



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2026 – 01:50 PM JST

PDB ID : 9V67 / pdb\_00009v67  
Title : The crystal structure of a ThDP-dependent enzyme PpBFD  
Authors : Hou, X.L.; Zhou, J.H.  
Deposited on : 2025-05-26  
Resolution : 2.25 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:

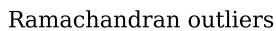
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

i

## X-RAY DIFFRACTION

A.

Metric	Percentile Banks	Value
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 $R_{free}$ 

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.

1

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	612	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16874 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 Benzoylformate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	4	0
			3942	2493	682	747	20			
1	B	508	Total	C	N	O	S	0	3	0
			3824	2415	665	725	19			
1	C	503	Total	C	N	O	S	0	4	0
			3788	2392	657	719	20			
1	D	523	Total	C	N	O	S	0	3	0
			3938	2490	682	747	19			

There are 8 discrepancies between the modelled and reference sequences:

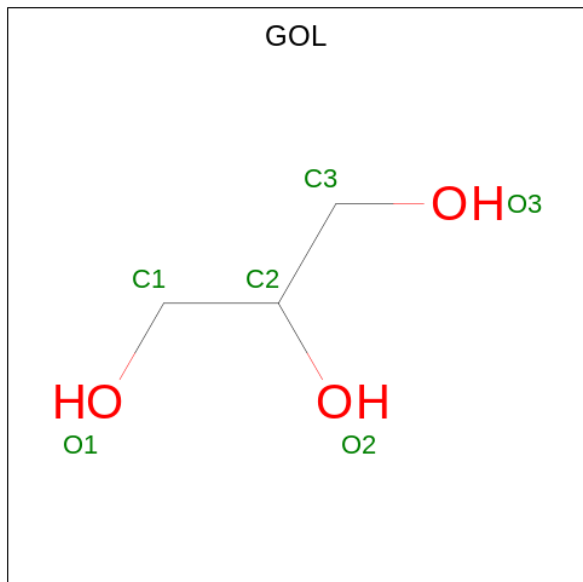
Chain	Residue	Modelled	Actual	Comment	Reference
A	529	LEU	-	expression tag	UNP P20906
A	530	GLU	-	expression tag	UNP P20906
B	529	LEU	-	expression tag	UNP P20906
B	530	GLU	-	expression tag	UNP P20906
C	529	LEU	-	expression tag	UNP P20906
C	530	GLU	-	expression tag	UNP P20906
D	529	LEU	-	expression tag	UNP P20906
D	530	GLU	-	expression tag	UNP P20906

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total	Mg	0	0
			11	11		
2	B	10	Total	Mg	0	0
			10	10		
2	C	8	Total	Mg	0	0
			8	8		
2	D	1	Total	Mg	0	0
			1	1		

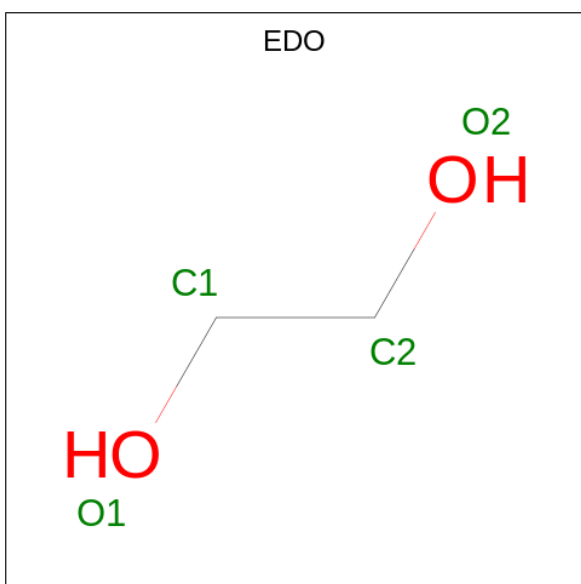
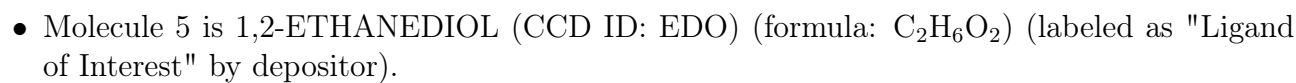


- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula:  $C_{12}H_{19}N_4O_7P_2S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0
6	C	1	Total Cl 1 1	0	0

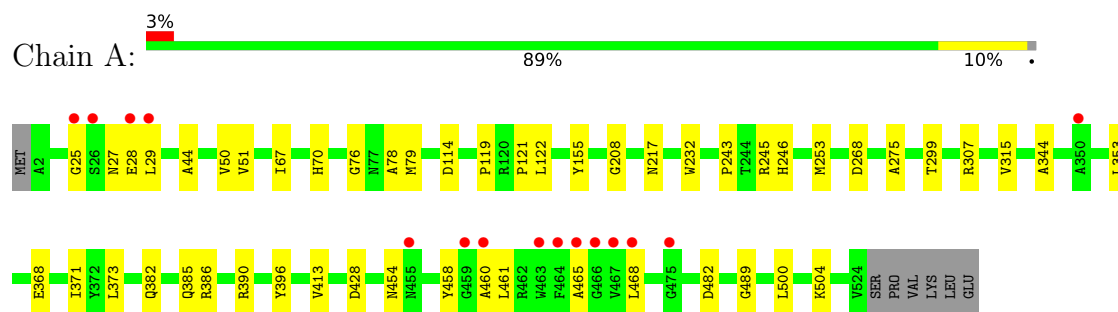
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	343	Total O 343 343	0	0
7	B	317	Total O 317 317	0	0
7	C	267	Total O 267 267	0	0
7	D	247	Total O 247 247	0	0

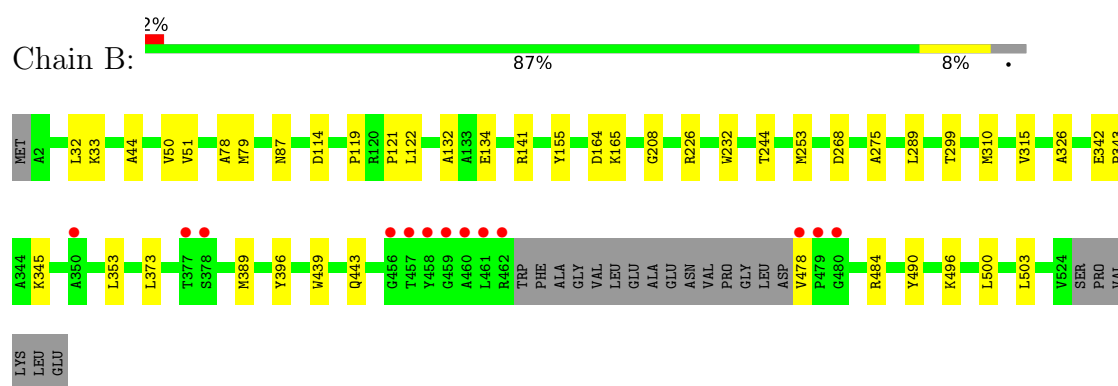
### 3 Residue-property plots [i](#)

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

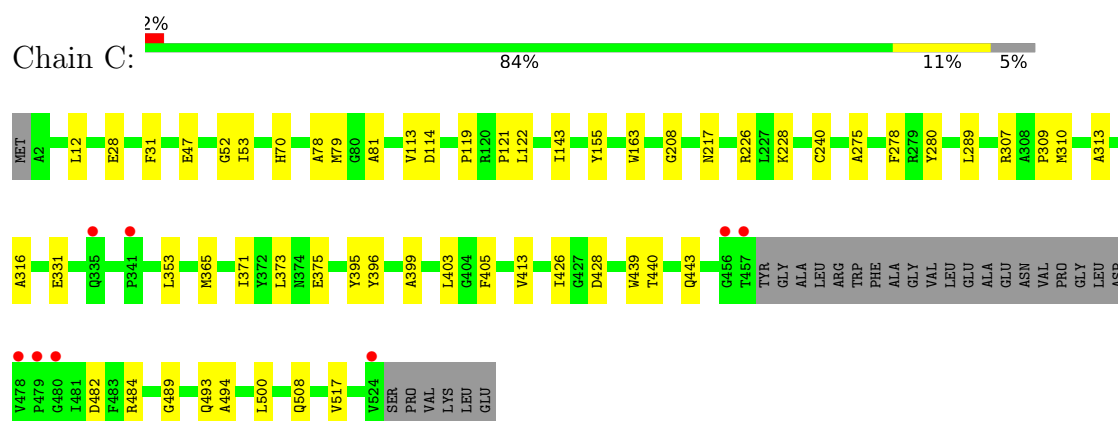
#### • Molecule 1: Benzoylformate decarboxylase



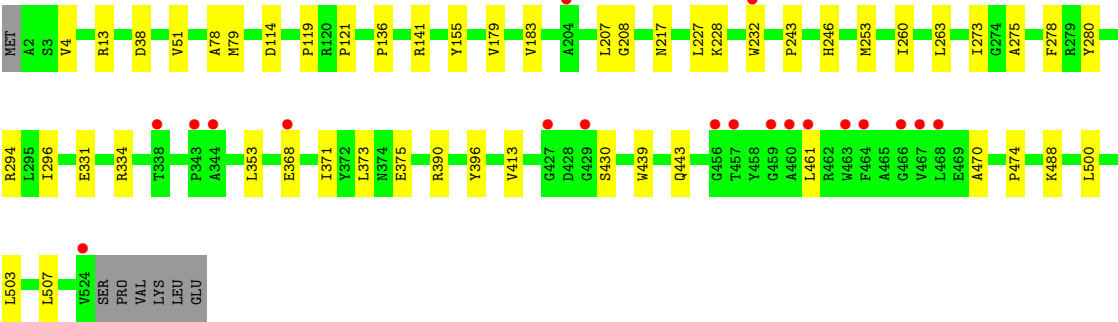
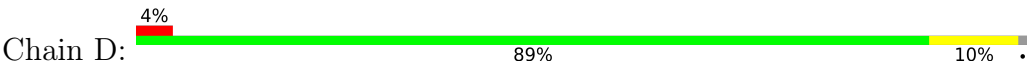
#### • Molecule 1: Benzoylformate decarboxylase



#### • Molecule 1: Benzoylformate decarboxylase



● Molecule 1: Benzoylformate decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.69Å 111.93Å 199.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.68 – 2.25 43.68 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.68-2.25) 99.8 (43.68-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.12_2829, PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.188 , 0.229 0.188 , 0.228	Depositor DCC
$R_{free}$ test set	5195 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16874	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: TPP, MG, EDO, CL, GOL

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	0.10	0/4053	0.30	0/5540
1	B	0.09	0/3926	0.29	0/5364
1	C	0.09	0/3893	0.28	0/5319
1	D	0.10	0/4045	0.28	0/5530
All	All	0.10	0/15917	0.29	0/21753

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3942	0	3871	36	0
1	B	3824	0	3761	34	0
1	C	3788	0	3725	41	0
1	D	3938	0	3865	37	0
2	A	11	0	0	0	0
2	B	10	0	0	0	0
2	C	8	0	0	0	0
2	D	1	0	0	0	0
3	A	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	24	3	0
3	C	24	0	32	7	0
3	D	6	0	8	0	0
4	A	26	0	16	2	0
4	C	26	0	16	2	0
4	D	26	0	16	2	0
5	A	12	0	18	0	0
5	B	12	0	18	1	0
5	C	4	0	6	1	0
5	D	4	0	6	0	0
6	B	1	0	0	0	0
6	C	1	0	0	1	0
7	A	343	0	0	0	0
7	B	317	0	0	0	0
7	C	267	0	0	0	0
7	D	247	0	0	1	0
All	All	16874	0	15406	135	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 4.

The worst 5 of 135 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:C:405:PHE:HA	3:C:612:GOL:H12	1.56	0.87
1:B:165:LYS:HE2	3:B:612:GOL:H11	1.68	0.75
1:B:132:ALA:HB2	3:B:612:GOL:H12	1.70	0.72
1:A:114:ASP:HB3	1:C:121:PRO:HG3	1.73	0.71
1:D:353:LEU:HD13	1:D:503:LEU:HD12	1.74	0.70

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	525/530 (99%)	518 (99%)	7 (1%)	0	100	100
1	B	507/530 (96%)	501 (99%)	6 (1%)	0	100	100
1	C	503/530 (95%)	496 (99%)	7 (1%)	0	100	100
1	D	524/530 (99%)	518 (99%)	6 (1%)	0	100	100
All	All	2059/2120 (97%)	2033 (99%)	26 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/416 (99%)	413 (100%)	0	100	100
1	B	401/416 (96%)	401 (100%)	0	100	100
1	C	399/416 (96%)	399 (100%)	0	100	100
1	D	412/416 (99%)	412 (100%)	0	100	100
All	All	1625/1664 (98%)	1625 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	68	ASN
1	D	151	GLN
1	D	281	HIS
1	B	445	ASN
1	C	178	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 54 ligands modelled in this entry, 32 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	A	614	-	5,5,5	1.03	0	5,5,5	0.81	0
4	TPP	A	615	2	25,27,27	1.78	6 (24%)	37,40,40	1.56	10 (27%)
5	EDO	B	616	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	B	617	-	3,3,3	0.46	0	2,2,2	0.30	0
3	GOL	C	611	-	5,5,5	0.87	0	5,5,5	1.00	0
5	EDO	D	604	-	3,3,3	0.45	0	2,2,2	0.35	0
3	GOL	A	612	-	5,5,5	0.93	0	5,5,5	0.99	0
5	EDO	B	615	-	3,3,3	0.45	0	2,2,2	0.30	0
3	GOL	D	602	-	5,5,5	0.92	0	5,5,5	0.95	0
5	EDO	A	616	2	3,3,3	0.43	0	2,2,2	0.29	0
3	GOL	B	612	-	5,5,5	0.95	0	5,5,5	0.98	0
5	EDO	C	615	-	3,3,3	0.44	0	2,2,2	0.35	0
5	EDO	A	618	-	3,3,3	0.45	0	2,2,2	0.33	0
3	GOL	C	612	-	5,5,5	0.98	0	5,5,5	0.97	0
4	TPP	D	603	2	25,27,27	1.79	8 (32%)	37,40,40	1.63	9 (24%)
3	GOL	B	614	-	5,5,5	0.91	0	5,5,5	1.00	0
3	GOL	B	613	-	5,5,5	0.90	0	5,5,5	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	C	610	-	5,5,5	0.92	0	5,5,5	0.95	0
3	GOL	A	613	-	5,5,5	0.86	0	5,5,5	1.01	0
3	GOL	C	613	-	5,5,5	0.87	0	5,5,5	1.06	0
5	EDO	A	617	-	3,3,3	0.46	0	2,2,2	0.30	0
4	TPP	C	614	2	25,27,27	1.79	7 (28%)	37,40,40	1.59	11 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	614	-	-	2/4/4/4	-
4	TPP	A	615	2	-	5/17/17/17	0/2/2/2
5	EDO	B	616	-	-	0/1/1/1	-
5	EDO	B	617	-	-	0/1/1/1	-
3	GOL	C	611	-	-	1/4/4/4	-
5	EDO	D	604	-	-	0/1/1/1	-
3	GOL	A	612	-	-	2/4/4/4	-
5	EDO	B	615	-	-	0/1/1/1	-
3	GOL	D	602	-	-	3/4/4/4	-
5	EDO	A	616	2	-	1/1/1/1	-
3	GOL	B	612	-	-	4/4/4/4	-
5	EDO	C	615	-	-	1/1/1/1	-
5	EDO	A	618	-	-	0/1/1/1	-
3	GOL	C	612	-	-	4/4/4/4	-
4	TPP	D	603	2	-	5/17/17/17	0/2/2/2
3	GOL	B	614	-	-	4/4/4/4	-
3	GOL	B	613	-	-	4/4/4/4	-
3	GOL	C	610	-	-	2/4/4/4	-
3	GOL	A	613	-	-	4/4/4/4	-
3	GOL	C	613	-	-	3/4/4/4	-
5	EDO	A	617	-	-	0/1/1/1	-
4	TPP	C	614	2	-	2/17/17/17	0/2/2/2

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	615	TPP	C5-S1	-5.04	1.59	1.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	614	TPP	C5-S1	-5.04	1.59	1.72
4	D	603	TPP	C5-S1	-4.99	1.59	1.72
4	A	615	TPP	C2-S1	-2.82	1.60	1.69
4	C	614	TPP	C2-S1	-2.79	1.60	1.69

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	603	TPP	N1'-C2'-N3'	-3.45	119.60	125.54
4	A	615	TPP	N1'-C2'-N3'	-3.16	120.09	125.54
4	C	614	TPP	N1'-C2'-N3'	-3.10	120.20	125.54
4	D	603	TPP	C6-C5-S1	-3.01	113.66	120.89
4	C	614	TPP	C6'-C5'-C4'	2.98	119.77	115.72

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	612	GOL	C1-C2-C3-O3
3	A	613	GOL	O1-C1-C2-O2
3	A	613	GOL	O1-C1-C2-C3
3	A	613	GOL	C1-C2-C3-O3
3	B	612	GOL	C1-C2-C3-O3

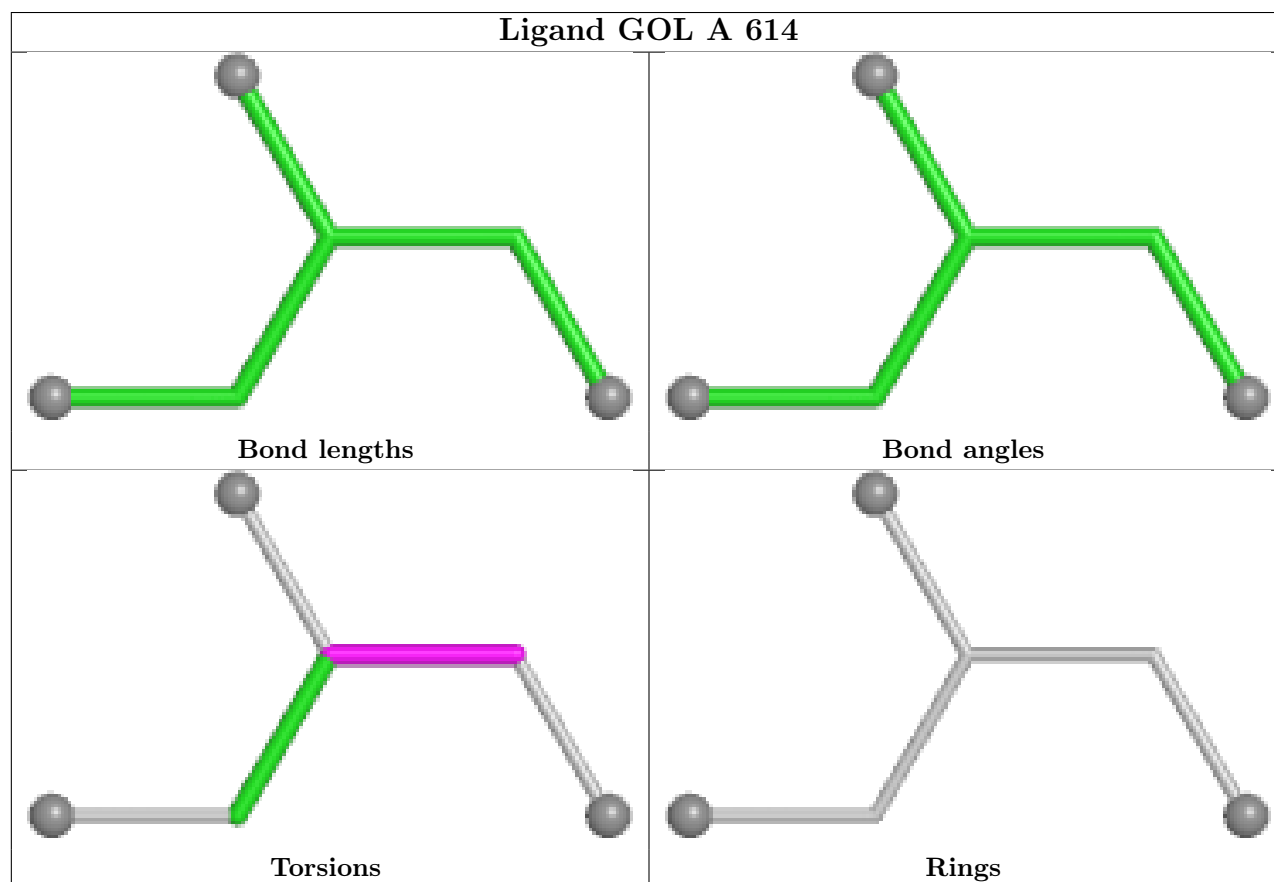
There are no ring outliers.

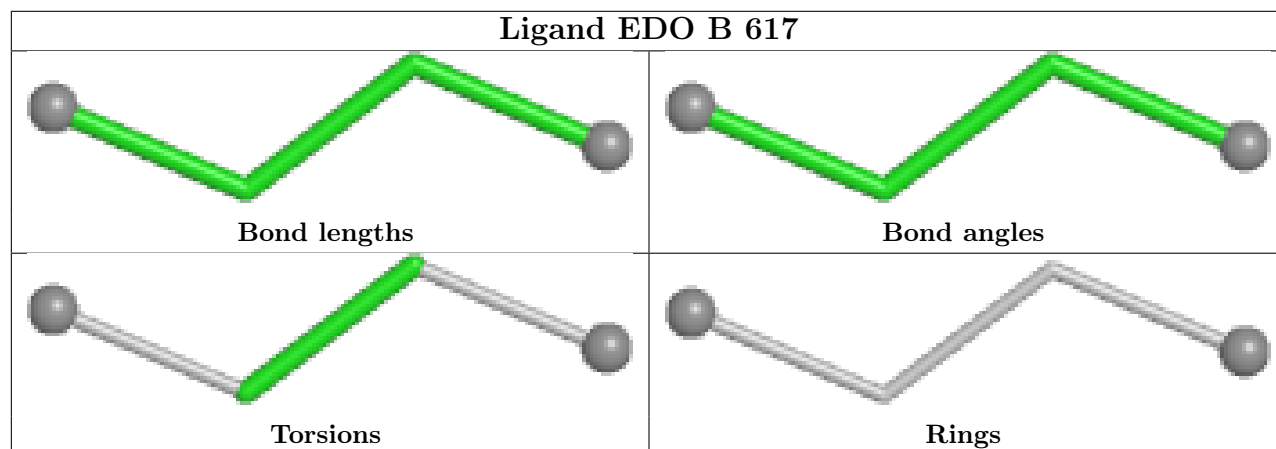
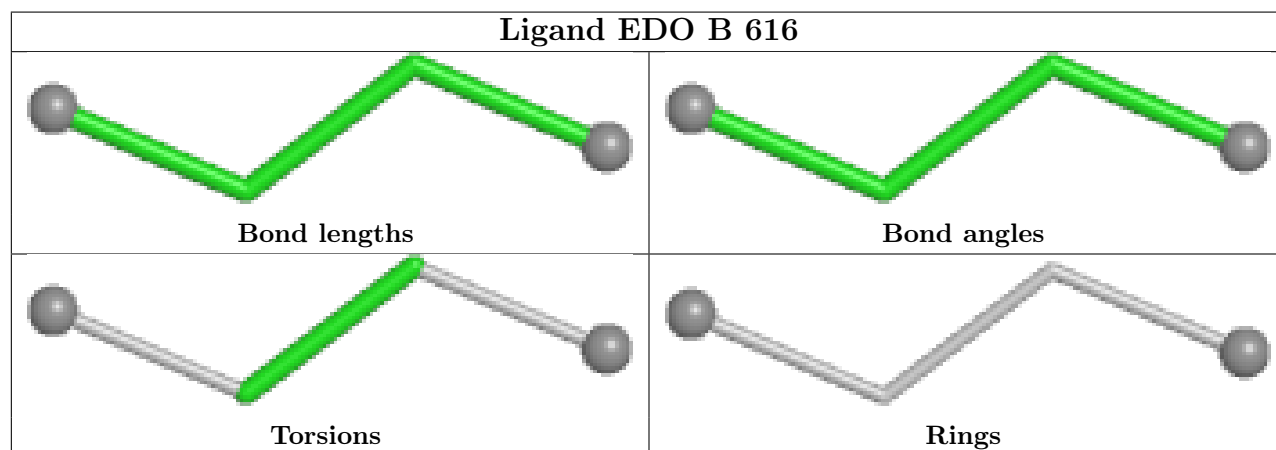
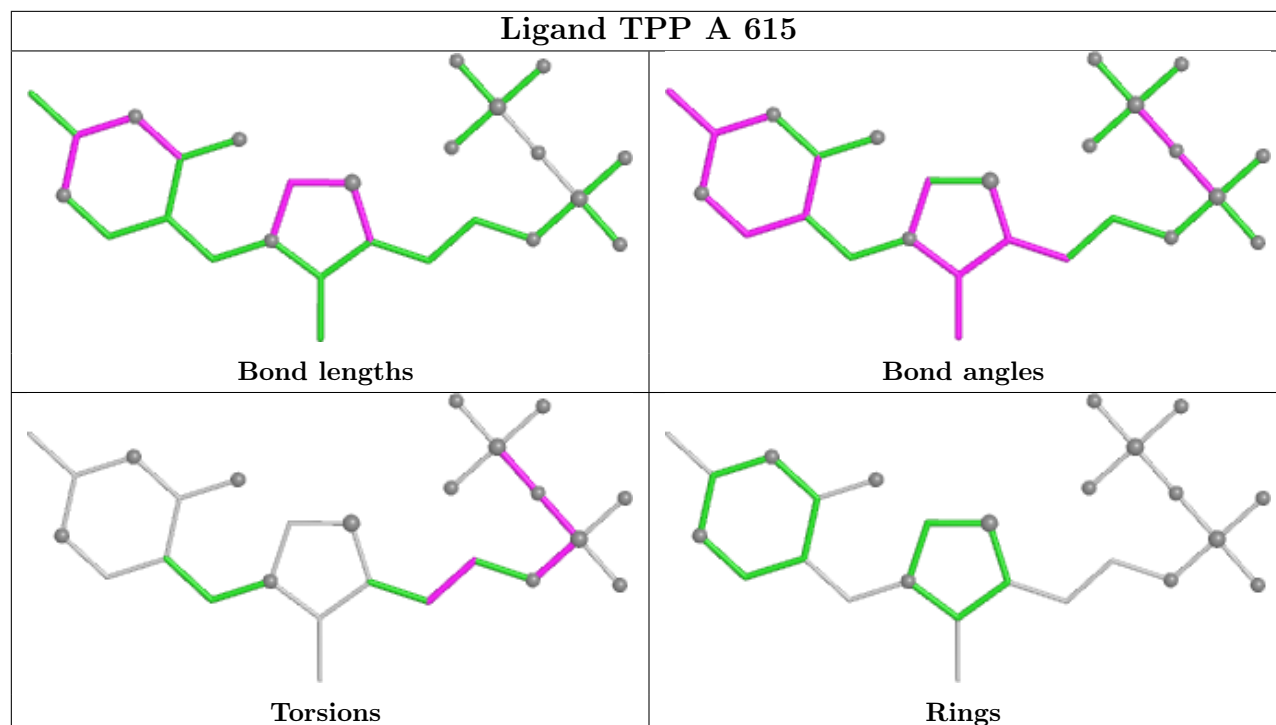
9 monomers are involved in 18 short contacts:

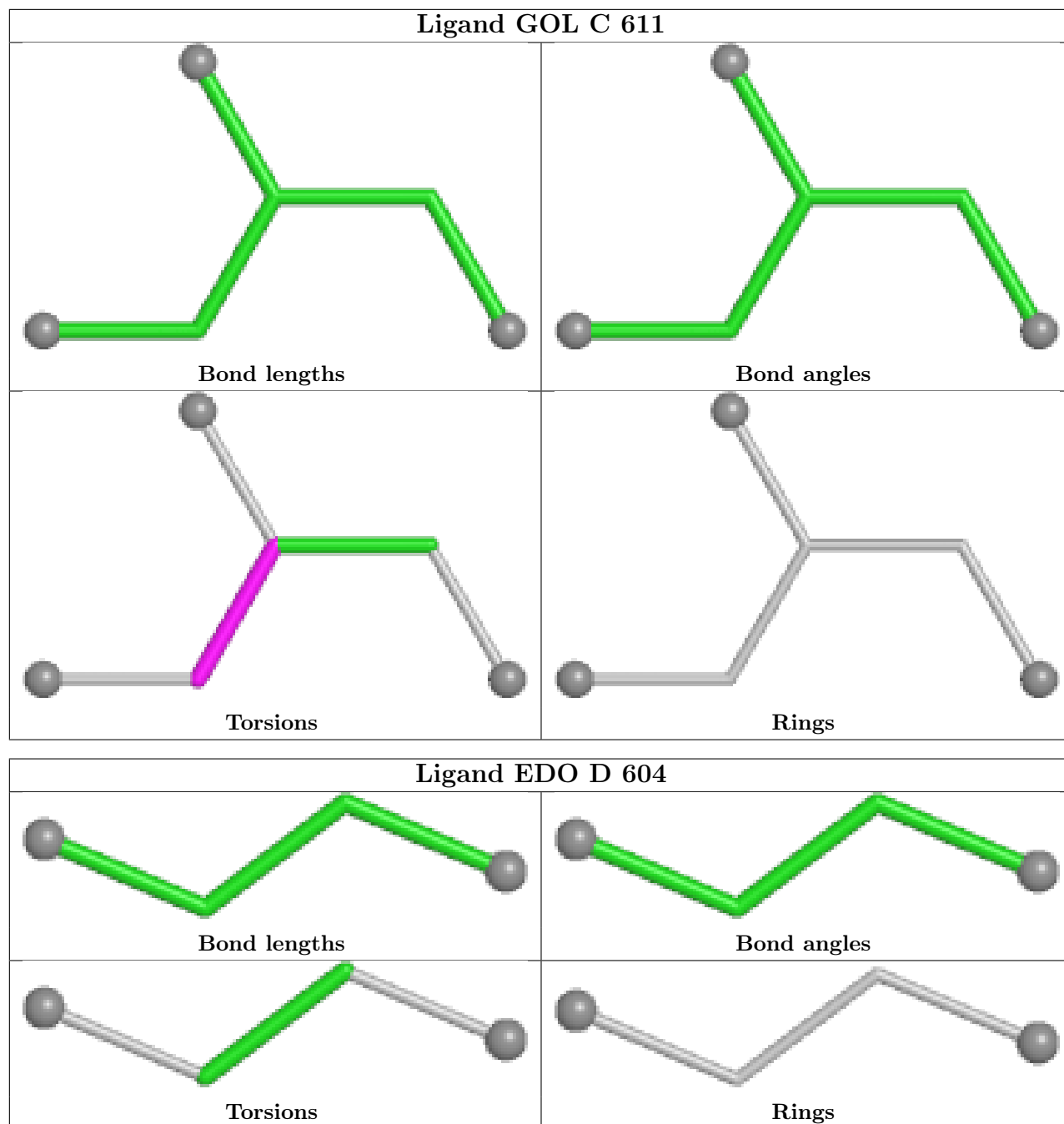
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	615	TPP	2	0
5	B	616	EDO	1	0
3	C	611	GOL	1	0
3	B	612	GOL	3	0
5	C	615	EDO	1	0
3	C	612	GOL	5	0
4	D	603	TPP	2	0
3	C	610	GOL	1	0
4	C	614	TPP	2	0

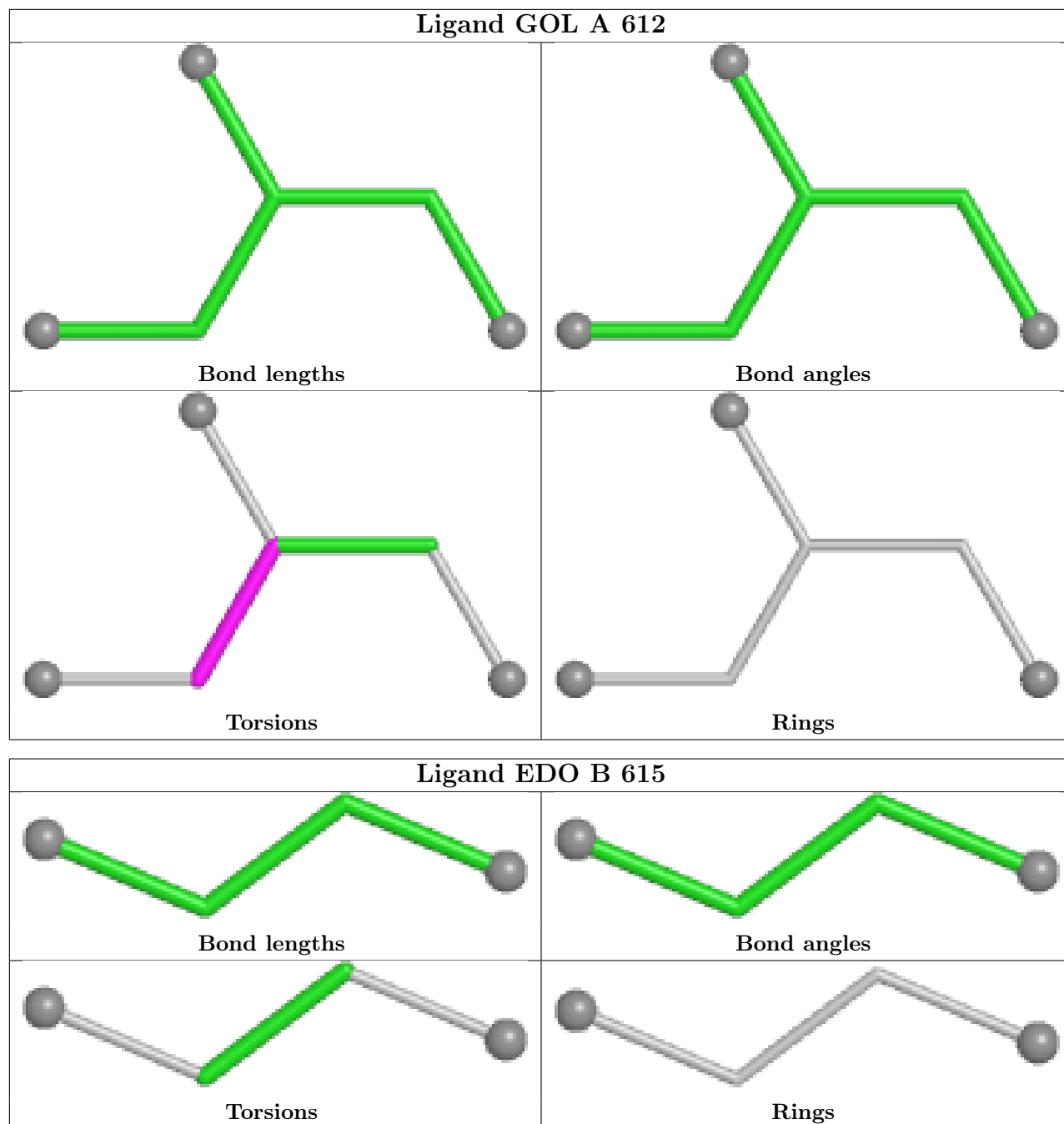
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

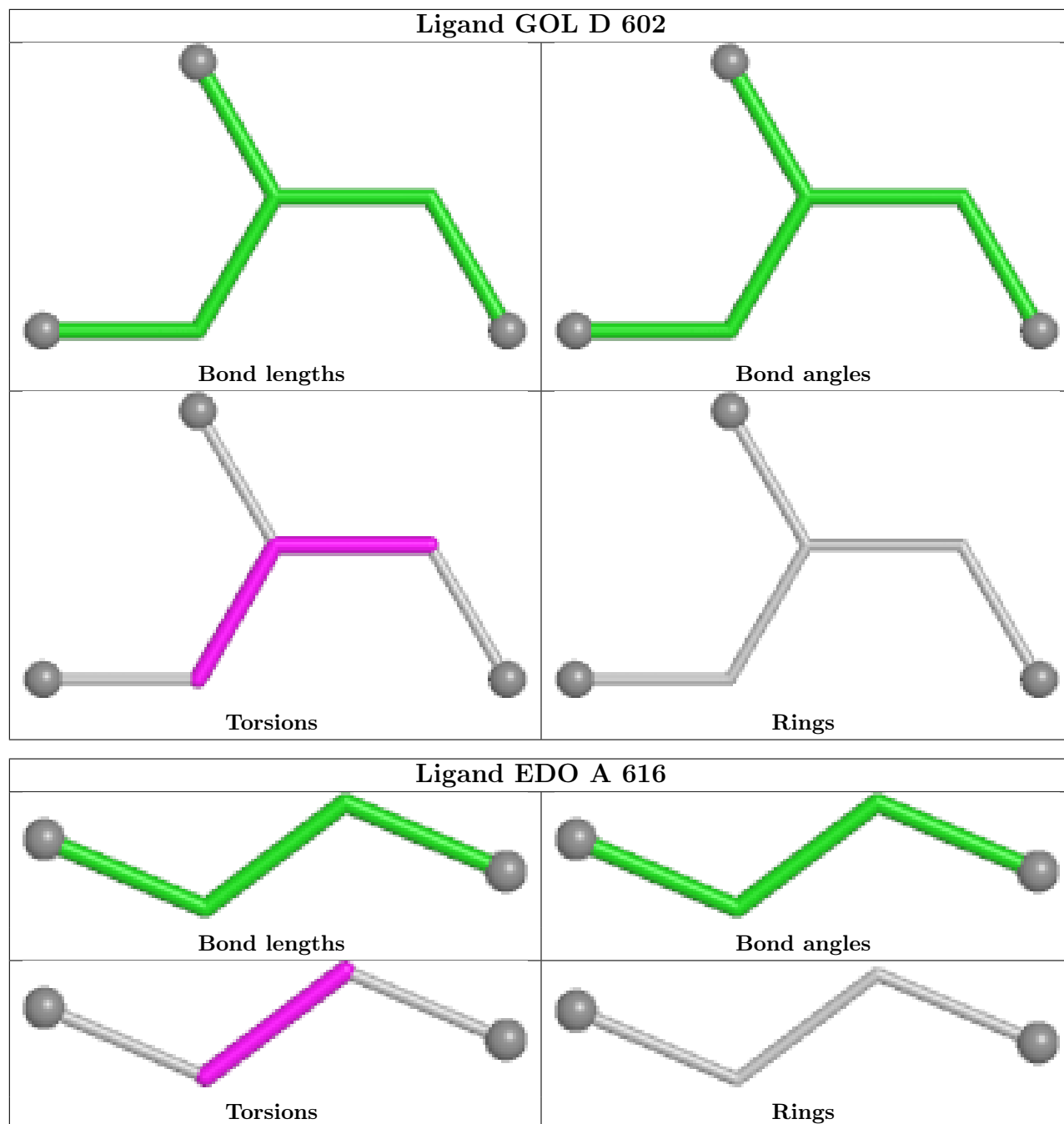


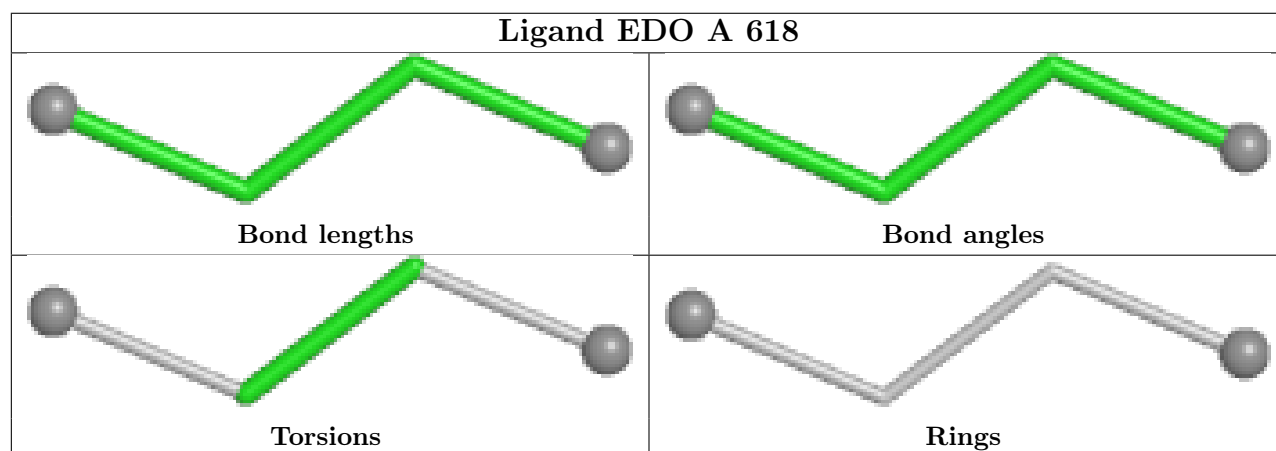
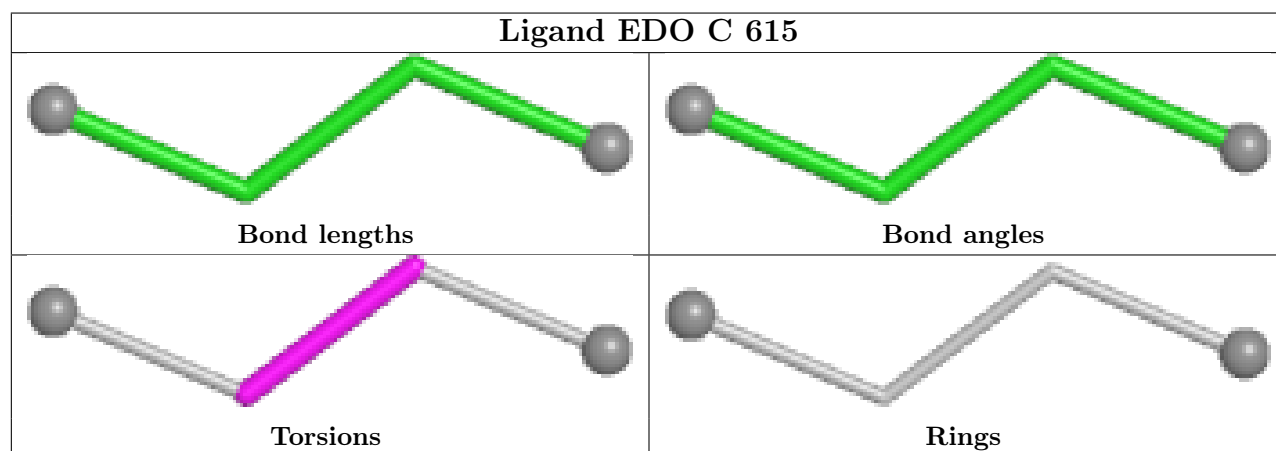
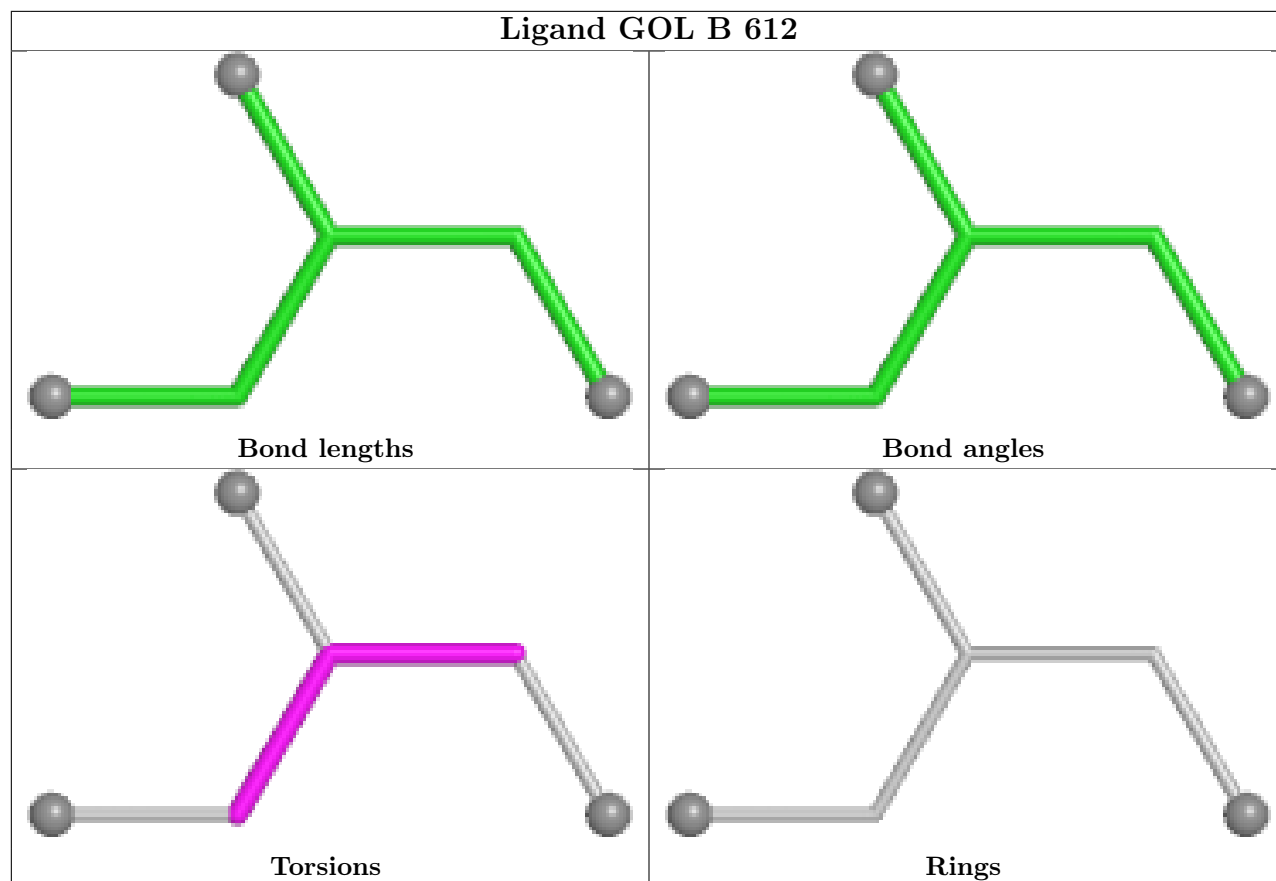


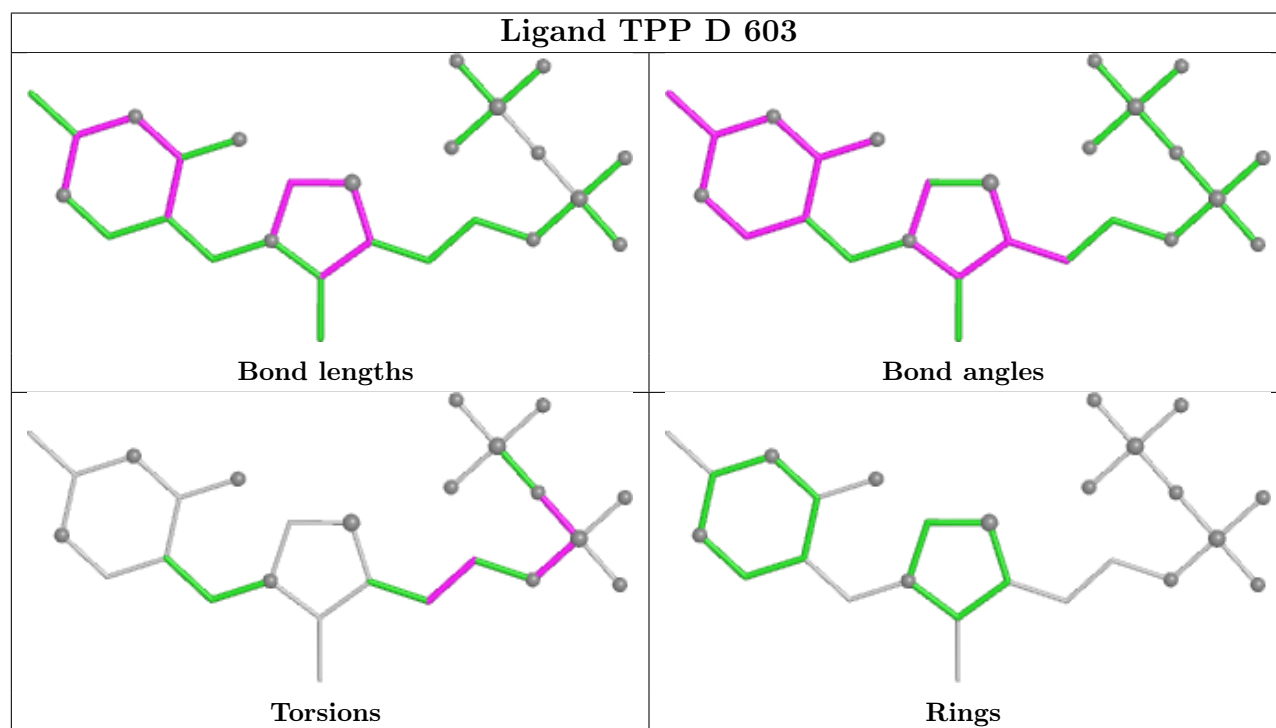
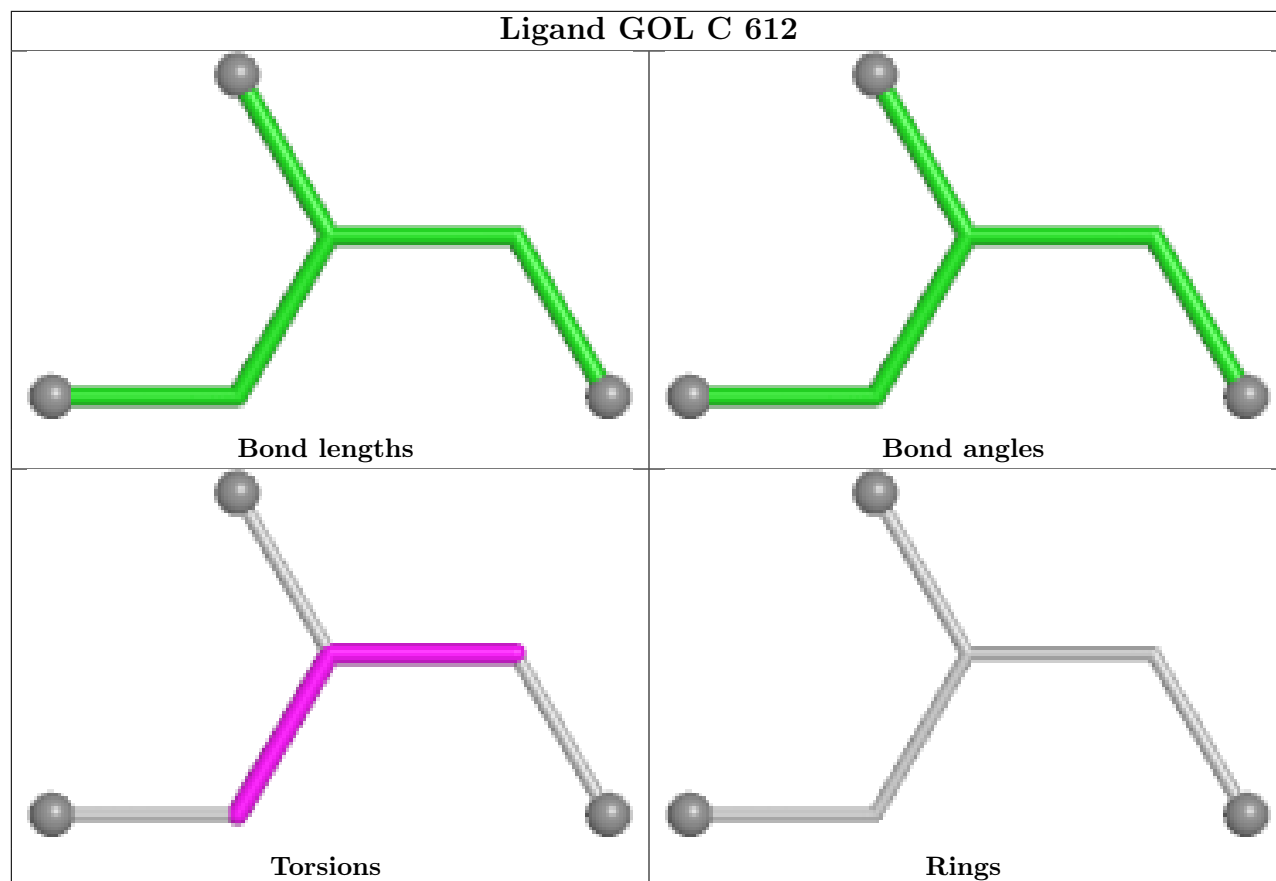


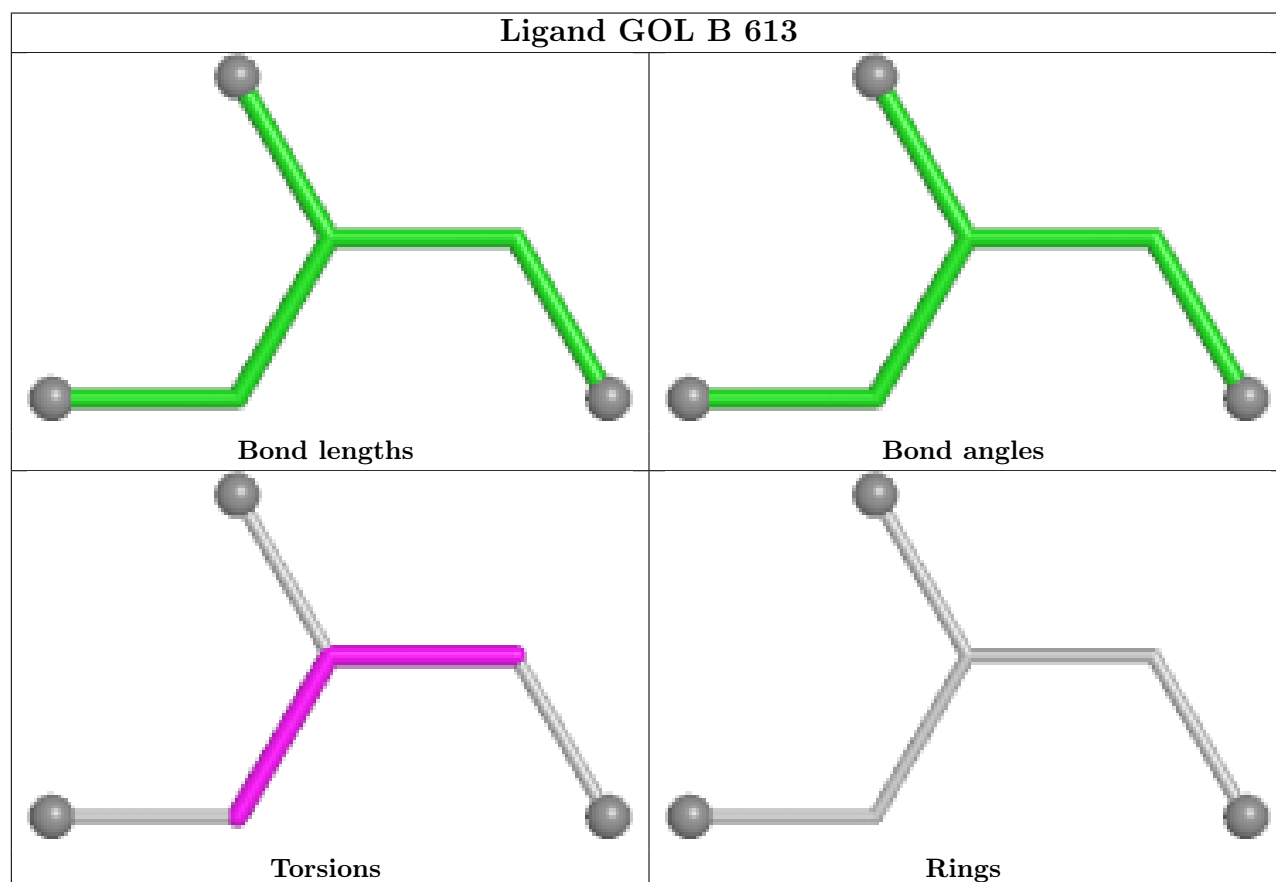
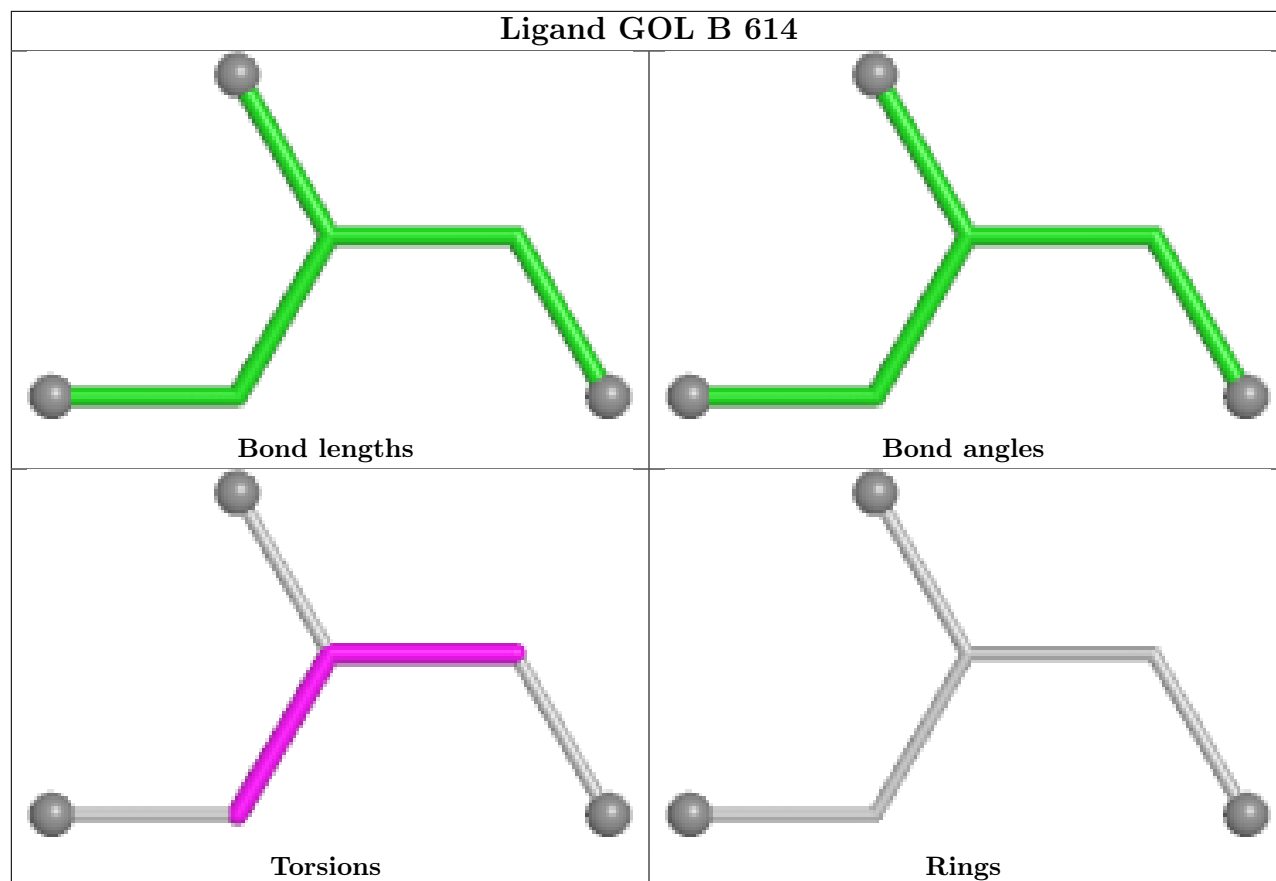


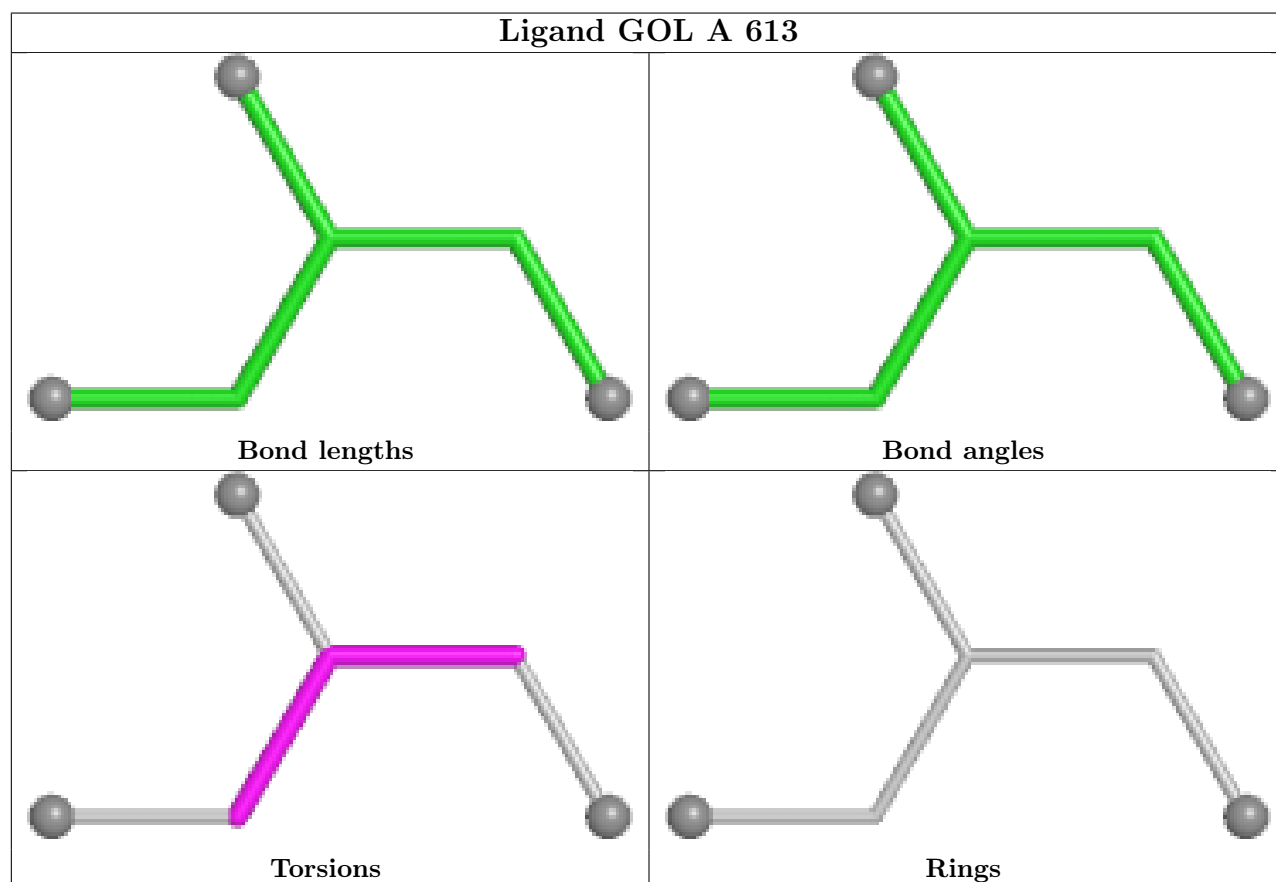
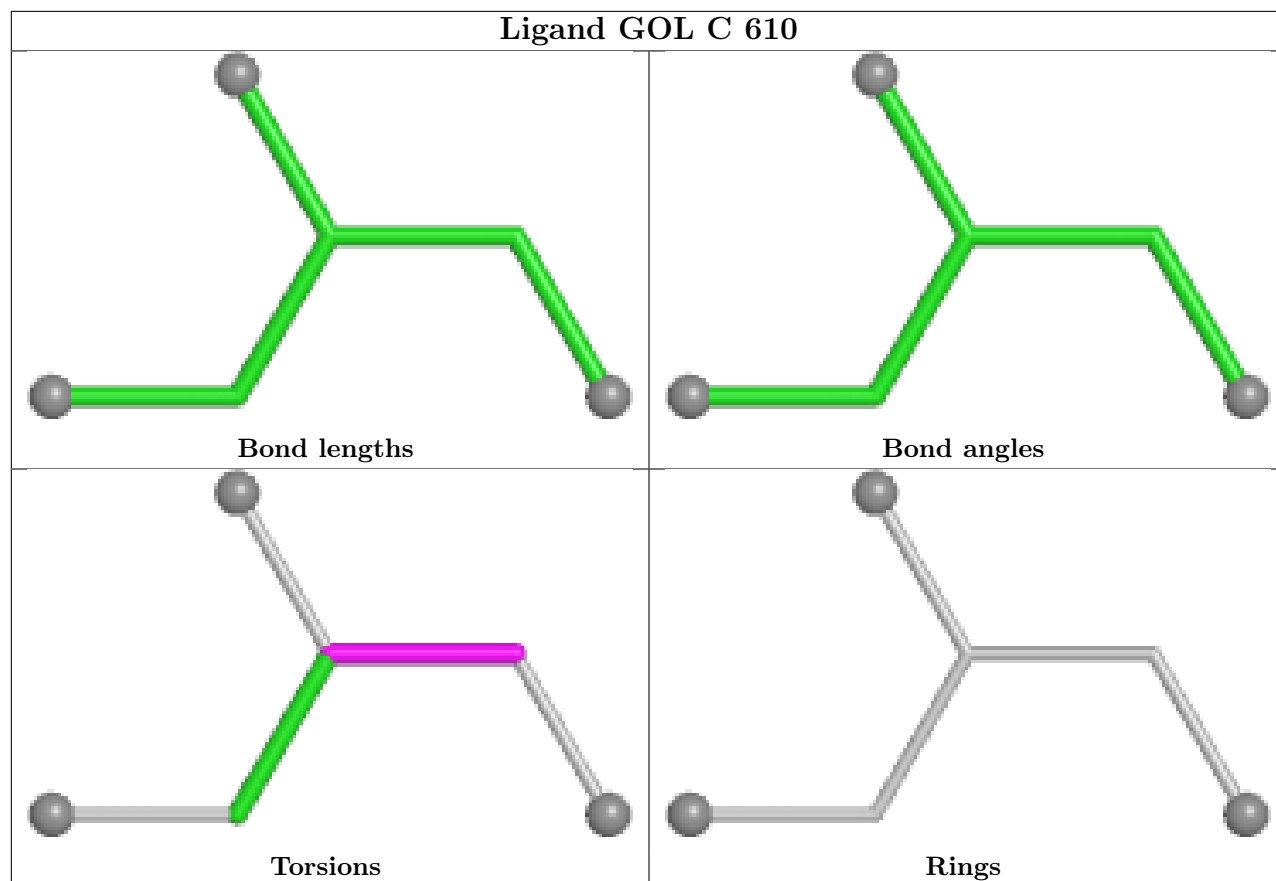


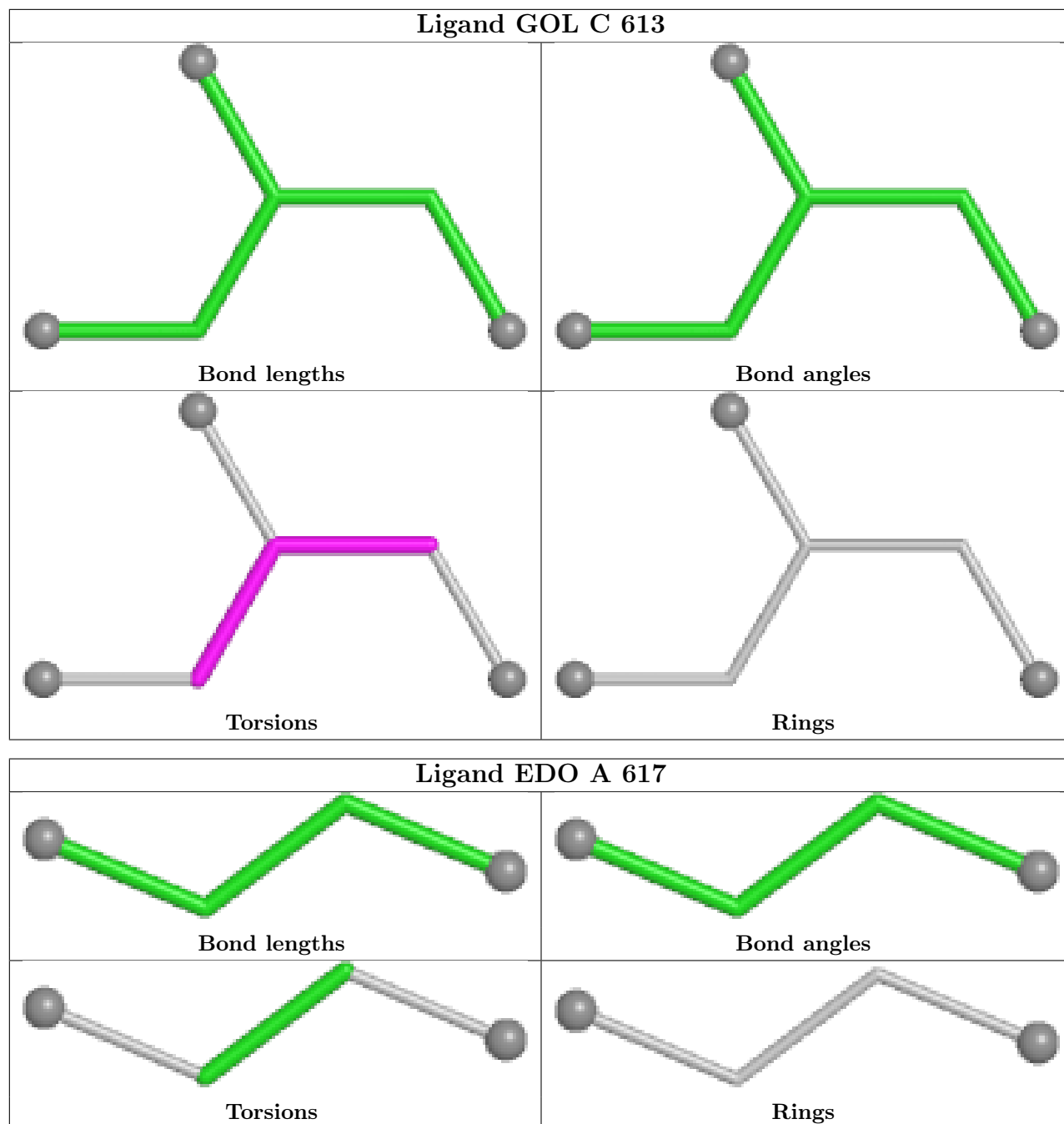


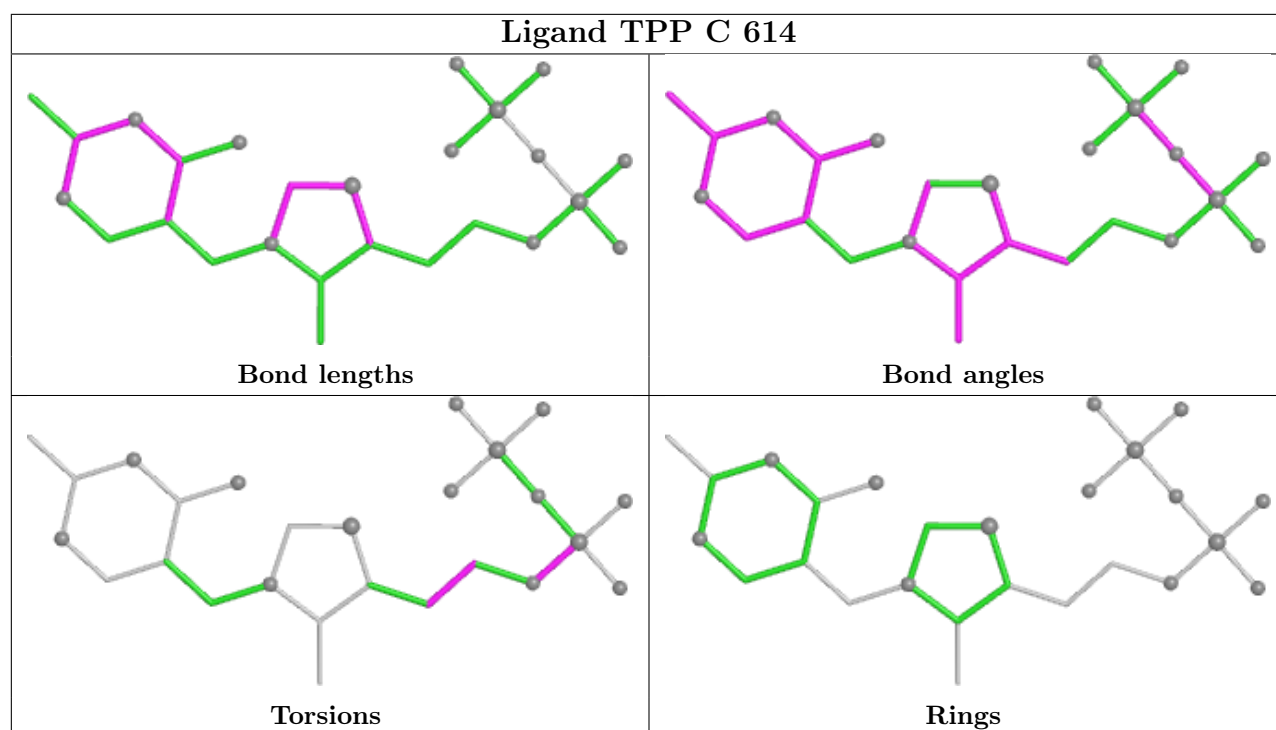












## 5.7 Other polymers [i](#)

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	523/530 (98%)	-0.16	15 (2%) 53 54	9, 21, 51, 86	4 (0%)
1	B	508/530 (95%)	-0.11	13 (2%) 57 58	12, 22, 45, 69	3 (0%)
1	C	503/530 (94%)	-0.02	8 (1%) 70 71	10, 27, 47, 60	4 (0%)
1	D	523/530 (98%)	0.38	19 (3%) 46 46	17, 35, 60, 86	4 (0%)
All	All	2057/2120 (97%)	0.02	55 (2%) 56 57	9, 26, 52, 86	15 (0%)

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	458	TYR	6.8
1	A	464	PHE	5.8
1	B	461	LEU	5.2
1	C	479	PRO	5.0
1	A	463	TRP	4.7

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.



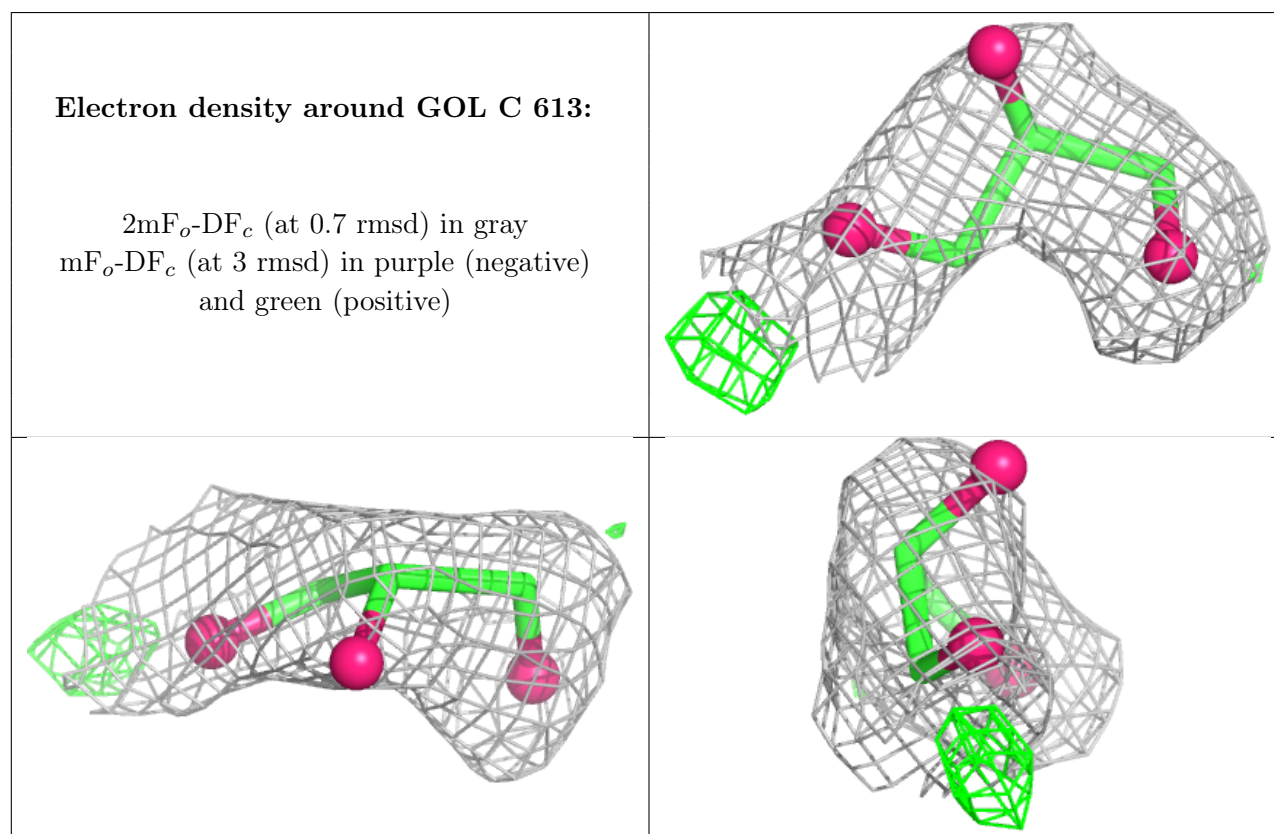
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	C	613	6/6	0.69	0.18	42,50,60,62	0
4	TPP	C	614	26/26	0.75	0.19	23,41,51,57	26
3	GOL	A	614	6/6	0.77	0.25	12,19,22,32	6
3	GOL	C	611	6/6	0.80	0.18	21,23,26,29	6
4	TPP	D	603	26/26	0.80	0.17	23,44,56,59	26
3	GOL	B	614	6/6	0.81	0.15	38,39,42,53	0
3	GOL	C	610	6/6	0.81	0.18	15,20,28,33	6
3	GOL	B	612	6/6	0.81	0.16	17,20,21,26	6
5	EDO	C	615	4/4	0.81	0.16	18,20,24,29	4
3	GOL	D	602	6/6	0.82	0.18	24,27,33,46	0
3	GOL	A	612	6/6	0.82	0.18	31,38,42,48	0
2	MG	D	601	1/1	0.83	0.11	56,56,56,56	0
3	GOL	A	613	6/6	0.84	0.20	20,30,36,38	0
3	GOL	B	613	6/6	0.84	0.18	16,27,32,34	0
5	EDO	B	616	4/4	0.85	0.16	21,25,26,27	4
5	EDO	B	617	4/4	0.86	0.13	28,31,32,34	0
4	TPP	A	615	26/26	0.87	0.14	20,34,40,49	26
2	MG	A	601	1/1	0.87	0.09	42,42,42,42	0
2	MG	C	606	1/1	0.89	0.21	47,47,47,47	0
3	GOL	C	612	6/6	0.90	0.17	11,15,17,21	6
5	EDO	A	616	4/4	0.91	0.20	19,25,26,30	0
5	EDO	B	615	4/4	0.92	0.09	19,20,26,27	0
5	EDO	A	617	4/4	0.92	0.14	23,26,28,43	0
2	MG	B	608	1/1	0.93	0.20	37,37,37,37	0
2	MG	C	601	1/1	0.94	0.07	49,49,49,49	0
2	MG	C	605	1/1	0.94	0.09	30,30,30,30	0
2	MG	B	610	1/1	0.94	0.07	38,38,38,38	0
2	MG	C	608	1/1	0.95	0.17	37,37,37,37	0
5	EDO	A	618	4/4	0.95	0.10	15,20,21,22	0
5	EDO	D	604	4/4	0.95	0.07	25,26,26,28	0
6	CL	C	609	1/1	0.95	0.23	38,38,38,38	0
2	MG	A	611	1/1	0.96	0.06	31,31,31,31	0
2	MG	C	602	1/1	0.96	0.08	26,26,26,26	0
2	MG	C	603	1/1	0.96	0.07	29,29,29,29	0
2	MG	A	606	1/1	0.96	0.12	29,29,29,29	0
2	MG	B	609	1/1	0.96	0.07	19,19,19,19	0
2	MG	A	609	1/1	0.96	0.13	24,24,24,24	0
2	MG	A	603	1/1	0.97	0.07	21,21,21,21	0
2	MG	C	607	1/1	0.97	0.19	27,27,27,27	0
6	CL	B	611	1/1	0.97	0.11	35,35,35,35	0
2	MG	A	604	1/1	0.97	0.10	22,22,22,22	0
2	MG	A	607	1/1	0.98	0.13	21,21,21,21	0
2	MG	A	605	1/1	0.98	0.13	19,19,19,19	0

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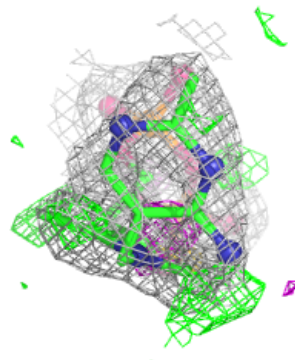
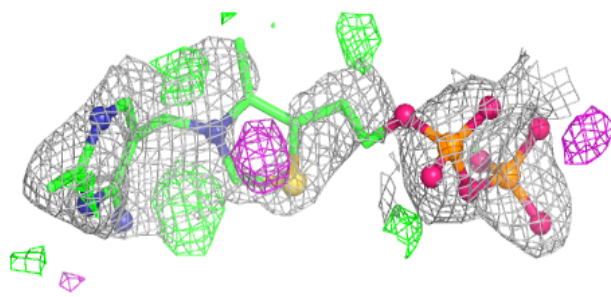
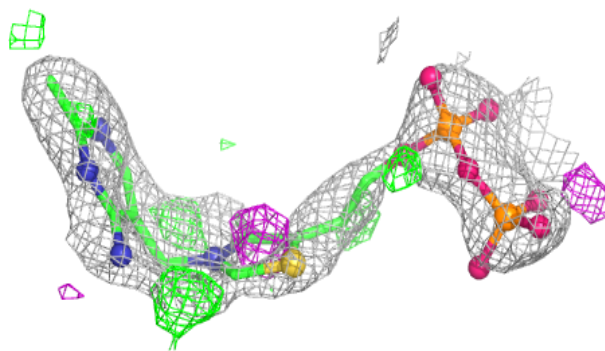
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	610	1/1	0.98	0.06	18,18,18,18	0
2	MG	A	602	1/1	0.98	0.05	18,18,18,18	0
2	MG	B	601	1/1	0.98	0.11	24,24,24,24	0
2	MG	B	604	1/1	0.98	0.09	19,19,19,19	0
2	MG	C	604	1/1	0.98	0.10	24,24,24,24	0
2	MG	B	606	1/1	0.98	0.04	25,25,25,25	0
2	MG	B	607	1/1	0.98	0.12	28,28,28,28	0
2	MG	A	608	1/1	0.99	0.08	19,19,19,19	0
2	MG	B	605	1/1	0.99	0.08	21,21,21,21	0
2	MG	B	602	1/1	0.99	0.05	25,25,25,25	0
2	MG	B	603	1/1	0.99	0.05	19,19,19,19	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.

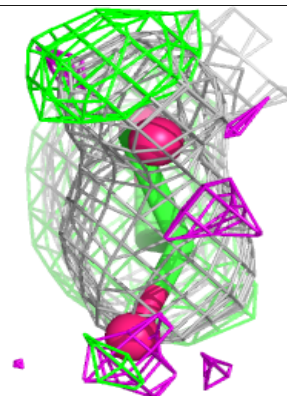
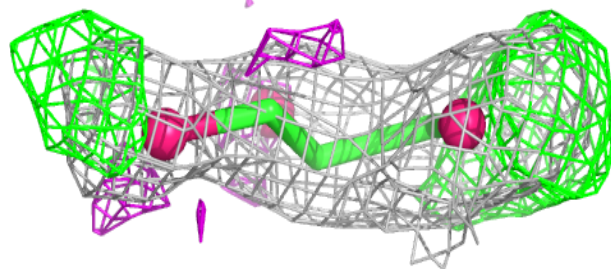
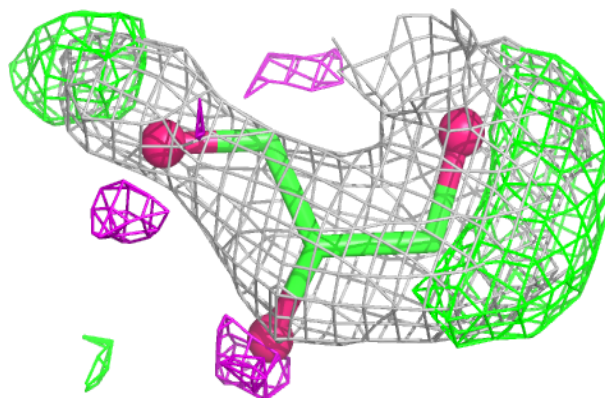


**Electron density around TPP C 614:**

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

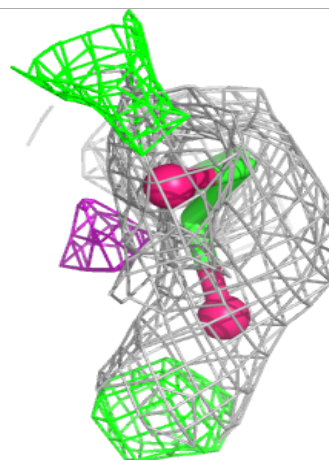
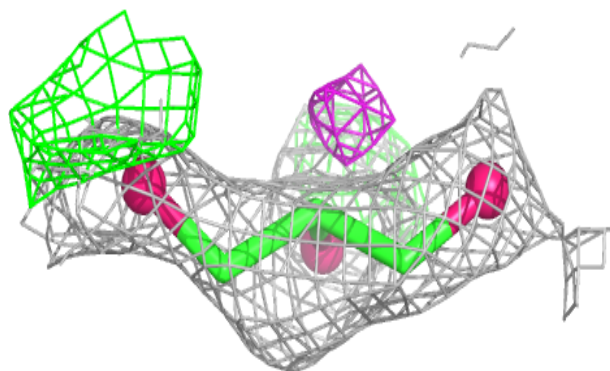
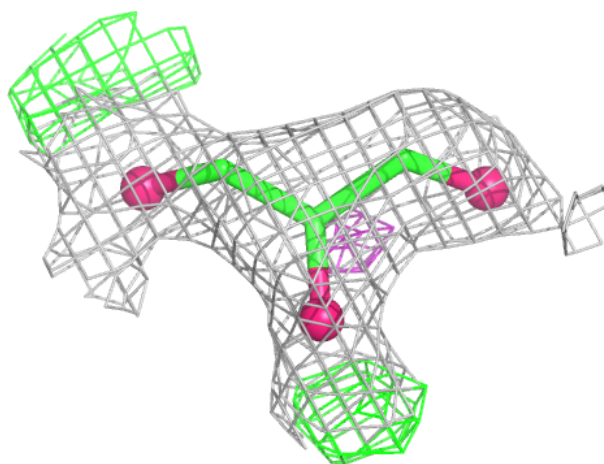
**Electron density around GOL A 614:**

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



**Electron density around GOL C 611:**

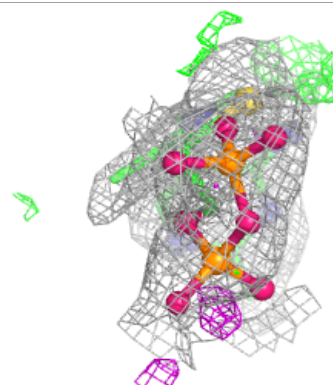
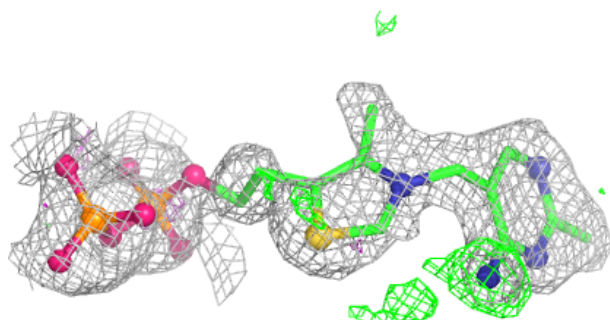
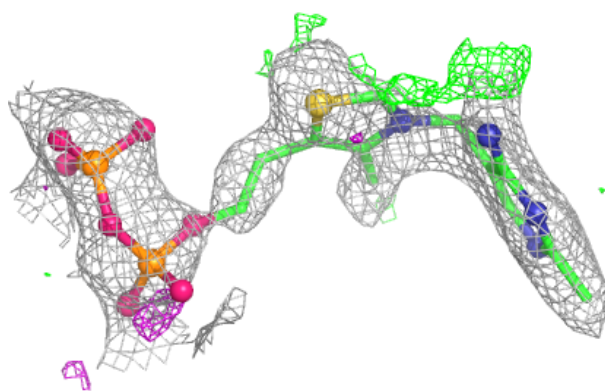
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



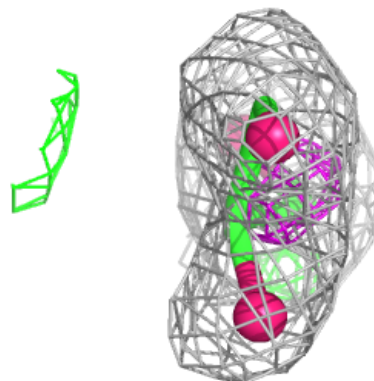
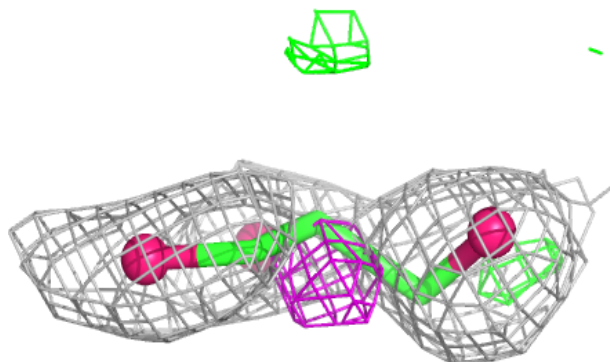
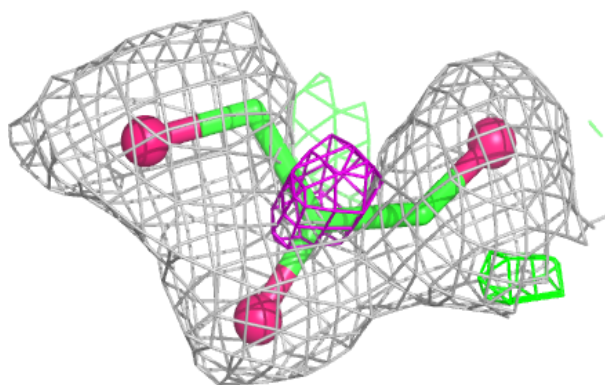


**Electron density around TPP D 603:**

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

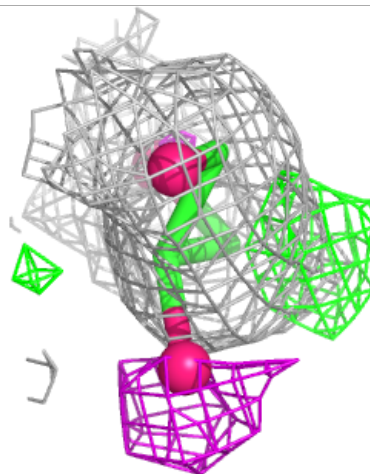
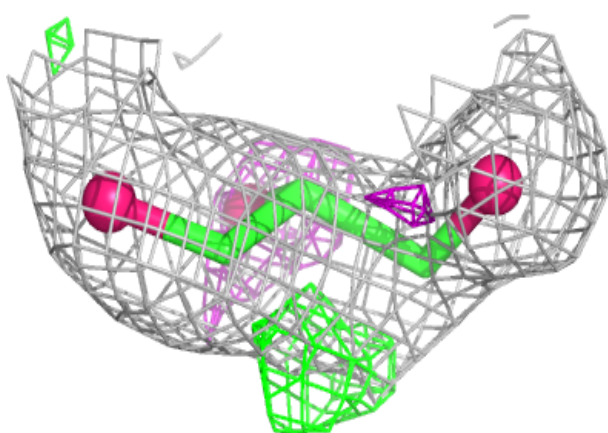
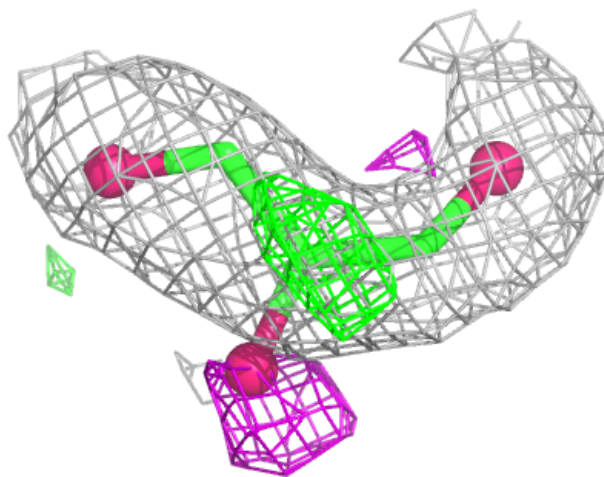
**Electron density around GOL B 614:**

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



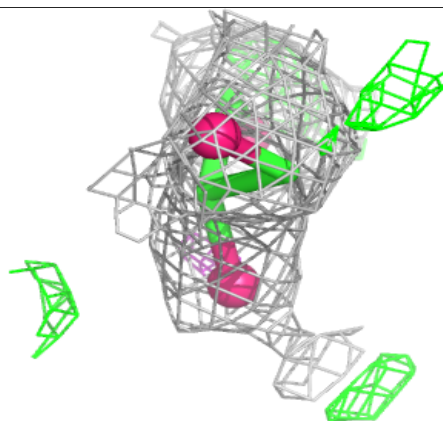
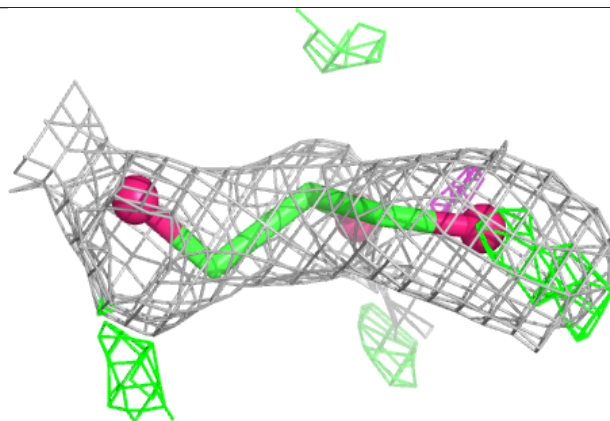
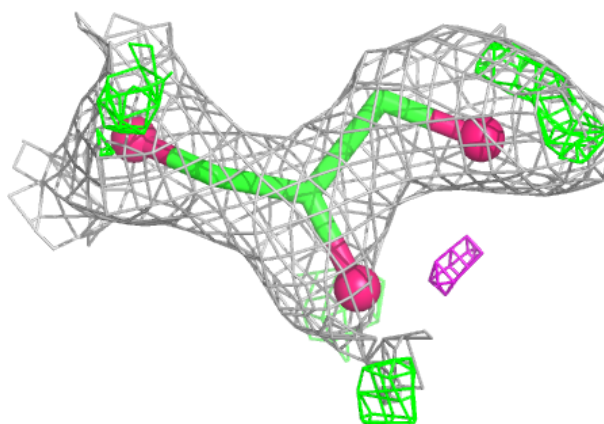
**Electron density around GOL C 610:**

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



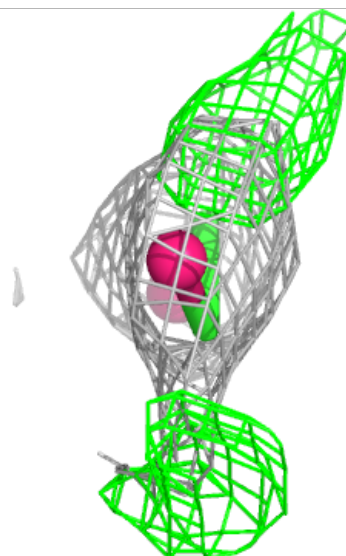
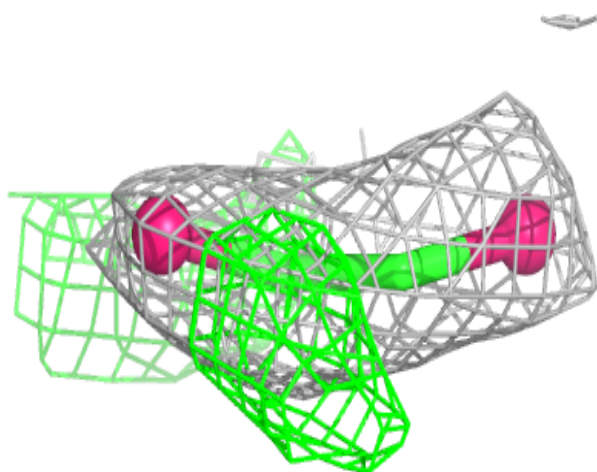
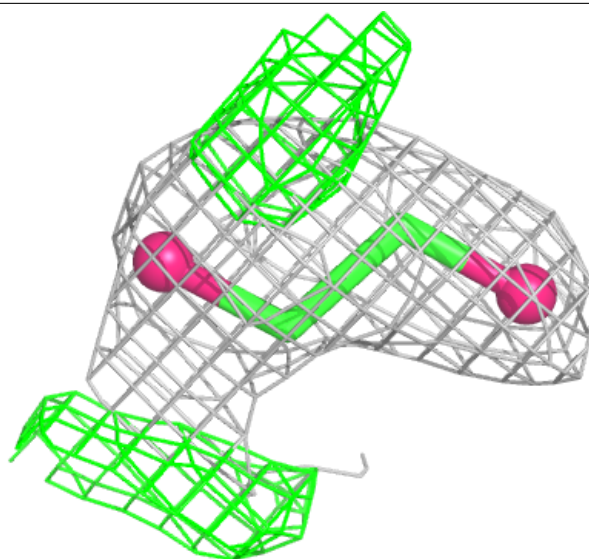
**Electron density around GOL B 612:**

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



**Electron density around EDO C 615:**

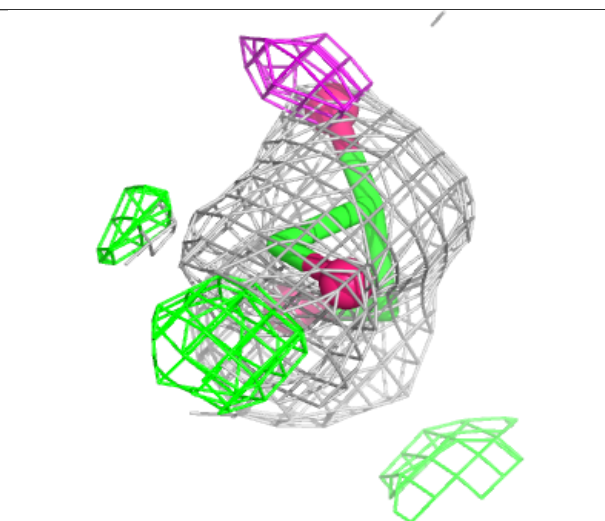
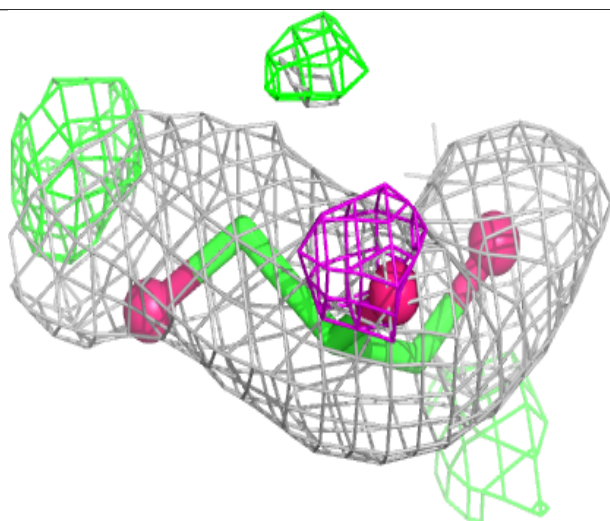
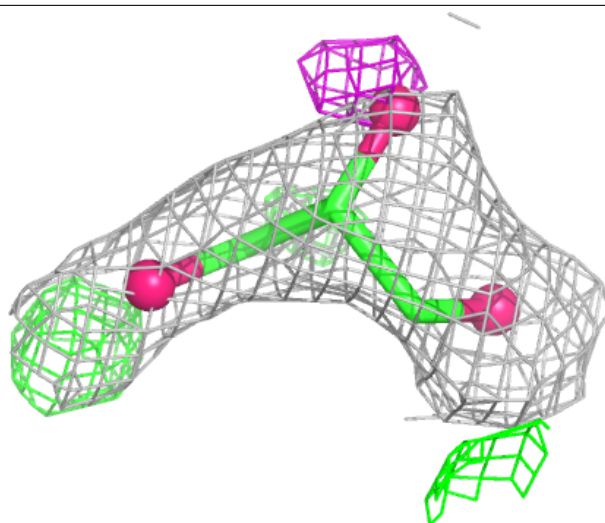
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





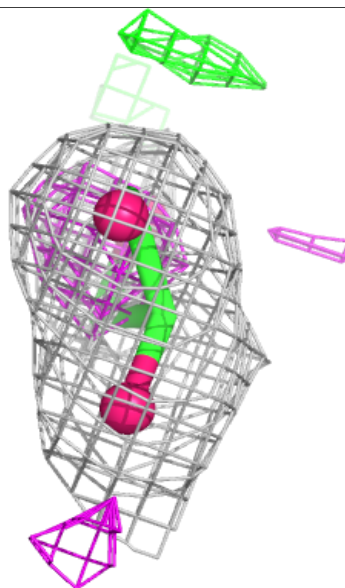
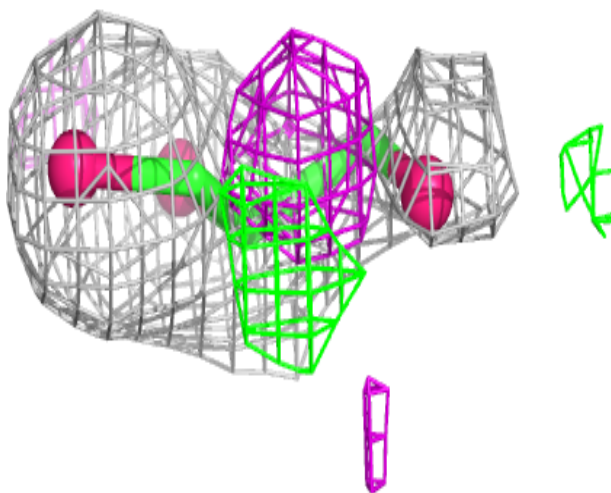
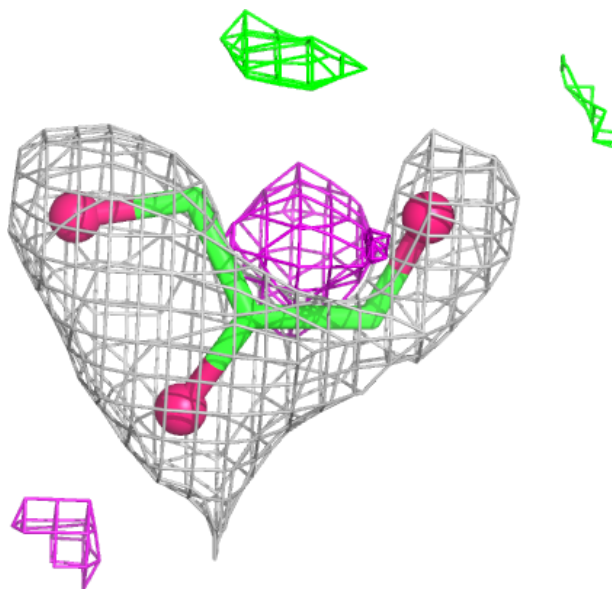
**Electron density around GOL D 602:**

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



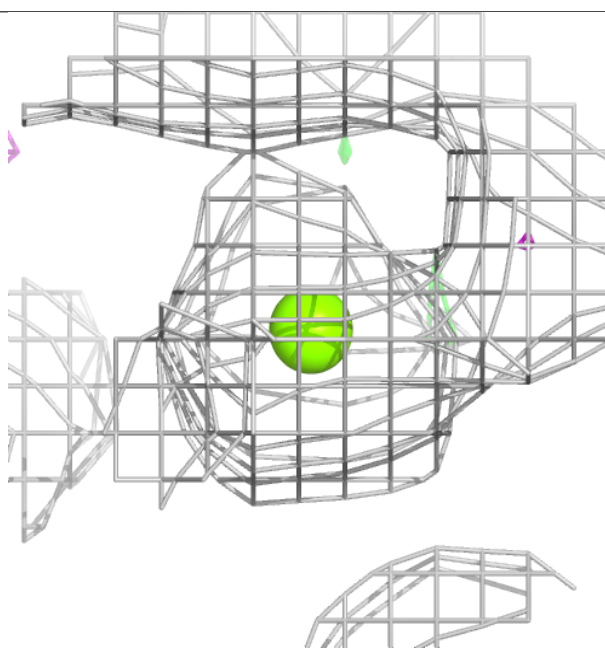
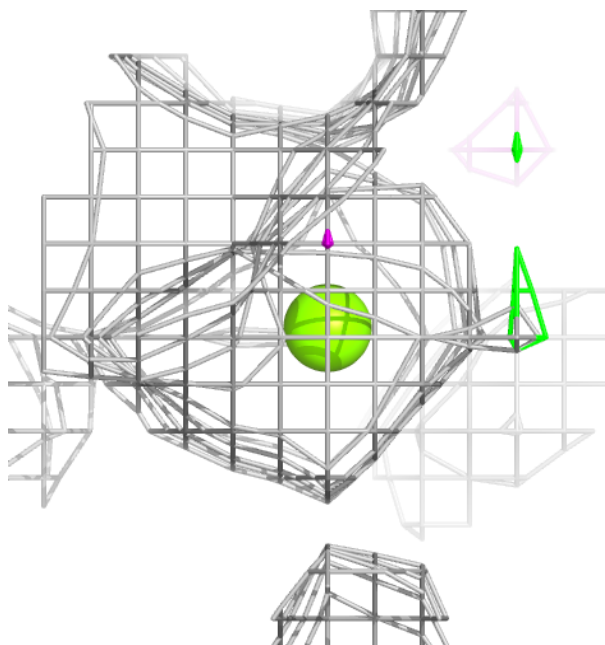
**Electron density around GOL A 612:**

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



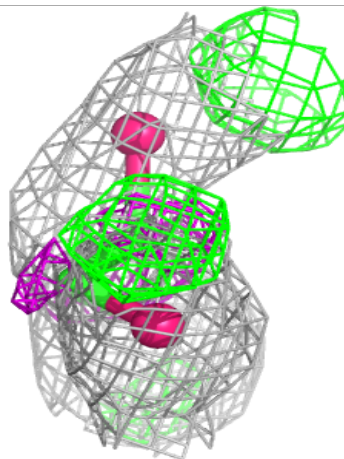
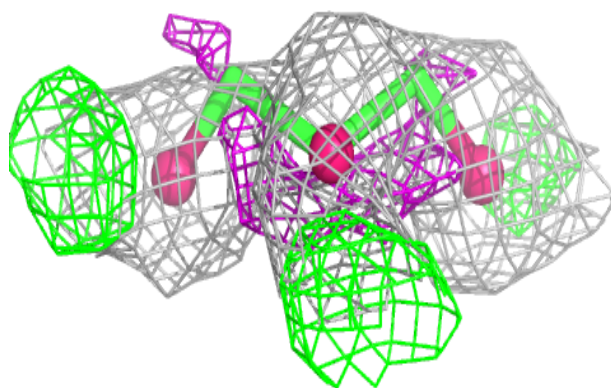
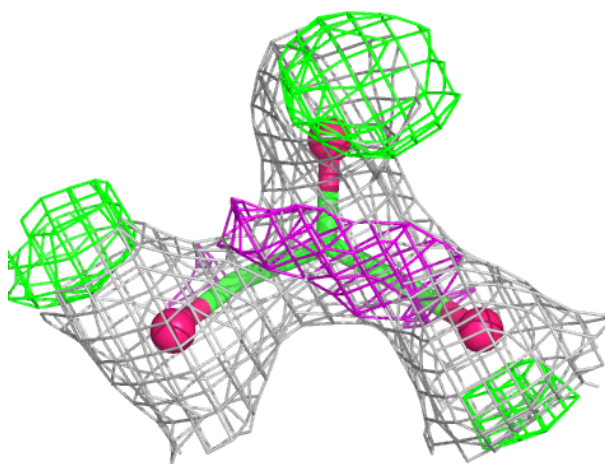
**Electron density around MG D 601:**

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



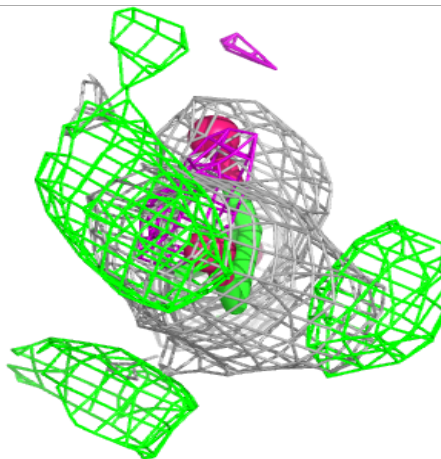
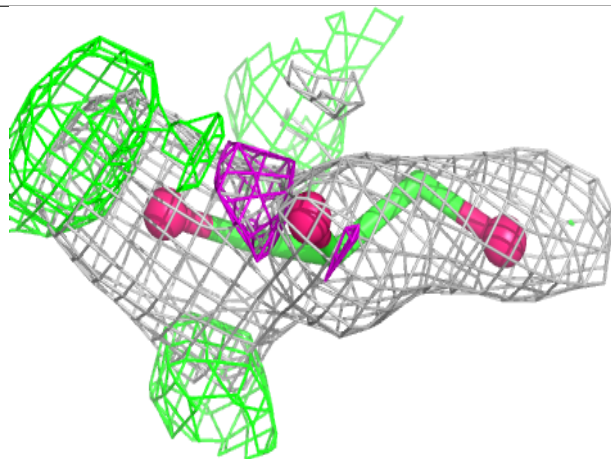
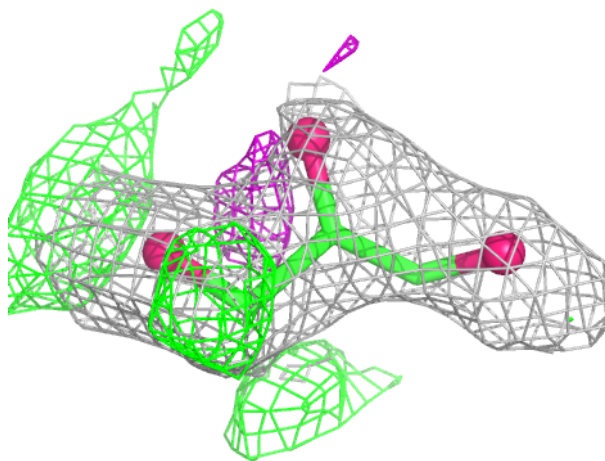
**Electron density around GOL A 613:**

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



**Electron density around GOL B 613:**

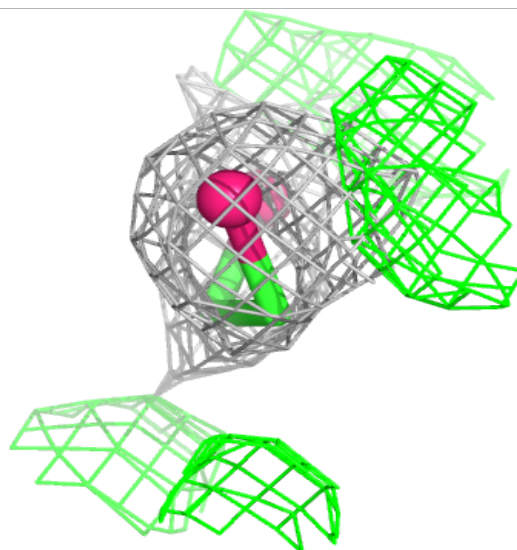
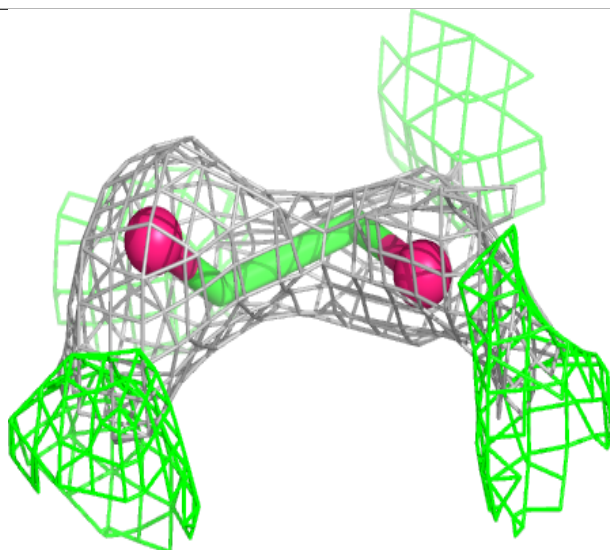
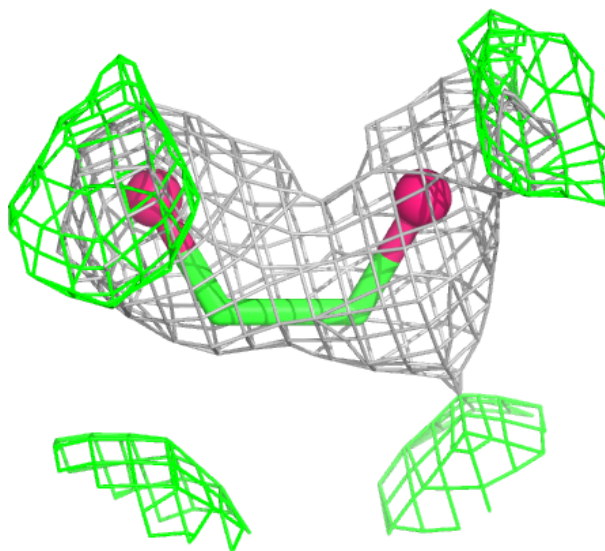
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





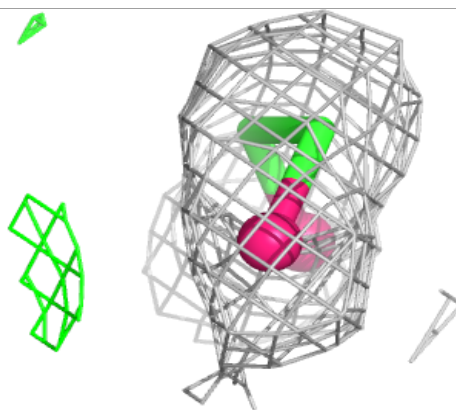
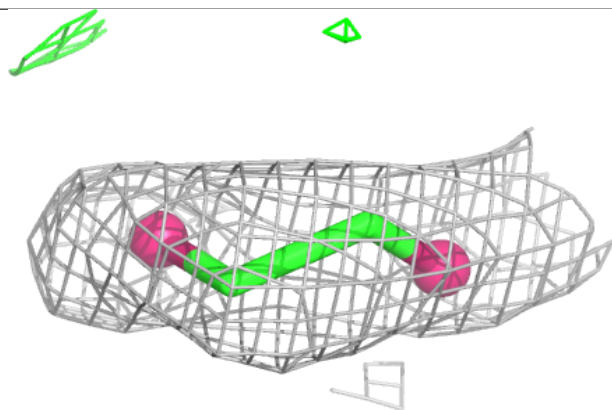
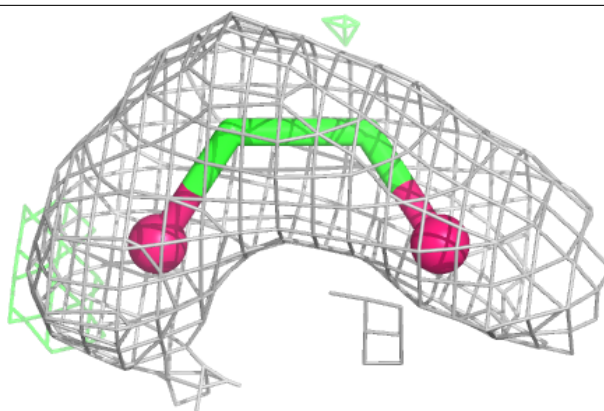
**Electron density around EDO B 616:**

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

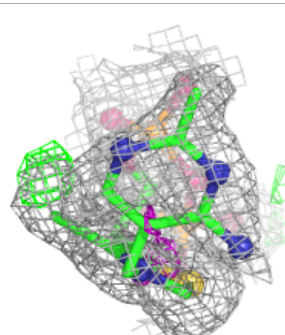
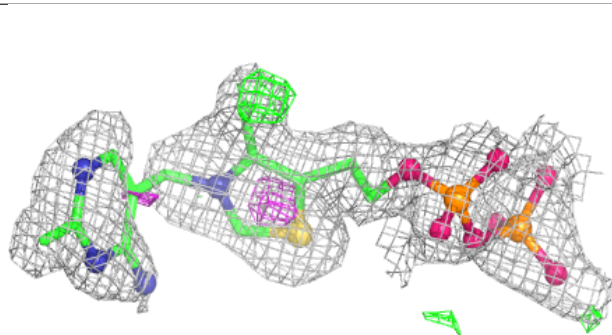
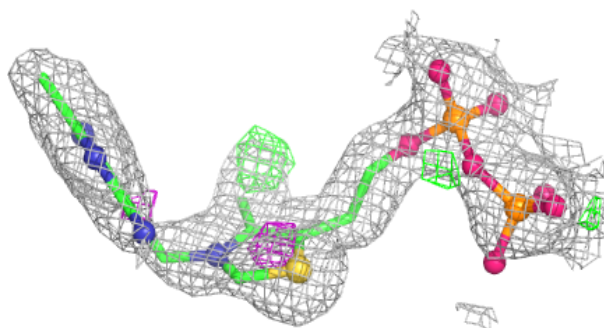


**Electron density around EDO B 617:**

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

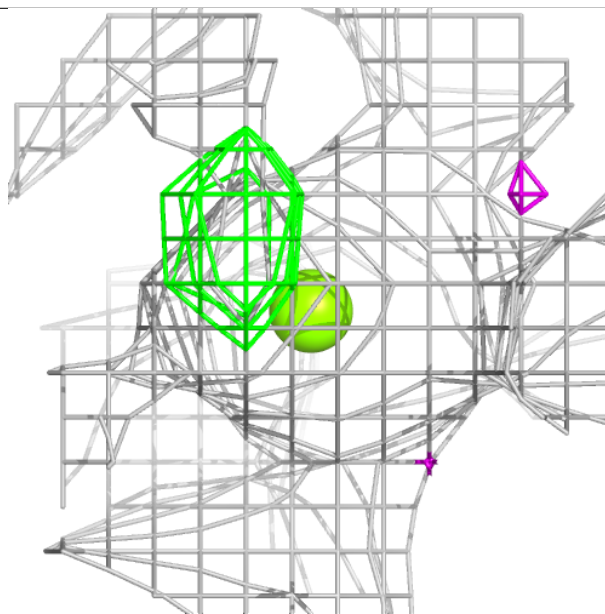
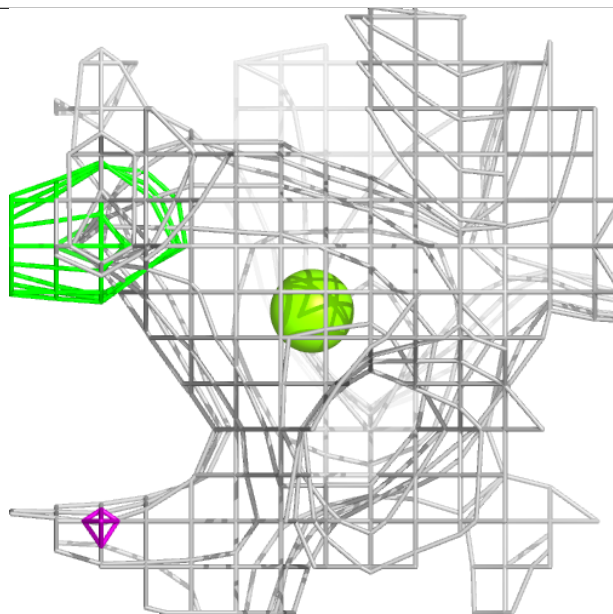
**Electron density around TPP A 615:**

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



**Electron density around MG A 601:**

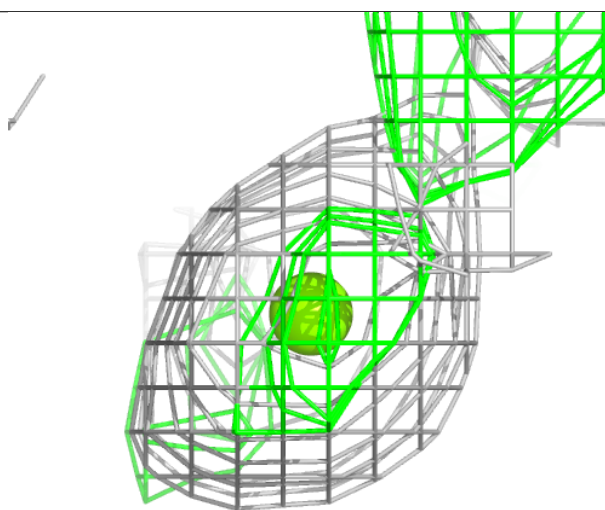
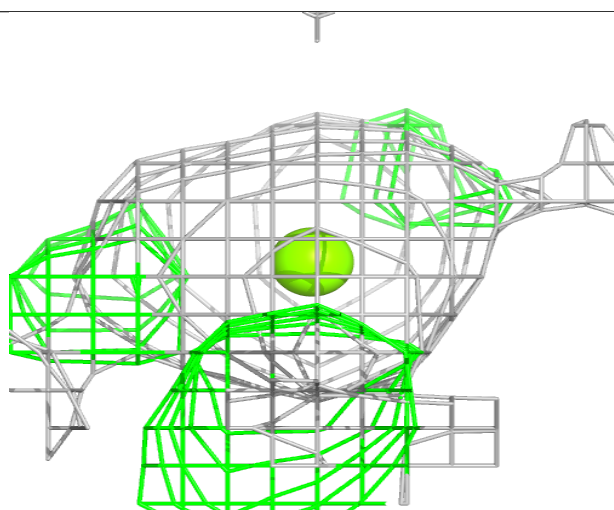
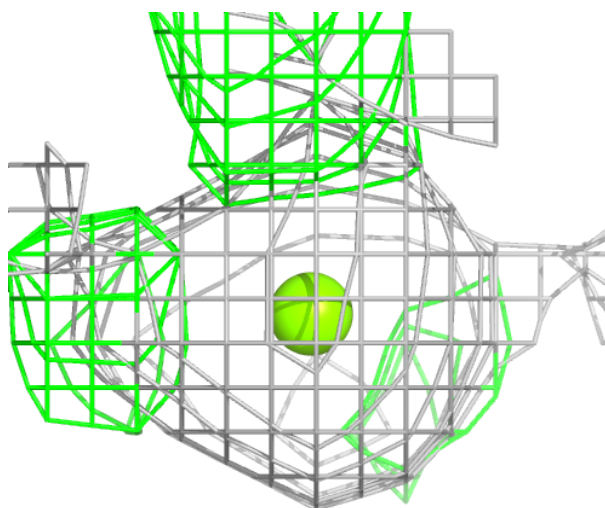
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





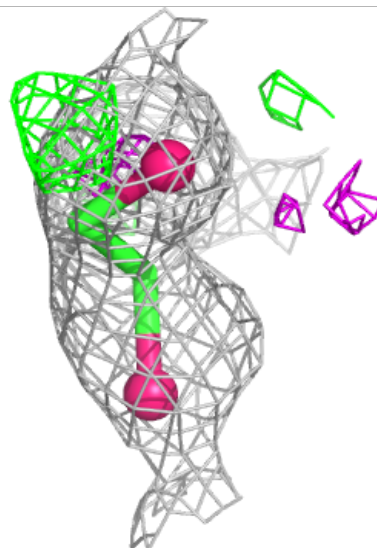
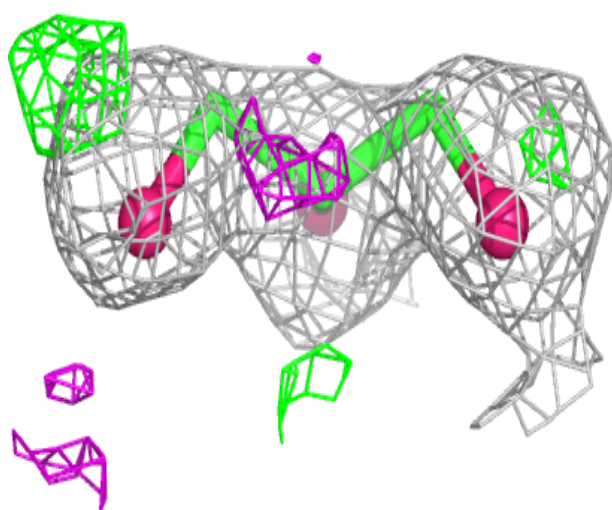
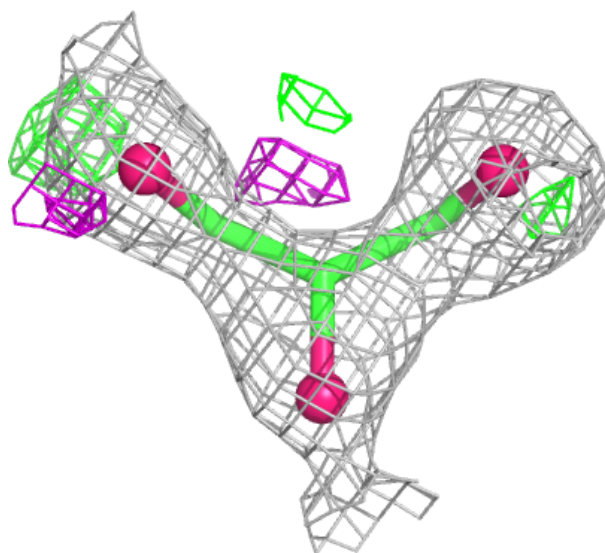
**Electron density around MG C 606:**

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



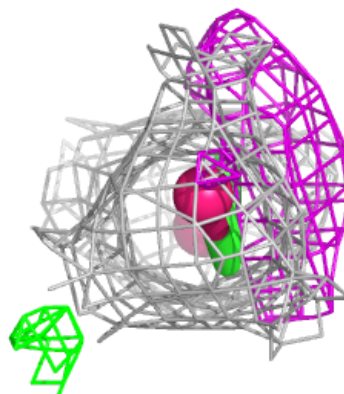
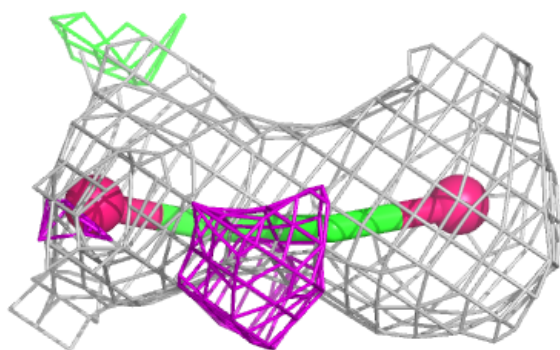
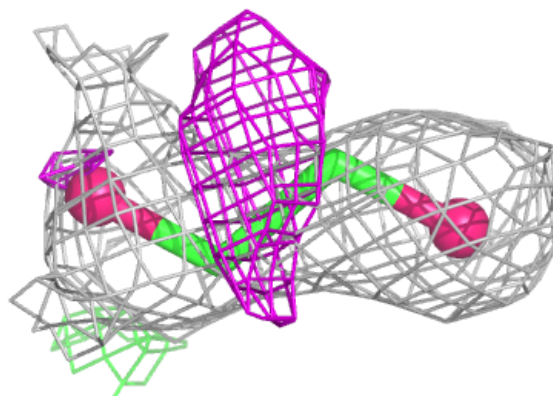
**Electron density around GOL C 612:**

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

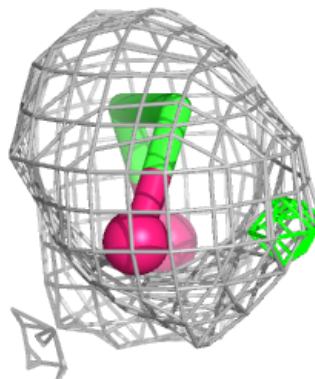
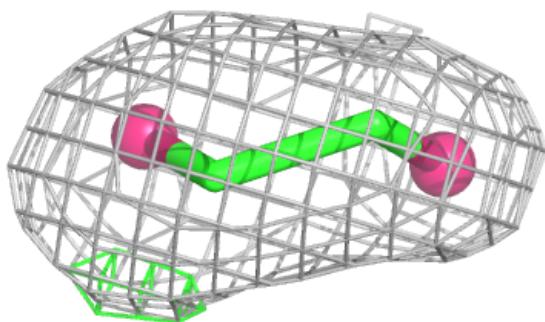
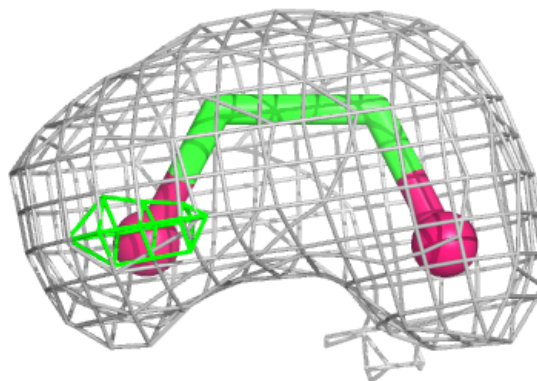


**Electron density around EDO A 616:**

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

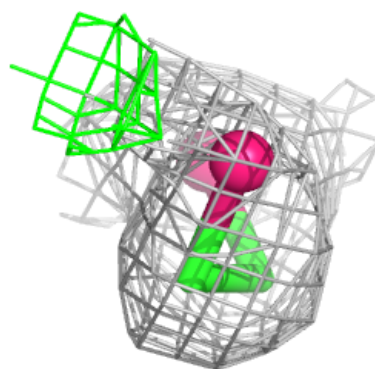
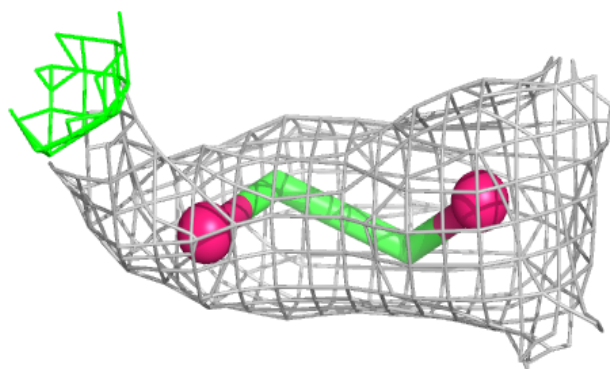
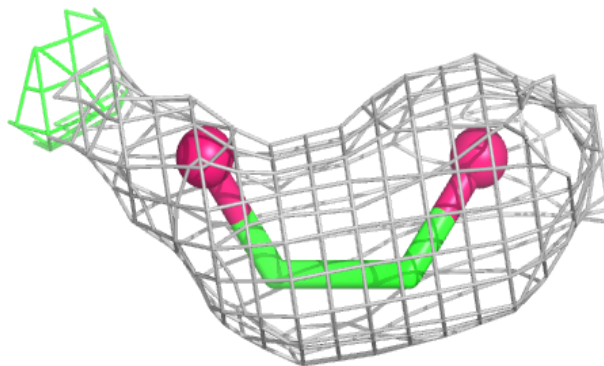
**Electron density around EDO B 615:**

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



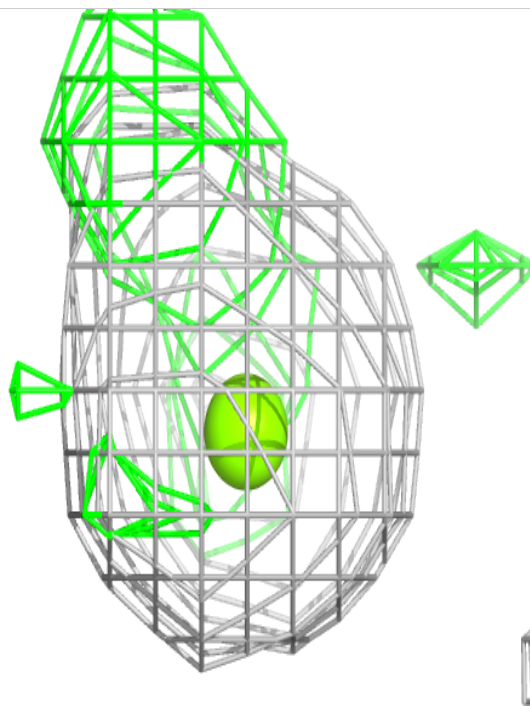
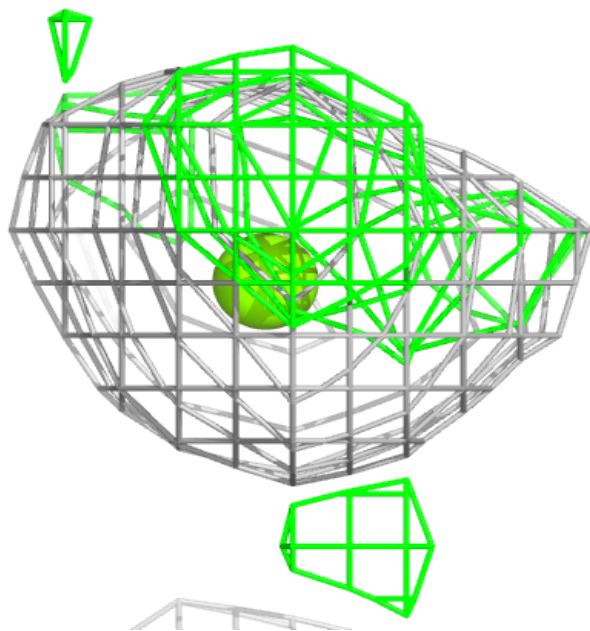
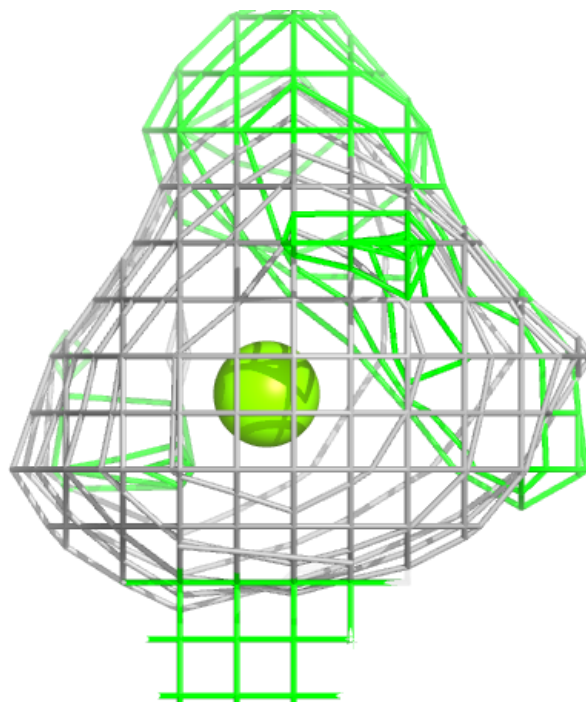
**Electron density around EDO A 617:**

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



**Electron density around MG B 608:**

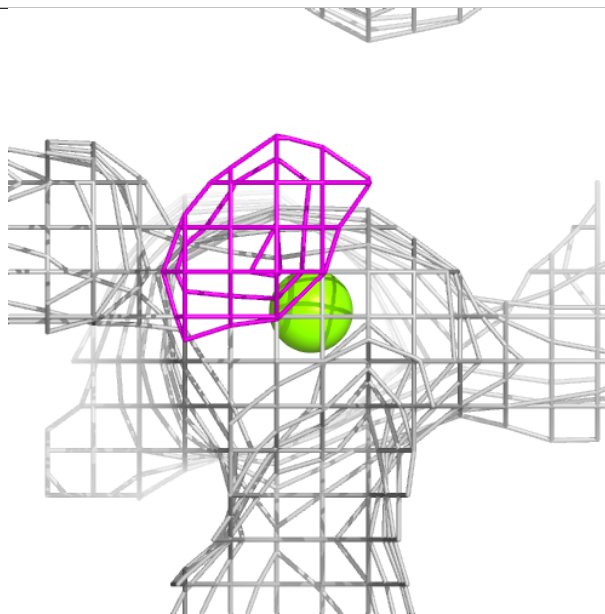
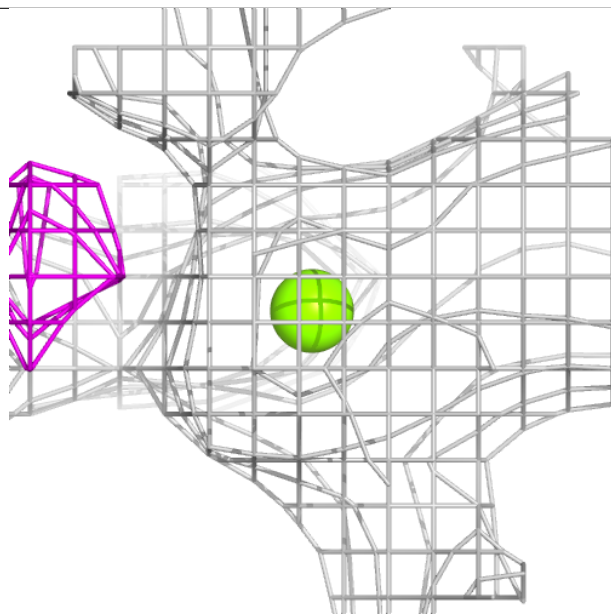
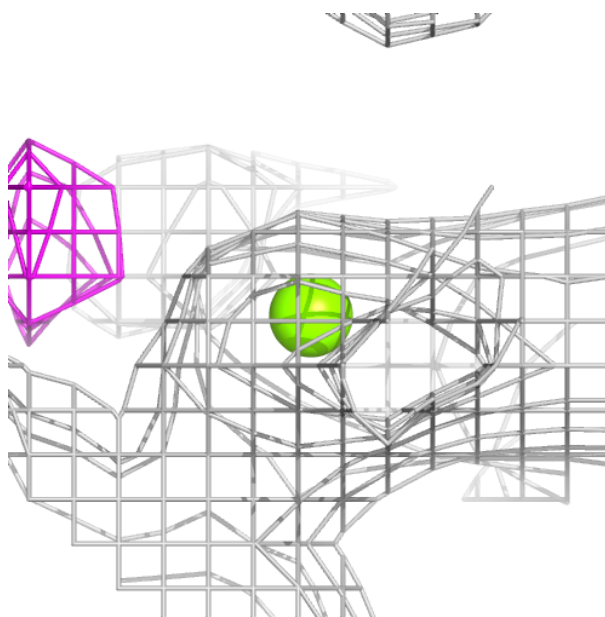
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





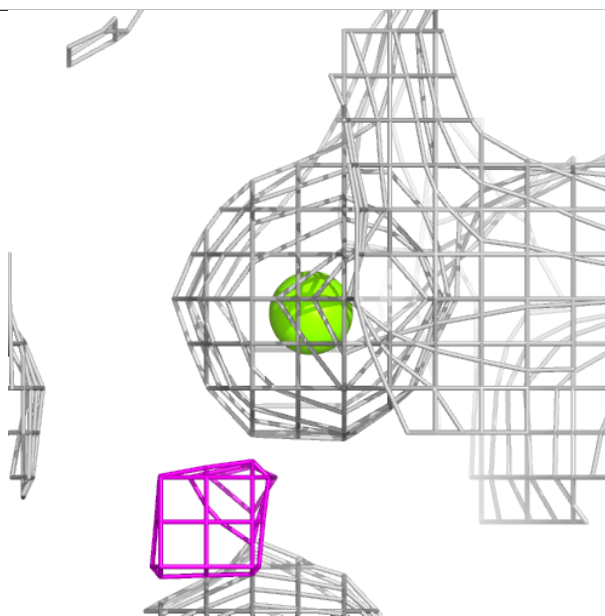
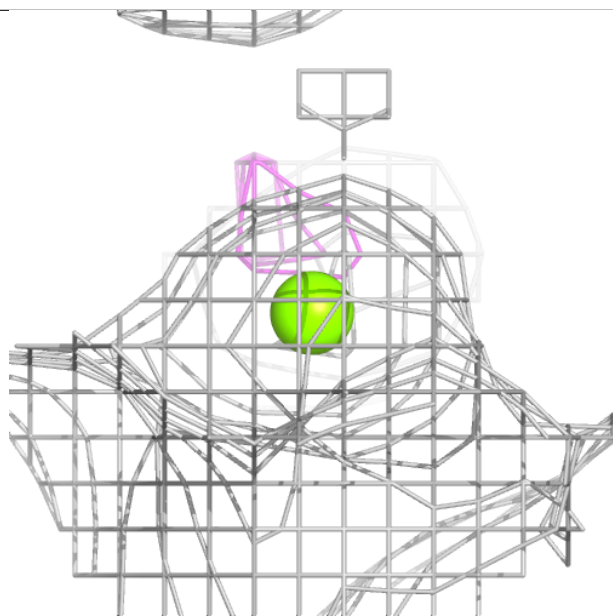
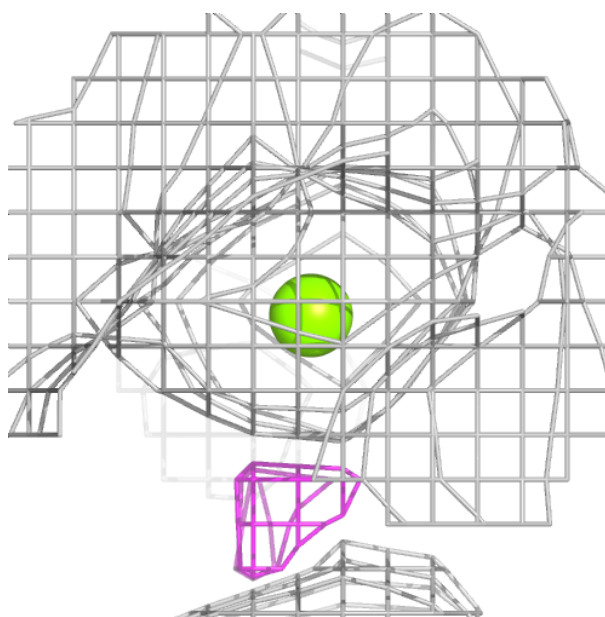
**Electron density around MG C 601:**

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



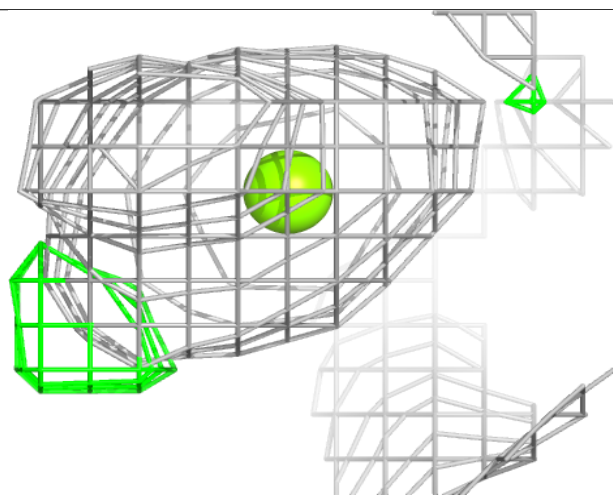
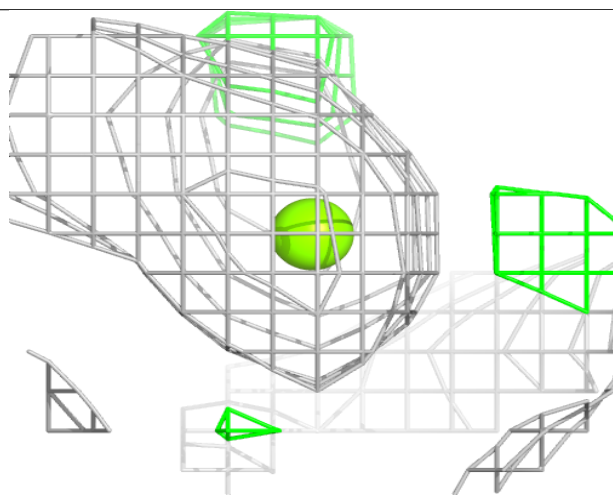
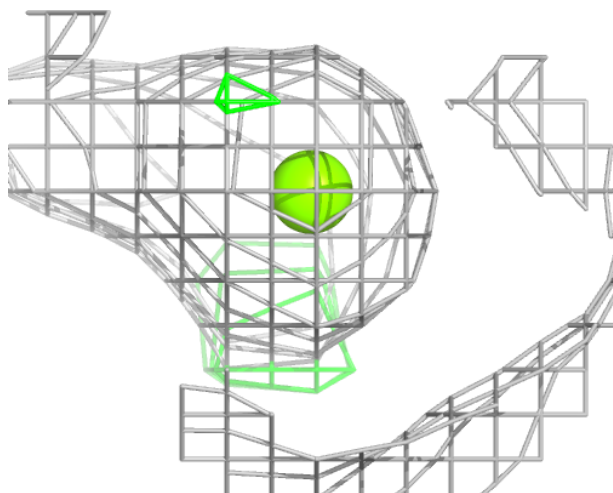
**Electron density around MG C 605:**

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



**Electron density around MG B 610:**

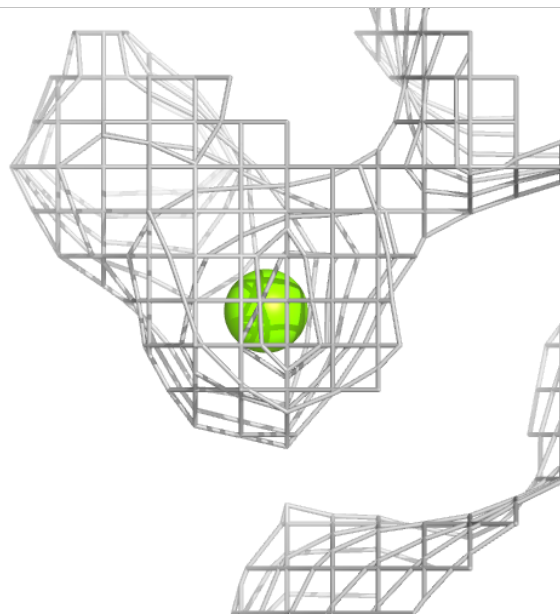
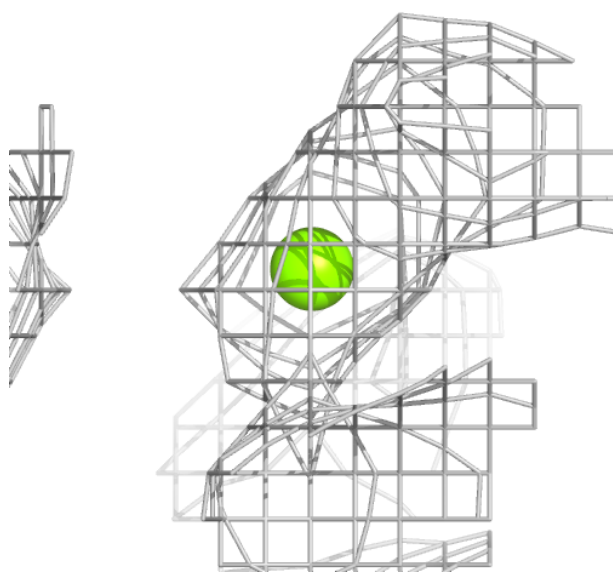
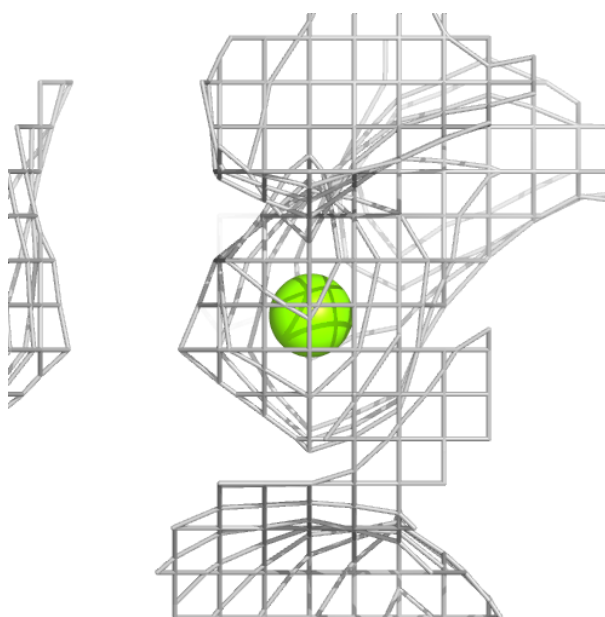
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





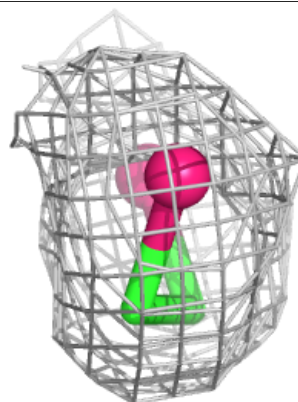
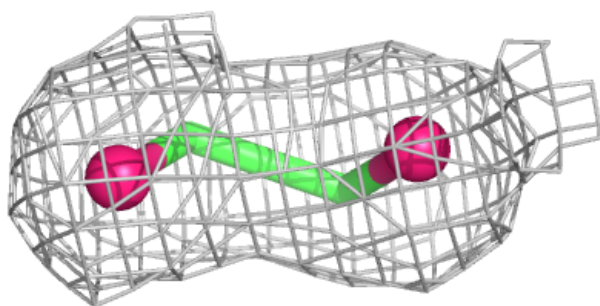
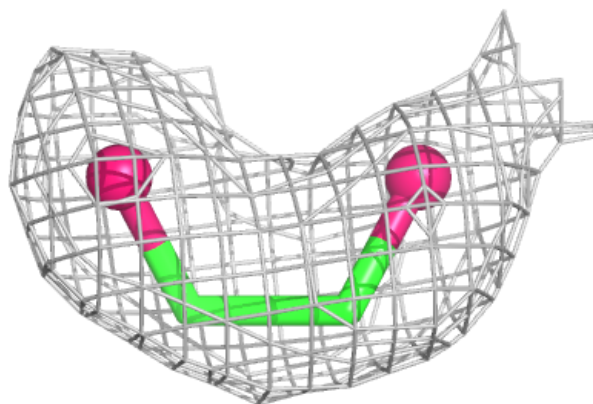
**Electron density around MG C 608:**

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

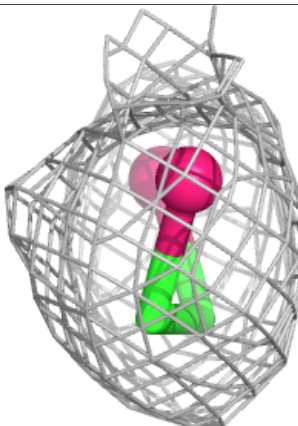
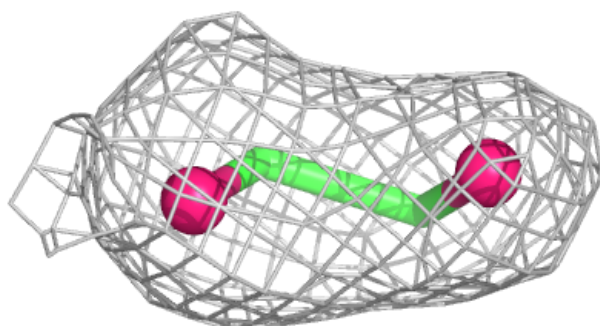
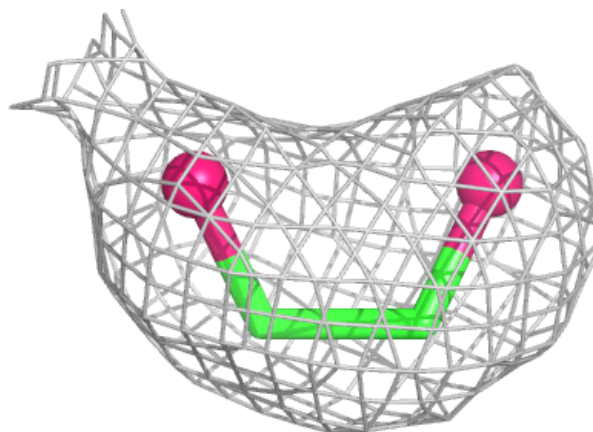


**Electron density around EDO A 618:**

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

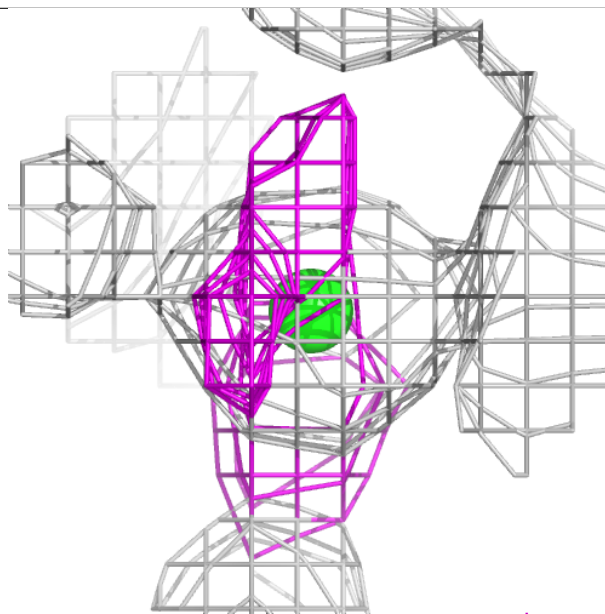
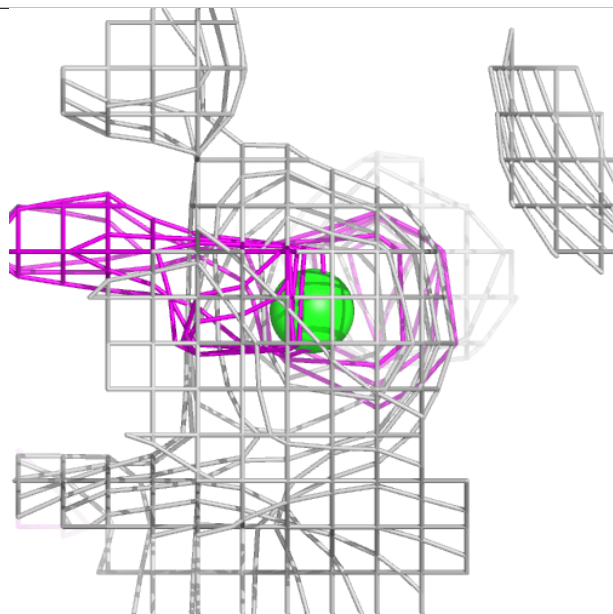
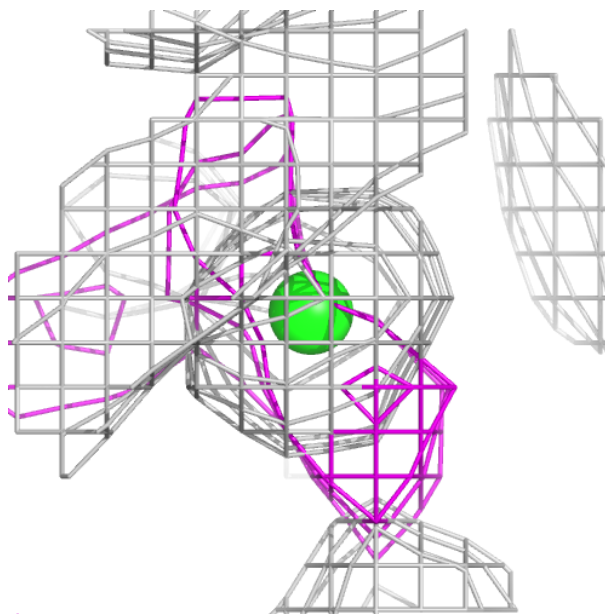
**Electron density around EDO D 604:**

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



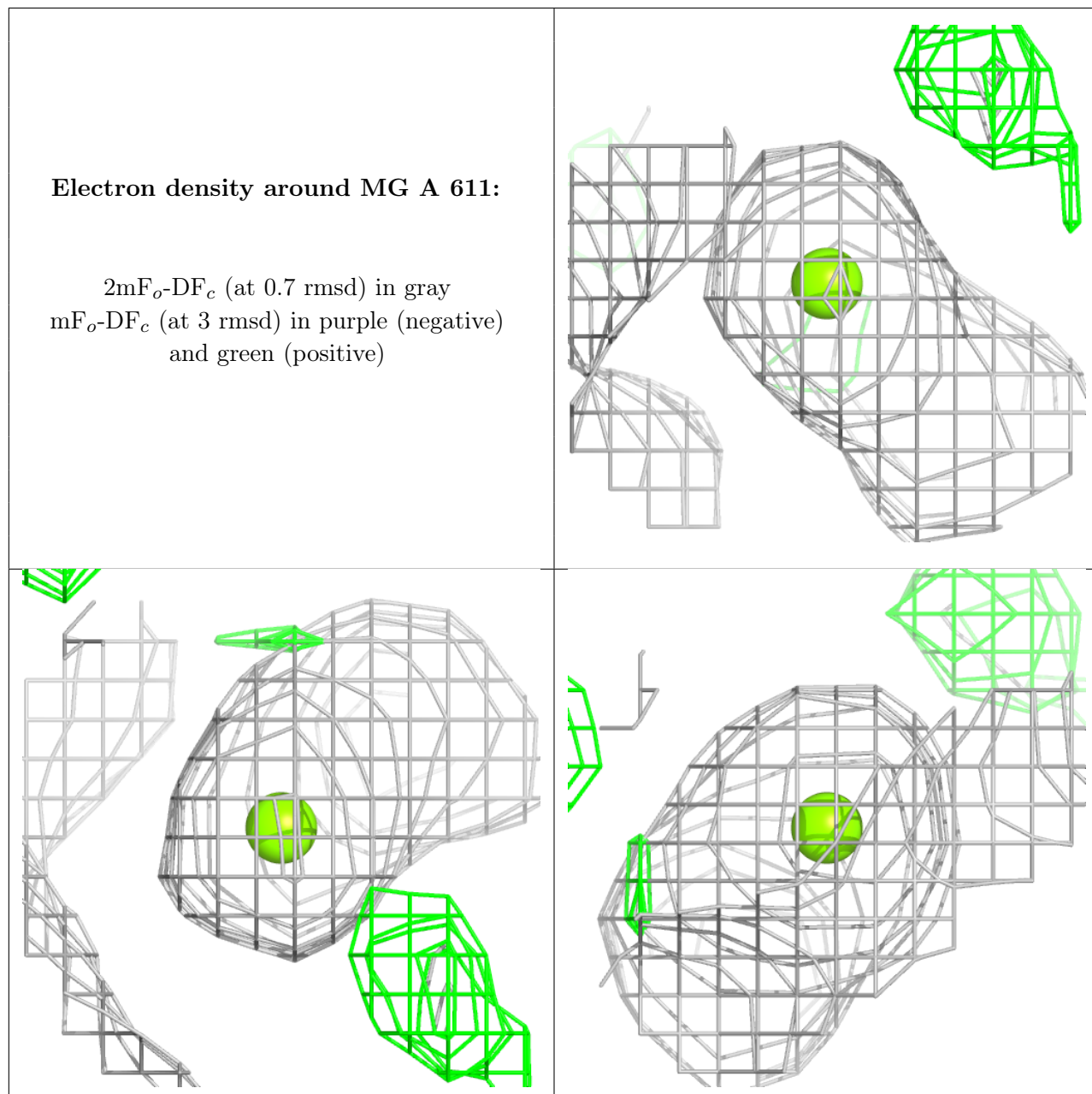
**Electron density around CL C 609:**

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



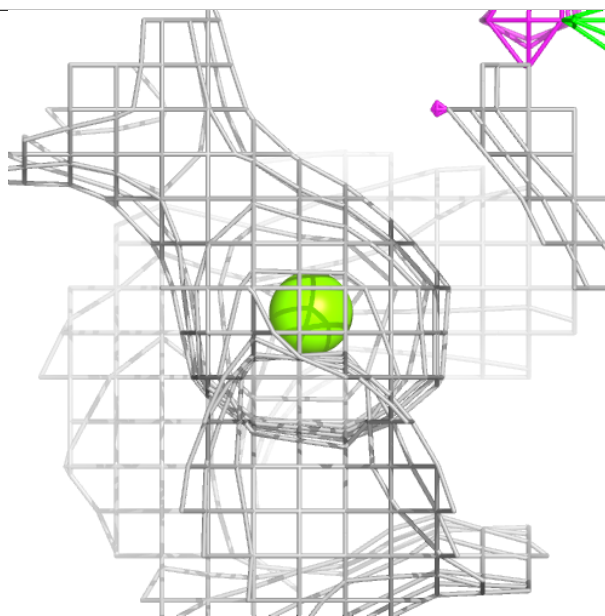
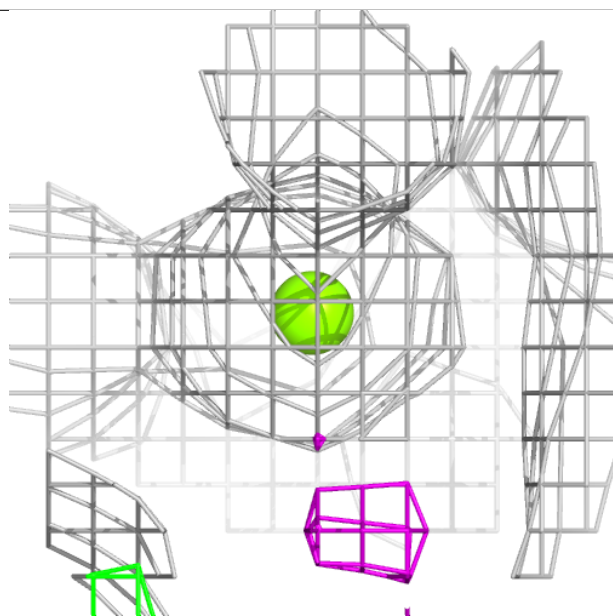
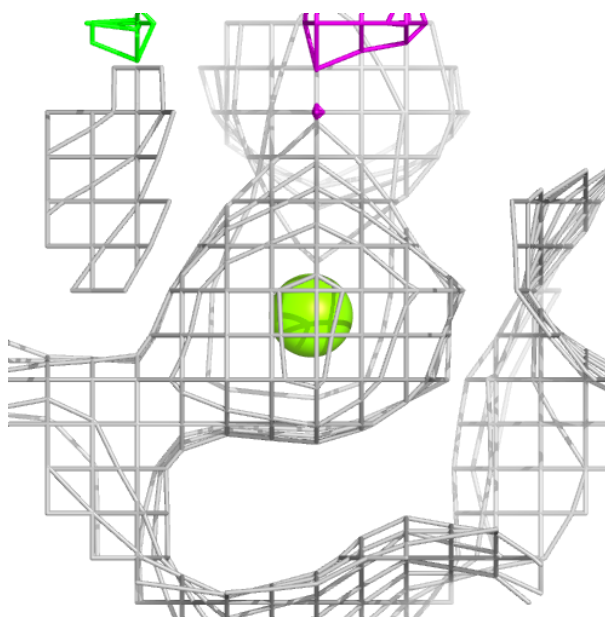
**Electron density around MG A 611:**

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



**Electron density around MG C 602:**

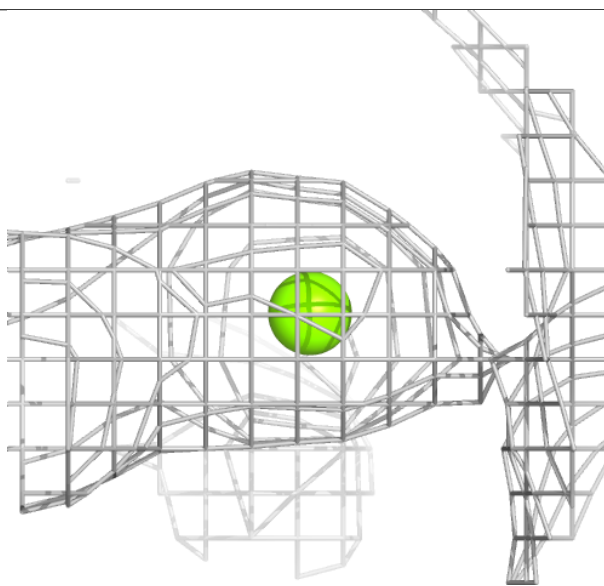
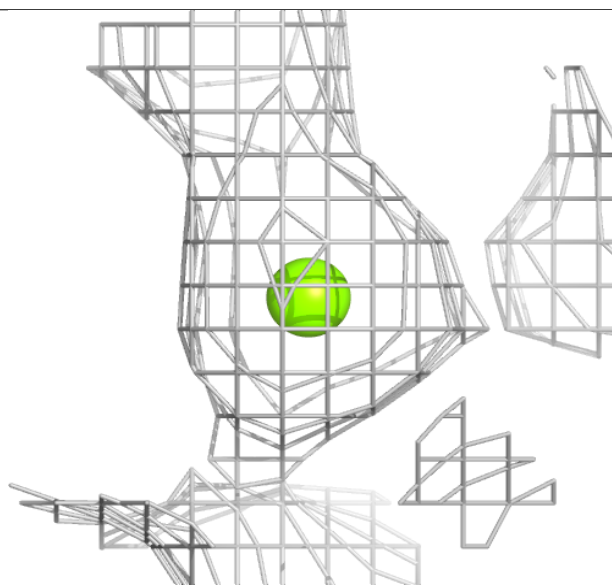
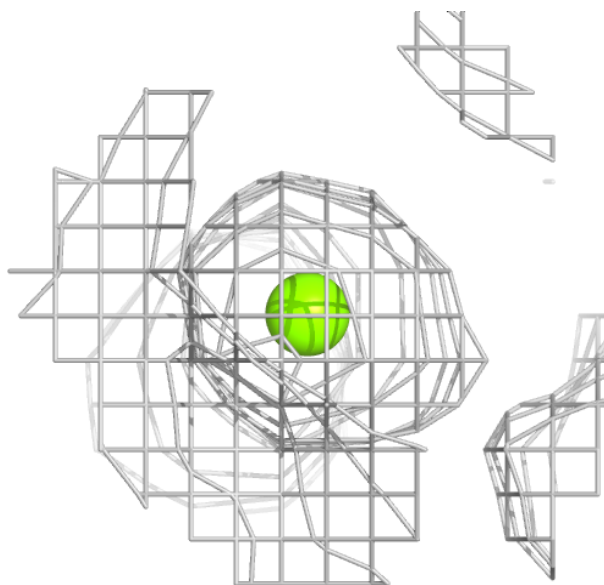
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





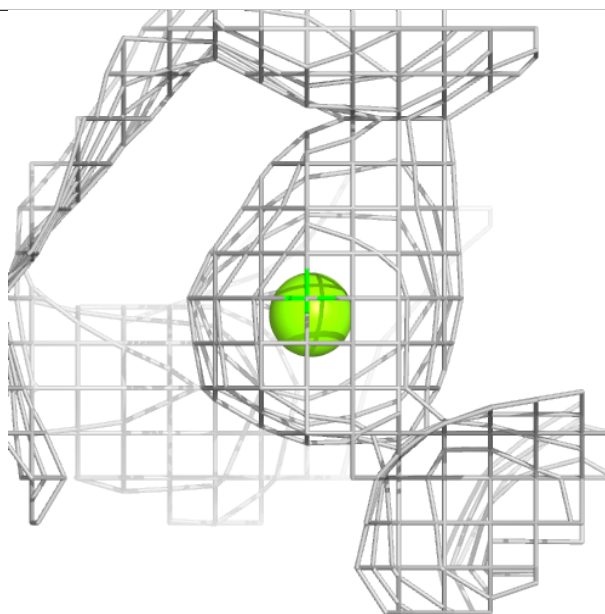
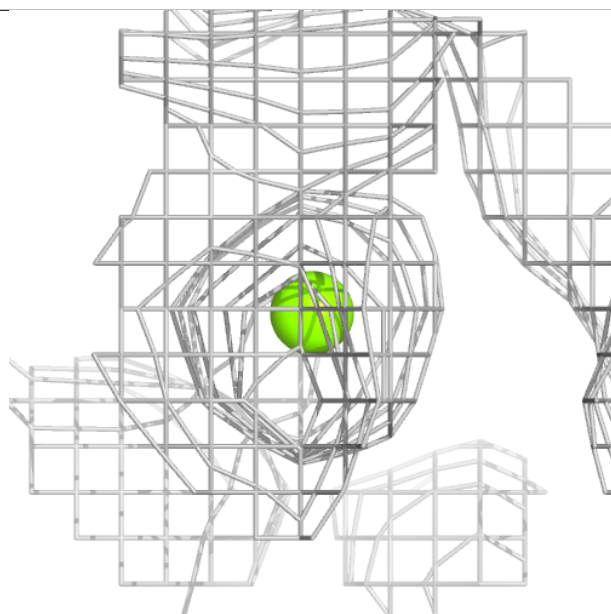
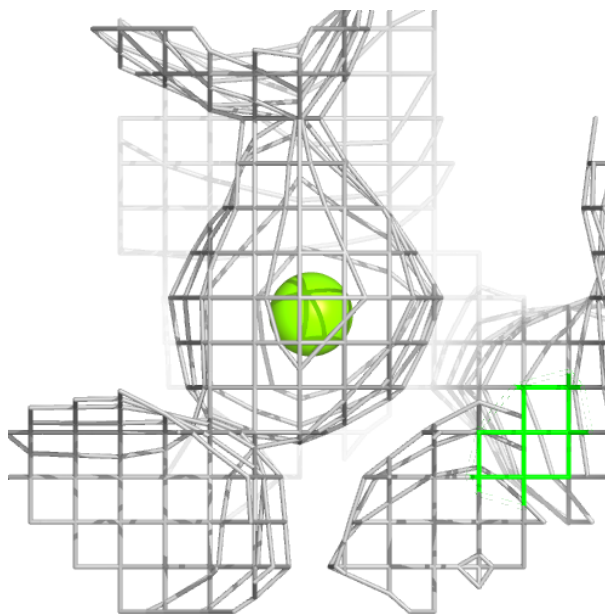
**Electron density around MG C 603:**

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



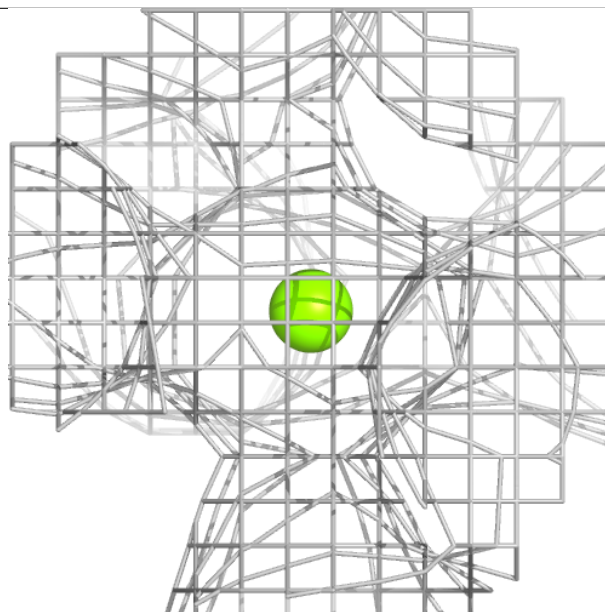
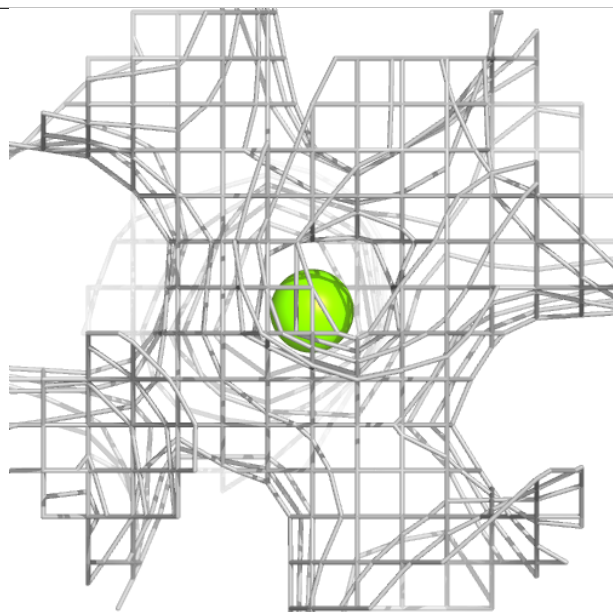
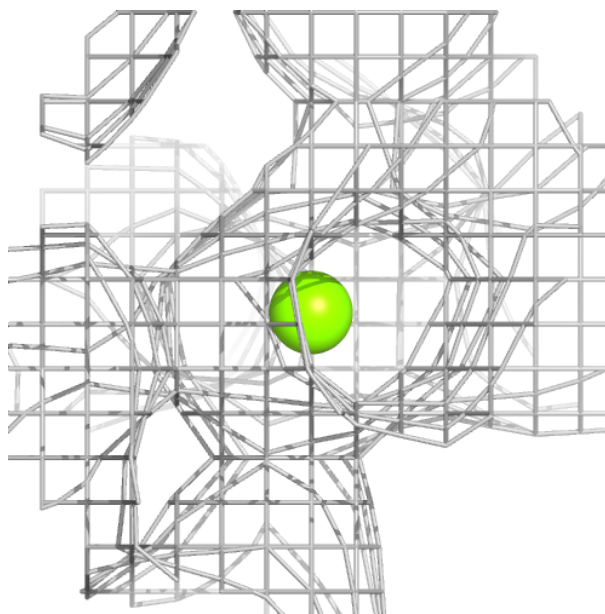
**Electron density around MG A 606:**

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



**Electron density around MG B 609:**

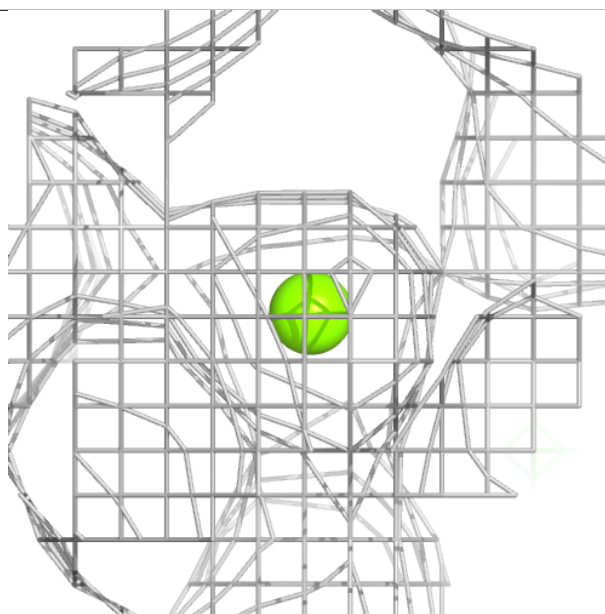
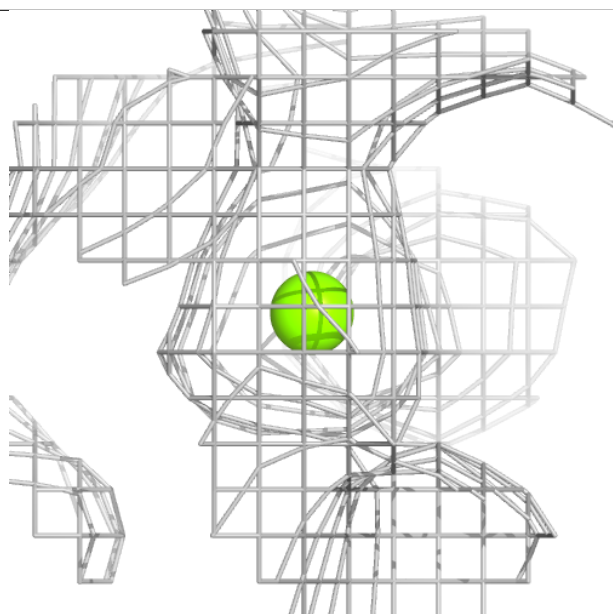
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





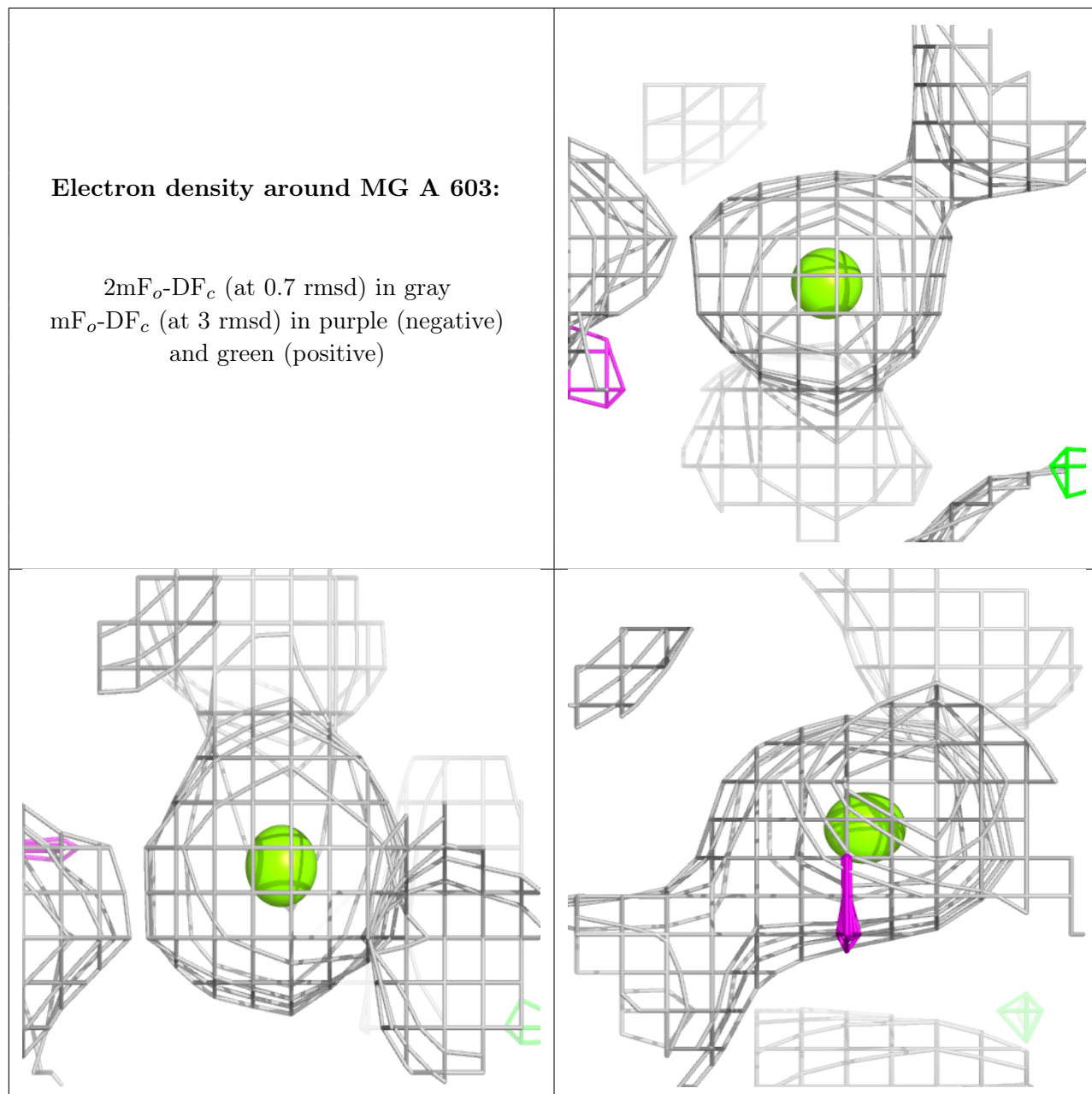
**Electron density around MG A 609:**

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



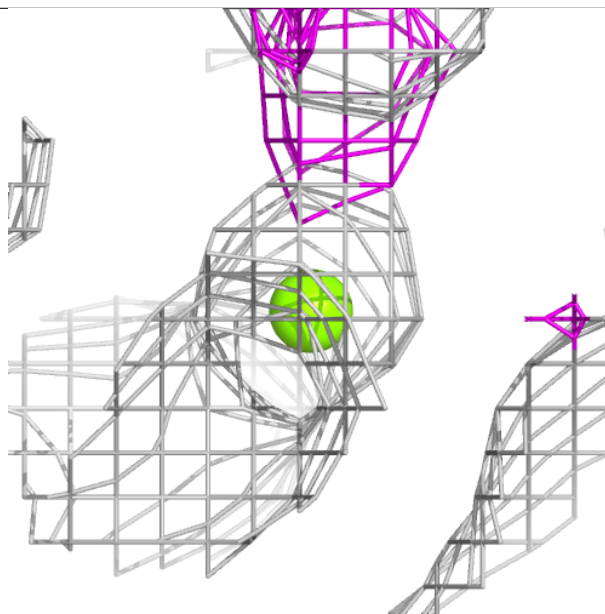
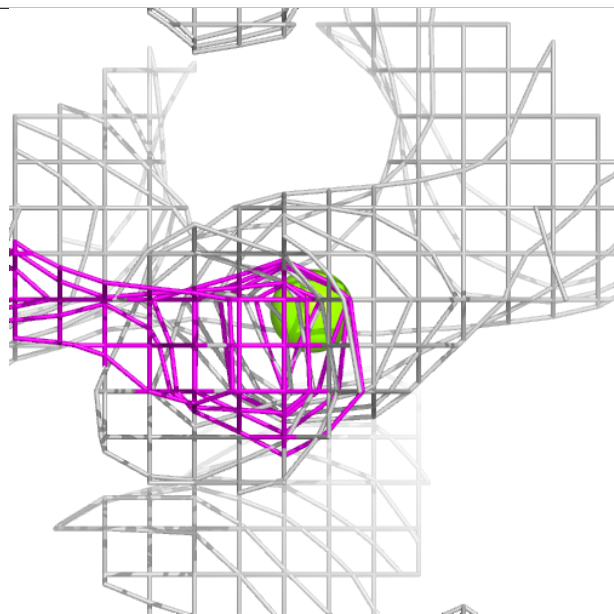
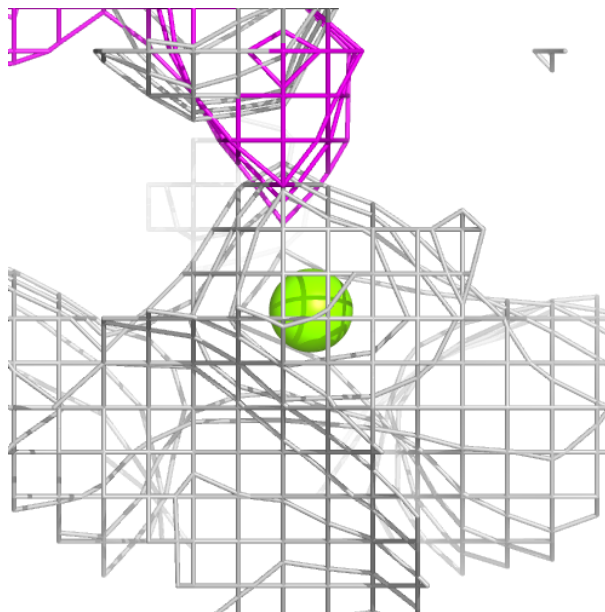
**Electron density around MG A 603:**

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



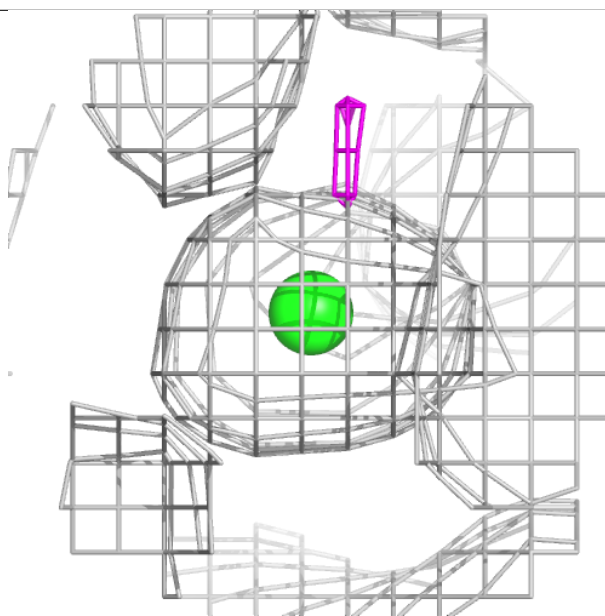
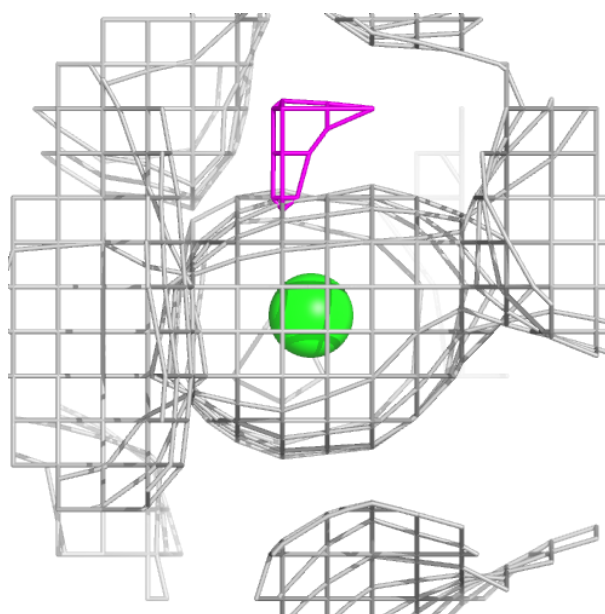
**Electron density around MG C 607:**

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



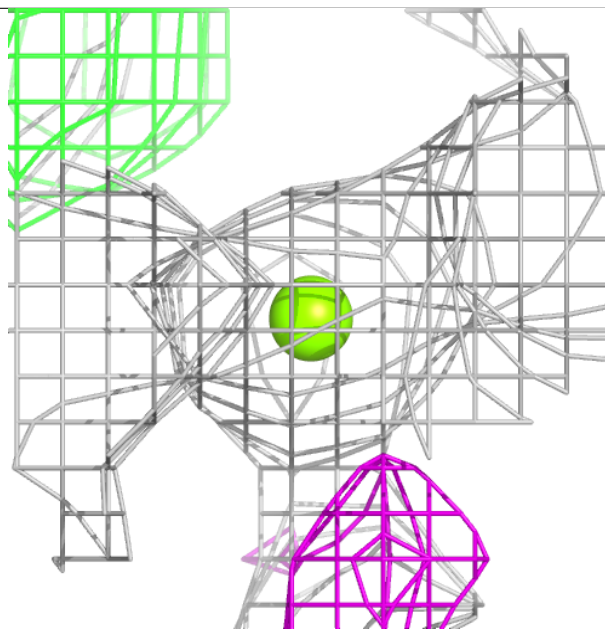
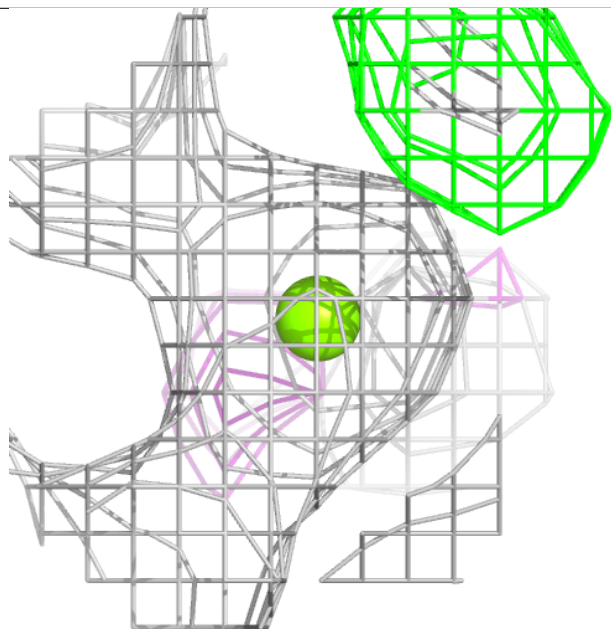
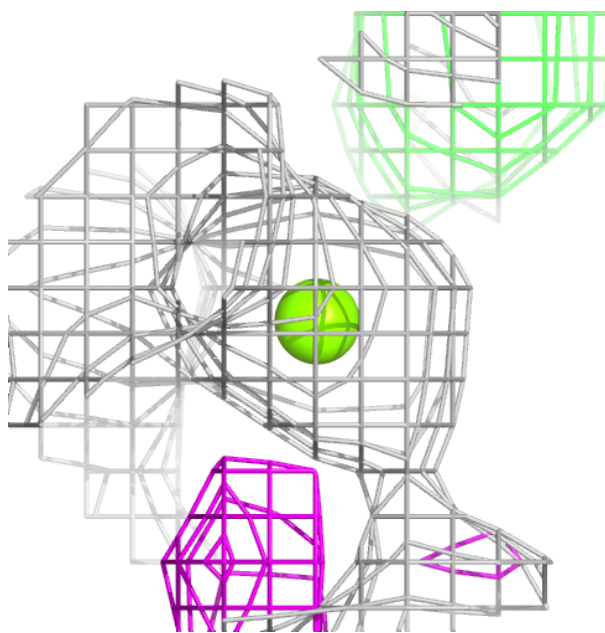
**Electron density around CL B 611:**

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



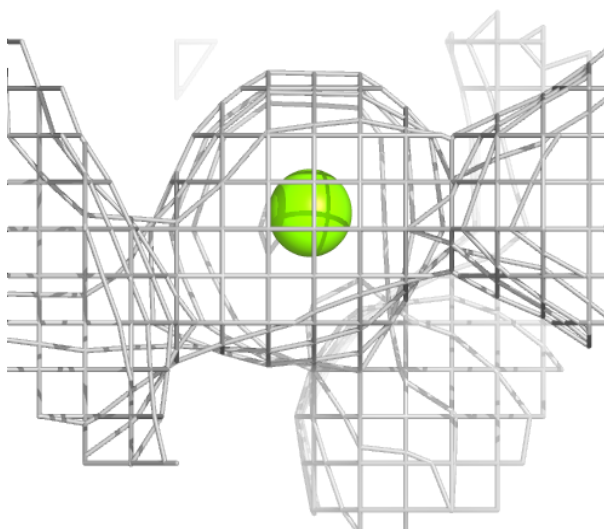
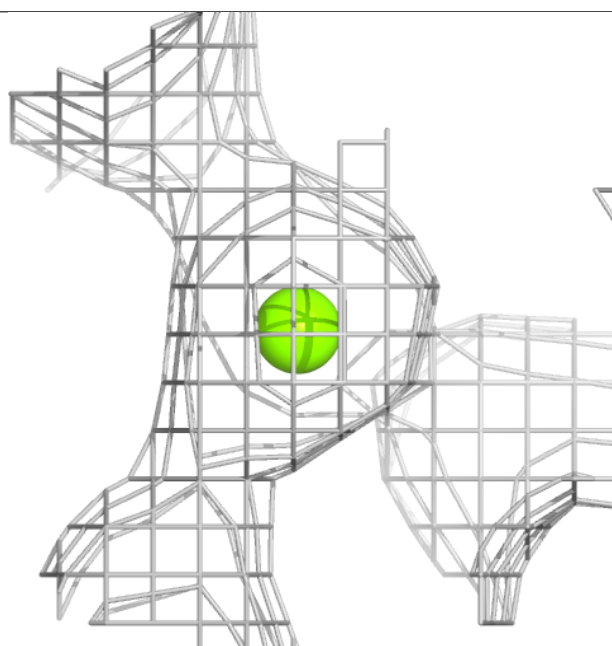
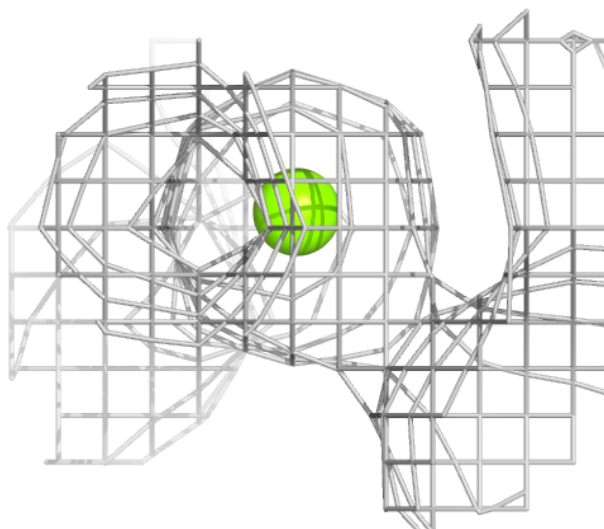
**Electron density around MG A 604:**

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



**Electron density around MG A 607:**

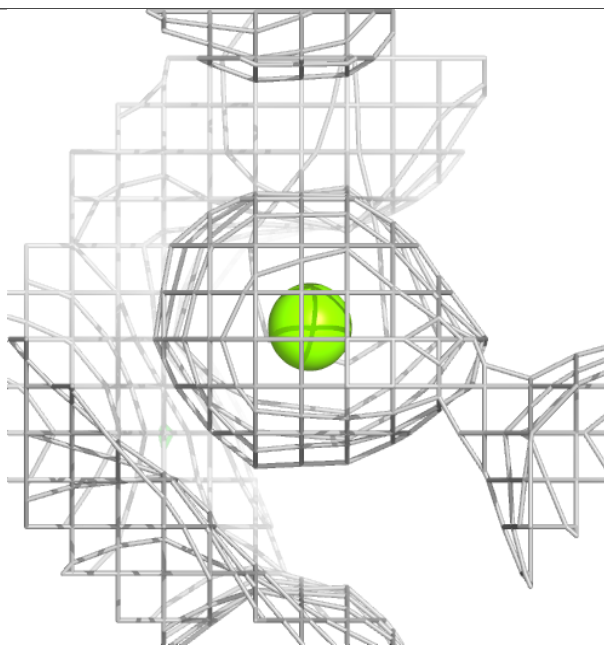
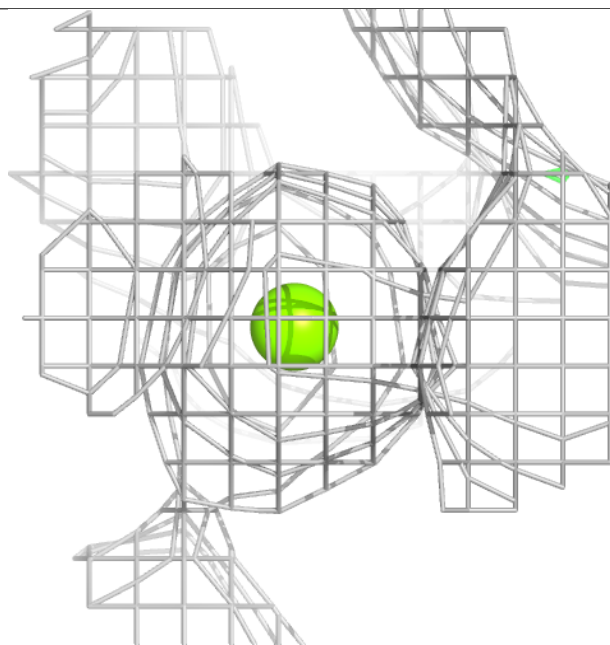
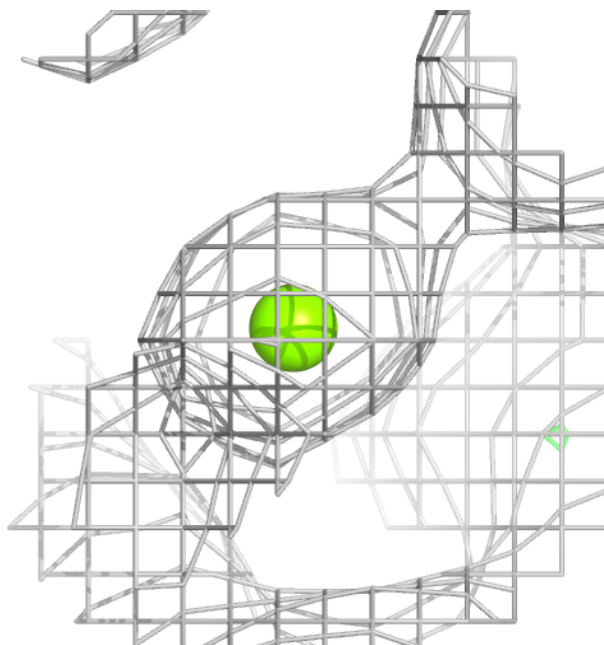
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





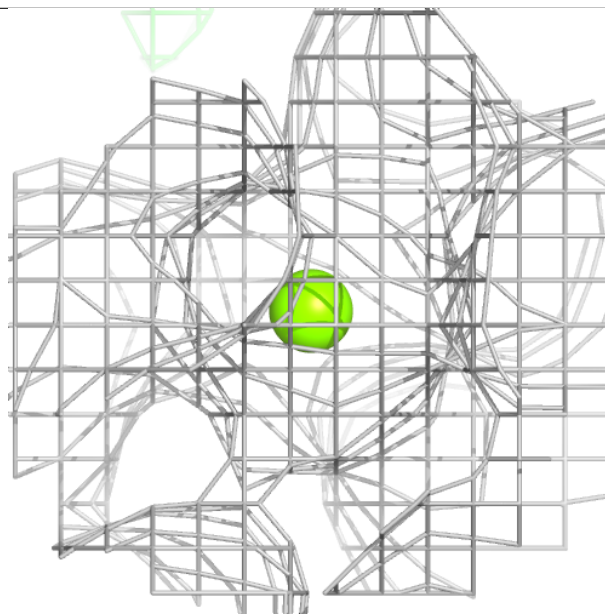
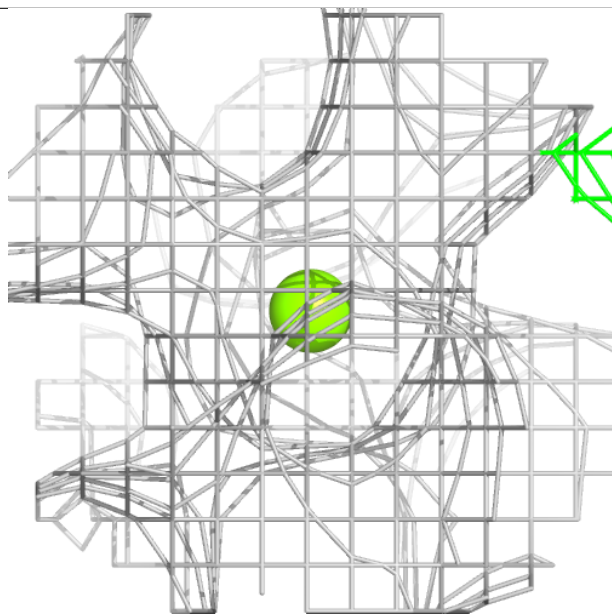
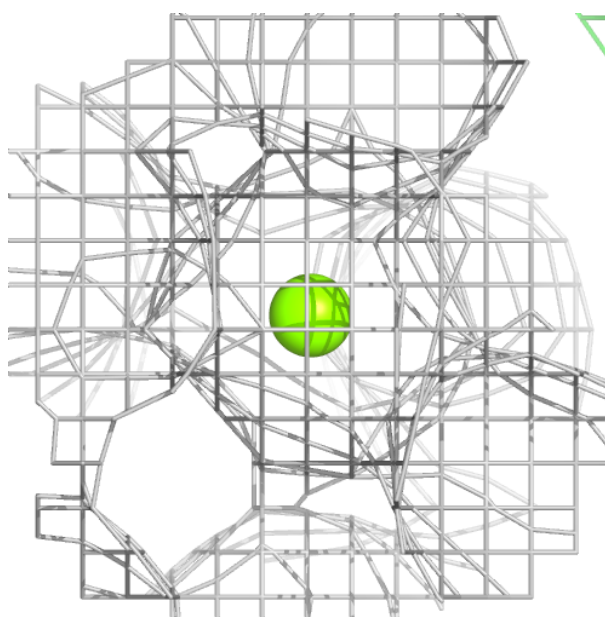
**Electron density around MG A 605:**

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



**Electron density around MG A 610:**

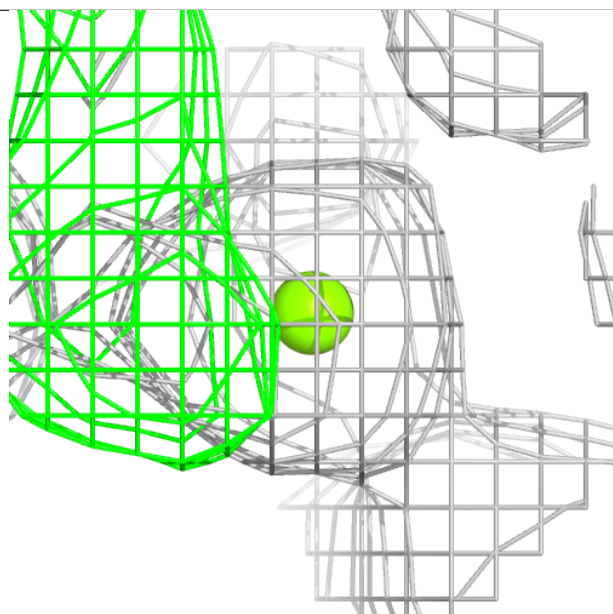
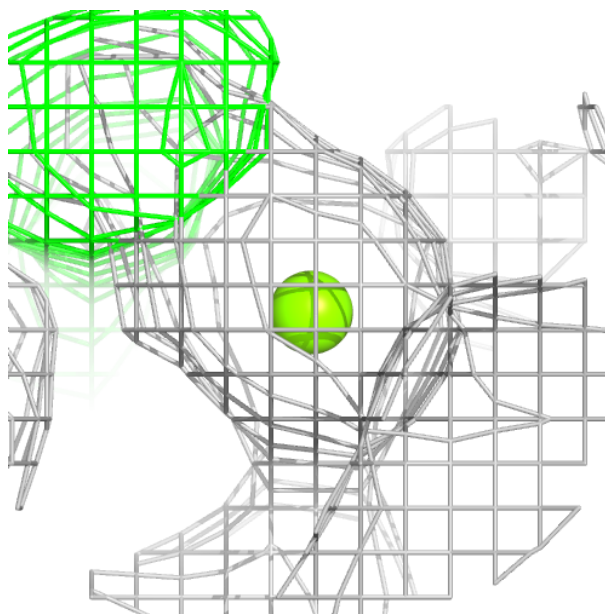
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





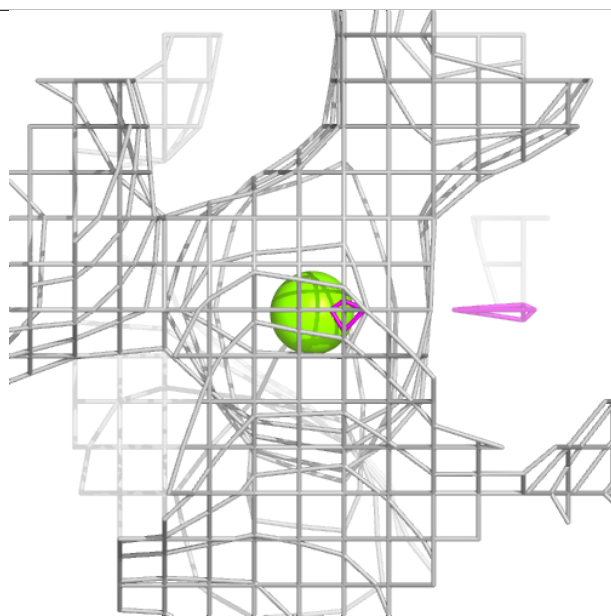
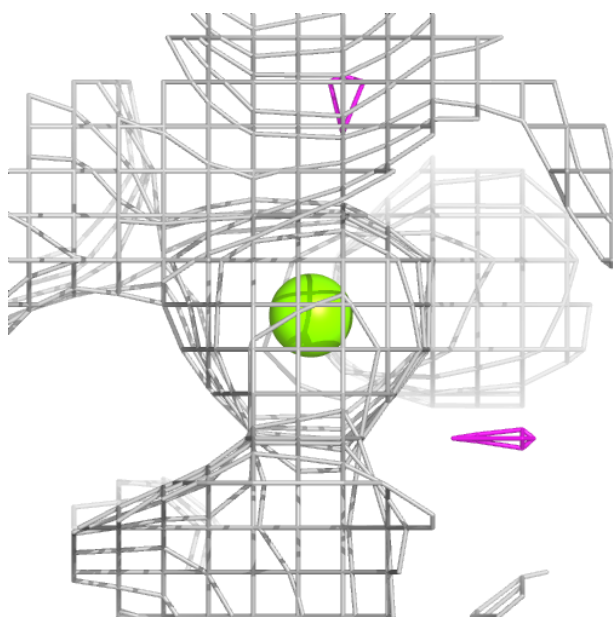
**Electron density around MG A 602:**

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



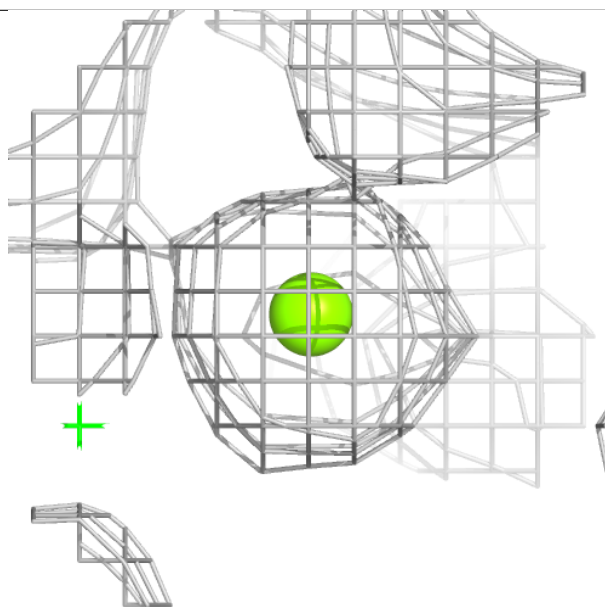
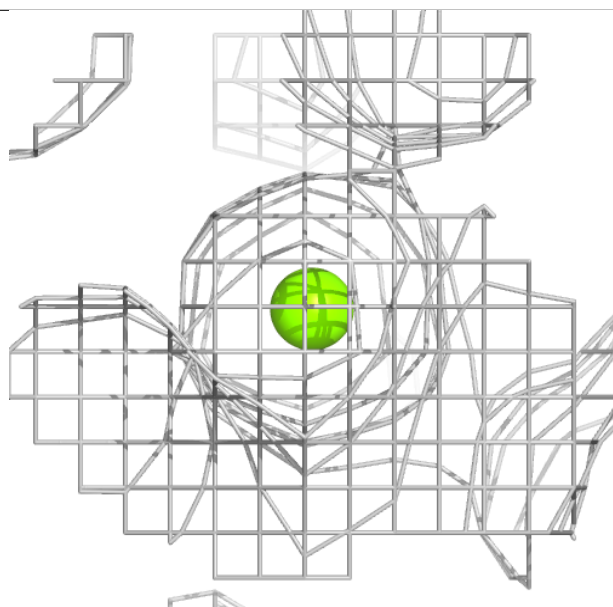
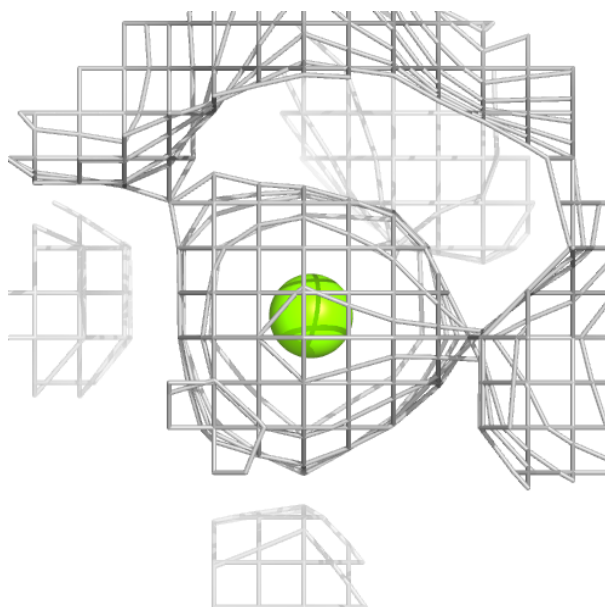
**Electron density around MG B 601:**

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



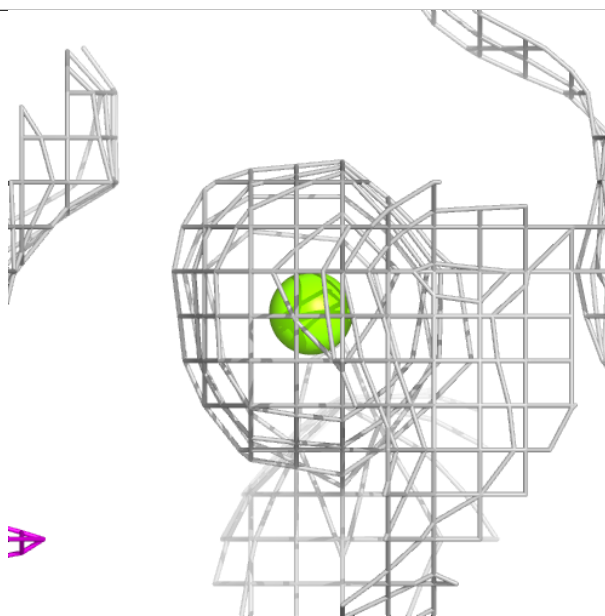
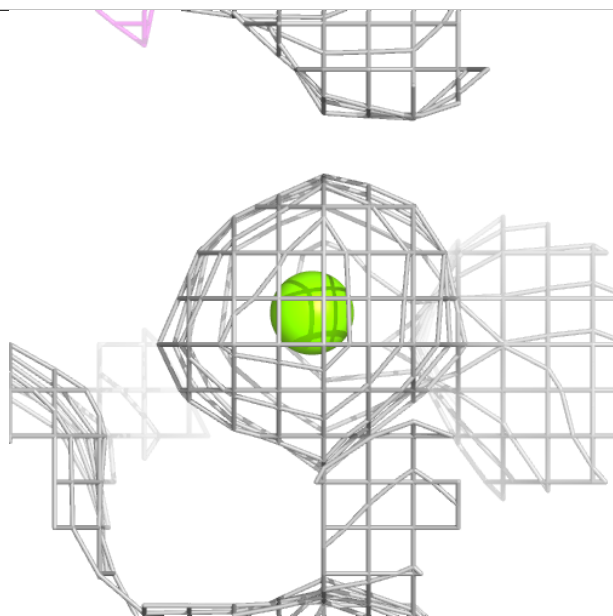
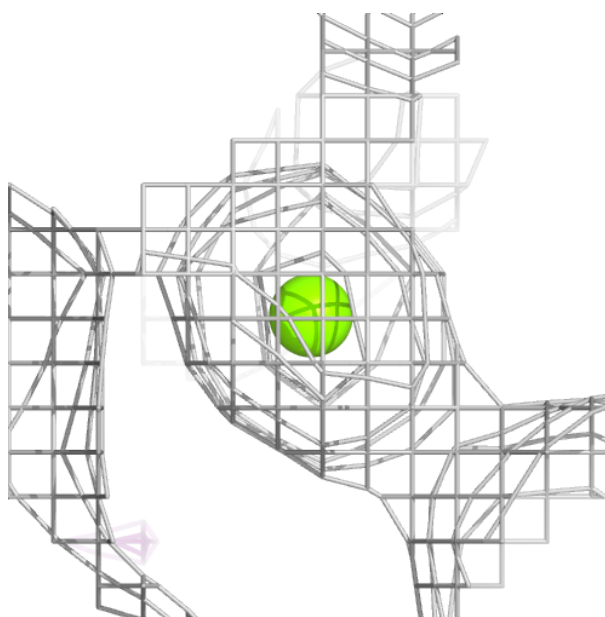
**Electron density around MG B 604:**

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



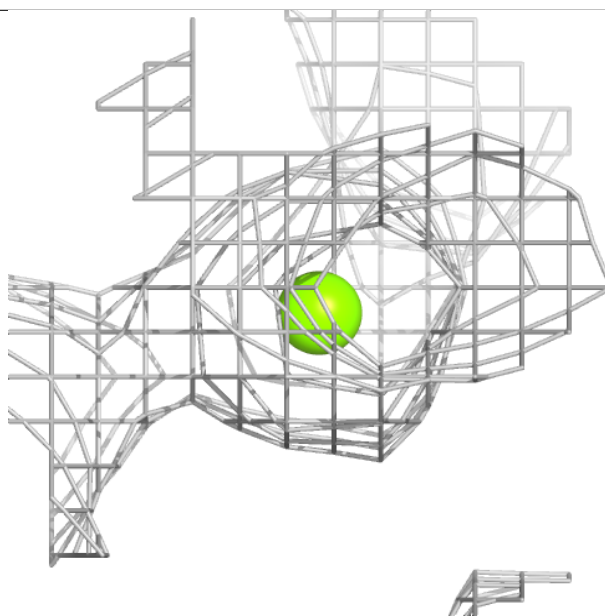
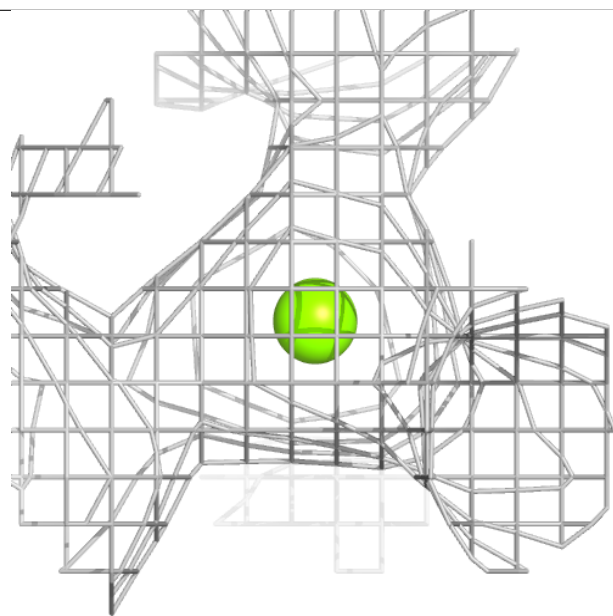
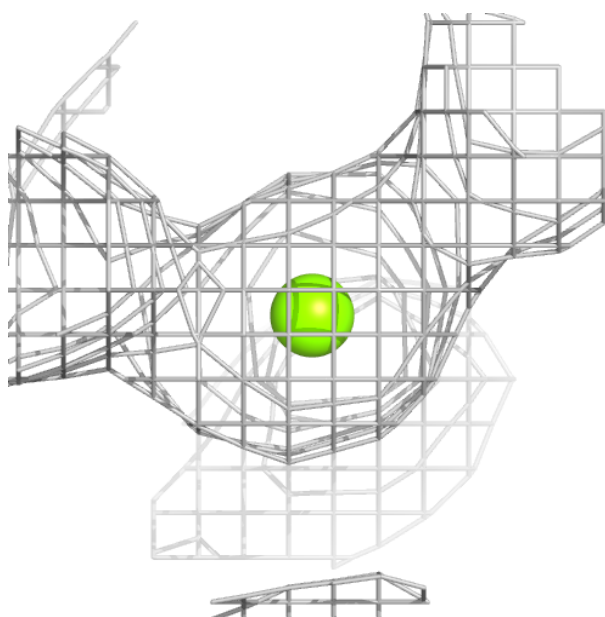
**Electron density around MG C 604:**

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



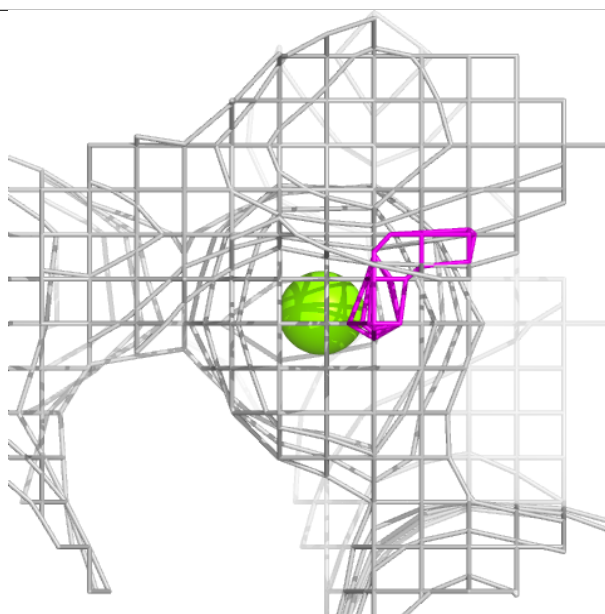
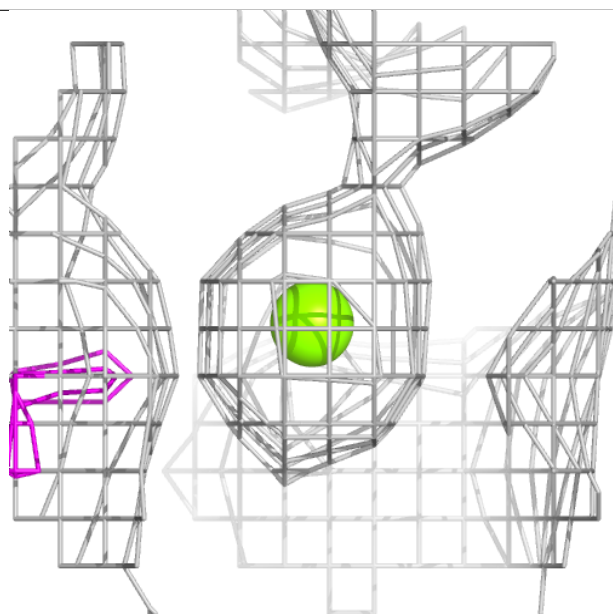
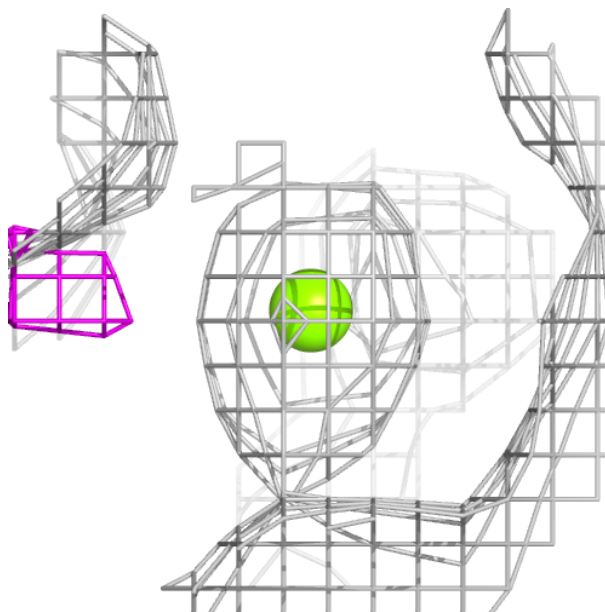
**Electron density around MG B 606:**

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



**Electron density around MG B 607:**

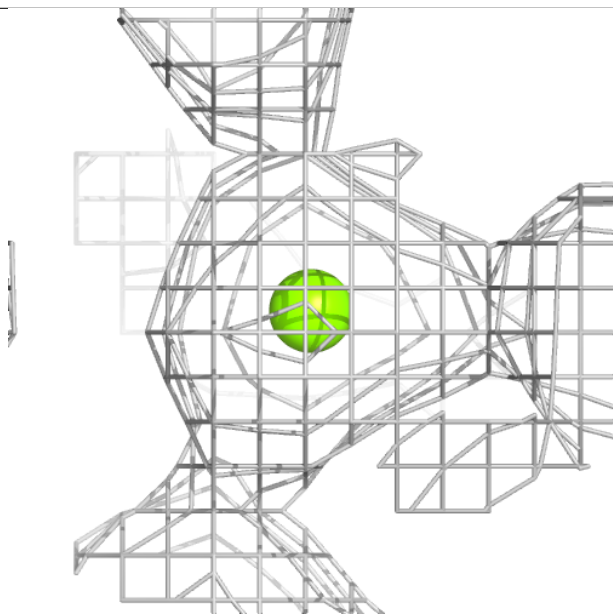
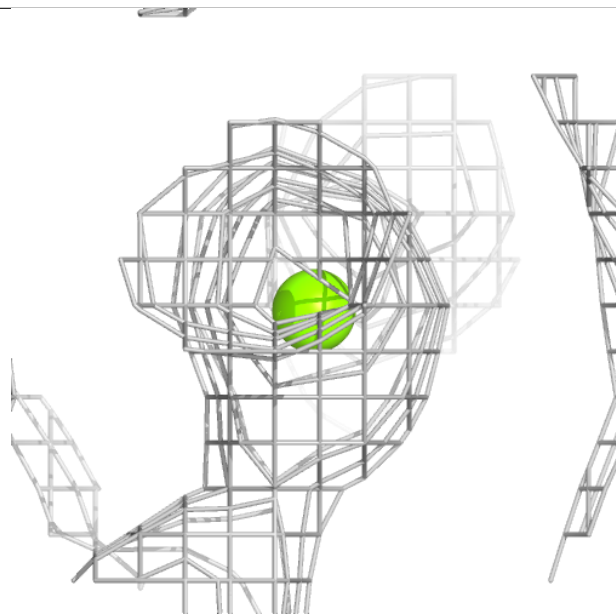
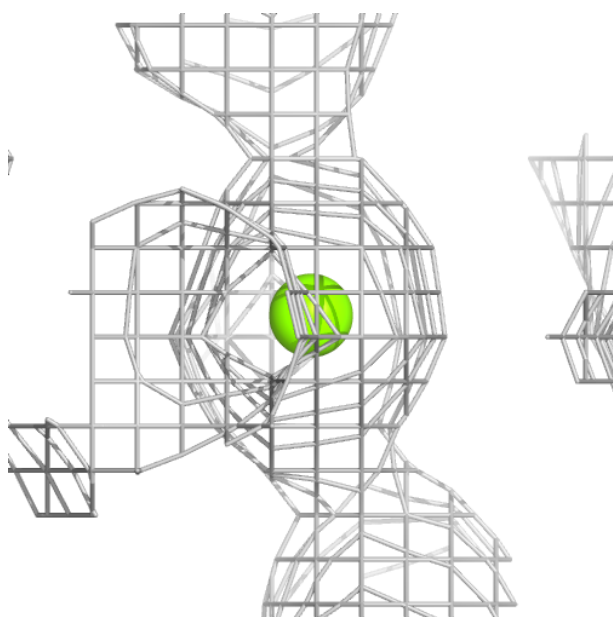
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





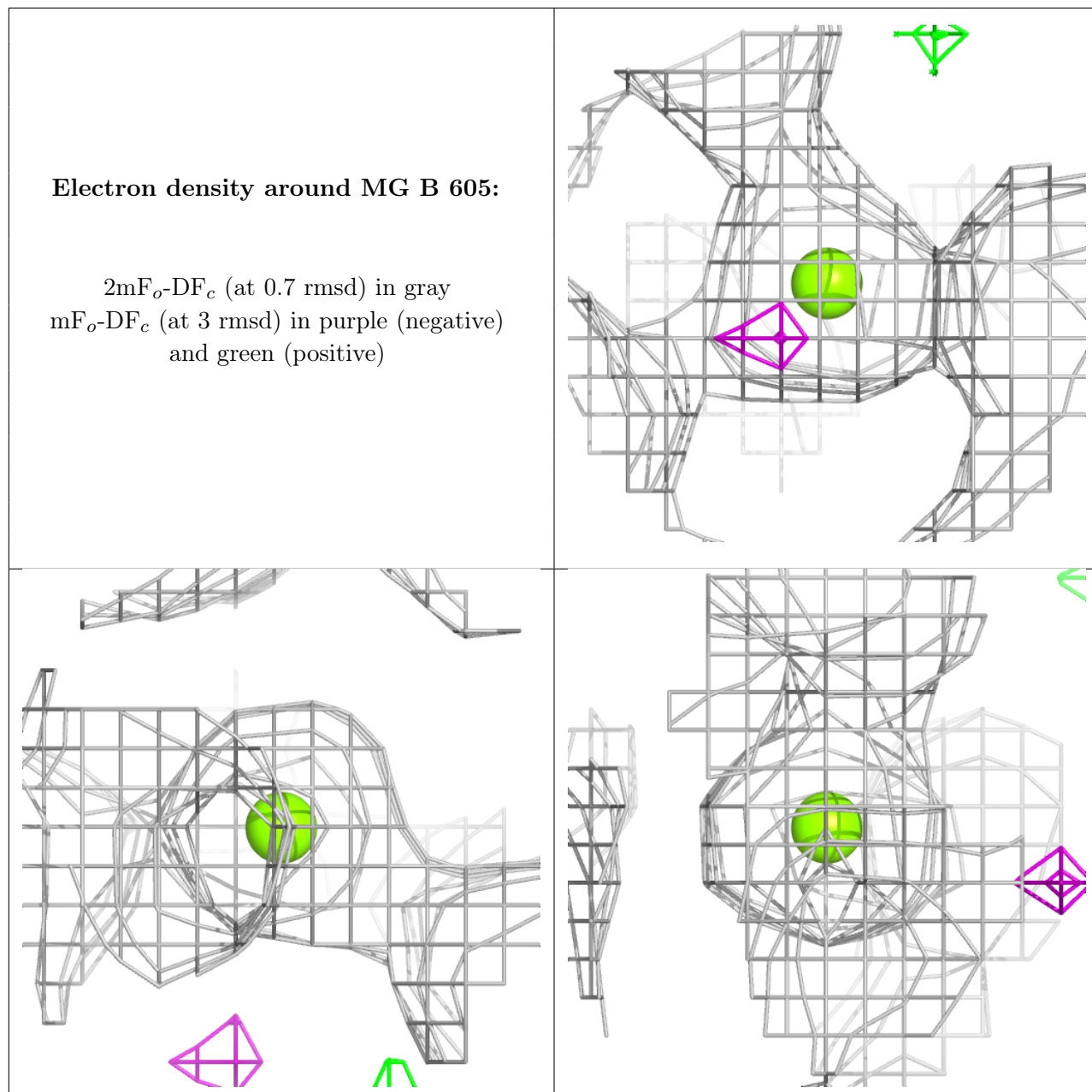
**Electron density around MG A 608:**

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



**Electron density around MG B 605:**

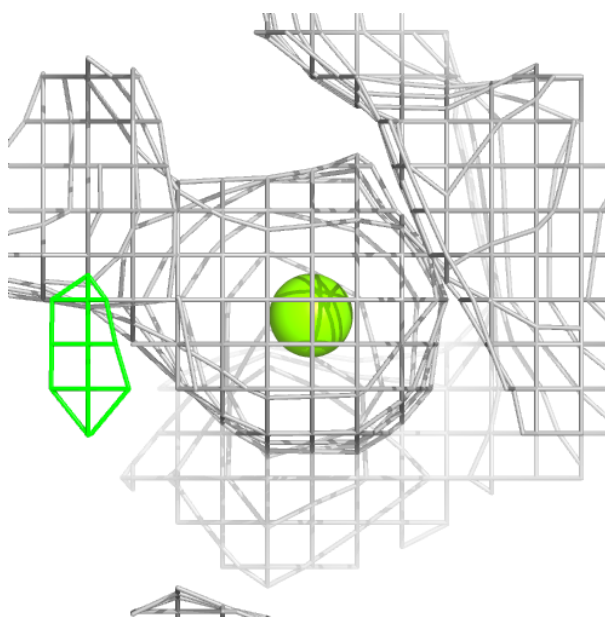
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





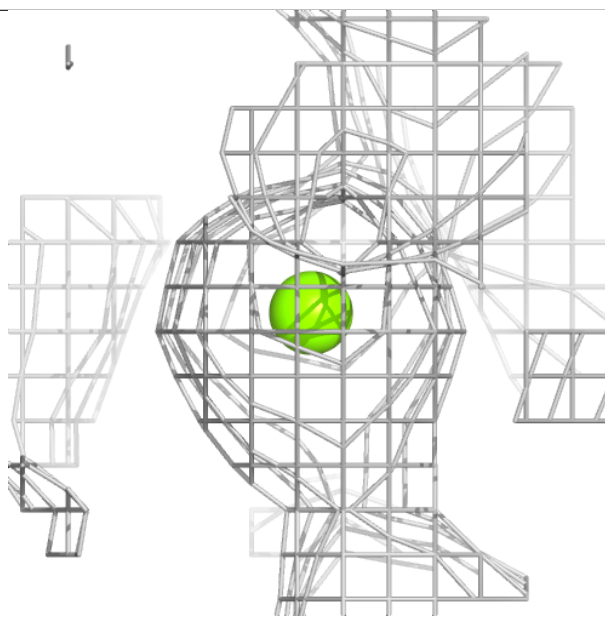
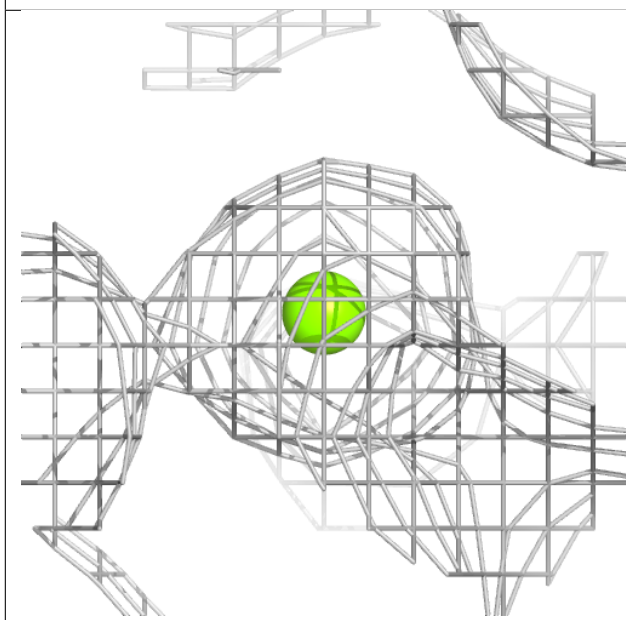
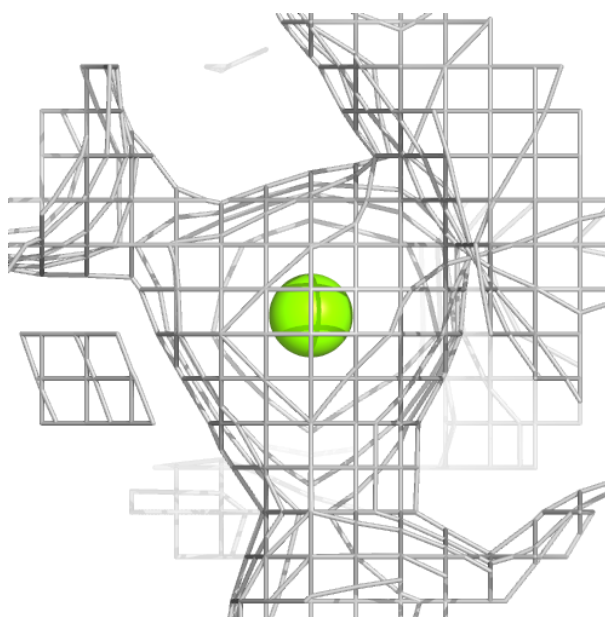
**Electron density around MG B 602:**

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



**Electron density around MG B 603:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.