



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2023 – 08:30 AM JST

PDB ID : 7FF9  
Title : Pseudomonas aeruginosa Virulence Factor Regulator with cAMP ligand and Cl(triethylphosphine)gold(I)  
Authors : Chew, B.L.A.; Luo, D.  
Deposited on : 2021-07-23  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

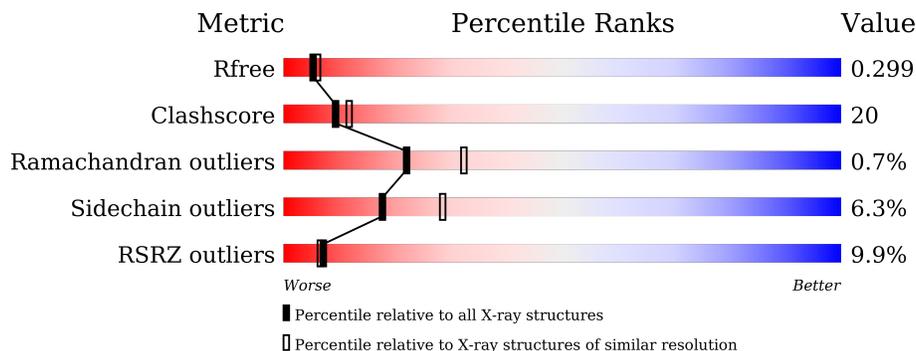
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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	210	
1	B	210	
1	C	210	
1	D	210	
1	E	210	
1	F	210	

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Mol	Chain	Length	Quality of chain
1	G	210	
1	H	210	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	307	-	-	X	-
4	CL	B	307	-	-	-	X
4	CL	B	308	-	-	X	-
4	CL	B	309	-	-	X	-
4	CL	C	308	-	-	X	-
4	CL	D	307	-	-	X	-
4	CL	E	307	-	-	X	-
4	CL	G	307	-	-	X	-
4	CL	H	305	-	-	X	-
5	SO4	C	302	-	-	X	-
5	SO4	E	302	-	-	X	-

## 2 Entry composition

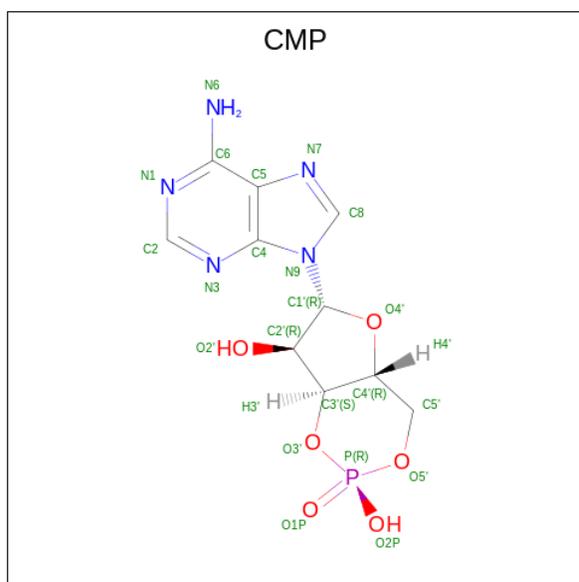
There are 6 unique types of molecules in this entry. The entry contains 23885 atoms, of which 11355 are hydrogens and 0 are deuteriums.

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 cAMP-activated global transcriptional regulator Vfr.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	197	2877	923	1413	256	274	11	0	0	0
1	B	195	2877	924	1412	250	281	10	0	0	0
1	C	197	2935	933	1452	260	279	11	0	0	0
1	D	198	2873	926	1406	249	282	10	0	0	0
1	E	194	2828	908	1389	251	269	11	0	0	0
1	F	188	2744	882	1347	240	267	8	0	0	0
1	G	197	3003	945	1495	269	283	11	0	0	0
1	H	186	2748	882	1353	235	269	9	0	0	0

- Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: C<sub>10</sub>H<sub>12</sub>N<sub>5</sub>O<sub>6</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	Total 33	C 10	H 11	N 5	O 6	P 1	0	0
2	B	1	Total 33	C 10	H 11	N 5	O 6	P 1	0	0
2	C	1	Total 33	C 10	H 11	N 5	O 6	P 1	0	0
2	D	1	Total 33	C 10	H 11	N 5	O 6	P 1	0	0
2	E	1	Total 33	C 10	H 11	N 5	O 6	P 1	0	0
2	F	1	Total 33	C 10	H 11	N 5	O 6	P 1	0	0
2	G	1	Total 33	C 10	H 11	N 5	O 6	P 1	0	0
2	H	1	Total 33	C 10	H 11	N 5	O 6	P 1	0	0

- Molecule 3 is GOLD ION (three-letter code: AU) (formula: Au) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Au 4 4	0	0
3	B	5	Total Au 5 5	0	0
3	C	5	Total Au 5 5	0	0

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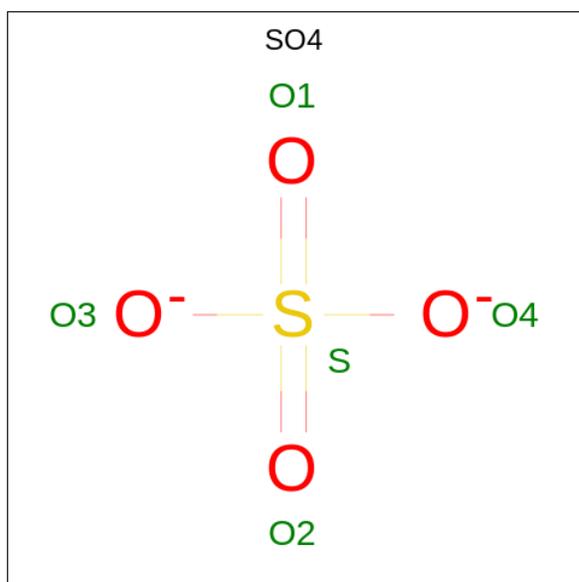
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	4	Total Au 4 4	0	0
3	E	4	Total Au 4 4	0	0
3	F	3	Total Au 3 3	0	0
3	G	3	Total Au 3 3	0	0
3	H	3	Total Au 3 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	B	3	Total Cl 3 3	0	0
4	C	2	Total Cl 2 2	0	0
4	D	2	Total Cl 2 2	0	0
4	E	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	G	2	Total Cl 2 2	0	0
4	H	1	Total Cl 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		

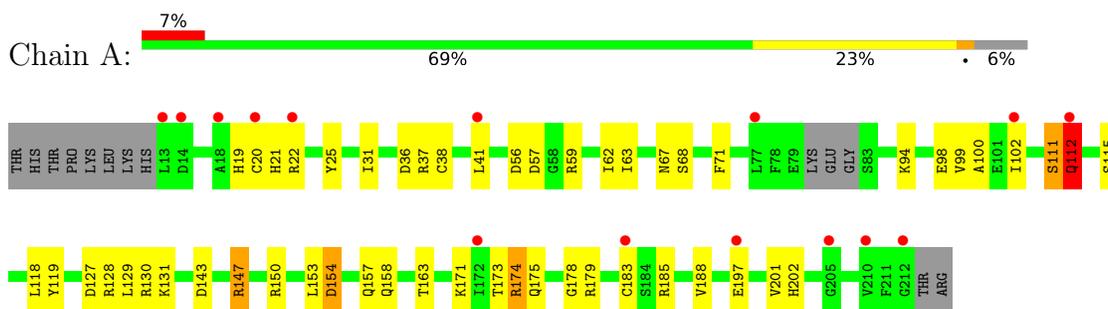
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	80	Total	O	0	0
			80	80		
6	B	69	Total	O	0	0
			69	69		
6	C	104	Total	O	0	0
			104	104		
6	D	91	Total	O	0	0
			91	91		
6	E	73	Total	O	0	0
			73	73		
6	F	58	Total	O	0	0
			58	58		
6	G	112	Total	O	0	0
			112	112		
6	H	89	Total	O	0	0
			89	89		

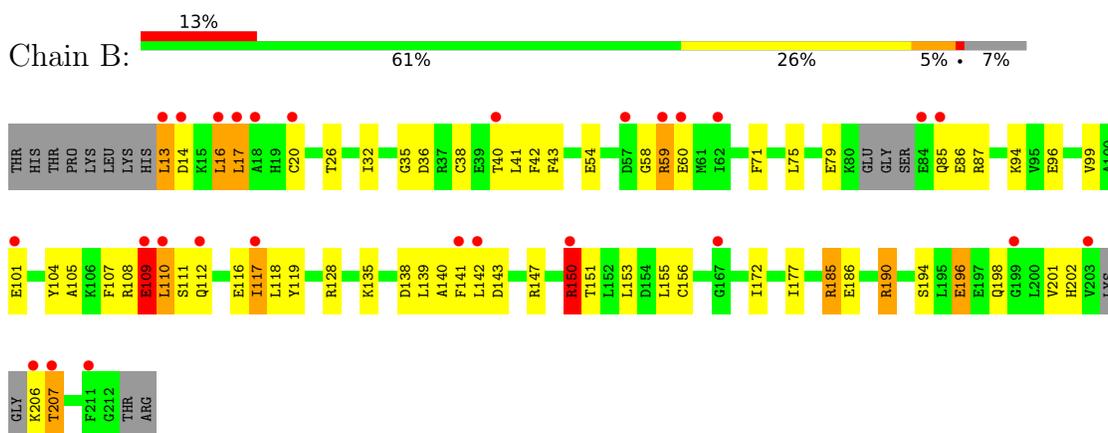
### 3 Residue-property plots [i](#)

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

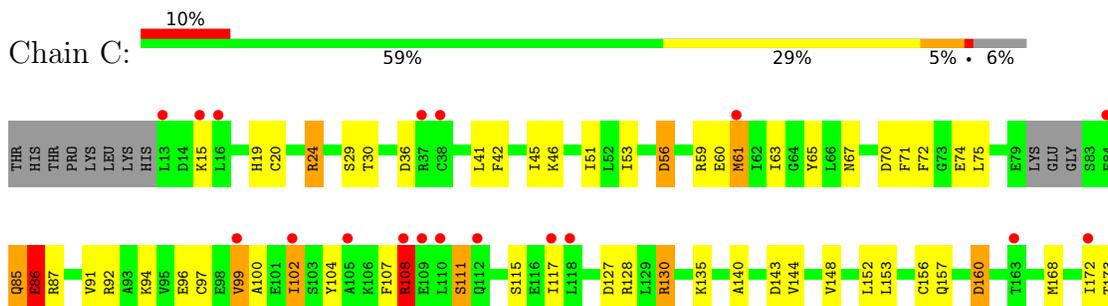
- Molecule 1: cAMP-activated global transcriptional regulator Vfr



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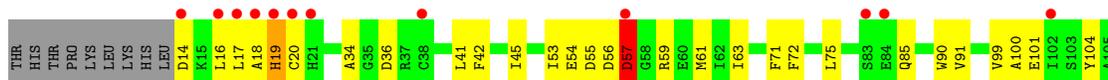


- Molecule 1: cAMP-activated global transcriptional regulator Vfr

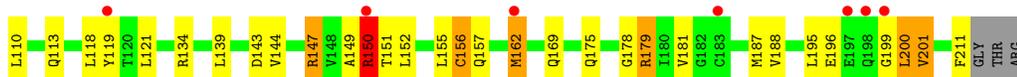




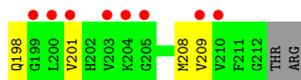
- Molecule 1: cAMP-activated global transcriptional regulator Vfr



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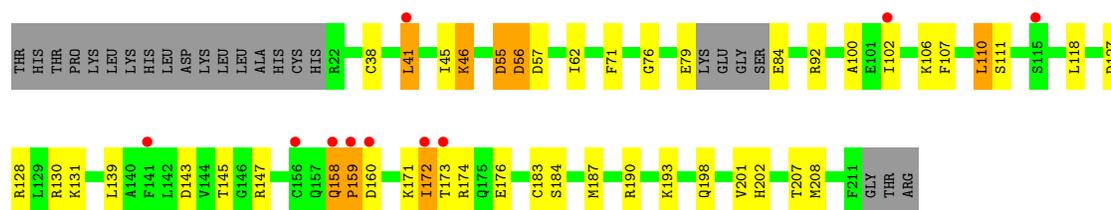


- Molecule 1: cAMP-activated global transcriptional regulator Vfr



- Molecule 1: cAMP-activated global transcriptional regulator Vfr

Chain H: 



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.74Å 87.61Å 104.97Å 79.04° 77.87° 75.40°	Depositor
Resolution (Å)	46.53 – 2.40 46.53 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.9 (46.53-2.40) 83.4 (46.53-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	83.78 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.264 , 0.293 0.273 , 0.299	Depositor DCC
$R_{free}$ test set	2962 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtrriage
Anisotropy	0.439	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 33.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.055 for h,h-k,h-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23885	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3798e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: AU, CL, CMP, SO4

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	0.34	0/1482	0.73	5/1999 (0.3%)
1	B	0.46	1/1482 (0.1%)	0.89	11/1999 (0.6%)
1	C	0.62	6/1500 (0.4%)	0.95	17/2020 (0.8%)
1	D	0.43	3/1486 (0.2%)	1.61	6/2008 (0.3%)
1	E	0.50	3/1456 (0.2%)	1.03	10/1965 (0.5%)
1	F	1.22	10/1413 (0.7%)	1.49	17/1907 (0.9%)
1	G	0.30	0/1525	0.61	0/2050
1	H	0.32	0/1411	0.65	2/1904 (0.1%)
All	All	0.59	23/11755 (0.2%)	1.05	68/15852 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	5
1	D	0	1
1	E	0	2
1	F	0	5
All	All	0	16

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	176	GLU	CG-CD	32.84	2.01	1.51
1	F	119	TYR	CD2-CE2	-12.53	1.20	1.39
1	C	197	GLU	CD-OE1	9.97	1.36	1.25
1	F	176	GLU	CD-OE1	9.75	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	176	GLU	CB-CG	9.37	1.70	1.52

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	57	ASP	CB-CG-OD2	-51.84	71.64	118.30
1	D	57	ASP	CB-CG-OD1	38.71	153.14	118.30
1	F	119	TYR	CB-CG-CD2	-31.82	101.91	121.00
1	F	119	TYR	CB-CG-CD1	20.54	133.32	121.00
1	F	119	TYR	N-CA-CB	-18.03	78.15	110.60

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	SER	Peptide
1	B	109	GLU	Sidechain
1	B	59	ARG	Peptide
1	C	108	ARG	Sidechain
1	C	86	GLU	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1464	1413	1412	49	0
1	B	1465	1412	1410	55	1
1	C	1483	1452	1451	77	0
1	D	1467	1406	1406	58	0
1	E	1439	1389	1389	52	1
1	F	1397	1347	1347	53	1
1	G	1508	1495	1495	62	0
1	H	1395	1353	1352	43	0
2	A	22	11	11	1	0
2	B	22	11	11	2	0
2	C	22	11	11	2	0
2	D	22	11	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	22	11	11	2	0
2	F	22	11	11	1	0
2	G	22	11	11	1	0
2	H	22	11	11	1	0
3	A	4	0	0	0	1
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	1
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
4	A	2	0	0	2	1
4	B	3	0	0	5	0
4	C	2	0	0	6	0
4	D	2	0	0	2	0
4	E	1	0	0	2	0
4	F	1	0	0	0	0
4	G	2	0	0	5	0
4	H	1	0	0	2	0
5	C	5	0	0	3	0
5	E	5	0	0	3	0
5	G	5	0	0	1	0
6	A	80	0	0	17	2
6	B	69	0	0	22	2
6	C	104	0	0	35	2
6	D	91	0	0	29	2
6	E	73	0	0	17	2
6	F	58	0	0	10	2
6	G	112	0	0	33	1
6	H	89	0	0	13	1
All	All	12530	11355	11350	457	10

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 20.

The worst 5 of 457 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:D:162:MET:CB	1:D:162:MET:CG	1.74	1.59
2:F:301:CMP:C2	2:F:301:CMP:H2	0.97	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:301:CMP:H2	2:H:301:CMP:C2	0.97	1.50
2:D:301:CMP:C2	2:D:301:CMP:H2	0.97	1.49
2:A:301:CMP:C2	2:A:301:CMP:H2	0.97	1.47

The worst 5 of 10 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:427:HOH:O	6:E:433:HOH:O[1_554]	1.80	0.40
6:A:460:HOH:O	6:E:453:HOH:O[1_554]	1.81	0.39
6:C:495:HOH:O	6:D:469:HOH:O[1_455]	1.83	0.37
6:C:495:HOH:O	6:D:470:HOH:O[1_455]	1.88	0.32
6:B:457:HOH:O	6:F:444:HOH:O[1_554]	1.95	0.25

## 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	193/210 (92%)	183 (95%)	8 (4%)	2 (1%)	15	23
1	B	189/210 (90%)	178 (94%)	10 (5%)	1 (0%)	29	41
1	C	193/210 (92%)	189 (98%)	4 (2%)	0	100	100
1	D	196/210 (93%)	184 (94%)	10 (5%)	2 (1%)	15	23
1	E	190/210 (90%)	179 (94%)	9 (5%)	2 (1%)	14	20
1	F	184/210 (88%)	170 (92%)	14 (8%)	0	100	100
1	G	193/210 (92%)	181 (94%)	10 (5%)	2 (1%)	15	23
1	H	182/210 (87%)	174 (96%)	6 (3%)	2 (1%)	14	20
All	All	1520/1680 (90%)	1438 (95%)	71 (5%)	11 (1%)	22	32

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	D	19	HIS
1	H	158	GLN
1	H	159	PRO
1	G	17	LEU

### 5.3.2 Protein sidechains [i](#)

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	146/181 (81%)	138 (94%)	8 (6%)	21	35
1	B	149/181 (82%)	136 (91%)	13 (9%)	10	15
1	C	151/181 (83%)	139 (92%)	12 (8%)	12	19
1	D	147/181 (81%)	139 (95%)	8 (5%)	22	36
1	E	143/181 (79%)	137 (96%)	6 (4%)	30	47
1	F	139/181 (77%)	134 (96%)	5 (4%)	35	54
1	G	157/181 (87%)	140 (89%)	17 (11%)	6	9
1	H	142/181 (78%)	137 (96%)	5 (4%)	36	55
All	All	1174/1448 (81%)	1100 (94%)	74 (6%)	18	28

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	38	CYS
1	H	55	ASP
1	G	46	LYS
1	G	176	GLU
1	C	86	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN

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Mol	Chain	Res	Type
1	A	158	GLN
1	B	112	GLN
1	C	67	ASN
1	E	175	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 45 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CMP	E	301	-	22,25,25	1.42	4 (18%)	24,39,39	1.53	4 (16%)
2	CMP	G	301	-	22,25,25	1.42	4 (18%)	24,39,39	1.49	4 (16%)
2	CMP	B	301	-	22,25,25	1.41	4 (18%)	24,39,39	1.58	5 (20%)
2	CMP	D	301	-	22,25,25	1.41	4 (18%)	24,39,39	1.55	5 (20%)
5	SO4	G	302	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	C	302	-	4,4,4	0.13	0	6,6,6	0.16	0
2	CMP	A	301	-	22,25,25	1.40	4 (18%)	24,39,39	1.55	5 (20%)
5	SO4	E	302	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CMP	C	301	-	22,25,25	1.40	4 (18%)	24,39,39	1.55	4 (16%)
2	CMP	H	301	-	22,25,25	1.42	4 (18%)	24,39,39	1.50	4 (16%)
2	CMP	F	301	-	22,25,25	1.40	5 (22%)	24,39,39	1.48	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CMP	E	301	-	-	0/0/31/31	0/4/4/4
2	CMP	G	301	-	-	0/0/31/31	0/4/4/4
2	CMP	B	301	-	-	0/0/31/31	0/4/4/4
2	CMP	D	301	-	-	0/0/31/31	0/4/4/4
2	CMP	A	301	-	-	0/0/31/31	0/4/4/4
2	CMP	C	301	-	-	0/0/31/31	0/4/4/4
2	CMP	H	301	-	-	0/0/31/31	0/4/4/4
2	CMP	F	301	-	-	0/0/31/31	0/4/4/4

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	CMP	P-O3'	3.44	1.63	1.57
2	H	301	CMP	P-O3'	3.42	1.63	1.57
2	E	301	CMP	P-O3'	3.40	1.63	1.57
2	B	301	CMP	P-O3'	3.37	1.63	1.57
2	C	301	CMP	P-O3'	3.29	1.63	1.57

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	CMP	N3-C2-N1	-3.83	122.69	128.68
2	C	301	CMP	N3-C2-N1	-3.81	122.72	128.68
2	F	301	CMP	N3-C2-N1	-3.81	122.73	128.68
2	H	301	CMP	N3-C2-N1	-3.79	122.76	128.68
2	B	301	CMP	N3-C2-N1	-3.78	122.78	128.68

There are no chirality outliers.

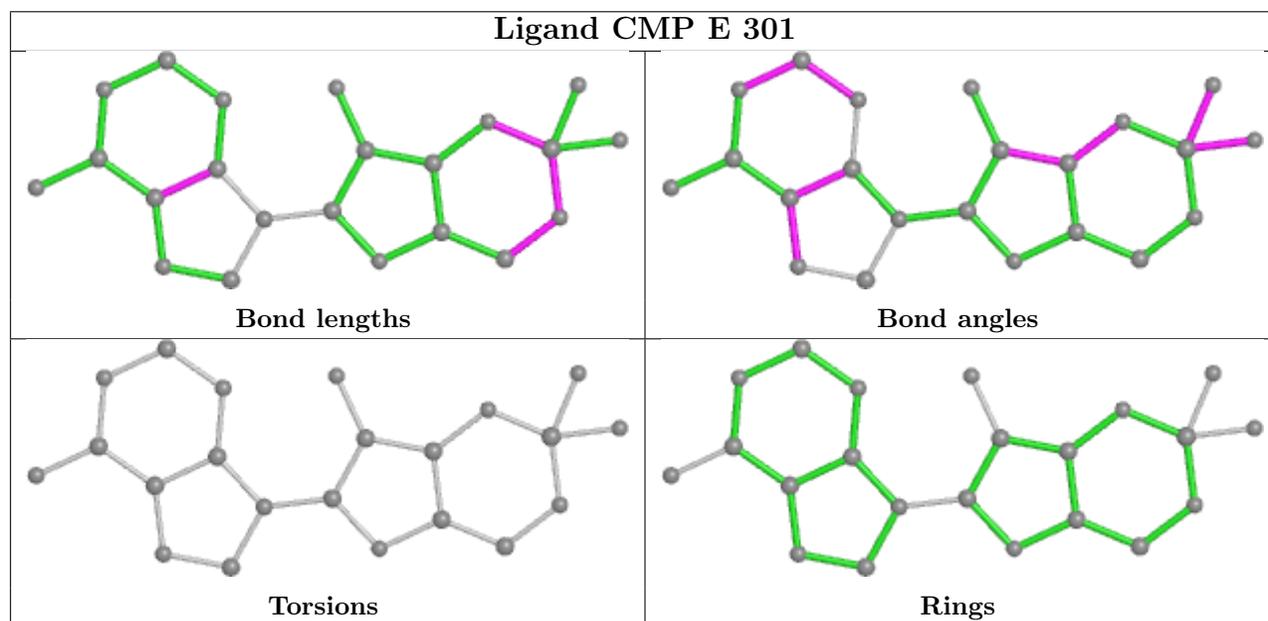
There are no torsion outliers.

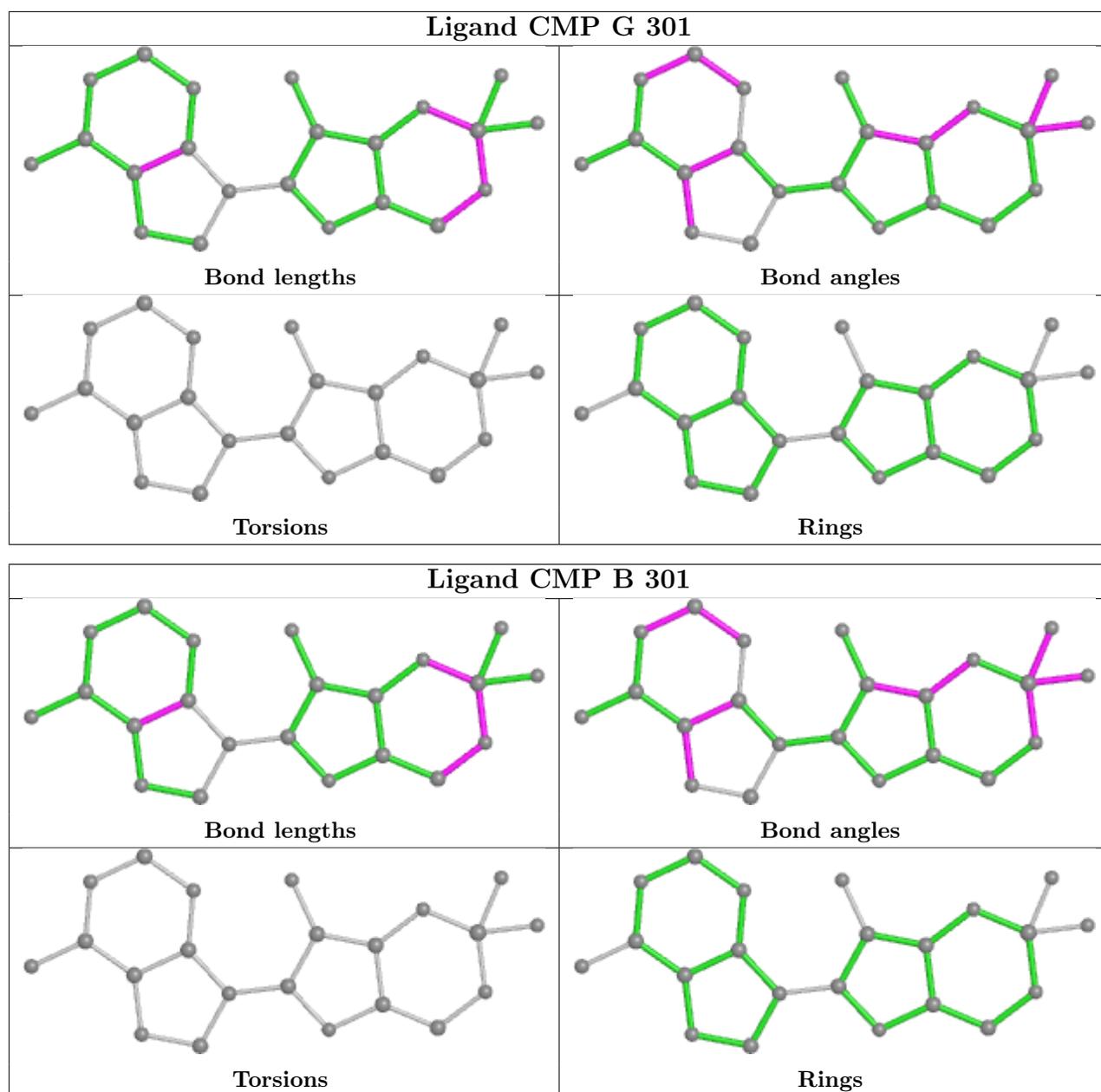
There are no ring outliers.

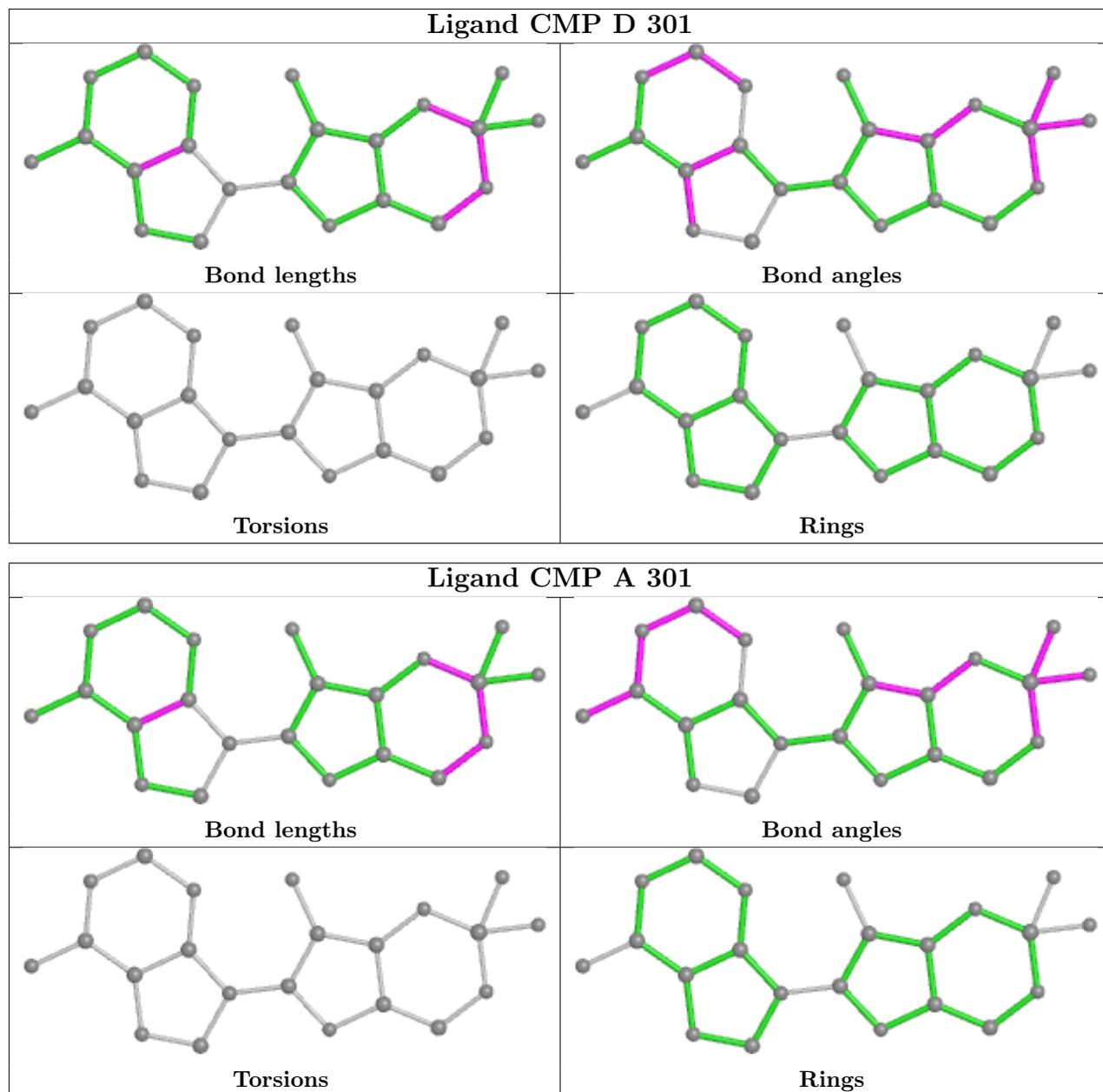
11 monomers are involved in 18 short contacts:

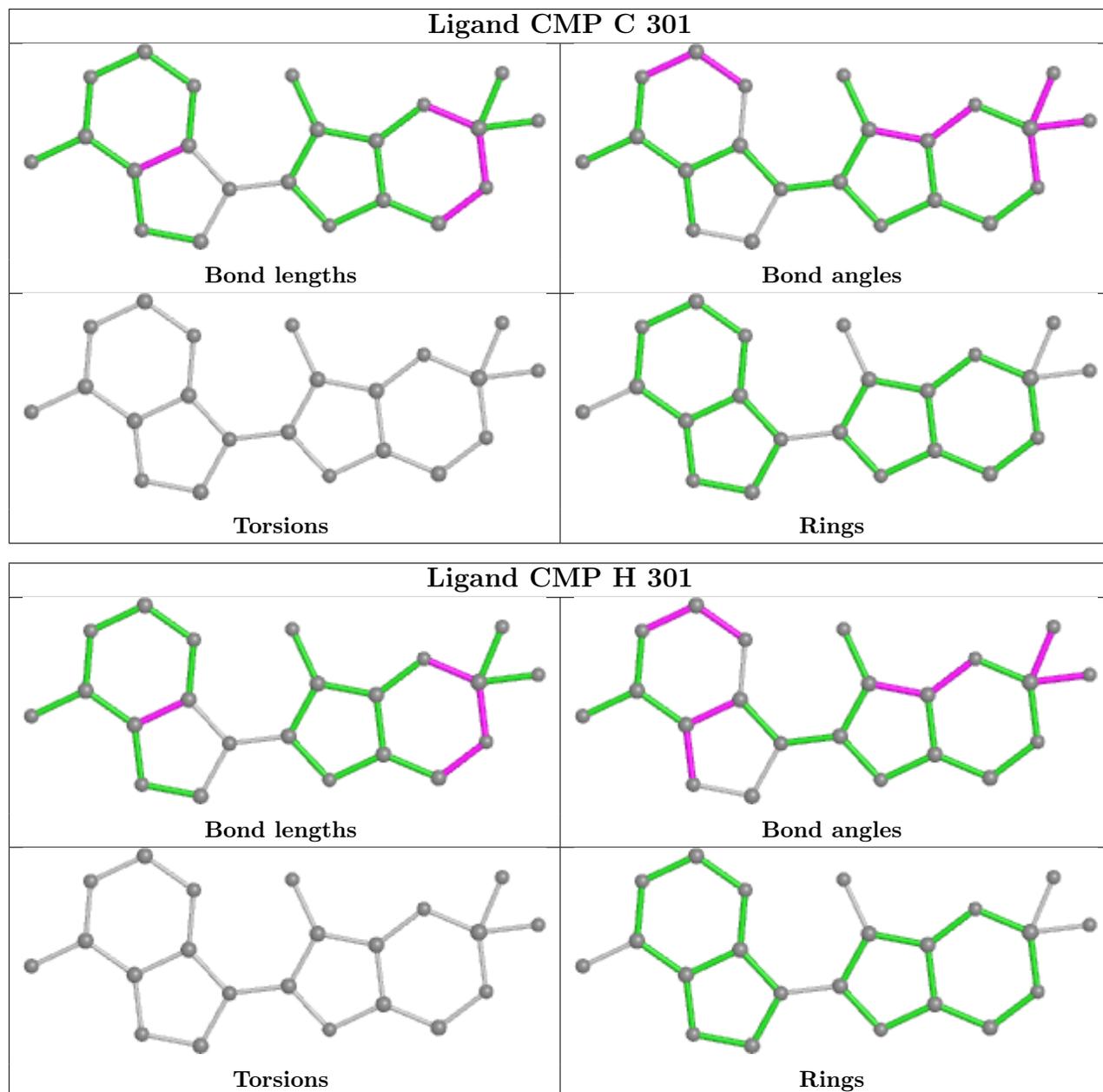
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	CMP	2	0
2	G	301	CMP	1	0
2	B	301	CMP	2	0
2	D	301	CMP	1	0
5	G	302	SO4	1	0
5	C	302	SO4	3	0
2	A	301	CMP	1	0
5	E	302	SO4	3	0
2	C	301	CMP	2	0
2	H	301	CMP	1	0
2	F	301	CMP	1	0

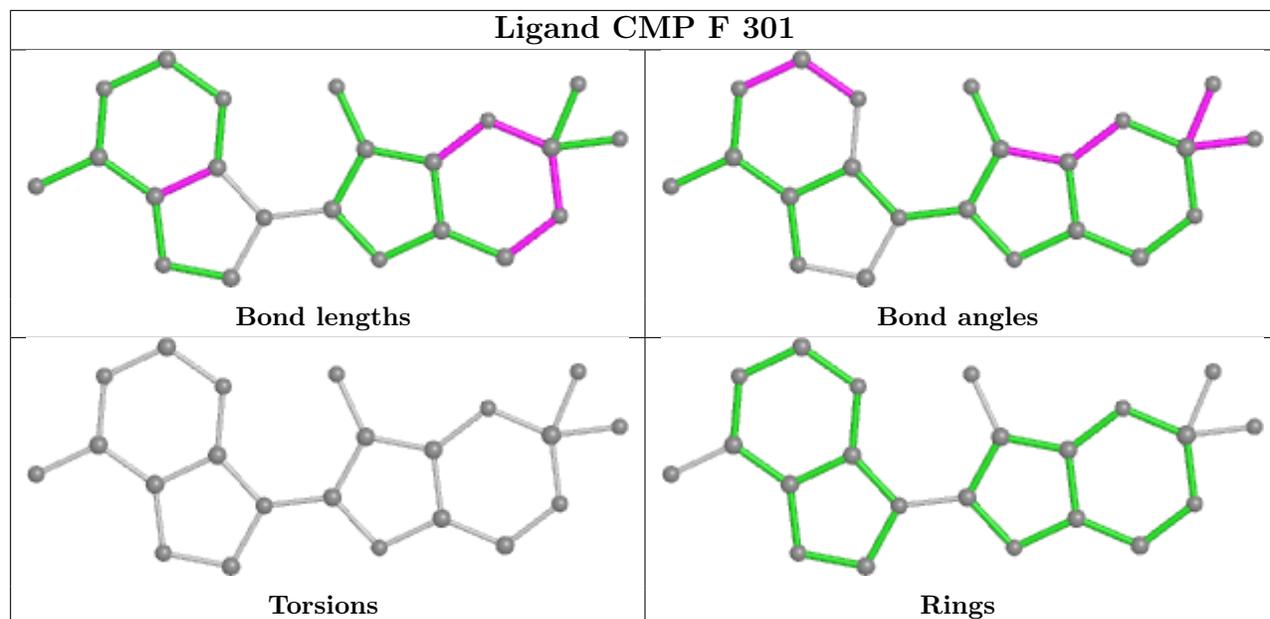
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	197/210 (93%)	0.66	15 (7%) 13 12	21, 30, 50, 69	0
1	B	195/210 (92%)	0.89	27 (13%) 2 2	22, 36, 56, 82	0
1	C	197/210 (93%)	0.71	20 (10%) 6 6	20, 28, 50, 59	0
1	D	198/210 (94%)	0.73	20 (10%) 7 6	21, 31, 51, 73	0
1	E	194/210 (92%)	0.68	13 (6%) 17 16	22, 30, 50, 56	0
1	F	188/210 (89%)	1.21	36 (19%) 1 0	22, 38, 78, 105	0
1	G	197/210 (93%)	0.62	12 (6%) 21 20	19, 27, 52, 80	0
1	H	186/210 (88%)	0.61	10 (5%) 25 24	19, 30, 46, 58	0
All	All	1552/1680 (92%)	0.76	153 (9%) 7 6	19, 31, 57, 105	0

The worst 5 of 153 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	161	ALA	13.7
1	F	160	ASP	8.4
1	E	17	LEU	6.7
1	G	38	CYS	6.4
1	G	13	LEU	6.3

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	AU	D	305	1/1	0.28	0.13	137,137,137,137	0
4	CL	B	307	1/1	0.34	0.46	52,52,52,52	0
3	AU	B	302	1/1	0.40	0.24	110,110,110,110	0
3	AU	C	305	1/1	0.41	0.23	119,119,119,119	0
3	AU	H	303	1/1	0.47	0.28	123,123,123,123	0
3	AU	F	304	1/1	0.49	0.12	141,141,141,141	0
3	AU	A	302	1/1	0.59	0.20	59,59,59,59	0
3	AU	C	304	1/1	0.62	0.14	71,71,71,71	0
4	CL	G	307	1/1	0.65	0.15	51,51,51,51	0
4	CL	G	306	1/1	0.68	0.23	41,41,41,41	0
4	CL	C	308	1/1	0.74	0.10	34,34,34,34	0
4	CL	A	307	1/1	0.75	0.25	40,40,40,40	0
3	AU	C	303	1/1	0.81	0.13	64,64,64,64	0
5	SO4	G	302	5/5	0.82	0.31	35,43,47,53	0
3	AU	B	306	1/1	0.83	0.06	114,114,114,114	0
4	CL	B	309	1/1	0.83	0.21	47,47,47,47	0
4	CL	H	305	1/1	0.84	0.24	43,43,43,43	0
4	CL	B	308	1/1	0.84	0.31	26,26,26,26	0
3	AU	F	302	1/1	0.85	0.12	103,103,103,103	0
5	SO4	C	302	5/5	0.85	0.33	30,30,38,41	0
3	AU	D	303	1/1	0.85	0.10	110,110,110,110	0
3	AU	B	304	1/1	0.86	0.05	96,96,96,96	0
4	CL	E	307	1/1	0.90	0.25	20,20,20,20	0
3	AU	B	303	1/1	0.91	0.09	111,111,111,111	0
3	AU	E	303	1/1	0.91	0.14	119,119,119,119	0
2	CMP	B	301	22/22	0.92	0.18	17,19,23,27	0
5	SO4	E	302	5/5	0.92	0.14	28,33,38,39	0
4	CL	D	307	1/1	0.92	0.34	43,43,43,43	0
2	CMP	H	301	22/22	0.93	0.16	16,19,25,27	0
2	CMP	G	301	22/22	0.94	0.16	13,18,24,29	0
3	AU	A	305	1/1	0.94	0.07	85,85,85,85	0
4	CL	C	309	1/1	0.94	0.23	54,54,54,54	0
4	CL	D	306	1/1	0.94	0.12	34,34,34,34	0
2	CMP	F	301	22/22	0.95	0.15	17,20,23,29	0
2	CMP	A	301	22/22	0.95	0.15	16,19,23,27	0
2	CMP	C	301	22/22	0.95	0.15	15,19,26,27	0
2	CMP	D	301	22/22	0.95	0.17	17,19,22,23	0

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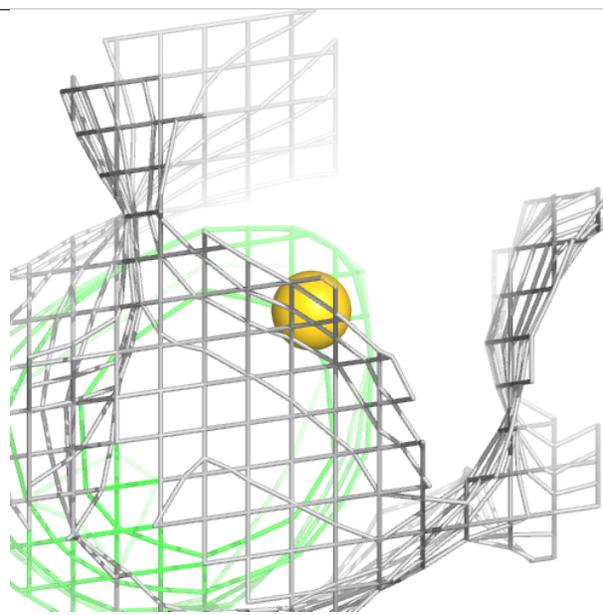
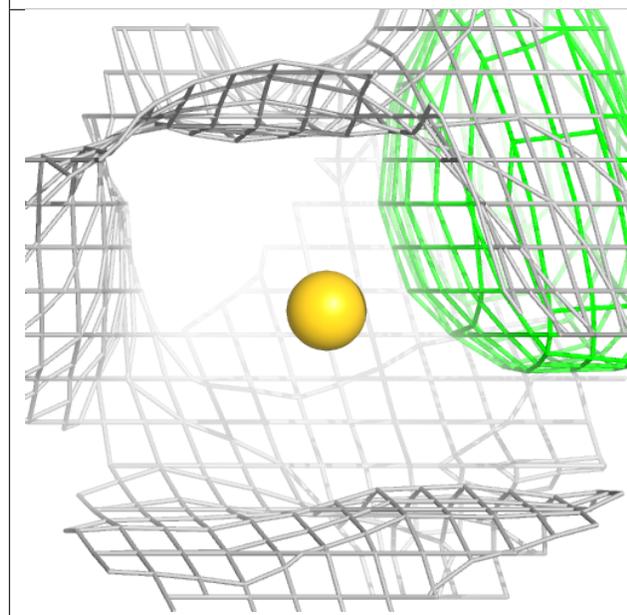
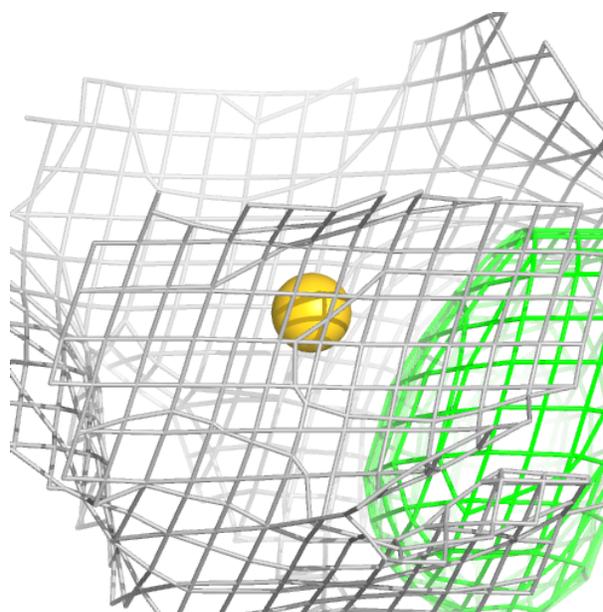
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CMP	E	301	22/22	0.95	0.17	16,19,22,23	0
3	AU	E	306	1/1	0.95	0.08	46,46,46,46	0
3	AU	H	304	1/1	0.96	0.06	65,65,65,65	0
3	AU	G	303	1/1	0.96	0.07	52,52,52,52	0
3	AU	G	304	1/1	0.96	0.06	49,49,49,49	0
3	AU	D	304	1/1	0.96	0.06	53,53,53,53	0
3	AU	B	305	1/1	0.97	0.10	52,52,52,52	0
3	AU	E	305	1/1	0.97	0.07	60,60,60,60	0
4	CL	F	305	1/1	0.97	0.13	32,32,32,32	0
3	AU	A	303	1/1	0.98	0.08	56,56,56,56	0
3	AU	C	306	1/1	0.98	0.07	90,90,90,90	0
3	AU	F	303	1/1	0.98	0.07	47,47,47,47	0
3	AU	D	302	1/1	0.98	0.07	42,42,42,42	0
3	AU	E	304	1/1	0.98	0.05	82,82,82,82	0
3	AU	A	304	1/1	0.98	0.05	85,85,85,85	0
3	AU	H	302	1/1	0.99	0.07	38,38,38,38	0
3	AU	C	307	1/1	0.99	0.11	27,27,27,27	0
3	AU	G	305	1/1	0.99	0.11	26,26,26,26	0
4	CL	A	306	1/1	0.99	0.16	15,15,15,15	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.

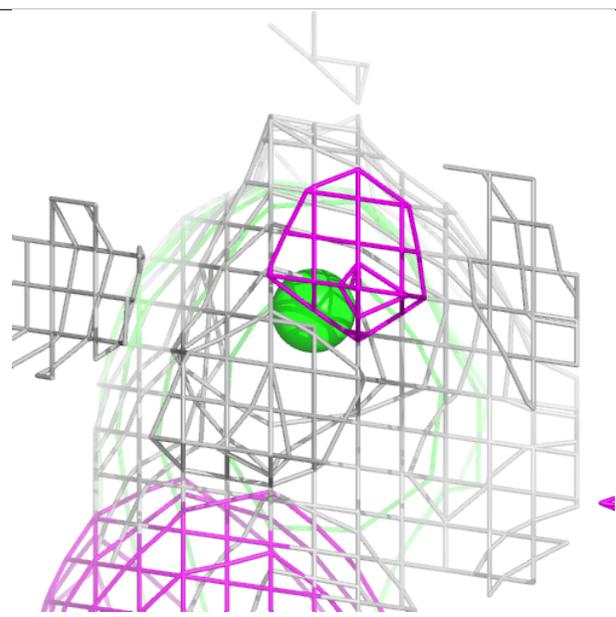
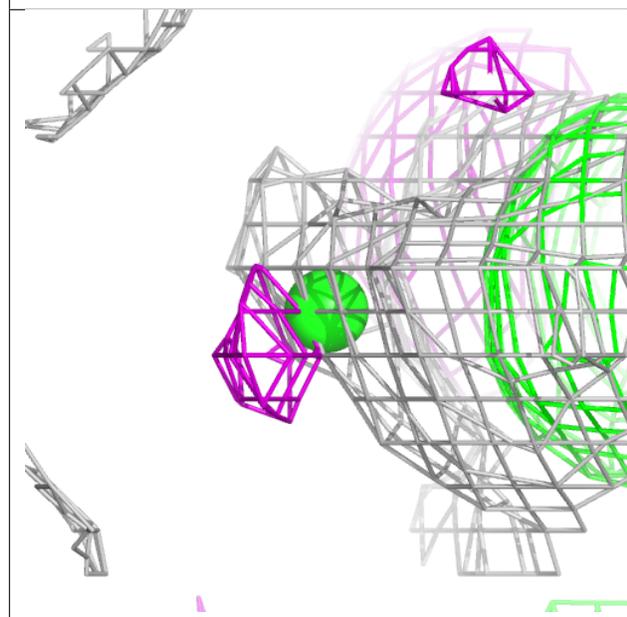
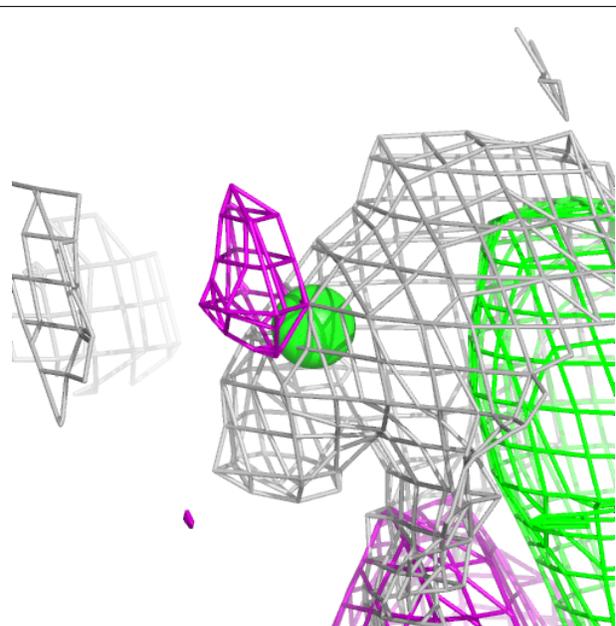
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and green (positive)



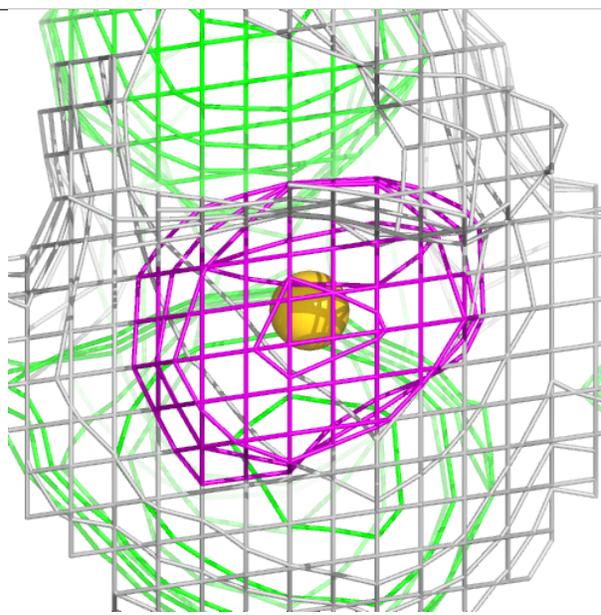
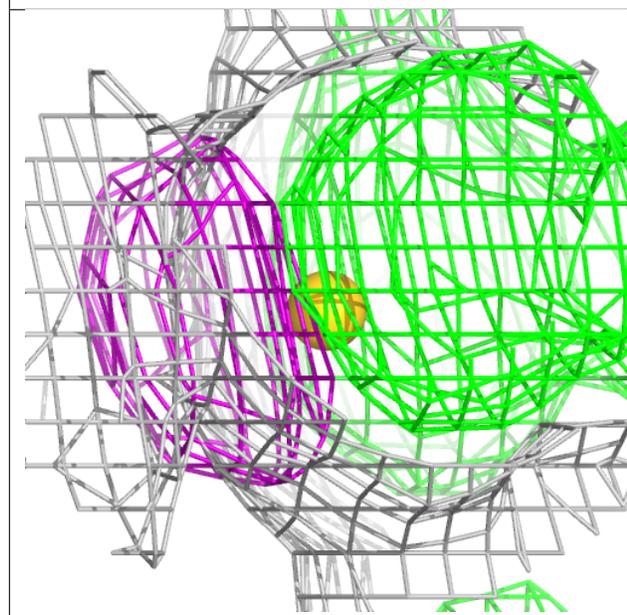
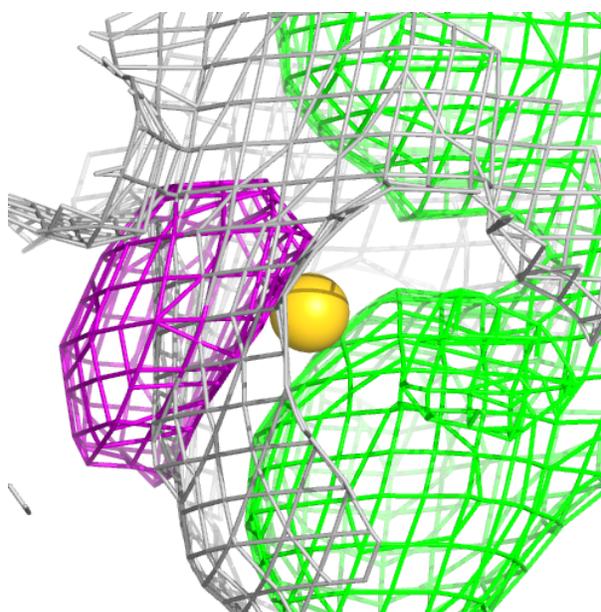
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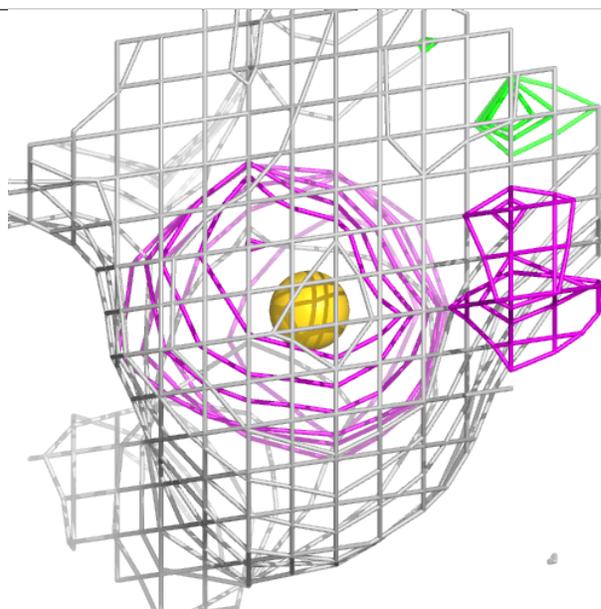
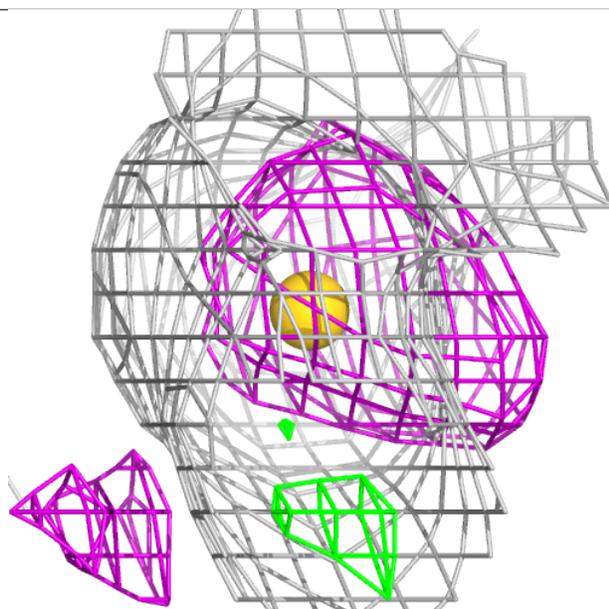
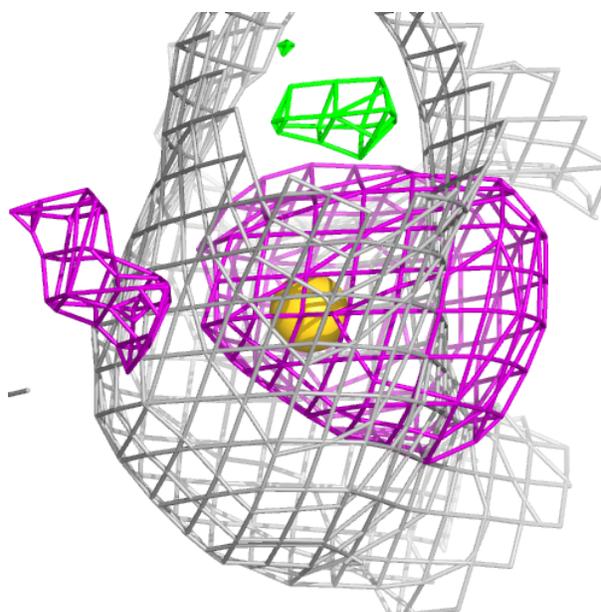
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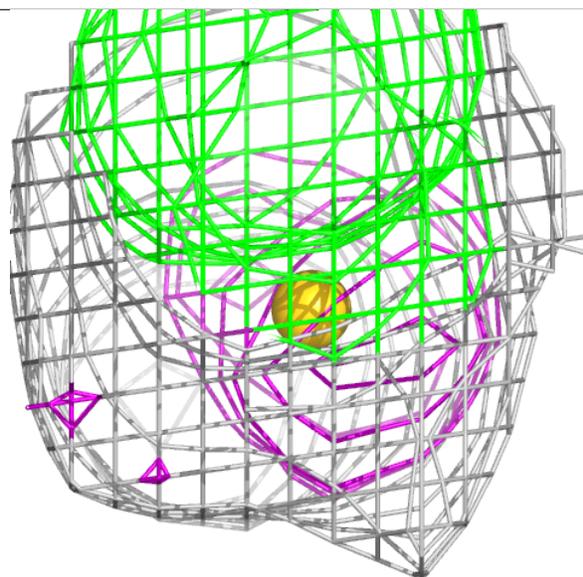
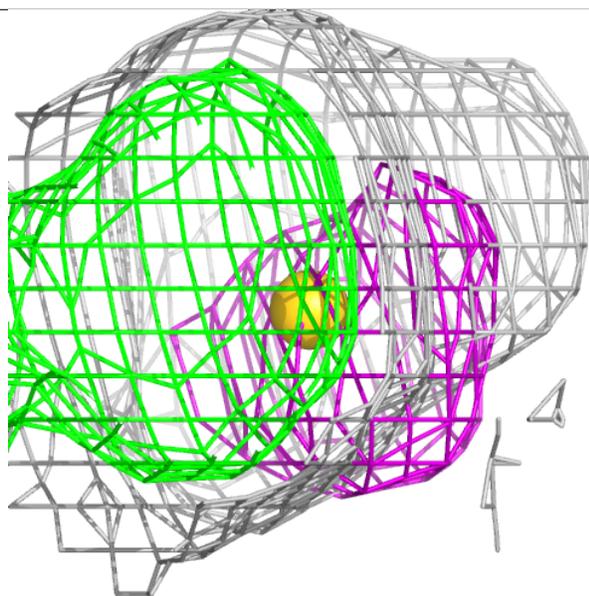
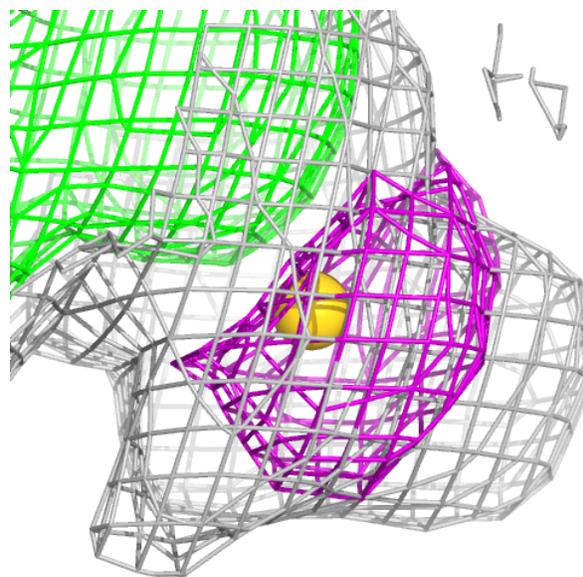
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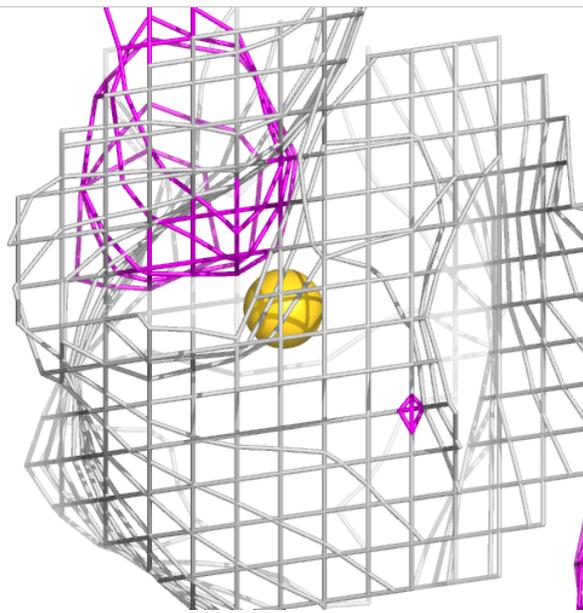
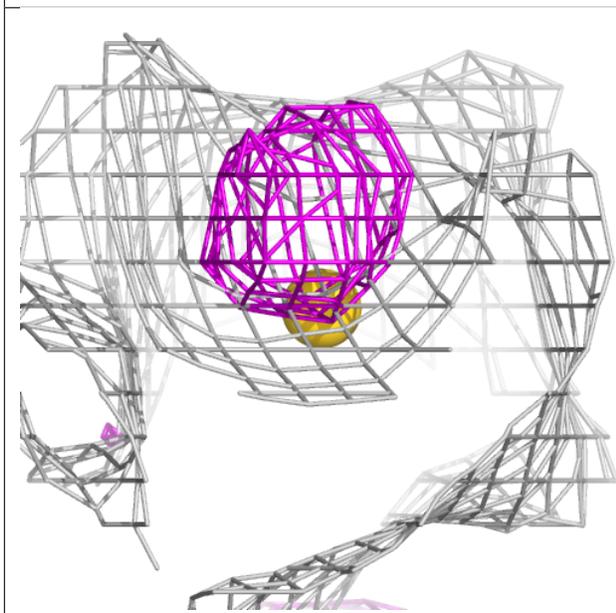
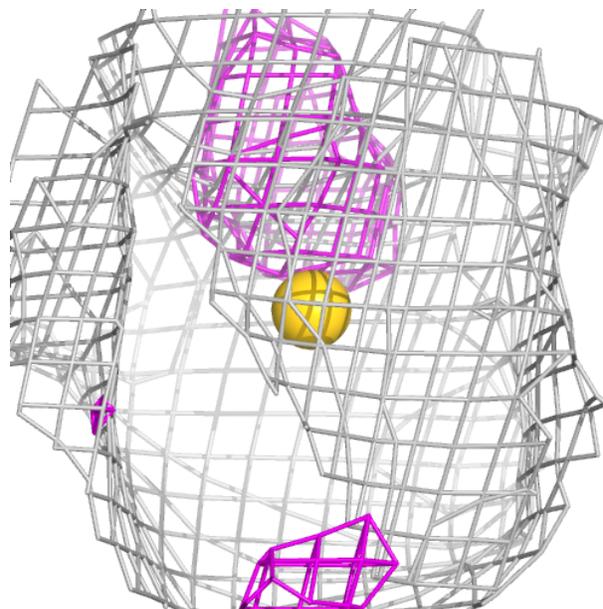
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and green (positive)



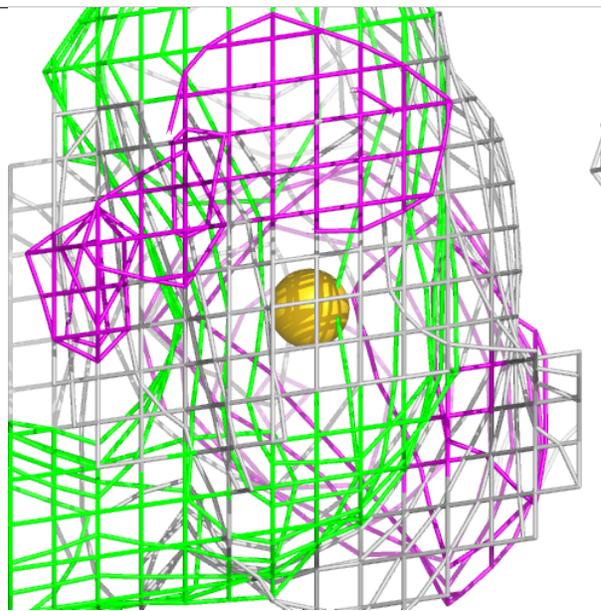
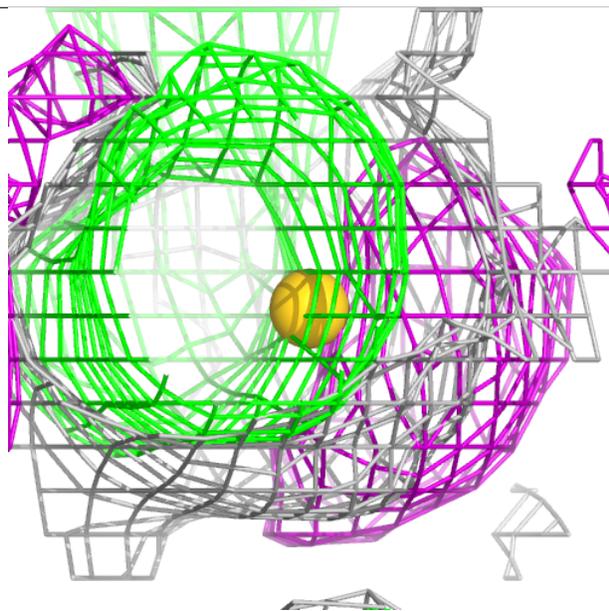
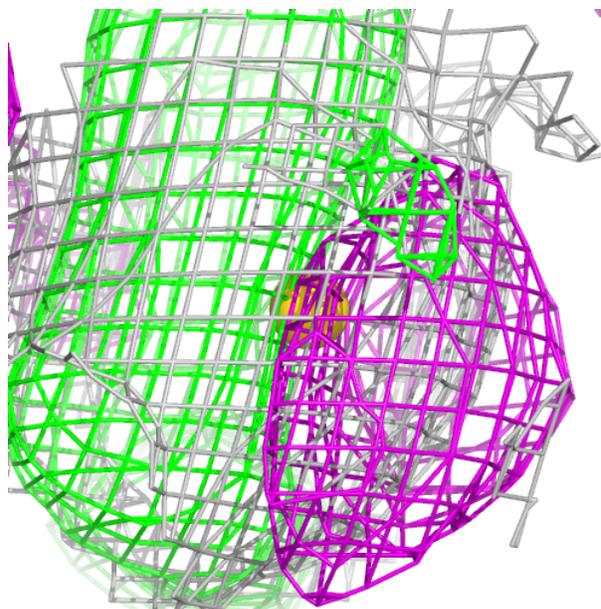
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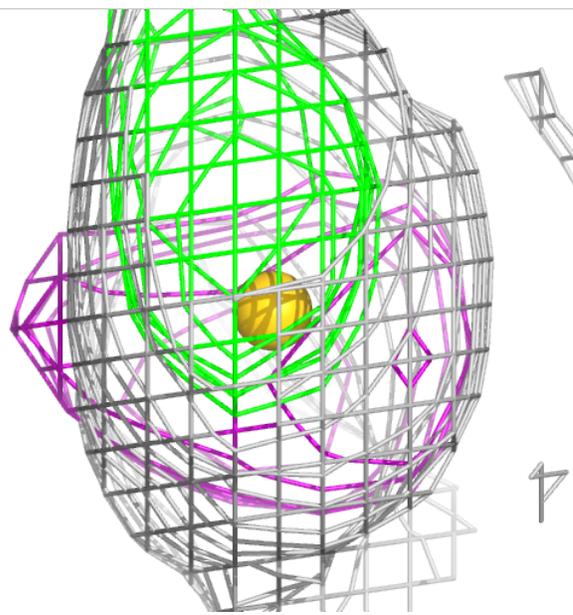
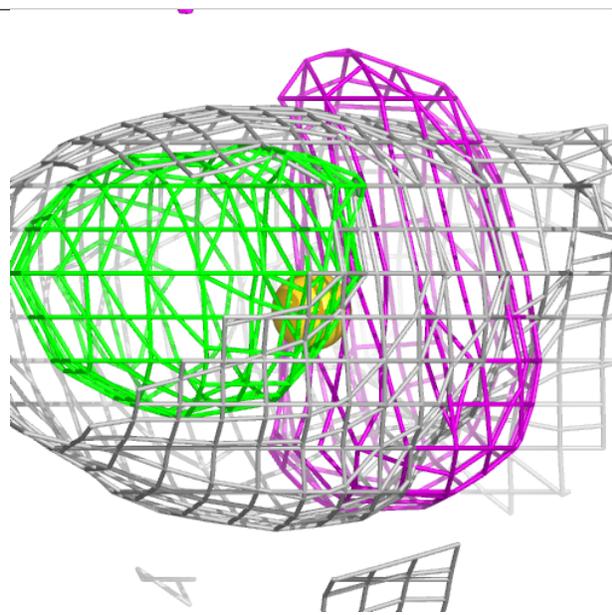
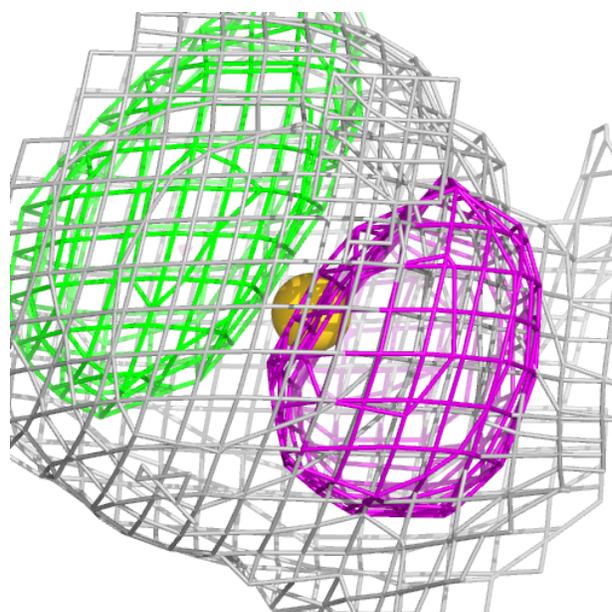
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and green (positive)



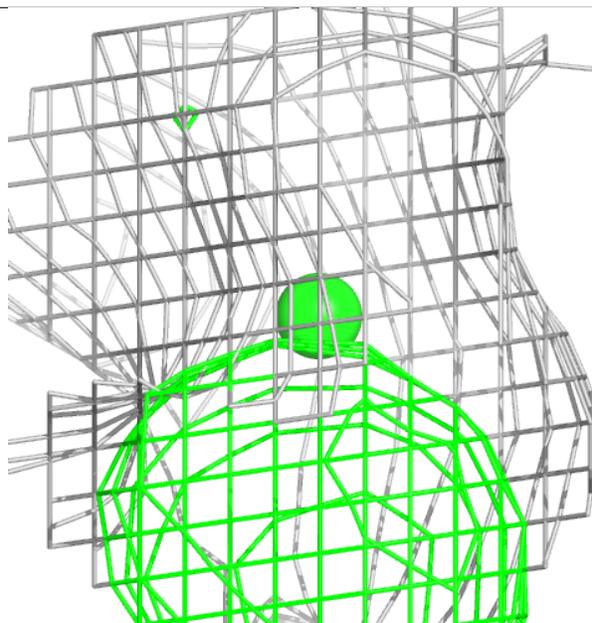
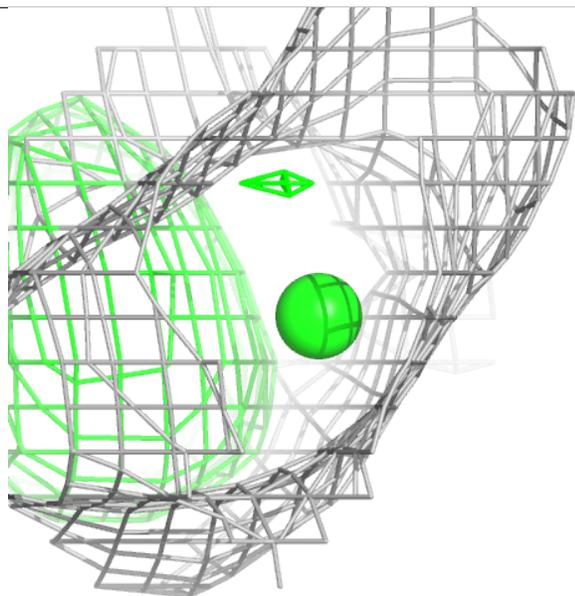
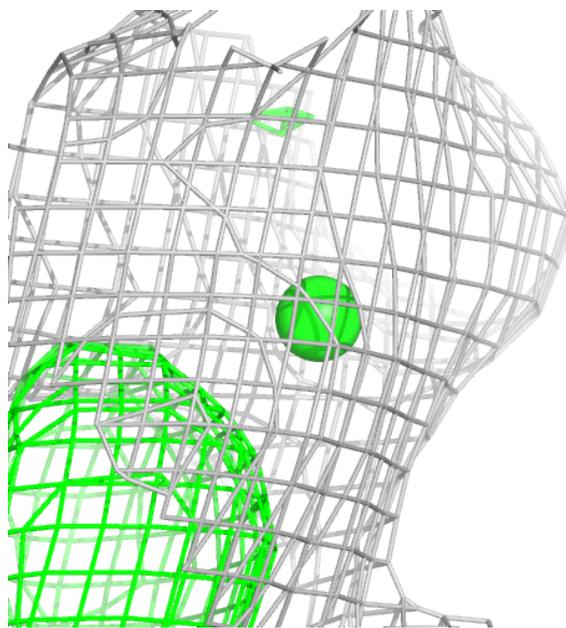
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and green (positive)



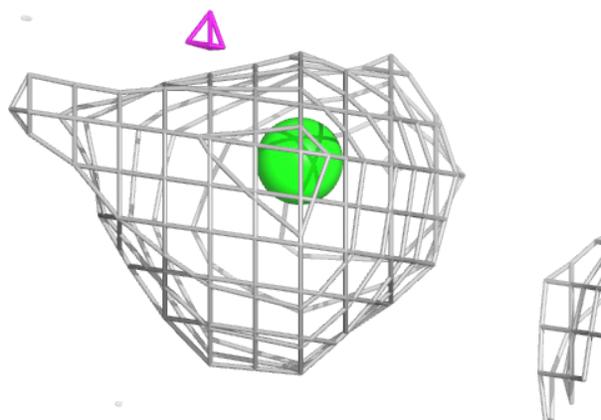
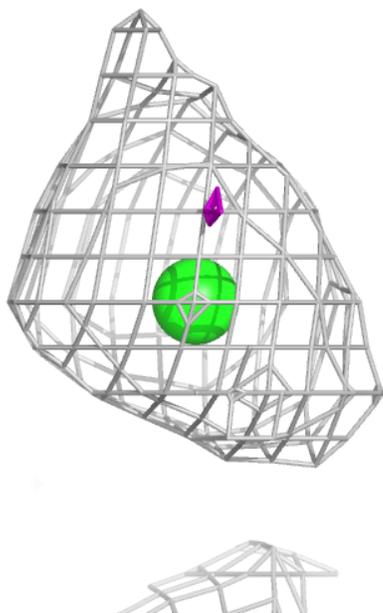
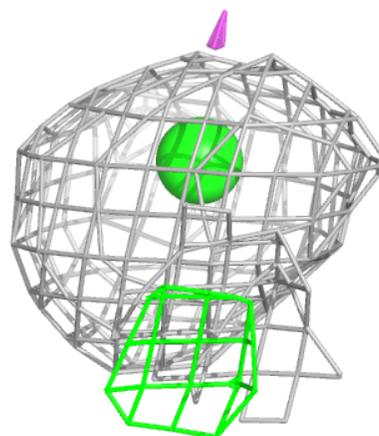
**Electron density around CL G 307:**

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



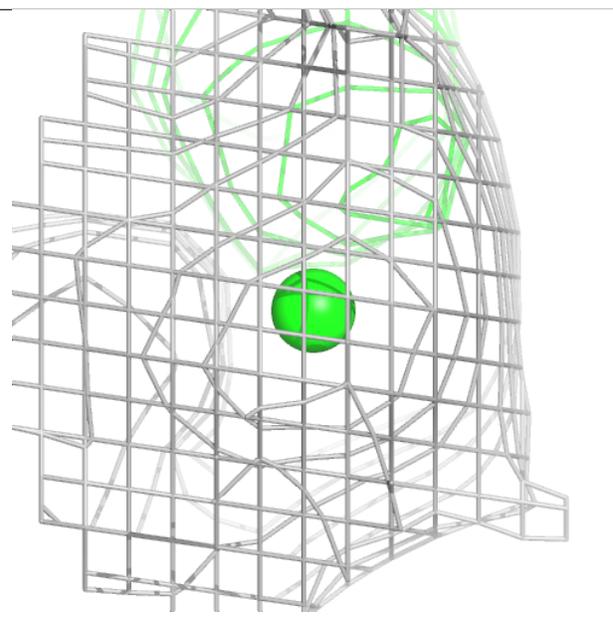
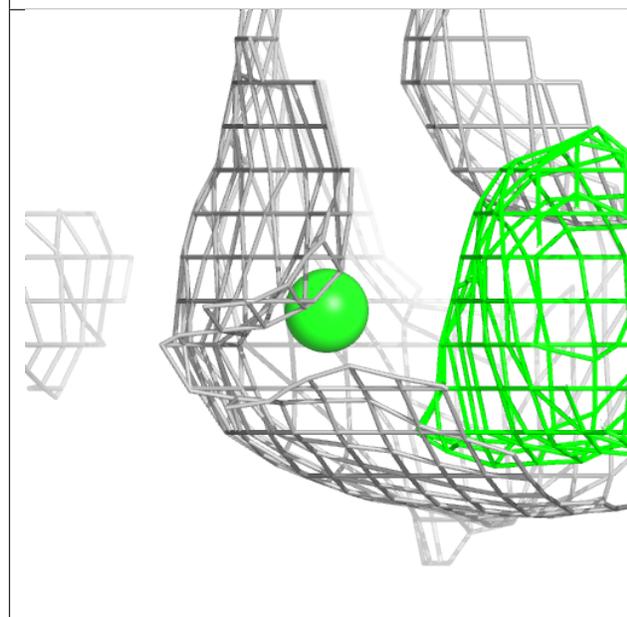
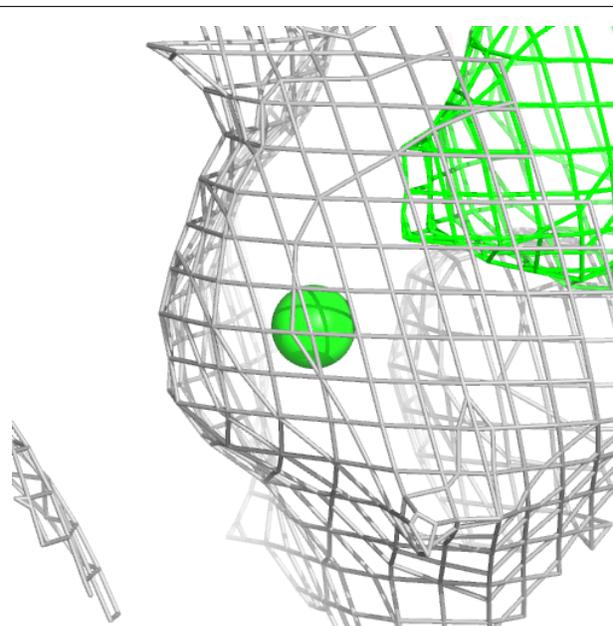
**Electron density around CL G 306:**

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



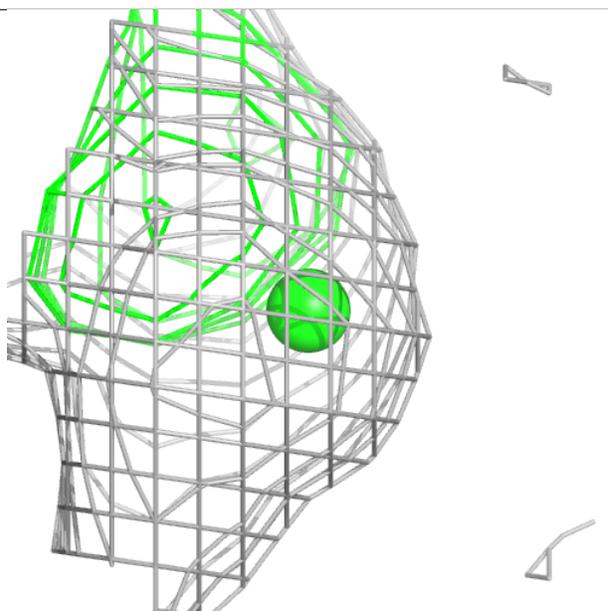
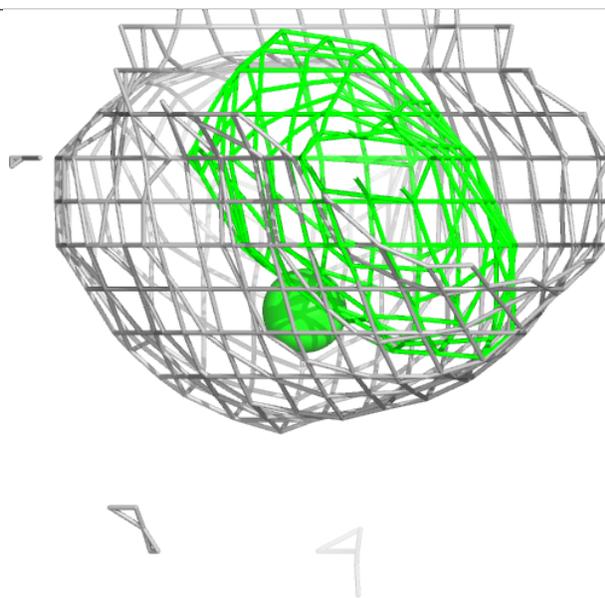
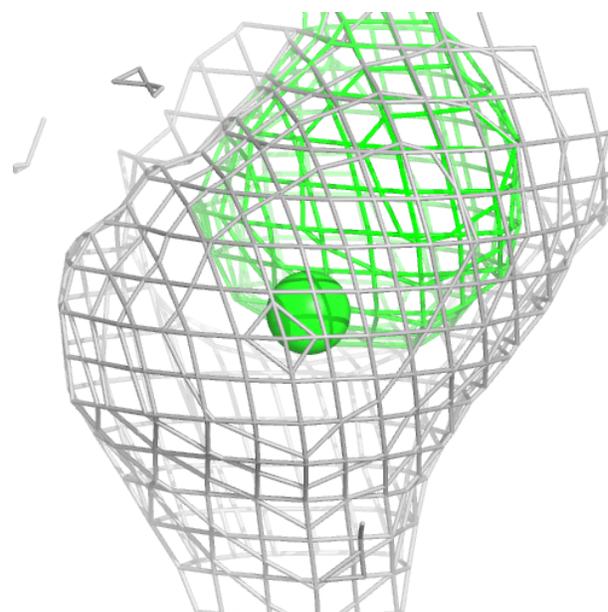
**Electron density around CL C 308:**

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



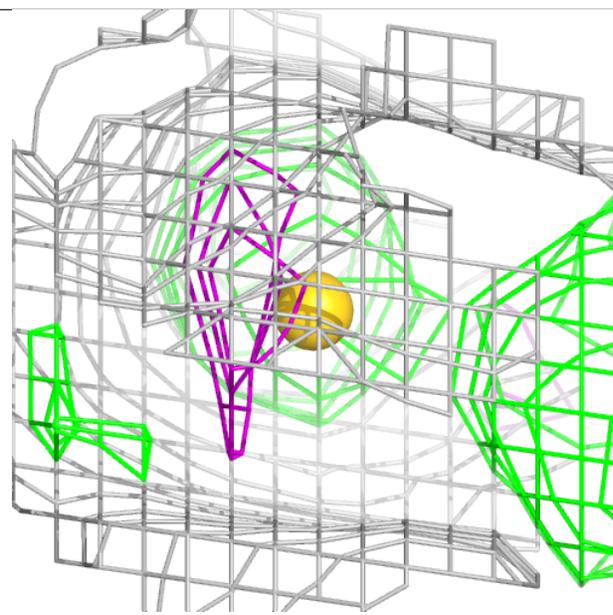
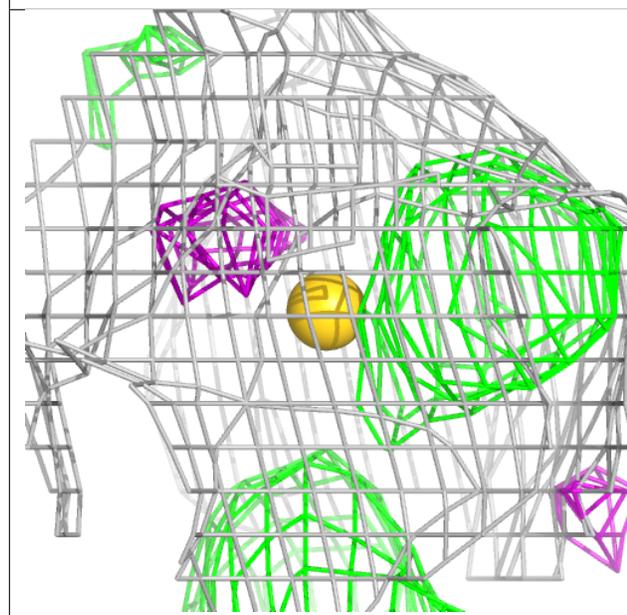
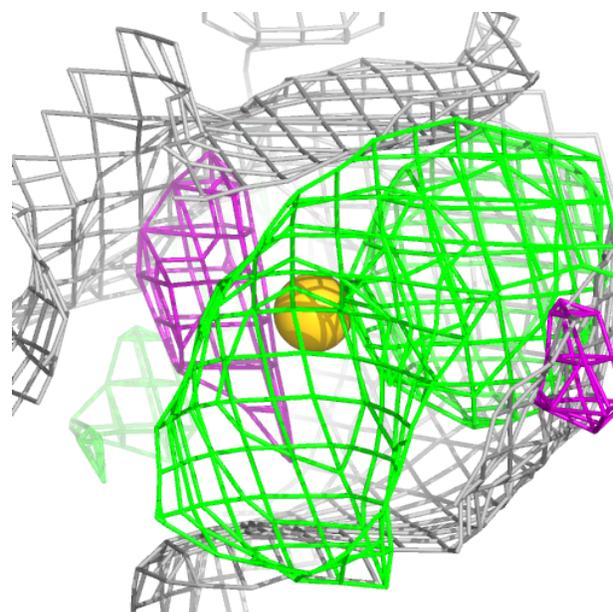
**Electron density around CL A 307:**

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



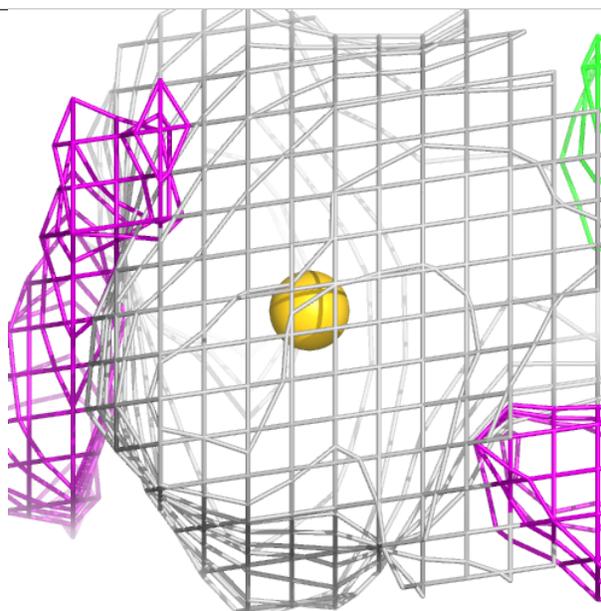
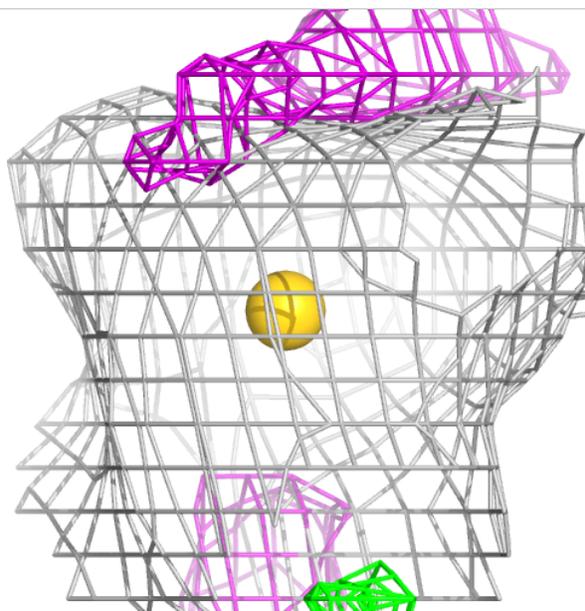
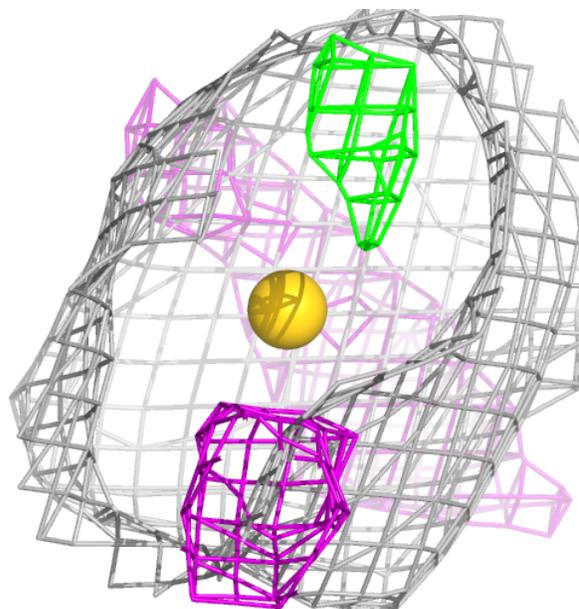
**Electron density around AU C 303:**

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



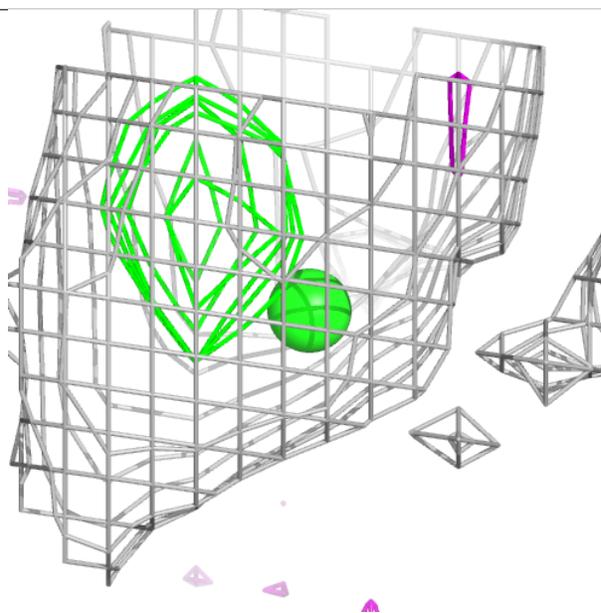
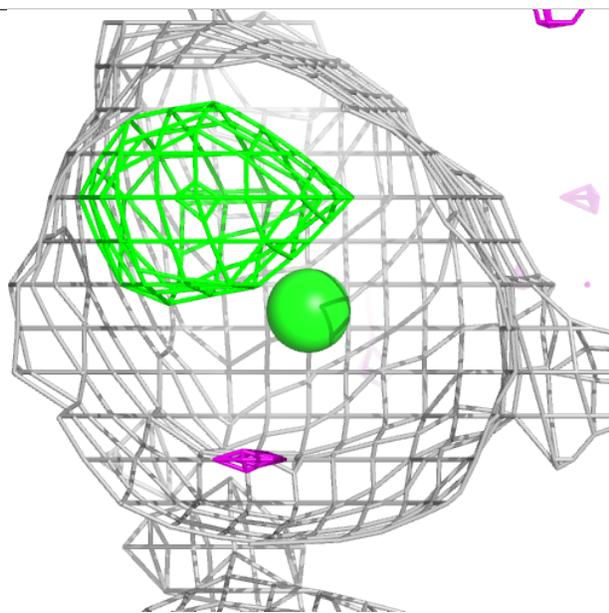
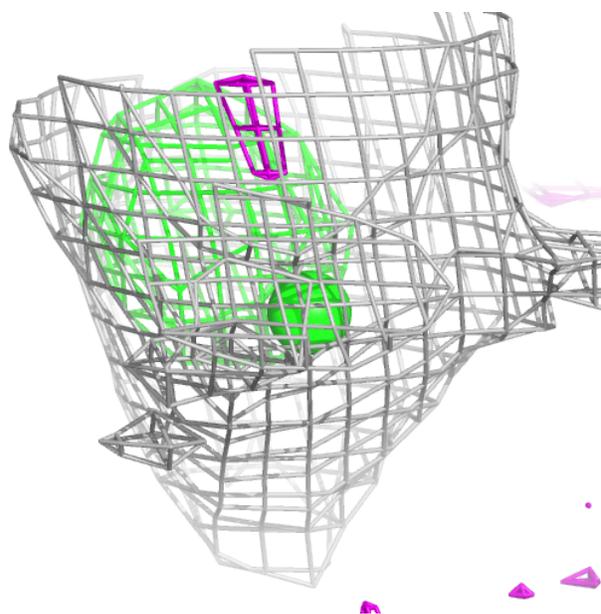
**Electron density around AU B 306:**

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



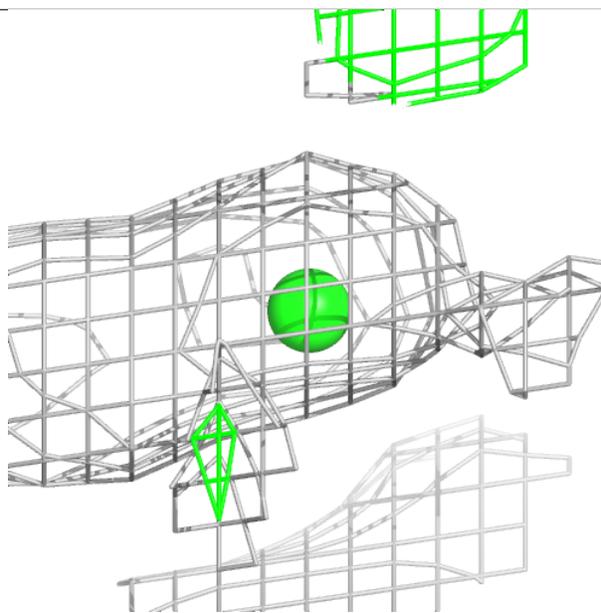
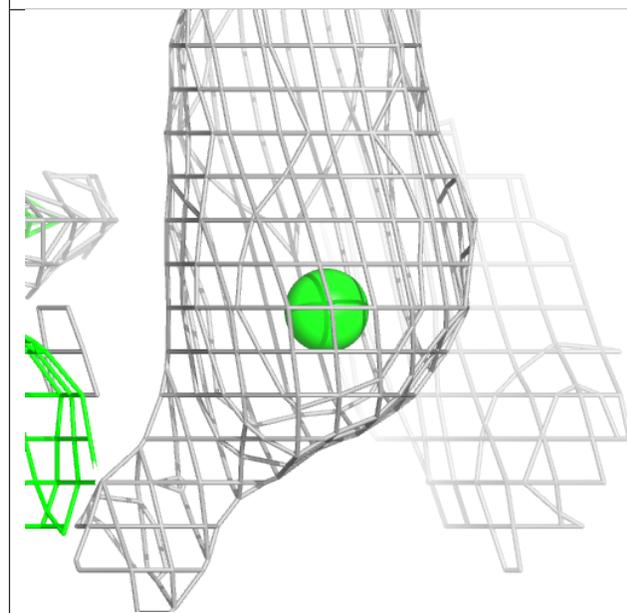
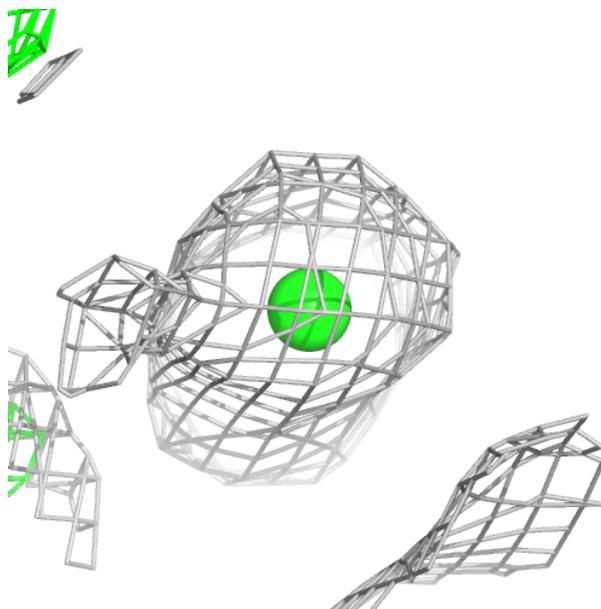
**Electron density around CL B 309:**

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



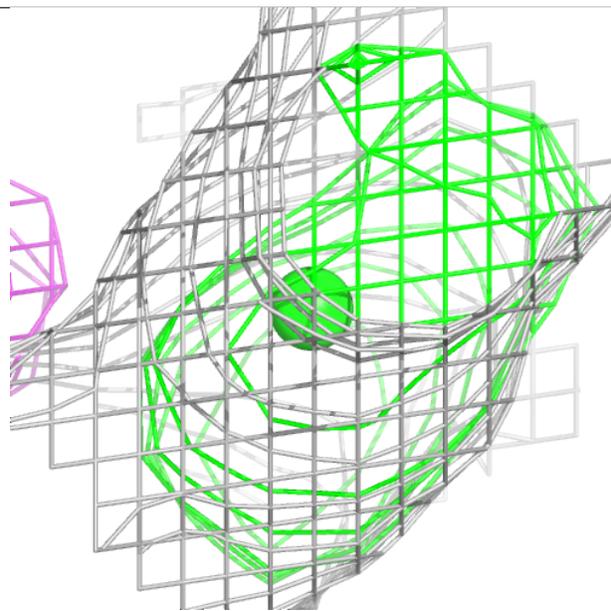
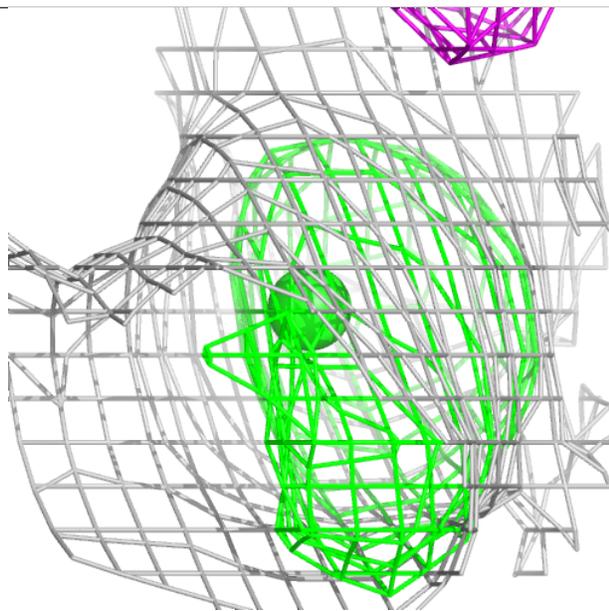
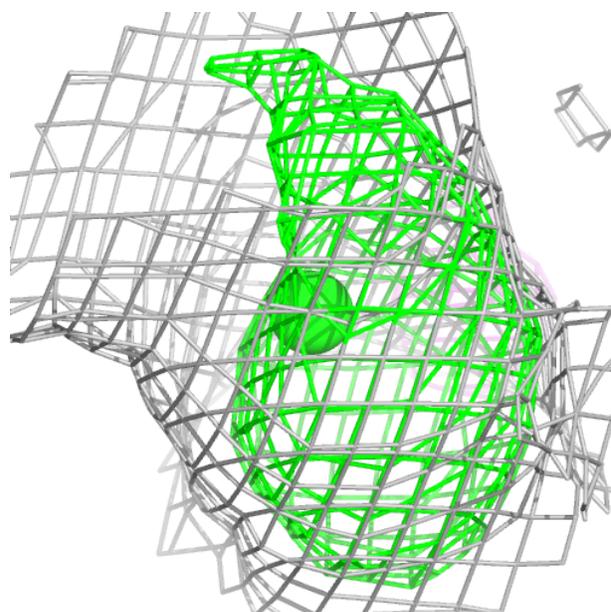
**Electron density around CL H 305:**

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



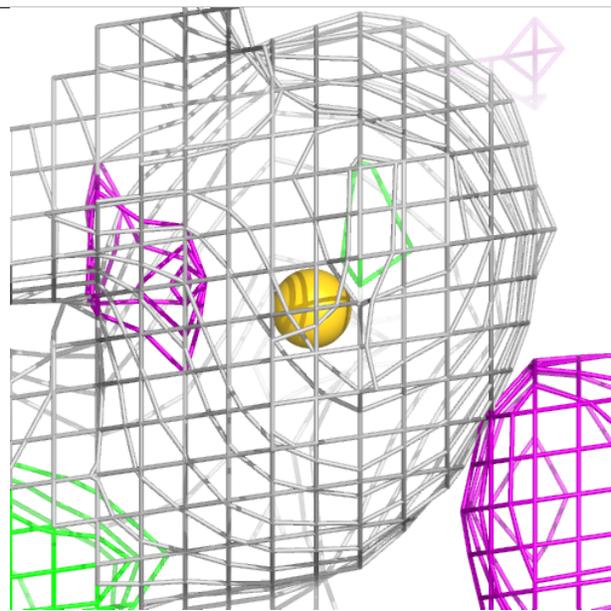
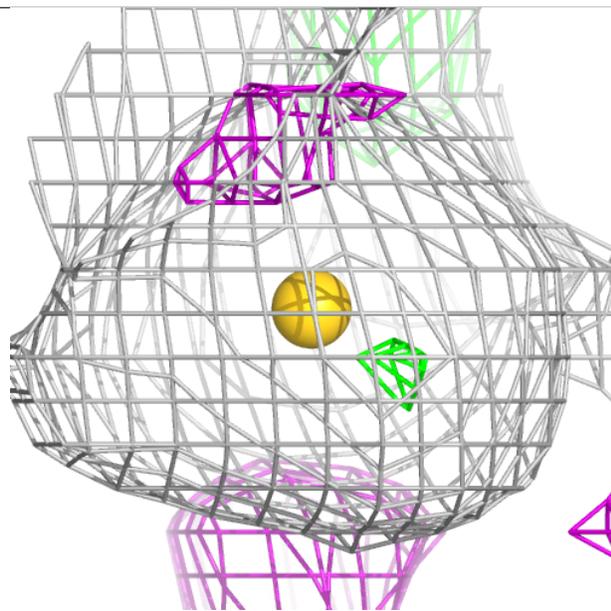
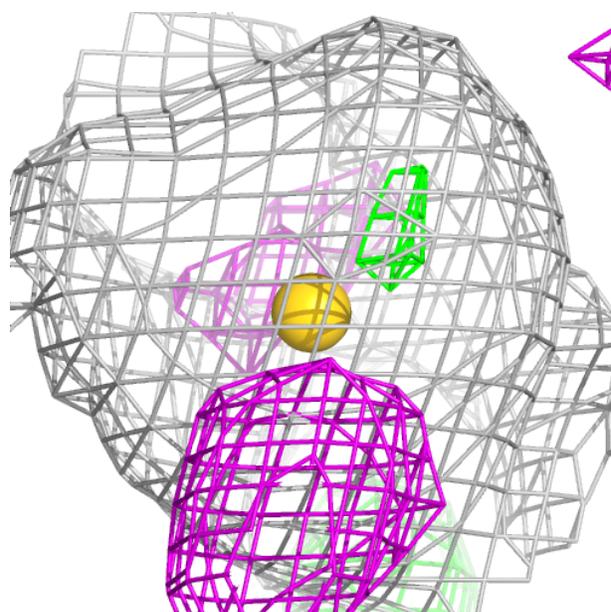
**Electron density around CL B 308:**

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



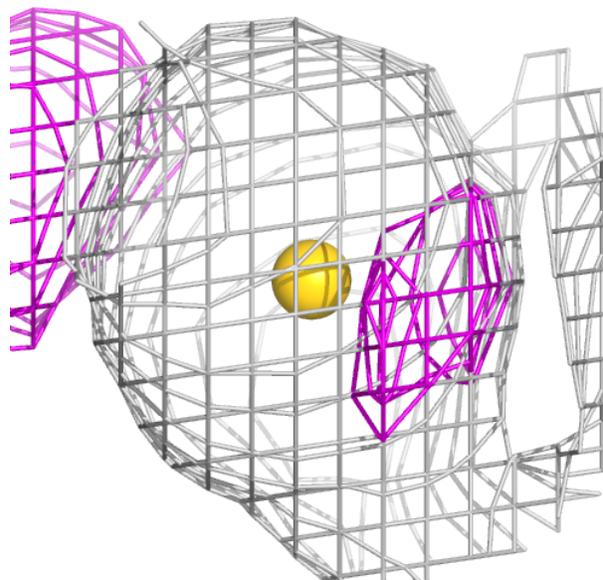
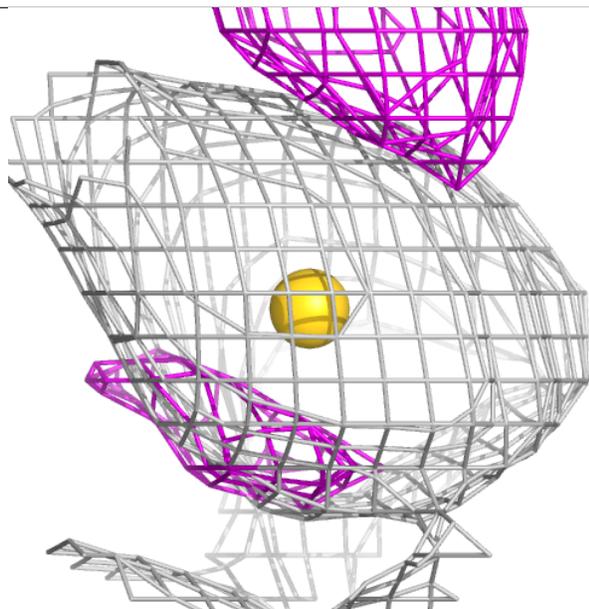
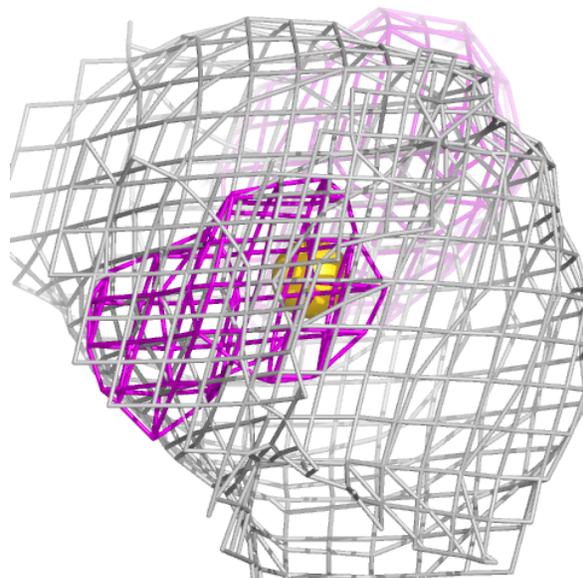
**Electron density around AU F 302:**

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



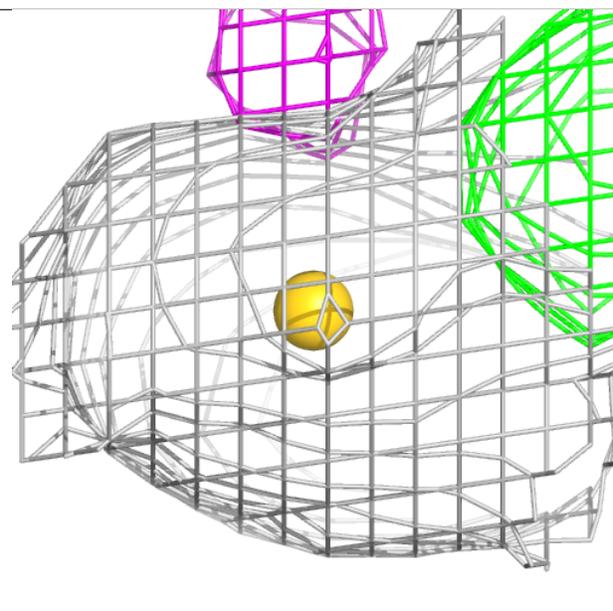
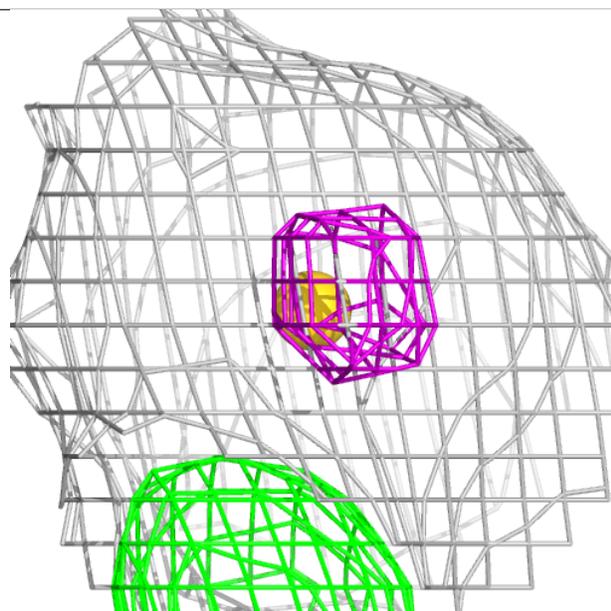
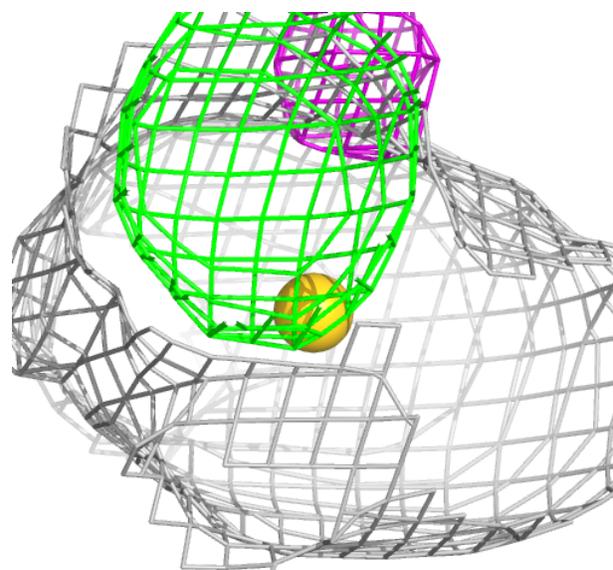
**Electron density around AU D 303:**

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



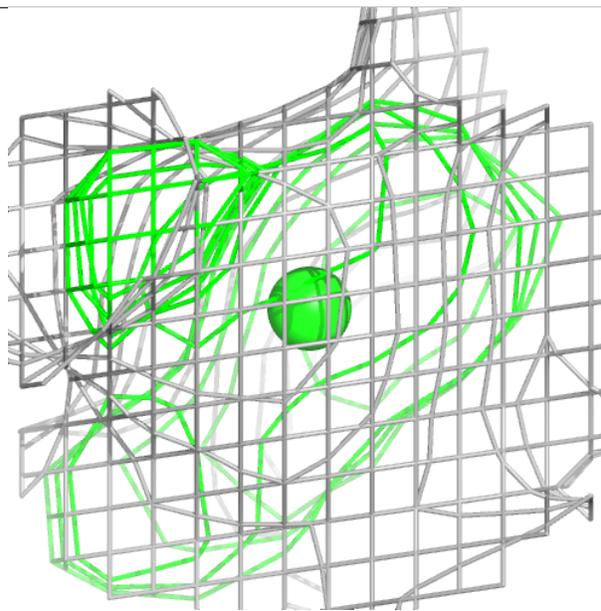
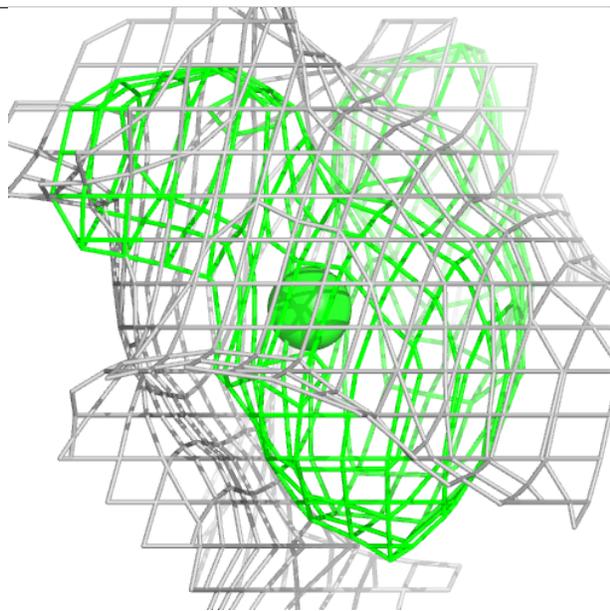
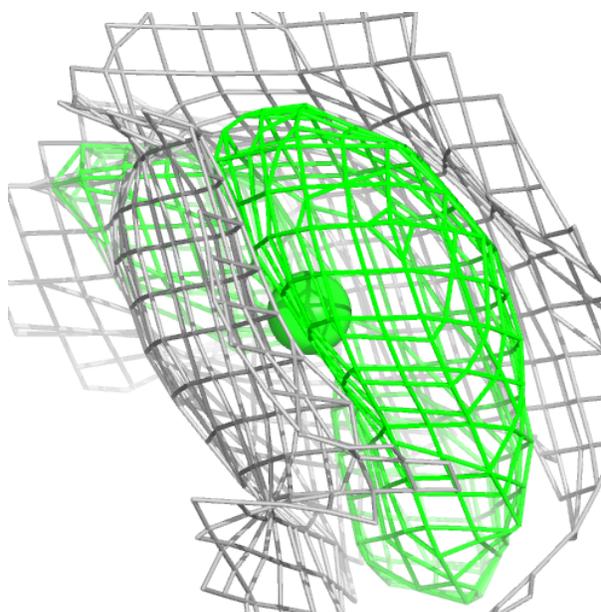
**Electron density around AU B 304:**

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



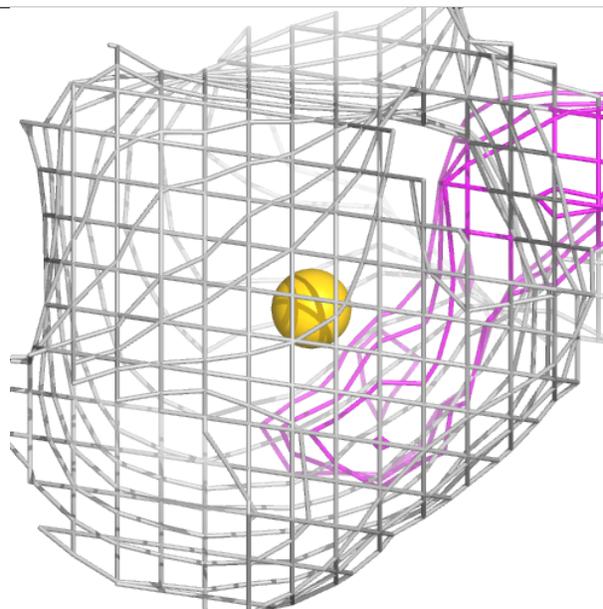
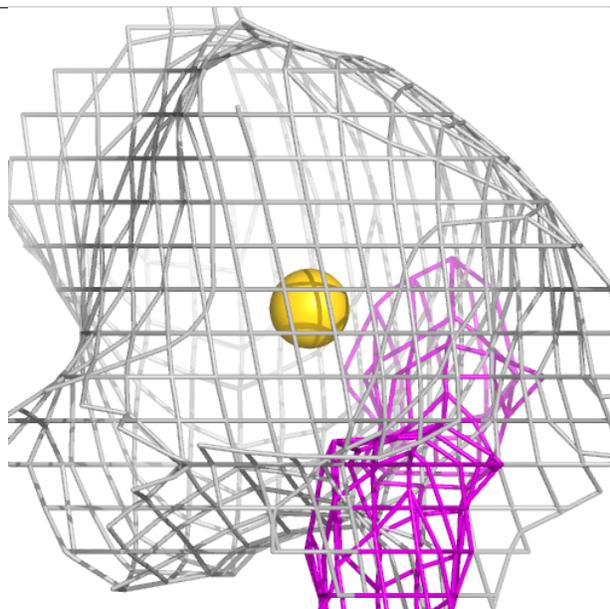
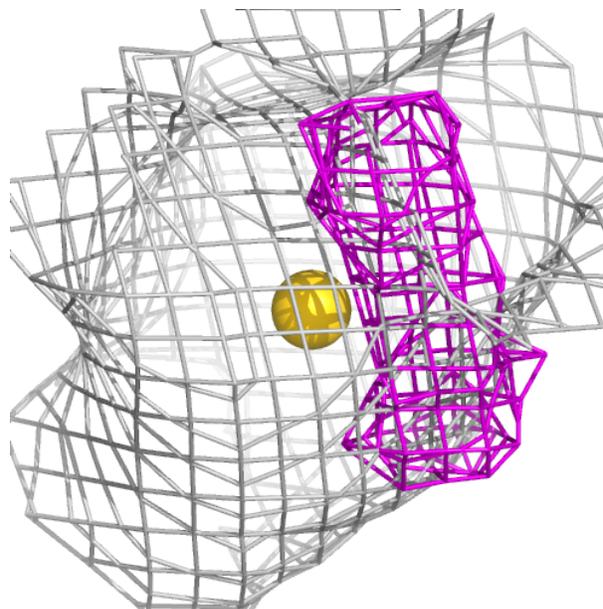
**Electron density around CL E 307:**

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



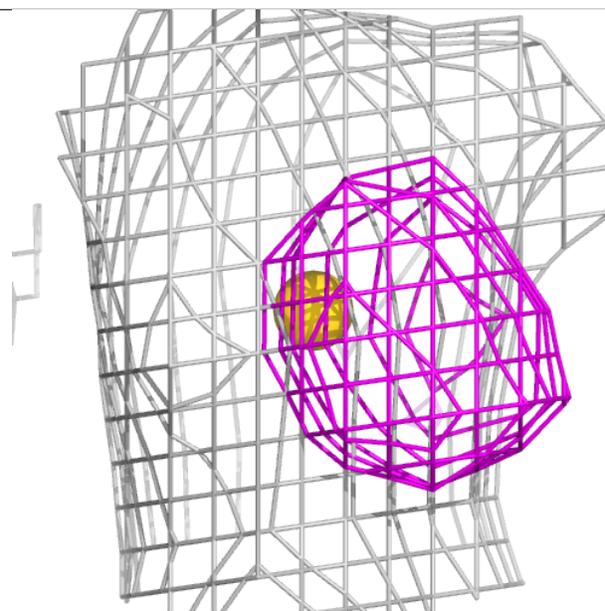
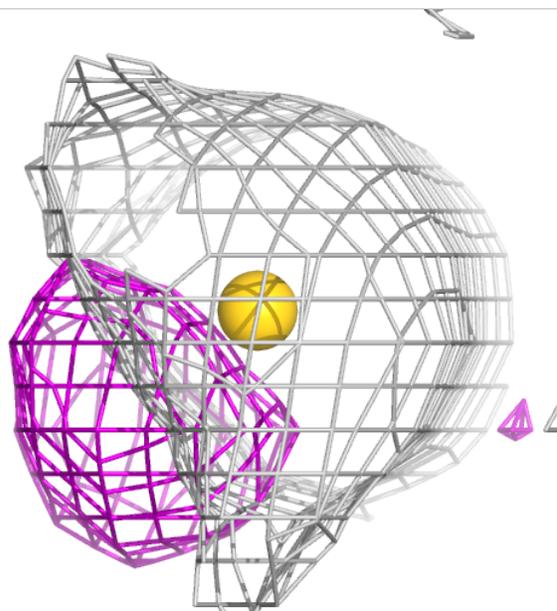
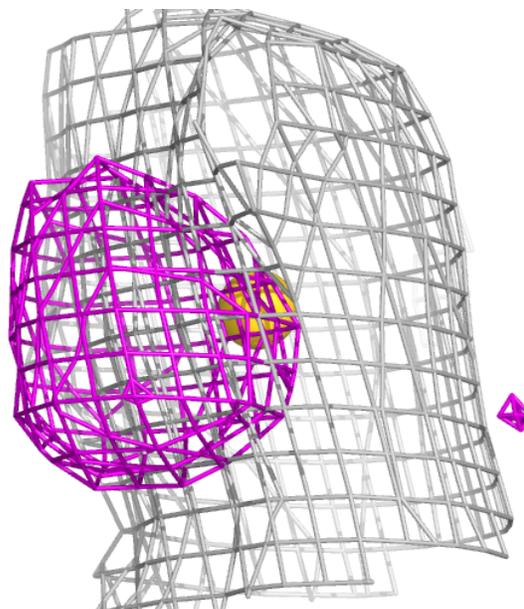
**Electron density around AU B 303:**

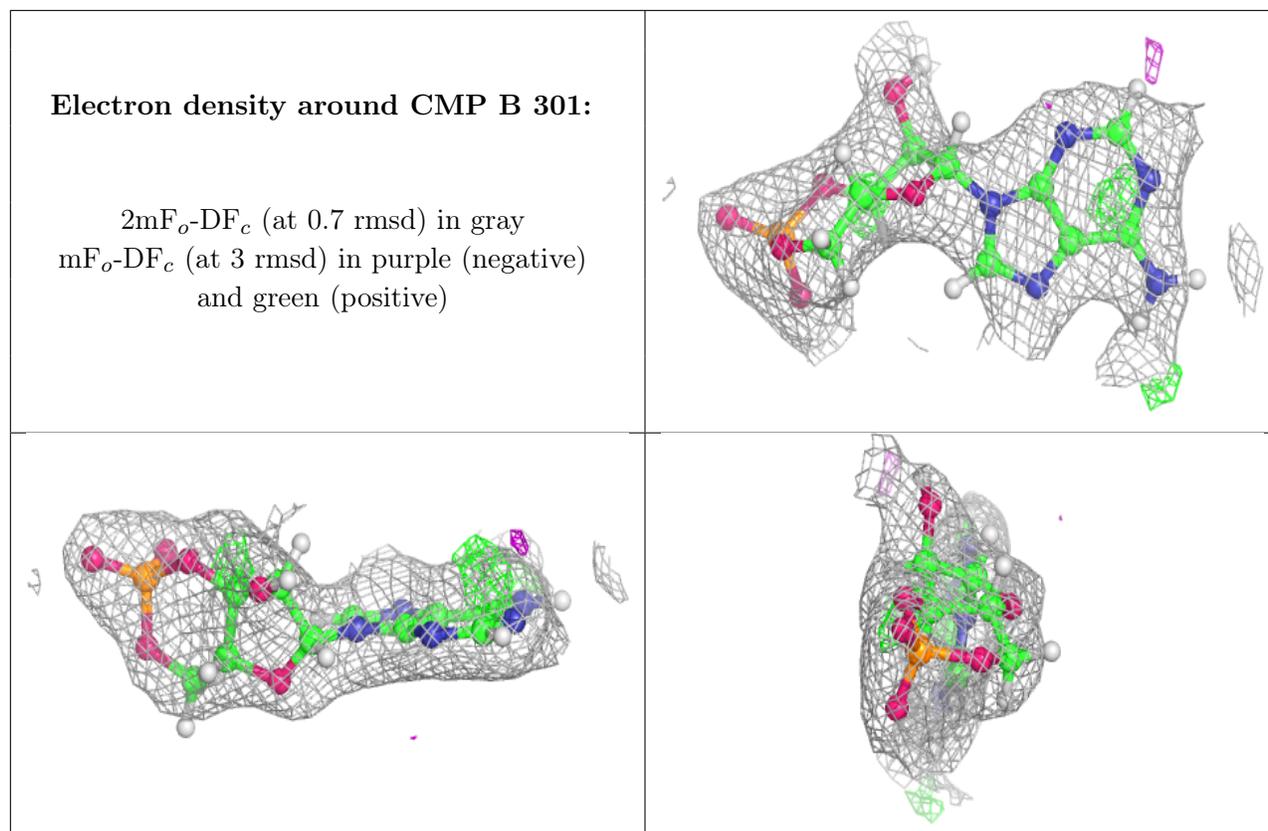
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around AU E 303:**

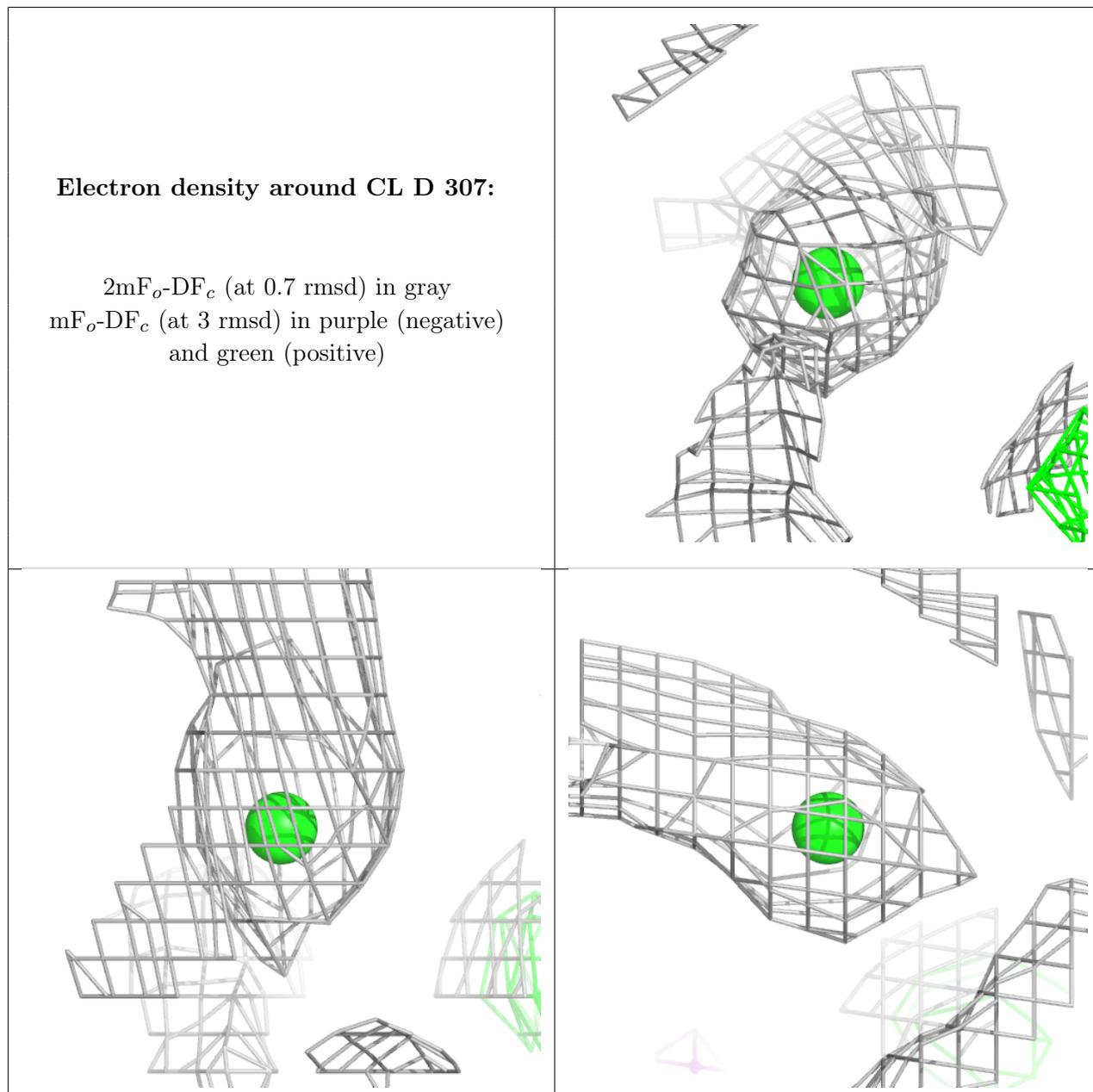
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





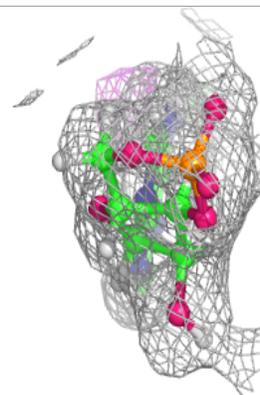
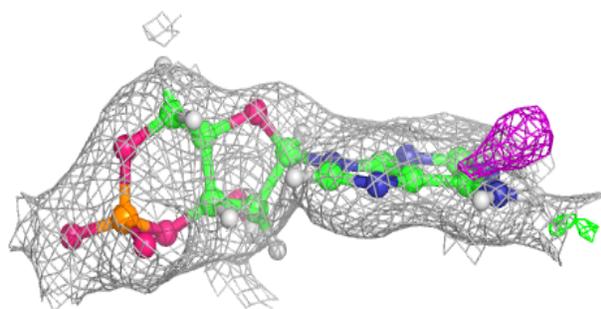
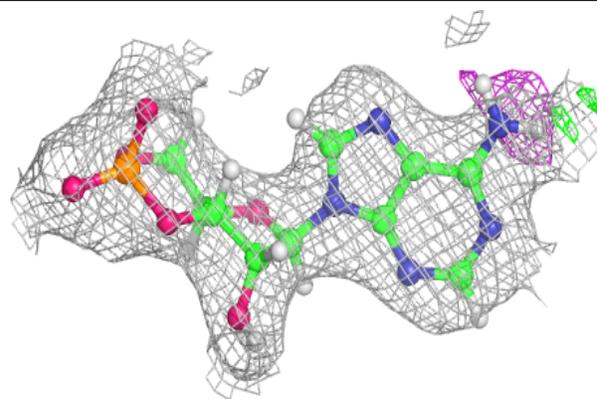
**Electron density around CL D 307:**

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

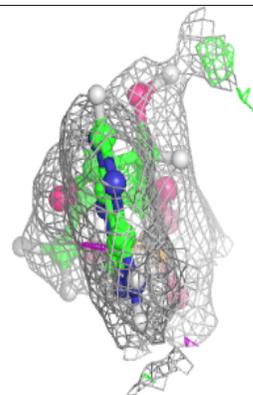
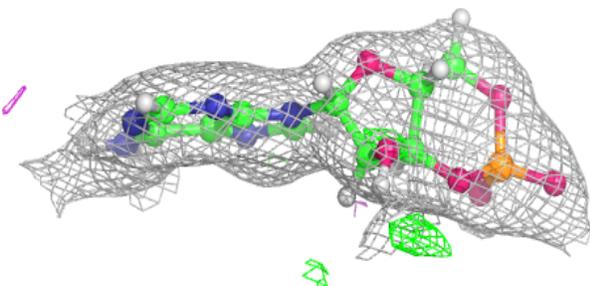
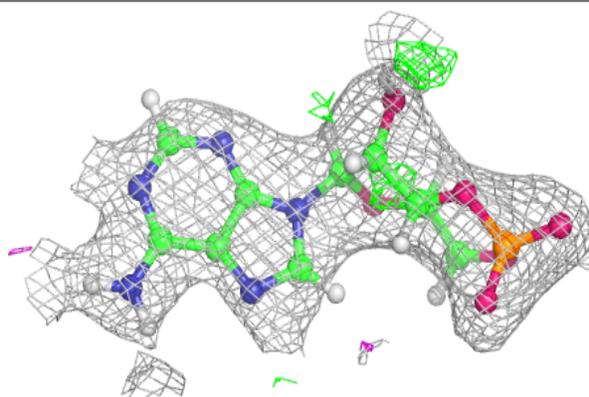


**Electron density around CMP H 301:**

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

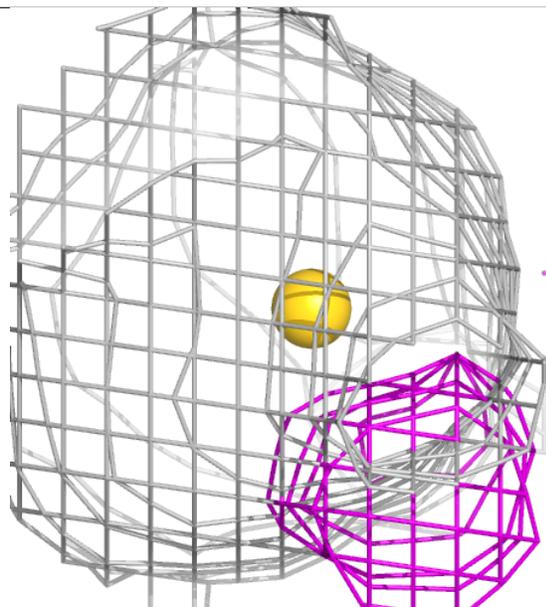
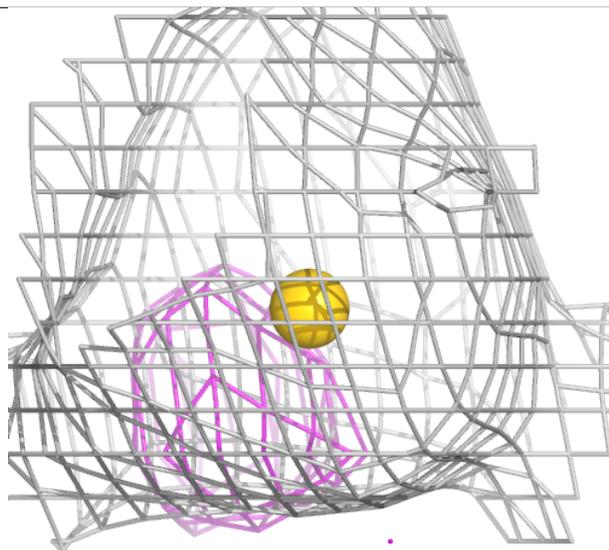
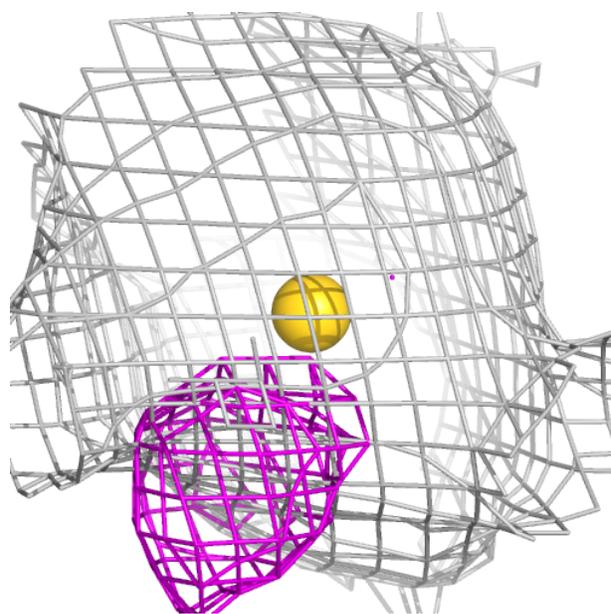
**Electron density around CMP G 301:**

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



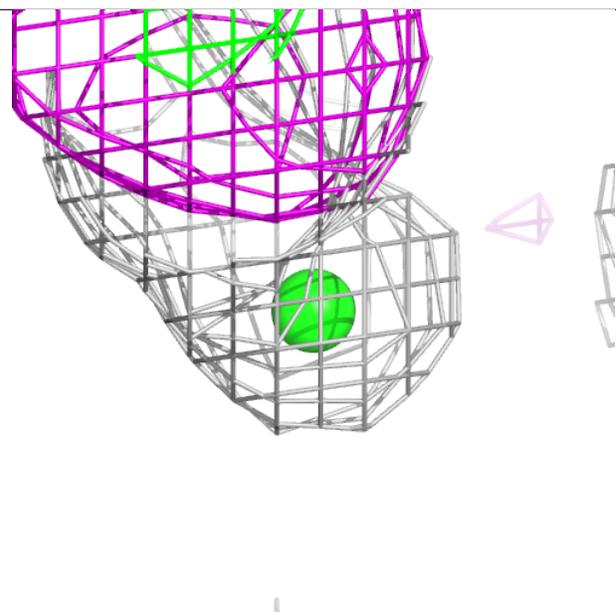
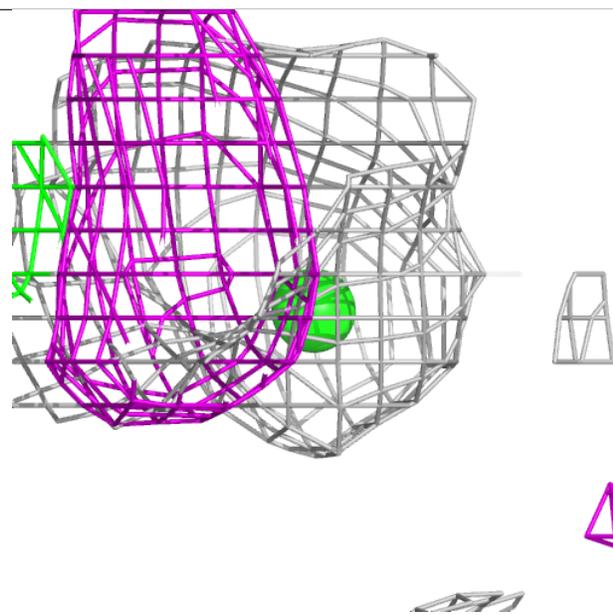
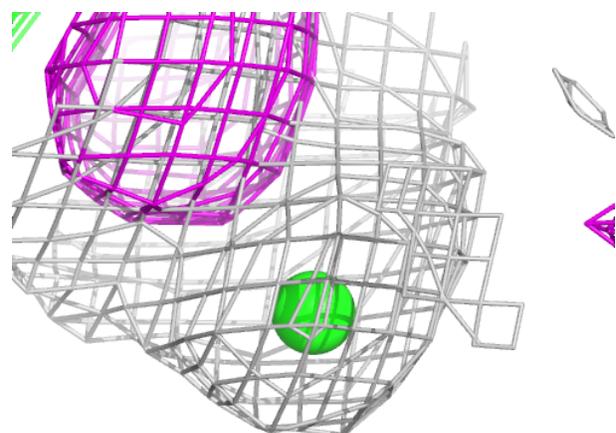
**Electron density around AU A 305:**

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



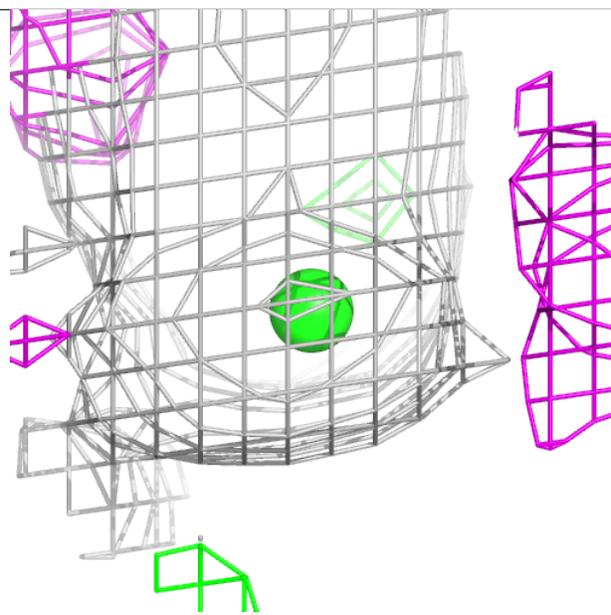
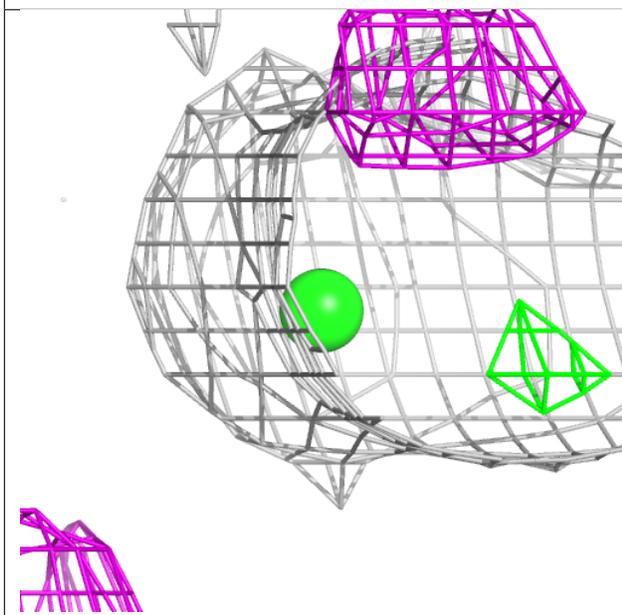
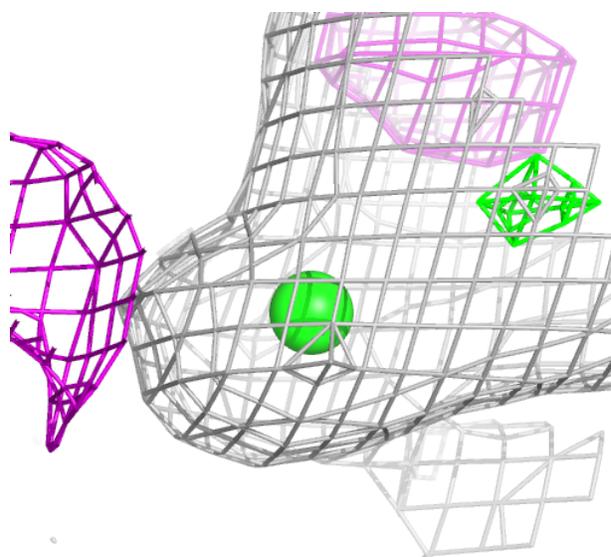
**Electron density around CL C 309:**

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



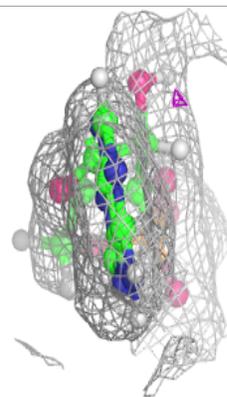
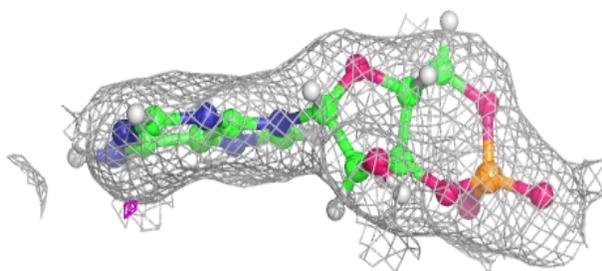
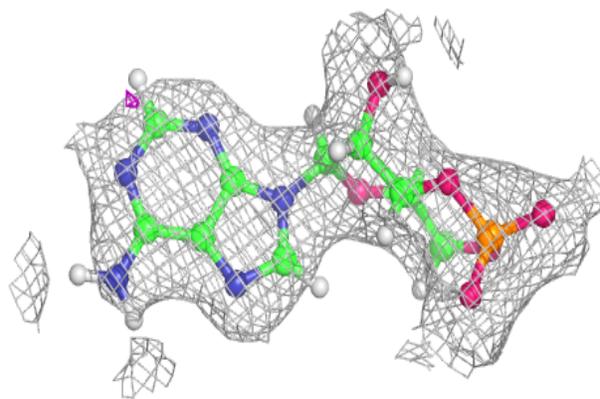
**Electron density around CL D 306:**

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

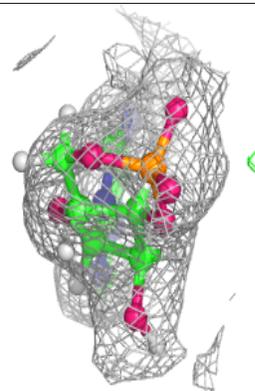
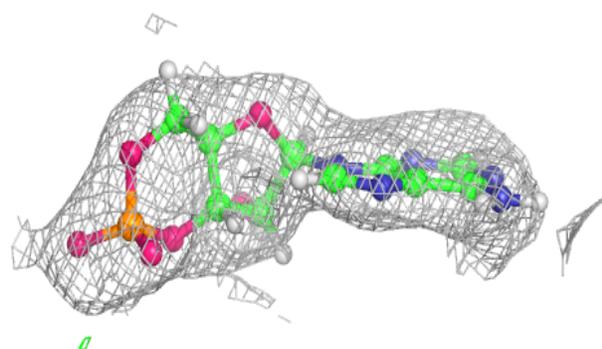
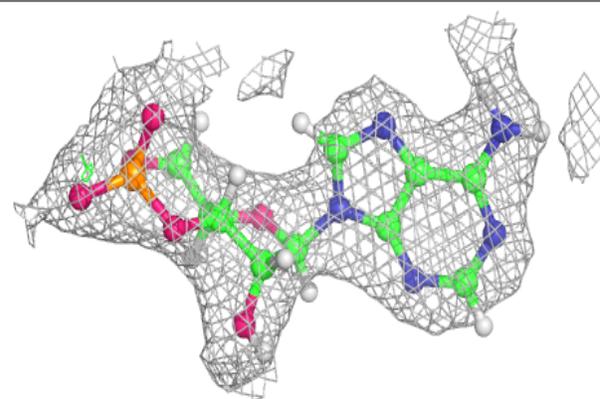


**Electron density around CMP F 301:**

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

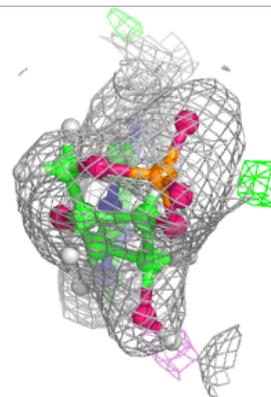
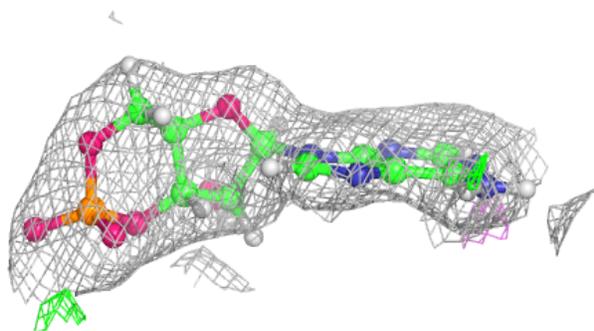
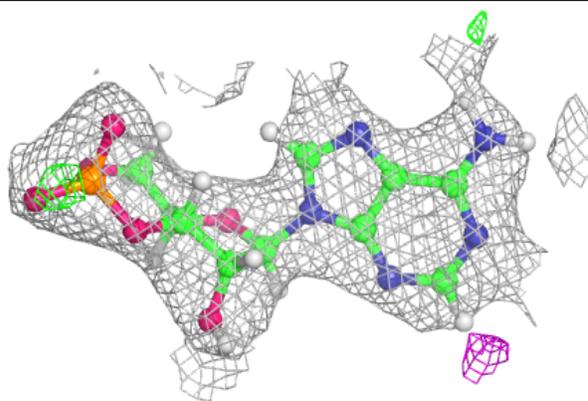
**Electron density around CMP A 301:**

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

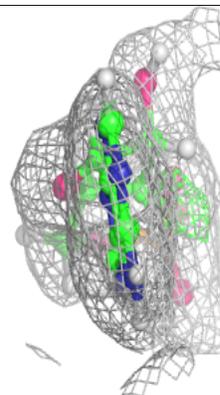
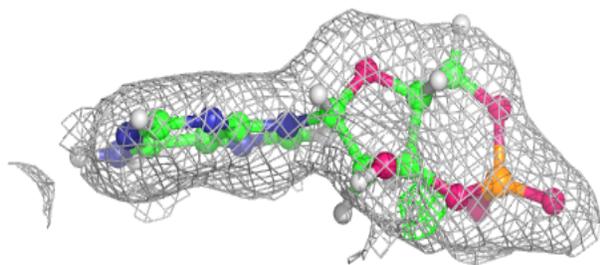
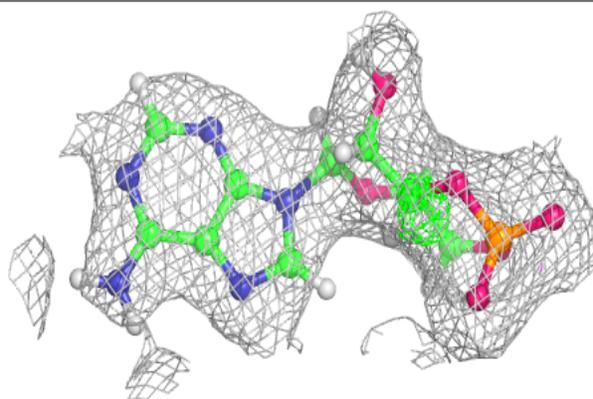


**Electron density around CMP C 301:**

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

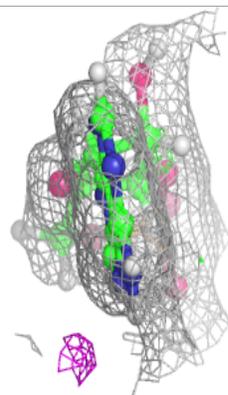
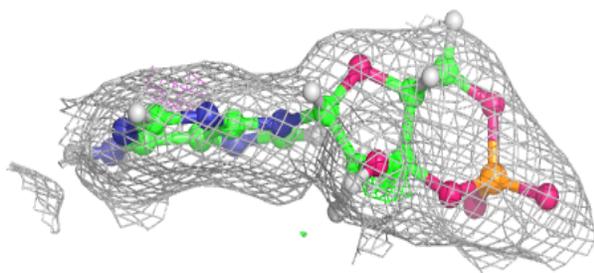
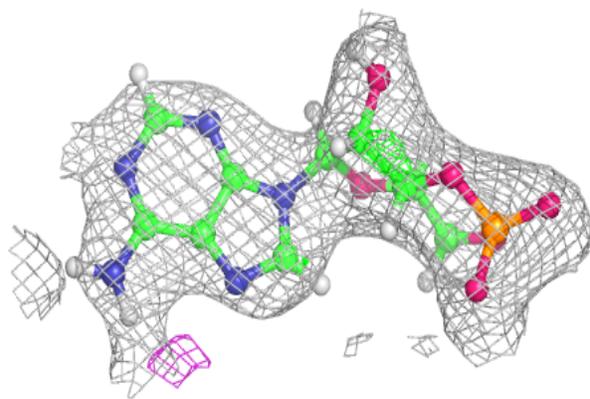
**Electron density around CMP D 301:**

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



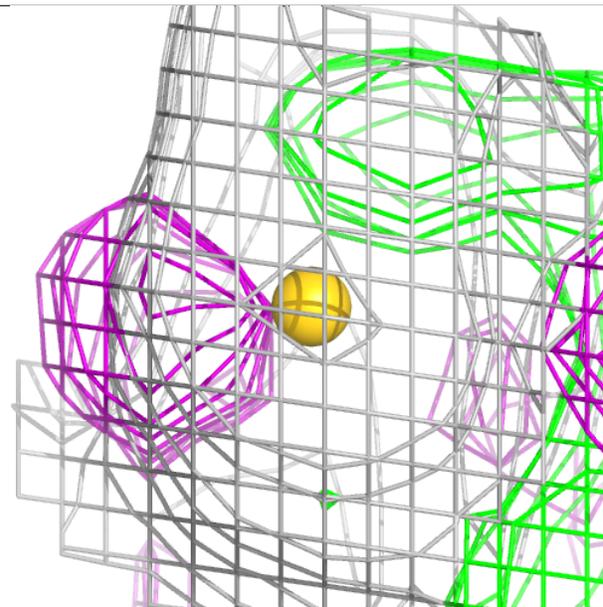
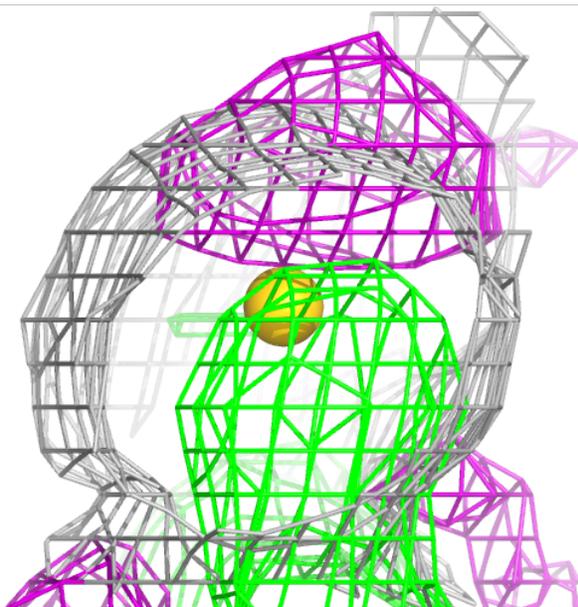
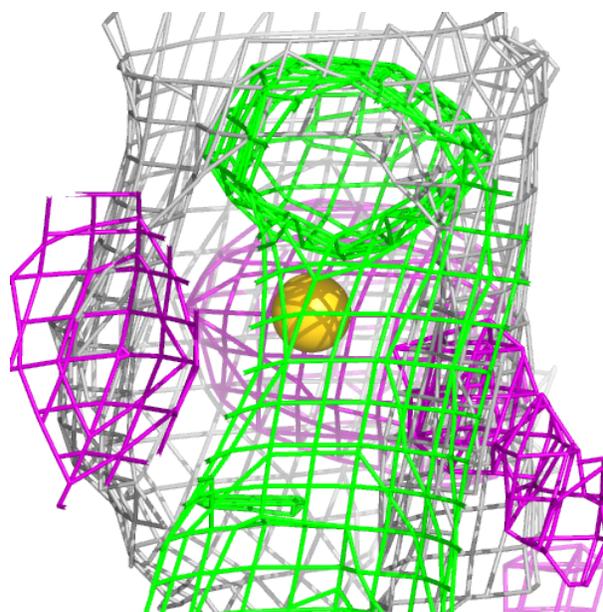
**Electron density around CMP E 301:**

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



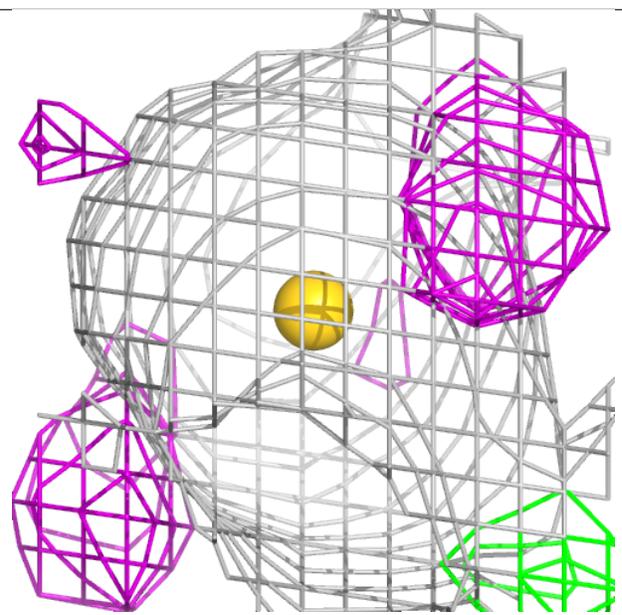
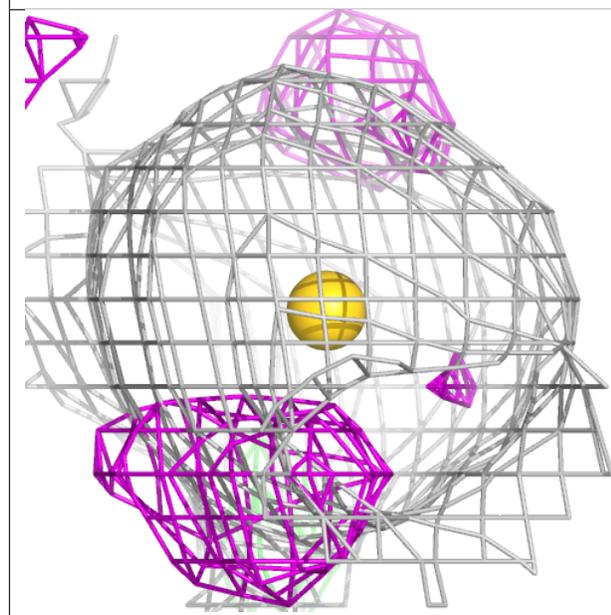
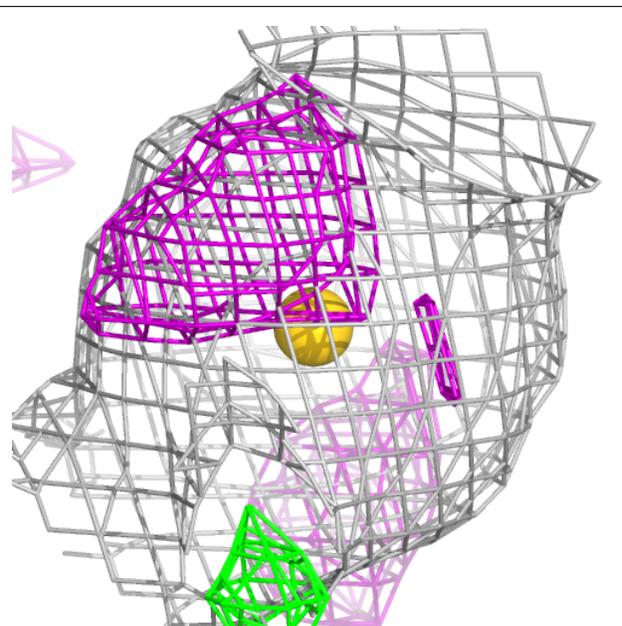
**Electron density around AU E 306:**

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



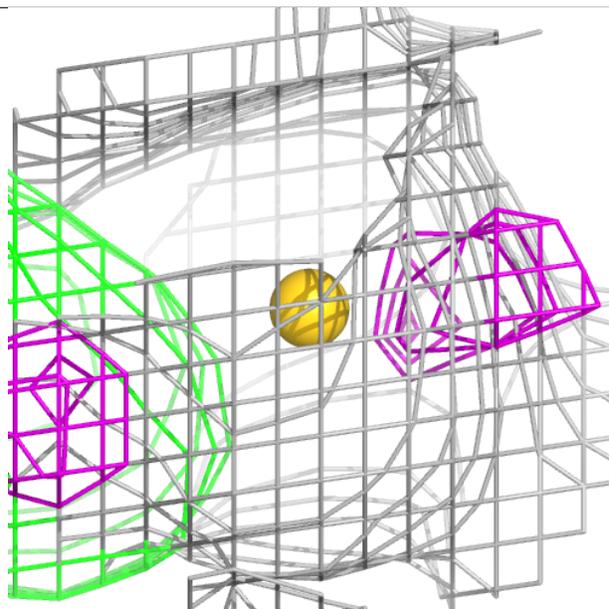
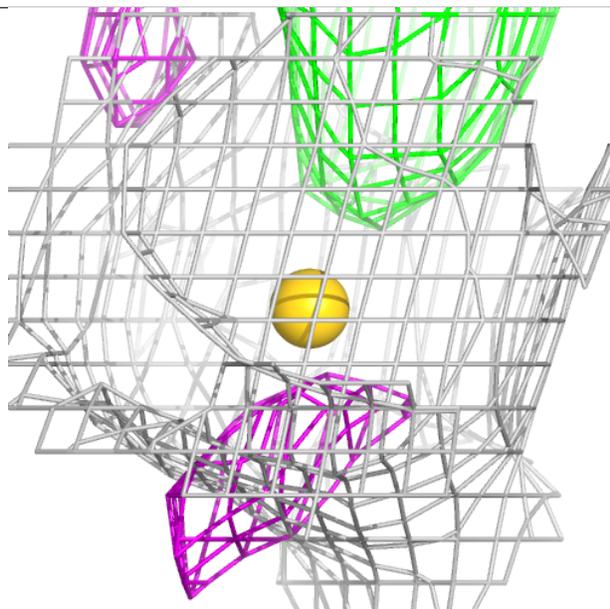
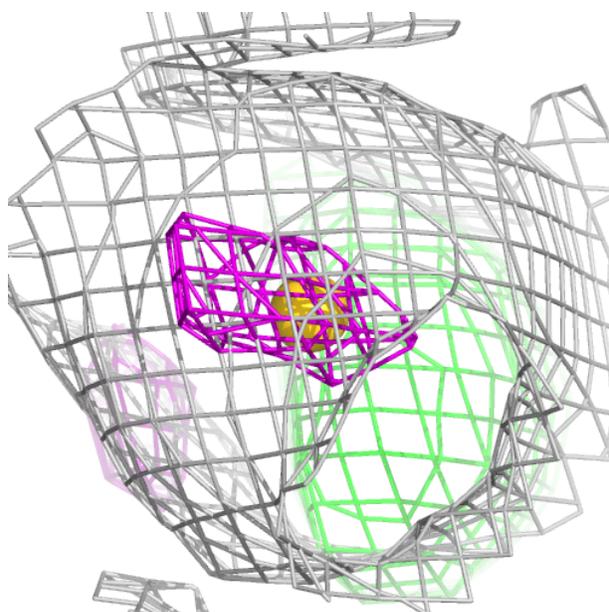
**Electron density around AU H 304:**

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



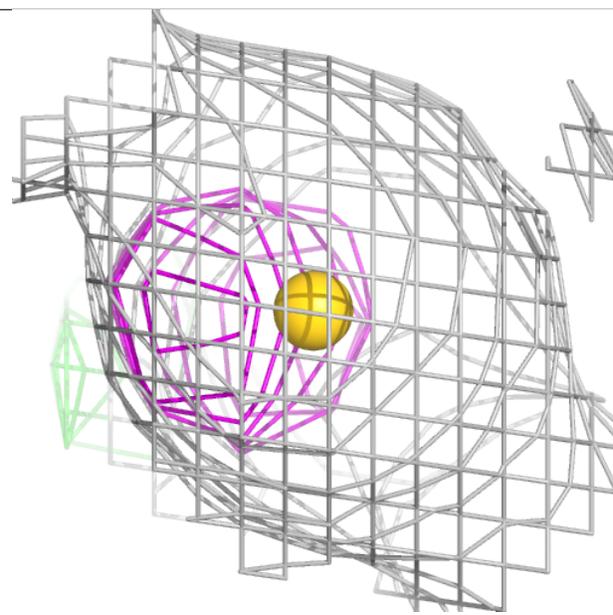
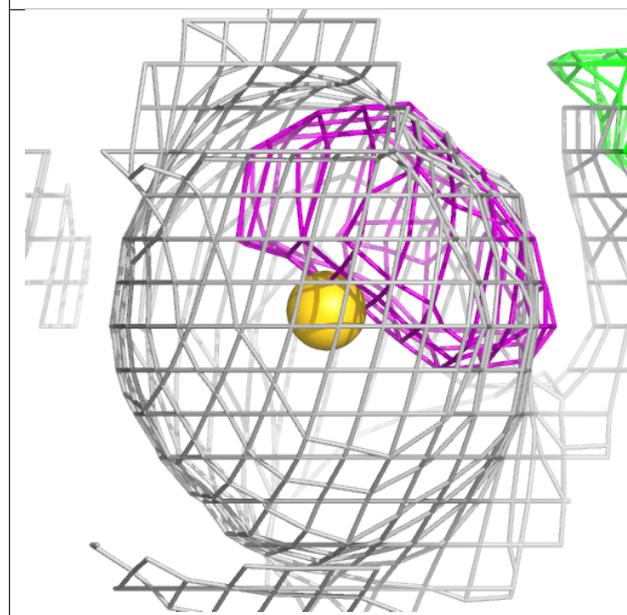
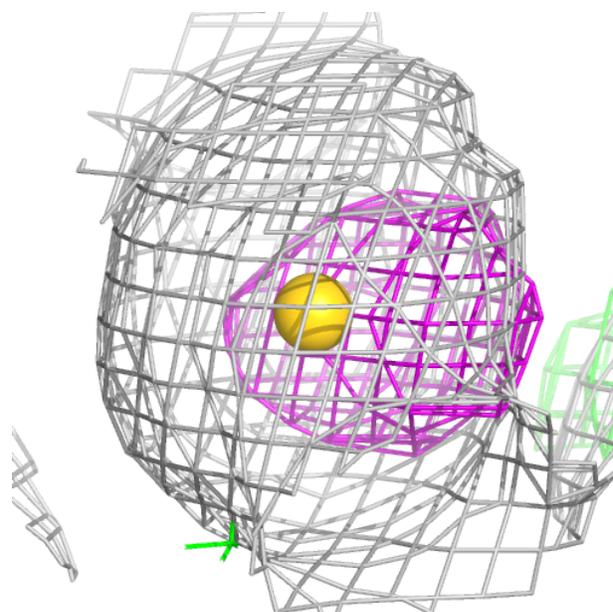
**Electron density around AU G 303:**

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



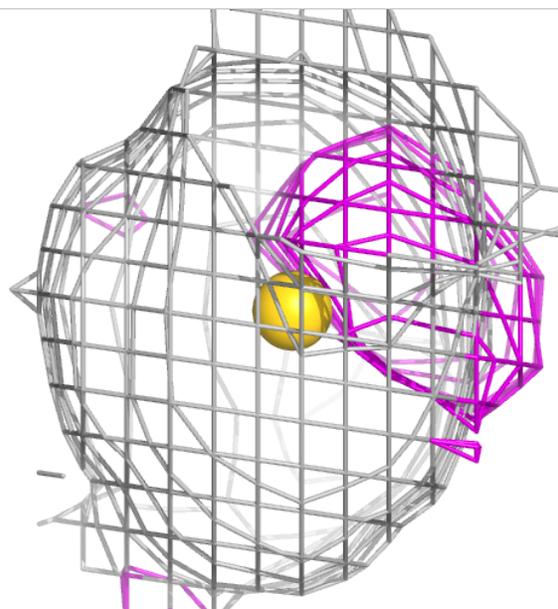
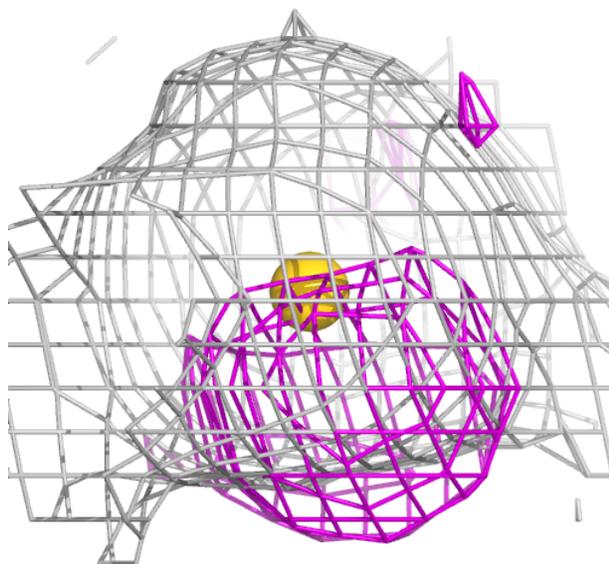
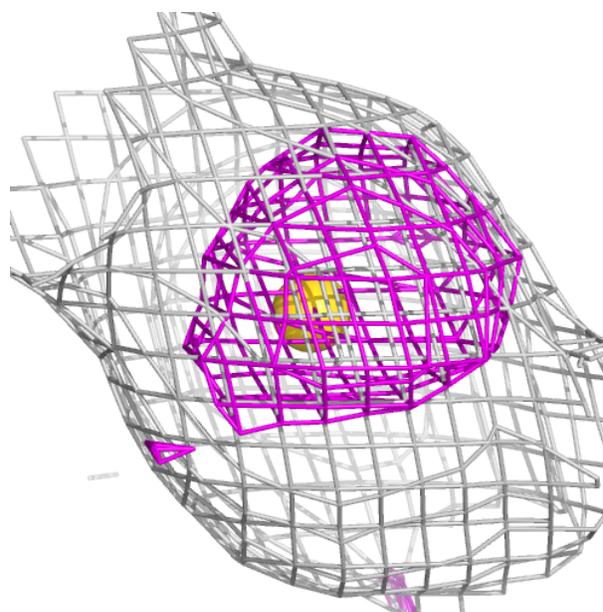
**Electron density around AU G 304:**

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



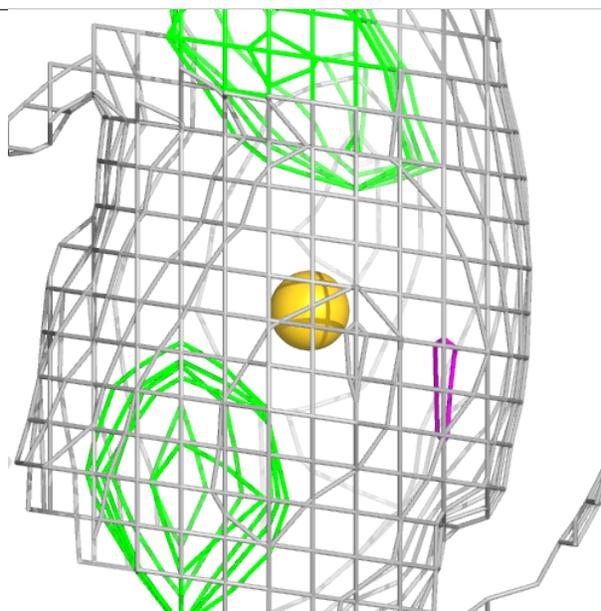
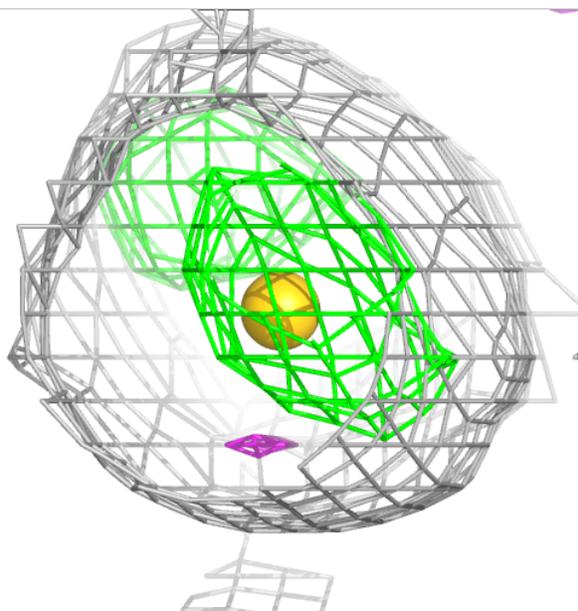
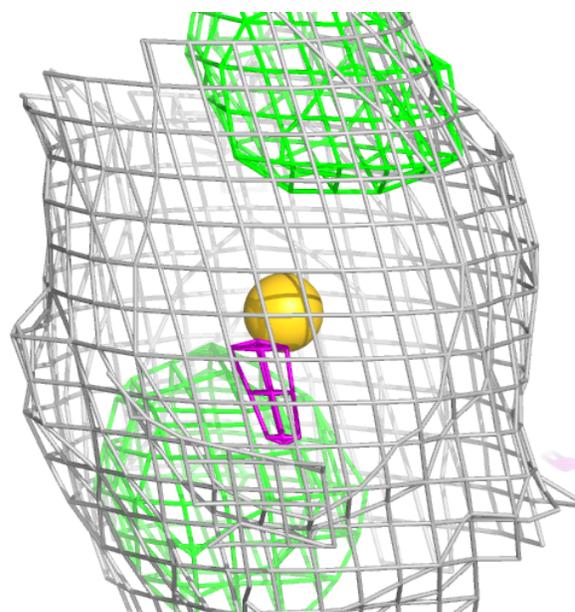
**Electron density around AU D 304:**

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



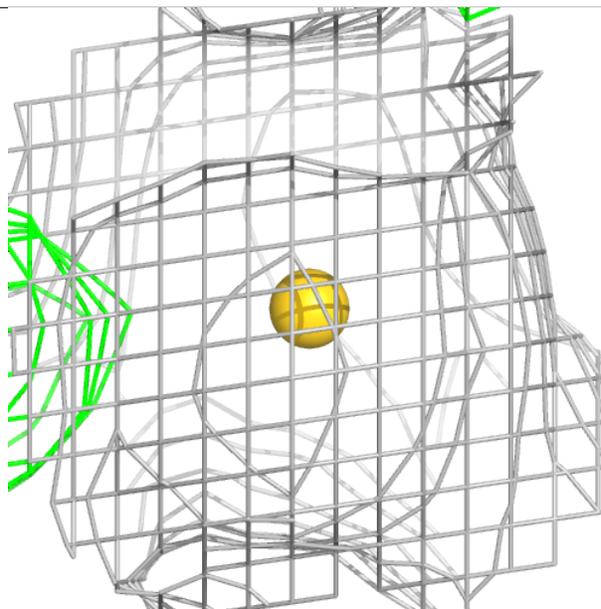
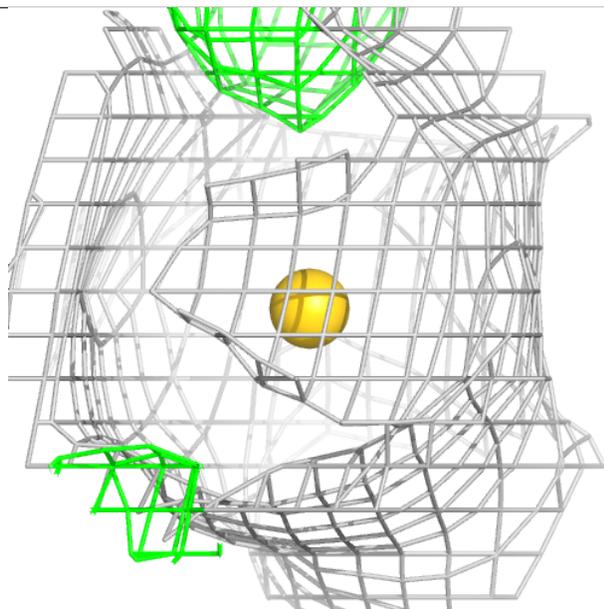
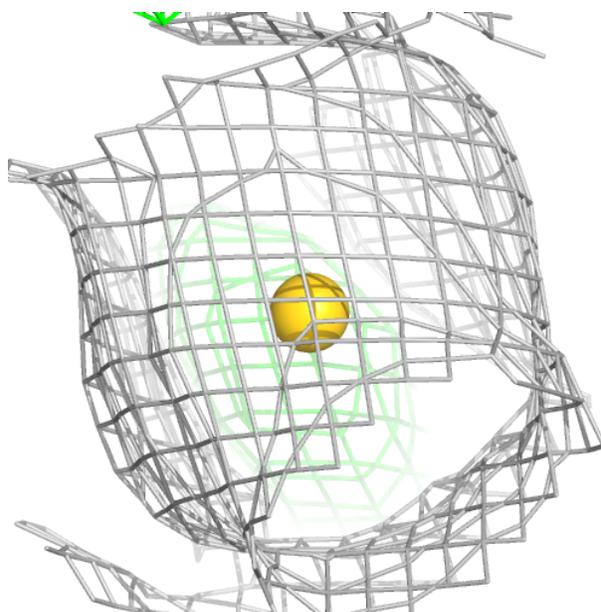
**Electron density around AU B 305:**

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



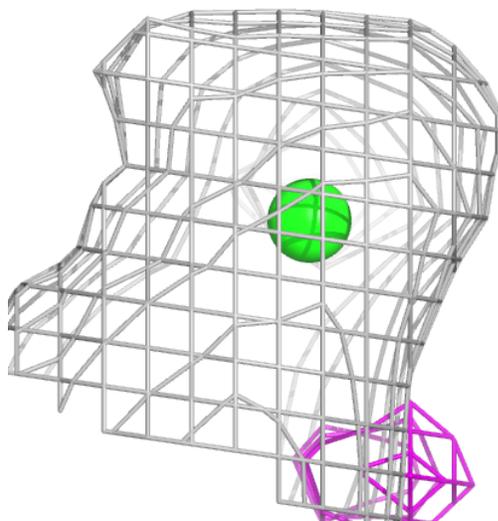
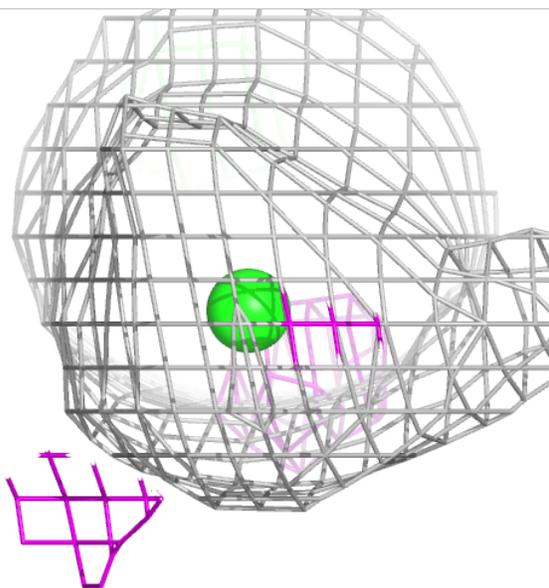
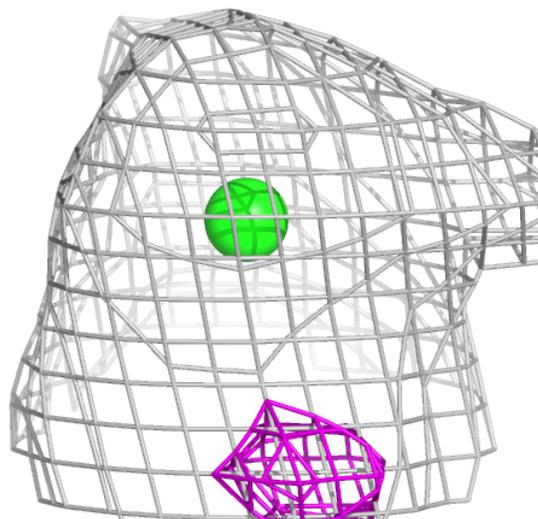
**Electron density around AU E 305:**

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



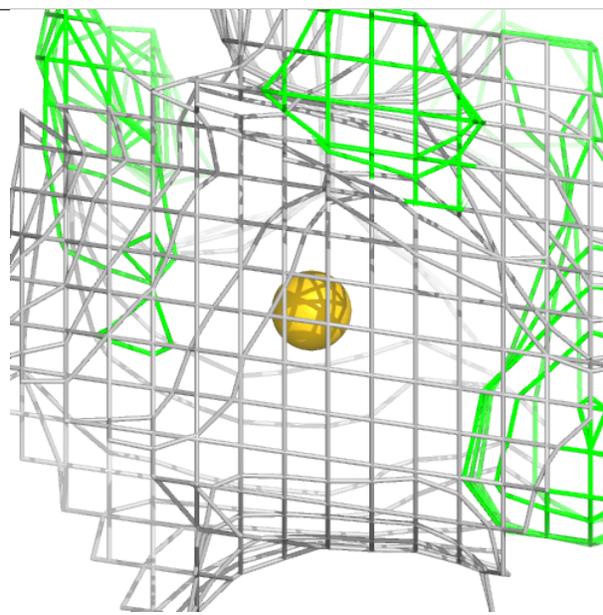
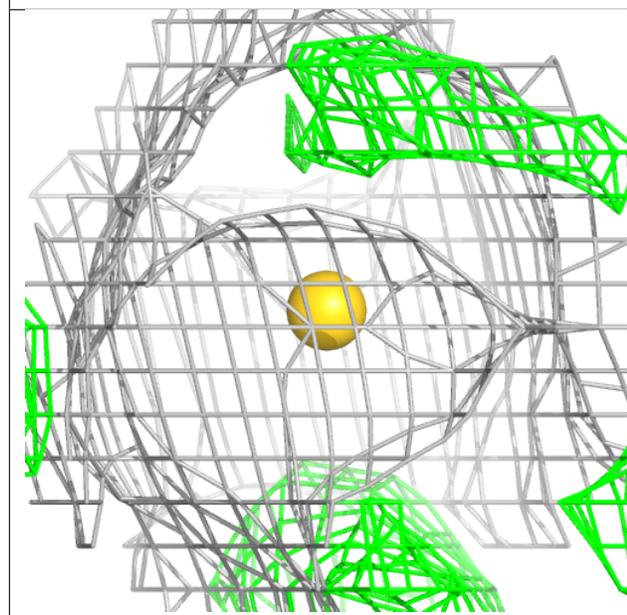
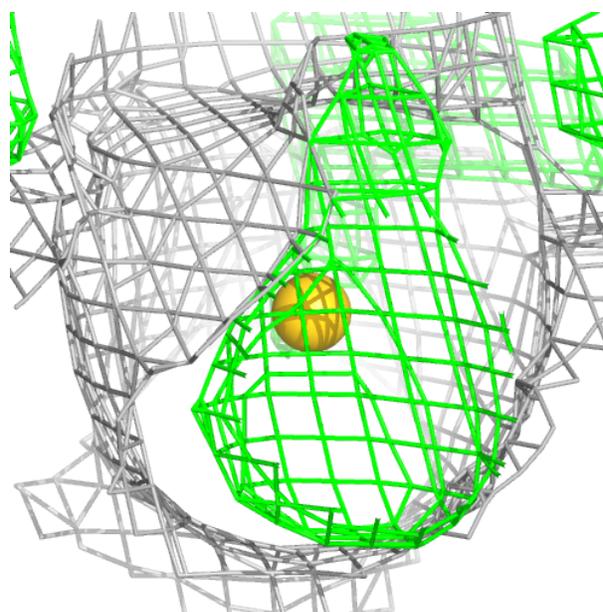
**Electron density around CL F 305:**

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



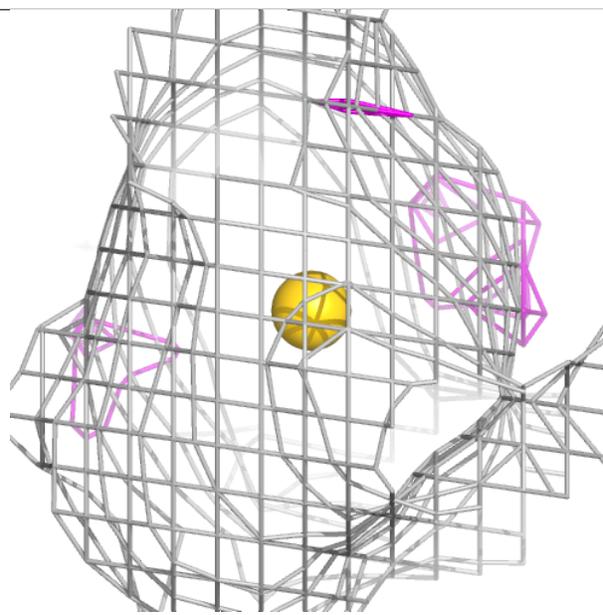
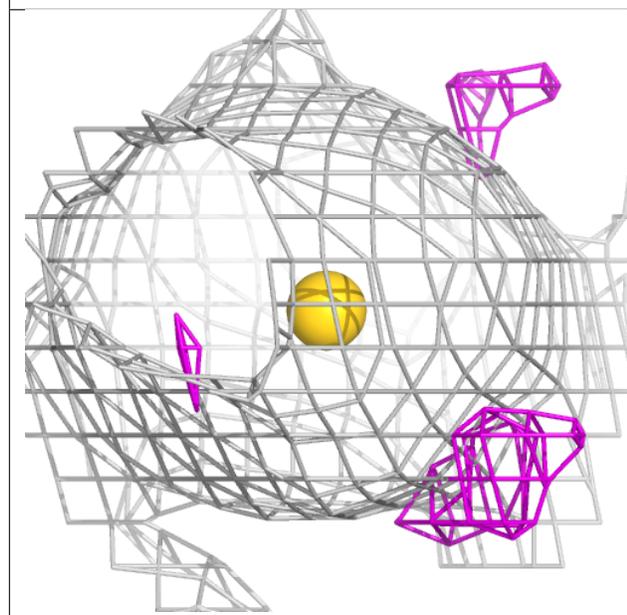
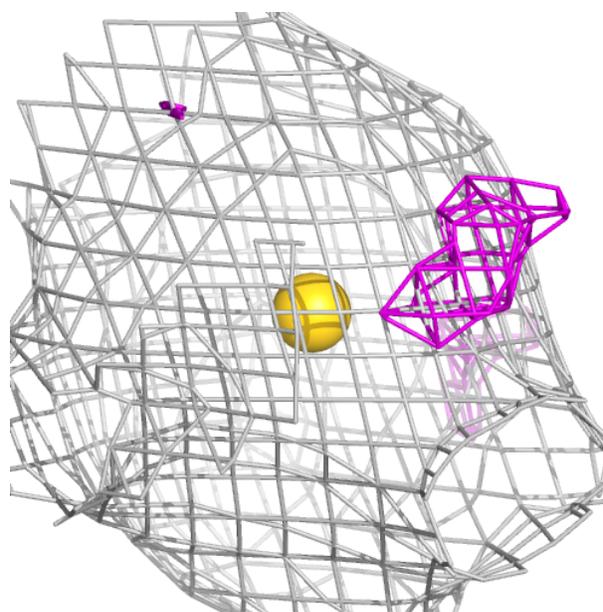
**Electron density around AU A 303:**

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



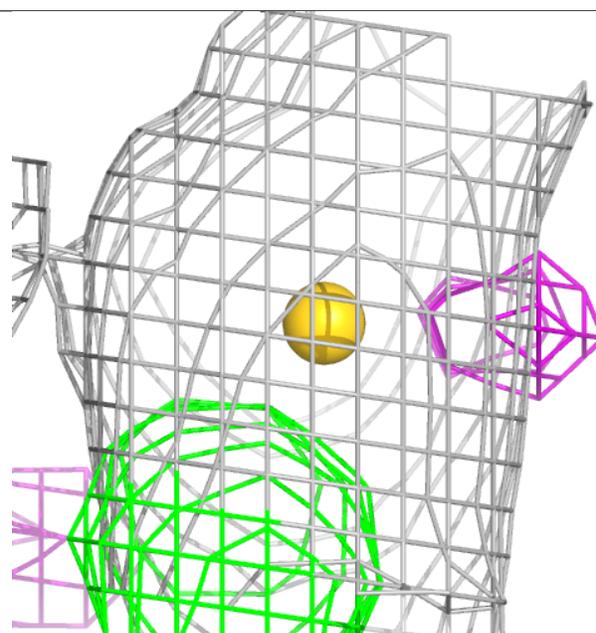
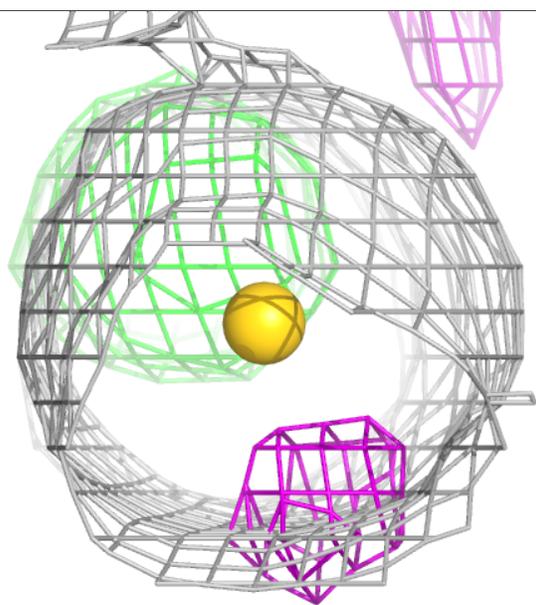
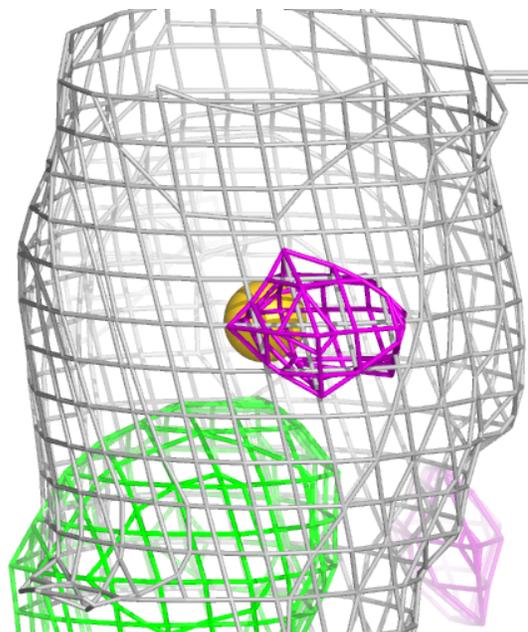
**Electron density around AU C 306:**

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



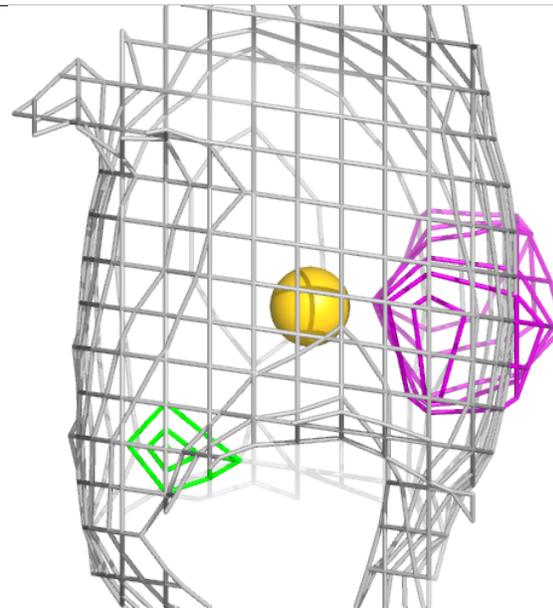
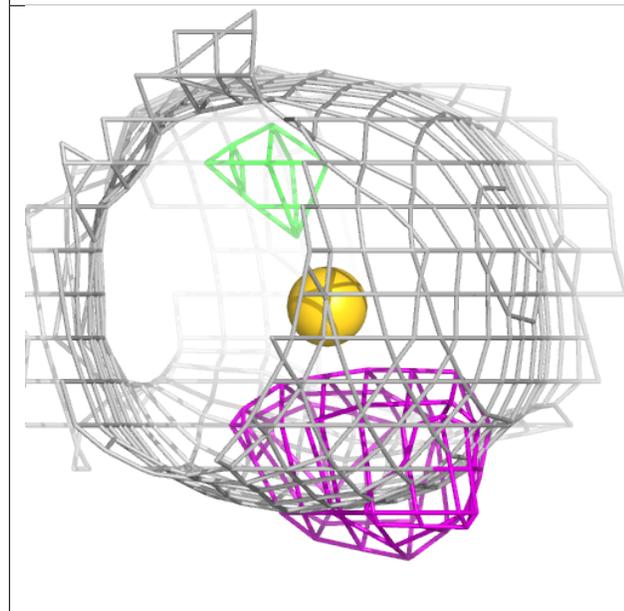
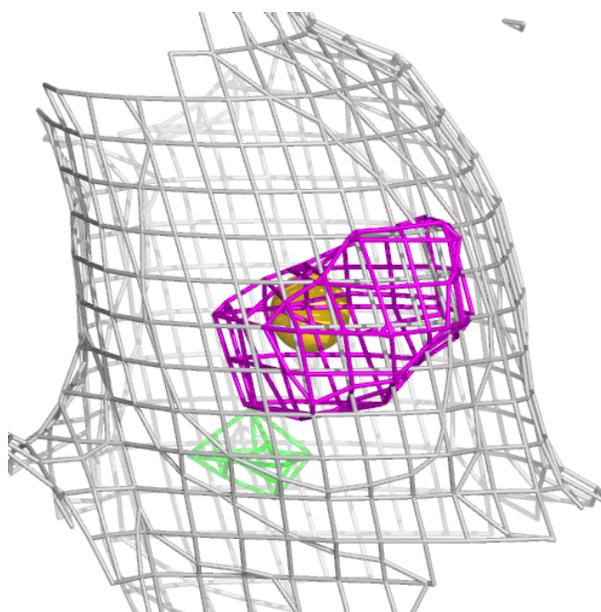
**Electron density around AU F 303:**

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



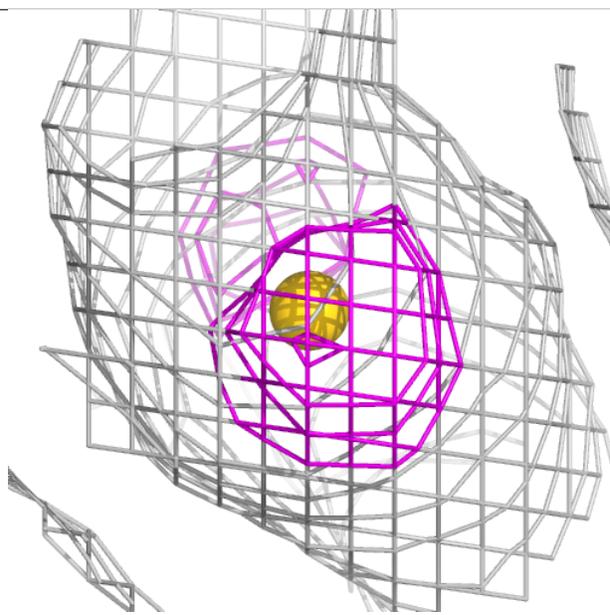
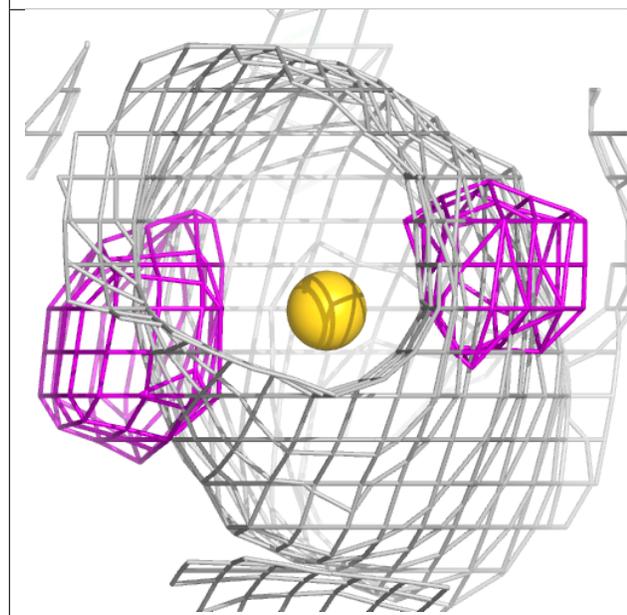
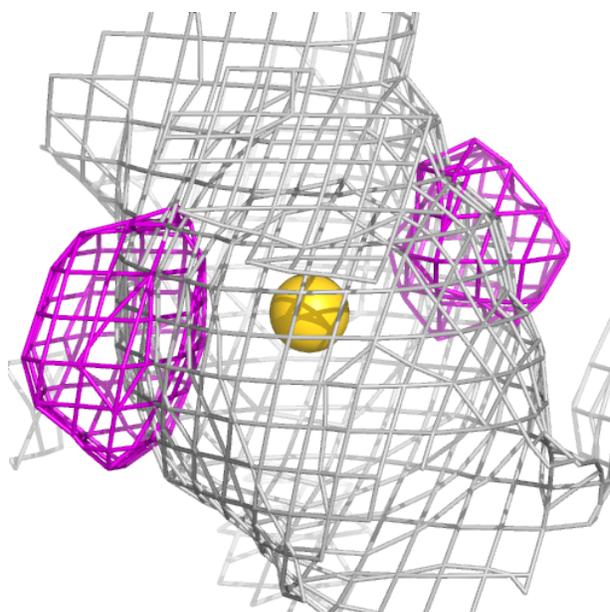
**Electron density around AU D 302:**

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



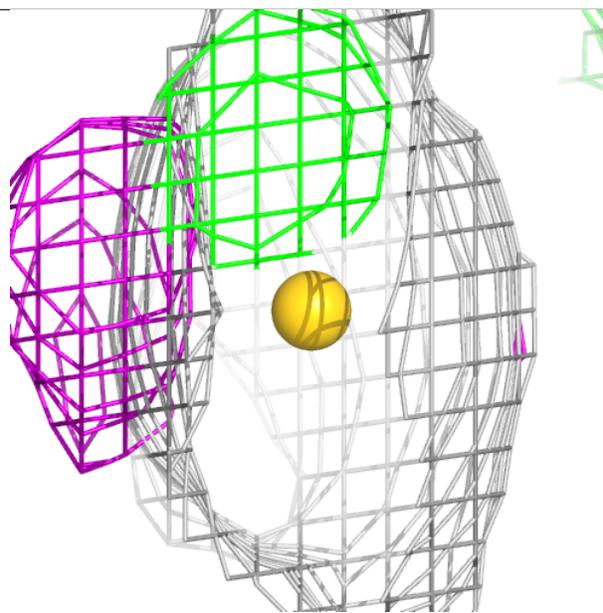
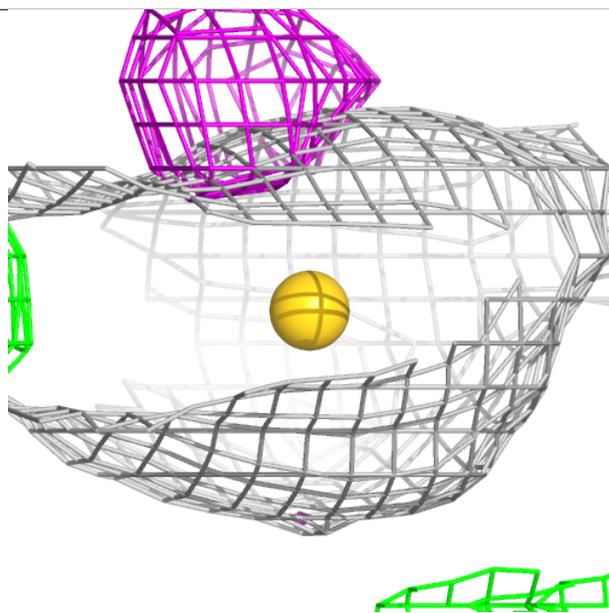
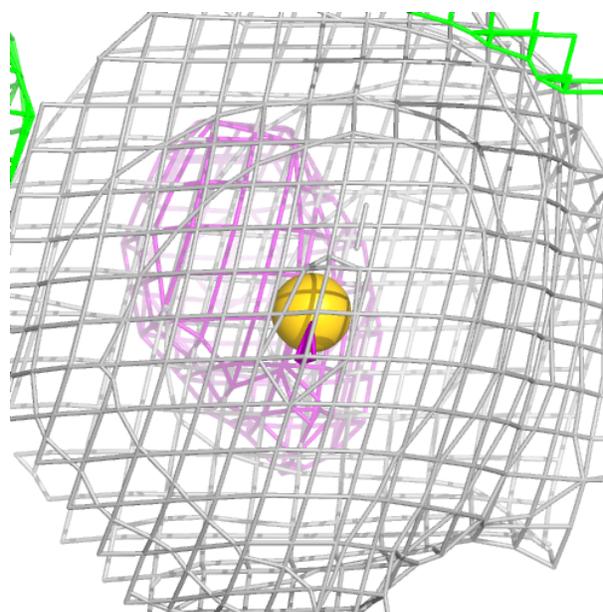
**Electron density around AU E 304:**

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



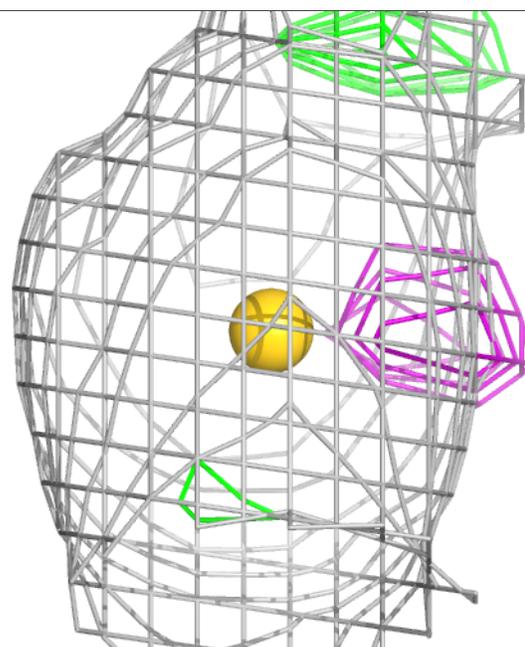
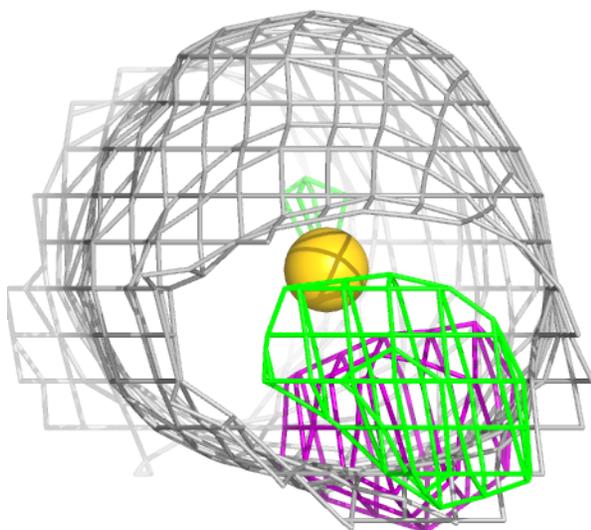
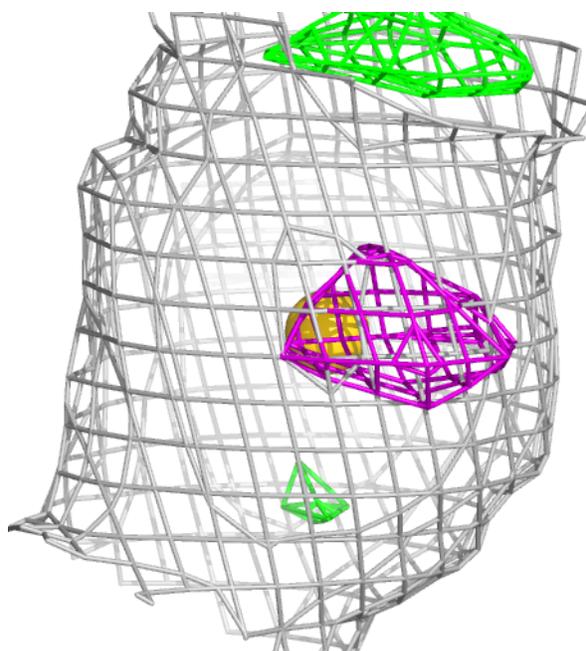
**Electron density around AU A 304:**

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



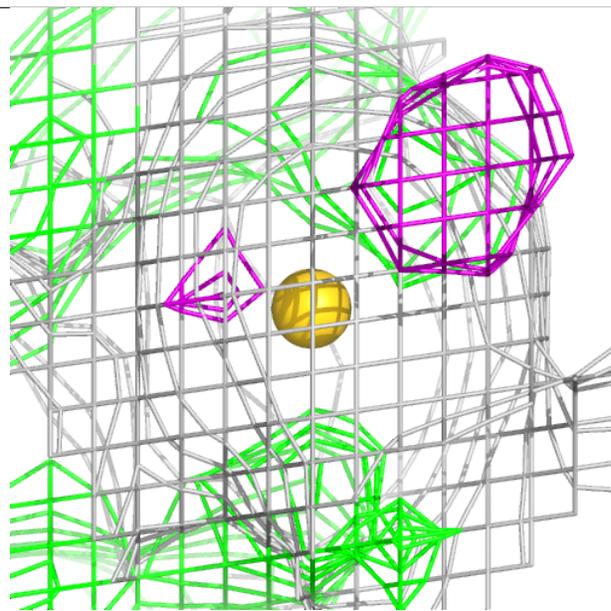
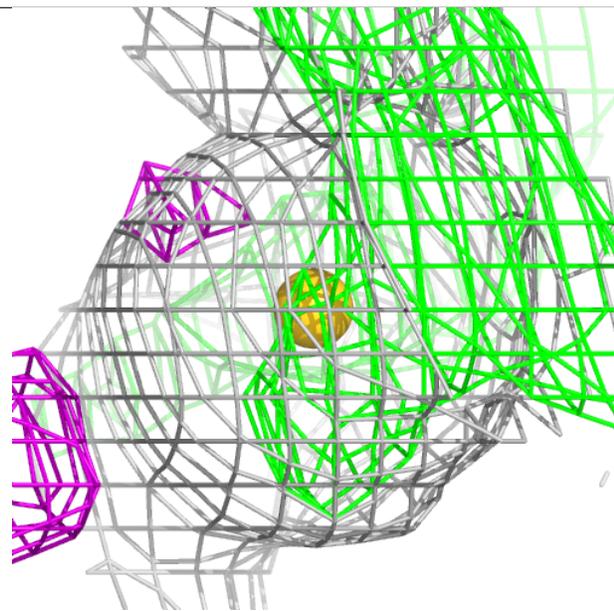
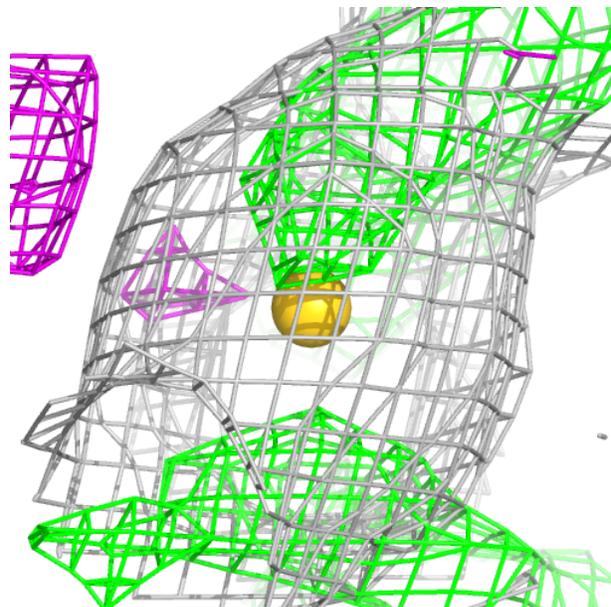
**Electron density around AU H 302:**

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



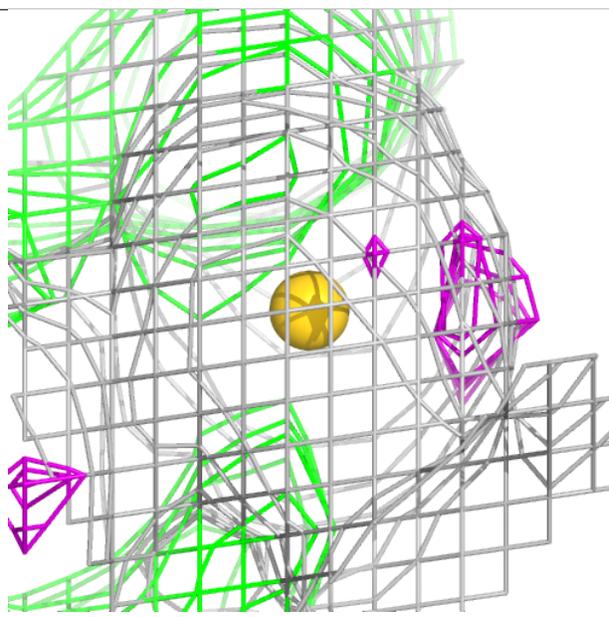
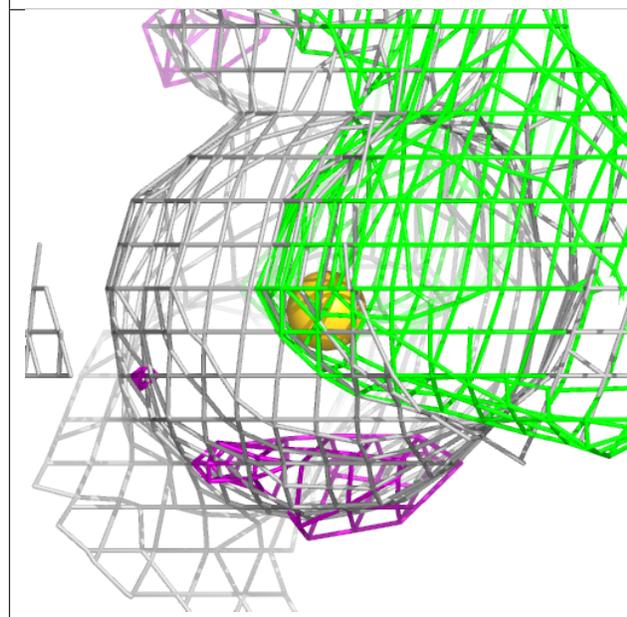
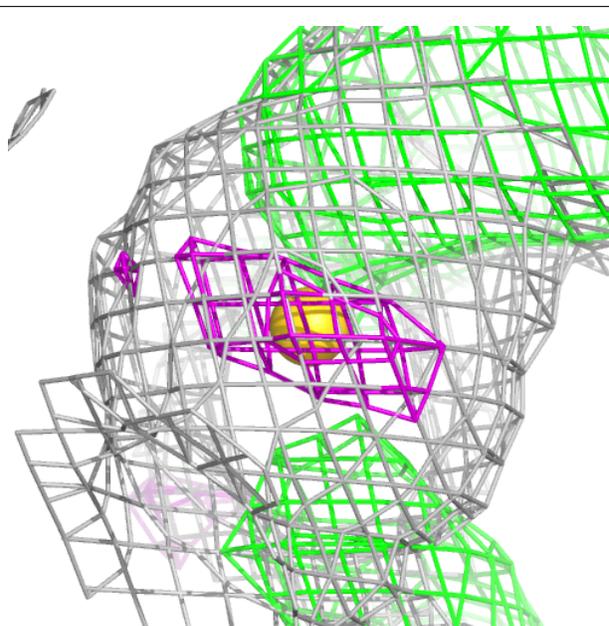
**Electron density around AU C 307:**

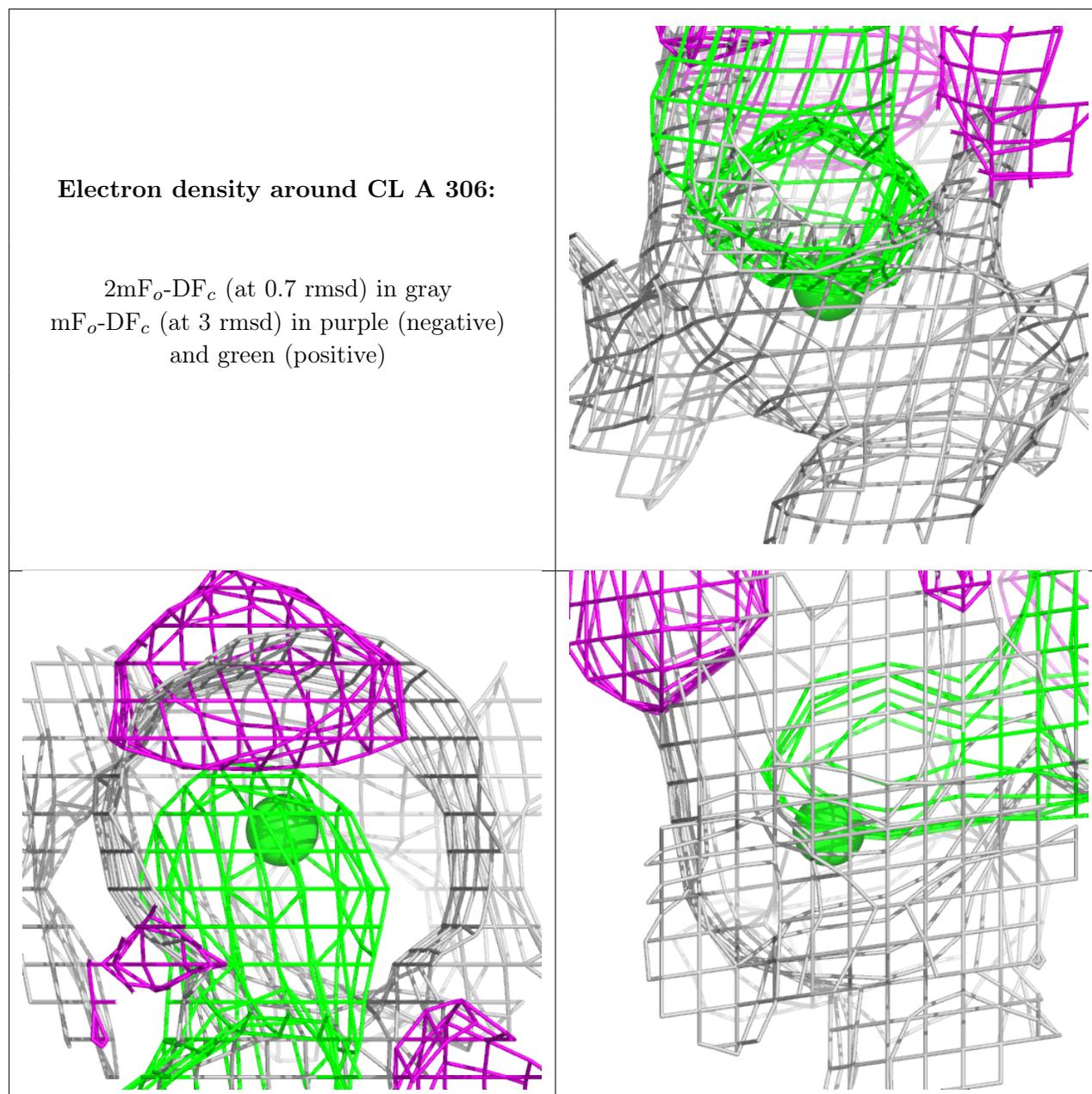
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around AU G 305:**

$2mF_o-DF_c$  (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.