



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 10:40 AM UTC

PDB ID : 8X8F / pdb_00008x8f
Title : Crystal structure of lipoygenase from *Enhygromyxa salina*
Authors : Kim, J.W.; Seo, P.W.; Kim, J.S.
Deposited on : 2023-11-27
Resolution : 2.80 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
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

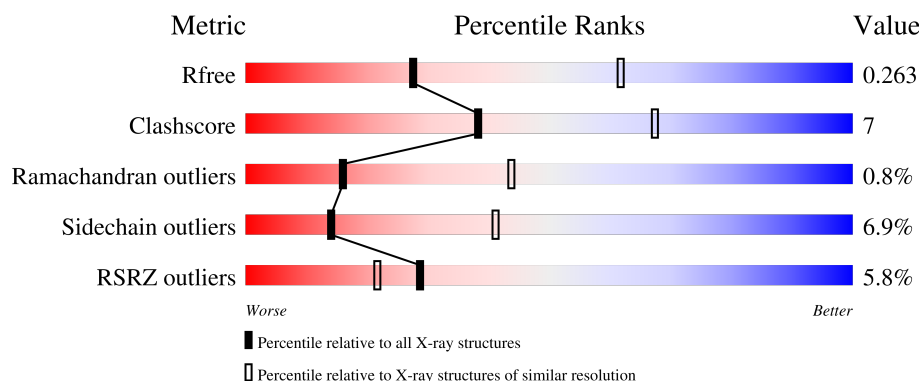
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



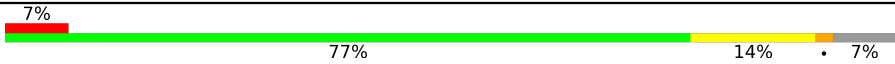
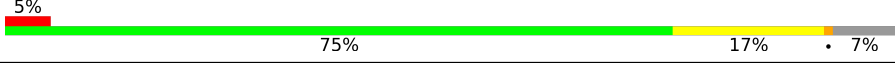
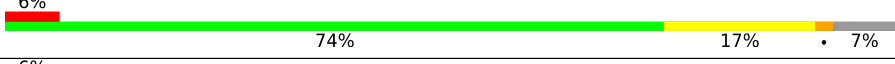
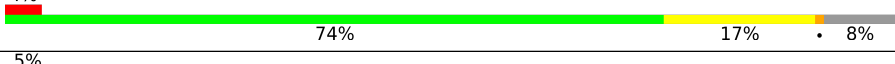
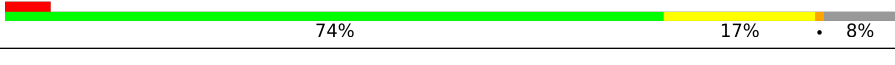
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	650	5% 70% 21% • 7%
1	B	650	6% 73% 17% • 8%
1	C	650	4% 75% 16% • 7%
1	D	650	6% 74% 18% • 7%
1	E	650	5% 73% 17% • 7%

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Mol	Chain	Length	Quality of chain
1	F	650	
1	G	650	
1	H	650	
1	I	650	
1	J	650	
1	K	650	
1	L	650	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 56680 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 Arachidonate 15-lipoxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	0	0
			4666	2974	802	879	11			
1	B	600	Total	C	N	O	S	0	0	0
			4615	2946	790	868	11			
1	C	602	Total	C	N	O	S	0	0	0
			4629	2954	792	872	11			
1	D	607	Total	C	N	O	S	0	0	0
			4677	2983	801	882	11			
1	E	604	Total	C	N	O	S	0	0	0
			4650	2966	797	876	11			
1	F	605	Total	C	N	O	S	0	0	0
			4657	2969	798	879	11			
1	G	603	Total	C	N	O	S	0	0	0
			4637	2955	797	874	11			
1	H	604	Total	C	N	O	S	0	0	0
			4646	2963	796	876	11			
1	I	603	Total	C	N	O	S	0	0	0
			4637	2958	794	874	11			
1	J	604	Total	C	N	O	S	0	0	0
			4651	2969	797	874	11			
1	K	600	Total	C	N	O	S	0	0	0
			4612	2944	788	869	11			
1	L	600	Total	C	N	O	S	0	0	0
			4605	2939	787	868	11			

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cd	0	0
			4	4		
2	B	4	Total	Cd	0	0
			4	4		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total 83	O 83	0	0
3	B	56	Total 56	O 56	0	0
3	C	89	Total 89	O 89	0	0
3	D	103	Total 103	O 103	0	0
3	E	103	Total 103	O 103	0	0
3	F	75	Total 75	O 75	0	0
3	G	82	Total 82	O 82	0	0
3	H	69	Total 69	O 69	0	0
3	I	62	Total 62	O 62	0	0

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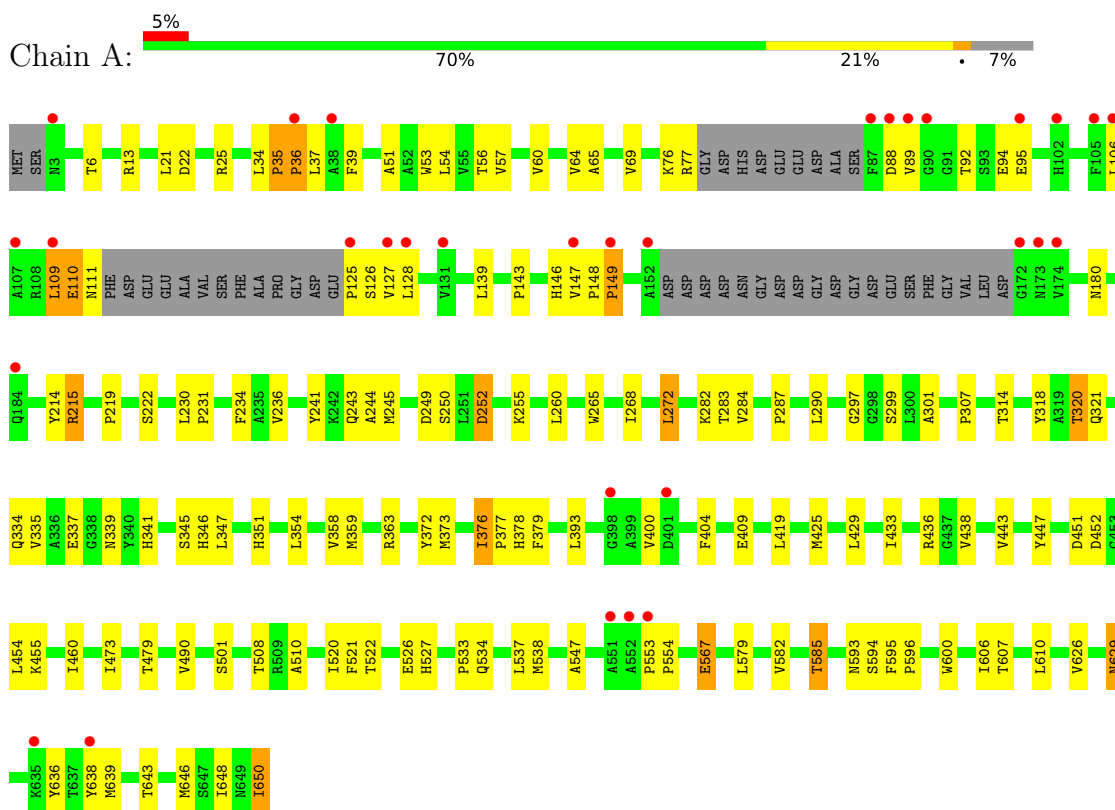
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	56	Total 56	O 56	0	0
3	K	79	Total 79	O 79	0	0
3	L	93	Total 93	O 93	0	0

3 Residue-property plots [i](#)

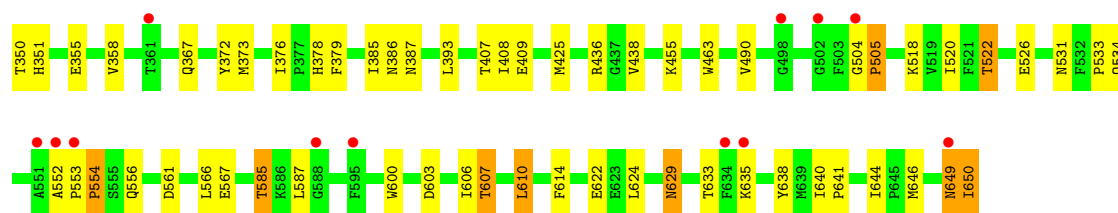
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Arachidonate 15-lipoxygenase

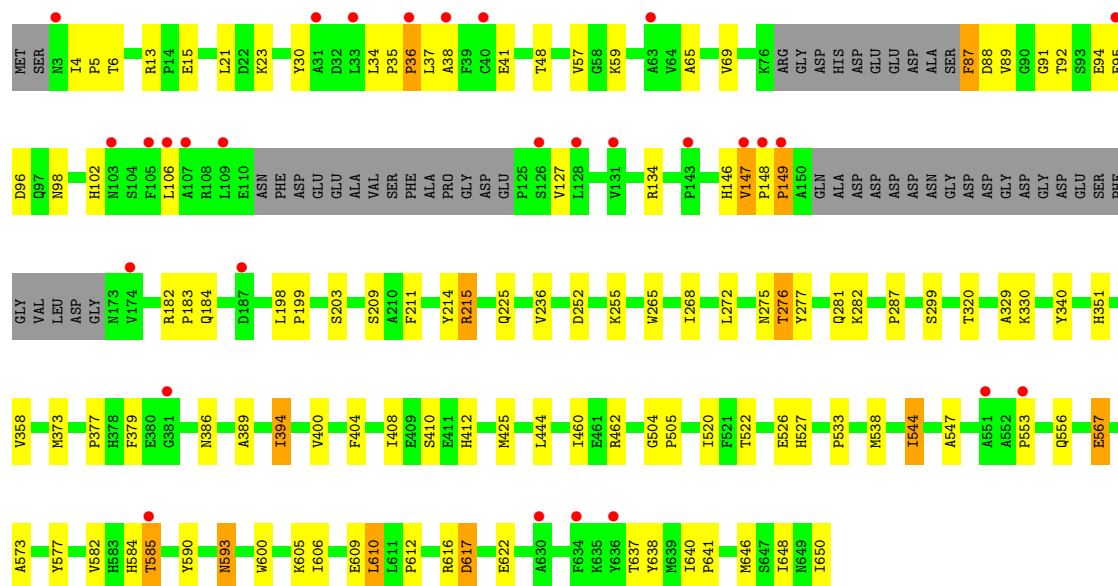
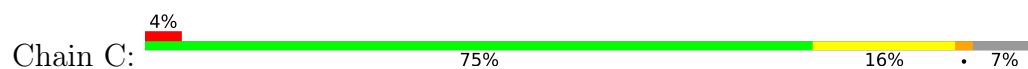


• Molecule 1: Arachidonate 15-lipoxygenase

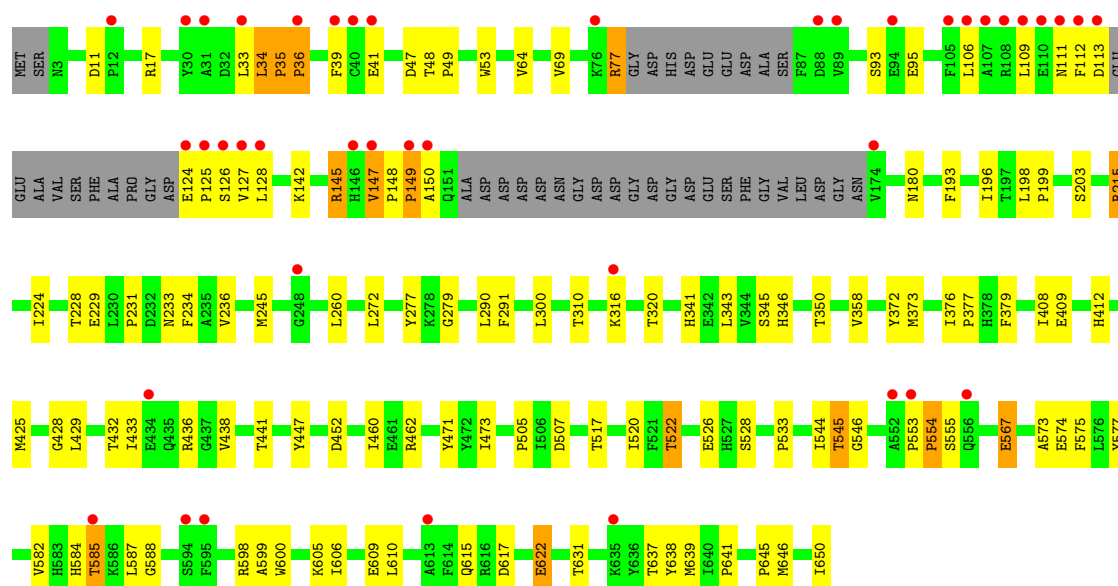
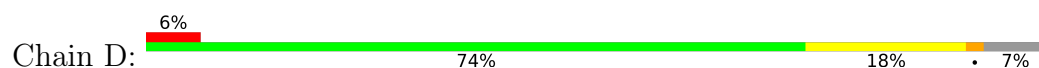




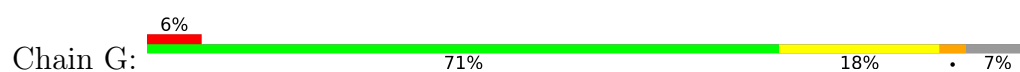
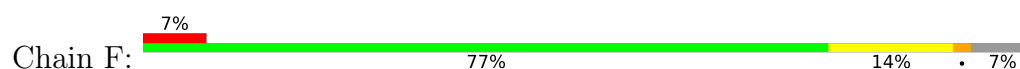
• Molecule 1: Arachidonate 15-lipoxygenase

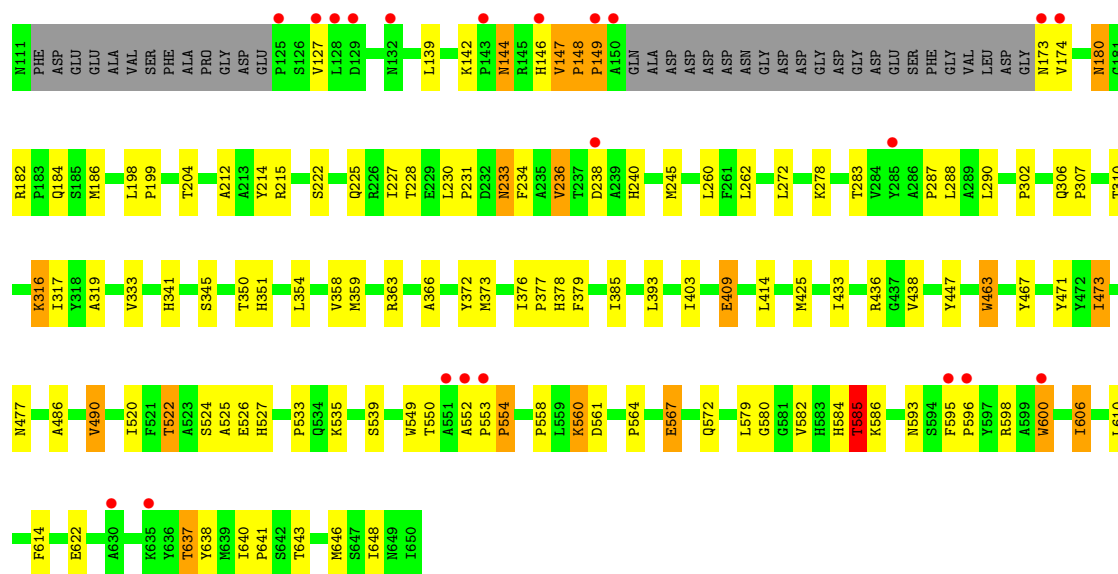


• Molecule 1: Arachidonate 15-lipoxygenase

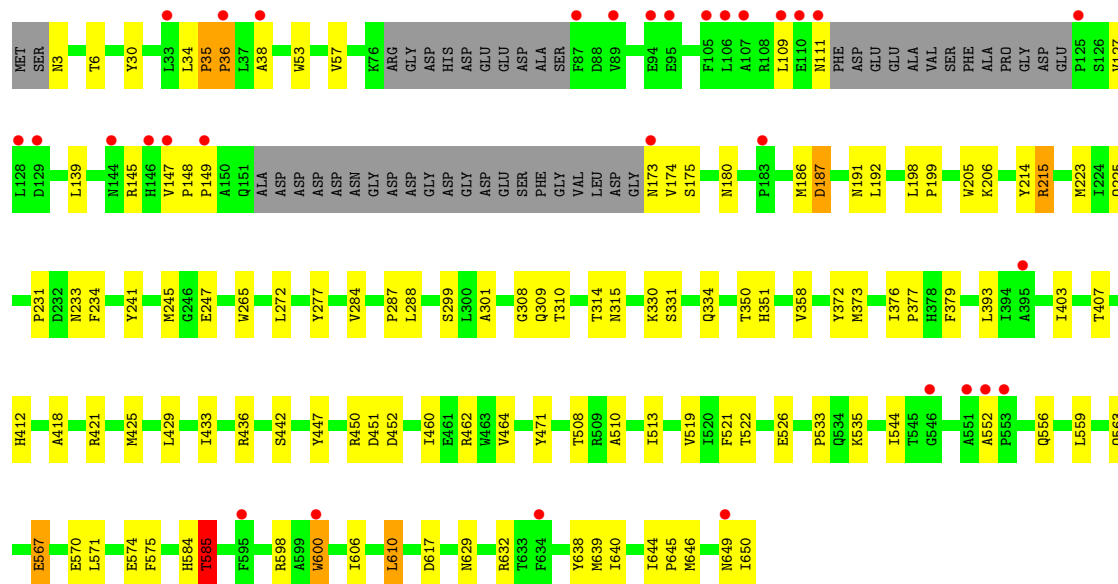
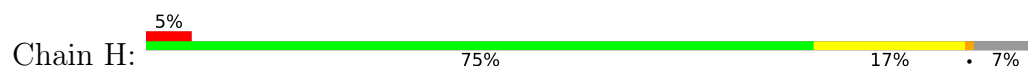


Chain E: 5% 73% 17% 7%

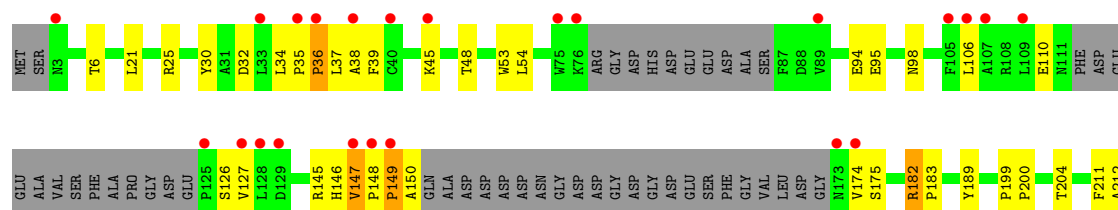
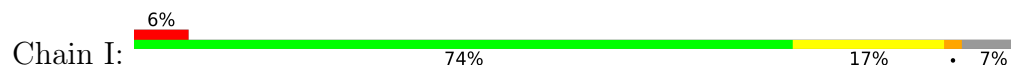


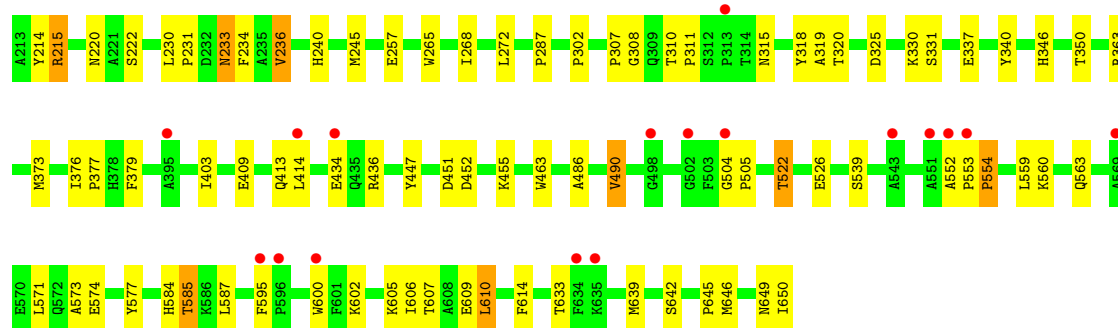


• Molecule 1: Arachidonate 15-lipoxygenase

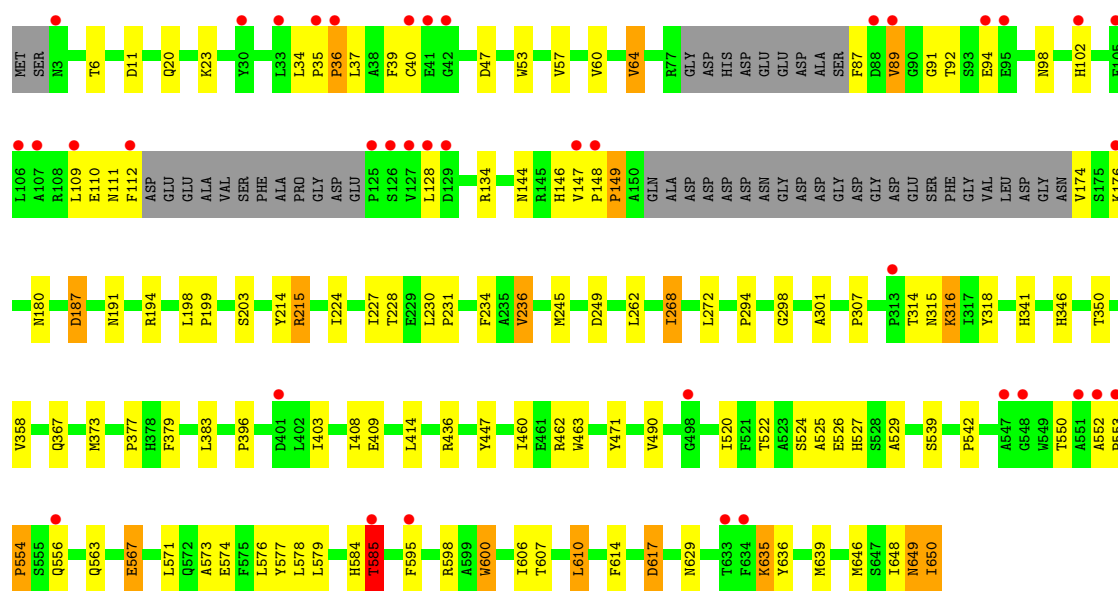
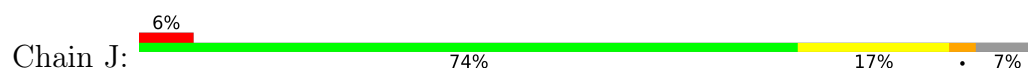


• Molecule 1: Arachidonate 15-lipoxygenase

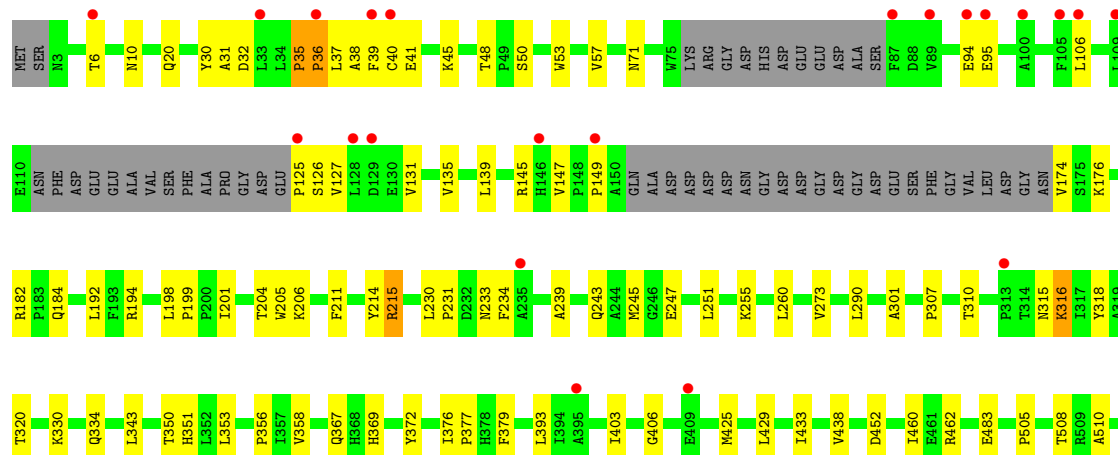
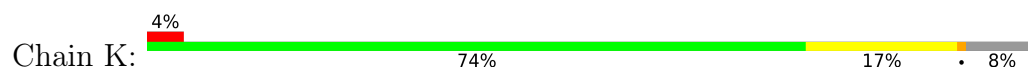




• Molecule 1: Arachidonate 15-lipoxygenase

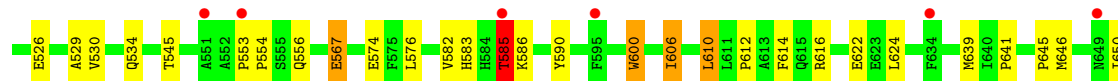
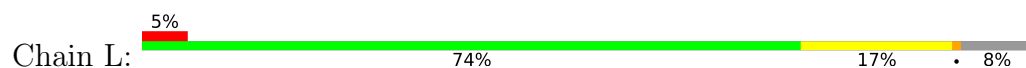


• Molecule 1: Arachidonate 15-lipoxygenase





• Molecule 1: Arachidonate 15-lipoxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	164.73Å 248.59Å 164.09Å 90.00° 119.86° 90.00°	Depositor
Resolution (Å)	49.61 – 2.80 49.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.9 (49.61-2.80) 91.9 (49.61-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.227 , 0.254 0.238 , 0.263	Depositor DCC
R_{free} test set	9992 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.145 for l,k,-h-l 0.145 for -h-l,k,h 0.418 for -h-l,-k,l 0.124 for h,-k,-h-l 0.176 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	56680	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.51% 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:
CD

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	0.14	0/4787	0.37	0/6535
1	B	0.13	0/4736	0.33	0/6467
1	C	0.13	0/4750	0.35	0/6486
1	D	0.14	0/4799	0.35	0/6552
1	E	0.14	0/4771	0.34	0/6514
1	F	0.13	0/4778	0.35	0/6524
1	G	0.14	0/4757	0.36	0/6495
1	H	0.14	0/4767	0.35	0/6509
1	I	0.13	0/4758	0.34	0/6497
1	J	0.16	0/4773	0.38	2/6516 (0.0%)
1	K	0.13	0/4733	0.35	0/6464
1	L	0.14	0/4726	0.34	0/6454
All	All	0.14	0/57135	0.35	2/78013 (0.0%)

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	D	0	1
1	E	0	1
1	H	0	2
1	K	0	1
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	550	THR	CA-C-O	6.15	121.51	117.94
1	J	550	THR	CB-CA-C	-5.26	109.50	117.07

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	PRO	Peptide
1	D	35	PRO	Peptide
1	E	35	PRO	Peptide
1	H	35	PRO	Peptide
1	H	552	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4666	0	4577	80	0
1	B	4615	0	4531	62	0
1	C	4629	0	4542	57	0
1	D	4677	0	4581	64	0
1	E	4650	0	4562	61	0
1	F	4657	0	4564	51	0
1	G	4637	0	4552	72	0
1	H	4646	0	4556	63	0
1	I	4637	0	4548	65	0
1	J	4651	0	4564	73	0
1	K	4612	0	4523	61	0
1	L	4605	0	4515	61	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
2	I	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	83	0	0	0	0
3	B	56	0	0	0	0
3	C	89	0	0	0	0
3	D	103	0	0	0	0
3	E	103	0	0	1	0
3	F	75	0	0	0	0
3	G	82	0	0	1	0
3	H	69	0	0	1	0
3	I	62	0	0	0	0
3	J	56	0	0	0	0
3	K	79	0	0	1	0
3	L	93	0	0	0	0
All	All	56680	0	54615	765	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 765 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:G:148:PRO:HB2	1:G:149:PRO:HD2	1.54	0.89
1:D:148:PRO:HB2	1:D:149:PRO:HD2	1.57	0.87
1:I:585:THR:HG23	1:I:646:MET:H	1.40	0.86
1:B:385:ILE:HG12	1:B:650:ILE:HA	1.58	0.86
1:D:585:THR:HG23	1:D:646:MET:H	1.45	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	599/650 (92%)	558 (93%)	33 (6%)	8 (1%)	9	31
1	B	592/650 (91%)	558 (94%)	29 (5%)	5 (1%)	16	44
1	C	594/650 (91%)	559 (94%)	33 (6%)	2 (0%)	36	66
1	D	599/650 (92%)	569 (95%)	23 (4%)	7 (1%)	10	34
1	E	596/650 (92%)	562 (94%)	27 (4%)	7 (1%)	10	34
1	F	597/650 (92%)	559 (94%)	32 (5%)	6 (1%)	12	38
1	G	595/650 (92%)	564 (95%)	25 (4%)	6 (1%)	12	38
1	H	596/650 (92%)	555 (93%)	37 (6%)	4 (1%)	18	47
1	I	595/650 (92%)	568 (96%)	23 (4%)	4 (1%)	18	47
1	J	596/650 (92%)	562 (94%)	30 (5%)	4 (1%)	18	47
1	K	592/650 (91%)	559 (94%)	30 (5%)	3 (0%)	24	55
1	L	592/650 (91%)	565 (95%)	24 (4%)	3 (0%)	24	55
All	All	7143/7800 (92%)	6738 (94%)	346 (5%)	59 (1%)	16	44

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	PRO
1	A	149	PRO
1	A	585	THR
1	B	36	PRO
1	B	585	THR

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	484/518 (93%)	446 (92%)	38 (8%)	11	35
1	B	480/518 (93%)	443 (92%)	37 (8%)	12	36
1	C	481/518 (93%)	446 (93%)	35 (7%)	13	38
1	D	486/518 (94%)	452 (93%)	34 (7%)	14	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	483/518 (93%)	441 (91%)	42 (9%)	9	30
1	F	484/518 (93%)	457 (94%)	27 (6%)	19	50
1	G	482/518 (93%)	440 (91%)	42 (9%)	9	30
1	H	483/518 (93%)	458 (95%)	25 (5%)	21	53
1	I	482/518 (93%)	453 (94%)	29 (6%)	17	47
1	J	483/518 (93%)	449 (93%)	34 (7%)	14	40
1	K	479/518 (92%)	454 (95%)	25 (5%)	21	53
1	L	478/518 (92%)	446 (93%)	32 (7%)	15	42
All	All	5785/6216 (93%)	5385 (93%)	400 (7%)	14	41

5 of 400 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	236	VAL
1	I	146	HIS
1	L	624	LEU
1	G	354	LEU
1	H	225	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	584	HIS
1	L	191	ASN
1	L	392	ASN
1	E	281	GLN
1	D	649	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 48 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	607/650 (93%)	0.46	31 (5%)	33	25	27, 47, 95, 192	0
1	B	600/650 (92%)	0.56	37 (6%)	26	20	29, 53, 98, 148	0
1	C	602/650 (92%)	0.44	29 (4%)	35	28	27, 46, 95, 150	0
1	D	607/650 (93%)	0.43	42 (6%)	23	16	26, 44, 96, 215	0
1	E	604/650 (92%)	0.39	32 (5%)	32	24	27, 44, 92, 178	0
1	F	605/650 (93%)	0.66	45 (7%)	20	15	29, 54, 106, 173	0
1	G	603/650 (92%)	0.48	37 (6%)	27	20	28, 48, 92, 180	0
1	H	604/650 (92%)	0.49	31 (5%)	33	25	28, 46, 93, 179	0
1	I	603/650 (92%)	0.58	40 (6%)	24	18	30, 53, 98, 188	0
1	J	604/650 (92%)	0.61	39 (6%)	25	18	29, 53, 101, 191	0
1	K	600/650 (92%)	0.46	26 (4%)	40	31	27, 47, 92, 168	0
1	L	600/650 (92%)	0.47	34 (5%)	29	22	27, 46, 88, 199	0
All	All	7239/7800 (92%)	0.50	423 (5%)	29	22	26, 49, 96, 215	0

The worst 5 of 423 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	36	PRO	8.1
1	D	106	LEU	8.0
1	K	106	LEU	7.6
1	F	36	PRO	7.4
1	K	128	LEU	7.4

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 ⓘ

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
2	CD	F	704	1/1	0.81	0.11	161,161,161,161	0
2	CD	G	704	1/1	0.89	0.11	139,139,139,139	0
2	CD	J	704	1/1	0.89	0.12	155,155,155,155	0
2	CD	B	704	1/1	0.90	0.11	133,133,133,133	0
2	CD	A	704	1/1	0.90	0.14	132,132,132,132	0
2	CD	C	704	1/1	0.91	0.12	119,119,119,119	0
2	CD	K	701	1/1	0.91	0.07	73,73,73,73	0
2	CD	I	704	1/1	0.92	0.11	126,126,126,126	0
2	CD	E	701	1/1	0.92	0.07	61,61,61,61	0
2	CD	I	701	1/1	0.92	0.06	78,78,78,78	0
2	CD	L	701	1/1	0.93	0.05	68,68,68,68	0
2	CD	L	704	1/1	0.93	0.10	110,110,110,110	0
2	CD	D	701	1/1	0.95	0.05	58,58,58,58	0
2	CD	D	703	1/1	0.95	0.06	76,76,76,76	0
2	CD	H	702	1/1	0.95	0.08	48,48,48,48	0
2	CD	K	704	1/1	0.95	0.06	94,94,94,94	0
2	CD	H	704	1/1	0.95	0.09	98,98,98,98	0
2	CD	B	703	1/1	0.95	0.06	85,85,85,85	0
2	CD	G	702	1/1	0.96	0.07	50,50,50,50	0
2	CD	F	701	1/1	0.96	0.04	62,62,62,62	0
2	CD	I	703	1/1	0.96	0.05	84,84,84,84	0
2	CD	A	702	1/1	0.96	0.06	45,45,45,45	0
2	CD	J	701	1/1	0.96	0.05	68,68,68,68	0
2	CD	E	704	1/1	0.97	0.05	94,94,94,94	0
2	CD	H	701	1/1	0.97	0.05	67,67,67,67	0
2	CD	B	701	1/1	0.97	0.04	75,75,75,75	0
2	CD	D	704	1/1	0.97	0.05	88,88,88,88	0
2	CD	K	702	1/1	0.97	0.09	49,49,49,49	0
2	CD	G	701	1/1	0.97	0.04	62,62,62,62	0
2	CD	I	702	1/1	0.97	0.06	50,50,50,50	0
2	CD	B	702	1/1	0.97	0.06	51,51,51,51	0
2	CD	C	702	1/1	0.98	0.07	47,47,47,47	0

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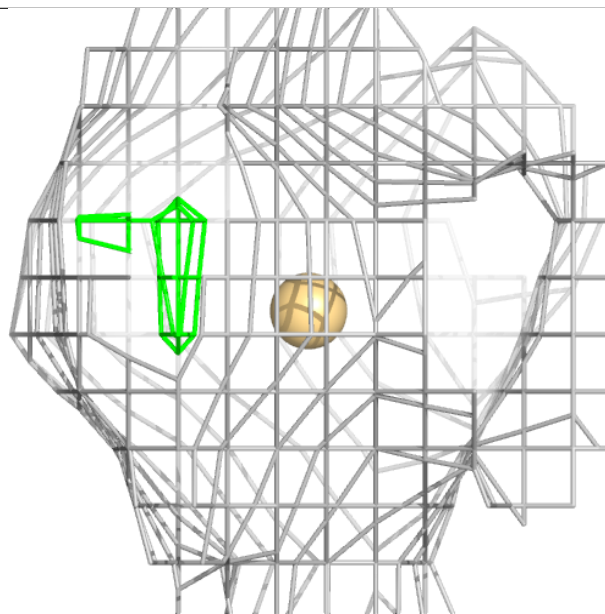
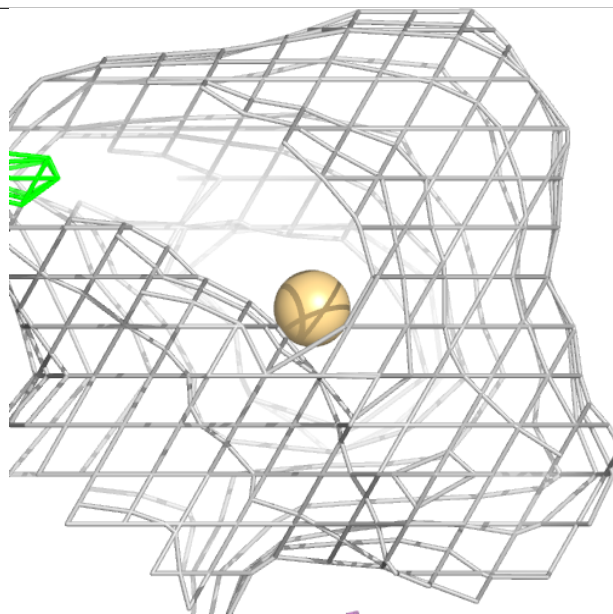
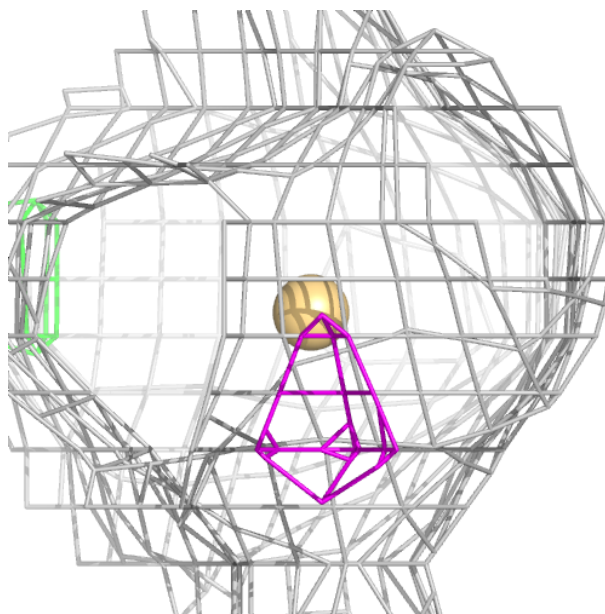
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CD	F	702	1/1	0.98	0.07	50,50,50,50	0
2	CD	J	703	1/1	0.98	0.04	80,80,80,80	0
2	CD	F	703	1/1	0.98	0.04	87,87,87,87	0
2	CD	H	703	1/1	0.98	0.05	82,82,82,82	0
2	CD	C	703	1/1	0.98	0.03	77,77,77,77	0
2	CD	A	703	1/1	0.98	0.04	96,96,96,96	0
2	CD	C	701	1/1	0.98	0.03	64,64,64,64	0
2	CD	L	702	1/1	0.98	0.06	49,49,49,49	0
2	CD	G	703	1/1	0.98	0.04	85,85,85,85	0
2	CD	K	703	1/1	0.99	0.04	82,82,82,82	0
2	CD	E	702	1/1	0.99	0.05	45,45,45,45	0
2	CD	E	703	1/1	0.99	0.03	78,78,78,78	0
2	CD	D	702	1/1	0.99	0.05	47,47,47,47	0
2	CD	L	703	1/1	0.99	0.03	74,74,74,74	0
2	CD	A	701	1/1	0.99	0.03	69,69,69,69	0
2	CD	J	702	1/1	1.00	0.06	47,47,47,47	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.

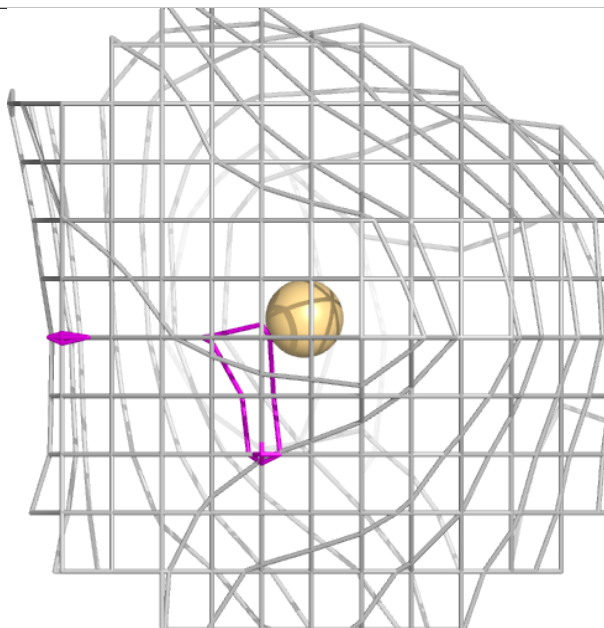
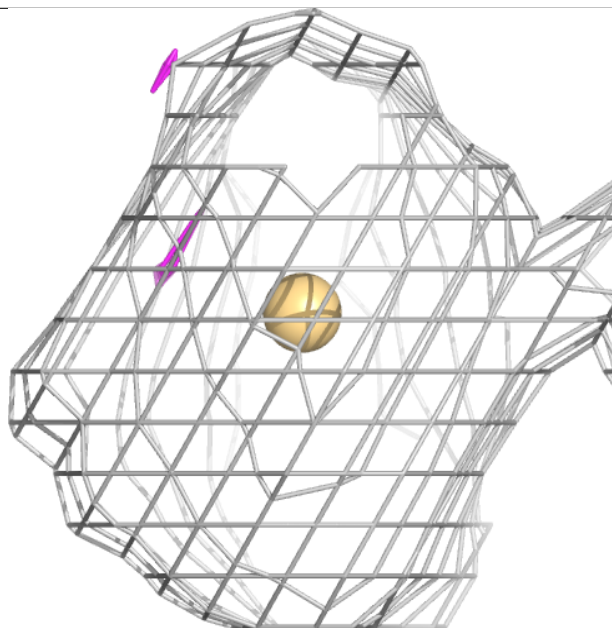
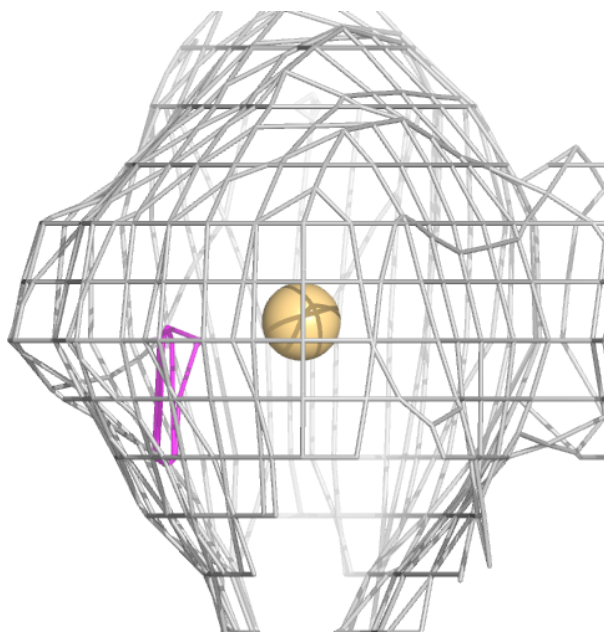
Electron density around CD F 704:

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and green (positive)



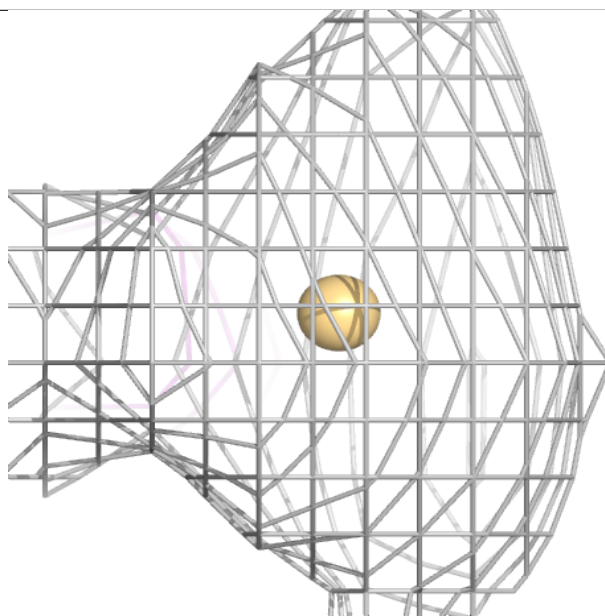
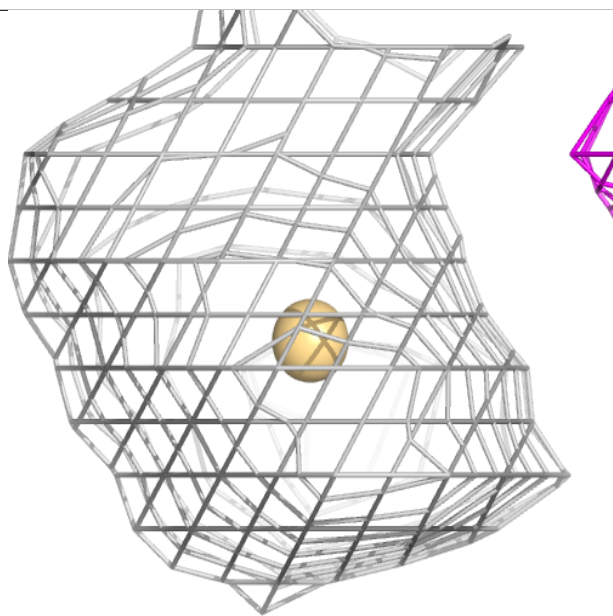
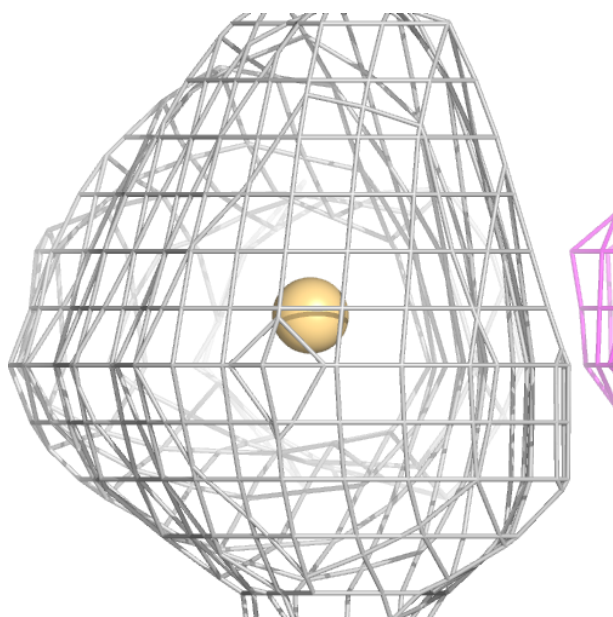
Electron density around CD G 704:

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and green (positive)



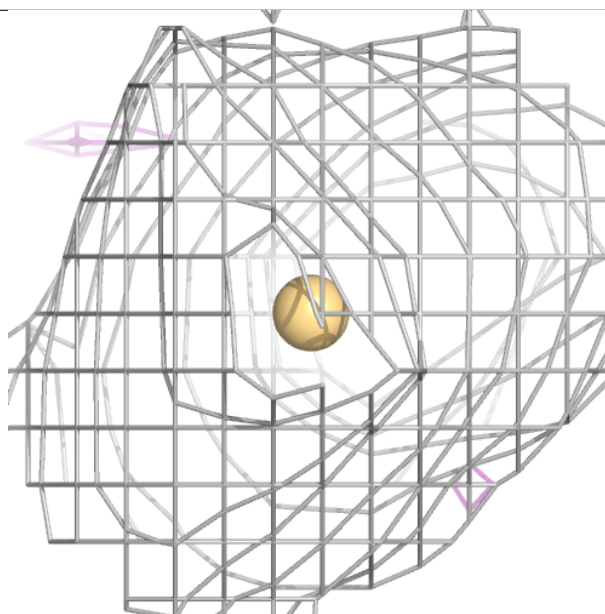
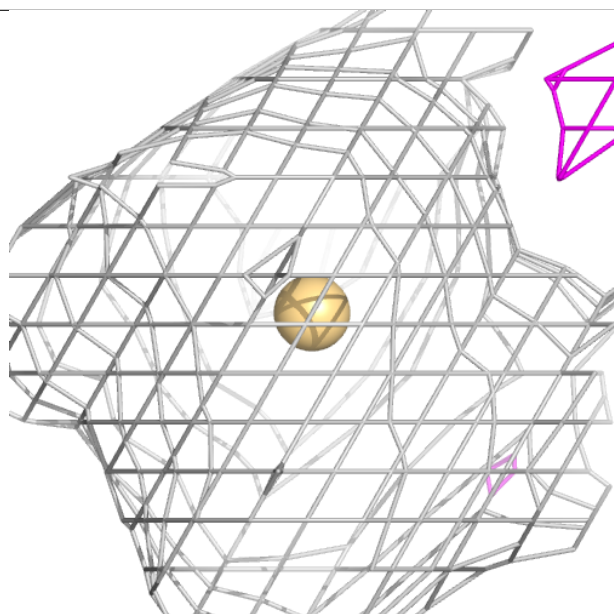
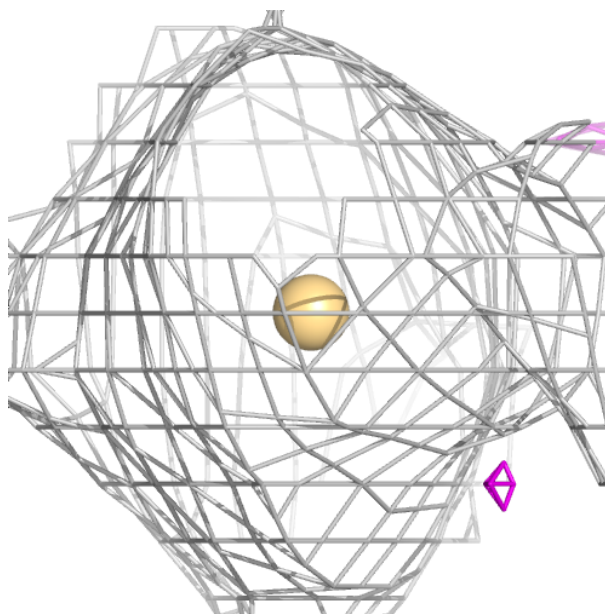
Electron density around CD J 704:

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and green (positive)



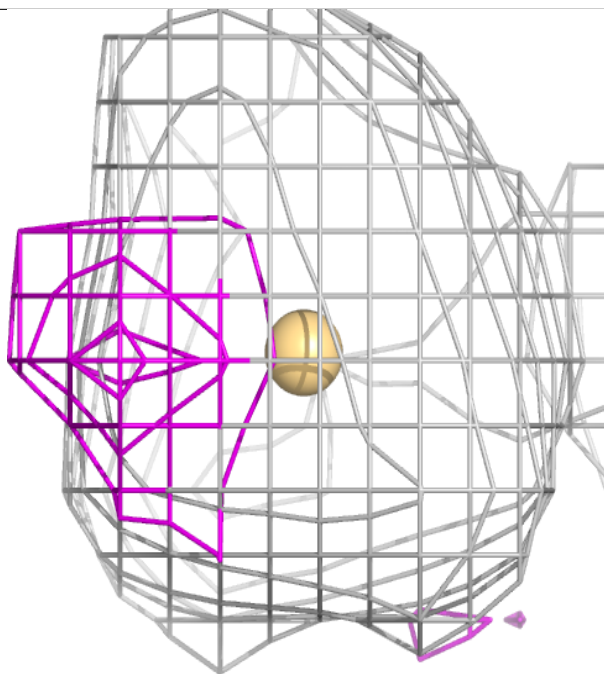
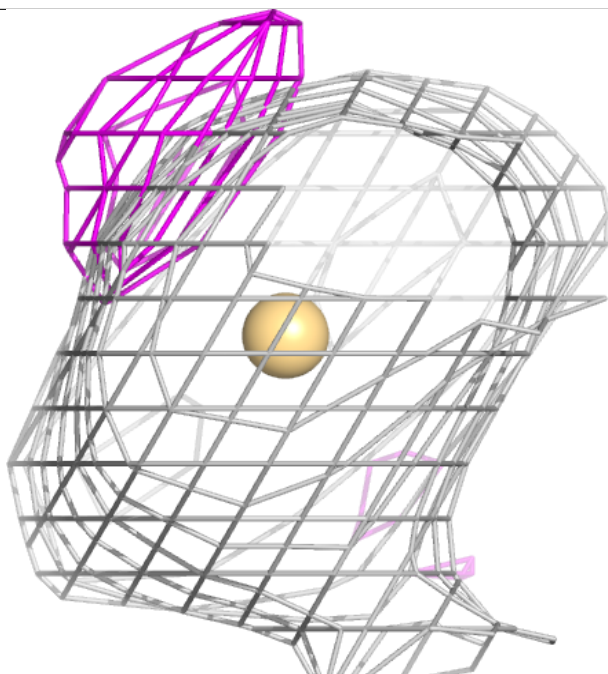
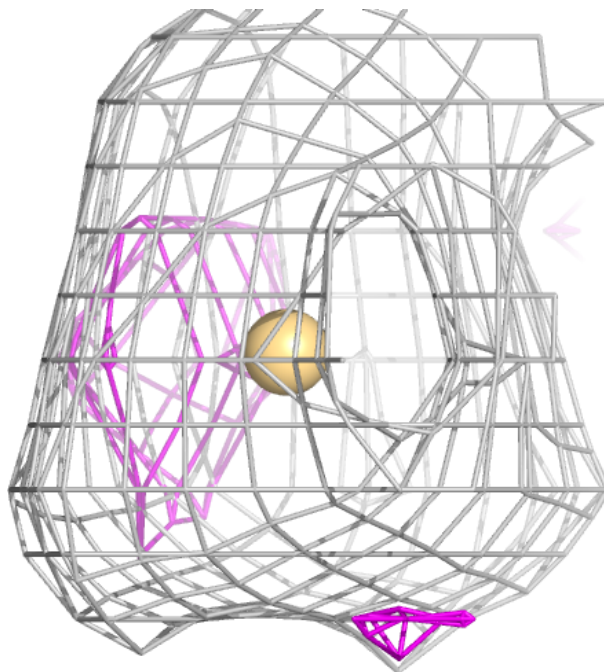
Electron density around CD B 704:

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and green (positive)



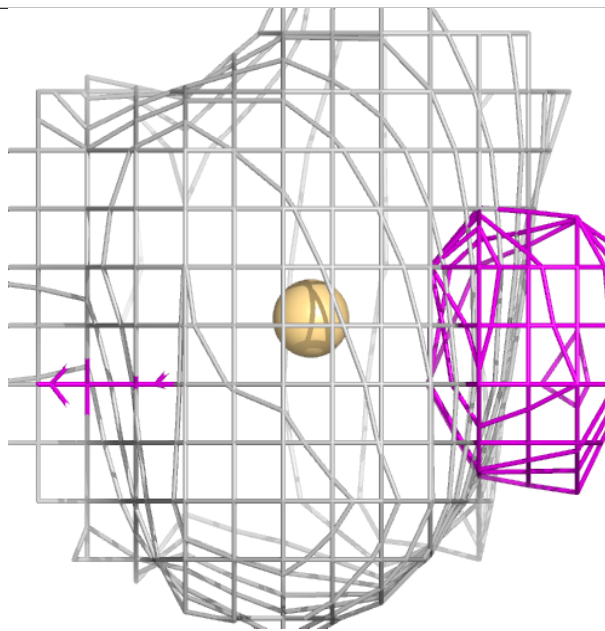
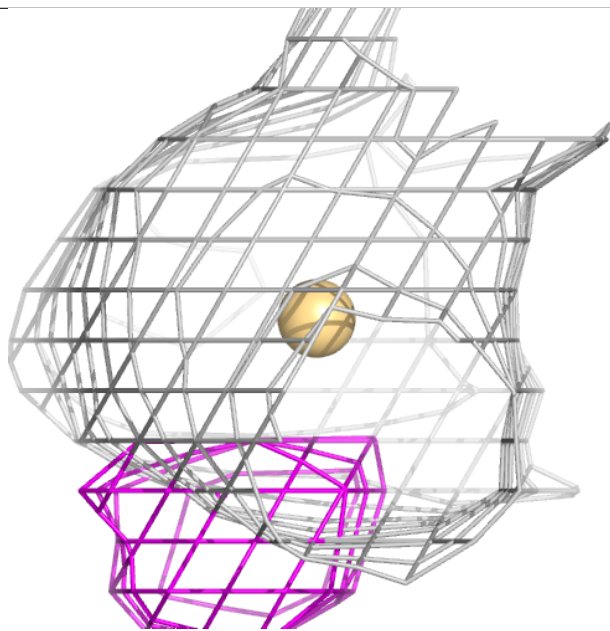
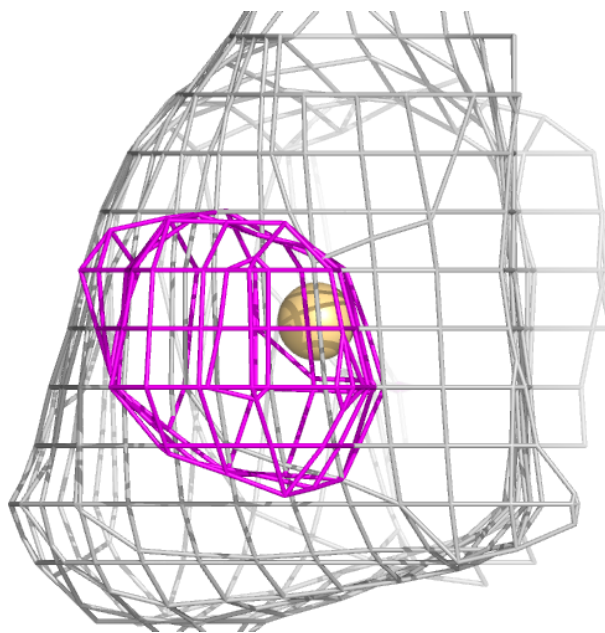
Electron density around CD A 704:

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and green (positive)



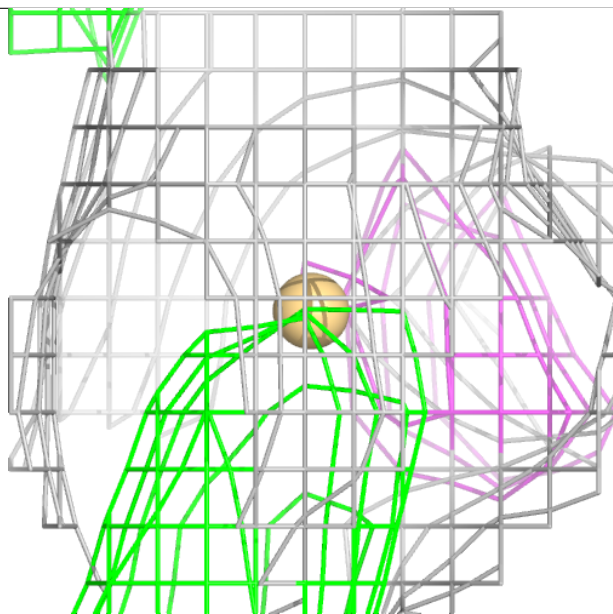
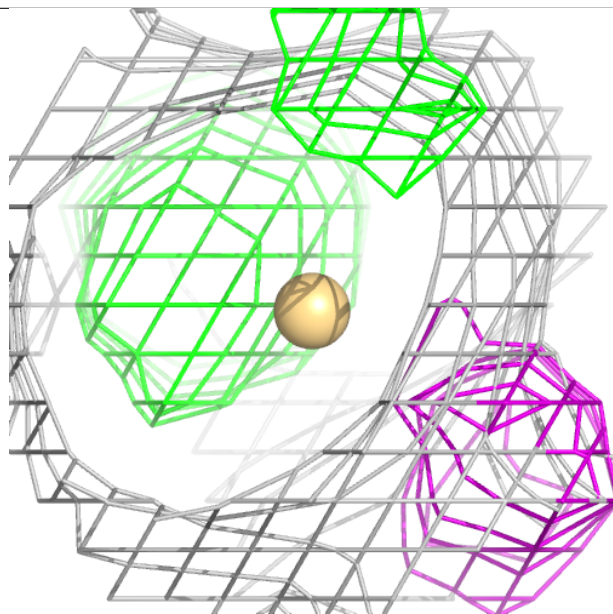
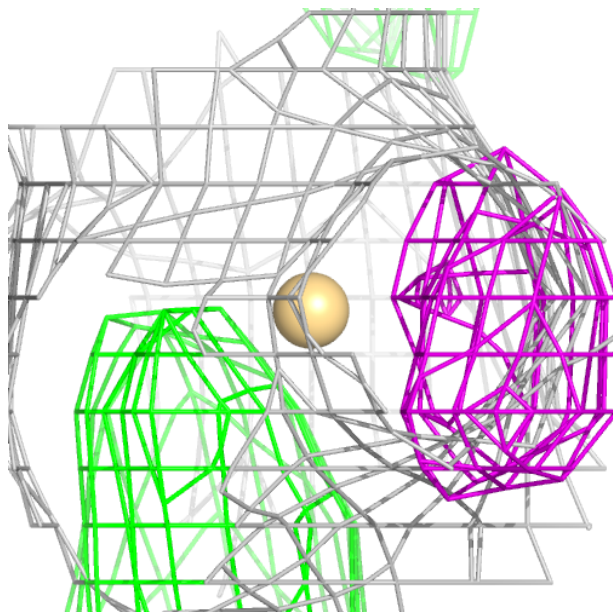
Electron density around CD C 704:

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and green (positive)



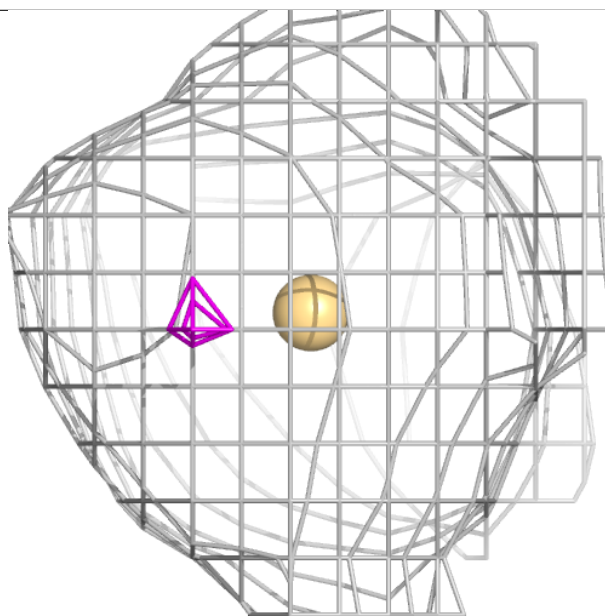
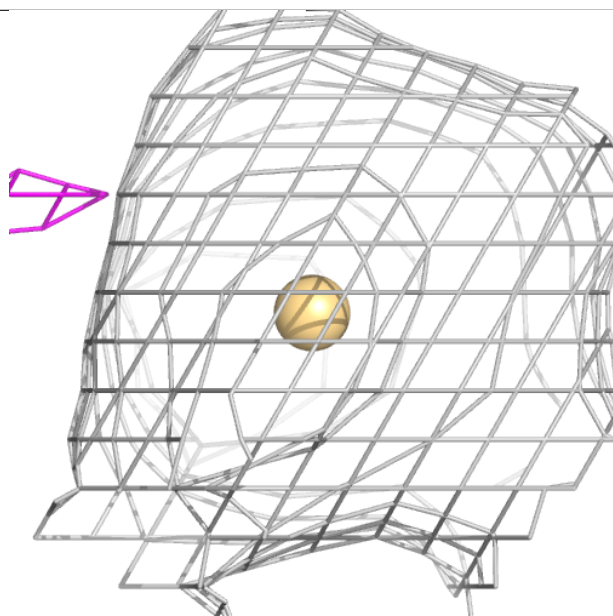
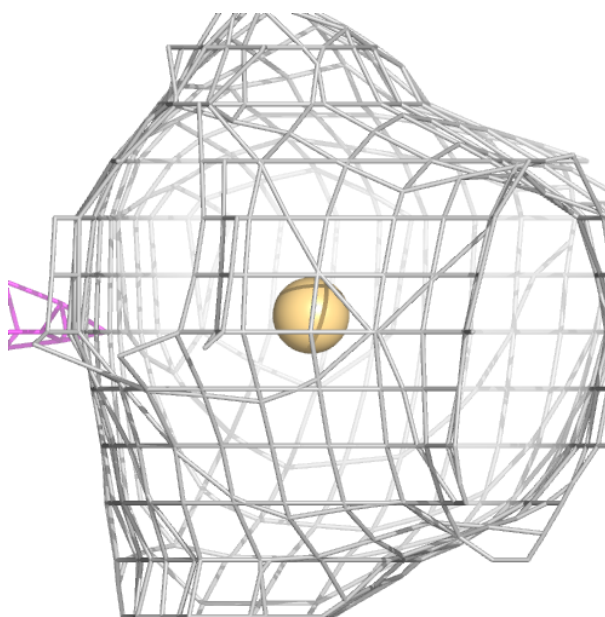
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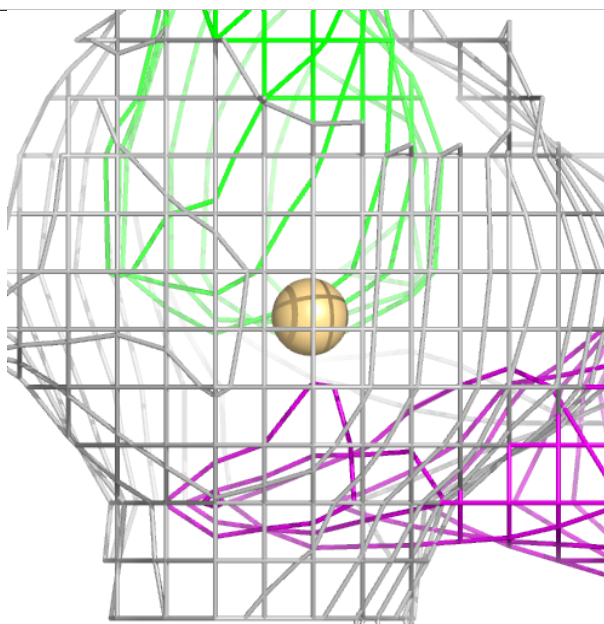
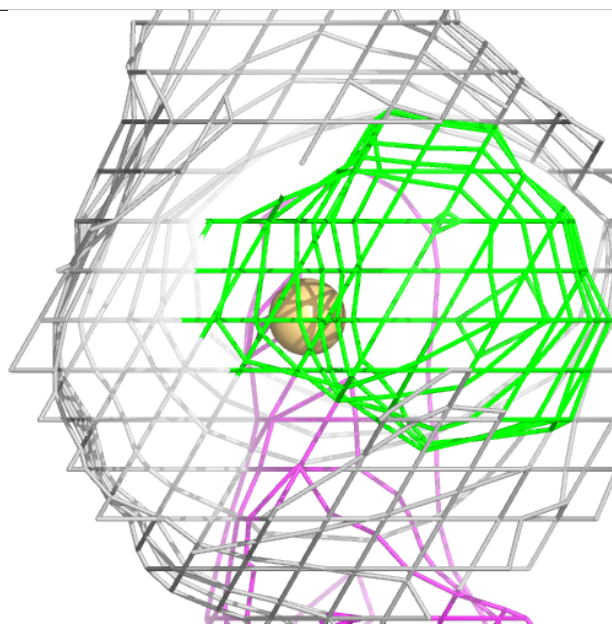
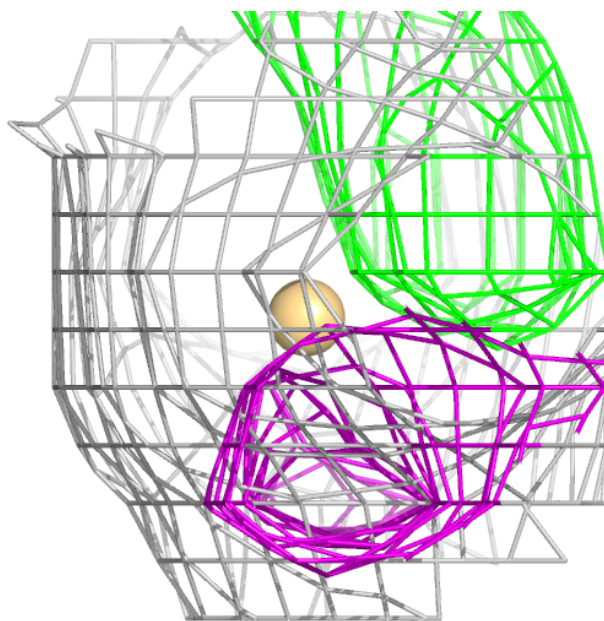
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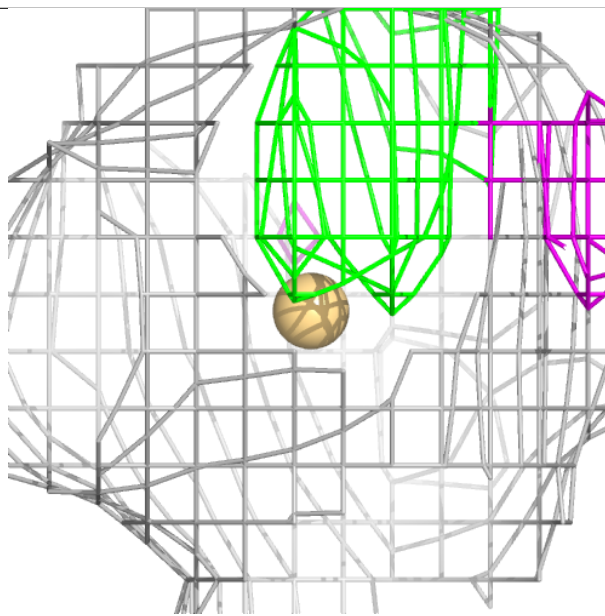
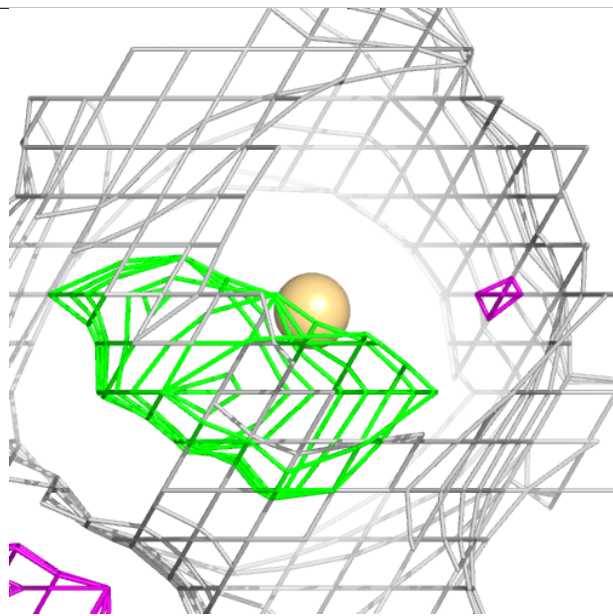
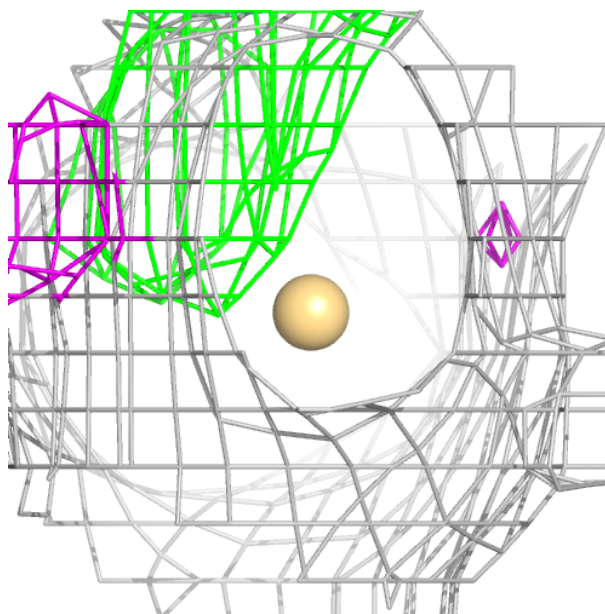
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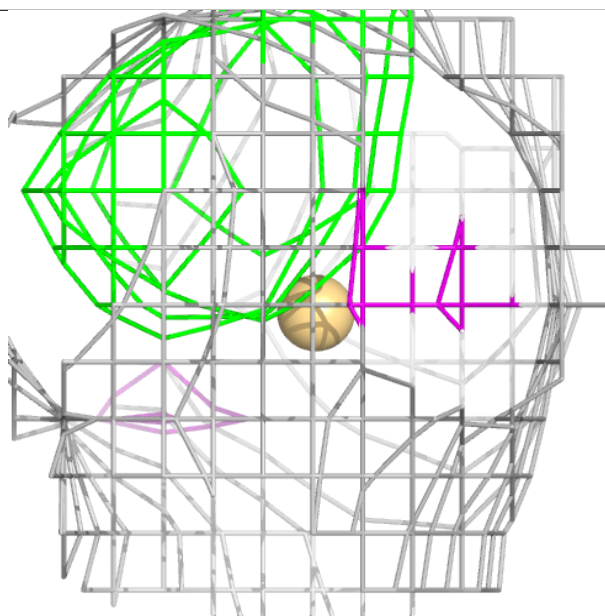
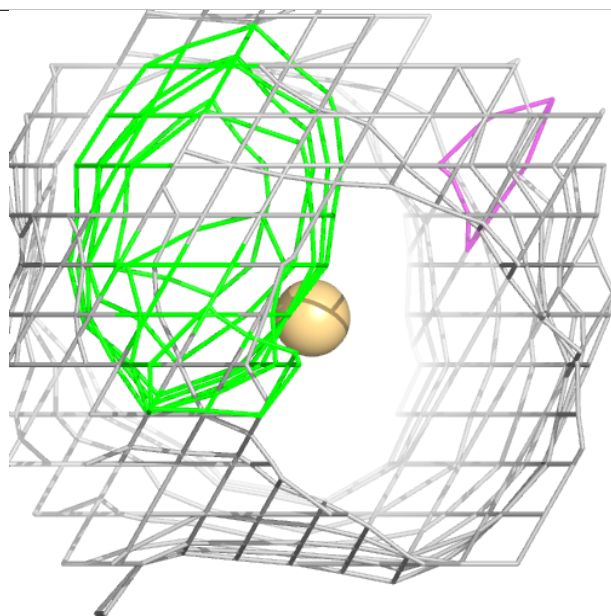
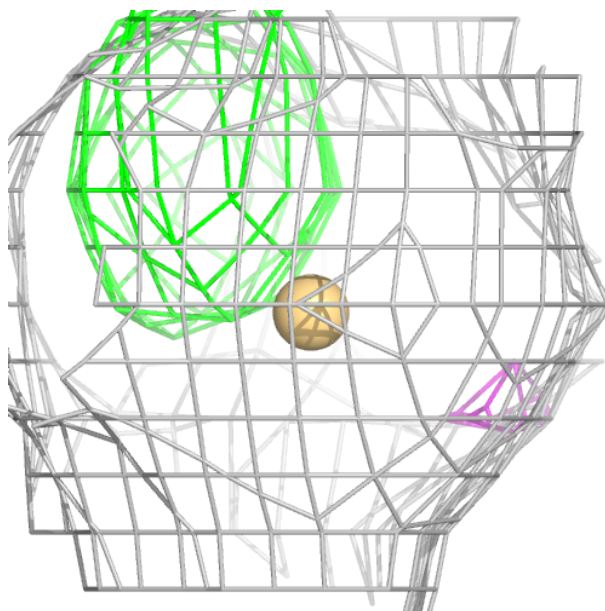
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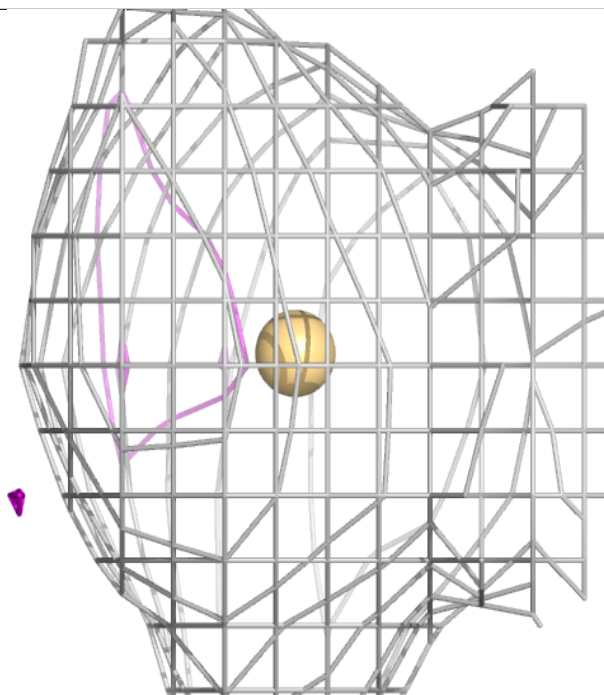
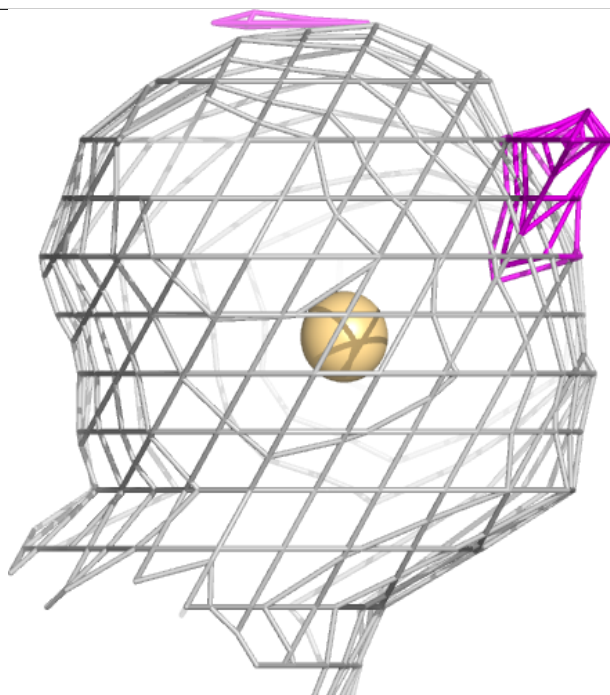
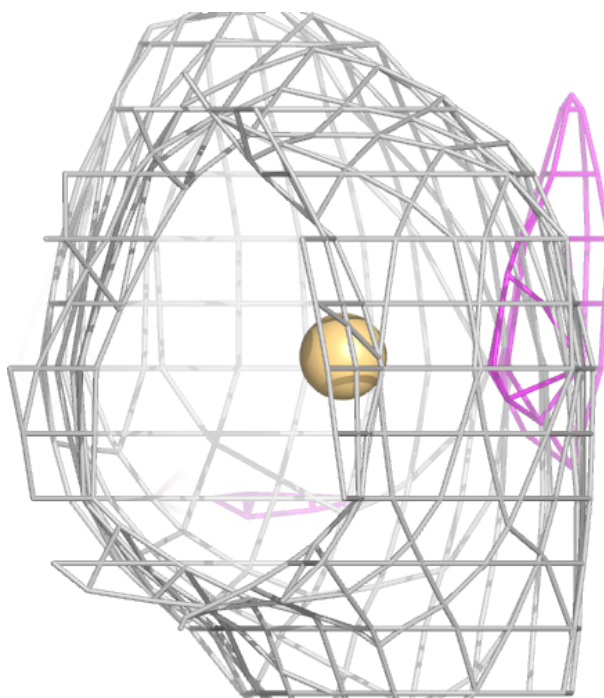
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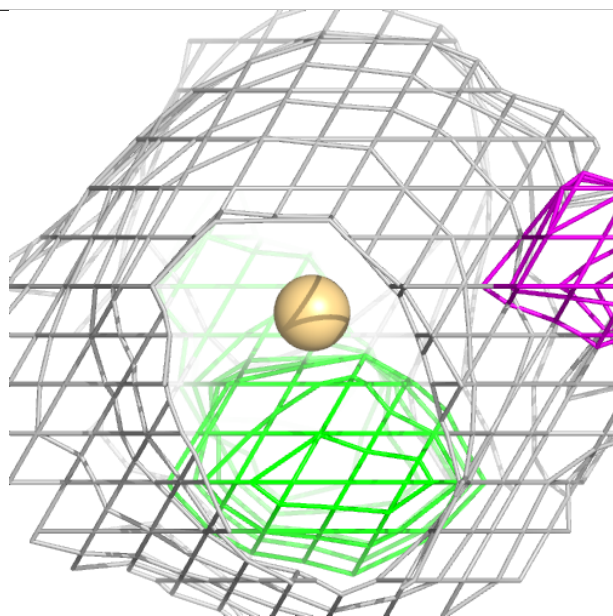
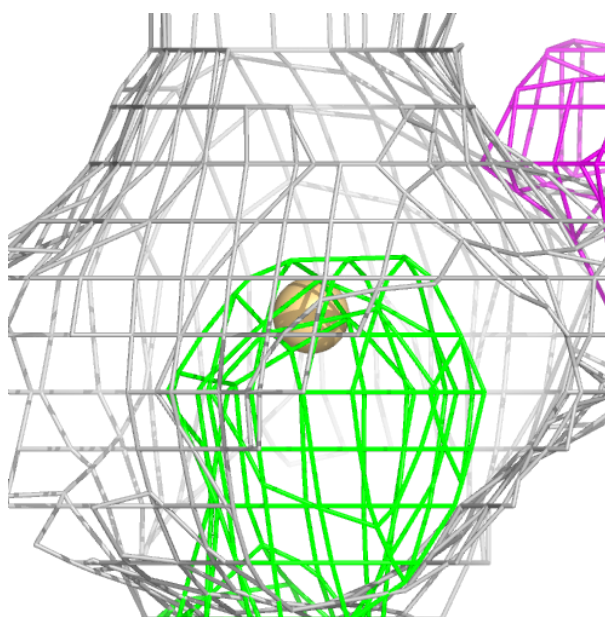
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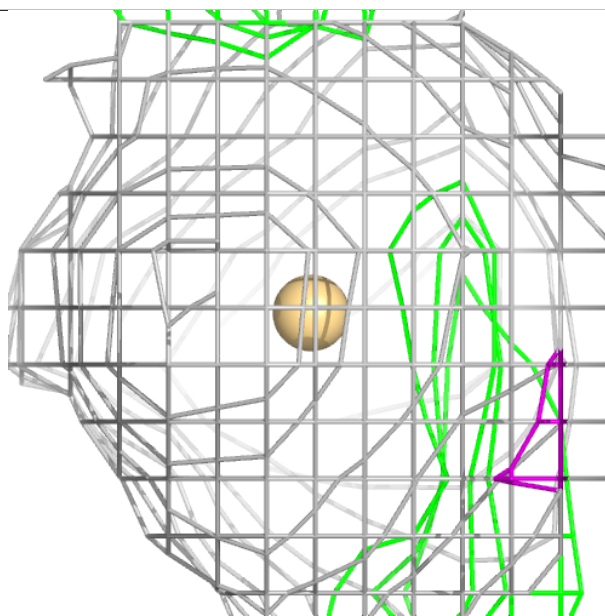
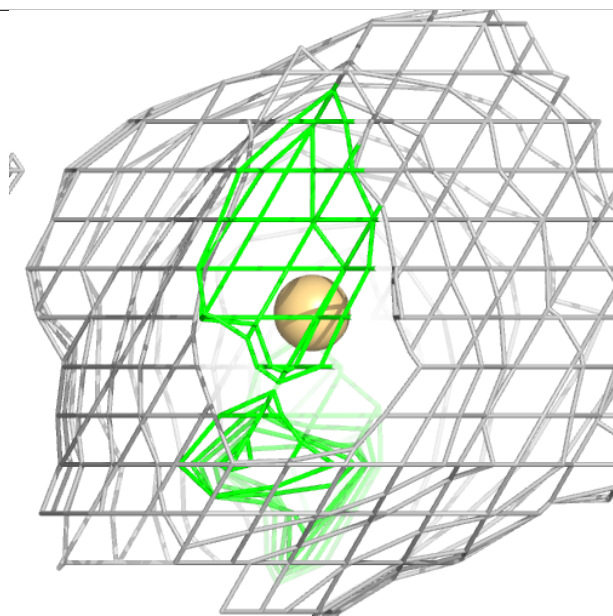
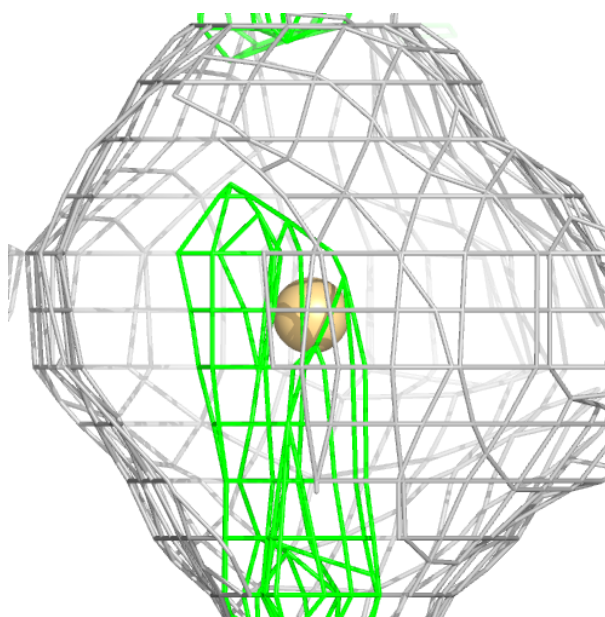
Electron density around CD D 701:

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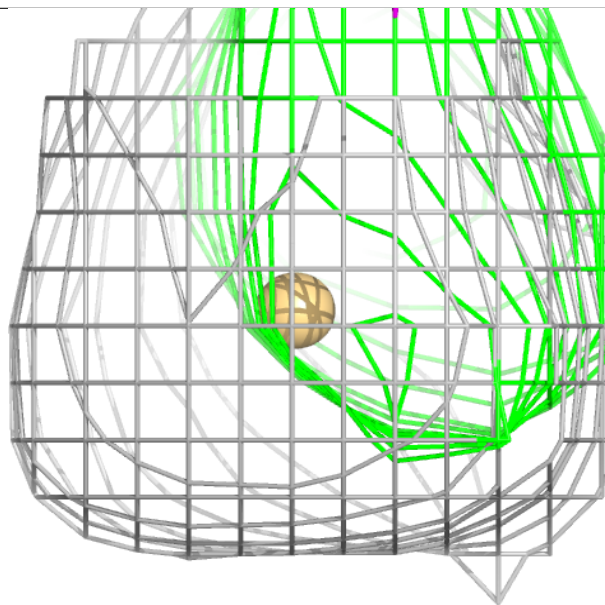
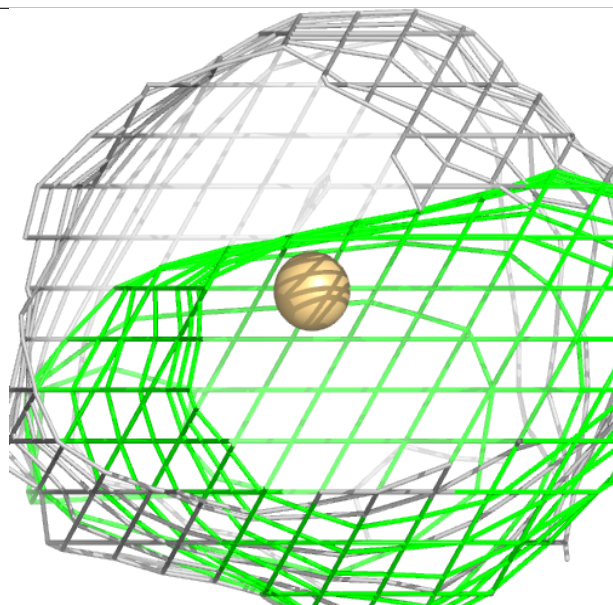
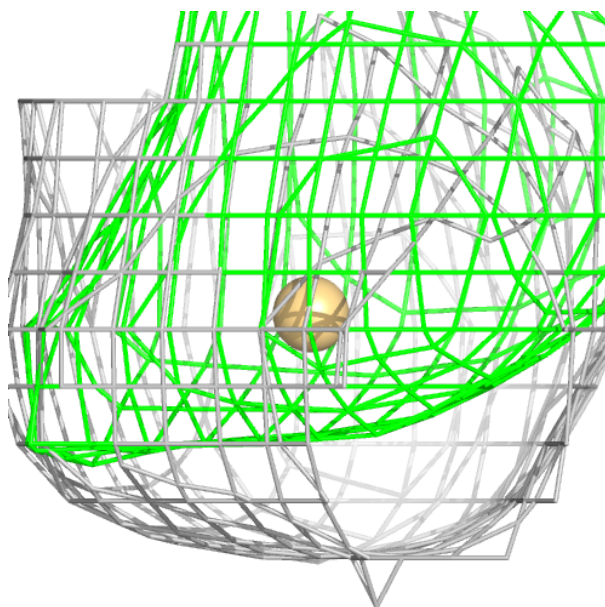
Electron density around CD D 703:

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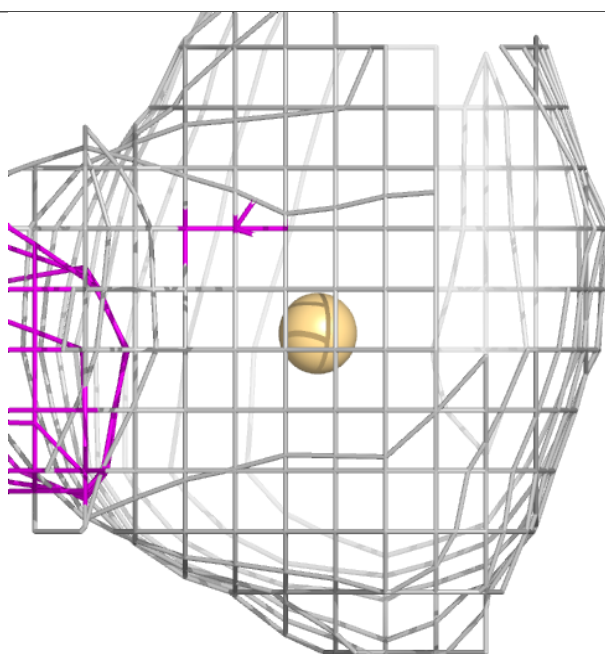
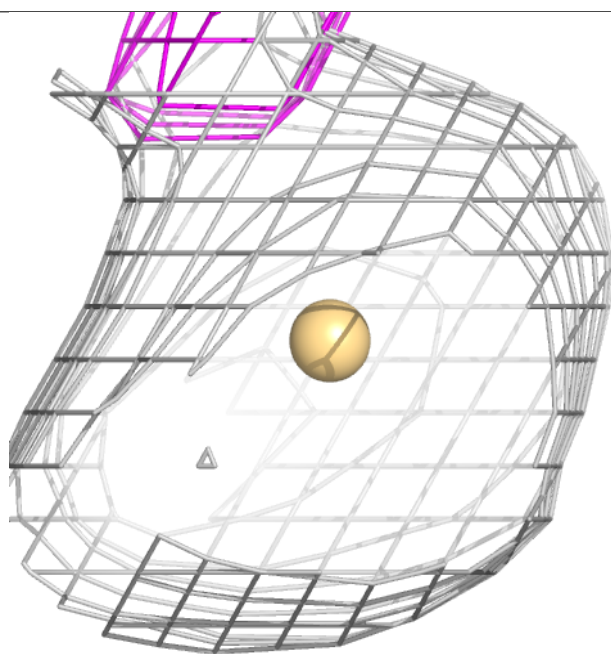
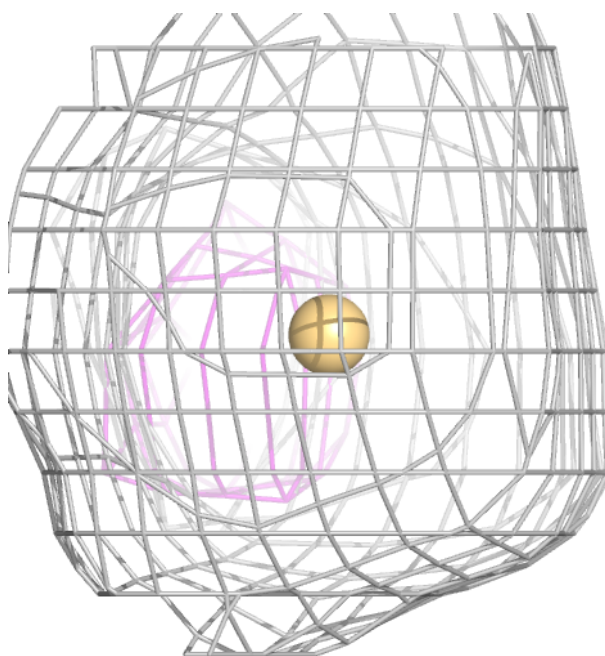
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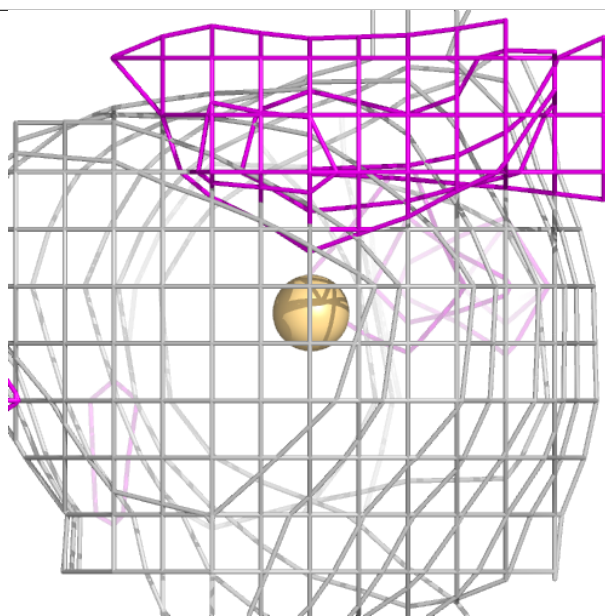
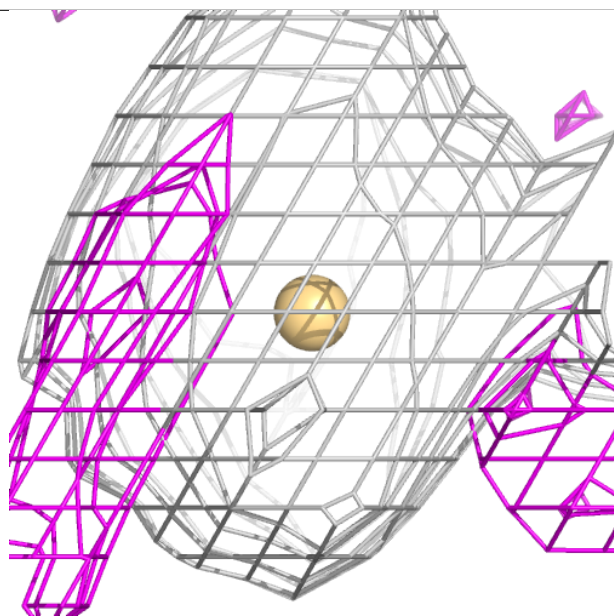
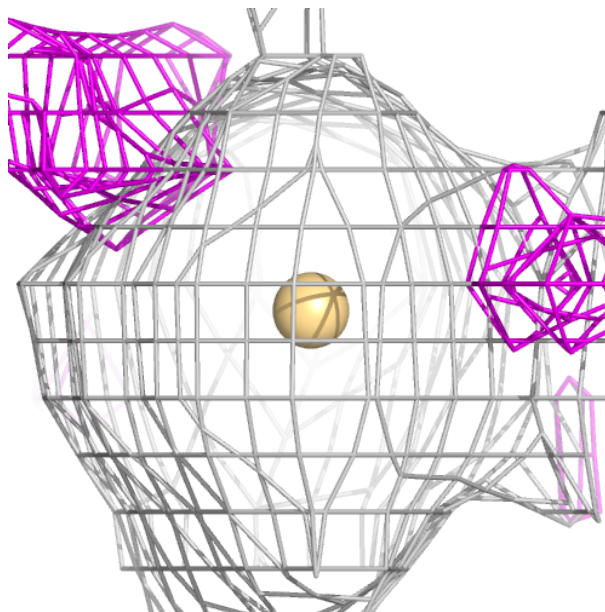
Electron density around CD K 704:

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and green (positive)



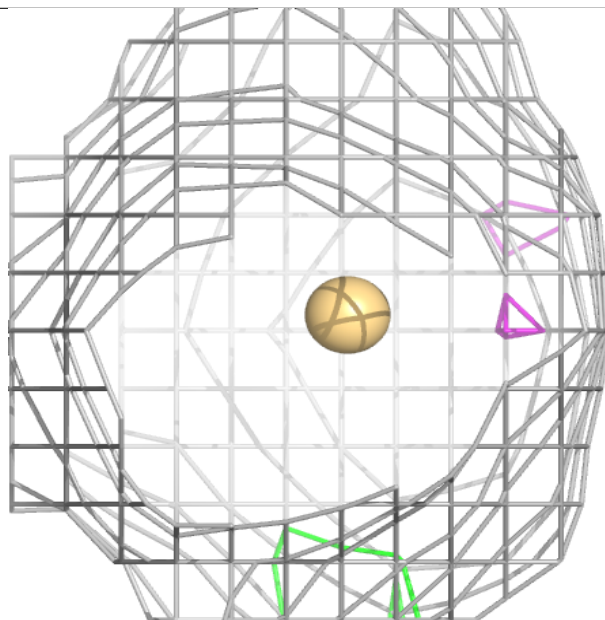
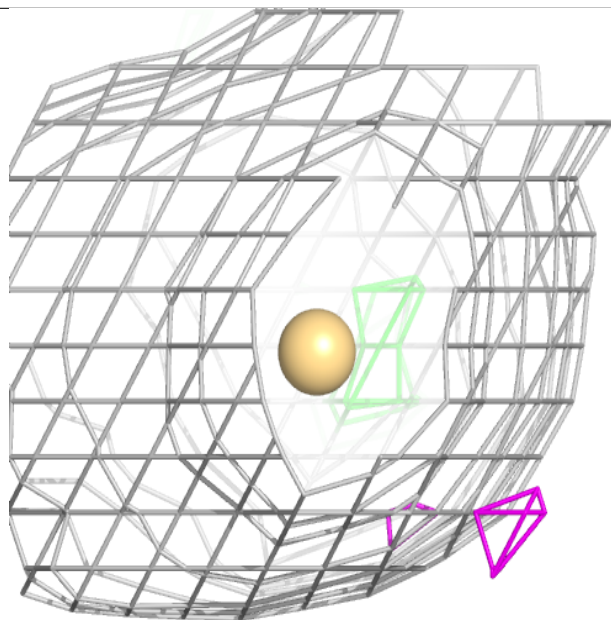
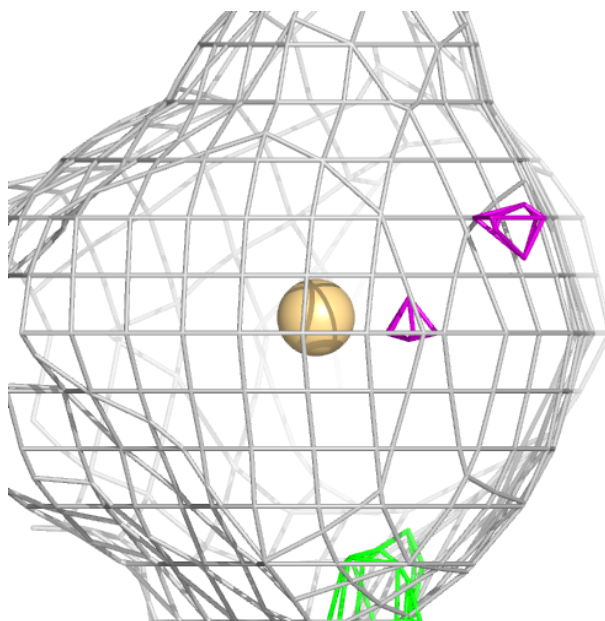
Electron density around CD H 704:

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



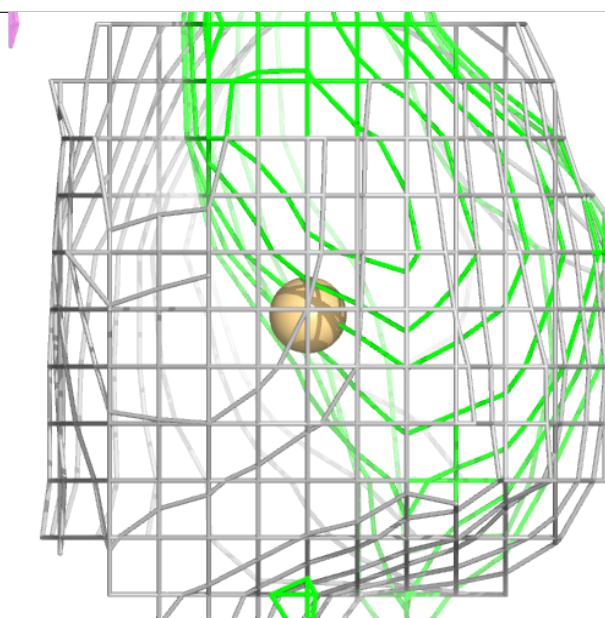
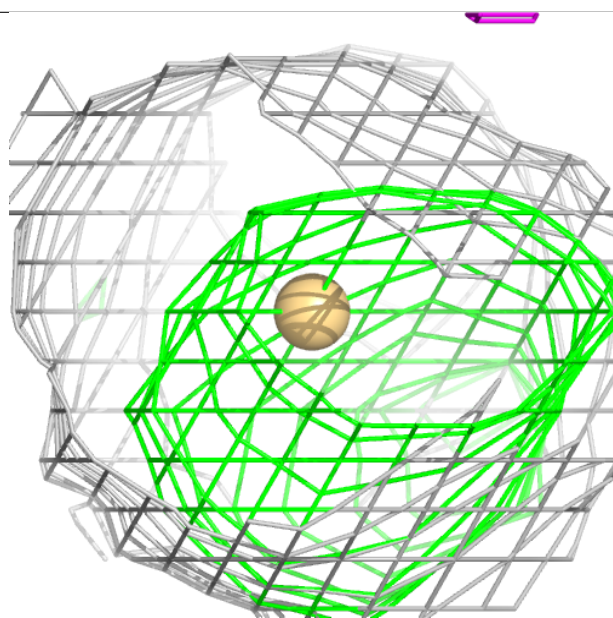
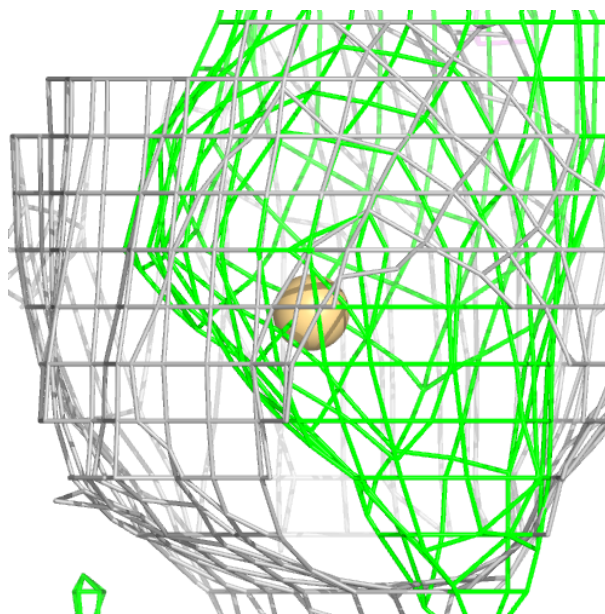
Electron density around CD B 703:

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



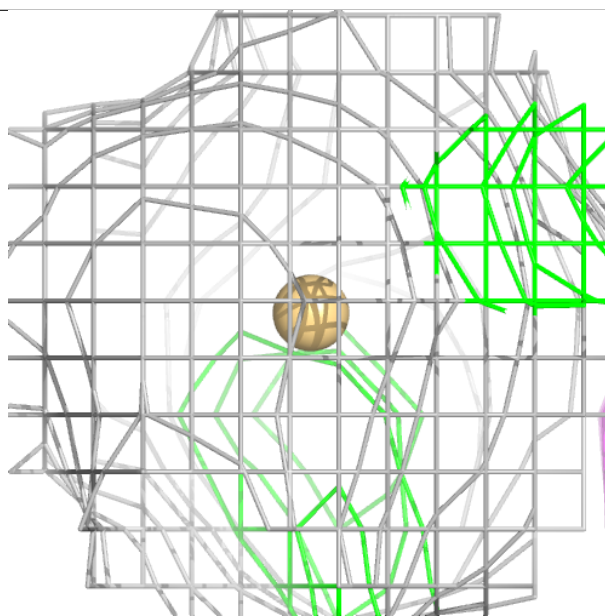
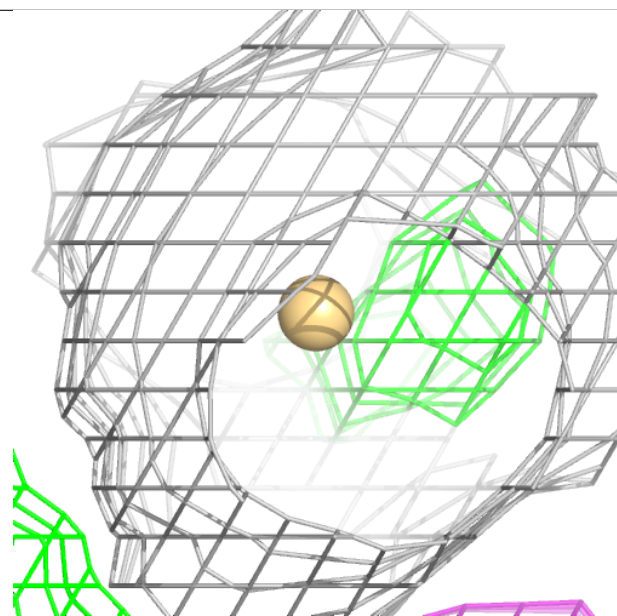
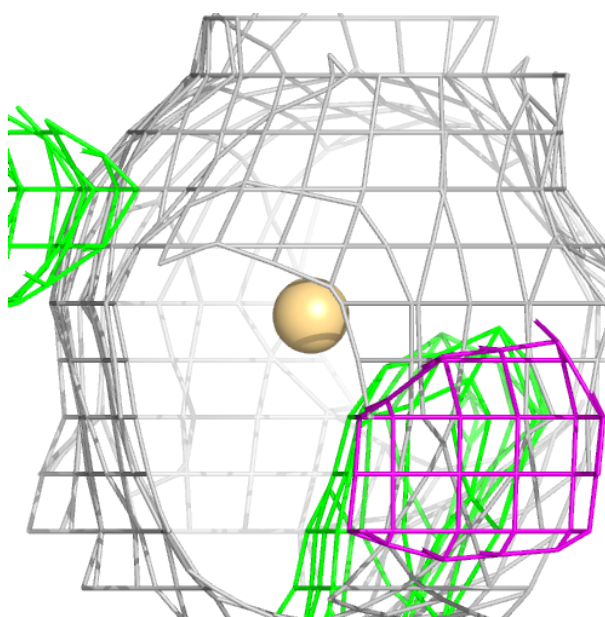
Electron density around CD G 702:

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



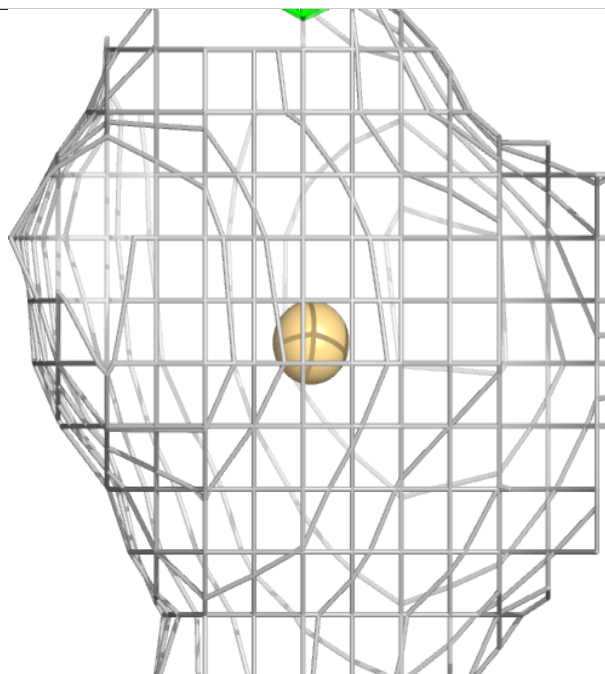
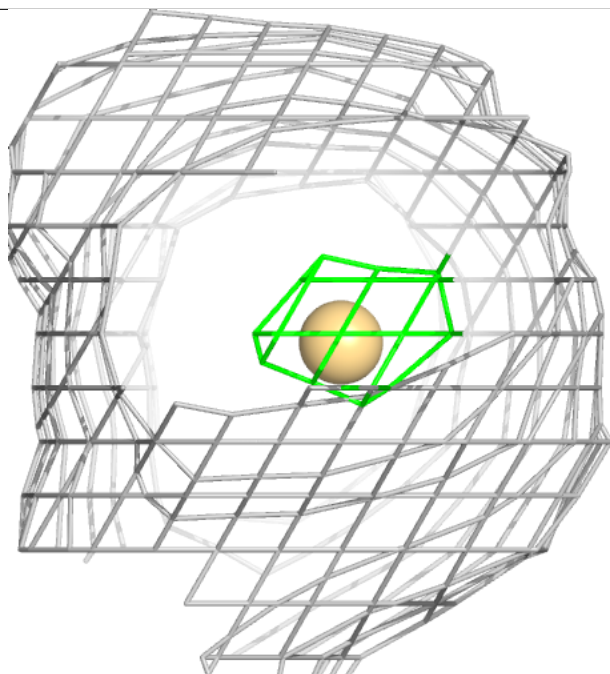
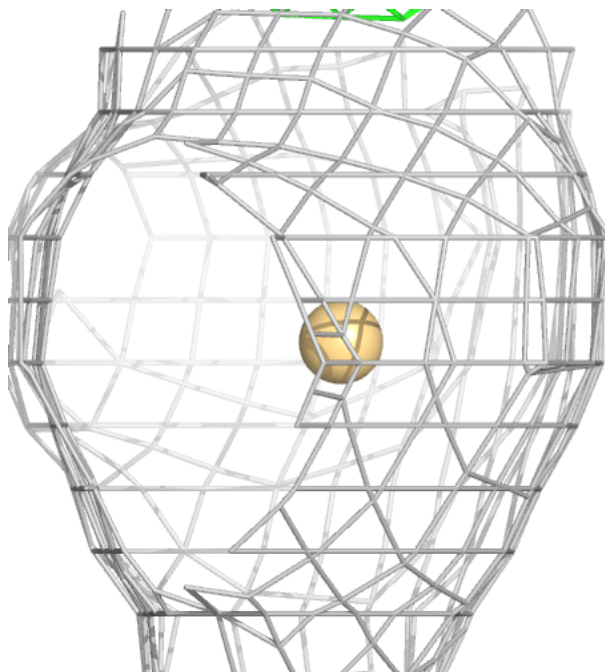
Electron density around CD F 701:

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



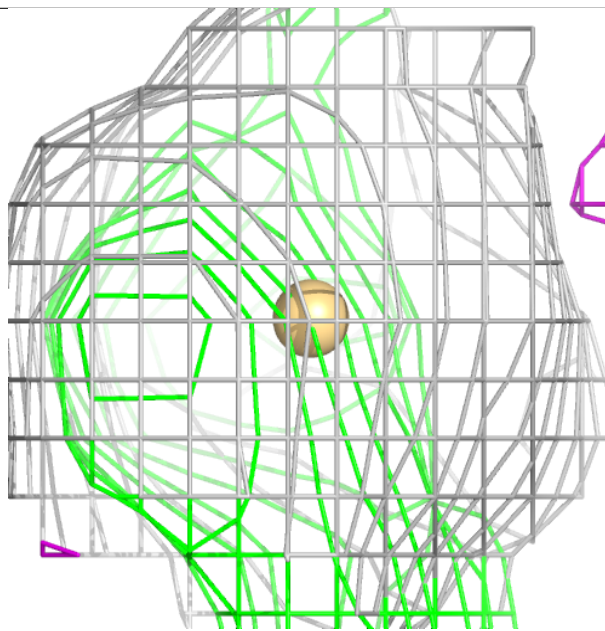
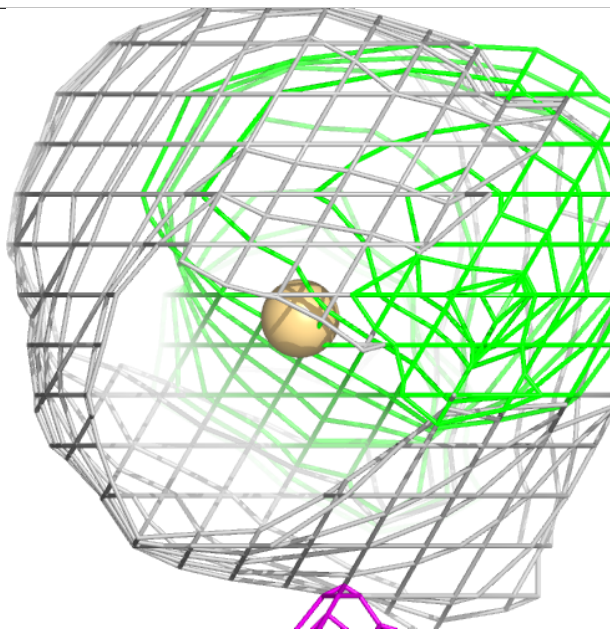
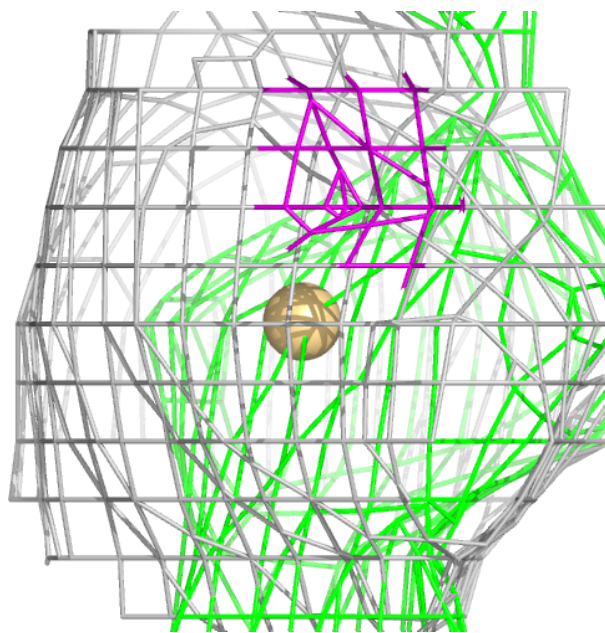
Electron density around CD I 703:

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



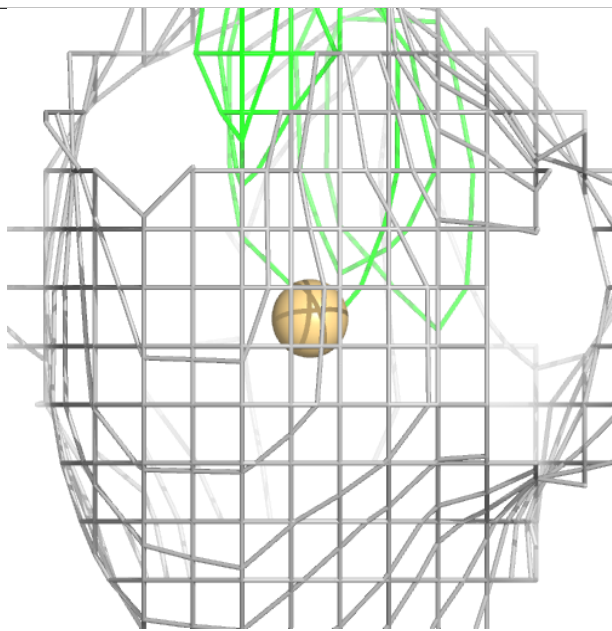
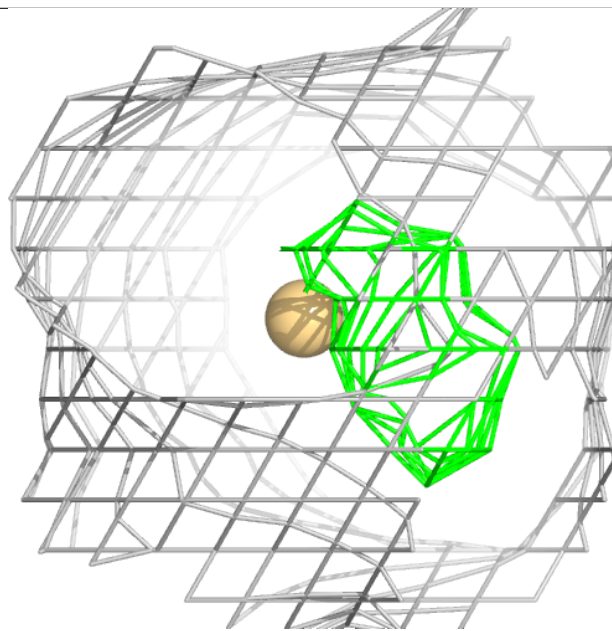
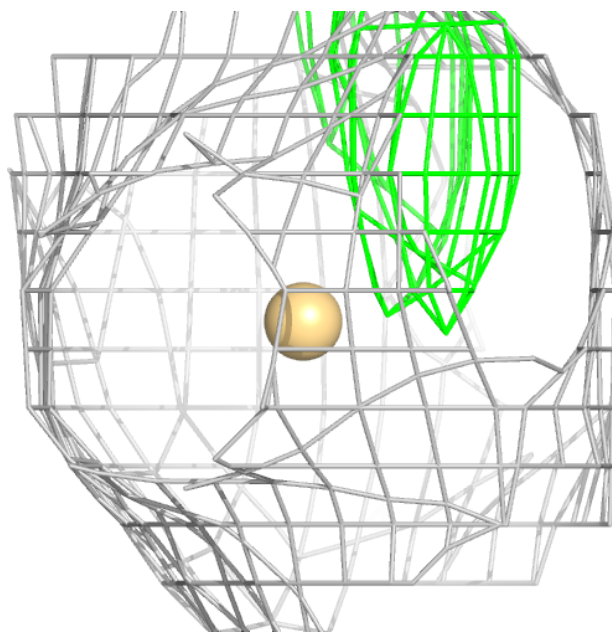
Electron density around CD A 702:

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



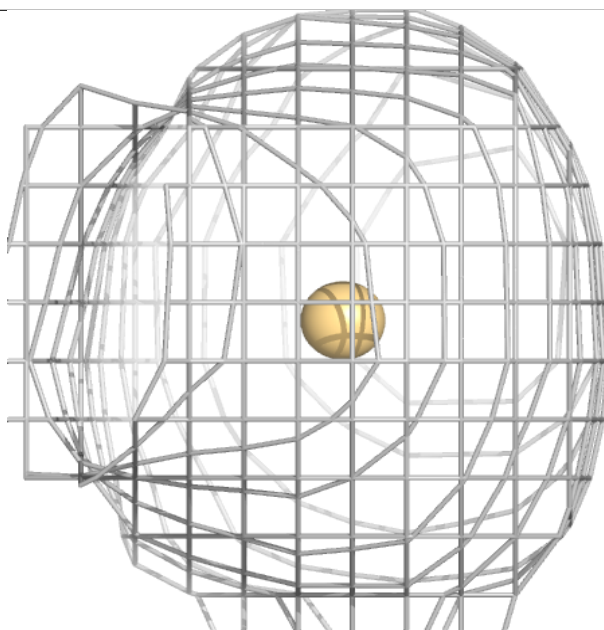
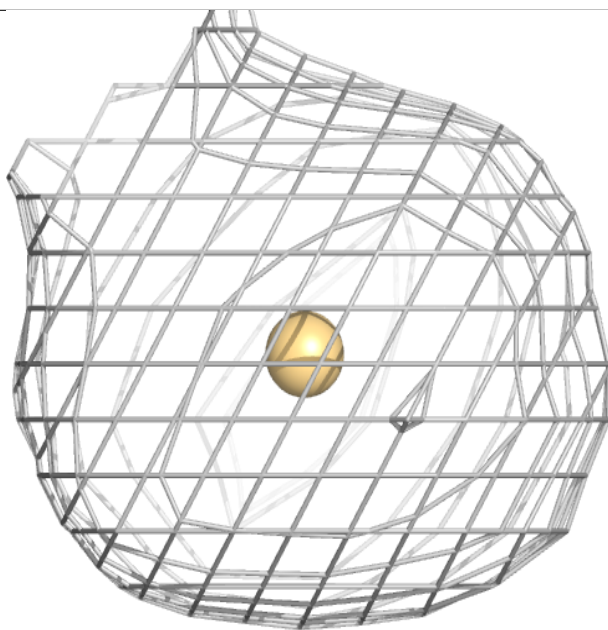
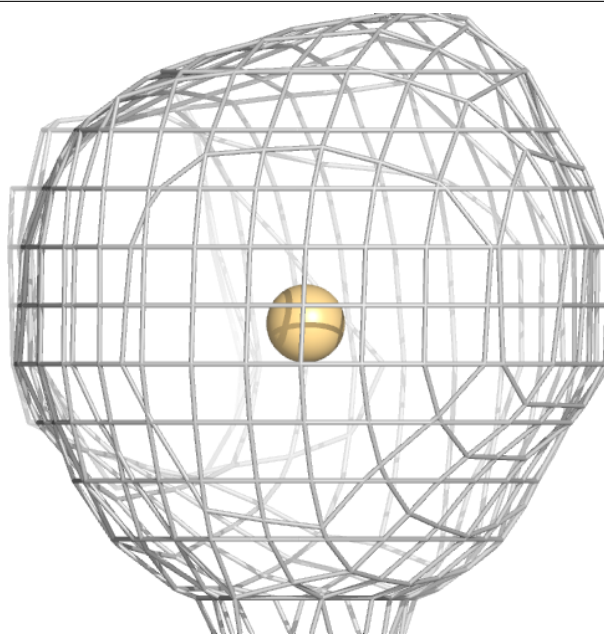
Electron density around CD J 701:

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



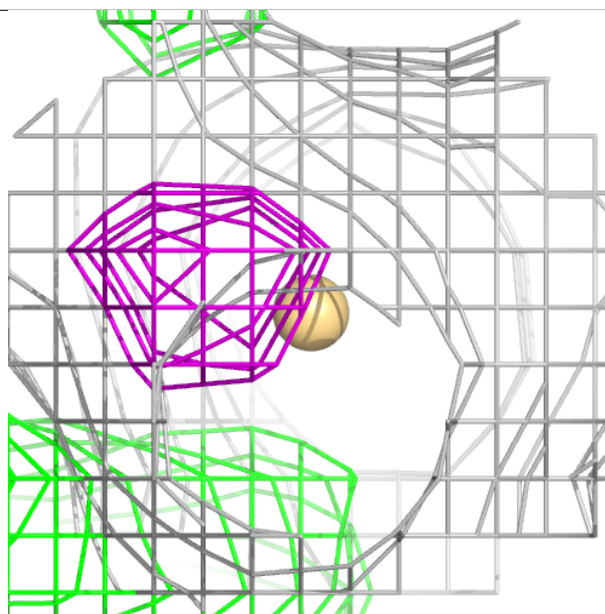
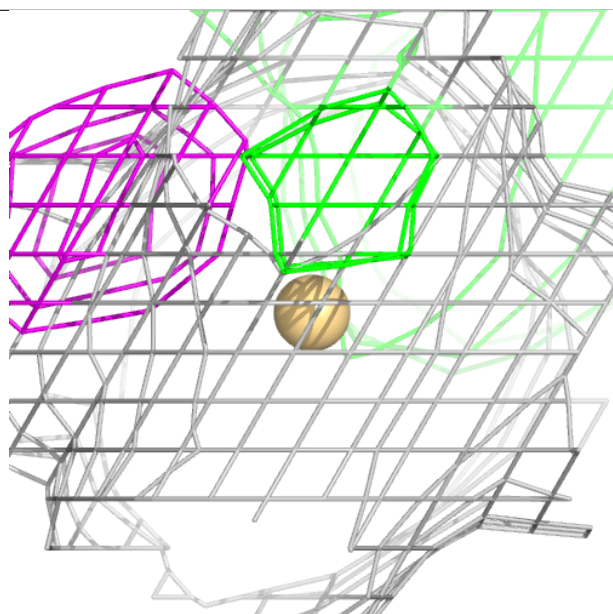
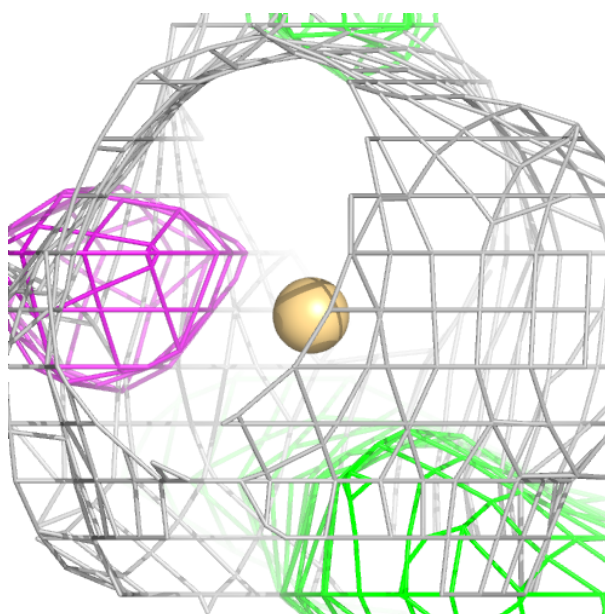
Electron density around CD E 704:

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



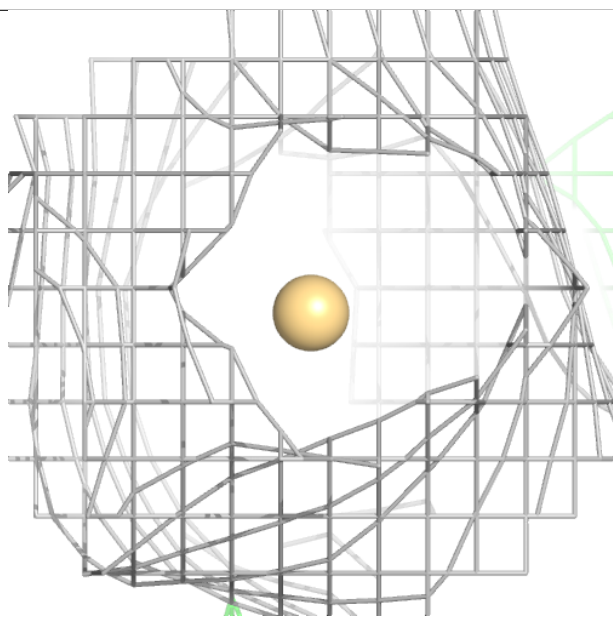
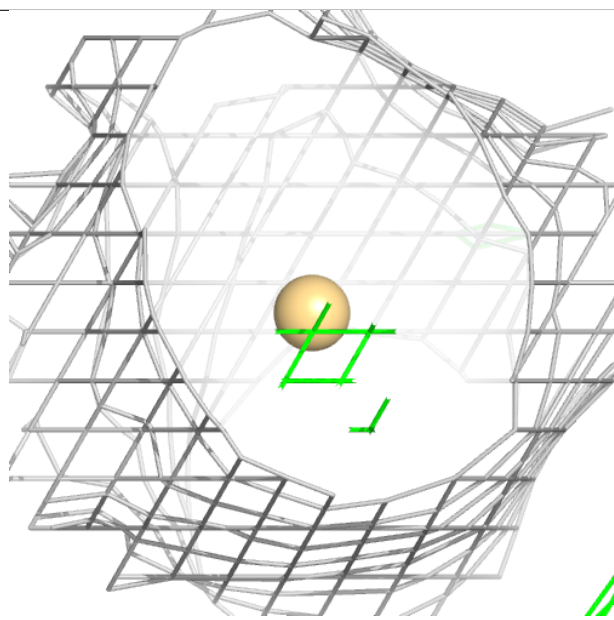
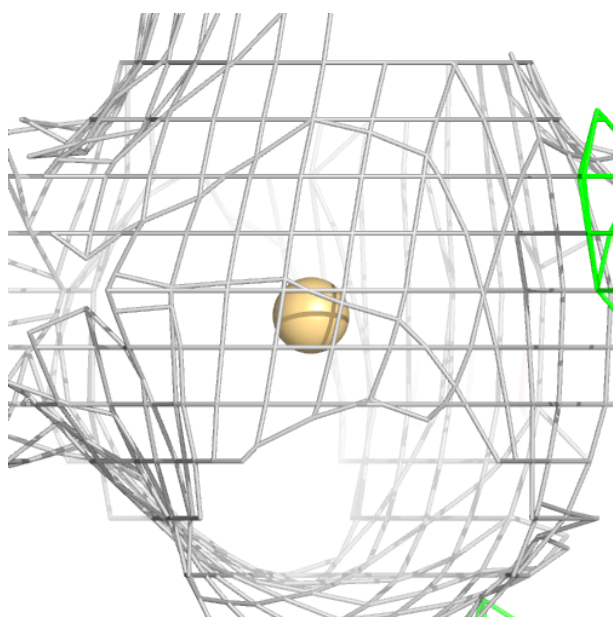
Electron density around CD H 701:

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



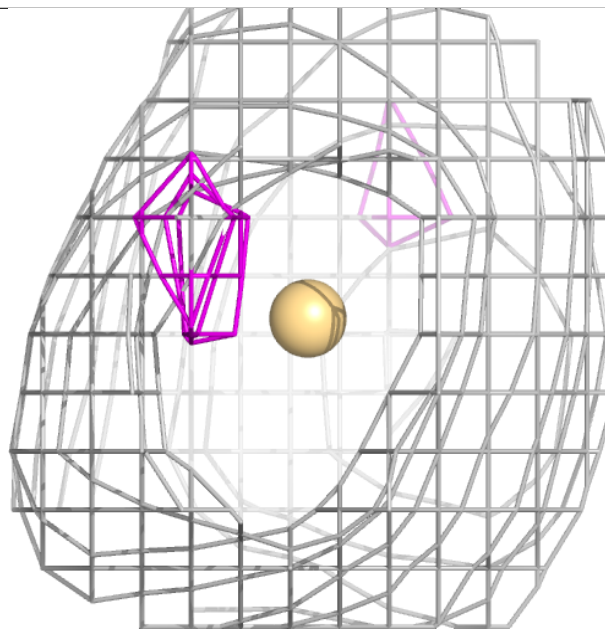
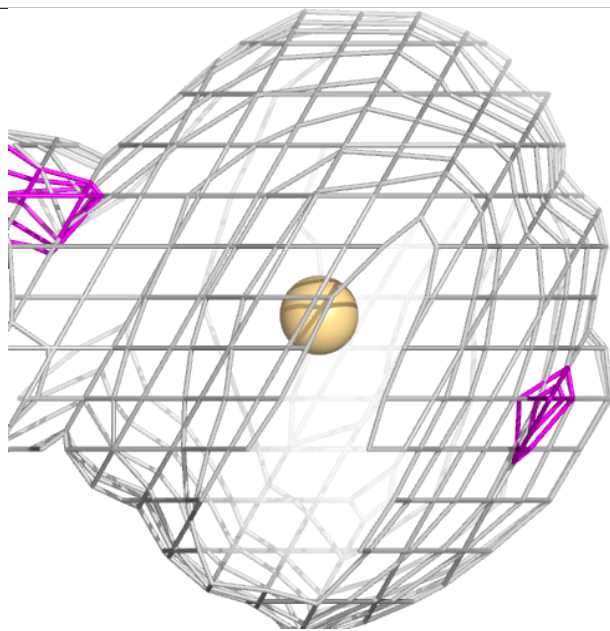
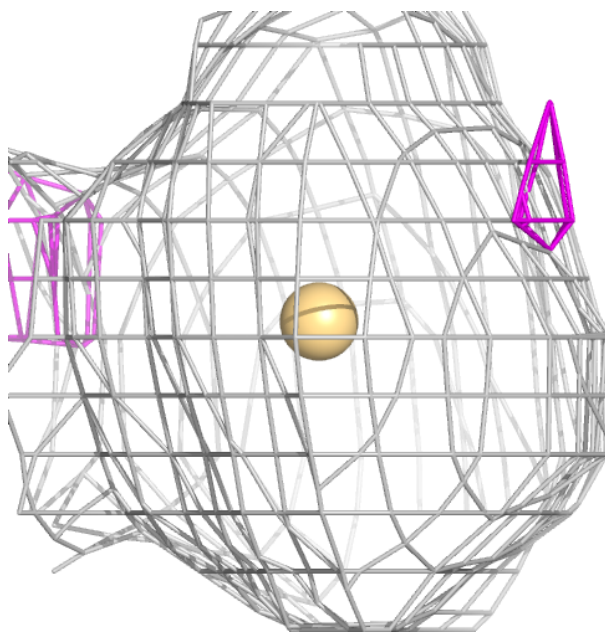
Electron density around CD B 701:

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



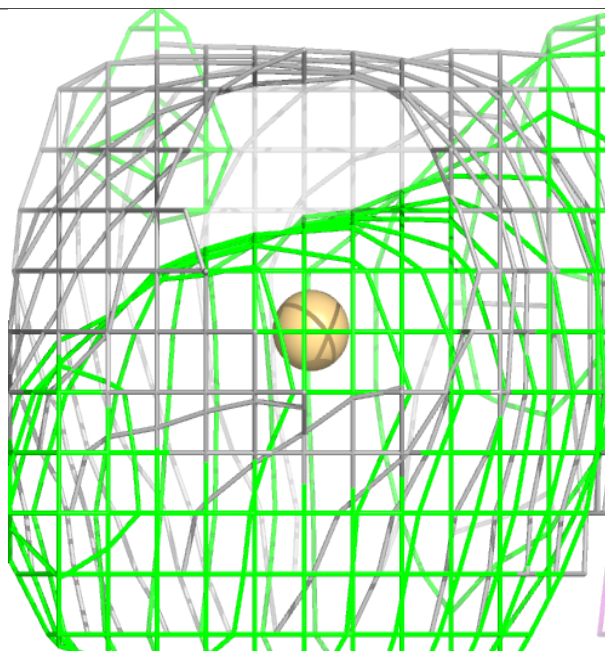
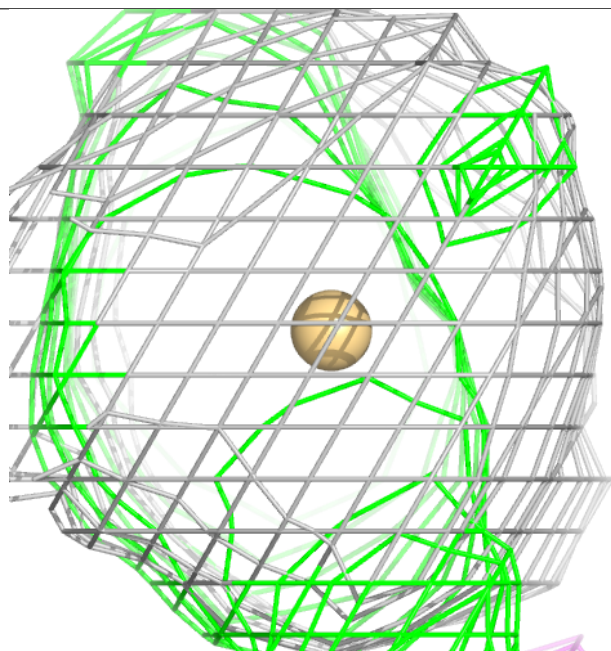
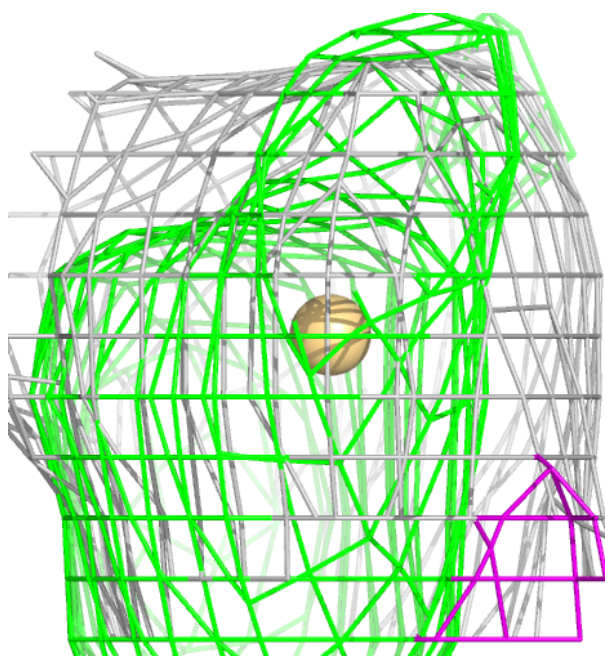
Electron density around CD D 704:

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



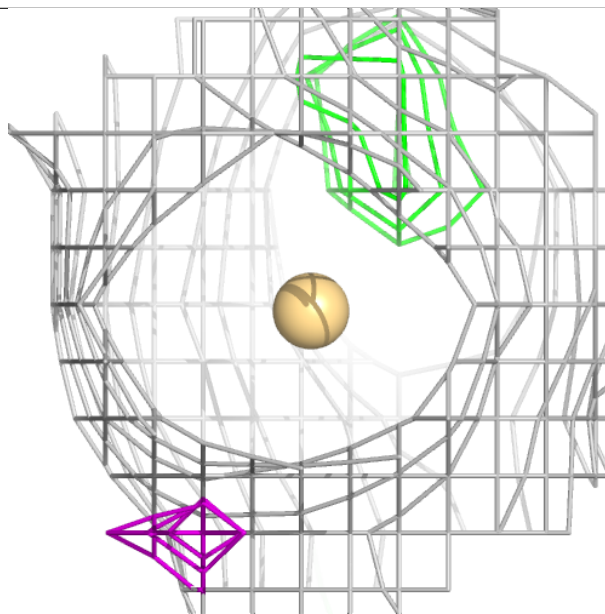
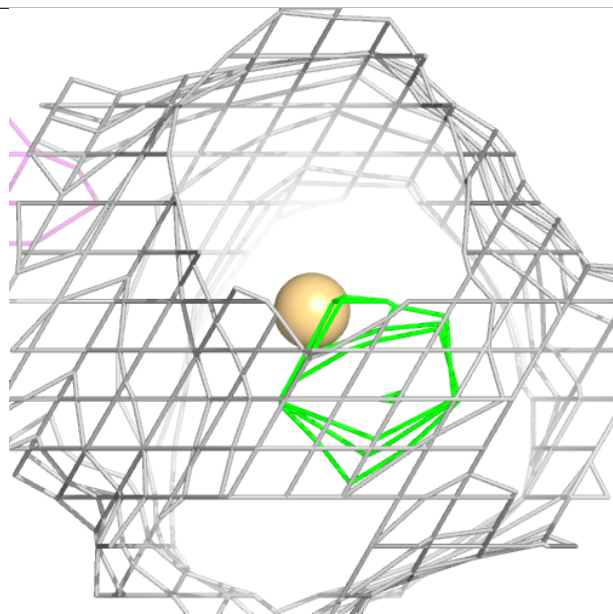
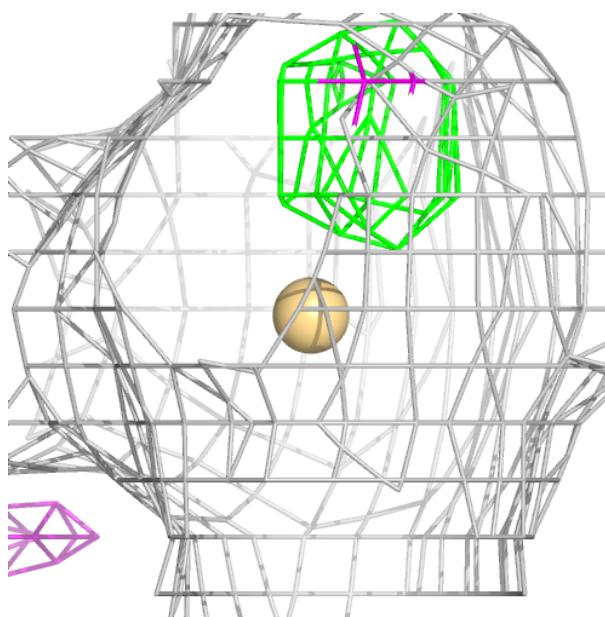
Electron density around CD K 702:

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



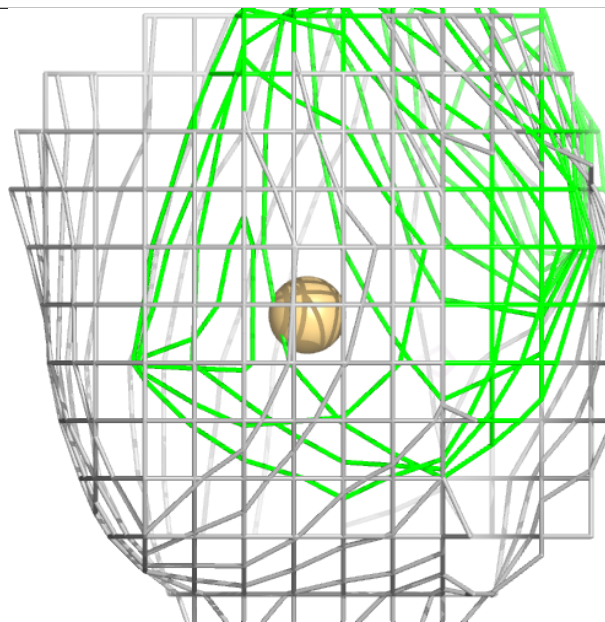
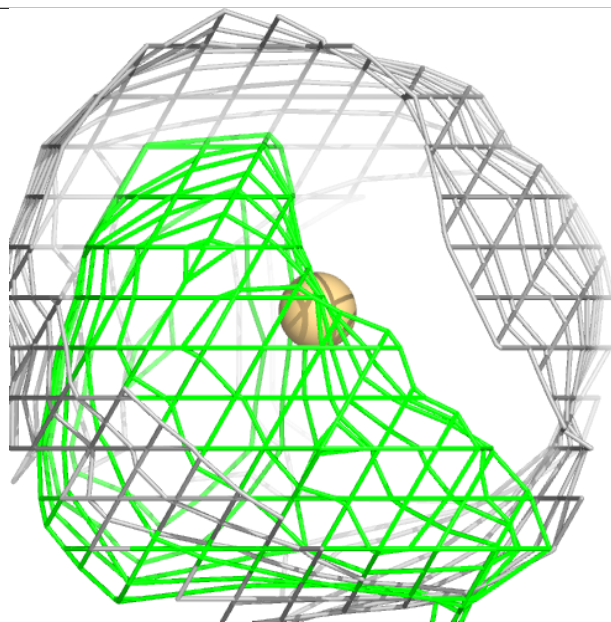
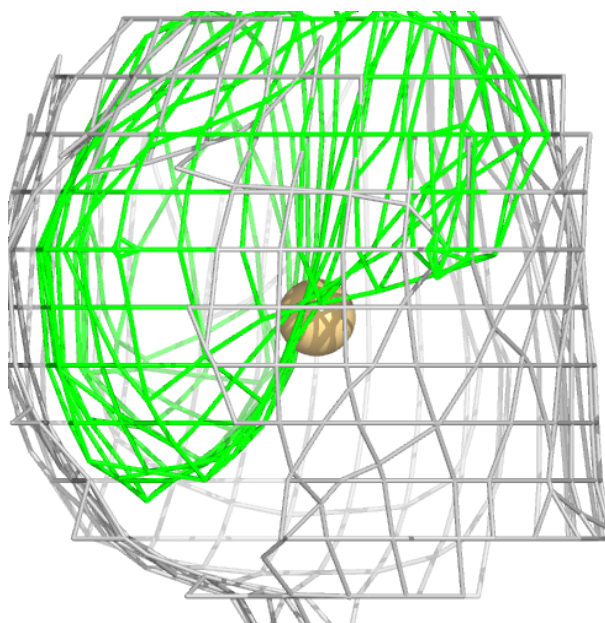
Electron density around CD G 701:

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



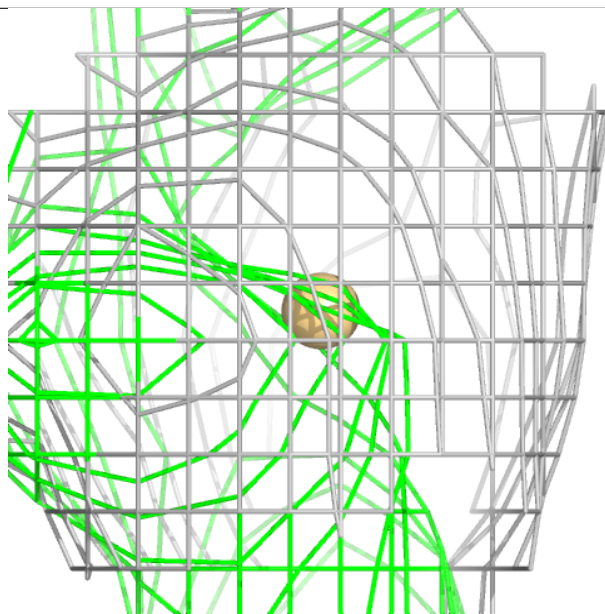
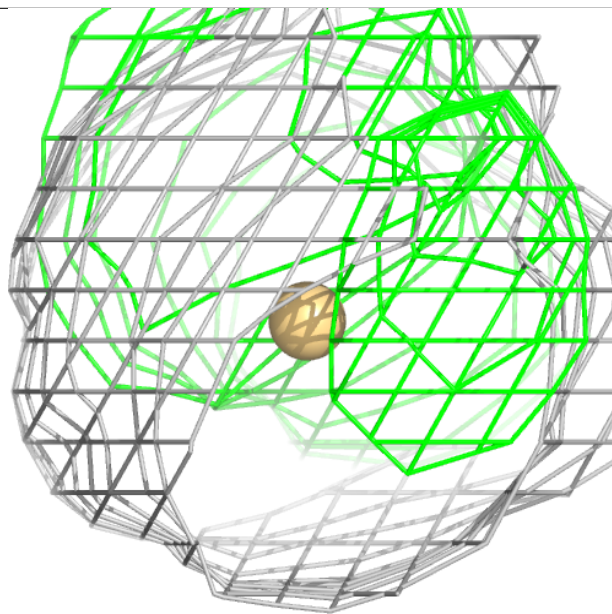
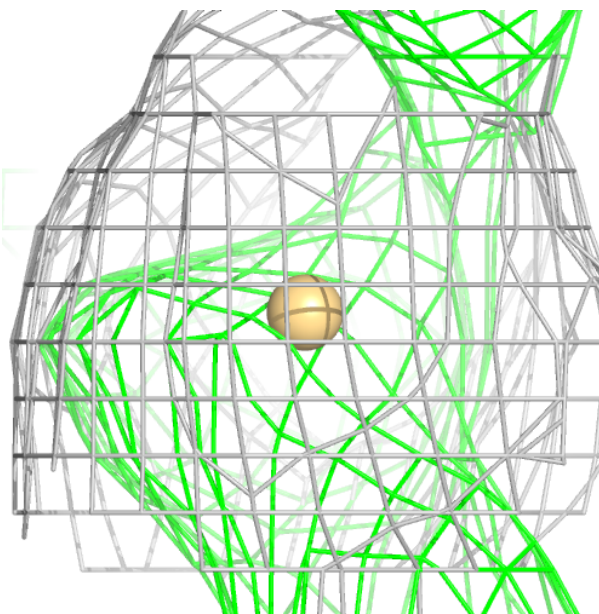
Electron density around CD I 702:

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



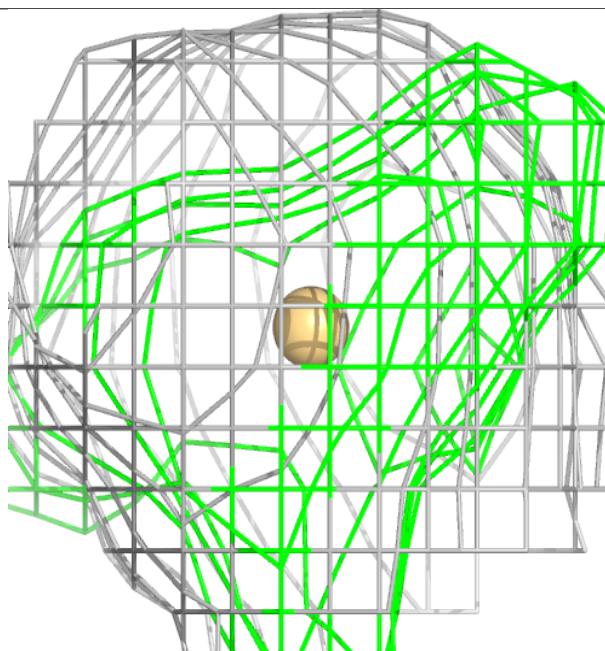
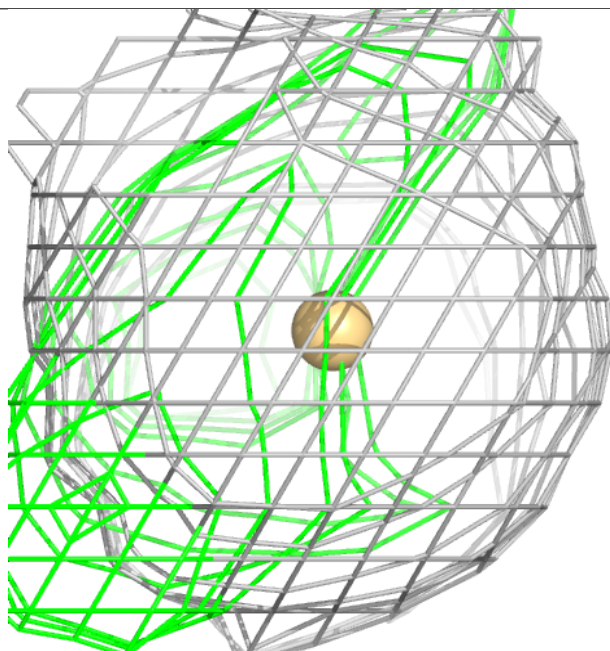
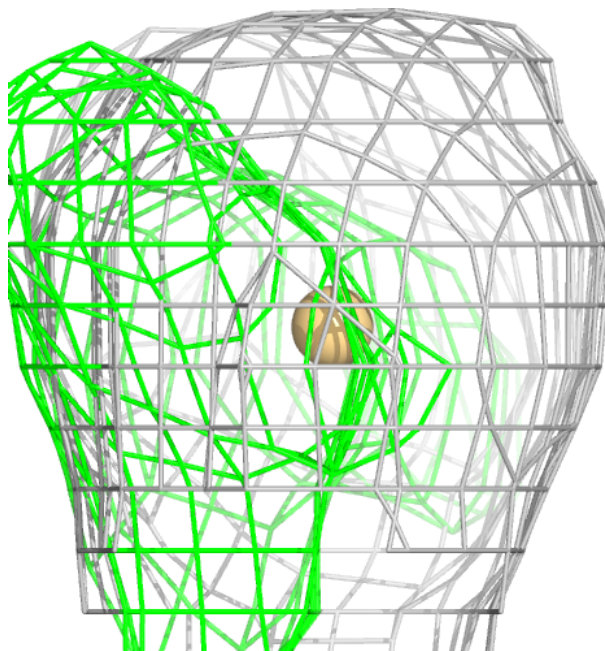
Electron density around CD B 702:

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



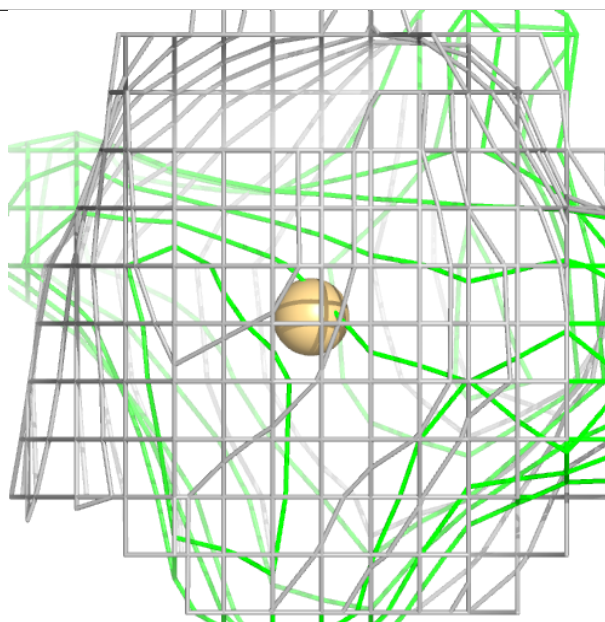
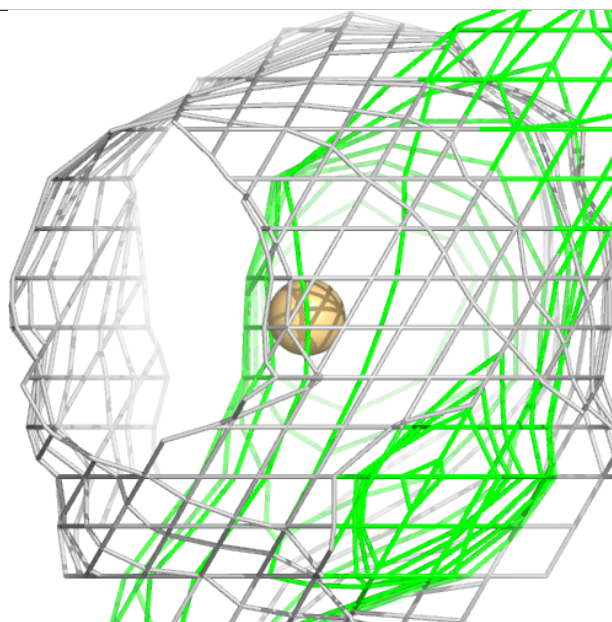
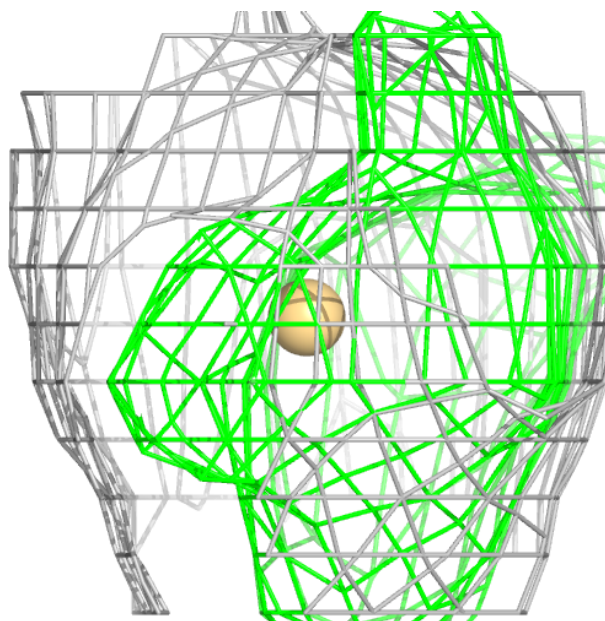
Electron density around CD C 702:

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



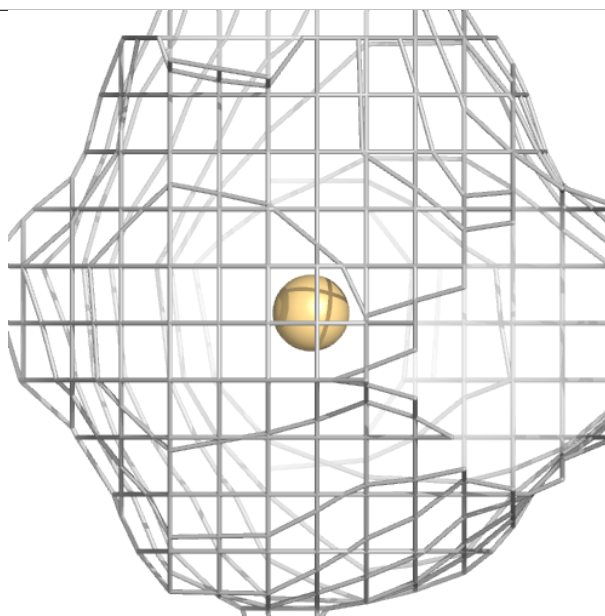
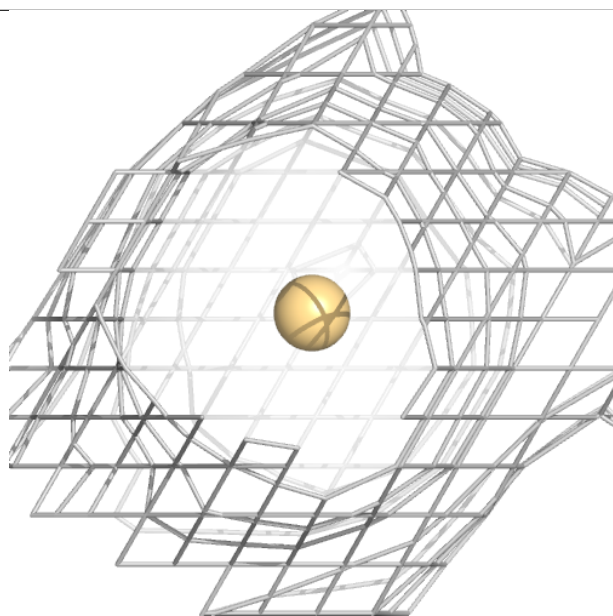
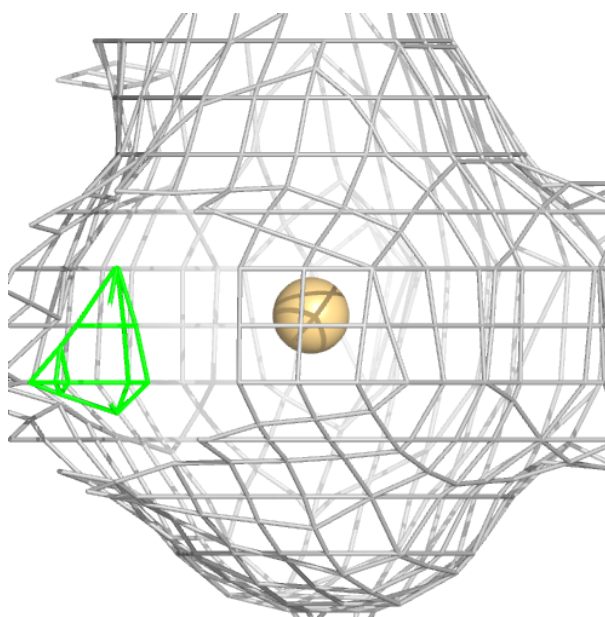
Electron density around CD F 702:

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



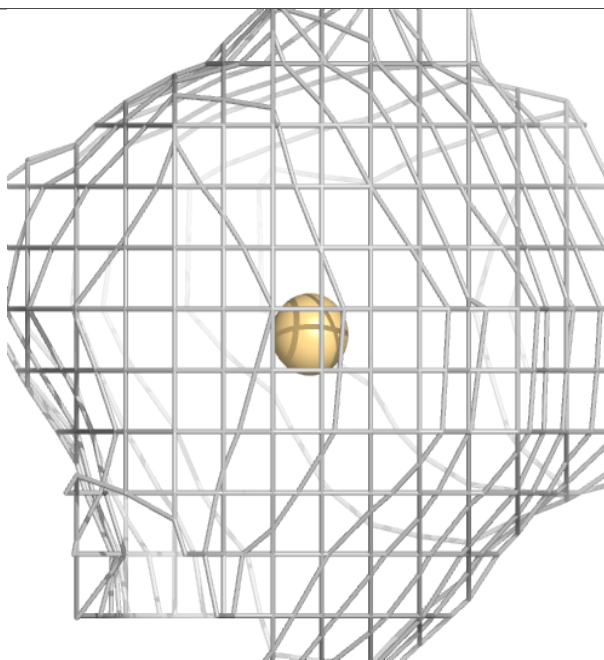
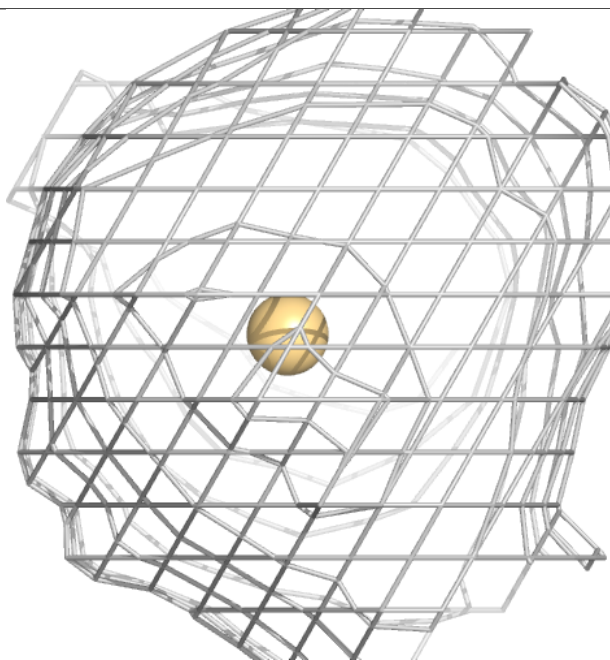
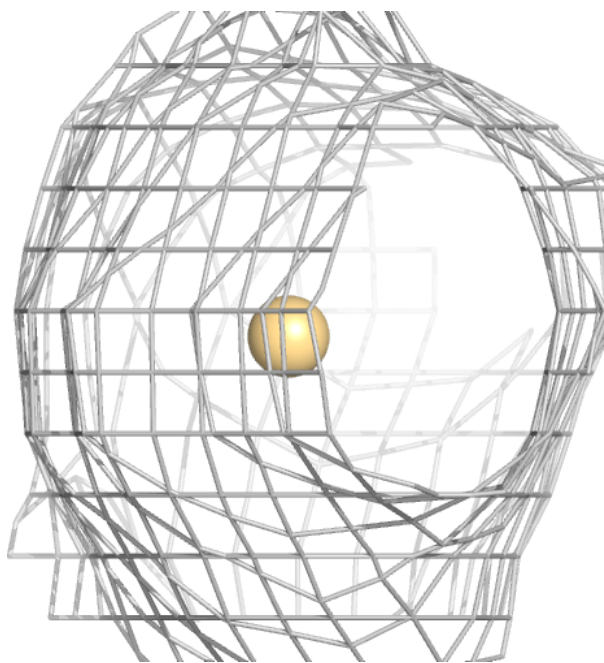
Electron density around CD J 703:

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



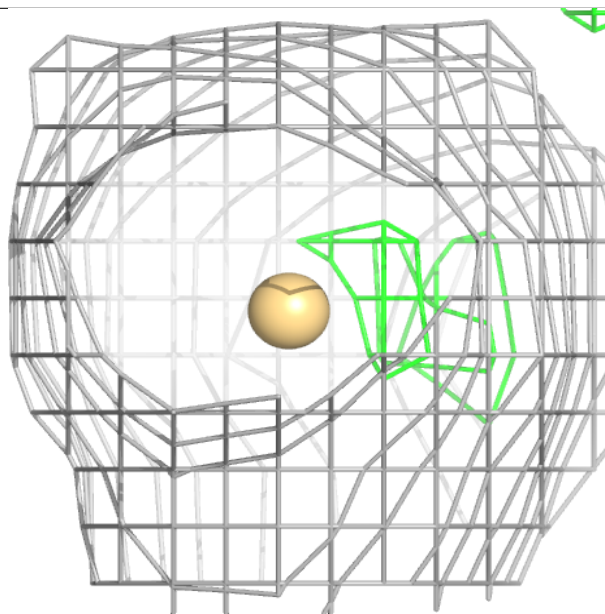
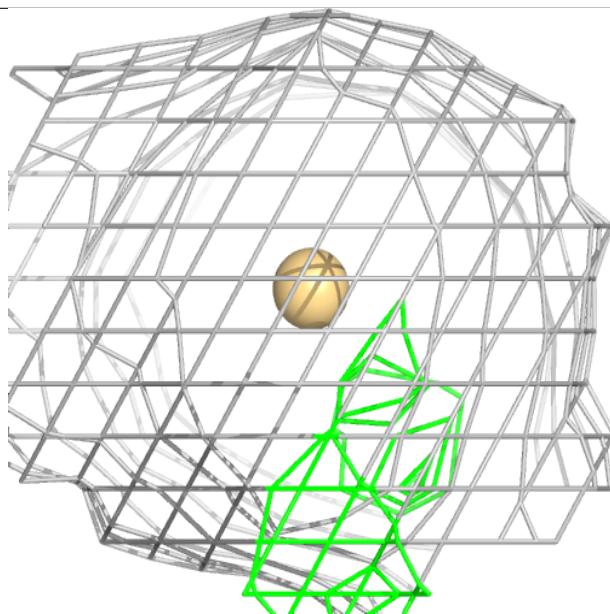
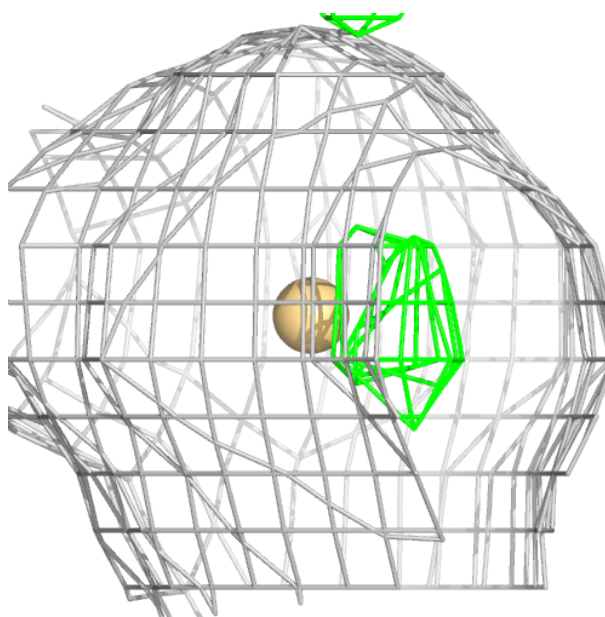
Electron density around CD F 703:

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



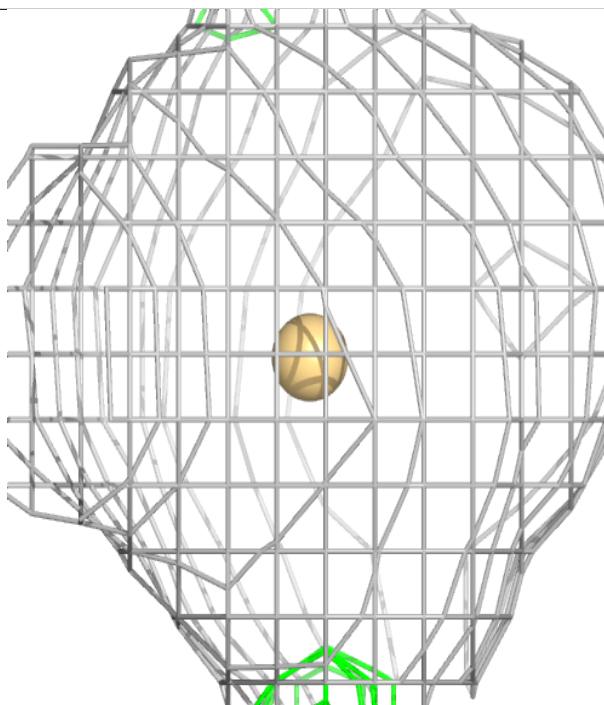
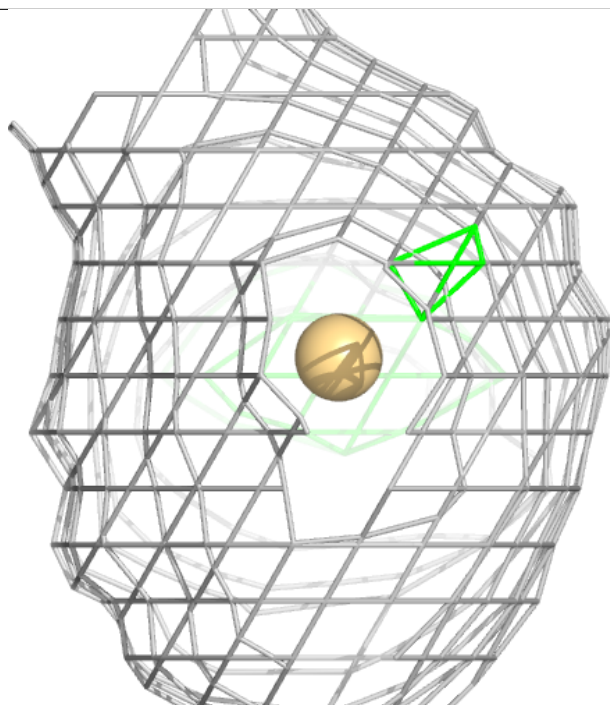
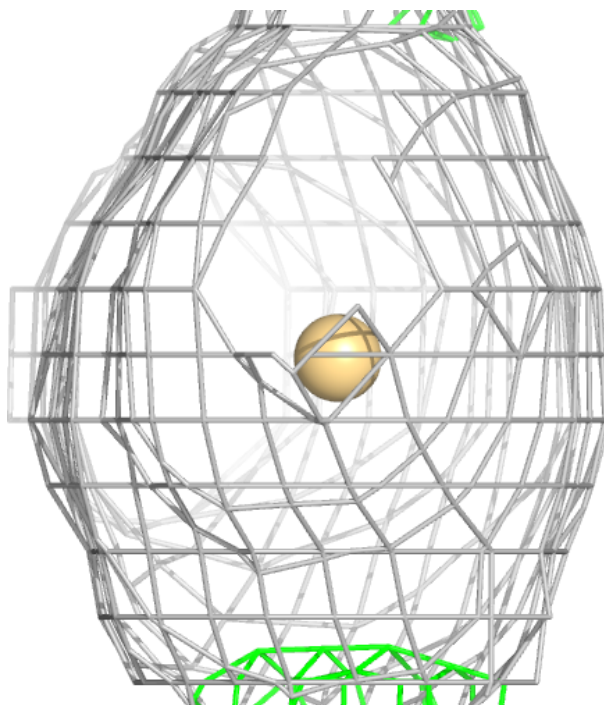
Electron density around CD H 703:

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



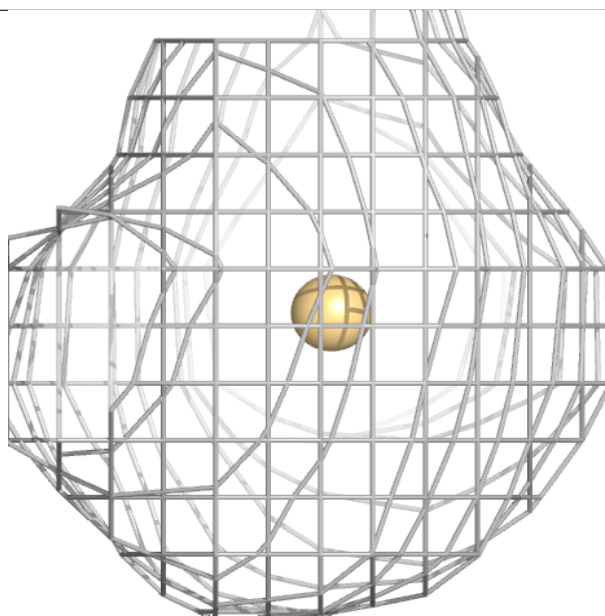
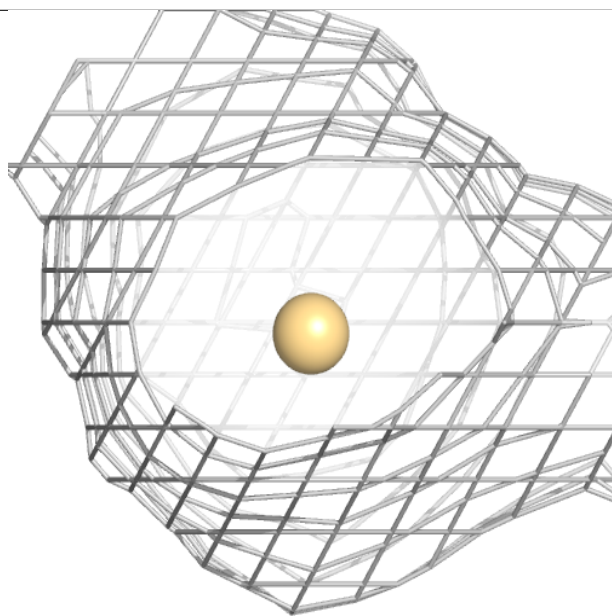
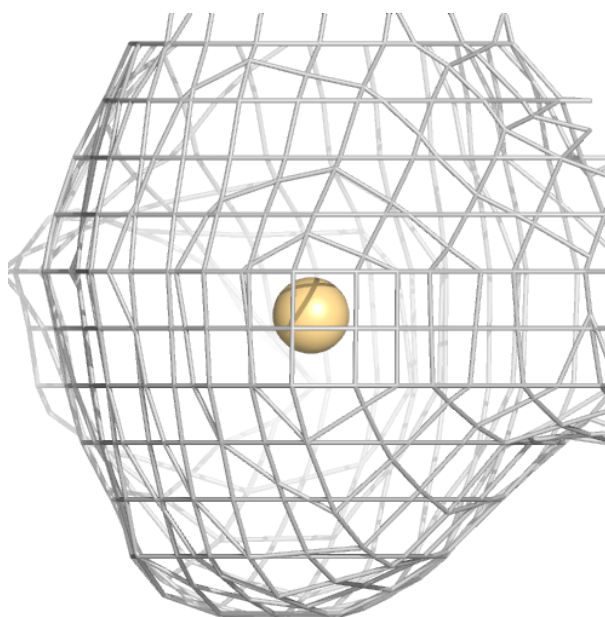
Electron density around CD C 703:

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



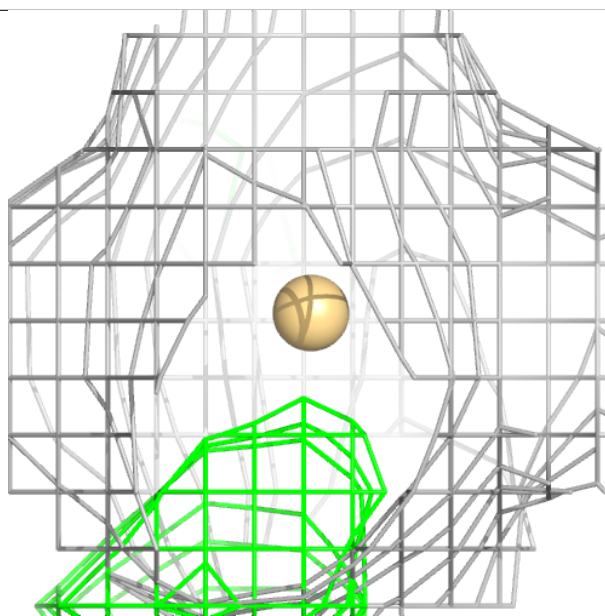
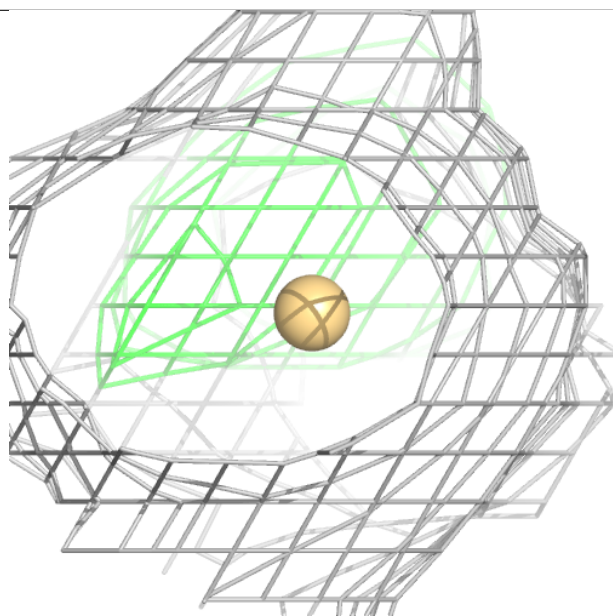
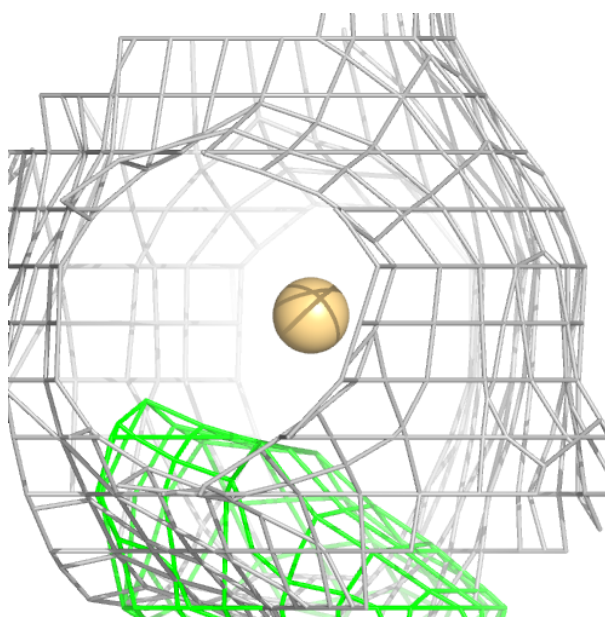
Electron density around CD A 703:

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



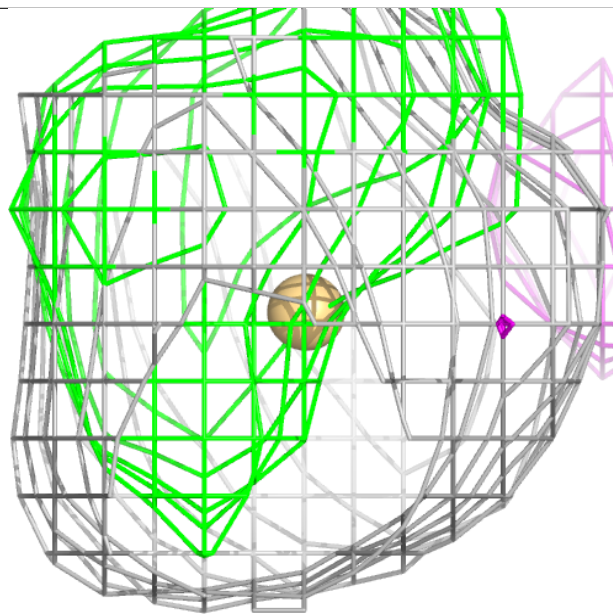
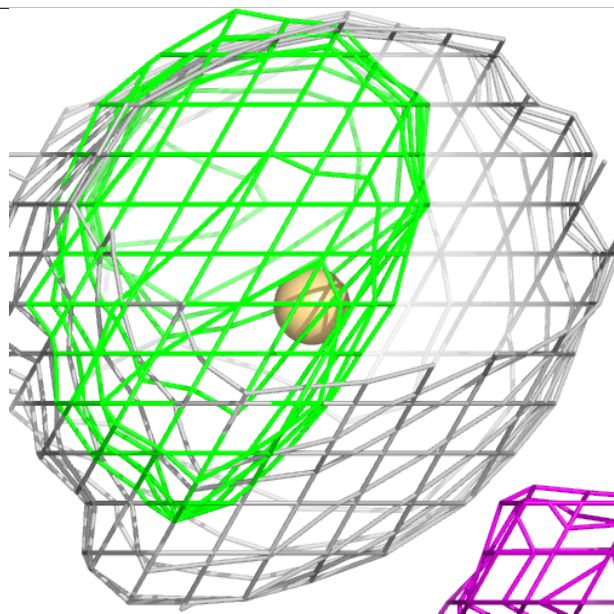
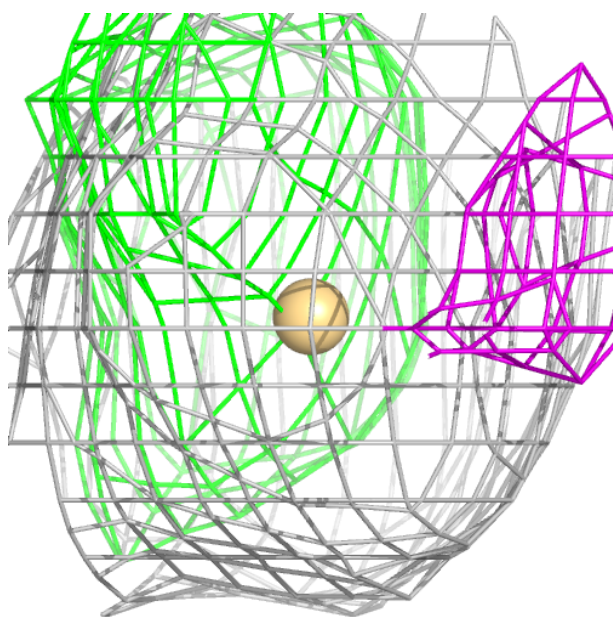
Electron density around CD C 701:

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



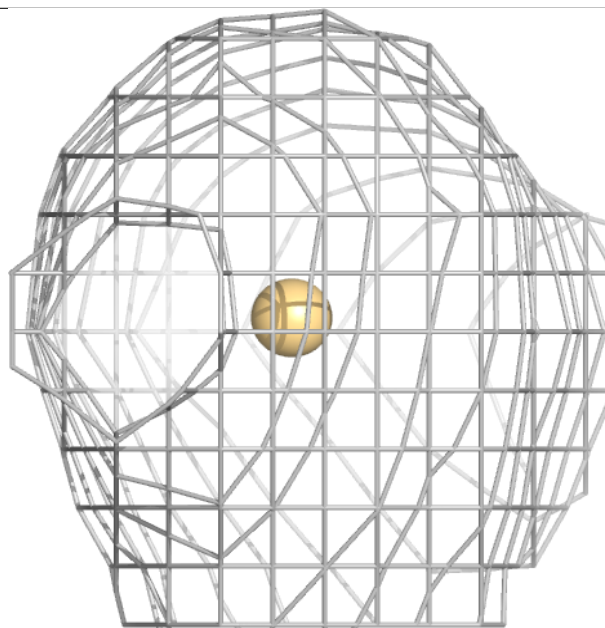
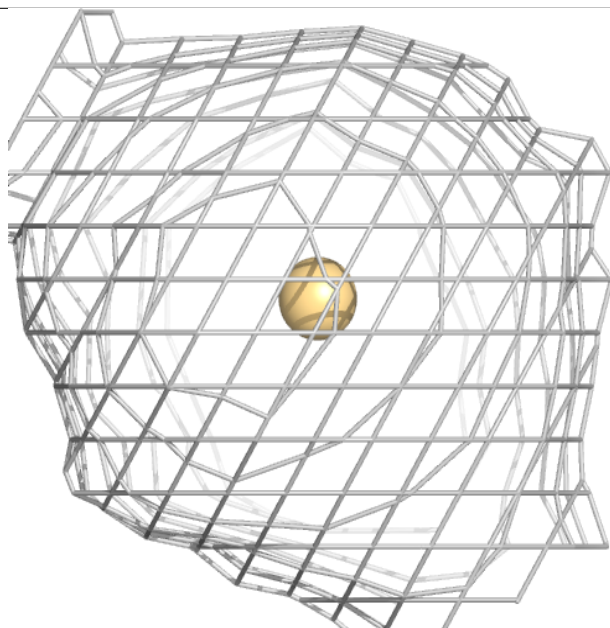
Electron density around CD L 702:

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



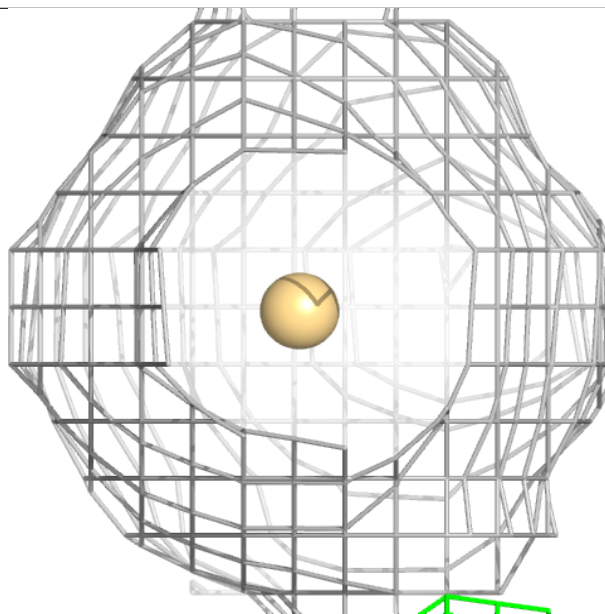
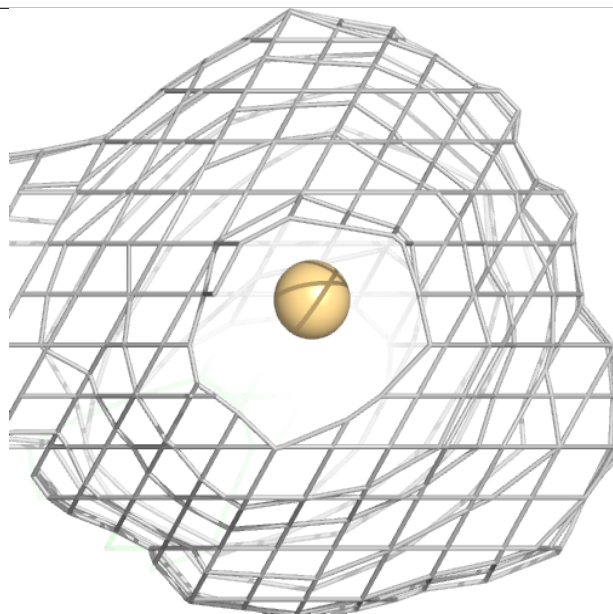
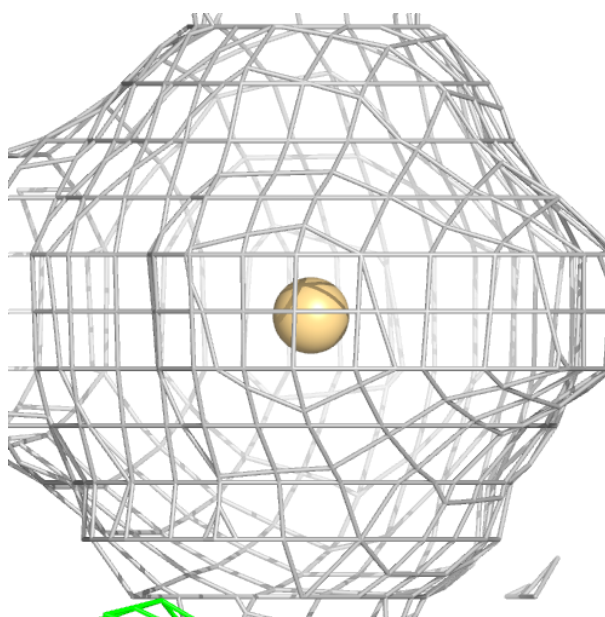
Electron density around CD G 703:

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



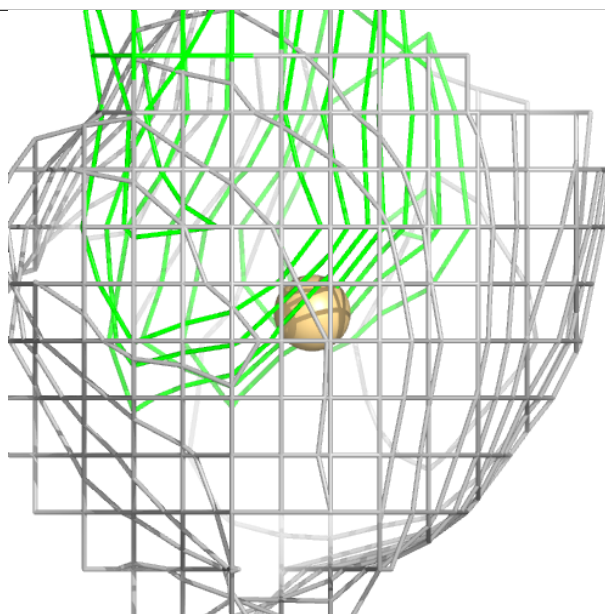
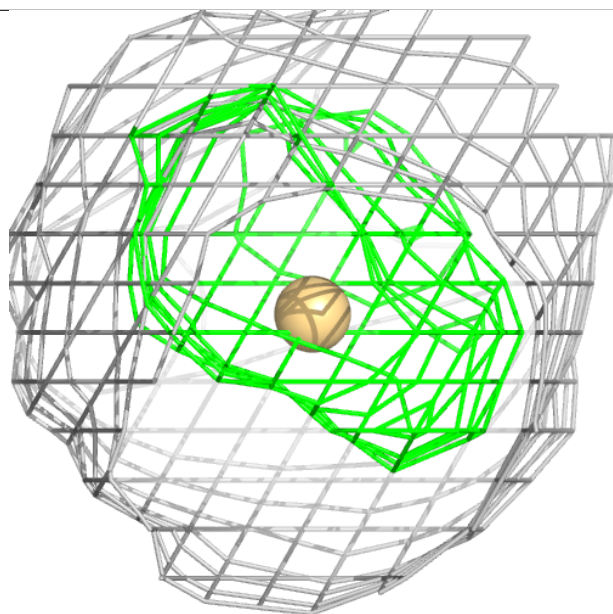
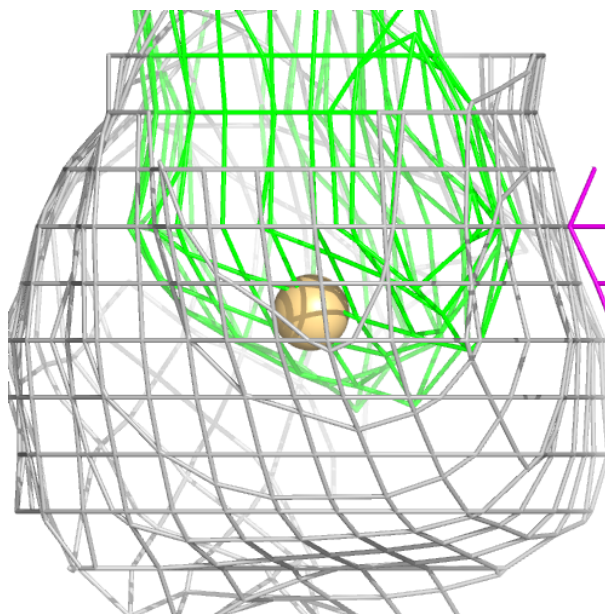
Electron density around CD K 703:

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



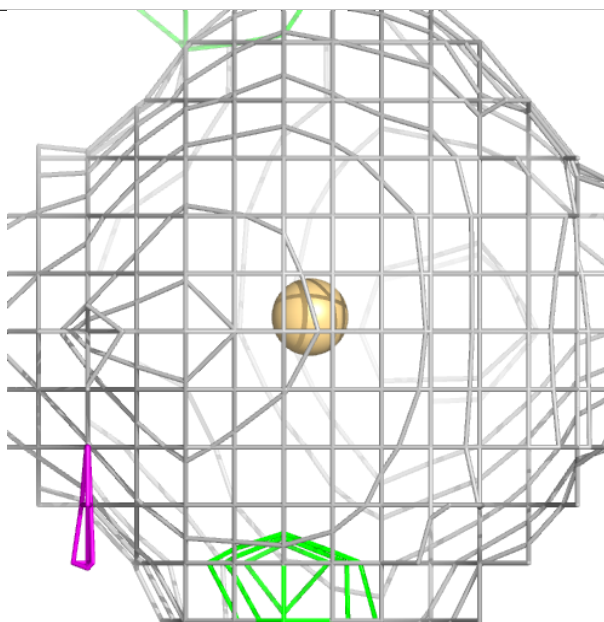
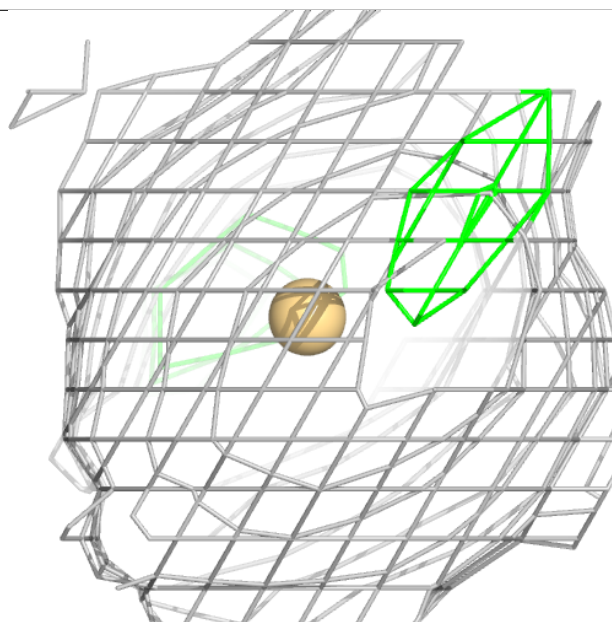
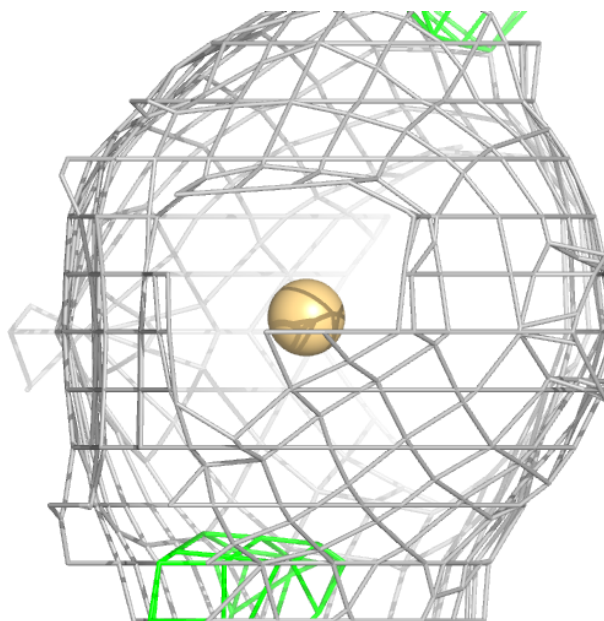
Electron density around CD E 702:

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



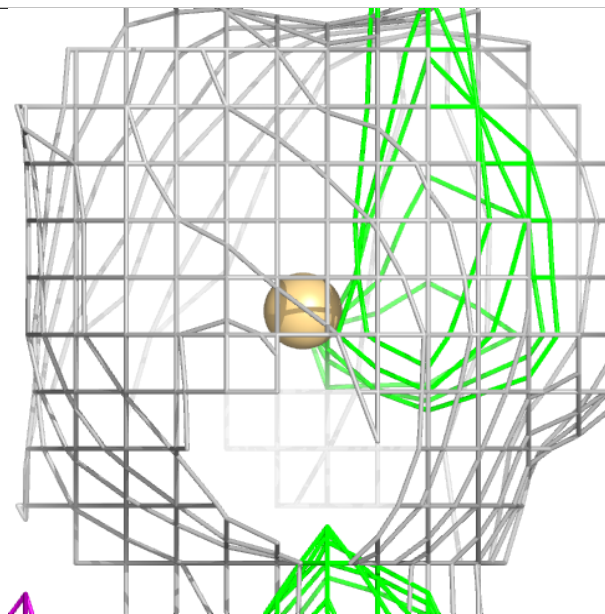
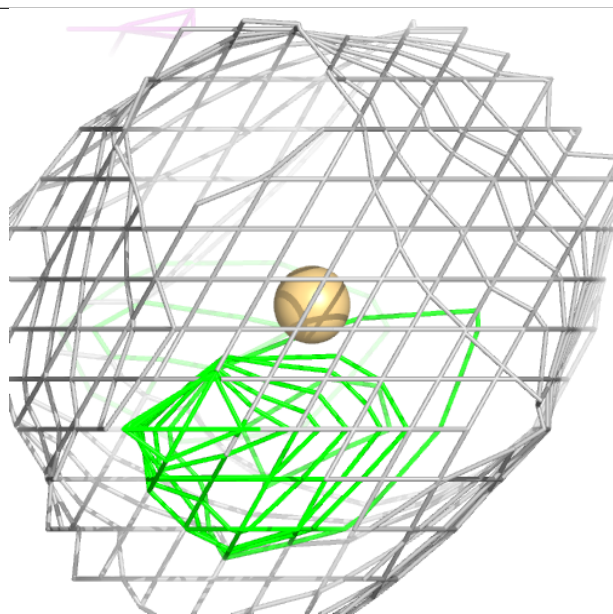
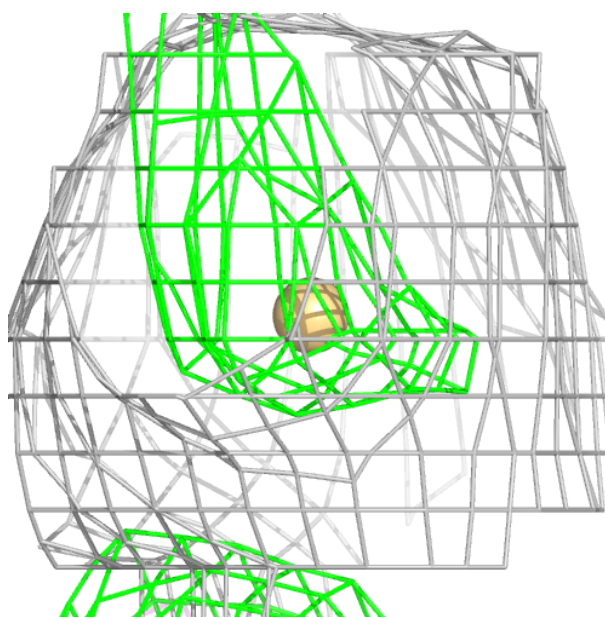
Electron density around CD E 703:

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



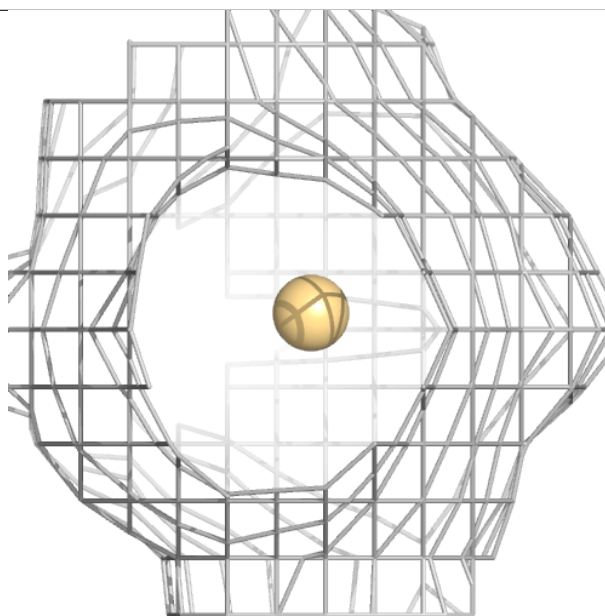
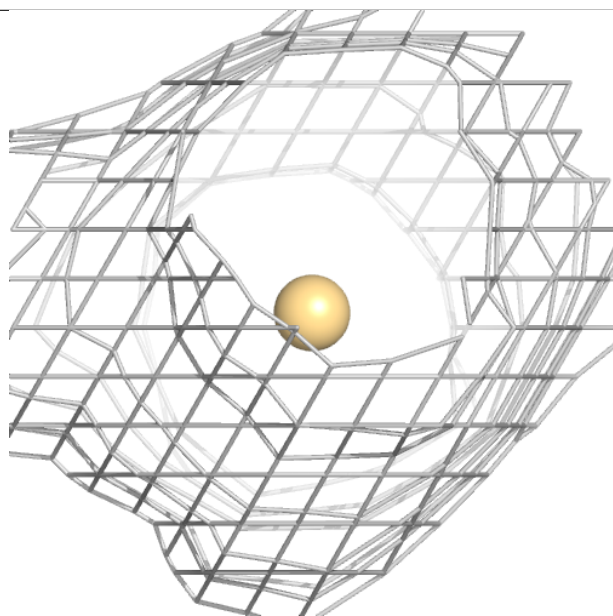
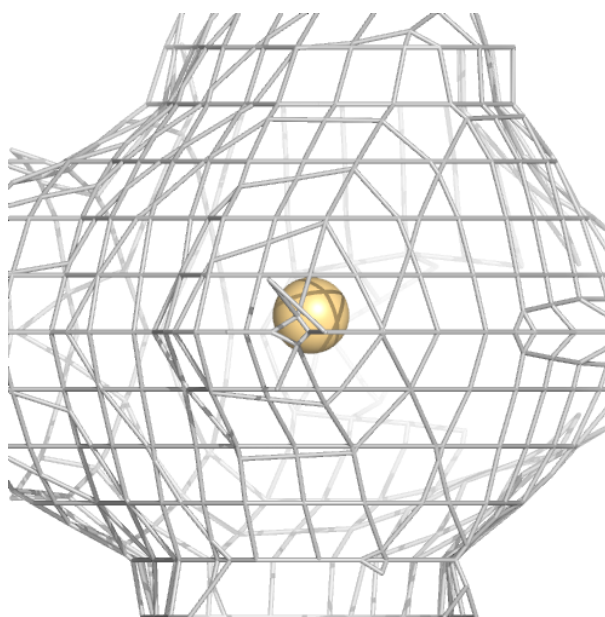
Electron density around CD D 702:

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



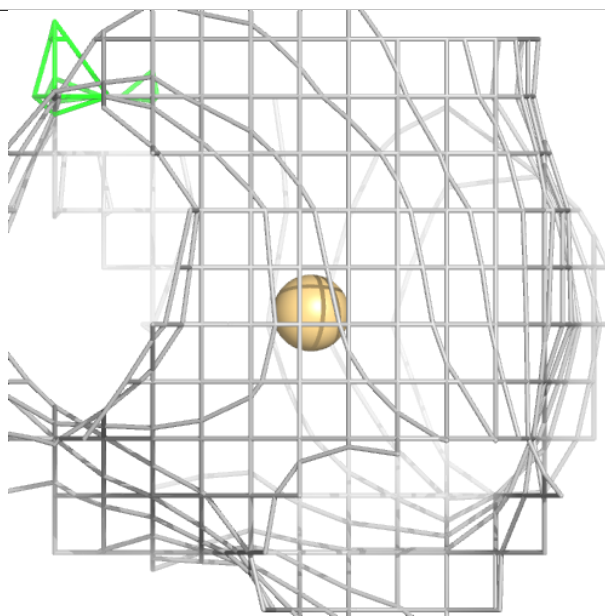
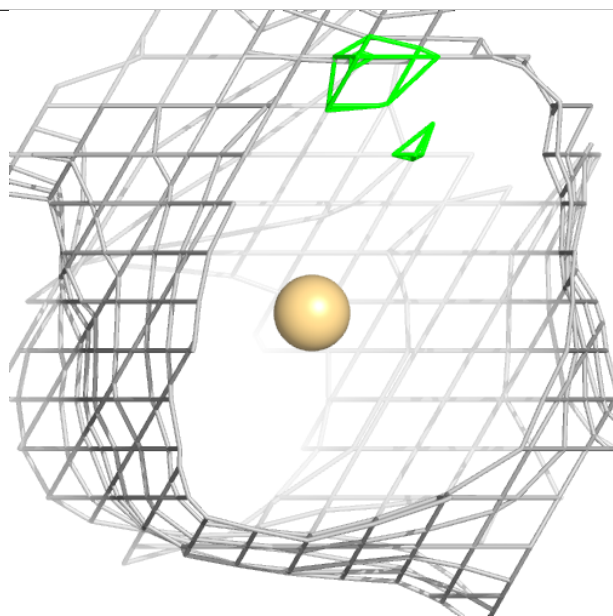
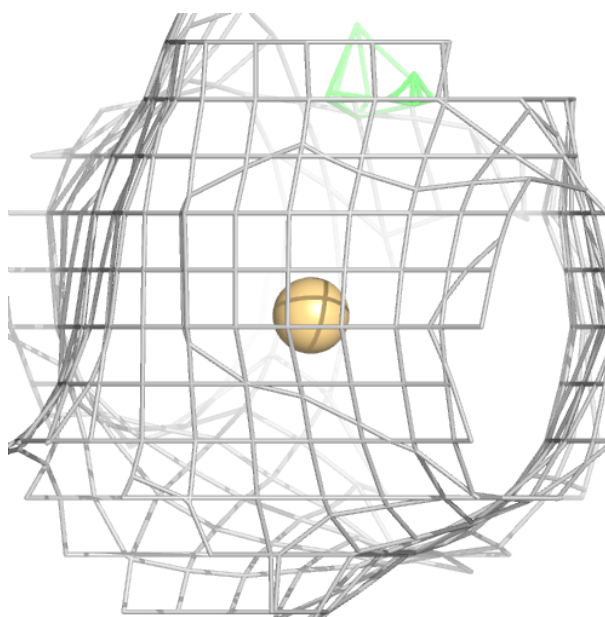
Electron density around CD L 703:

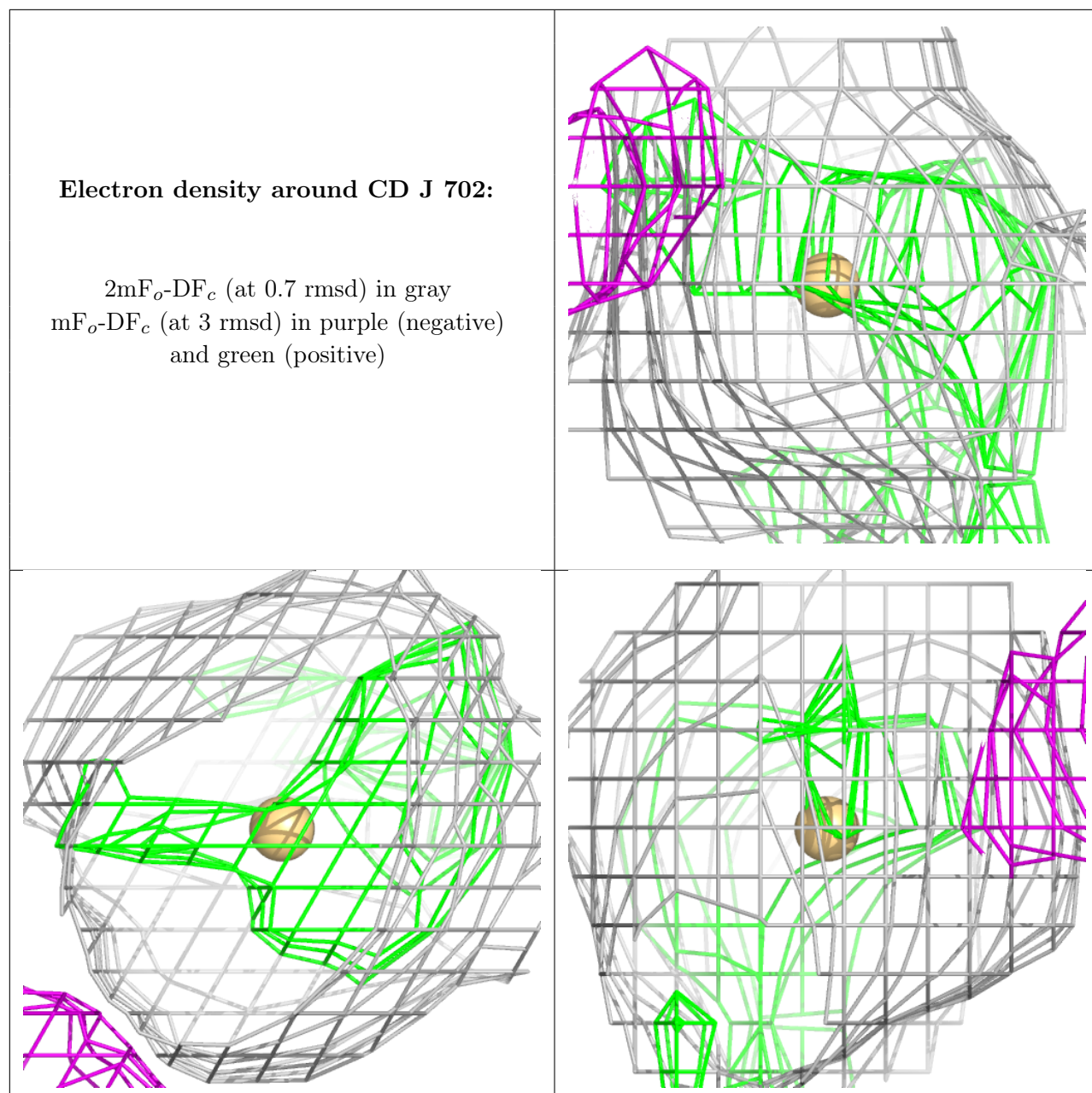
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CD 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.