



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 10:48 AM UTC

PDB ID : 8X8F / pdb_00008x8f
Title : Crystal structure of lipoyxygenase 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 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

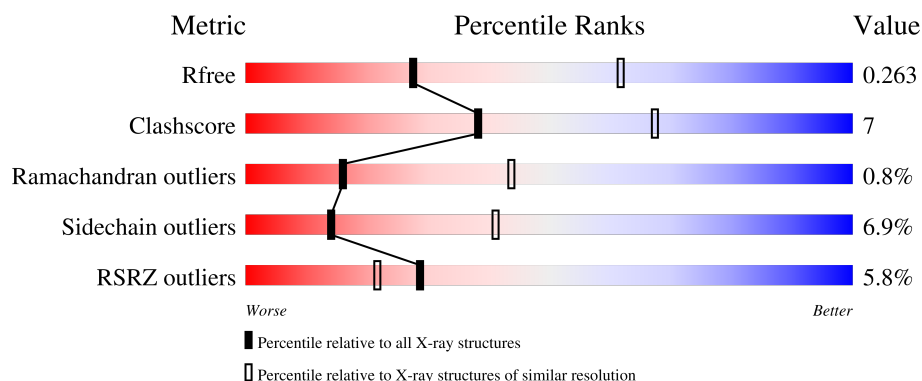
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	77%14%7%
1	G	650	71%18%7%
1	H	650	75%17%7%
1	I	650	74%17%7%
1	J	650	74%17%7%
1	K	650	74%17%8%
1	L	650	74%17%8%

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

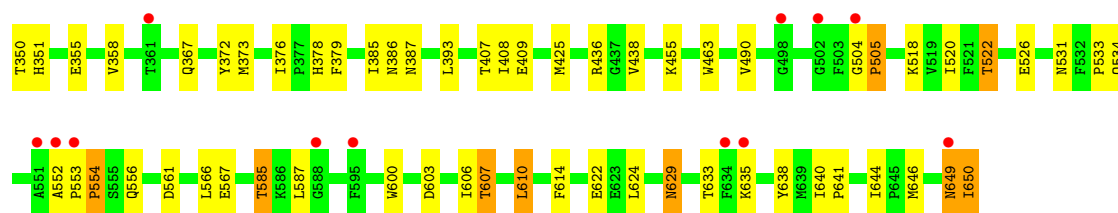
- Molecule 3 is water.

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

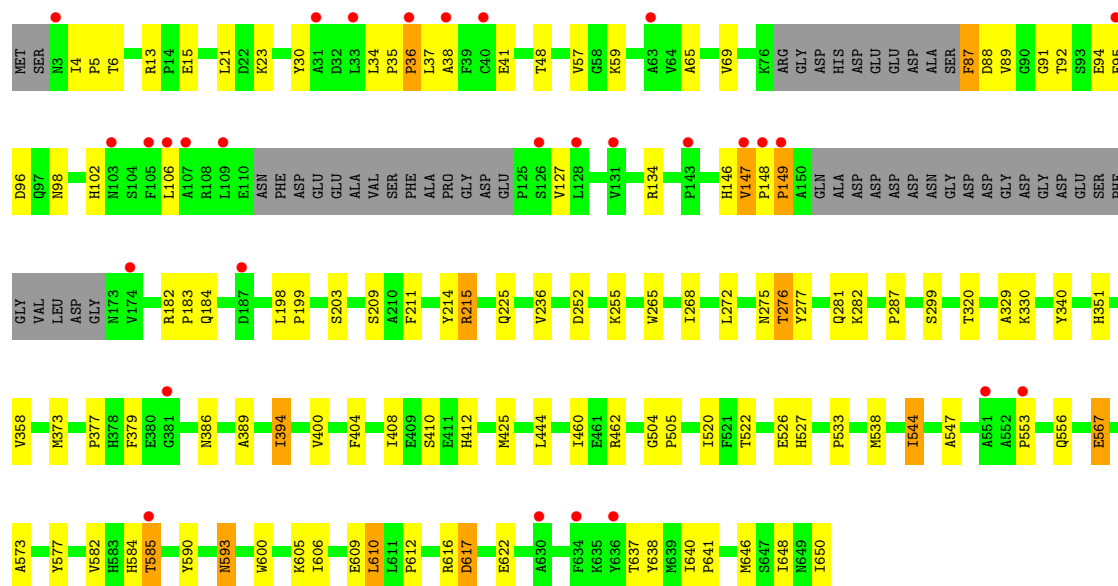
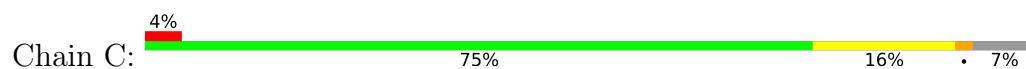
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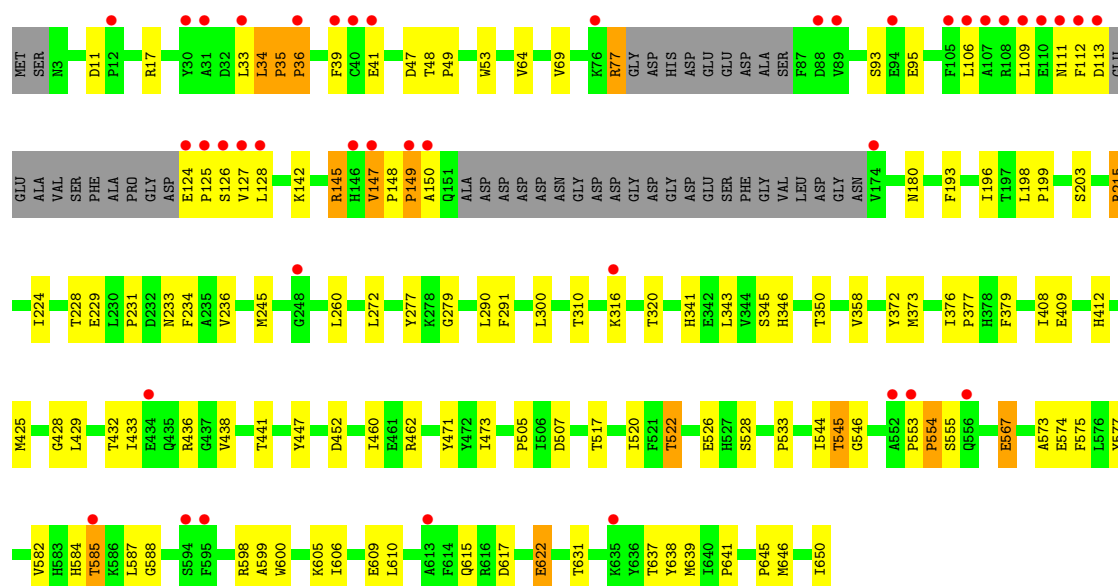
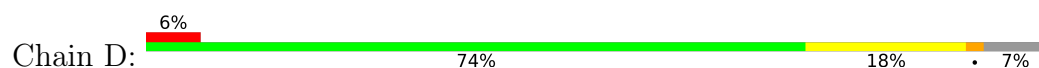
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	56	Total 56	O 56	0	0
3	K	79	Total 79	O 79	0	0
3	L	93	Total 93	O 93	0	0



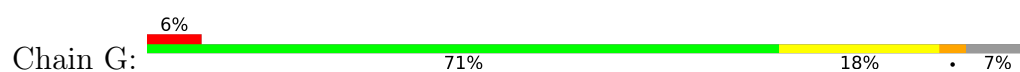
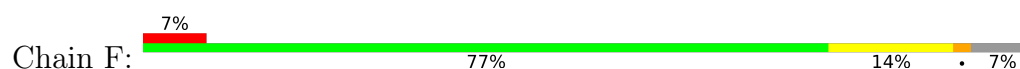
• Molecule 1: Arachidonate 15-lipoxygenase

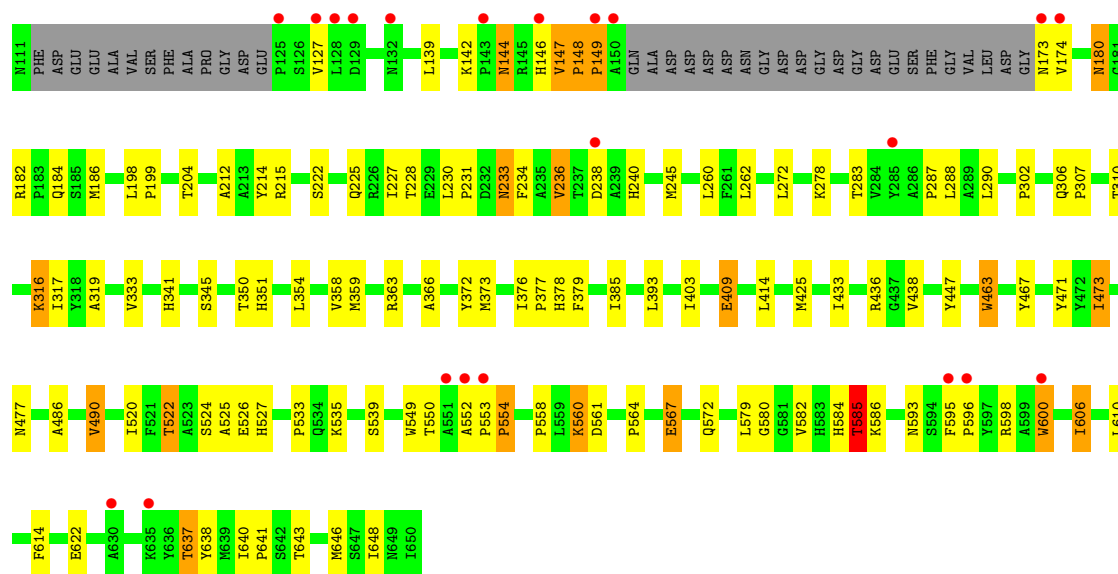


• Molecule 1: Arachidonate 15-lipoxygenase

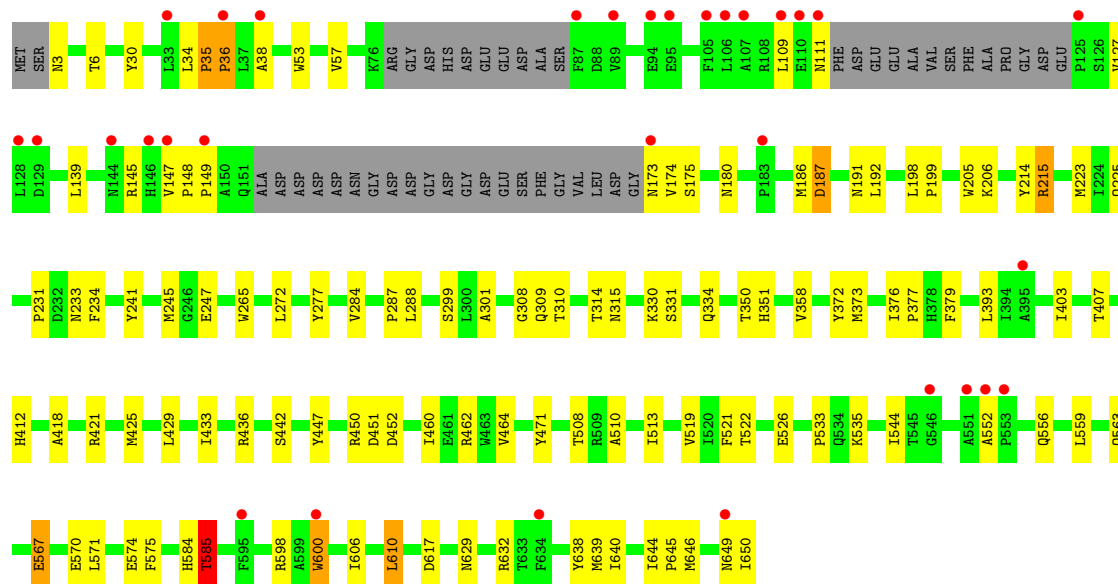
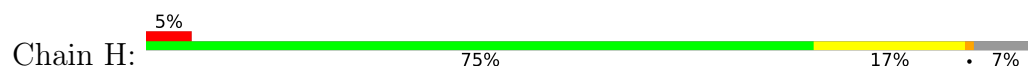


Chain E: 5% 73% 17% 7%

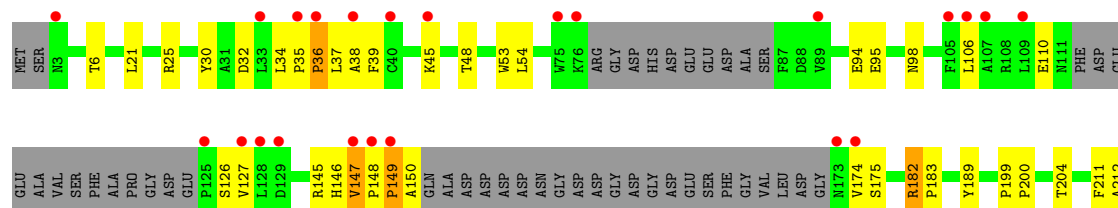
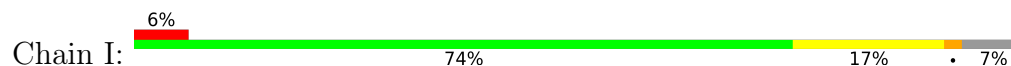


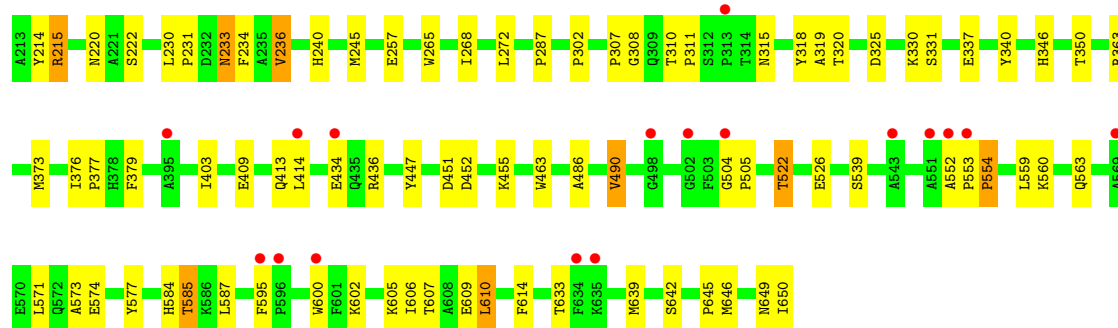


• Molecule 1: Arachidonate 15-lipoxygenase

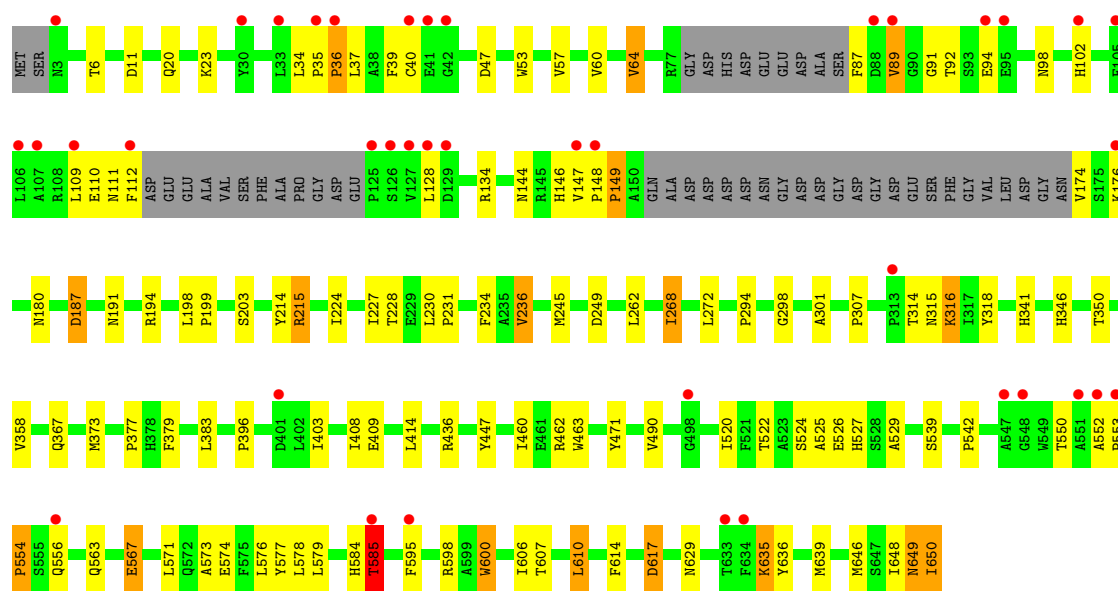
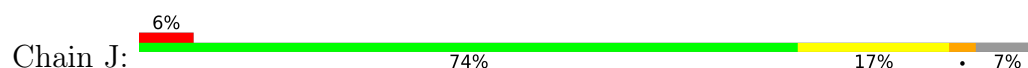


• Molecule 1: Arachidonate 15-lipoxygenase

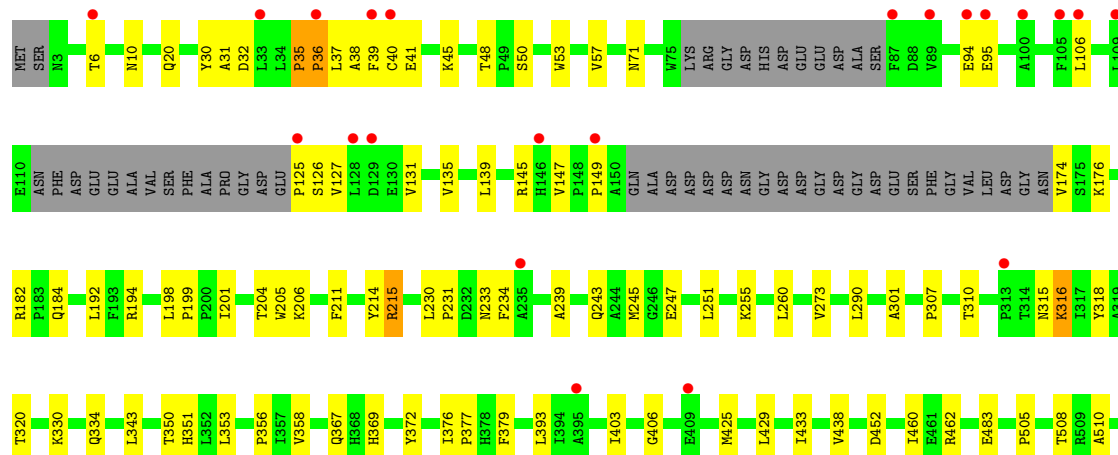
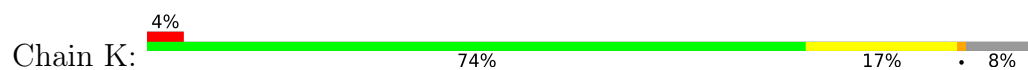




• Molecule 1: Arachidonate 15-lipoxygenase

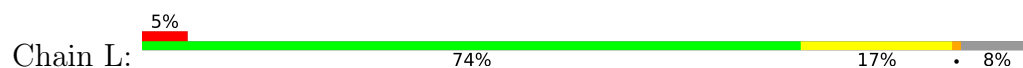


• Molecule 1: Arachidonate 15-lipoxygenase





• 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.

All (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
1	K	35	PRO	Peptide

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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	4	0	0	0	0
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.

All (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
1:J:148:PRO:HB2	1:J:149:PRO:HD2	1.62	0.81
1:J:35:PRO:O	1:J:37:LEU:N	2.14	0.79
1:E:585:THR:HG23	1:E:646:MET:H	1.48	0.79
1:H:585:THR:HG23	1:H:646:MET:H	1.47	0.78
1:B:585:THR:HG23	1:B:646:MET:H	1.46	0.78
1:G:585:THR:HG23	1:G:646:MET:H	1.46	0.77
1:A:522:THR:HA	1:A:526:GLU:HB3	1.64	0.77
1:B:220:ASN:HD21	1:B:223:MET:HG3	1.50	0.76
1:C:585:THR:HG23	1:C:646:MET:H	1.50	0.76
1:A:585:THR:HG23	1:A:646:MET:H	1.50	0.75
1:E:148:PRO:HB2	1:E:149:PRO:HD2	1.69	0.75
1:K:585:THR:HG23	1:K:646:MET:H	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:522:THR:HA	1:K:526:GLU:HB3	1.67	0.75
1:L:11:ASP:OD2	1:L:17:ARG:NH1	2.20	0.74
1:F:585:THR:HG23	1:F:646:MET:H	1.52	0.74
1:A:148:PRO:HB2	1:A:149:PRO:HD2	1.69	0.74
1:D:522:THR:HA	1:D:526:GLU:HB3	1.70	0.73
1:K:31:ALA:HB2	1:K:41:GLU:HG2	1.71	0.73
1:G:552:ALA:HB1	1:G:554:PRO:HD2	1.71	0.72
1:D:587:LEU:HA	1:D:646:MET:HG2	1.70	0.72
1:A:92:THR:HG23	1:A:147:VAL:HG23	1.72	0.72
1:E:252:ASP:HA	1:E:255:LYS:HE3	1.71	0.72
1:C:148:PRO:HB2	1:C:149:PRO:HD2	1.71	0.72
1:A:436:ARG:NH2	1:A:447:TYR:OH	2.22	0.71
1:K:35:PRO:HB2	1:K:36:PRO:HD2	1.74	0.70
1:I:346:HIS:O	1:I:350:THR:OG1	2.11	0.69
1:F:148:PRO:HB2	1:F:149:PRO:HD2	1.75	0.69
1:I:522:THR:HA	1:I:526:GLU:HB3	1.75	0.68
1:G:522:THR:HA	1:G:526:GLU:HB3	1.75	0.68
1:H:522:THR:HA	1:H:526:GLU:HB3	1.76	0.68
1:G:307:PRO:HB3	1:G:553:PRO:HG2	1.74	0.68
1:J:522:THR:HA	1:J:526:GLU:HB3	1.76	0.68
1:B:182:ARG:HH22	1:B:561:ASP:HA	1.59	0.67
1:H:35:PRO:HB2	1:H:36:PRO:HD2	1.77	0.67
1:K:71:ASN:HA	1:K:194:ARG:HE	1.60	0.67
1:G:230:LEU:HD11	1:G:236:VAL:HG22	1.77	0.67
1:G:436:ARG:NH2	1:G:447:TYR:OH	2.28	0.67
1:J:272:LEU:HD11	1:J:414:LEU:HD22	1.77	0.67
1:I:240:HIS:HD2	1:I:319:ALA:HB2	1.60	0.66
1:D:436:ARG:NH2	1:D:447:TYR:OH	2.27	0.66
1:C:522:THR:HA	1:C:526:GLU:HB3	1.77	0.66
1:J:373:MET:HA	1:J:600:TRP:HZ3	1.61	0.66
1:D:433:ILE:HG23	1:D:438:VAL:HG23	1.77	0.65
1:I:34:LEU:HD23	1:I:37:LEU:HD12	1.78	0.65
1:G:272:LEU:HD11	1:G:414:LEU:HD22	1.78	0.65
1:B:587:LEU:HA	1:B:646:MET:HG2	1.78	0.65
1:L:57:VAL:HG22	1:L:582:VAL:HG21	1.79	0.64
1:A:272:LEU:HD23	1:A:284:VAL:HG11	1.80	0.64
1:D:215:ARG:HG2	1:D:224:ILE:HG23	1.78	0.64
1:G:57:VAL:HG22	1:G:582:VAL:HG21	1.79	0.64
1:J:180:ASN:HA	1:J:567:GLU:HG3	1.79	0.64
1:B:347:LEU:HA	1:B:351:HIS:HB2	1.80	0.63
1:B:518:LYS:O	1:B:522:THR:OG1	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:LYS:HE2	1:E:405:ALA:HA	1.79	0.63
1:H:186:MET:HE2	1:H:559:LEU:HB3	1.80	0.63
1:G:21:LEU:HD21	1:G:366:ALA:HA	1.79	0.63
1:K:462:ARG:NH1	1:K:617:ASP:OD2	2.31	0.63
1:A:335:VAL:O	1:A:339:ASN:ND2	2.32	0.63
1:E:92:THR:HG23	1:E:147:VAL:HB	1.81	0.63
1:K:452:ASP:OD2	1:K:632:ARG:NH2	2.31	0.63
1:D:35:PRO:HB2	1:D:36:PRO:HD2	1.80	0.62
1:A:363:ARG:NH2	1:D:279:GLY:O	2.32	0.62
1:F:106:LEU:HD21	1:F:125:PRO:HG2	1.81	0.62
1:E:198:LEU:HD12	1:E:199:PRO:HD2	1.81	0.62
1:E:436:ARG:NH2	1:E:447:TYR:OH	2.32	0.62
1:F:34:LEU:HD23	1:F:37:LEU:HD12	1.81	0.62
1:L:95:GLU:HB2	1:L:147:VAL:HG21	1.79	0.62
1:E:242:LYS:HE3	1:E:247:GLU:HG3	1.80	0.62
1:I:212:ALA:HB2	1:I:302:PRO:HD3	1.82	0.62
1:G:110:GLU:HB3	1:G:595:PHE:CD1	2.35	0.62
1:D:111:ASN:O	1:D:113:ASP:N	2.33	0.61
1:K:198:LEU:HD12	1:K:199:PRO:HD2	1.81	0.61
1:H:109:LEU:HG	1:H:111:ASN:H	1.63	0.61
1:D:124:GLU:HB2	1:D:128:LEU:HB2	1.81	0.61
1:A:252:ASP:OD1	1:A:252:ASP:N	2.32	0.60
1:F:180:ASN:HA	1:F:567:GLU:HG3	1.83	0.60
1:K:95:GLU:HB2	1:K:147:VAL:HG21	1.82	0.60
1:G:198:LEU:HD12	1:G:199:PRO:HD2	1.83	0.60
1:E:279:GLY:O	1:G:363:ARG:NH2	2.34	0.60
1:F:373:MET:HA	1:F:600:TRP:HZ3	1.66	0.60
1:I:110:GLU:HB3	1:I:595:PHE:CE1	2.36	0.60
1:L:522:THR:HA	1:L:526:GLU:HB3	1.83	0.60
1:I:233:ASN:OD1	1:I:233:ASN:N	2.35	0.59
1:D:34:LEU:HD21	1:D:412:HIS:CE1	2.38	0.59
1:D:462:ARG:NH1	1:D:617:ASP:OD2	2.35	0.59
1:F:463:TRP:HZ3	1:F:610:LEU:HB3	1.68	0.59
1:G:373:MET:HA	1:G:600:TRP:HZ3	1.66	0.59
1:H:350:THR:OG1	1:H:351:HIS:N	2.35	0.59
1:J:174:VAL:HG11	1:J:567:GLU:HG2	1.84	0.59
1:F:522:THR:HA	1:F:526:GLU:HB3	1.83	0.59
1:J:585:THR:HG23	1:J:646:MET:H	1.68	0.59
1:G:596:PRO:HB2	1:G:598:ARG:HG3	1.84	0.59
1:A:214:TYR:OH	1:A:537:LEU:O	2.20	0.58
1:L:307:PRO:HB3	1:L:553:PRO:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:HIS:O	1:F:350:THR:OG1	2.16	0.58
1:B:346:HIS:O	1:B:350:THR:OG1	2.20	0.57
1:H:508:THR:HG22	1:H:510:ALA:H	1.67	0.57
1:H:418:ALA:HA	1:H:421:ARG:HG2	1.85	0.57
1:I:552:ALA:HB1	1:I:554:PRO:HD2	1.86	0.57
1:F:245:MET:HE1	1:F:301:ALA:HB3	1.85	0.57
1:I:587:LEU:HA	1:I:646:MET:HG2	1.85	0.57
1:J:346:HIS:O	1:J:350:THR:OG1	2.21	0.57
1:K:30:TYR:CE1	1:K:38:ALA:HB1	2.40	0.57
1:L:35:PRO:HB2	1:L:36:PRO:HD2	1.86	0.57
1:A:606:ILE:HA	1:A:610:LEU:HB2	1.85	0.57
1:L:260:LEU:HD22	1:L:290:LEU:HD11	1.85	0.57
1:A:109:LEU:O	1:A:111:ASN:N	2.38	0.57
1:L:215:ARG:N	1:L:215:ARG:HD2	2.20	0.57
1:C:96:ASP:OD1	1:C:134:ARG:NH2	2.36	0.56
1:B:455:LYS:HD3	1:B:624:LEU:HD23	1.86	0.56
1:A:243:GLN:HB3	1:A:321:GLN:HG2	1.87	0.56
1:G:580:GLY:O	3:G:801:HOH:O	2.18	0.56
1:B:552:ALA:HB1	1:B:554:PRO:HD2	1.87	0.56
1:G:231:PRO:HG2	1:G:234:PHE:HB3	1.86	0.56
1:C:215:ARG:N	1:C:215:ARG:HD2	2.21	0.56
1:C:408:ILE:O	1:C:412:HIS:ND1	2.38	0.56
1:F:64:VAL:HG13	1:F:574:GLU:HB3	1.88	0.56
1:F:198:LEU:HD12	1:F:199:PRO:HD2	1.87	0.56
1:G:180:ASN:HA	1:G:567:GLU:HG2	1.88	0.56
1:A:215:ARG:NH2	1:A:334:GLN:OE1	2.39	0.56
1:F:260:LEU:HD22	1:F:290:LEU:HD11	1.87	0.55
1:J:230:LEU:HD11	1:J:236:VAL:HG22	1.87	0.55
1:L:145:ARG:NH1	1:L:574:GLU:OE1	2.39	0.55
1:L:463:TRP:HZ3	1:L:610:LEU:HB3	1.70	0.55
1:G:433:ILE:HG23	1:G:438:VAL:HG23	1.89	0.55
1:K:522:THR:HG22	1:K:526:GLU:HG2	1.88	0.55
1:I:559:LEU:HG	1:I:563:GLN:HE21	1.70	0.55
1:J:403:ILE:HD11	1:J:571:LEU:HG	1.88	0.55
1:B:378:HIS:HD2	1:B:520:ILE:HG12	1.71	0.55
1:A:260:LEU:HD22	1:A:290:LEU:HD11	1.88	0.55
1:K:53:TRP:CD1	1:K:649:ASN:HD22	2.25	0.55
1:L:508:THR:HG22	1:L:510:ALA:H	1.72	0.55
1:B:89:VAL:HA	1:B:92:THR:HG22	1.87	0.55
1:J:57:VAL:HG22	1:J:650:ILE:HD11	1.89	0.55
1:H:53:TRP:CD1	1:H:649:ASN:HD22	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:452:ASP:HB3	1:I:639:MET:HB2	1.89	0.55
1:A:341:HIS:HA	1:A:345:SER:HB2	1.89	0.54
1:E:341:HIS:HA	1:E:345:SER:HB2	1.89	0.54
1:H:187:ASP:O	1:H:191:ASN:ND2	2.41	0.54
1:J:358:VAL:HG22	1:J:379:PHE:CG	2.42	0.54
1:G:584:HIS:O	1:G:585:THR:HG22	2.07	0.54
1:H:436:ARG:NH2	1:H:447:TYR:OH	2.39	0.54
1:J:198:LEU:HD12	1:J:199:PRO:HD2	1.88	0.54
1:B:220:ASN:ND2	1:B:223:MET:HG3	2.21	0.54
1:G:341:HIS:HA	1:G:345:SER:HB2	1.88	0.54
1:J:92:THR:OG1	1:J:147:VAL:HB	2.08	0.54
1:K:230:LEU:HD11	1:K:251:LEU:HD21	1.90	0.54
1:L:214:TYR:HB3	1:L:215:ARG:NH1	2.22	0.54
1:D:373:MET:HA	1:D:600:TRP:CZ3	2.43	0.54
1:E:462:ARG:NH1	1:E:617:ASP:OD2	2.40	0.54
1:J:373:MET:HA	1:J:600:TRP:CZ3	2.43	0.54
1:K:39:PHE:HD1	1:K:40:CYS:H	1.56	0.54
1:B:629:ASN:HD21	1:B:635:LYS:HB3	1.73	0.54
1:B:234:PHE:HD2	1:B:262:LEU:HD11	1.72	0.54
1:B:622:GLU:HB2	1:B:641:PRO:HD2	1.89	0.54
1:C:268:ILE:HD11	1:C:340:TYR:HB2	1.89	0.54
1:C:584:HIS:O	1:C:585:THR:HG22	2.08	0.54
1:E:35:PRO:O	1:E:37:LEU:N	2.35	0.54
1:K:231:PRO:HG2	1:K:234:PHE:HB3	1.89	0.54
1:K:316:LYS:HB3	1:K:316:LYS:HZ2	1.72	0.54
1:J:584:HIS:O	1:J:585:THR:HG22	2.07	0.54
1:C:462:ARG:NH1	1:C:617:ASP:OD2	2.41	0.53
1:D:95:GLU:HB2	1:D:147:VAL:HG21	1.90	0.53
1:D:373:MET:HA	1:D:600:TRP:HZ3	1.72	0.53
1:A:527:HIS:CG	1:A:648:ILE:HG12	2.42	0.53
1:B:231:PRO:HG2	1:B:234:PHE:HB3	1.90	0.53
1:D:585:THR:CG2	1:D:646:MET:H	2.17	0.53
1:F:272:LEU:HD11	1:F:414:LEU:HD22	1.90	0.53
1:H:452:ASP:HB3	1:H:639:MET:HB2	1.90	0.53
1:I:584:HIS:O	1:I:585:THR:HG22	2.08	0.53
1:E:35:PRO:HB2	1:E:36:PRO:HD2	1.90	0.53
1:F:385:ILE:HG12	1:F:650:ILE:C	2.33	0.53
1:H:198:LEU:HD12	1:H:199:PRO:HD2	1.90	0.53
1:J:462:ARG:NH1	1:J:617:ASP:OD2	2.41	0.53
1:F:215:ARG:HD2	1:F:215:ARG:N	2.24	0.53
1:G:240:HIS:CD2	1:G:319:ALA:HB2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:373:MET:HA	1:G:600:TRP:CZ3	2.42	0.53
1:I:147:VAL:HB	1:I:150:ALA:HB3	1.90	0.53
1:I:268:ILE:HG23	1:I:272:LEU:HD22	1.91	0.53
1:L:385:ILE:HG12	1:L:650:ILE:HA	1.90	0.53
1:A:110:GLU:HB3	1:A:595:PHE:CE1	2.44	0.53
1:D:198:LEU:HD12	1:D:199:PRO:HD2	1.91	0.53
1:G:214:TYR:HB3	1:G:215:ARG:NH1	2.24	0.53
1:J:6:THR:OG1	1:J:11:ASP:OD1	2.27	0.53
1:A:25:ARG:HG2	1:A:363:ARG:HB3	1.90	0.53
1:B:215:ARG:HD2	1:B:215:ARG:N	2.24	0.53
1:C:268:ILE:HG23	1:C:272:LEU:HD22	1.91	0.53
1:A:534:GLN:HG2	1:A:538:MET:HE2	1.91	0.53
1:I:308:GLY:N	1:I:315:ASN:OD1	2.37	0.53
1:A:35:PRO:HB2	1:A:36:PRO:HD2	1.91	0.52
1:H:187:ASP:OD1	1:H:187:ASP:N	2.42	0.52
1:E:606:ILE:HA	1:E:610:LEU:HB2	1.91	0.52
1:G:524:SER:OG	1:G:525:ALA:N	2.39	0.52
1:H:358:VAL:HG22	1:H:379:PHE:CG	2.44	0.52
1:J:268:ILE:HG23	1:J:272:LEU:HD13	1.89	0.52
1:L:272:LEU:HA	1:L:410:SER:HB2	1.91	0.52
1:C:637:THR:HA	1:C:640:ILE:HD13	1.90	0.52
1:J:89:VAL:HA	1:J:92:THR:HG22	1.90	0.52
1:L:318:TYR:OH	1:L:554:PRO:HD3	2.10	0.52
1:C:57:VAL:HG22	1:C:582:VAL:HG21	1.91	0.52
1:J:187:ASP:N	1:J:187:ASP:OD1	2.42	0.52
1:F:584:HIS:O	1:F:585:THR:HG22	2.10	0.52
1:I:606:ILE:HA	1:I:610:LEU:HB2	1.92	0.52
1:J:109:LEU:O	1:J:111:ASN:N	2.41	0.52
1:K:318:TYR:OH	1:K:554:PRO:HD3	2.10	0.52
1:B:378:HIS:CD2	1:B:520:ILE:HG12	2.43	0.52
1:H:272:LEU:HD23	1:H:284:VAL:HG11	1.92	0.52
1:C:211:PHE:CG	1:C:330:LYS:HD2	2.44	0.51
1:G:527:HIS:CG	1:G:648:ILE:HG12	2.43	0.51
1:J:318:TYR:OH	1:J:554:PRO:HD3	2.09	0.51
1:K:433:ILE:HG23	1:K:438:VAL:HG23	1.92	0.51
1:A:318:TYR:OH	1:A:554:PRO:HD3	2.11	0.51
1:B:174:VAL:HG22	1:B:175:SER:H	1.75	0.51
1:G:260:LEU:HD22	1:G:290:LEU:HD11	1.93	0.51
1:H:373:MET:HA	1:H:600:TRP:HZ3	1.74	0.51
1:A:215:ARG:HD2	1:A:215:ARG:N	2.25	0.51
1:F:307:PRO:HB3	1:F:553:PRO:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:LEU:HD22	1:H:393:LEU:HD13	1.92	0.51
1:L:373:MET:HA	1:L:600:TRP:HZ3	1.75	0.51
1:B:53:TRP:HE1	1:B:649:ASN:HB2	1.75	0.51
1:H:241:TYR:CZ	1:H:245:MET:HG3	2.46	0.51
1:H:584:HIS:O	1:H:585:THR:HG22	2.10	0.51
1:B:265:TRP:HB2	1:B:287:PRO:HD2	1.91	0.51
1:B:522:THR:HA	1:B:526:GLU:HB3	1.93	0.51
1:H:180:ASN:HA	1:H:567:GLU:HG2	1.93	0.51
1:K:255:LYS:HB3	1:K:260:LEU:HD12	1.93	0.51
1:C:214:TYR:HB3	1:C:215:ARG:NH1	2.25	0.51
1:D:231:PRO:HG2	1:D:234:PHE:HB3	1.91	0.51
1:C:282:LYS:HB3	1:C:547:ALA:HB1	1.93	0.51
1:E:460:ILE:HD13	1:E:520:ILE:HG22	1.92	0.51
1:E:471:TYR:HE2	1:E:606:ILE:HD11	1.76	0.51
1:E:649:ASN:ND2	3:E:801:HOH:O	2.44	0.51
1:F:135:VAL:HG22	1:F:578:LEU:HD21	1.92	0.51
1:I:272:LEU:HD11	1:I:414:LEU:HD22	1.93	0.51
1:K:215:ARG:HD2	1:K:215:ARG:N	2.25	0.51
1:L:147:VAL:HB	1:L:150:ALA:HB2	1.92	0.51
1:C:182:ARG:HE	1:C:183:PRO:HD2	1.75	0.51
1:C:272:LEU:HA	1:C:410:SER:HB2	1.93	0.51
1:A:231:PRO:HG2	1:A:234:PHE:HB3	1.93	0.50
1:E:182:ARG:HH21	1:E:561:ASP:HA	1.76	0.50
1:F:264:ASP:OD1	1:F:265:TRP:N	2.44	0.50
1:K:145:ARG:NH1	3:K:801:HOH:O	2.43	0.50
1:C:622:GLU:HB2	1:C:641:PRO:HD2	1.93	0.50
1:K:307:PRO:HB3	1:K:553:PRO:HG2	1.93	0.50
1:D:260:LEU:HD22	1:D:290:LEU:HD11	1.93	0.50
1:H:373:MET:HA	1:H:600:TRP:CZ3	2.46	0.50
1:J:134:ARG:HH21	1:J:148:PRO:HG3	1.77	0.50
1:D:573:ALA:O	1:D:577:TYR:HB2	2.11	0.50
1:H:215:ARG:HD2	1:H:215:ARG:N	2.26	0.50
1:J:552:ALA:HB1	1:J:554:PRO:HD2	1.92	0.50
1:A:522:THR:HG22	1:A:526:GLU:HG2	1.93	0.50
1:A:373:MET:HA	1:A:600:TRP:CH2	2.47	0.50
1:J:64:VAL:HG13	1:J:574:GLU:HB3	1.94	0.50
1:J:134:ARG:NH2	1:J:148:PRO:HG3	2.27	0.50
1:E:215:ARG:N	1:E:215:ARG:HD2	2.27	0.50
1:G:35:PRO:HB3	1:G:36:PRO:HD2	1.93	0.50
1:A:139:LEU:HD22	1:A:393:LEU:HD13	1.94	0.49
1:F:30:TYR:CE1	1:F:38:ALA:HB1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:436:ARG:NH2	1:I:447:TYR:OH	2.45	0.49
1:F:54:LEU:HD13	1:F:127:VAL:HB	1.94	0.49
1:K:245:MET:HE1	1:K:301:ALA:HB3	1.94	0.49
1:A:460:ILE:HD13	1:A:520:ILE:HG22	1.95	0.49
1:L:198:LEU:HD12	1:L:199:PRO:HD2	1.93	0.49
1:A:241:TYR:CZ	1:A:245:MET:HG3	2.47	0.49
1:C:277:TYR:OH	1:C:567:GLU:OE1	2.18	0.49
1:D:106:LEU:HD22	1:D:126:SER:HB3	1.93	0.49
1:G:463:TRP:HB2	1:G:614:PHE:HB2	1.94	0.49
1:H:34:LEU:HD11	1:H:412:HIS:CE1	2.47	0.49
1:J:471:TYR:HE2	1:J:606:ILE:HD11	1.77	0.49
1:G:403:ILE:HG21	1:G:572:GLN:HB2	1.94	0.49
1:I:215:ARG:HD2	1:I:215:ARG:N	2.28	0.49
1:L:275:ASN:HB2	1:L:407:THR:HG22	1.94	0.49
1:A:268:ILE:HG23	1:A:272:LEU:HD22	1.94	0.49
1:E:241:TYR:CZ	1:E:245:MET:HG3	2.48	0.49
1:E:316:LYS:NZ	1:E:317:ILE:H	2.10	0.49
1:B:92:THR:OG1	1:B:147:VAL:HB	2.13	0.49
1:L:358:VAL:HG22	1:L:379:PHE:CG	2.47	0.49
1:G:471:TYR:OH	1:G:606:ILE:HD11	2.13	0.49
1:I:265:TRP:HB2	1:I:287:PRO:HD2	1.95	0.49
1:J:245:MET:HE1	1:J:301:ALA:HB3	1.95	0.49
1:K:377:PRO:HD3	1:K:600:TRP:CZ3	2.47	0.49
1:C:351:HIS:ND1	1:C:386:ASN:OD1	2.42	0.49
1:G:92:THR:HG23	1:G:147:VAL:HB	1.95	0.49
1:D:109:LEU:O	1:D:111:ASN:N	2.40	0.49
1:F:214:TYR:HB3	1:F:215:ARG:NH1	2.28	0.49
1:A:433:ILE:HG23	1:A:438:VAL:HG23	1.93	0.48
1:D:69:VAL:HG11	1:D:93:SER:HB2	1.93	0.48
1:J:294:PRO:HG2	1:J:298:GLY:HA3	1.94	0.48
1:B:214:TYR:HB3	1:B:215:ARG:NH1	2.28	0.48
1:G:227:ILE:HD13	1:G:262:LEU:HB2	1.95	0.48
1:B:212:ALA:HB2	1:B:302:PRO:HD3	1.94	0.48
1:B:215:ARG:HD2	1:B:215:ARG:H	1.78	0.48
1:F:373:MET:HA	1:F:600:TRP:CZ3	2.47	0.48
1:I:94:GLU:O	1:I:98:ASN:N	2.45	0.48
1:H:174:VAL:HG11	1:H:567:GLU:HB3	1.94	0.48
1:K:372:TYR:CZ	1:K:376:ILE:HG13	2.48	0.48
1:E:584:HIS:O	1:E:585:THR:HG22	2.13	0.48
1:B:372:TYR:CZ	1:B:376:ILE:HG13	2.49	0.48
1:I:486:ALA:O	1:I:490:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:60:VAL:HG12	1:J:578:LEU:HD12	1.94	0.48
1:D:11:ASP:OD2	1:D:17:ARG:NH1	2.43	0.48
1:D:346:HIS:O	1:D:350:THR:OG1	2.22	0.48
1:H:377:PRO:HD3	1:H:600:TRP:CZ3	2.49	0.48
1:I:373:MET:HA	1:I:600:TRP:CZ3	2.49	0.48
1:J:436:ARG:NH2	1:J:447:TYR:OH	2.47	0.48
1:A:245:MET:HE1	1:A:301:ALA:HB3	1.96	0.48
1:B:234:PHE:CD2	1:B:262:LEU:HD11	2.48	0.48
1:G:182:ARG:HH22	1:G:561:ASP:HA	1.79	0.48
1:I:373:MET:HA	1:I:600:TRP:HZ3	1.79	0.48
1:D:606:ILE:HA	1:D:610:LEU:HB2	1.95	0.48
1:J:629:ASN:OD1	1:J:636:TYR:N	2.47	0.48
1:B:225:GLN:HG3	1:B:436:ARG:HA	1.95	0.47
1:B:533:PRO:HG3	1:B:638:TYR:CE2	2.49	0.47
1:D:605:LYS:O	1:D:609:GLU:HB3	2.13	0.47
1:L:231:PRO:HG2	1:L:234:PHE:HB3	1.96	0.47
1:C:593:ASN:N	1:C:593:ASN:OD1	2.47	0.47
1:D:584:HIS:O	1:D:585:THR:HG22	2.13	0.47
1:E:433:ILE:HG23	1:E:438:VAL:HG23	1.96	0.47
1:E:463:TRP:HZ3	1:E:610:LEU:HB3	1.79	0.47
1:G:144:ASN:O	1:G:144:ASN:ND2	2.47	0.47
1:L:211:PHE:CG	1:L:330:LYS:HD2	2.49	0.47
1:A:35:PRO:C	1:A:37:LEU:H	2.21	0.47
1:L:389:ALA:O	1:L:394:ILE:HG12	2.14	0.47
1:L:456:ILE:HD11	1:L:641:PRO:HG3	1.96	0.47
1:L:585:THR:O	1:L:645:PRO:HA	2.14	0.47
1:D:528:SER:HB2	1:D:645:PRO:HD2	1.96	0.47
1:G:174:VAL:HG23	1:G:278:LYS:NZ	2.29	0.47
1:K:211:PHE:CG	1:K:330:LYS:HD2	2.50	0.47
1:D:553:PRO:O	1:D:555:SER:N	2.48	0.47
1:B:255:LYS:HB3	1:B:260:LEU:HD12	1.96	0.47
1:B:603:ASP:O	1:B:607:THR:OG1	2.32	0.47
1:D:64:VAL:HG13	1:D:574:GLU:HB3	1.96	0.47
1:G:586:LYS:HA	1:G:586:LYS:HD3	1.73	0.47
1:B:355:GLU:OE1	1:B:386:ASN:ND2	2.38	0.47
1:F:358:VAL:HG22	1:F:379:PHE:CG	2.50	0.47
1:G:558:PRO:HB2	1:G:560:LYS:HG3	1.96	0.47
1:J:227:ILE:HD13	1:J:262:LEU:HB2	1.97	0.47
1:K:584:HIS:O	1:K:585:THR:HG22	2.14	0.47
1:A:373:MET:HA	1:A:600:TRP:HH2	1.78	0.47
1:A:429:LEU:HD22	1:A:521:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:MET:HA	1:E:600:TRP:HZ3	1.79	0.47
1:H:452:ASP:OD2	1:H:632:ARG:NH2	2.48	0.47
1:L:268:ILE:HG23	1:L:272:LEU:HD22	1.97	0.47
1:A:347:LEU:HA	1:A:351:HIS:HB2	1.97	0.47
1:C:92:THR:HG23	1:C:147:VAL:HG22	1.96	0.47
1:H:231:PRO:HG2	1:H:234:PHE:HB3	1.97	0.47
1:A:377:PRO:HD3	1:A:600:TRP:CH2	2.49	0.47
1:C:358:VAL:HG22	1:C:379:PHE:CG	2.50	0.47
1:G:473:ILE:H	1:G:477:ASN:HD22	1.63	0.47
1:H:522:THR:HG22	1:H:526:GLU:HG2	1.97	0.47
1:I:268:ILE:HD11	1:I:340:TYR:HB2	1.97	0.47
1:J:110:GLU:HB3	1:J:595:PHE:HE1	1.79	0.47
1:C:533:PRO:HG3	1:C:638:TYR:CE2	2.50	0.46
1:G:377:PRO:HD3	1:G:600:TRP:CZ3	2.50	0.46
1:H:265:TRP:HB2	1:H:287:PRO:HD2	1.96	0.46
1:J:460:ILE:HD13	1:J:520:ILE:HG22	1.97	0.46
1:J:524:SER:OG	1:J:525:ALA:N	2.47	0.46
1:K:139:LEU:HD22	1:K:393:LEU:HD13	1.97	0.46
1:K:307:PRO:HG2	1:K:315:ASN:ND2	2.30	0.46
1:A:35:PRO:O	1:A:37:LEU:N	2.42	0.46
1:A:358:VAL:HG22	1:A:379:PHE:CG	2.50	0.46
1:F:318:TYR:OH	1:F:554:PRO:HD3	2.15	0.46
1:A:341:HIS:O	1:A:346:HIS:N	2.46	0.46
1:A:629:ASN:HD21	1:A:636:TYR:H	1.63	0.46
1:D:460:ILE:HD13	1:D:520:ILE:HG22	1.98	0.46
1:F:189:TYR:OH	1:F:563:GLN:HB2	2.14	0.46
1:F:211:PHE:CG	1:F:330:LYS:HD2	2.51	0.46
1:H:308:GLY:N	1:H:315:ASN:HD21	2.13	0.46
1:J:553:PRO:N	1:J:554:PRO:HD2	2.30	0.46
1:L:534:GLN:HB3	1:L:576:LEU:HD22	1.96	0.46
1:A:51:ALA:HA	1:A:54:LEU:HD12	1.97	0.46
1:K:205:TRP:CZ2	1:K:206:LYS:HE2	2.50	0.46
1:L:216:VAL:HB	1:L:447:TYR:HA	1.96	0.46
1:H:109:LEU:C	1:H:111:ASN:H	2.24	0.46
1:I:53:TRP:HE3	1:I:54:LEU:HD23	1.80	0.46
1:I:573:ALA:O	1:I:577:TYR:HB2	2.15	0.46
1:L:92:THR:OG1	1:L:146:HIS:HB3	2.15	0.46
1:A:508:THR:HG22	1:A:510:ALA:H	1.80	0.46
1:B:603:ASP:HB3	1:B:606:ILE:HD12	1.98	0.46
1:H:277:TYR:OH	1:H:567:GLU:OE1	2.12	0.46
1:K:508:THR:HG22	1:K:510:ALA:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:PRO:HB3	1:B:566:LEU:HD21	1.98	0.46
1:C:373:MET:HA	1:C:600:TRP:HZ3	1.79	0.46
1:C:408:ILE:HG13	1:C:412:HIS:CE1	2.51	0.46
1:D:49:PRO:HB3	1:D:53:TRP:CE3	2.51	0.46
1:H:30:TYR:HE1	1:H:38:ALA:HB1	1.81	0.46
1:L:341:HIS:HA	1:L:345:SER:HB2	1.98	0.46
1:A:452:ASP:HB3	1:A:639:MET:HB2	1.98	0.46
1:B:260:LEU:HD22	1:B:290:LEU:HD11	1.98	0.46
1:C:198:LEU:HD12	1:C:199:PRO:HD2	1.98	0.46
1:C:460:ILE:HD13	1:C:520:ILE:HG22	1.98	0.46
1:H:233:ASN:HB2	1:H:309:GLN:O	2.16	0.46
1:K:53:TRP:CZ2	1:K:57:VAL:HG21	2.50	0.46
1:A:180:ASN:HA	1:A:567:GLU:HG3	1.98	0.46
1:I:403:ILE:HD11	1:I:571:LEU:HG	1.98	0.46
1:B:20:GLN:NE2	1:B:367:GLN:HG3	2.31	0.46
1:B:504:GLY:HA2	1:B:505:PRO:HA	1.67	0.46
1:H:205:TRP:CZ2	1:H:206:LYS:HE2	2.51	0.46
1:E:358:VAL:HG22	1:E:379:PHE:CG	2.51	0.45
1:E:637:THR:HG22	1:E:640:ILE:HD12	1.97	0.45
1:F:403:ILE:HA	1:F:568:LEU:HD13	1.98	0.45
1:G:30:TYR:CE1	1:G:38:ALA:HB1	2.51	0.45
1:B:224:ILE:HG13	1:B:438:VAL:HG11	1.98	0.45
1:H:334:GLN:HE21	1:H:544:ILE:HB	1.80	0.45
1:J:191:ASN:O	1:J:194:ARG:HG3	2.16	0.45
1:B:307:PRO:HG3	1:B:553:PRO:HG2	1.98	0.45
1:B:372:TYR:CE2	1:B:376:ILE:HG13	2.51	0.45
1:C:389:ALA:O	1:C:394:ILE:HG12	2.16	0.45
1:D:533:PRO:HG3	1:D:638:TYR:CE2	2.52	0.45
1:G:637:THR:HG22	1:G:640:ILE:HD12	1.96	0.45
1:I:183:PRO:HG2	1:I:560:LYS:HB2	1.98	0.45
1:G:35:PRO:CB	1:G:36:PRO:HD2	2.45	0.45
1:G:378:HIS:CE1	1:G:520:ILE:HG23	2.52	0.45
1:J:606:ILE:HA	1:J:610:LEU:HB2	1.99	0.45
1:B:223:MET:HE1	1:B:264:ASP:O	2.17	0.45
1:D:452:ASP:HB3	1:D:639:MET:HB2	1.97	0.45
1:I:214:TYR:HB3	1:I:215:ARG:NH1	2.31	0.45
1:H:460:ILE:HD12	1:H:521:PHE:HD1	1.82	0.45
1:H:585:THR:O	1:H:645:PRO:HA	2.16	0.45
1:K:260:LEU:HD22	1:K:290:LEU:HD11	1.98	0.45
1:B:358:VAL:HG22	1:B:379:PHE:CG	2.52	0.45
1:D:377:PRO:HD3	1:D:600:TRP:CZ3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:ARG:HD2	1:E:215:ARG:H	1.80	0.45
1:J:215:ARG:N	1:J:215:ARG:HD2	2.31	0.45
1:K:460:ILE:HD13	1:K:520:ILE:HG22	1.98	0.45
1:L:346:HIS:HD2	1:L:530:VAL:HG23	1.82	0.45
1:L:583:HIS:HB3	1:L:586:LYS:NZ	2.32	0.45
1:H:471:TYR:OH	1:H:606:ILE:HD11	2.17	0.45
1:A:56:THR:HG22	1:A:582:VAL:HG13	1.99	0.45
1:A:451:ASP:O	1:A:455:LYS:HG3	2.17	0.45
1:B:606:ILE:HA	1:B:610:LEU:HB2	1.99	0.45
1:C:35:PRO:CB	1:C:36:PRO:HD2	2.47	0.45
1:C:606:ILE:HA	1:C:610:LEU:HB2	1.99	0.45
1:H:245:MET:HE1	1:H:301:ALA:HB3	1.98	0.45
1:I:174:VAL:HG22	1:I:175:SER:H	1.82	0.45
1:J:35:PRO:HB3	1:J:36:PRO:HD2	1.99	0.45
1:J:529:ALA:HB2	1:J:639:MET:HE2	1.99	0.45
1:L:245:MET:HE1	1:L:301:ALA:HB3	1.99	0.45
1:D:460:ILE:HG22	1:D:517:THR:HG23	1.98	0.45
1:E:346:HIS:O	1:E:350:THR:OG1	2.27	0.45
1:E:553:PRO:O	1:E:555:SER:N	2.50	0.45
1:I:30:TYR:CE1	1:I:38:ALA:HB1	2.52	0.45
1:L:463:TRP:HB2	1:L:614:PHE:HB2	1.97	0.45
1:A:429:LEU:O	1:A:433:ILE:HG12	2.17	0.44
1:A:582:VAL:HB	1:A:650:ILE:HD12	1.99	0.44
1:B:220:ASN:HB3	1:B:337:GLU:CD	2.42	0.44
1:D:429:LEU:O	1:D:433:ILE:HG12	2.17	0.44
1:E:330:LYS:HB2	1:E:330:LYS:HE3	1.83	0.44
1:F:264:ASP:OD1	1:F:266:LYS:N	2.51	0.44
1:K:131:VAL:O	1:K:135:VAL:HG23	2.18	0.44
1:L:180:ASN:HA	1:L:567:GLU:HG3	2.00	0.44
1:L:529:ALA:HB2	1:L:639:MET:HE2	1.98	0.44
1:C:215:ARG:HD2	1:C:215:ARG:H	1.81	0.44
1:C:329:ALA:HA	1:C:553:PRO:HB3	1.99	0.44
1:E:188:ASP:O	1:E:192:LEU:HG	2.17	0.44
1:G:28:TYR:HB3	1:G:359:MET:HE1	1.99	0.44
1:G:358:VAL:HG22	1:G:379:PHE:CG	2.52	0.44
1:J:307:PRO:HG2	1:J:315:ASN:ND2	2.33	0.44
1:J:377:PRO:HD3	1:J:600:TRP:CZ3	2.52	0.44
1:B:30:TYR:CE1	1:B:38:ALA:HB1	2.52	0.44
1:G:225:GLN:HG3	1:G:436:ARG:HA	2.00	0.44
1:J:573:ALA:O	1:J:577:TYR:HB2	2.18	0.44
1:L:377:PRO:HD3	1:L:600:TRP:CZ3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:MET:O	1:B:600:TRP:HZ3	2.01	0.44
1:C:276:THR:HG22	1:C:281:GLN:HA	2.00	0.44
1:F:606:ILE:HA	1:F:610:LEU:HB2	1.99	0.44
1:G:287:PRO:HG2	1:G:333:VAL:HA	2.00	0.44
1:I:376:ILE:HD13	1:I:379:PHE:HD2	1.81	0.44
1:I:463:TRP:HB2	1:I:614:PHE:CD1	2.52	0.44
1:I:377:PRO:HD3	1:I:600:TRP:CZ3	2.53	0.44
1:K:334:GLN:HE21	1:K:544:ILE:HB	1.82	0.44
1:K:552:ALA:HB1	1:K:554:PRO:HD2	1.98	0.44
1:E:11:ASP:OD2	1:E:17:ARG:NH1	2.48	0.44
1:G:372:TYR:CZ	1:G:376:ILE:HG13	2.53	0.44
1:J:110:GLU:HB3	1:J:595:PHE:CE1	2.52	0.44
1:J:214:TYR:HB3	1:J:215:ARG:NH1	2.33	0.44
1:A:594:SER:HB3	1:A:596:PRO:HD2	1.98	0.44
1:B:640:ILE:O	1:B:644:ILE:HG13	2.18	0.44
1:D:291:PHE:HB3	1:D:300:LEU:HG	2.00	0.44
1:H:147:VAL:HG12	1:H:148:PRO:O	2.18	0.44
1:H:450:ARG:NE	1:H:451:ASP:OD1	2.48	0.44
1:I:230:LEU:HD13	1:I:236:VAL:HG13	1.99	0.44
1:L:34:LEU:HD11	1:L:412:HIS:CE1	2.53	0.44
1:E:573:ALA:O	1:E:577:TYR:HB2	2.18	0.44
1:G:622:GLU:HB2	1:G:641:PRO:HD2	2.00	0.44
1:H:214:TYR:HB3	1:H:215:ARG:NH1	2.33	0.44
1:I:240:HIS:CD2	1:I:319:ALA:HB2	2.47	0.44
1:I:409:GLU:O	1:I:413:GLN:HG2	2.18	0.44
1:L:95:GLU:HB3	1:L:147:VAL:HG11	2.00	0.44
1:A:265:TRP:HB2	1:A:287:PRO:HD2	2.00	0.43
1:D:142:LYS:HA	1:D:142:LYS:HD3	1.64	0.43
1:L:590:TYR:CE2	1:L:646:MET:HE1	2.53	0.43
1:G:215:ARG:HD2	1:G:215:ARG:N	2.32	0.43
1:I:233:ASN:O	1:I:311:PRO:HG3	2.19	0.43
1:K:567:GLU:H	1:K:567:GLU:HG3	1.38	0.43
1:L:144:ASN:O	1:L:144:ASN:ND2	2.52	0.43
1:L:265:TRP:HB2	1:L:287:PRO:HD2	1.99	0.43
1:A:92:THR:HG21	1:A:146:HIS:HB3	1.99	0.43
1:D:545:THR:OG1	1:D:546:GLY:N	2.50	0.43
1:E:534:GLN:HA	1:E:538:MET:HB2	2.01	0.43
1:F:409:GLU:O	1:F:413:GLN:HG2	2.18	0.43
1:H:533:PRO:HG3	1:H:638:TYR:CE2	2.53	0.43
1:I:21:LEU:HD23	1:I:21:LEU:HA	1.80	0.43
1:I:106:LEU:HD22	1:I:126:SER:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:HIS:O	1:L:106:LEU:HB2	2.17	0.43
1:E:174:VAL:HG21	1:E:567:GLU:HB3	1.99	0.43
1:G:173:ASN:HD22	1:L:29:LYS:NZ	2.16	0.43
1:B:531:ASN:ND2	1:B:534:GLN:OE1	2.52	0.43
1:C:527:HIS:NE2	1:C:648:ILE:HG23	2.33	0.43
1:G:212:ALA:HB2	1:G:302:PRO:HD3	2.00	0.43
1:J:635:LYS:HE3	1:J:635:LYS:HB3	1.87	0.43
1:B:216:VAL:HG13	1:B:300:LEU:HD22	2.01	0.43
1:I:231:PRO:HG2	1:I:234:PHE:HB3	2.01	0.43
1:J:316:LYS:HE2	1:J:316:LYS:HA	2.00	0.43
1:K:358:VAL:HG22	1:K:379:PHE:CG	2.54	0.43
1:K:429:LEU:O	1:K:433:ILE:HG12	2.18	0.43
1:A:53:TRP:CE3	1:A:54:LEU:HD23	2.53	0.43
1:A:230:LEU:HD11	1:A:236:VAL:HG22	2.01	0.43
1:A:282:LYS:HB3	1:A:547:ALA:HB1	2.01	0.43
1:B:134:ARG:CZ	1:B:148:PRO:HG2	2.49	0.43
1:C:373:MET:HA	1:C:600:TRP:CZ3	2.53	0.43
1:H:559:LEU:O	1:H:563:GLN:HG2	2.19	0.43
1:J:463:TRP:HB2	1:J:614:PHE:CD1	2.53	0.43
1:J:527:HIS:CG	1:J:648:ILE:HG12	2.54	0.43
1:K:201:ILE:HG12	1:K:214:TYR:OH	2.18	0.43
1:L:35:PRO:CB	1:L:36:PRO:HD2	2.47	0.43
1:L:372:TYR:CE2	1:L:376:ILE:HG13	2.54	0.43
1:C:21:LEU:HD23	1:C:21:LEU:HA	1.82	0.43
1:C:408:ILE:HG13	1:C:412:HIS:HE1	1.84	0.43
1:E:57:VAL:HG22	1:E:582:VAL:HG21	1.99	0.43
1:G:533:PRO:HG3	1:G:638:TYR:CE2	2.54	0.43
1:I:211:PHE:CG	1:I:330:LYS:HD2	2.53	0.43
1:I:585:THR:O	1:I:645:PRO:HA	2.18	0.43
1:L:174:VAL:HG11	1:L:567:GLU:HB3	2.01	0.43
1:A:95:GLU:CD	1:A:147:VAL:HG11	2.44	0.43
1:C:102:HIS:O	1:C:106:LEU:HB2	2.19	0.43
1:C:612:PRO:O	1:C:616:ARG:HG3	2.19	0.43
1:D:145:ARG:H	1:D:145:ARG:HG3	1.41	0.43
1:D:358:VAL:HG22	1:D:379:PHE:CG	2.54	0.43
1:F:215:ARG:HD2	1:F:215:ARG:H	1.84	0.43
1:G:139:LEU:HD22	1:G:393:LEU:HD13	2.00	0.43
1:L:373:MET:HA	1:L:600:TRP:CZ3	2.54	0.43
1:B:69:VAL:HG11	1:B:93:SER:HB2	2.00	0.43
1:F:20:GLN:NE2	1:F:367:GLN:HG3	2.34	0.43
1:F:585:THR:O	1:F:645:PRO:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:233:ASN:O	1:G:306:GLN:NE2	2.45	0.43
1:G:316:LYS:NZ	1:G:317:ILE:H	2.17	0.43
1:H:462:ARG:NH1	1:H:617:ASP:OD2	2.47	0.43
1:I:504:GLY:HA2	1:I:505:PRO:HA	1.70	0.43
1:J:341:HIS:O	1:J:346:HIS:N	2.50	0.43
1:A:35:PRO:CB	1:A:36:PRO:HD2	2.49	0.42
1:A:307:PRO:HB3	1:A:553:PRO:HG2	2.01	0.42
1:B:125:PRO:HB2	1:B:126:SER:H	1.52	0.42
1:B:408:ILE:HD12	1:B:408:ILE:HA	1.91	0.42
1:C:37:LEU:HD23	1:C:37:LEU:HA	1.87	0.42
1:I:37:LEU:HD23	1:I:37:LEU:HA	1.82	0.42
1:J:408:ILE:HD12	1:J:408:ILE:HA	1.85	0.42
1:C:65:ALA:O	1:C:69:VAL:HG23	2.19	0.42
1:D:203:SER:O	1:K:10:ASN:HB3	2.19	0.42
1:E:429:LEU:O	1:E:433:ILE:HG12	2.19	0.42
1:G:76:LYS:HB3	1:G:76:LYS:HE2	1.78	0.42
1:I:220:ASN:HB3	1:I:337:GLU:CD	2.44	0.42
1:J:87:PHE:O	1:J:91:GLY:N	2.45	0.42
1:L:553:PRO:N	1:L:554:PRO:HD2	2.34	0.42
1:L:612:PRO:O	1:L:616:ARG:HG3	2.19	0.42
1:C:538:MET:HG2	1:C:544:ILE:HD13	2.01	0.42
1:F:533:PRO:HG3	1:F:638:TYR:CE2	2.54	0.42
1:F:586:LYS:HA	1:F:586:LYS:HD3	1.74	0.42
1:G:606:ILE:HA	1:G:610:LEU:HB2	2.00	0.42
1:H:610:LEU:HA	1:H:610:LEU:HD12	1.73	0.42
1:H:646:MET:HE3	1:H:646:MET:HB3	1.80	0.42
1:K:125:PRO:HB2	1:K:126:SER:H	1.63	0.42
1:A:553:PRO:N	1:A:554:PRO:HD2	2.34	0.42
1:B:147:VAL:HG22	1:B:148:PRO:O	2.20	0.42
1:C:377:PRO:HD3	1:C:600:TRP:CZ3	2.54	0.42
1:D:582:VAL:HB	1:D:650:ILE:HG13	2.02	0.42
1:E:646:MET:HE3	1:E:646:MET:HB3	1.92	0.42
1:F:33:LEU:HD12	1:F:39:PHE:CD1	2.54	0.42
1:F:35:PRO:CB	1:F:36:PRO:HD2	2.49	0.42
1:F:316:LYS:HD2	1:F:316:LYS:HA	1.66	0.42
1:G:186:MET:HE3	1:G:186:MET:HB3	1.95	0.42
1:G:409:GLU:CD	1:G:409:GLU:H	2.28	0.42
1:G:467:TYR:HE2	1:G:606:ILE:HD13	1.84	0.42
1:G:646:MET:HE3	1:G:646:MET:HB3	1.83	0.42
1:H:30:TYR:CE1	1:H:38:ALA:HB1	2.53	0.42
1:D:376:ILE:HD13	1:D:376:ILE:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:GLU:H	1:D:567:GLU:HG3	1.47	0.42
1:E:604:PRO:HA	1:E:607:THR:HB	2.02	0.42
1:F:307:PRO:HG2	1:F:315:ASN:ND2	2.35	0.42
1:K:174:VAL:HG11	1:K:567:GLU:HB3	2.01	0.42
1:K:353:LEU:O	1:K:356:PRO:HD2	2.19	0.42
1:L:422:HIS:O	1:L:501:SER:HB2	2.20	0.42
1:A:139:LEU:HD21	1:A:579:LEU:HD21	2.01	0.42
1:D:34:LEU:HA	1:D:34:LEU:HD22	1.68	0.42
1:G:376:ILE:N	1:G:377:PRO:HD2	2.35	0.42
1:J:635:LYS:H	1:J:635:LYS:HG2	1.53	0.42
1:K:53:TRP:CE2	1:K:57:VAL:HG21	2.54	0.42
1:B:284:VAL:HG23	1:B:335:VAL:HG12	2.02	0.42
1:C:87:PHE:HD1	1:C:87:PHE:HA	1.71	0.42
1:D:553:PRO:N	1:D:554:PRO:HD2	2.35	0.42
1:E:110:GLU:HB3	1:E:595:PHE:CD1	2.55	0.42
1:H:223:MET:HE2	1:H:265:TRP:CE2	2.54	0.42
1:H:330:LYS:HE3	1:H:330:LYS:HB2	1.76	0.42
1:L:438:VAL:O	1:L:450:ARG:NH1	2.43	0.42
1:C:252:ASP:HA	1:C:255:LYS:HG2	2.01	0.42
1:C:573:ALA:O	1:C:577:TYR:HB2	2.20	0.42
1:E:51:ALA:O	1:E:55:VAL:HG23	2.20	0.42
1:E:307:PRO:HB3	1:E:553:PRO:HG2	2.01	0.42
1:H:192:LEU:HD22	1:H:570:GLU:HB2	2.02	0.42
1:K:20:GLN:NE2	1:K:367:GLN:HG3	2.35	0.42
1:C:30:TYR:CE1	1:C:38:ALA:HB1	2.55	0.42
1:D:341:HIS:HA	1:D:345:SER:HB2	2.02	0.42
1:E:145:ARG:NH1	1:E:574:GLU:OE1	2.53	0.42
1:E:307:PRO:HG2	1:E:315:ASN:ND2	2.34	0.42
1:G:173:ASN:CG	1:G:174:VAL:H	2.26	0.42
1:K:57:VAL:HG22	1:K:582:VAL:HG21	2.02	0.42
1:K:273:VAL:O	1:K:406:GLY:HA2	2.20	0.42
1:L:45:LYS:HA	1:L:45:LYS:HD2	1.87	0.42
1:L:606:ILE:HA	1:L:610:LEU:HB2	2.02	0.42
1:A:567:GLU:HG3	1:A:567:GLU:H	1.44	0.42
1:D:77:ARG:H	1:D:77:ARG:HG3	1.53	0.42
1:D:588:GLY:O	1:D:615:GLN:NE2	2.51	0.42
1:E:471:TYR:CE2	1:E:606:ILE:HD11	2.53	0.42
1:E:533:PRO:HG3	1:E:638:TYR:CE2	2.55	0.42
1:F:87:PHE:O	1:F:91:GLY:N	2.44	0.42
1:F:144:ASN:C	1:F:146:HIS:H	2.28	0.42
1:G:139:LEU:HD21	1:G:579:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:ASP:N	1:E:187:ASP:OD1	2.53	0.41
1:G:72:ARG:HD2	1:G:146:HIS:CE1	2.54	0.41
1:G:549:TRP:CD1	1:G:564:PRO:HA	2.54	0.41
1:I:45:LYS:HA	1:I:45:LYS:HD2	1.94	0.41
1:I:182:ARG:HE	1:I:182:ARG:HA	1.84	0.41
1:J:53:TRP:HE1	1:J:649:ASN:HB2	1.84	0.41
1:K:182:ARG:NH2	1:K:563:GLN:O	2.53	0.41
1:A:297:GLY:HA2	1:A:443:VAL:O	2.20	0.41
1:C:400:VAL:HA	1:C:404:PHE:CD1	2.55	0.41
1:C:504:GLY:HA2	1:C:505:PRO:HA	1.85	0.41
1:D:372:TYR:CZ	1:D:376:ILE:HG13	2.55	0.41
1:D:428:GLY:O	1:D:432:THR:HG23	2.20	0.41
1:H:372:TYR:CZ	1:H:376:ILE:HG13	2.55	0.41
1:I:145:ARG:NH1	1:I:574:GLU:OE1	2.53	0.41
1:J:231:PRO:HG2	1:J:234:PHE:HB3	2.03	0.41
1:J:646:MET:HE3	1:J:646:MET:HB3	1.93	0.41
1:B:463:TRP:HB2	1:B:614:PHE:CG	2.54	0.41
1:D:471:TYR:HE2	1:D:606:ILE:HD11	1.85	0.41
1:E:378:HIS:CE1	1:E:520:ILE:HG23	2.55	0.41
1:E:605:LYS:O	1:E:609:GLU:HB3	2.20	0.41
1:F:359:MET:O	1:F:363:ARG:HG3	2.20	0.41
1:H:464:VAL:HG12	1:H:513:ILE:HG23	2.02	0.41
1:I:376:ILE:HD13	1:I:376:ILE:HA	1.95	0.41
1:J:35:PRO:CB	1:J:36:PRO:HD2	2.51	0.41
1:J:47:ASP:OD2	1:J:383:LEU:HD12	2.20	0.41
1:A:77:ARG:HE	1:A:77:ARG:HB3	1.69	0.41
1:D:622:GLU:HB2	1:D:641:PRO:HD2	2.01	0.41
1:F:182:ARG:HH21	1:F:561:ASP:HA	1.85	0.41
1:F:486:ALA:O	1:F:490:VAL:HG12	2.20	0.41
1:G:385:ILE:HD12	1:G:385:ILE:HA	1.92	0.41
1:I:377:PRO:HB2	1:I:646:MET:HE1	2.02	0.41
1:I:605:LYS:O	1:I:609:GLU:HB3	2.21	0.41
1:J:358:VAL:HG11	1:J:383:LEU:HG	2.02	0.41
1:K:403:ILE:HD11	1:K:571:LEU:HG	2.02	0.41
1:K:553:PRO:N	1:K:554:PRO:HD2	2.35	0.41
1:L:241:TYR:CZ	1:L:245:MET:HG3	2.55	0.41
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.82	0.41
1:A:400:VAL:O	1:A:404:PHE:HB2	2.19	0.41
1:C:590:TYR:CE2	1:C:646:MET:HE1	2.56	0.41
1:E:33:LEU:HD12	1:E:39:PHE:HD2	1.84	0.41
1:E:552:ALA:HB1	1:E:554:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:576:LEU:HD23	1:E:576:LEU:HA	1.93	0.41
1:F:330:LYS:O	1:F:334:GLN:HG2	2.20	0.41
1:F:378:HIS:CE1	1:F:520:ILE:HG23	2.55	0.41
1:F:567:GLU:HG3	1:F:567:GLU:H	1.57	0.41
1:K:369:HIS:HD2	1:K:483:GLU:OE1	2.03	0.41
1:C:92:THR:HG21	1:C:146:HIS:HB3	2.02	0.41
1:C:265:TRP:HB2	1:C:287:PRO:HD2	2.03	0.41
1:D:193:PHE:HB3	1:D:196:ILE:O	2.20	0.41
1:E:640:ILE:O	1:E:644:ILE:HG13	2.21	0.41
1:G:110:GLU:HB3	1:G:595:PHE:CE1	2.55	0.41
1:I:25:ARG:NH1	1:I:363:ARG:O	2.54	0.41
1:I:307:PRO:HB3	1:I:553:PRO:HG2	2.02	0.41
1:J:20:GLN:NE2	1:J:367:GLN:HG3	2.36	0.41
1:A:110:GLU:HB3	1:A:595:PHE:CD1	2.55	0.41
1:A:646:MET:HE3	1:A:646:MET:HB3	1.87	0.41
1:D:233:ASN:OD1	1:D:233:ASN:N	2.46	0.41
1:E:77:ARG:H	1:E:77:ARG:HG3	1.35	0.41
1:I:148:PRO:CB	1:I:149:PRO:HD2	2.51	0.41
1:I:602:LYS:HD3	1:I:602:LYS:HA	1.79	0.41
1:J:144:ASN:C	1:J:146:HIS:H	2.28	0.41
1:K:192:LEU:HD22	1:K:570:GLU:HB2	2.02	0.41
1:A:57:VAL:O	1:A:60:VAL:N	2.53	0.41
1:A:252:ASP:HA	1:A:255:LYS:HE3	2.03	0.41
1:A:378:HIS:CE1	1:A:520:ILE:HG23	2.56	0.41
1:A:533:PRO:HG3	1:A:638:TYR:CE2	2.55	0.41
1:D:34:LEU:HD21	1:D:412:HIS:HE1	1.86	0.41
1:E:145:ARG:H	1:E:145:ARG:HG3	1.57	0.41
1:E:590:TYR:CE2	1:E:646:MET:HE1	2.56	0.41
1:G:486:ALA:O	1:G:490:VAL:HG12	2.20	0.41
1:H:145:ARG:NH1	1:H:574:GLU:OE1	2.54	0.41
1:A:125:PRO:HB2	1:A:126:SER:H	1.72	0.41
1:A:359:MET:O	1:A:363:ARG:HG3	2.21	0.41
1:A:372:TYR:CZ	1:A:376:ILE:HG13	2.55	0.41
1:B:316:LYS:HD2	1:B:316:LYS:HA	1.83	0.41
1:C:91:GLY:O	1:C:95:GLU:HG3	2.21	0.41
1:D:180:ASN:HA	1:D:567:GLU:HG3	2.02	0.41
1:D:408:ILE:O	1:D:412:HIS:HD2	2.04	0.41
1:E:528:SER:OG	1:E:638:TYR:O	2.36	0.41
1:H:53:TRP:CZ2	1:H:57:VAL:HG21	2.55	0.41
1:H:234:PHE:HB2	1:H:288:LEU:HD22	2.03	0.41
1:H:376:ILE:HD13	1:H:376:ILE:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:199:PRO:HA	1:I:200:PRO:HD3	1.97	0.41
1:I:376:ILE:N	1:I:377:PRO:HD2	2.36	0.41
1:I:451:ASP:O	1:I:455:LYS:HG3	2.21	0.41
1:J:542:PRO:HA	1:J:563:GLN:OE1	2.21	0.41
1:J:579:LEU:HA	1:J:650:ILE:HG21	2.03	0.41
1:K:35:PRO:C	1:K:37:LEU:H	2.29	0.41
1:K:350:THR:OG1	1:K:351:HIS:N	2.54	0.41
1:K:585:THR:CG2	1:K:646:MET:H	2.26	0.41
1:L:21:LEU:HD23	1:L:21:LEU:HA	1.84	0.41
1:L:567:GLU:HG3	1:L:567:GLU:H	1.55	0.41
1:L:586:LYS:C	1:L:646:MET:HG2	2.46	0.41
1:A:65:ALA:O	1:A:69:VAL:HG23	2.21	0.41
1:A:534:GLN:HA	1:A:538:MET:HE2	2.01	0.41
1:D:598:ARG:HG3	1:D:599:ALA:H	1.86	0.41
1:G:350:THR:OG1	1:G:351:HIS:N	2.54	0.41
1:H:173:ASN:N	3:H:806:HOH:O	2.53	0.41
1:I:189:TYR:CZ	1:I:563:GLN:HB2	2.56	0.41
1:B:139:LEU:HD22	1:B:393:LEU:HD13	2.03	0.40
1:F:429:LEU:O	1:F:433:ILE:HG12	2.20	0.40
1:H:403:ILE:HD11	1:H:571:LEU:HG	2.02	0.40
1:H:429:LEU:O	1:H:433:ILE:HG12	2.21	0.40
1:J:40:CYS:HB2	1:J:383:LEU:HD22	2.01	0.40
1:J:396:PRO:HG3	1:J:408:ILE:HG21	2.03	0.40
1:J:585:THR:CG2	1:J:646:MET:H	2.33	0.40
1:K:45:LYS:HD2	1:K:45:LYS:HA	1.85	0.40
1:L:273:VAL:O	1:L:407:THR:HG23	2.21	0.40
1:B:21:LEU:HD23	1:B:21:LEU:HA	1.96	0.40
1:E:10:ASN:HB3	1:J:203:SER:O	2.20	0.40
1:F:287:PRO:HG2	1:F:333:VAL:HA	2.03	0.40
1:H:640:ILE:O	1:H:644:ILE:HG13	2.22	0.40
1:J:383:LEU:HD23	1:J:383:LEU:HA	1.95	0.40
1:J:576:LEU:HD23	1:J:576:LEU:HA	1.92	0.40
1:L:335:VAL:HA	1:L:545:THR:O	2.21	0.40
1:L:622:GLU:HB2	1:L:641:PRO:HD2	2.03	0.40
1:A:214:TYR:HB3	1:A:215:ARG:NH1	2.36	0.40
1:A:244:ALA:HB2	1:A:320:THR:OG1	2.21	0.40
1:C:4:ILE:HA	1:C:5:PRO:HD3	1.98	0.40
1:E:144:ASN:C	1:E:146:HIS:H	2.30	0.40
1:I:35:PRO:CB	1:I:36:PRO:HD2	2.51	0.40
1:K:624:LEU:HD12	1:K:624:LEU:HA	1.93	0.40
1:A:249:ASP:OD1	1:A:250:SER:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASN:O	1:B:144:ASN:ND2	2.53	0.40
1:D:277:TYR:OH	1:D:567:GLU:OE1	2.25	0.40
1:E:277:TYR:HB2	1:E:282:LYS:HD2	2.03	0.40
1:I:21:LEU:HB3	1:I:25:ARG:NH2	2.37	0.40
1:K:239:ALA:O	1:K:243:GLN:HG3	2.22	0.40
1:K:376:ILE:HD13	1:K:376:ILE:HA	1.92	0.40
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.89	0.40
1:C:275:ASN:CG	1:C:276:THR:H	2.28	0.40
1:C:605:LYS:O	1:C:609:GLU:HB3	2.21	0.40
1:I:318:TYR:CE1	1:I:325:ASP:HB3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7143/7800 (92%)	6738 (94%)	346 (5%)	59 (1%)	16	44

All (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
1	C	36	PRO
1	C	149	PRO
1	D	36	PRO
1	D	125	PRO
1	D	149	PRO
1	E	36	PRO
1	E	149	PRO
1	F	36	PRO
1	F	125	PRO
1	F	149	PRO
1	G	36	PRO
1	G	149	PRO
1	H	36	PRO
1	H	149	PRO
1	I	36	PRO
1	I	149	PRO
1	J	36	PRO
1	J	149	PRO
1	K	36	PRO
1	K	149	PRO
1	L	36	PRO
1	L	149	PRO
1	D	112	PHE
1	H	175	SER
1	I	585	THR
1	G	585	THR
1	J	585	THR
1	A	106	LEU
1	A	143	PRO
1	D	554	PRO
1	E	554	PRO
1	E	585	THR

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Mol	Chain	Res	Type
1	G	550	THR
1	H	585	THR
1	I	554	PRO
1	L	585	THR
1	E	609	GLU
1	F	148	PRO
1	F	585	THR
1	G	148	PRO
1	A	110	GLU
1	A	128	LEU
1	A	219	PRO
1	D	150	ALA
1	E	344	VAL
1	B	554	PRO
1	B	307	PRO
1	G	554	PRO
1	J	554	PRO
1	E	505	PRO
1	B	505	PRO
1	K	505	PRO
1	D	505	PRO
1	F	505	PRO

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (400) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	13	ARG
1	A	22	ASP
1	A	34	LEU
1	A	39	PHE
1	A	64	VAL
1	A	76	LYS
1	A	88	ASP
1	A	89	VAL
1	A	94	GLU
1	A	109	LEU
1	A	127	VAL
1	A	215	ARG
1	A	222	SER
1	A	252	ASP
1	A	272	LEU
1	A	283	THR
1	A	299	SER
1	A	314	THR
1	A	320	THR
1	A	337	GLU
1	A	354	LEU
1	A	376	ILE
1	A	409	GLU
1	A	419	LEU
1	A	425	MET
1	A	454	LEU
1	A	473	ILE
1	A	479	THR
1	A	490	VAL

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Mol	Chain	Res	Type
1	A	501	SER
1	A	567	GLU
1	A	593	ASN
1	A	607	THR
1	A	626	VAL
1	A	629	ASN
1	A	643	THR
1	A	650	ILE
1	B	27	THR
1	B	34	LEU
1	B	39	PHE
1	B	47	ASP
1	B	64	VAL
1	B	87	PHE
1	B	105	PHE
1	B	109	LEU
1	B	127	VAL
1	B	146	HIS
1	B	176	LYS
1	B	209	SER
1	B	215	ARG
1	B	223	MET
1	B	229	GLU
1	B	236	VAL
1	B	245	MET
1	B	262	LEU
1	B	272	LEU
1	B	310	THR
1	B	314	THR
1	B	320	THR
1	B	321	GLN
1	B	387	ASN
1	B	407	THR
1	B	409	GLU
1	B	425	MET
1	B	490	VAL
1	B	522	THR
1	B	556	GLN
1	B	567	GLU
1	B	607	THR
1	B	610	LEU
1	B	629	ASN

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Mol	Chain	Res	Type
1	B	633	THR
1	B	649	ASN
1	B	650	ILE
1	C	6	THR
1	C	13	ARG
1	C	15	GLU
1	C	23	LYS
1	C	34	LEU
1	C	41	GLU
1	C	48	THR
1	C	59	LYS
1	C	87	PHE
1	C	88	ASP
1	C	89	VAL
1	C	94	GLU
1	C	98	ASN
1	C	127	VAL
1	C	147	VAL
1	C	184	GLN
1	C	203	SER
1	C	209	SER
1	C	215	ARG
1	C	225	GLN
1	C	236	VAL
1	C	276	THR
1	C	299	SER
1	C	320	THR
1	C	394	ILE
1	C	425	MET
1	C	444	LEU
1	C	544	ILE
1	C	556	GLN
1	C	567	GLU
1	C	585	THR
1	C	593	ASN
1	C	610	LEU
1	C	617	ASP
1	C	650	ILE
1	D	33	LEU
1	D	34	LEU
1	D	39	PHE
1	D	41	GLU

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Mol	Chain	Res	Type
1	D	47	ASP
1	D	48	THR
1	D	77	ARG
1	D	127	VAL
1	D	145	ARG
1	D	147	VAL
1	D	215	ARG
1	D	228	THR
1	D	229	GLU
1	D	236	VAL
1	D	245	MET
1	D	272	LEU
1	D	310	THR
1	D	316	LYS
1	D	320	THR
1	D	343	LEU
1	D	409	GLU
1	D	425	MET
1	D	441	THR
1	D	473	ILE
1	D	507	ASP
1	D	522	THR
1	D	544	ILE
1	D	545	THR
1	D	567	GLU
1	D	575	PHE
1	D	585	THR
1	D	622	GLU
1	D	631	THR
1	D	637	THR
1	E	22	ASP
1	E	27	THR
1	E	48	THR
1	E	77	ARG
1	E	87	PHE
1	E	89	VAL
1	E	94	GLU
1	E	102	HIS
1	E	105	PHE
1	E	127	VAL
1	E	145	ARG
1	E	176	LYS

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Mol	Chain	Res	Type
1	E	204	THR
1	E	215	ARG
1	E	222	SER
1	E	225	GLN
1	E	228	THR
1	E	229	GLU
1	E	236	VAL
1	E	247	GLU
1	E	278	LYS
1	E	314	THR
1	E	316	LYS
1	E	320	THR
1	E	331	SER
1	E	343	LEU
1	E	391	THR
1	E	409	GLU
1	E	425	MET
1	E	441	THR
1	E	490	VAL
1	E	556	GLN
1	E	567	GLU
1	E	575	PHE
1	E	585	THR
1	E	586	LYS
1	E	600	TRP
1	E	610	LEU
1	E	624	LEU
1	E	631	THR
1	E	637	THR
1	E	650	ILE
1	F	6	THR
1	F	32	ASP
1	F	89	VAL
1	F	94	GLU
1	F	106	LEU
1	F	109	LEU
1	F	144	ASN
1	F	204	THR
1	F	215	ARG
1	F	233	ASN
1	F	236	VAL
1	F	276	THR

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Mol	Chain	Res	Type
1	F	300	LEU
1	F	314	THR
1	F	320	THR
1	F	409	GLU
1	F	425	MET
1	F	461	GLU
1	F	490	VAL
1	F	508	THR
1	F	522	THR
1	F	544	ILE
1	F	567	GLU
1	F	575	PHE
1	F	585	THR
1	F	642	SER
1	F	650	ILE
1	G	26	GLU
1	G	39	PHE
1	G	47	ASP
1	G	64	VAL
1	G	77	ARG
1	G	89	VAL
1	G	103	ASN
1	G	105	PHE
1	G	127	VAL
1	G	142	LYS
1	G	144	ASN
1	G	147	VAL
1	G	180	ASN
1	G	184	GLN
1	G	204	THR
1	G	222	SER
1	G	228	THR
1	G	233	ASN
1	G	236	VAL
1	G	238	ASP
1	G	245	MET
1	G	283	THR
1	G	288	LEU
1	G	310	THR
1	G	316	LYS
1	G	354	LEU
1	G	409	GLU

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Mol	Chain	Res	Type
1	G	425	MET
1	G	463	TRP
1	G	473	ILE
1	G	490	VAL
1	G	522	THR
1	G	535	LYS
1	G	539	SER
1	G	560	LYS
1	G	567	GLU
1	G	585	THR
1	G	593	ASN
1	G	600	TRP
1	G	606	ILE
1	G	637	THR
1	G	643	THR
1	H	3	ASN
1	H	6	THR
1	H	127	VAL
1	H	187	ASP
1	H	215	ARG
1	H	225	GLN
1	H	247	GLU
1	H	299	SER
1	H	310	THR
1	H	314	THR
1	H	331	SER
1	H	407	THR
1	H	425	MET
1	H	442	SER
1	H	519	VAL
1	H	535	LYS
1	H	556	GLN
1	H	567	GLU
1	H	575	PHE
1	H	585	THR
1	H	598	ARG
1	H	600	TRP
1	H	610	LEU
1	H	629	ASN
1	H	650	ILE
1	I	6	THR
1	I	32	ASP

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Mol	Chain	Res	Type
1	I	39	PHE
1	I	48	THR
1	I	95	GLU
1	I	127	VAL
1	I	146	HIS
1	I	147	VAL
1	I	182	ARG
1	I	204	THR
1	I	215	ARG
1	I	222	SER
1	I	233	ASN
1	I	236	VAL
1	I	245	MET
1	I	257	GLU
1	I	310	THR
1	I	320	THR
1	I	331	SER
1	I	434	GLU
1	I	490	VAL
1	I	522	THR
1	I	539	SER
1	I	607	THR
1	I	610	LEU
1	I	633	THR
1	I	642	SER
1	I	649	ASN
1	I	650	ILE
1	J	23	LYS
1	J	34	LEU
1	J	39	PHE
1	J	64	VAL
1	J	89	VAL
1	J	94	GLU
1	J	98	ASN
1	J	102	HIS
1	J	112	PHE
1	J	128	LEU
1	J	176	LYS
1	J	187	ASP
1	J	215	ARG
1	J	224	ILE
1	J	228	THR

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Mol	Chain	Res	Type
1	J	236	VAL
1	J	249	ASP
1	J	268	ILE
1	J	314	THR
1	J	316	LYS
1	J	409	GLU
1	J	490	VAL
1	J	539	SER
1	J	556	GLN
1	J	567	GLU
1	J	585	THR
1	J	598	ARG
1	J	600	TRP
1	J	607	THR
1	J	610	LEU
1	J	617	ASP
1	J	635	LYS
1	J	649	ASN
1	J	650	ILE
1	K	6	THR
1	K	32	ASP
1	K	48	THR
1	K	50	SER
1	K	94	GLU
1	K	106	LEU
1	K	127	VAL
1	K	176	LYS
1	K	184	GLN
1	K	204	THR
1	K	215	ARG
1	K	233	ASN
1	K	247	GLU
1	K	310	THR
1	K	316	LYS
1	K	320	THR
1	K	343	LEU
1	K	425	MET
1	K	535	LYS
1	K	567	GLU
1	K	575	PHE
1	K	585	THR
1	K	600	TRP

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Mol	Chain	Res	Type
1	K	607	THR
1	K	643	THR
1	L	6	THR
1	L	22	ASP
1	L	33	LEU
1	L	34	LEU
1	L	47	ASP
1	L	88	ASP
1	L	89	VAL
1	L	94	GLU
1	L	173	ASN
1	L	176	LYS
1	L	203	SER
1	L	215	ARG
1	L	222	SER
1	L	225	GLN
1	L	229	GLU
1	L	236	VAL
1	L	247	GLU
1	L	272	LEU
1	L	278	LYS
1	L	314	THR
1	L	316	LYS
1	L	320	THR
1	L	425	MET
1	L	438	VAL
1	L	513	ILE
1	L	556	GLN
1	L	567	GLU
1	L	585	THR
1	L	600	TRP
1	L	606	ILE
1	L	610	LEU
1	L	624	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	191	ASN
1	A	387	ASN
1	A	392	ASN

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Mol	Chain	Res	Type
1	A	534	GLN
1	A	584	HIS
1	B	387	ASN
1	B	584	HIS
1	B	591	ASN
1	B	649	ASN
1	C	191	ASN
1	C	225	GLN
1	C	306	GLN
1	C	339	ASN
1	C	435	GLN
1	C	531	ASN
1	C	534	GLN
1	C	591	ASN
1	D	346	HIS
1	D	459	ASN
1	D	556	GLN
1	D	584	HIS
1	D	591	ASN
1	D	649	ASN
1	E	281	GLN
1	E	435	GLN
1	E	459	ASN
1	E	531	ASN
1	E	534	GLN
1	E	584	HIS
1	F	146	HIS
1	G	111	ASN
1	G	173	ASN
1	G	180	ASN
1	G	243	GLN
1	G	531	ASN
1	G	584	HIS
1	H	144	ASN
1	H	180	ASN
1	H	274	ASN
1	H	334	GLN
1	H	387	ASN
1	H	531	ASN
1	H	584	HIS
1	I	103	ASN
1	I	309	GLN

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Mol	Chain	Res	Type
1	I	534	GLN
1	I	563	GLN
1	J	364	GLN
1	J	531	ASN
1	K	98	ASN
1	K	180	ASN
1	K	240	HIS
1	K	306	GLN
1	K	334	GLN
1	K	387	ASN
1	K	477	ASN
1	K	584	HIS
1	L	144	ASN
1	L	191	ASN
1	L	243	GLN
1	L	306	GLN
1	L	346	HIS
1	L	364	GLN
1	L	368	HIS
1	L	392	ASN
1	L	459	ASN
1	L	534	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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

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	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

All (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
1	I	106	LEU	7.3
1	J	585	THR	7.2
1	J	106	LEU	6.9
1	F	553	PRO	6.9
1	H	106	LEU	6.6
1	G	553	PRO	6.4

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Mol	Chain	Res	Type	RSRZ
1	D	553	PRO	6.3
1	C	553	PRO	6.2
1	L	128	LEU	6.2
1	G	106	LEU	6.1
1	B	106	LEU	6.0
1	H	128	LEU	6.0
1	H	553	PRO	5.8
1	G	109	LEU	5.8
1	B	173	ASN	5.7
1	H	146	HIS	5.7
1	I	107	ALA	5.6
1	J	112	PHE	5.6
1	G	36	PRO	5.6
1	K	36	PRO	5.5
1	L	553	PRO	5.5
1	D	33	LEU	5.4
1	A	551	ALA	5.4
1	D	112	PHE	5.4
1	A	106	LEU	5.4
1	F	106	LEU	5.4
1	J	553	PRO	5.3
1	K	553	PRO	5.3
1	K	33	LEU	5.3
1	A	128	LEU	5.2
1	E	128	LEU	5.1
1	C	36	PRO	5.1
1	F	585	THR	5.1
1	F	147	VAL	5.0
1	B	109	LEU	5.0
1	I	128	LEU	5.0
1	B	36	PRO	4.9
1	C	551	ALA	4.9
1	J	109	LEU	4.8
1	L	595	PHE	4.8
1	E	553	PRO	4.8
1	H	33	LEU	4.8
1	E	595	PHE	4.7
1	D	36	PRO	4.7
1	E	125	PRO	4.7
1	G	125	PRO	4.7
1	D	89	VAL	4.7
1	C	33	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	G	128	LEU	4.6
1	E	106	LEU	4.6
1	I	634	PHE	4.6
1	K	89	VAL	4.6
1	H	36	PRO	4.5
1	H	634	PHE	4.5
1	A	172	GLY	4.5
1	I	89	VAL	4.5
1	F	109	LEU	4.4
1	L	146	HIS	4.4
1	H	552	ALA	4.3
1	A	553	PRO	4.2
1	D	105	PHE	4.2
1	E	105	PHE	4.2
1	H	105	PHE	4.2
1	K	149	PRO	4.2
1	E	551	ALA	4.2
1	D	174	VAL	4.2
1	K	125	PRO	4.1
1	I	36	PRO	4.1
1	A	552	ALA	4.1
1	J	128	LEU	4.1
1	A	36	PRO	4.0
1	A	149	PRO	4.0
1	B	588	GLY	4.0
1	A	109	LEU	4.0
1	F	126	SER	4.0
1	B	635	LYS	3.9
1	E	109	LEU	3.9
1	I	551	ALA	3.9
1	F	42	GLY	3.9
1	B	105	PHE	3.8
1	B	174	VAL	3.8
1	D	585	THR	3.8
1	L	106	LEU	3.8
1	G	552	ALA	3.8
1	C	105	PHE	3.7
1	E	552	ALA	3.7
1	B	504	GLY	3.7
1	J	125	PRO	3.7
1	K	94	GLU	3.7
1	C	128	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	551	ALA	3.7
1	J	176	LYS	3.7
1	H	125	PRO	3.7
1	B	3	ASN	3.7
1	B	89	VAL	3.7
1	B	125	PRO	3.7
1	G	95	GLU	3.7
1	H	94	GLU	3.7
1	C	109	LEU	3.6
1	E	33	LEU	3.6
1	H	109	LEU	3.6
1	L	105	PHE	3.6
1	F	33	LEU	3.6
1	C	147	VAL	3.6
1	I	147	VAL	3.6
1	J	148	PRO	3.6
1	I	109	LEU	3.6
1	B	553	PRO	3.5
1	C	106	LEU	3.5
1	D	128	LEU	3.5
1	B	551	ALA	3.5
1	G	105	PHE	3.5
1	D	146	HIS	3.5
1	I	148	PRO	3.5
1	J	147	VAL	3.5
1	K	109	LEU	3.5
1	J	107	ALA	3.5
1	A	95	GLU	3.5
1	K	146	HIS	3.5
1	A	131	VAL	3.4
1	E	31	ALA	3.4
1	F	128	LEU	3.4
1	D	127	VAL	3.4
1	F	636	TYR	3.3
1	B	149	PRO	3.3
1	G	127	VAL	3.3
1	C	149	PRO	3.3
1	E	94	GLU	3.3
1	A	152	ALA	3.3
1	C	634	PHE	3.3
1	C	40	CYS	3.3
1	I	553	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	88	ASP	3.3
1	F	102	HIS	3.2
1	L	89	VAL	3.2
1	D	109	LEU	3.2
1	H	600	TRP	3.2
1	F	30	TYR	3.2
1	C	131	VAL	3.2
1	F	634	PHE	3.2
1	E	585	THR	3.2
1	L	126	SER	3.2
1	B	30	TYR	3.2
1	B	595	PHE	3.2
1	F	89	VAL	3.2
1	D	113	ASP	3.2
1	B	498	GLY	3.2
1	A	107	ALA	3.2
1	L	551	ALA	3.2
1	H	173	ASN	3.1
1	F	125	PRO	3.1
1	C	187	ASP	3.1
1	F	401	ASP	3.1
1	H	89	VAL	3.1
1	H	129	ASP	3.1
1	J	102	HIS	3.1
1	B	146	HIS	3.1
1	C	107	ALA	3.1
1	F	556	GLN	3.0
1	G	174	VAL	3.0
1	I	173	ASN	3.0
1	L	149	PRO	3.0
1	D	635	LYS	3.0
1	J	552	ALA	3.0
1	E	147	VAL	3.0
1	L	634	PHE	3.0
1	D	94	GLU	3.0
1	A	125	PRO	3.0
1	C	148	PRO	3.0
1	I	3	ASN	3.0
1	A	638	TYR	3.0
1	E	89	VAL	3.0
1	J	33	LEU	2.9
1	C	126	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	498	GLY	2.9
1	G	89	VAL	2.9
1	H	87	PHE	2.9
1	H	147	VAL	2.9
1	I	174	VAL	2.9
1	G	3	ASN	2.9
1	K	105	PHE	2.9
1	G	143	PRO	2.9
1	I	125	PRO	2.9
1	F	129	ASP	2.9
1	I	129	ASP	2.9
1	F	140	GLY	2.9
1	F	39	PHE	2.9
1	I	33	LEU	2.9
1	E	32	ASP	2.9
1	I	504	GLY	2.9
1	D	39	PHE	2.9
1	B	128	LEU	2.8
1	K	235	ALA	2.8
1	F	313	PRO	2.8
1	G	596	PRO	2.8
1	I	596	PRO	2.8
1	K	313	PRO	2.8
1	K	600	TRP	2.8
1	H	111	ASN	2.8
1	C	63	ALA	2.8
1	D	124	GLU	2.8
1	C	103	ASN	2.8
1	A	102	HIS	2.8
1	D	107	ALA	2.8
1	E	102	HIS	2.8
1	G	129	ASP	2.8
1	G	6	THR	2.8
1	L	395	ALA	2.8
1	I	595	PHE	2.8
1	D	40	CYS	2.7
1	F	111	ASN	2.7
1	B	147	VAL	2.7
1	I	127	VAL	2.7
1	D	125	PRO	2.7
1	J	36	PRO	2.7
1	K	409	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	434	GLU	2.7
1	B	38	ALA	2.7
1	E	174	VAL	2.7
1	F	314	THR	2.7
1	H	595	PHE	2.7
1	J	105	PHE	2.7
1	E	110	GLU	2.7
1	D	552	ALA	2.7
1	I	395	ALA	2.7
1	F	219	PRO	2.7
1	J	35	PRO	2.7
1	G	103	ASN	2.7
1	H	551	ALA	2.7
1	L	39	PHE	2.7
1	L	174	VAL	2.7
1	H	149	PRO	2.7
1	B	107	ALA	2.6
1	B	148	PRO	2.6
1	K	87	PHE	2.6
1	L	585	THR	2.6
1	K	129	ASP	2.6
1	A	173	ASN	2.6
1	J	634	PHE	2.6
1	I	76	LYS	2.6
1	H	107	ALA	2.6
1	L	184	GLN	2.6
1	K	39	PHE	2.6
1	L	31	ALA	2.6
1	L	173	ASN	2.6
1	J	401	ASP	2.5
1	F	37	LEU	2.5
1	L	176	LYS	2.5
1	E	42	GLY	2.5
1	A	89	VAL	2.5
1	B	183	PRO	2.5
1	E	87	PHE	2.5
1	D	434	GLU	2.5
1	B	313	PRO	2.5
1	A	174	VAL	2.5
1	D	31	ALA	2.5
1	E	244	ALA	2.5
1	F	105	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	40	CYS	2.5
1	F	40	CYS	2.5
1	J	126	SER	2.5
1	G	635	LYS	2.5
1	D	41	GLU	2.5
1	J	41	GLU	2.5
1	L	127	VAL	2.5
1	I	40	CYS	2.5
1	E	129	ASP	2.5
1	E	252	ASP	2.5
1	A	90	GLY	2.5
1	F	148	PRO	2.5
1	J	30	TYR	2.5
1	G	238	ASP	2.4
1	H	95	GLU	2.4
1	C	381	GLY	2.4
1	C	174	VAL	2.4
1	J	127	VAL	2.4
1	G	595	PHE	2.4
1	J	595	PHE	2.4
1	L	76	LYS	2.4
1	F	551	ALA	2.4
1	K	100	ALA	2.4
1	K	551	ALA	2.4
1	G	146	HIS	2.4
1	D	88	ASP	2.4
1	H	110	GLU	2.4
1	G	149	PRO	2.4
1	I	149	PRO	2.4
1	D	316	LYS	2.4
1	D	613	ALA	2.4
1	C	3	ASN	2.4
1	L	649	ASN	2.4
1	B	94	GLU	2.4
1	E	95	GLU	2.4
1	L	94	GLU	2.4
1	I	45	LYS	2.4
1	F	398	GLY	2.4
1	I	502	GLY	2.4
1	C	636	TYR	2.4
1	I	38	ALA	2.4
1	J	633	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	95	GLU	2.4
1	C	95	GLU	2.4
1	F	442	SER	2.4
1	J	42	GLY	2.4
1	A	87	PHE	2.4
1	I	552	ALA	2.4
1	I	569	ALA	2.4
1	L	87	PHE	2.4
1	F	146	HIS	2.3
1	G	173	ASN	2.3
1	A	88	ASP	2.3
1	J	40	CYS	2.3
1	L	19	GLN	2.3
1	A	105	PHE	2.3
1	B	552	ALA	2.3
1	D	110	GLU	2.3
1	E	41	GLU	2.3
1	J	95	GLU	2.3
1	C	143	PRO	2.3
1	F	600	TRP	2.3
1	I	75	TRP	2.3
1	L	125	PRO	2.3
1	A	398	GLY	2.3
1	L	502	GLY	2.3
1	I	105	PHE	2.3
1	H	395	ALA	2.3
1	J	547	ALA	2.3
1	G	76	LYS	2.3
1	I	635	LYS	2.3
1	D	594	SER	2.3
1	J	313	PRO	2.3
1	J	498	GLY	2.3
1	D	150	ALA	2.3
1	D	111	ASN	2.3
1	D	556	GLN	2.3
1	J	548	GLY	2.3
1	L	147	VAL	2.3
1	E	253	ALA	2.2
1	F	552	ALA	2.2
1	B	361	THR	2.2
1	I	434	GLU	2.2
1	K	95	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	30	TYR	2.2
1	L	189	TYR	2.2
1	F	35	PRO	2.2
1	D	248	GLY	2.2
1	E	600	TRP	2.2
1	L	131	VAL	2.2
1	C	630	ALA	2.2
1	G	38	ALA	2.2
1	K	395	ALA	2.2
1	E	633	THR	2.2
1	D	126	SER	2.2
1	H	546	GLY	2.2
1	J	129	ASP	2.2
1	D	147	VAL	2.2
1	D	595	PHE	2.2
1	F	608	ALA	2.2
1	K	40	CYS	2.2
1	D	108	ARG	2.2
1	H	649	ASN	2.2
1	D	12	PRO	2.2
1	A	635	LYS	2.2
1	F	22	ASP	2.2
1	F	107	ALA	2.2
1	B	649	ASN	2.2
1	B	502	GLY	2.2
1	A	401	ASP	2.2
1	A	127	VAL	2.2
1	B	127	VAL	2.2
1	E	127	VAL	2.2
1	A	38	ALA	2.1
1	F	256	ALA	2.1
1	G	600	TRP	2.1
1	H	144	ASN	2.1
1	J	3	ASN	2.1
1	I	498	GLY	2.1
1	E	146	HIS	2.1
1	F	650	ILE	2.1
1	G	100	ALA	2.1
1	F	607	THR	2.1
1	H	183	PRO	2.1
1	E	40	CYS	2.1
1	F	249	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	89	VAL	2.1
1	K	595	PHE	2.1
1	C	38	ALA	2.1
1	G	630	ALA	2.1
1	J	94	GLU	2.1
1	I	35	PRO	2.1
1	A	184	GLN	2.1
1	F	578	LEU	2.1
1	G	33	LEU	2.1
1	G	150	ALA	2.1
1	C	585	THR	2.1
1	K	6	THR	2.1
1	D	149	PRO	2.1
1	I	313	PRO	2.1
1	I	414	LEU	2.1
1	A	3	ASN	2.1
1	G	40	CYS	2.1
1	B	96	ASP	2.0
1	B	634	PHE	2.1
1	F	409	GLU	2.0
1	I	543	ALA	2.0
1	J	551	ALA	2.0
1	I	600	TRP	2.0
1	B	14	PRO	2.0
1	A	147	VAL	2.0
1	G	285	TYR	2.0
1	L	40	CYS	2.0
1	C	31	ALA	2.0
1	D	76	LYS	2.0
1	G	107	ALA	2.0
1	H	38	ALA	2.0
1	J	88	ASP	2.0
1	J	556	GLN	2.0
1	G	132	ASN	2.0

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

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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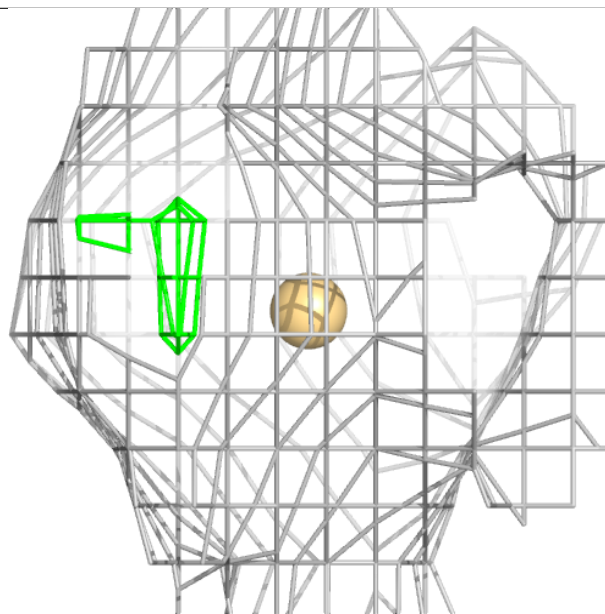
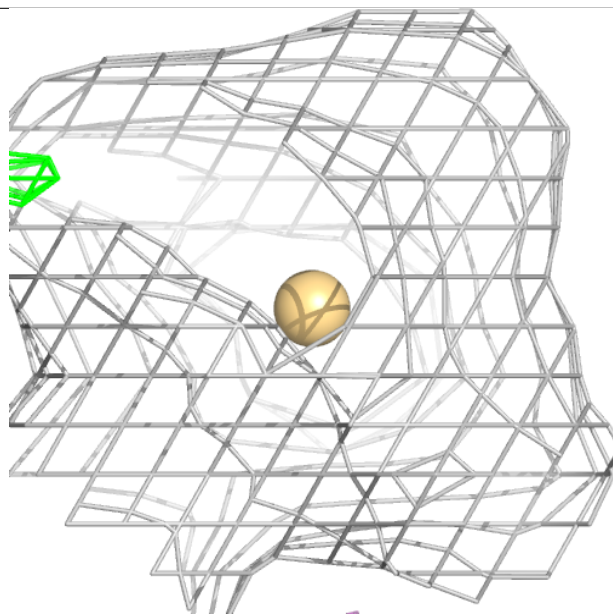
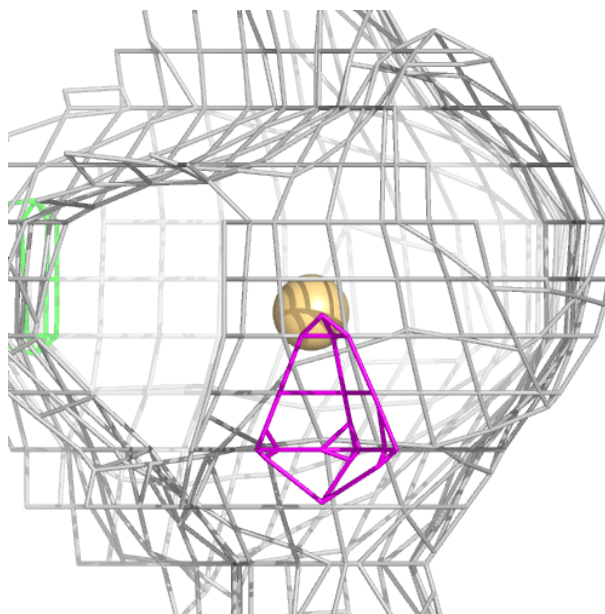
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CD	F	702	1/1	0.98	0.07	50,50,50,50	0
2	CD	J	703	1/1	0.98	0.04	80,80,80,80	0
2	CD	F	703	1/1	0.98	0.04	87,87,87,87	0
2	CD	H	703	1/1	0.98	0.05	82,82,82,82	0
2	CD	C	703	1/1	0.98	0.03	77,77,77,77	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.

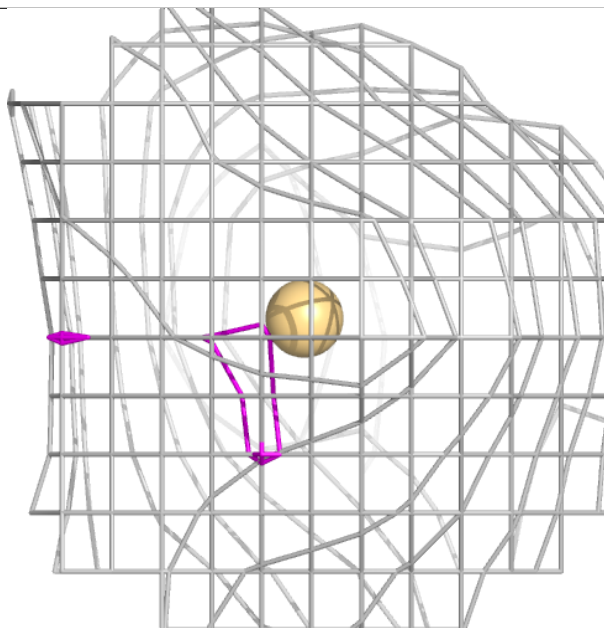
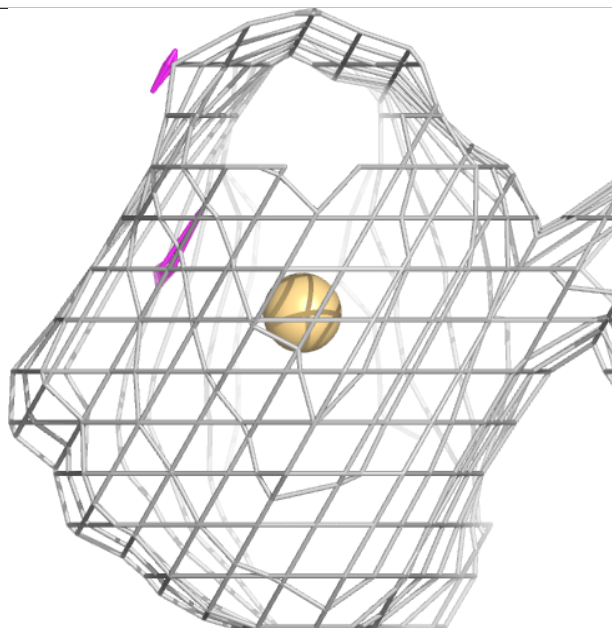
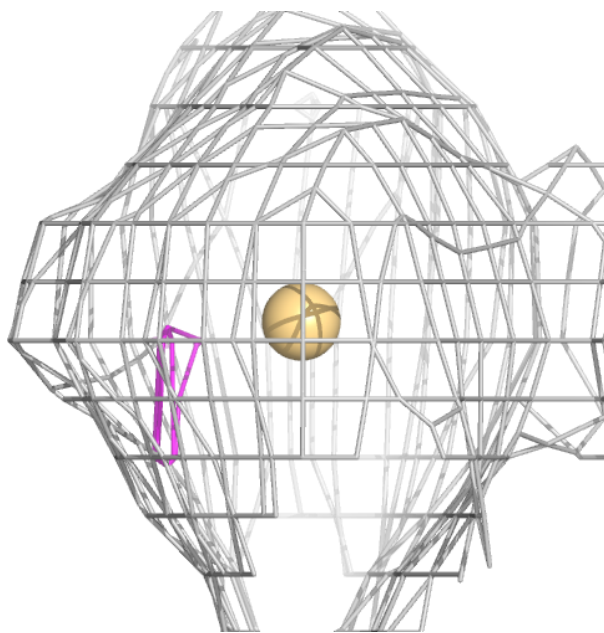
Electron density around CD F 704:

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



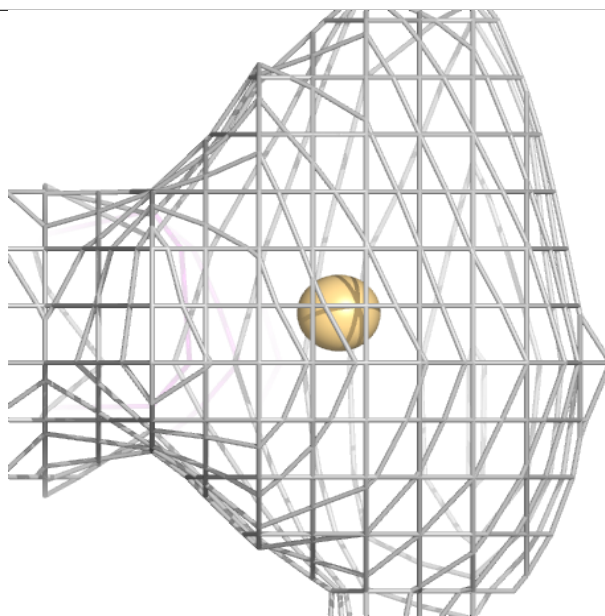
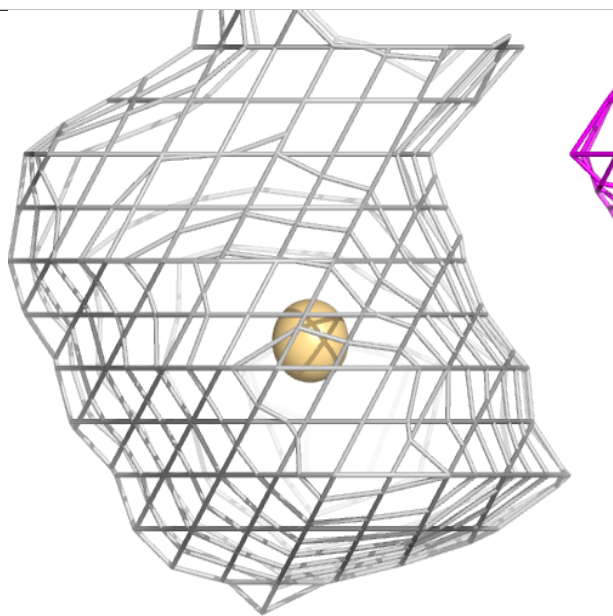
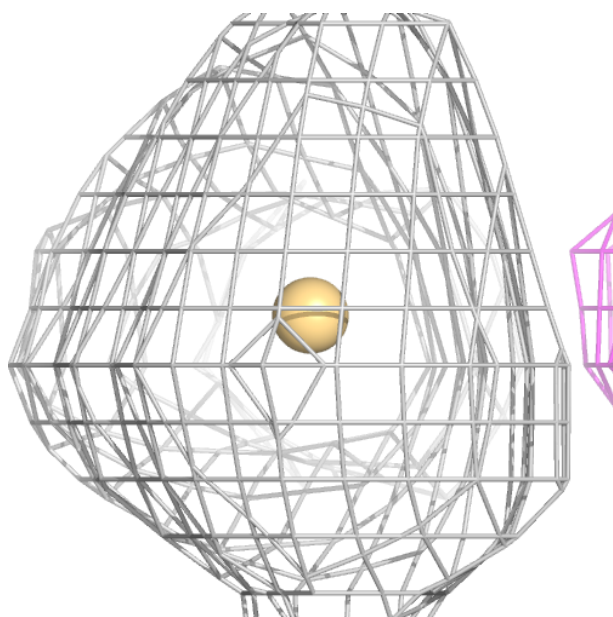
Electron density around CD G 704:

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



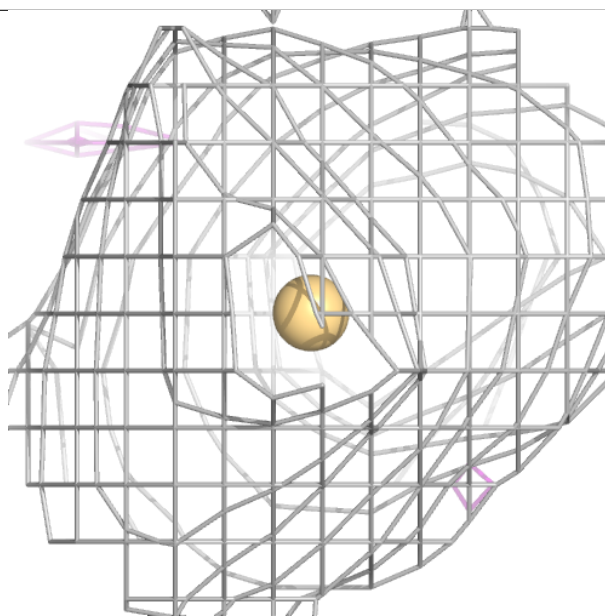
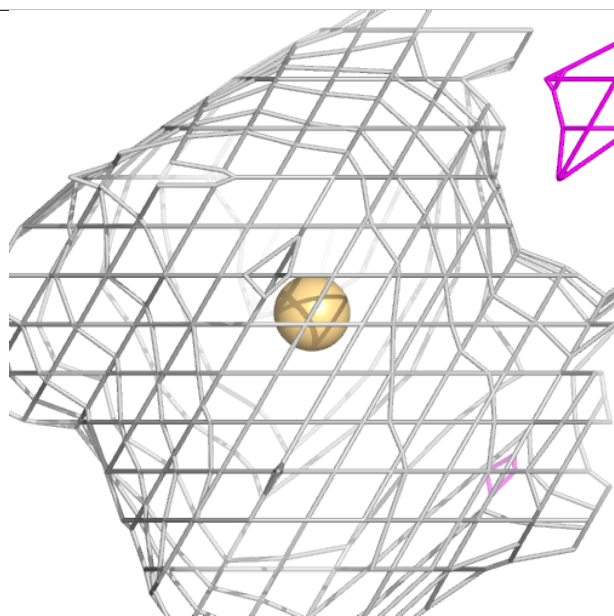
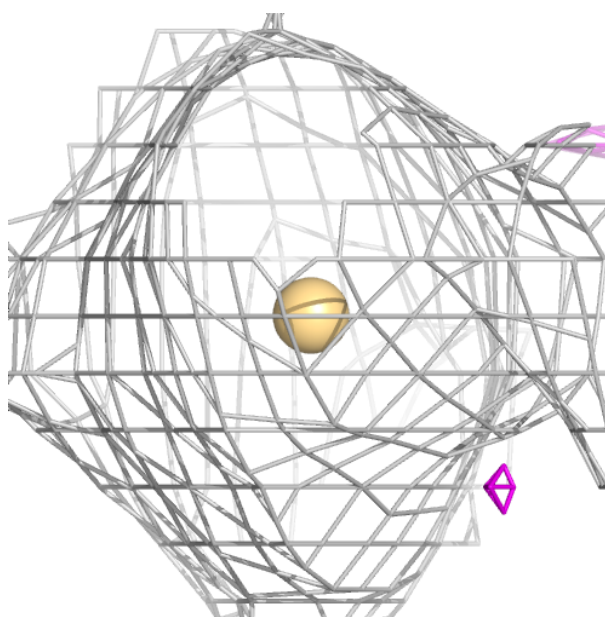
Electron density around CD J 704:

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



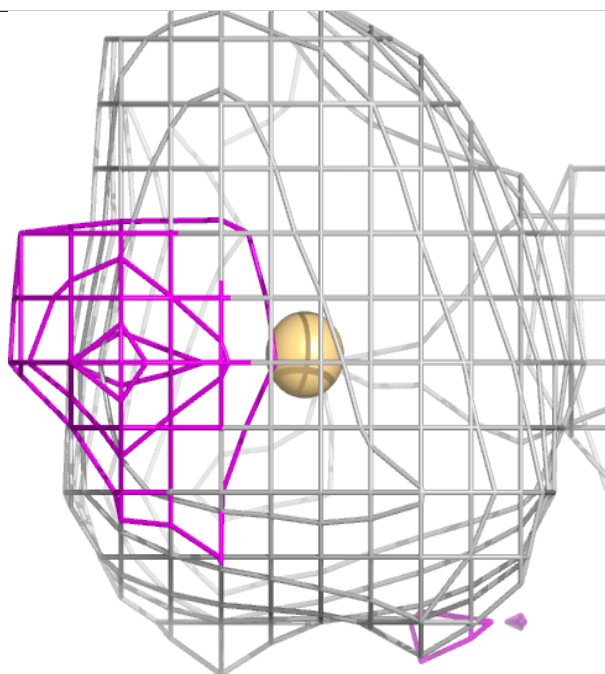
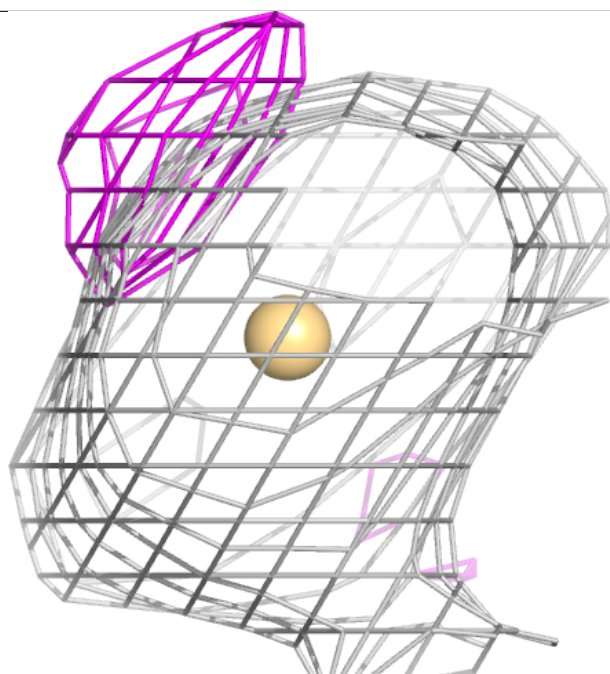
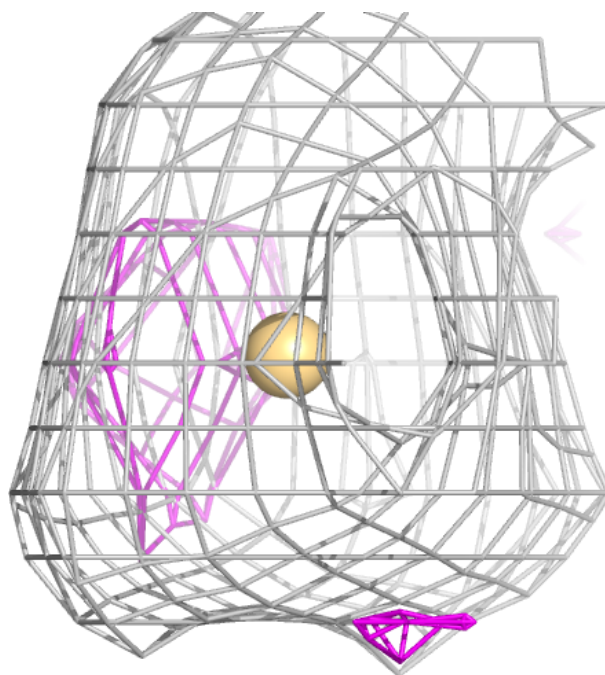
Electron density around CD B 704:

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



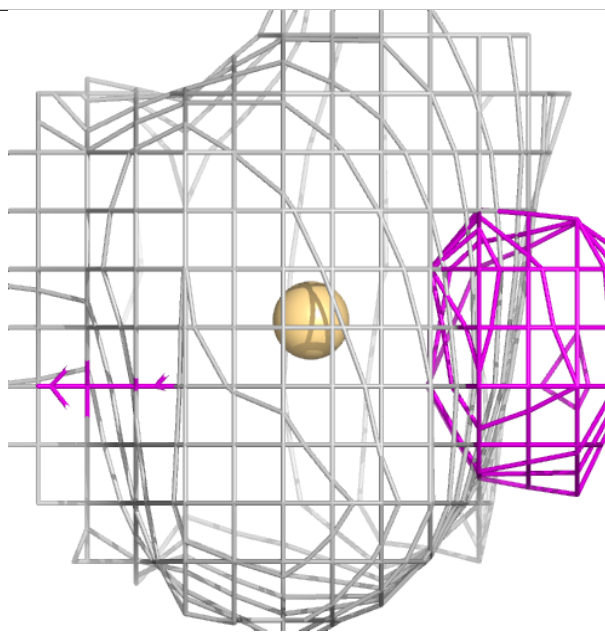
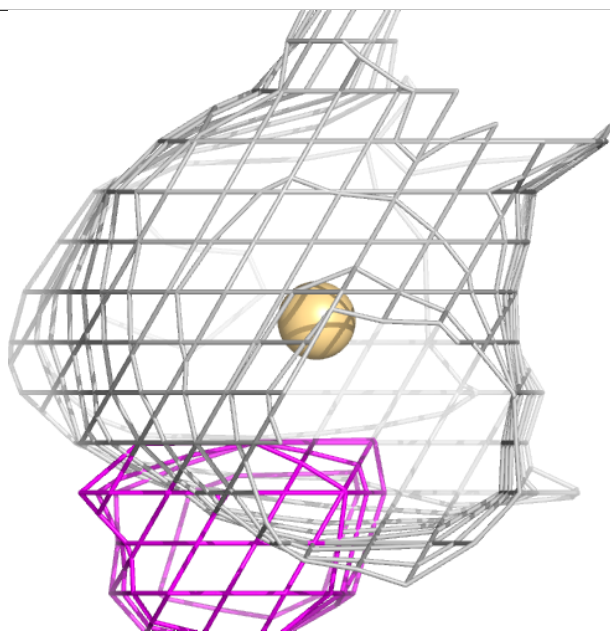
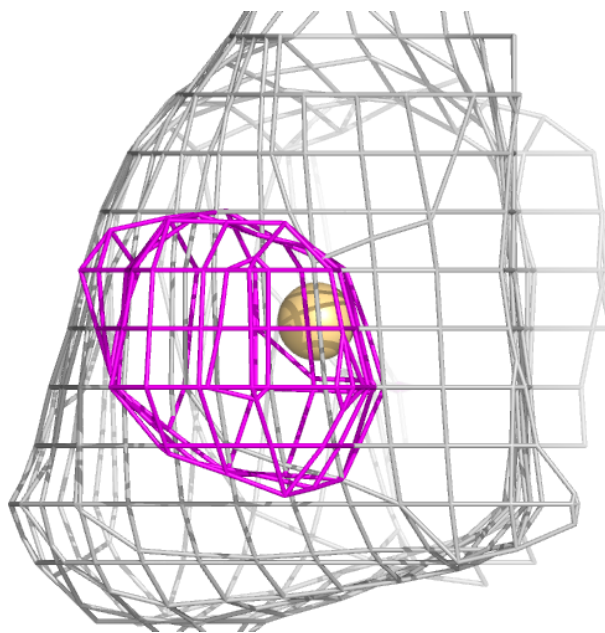
Electron density around CD A 704:

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



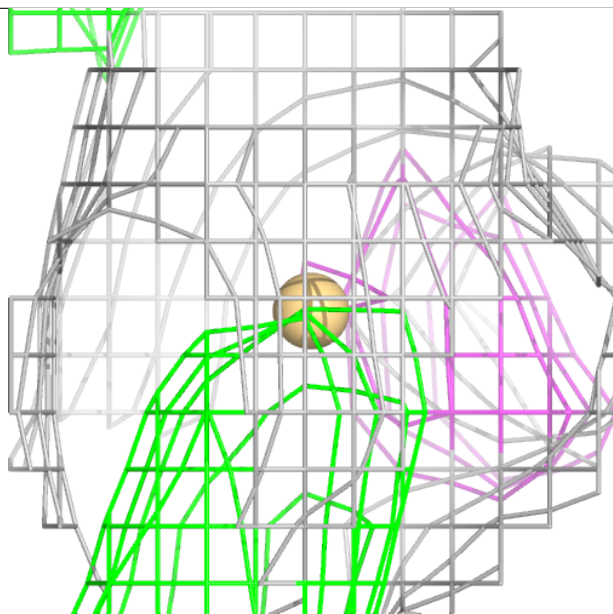
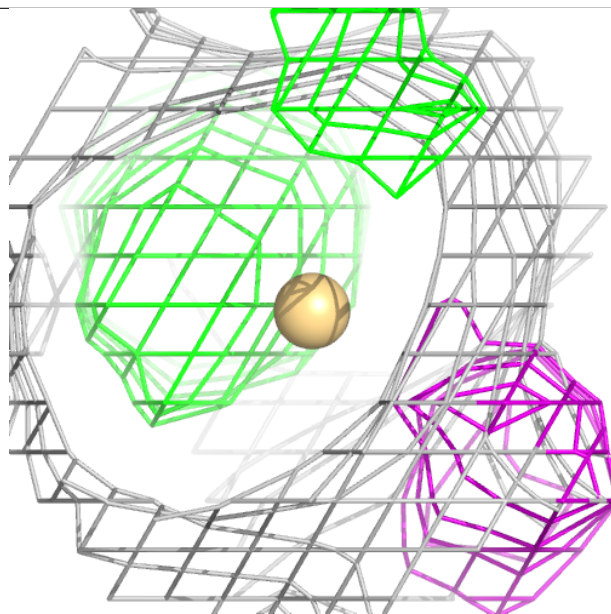
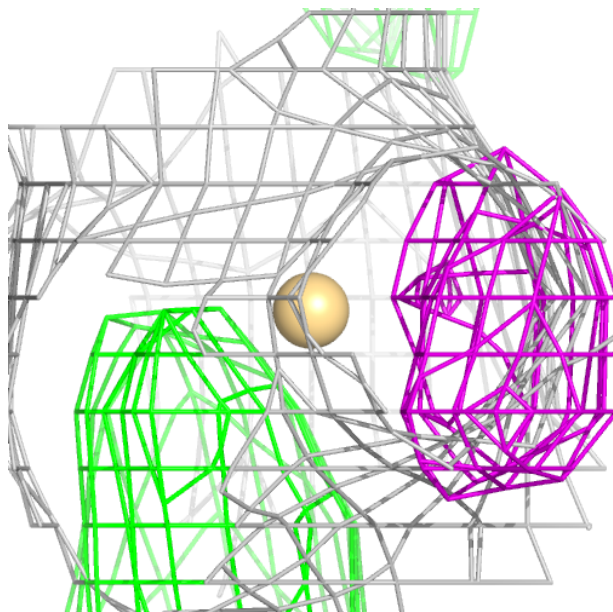
Electron density around CD C 704:

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



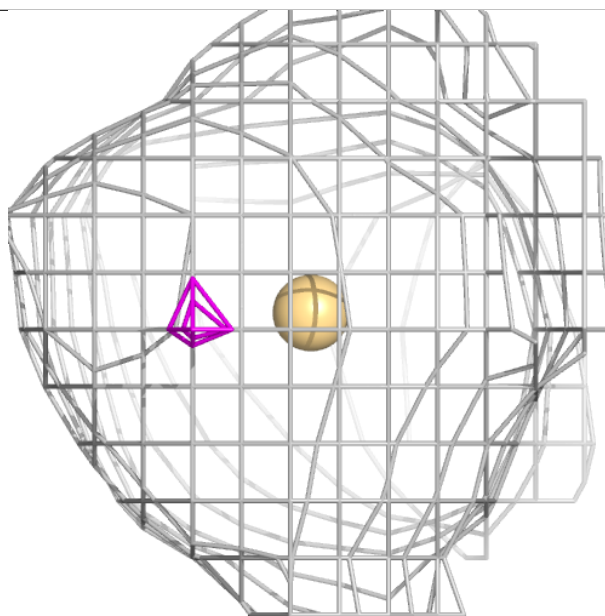
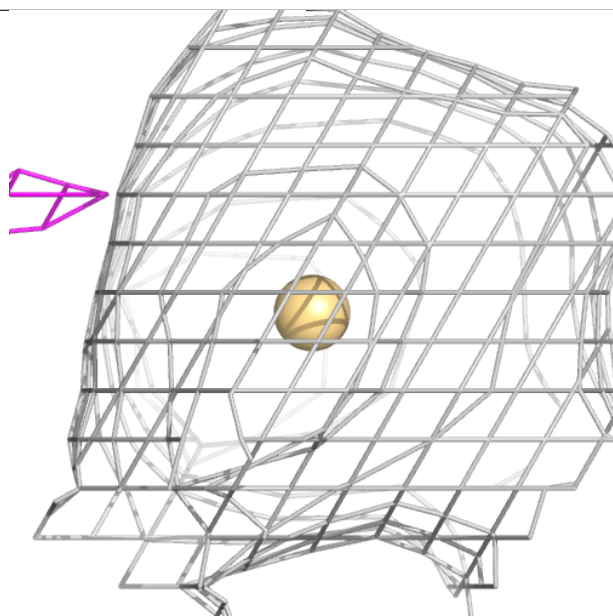
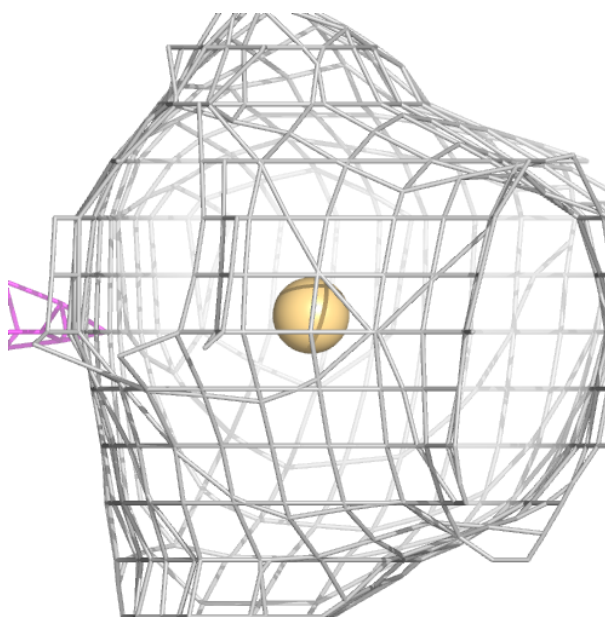
Electron density around CD K 701:

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



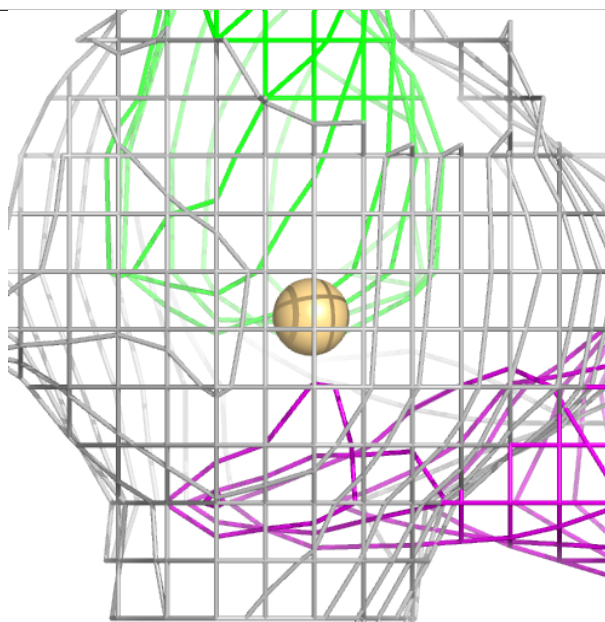
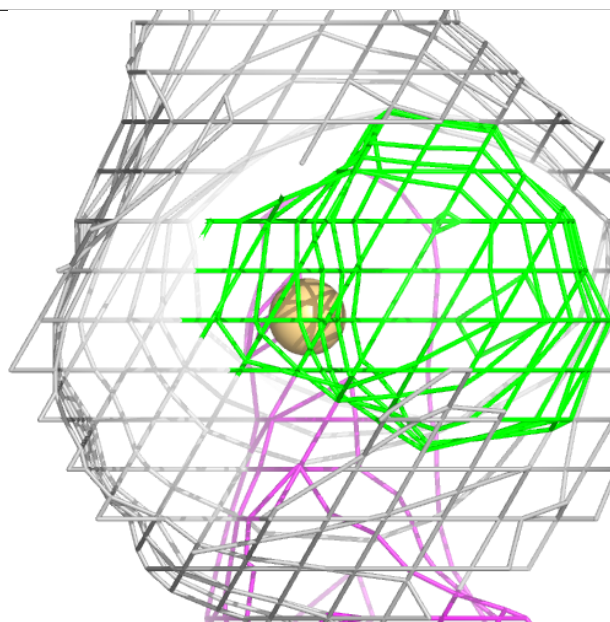
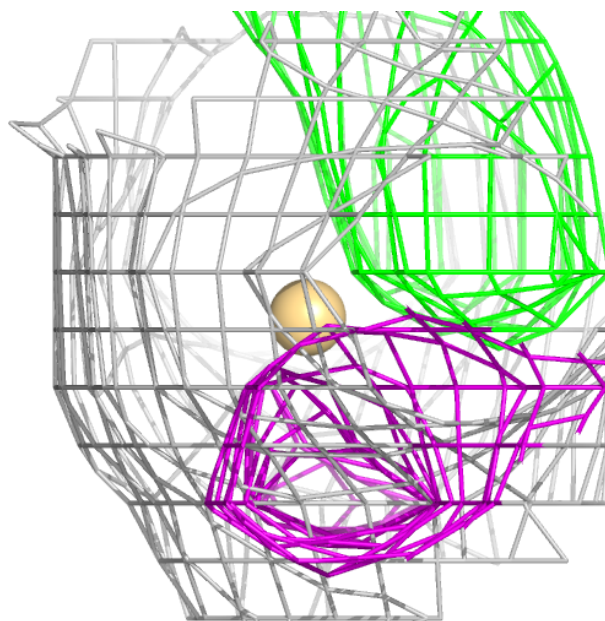
Electron density around CD I 704:

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



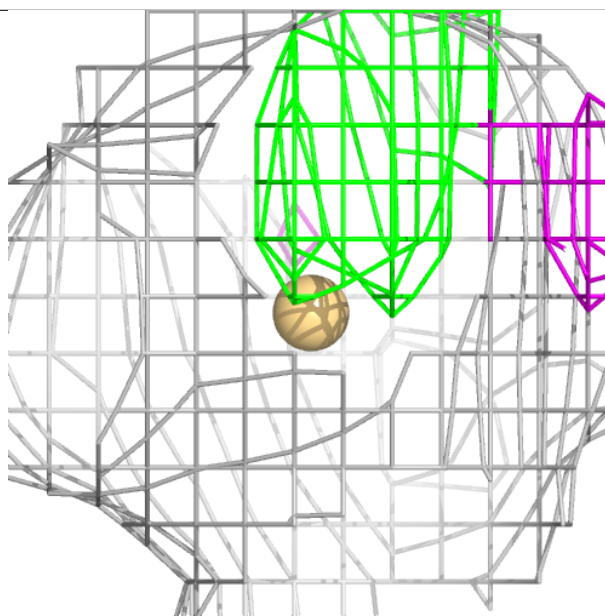
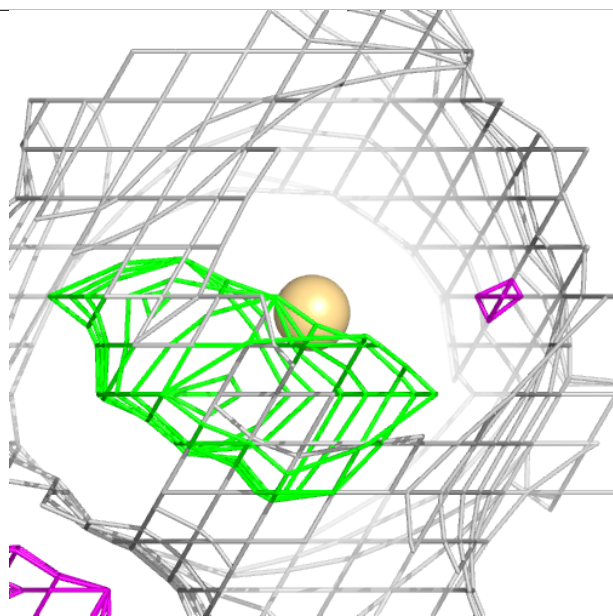
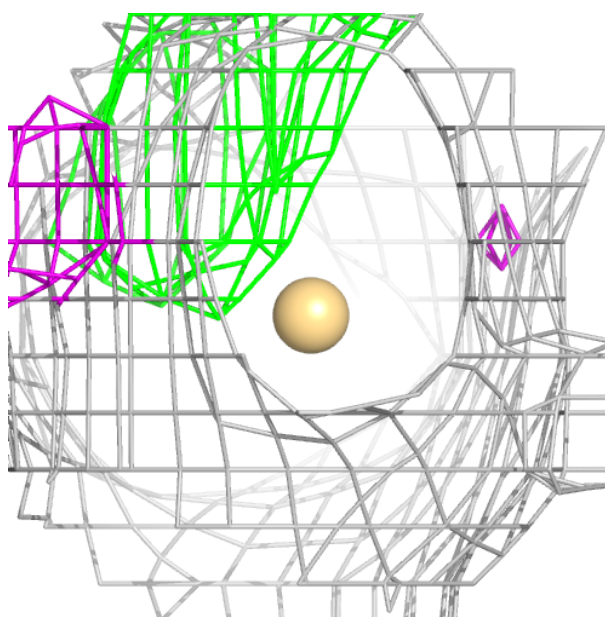
Electron density around CD E 701:

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



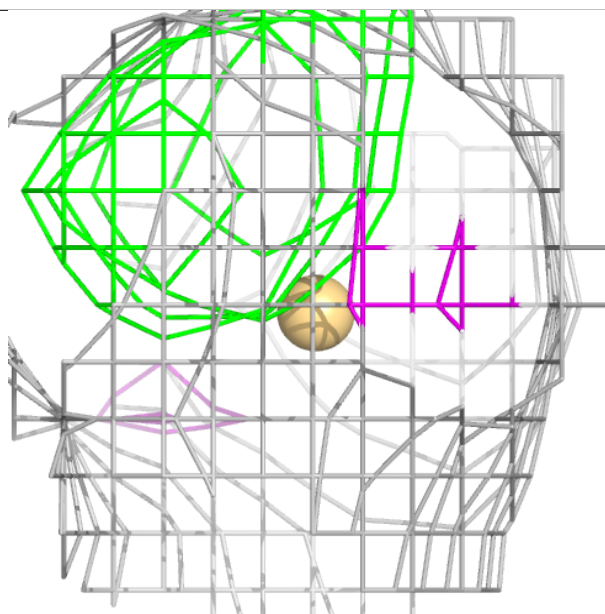
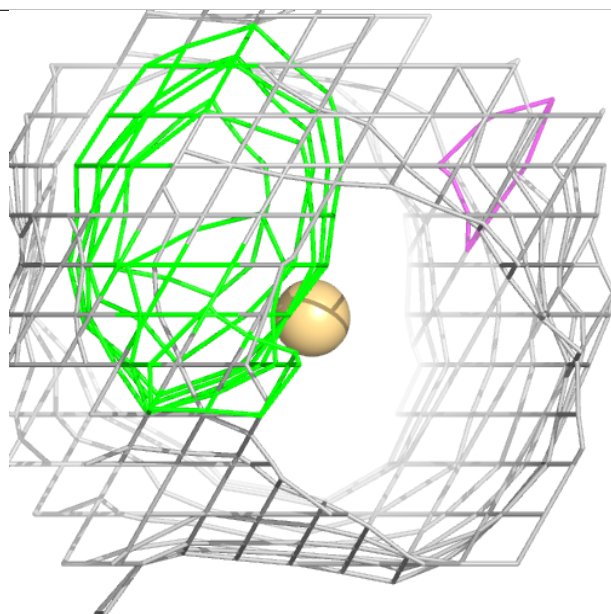
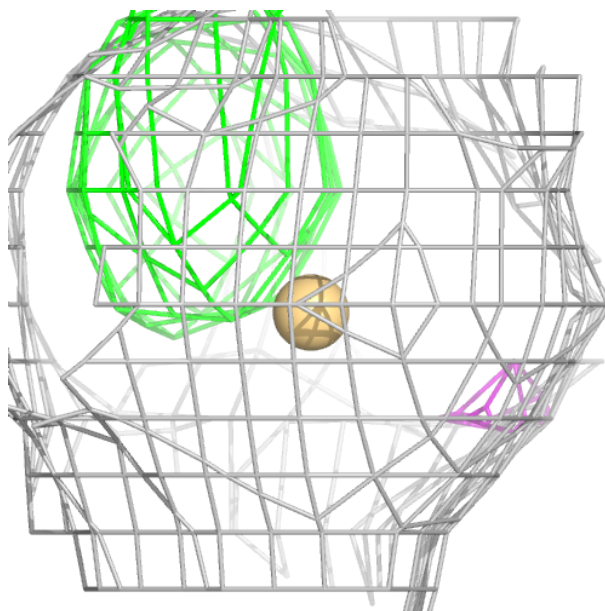
Electron density around CD I 701:

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



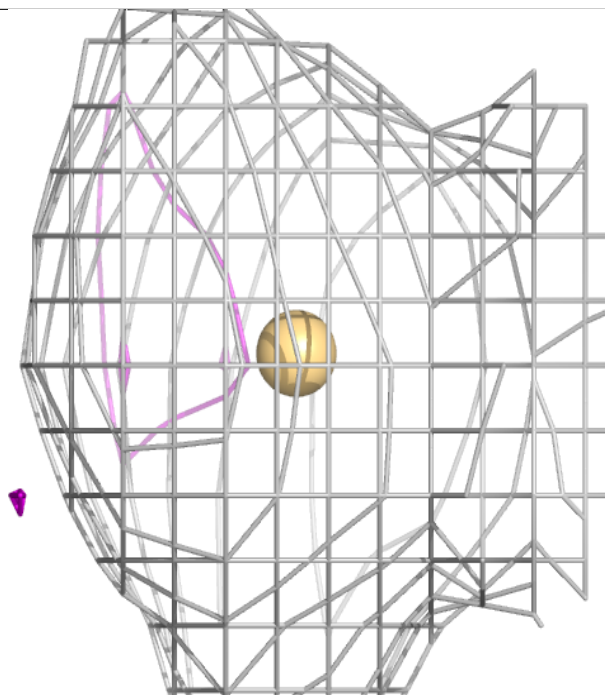
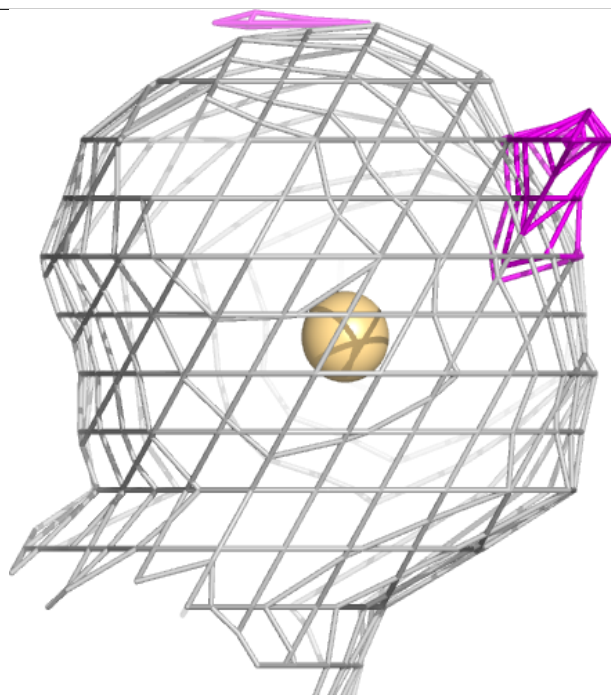
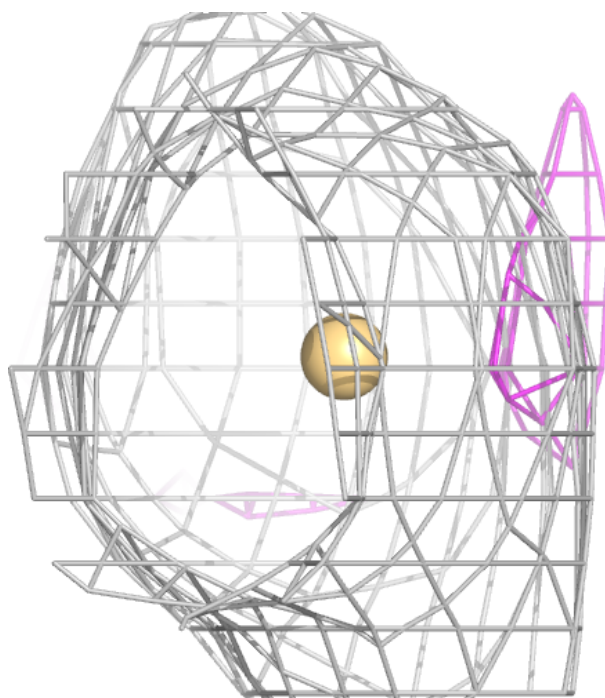
Electron density around CD L 701:

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



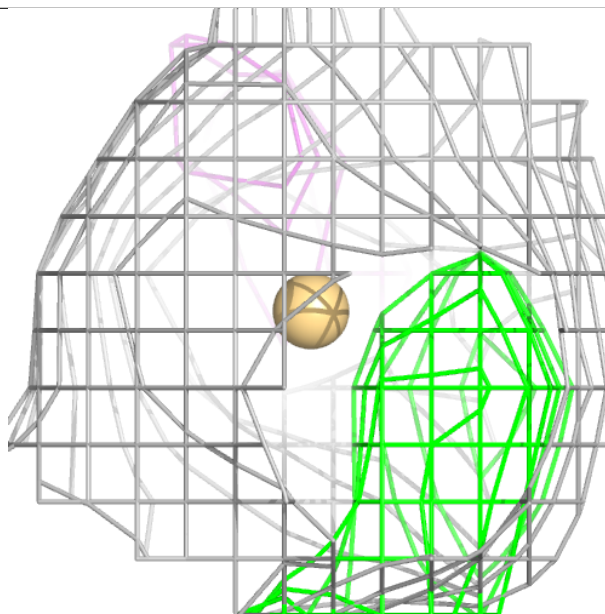
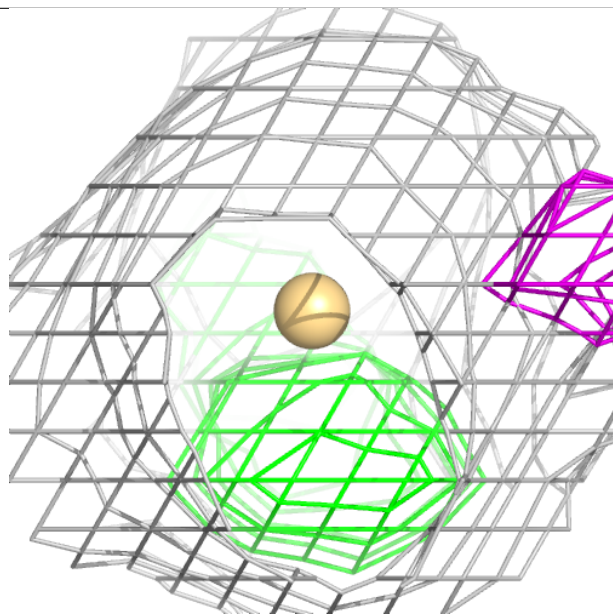
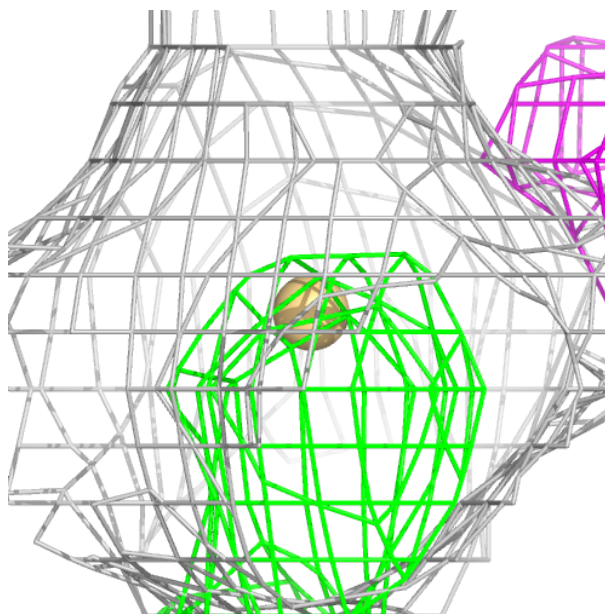
Electron density around CD L 704:

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



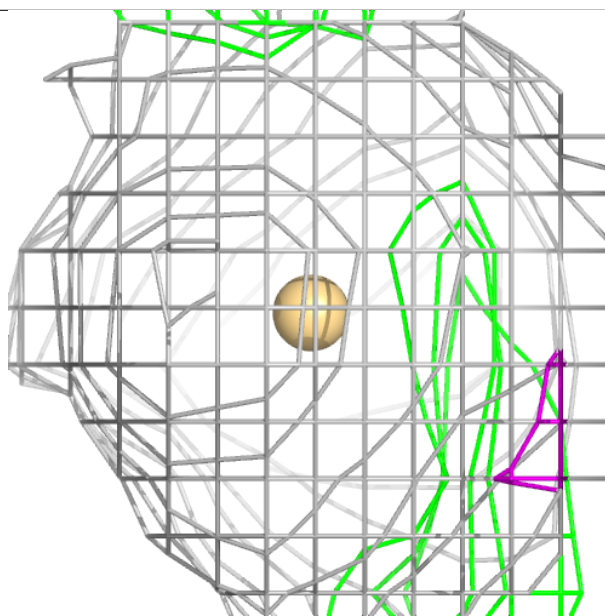
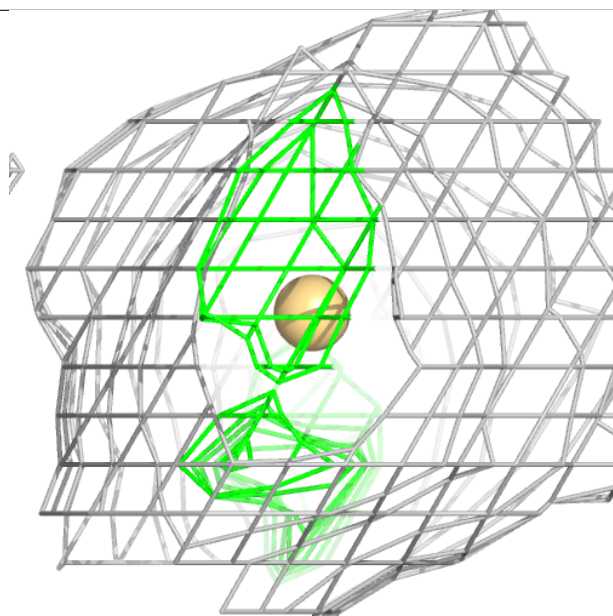
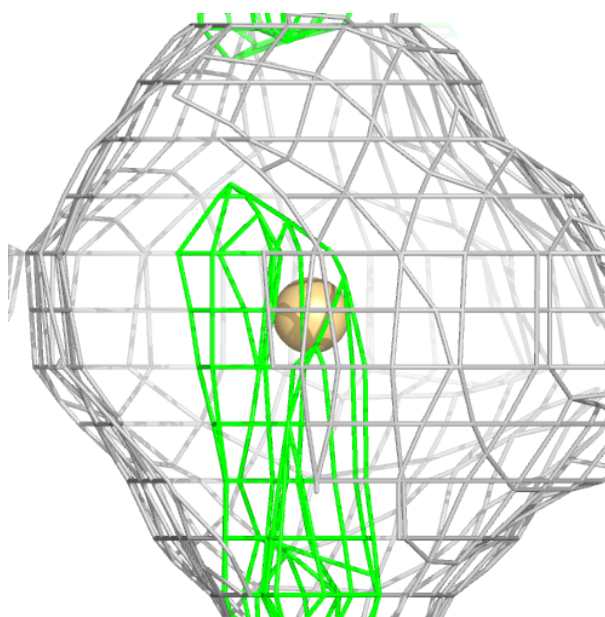
Electron density around CD D 701:

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



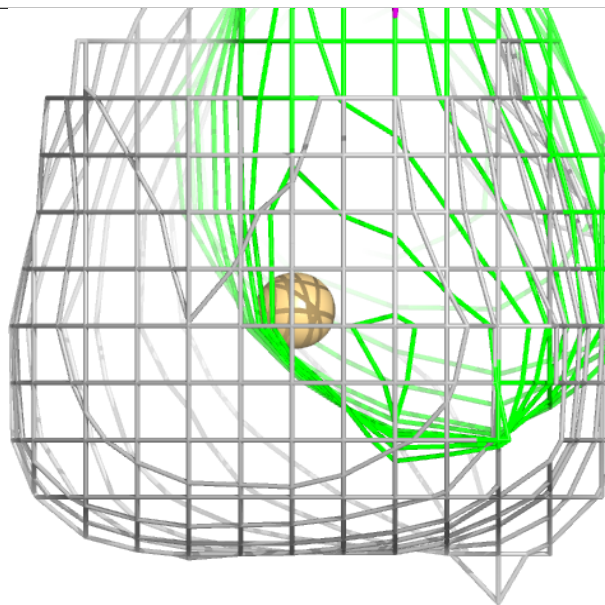
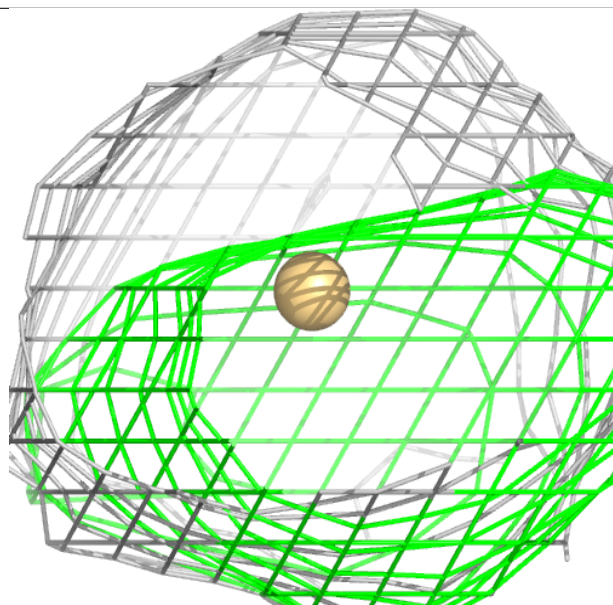
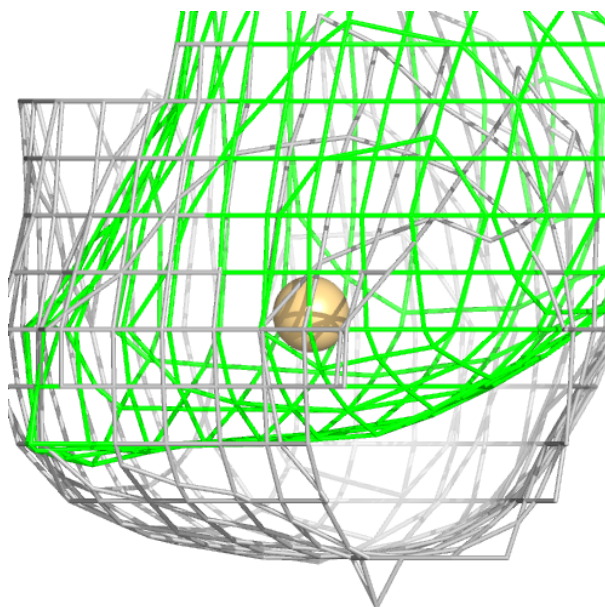
Electron density around CD D 703:

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



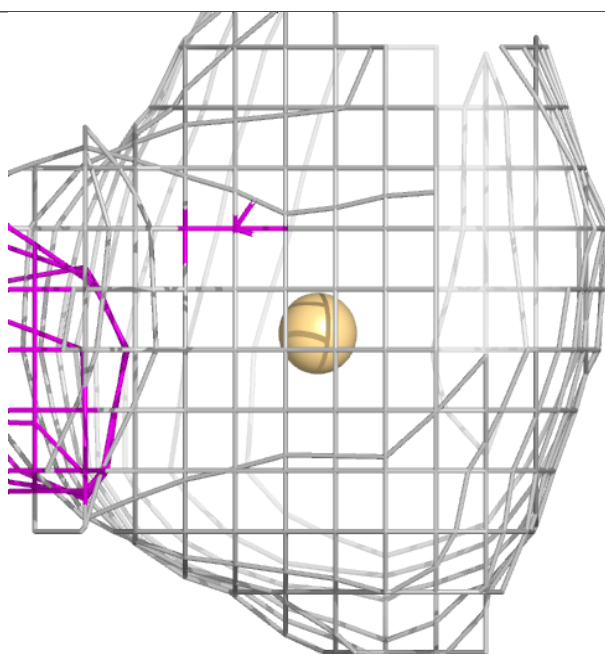
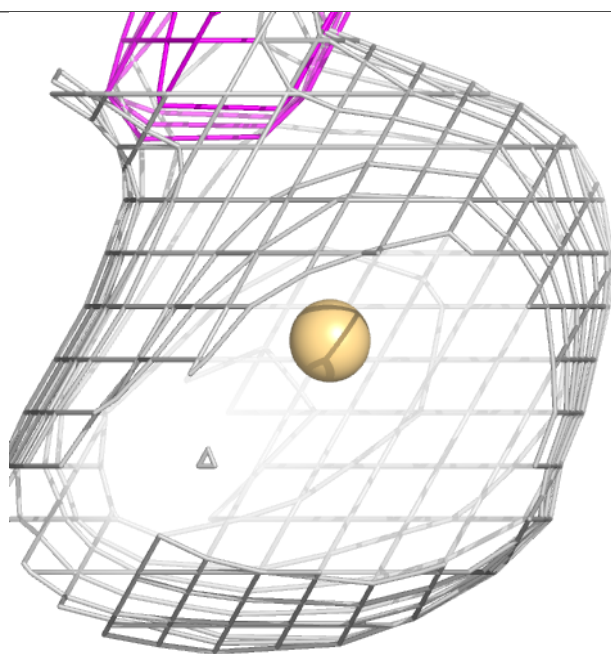
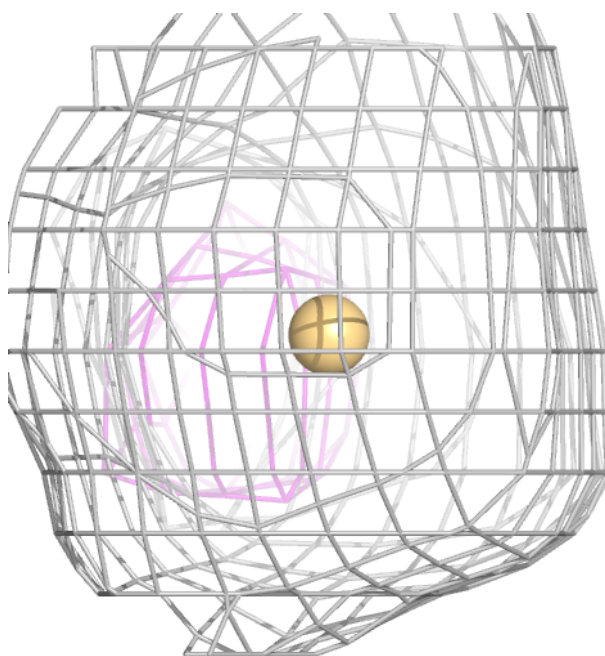
Electron density around CD H 702:

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



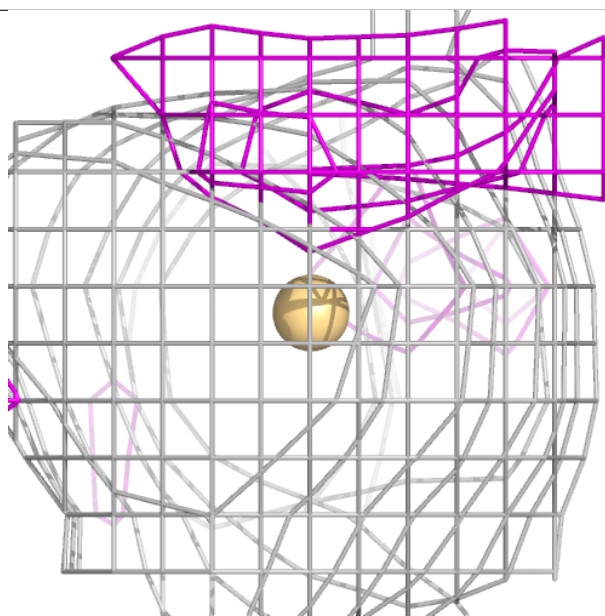
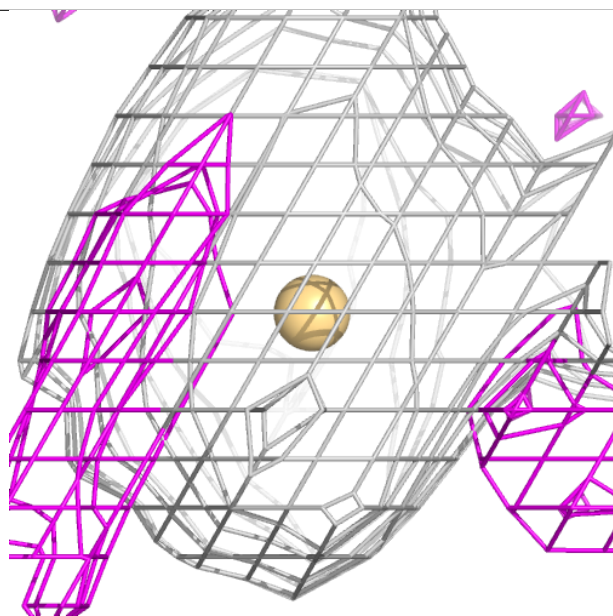
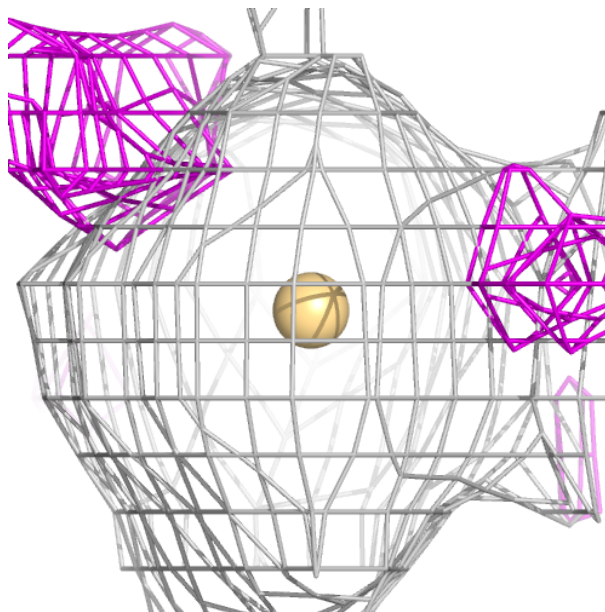
Electron density around CD K 704:

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



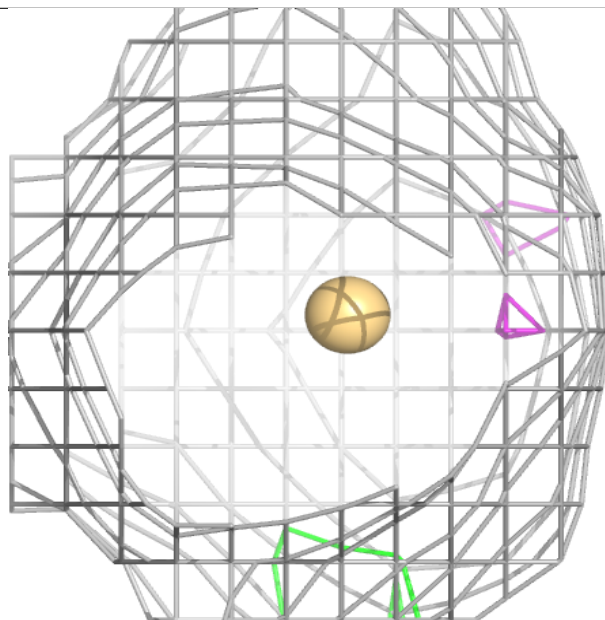
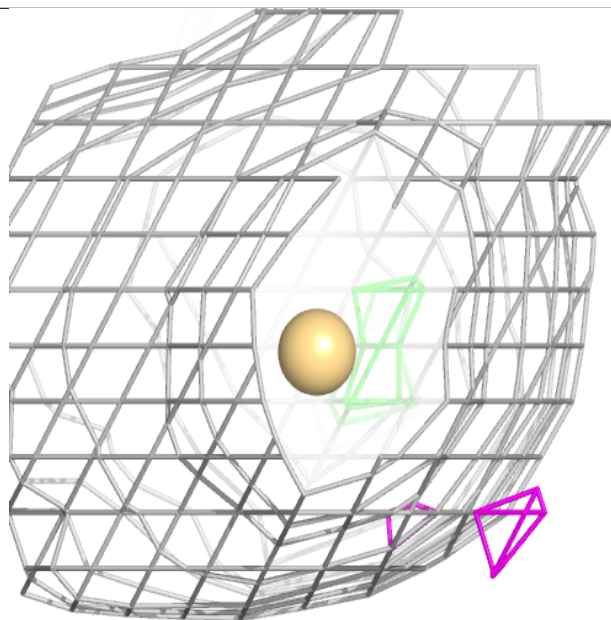
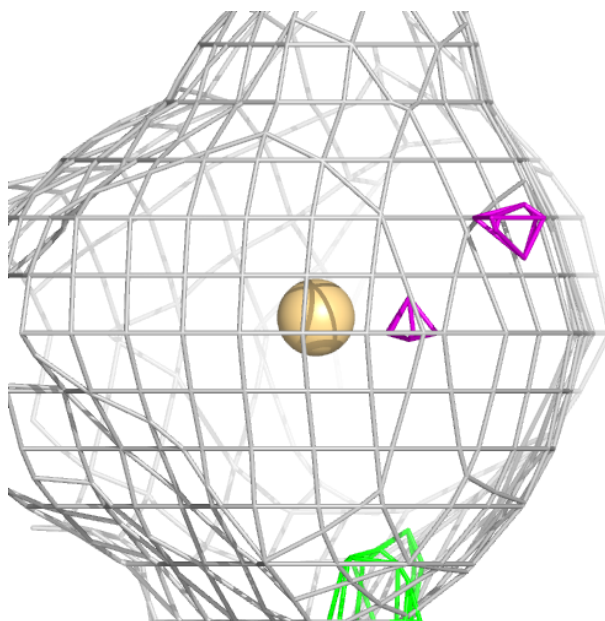
Electron density around CD H 704:

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



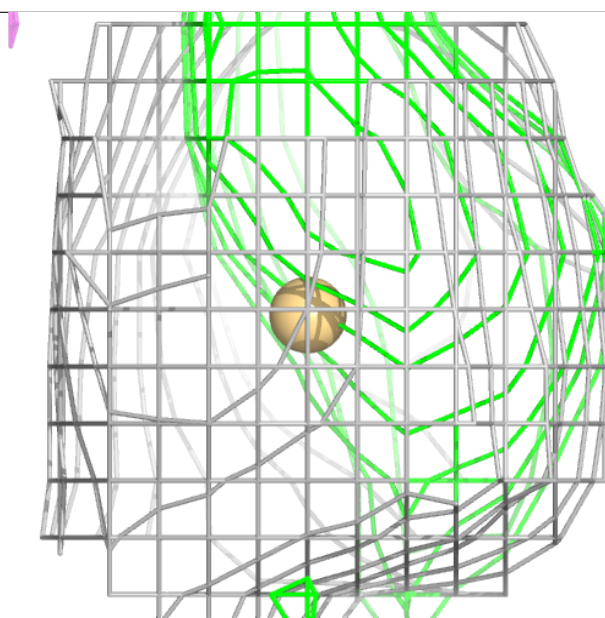
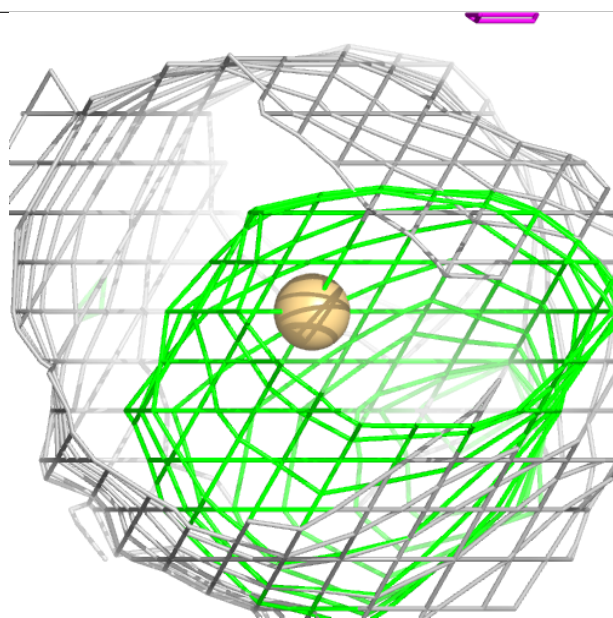
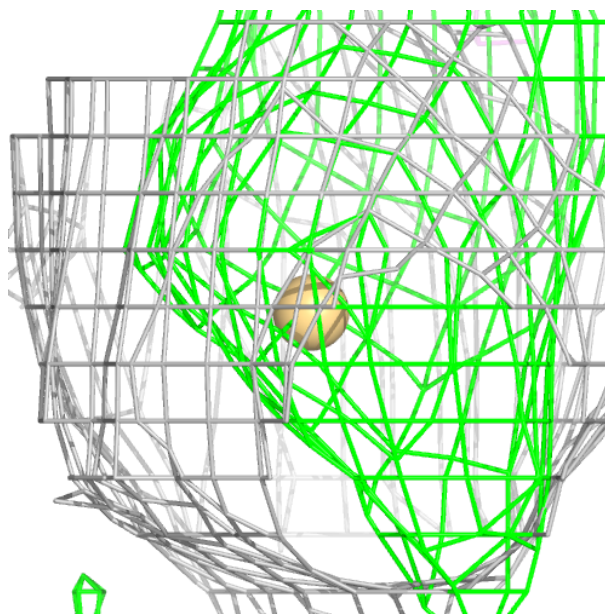
Electron density around CD B 703:

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



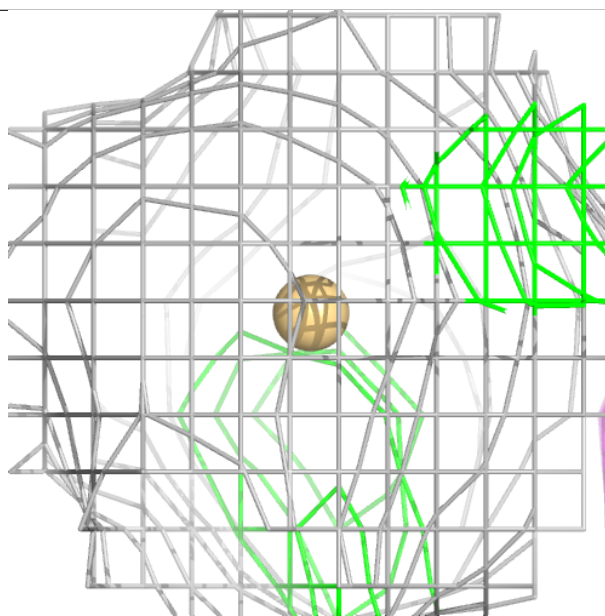
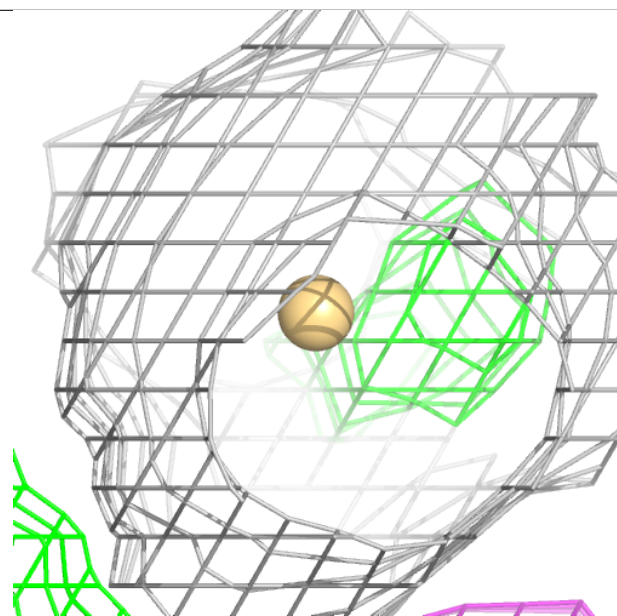
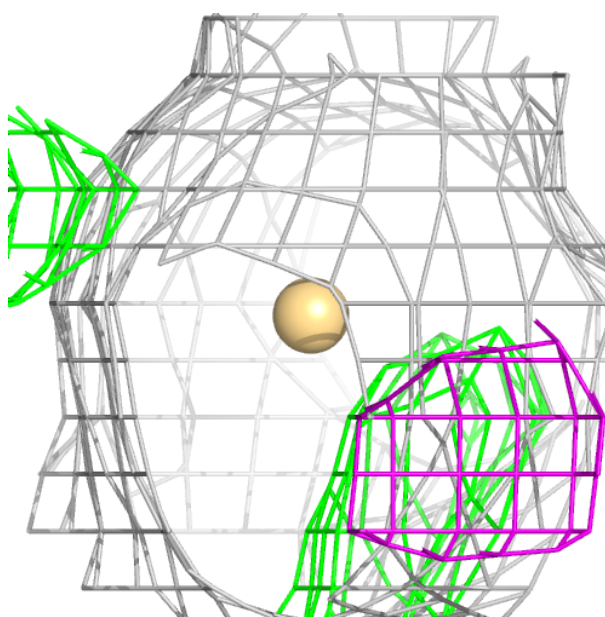
Electron density around CD G 702:

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



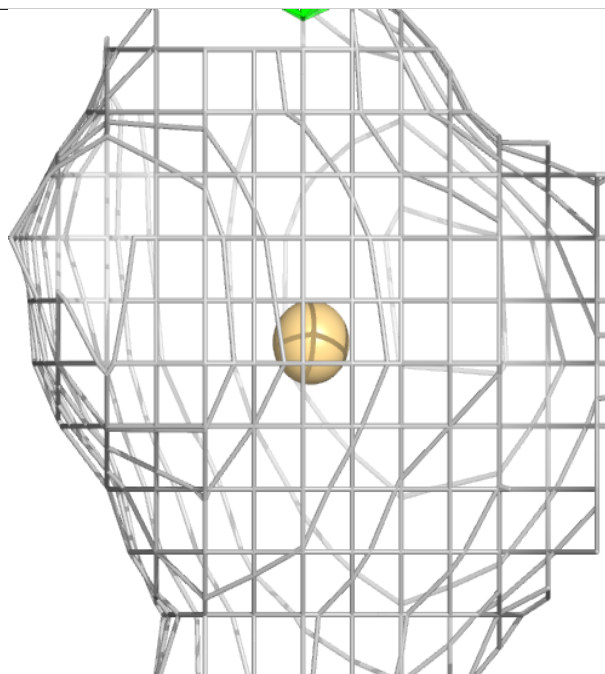
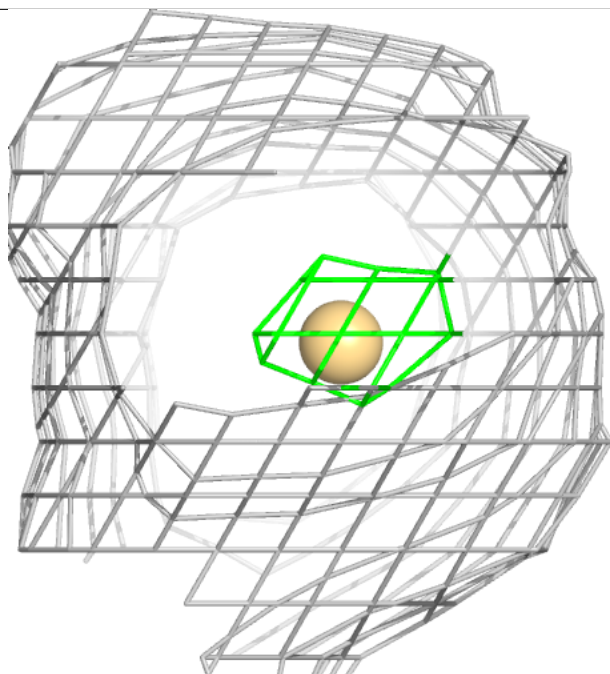
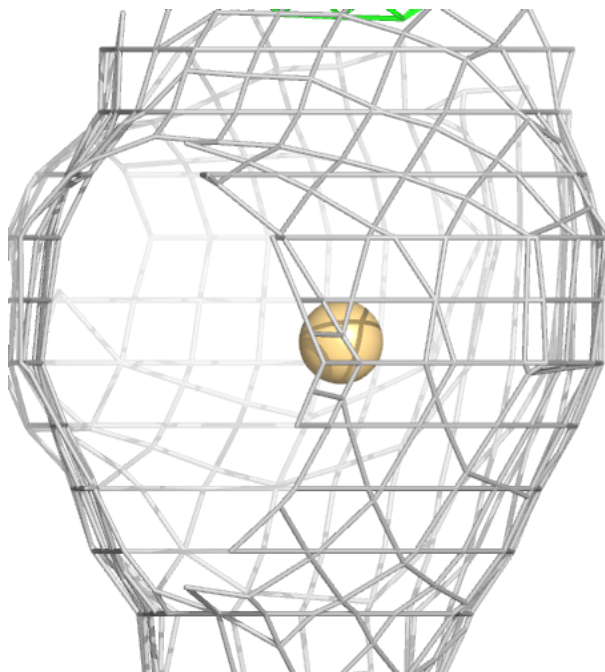
Electron density around CD F 701:

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



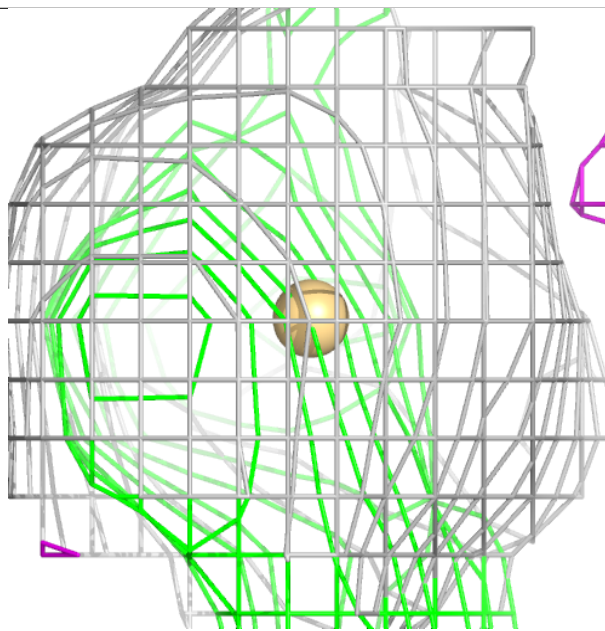
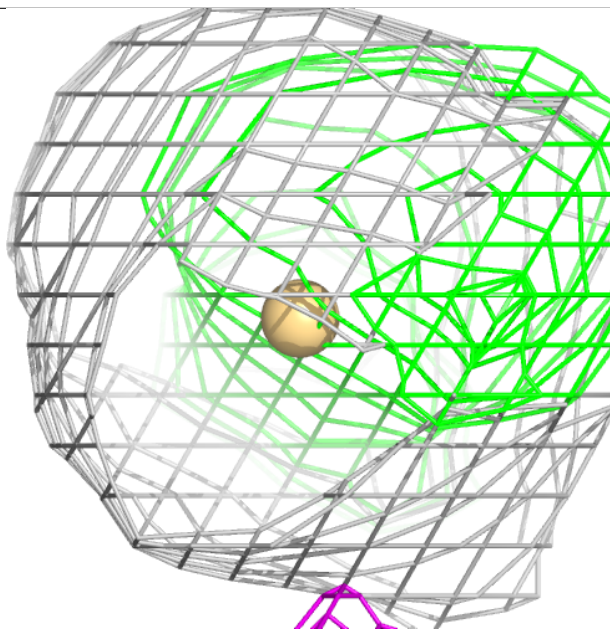
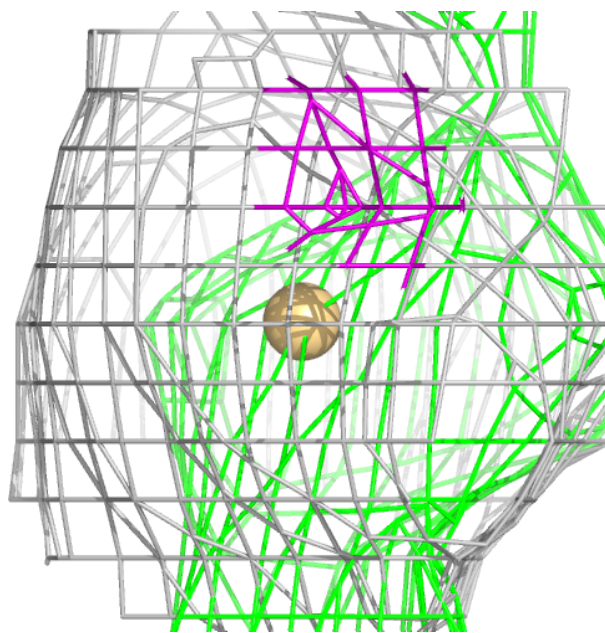
Electron density around CD I 703:

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



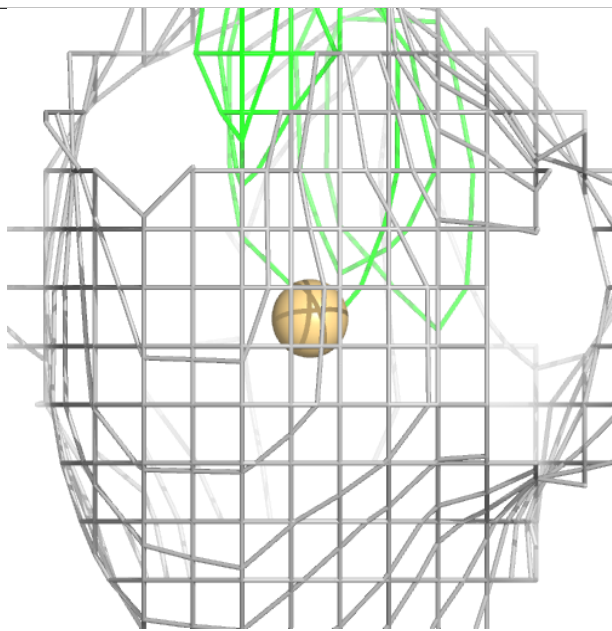
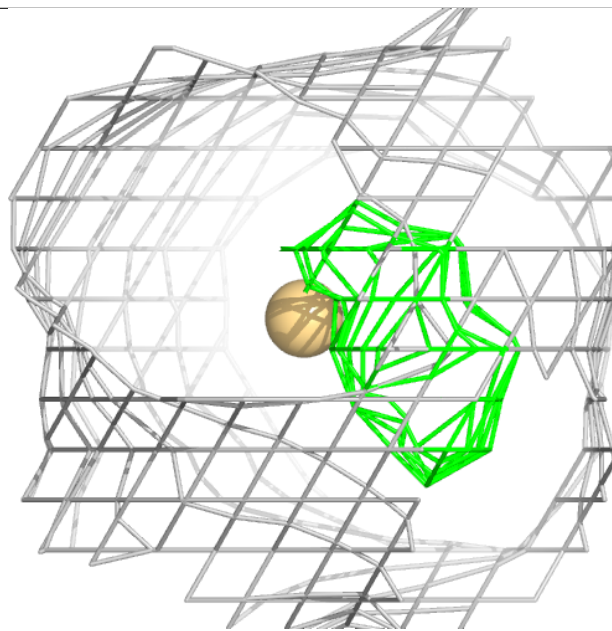
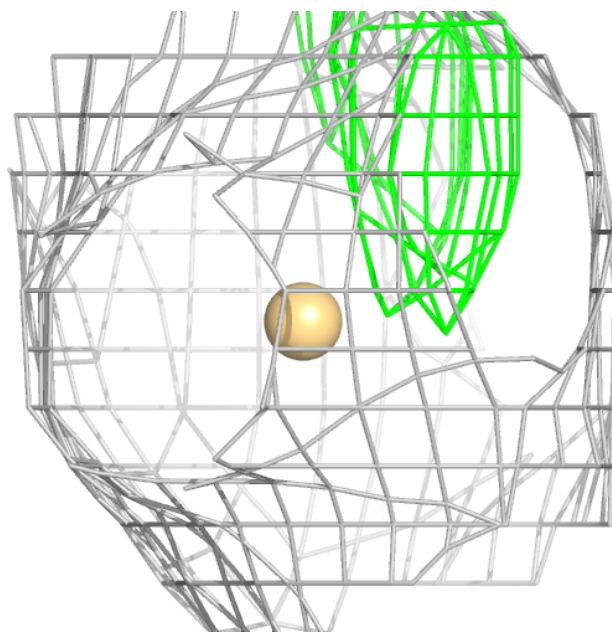
Electron density around CD A 702:

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



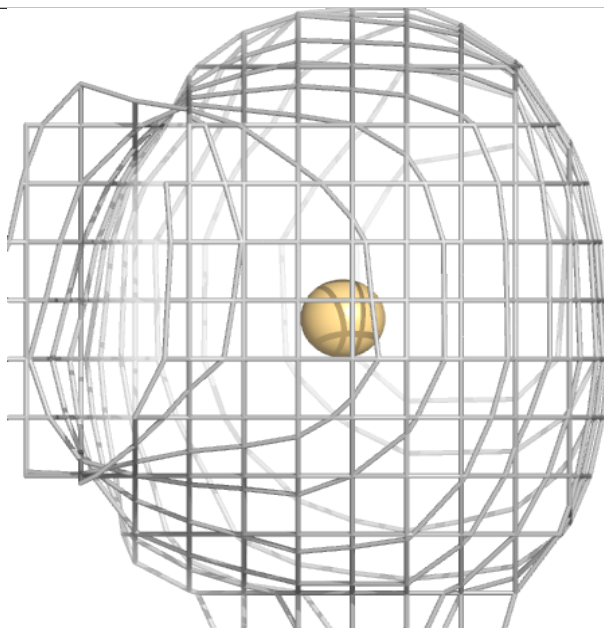
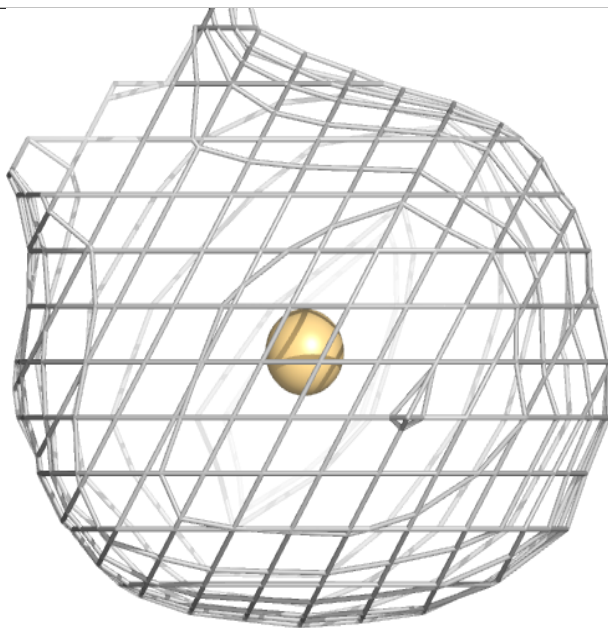
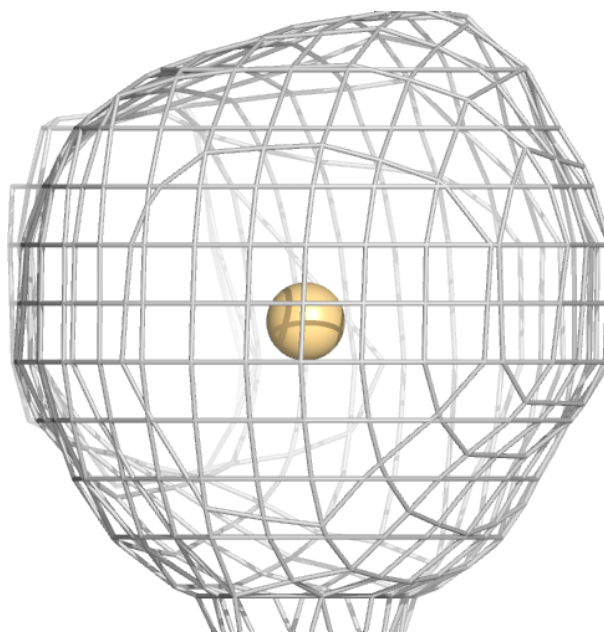
Electron density around CD J 701:

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



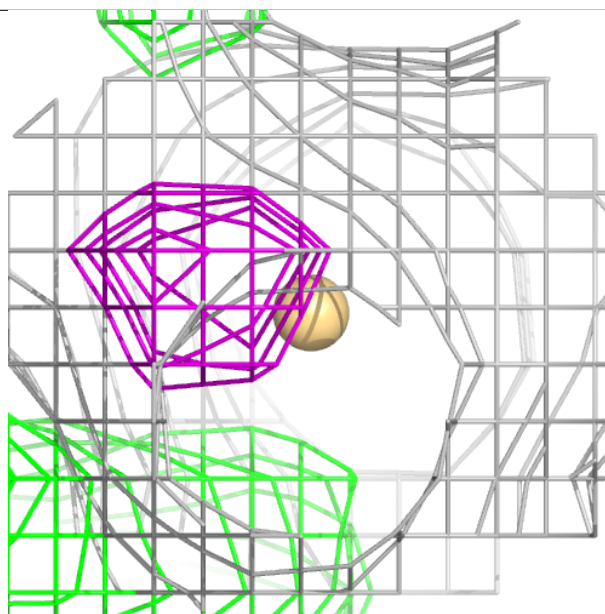
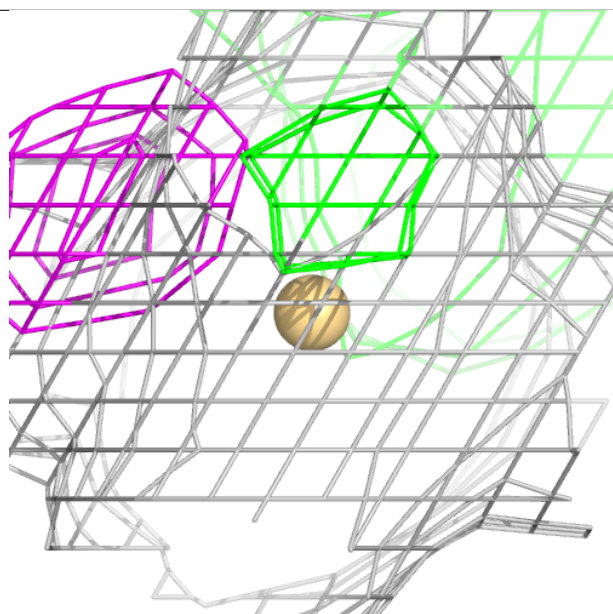
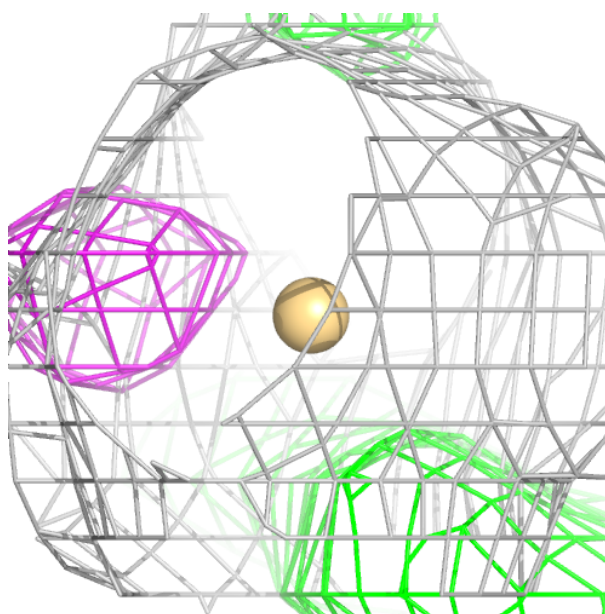
Electron density around CD E 704:

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



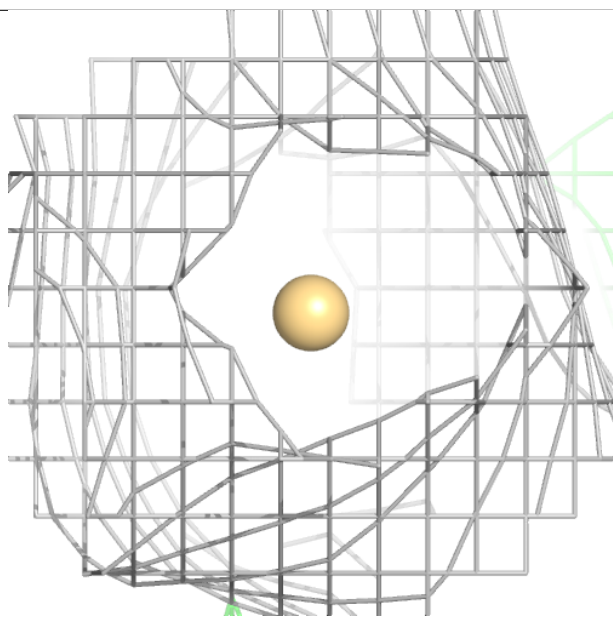
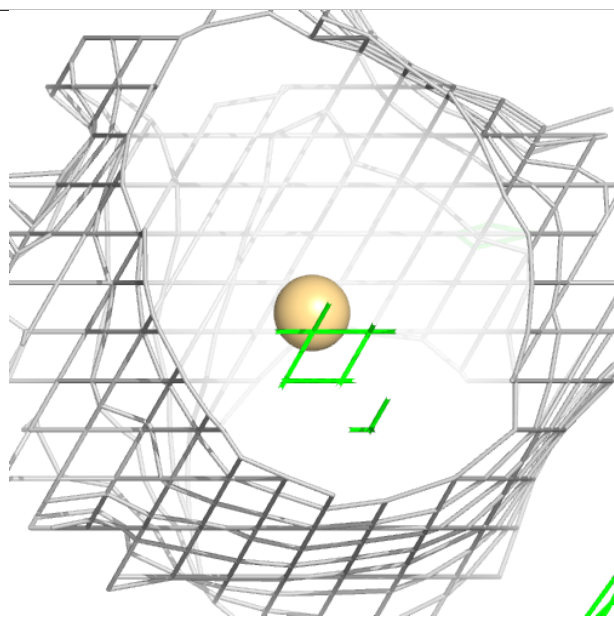
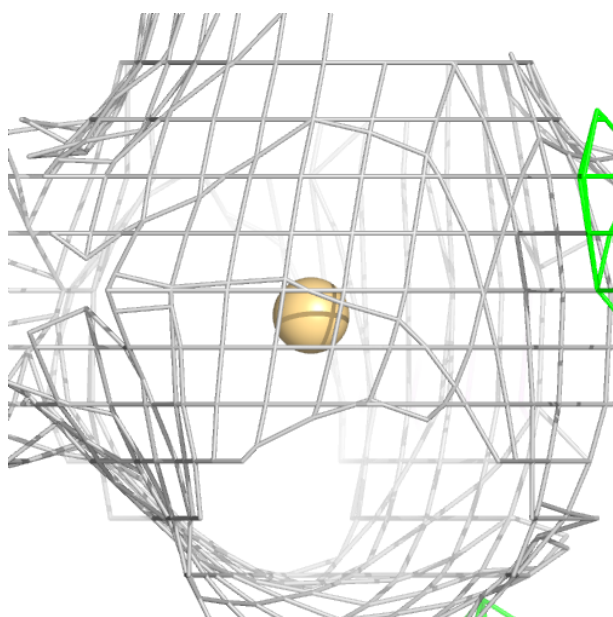
Electron density around CD H 701:

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



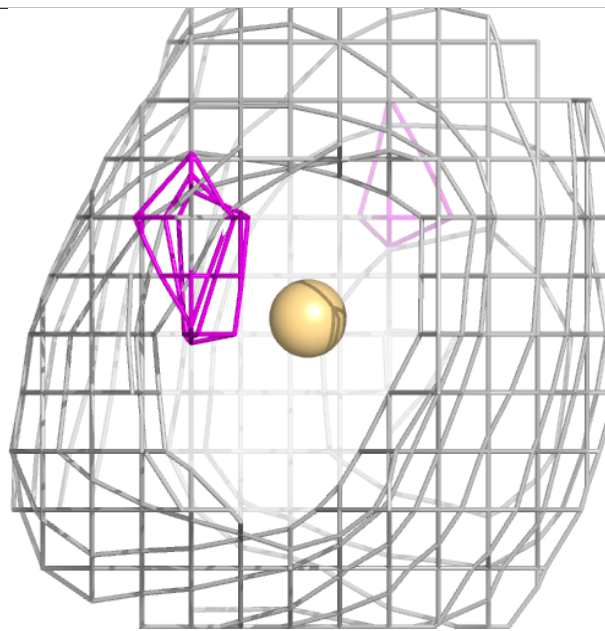
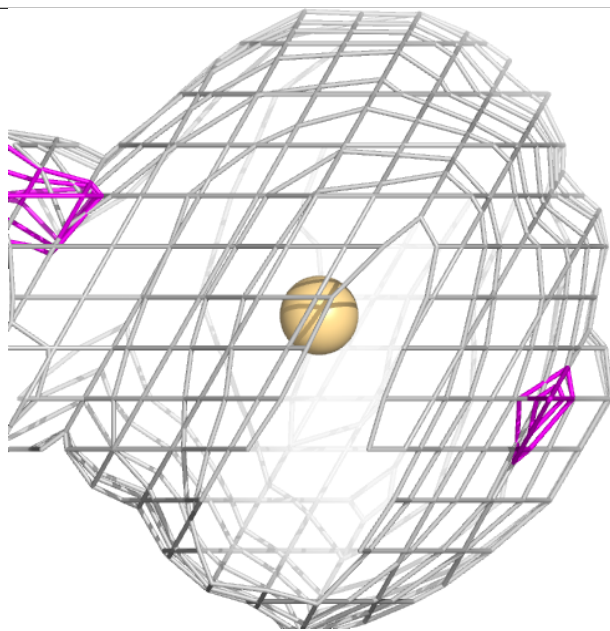
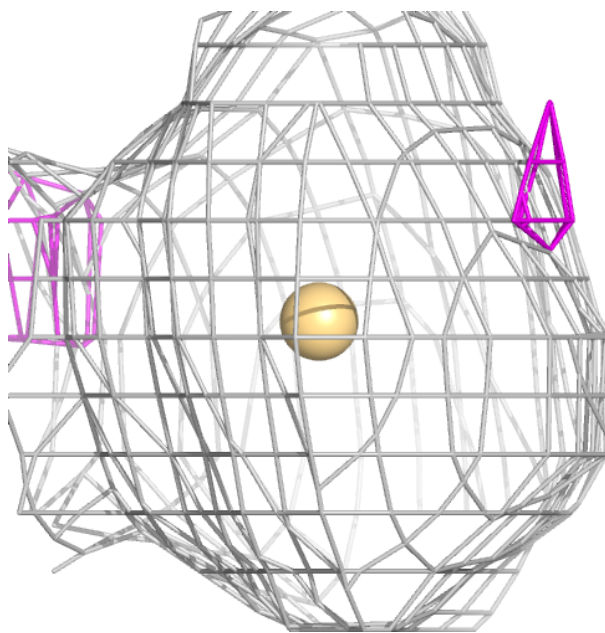
Electron density around CD B 701:

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



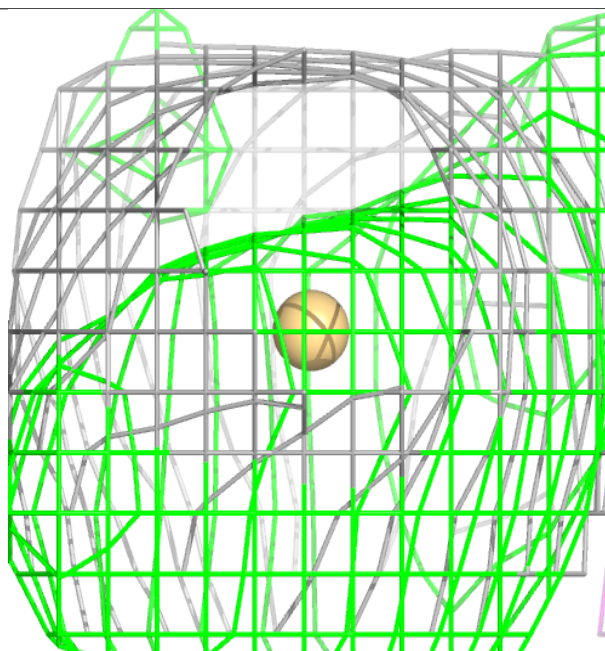
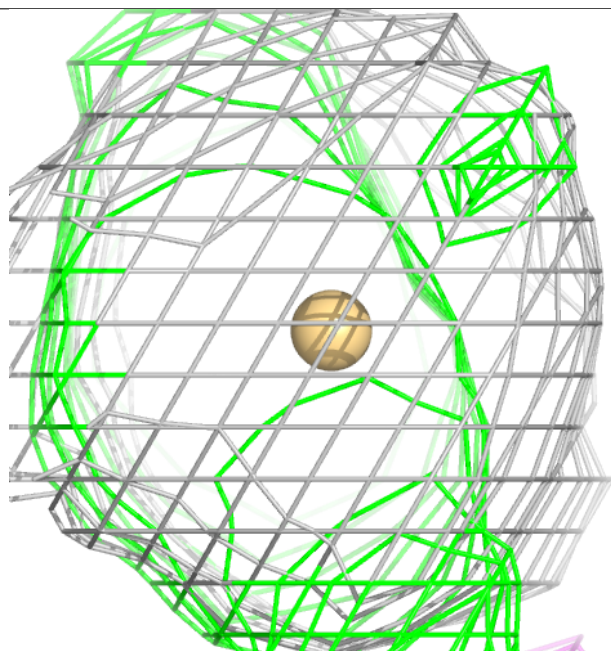
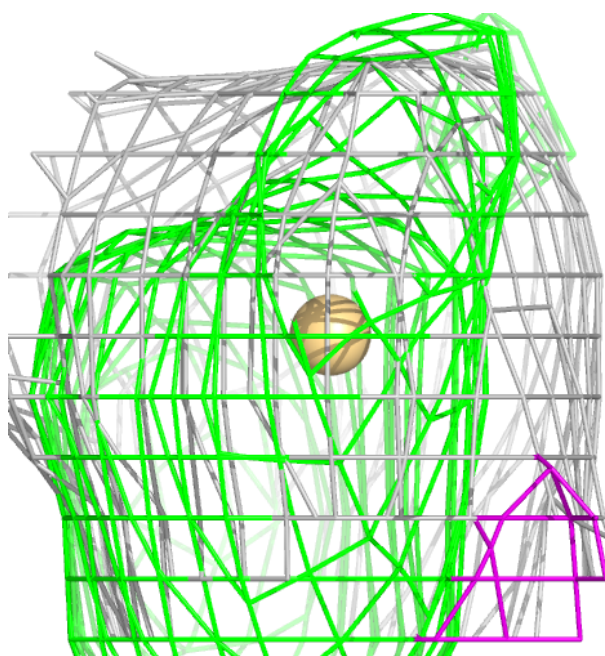
Electron density around CD D 704:

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



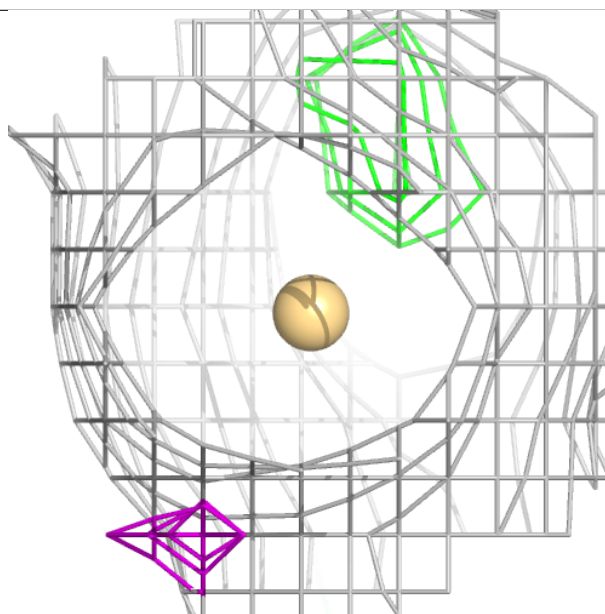
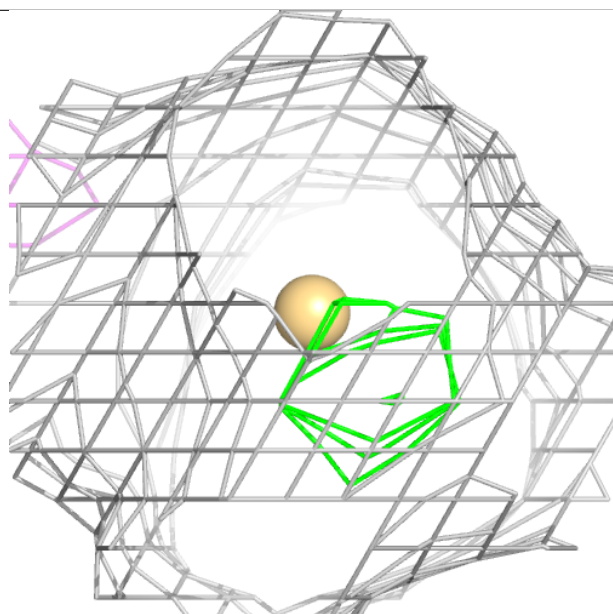
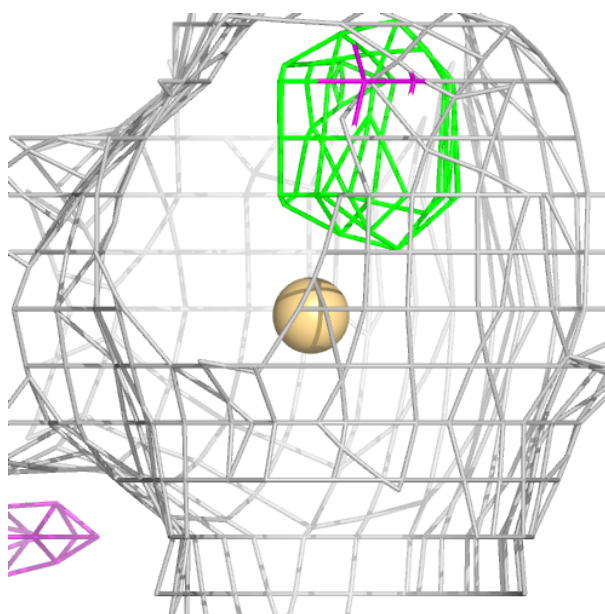
Electron density around CD K 702:

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



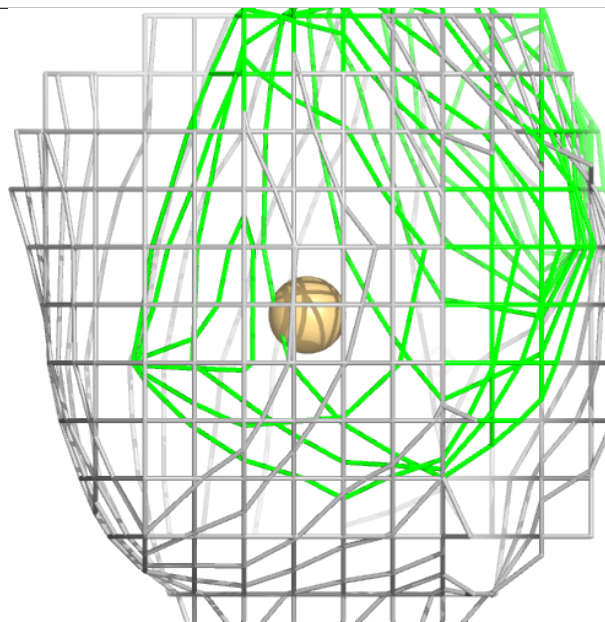
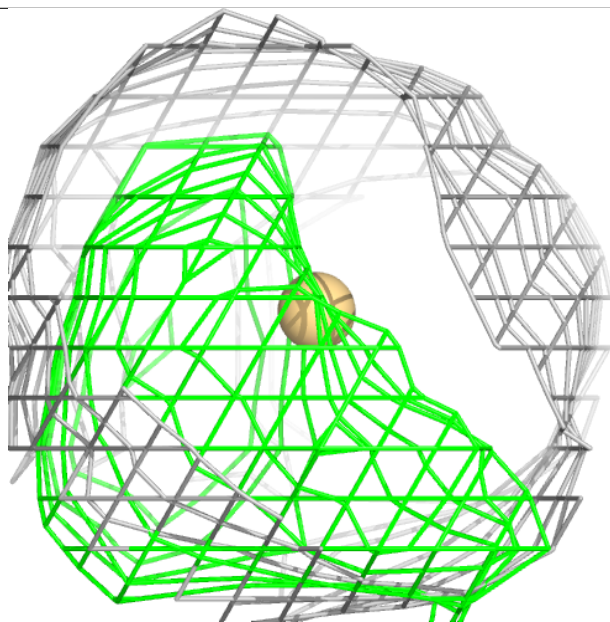
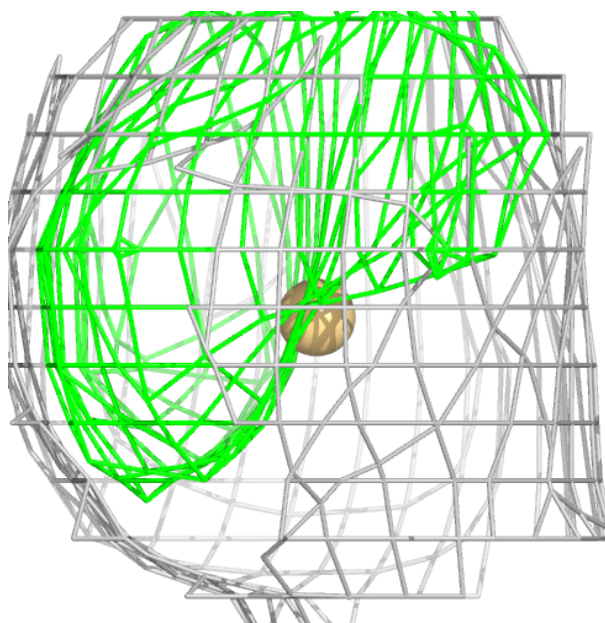
Electron density around CD G 701:

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



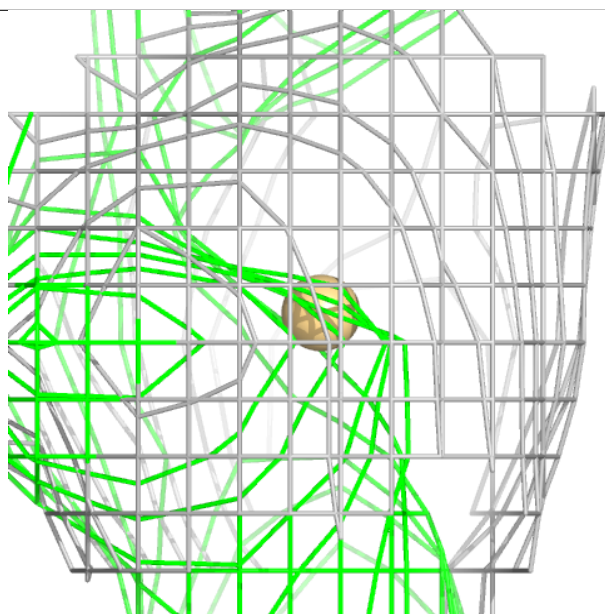
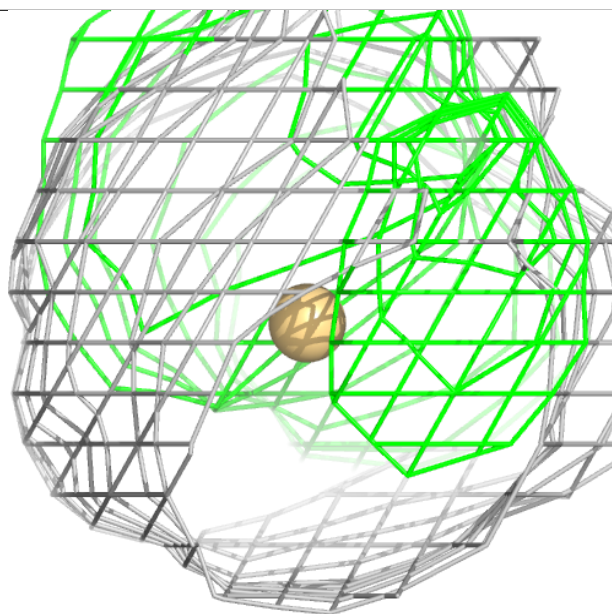
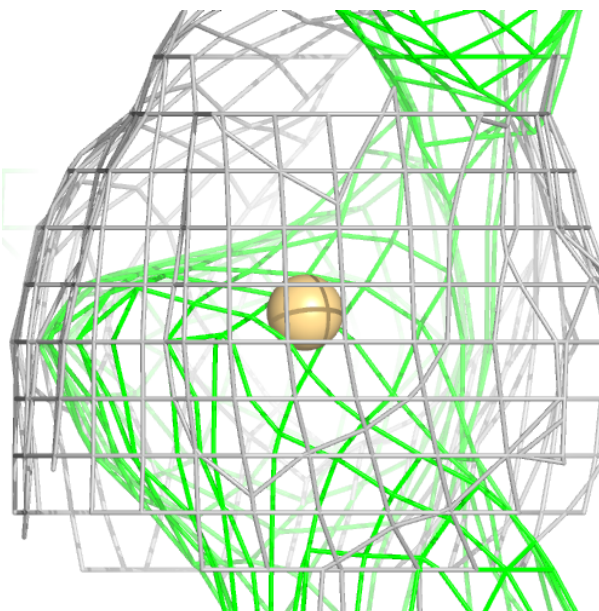
Electron density around CD I 702:

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



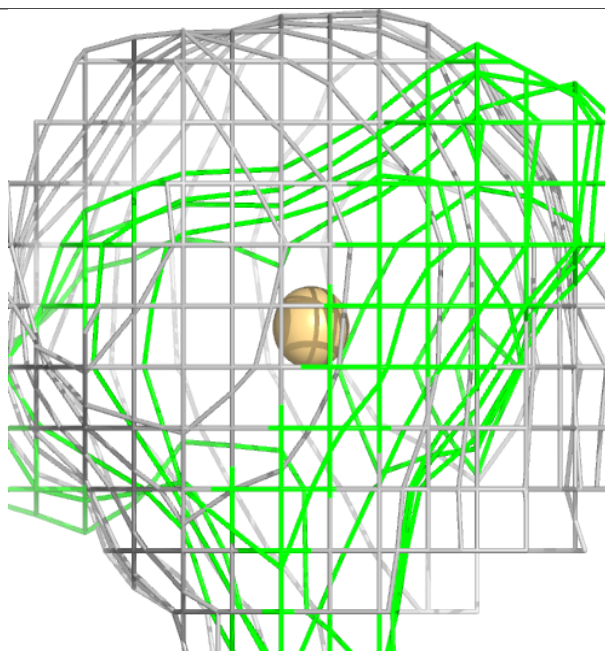
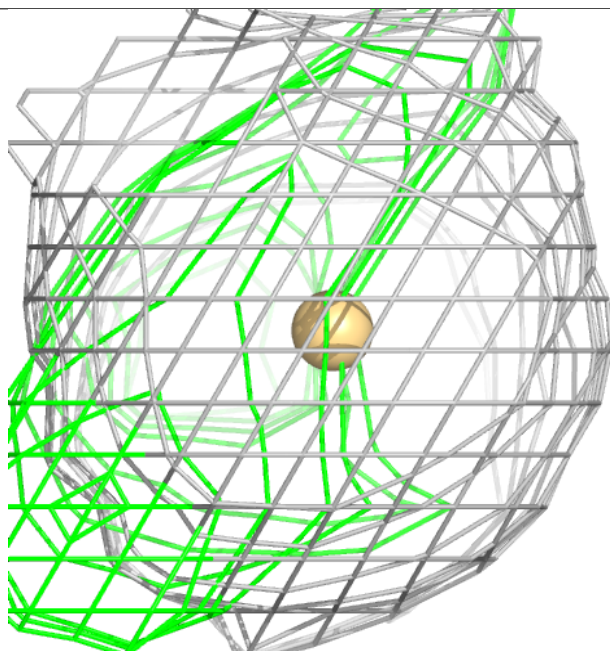
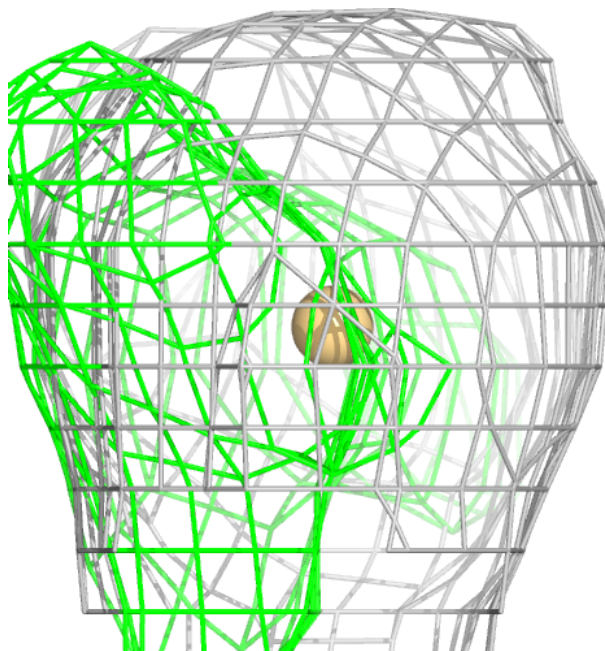
Electron density around CD B 702:

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



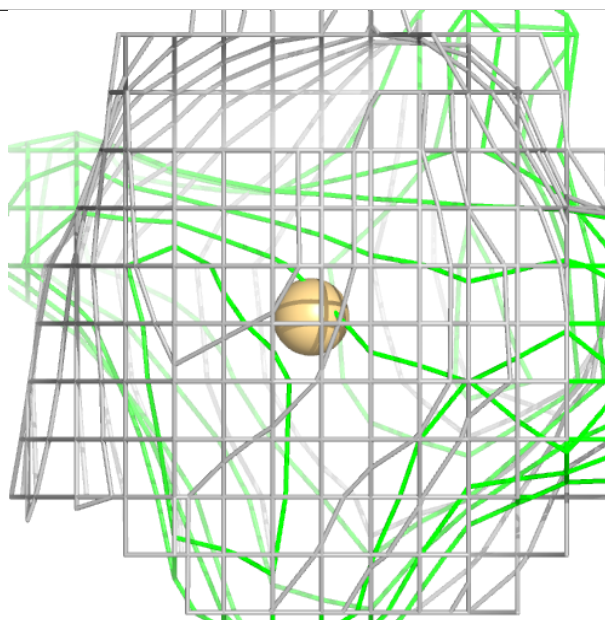
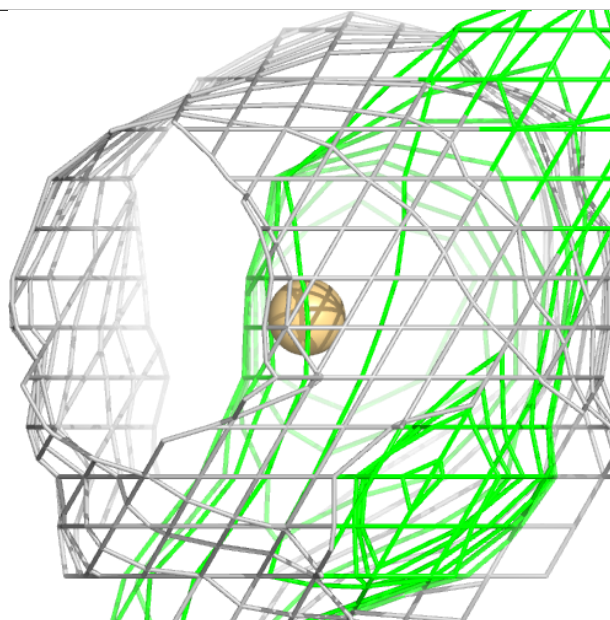
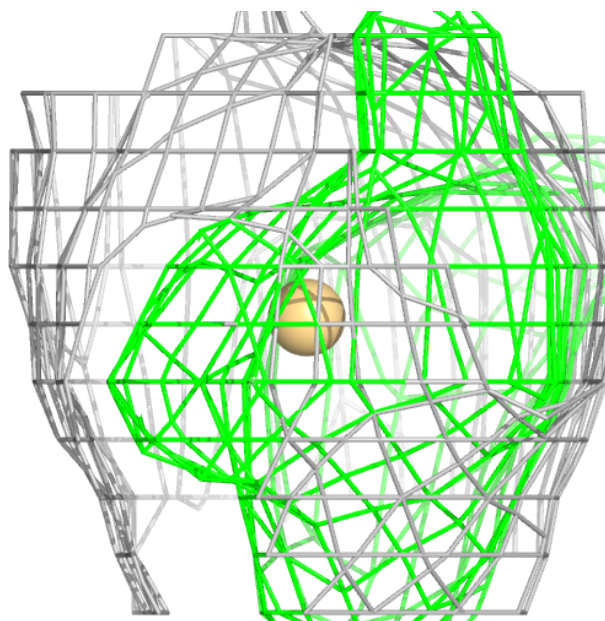
Electron density around CD C 702:

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



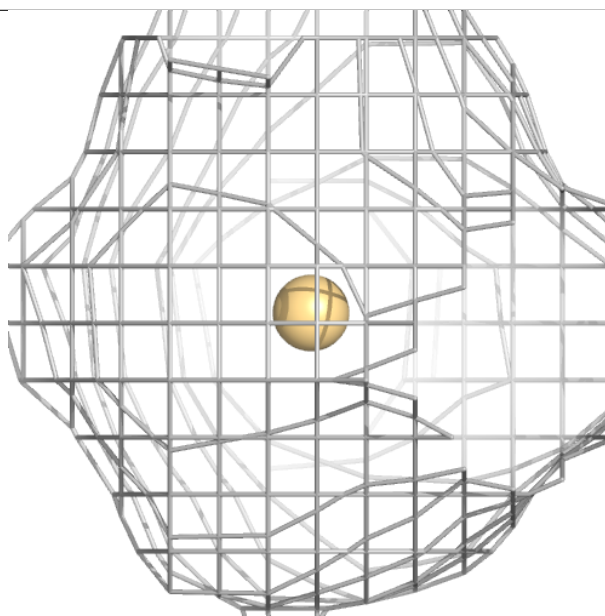
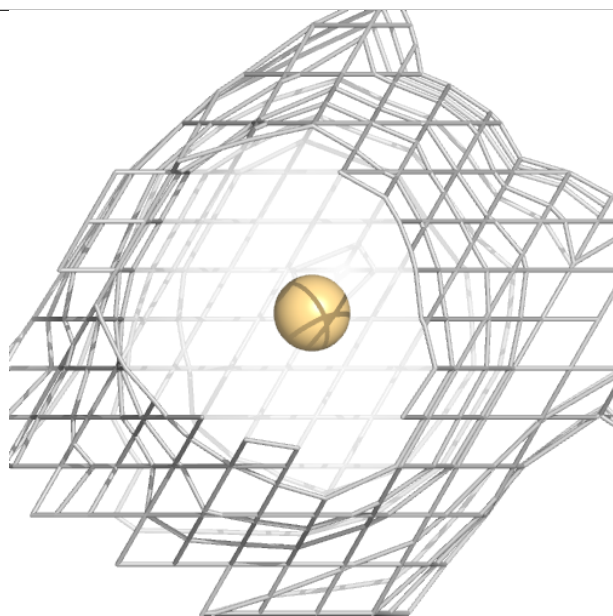
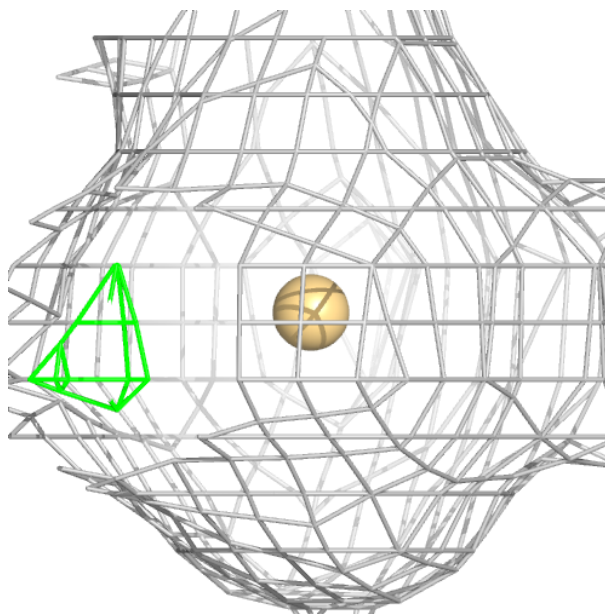
Electron density around CD F 702:

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



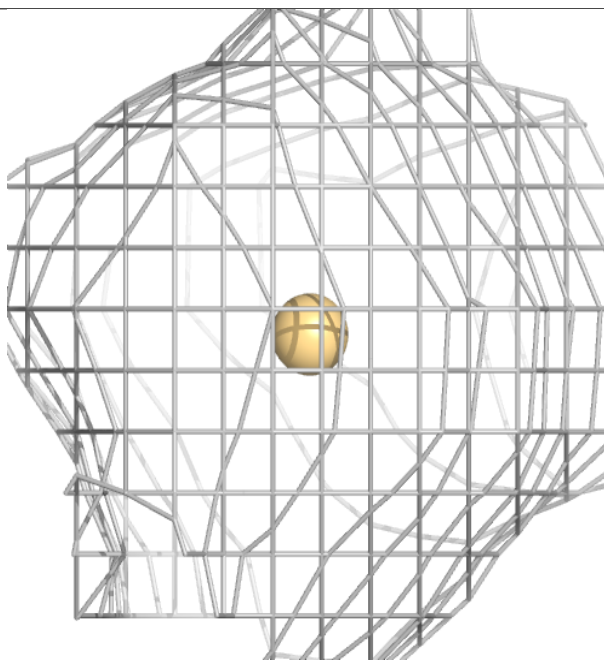
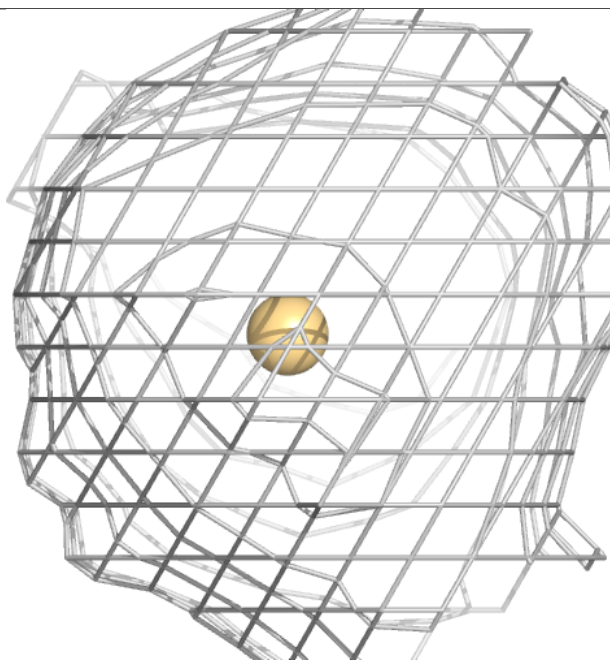
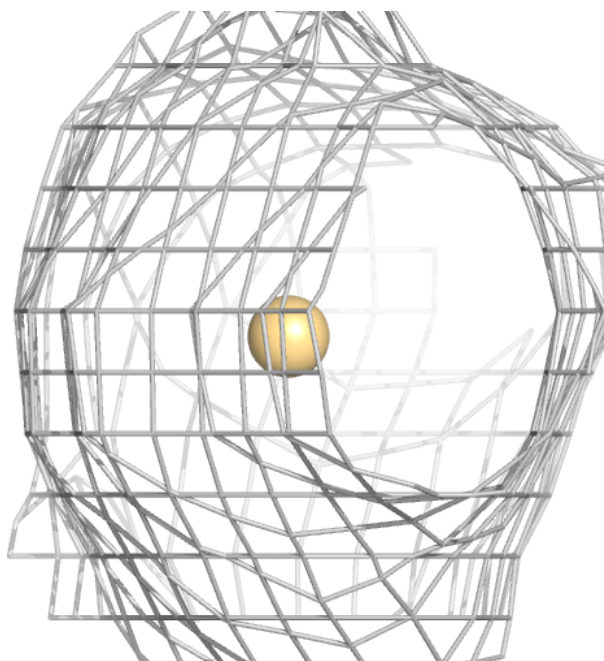
Electron density around CD J 703:

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



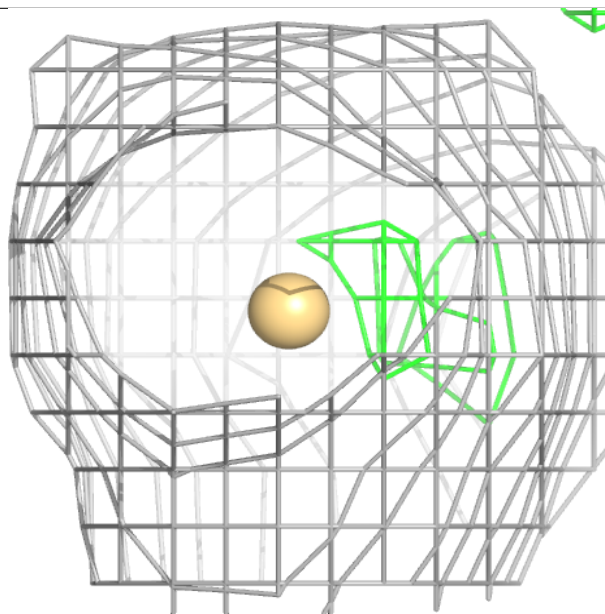
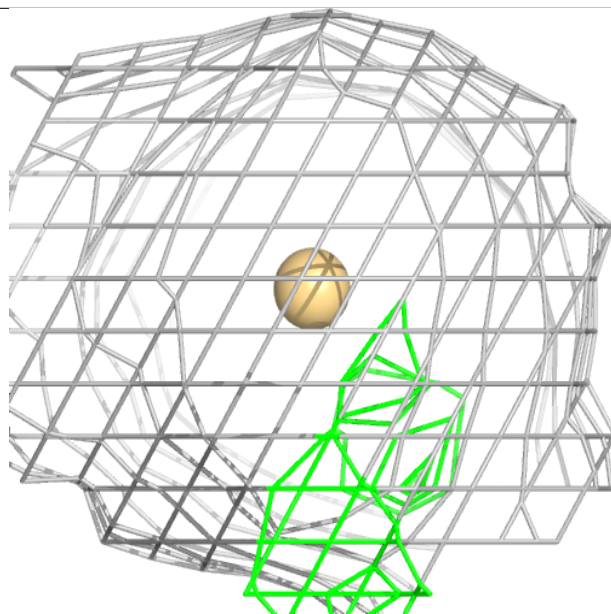
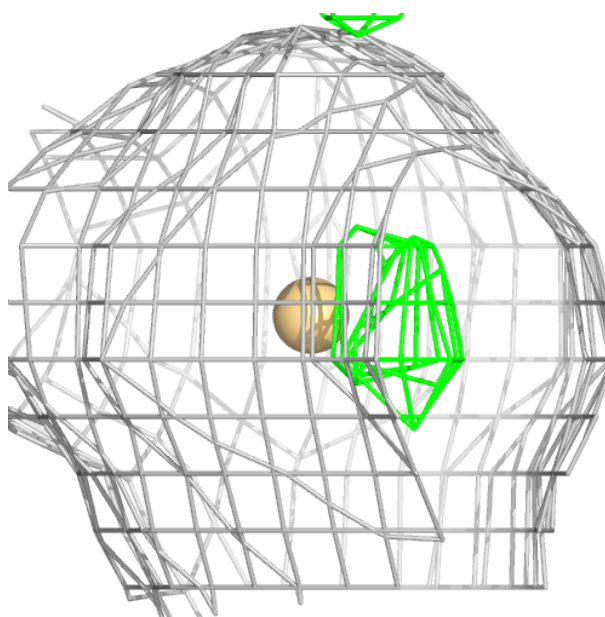
Electron density around CD F 703:

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



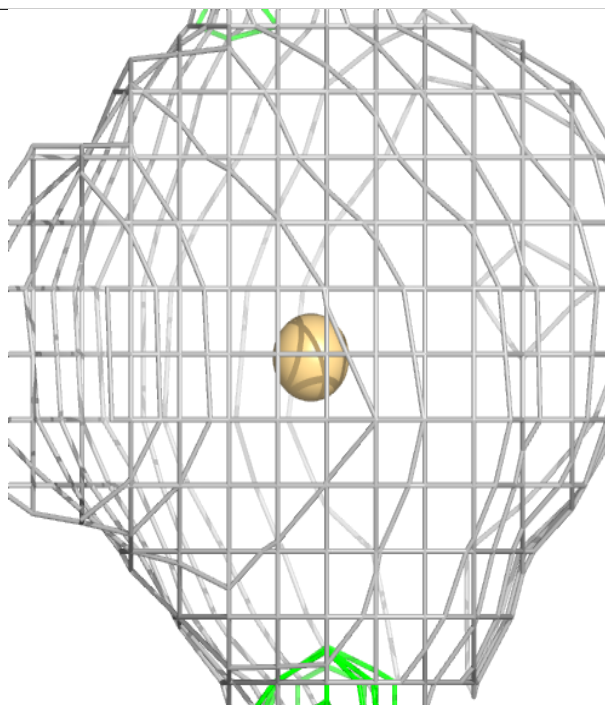
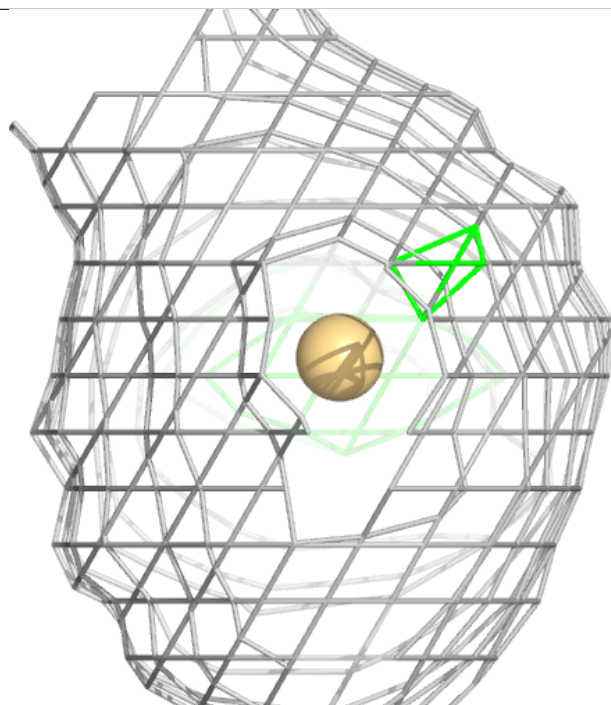
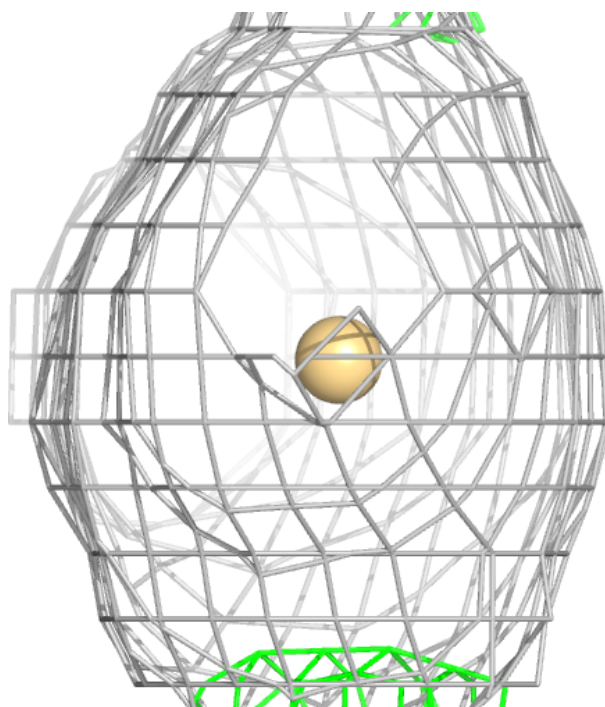
Electron density around CD H 703:

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



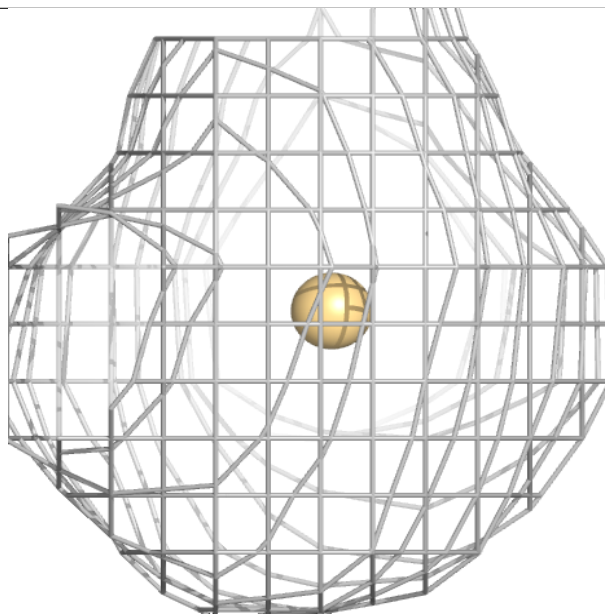
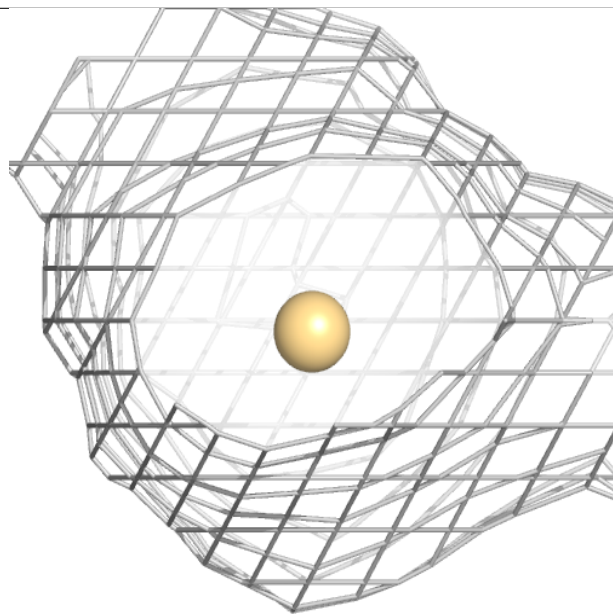
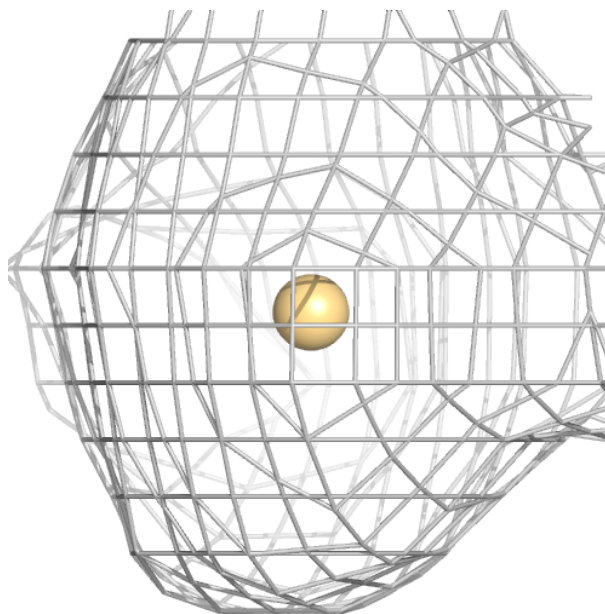
Electron density around CD C 703:

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



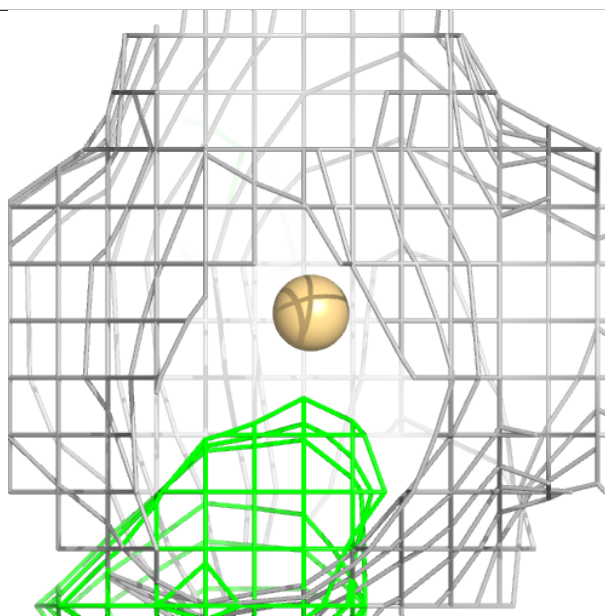
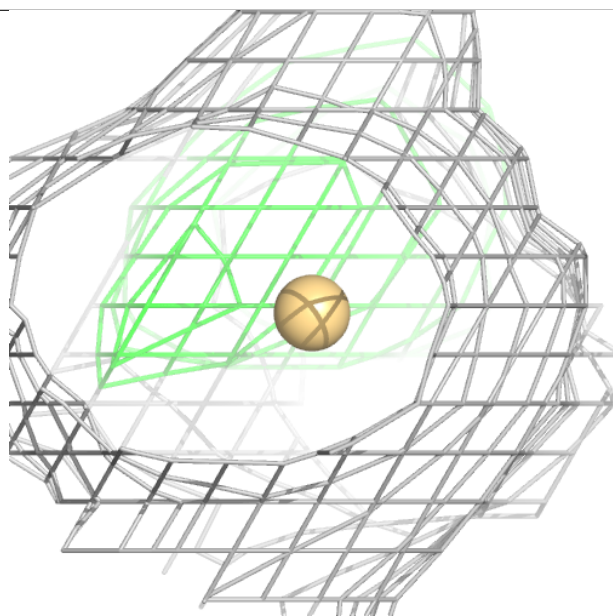
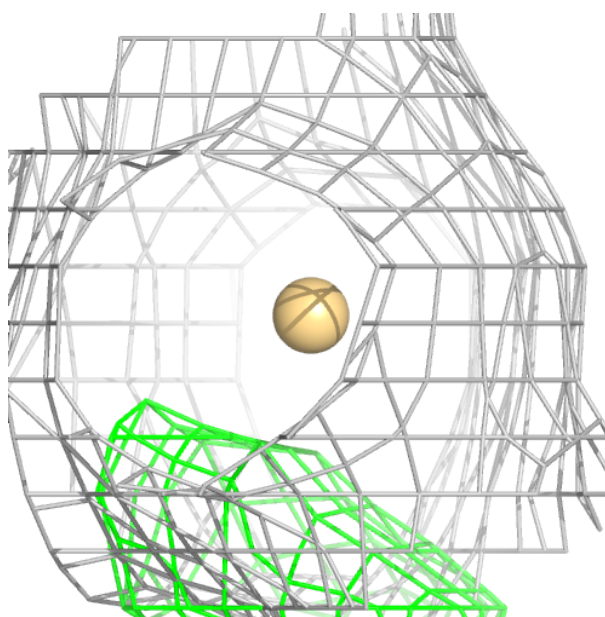
Electron density around CD A 703:

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



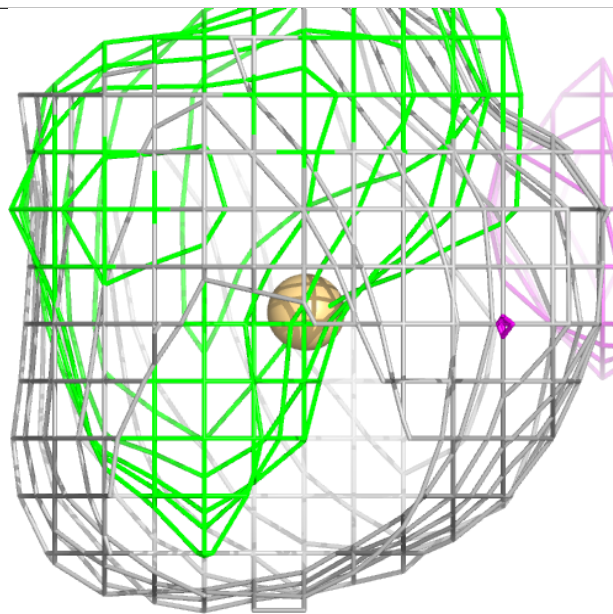
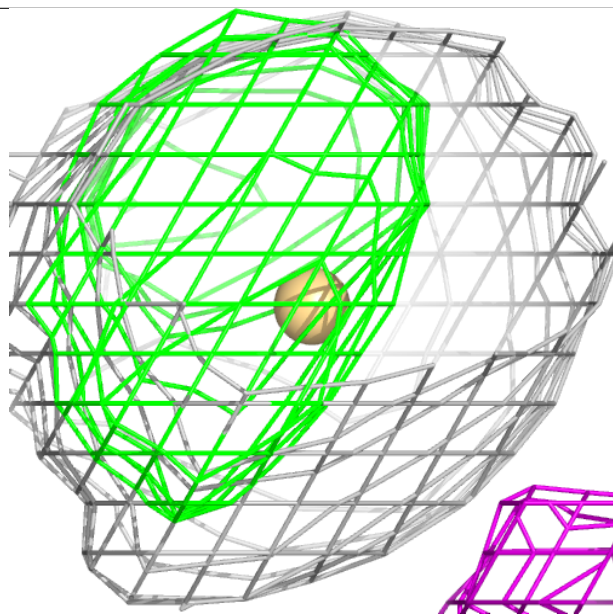
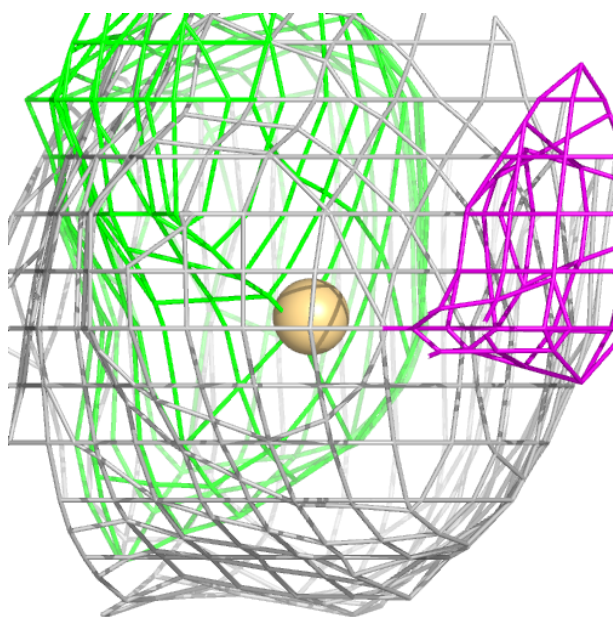
Electron density around CD C 701:

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



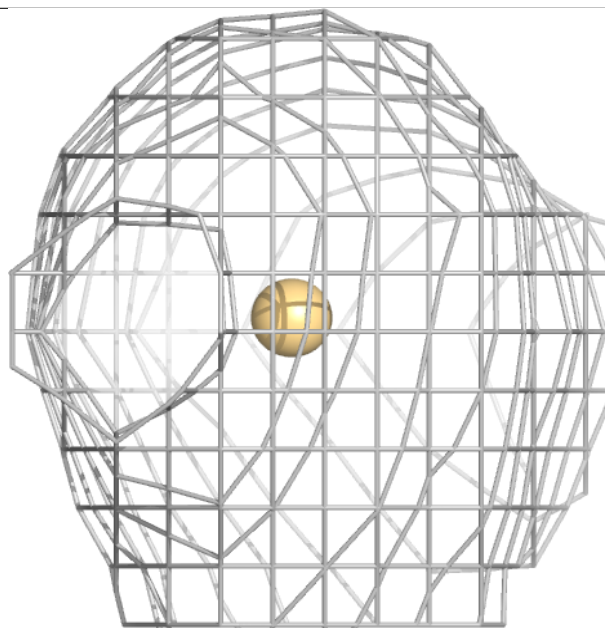
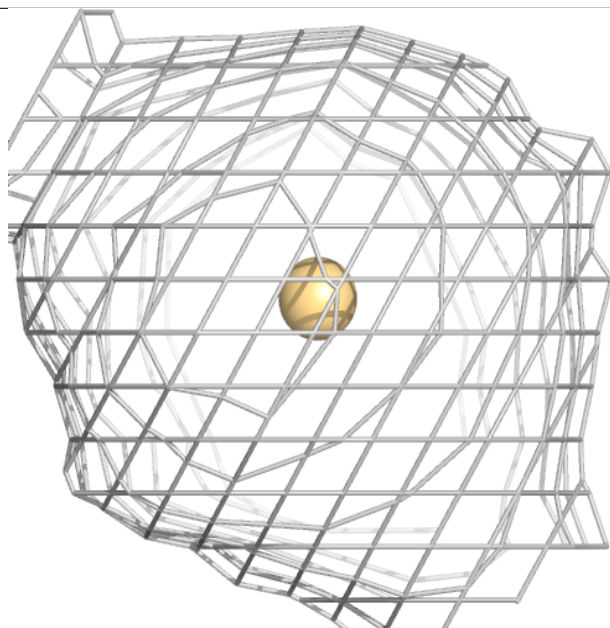
Electron density around CD L 702:

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



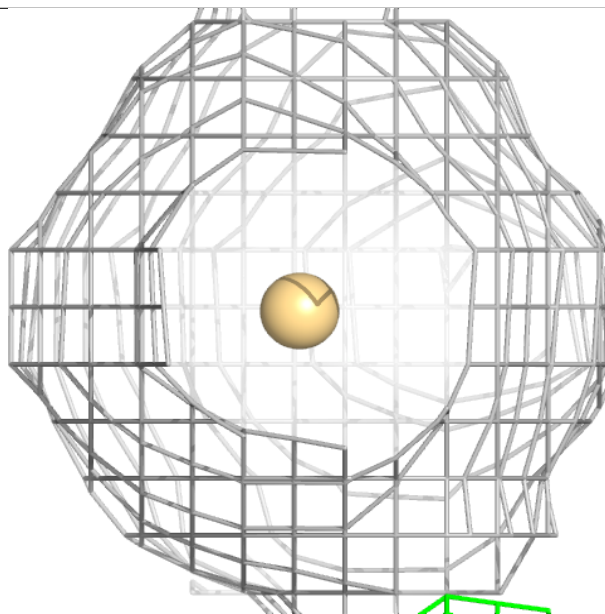
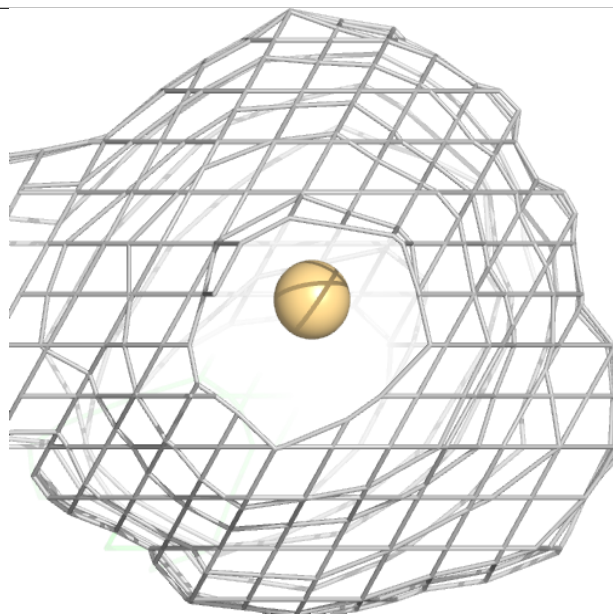
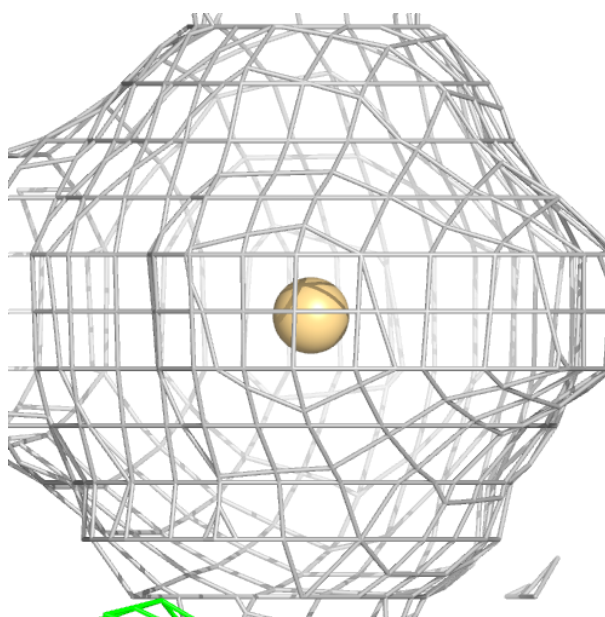
Electron density around CD G 703:

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



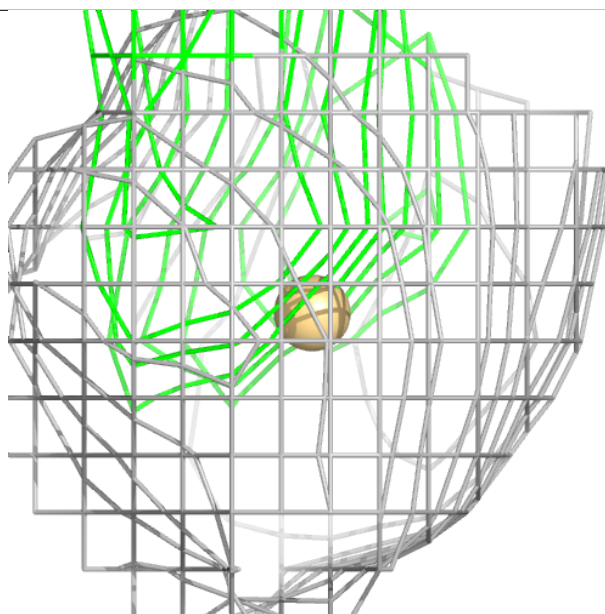
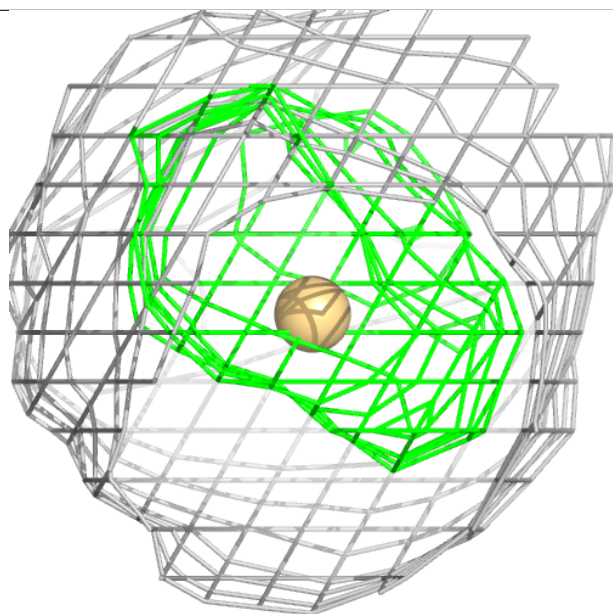
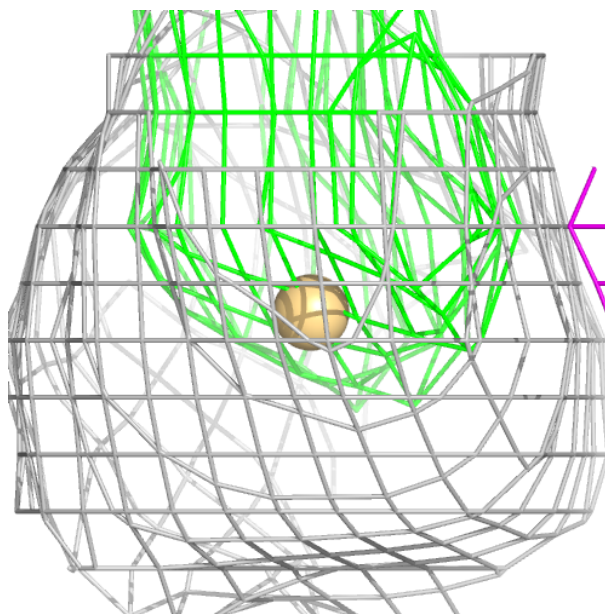
Electron density around CD K 703:

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



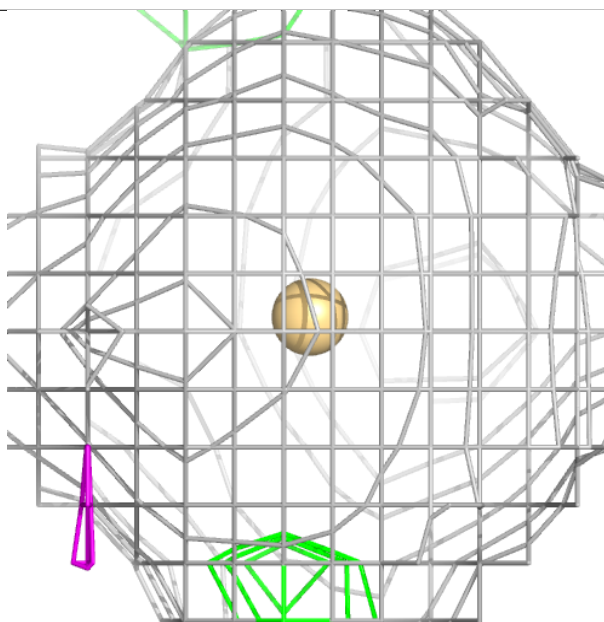
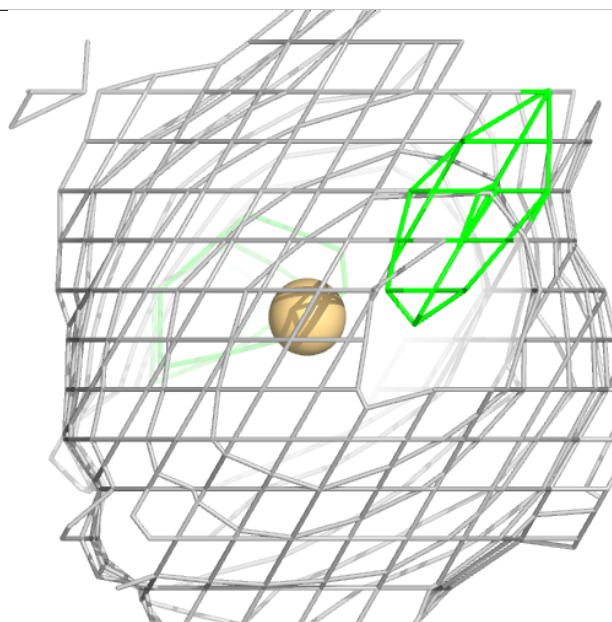
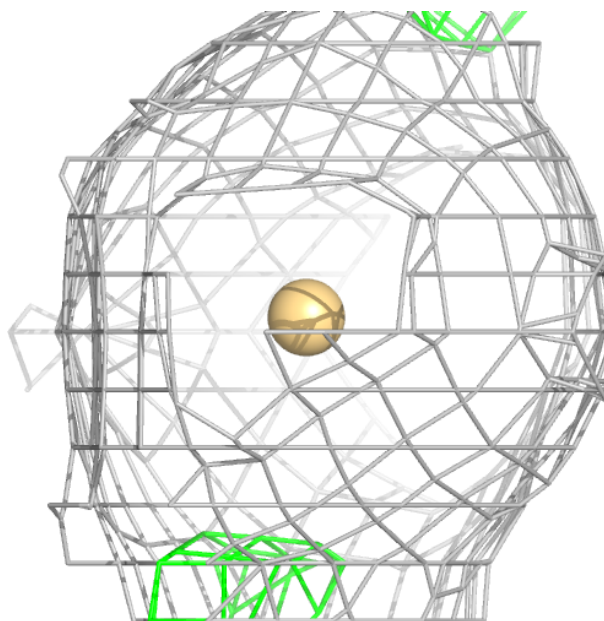
Electron density around CD E 702:

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



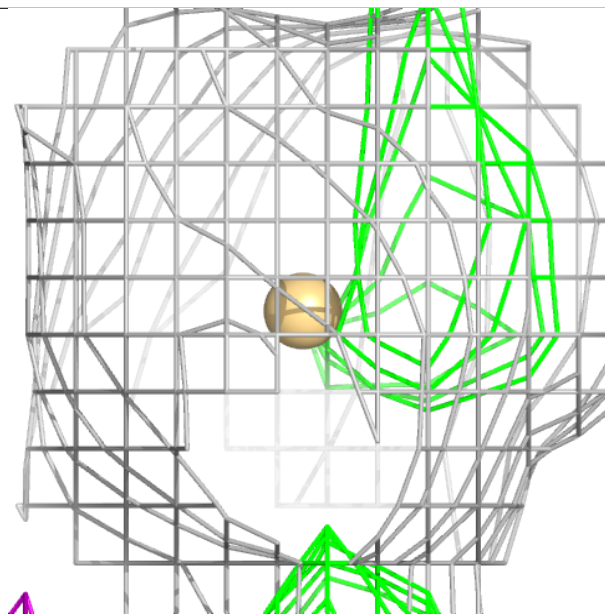
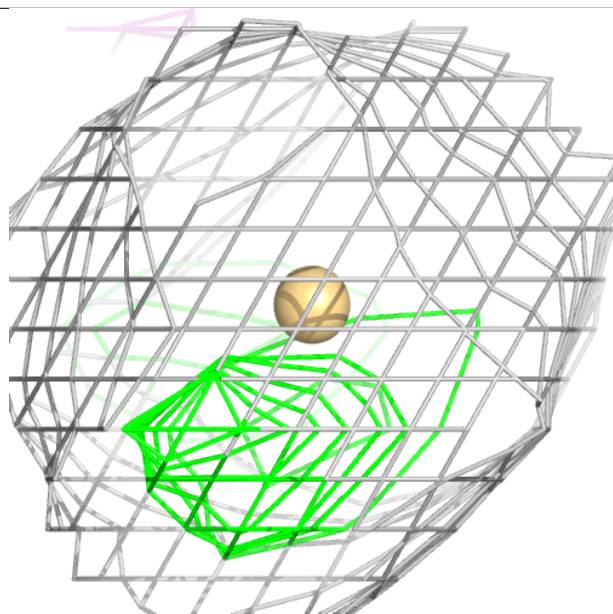
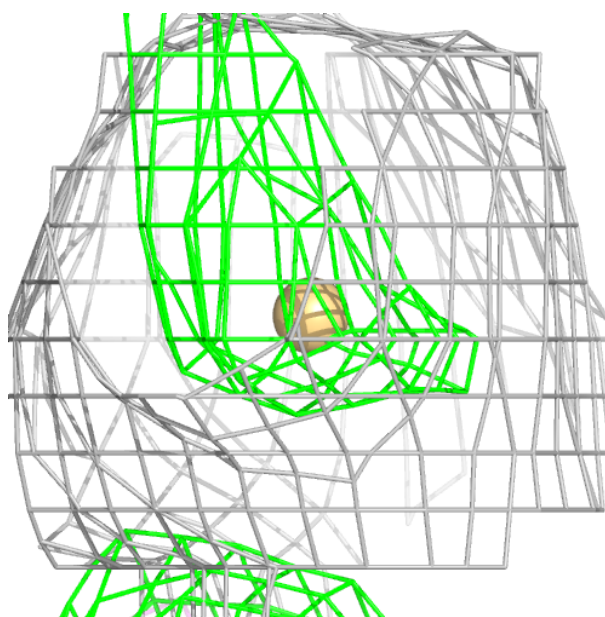
Electron density around CD E 703:

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



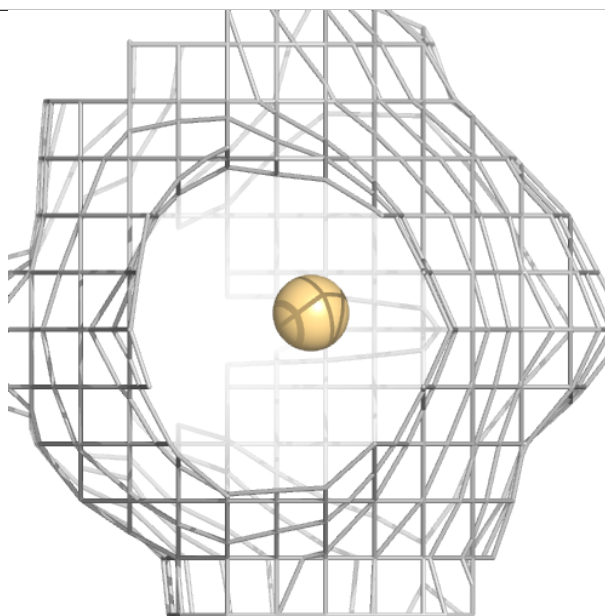
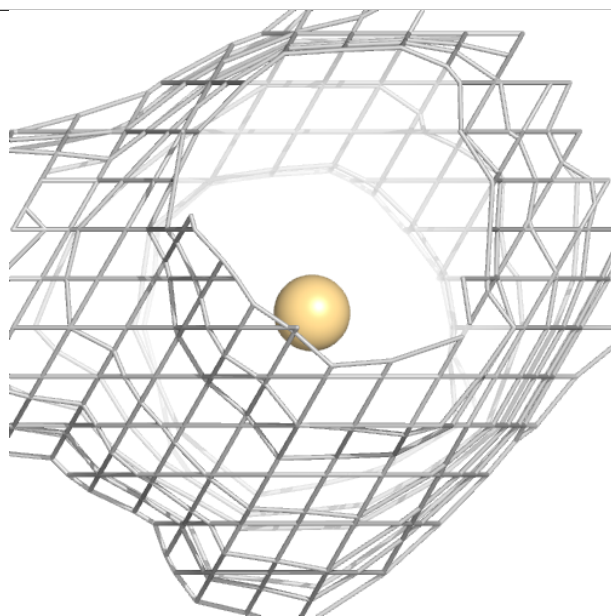
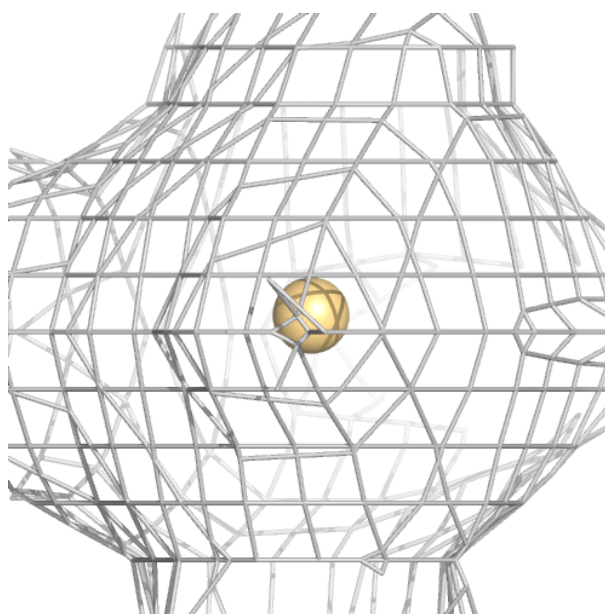
Electron density around CD D 702:

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



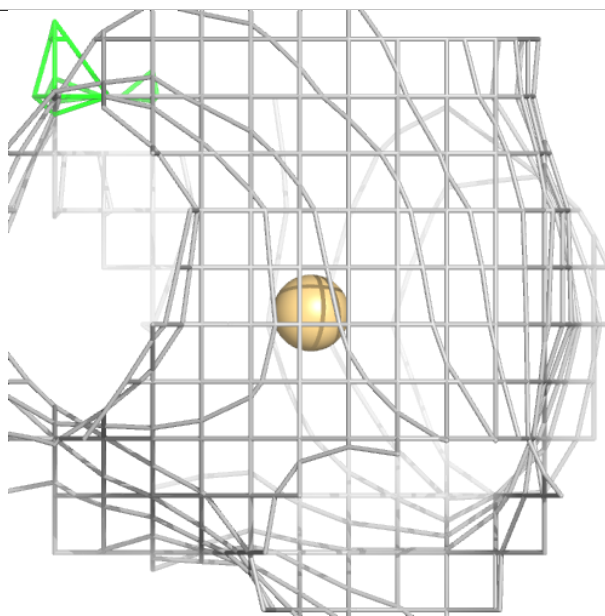
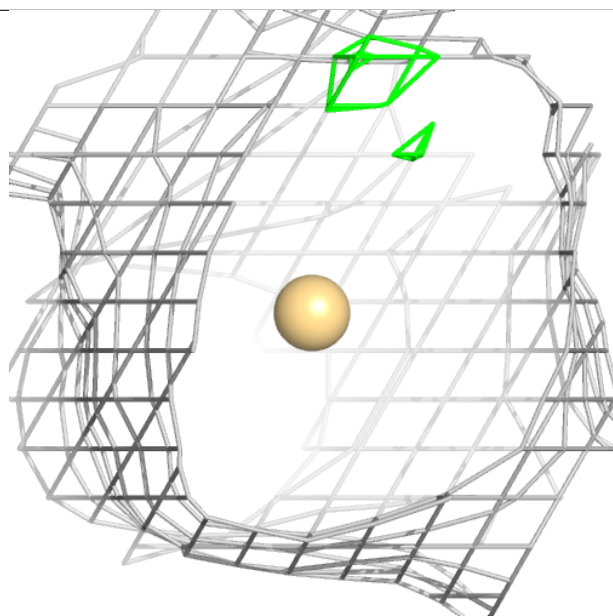
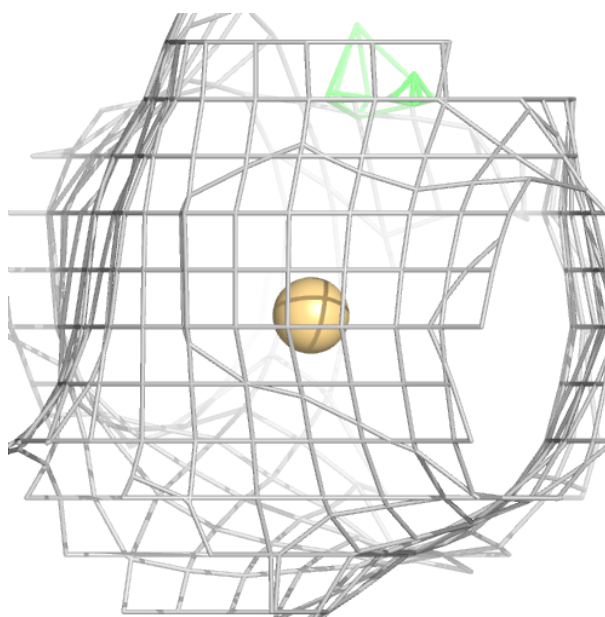
Electron density around CD L 703:

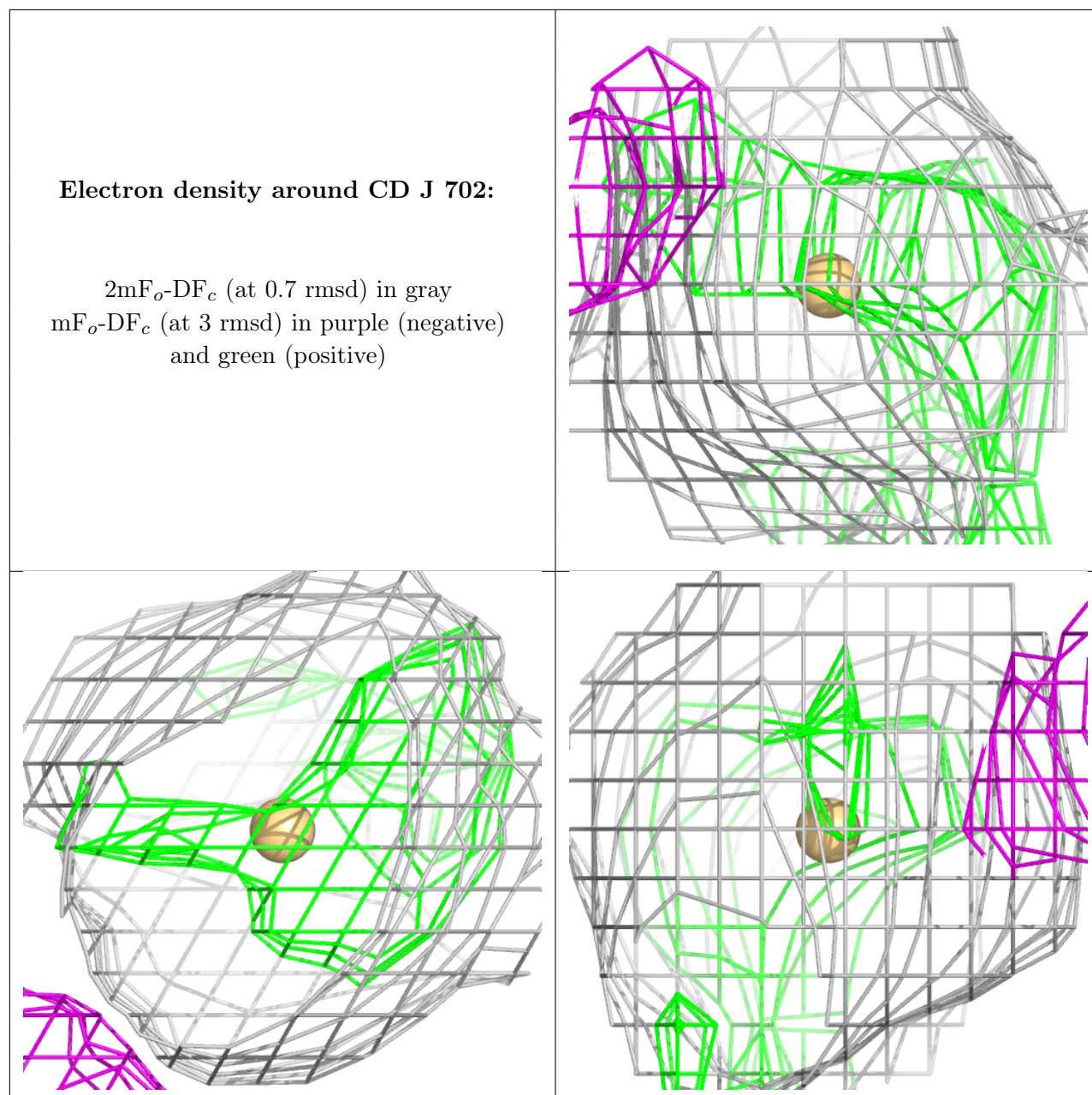
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.