



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 03:36 PM EDT

PDB ID : 8JIB / pdb_00008jib
Title : Crystal Structure of Prophenoloxidase PPO6 from Aedes aegypti
Authors : Zhu, X.; Zhang, L.; Yang, X.; Bao, P.; Ren, D.; Han, Q.
Deposited on : 2023-05-26
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

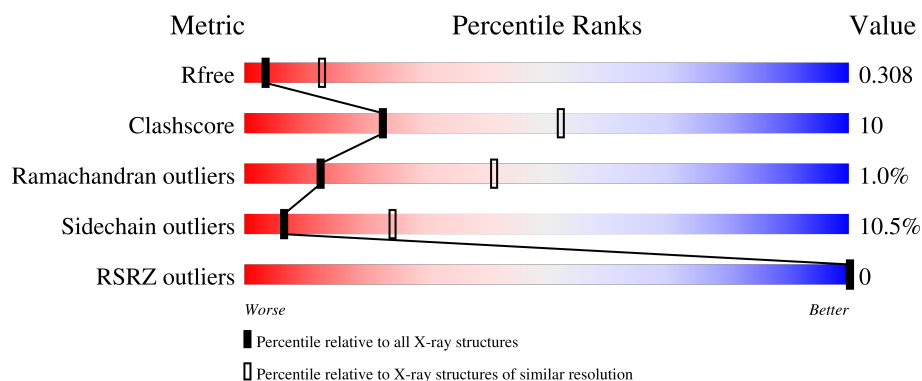
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	681	 71% 20% 5% .
1	B	681	 70% 20% . . 5%
1	C	681	 69% 21% . . 5%
1	D	681	 72% 19% . . 5%
1	E	681	 72% 20% . . .

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Mol	Chain	Length	Quality of chain
1	F	681	
1	G	681	
1	H	681	
1	I	681	
1	J	681	
1	K	681	
1	L	681	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 65153 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 TK receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			5377	3422	969	961	25			
1	B	645	Total	C	N	O	S	0	0	0
			5330	3395	960	952	23			
1	C	648	Total	C	N	O	S	0	0	0
			5358	3412	966	955	25			
1	D	650	Total	C	N	O	S	0	0	0
			5373	3420	968	960	25			
1	E	661	Total	C	N	O	S	0	0	0
			5450	3466	981	976	27			
1	F	657	Total	C	N	O	S	0	0	0
			5421	3448	976	971	26			
1	G	659	Total	C	N	O	S	0	0	0
			5431	3453	978	973	27			
1	H	661	Total	C	N	O	S	0	0	0
			5450	3466	981	976	27			
1	I	660	Total	C	N	O	S	0	0	0
			5442	3462	979	974	27			
1	J	659	Total	C	N	O	S	0	0	0
			5431	3453	978	973	27			
1	K	660	Total	C	N	O	S	0	0	0
			5442	3462	979	974	27			
1	L	659	Total	C	N	O	S	0	0	0
			5431	3453	978	973	27			

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

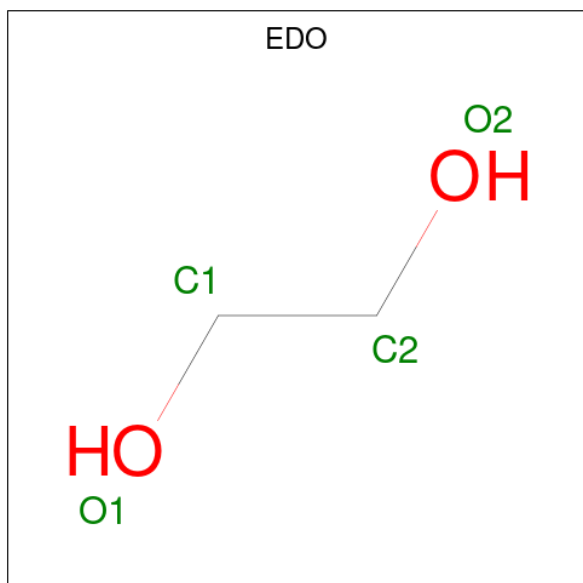
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		
2	B	2	Total	Cu	0	0
			2	2		

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	F	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0

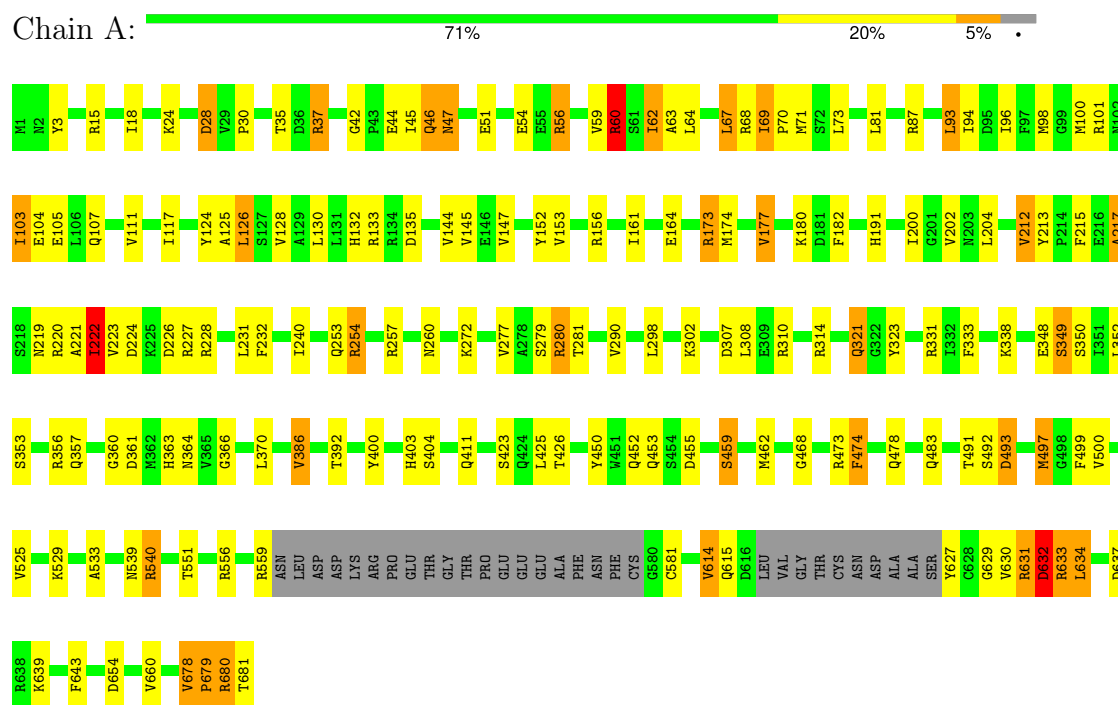
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total 31	O 31	0	0
4	B	25	Total 25	O 25	0	0
4	C	23	Total 23	O 23	0	0
4	D	13	Total 13	O 13	0	0
4	E	14	Total 14	O 14	0	0
4	F	12	Total 12	O 12	0	0
4	G	8	Total 8	O 8	0	0
4	H	6	Total 6	O 6	0	0
4	I	8	Total 8	O 8	0	0
4	J	6	Total 6	O 6	0	0
4	K	1	Total 1	O 1	0	0
4	L	18	Total 18	O 18	0	0

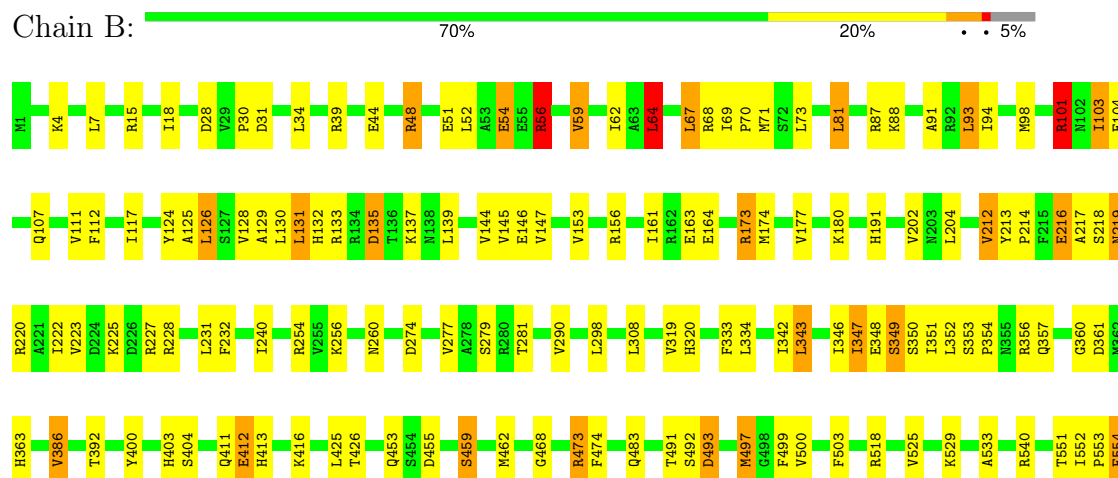
3 Residue-property plots

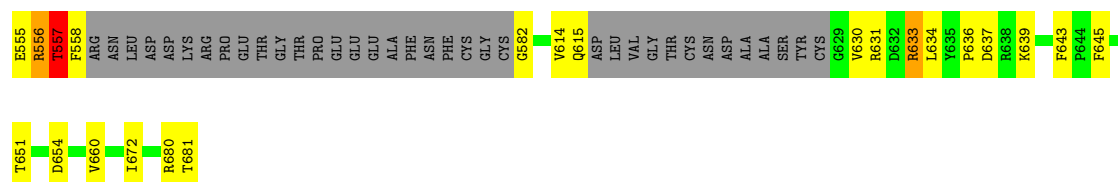
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: TK receptor



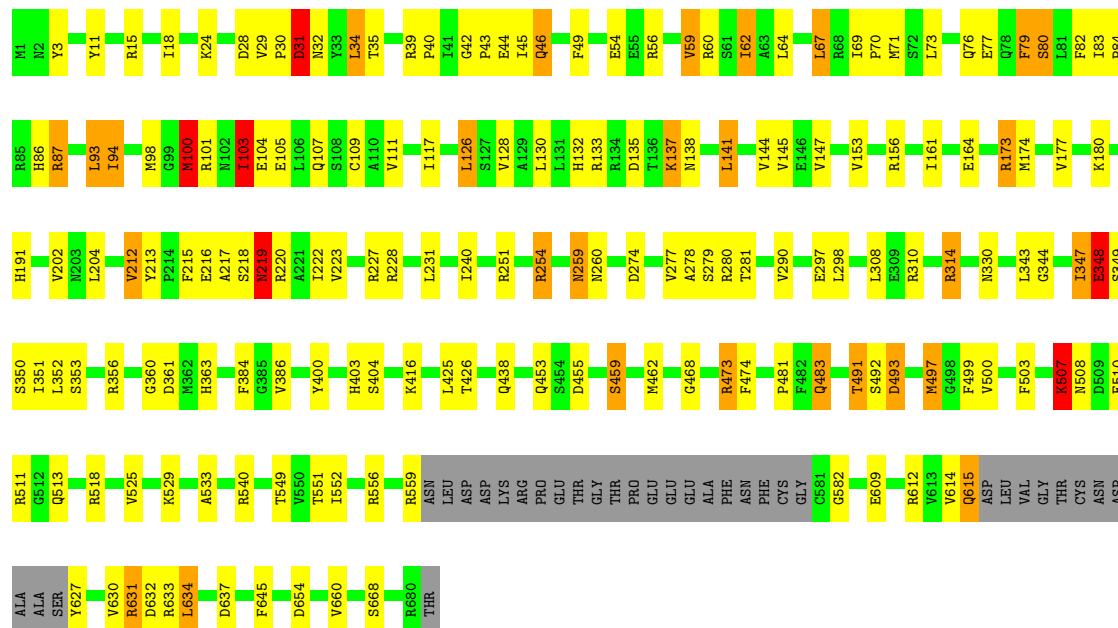
• Molecule 1: TK receptor





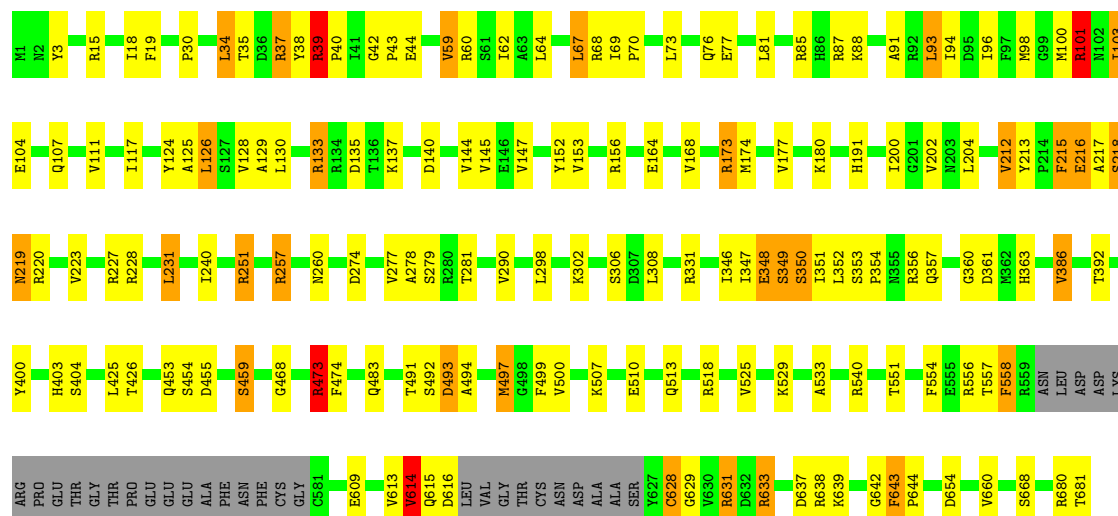
• Molecule 1: TK receptor

Chain C: 69% 21% 5%



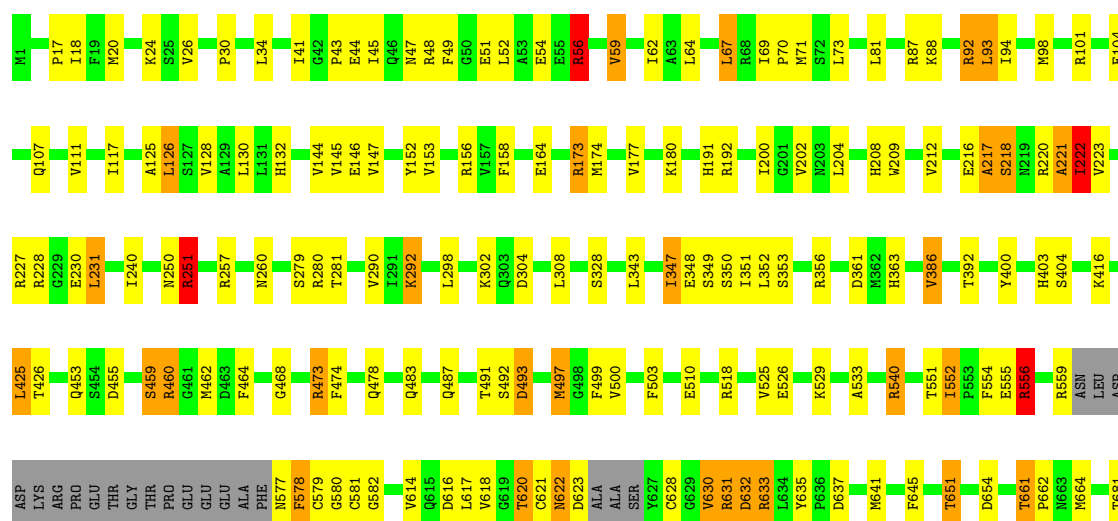
• Molecule 1: TK receptor

Chain D: 72% 19% 5%



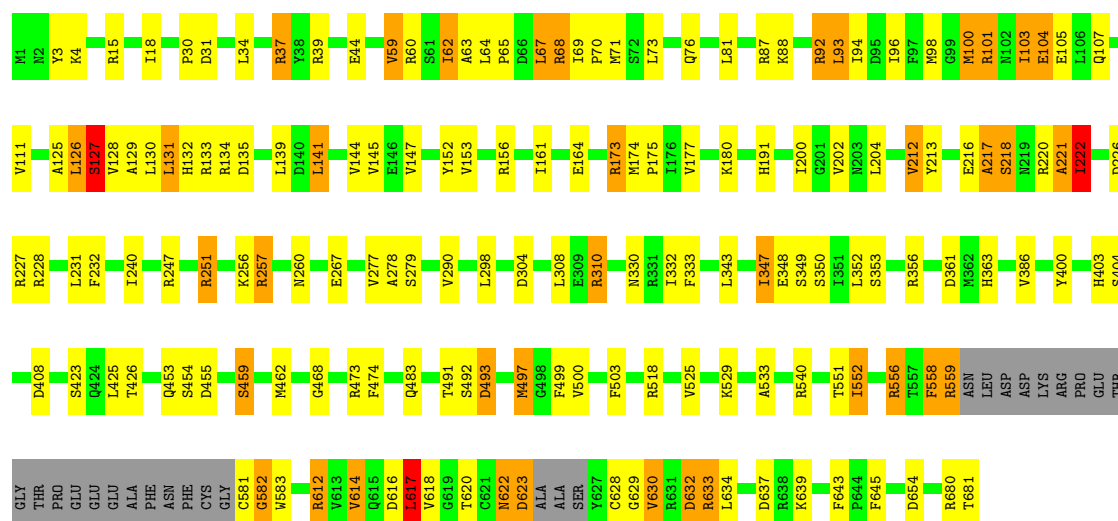
• Molecule 1: TK receptor

Chain E:  72% 20% . . .



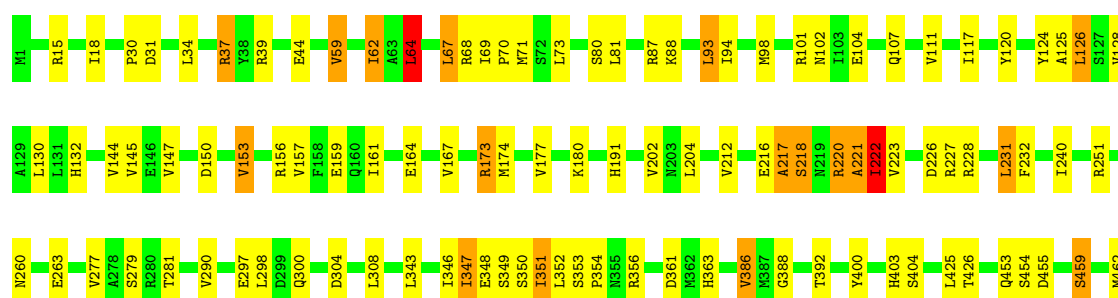
• Molecule 1: TK receptor

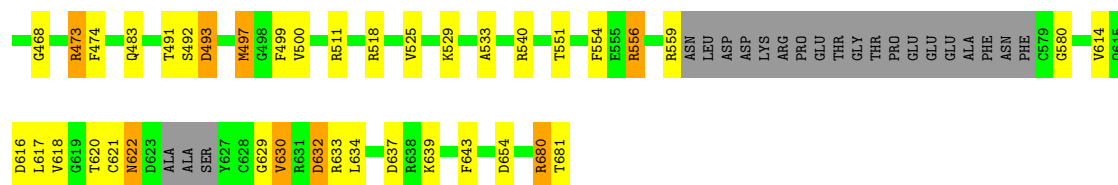
Chain F:  72% 19% 6% .



• Molecule 1: TK receptor

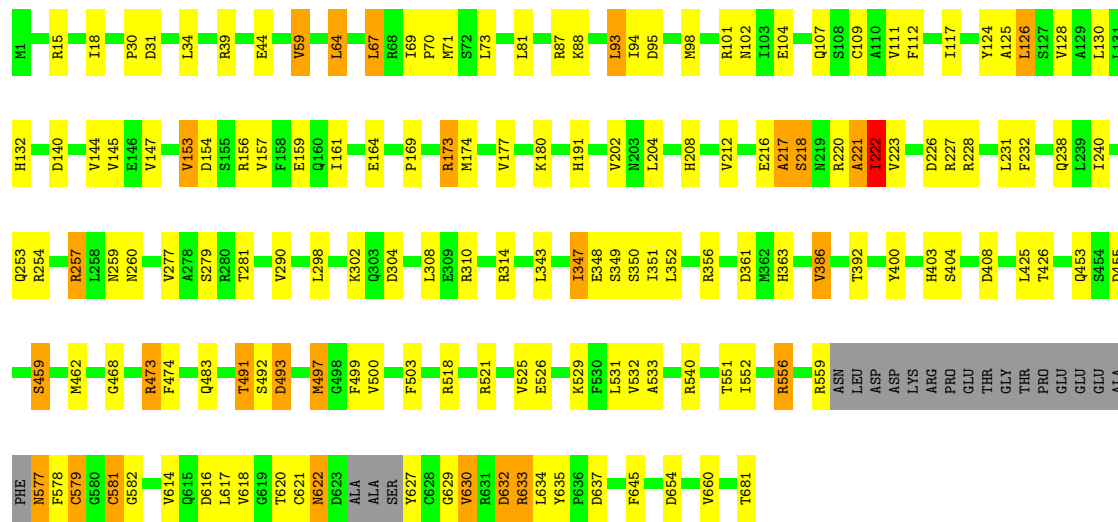
Chain G:  75% 17% . . .





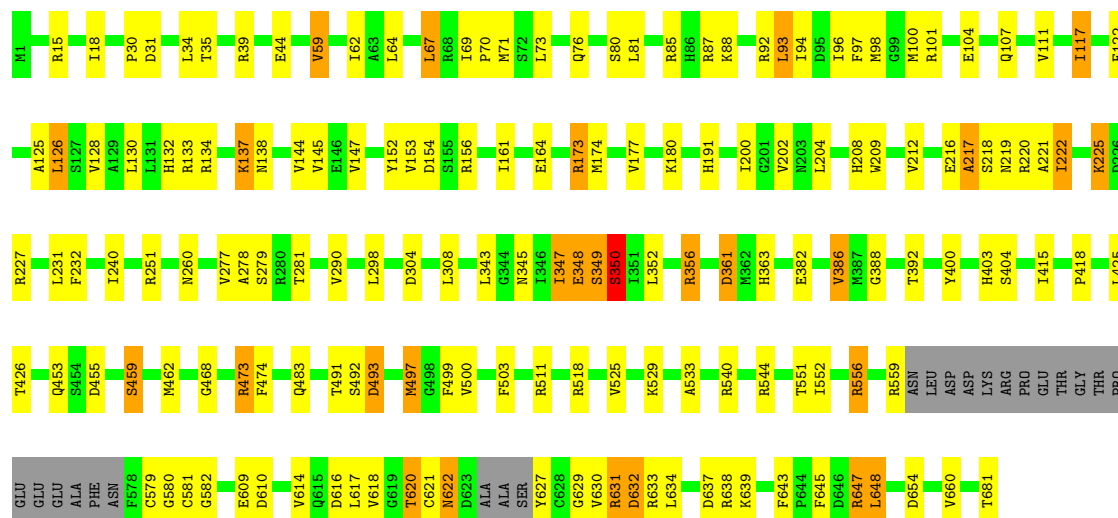
• Molecule 1: TK receptor

Chain H: 74% 19%



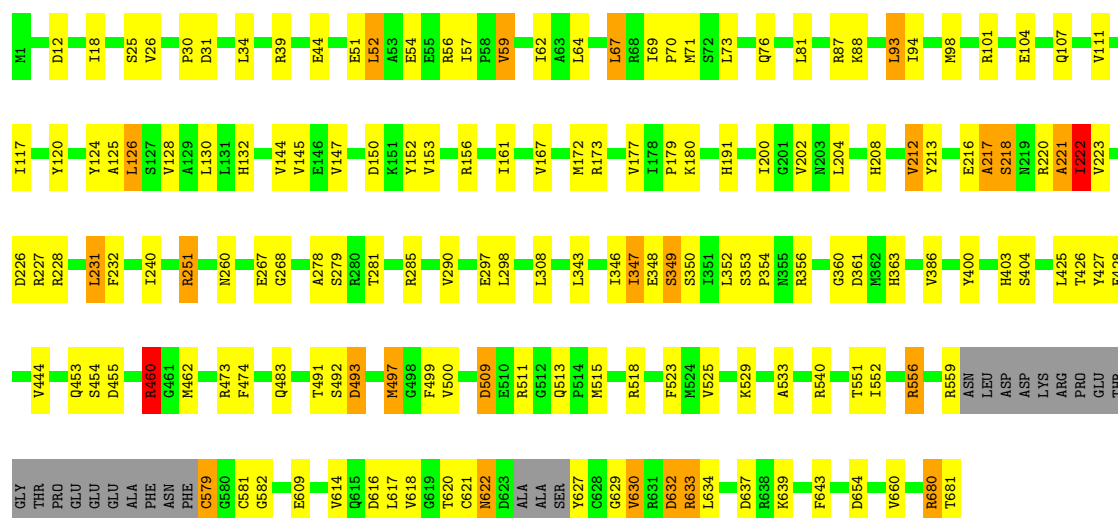
• Molecule 1: TK receptor

Chain I: 73% 20%



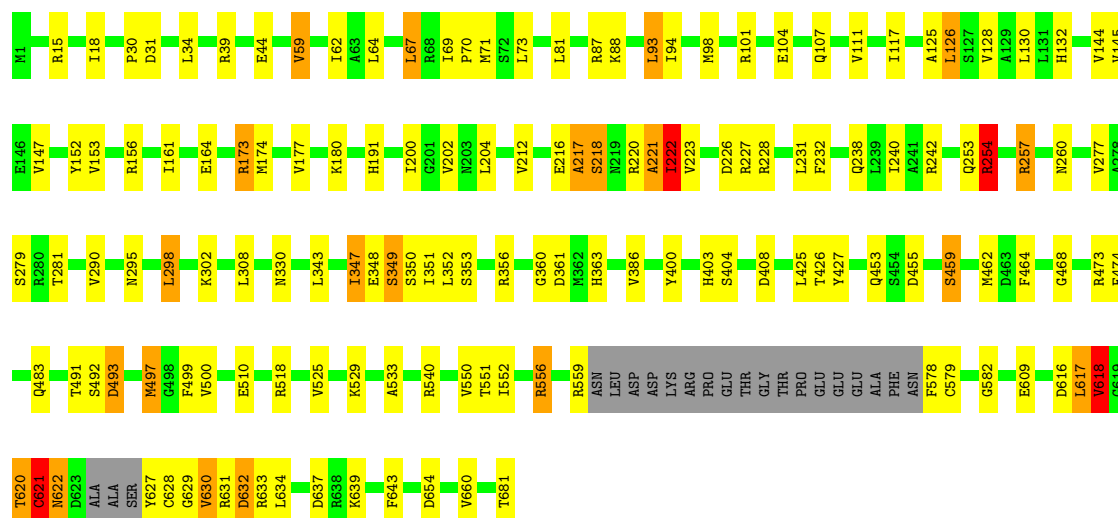
• Molecule 1: TK receptor

Chain J: 73% 20%



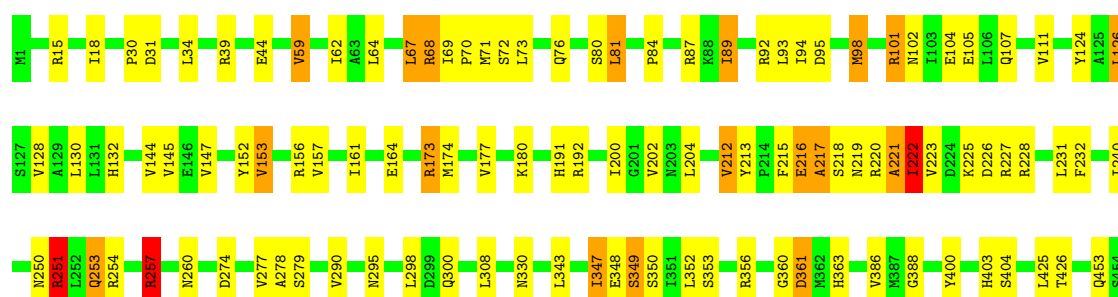
• Molecule 1: TK receptor

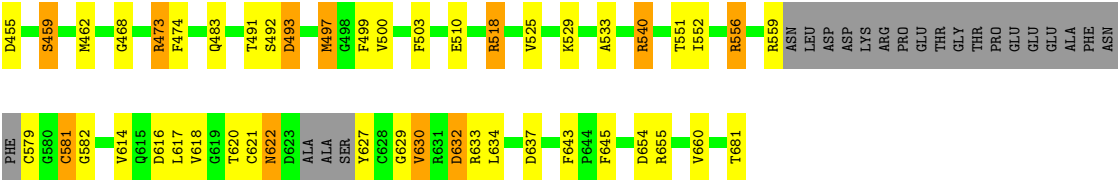
Chain K: 75% 18%



• Molecule 1: TK receptor

Chain L: 74% 18%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.04Å 364.15Å 125.52Å 90.00° 118.95° 90.00°	Depositor
Resolution (Å)	48.66 – 3.15 48.66 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.66-3.15) 98.2 (48.66-3.15)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.269 , 0.310 0.269 , 0.308	Depositor DCC
R_{free} test set	7921 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.046 for l,k,-h-l 0.046 for -h-l,k,h 0.387 for h,-k,-h-l 0.047 for l,-k,h 0.047 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	65153	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.38% 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: EDO, 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	0.55	0/5513	1.07	10/7461 (0.1%)
1	B	0.54	0/5465	1.03	5/7397 (0.1%)
1	C	0.54	0/5494	1.06	15/7435 (0.2%)
1	D	0.57	0/5509	1.04	9/7456 (0.1%)
1	E	0.53	0/5587	1.02	6/7562 (0.1%)
1	F	0.53	0/5557	1.05	12/7522 (0.2%)
1	G	0.51	0/5567	0.98	1/7535 (0.0%)
1	H	0.51	0/5587	0.99	3/7562 (0.0%)
1	I	0.52	0/5579	1.01	8/7551 (0.1%)
1	J	0.51	0/5567	1.00	4/7535 (0.1%)
1	K	0.50	0/5579	0.98	4/7551 (0.1%)
1	L	0.51	0/5567	0.99	7/7535 (0.1%)
All	All	0.53	0/66571	1.02	84/90102 (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	A	0	1
1	B	0	1
1	D	0	3
1	E	0	3
1	F	0	4
1	G	0	1
1	H	0	2
1	J	0	2
1	K	0	1
1	L	0	2
All	All	0	20

There are no bond length outliers.

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	PHE	CB-CA-C	10.70	131.72	110.42
1	F	228	ARG	CG-CD-NE	-9.28	91.59	112.00
1	F	247	ARG	CG-CD-NE	-9.01	92.18	112.00
1	K	620	THR	CA-CB-OG1	-8.39	97.01	109.60
1	H	408	ASP	CA-CB-CG	7.70	120.30	112.60

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ARG	Sidechain
1	B	56	ARG	Sidechain
1	D	34	LEU	Mainchain
1	D	473	ARG	Sidechain
1	D	631	ARG	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	5377	0	5284	136	3
1	B	5330	0	5242	111	0
1	C	5358	0	5270	133	3
1	D	5373	0	5281	120	1
1	E	5450	0	5348	142	0
1	F	5421	0	5324	152	0
1	G	5431	0	5334	98	1
1	H	5450	0	5348	99	1
1	I	5442	0	5341	108	0
1	J	5431	0	5334	113	1
1	K	5442	0	5342	106	1
1	L	5431	0	5333	119	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	12	0	18	0	0
3	D	8	0	12	0	0
3	F	4	0	6	0	0
3	H	4	0	6	0	0
4	A	31	0	0	0	0
4	B	25	0	0	0	0
4	C	23	0	0	1	0
4	D	13	0	0	0	0
4	E	14	0	0	2	0
4	F	12	0	0	1	0
4	G	8	0	0	0	0
4	H	6	0	0	0	0
4	I	8	0	0	1	0
4	J	6	0	0	1	0
4	K	1	0	0	0	0
4	L	18	0	0	1	0
All	All	65153	0	63823	1343	6

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 10.

The worst 5 of 1343 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:J:208:HIS:HB3	1:J:581:CYS:SG	1.38	1.60
1:A:132:HIS:CG	1:A:222:ILE:HD11	1.41	1.50
1:J:581:CYS:SG	1:J:622:ASN:HB3	1.55	1.46
1:B:28:ASP:OD1	1:B:56:ARG:NH1	1.60	1.33
1:B:493:ASP:O	1:D:101:ARG:HG2	1.34	1.27

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:GLU:OE2	1:J:444:VAL:CG1[1_655]	1.59	0.61
1:A:47:ASN:OD1	1:C:438:GLN:NE2[1_656]	1.60	0.60
1:G:102:ASN:OD1	1:K:330:ASN:ND2[2_645]	1.95	0.25
1:A:47:ASN:OD1	1:C:438:GLN:CD[1_656]	1.96	0.24
1:H:102:ASN:OD1	1:L:330:ASN:ND2[2_555]	2.03	0.17

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	645/681 (95%)	608 (94%)	30 (5%)	7 (1%)	11	39
1	B	639/681 (94%)	602 (94%)	32 (5%)	5 (1%)	16	46
1	C	642/681 (94%)	609 (95%)	27 (4%)	6 (1%)	14	43
1	D	644/681 (95%)	610 (95%)	29 (4%)	5 (1%)	16	46
1	E	655/681 (96%)	620 (95%)	30 (5%)	5 (1%)	16	46
1	F	651/681 (96%)	614 (94%)	29 (4%)	8 (1%)	10	37
1	G	653/681 (96%)	615 (94%)	32 (5%)	6 (1%)	14	43
1	H	655/681 (96%)	616 (94%)	32 (5%)	7 (1%)	11	39
1	I	654/681 (96%)	618 (94%)	30 (5%)	6 (1%)	14	43
1	J	653/681 (96%)	614 (94%)	33 (5%)	6 (1%)	14	43
1	K	654/681 (96%)	617 (94%)	29 (4%)	8 (1%)	10	37
1	L	653/681 (96%)	616 (94%)	31 (5%)	6 (1%)	14	43
All	All	7798/8172 (95%)	7359 (94%)	364 (5%)	75 (1%)	12	41

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	SER
1	B	630	VAL
1	D	614	VAL

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Mol	Chain	Res	Type
1	D	643	PHE
1	E	217	ALA

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	585/610 (96%)	520 (89%)	65 (11%)	6	22
1	B	580/610 (95%)	512 (88%)	68 (12%)	5	20
1	C	583/610 (96%)	511 (88%)	72 (12%)	4	19
1	D	585/610 (96%)	526 (90%)	59 (10%)	7	26
1	E	594/610 (97%)	527 (89%)	67 (11%)	5	21
1	F	591/610 (97%)	527 (89%)	64 (11%)	6	23
1	G	592/610 (97%)	535 (90%)	57 (10%)	8	28
1	H	594/610 (97%)	539 (91%)	55 (9%)	8	29
1	I	593/610 (97%)	530 (89%)	63 (11%)	6	24
1	J	592/610 (97%)	535 (90%)	57 (10%)	8	28
1	K	593/610 (97%)	540 (91%)	53 (9%)	9	30
1	L	592/610 (97%)	531 (90%)	61 (10%)	7	25
All	All	7074/7320 (97%)	6333 (90%)	741 (10%)	6	24

5 of 741 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	174	MET
1	J	59	VAL
1	H	298	LEU
1	H	173	ARG
1	I	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	615	GLN
1	K	295	ASN
1	G	303	GLN
1	K	253	GLN
1	L	295	ASN

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 31 ligands modelled in this entry, 24 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	D	704	-	3,3,3	0.24	0	2,2,2	0.40	0
3	EDO	D	703	-	3,3,3	0.59	0	2,2,2	0.50	0
3	EDO	A	704	-	3,3,3	0.34	0	2,2,2	0.47	0
3	EDO	H	703	-	3,3,3	0.18	0	2,2,2	0.25	0
3	EDO	A	705	-	3,3,3	0.20	0	2,2,2	0.33	0
3	EDO	F	703	-	3,3,3	0.08	0	2,2,2	0.09	0
3	EDO	A	703	-	3,3,3	0.24	0	2,2,2	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	704	-	-	0/1/1/1	-
3	EDO	D	703	-	-	1/1/1/1	-
3	EDO	A	704	-	-	1/1/1/1	-
3	EDO	H	703	-	-	1/1/1/1	-
3	EDO	A	705	-	-	0/1/1/1	-
3	EDO	F	703	-	-	1/1/1/1	-
3	EDO	A	703	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	704	EDO	O1-C1-C2-O2
3	H	703	EDO	O1-C1-C2-O2
3	D	703	EDO	O1-C1-C2-O2
3	F	703	EDO	O1-C1-C2-O2

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	651/681 (95%)	-1.58	0 100 100	26, 55, 102, 177	0
1	B	645/681 (94%)	-1.55	0 100 100	27, 62, 105, 177	0
1	C	648/681 (95%)	-1.55	0 100 100	21, 60, 107, 194	0
1	D	650/681 (95%)	-1.56	0 100 100	23, 59, 105, 181	0
1	E	661/681 (97%)	-1.56	0 100 100	28, 62, 113, 160	0
1	F	657/681 (96%)	-1.53	0 100 100	29, 64, 115, 177	0
1	G	659/681 (96%)	-1.58	0 100 100	27, 59, 109, 192	0
1	H	661/681 (97%)	-1.58	0 100 100	28, 60, 117, 214	0
1	I	660/681 (96%)	-1.52	0 100 100	28, 66, 127, 189	0
1	J	659/681 (96%)	-1.54	0 100 100	26, 67, 124, 219	0
1	K	660/681 (96%)	-1.53	0 100 100	32, 69, 128, 181	0
1	L	659/681 (96%)	-1.49	0 100 100	26, 70, 127, 198	0
All	All	7870/8172 (96%)	-1.55	0 100 100	21, 63, 116, 219	0

There are no RSRZ outliers to report.

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

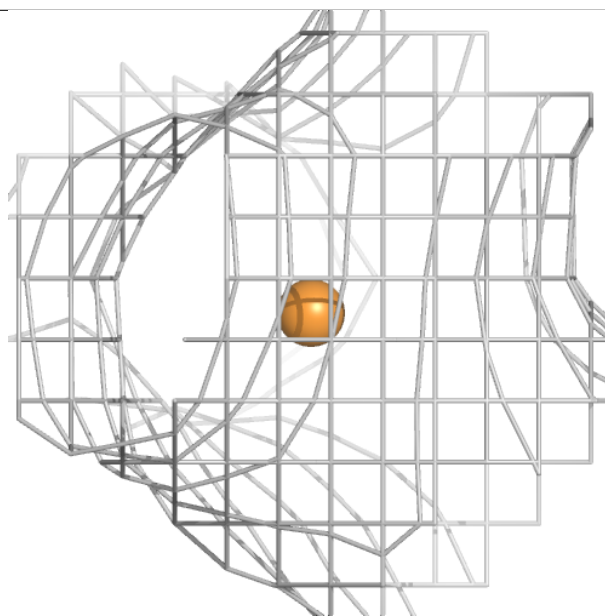
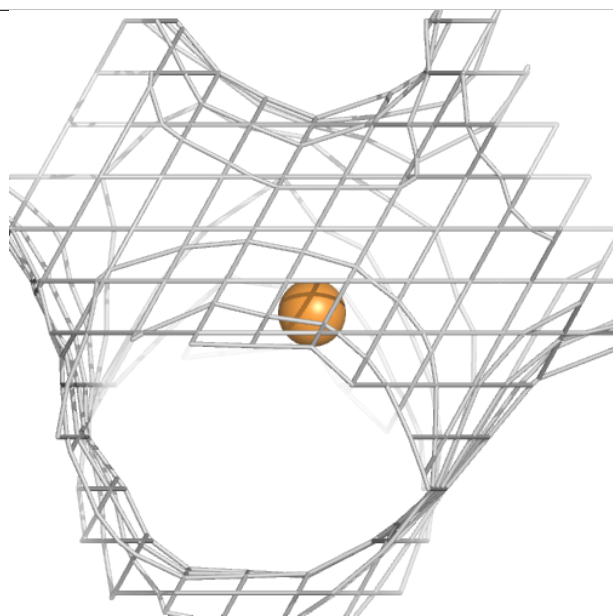
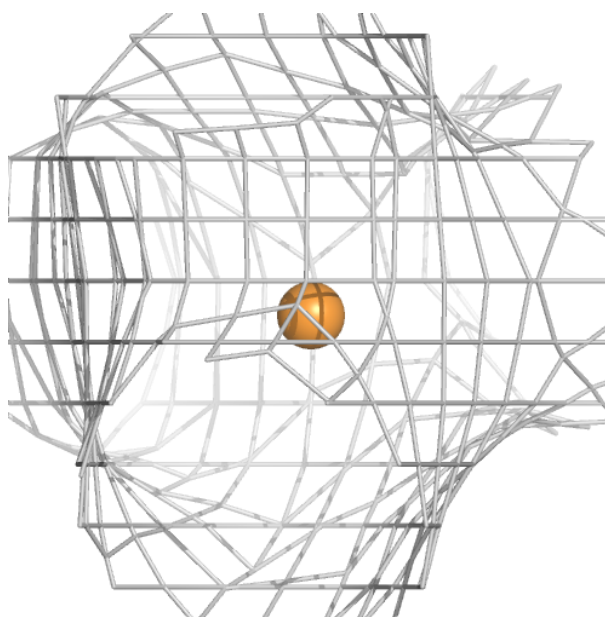
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	F	703	4/4	0.95	0.09	57,61,61,62	0
3	EDO	D	704	4/4	0.97	0.06	46,47,48,49	0
3	EDO	A	705	4/4	0.98	0.04	56,58,60,61	0
3	EDO	D	703	4/4	0.98	0.05	21,24,25,25	0
3	EDO	A	703	4/4	0.99	0.04	23,25,27,28	0
3	EDO	A	704	4/4	0.99	0.04	33,36,39,39	0
3	EDO	H	703	4/4	0.99	0.07	50,51,51,51	0
2	CU	D	702	1/1	1.00	0.02	65,65,65,65	0
2	CU	E	701	1/1	1.00	0.03	81,81,81,81	0
2	CU	E	702	1/1	1.00	0.03	56,56,56,56	0
2	CU	F	701	1/1	1.00	0.02	62,62,62,62	0
2	CU	F	702	1/1	1.00	0.01	57,57,57,57	0
2	CU	G	701	1/1	1.00	0.01	56,56,56,56	0
2	CU	G	702	1/1	1.00	0.02	66,66,66,66	0
2	CU	H	701	1/1	1.00	0.01	52,52,52,52	0
2	CU	H	702	1/1	1.00	0.01	47,47,47,47	0
2	CU	I	701	1/1	1.00	0.02	60,60,60,60	0
2	CU	I	702	1/1	1.00	0.02	73,73,73,73	0
2	CU	J	701	1/1	1.00	0.01	73,73,73,73	0
2	CU	J	702	1/1	1.00	0.01	66,66,66,66	0
2	CU	K	701	1/1	1.00	0.01	75,75,75,75	0
2	CU	K	702	1/1	1.00	0.01	57,57,57,57	0
2	CU	L	701	1/1	1.00	0.02	66,66,66,66	0
2	CU	L	702	1/1	1.00	0.01	53,53,53,53	0
2	CU	A	701	1/1	1.00	0.03	55,55,55,55	0
2	CU	A	702	1/1	1.00	0.03	61,61,61,61	0
2	CU	B	701	1/1	1.00	0.01	64,64,64,64	0
2	CU	B	702	1/1	1.00	0.03	56,56,56,56	0
2	CU	C	701	1/1	1.00	0.02	59,59,59,59	0
2	CU	C	702	1/1	1.00	0.03	46,46,46,46	0
2	CU	D	701	1/1	1.00	0.01	44,44,44,44	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.

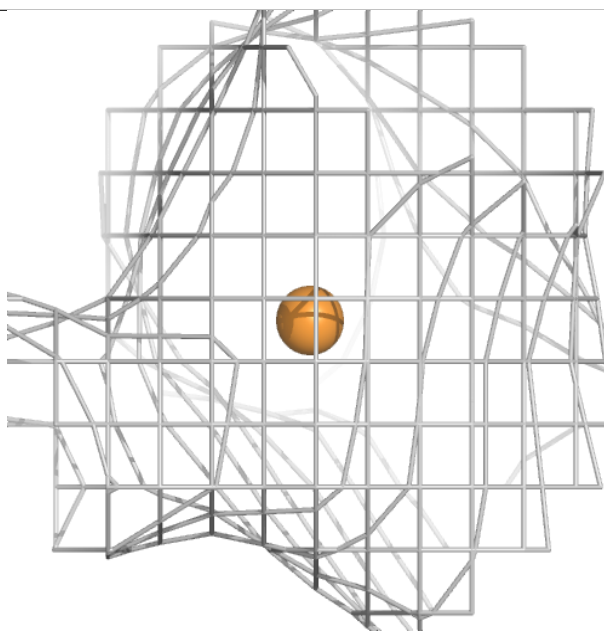
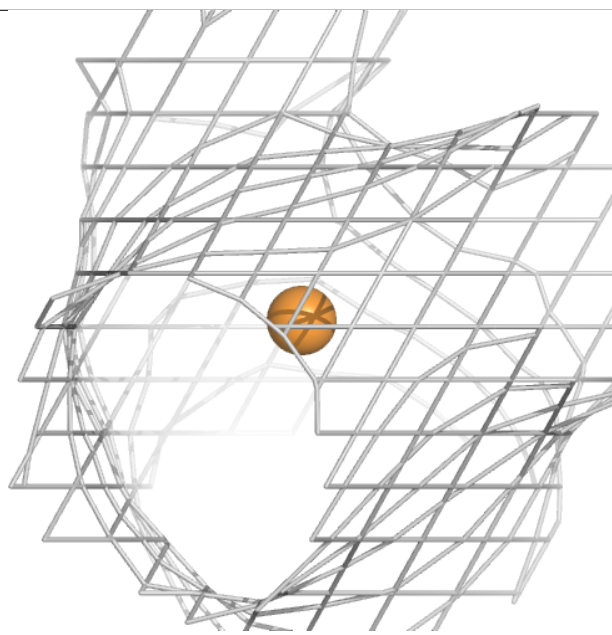
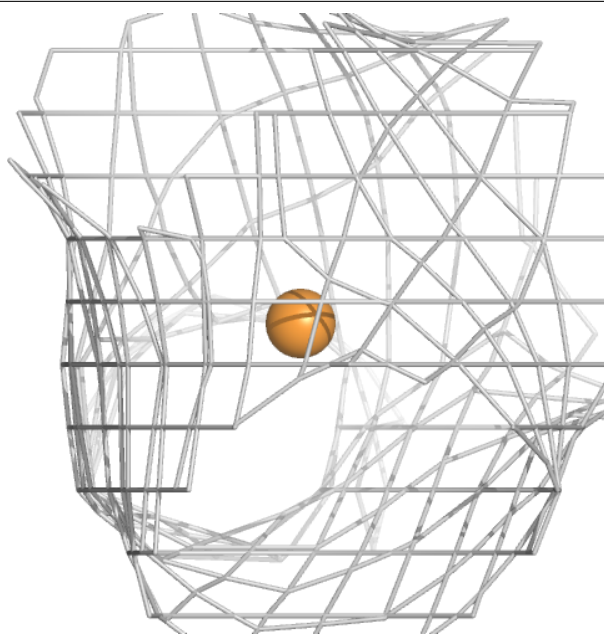
Electron density around CU D 702:

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and green (positive)



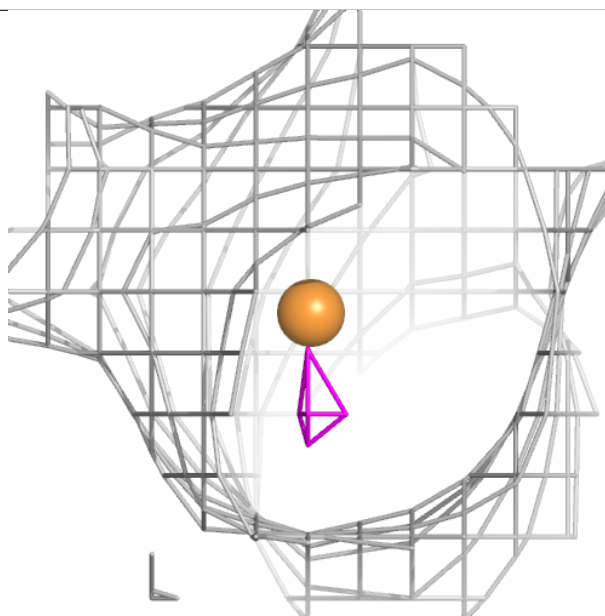
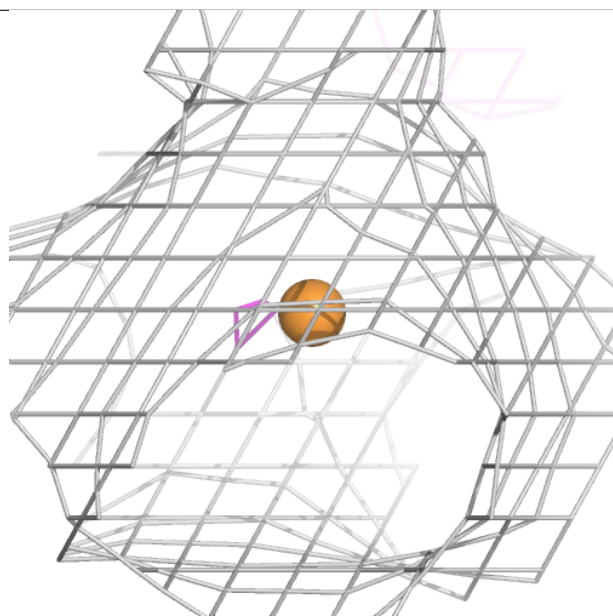
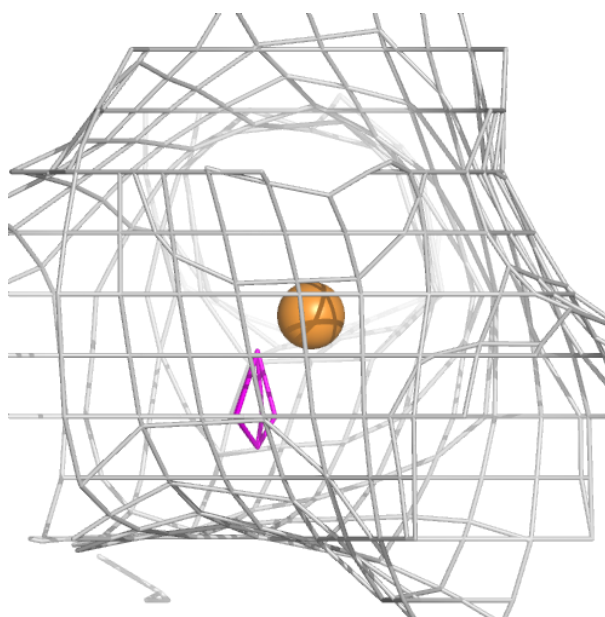
Electron density around CU E 701:

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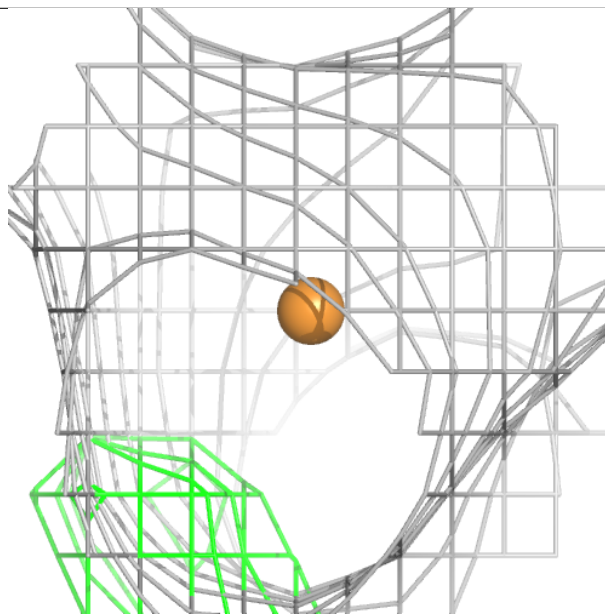
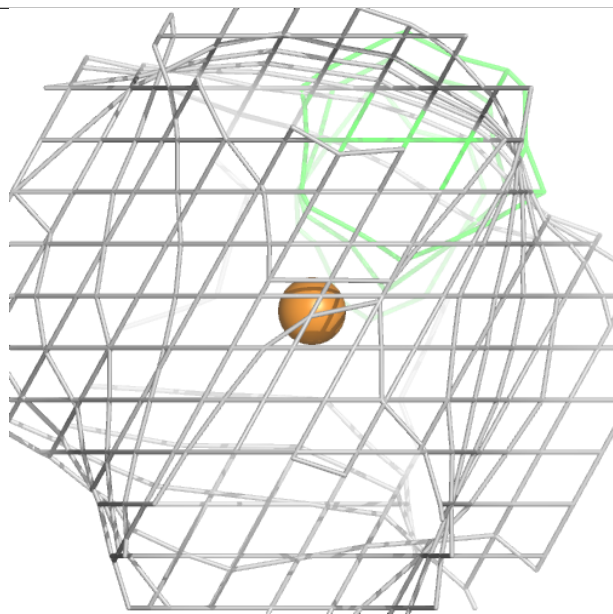
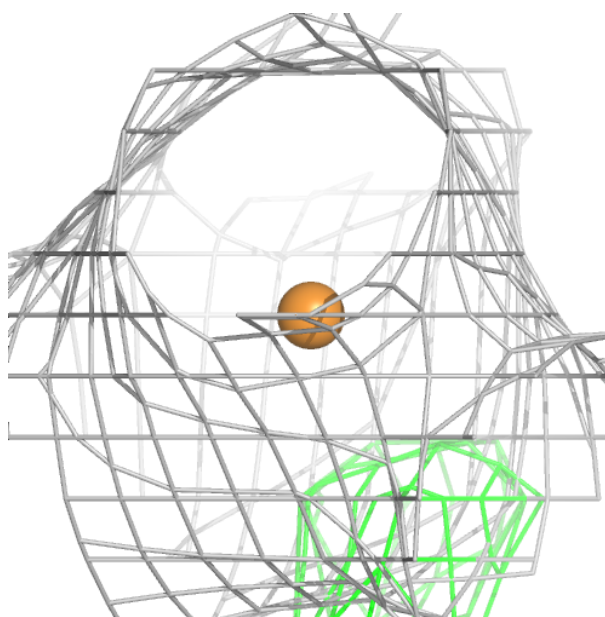
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and green (positive)



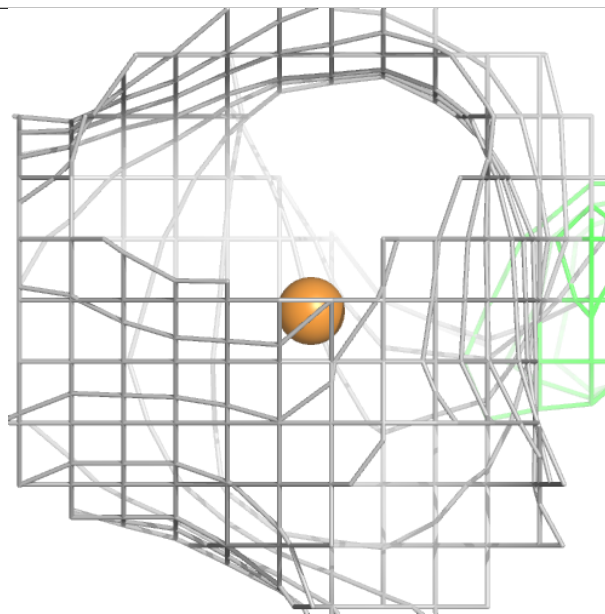
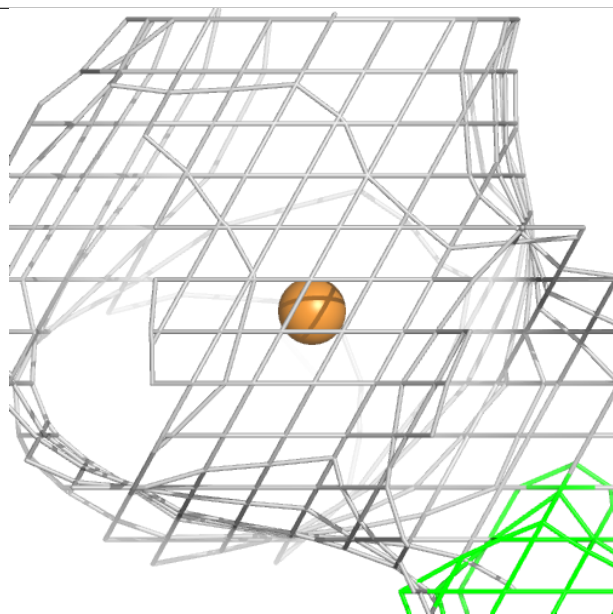
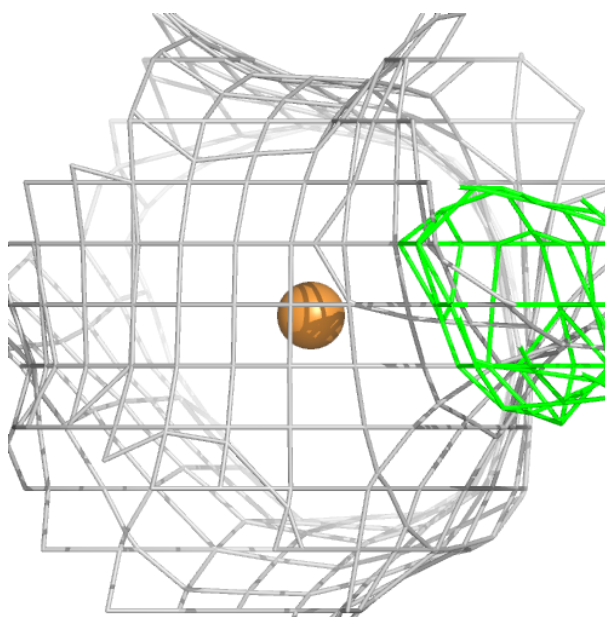
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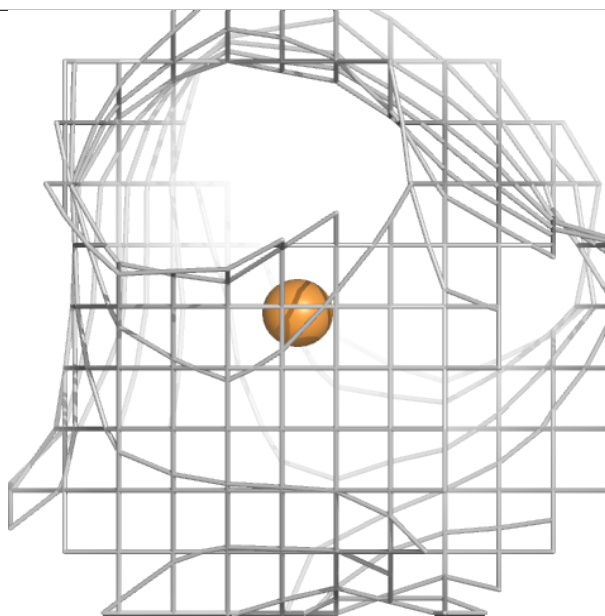
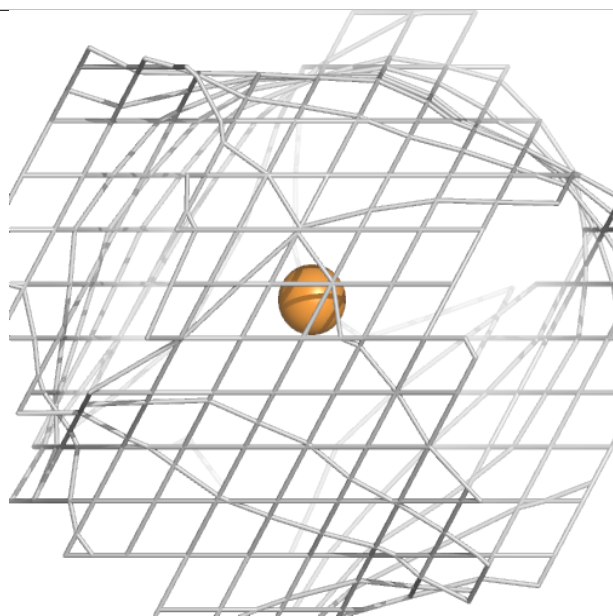
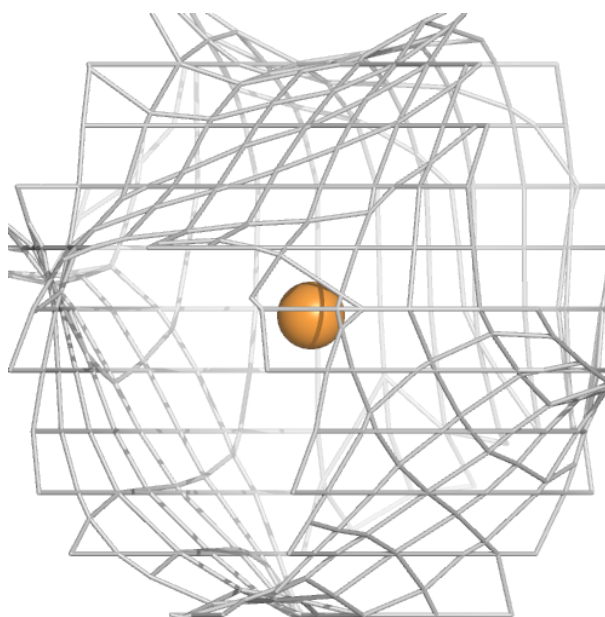
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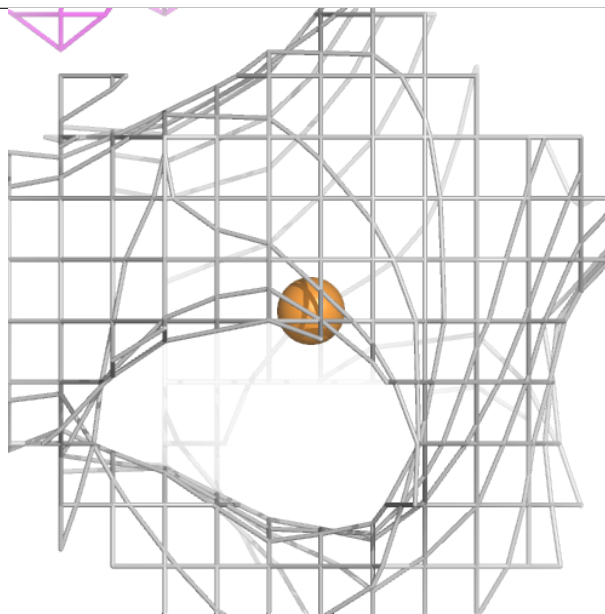
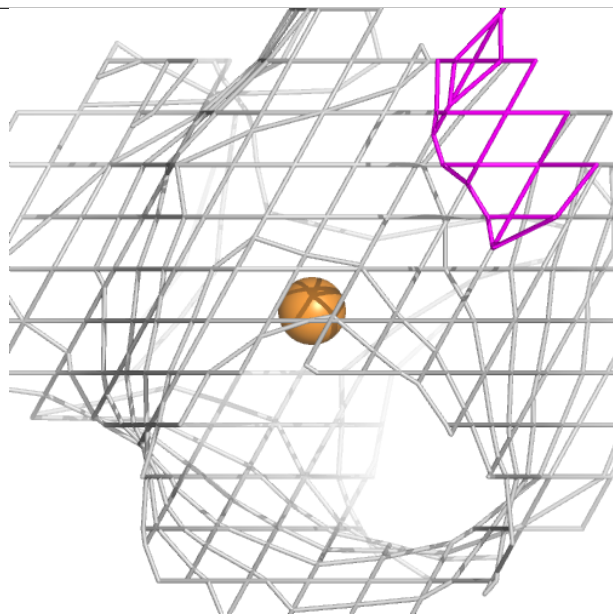
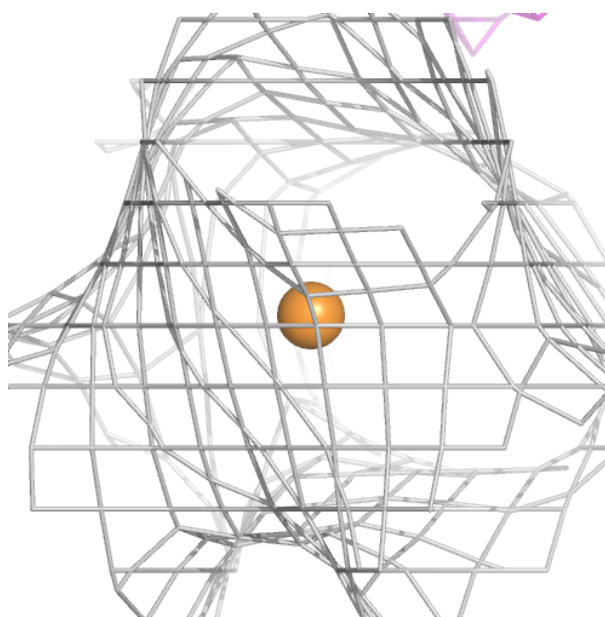
Electron density around CU G 701:

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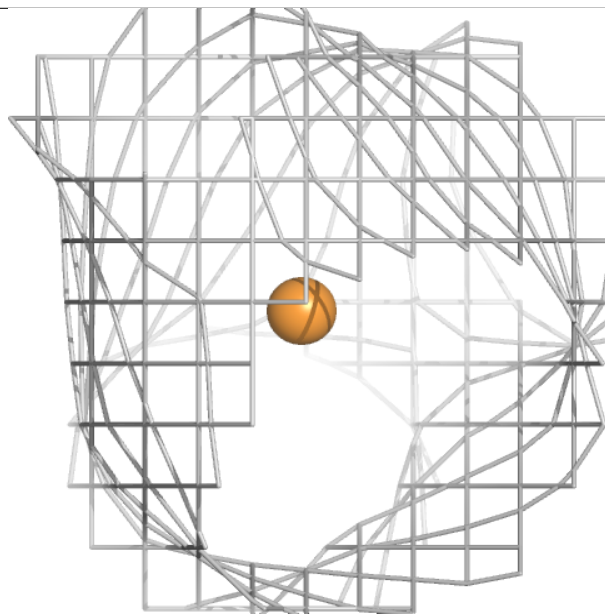
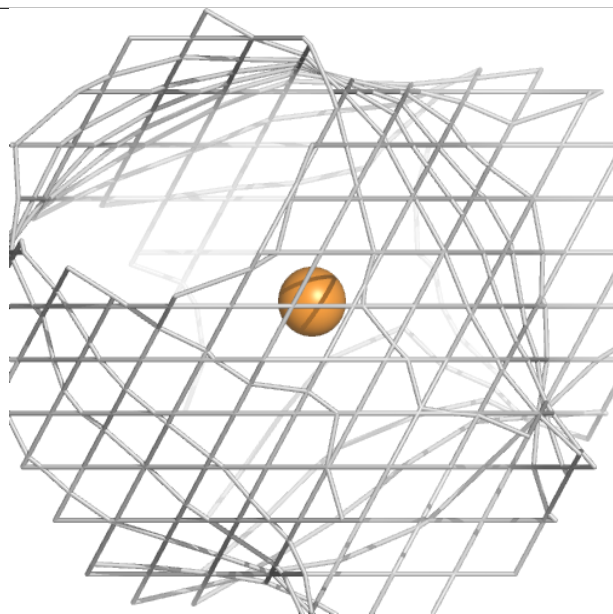
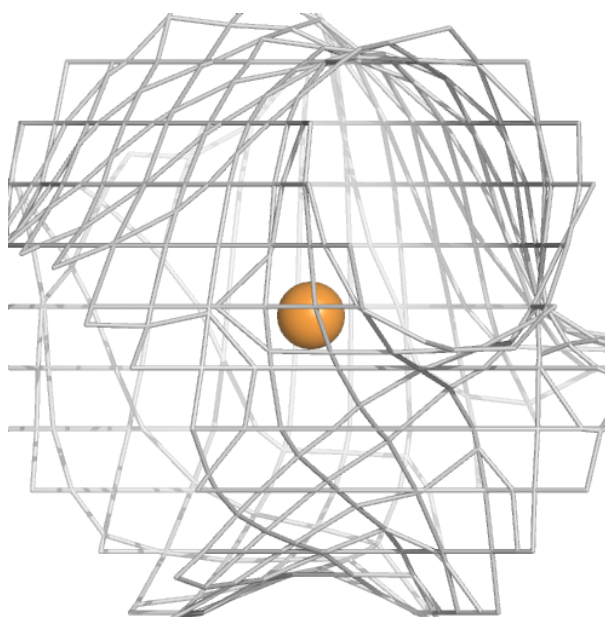
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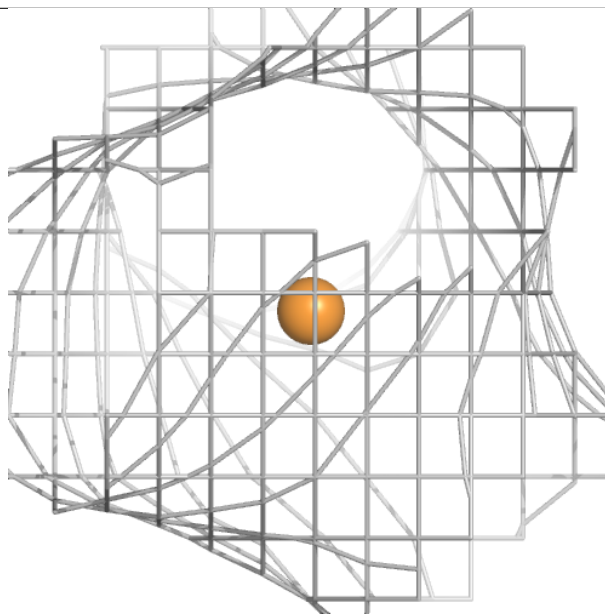
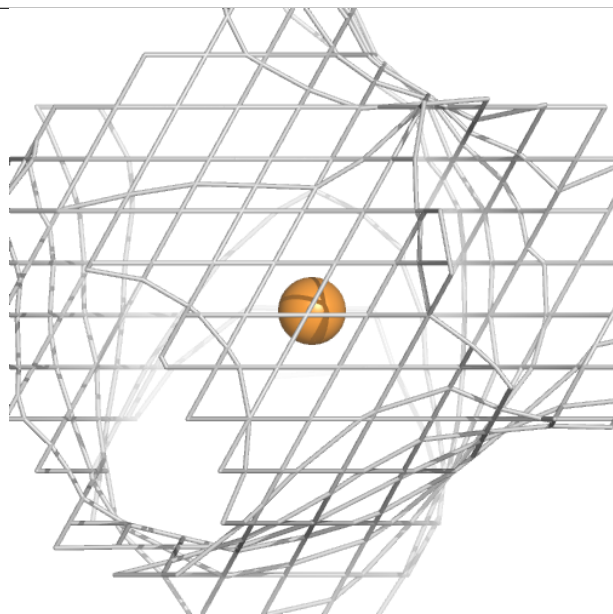
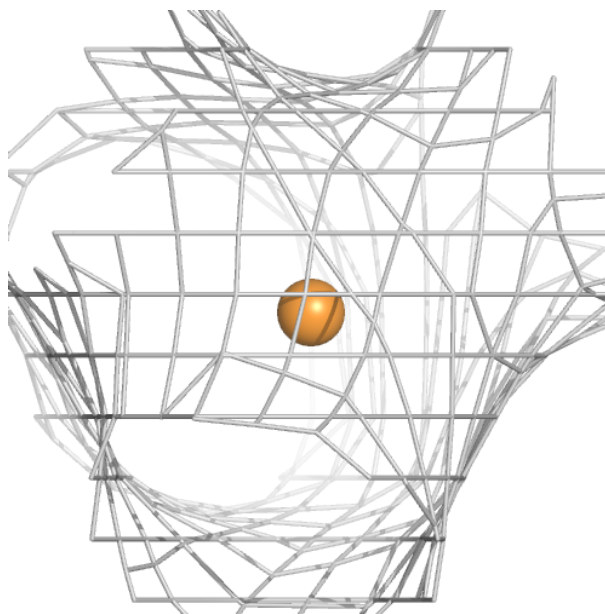
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and green (positive)



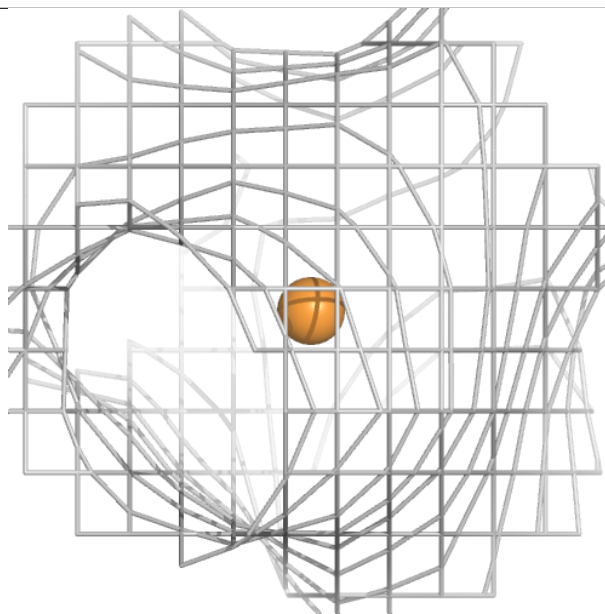
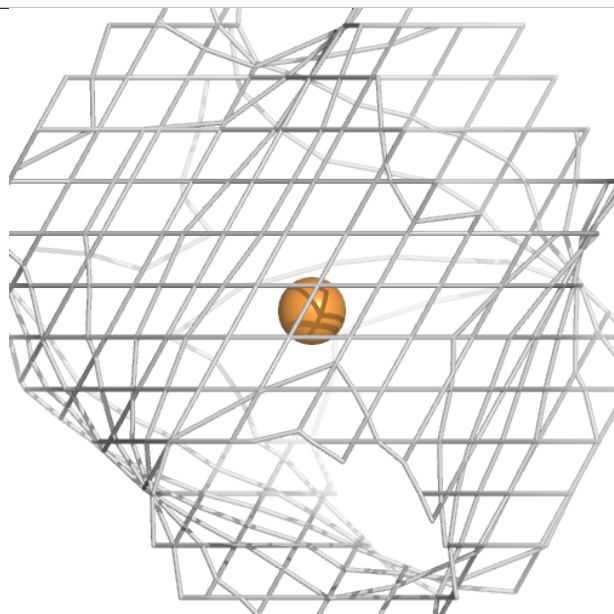
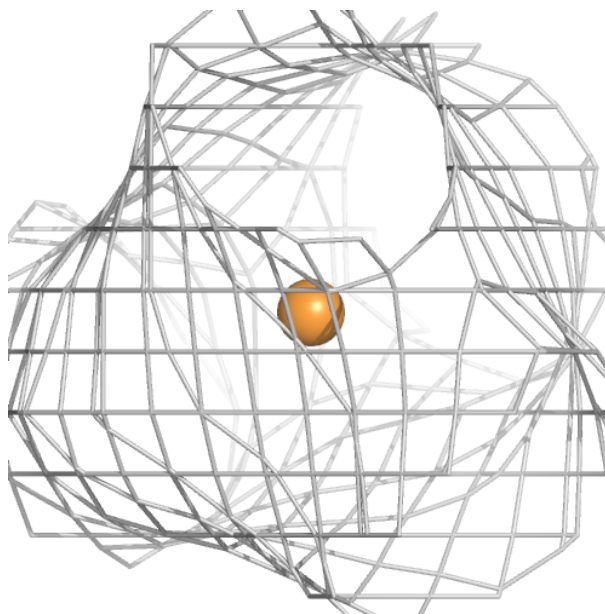
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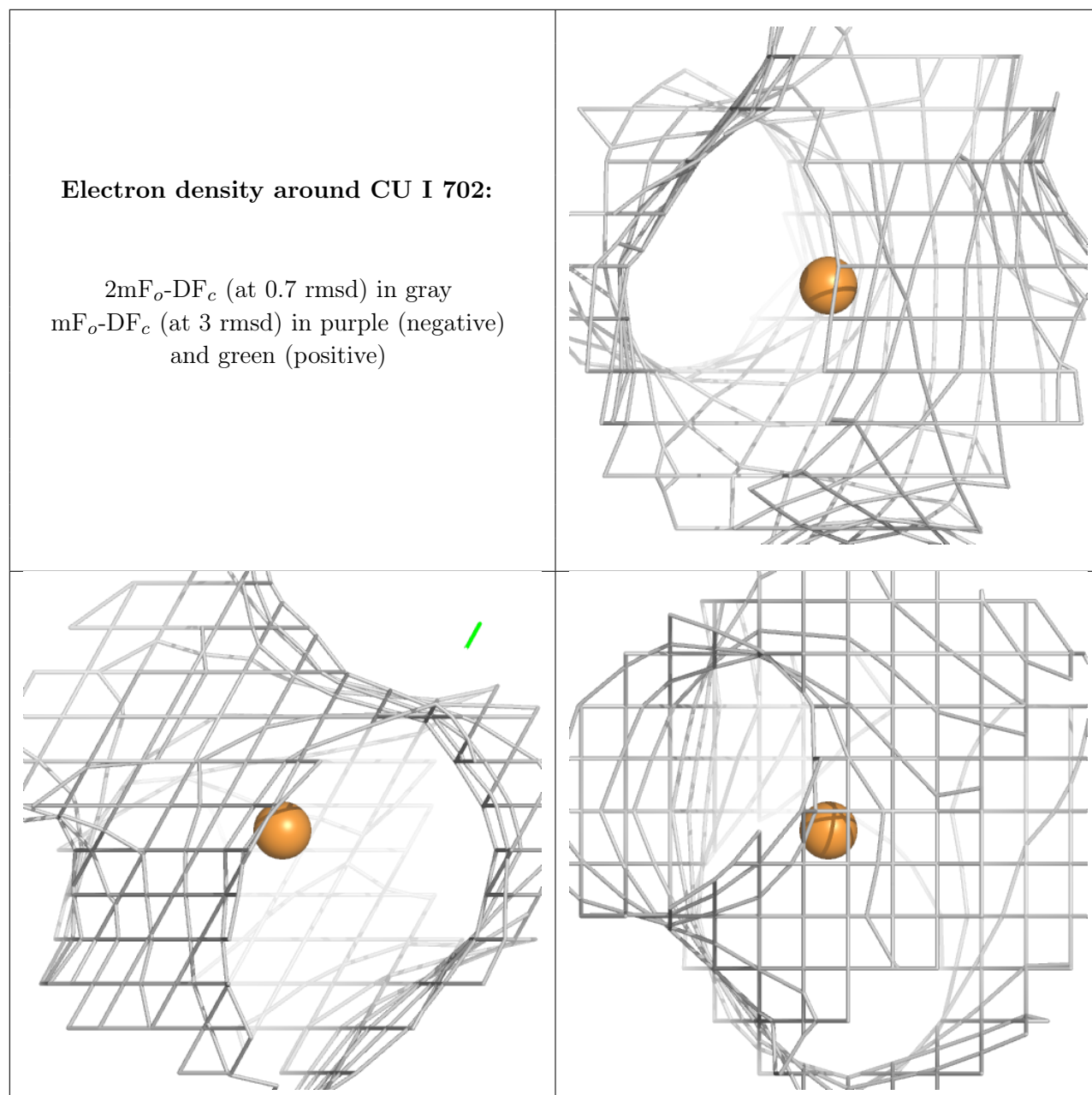
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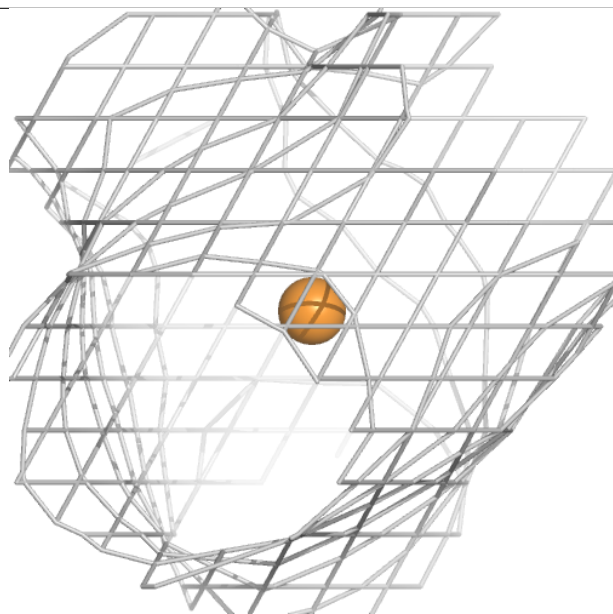
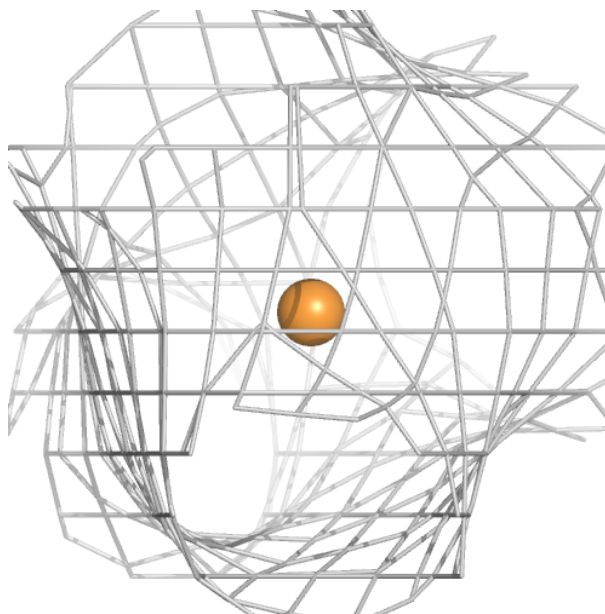
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and green (positive)





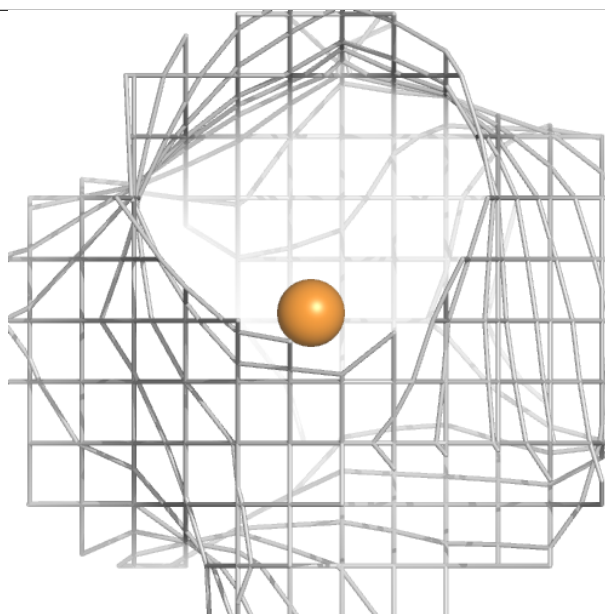
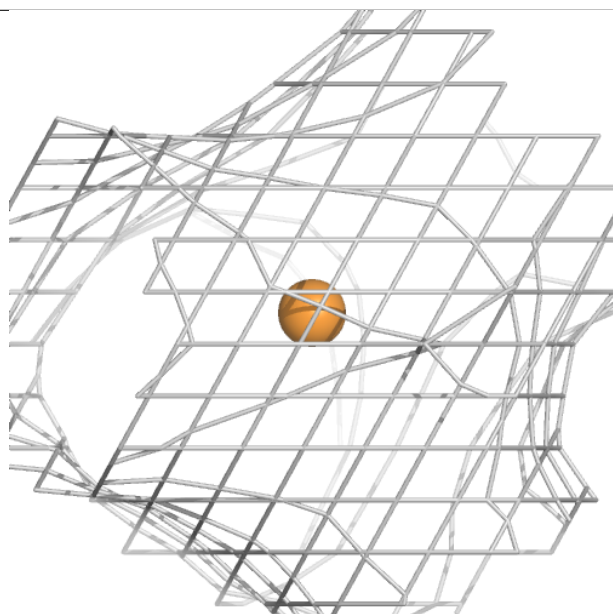
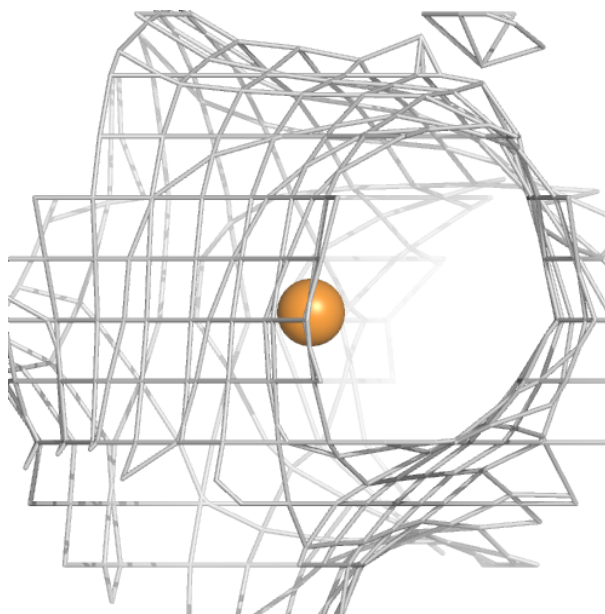
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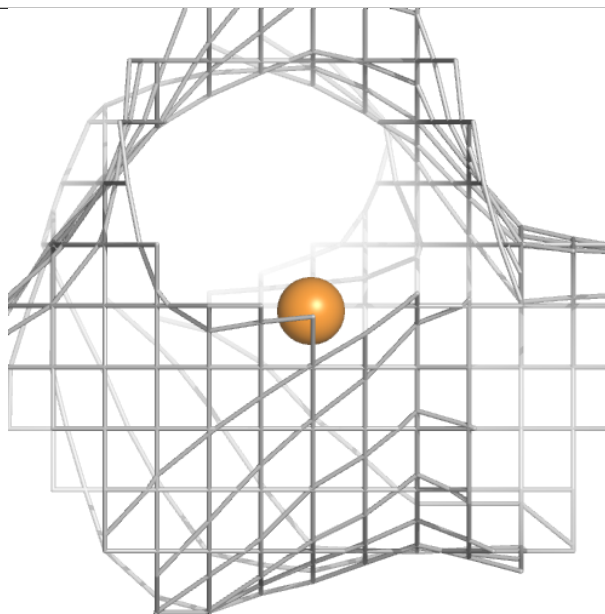
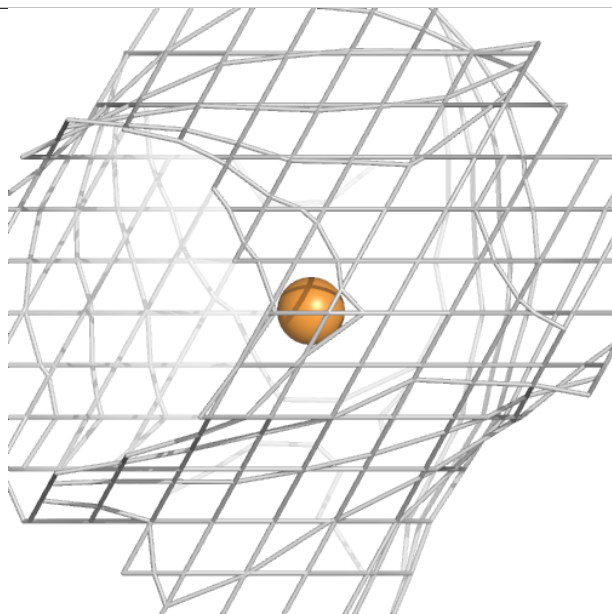
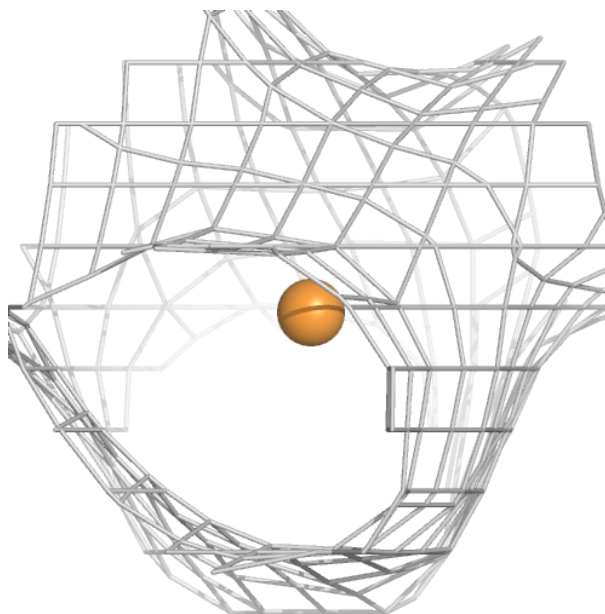
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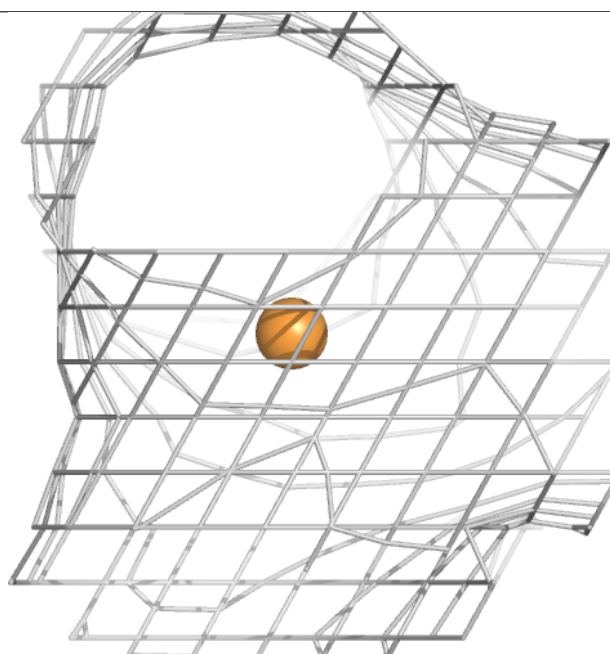
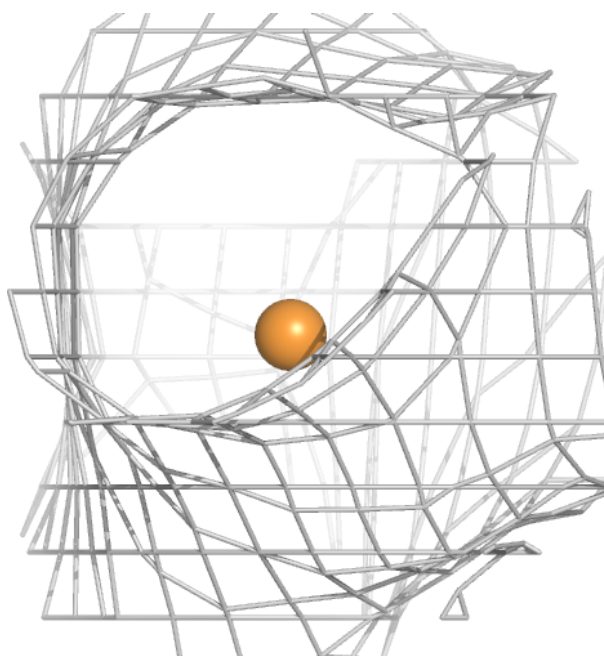
Electron density around CU K 701:

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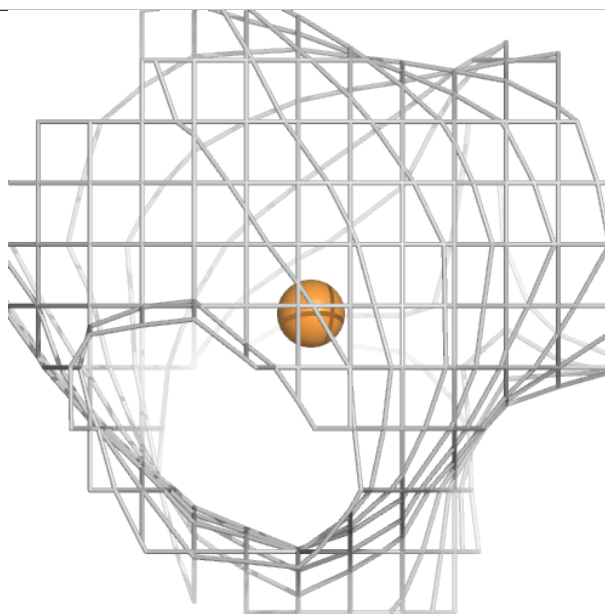
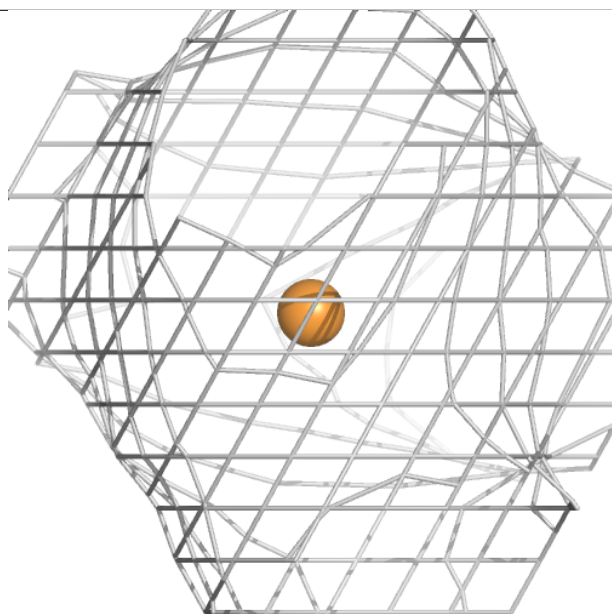
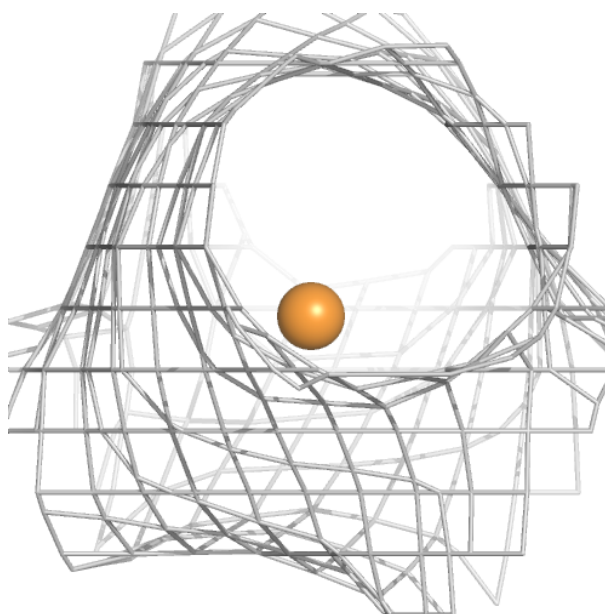
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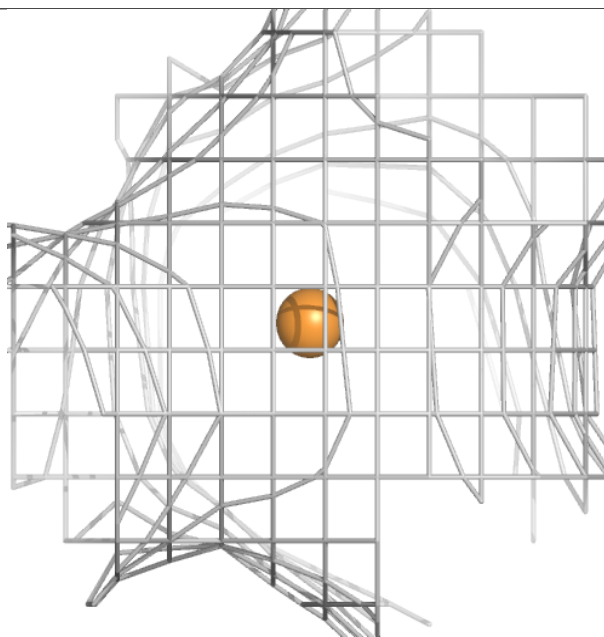
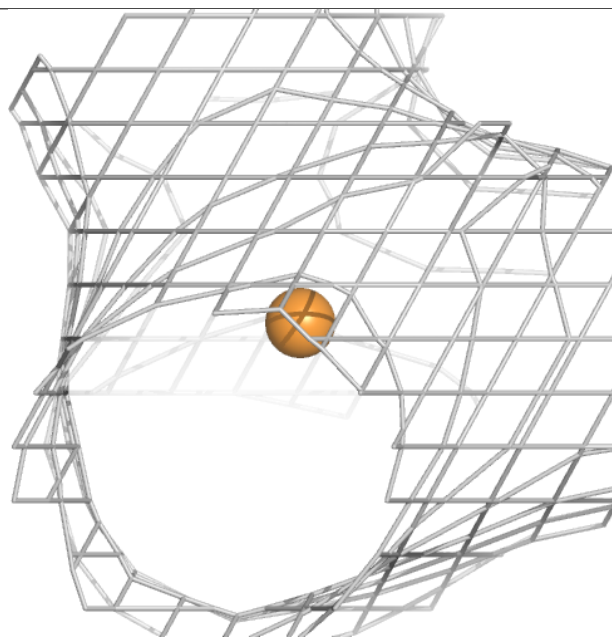
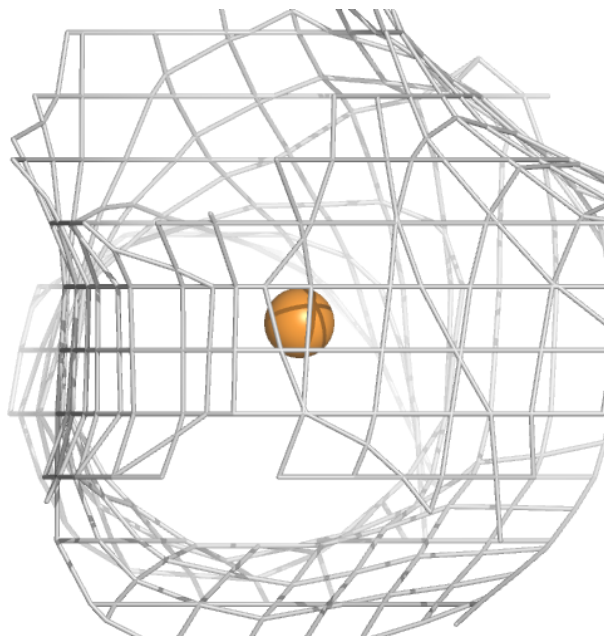
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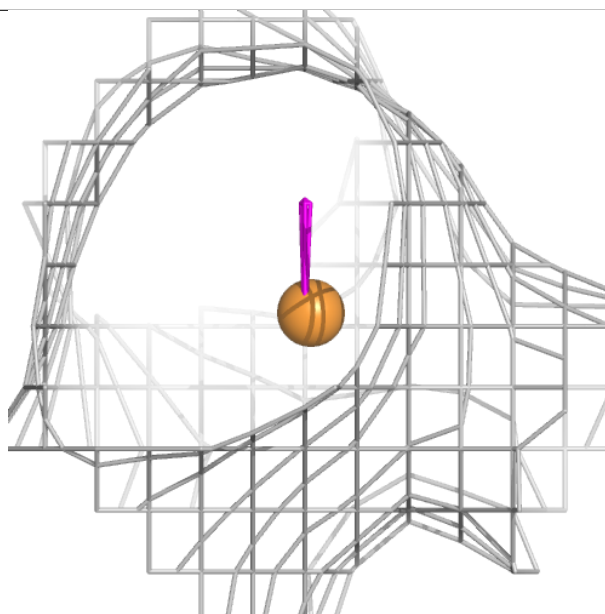
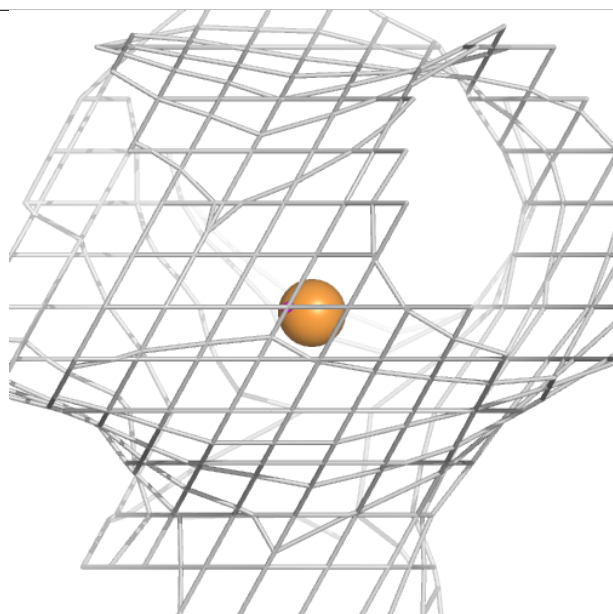
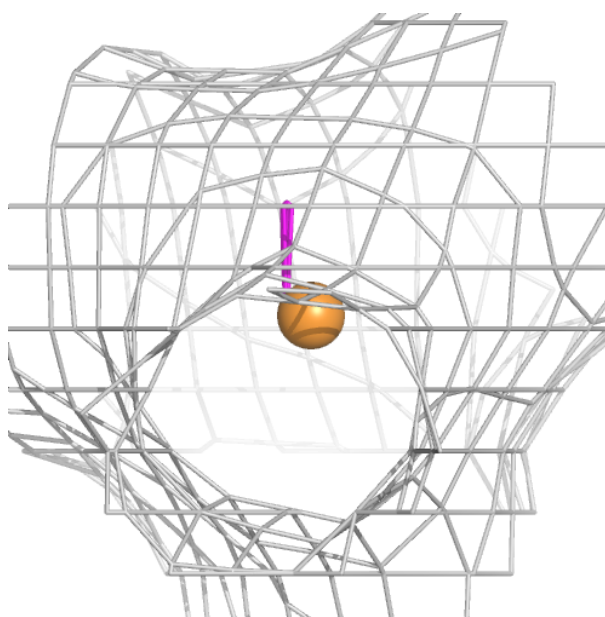
Electron density around CU L 702:

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



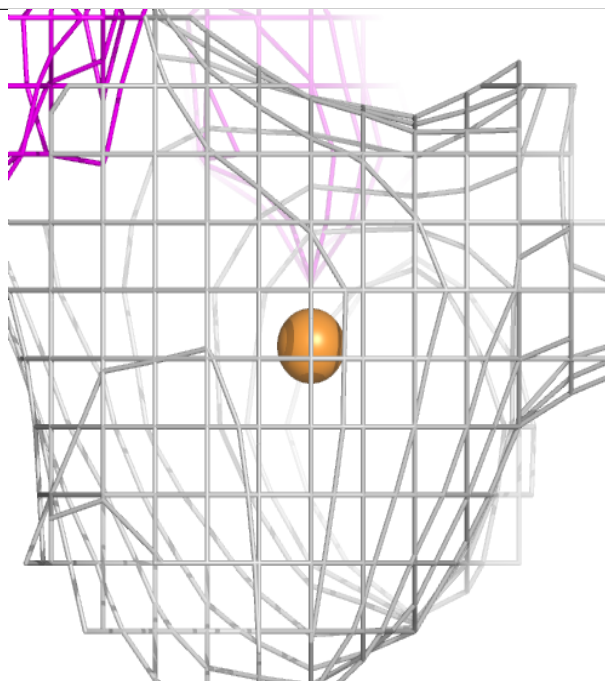
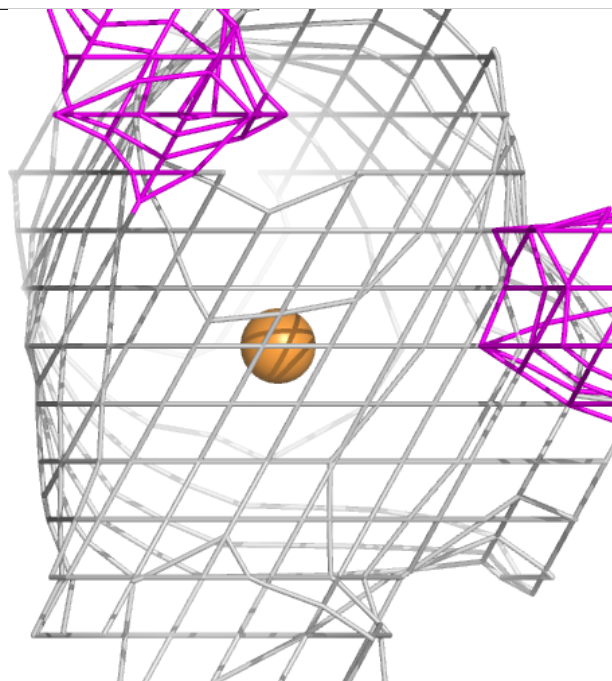
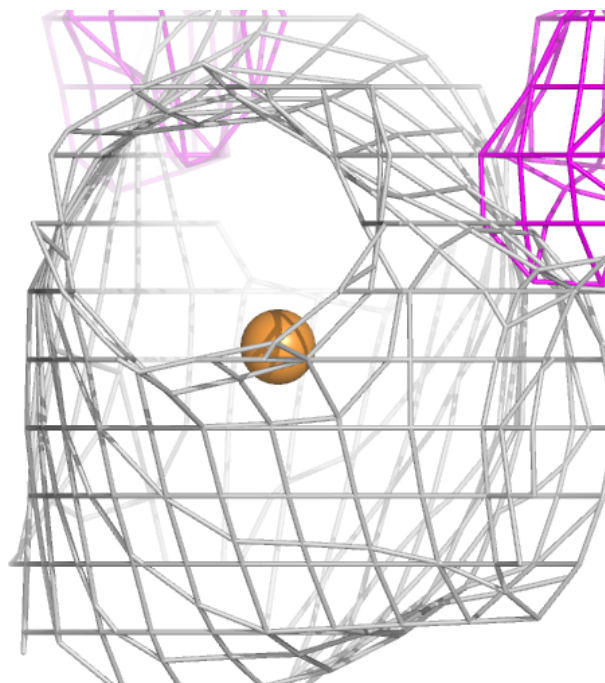
Electron density around CU A 701:

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



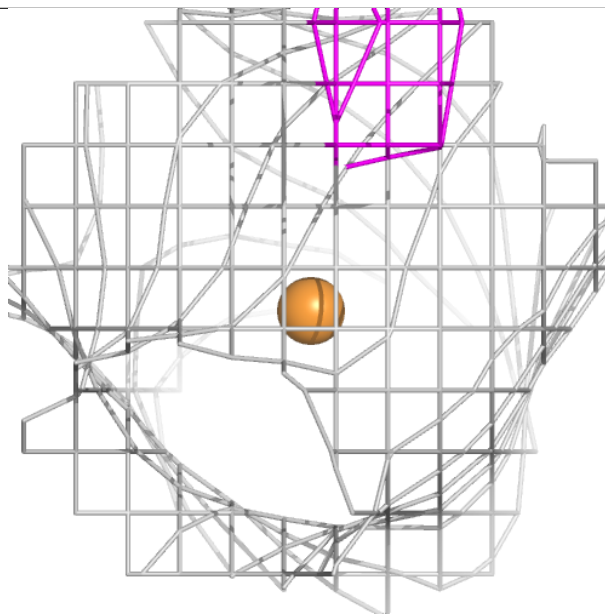
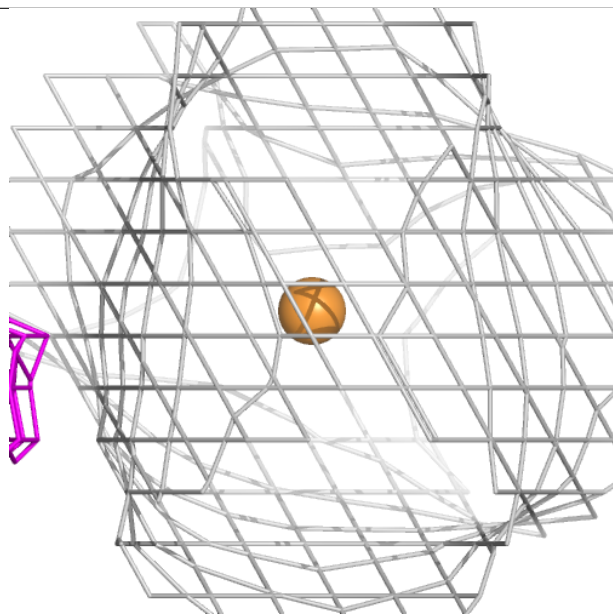
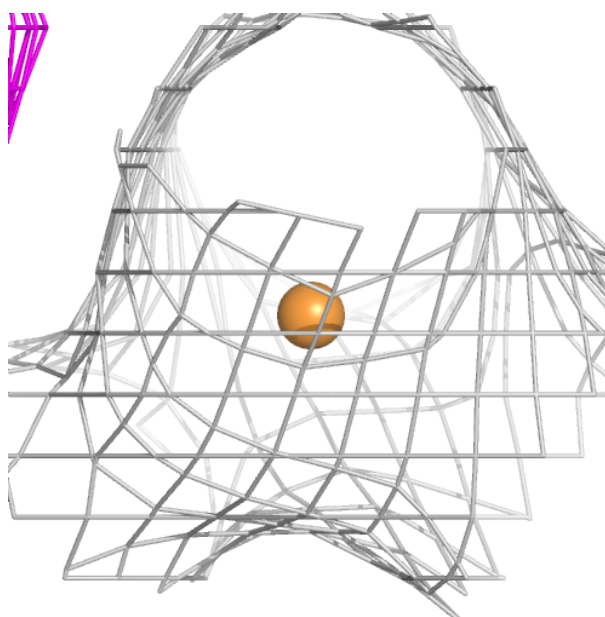
Electron density around CU A 702:

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



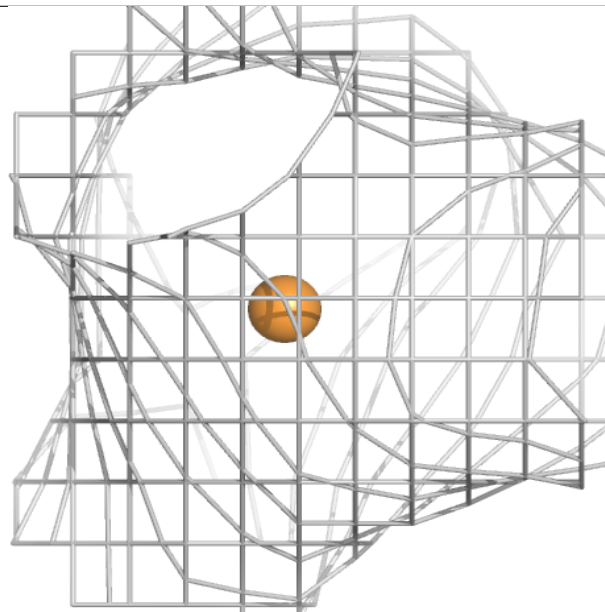
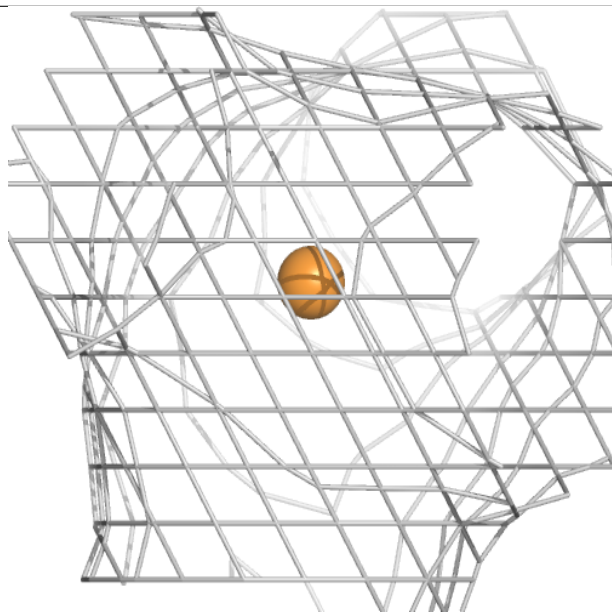
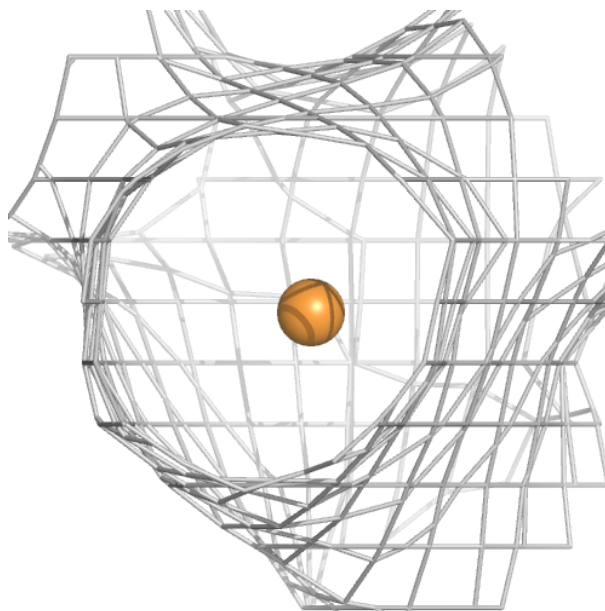
Electron density around CU B 701:

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



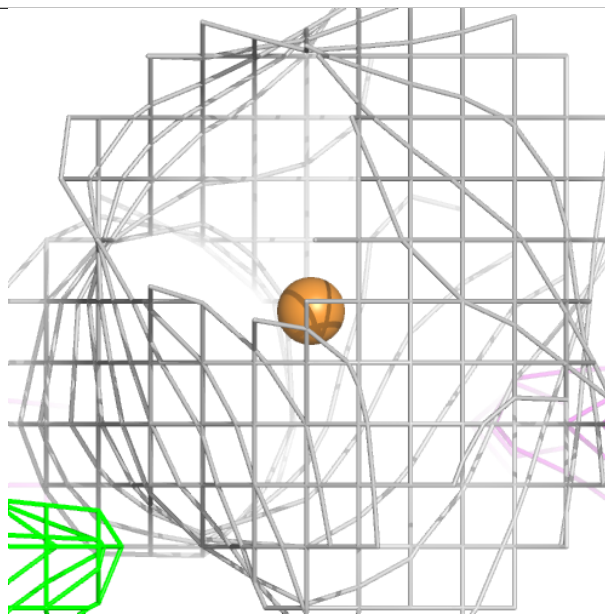
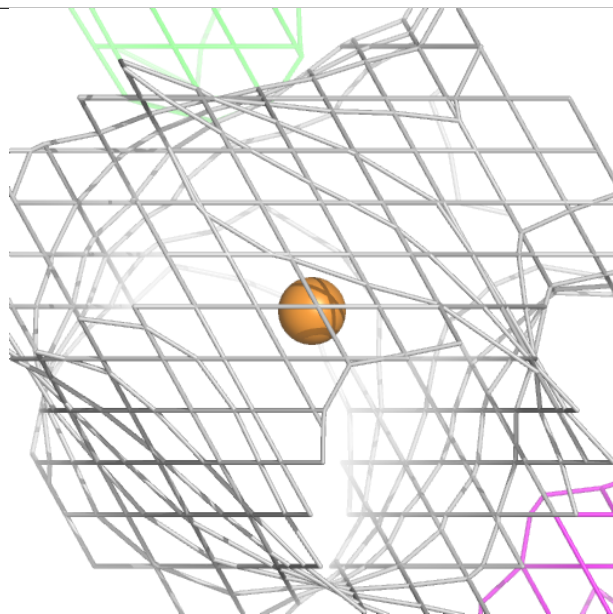
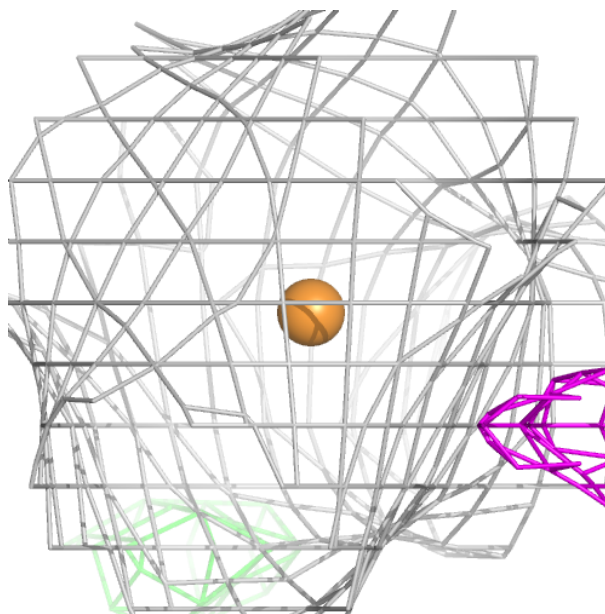
Electron density around CU B 702:

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



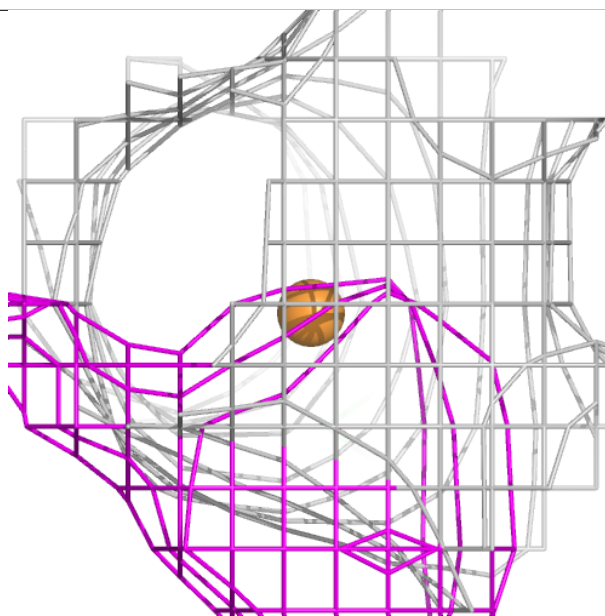
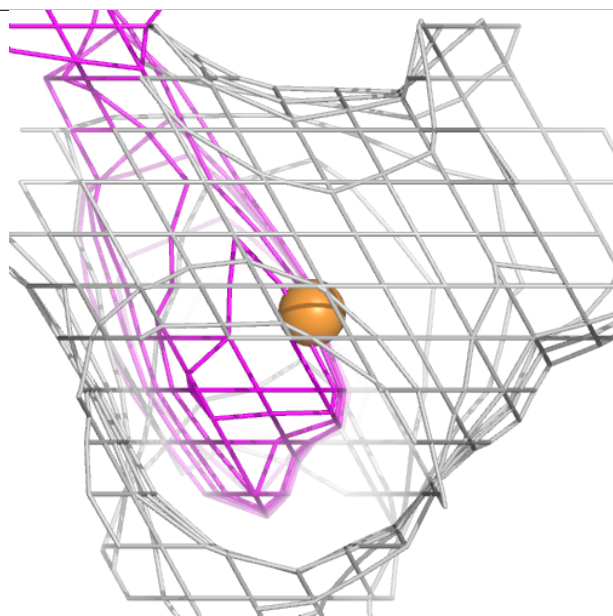
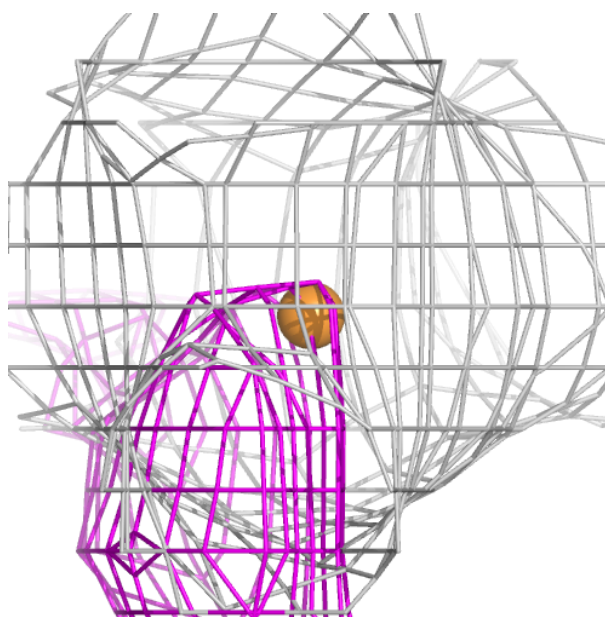
Electron density around CU C 701:

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



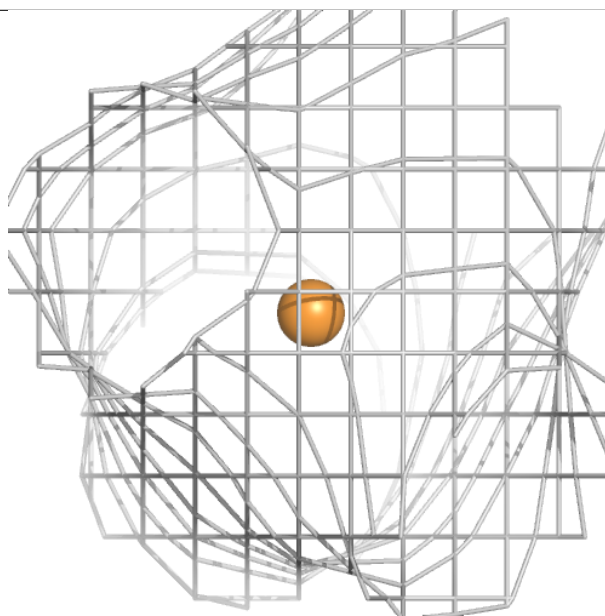
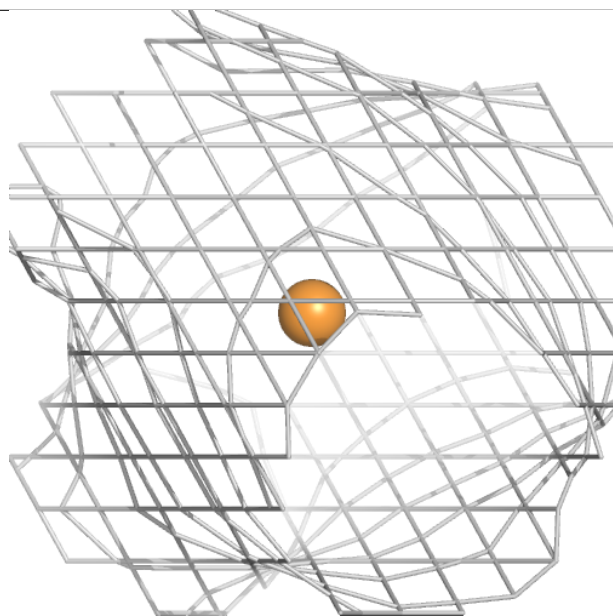
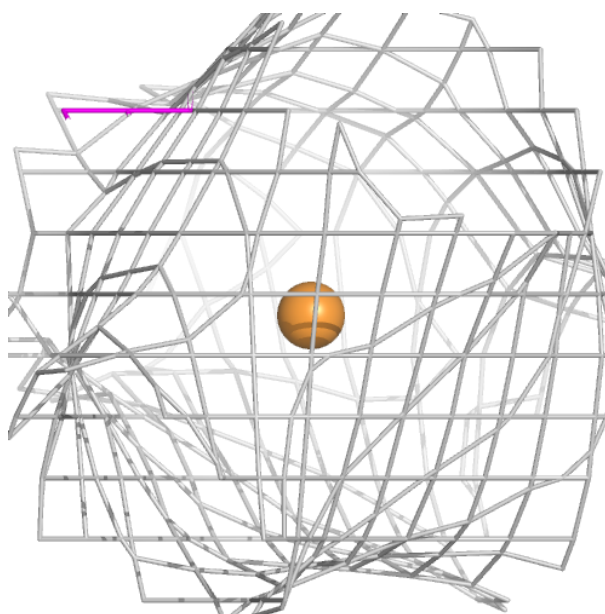
Electron density around CU C 702:

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



Electron density around CU D 701:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.