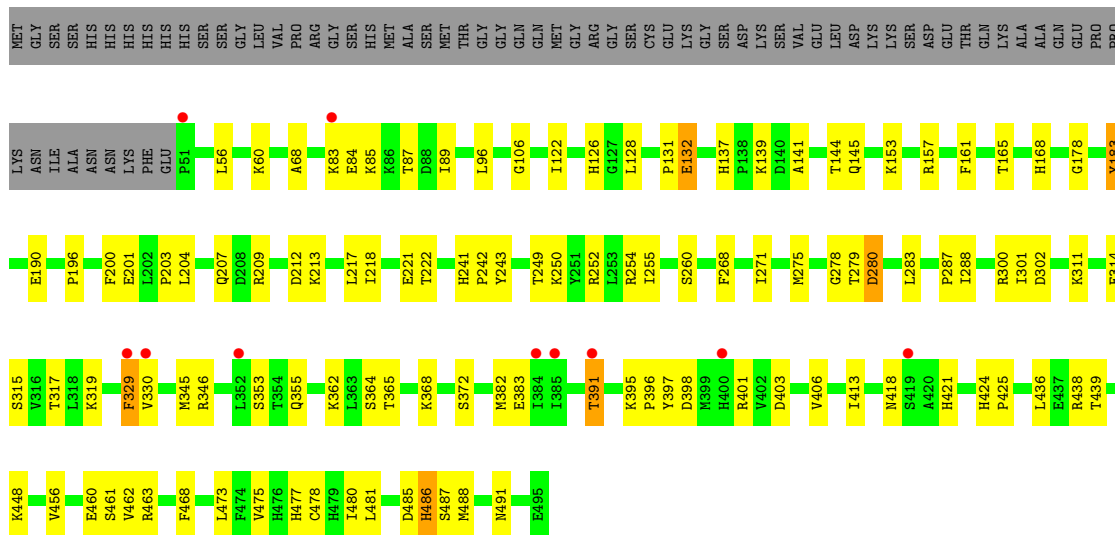


• Molecule 1: Bilirubin oxidase

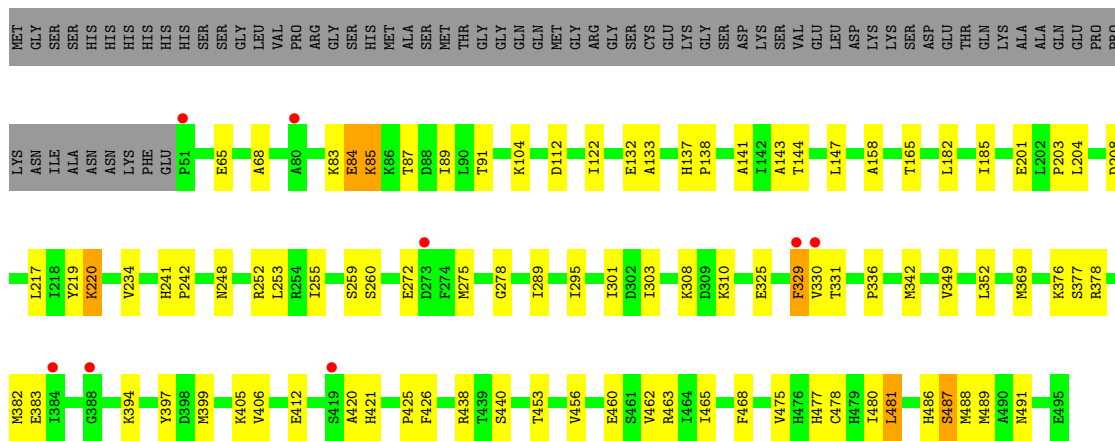


V494
E495

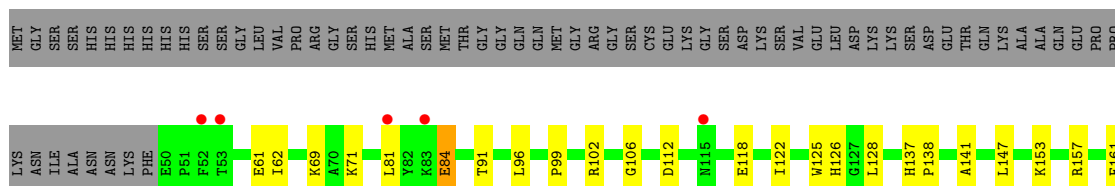
• Molecule 1: Bilirubin oxidase

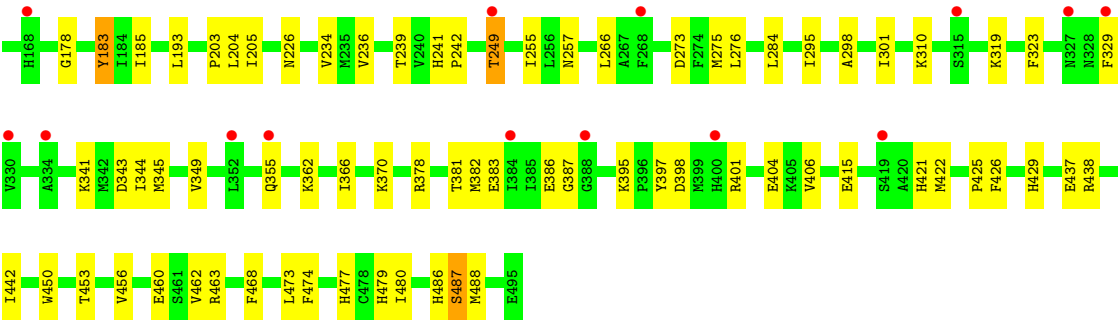
Chain F: 

• Molecule 1: Bilirubin oxidase

Chain G: 

• Molecule 1: Bilirubin oxidase

Chain H: 



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	2000 reflections (1.51%)	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 , 40.1	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	0.76	2/3667 (0.1%)	0.85	12/4955 (0.2%)
1	B	0.82	3/3658 (0.1%)	0.91	14/4942 (0.3%)
1	C	0.79	1/3658 (0.0%)	0.86	11/4942 (0.2%)
1	D	0.74	1/3667 (0.0%)	0.89	14/4955 (0.3%)
1	E	0.75	1/3658 (0.0%)	0.90	16/4942 (0.3%)
1	F	0.73	5/3658 (0.1%)	0.89	15/4942 (0.3%)
1	G	0.79	3/3658 (0.1%)	0.91	18/4942 (0.4%)
1	H	0.76	1/3667 (0.0%)	0.89	10/4955 (0.2%)
All	All	0.77	17/29291 (0.1%)	0.89	110/39575 (0.3%)

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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	HIS	CA-C	-8.48	1.47	1.53
1	E	241	HIS	CA-C	-8.02	1.46	1.53
1	C	241	HIS	CA-C	-8.02	1.47	1.53
1	G	241	HIS	CA-C	-7.91	1.47	1.53
1	H	241	HIS	CA-C	-7.88	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	241	HIS	CA-C	-7.68	1.47	1.53
1	D	241	HIS	CA-C	-7.07	1.48	1.53
1	F	241	HIS	CA-C	-7.06	1.47	1.53
1	F	85	LYS	CA-C	-6.26	1.45	1.52
1	F	279	THR	C-O	-6.15	1.16	1.23
1	B	180	ALA	C-O	-5.33	1.17	1.23
1	F	83	LYS	CA-C	-5.31	1.48	1.53
1	G	463	ARG	CD-NE	5.30	1.53	1.46
1	F	279	THR	CA-C	-5.23	1.46	1.52
1	G	463	ARG	NE-CZ	5.14	1.38	1.33
1	A	85	LYS	CA-C	-5.07	1.46	1.52
1	B	463	ARG	CB-CG	-5.00	1.37	1.52

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	487	SER	N-CA-C	11.74	129.87	113.56
1	D	487	SER	N-CA-C	11.52	127.29	113.23
1	G	487	SER	N-CA-C	10.73	125.97	112.24
1	E	487	SER	N-CA-C	10.61	128.31	113.56
1	H	487	SER	N-CA-C	10.34	125.84	113.23
1	D	421	HIS	N-CA-C	10.20	121.98	111.07
1	C	487	SER	N-CA-C	9.89	127.30	113.56
1	G	421	HIS	N-CA-C	9.80	121.56	111.07
1	E	421	HIS	N-CA-C	9.51	121.34	110.97
1	F	421	HIS	N-CA-C	9.35	121.23	111.14
1	A	421	HIS	N-CA-C	8.69	120.37	111.07
1	C	242	PRO	N-CA-C	8.36	123.59	111.13
1	D	118	GLU	CA-CB-CG	8.29	130.68	114.10
1	F	242	PRO	N-CA-C	8.24	123.41	111.13
1	B	421	HIS	N-CA-C	8.18	119.98	111.14
1	D	84	GLU	N-CA-C	-8.02	100.50	111.56
1	G	242	PRO	N-CA-C	8.01	123.06	111.13
1	G	329	PHE	N-CA-C	7.95	120.47	109.18
1	E	242	PRO	N-CA-C	7.83	122.79	111.13
1	H	84	GLU	N-CA-C	-7.61	102.21	112.94
1	E	83	LYS	CB-CA-C	-7.51	107.90	116.54
1	F	85	LYS	N-CA-C	7.47	121.42	109.24
1	B	84	GLU	N-CA-C	-7.45	101.34	110.88
1	B	242	PRO	N-CA-C	7.22	121.89	111.13
1	B	463	ARG	CD-NE-CZ	7.22	134.51	124.40
1	A	420	ALA	N-CA-C	7.21	120.19	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	421	HIS	N-CA-C	7.12	118.83	111.14
1	H	266	LEU	N-CA-C	7.11	121.43	110.20
1	E	420	ALA	N-CA-C	6.92	119.84	111.82
1	B	397	TYR	N-CA-C	6.90	120.23	110.23
1	H	275	MET	N-CA-C	6.87	119.71	108.52
1	F	280	ASP	N-CA-C	6.80	120.46	111.75
1	B	398	ASP	N-CA-C	-6.78	97.30	108.76
1	G	420	ALA	N-CA-C	6.75	119.65	111.82
1	E	407	LYS	CA-CB-CG	-6.52	101.06	114.10
1	F	372	SER	CA-C-N	-6.50	109.98	122.06
1	F	372	SER	C-N-CA	-6.50	109.98	122.06
1	G	330	VAL	N-CA-C	6.48	118.97	109.63
1	G	481	LEU	N-CA-C	6.45	118.31	111.28
1	C	84	GLU	N-CA-C	-6.45	103.85	112.94
1	A	422	MET	N-CA-C	6.43	119.75	108.75
1	B	75	GLN	N-CA-C	6.41	118.91	109.24
1	G	220	LYS	CA-C-N	-6.39	109.42	121.63
1	G	220	LYS	C-N-CA	-6.39	109.42	121.63
1	F	329	PHE	N-CA-C	-6.35	99.76	109.41
1	A	118	GLU	N-CA-CB	-6.34	100.55	110.06
1	H	421	HIS	N-CA-C	6.26	117.77	111.07
1	D	75	GLN	N-CA-C	6.21	118.86	109.23
1	A	242	PRO	N-CA-C	6.17	122.08	111.77
1	B	463	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	D	241	HIS	CB-CA-C	6.13	116.33	111.00
1	F	391	THR	N-CA-C	6.04	118.14	109.14
1	F	84	GLU	N-CA-C	-6.03	104.10	112.30
1	B	241	HIS	CB-CA-C	6.03	116.24	111.00
1	D	242	PRO	N-CA-C	5.95	120.62	111.57
1	F	418	ASN	N-CA-C	5.90	119.17	109.72
1	B	361	LYS	CB-CG-CD	-5.87	97.81	111.30
1	B	463	ARG	CB-CA-C	5.87	119.48	110.62
1	H	242	PRO	N-CA-C	5.87	119.87	111.13
1	E	310	LYS	CG-CD-CE	-5.86	97.82	111.30
1	A	241	HIS	CB-CA-C	5.86	116.10	111.00
1	C	183	TYR	CA-CB-CG	5.83	124.40	113.90
1	G	84	GLU	N-CA-C	-5.80	103.55	111.56
1	G	463	ARG	CA-C-O	5.76	126.71	120.32
1	D	418	ASN	N-CA-C	5.69	118.50	109.50
1	D	326	ALA	N-CA-C	5.69	117.56	111.36
1	E	329	PHE	N-CA-C	-5.68	102.35	110.59
1	D	262	ARG	N-CA-C	5.67	118.45	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	52	PHE	N-CA-C	5.65	119.37	111.74
1	A	341	LYS	CB-CG-CD	-5.64	98.32	111.30
1	E	406	VAL	CA-C-N	-5.64	113.74	122.09
1	E	406	VAL	C-N-CA	-5.64	113.74	122.09
1	H	370	LYS	CG-CD-CE	-5.62	98.38	111.30
1	G	325	GLU	N-CA-C	5.59	119.61	112.34
1	A	217	LEU	N-CA-C	5.55	118.49	110.28
1	C	340	ALA	N-CA-C	5.52	118.45	110.28
1	D	278	GLY	N-CA-C	5.51	121.07	111.14
1	F	241	HIS	CB-CA-C	5.51	115.11	111.20
1	C	357	SER	N-CA-C	-5.50	100.05	109.24
1	G	278	GLY	N-CA-C	5.42	120.90	111.14
1	G	85	LYS	N-CA-C	5.41	118.05	109.24
1	H	226	ASN	CB-CG-OD1	-5.40	110.00	120.80
1	B	83	LYS	CB-CA-C	-5.39	110.34	116.54
1	G	241	HIS	CB-CA-C	5.37	115.67	111.00
1	H	273	ASP	N-CA-C	5.33	117.79	109.52
1	A	329	PHE	N-CA-C	-5.33	102.11	110.36
1	C	391	THR	N-CA-C	5.32	117.27	109.24
1	E	183	TYR	CA-CB-CG	5.32	123.47	113.90
1	G	336	PRO	N-CA-C	5.28	119.60	111.21
1	D	282	GLY	N-CA-C	5.25	117.51	110.43
1	E	240	VAL	N-CA-C	5.25	116.30	108.54
1	B	179	LEU	N-CA-C	5.24	117.72	109.39
1	F	83	LYS	CB-CA-C	-5.21	110.58	116.63
1	F	132	GLU	CA-C-O	-5.19	115.04	120.55
1	G	91	THR	N-CA-C	5.18	117.55	109.52
1	C	323	PHE	CA-C-N	-5.17	113.66	122.56
1	C	323	PHE	C-N-CA	-5.17	113.66	122.56
1	F	486	HIS	CA-C-N	5.14	129.85	122.35
1	F	486	HIS	C-N-CA	5.14	129.85	122.35
1	E	84	GLU	N-CA-C	-5.13	105.32	112.30
1	E	261	ALA	N-CA-C	5.13	121.73	110.80
1	A	51	PRO	CA-N-CD	-5.10	104.86	112.00
1	G	272	GLU	N-CA-C	5.10	116.92	111.36
1	H	178	GLY	N-CA-C	5.09	125.24	113.18
1	B	420	ALA	N-CA-C	5.08	119.48	113.28
1	A	118	GLU	CA-CB-CG	5.04	124.19	114.10
1	D	420	ALA	N-CA-C	5.04	118.69	112.54
1	D	395	LYS	CA-CB-CG	5.03	124.17	114.10
1	E	262	ARG	N-CA-C	5.03	117.60	110.10
1	E	241	HIS	CB-CA-C	5.01	114.75	111.20

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	44	0
1	B	3575	0	3586	65	0
1	C	3575	0	3586	50	0
1	D	3584	0	3591	76	0
1	E	3575	0	3586	59	0
1	F	3575	0	3586	72	0
1	G	3575	0	3586	47	0
1	H	3584	0	3591	60	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	5	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	464	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 (464) 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
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	0.79
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:F:424:HIS:CE1	1:F:488:MET:HE1	2.22	0.74
1:C:209:ARG:HG3	1:C:235:MET:HE2	1.71	0.73
1:H:319:LYS:NZ	1:H:341:LYS:HG2	2.03	0.73
1:D:407:LYS:NZ	3:D:703:HOH:O	1.97	0.71
1:H:249:THR:HG21	1:H:355:GLN:HB3	1.70	0.71
1:B:227:ASN:HB3	1:B:422:MET:HE1	1.72	0.71
1:F:486:HIS:HB3	3:F:704:HOH:O	1.90	0.70
1:E:467:LYS:NZ	3:E:704:HOH:O	2.21	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:F:319:LYS:NZ	3:F:705:HOH:O	2.26	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:138:PRO:HB2	1:A:399:MET:HE2	1.76	0.66
1:E:269:GLU:HG3	1:E:317:THR:HB	1.77	0.66
1:A:369:MET:HE2	1:A:465:ILE:HG12	1.75	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:D:56:LEU:HD22	1:D:345:MET:HE1	1.78	0.65
1:B:138:PRO:HG2	1:B:489:MET:HE1	1.78	0.65
1:G:397:TYR:H	1:G:487:SER:HB3	1.62	0.64
1:E:382:MET:HE1	1:E:426:PHE:HB2	1.79	0.64
1:F:122:ILE:HB	1:F:141:ALA:HA	1.78	0.64
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:E:319:LYS:HD2	1:E:341:LYS:HZ2	1.62	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: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:B:382:MET:HB3	1:B:488:MET:HE2	1.82	0.62
1:F:368:LYS:NZ	3:F:706:HOH:O	2.26	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:G:378:ARG:HH21	1:G:412:GLU:CD	2.07	0.61
1:H:381:THR:OG1	1:H:383:GLU:OE2	2.17	0.61
1:H:382:MET:HB3	1:H:488:MET:HE2	1.83	0.61
1:A:394:LYS:NZ	3:A:703:HOH:O	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:397:TYR:H	1:F:487:SER:HB2	1.66	0.60
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:C:275:MET:HE2	1:C:289:ILE:HD11	1.84	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:THR:H	1:D:307:PHE:HB2	1.69	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: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
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: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:382:MET:HE1	1:D:424:HIS:HB2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:236:VAL:HG21	1:H:345:MET:HE3	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
1:B:128:LEU:HB3	1:B:130:VAL:HG13	1.94	0.50
1:E:270:GLY:O	1:E:310:LYS:NZ	2.30	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:F:106:GLY:O	1:F:153:LYS:NZ	2.41	0.50
1:F:56:LEU:HD22	1:F:345:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:HIS:O	1:B:161:PHE:HB3	2.12	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:A:382:MET:HE1	1:A:456:VAL:HB	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:A:231:GLY:O	1:A:342:MET:HE1	2.12	0.48
1:F:317:THR:OG1	1:F:346:ARG:HG3	2.13	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: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:D:369:MET:HE3	1:D:465:ILE:HG23	1.96	0.48
1:A:187:ASP:O	1:A:191:LYS:HG3	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
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:B:145:GLN:HG2	1:B:145:GLN:O	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:478:CYS:HB2	1:F:488:MET:HE3	1.97	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:G:234:VAL:HG23	1:G:342:MET:HE2	1.97	0.46
1:H:137:HIS:ND1	1:H:138:PRO:HD2	2.30	0.46
1:A:336:PRO:HG2	1:A:342:MET:HE3	1.98	0.46
1:G:144:THR:N	3:G:702:HOH:O	2.22	0.46
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: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: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:B:369:MET:HE3	1:B:465:ILE:HG23	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:485:ASP:C	1:F:487:SER:H	2.25	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
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:382:MET:HB3	1:B:488:MET:CE	2.46	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:D:250:LYS:HG2	1:D:306:ASP:CG	2.42	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:A:457:MET:HE3	1:A:458:PRO:HD2	1.99	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:F:213:LYS:HD2	1:F:213:LYS:C	2.42	0.44
1:H:62:ILE:HG13	1:H:99:PRO:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:428:MET:HE2	1:D:431:VAL:HG21	2.01	0.43
1:E:397:TYR:H	1:E:487:SER:HB3	1.82	0.43
1:F:382:MET:HE3	1:F:382:MET:HB2	1.77	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
1:B:362:LYS:HD2	1:B:362:LYS:HA	1.76	0.42
1:E:337:ASP:C	1:E:339:GLY:H	2.27	0.42
1:H:422:MET:HE3	1:H:422:MET:HB2	1.90	0.42
1:B:475:VAL:HG21	1:B:489:MET:HE3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:GLU:CG	1:G:133:ALA:N	2.81	0.42
1:G:382:MET:HB3	1:G:488:MET:HE2	2.01	0.42
1:H:118:GLU:H	1:H:118:GLU:CD	2.26	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:A:365:THR:OG1	1:B:118:GLU:OE2	2.32	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:A:166:HIS:HE1	1:A:489:MET:HE1	1.85	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:61:GLU:CD	1:H:102:ARG:HE	2.29	0.41
1:H:157:ARG:HH11	1:H:450:TRP:CD1	2.39	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:G:399:MET:HE3	1:G:399:MET:HB2	1.75	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:63:ASP:OD1	1:E:63:ASP:C	2.63	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:138:PRO:HG2	1:E:489:MET:HE1	2.04	0.40
1:E:269:GLU:CG	1:E:317:THR:HB	2.50	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: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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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
1	F	443/514 (86%)	420 (95%)	23 (5%)	0	100	100
1	G	443/514 (86%)	421 (95%)	22 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	391 (99%)	5 (1%)	61	81
1	B	395/452 (87%)	387 (98%)	8 (2%)	48	72
1	C	395/452 (87%)	388 (98%)	7 (2%)	51	74
1	D	396/452 (88%)	390 (98%)	6 (2%)	57	78
1	E	395/452 (87%)	388 (98%)	7 (2%)	51	74
1	F	395/452 (87%)	391 (99%)	4 (1%)	68	84
1	G	395/452 (87%)	388 (98%)	7 (2%)	51	74
1	H	396/452 (88%)	389 (98%)	7 (2%)	51	74
All	All	3163/3616 (88%)	3112 (98%)	51 (2%)	55	77

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	GLU
1	A	218	ILE
1	A	239	THR
1	A	331	THR
1	A	486	HIS
1	B	81	LEU
1	B	84	GLU
1	B	221	GLU
1	B	239	THR
1	B	329	PHE

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Mol	Chain	Res	Type
1	B	331	THR
1	B	383	GLU
1	B	446	THR
1	C	81	LEU
1	C	239	THR
1	C	355	GLN
1	C	356	ASN
1	C	357	SER
1	C	383	GLU
1	C	386	GLU
1	D	78	LEU
1	D	85	LYS
1	D	239	THR
1	D	272	GLU
1	D	329	PHE
1	D	331	THR
1	E	84	GLU
1	E	85	LYS
1	E	95	ASP
1	E	239	THR
1	E	260	SER
1	E	330	VAL
1	E	422	MET
1	F	329	PHE
1	F	330	VAL
1	F	383	GLU
1	F	391	THR
1	G	85	LYS
1	G	89	ILE
1	G	182	LEU
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	193	LEU
1	H	239	THR
1	H	249	THR
1	H	329	PHE
1	H	486	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	358	GLN
1	A	486	HIS
1	B	54	GLN
1	B	245	ASN
1	B	358	GLN
1	B	400	HIS
1	B	486	HIS
1	D	245	ASN
1	D	477	HIS
1	D	486	HIS
1	E	66	HIS
1	E	75	GLN
1	E	93	GLN
1	E	145	GLN
1	E	207	GLN
1	E	224	GLN
1	E	327	ASN
1	F	245	ASN
1	G	75	GLN
1	G	421	HIS
1	G	491	ASN
1	H	54	GLN
1	H	66	HIS
1	H	93	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.07	3 (0%) 84 82	26, 42, 69, 96	0
1	B	445/514 (86%)	0.04	4 (0%) 81 79	27, 45, 67, 102	0
1	C	445/514 (86%)	-0.02	5 (1%) 78 75	25, 42, 64, 96	0
1	D	446/514 (86%)	0.25	16 (3%) 46 41	30, 48, 72, 108	0
1	E	445/514 (86%)	0.19	7 (1%) 70 67	31, 48, 75, 109	0
1	F	445/514 (86%)	0.24	10 (2%) 62 58	32, 50, 72, 105	0
1	G	445/514 (86%)	0.35	8 (1%) 67 64	31, 55, 77, 105	0
1	H	446/514 (86%)	0.62	19 (4%) 40 35	39, 62, 86, 114	0
All	All	3563/4112 (86%)	0.20	72 (2%) 65 61	25, 48, 75, 114	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	330	VAL	4.4
1	G	329	PHE	4.4
1	E	330	VAL	4.1
1	C	330	VAL	4.1
1	H	330	VAL	4.0
1	F	330	VAL	3.9
1	B	356	ASN	3.5
1	E	51	PRO	3.3
1	F	51	PRO	3.2
1	D	357	SER	3.2
1	E	331	THR	3.1
1	D	51	PRO	3.1
1	D	419	SER	3.1
1	B	400	HIS	3.0
1	D	361	LYS	3.0
1	D	356	ASN	3.0

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

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Mol	Chain	Res	Type	RSRZ
1	G	384	ILE	2.1
1	E	487	SER	2.1
1	H	52	PHE	2.1
1	D	331	THR	2.1
1	H	249	THR	2.1
1	B	51	PRO	2.1
1	D	396	PRO	2.1
1	A	349	VAL	2.0
1	H	388	GLY	2.0
1	H	83	LYS	2.0
1	C	419	SER	2.0
1	F	400	HIS	2.0
1	E	389	VAL	2.0
1	D	84	GLU	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 oligosaccharides 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($\text{\AA}^2$)	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	0.06	38,38,38,38	1
2	CU	D	601	1/1	0.97	0.04	56,56,56,56	1

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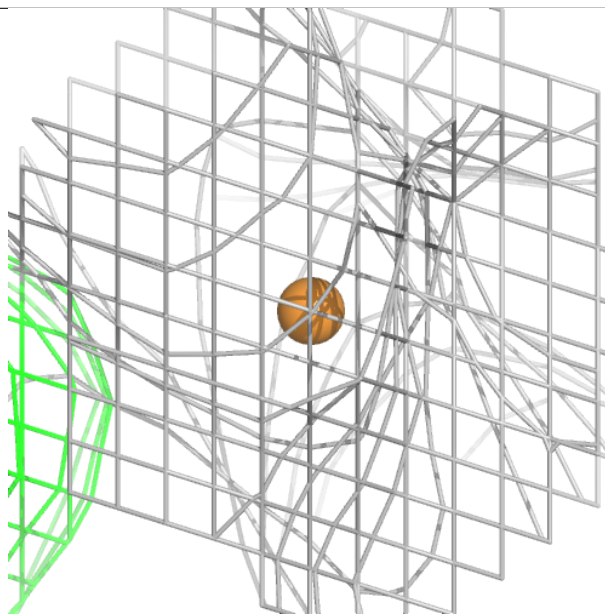
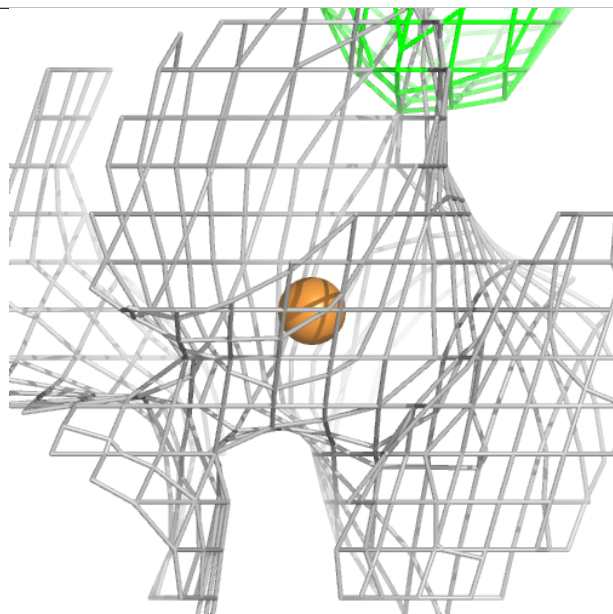
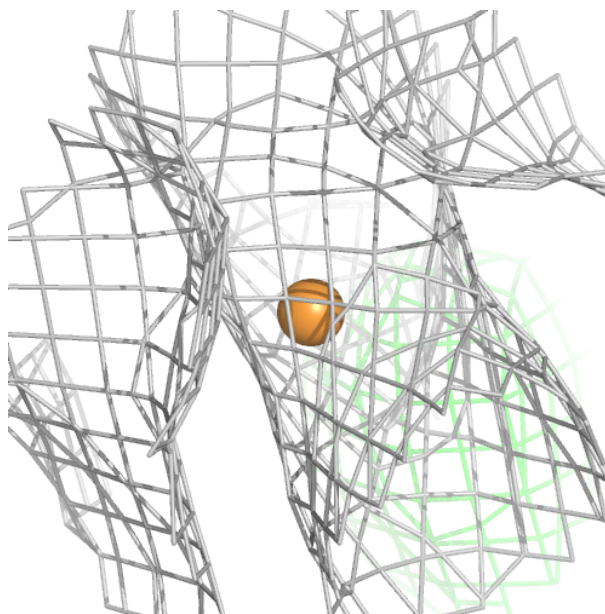
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CU	B	603	1/1	0.97	0.06	41,41,41,41	1
2	CU	E	603	1/1	0.98	0.10	47,47,47,47	1
2	CU	E	604	1/1	0.98	0.05	63,63,63,63	0
2	CU	A	603	1/1	0.98	0.04	38,38,38,38	1
2	CU	F	602	1/1	0.98	0.04	51,51,51,51	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
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	0.02	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	0.03	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.

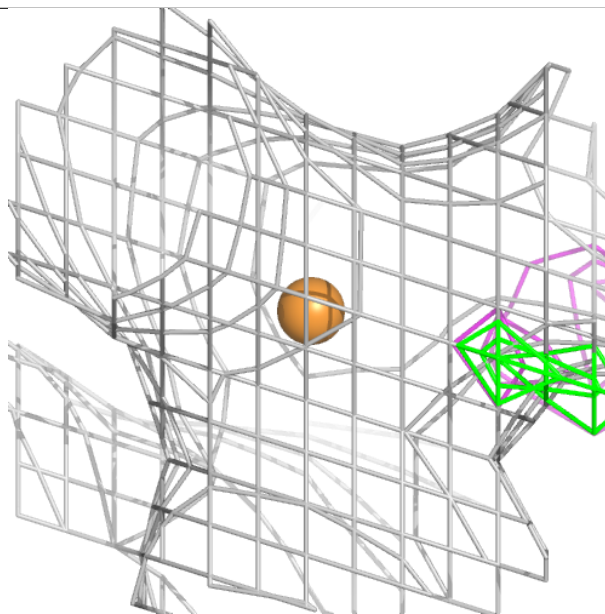
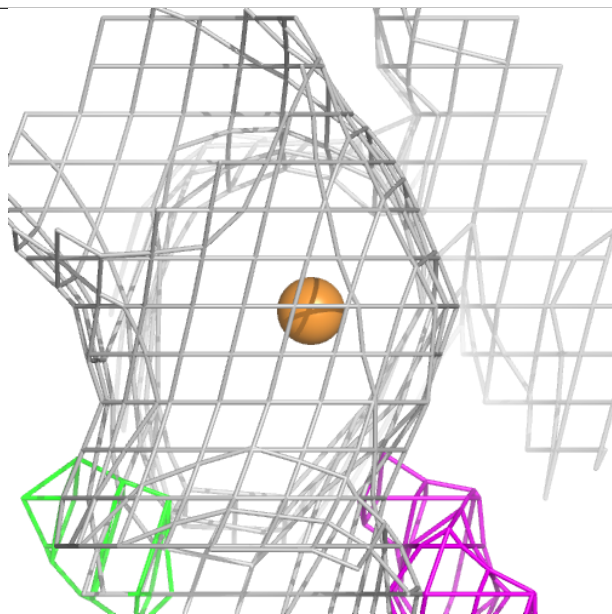
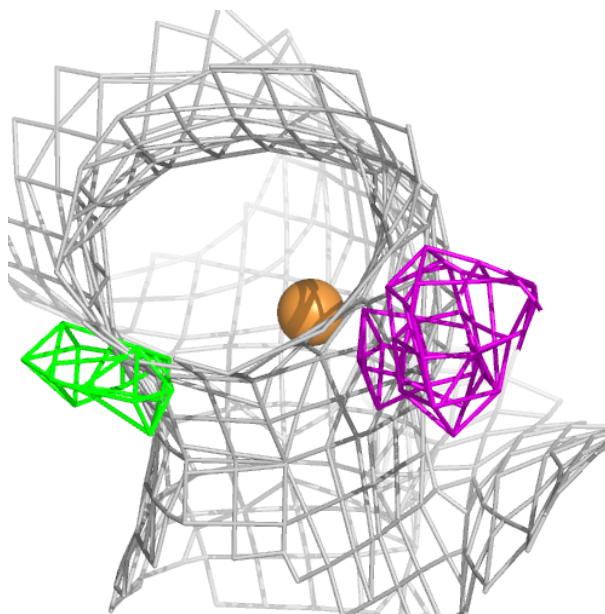
Electron density around CU H 603:

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



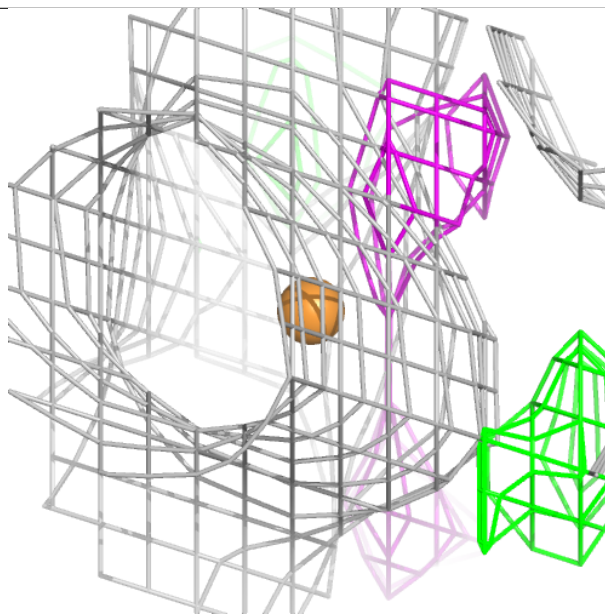
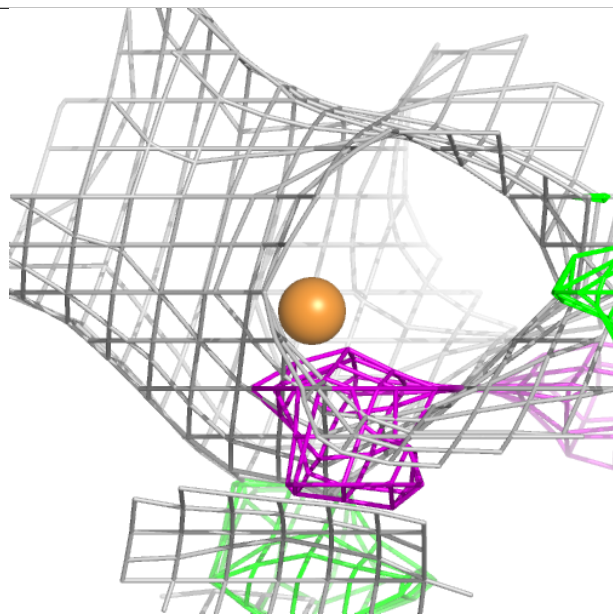
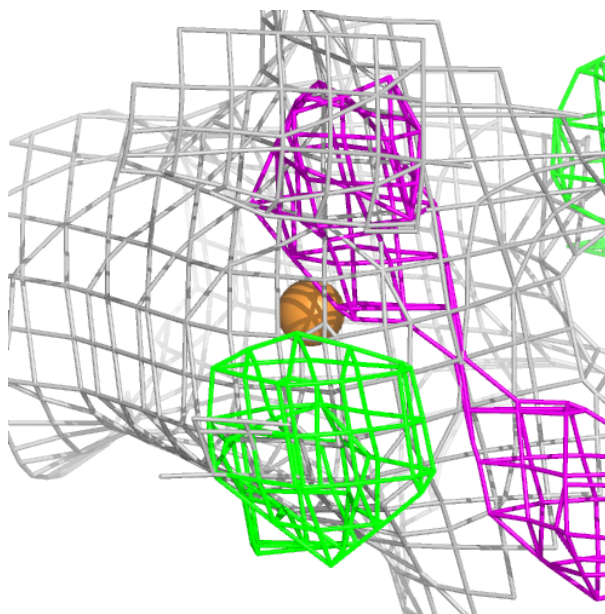
Electron density around CU G 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



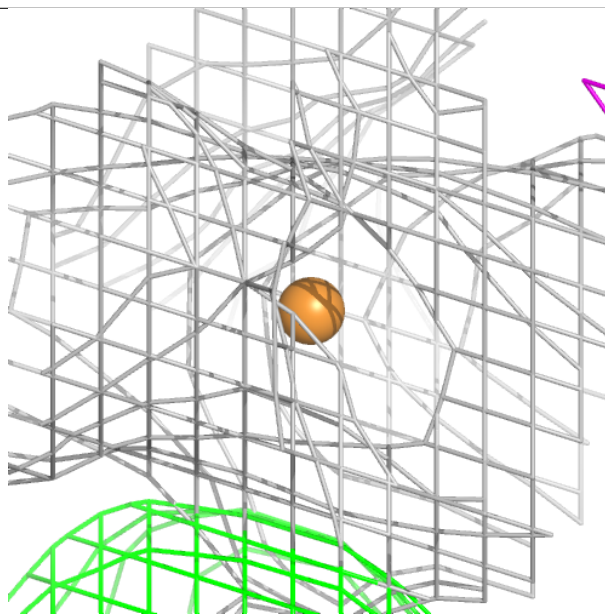
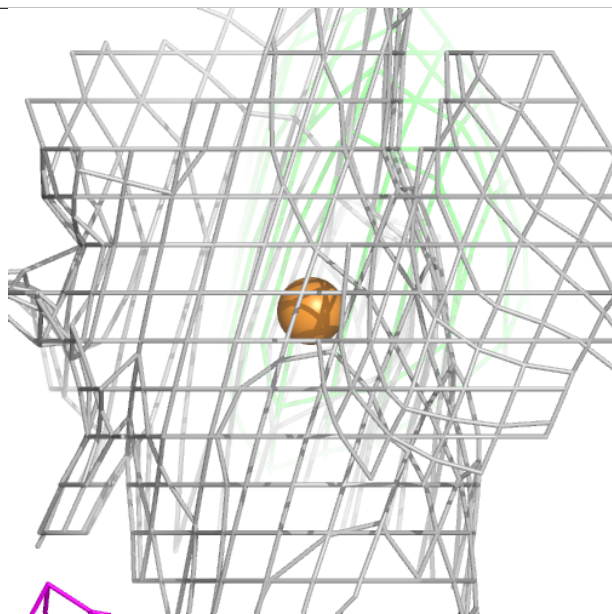
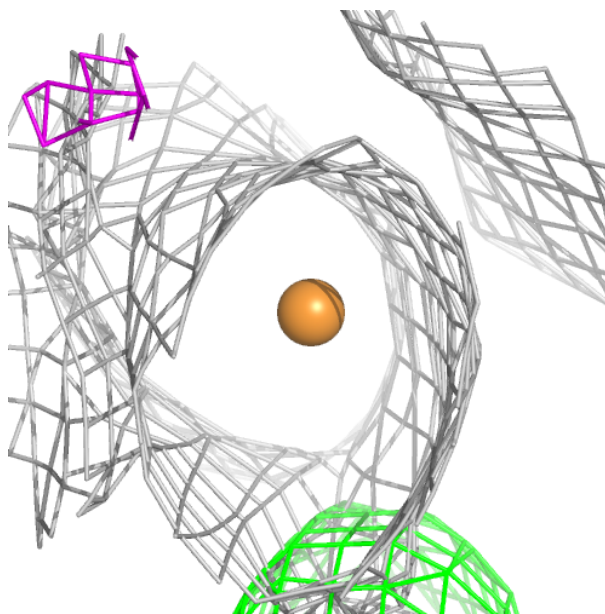
Electron density around CU A 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



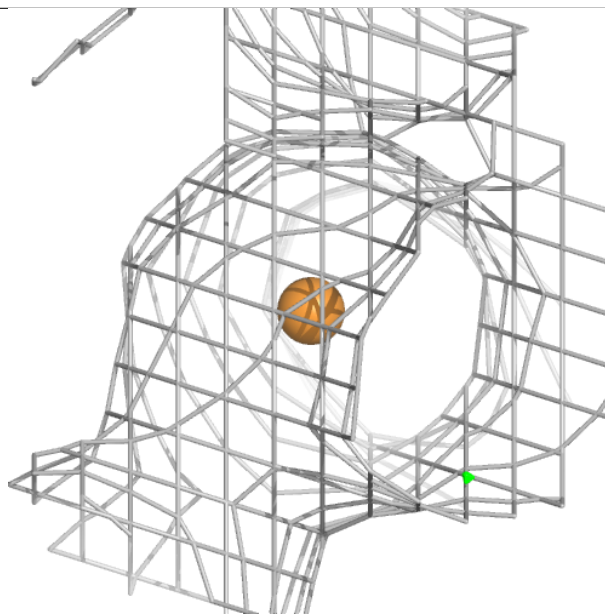
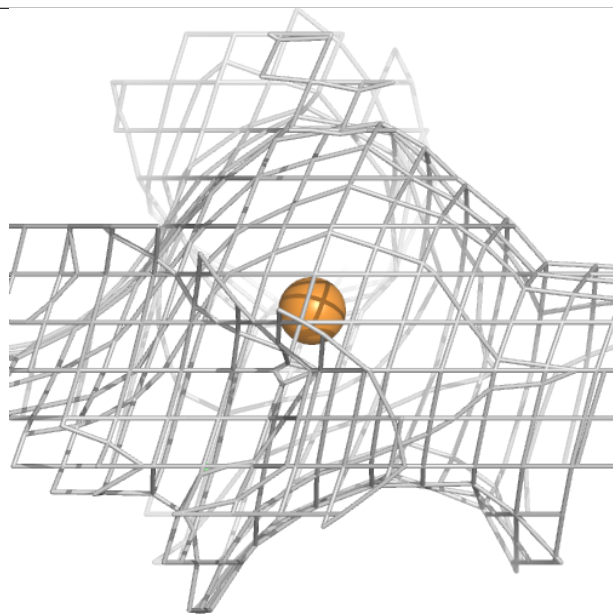
Electron density around CU G 603:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



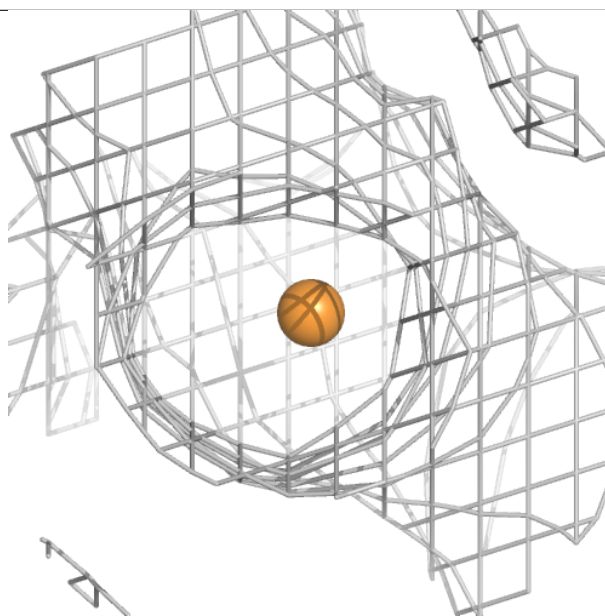
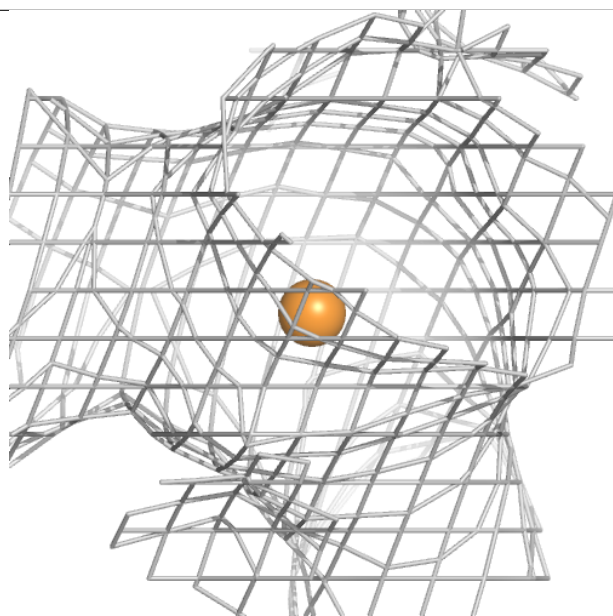
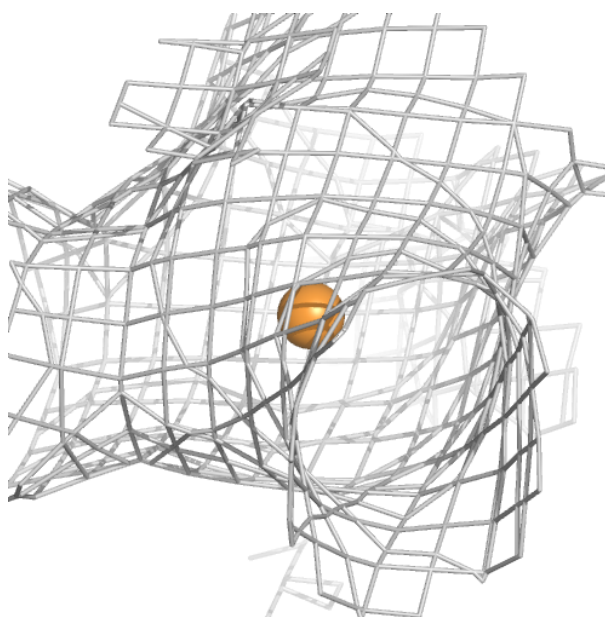
Electron density around CU E 601:

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and green (positive)



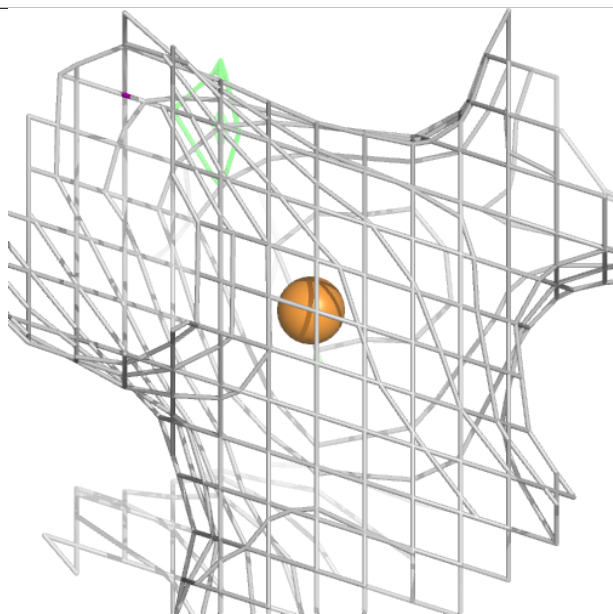
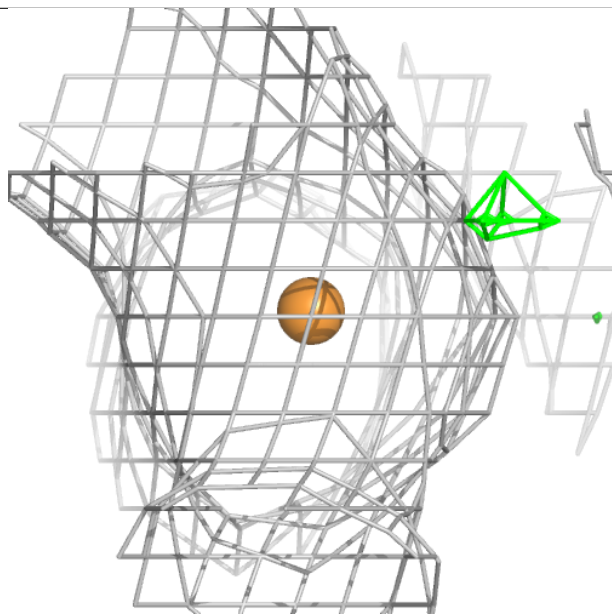
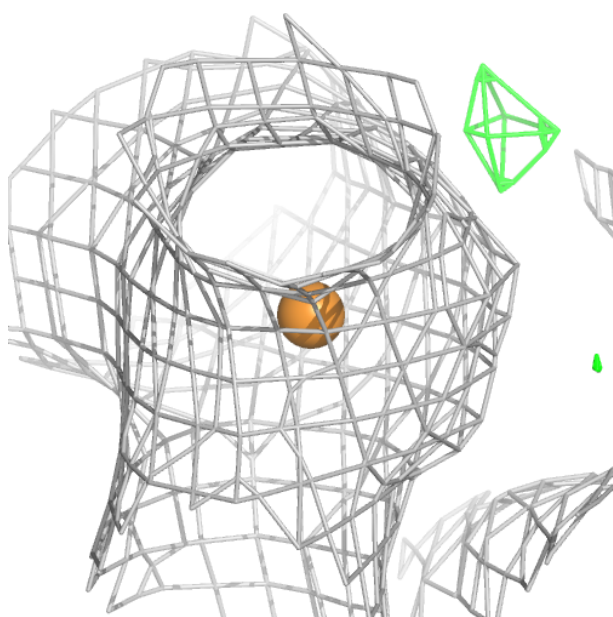
Electron density around CU E 602:

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and green (positive)



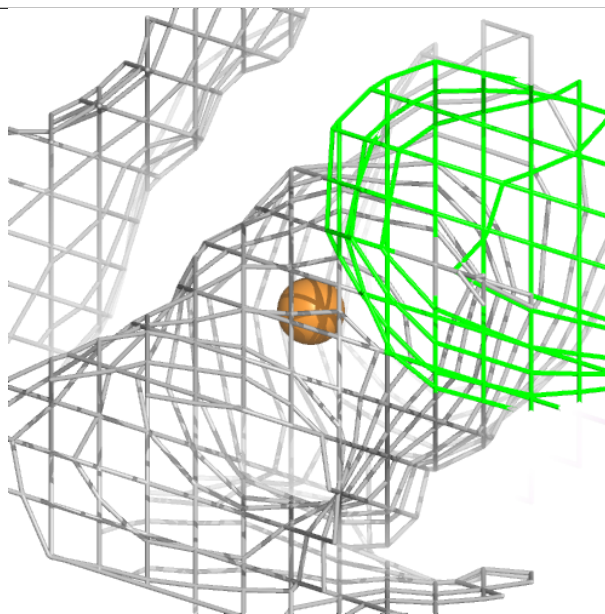
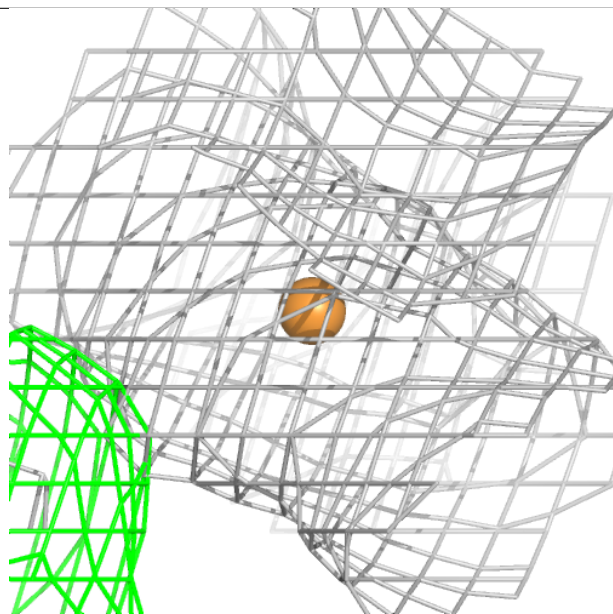
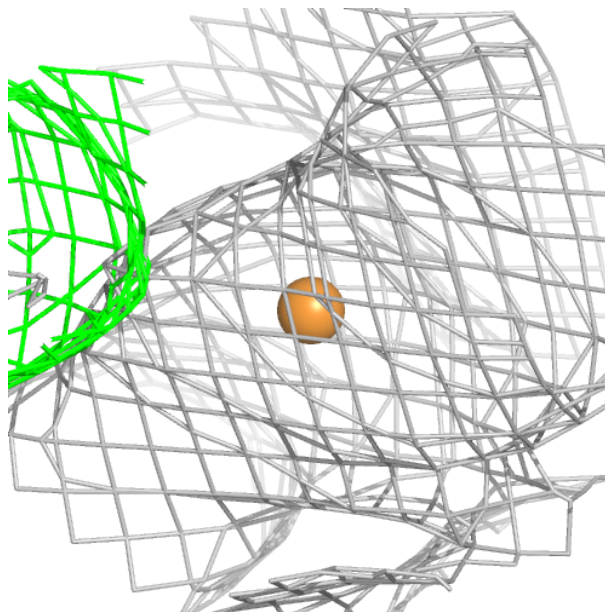
Electron density around CU F 601:

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and green (positive)



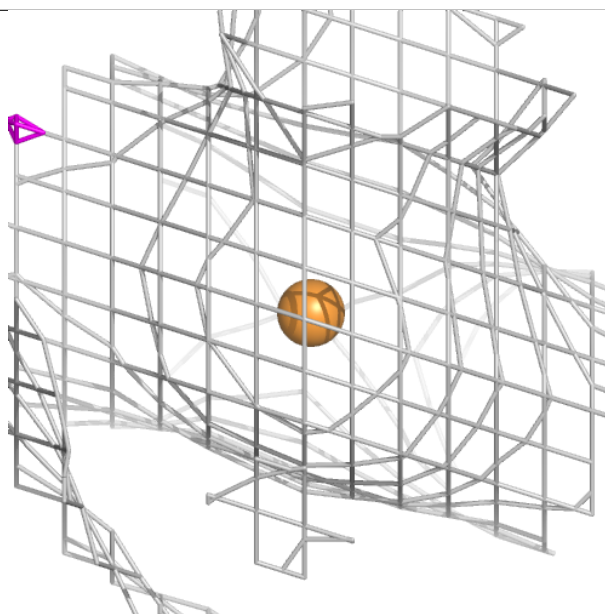
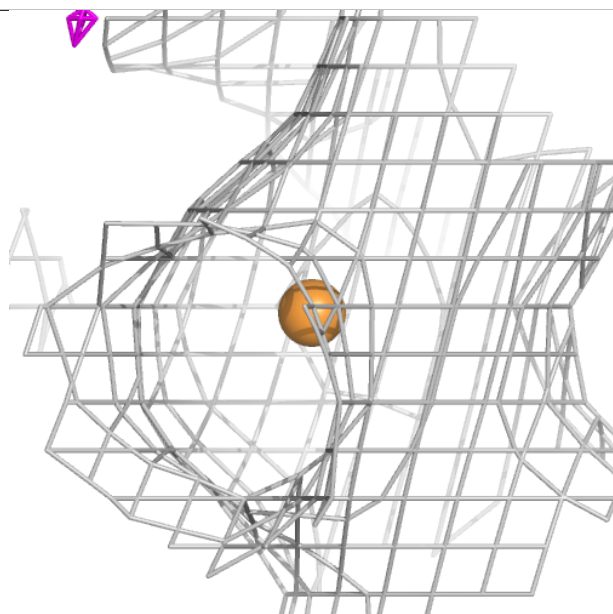
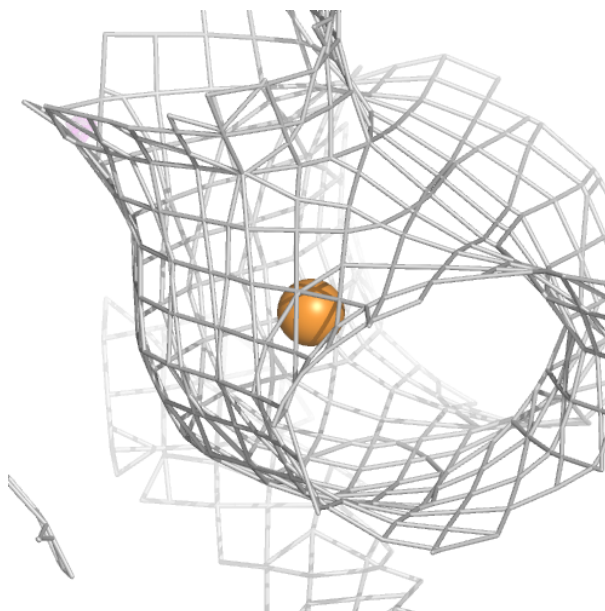
Electron density around CU C 603:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



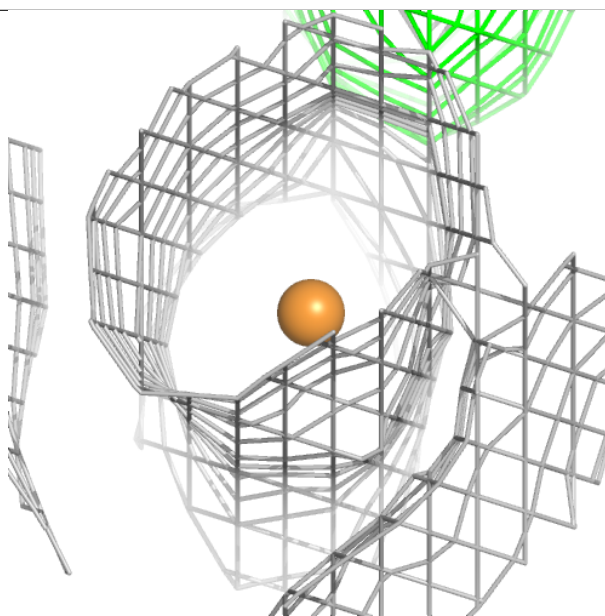
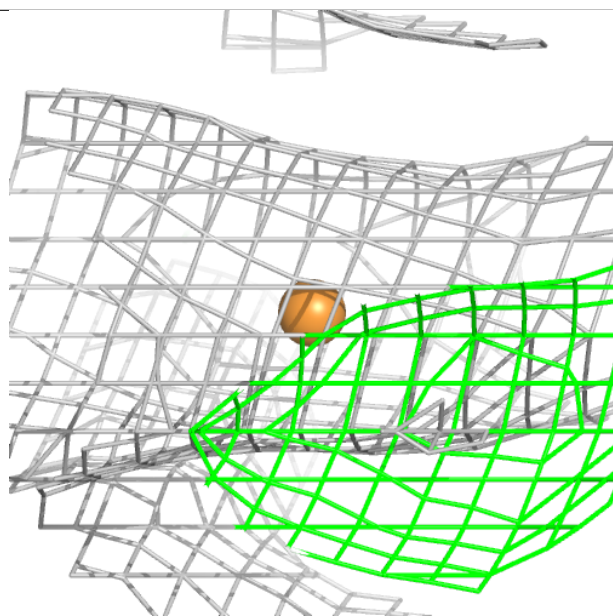
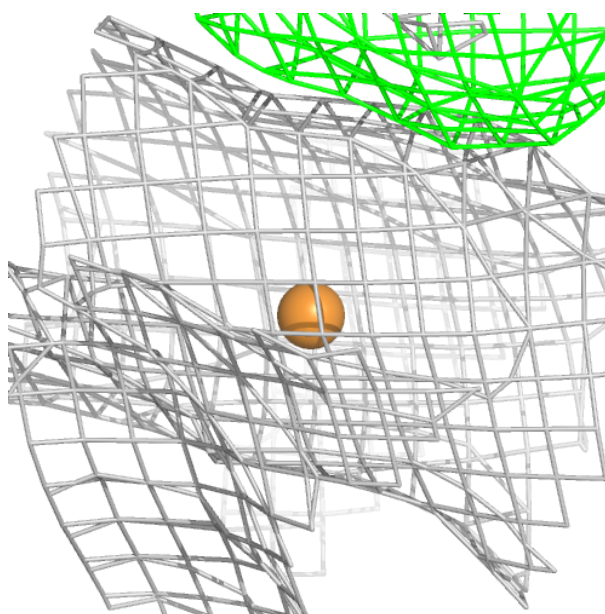
Electron density around CU D 601:

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and green (positive)



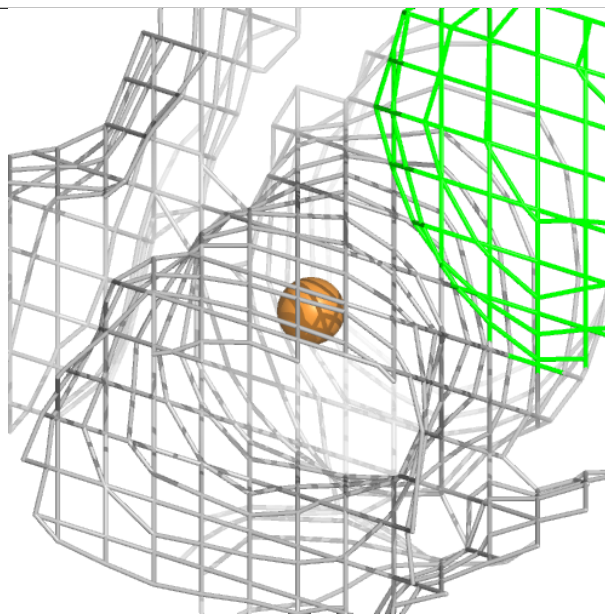
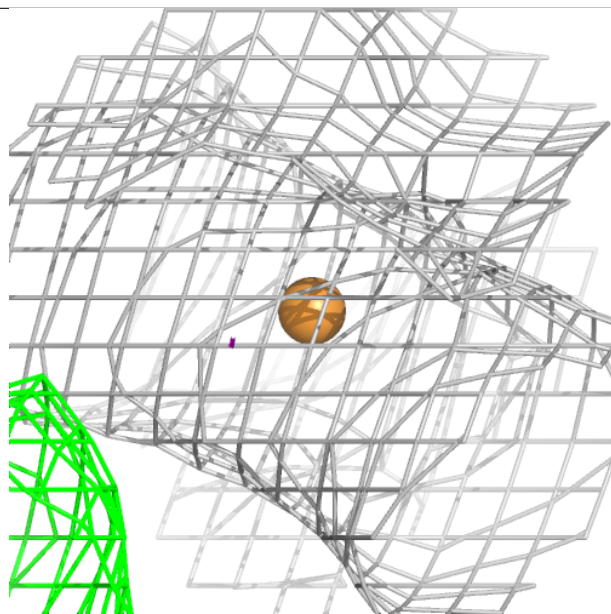
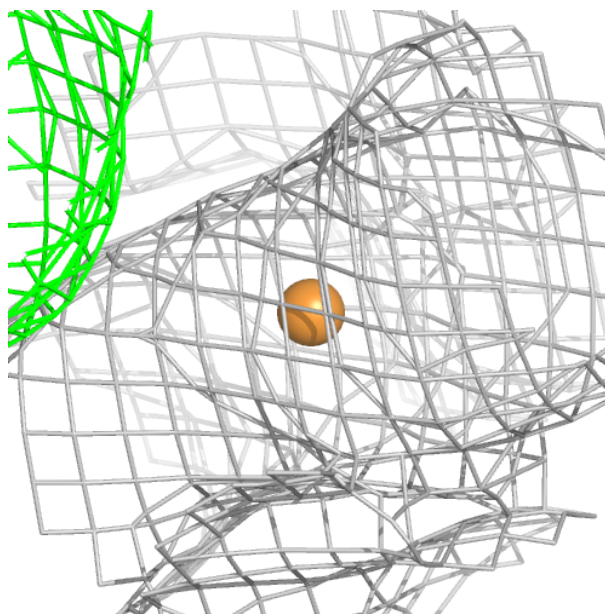
Electron density around CU B 603:

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and green (positive)



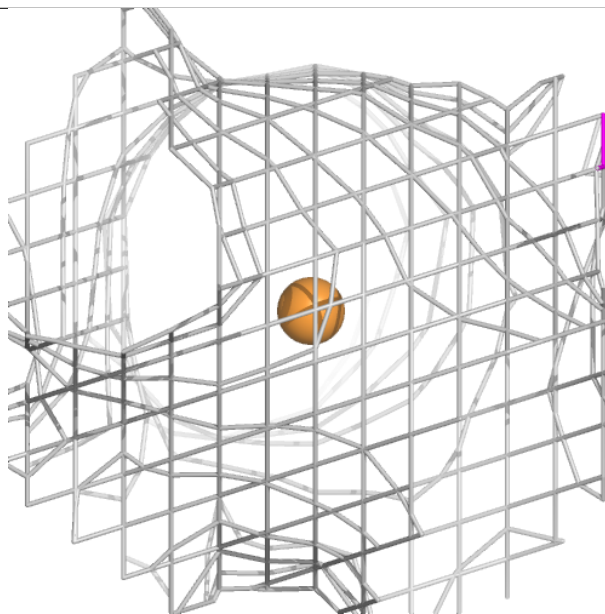
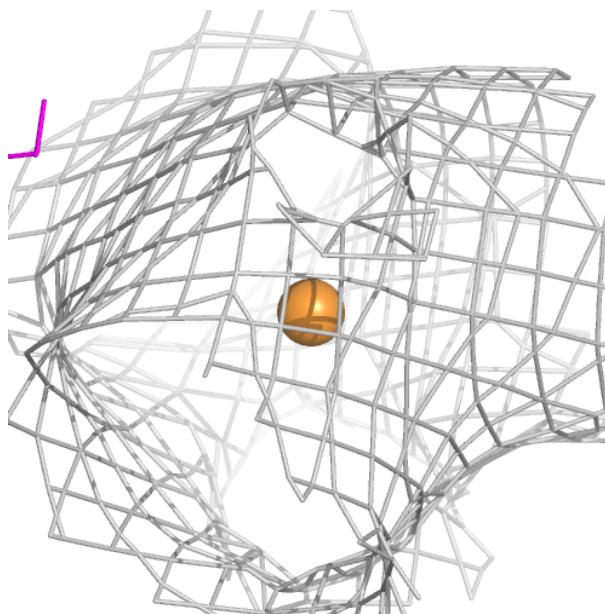
Electron density around CU E 603:

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and green (positive)



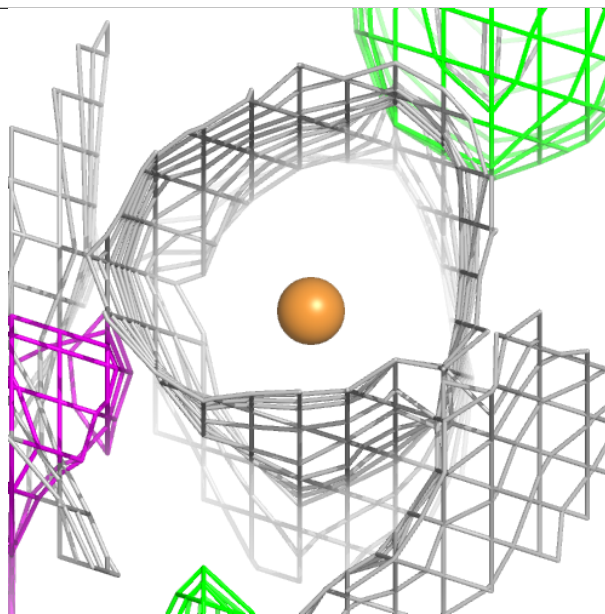
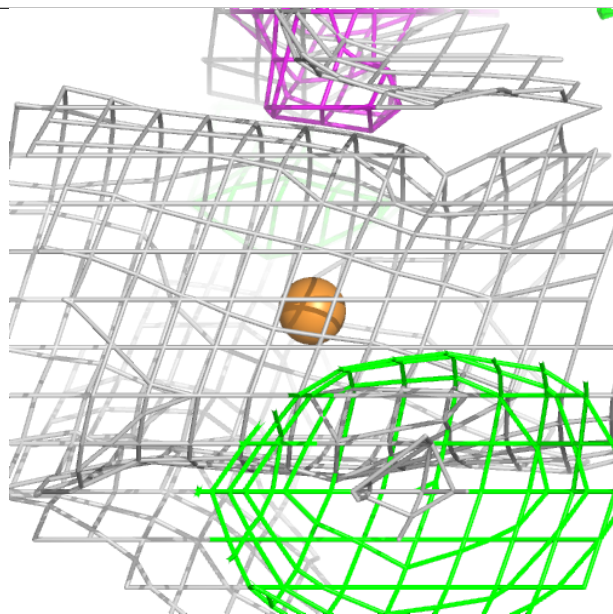
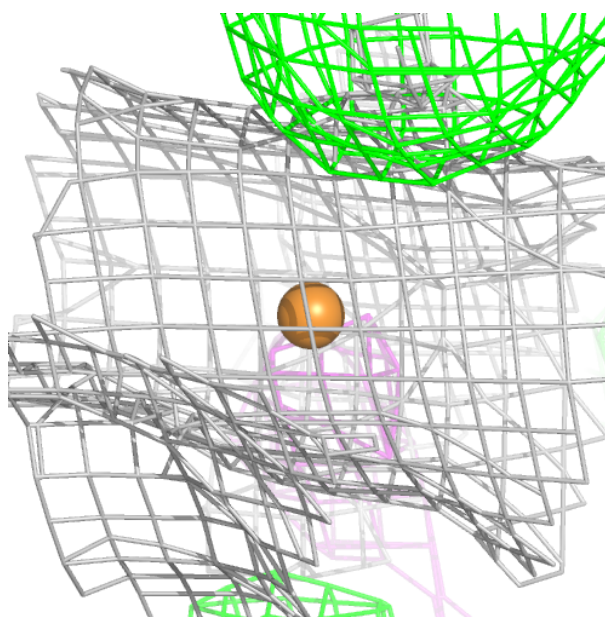
Electron density around CU E 604:

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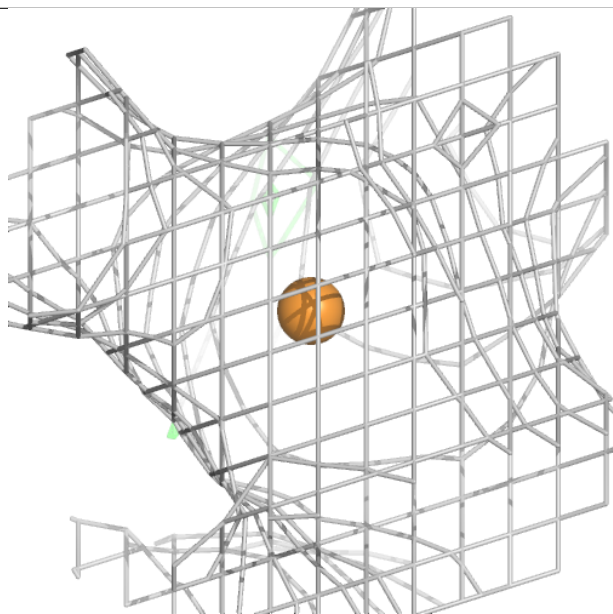
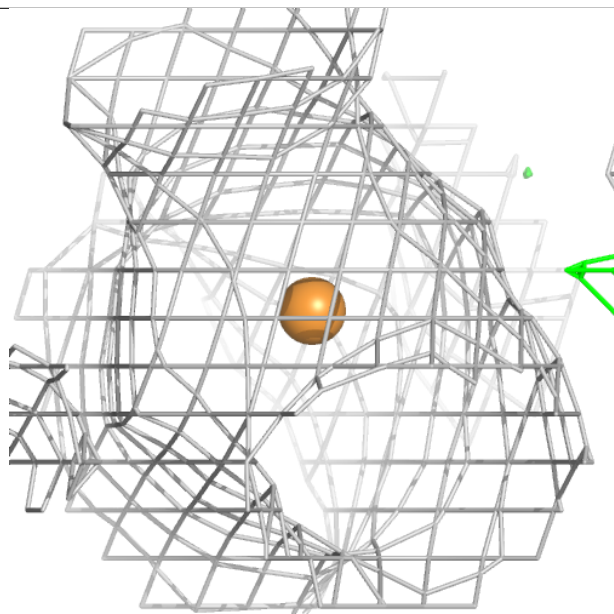
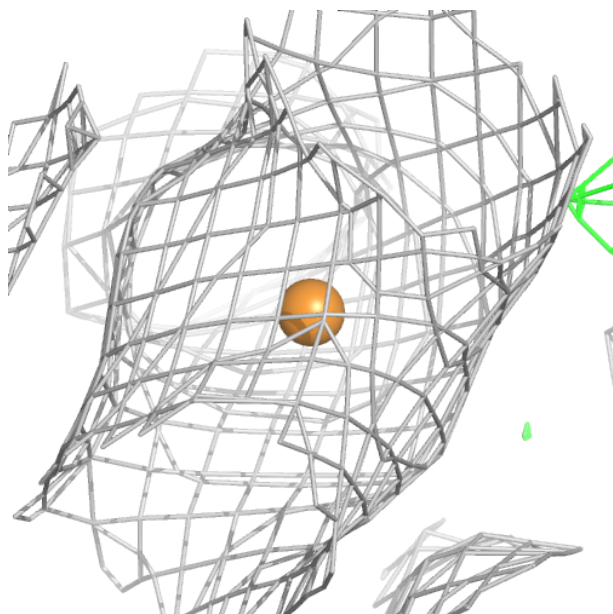
Electron density around CU A 603:

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and green (positive)



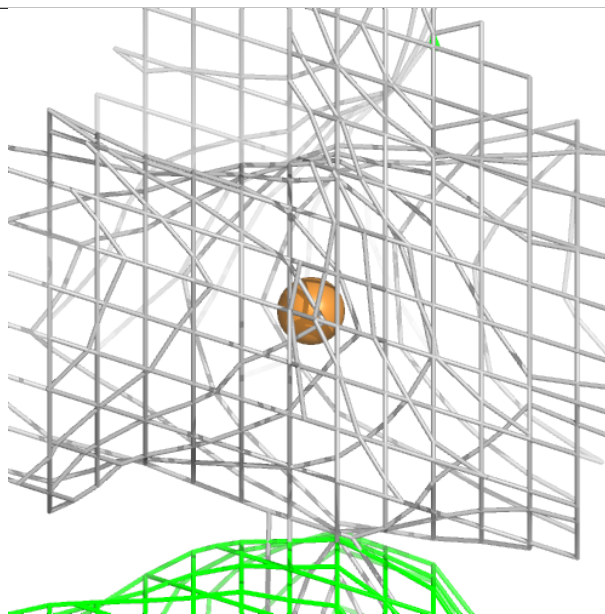
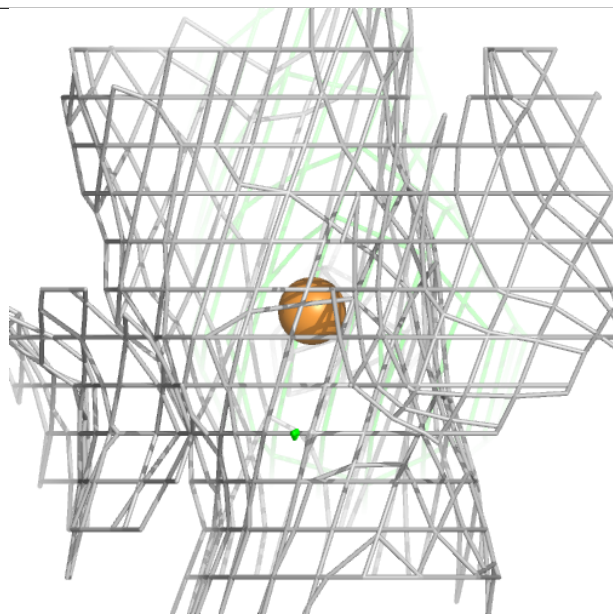
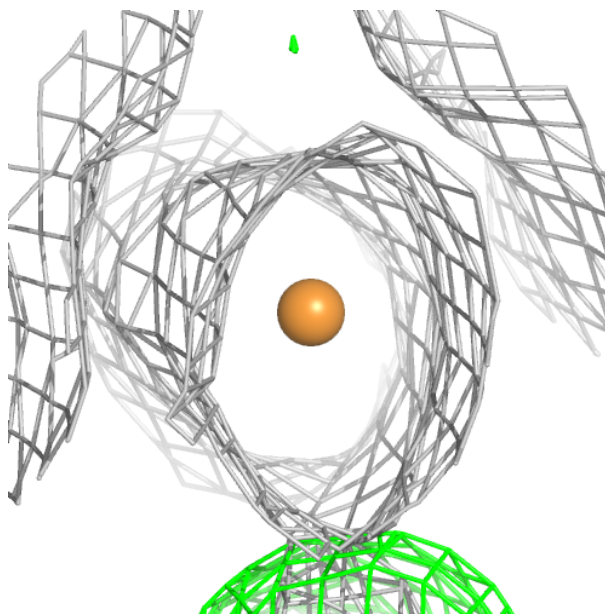
Electron density around CU F 602:

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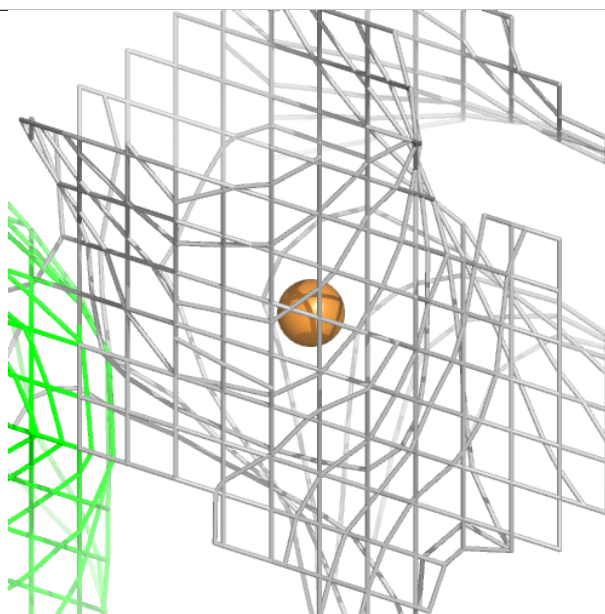
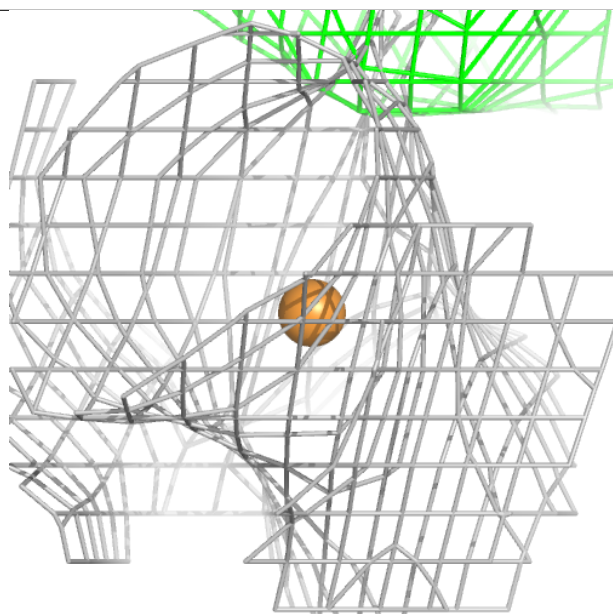
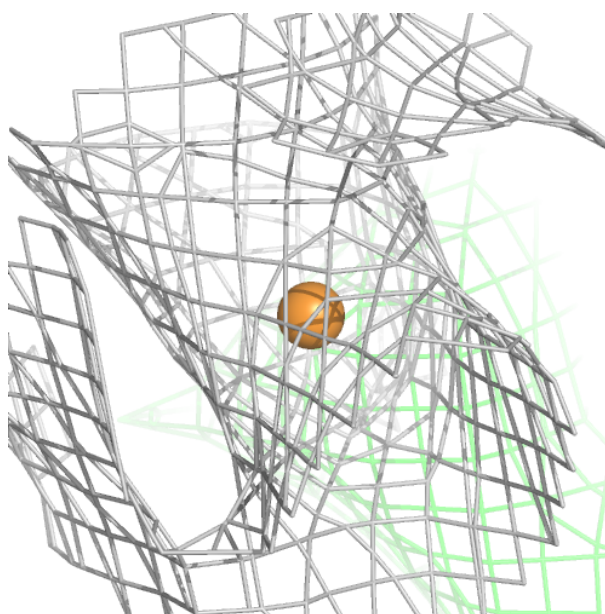
Electron density around CU F 603:

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and green (positive)



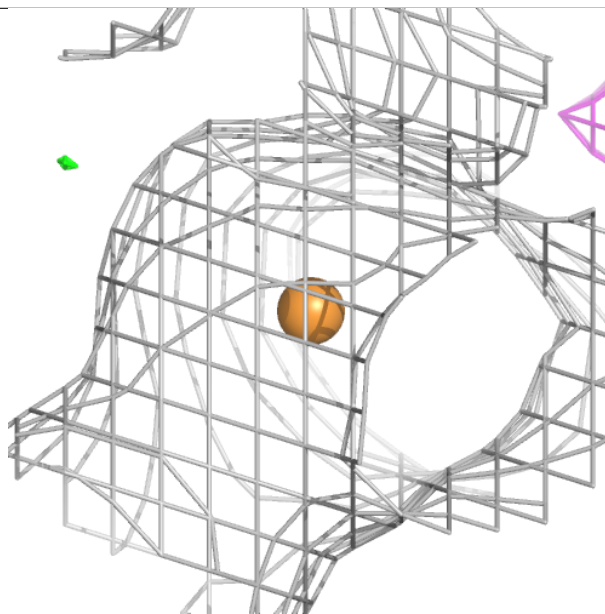
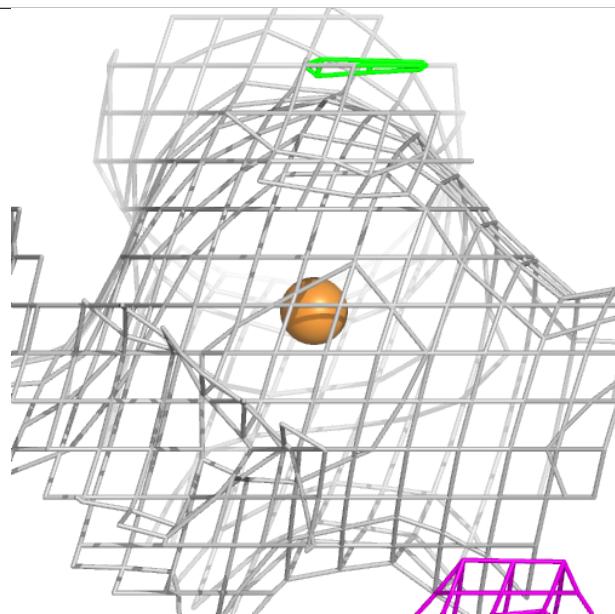
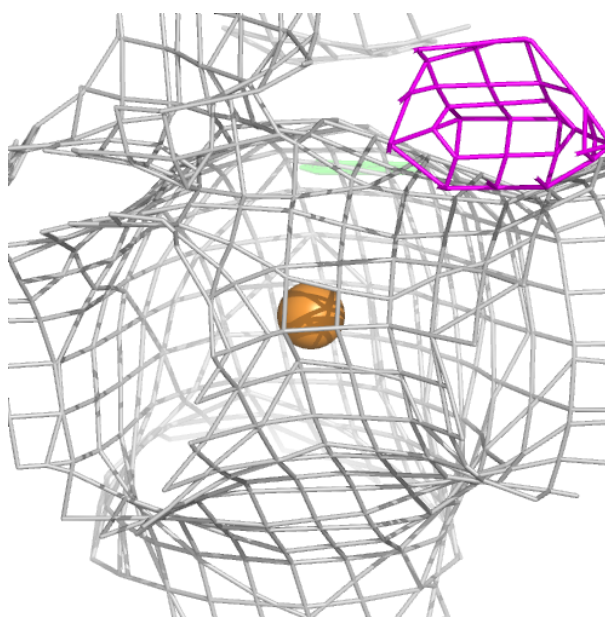
Electron density around CU D 603:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



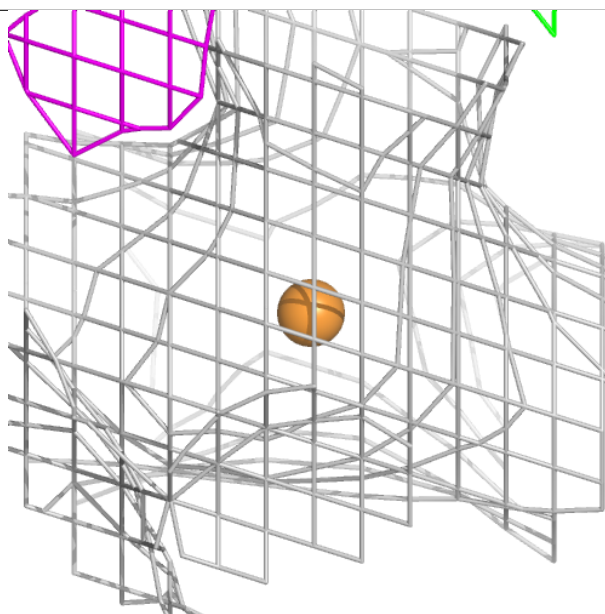
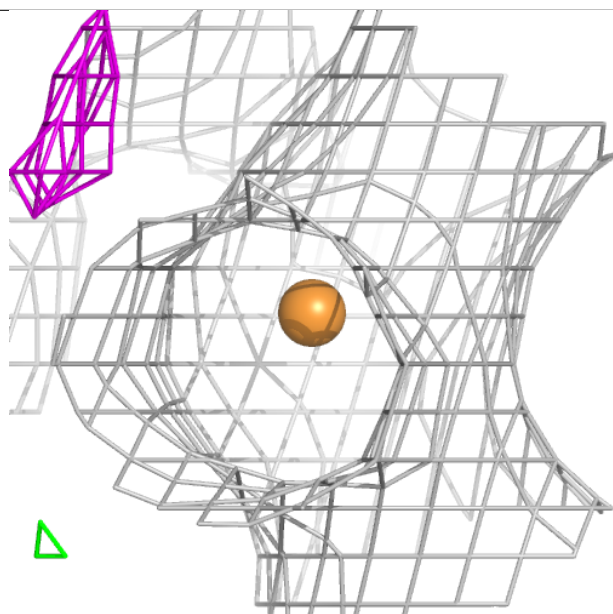
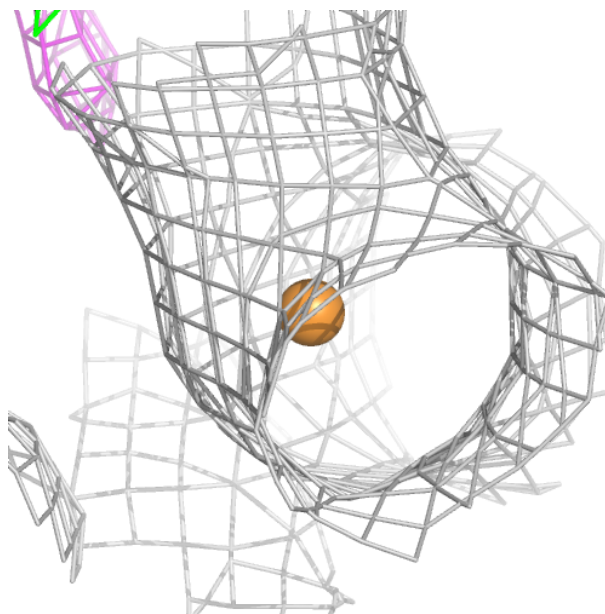
Electron density around CU C 601:

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



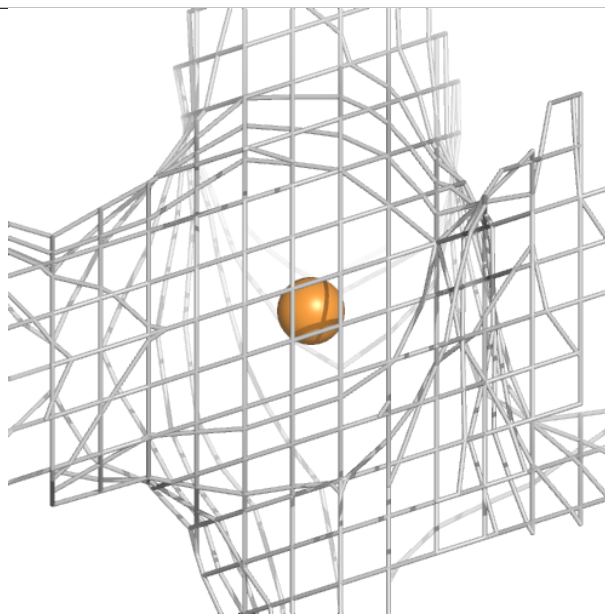
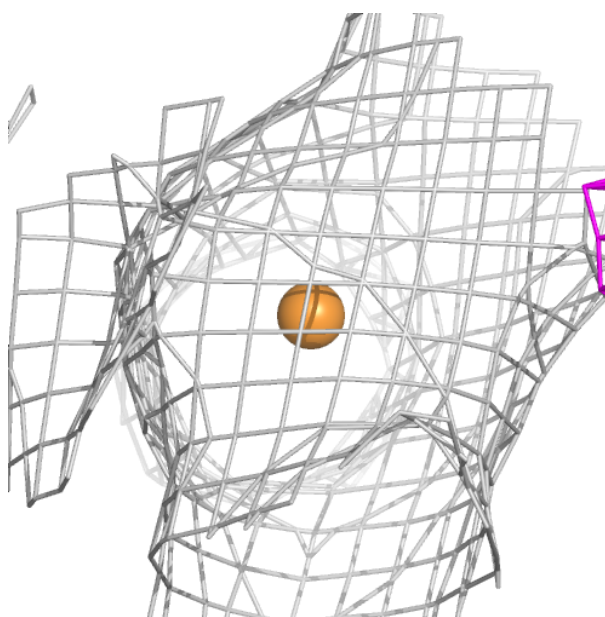
Electron density around CU H 601:

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



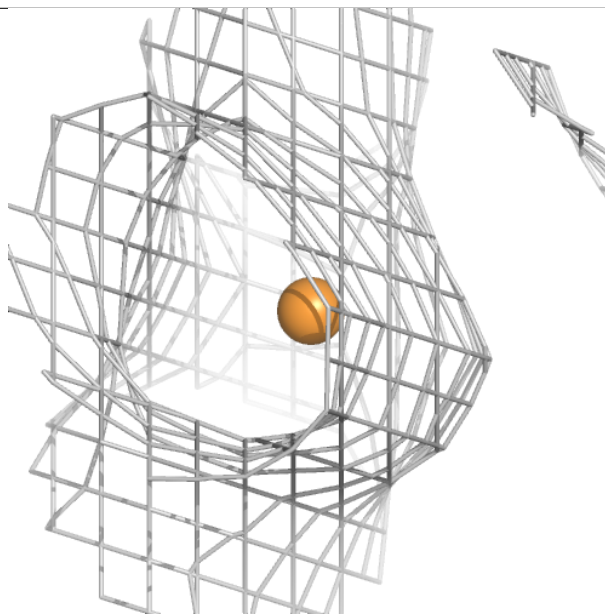
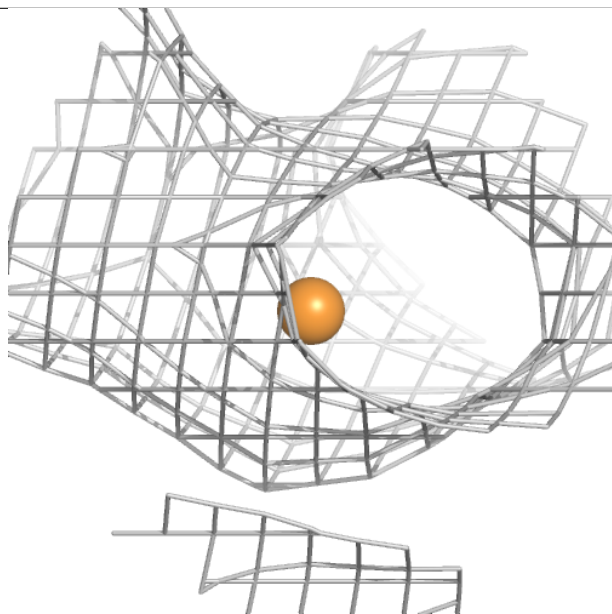
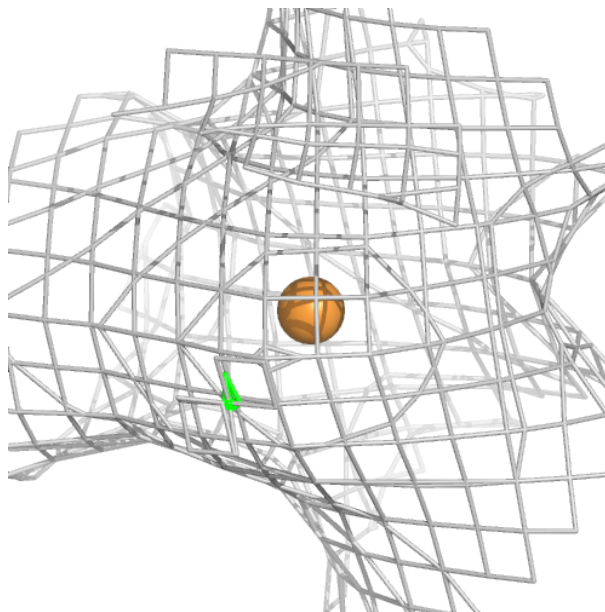
Electron density around CU H 602:

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



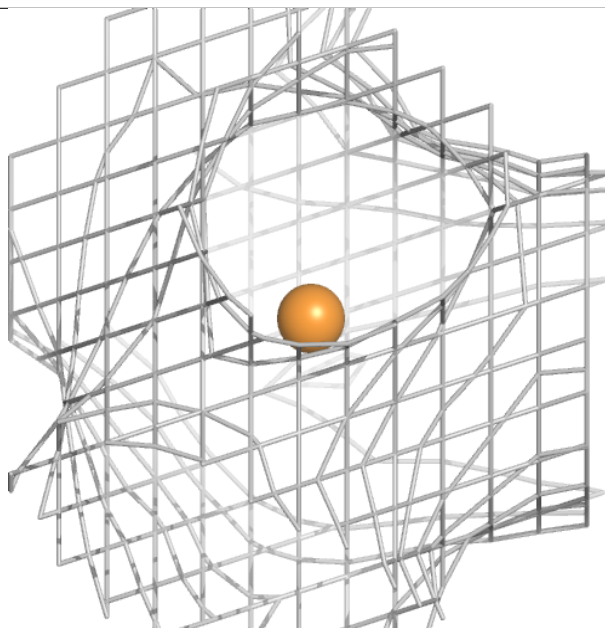
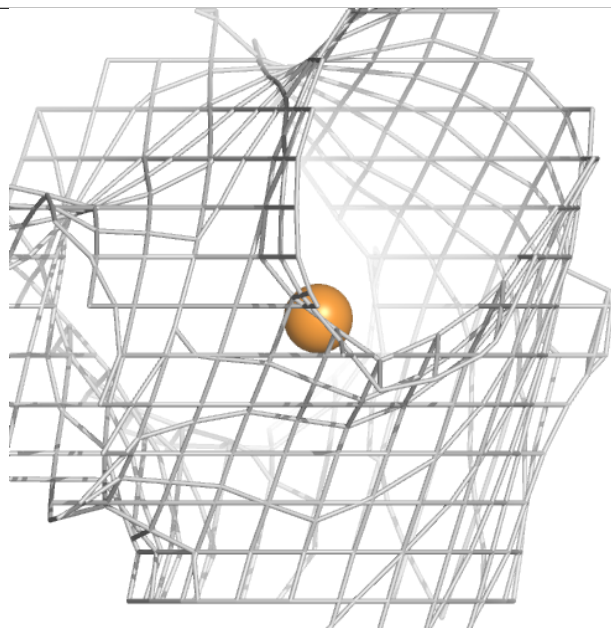
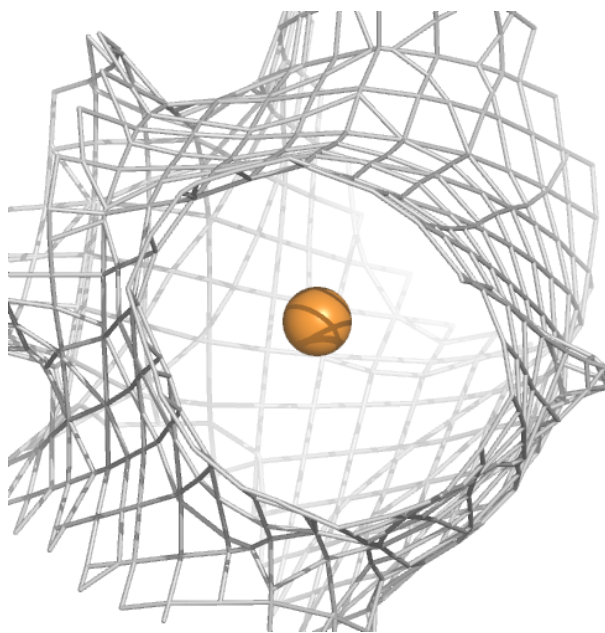
Electron density around CU B 601:

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



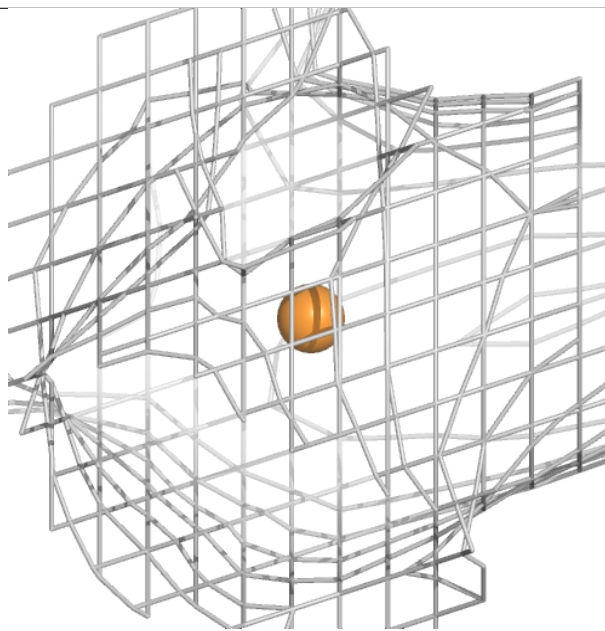
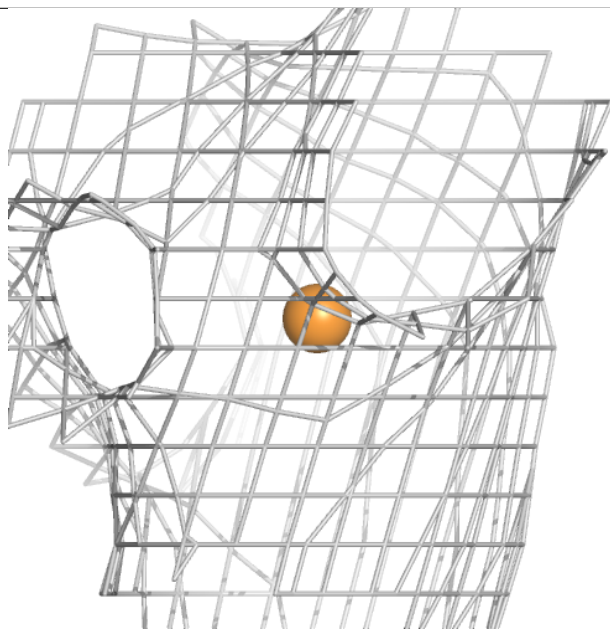
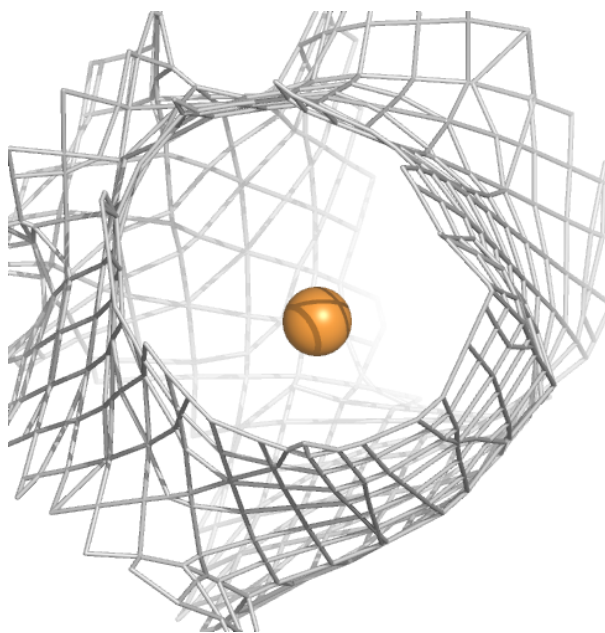
Electron density around CU H 604:

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



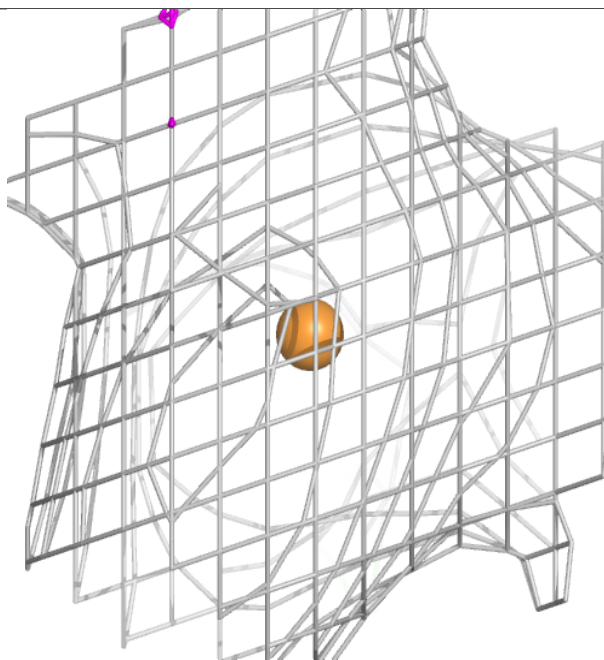
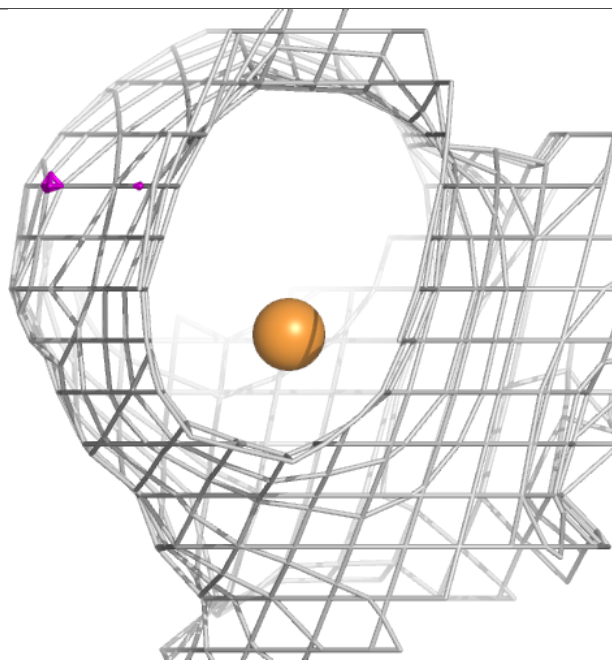
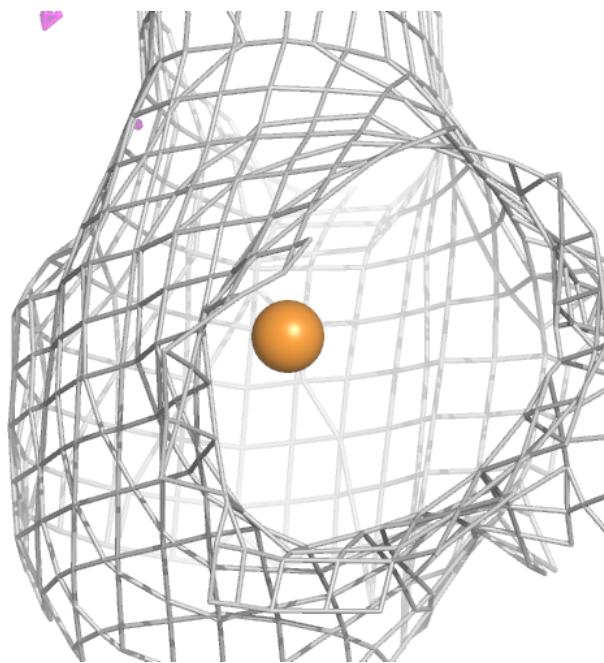
Electron density around CU D 604:

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



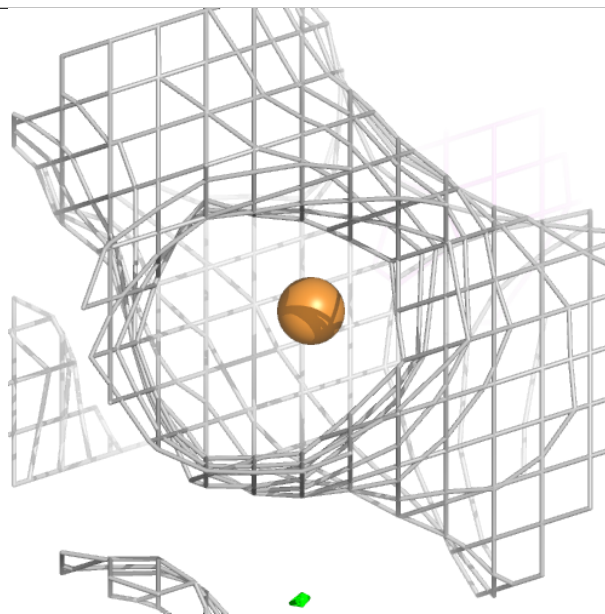
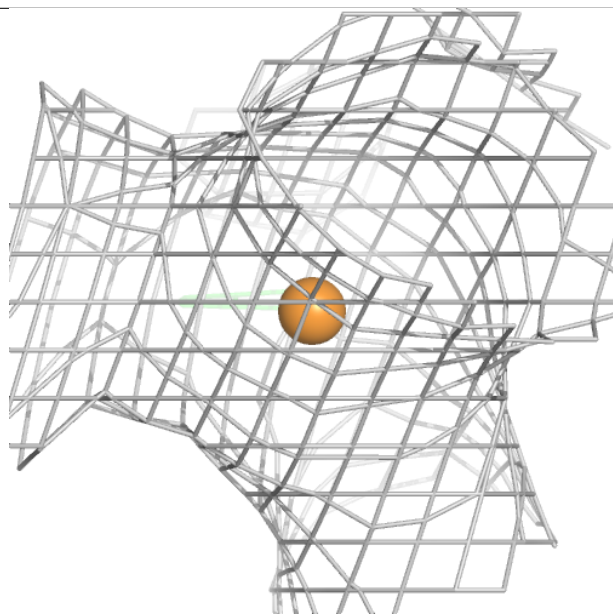
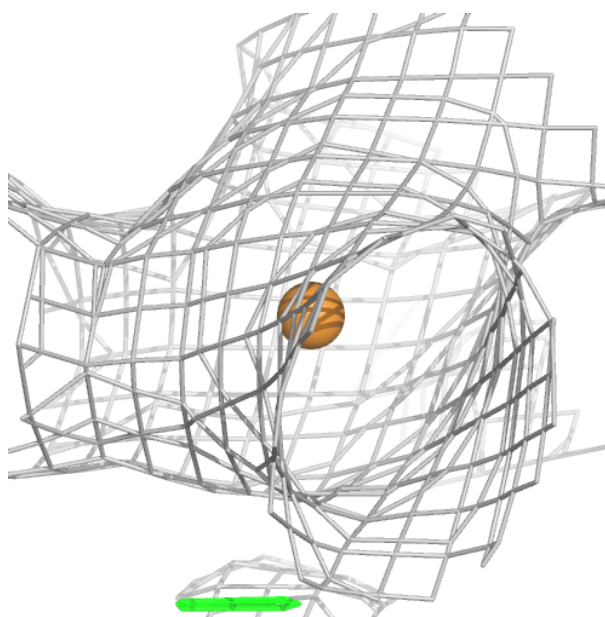
Electron density around CU F 604:

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



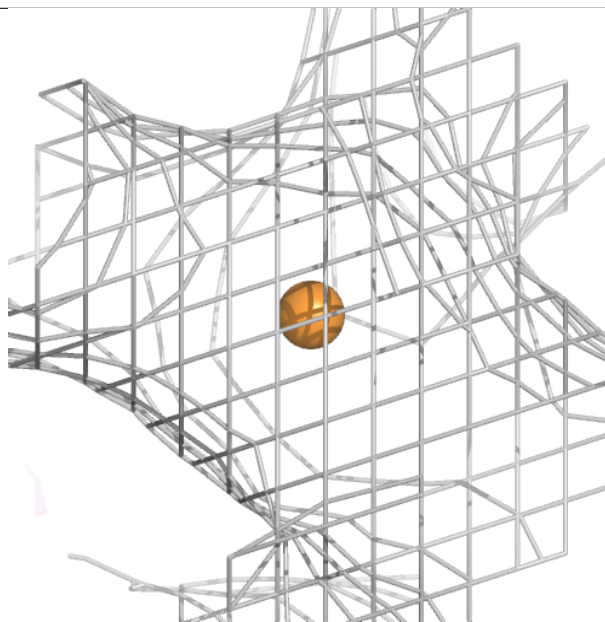
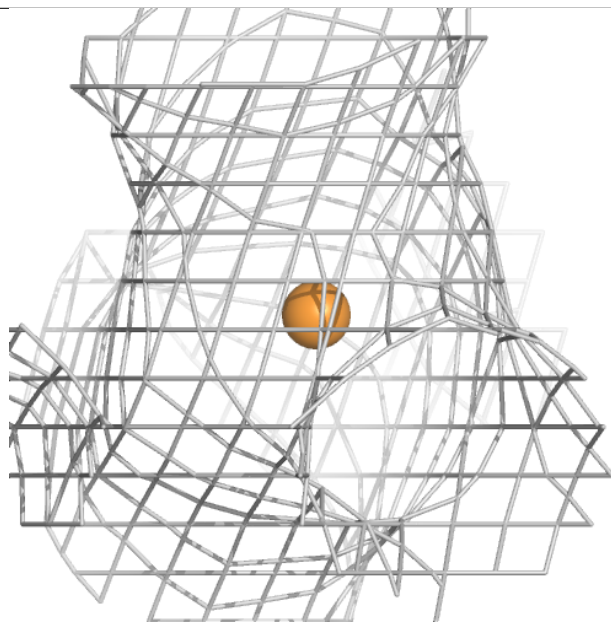
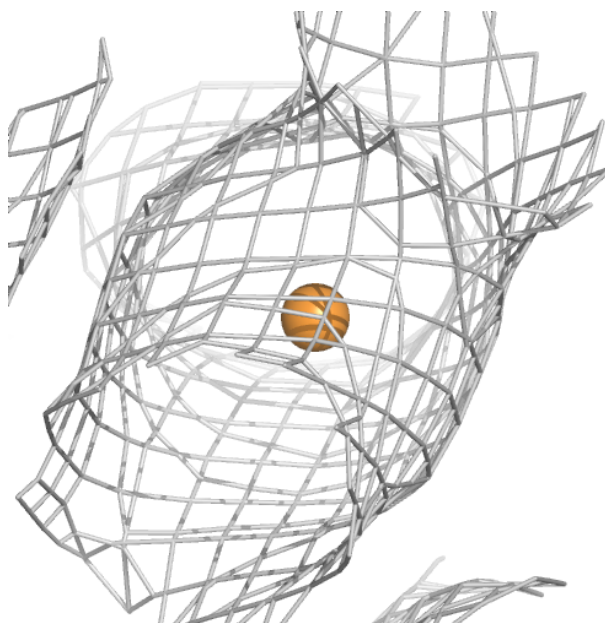
Electron density around CU C 602:

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



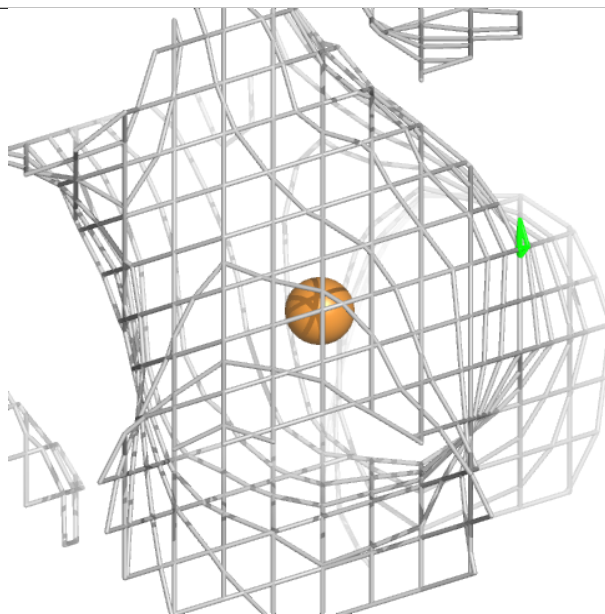
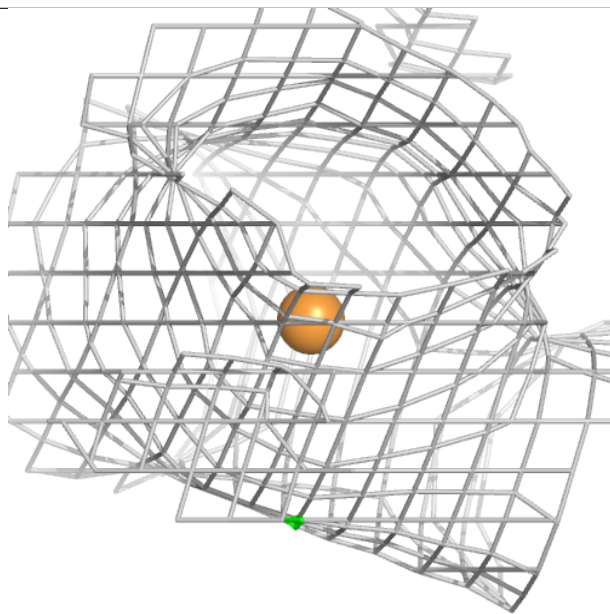
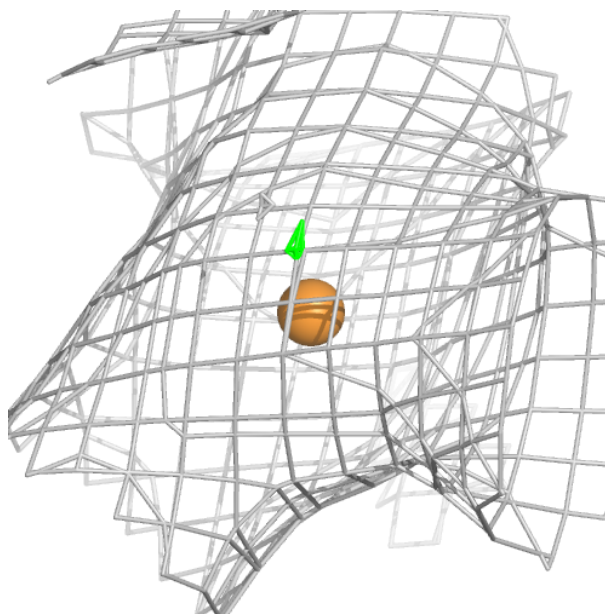
Electron density around CU G 602:

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



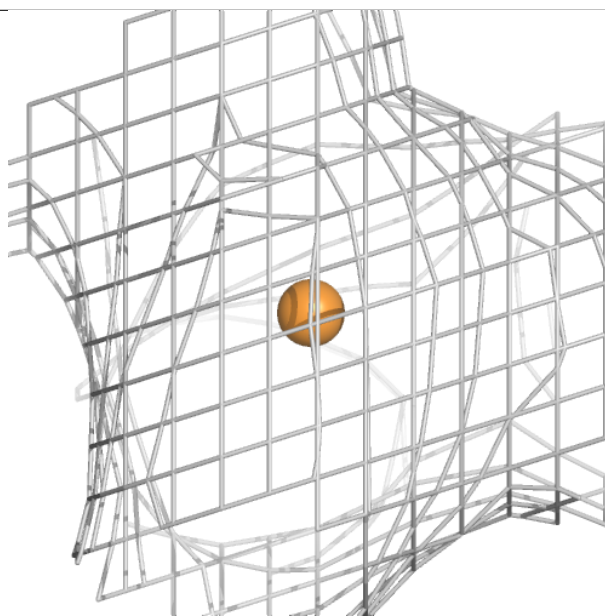
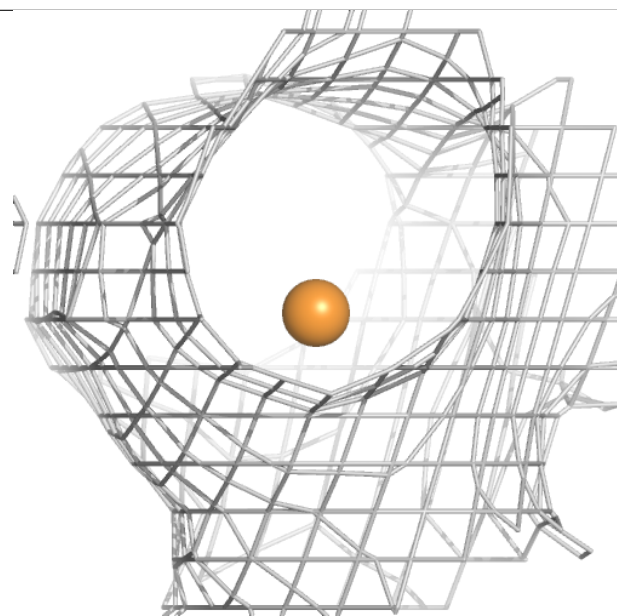
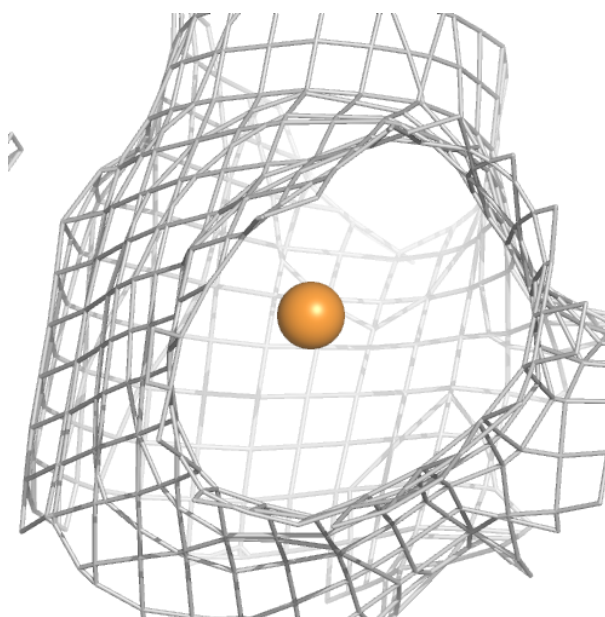
Electron density around CU B 602:

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



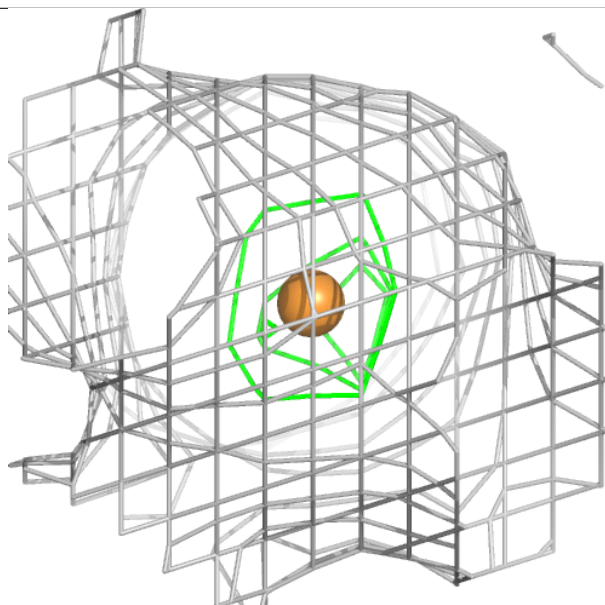
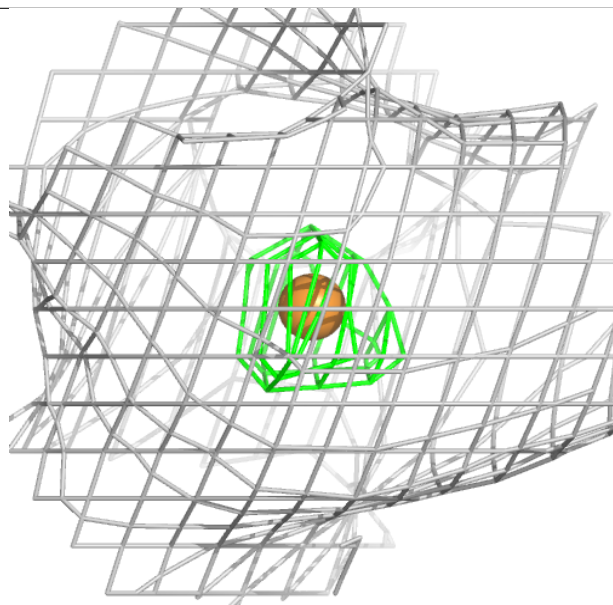
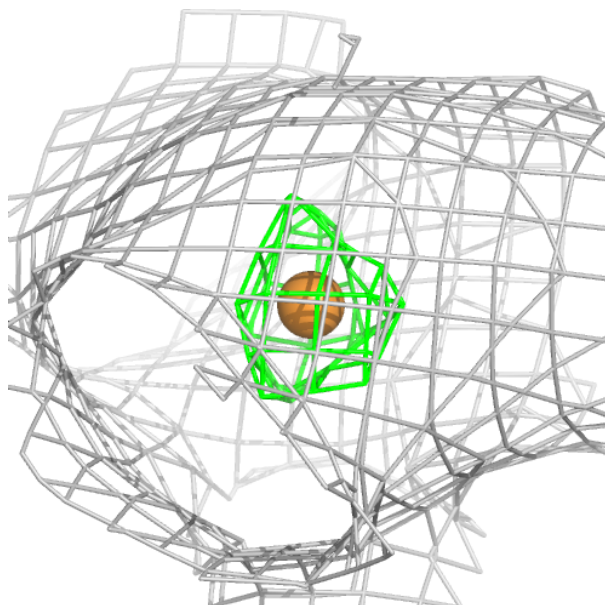
Electron density around CU G 604:

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



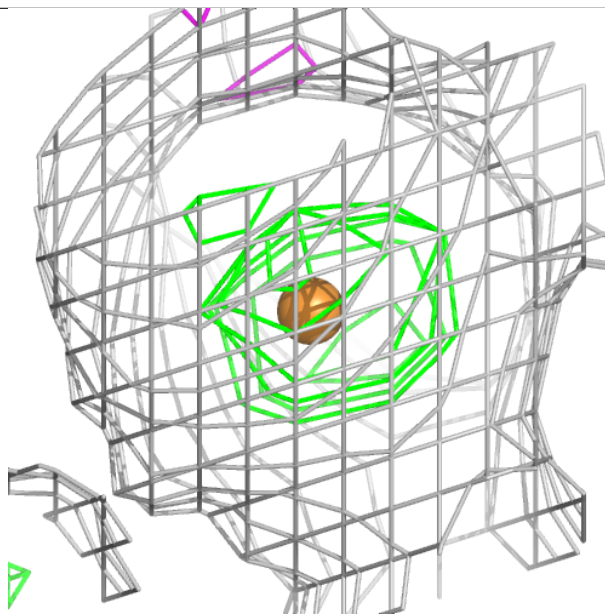
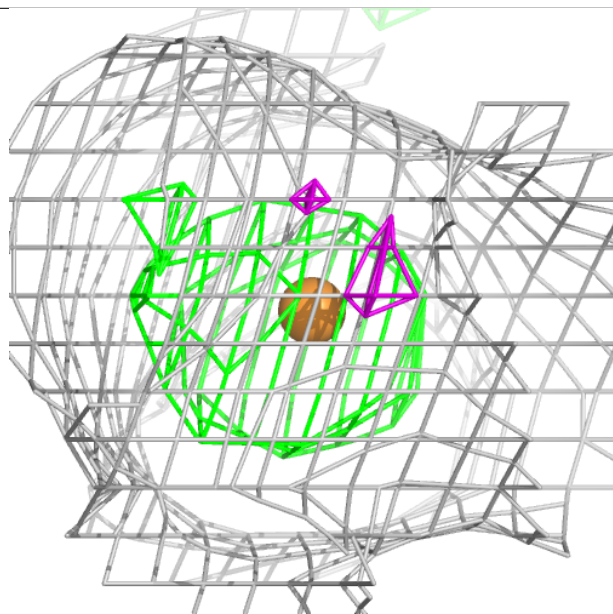
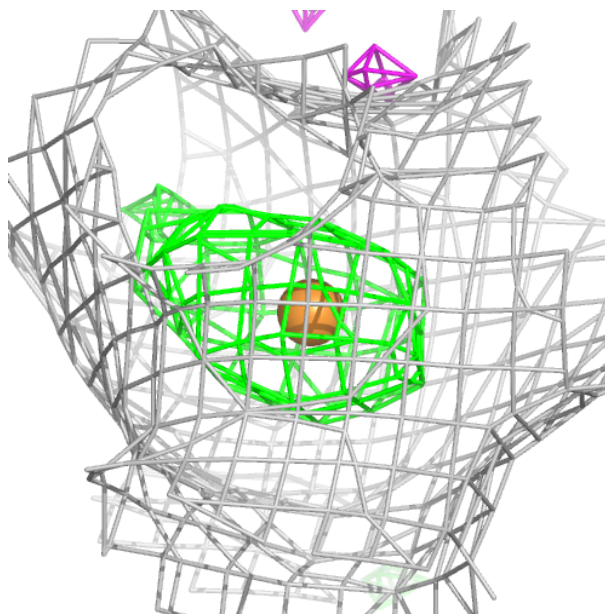
Electron density around CU C 604:

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



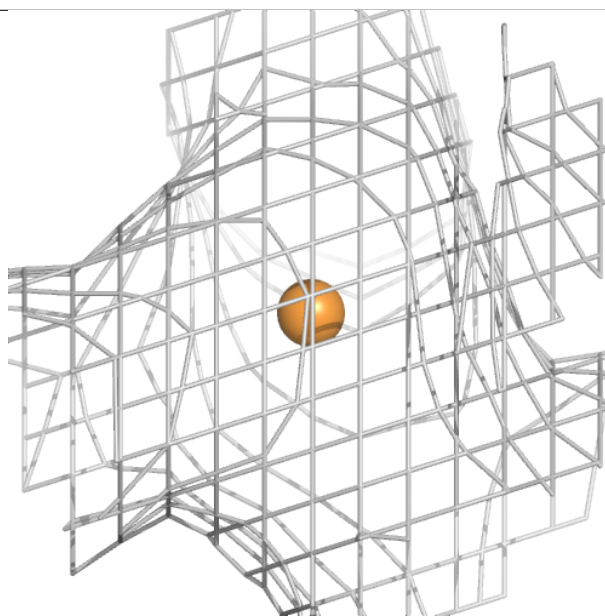
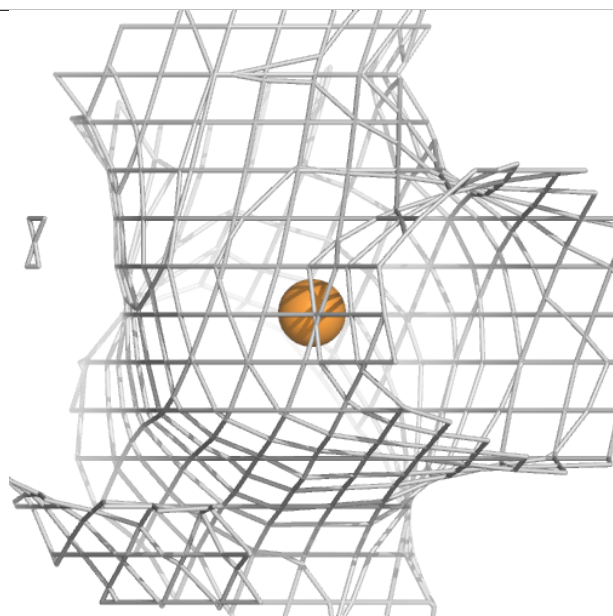
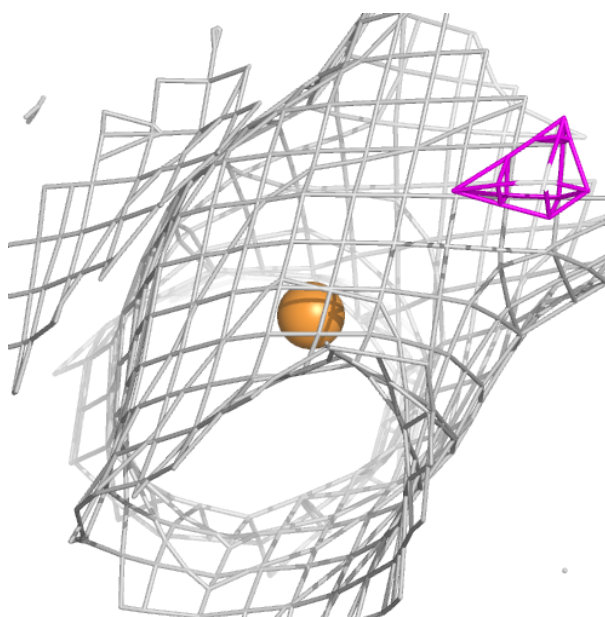
Electron density around CU A 604:

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



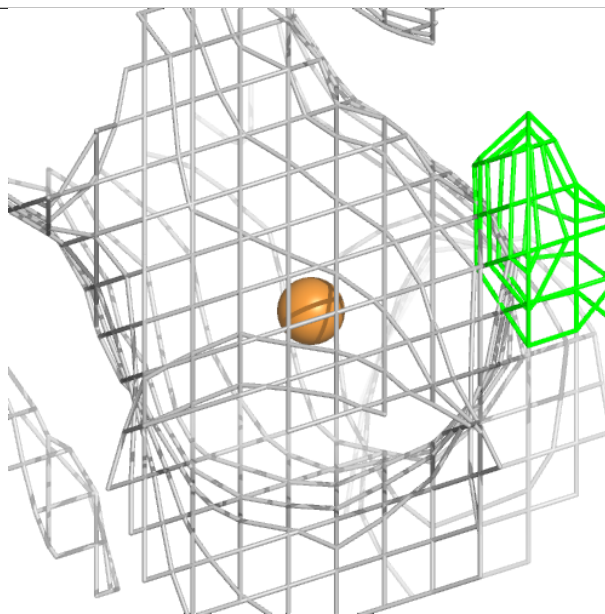
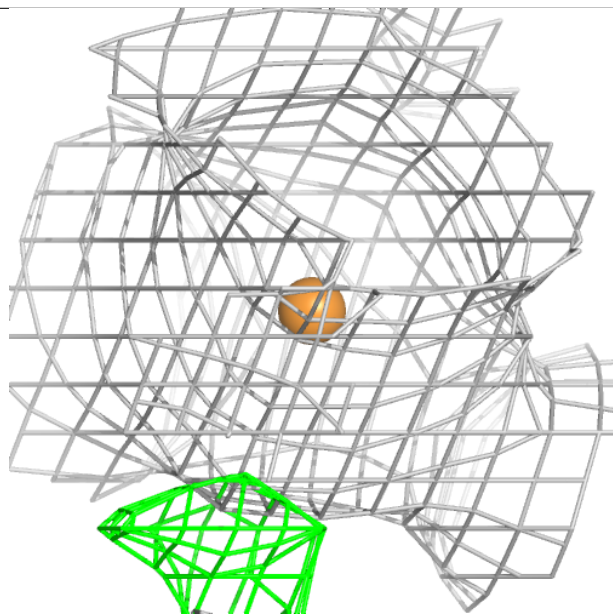
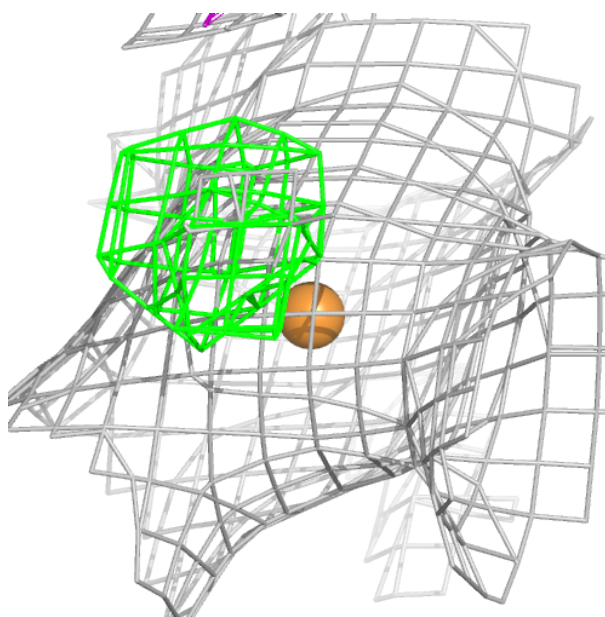
Electron density around CU D 602:

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



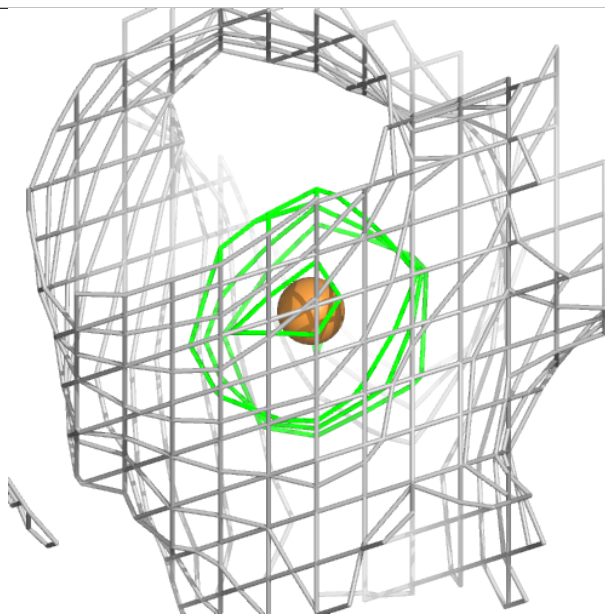
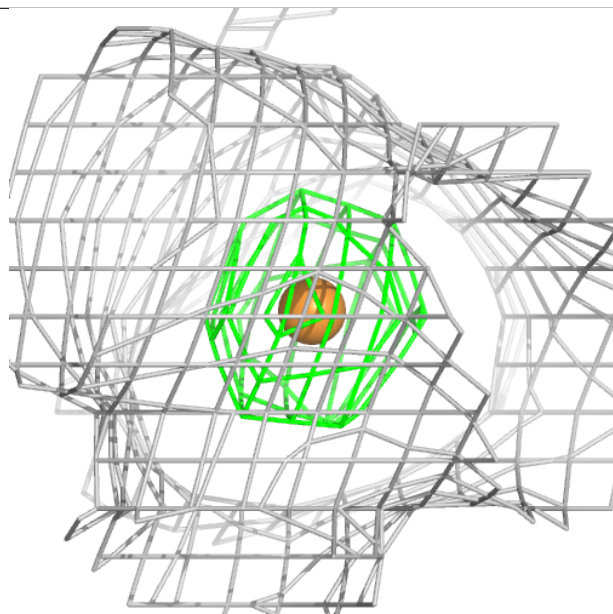
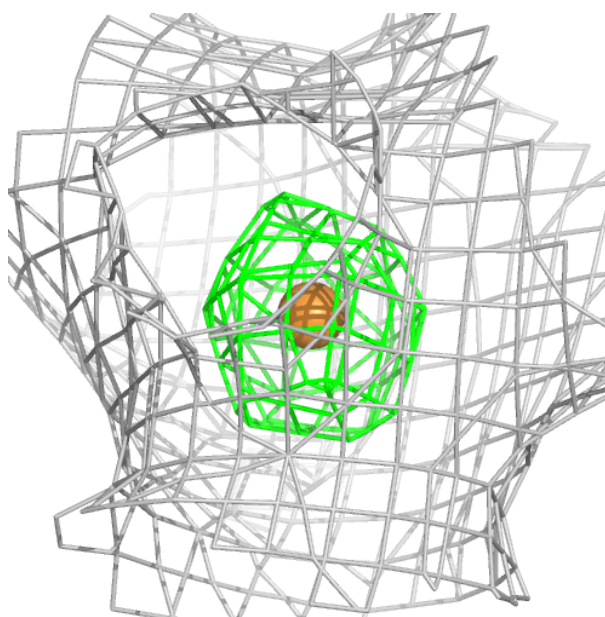
Electron density around CU A 602:

$2mF_o-DF_c$ (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.