



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 4, 2023 – 12:23 PM JST

PDB ID : 8GT7
Title : Structure of falcipain and human Stefin A mutant complex
Authors : Chakraborty, S.; Biswas, S.
Deposited on : 2022-09-07
Resolution : 3.28 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

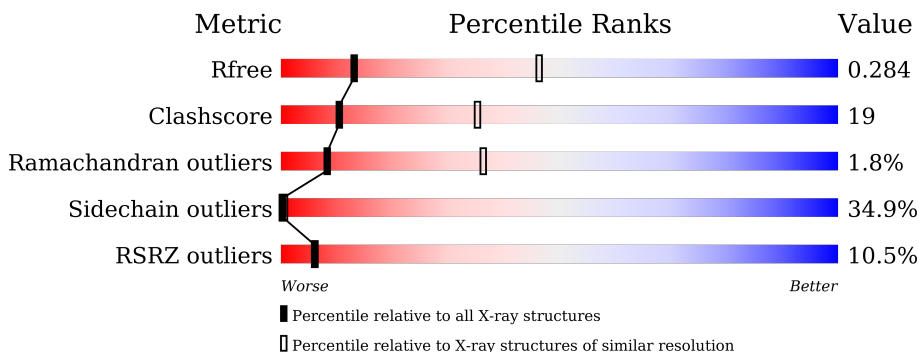
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	241	
1	C	241	
2	B	98	
2	D	98	
3	E	9	
4	F	9	

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
11	EDO	B	143	-	-	-	X
5	GOL	C	305	-	-	-	X
6	NA	A	356	-	-	-	X
6	NA	B	114	-	-	-	X
6	NA	B	115	-	-	-	X
6	NA	B	141	-	-	-	X
6	NA	C	341	-	-	-	X
6	NA	D	114	-	-	-	X
7	PG4	A	326	-	-	-	X
9	PEG	B	129	-	-	-	X
9	PEG	D	104	-	-	-	X
9	PEG	D	105	-	-	-	X

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 7507 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 Cysteine proteinase falcipain 2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	241	1914	1213	315	372	14	0	1	0
1	C	241	1909	1210	314	371	14	0	0	0

- Molecule 2 is a protein called Cystatin-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	98	777	492	128	155	2	0	0	0
2	D	98	777	492	128	155	2	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	68	ARG	LYS	engineered mutation	UNP P01040
D	68	ARG	LYS	engineered mutation	UNP P01040

- Molecule 3 is a protein called LYS-GLU-ILE-VAL-ASN-PRO-LEU-THR-LYS.

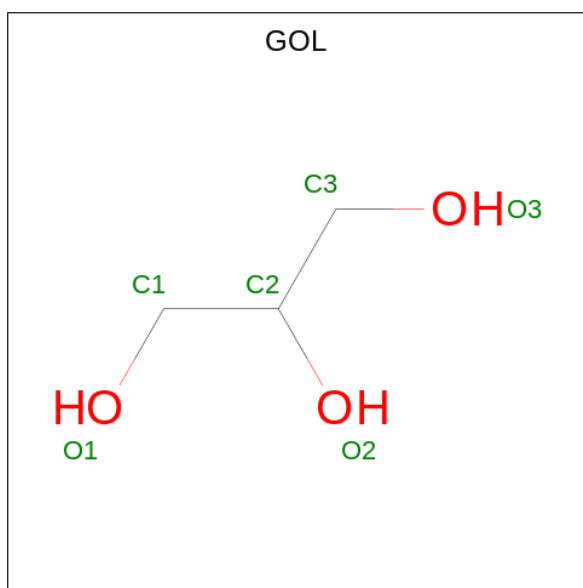
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	9	73	47	12	14	0	0	0

- Molecule 4 is a protein called VAL-ASN-PRO-LEU-THR-LYS-LYS-GLY-GLU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	9	69	43	12	14	0	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃) (labeled as "Ligand

of Interest" by depositor).



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

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

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

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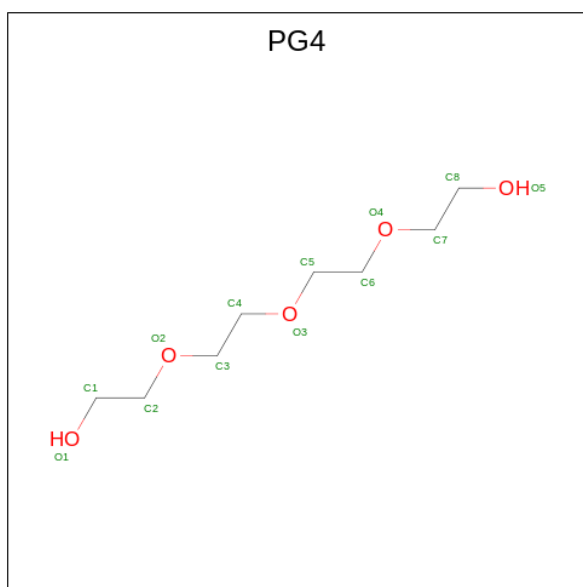
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	14	Total Na 14 14	0	0
6	B	11	Total Na 11 11	0	0
6	C	8	Total Na 8 8	0	0
6	D	8	Total Na 8 8	0	0
6	E	1	Total Na 1 1	0	0
6	F	2	Total Na 2 2	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0
7	A	1	Total C O 13 8 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	C	1	Total	C	O	0	0
			13	8	5		
7	C	1	Total	C	O	0	0
			13	8	5		
7	C	1	Total	C	O	0	0
			13	8	5		
7	C	1	Total	C	O	0	0
			13	8	5		
7	C	1	Total	C	O	0	0
			13	8	5		
7	C	1	Total	C	O	0	0
			13	8	5		
7	C	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		
7	F	1	Total	C	O	0	0
			13	8	5		
7	F	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		

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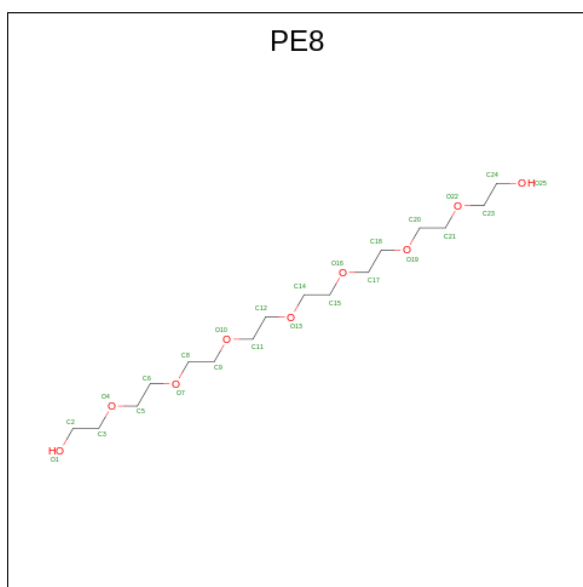
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	C	1	Total	C	O	0	0
			7	4	3		
9	C	1	Total	C	O	0	0
			7	4	3		

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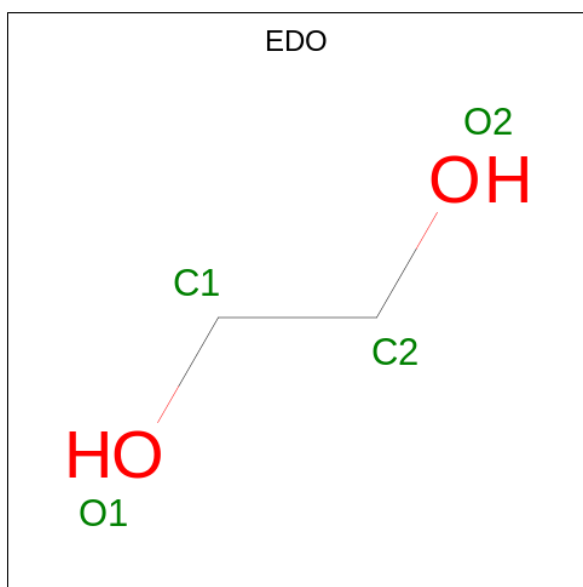
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			7	4	3		
9	C	1	Total	C	O	0	0
			7	4	3		
9	C	1	Total	C	O	0	0
			7	4	3		
9	C	1	Total	C	O	0	0
			7	4	3		
9	C	1	Total	C	O	0	0
			7	4	3		
9	C	1	Total	C	O	0	0
			7	4	3		
9	D	1	Total	C	O	0	0
			7	4	3		
9	D	1	Total	C	O	0	0
			7	4	3		
9	D	1	Total	C	O	0	0
			7	4	3		
9	D	1	Total	C	O	0	0
			7	4	3		
9	D	1	Total	C	O	0	0
			7	4	3		
9	D	1	Total	C	O	0	0
			7	4	3		
9	D	1	Total	C	O	0	0
			7	4	3		
9	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: C₁₆H₃₄O₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 25 16 9	0	0
10	A	1	Total C O 25 16 9	0	0
10	A	1	Total C O 25 16 9	0	0
10	B	1	Total C O 25 16 9	0	0
10	B	1	Total C O 25 16 9	0	0
10	B	1	Total C O 25 16 9	0	0
10	B	1	Total C O 25 16 9	0	0
10	B	1	Total C O 25 16 9	0	0
10	C	1	Total C O 25 16 9	0	0
10	E	1	Total C O 25 16 9	0	0
10	E	1	Total C O 25 16 9	0	0
10	F	1	Total C O 25 16 9	0	0
10	F	1	Total C O 25 16 9	0	0

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	67	Total O 67 67	0	0
12	B	42	Total O 42 42	0	0
12	C	41	Total O 41 41	0	0
12	D	27	Total O 27 27	0	0

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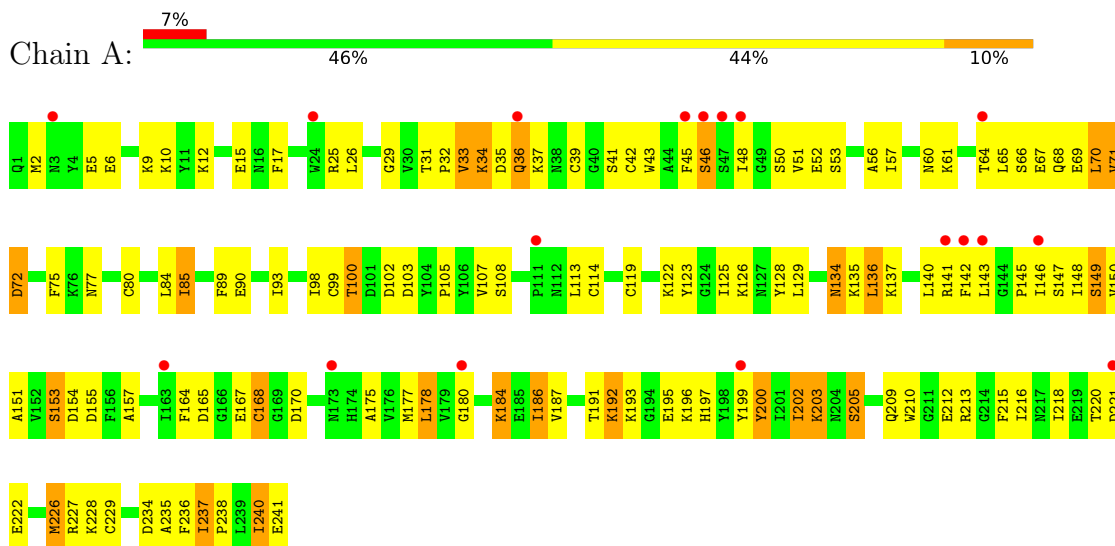
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	E	11	Total	O	0	0
			11	11		
12	F	7	Total	O	0	0
			7	7		

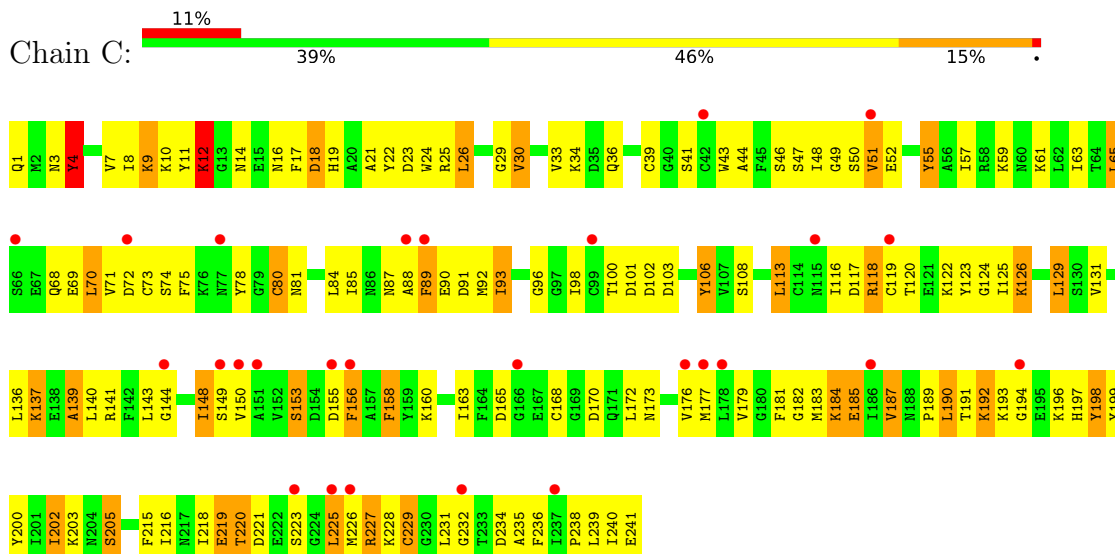
3 Residue-property plots

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

- Molecule 1: Cysteine proteinase falcipain 2a

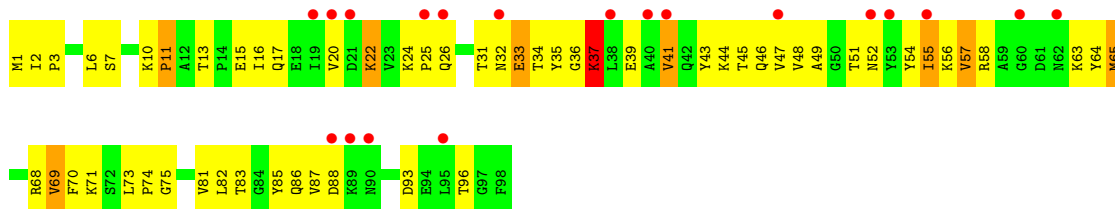


- Molecule 1: Cysteine proteinase falcipain 2a



- Molecule 2: Cystatin-A





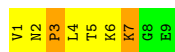
- Molecule 2: Cystatin-A



- Molecule 3: LYS-GLU-ILE-VAL-ASN-PRO-LEU-THR-LYS



- Molecule 4: VAL-ASN-PRO-LEU-THR-LYS-LYS-GLY-GLU



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.46Å 119.62Å 65.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.09 – 3.28 44.02 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.09-3.28) 99.7 (44.02-3.28)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.25Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.272 , 0.300 0.275 , 0.284	Depositor DCC
R_{free} test set	715 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	90.7	Xtrriage
Anisotropy	0.515	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.046 for k,h,-l	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	7507	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EDO, GOL, PE8, SO4, NA, PG4

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	0/1959	0.70	0/2641
1	C	0.37	0/1951	0.74	0/2630
2	B	0.44	0/790	0.77	0/1065
2	D	0.45	0/790	0.80	1/1065 (0.1%)
3	E	0.34	0/73	0.72	0/96
4	F	0.40	0/69	0.85	0/90
All	All	0.39	0/5632	0.74	1/7587 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	54	TYR	CA-CB-CG	5.47	123.80	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	16	ASN	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	1914	0	1834	70	0
1	C	1909	0	1830	89	0
2	B	777	0	780	31	0
2	D	777	0	780	50	0
3	E	73	0	85	3	0
4	F	69	0	77	5	0
5	A	120	0	160	4	0
5	B	84	0	112	2	0
5	C	96	0	128	5	0
5	D	60	0	80	3	0
5	E	24	0	32	1	0
5	F	6	0	8	0	0
6	A	14	0	0	0	0
6	B	11	0	0	0	0
6	C	8	0	0	0	0
6	D	8	0	0	0	0
6	E	1	0	0	0	0
6	F	2	0	0	0	0
7	A	182	0	252	5	0
7	B	156	0	216	7	0
7	C	117	0	162	13	0
7	D	78	0	108	3	0
7	E	65	0	90	2	0
7	F	26	0	36	2	0
8	A	10	0	0	0	0
8	C	10	0	0	0	0
8	E	5	0	0	0	0
9	A	126	0	180	5	0
9	B	105	0	150	2	0
9	C	77	0	110	2	0
9	D	70	0	100	0	0
10	A	75	0	102	2	0
10	B	100	0	136	5	0
10	C	25	0	34	2	0
10	E	50	0	68	4	0
10	F	50	0	68	4	0
11	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	8	0	12	0	0
11	D	12	0	18	2	0
11	E	8	0	12	0	0
12	A	67	0	0	1	0
12	B	42	0	0	0	0
12	C	41	0	0	2	0
12	D	27	0	0	1	0
12	E	11	0	0	1	0
12	F	7	0	0	0	0
All	All	7507	0	7766	280	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 19.

The worst 5 of 280 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:227:ARG:HD2	1:C:228:LYS:H	1.37	0.87
2:D:21:ASP:O	2:D:25:PRO:HD2	1.78	0.83
1:C:29:GLY:HA2	1:C:57:ILE:HD11	1.60	0.83
2:D:22:LYS:HD2	2:D:80:LEU:HD11	1.65	0.79
1:C:68:GLN:HA	1:C:71:VAL:HG12	1.66	0.78

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	240/241 (100%)	196 (82%)	42 (18%)	2 (1%)	19 52
1	C	239/241 (99%)	180 (75%)	55 (23%)	4 (2%)	9 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	96/98 (98%)	63 (66%)	31 (32%)	2 (2%)	7	33
2	D	96/98 (98%)	63 (66%)	30 (31%)	3 (3%)	4	24
3	E	7/9 (78%)	3 (43%)	4 (57%)	0	100	100
4	F	7/9 (78%)	4 (57%)	2 (29%)	1 (14%)	0	1
All	All	685/696 (98%)	509 (74%)	164 (24%)	12 (2%)	8	36

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	VAL
2	B	37	LYS
1	C	4	TYR
1	C	139	ALA
2	D	64	TYR

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	208/207 (100%)	139 (67%)	69 (33%)	0	0
1	C	207/207 (100%)	133 (64%)	74 (36%)	0	0
2	B	85/85 (100%)	55 (65%)	30 (35%)	0	0
2	D	85/85 (100%)	51 (60%)	34 (40%)	0	0
3	E	9/9 (100%)	8 (89%)	1 (11%)	6	24
4	F	8/8 (100%)	5 (62%)	3 (38%)	0	0
All	All	602/601 (100%)	391 (65%)	211 (35%)	0	0

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	65	LEU
1	C	158	PHE

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Mol	Chain	Res	Type
2	D	80	LEU
1	C	81	ASN
1	C	117	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	36	GLN
1	C	204	ASN
2	D	26	GLN
2	D	17	GLN
1	A	174	HIS

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 236 ligands modelled in this entry, 44 are monoatomic - leaving 192 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	$\# Z > 2$
5	GOL	C	347	-	5,5,5	0.94	0	5,5,5	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PEG	A	339	-	6,6,6	0.10	0	5,5,5	0.08	0
5	GOL	B	107	-	5,5,5	0.96	0	5,5,5	1.07	0
7	PG4	D	120	-	12,12,12	0.11	0	11,11,11	0.66	0
7	PG4	A	325	-	12,12,12	0.16	0	11,11,11	0.54	0
9	PEG	B	131	-	6,6,6	0.12	0	5,5,5	0.05	0
9	PEG	A	340	-	6,6,6	0.12	0	5,5,5	0.08	0
11	EDO	B	144	-	3,3,3	0.50	0	2,2,2	0.37	0
11	EDO	A	351	-	3,3,3	0.46	0	2,2,2	0.36	0
5	GOL	A	313	-	5,5,5	0.97	0	5,5,5	1.06	0
5	GOL	C	306	-	5,5,5	0.98	0	5,5,5	1.18	1 (20%)
9	PEG	C	339	-	6,6,6	0.09	0	5,5,5	0.11	0
9	PEG	A	330	-	6,6,6	0.11	0	5,5,5	0.07	0
5	GOL	A	312	-	5,5,5	1.01	0	5,5,5	0.95	0
9	PEG	D	127	-	6,6,6	0.10	0	5,5,5	0.10	0
10	PE8	A	342	-	24,24,24	0.49	0	23,23,23	0.24	0
7	PG4	D	118	-	12,12,12	0.12	0	11,11,11	0.73	0
5	GOL	A	305	-	5,5,5	0.96	0	5,5,5	1.05	0
9	PEG	B	132	-	6,6,6	0.10	0	5,5,5	0.10	0
9	PEG	C	333	-	6,6,6	0.09	0	5,5,5	0.14	0
5	GOL	A	362	-	5,5,5	0.94	0	5,5,5	1.10	0
9	PEG	D	123	-	6,6,6	0.10	0	5,5,5	0.07	0
9	PEG	A	336	-	6,6,6	0.10	0	5,5,5	0.12	0
9	PEG	D	105	-	6,6,6	0.10	0	5,5,5	0.10	0
7	PG4	F	105	-	12,12,12	0.15	0	11,11,11	0.58	0
9	PEG	A	332	-	6,6,6	0.10	0	5,5,5	0.07	0
11	EDO	E	111	-	3,3,3	0.46	0	2,2,2	0.42	0
5	GOL	D	131	-	5,5,5	0.95	0	5,5,5	1.17	1 (20%)
5	GOL	E	104	-	5,5,5	0.93	0	5,5,5	1.13	1 (20%)
5	GOL	D	111	-	5,5,5	0.96	0	5,5,5	1.08	0
5	GOL	C	314	-	5,5,5	0.89	0	5,5,5	1.08	0
5	GOL	F	103	-	5,5,5	0.95	0	5,5,5	1.12	0
7	PG4	D	119	-	12,12,12	0.13	0	11,11,11	0.69	0
9	PEG	A	329	-	6,6,6	0.11	0	5,5,5	0.09	0
11	EDO	D	101	-	3,3,3	0.41	0	2,2,2	0.40	0
9	PEG	A	337	-	6,6,6	0.10	0	5,5,5	0.09	0
9	PEG	A	333	-	6,6,6	0.10	0	5,5,5	0.10	0
9	PEG	B	156	-	6,6,6	0.09	0	5,5,5	0.13	0
7	PG4	A	321	-	12,12,12	0.11	0	11,11,11	0.66	0
7	PG4	B	120	-	12,12,12	0.12	0	11,11,11	0.77	0
7	PG4	B	101	-	12,12,12	0.10	0	11,11,11	0.67	0
9	PEG	B	133	-	6,6,6	0.11	0	5,5,5	0.08	0
7	PG4	B	123	-	12,12,12	0.10	0	11,11,11	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PEG	B	127	-	6,6,6	0.10	0	5,5,5	0.06	0
9	PEG	A	341	-	6,6,6	0.11	0	5,5,5	0.05	0
5	GOL	A	373	-	5,5,5	0.89	0	5,5,5	0.98	0
5	GOL	D	113	-	5,5,5	1.00	0	5,5,5	1.00	0
9	PEG	C	334	-	6,6,6	0.16	0	5,5,5	0.19	0
7	PG4	E	105	-	12,12,12	0.13	0	11,11,11	0.62	0
11	EDO	D	102	2	3,3,3	0.34	0	2,2,2	0.61	0
9	PEG	A	371	-	6,6,6	0.10	0	5,5,5	0.08	0
7	PG4	C	302	-	12,12,12	0.13	0	11,11,11	0.53	0
5	GOL	B	112	-	5,5,5	0.92	0	5,5,5	1.18	1 (20%)
7	PG4	E	106	-	12,12,12	0.10	0	11,11,11	0.70	0
7	PG4	B	117	-	12,12,12	0.13	0	11,11,11	0.62	0
5	GOL	C	344	-	5,5,5	0.97	0	5,5,5	1.06	0
7	PG4	F	101	-	12,12,12	0.13	0	11,11,11	0.59	0
5	GOL	D	109	-	5,5,5	0.97	0	5,5,5	1.08	0
5	GOL	B	106	-	5,5,5	0.98	0	5,5,5	1.13	0
8	SO4	E	108	-	4,4,4	0.14	0	6,6,6	0.05	0
5	GOL	C	305	-	5,5,5	1.03	0	5,5,5	0.95	0
9	PEG	C	328	-	6,6,6	0.11	0	5,5,5	0.06	0
5	GOL	B	153	-	5,5,5	0.97	0	5,5,5	1.07	0
9	PEG	B	157	-	6,6,6	0.15	0	5,5,5	0.24	0
5	GOL	A	303	-	5,5,5	0.95	0	5,5,5	1.07	0
10	PE8	E	109	-	24,24,24	0.48	0	23,23,23	0.27	0
10	PE8	E	110	-	24,24,24	0.48	0	23,23,23	0.31	0
7	PG4	A	366	-	12,12,12	0.11	0	11,11,11	0.73	0
5	GOL	D	110	-	5,5,5	0.99	0	5,5,5	1.13	0
9	PEG	B	158	-	6,6,6	0.10	0	5,5,5	0.10	0
5	GOL	B	104	-	5,5,5	0.94	0	5,5,5	1.11	1 (20%)
5	GOL	C	313	-	5,5,5	0.90	0	5,5,5	1.07	0
7	PG4	A	365	-	12,12,12	0.10	0	11,11,11	0.60	0
9	PEG	D	104	-	6,6,6	0.10	0	5,5,5	0.08	0
10	PE8	B	102	-	24,24,24	0.48	0	23,23,23	0.27	0
7	PG4	C	322	-	12,12,12	0.09	0	11,11,11	0.66	0
9	PEG	C	329	-	6,6,6	0.12	0	5,5,5	0.08	0
5	GOL	C	345	-	5,5,5	0.97	0	5,5,5	1.10	0
5	GOL	A	304	-	5,5,5	0.97	0	5,5,5	1.06	0
9	PEG	A	346	-	6,6,6	0.12	0	5,5,5	0.08	0
7	PG4	A	369	-	12,12,12	0.09	0	11,11,11	0.70	0
7	PG4	E	114	-	12,12,12	0.10	0	11,11,11	0.65	0
5	GOL	A	308	-	5,5,5	0.94	0	5,5,5	1.10	0
5	GOL	C	309	-	5,5,5	0.94	0	5,5,5	1.20	1 (20%)
5	GOL	C	312	-	5,5,5	0.90	0	5,5,5	1.14	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PG4	C	321	-	12,12,12	0.10	0	11,11,11	0.70	0
10	PE8	C	335	-	24,24,24	0.48	0	23,23,23	0.23	0
5	GOL	C	311	-	5,5,5	0.95	0	5,5,5	1.14	1 (20%)
7	PG4	B	118	-	12,12,12	0.14	0	11,11,11	0.71	0
5	GOL	A	307	-	5,5,5	0.99	0	5,5,5	1.17	0
5	GOL	D	106	-	5,5,5	1.02	0	5,5,5	0.96	0
8	SO4	C	326	-	4,4,4	0.13	0	6,6,6	0.06	0
10	PE8	F	106	-	24,24,24	0.47	0	23,23,23	0.27	0
5	GOL	B	154	-	5,5,5	0.97	0	5,5,5	1.08	0
5	GOL	A	347	-	5,5,5	0.78	0	5,5,5	1.22	1 (20%)
5	GOL	A	311	-	5,5,5	0.89	0	5,5,5	1.05	0
5	GOL	A	345	-	5,5,5	0.96	0	5,5,5	1.16	1 (20%)
5	GOL	C	307	-	5,5,5	0.95	0	5,5,5	1.12	0
5	GOL	B	110	-	5,5,5	0.95	0	5,5,5	1.18	1 (20%)
5	GOL	E	102	-	5,5,5	0.96	0	5,5,5	1.18	0
7	PG4	B	119	-	12,12,12	0.12	0	11,11,11	0.71	0
9	PEG	A	331	-	6,6,6	0.16	0	5,5,5	0.26	0
10	PE8	A	344	-	24,24,24	0.48	0	23,23,23	0.23	0
9	PEG	C	303	-	6,6,6	0.10	0	5,5,5	0.10	0
9	PEG	B	128	-	6,6,6	0.11	0	5,5,5	0.10	0
5	GOL	D	107	-	5,5,5	0.92	0	5,5,5	1.09	0
7	PG4	D	117	-	12,12,12	0.11	0	11,11,11	0.70	0
10	PE8	B	137	-	24,24,24	0.47	0	23,23,23	0.26	0
7	PG4	B	122	-	12,12,12	0.10	0	11,11,11	0.67	0
9	PEG	D	125	-	6,6,6	0.11	0	5,5,5	0.10	0
9	PEG	D	121	-	6,6,6	0.10	0	5,5,5	0.10	0
7	PG4	C	325	-	12,12,12	0.11	0	11,11,11	0.73	0
11	EDO	B	143	-	3,3,3	0.43	0	2,2,2	0.35	0
5	GOL	B	111	-	5,5,5	0.96	0	5,5,5	0.97	0
5	GOL	C	337	-	5,5,5	0.93	0	5,5,5	1.18	1 (20%)
9	PEG	B	134	-	6,6,6	0.10	0	5,5,5	0.10	0
10	PE8	A	343	-	24,24,24	0.49	0	23,23,23	0.26	0
11	EDO	E	101	-	3,3,3	0.41	0	2,2,2	0.40	0
9	PEG	D	128	-	6,6,6	0.11	0	5,5,5	0.07	0
7	PG4	C	324	-	12,12,12	0.12	0	11,11,11	0.65	0
5	GOL	B	105	-	5,5,5	0.99	0	5,5,5	1.00	0
5	GOL	C	304	-	5,5,5	0.94	0	5,5,5	1.16	1 (20%)
9	PEG	C	332	-	6,6,6	0.11	0	5,5,5	0.09	0
5	GOL	B	103	-	5,5,5	0.96	0	5,5,5	1.15	0
7	PG4	D	103	-	12,12,12	0.10	0	11,11,11	0.65	0
10	PE8	B	136	-	24,24,24	0.48	0	23,23,23	0.32	0
9	PEG	C	331	-	6,6,6	0.17	0	5,5,5	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	D	137	-	5,5,5	0.88	0	5,5,5	0.97	0
9	PEG	B	129	-	6,6,6	0.12	0	5,5,5	0.07	0
8	SO4	C	301	-	4,4,4	0.14	0	6,6,6	0.05	0
10	PE8	F	102	-	24,24,24	0.48	0	23,23,23	0.23	0
9	PEG	A	335	-	6,6,6	0.10	0	5,5,5	0.11	0
5	GOL	B	140	-	5,5,5	0.96	0	5,5,5	1.17	1 (20%)
7	PG4	A	324	-	12,12,12	0.10	0	11,11,11	0.68	0
9	PEG	A	353	-	6,6,6	0.11	0	5,5,5	0.09	0
5	GOL	D	108	-	5,5,5	0.94	0	5,5,5	1.19	1 (20%)
9	PEG	C	327	-	6,6,6	0.10	0	5,5,5	0.12	0
9	PEG	C	330	-	6,6,6	0.10	0	5,5,5	0.11	0
5	GOL	A	310	-	5,5,5	1.01	0	5,5,5	0.98	0
9	PEG	A	334	-	6,6,6	0.10	0	5,5,5	0.08	0
9	PEG	A	370	-	6,6,6	0.12	0	5,5,5	0.09	0
7	PG4	A	320	-	12,12,12	0.10	0	11,11,11	0.69	0
5	GOL	A	306	-	5,5,5	0.95	0	5,5,5	1.06	0
5	GOL	A	302	-	5,5,5	0.91	0	5,5,5	1.15	0
5	GOL	A	363	-	5,5,5	0.96	0	5,5,5	1.06	0
7	PG4	A	352	-	12,12,12	0.10	0	11,11,11	0.69	0
7	PG4	B	155	-	12,12,12	0.09	0	11,11,11	0.69	0
7	PG4	B	124	-	12,12,12	0.11	0	11,11,11	0.65	0
5	GOL	A	301	-	5,5,5	0.93	0	5,5,5	1.11	1 (20%)
5	GOL	A	314	-	5,5,5	0.94	0	5,5,5	1.16	1 (20%)
7	PG4	A	326	-	12,12,12	0.12	0	11,11,11	0.62	0
5	GOL	B	109	-	5,5,5	0.95	0	5,5,5	1.12	1 (20%)
9	PEG	B	126	-	6,6,6	0.11	0	5,5,5	0.09	0
9	PEG	C	346	-	6,6,6	0.09	0	5,5,5	0.11	0
5	GOL	A	364	-	5,5,5	0.96	0	5,5,5	1.11	0
7	PG4	B	125	-	12,12,12	0.13	0	11,11,11	0.75	0
5	GOL	B	108	-	5,5,5	0.95	0	5,5,5	1.16	1 (20%)
7	PG4	B	121	-	12,12,12	0.10	0	11,11,11	0.74	0
7	PG4	A	322	-	12,12,12	0.12	0	11,11,11	0.64	0
7	PG4	A	368	-	12,12,12	0.08	0	11,11,11	0.71	0
9	PEG	A	338	-	6,6,6	0.11	0	5,5,5	0.09	0
9	PEG	D	124	-	6,6,6	0.11	0	5,5,5	0.08	0
7	PG4	B	116	-	12,12,12	0.11	0	11,11,11	0.68	0
5	GOL	E	113	-	5,5,5	0.93	0	5,5,5	0.93	0
7	PG4	C	319	-	12,12,12	0.12	0	11,11,11	0.71	0
7	PG4	A	323	-	12,12,12	0.14	0	11,11,11	0.66	0
9	PEG	B	142	-	6,6,6	0.10	0	5,5,5	0.10	0
9	PEG	D	122	-	6,6,6	0.07	0	5,5,5	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	C	338	-	5,5,5	0.93	0	5,5,5	1.12	1 (20%)
11	EDO	D	130	-	3,3,3	0.47	0	2,2,2	0.36	0
5	GOL	D	112	-	5,5,5	0.97	0	5,5,5	1.17	1 (20%)
9	PEG	A	372	-	6,6,6	0.10	0	5,5,5	0.10	0
7	PG4	E	107	-	12,12,12	0.11	0	11,11,11	0.64	0
5	GOL	B	152	-	5,5,5	0.93	0	5,5,5	1.13	1 (20%)
9	PEG	B	130	-	6,6,6	0.11	0	5,5,5	0.08	0
7	PG4	C	323	-	12,12,12	0.14	0	11,11,11	0.60	0
7	PG4	D	116	-	12,12,12	0.12	0	11,11,11	0.62	0
7	PG4	C	336	-	12,12,12	0.10	0	11,11,11	0.65	0
9	PEG	B	139	-	6,6,6	0.09	0	5,5,5	0.09	0
5	GOL	C	308	-	5,5,5	0.98	0	5,5,5	1.06	0
8	SO4	A	328	-	4,4,4	0.14	0	6,6,6	0.04	0
10	PE8	B	138	-	24,24,24	0.47	0	23,23,23	0.28	0
5	GOL	C	310	-	5,5,5	0.93	0	5,5,5	1.09	0
7	PG4	E	115	-	12,12,12	0.12	0	11,11,11	0.57	0
9	PEG	B	135	-	6,6,6	0.12	0	5,5,5	0.08	0
7	PG4	C	320	-	12,12,12	0.12	0	11,11,11	0.50	0
7	PG4	A	319	-	12,12,12	0.10	0	11,11,11	0.67	0
7	PG4	A	367	-	12,12,12	0.10	0	11,11,11	0.69	0
9	PEG	D	126	-	6,6,6	0.10	0	5,5,5	0.09	0
5	GOL	E	103	-	5,5,5	0.92	0	5,5,5	1.12	0
8	SO4	A	327	-	4,4,4	0.13	0	6,6,6	0.06	0
5	GOL	A	309	-	5,5,5	0.96	0	5,5,5	1.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	347	-	-	2/4/4/4	-
9	PEG	A	339	-	-	3/4/4/4	-
5	GOL	B	107	-	-	0/4/4/4	-
7	PG4	D	120	-	-	7/10/10/10	-
7	PG4	A	325	-	-	8/10/10/10	-
9	PEG	B	131	-	-	2/4/4/4	-
9	PEG	A	340	-	-	4/4/4/4	-
11	EDO	B	144	-	-	1/1/1/1	-
11	EDO	A	351	-	-	1/1/1/1	-
5	GOL	A	313	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	306	-	-	2/4/4/4	-
9	PEG	C	339	-	-	3/4/4/4	-
9	PEG	A	330	-	-	2/4/4/4	-
5	GOL	A	312	-	-	4/4/4/4	-
9	PEG	D	127	-	-	2/4/4/4	-
10	PE8	A	342	-	-	13/22/22/22	-
7	PG4	D	118	-	-	8/10/10/10	-
5	GOL	A	305	-	-	0/4/4/4	-
9	PEG	B	132	-	-	3/4/4/4	-
9	PEG	C	333	-	-	2/4/4/4	-
5	GOL	A	362	-	-	4/4/4/4	-
9	PEG	D	123	-	-	2/4/4/4	-
9	PEG	A	336	-	-	2/4/4/4	-
9	PEG	D	105	-	-	3/4/4/4	-
7	PG4	F	105	-	-	5/10/10/10	-
9	PEG	A	332	-	-	3/4/4/4	-
11	EDO	E	111	-	-	1/1/1/1	-
5	GOL	D	131	-	-	4/4/4/4	-
5	GOL	E	104	-	-	2/4/4/4	-
5	GOL	D	111	-	-	2/4/4/4	-
5	GOL	C	314	-	-	4/4/4/4	-
5	GOL	F	103	-	-	2/4/4/4	-
7	PG4	D	119	-	-	4/10/10/10	-
9	PEG	A	329	-	-	1/4/4/4	-
11	EDO	D	101	-	-	0/1/1/1	-
9	PEG	A	337	-	-	4/4/4/4	-
9	PEG	A	333	-	-	3/4/4/4	-
9	PEG	B	156	-	-	2/4/4/4	-
7	PG4	A	321	-	-	8/10/10/10	-
7	PG4	B	120	-	-	4/10/10/10	-
7	PG4	B	101	-	-	3/10/10/10	-
9	PEG	B	133	-	-	3/4/4/4	-
7	PG4	B	123	-	-	8/10/10/10	-
9	PEG	B	127	-	-	3/4/4/4	-
9	PEG	A	341	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	373	-	-	2/4/4/4	-
5	GOL	D	113	-	-	0/4/4/4	-
9	PEG	C	334	-	-	2/4/4/4	-
7	PG4	E	105	-	-	4/10/10/10	-
11	EDO	D	102	2	-	1/1/1/1	-
9	PEG	A	371	-	-	1/4/4/4	-
7	PG4	C	302	-	-	5/10/10/10	-
5	GOL	B	112	-	-	2/4/4/4	-
7	PG4	E	106	-	-	7/10/10/10	-
7	PG4	B	117	-	-	7/10/10/10	-
5	GOL	C	344	-	-	2/4/4/4	-
7	PG4	F	101	-	-	6/10/10/10	-
5	GOL	D	109	-	-	2/4/4/4	-
5	GOL	B	106	-	-	0/4/4/4	-
5	GOL	C	305	-	-	2/4/4/4	-
9	PEG	C	328	-	-	2/4/4/4	-
5	GOL	B	153	-	-	0/4/4/4	-
9	PEG	B	157	-	-	3/4/4/4	-
5	GOL	A	303	-	-	1/4/4/4	-
10	PE8	E	109	-	-	11/22/22/22	-
10	PE8	E	110	-	-	16/22/22/22	-
7	PG4	A	366	-	-	5/10/10/10	-
5	GOL	D	110	-	-	2/4/4/4	-
9	PEG	B	158	-	-	2/4/4/4	-
5	GOL	B	104	-	-	2/4/4/4	-
5	GOL	C	313	-	-	2/4/4/4	-
7	PG4	A	365	-	-	8/10/10/10	-
9	PEG	D	104	-	-	1/4/4/4	-
10	PE8	B	102	-	-	9/22/22/22	-
7	PG4	C	322	-	-	5/10/10/10	-
9	PEG	C	329	-	-	3/4/4/4	-
5	GOL	C	345	-	-	2/4/4/4	-
5	GOL	A	304	-	-	2/4/4/4	-
9	PEG	A	346	-	-	3/4/4/4	-
7	PG4	A	369	-	-	6/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	E	114	-	-	7/10/10/10	-
5	GOL	A	308	-	-	0/4/4/4	-
5	GOL	C	309	-	-	4/4/4/4	-
5	GOL	C	312	-	-	4/4/4/4	-
7	PG4	C	321	-	-	6/10/10/10	-
10	PE8	C	335	-	-	13/22/22/22	-
5	GOL	C	311	-	-	4/4/4/4	-
7	PG4	B	118	-	-	5/10/10/10	-
5	GOL	A	307	-	-	2/4/4/4	-
5	GOL	D	106	-	-	3/4/4/4	-
10	PE8	F	106	-	-	16/22/22/22	-
5	GOL	B	154	-	-	0/4/4/4	-
5	GOL	A	347	-	-	2/4/4/4	-
5	GOL	A	311	-	-	4/4/4/4	-
5	GOL	A	345	-	-	4/4/4/4	-
5	GOL	C	307	-	-	4/4/4/4	-
5	GOL	B	110	-	-	1/4/4/4	-
5	GOL	E	102	-	-	4/4/4/4	-
7	PG4	B	119	-	-	7/10/10/10	-
9	PEG	A	331	-	-	3/4/4/4	-
10	PE8	A	344	-	-	12/22/22/22	-
9	PEG	C	303	-	-	3/4/4/4	-
9	PEG	B	128	-	-	2/4/4/4	-
5	GOL	D	107	-	-	4/4/4/4	-
7	PG4	D	117	-	-	7/10/10/10	-
10	PE8	B	137	-	-	12/22/22/22	-
7	PG4	B	122	-	-	7/10/10/10	-
9	PEG	D	125	-	-	2/4/4/4	-
9	PEG	D	121	-	-	3/4/4/4	-
7	PG4	C	325	-	-	7/10/10/10	-
11	EDO	B	143	-	-	0/1/1/1	-
5	GOL	B	111	-	-	4/4/4/4	-
5	GOL	C	337	-	-	2/4/4/4	-
9	PEG	B	134	-	-	3/4/4/4	-
10	PE8	A	343	-	-	15/22/22/22	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	EDO	E	101	-	-	0/1/1/1	-
9	PEG	D	128	-	-	2/4/4/4	-
7	PG4	C	324	-	-	7/10/10/10	-
5	GOL	B	105	-	-	0/4/4/4	-
5	GOL	C	304	-	-	4/4/4/4	-
9	PEG	C	332	-	-	3/4/4/4	-
5	GOL	B	103	-	-	4/4/4/4	-
7	PG4	D	103	-	-	7/10/10/10	-
10	PE8	B	136	-	-	13/22/22/22	-
9	PEG	C	331	-	-	3/4/4/4	-
5	GOL	D	137	-	-	2/4/4/4	-
9	PEG	B	129	-	-	2/4/4/4	-
10	PE8	F	102	-	-	14/22/22/22	-
9	PEG	A	335	-	-	3/4/4/4	-
5	GOL	B	140	-	-	2/4/4/4	-
7	PG4	A	324	-	-	7/10/10/10	-
9	PEG	A	353	-	-	3/4/4/4	-
5	GOL	D	108	-	-	1/4/4/4	-
9	PEG	C	327	-	-	2/4/4/4	-
9	PEG	C	330	-	-	3/4/4/4	-
5	GOL	A	310	-	-	2/4/4/4	-
9	PEG	A	334	-	-	2/4/4/4	-
9	PEG	A	370	-	-	2/4/4/4	-
7	PG4	A	320	-	-	5/10/10/10	-
5	GOL	A	306	-	-	2/4/4/4	-
5	GOL	A	302	-	-	2/4/4/4	-
5	GOL	A	363	-	-	2/4/4/4	-
7	PG4	A	352	-	-	8/10/10/10	-
7	PG4	B	155	-	-	6/10/10/10	-
7	PG4	B	124	-	-	4/10/10/10	-
5	GOL	A	301	-	-	4/4/4/4	-
5	GOL	A	314	-	-	2/4/4/4	-
7	PG4	A	326	-	-	8/10/10/10	-
5	GOL	B	109	-	-	2/4/4/4	-
9	PEG	B	126	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PEG	C	346	-	-	2/4/4/4	-
5	GOL	A	364	-	-	3/4/4/4	-
7	PG4	B	125	-	-	7/10/10/10	-
5	GOL	B	108	-	-	2/4/4/4	-
7	PG4	B	121	-	-	7/10/10/10	-
7	PG4	A	322	-	-	3/10/10/10	-
7	PG4	A	368	-	-	7/10/10/10	-
9	PEG	A	338	-	-	2/4/4/4	-
9	PEG	D	124	-	-	2/4/4/4	-
7	PG4	B	116	-	-	7/10/10/10	-
5	GOL	E	113	-	-	3/4/4/4	-
7	PG4	C	319	-	-	6/10/10/10	-
7	PG4	A	323	-	-	6/10/10/10	-
9	PEG	B	142	-	-	1/4/4/4	-
9	PEG	D	122	-	-	1/4/4/4	-
5	GOL	C	338	-	-	2/4/4/4	-
11	EDO	D	130	-	-	1/1/1/1	-
5	GOL	D	112	-	-	3/4/4/4	-
9	PEG	A	372	-	-	3/4/4/4	-
7	PG4	E	107	-	-	2/10/10/10	-
5	GOL	B	152	-	-	3/4/4/4	-
9	PEG	B	130	-	-	4/4/4/4	-
7	PG4	C	323	-	-	6/10/10/10	-
7	PG4	D	116	-	-	3/10/10/10	-
7	PG4	C	336	-	-	4/10/10/10	-
9	PEG	B	139	-	-	3/4/4/4	-
5	GOL	C	308	-	-	4/4/4/4	-
10	PE8	B	138	-	-	15/22/22/22	-
5	GOL	C	310	-	-	4/4/4/4	-
7	PG4	E	115	-	-	5/10/10/10	-
9	PEG	B	135	-	-	1/4/4/4	-
7	PG4	C	320	-	-	7/10/10/10	-
7	PG4	A	319	-	-	5/10/10/10	-
7	PG4	A	367	-	-	6/10/10/10	-
9	PEG	D	126	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	E	103	-	-	2/4/4/4	-
5	GOL	A	309	-	-	2/4/4/4	-

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	347	GOL	C3-C2-C1	-2.41	102.34	111.70
5	C	309	GOL	C3-C2-C1	-2.20	103.15	111.70
5	B	104	GOL	C3-C2-C1	-2.11	103.51	111.70
5	C	304	GOL	C3-C2-C1	-2.11	103.51	111.70
5	C	337	GOL	C3-C2-C1	-2.10	103.55	111.70

There are no chirality outliers.

5 of 731 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	306	GOL	C1-C2-C3-O3
5	A	309	GOL	C1-C2-C3-O3
5	A	310	GOL	C1-C2-C3-O3
5	A	310	GOL	O2-C2-C3-O3
5	A	312	GOL	O1-C1-C2-C3

There are no ring outliers.

54 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	325	PG4	2	0
10	A	342	PE8	2	0
9	C	333	PEG	1	0
9	A	336	PEG	1	0
7	F	105	PG4	1	0
7	D	119	PG4	1	0
9	A	329	PEG	1	0
7	B	101	PG4	1	0
9	A	341	PEG	1	0
11	D	102	EDO	2	0
7	C	302	PG4	2	0
7	E	106	PG4	1	0
7	B	117	PG4	1	0

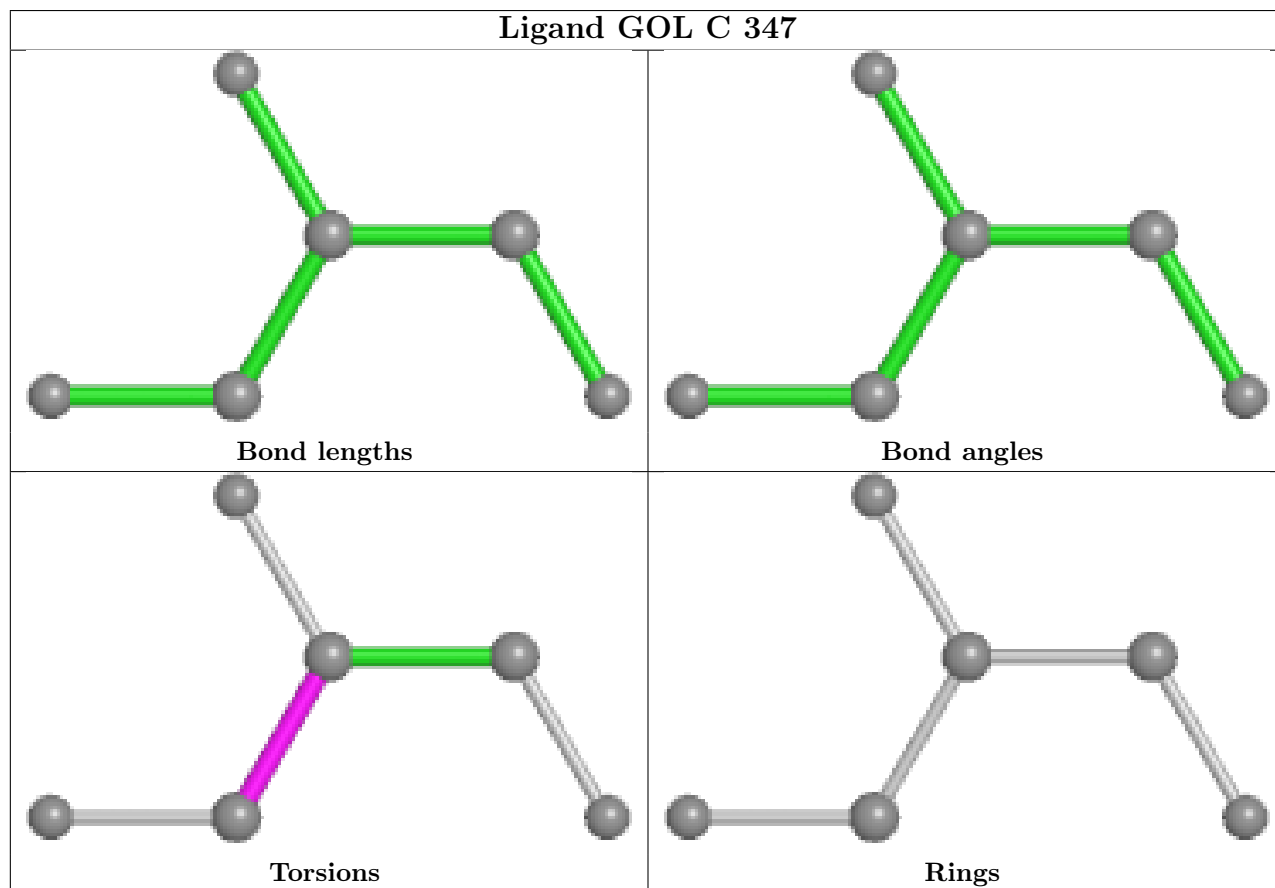
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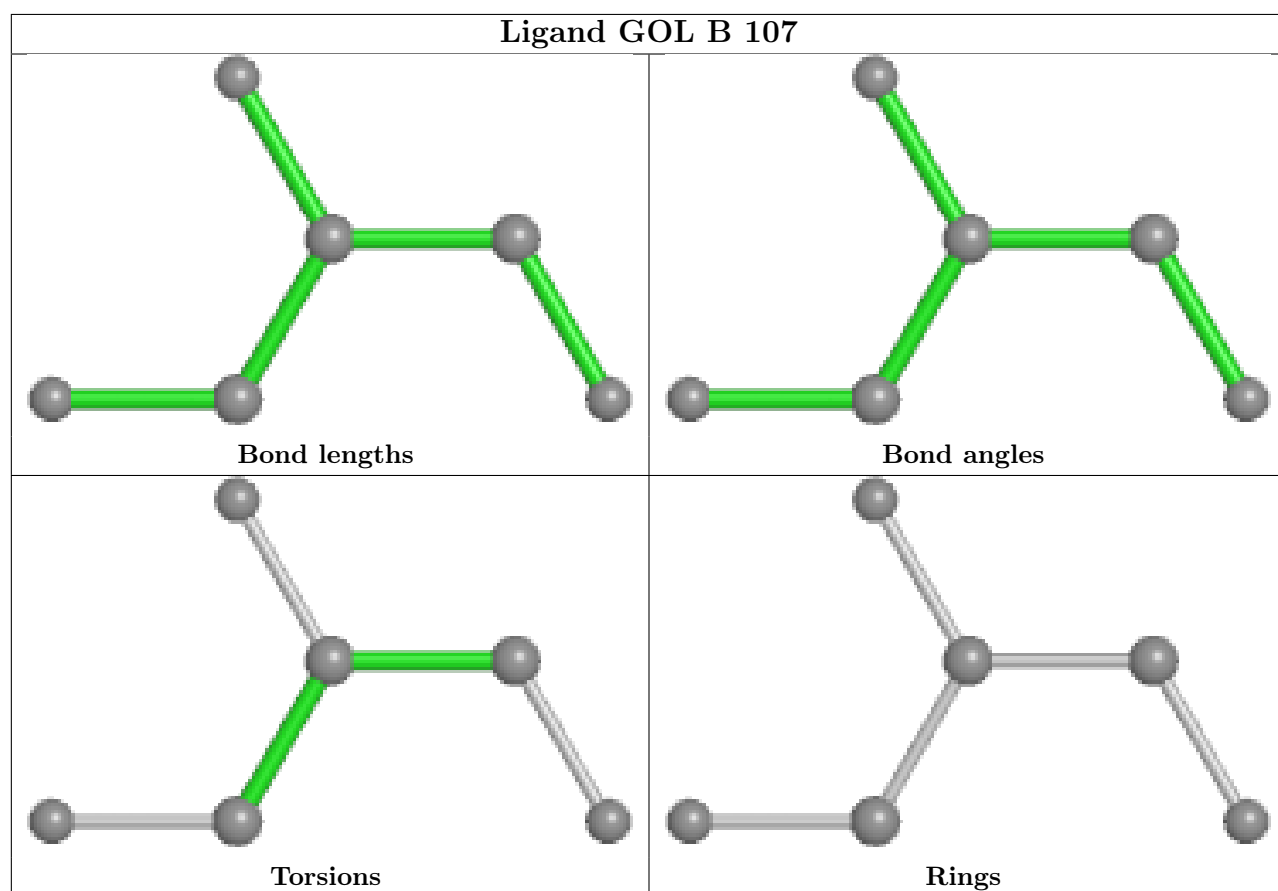
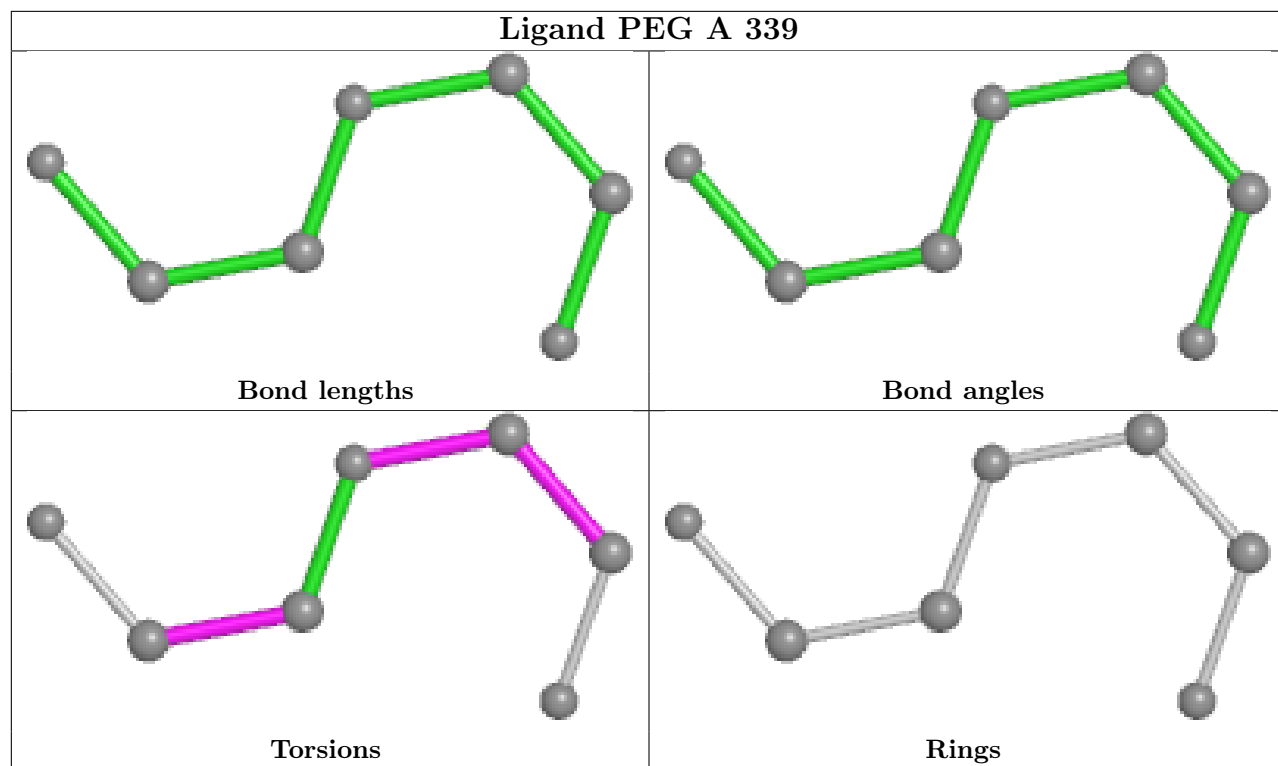
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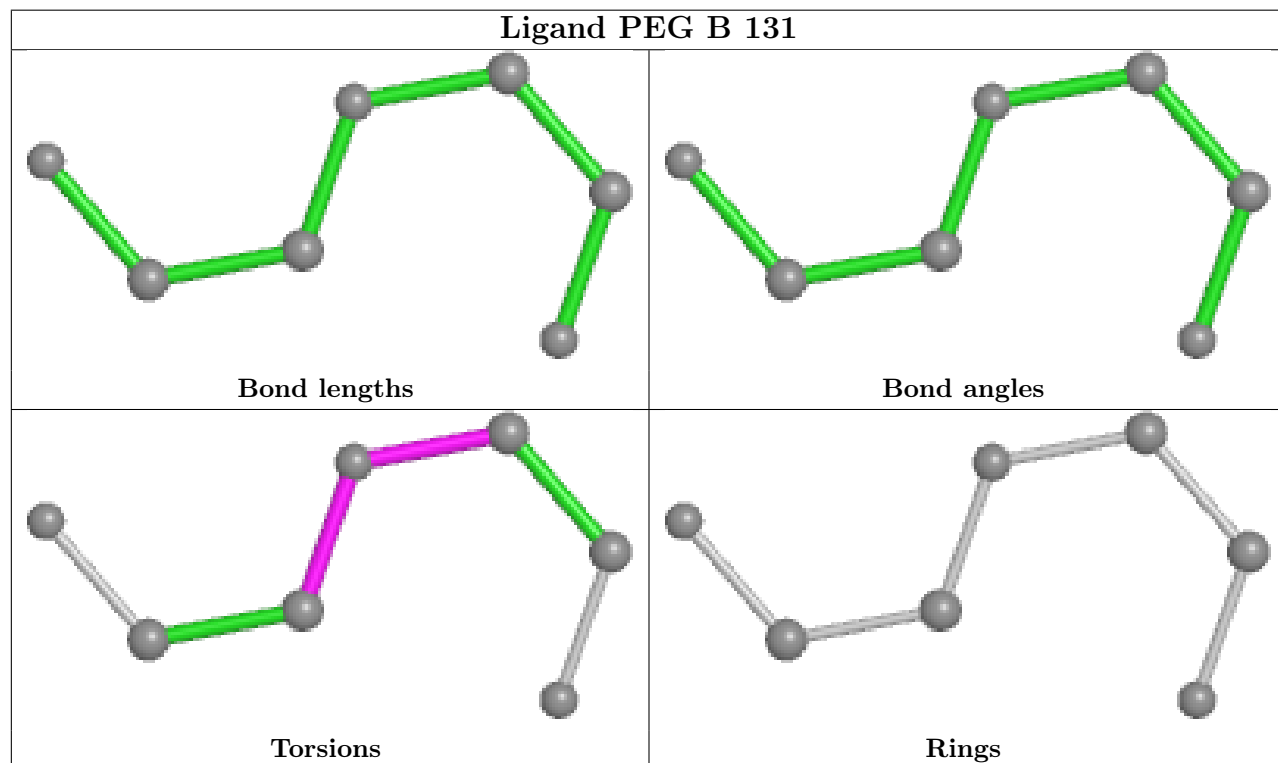
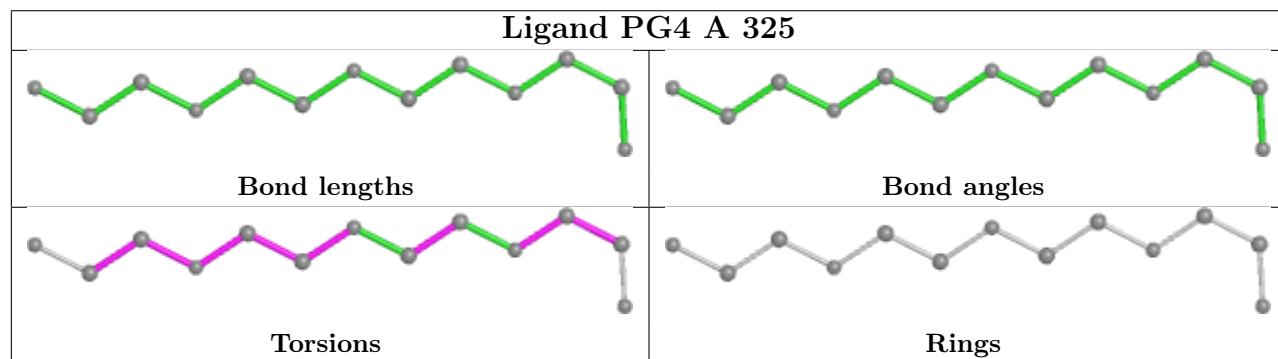
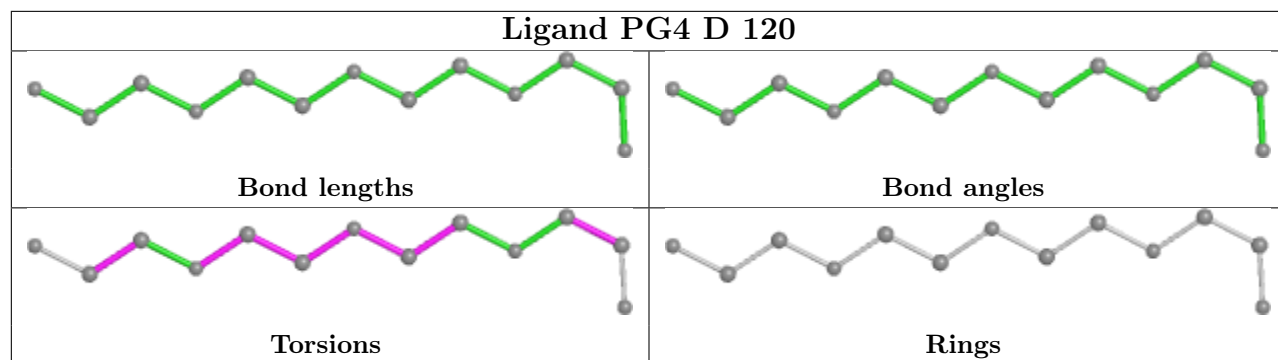
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	344	GOL	1	0
7	F	101	PG4	1	0
9	B	157	PEG	1	0
5	A	303	GOL	1	0
10	E	109	PE8	2	0
10	E	110	PE8	2	0
7	A	366	PG4	1	0
7	A	365	PG4	1	0
7	C	322	PG4	3	0
5	C	345	GOL	2	0
5	C	309	GOL	1	0
7	C	321	PG4	2	0
10	C	335	PE8	2	0
7	B	118	PG4	2	0
5	D	106	GOL	2	0
10	F	106	PE8	2	0
5	A	347	GOL	1	0
9	A	331	PEG	2	0
10	B	137	PE8	1	0
7	B	122	PG4	2	0
7	C	325	PG4	3	0
7	C	324	PG4	1	0
7	D	103	PG4	2	0
10	B	136	PE8	3	0
9	C	331	PEG	1	0
10	F	102	PE8	2	0
5	B	140	GOL	2	0
5	D	108	GOL	1	0
5	A	310	GOL	1	0
5	A	363	GOL	1	0
7	B	155	PG4	1	0
7	B	125	PG4	1	0
5	E	113	GOL	1	0
7	A	323	PG4	1	0
5	C	338	GOL	1	0
9	B	130	PEG	1	0
7	C	323	PG4	2	0
10	B	138	PE8	2	0
7	E	115	PG4	1	0
7	C	320	PG4	2	0
5	E	103	GOL	1	0

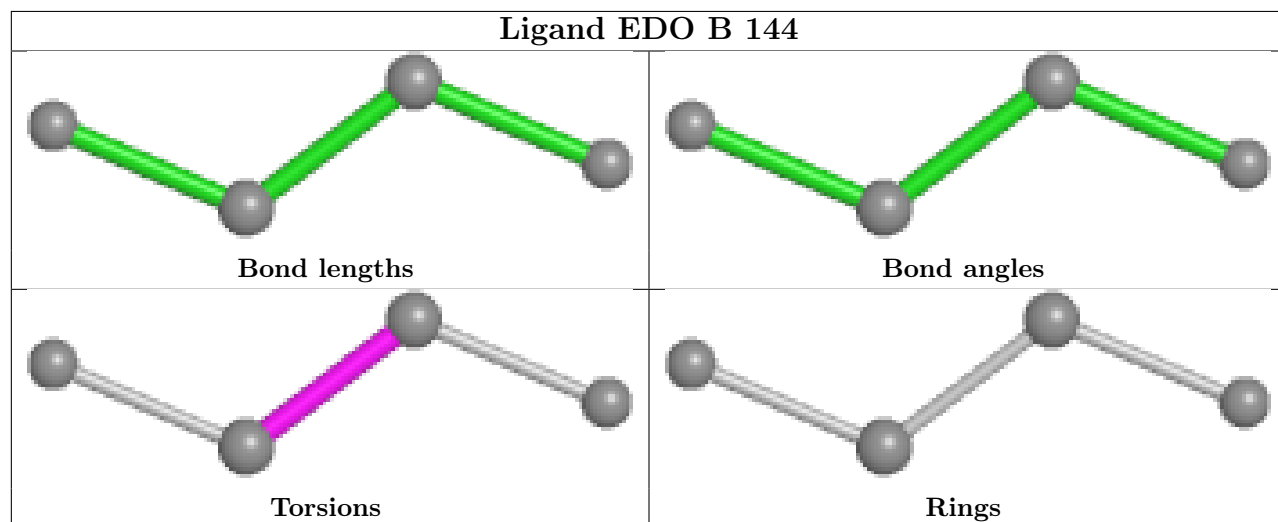
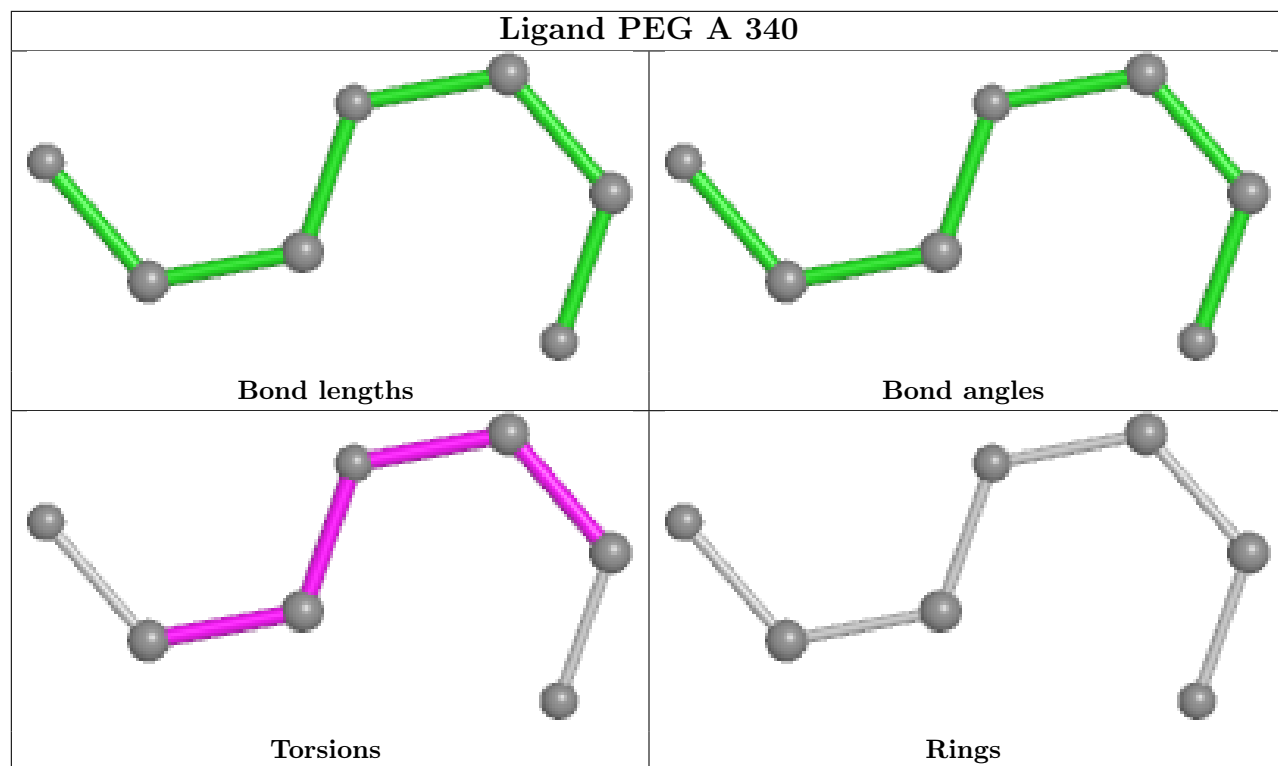
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

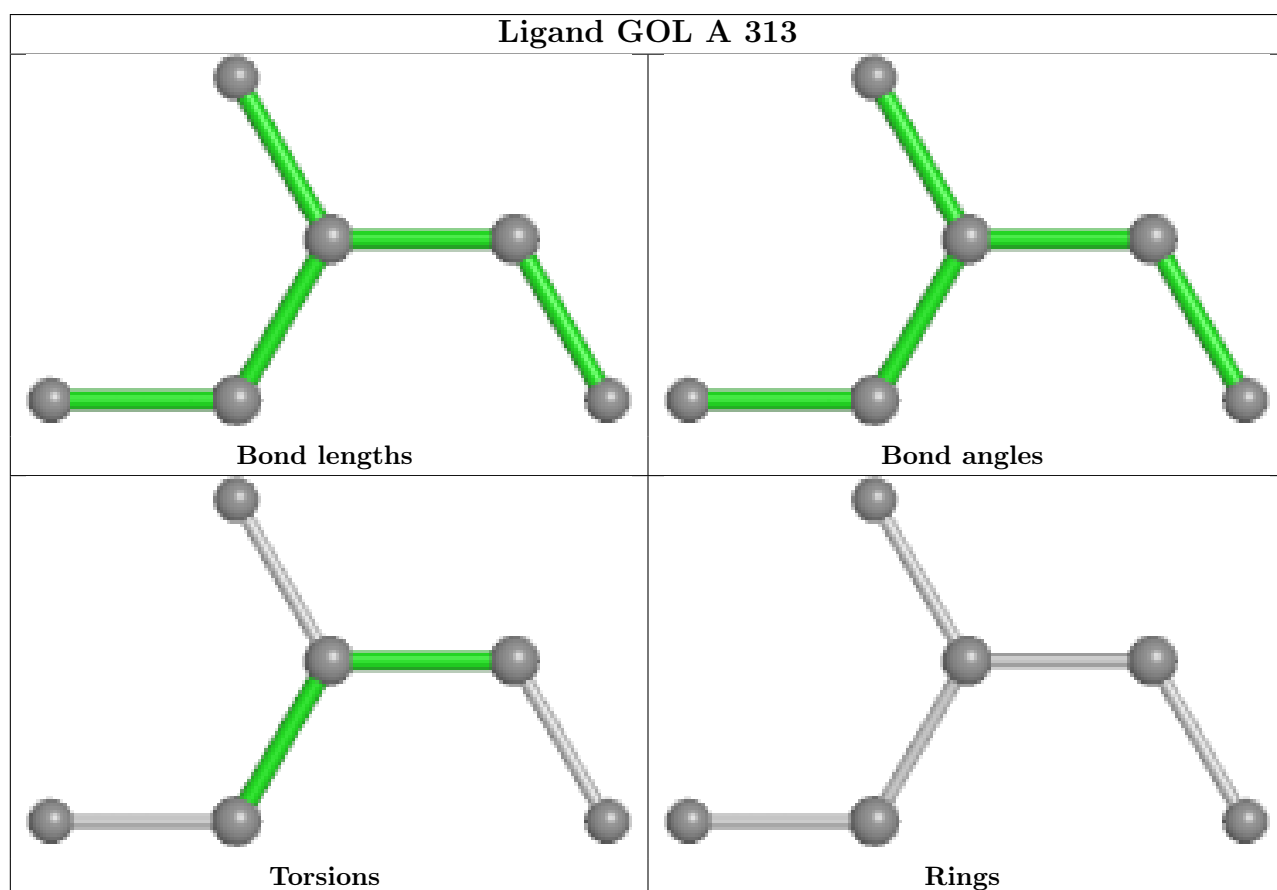
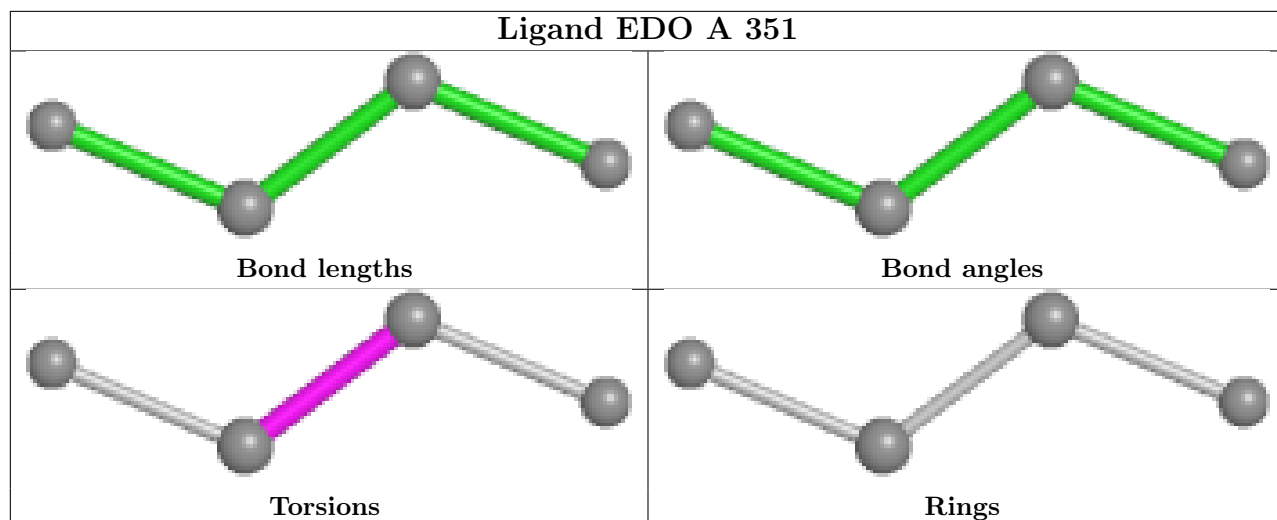
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

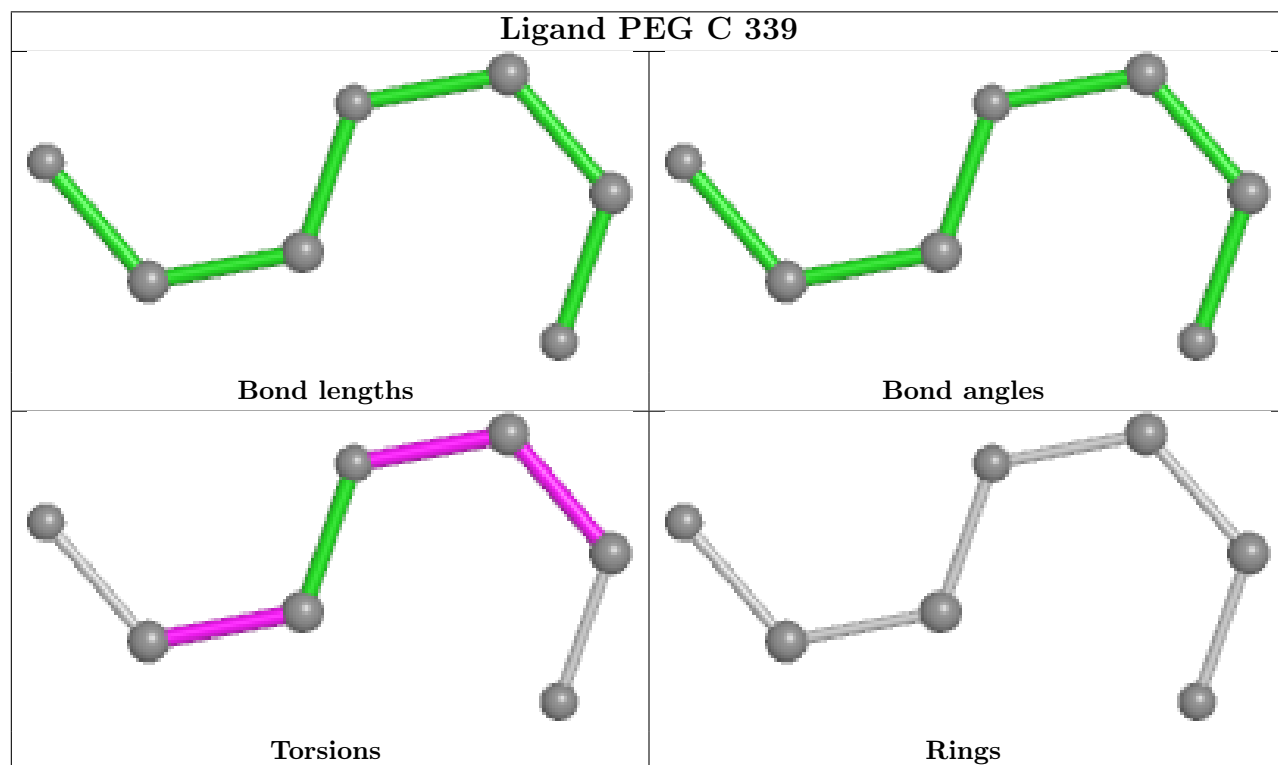
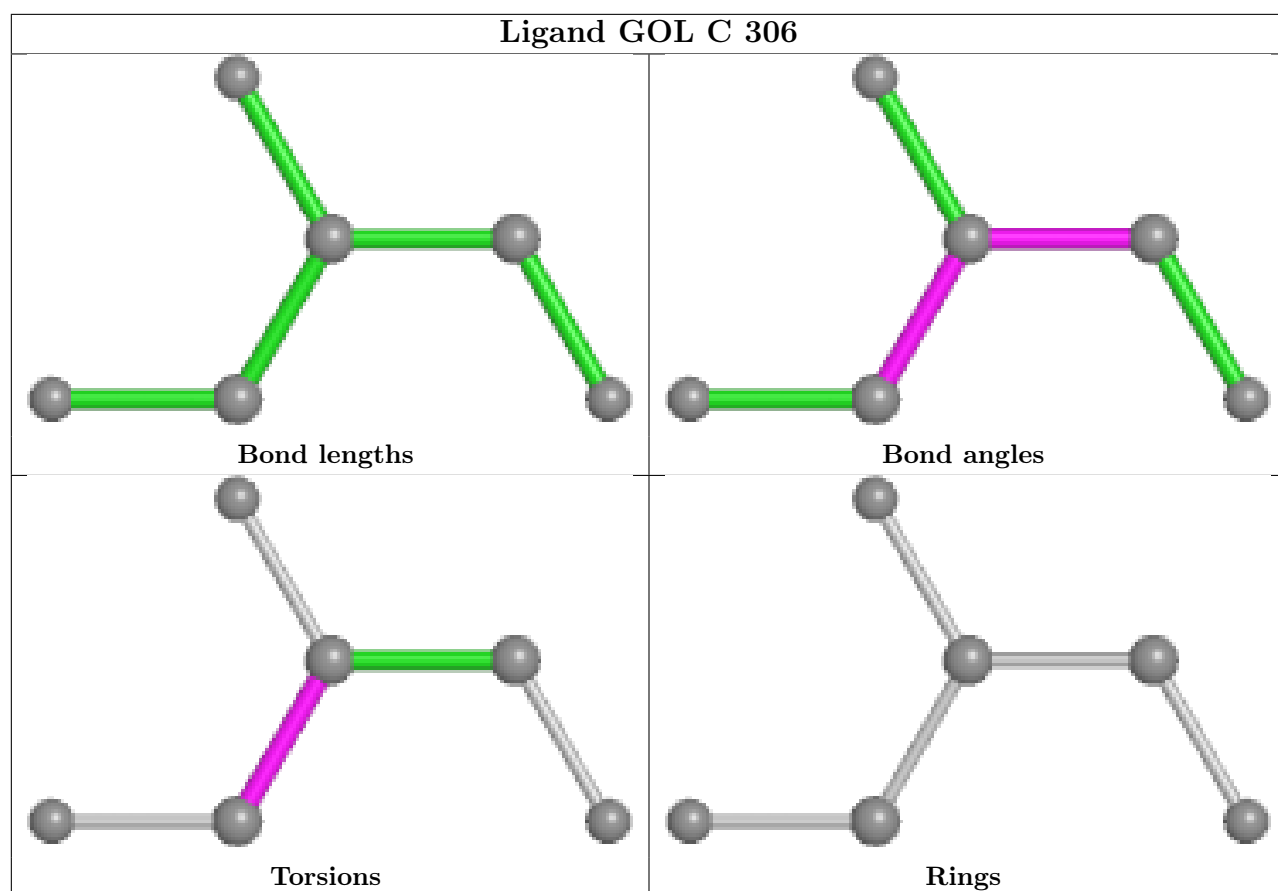


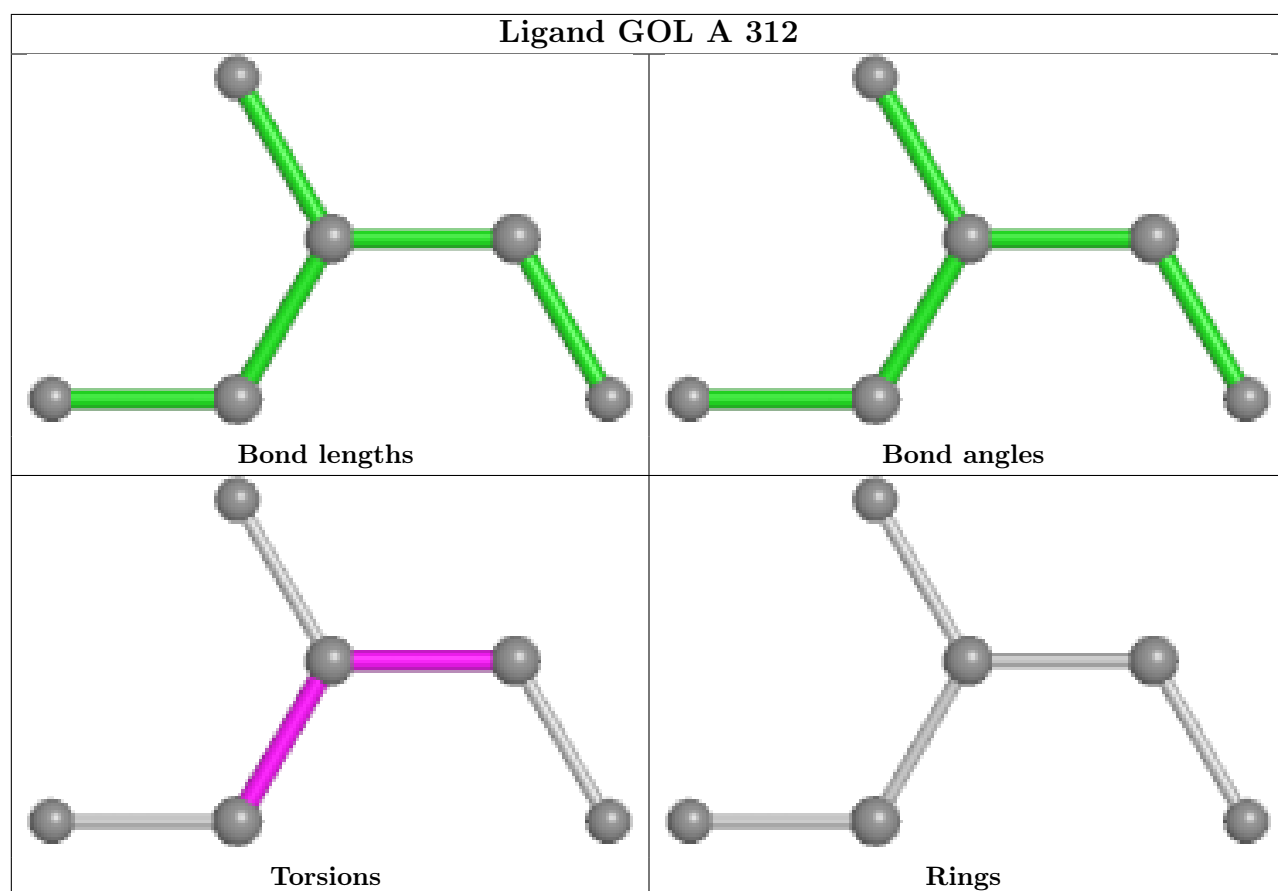
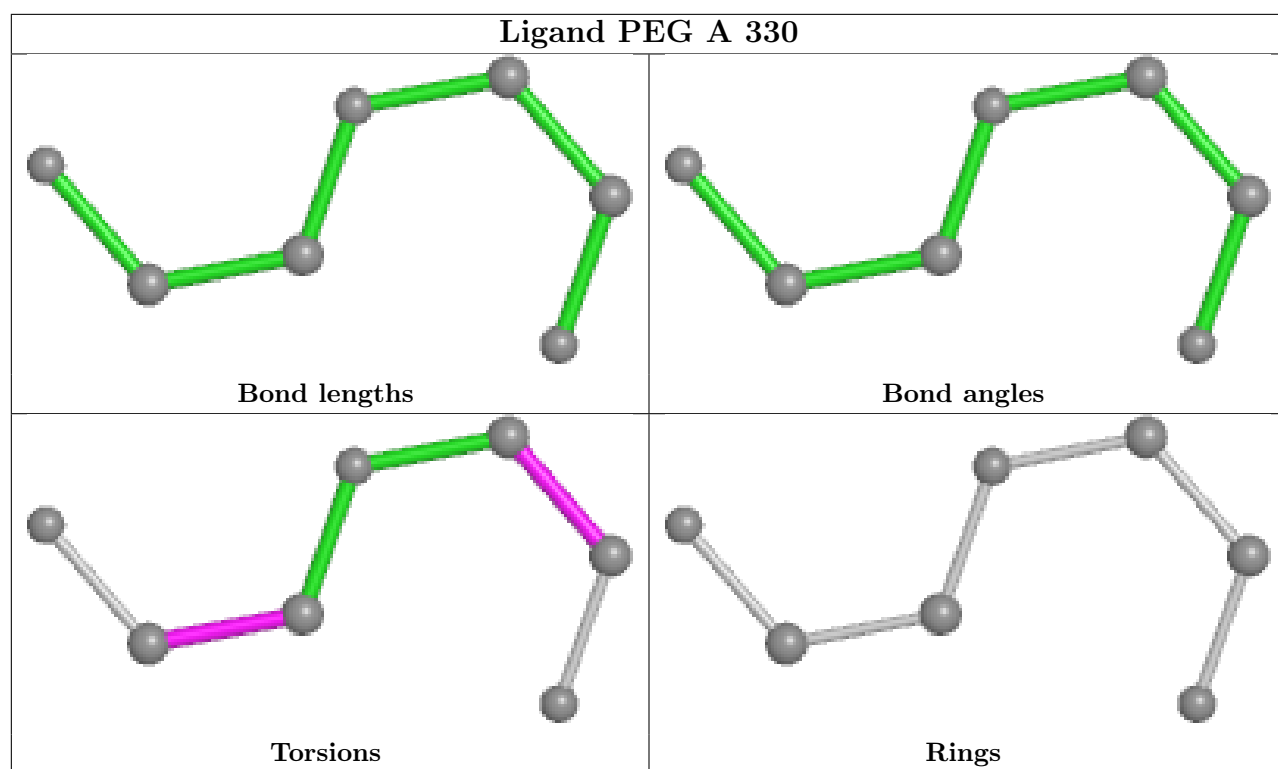


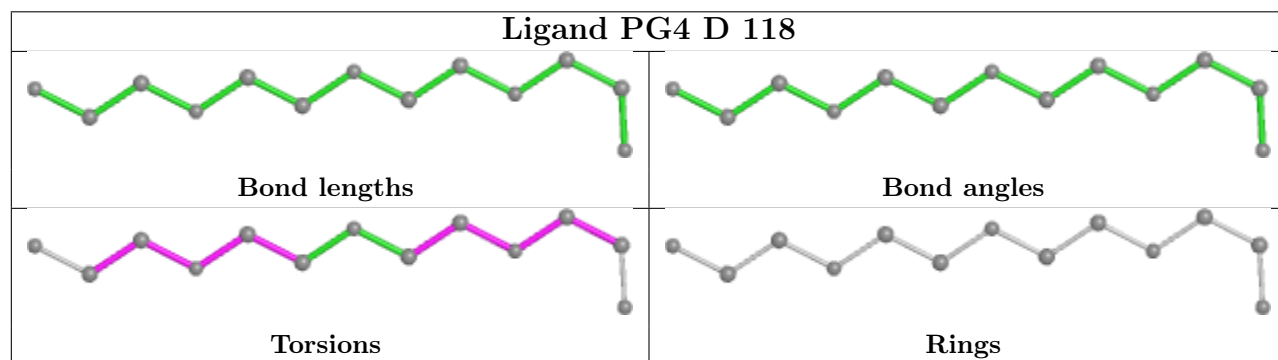
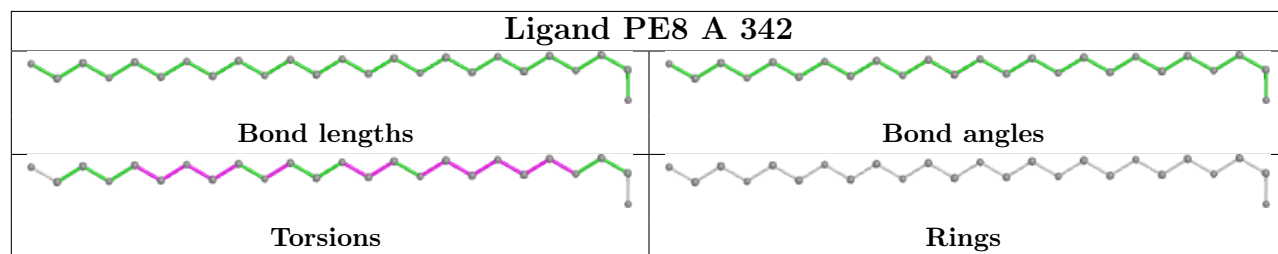
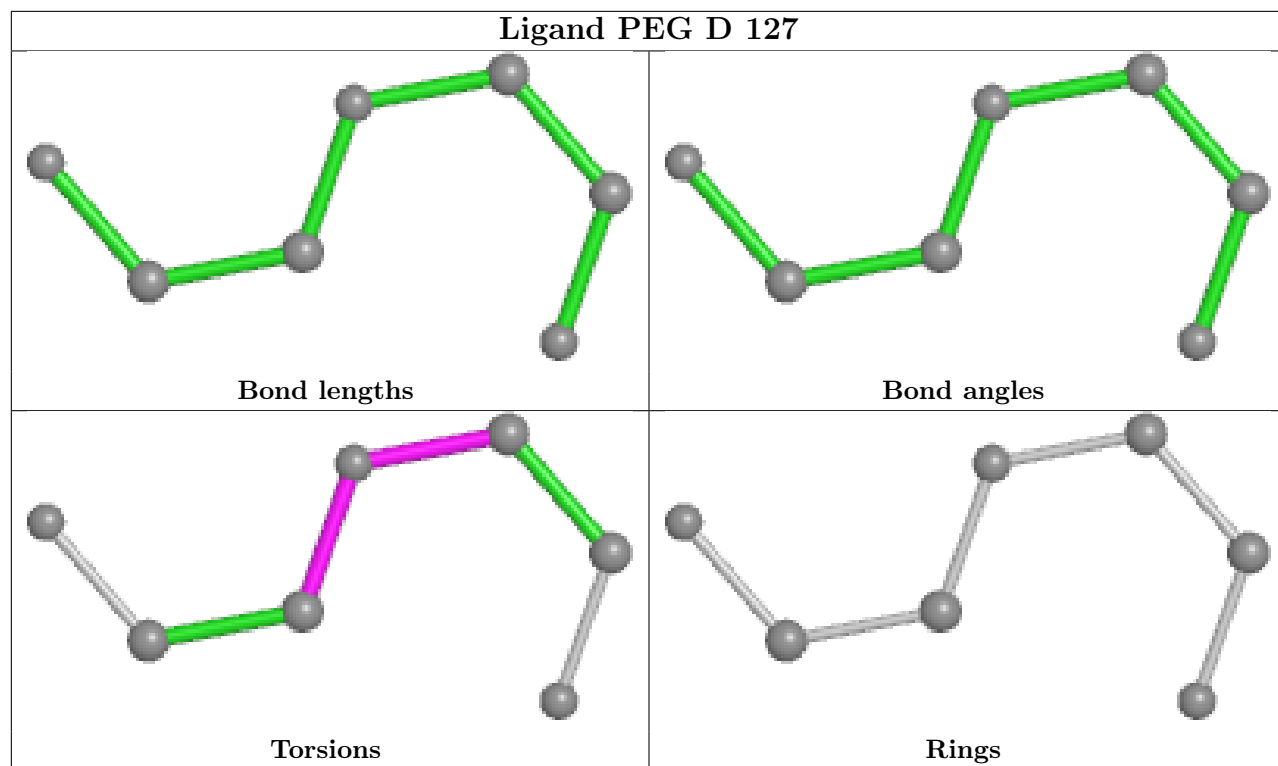


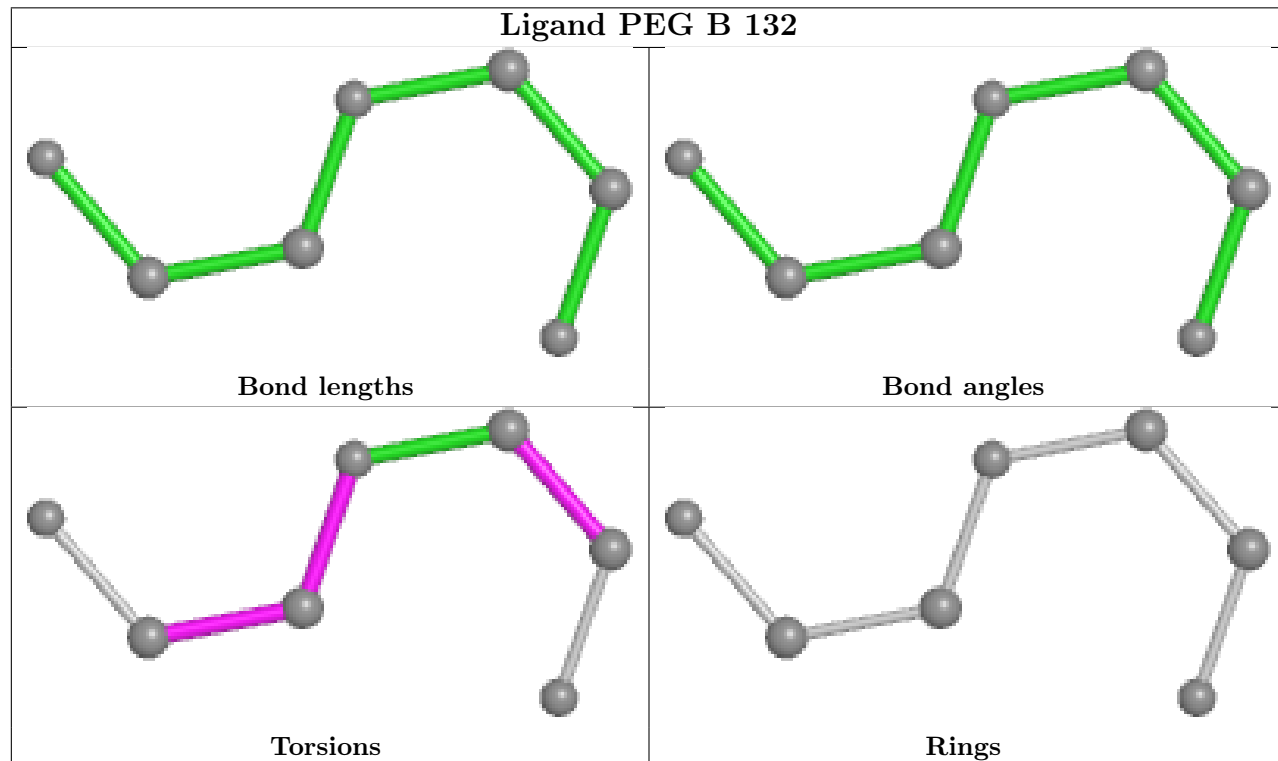
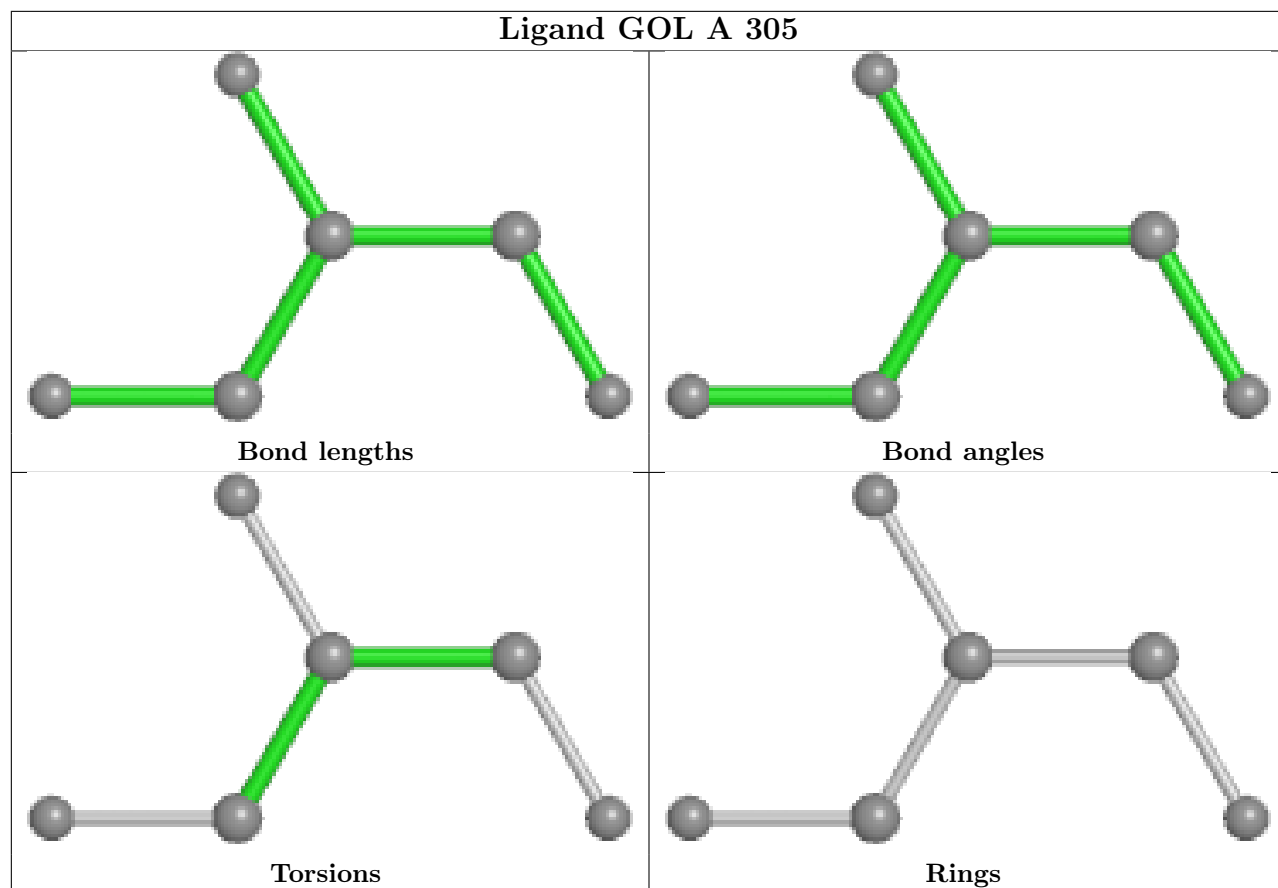


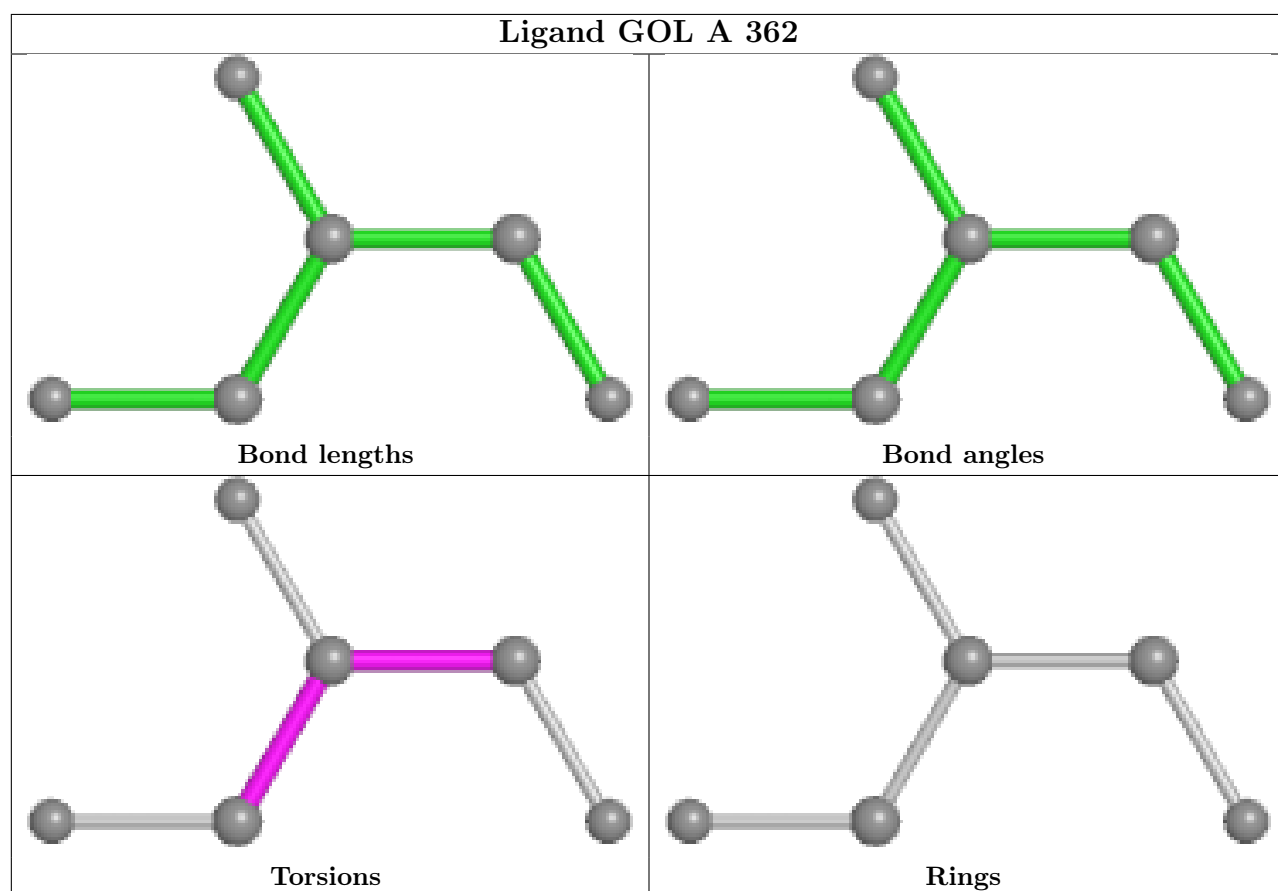
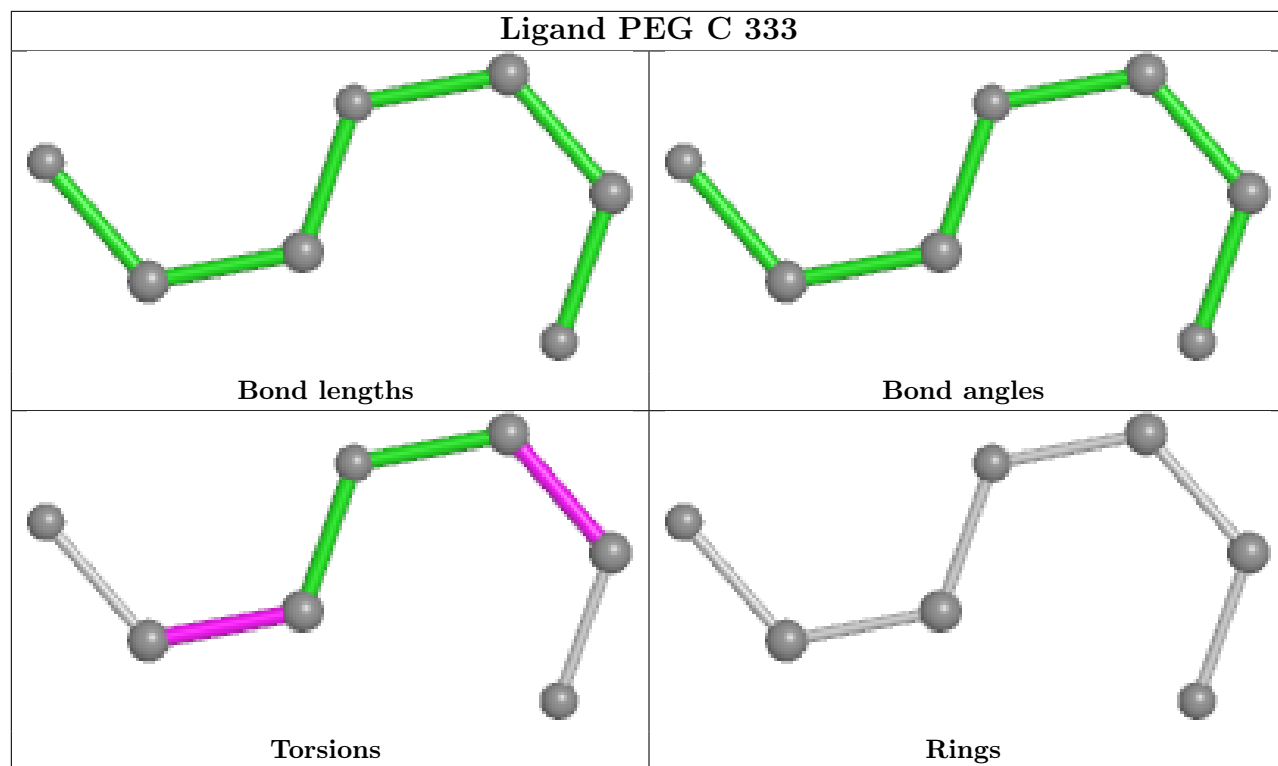


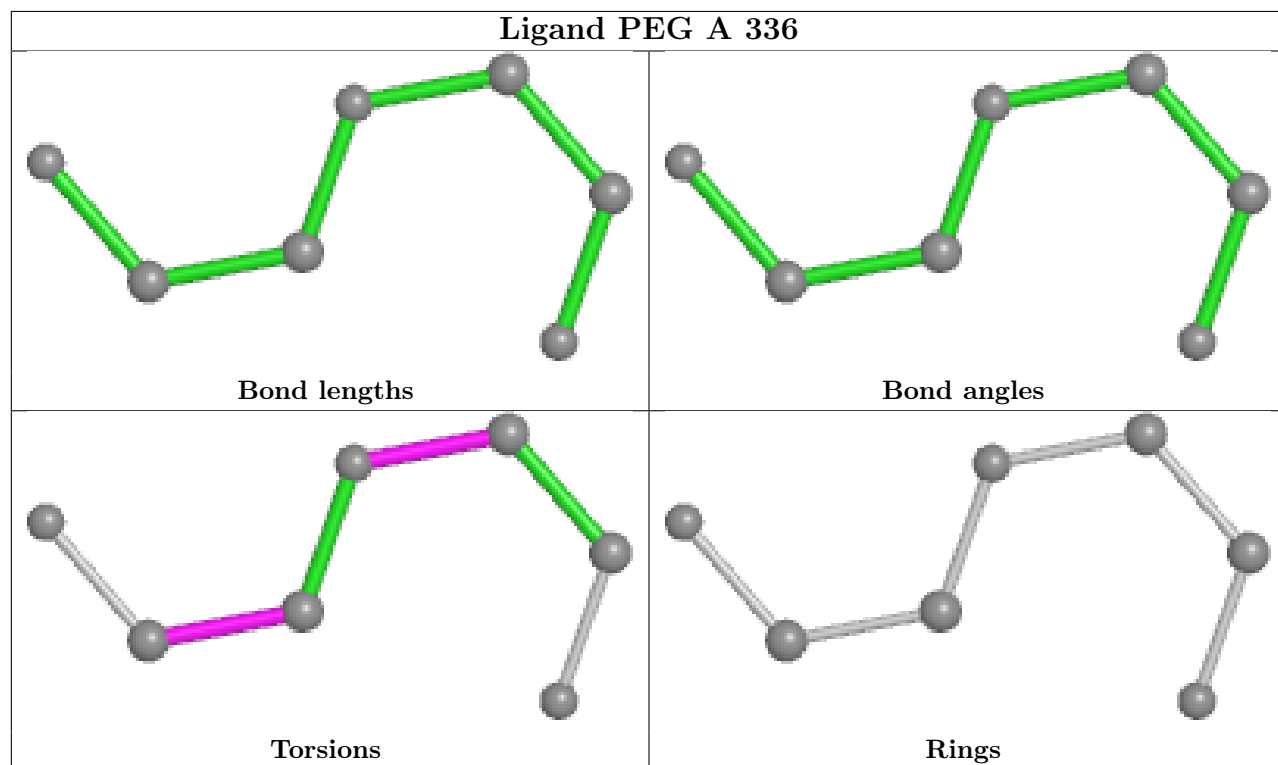
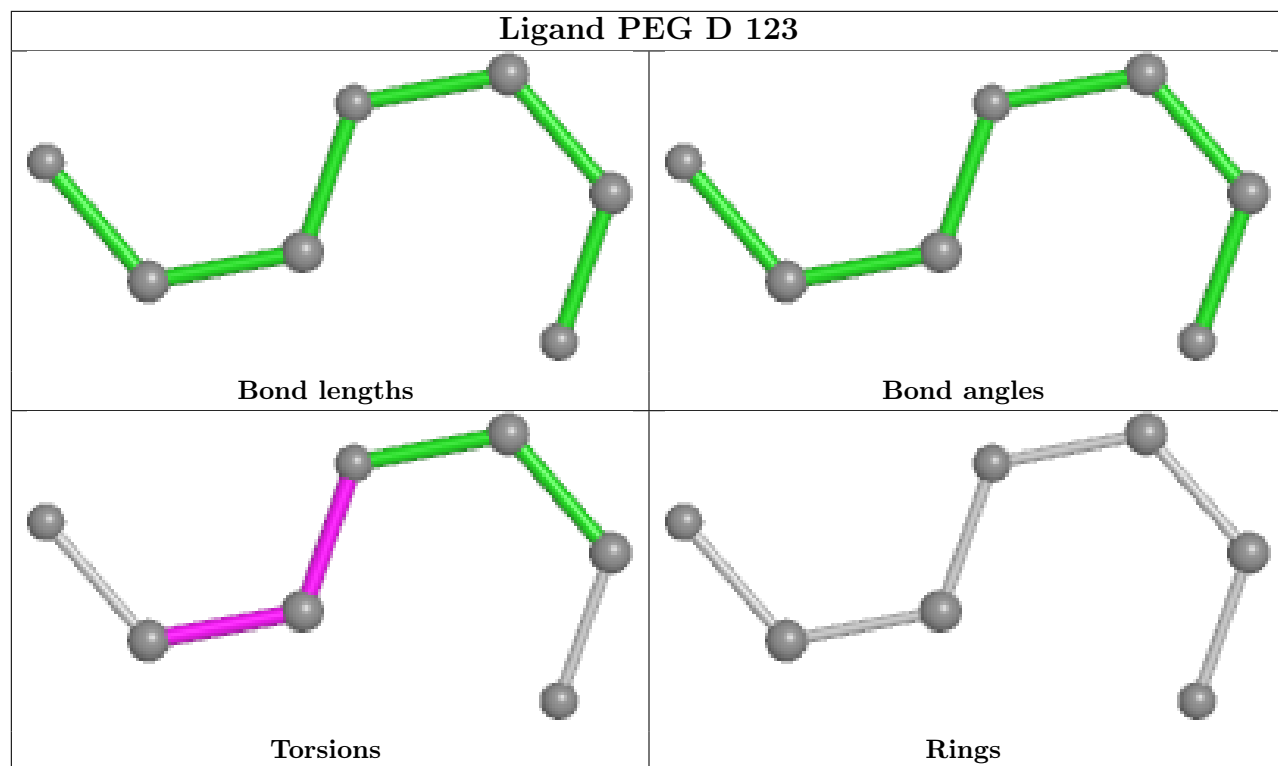


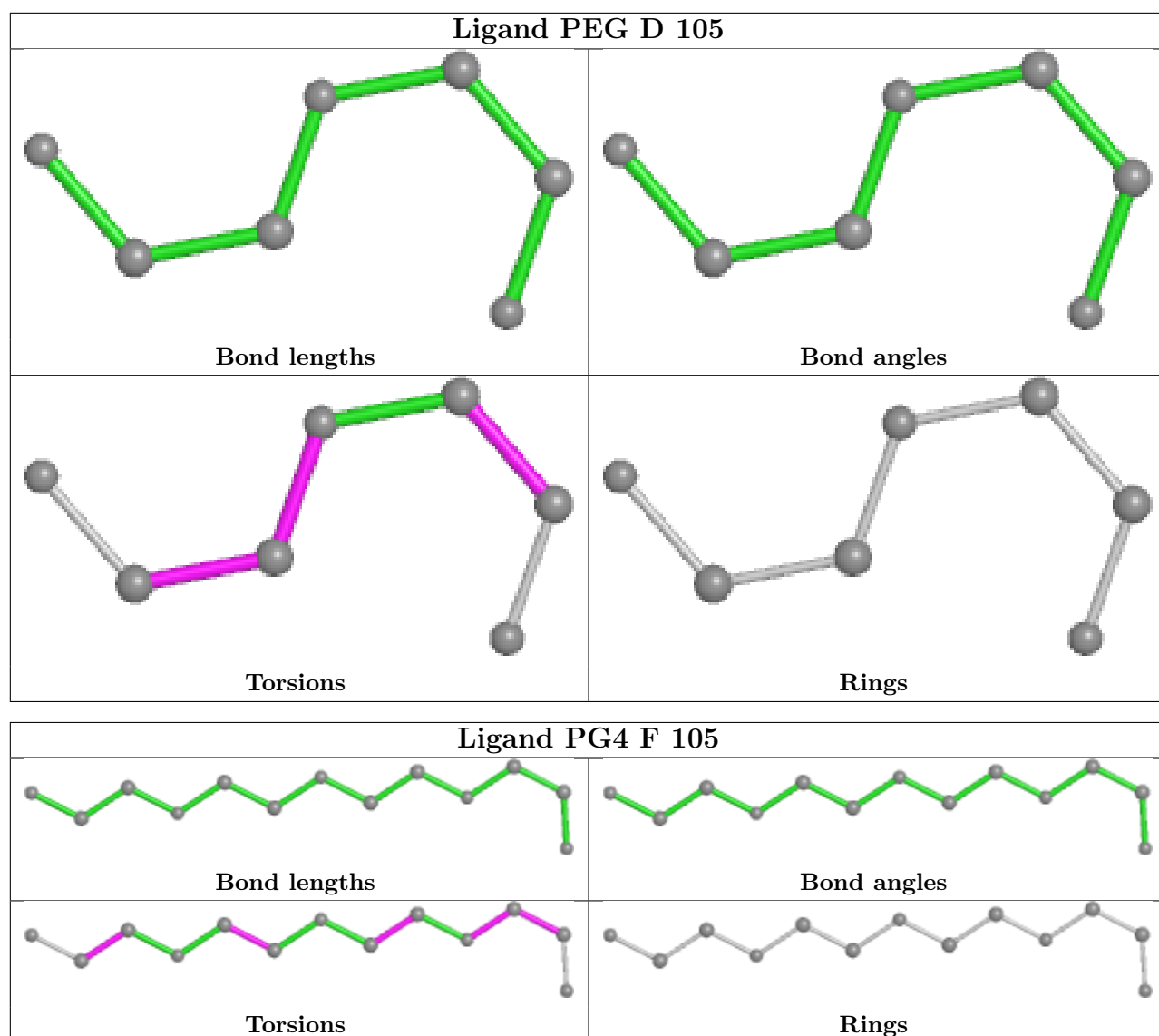


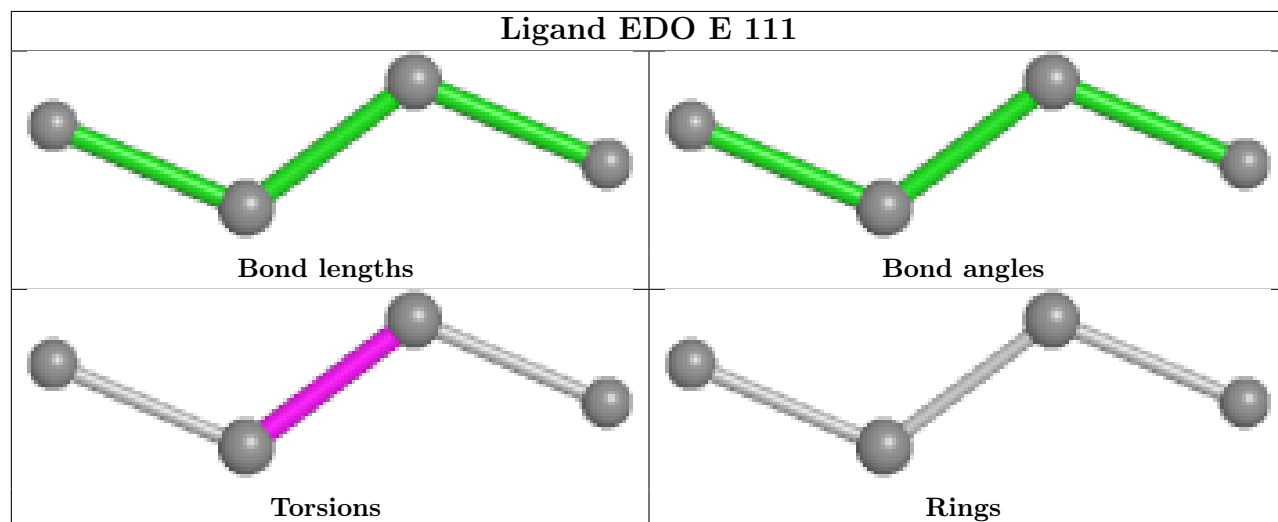
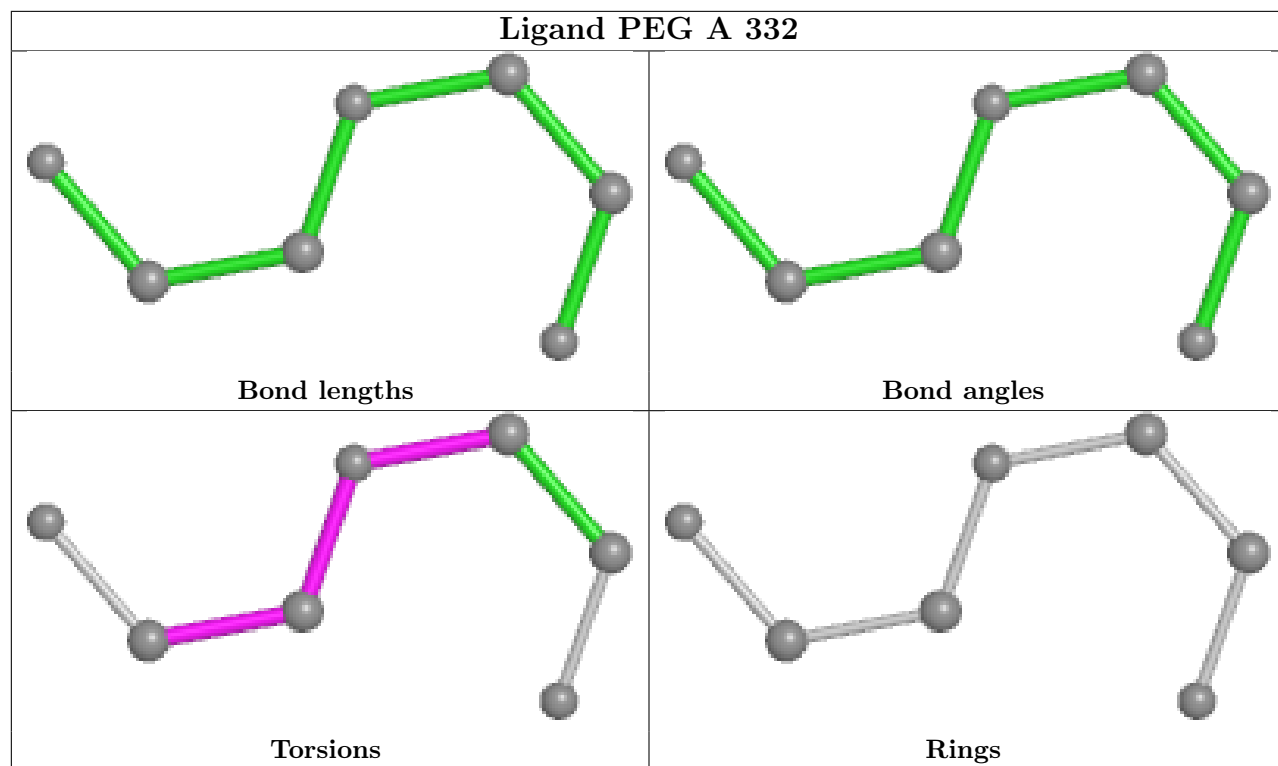


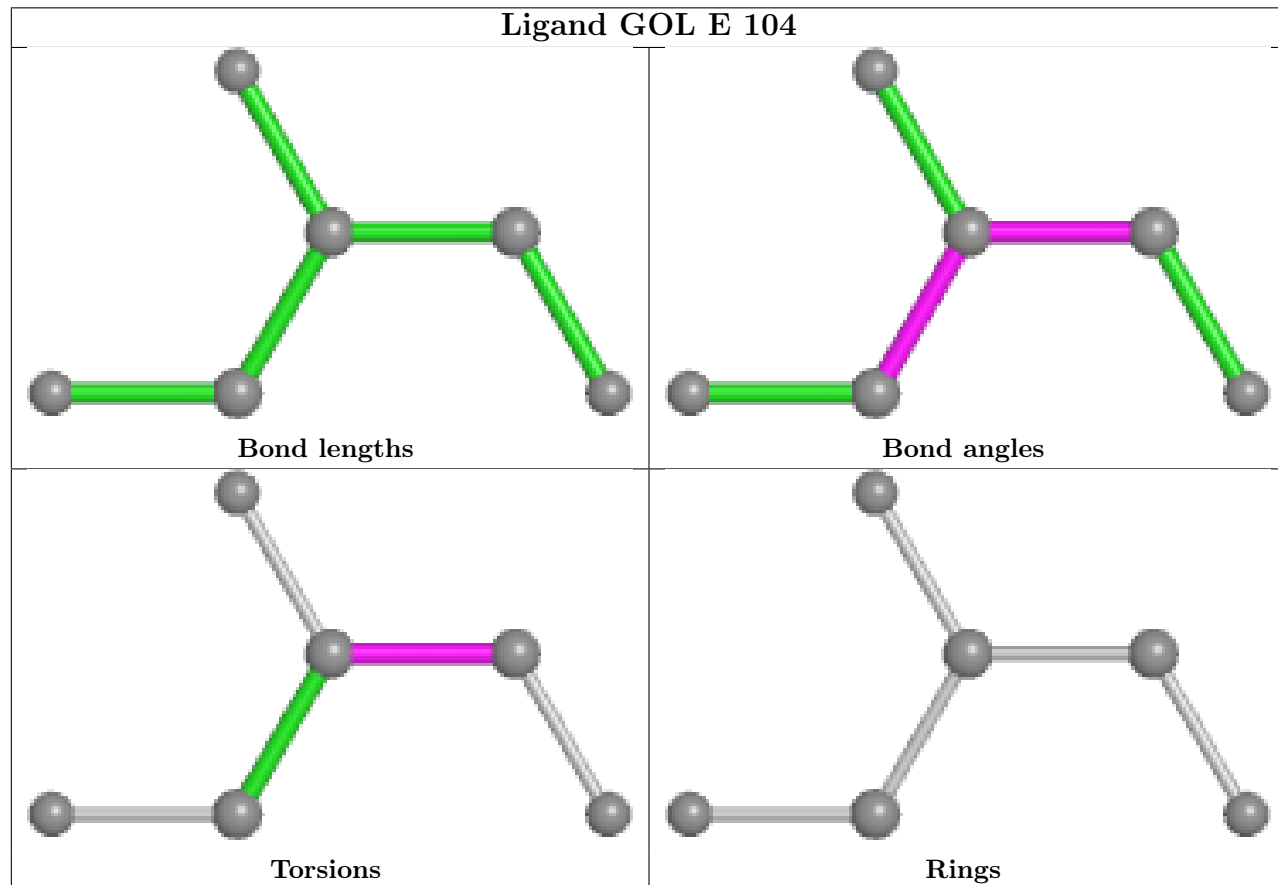
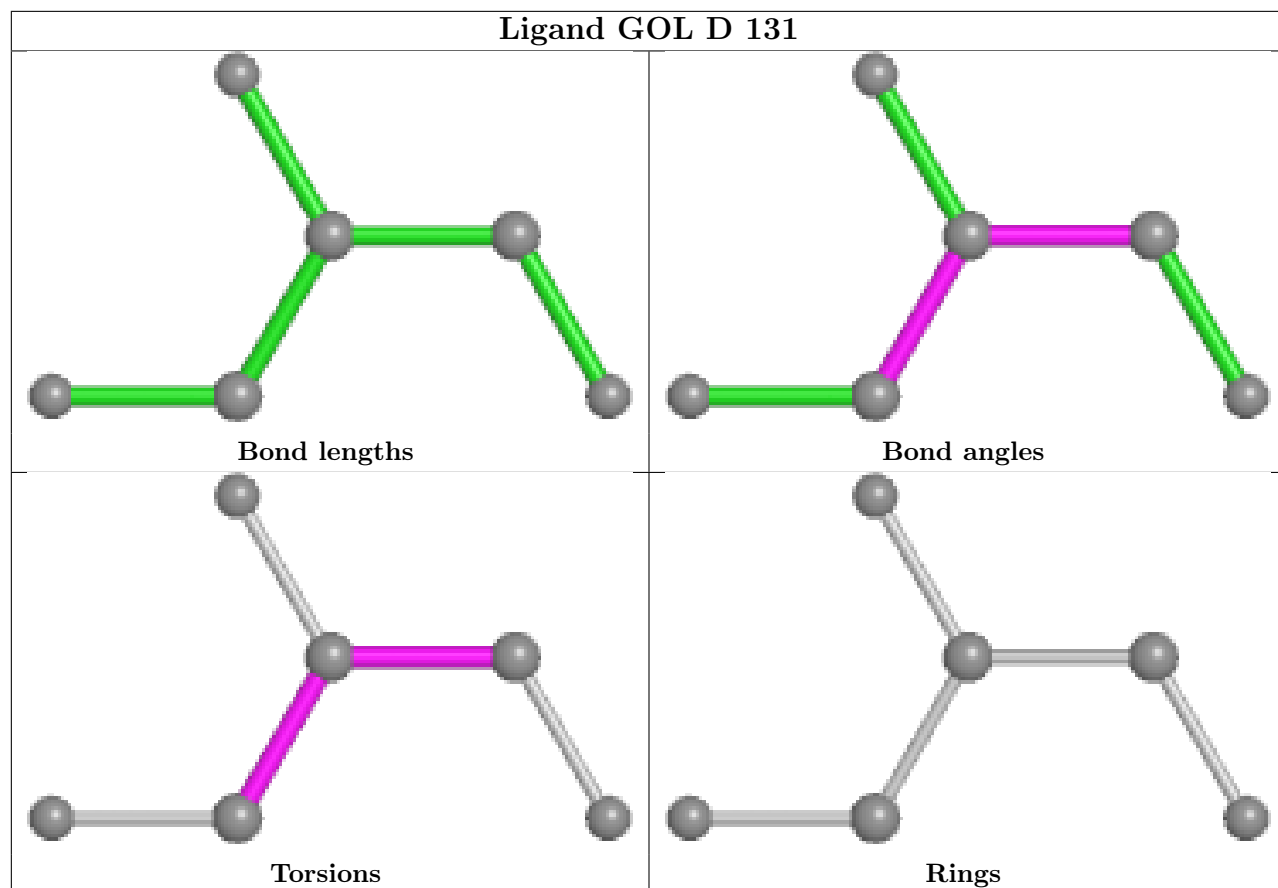


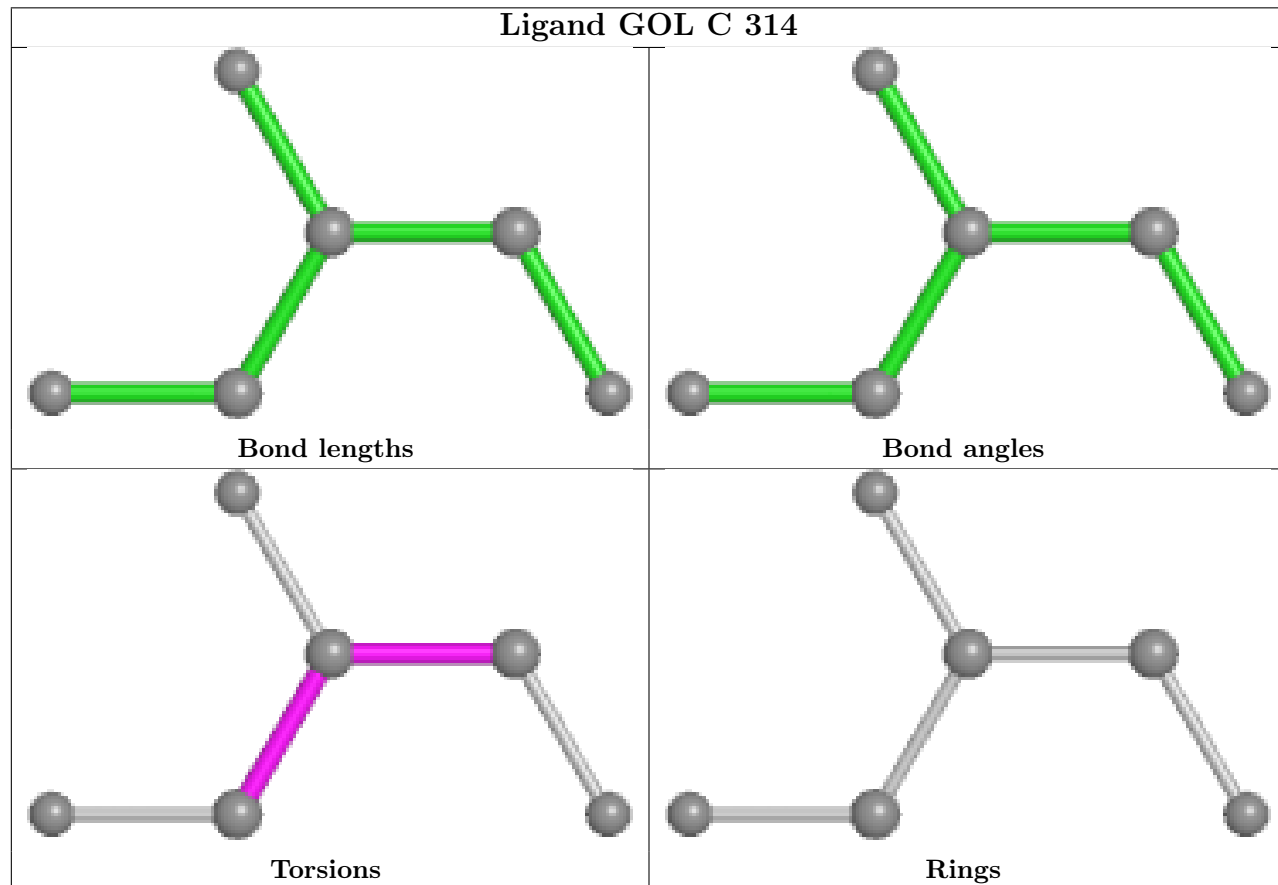
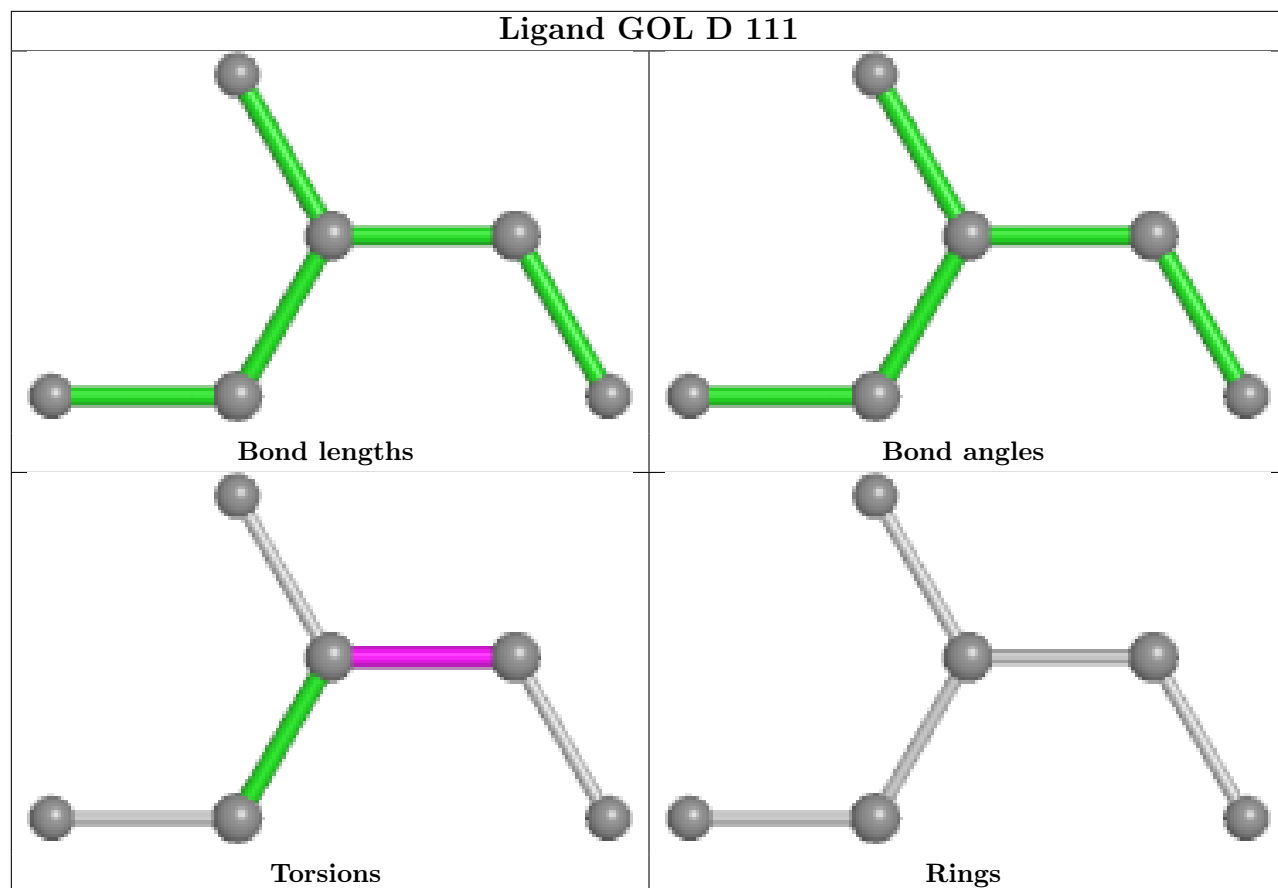


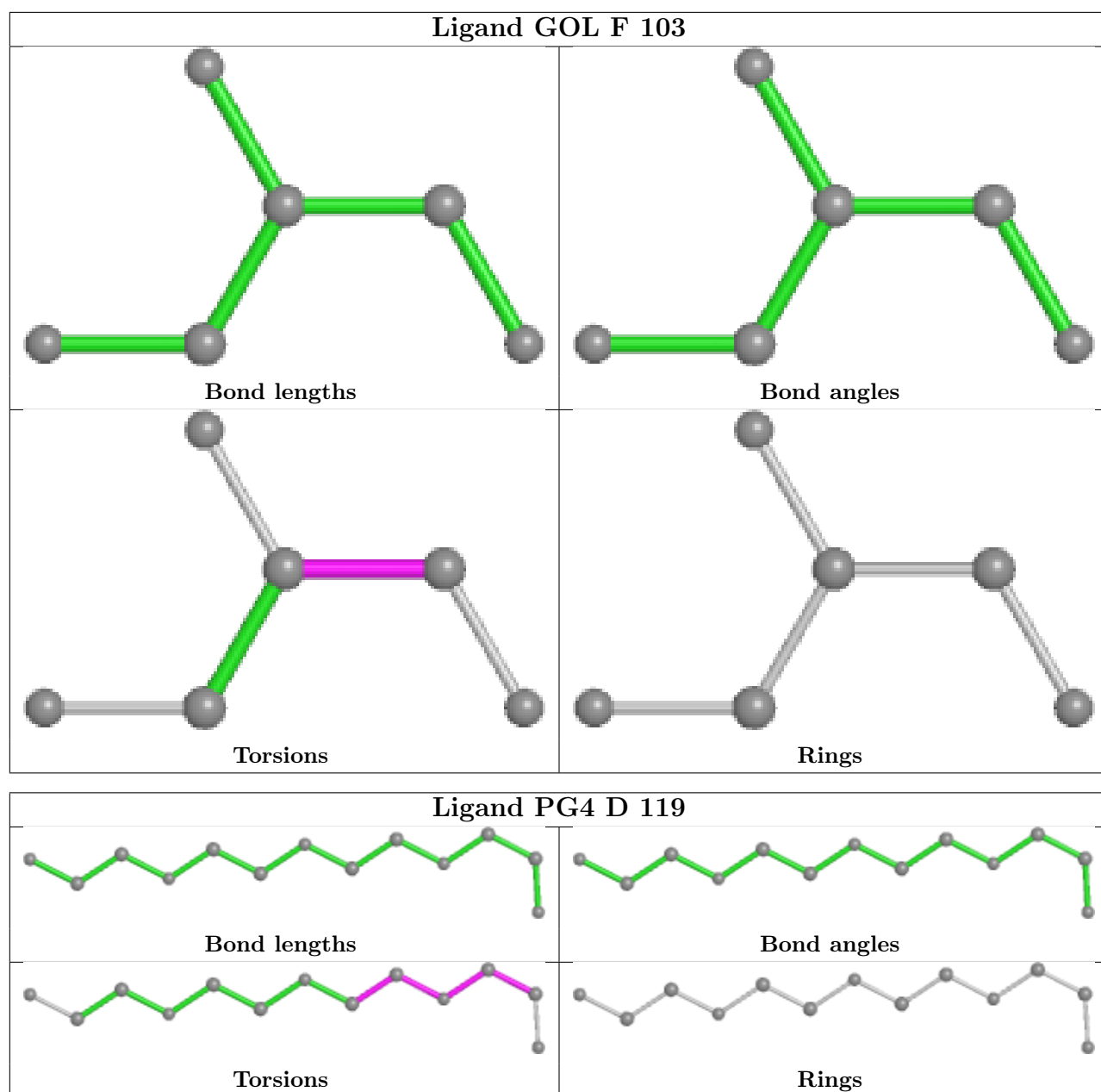


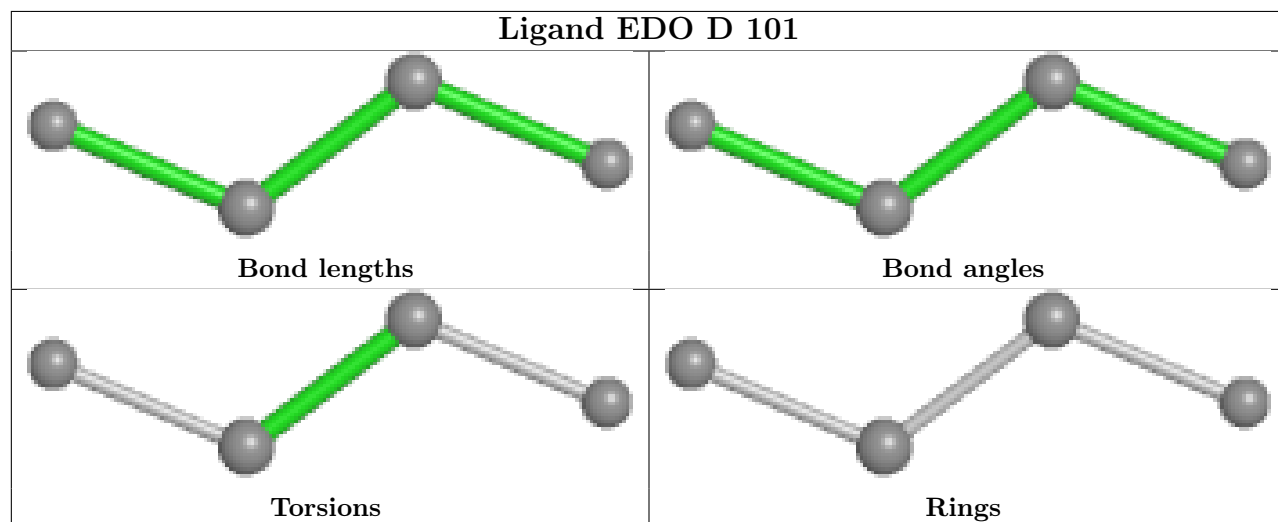
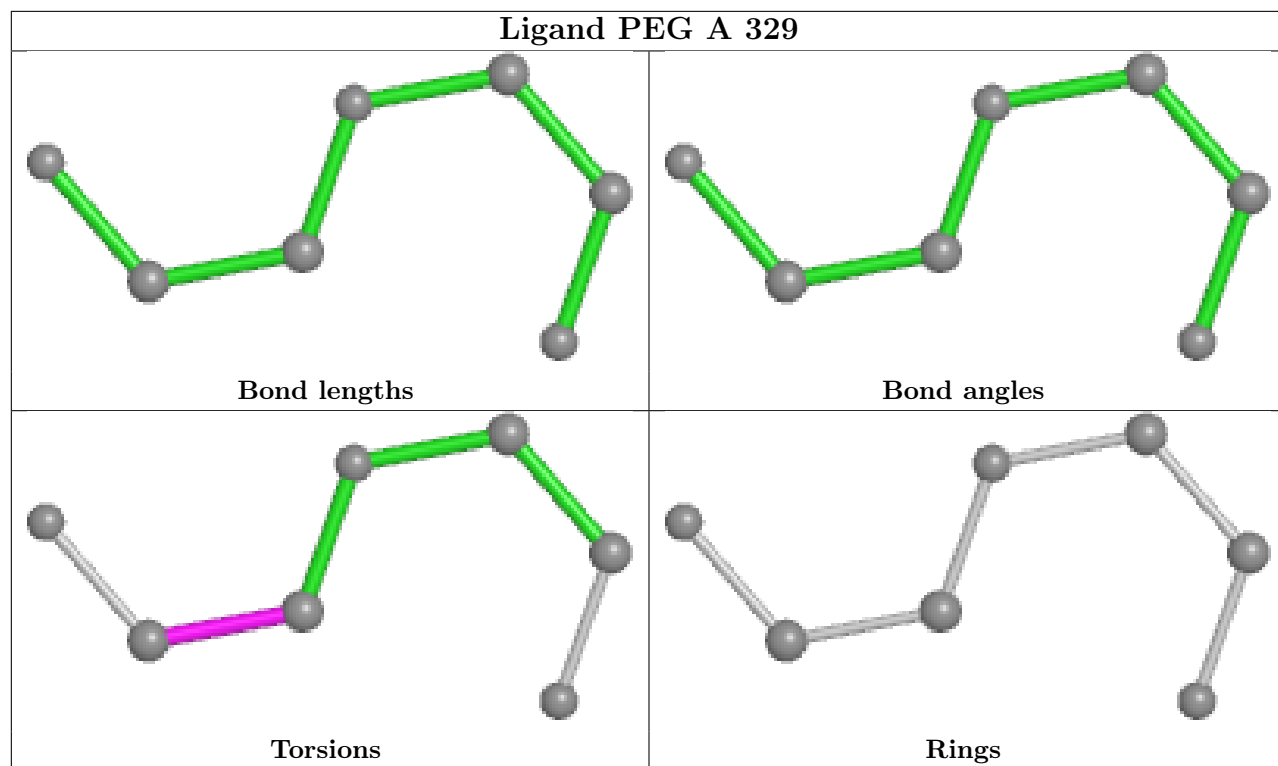


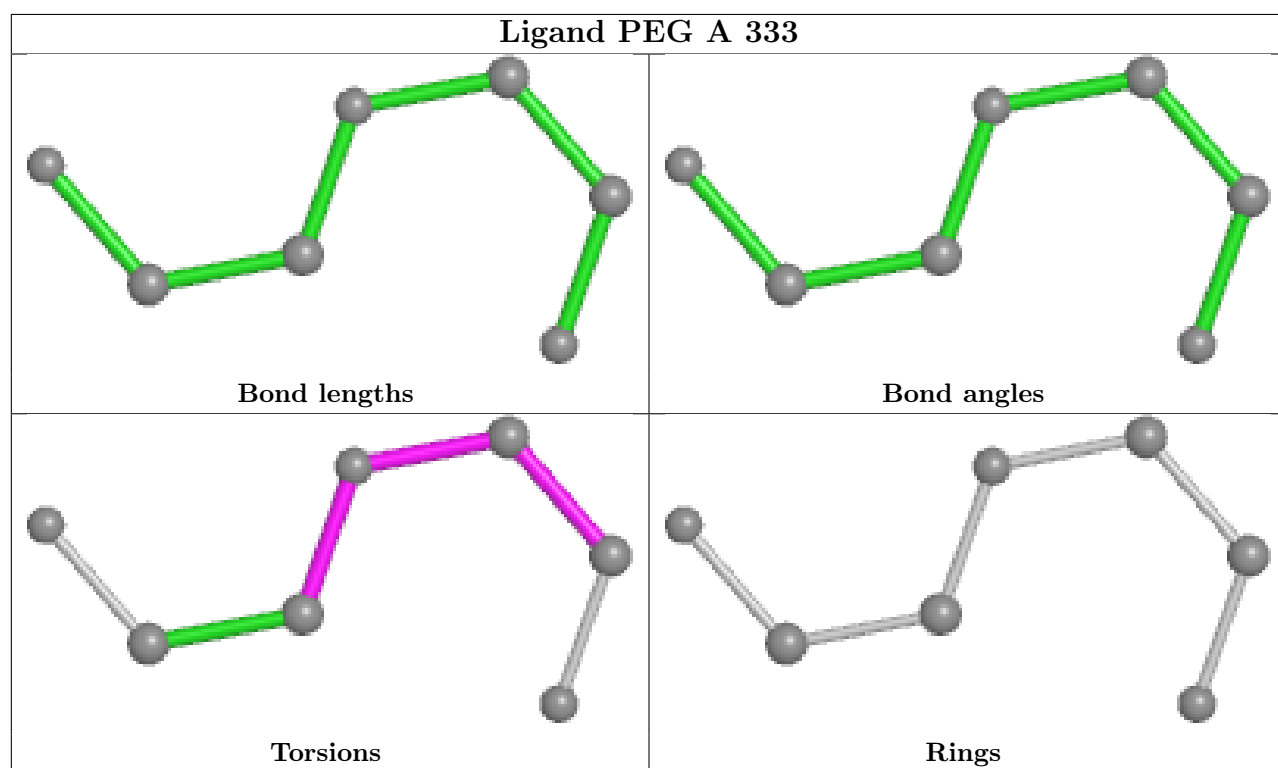
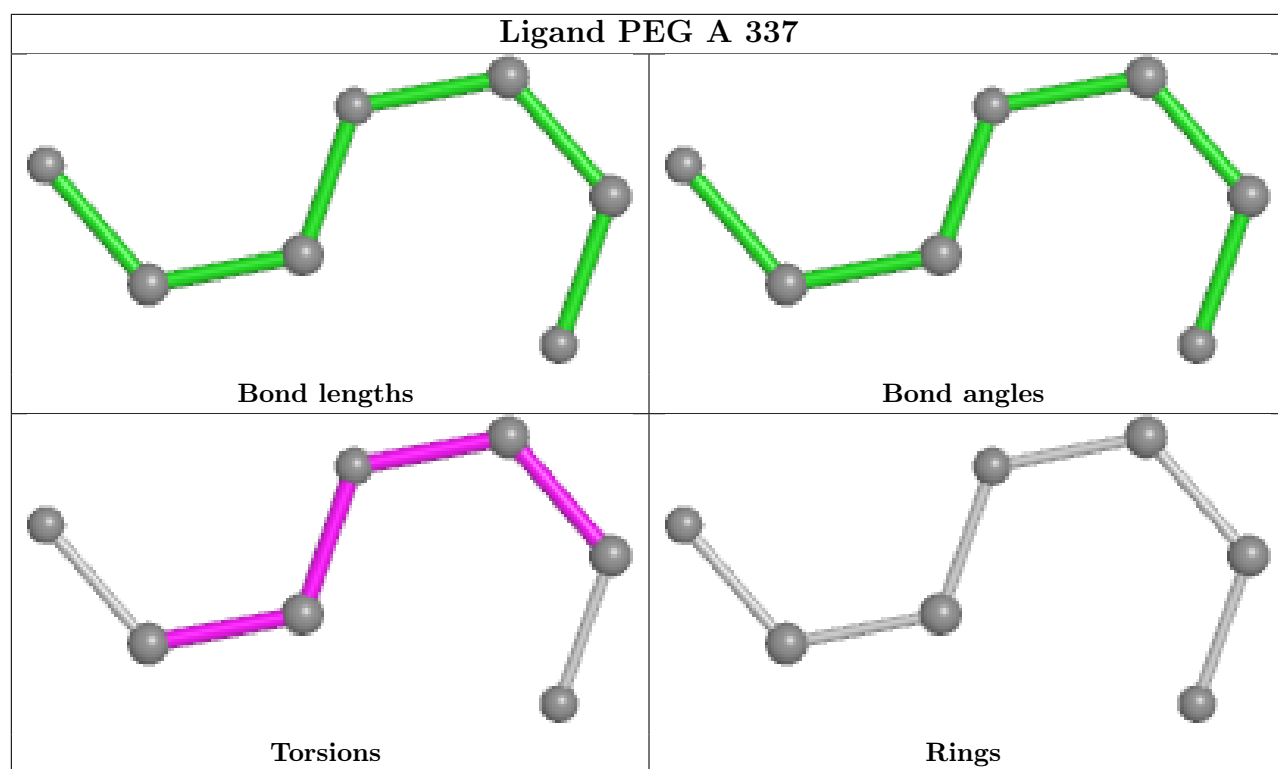


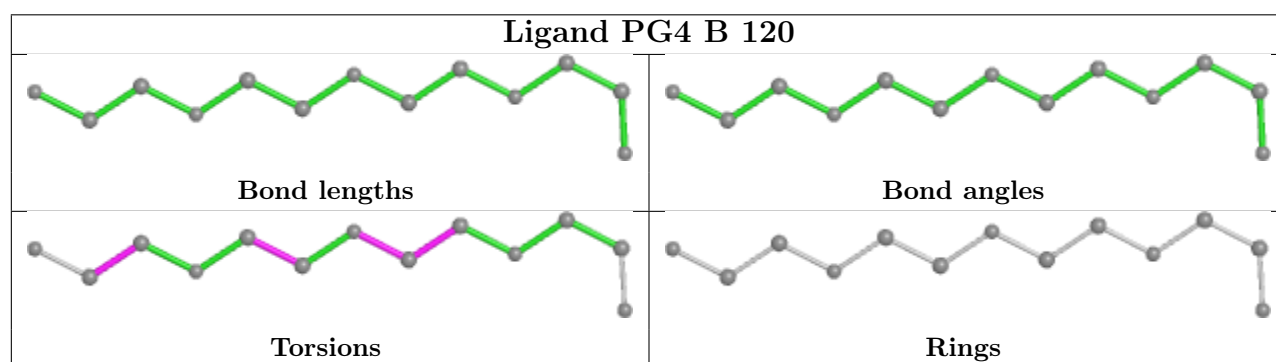
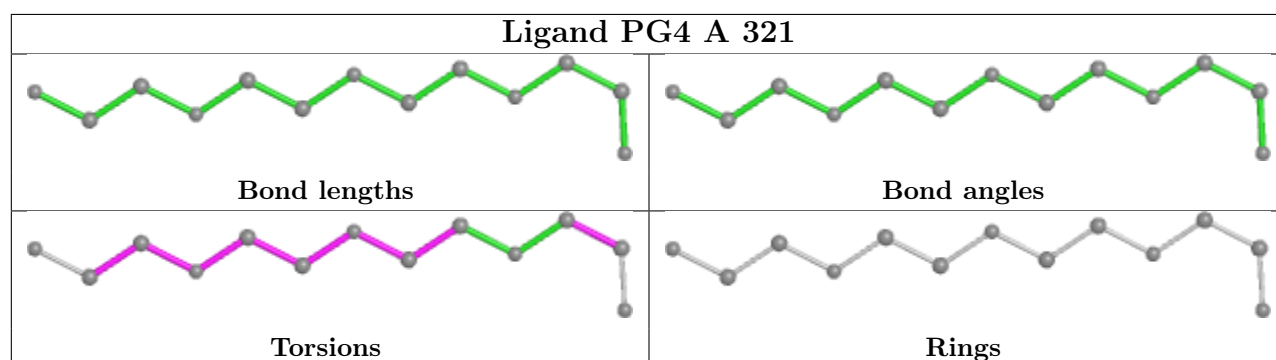
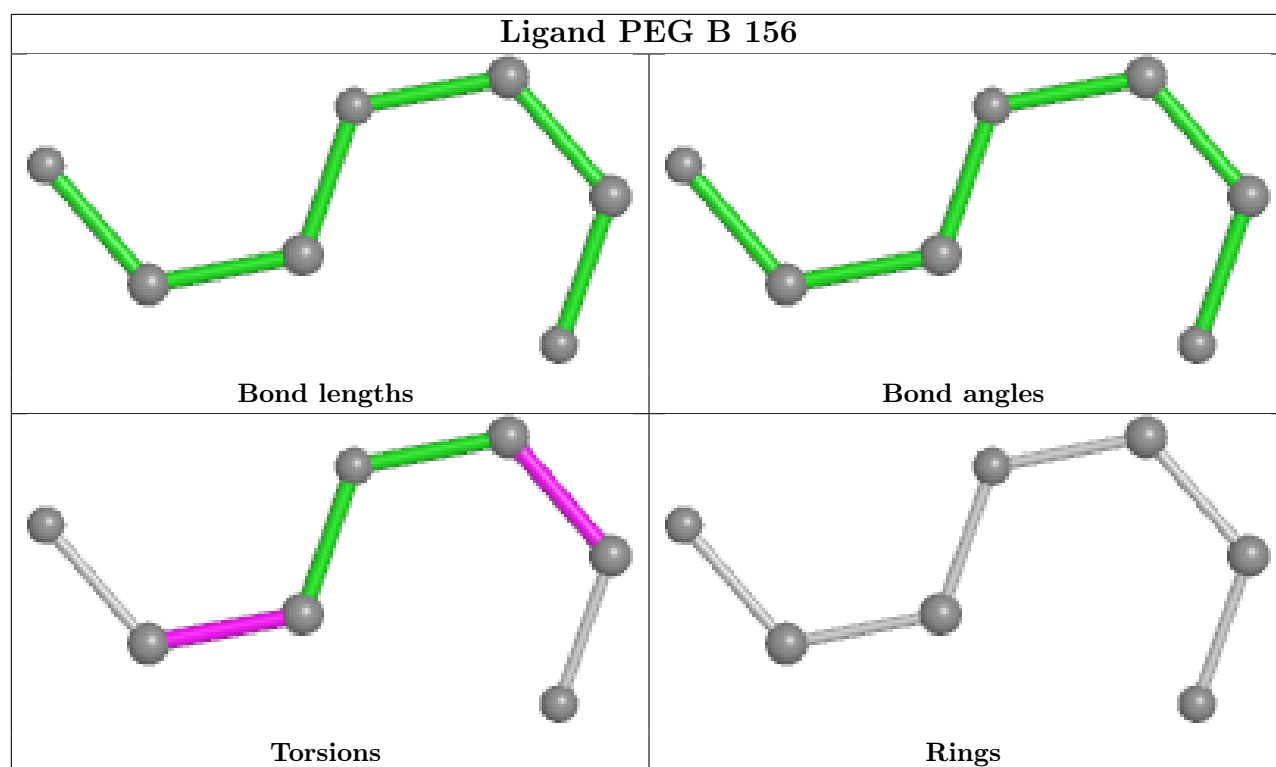


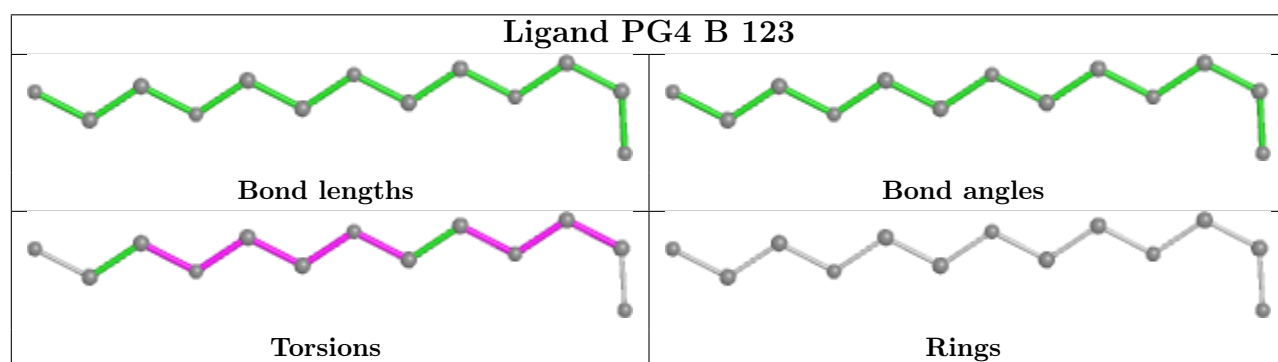
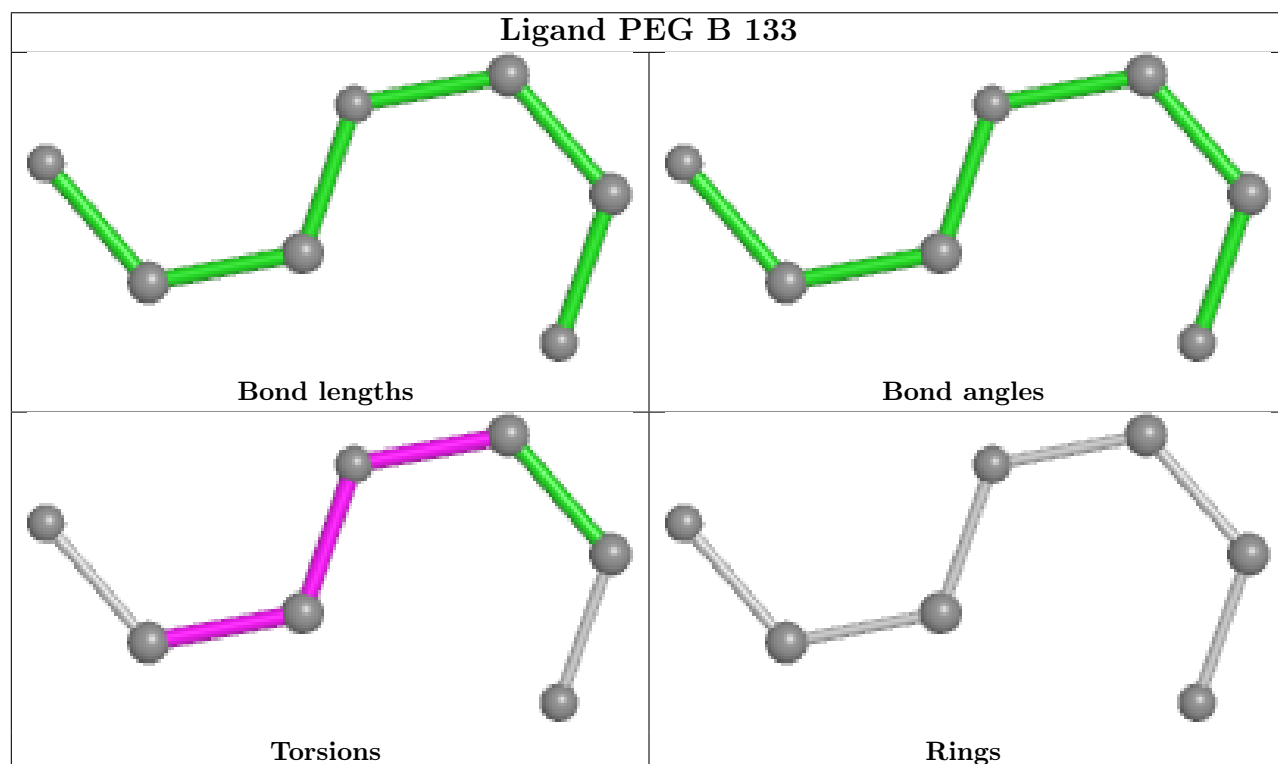
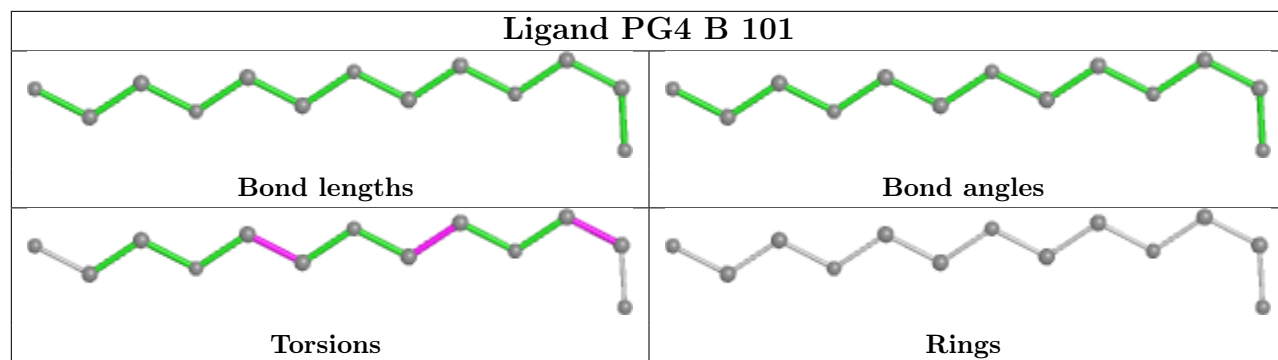


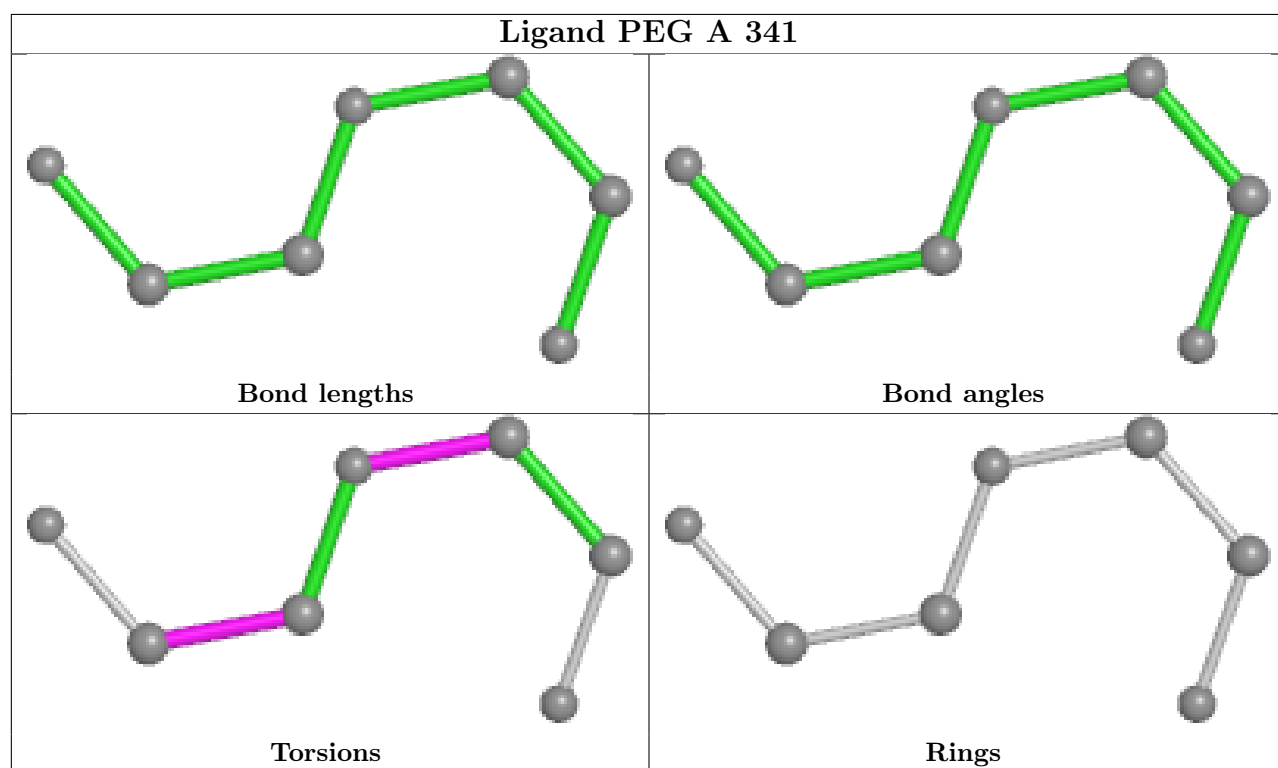
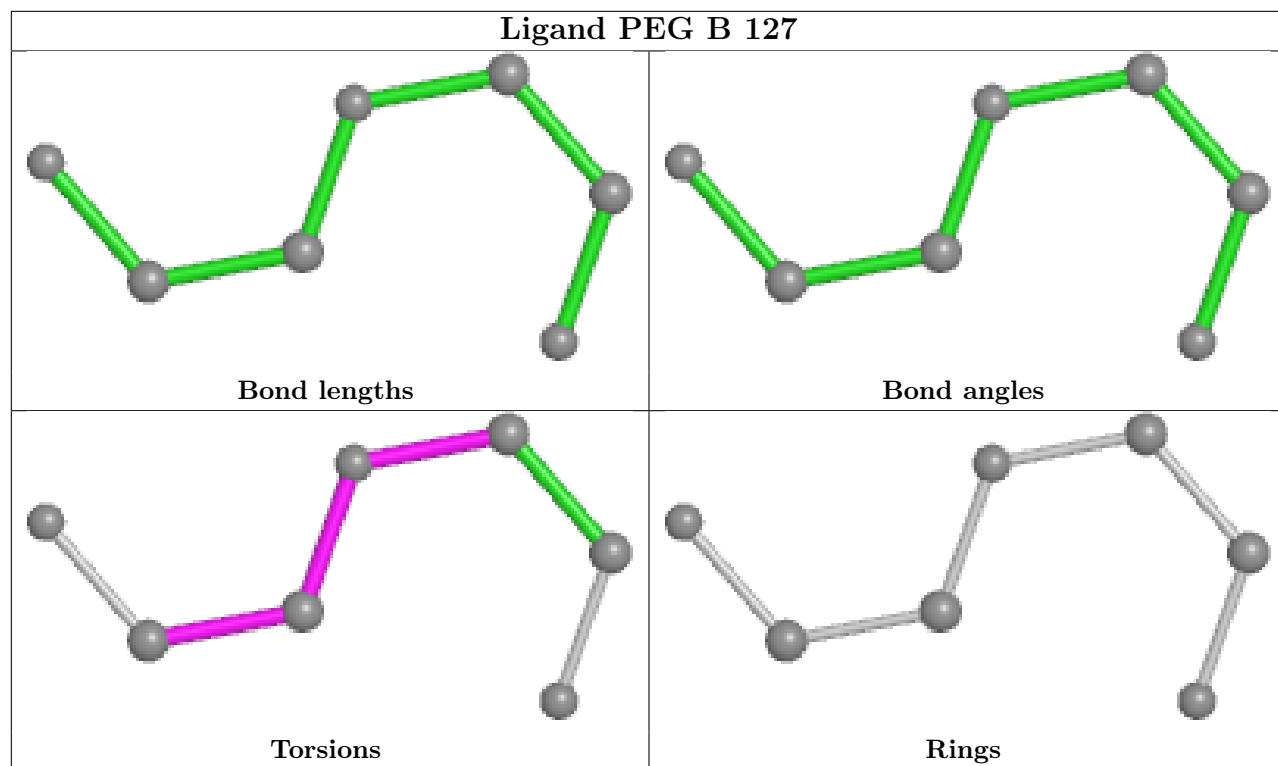


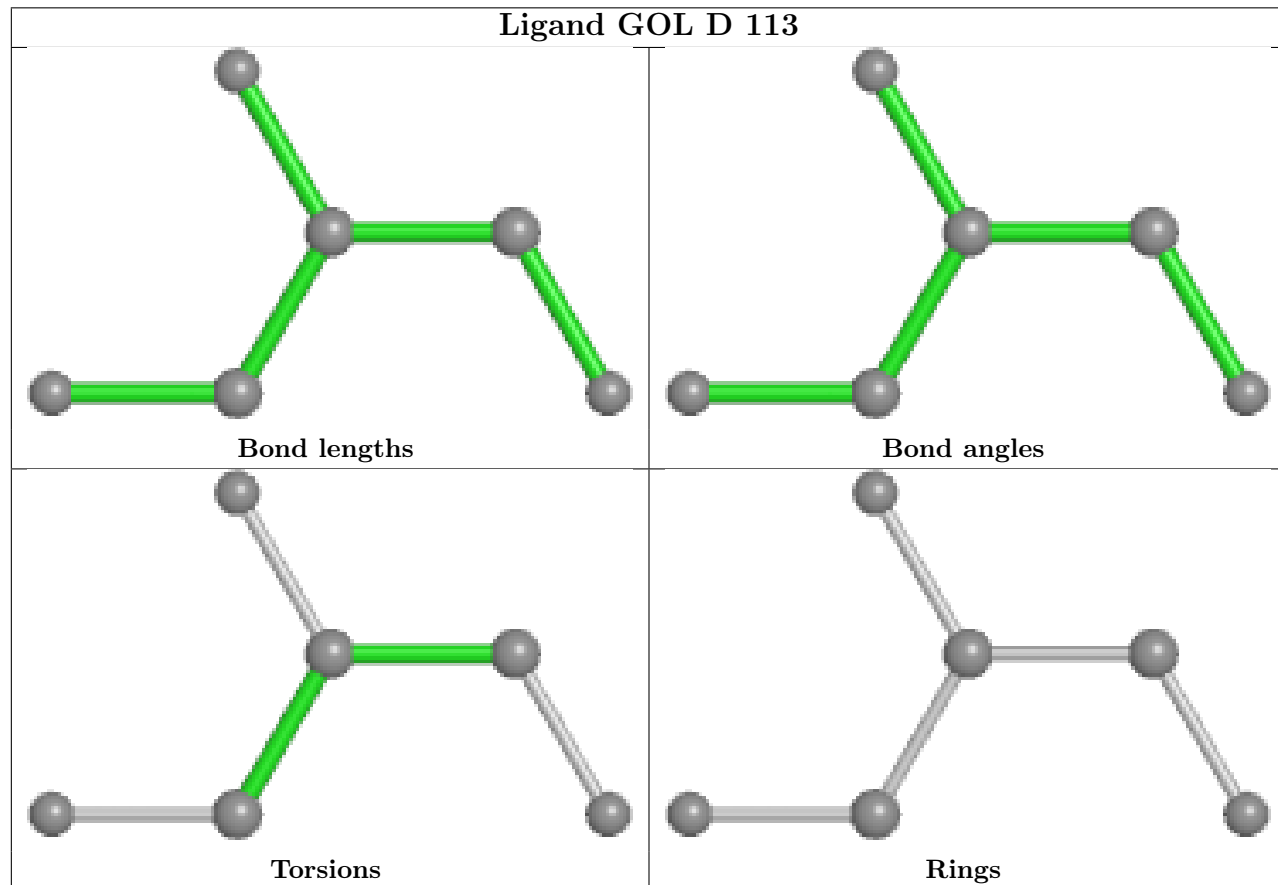
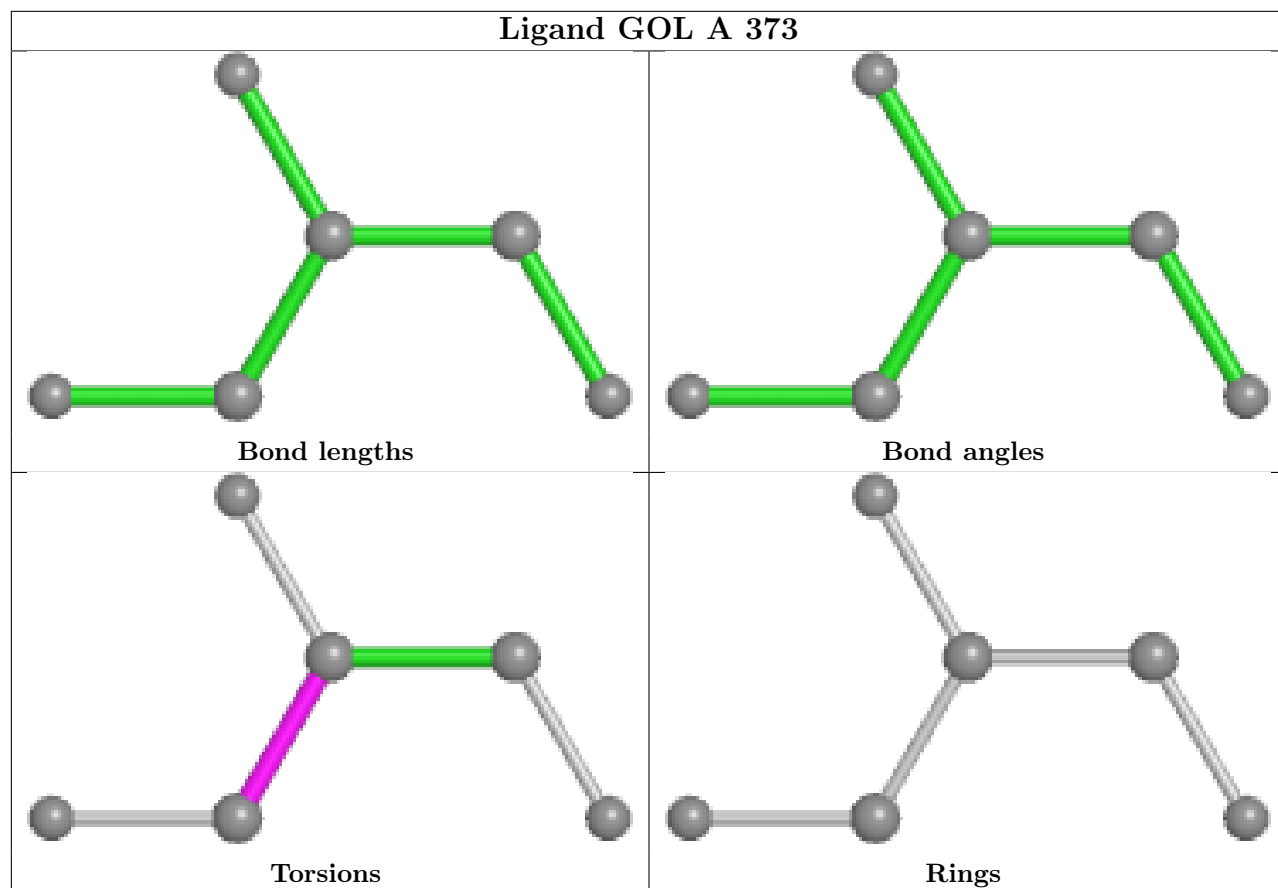


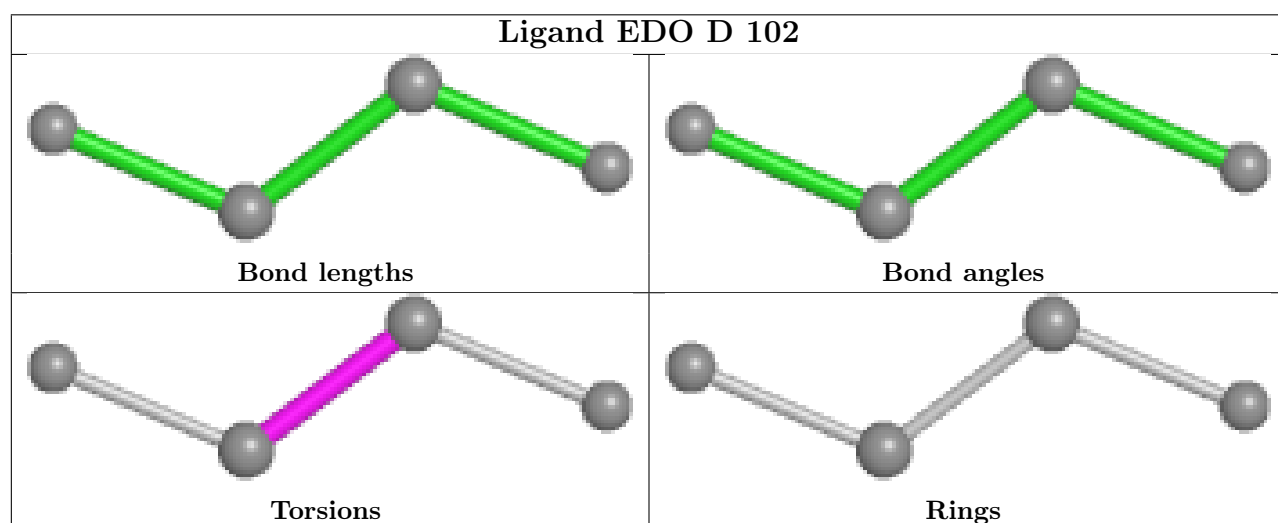
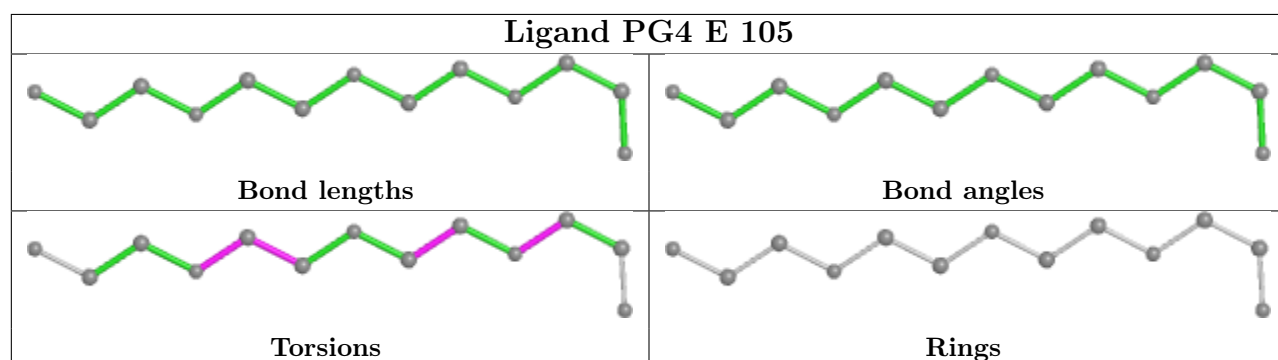
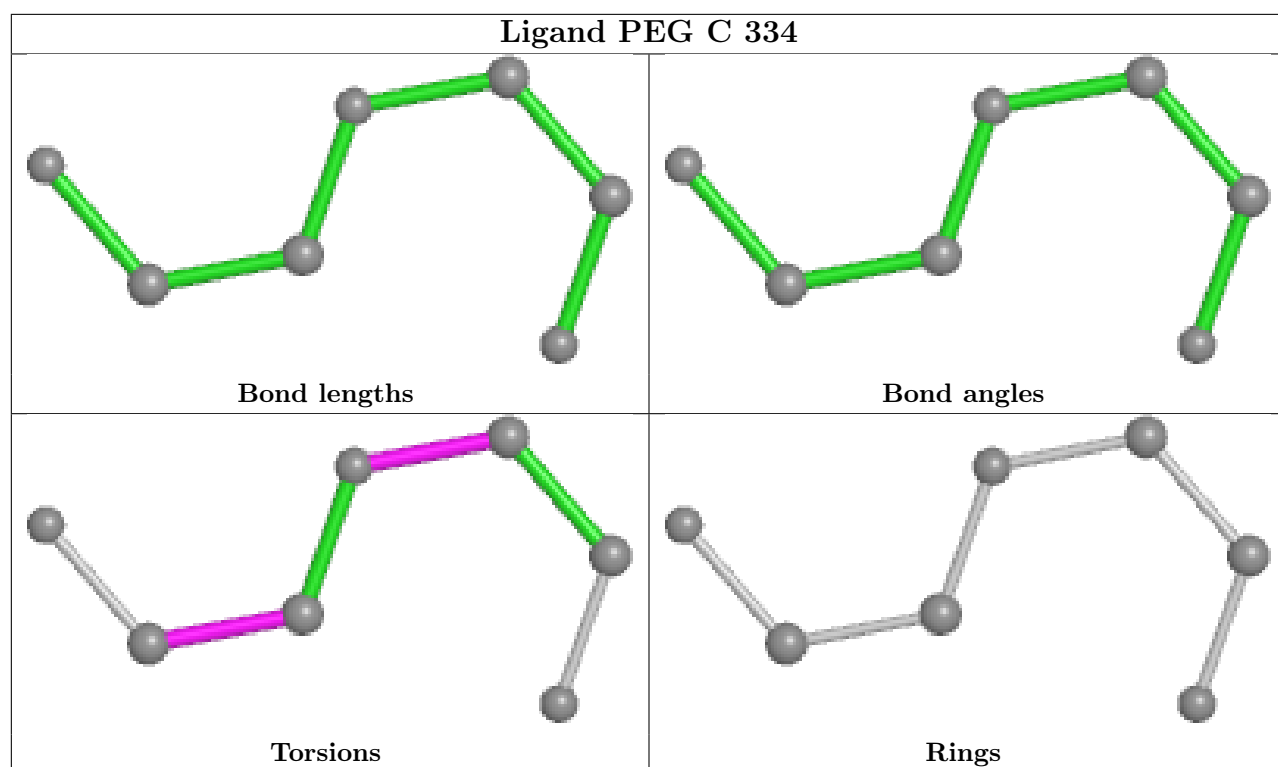


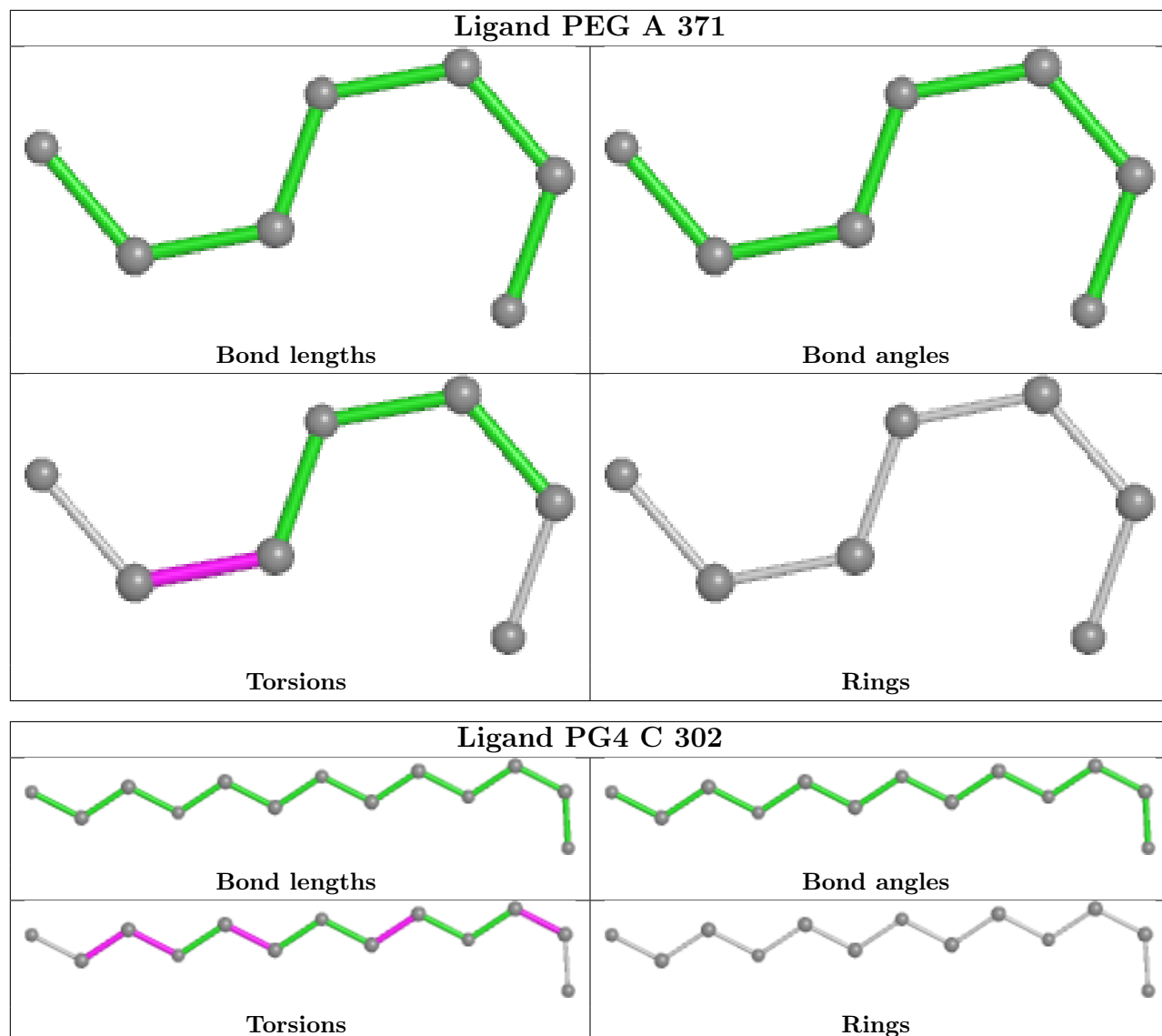


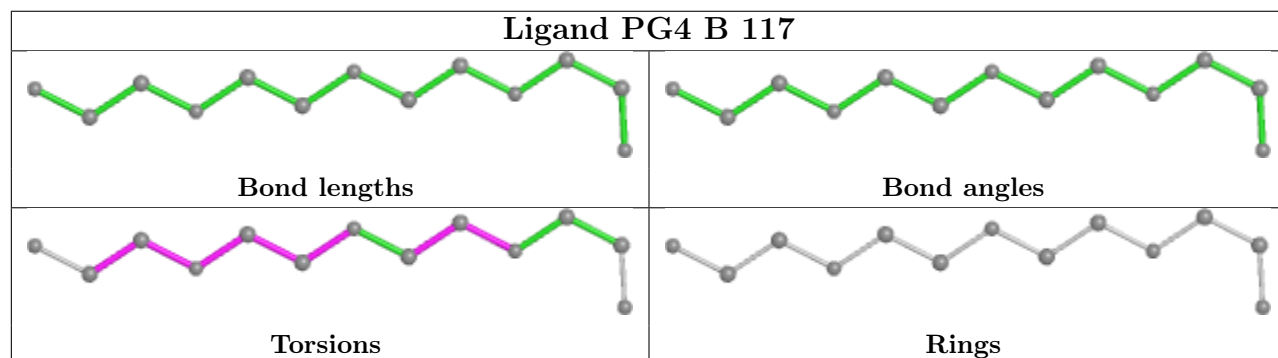
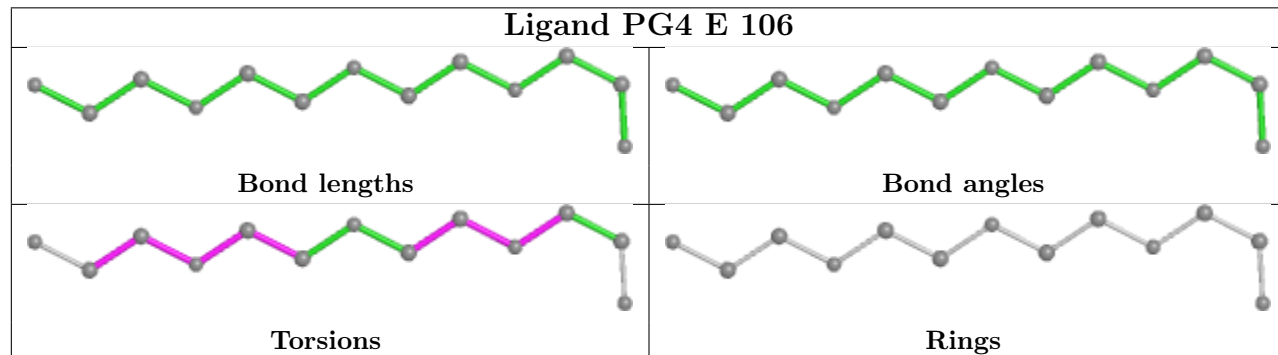
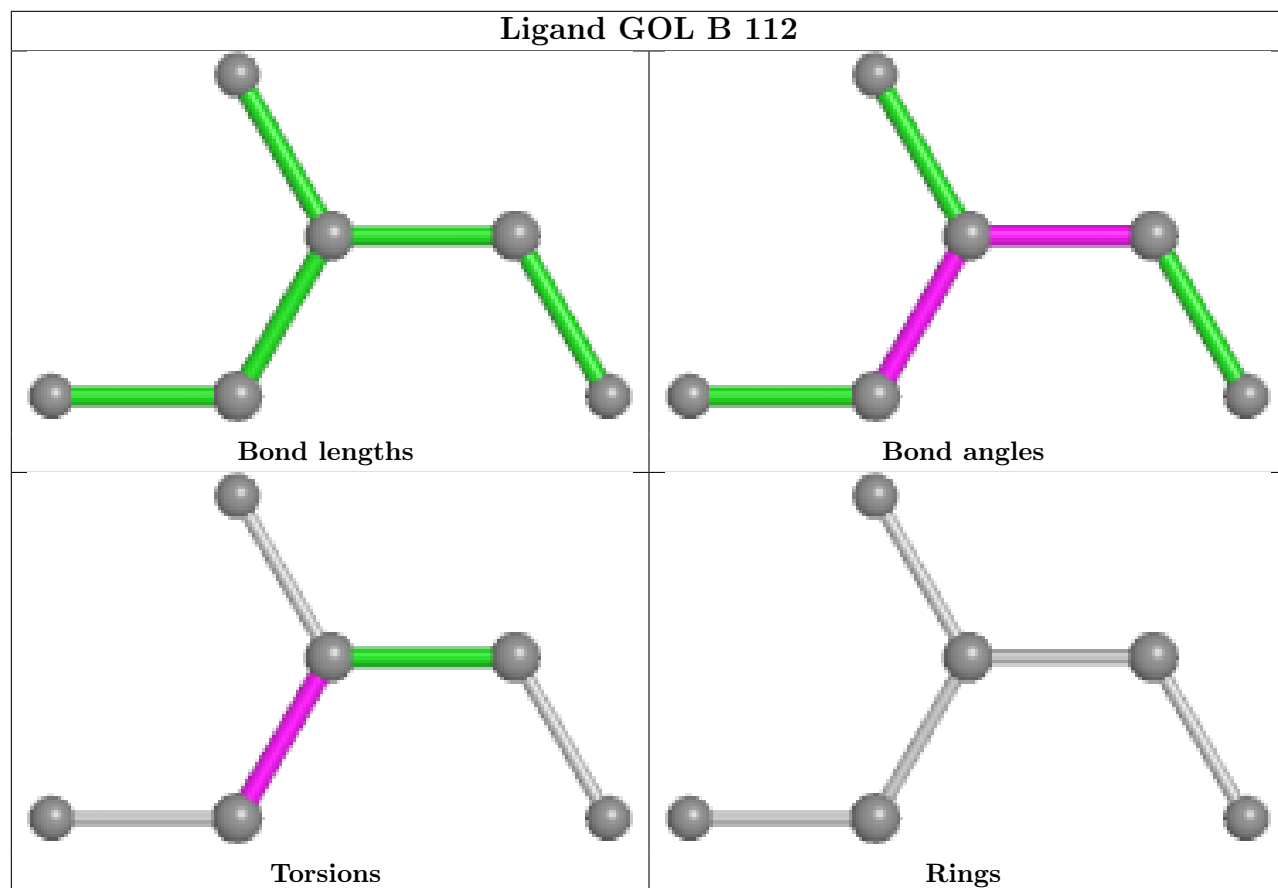


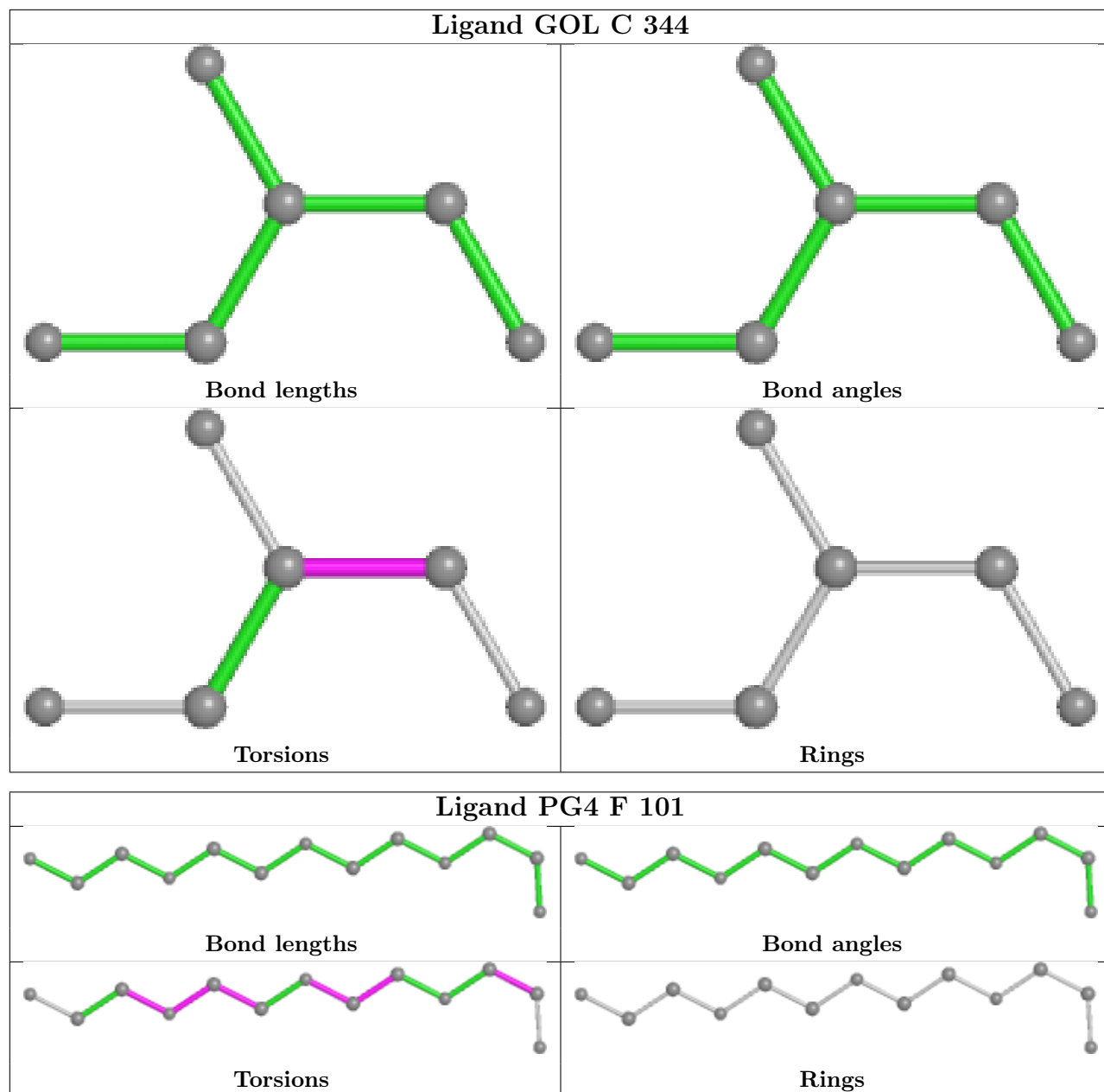


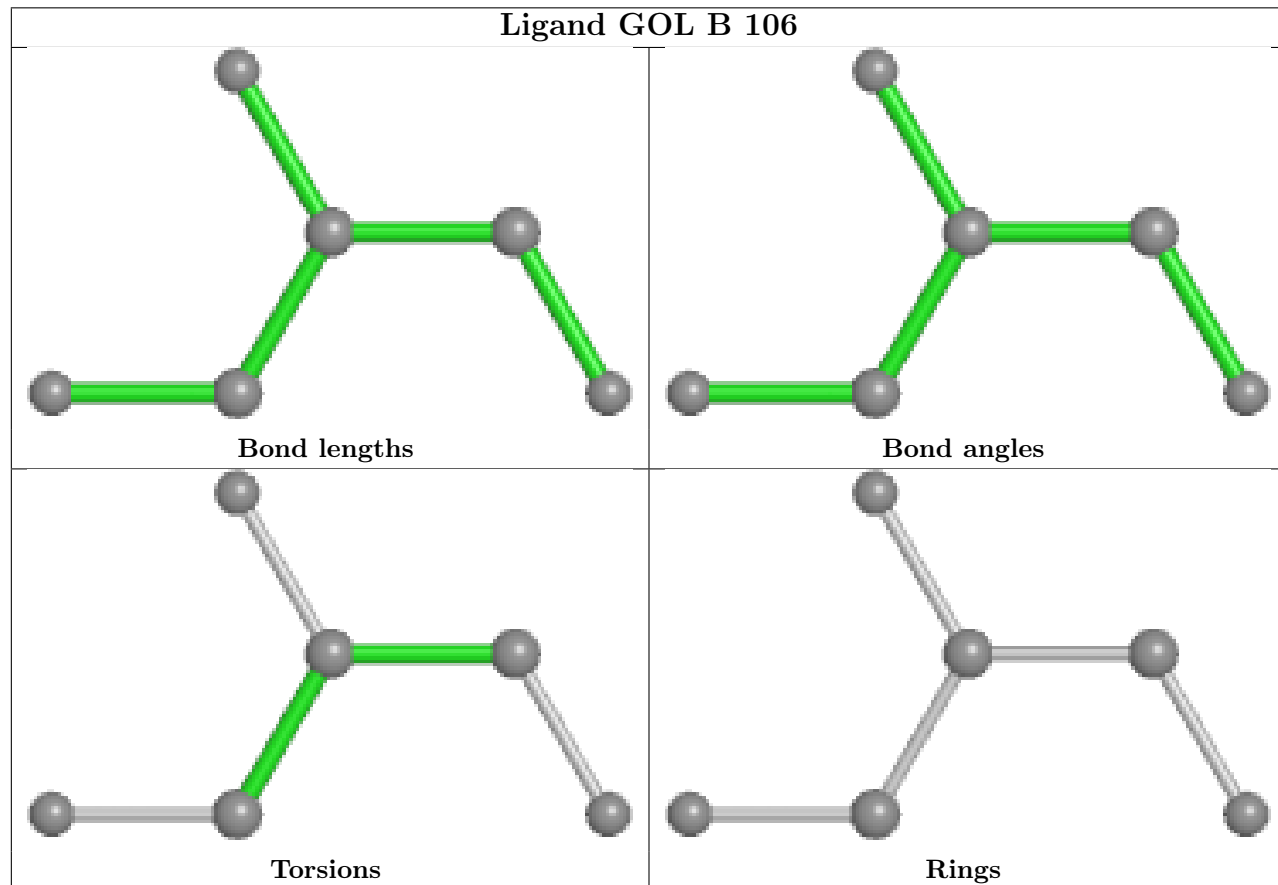
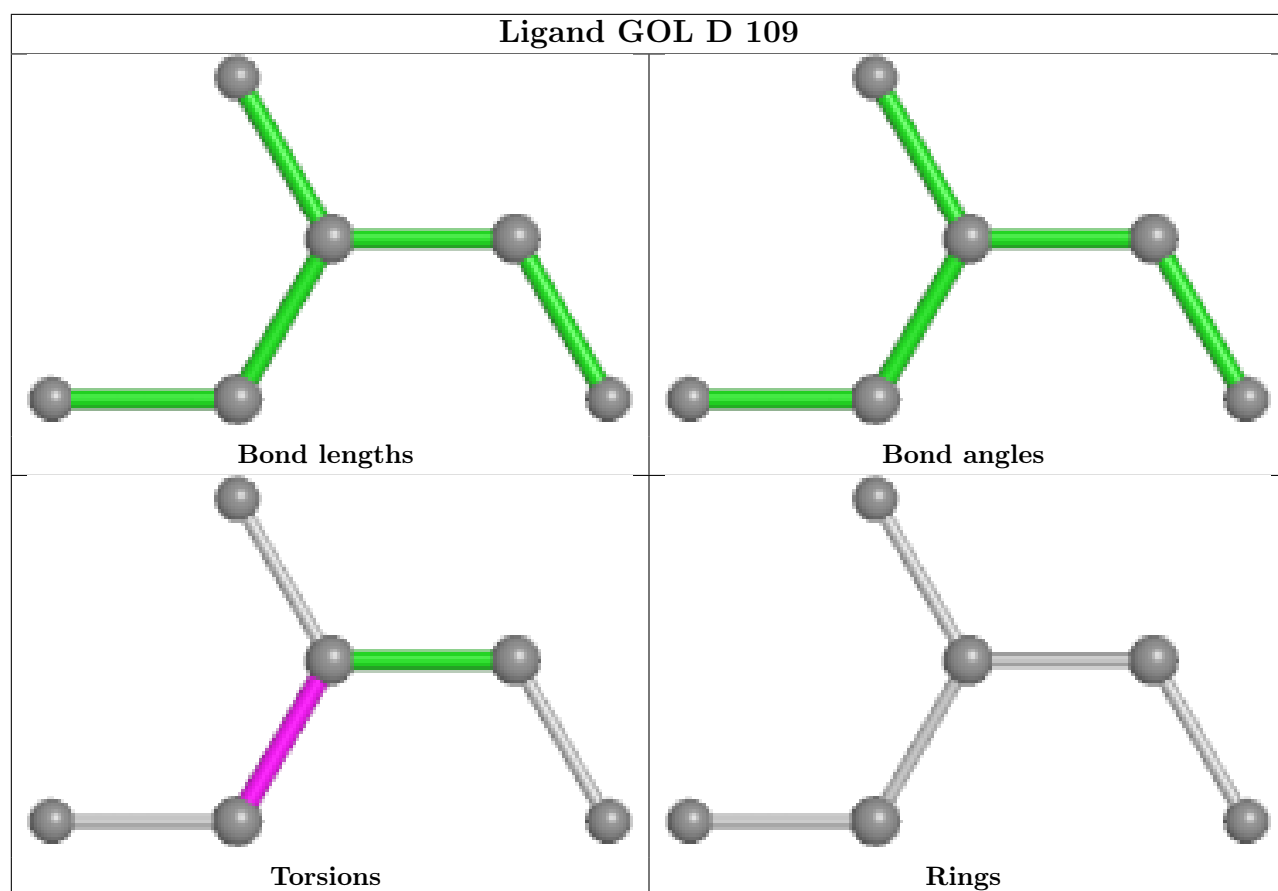


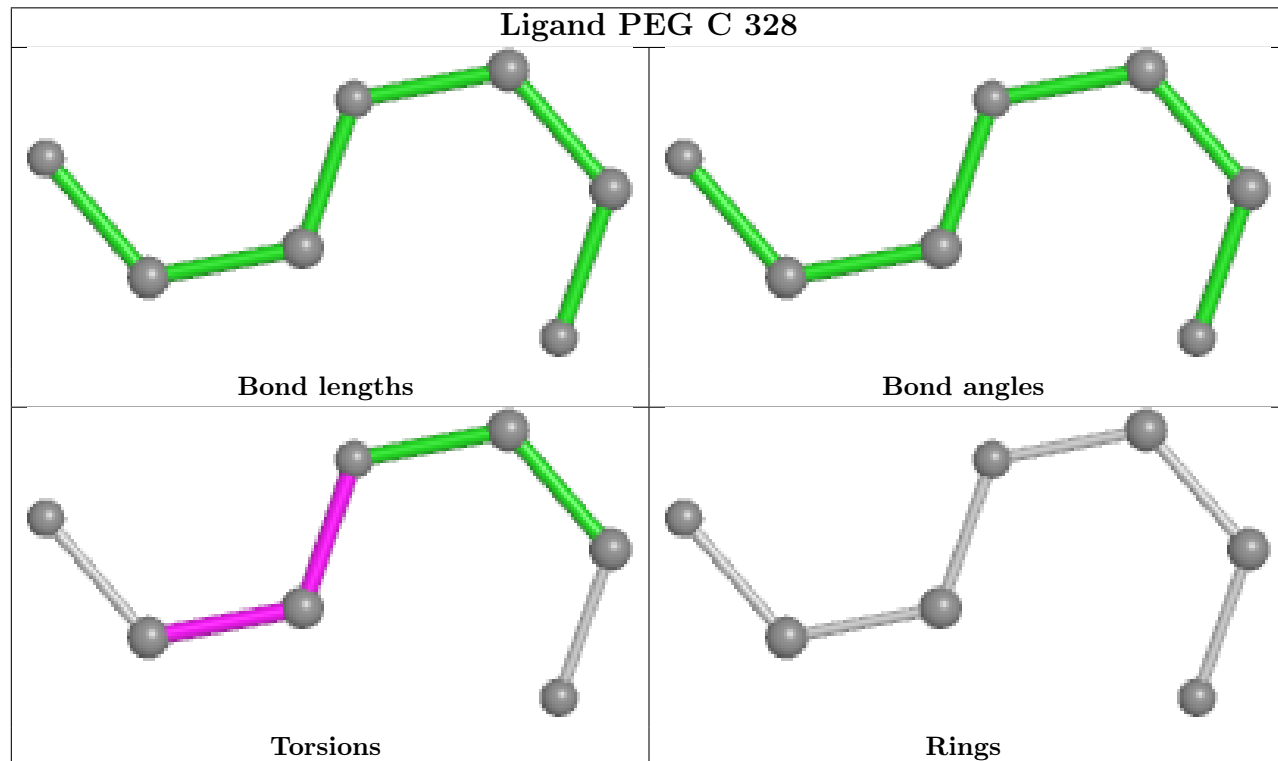
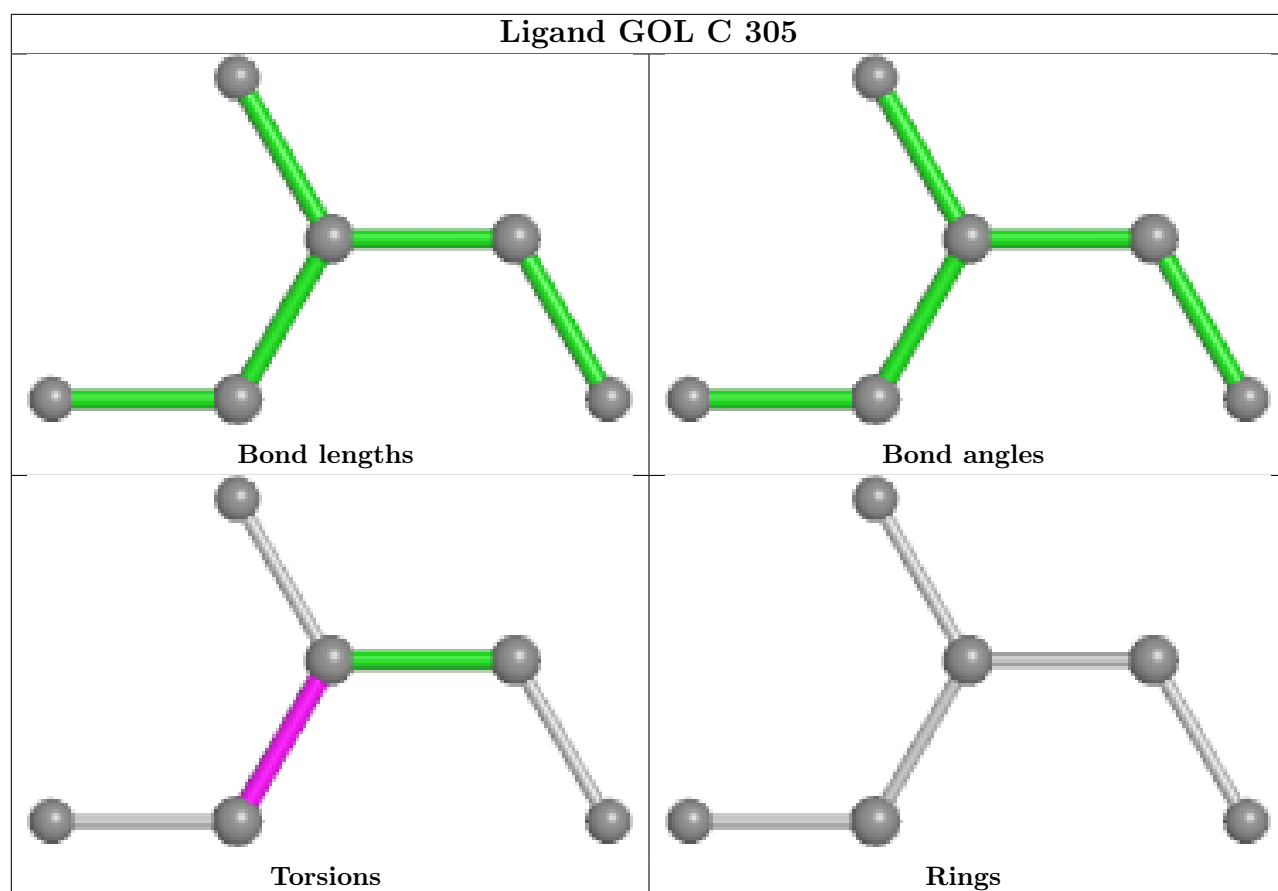


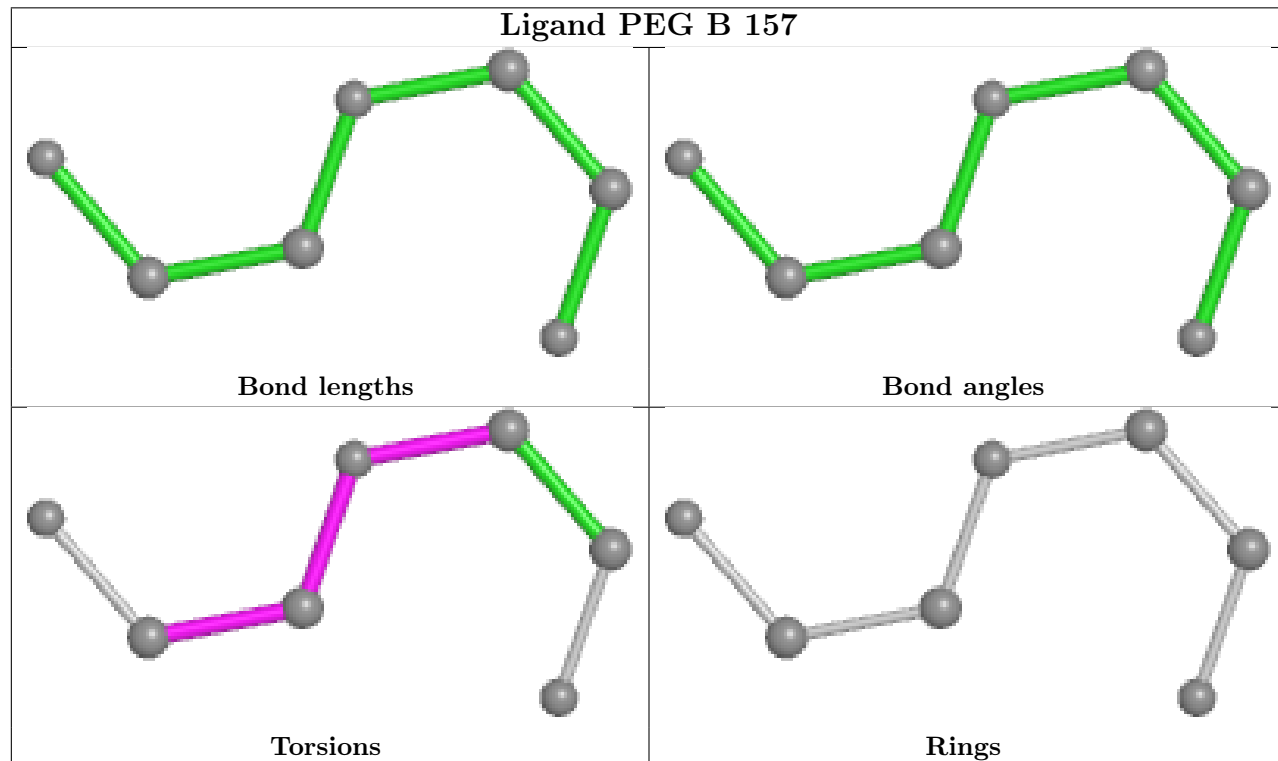
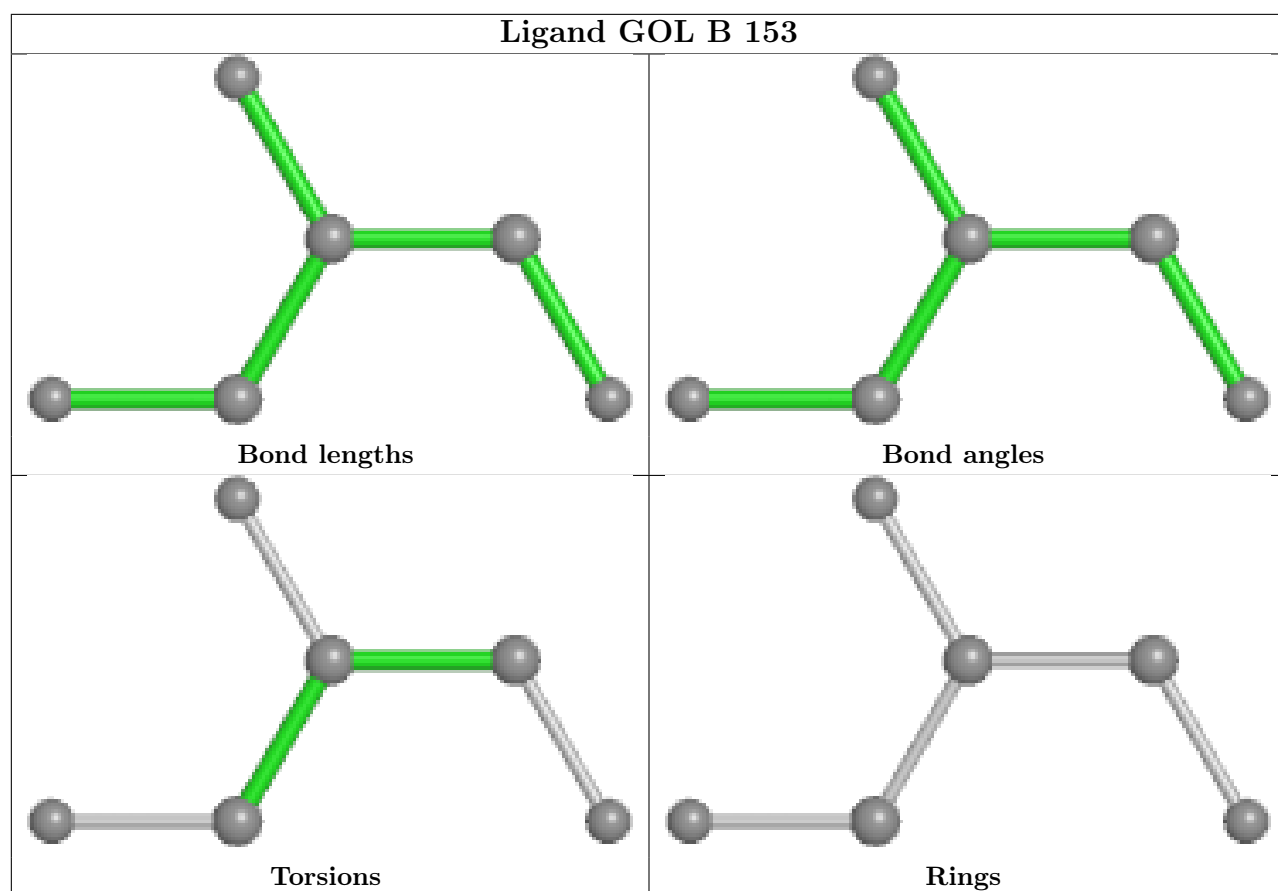


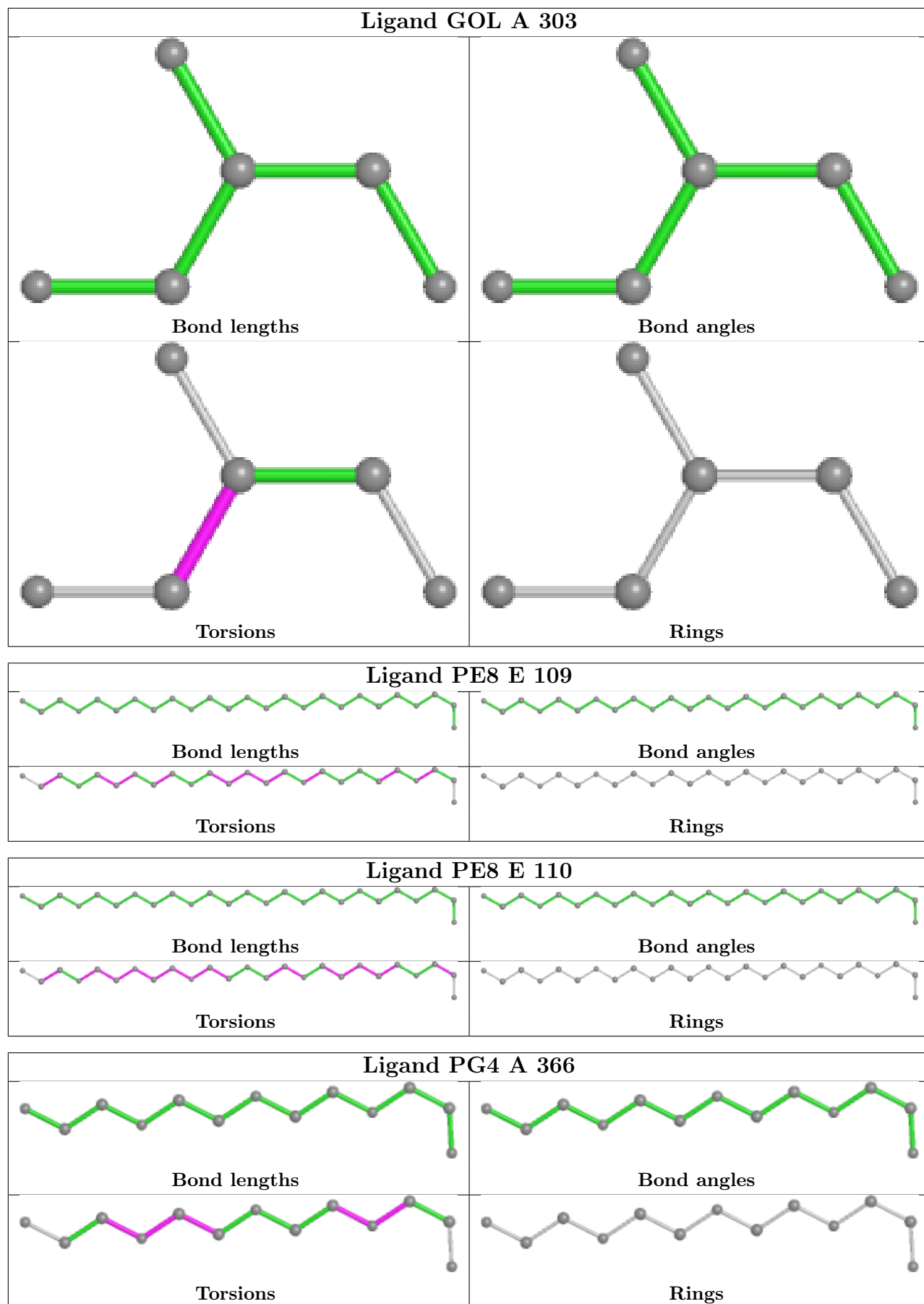


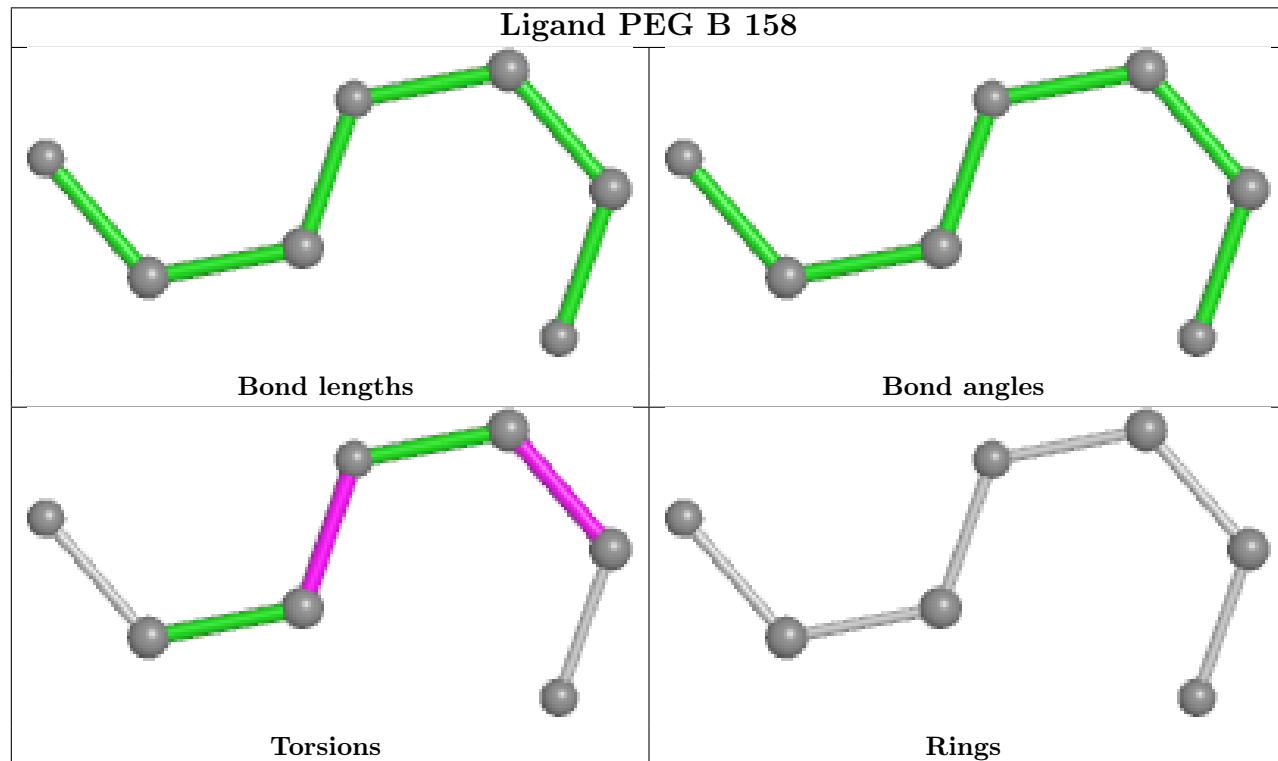
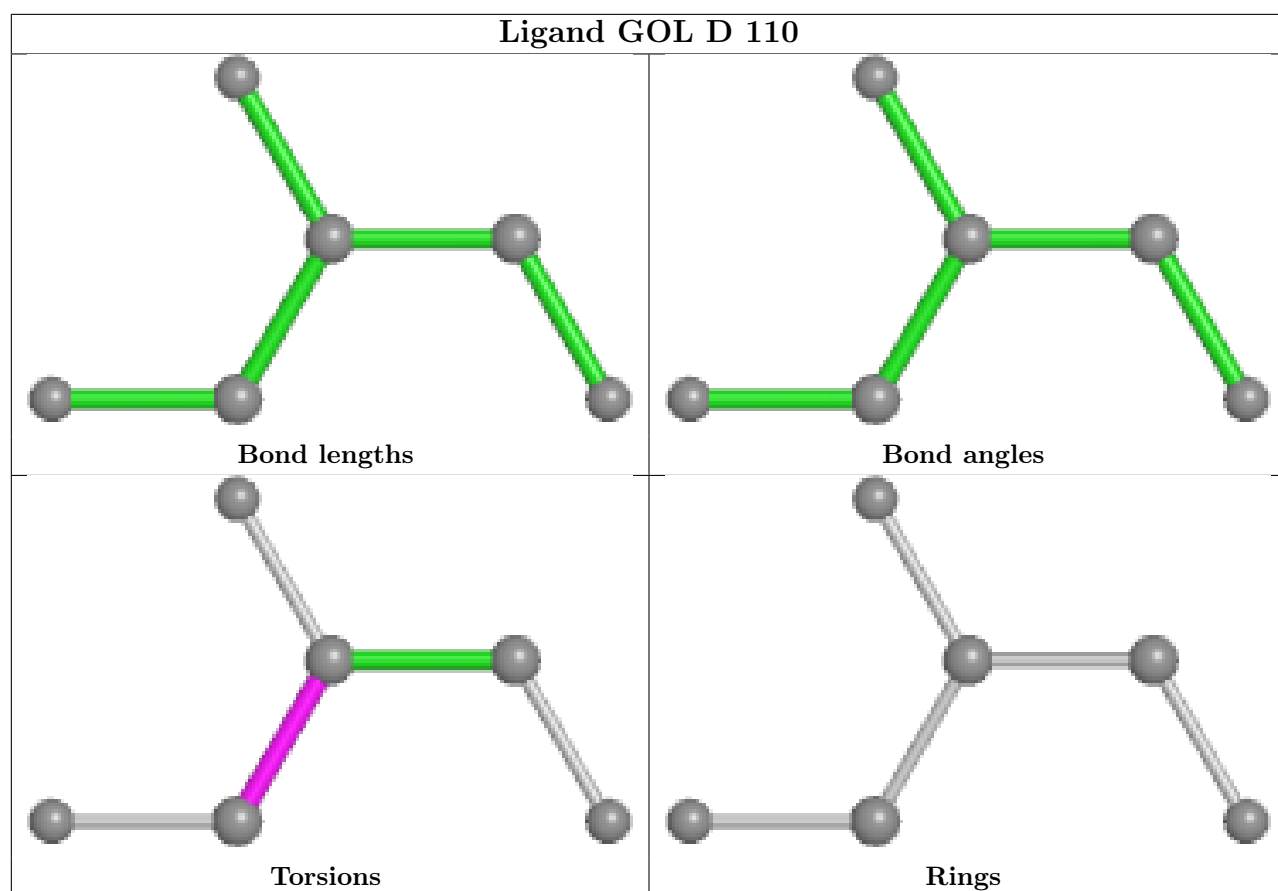


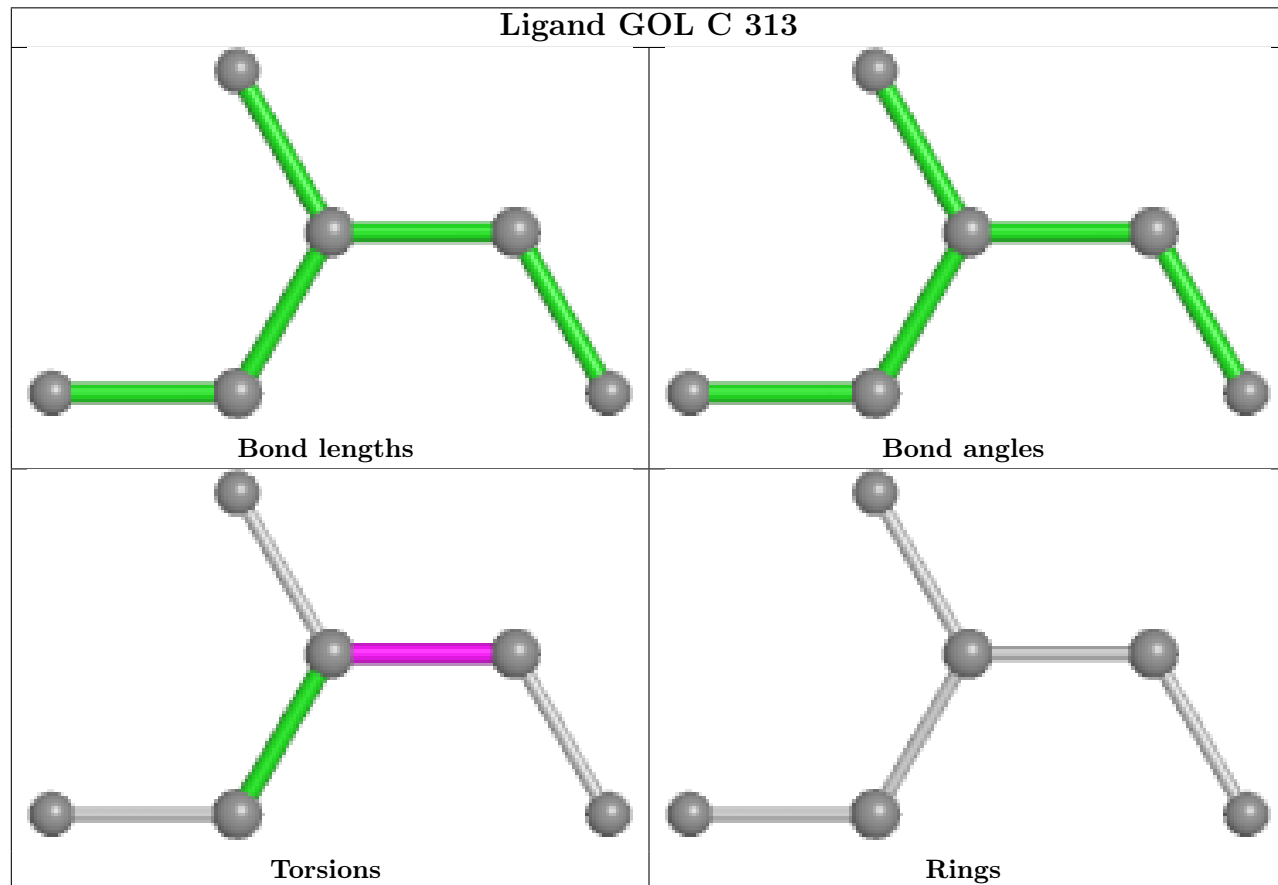
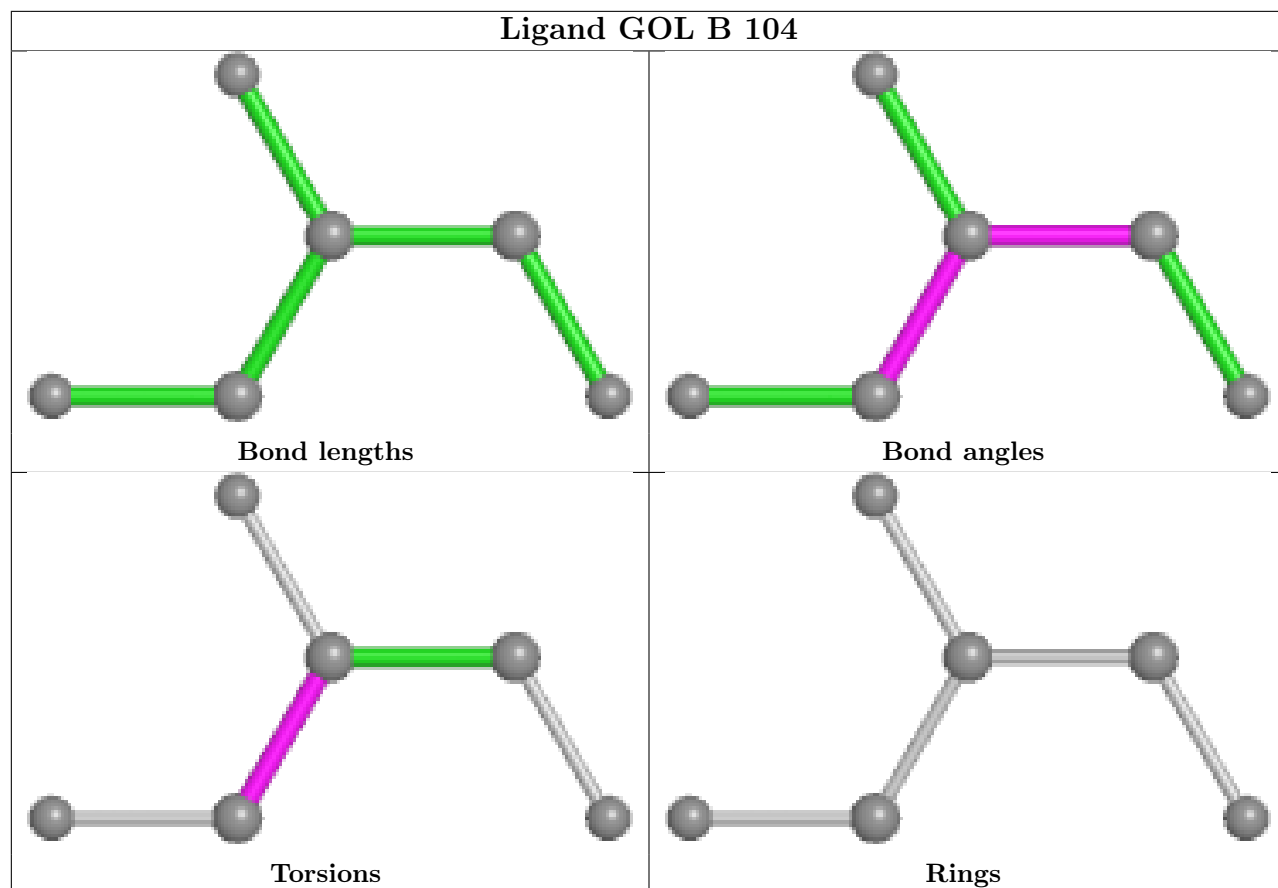


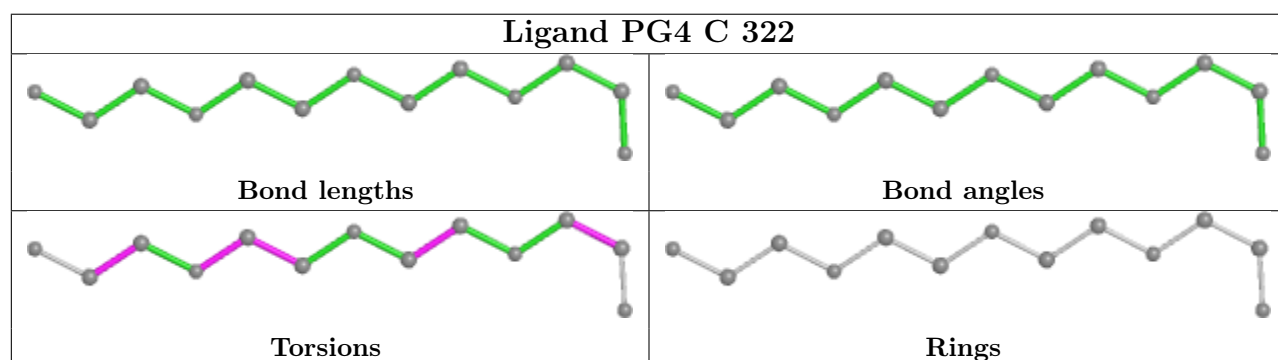
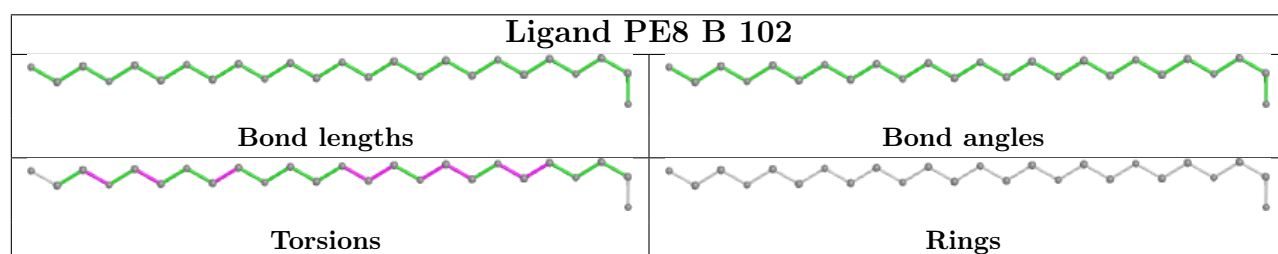
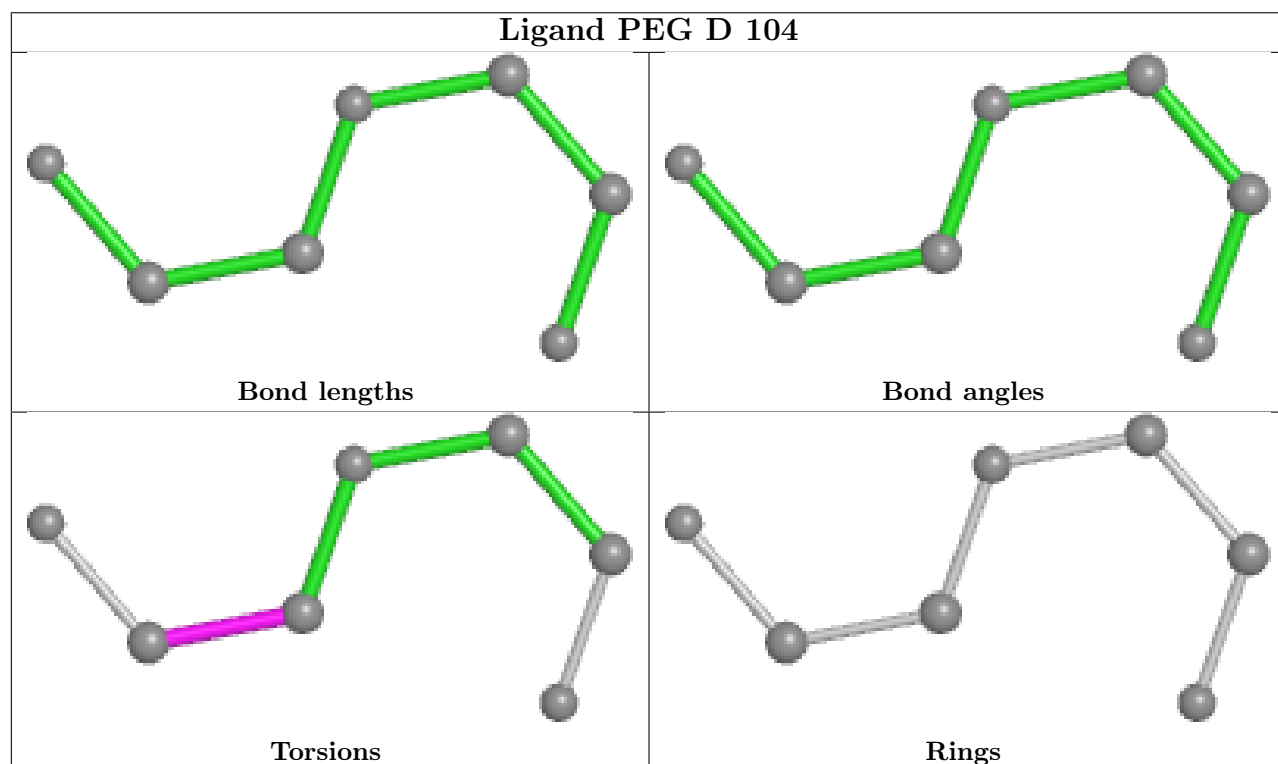
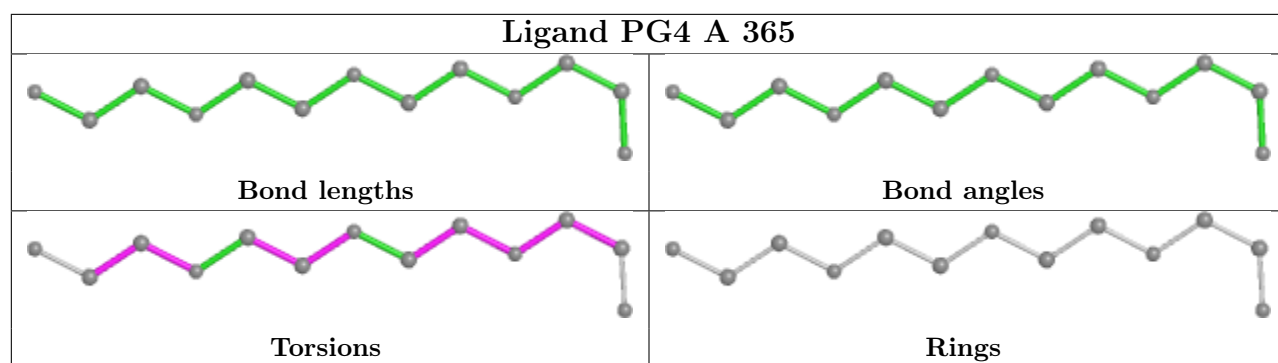


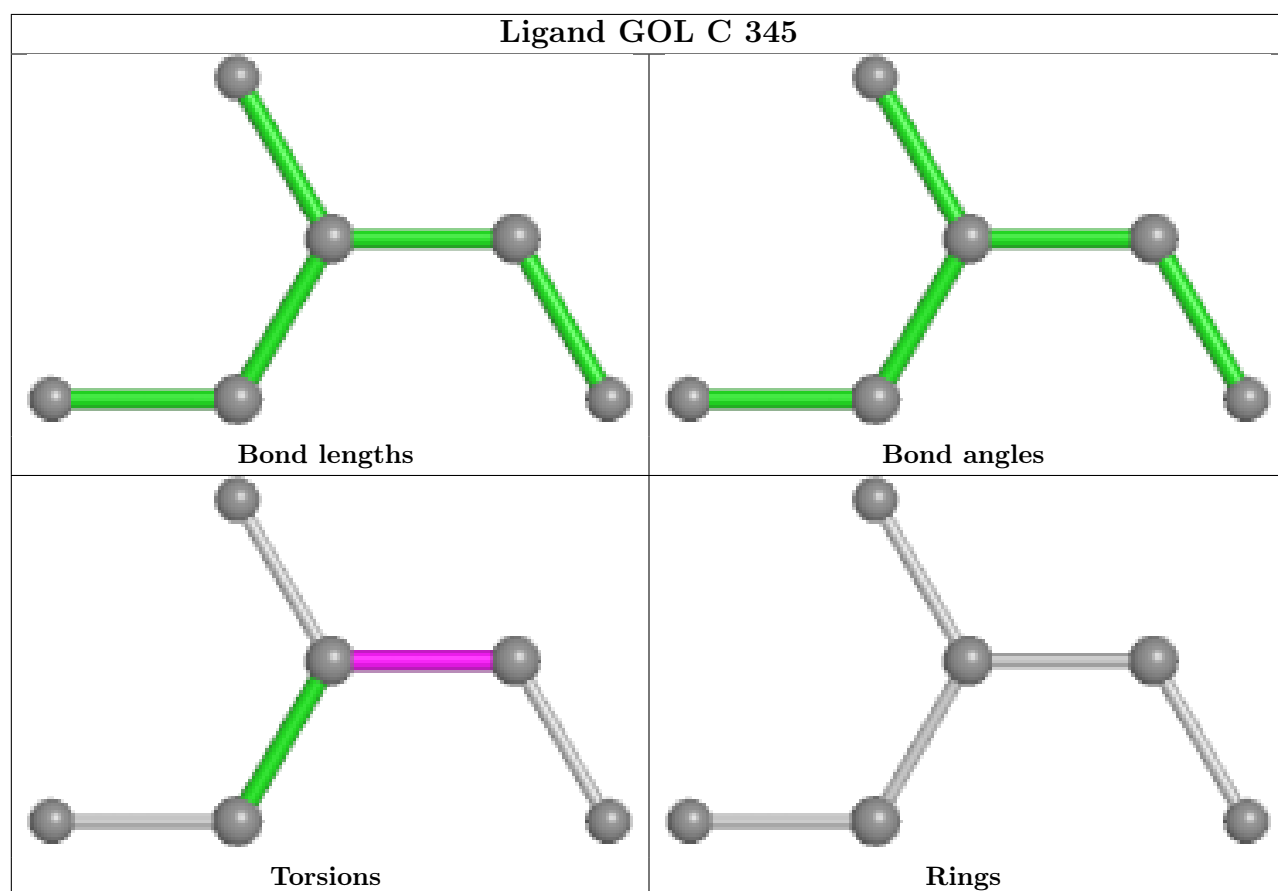
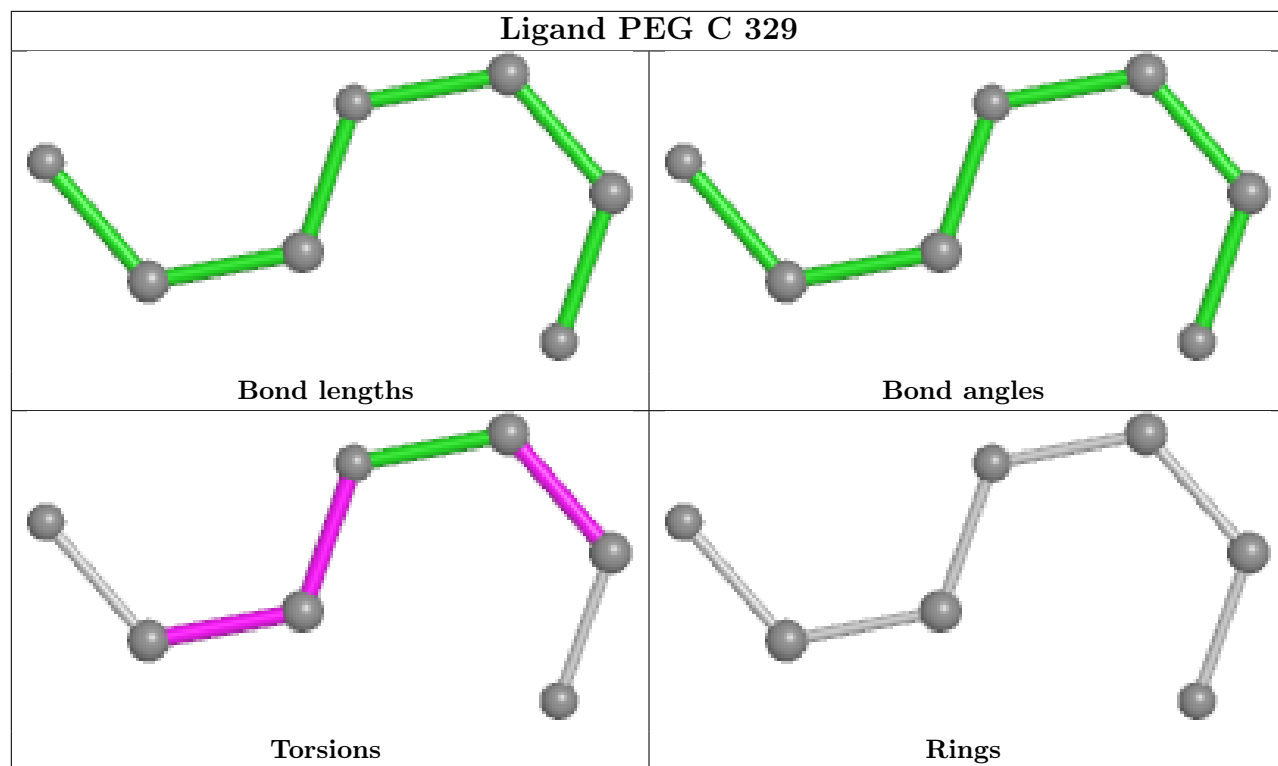


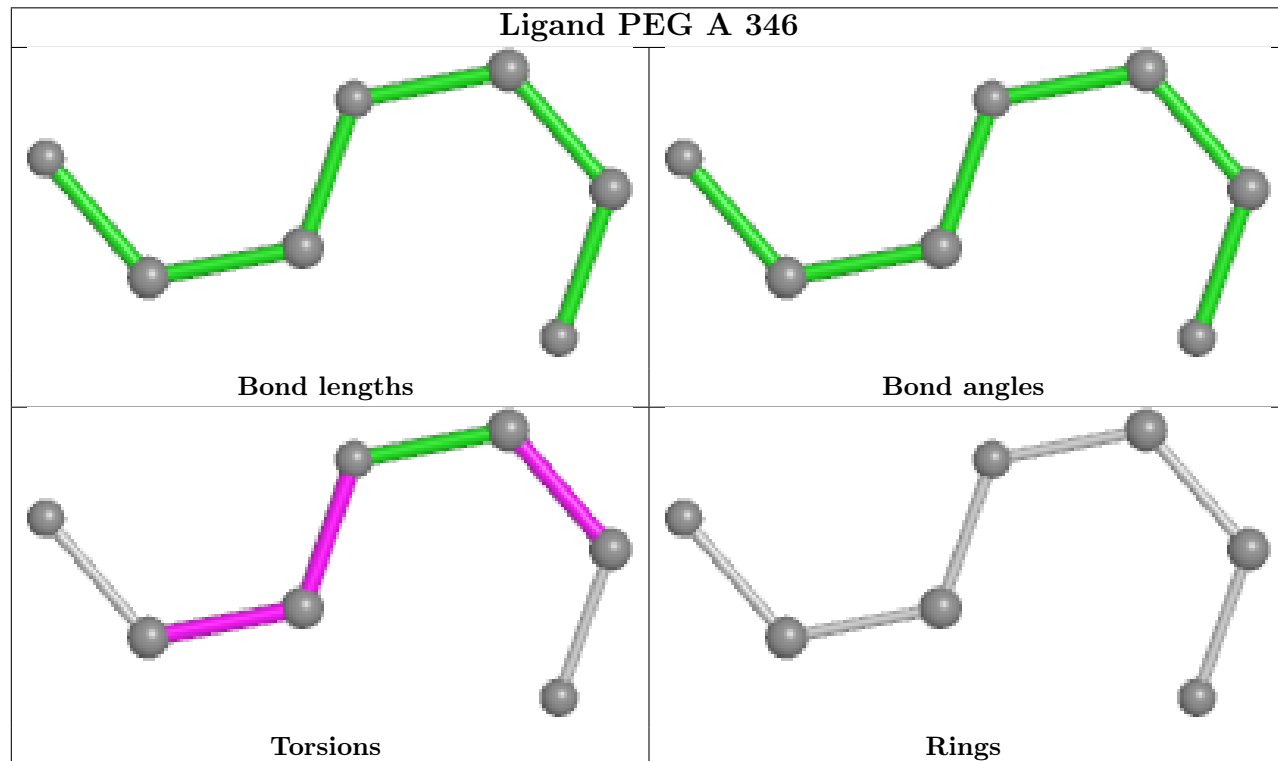
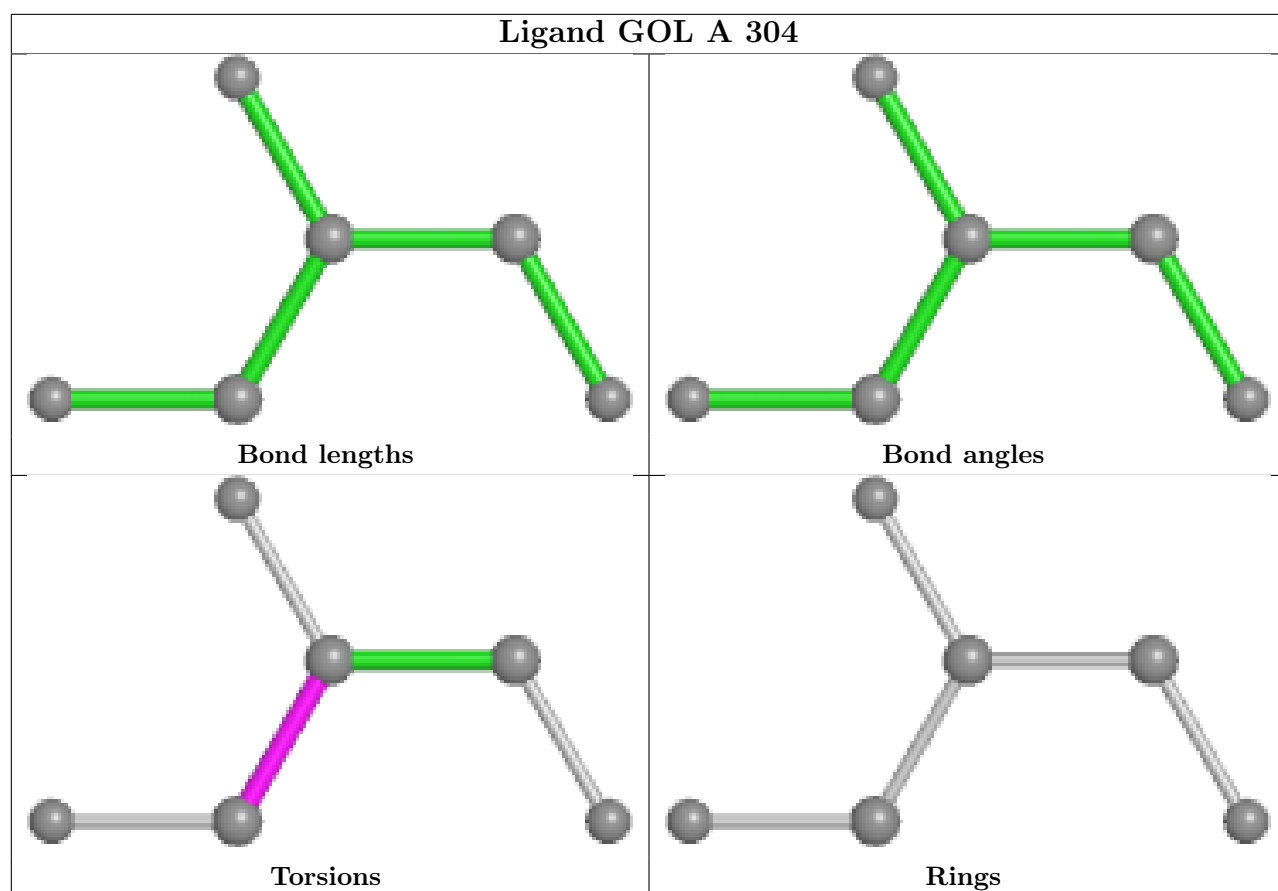


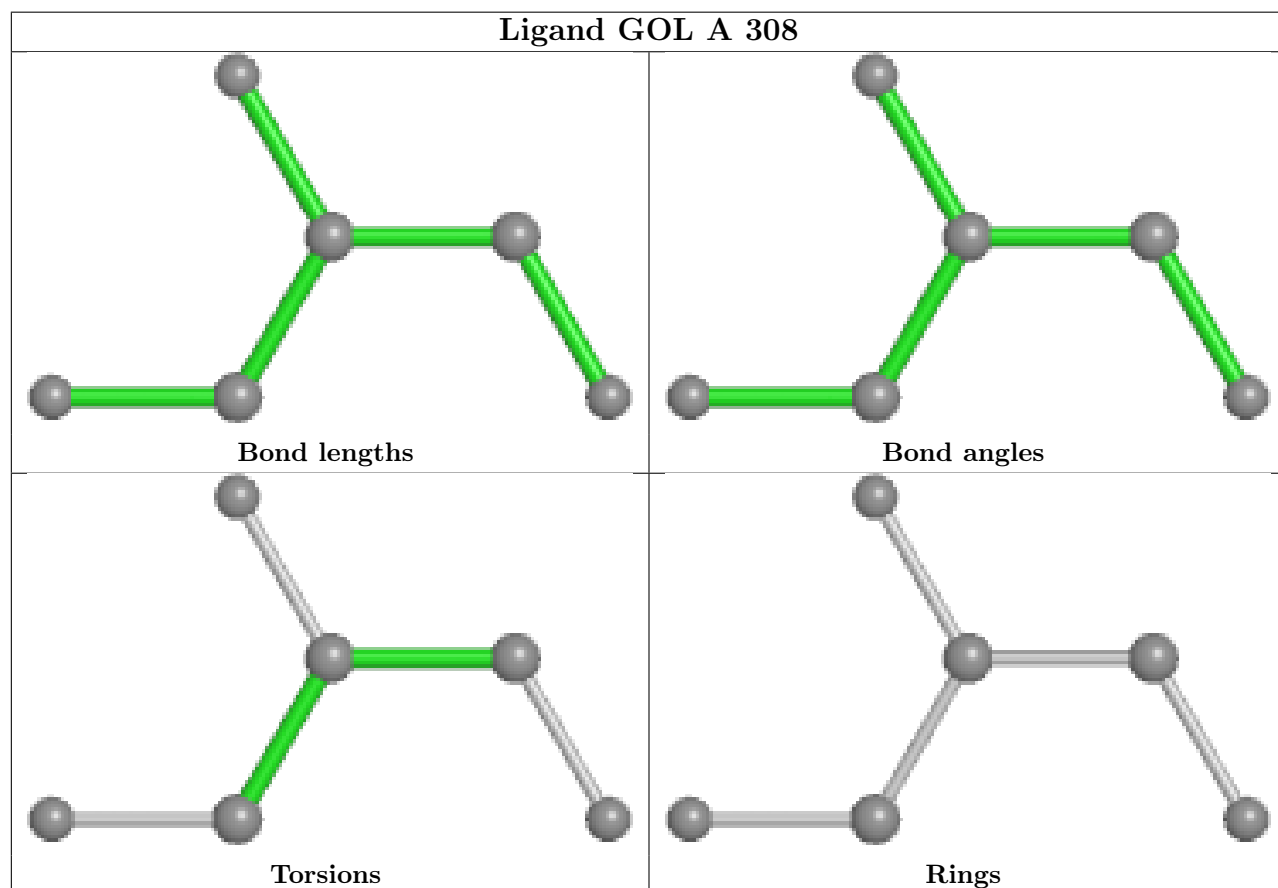
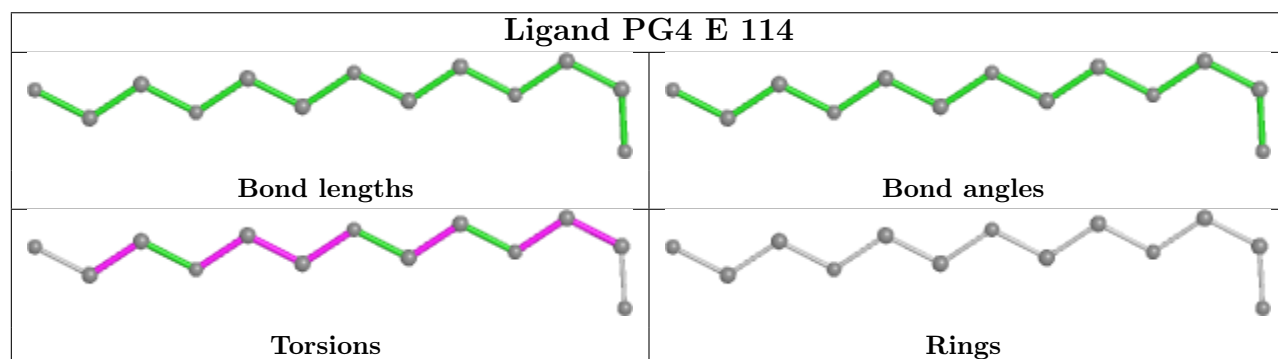
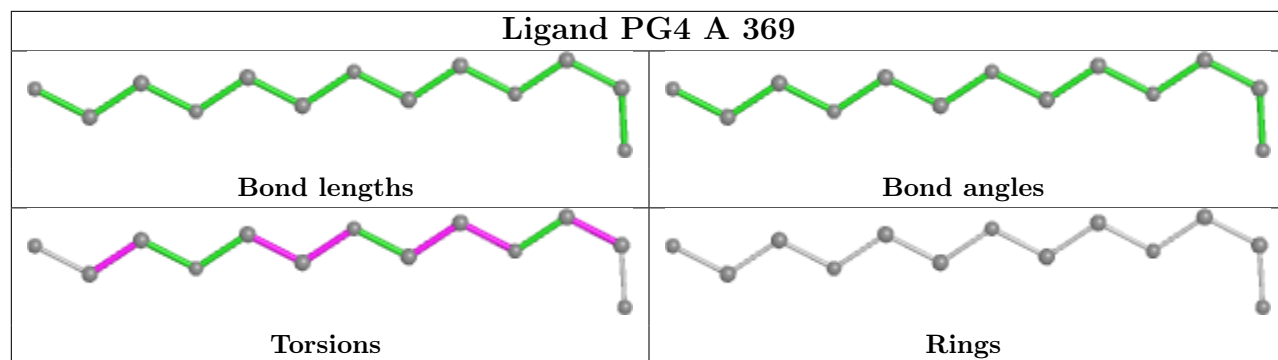


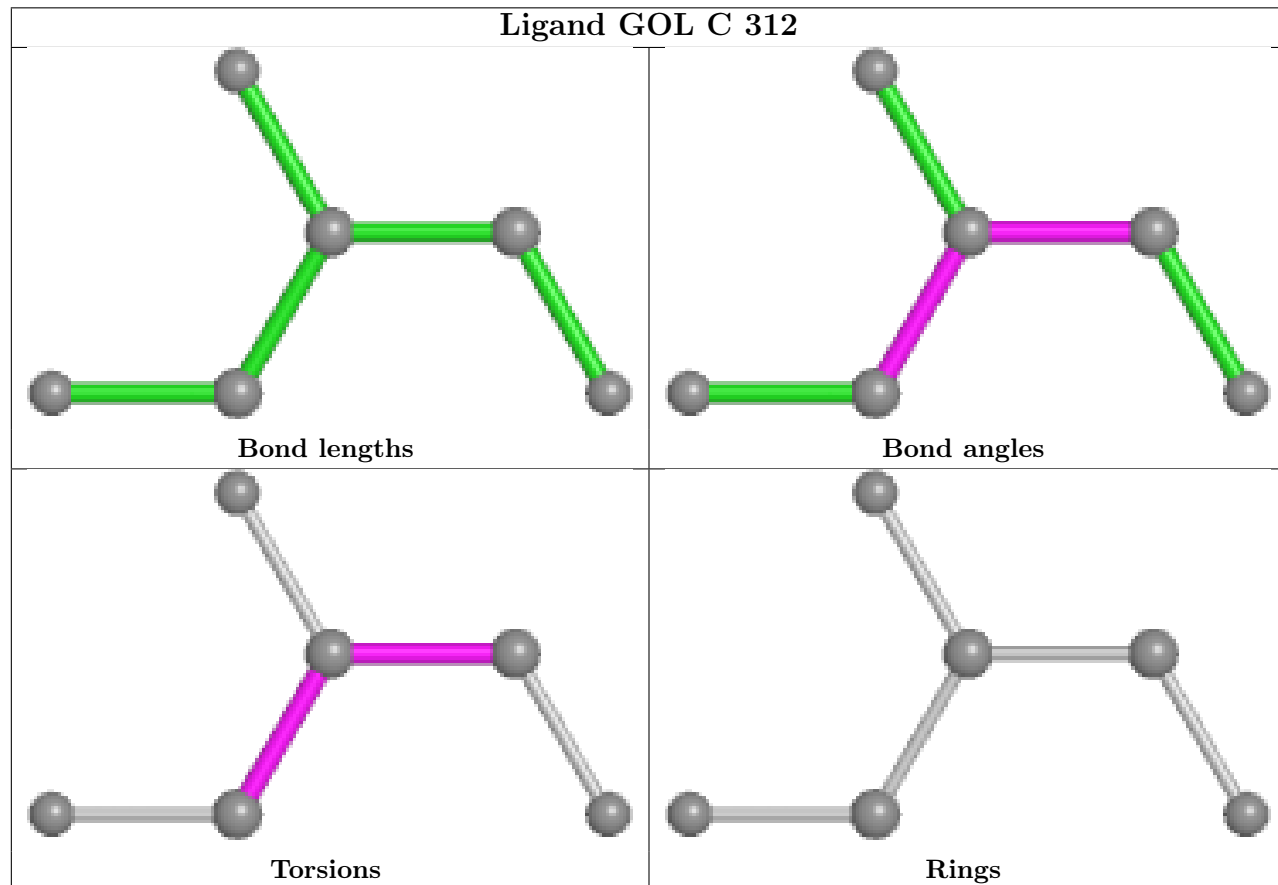
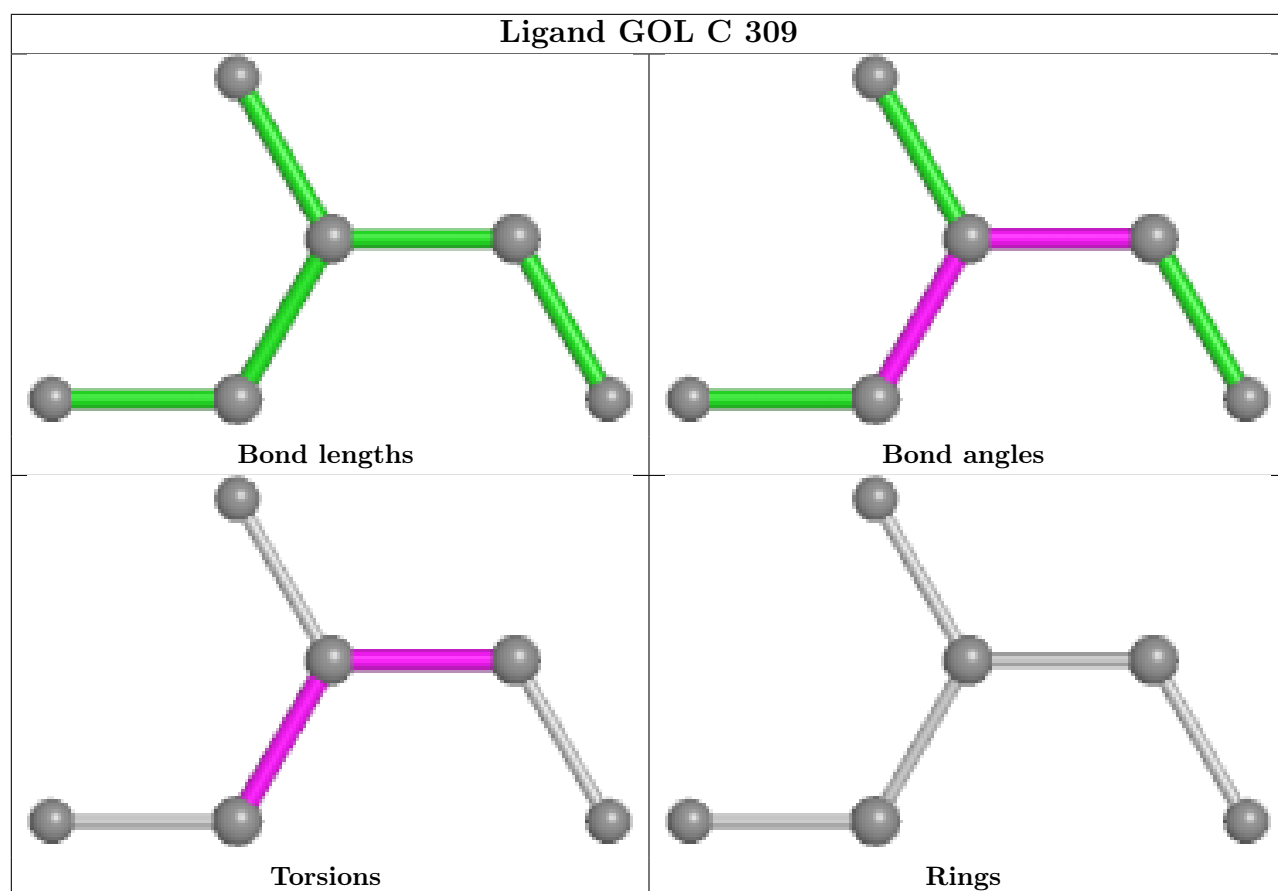


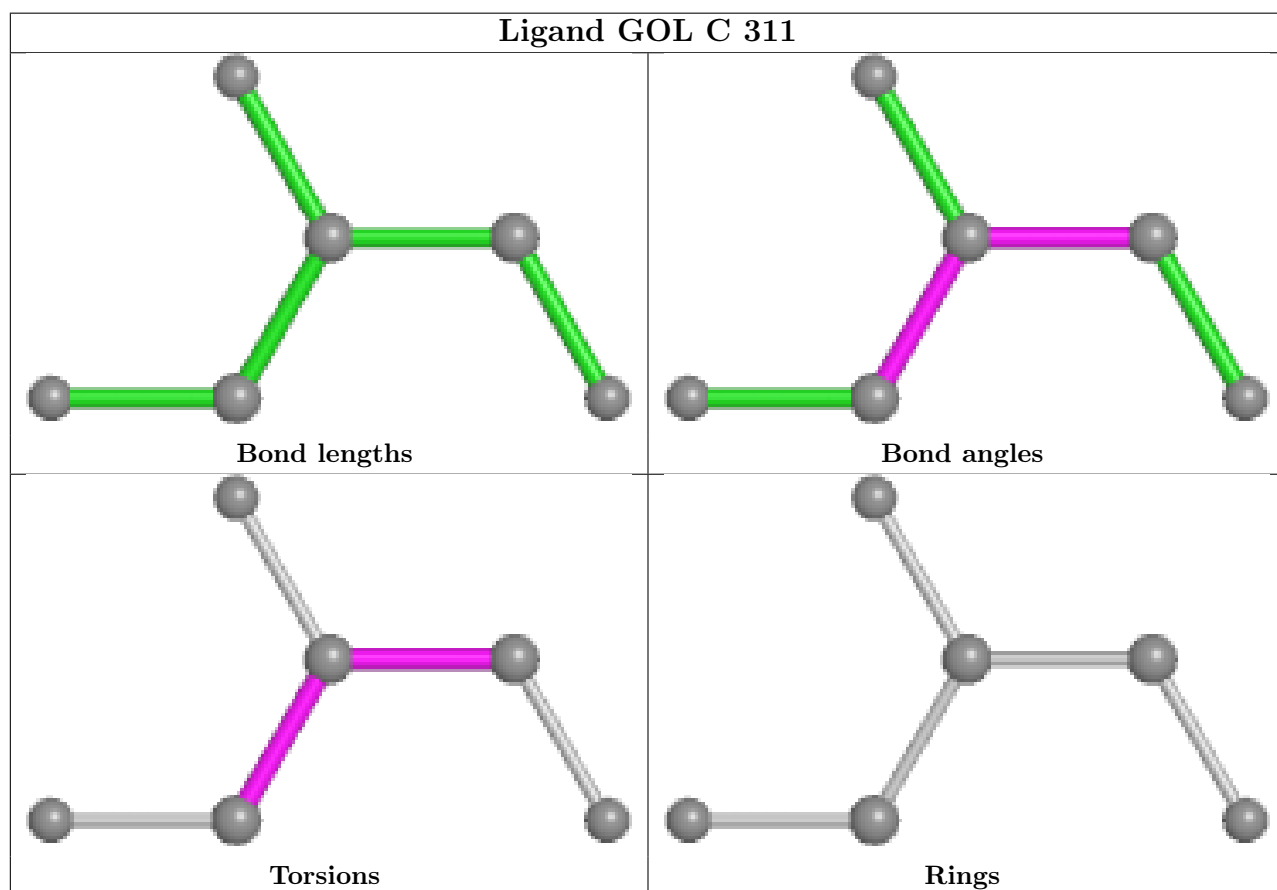
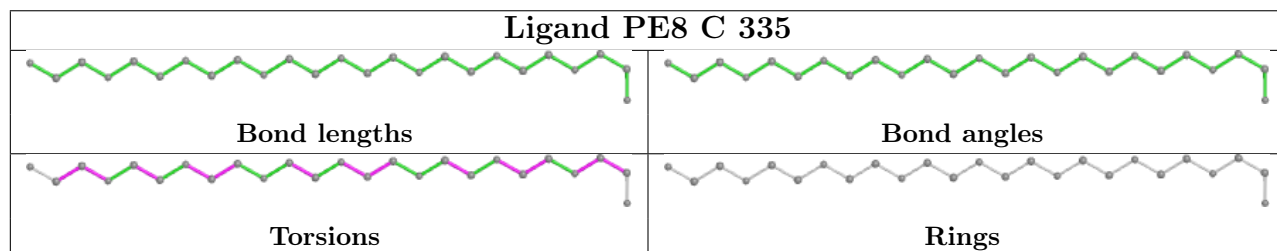
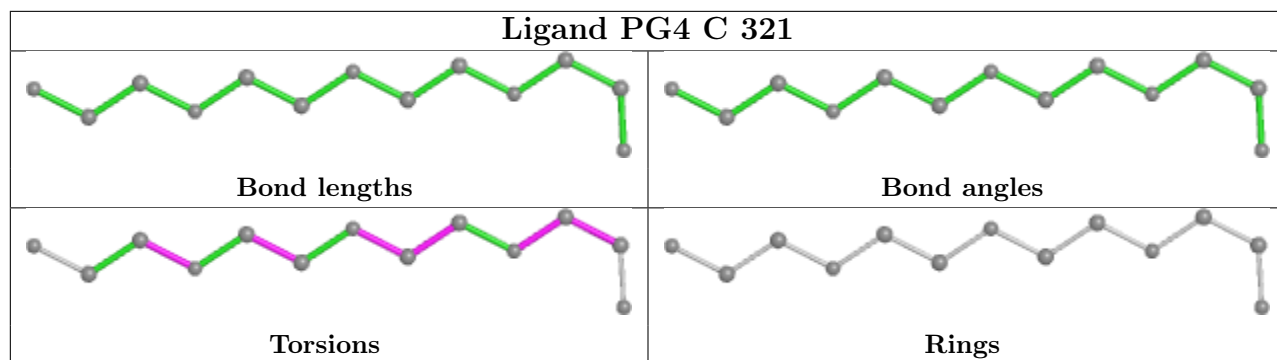


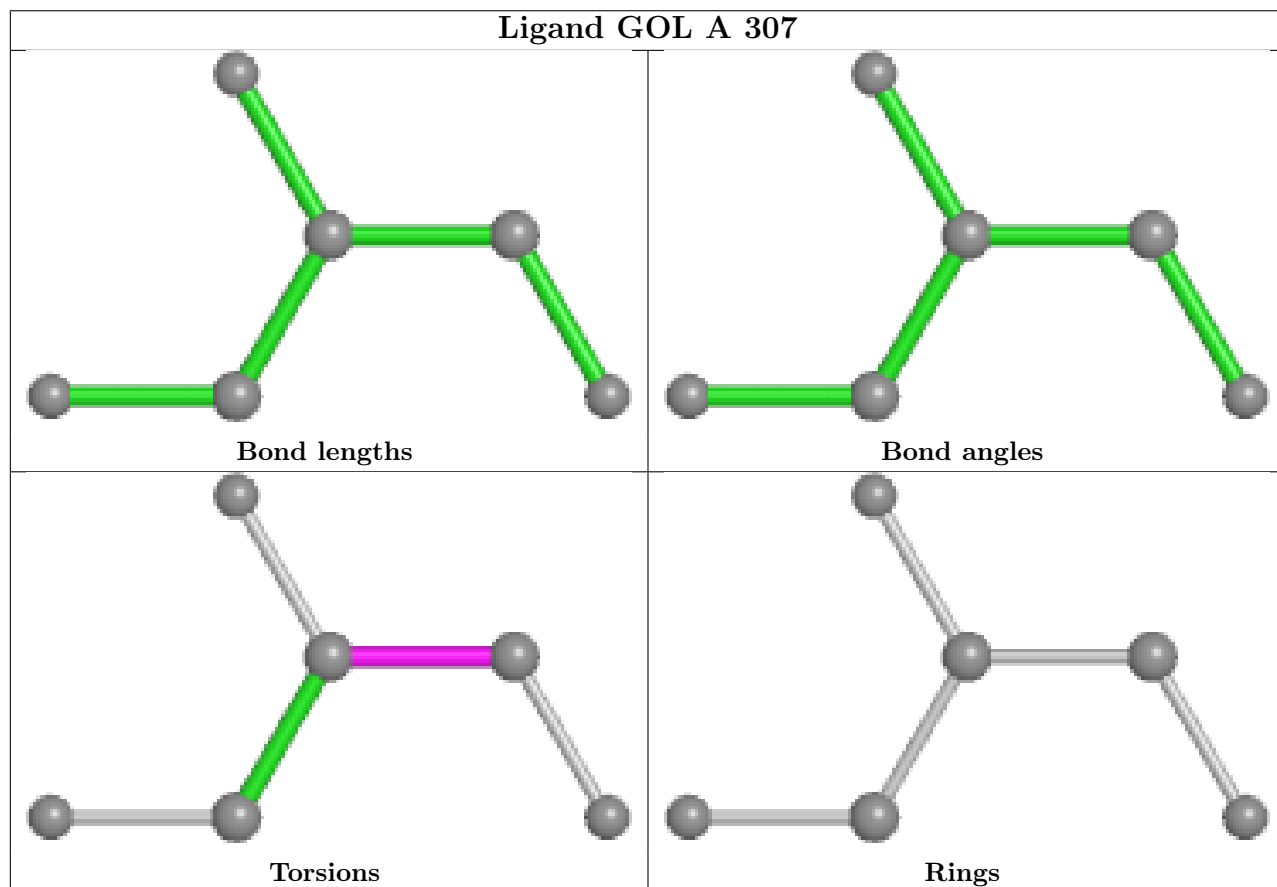
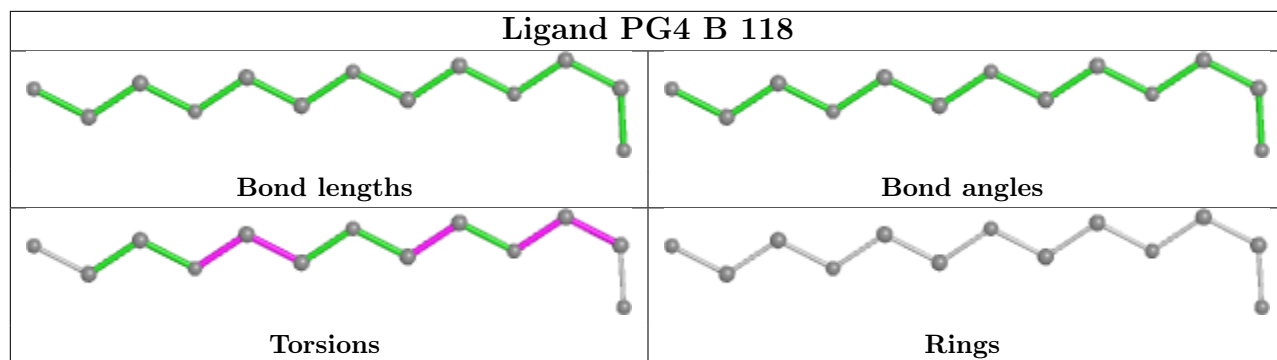


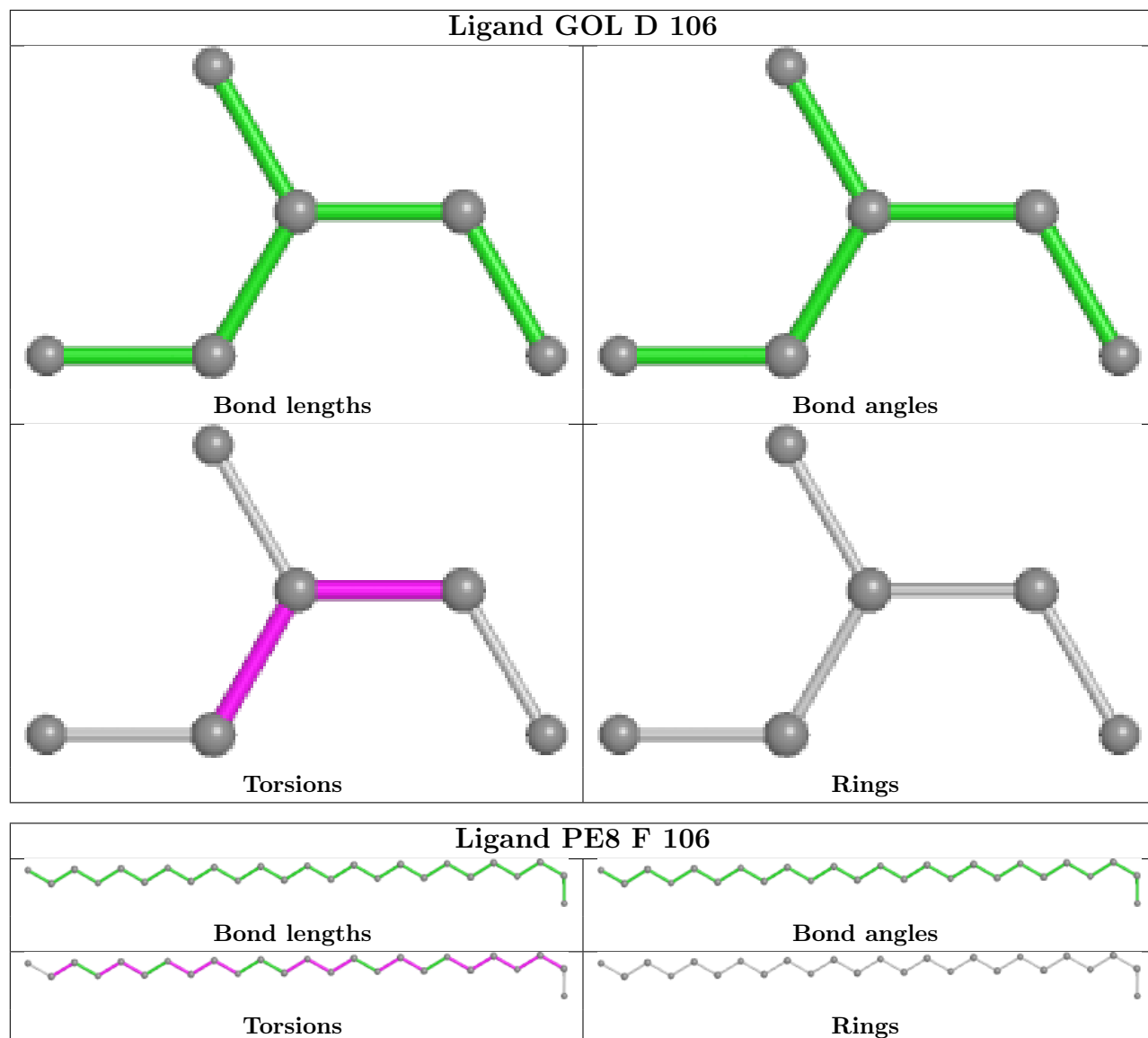


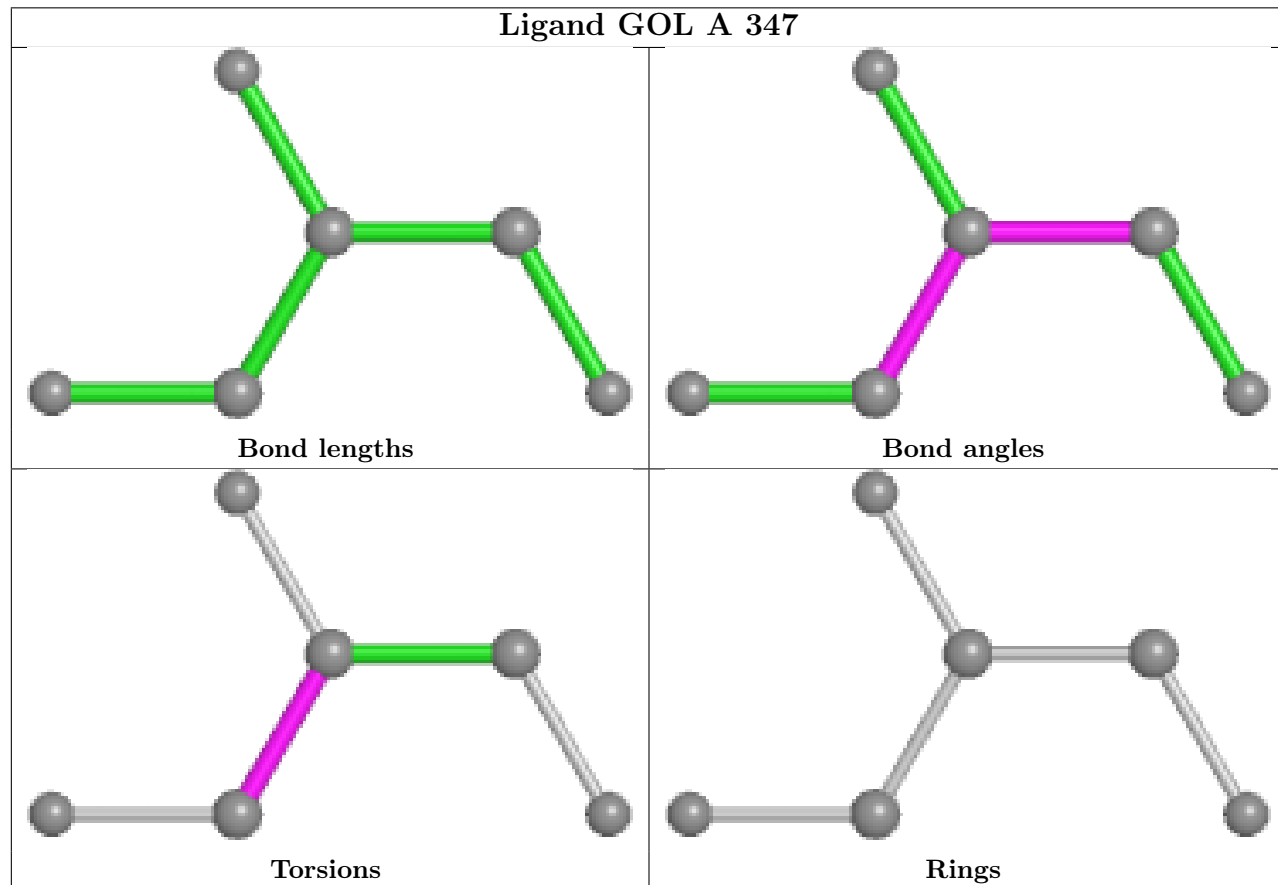
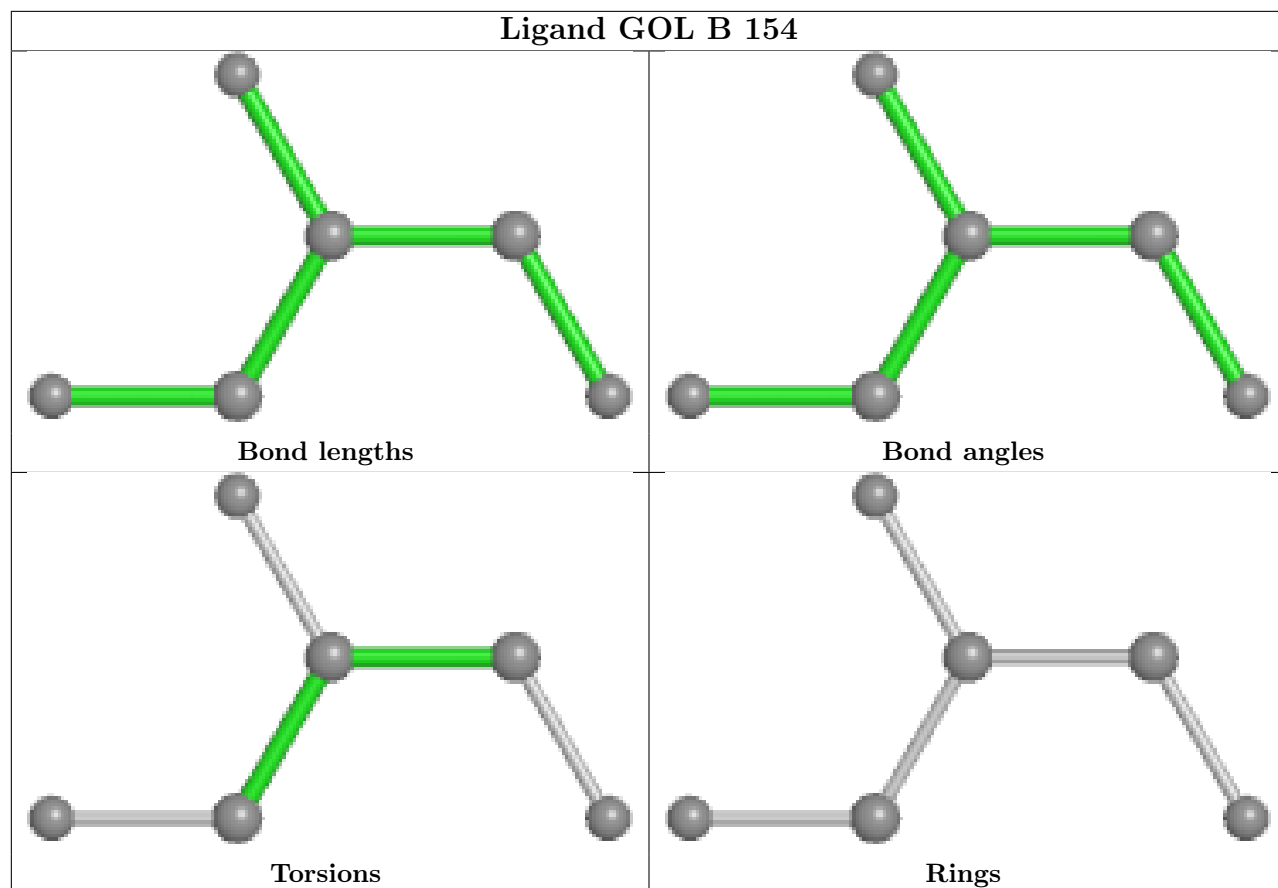


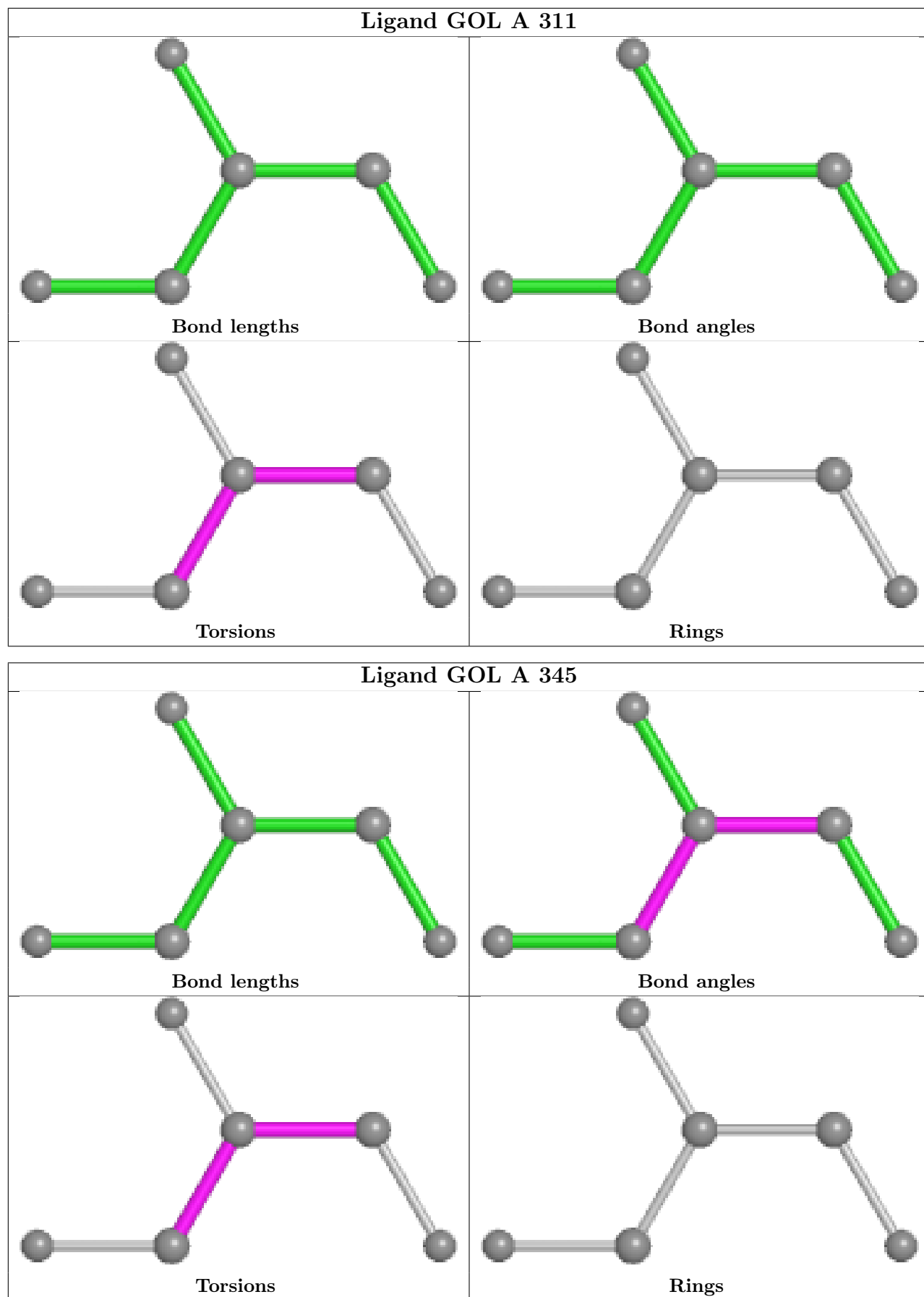


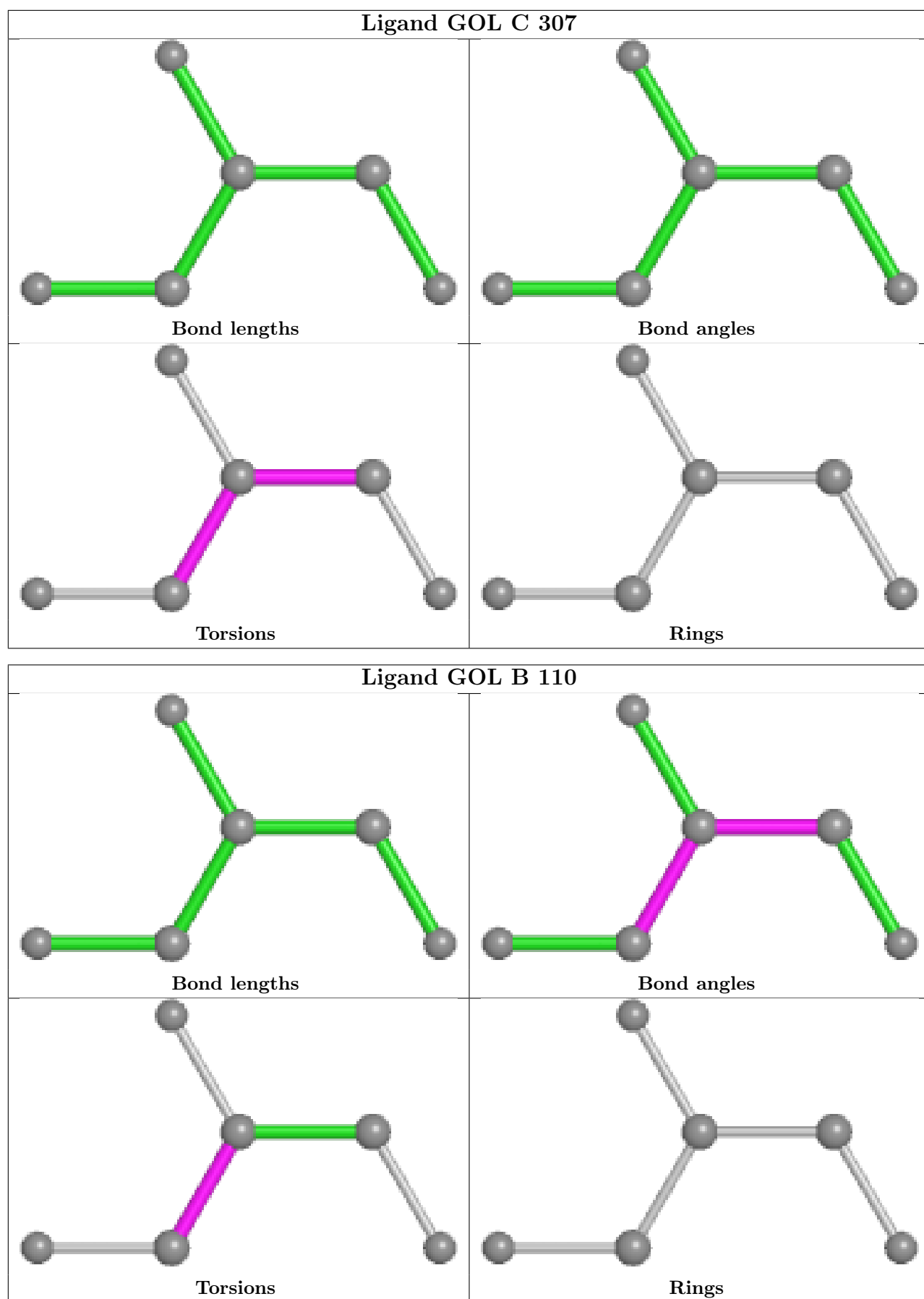


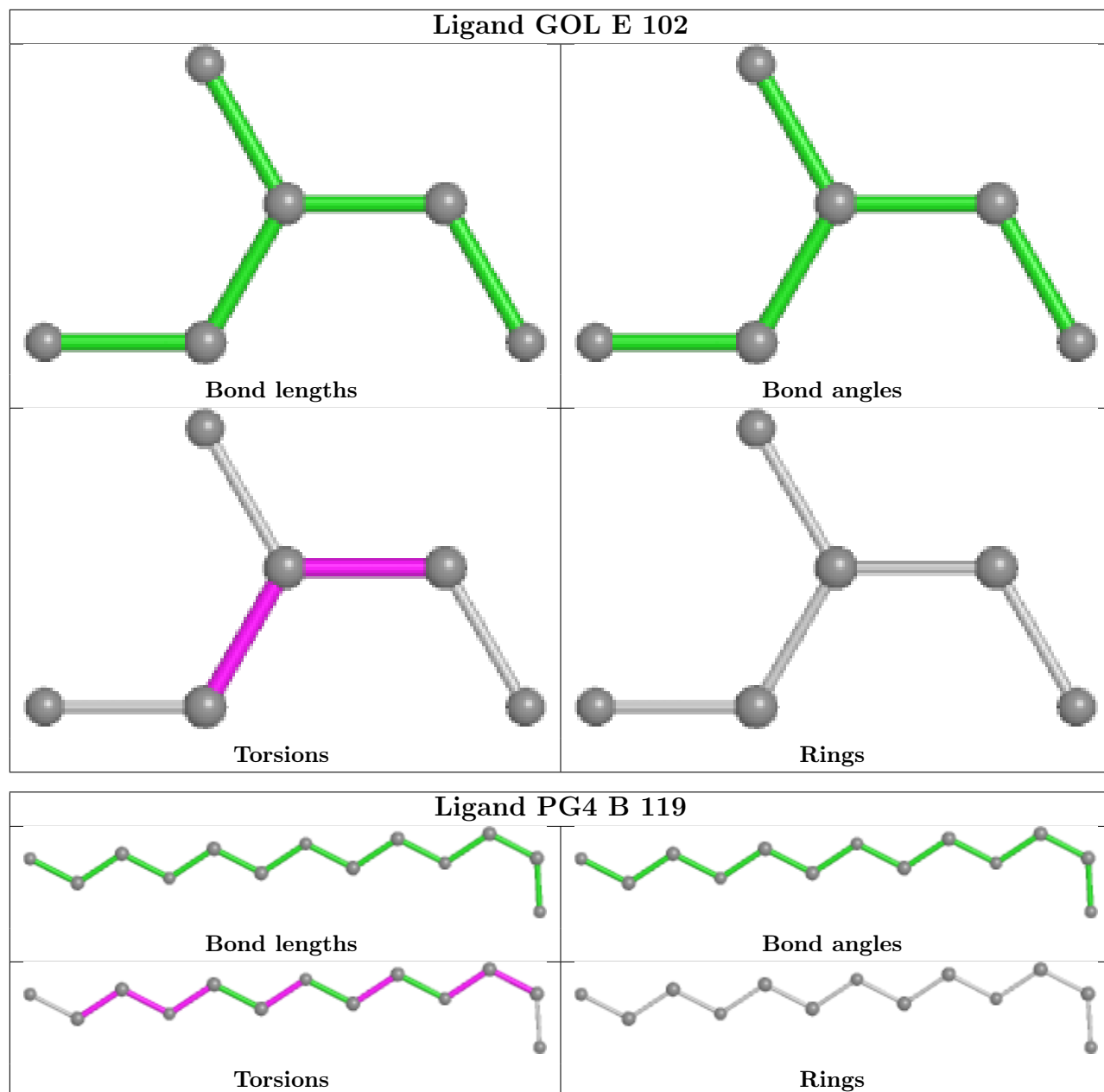


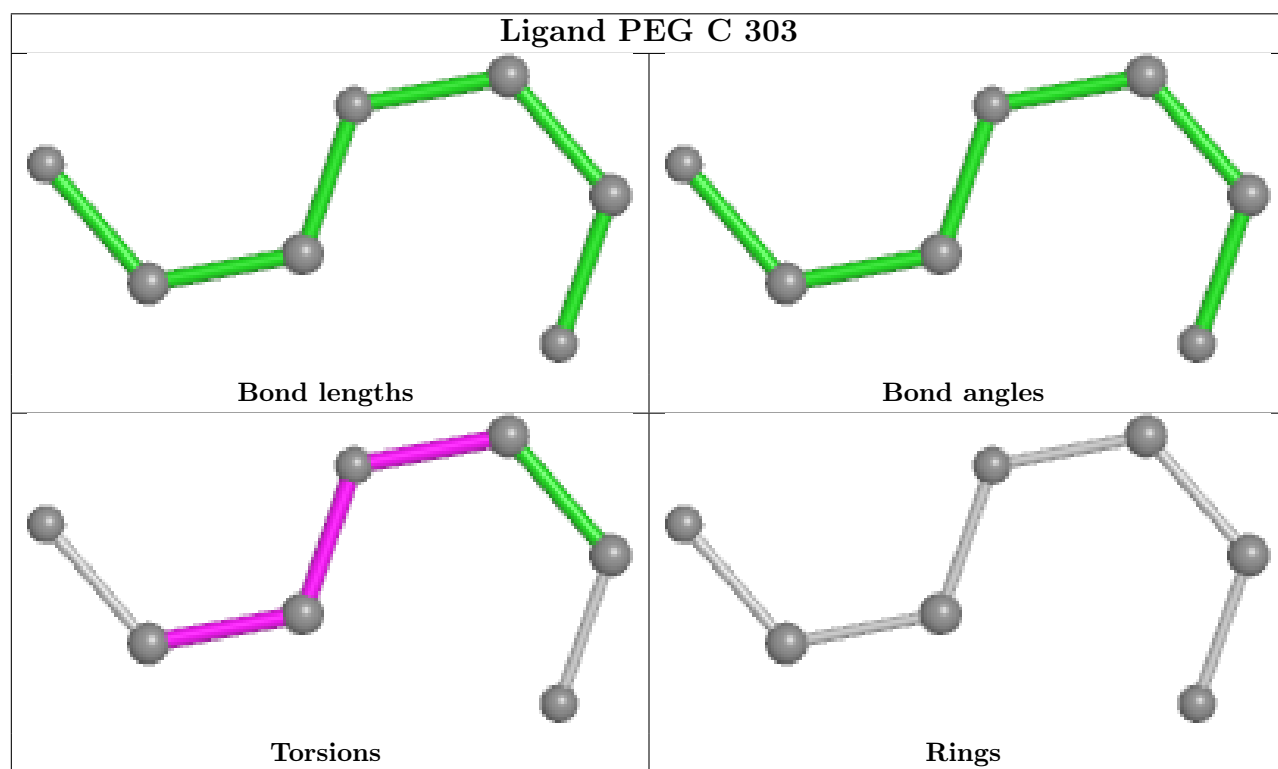
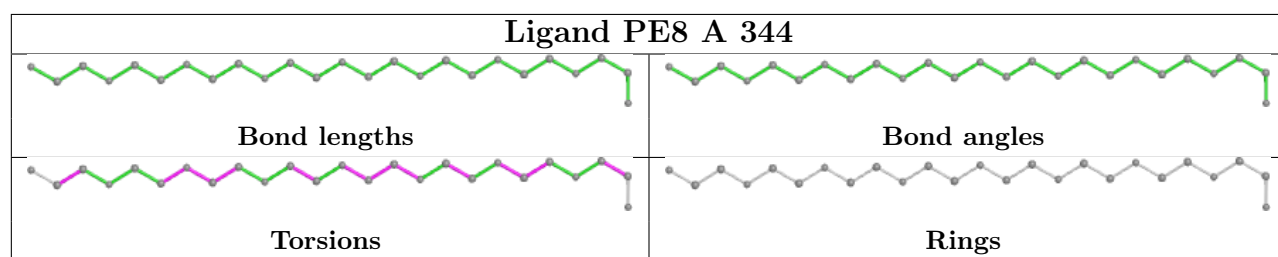
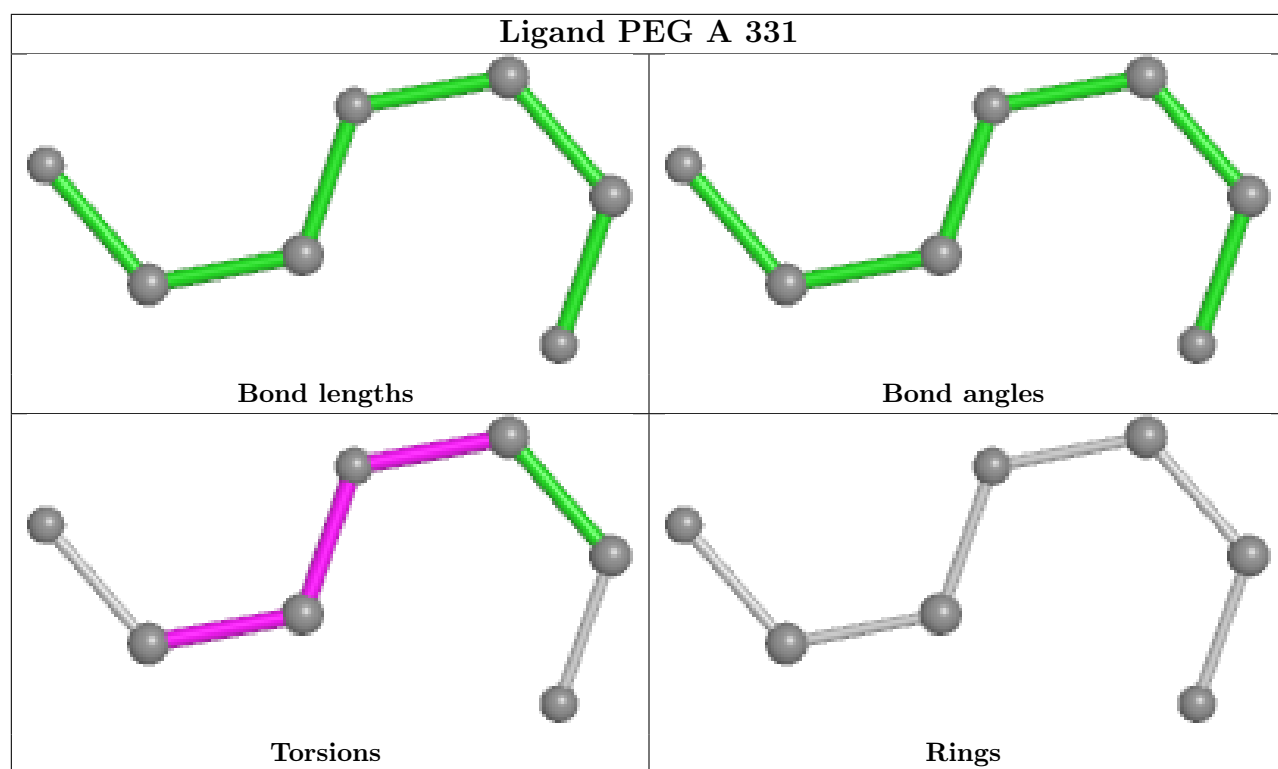


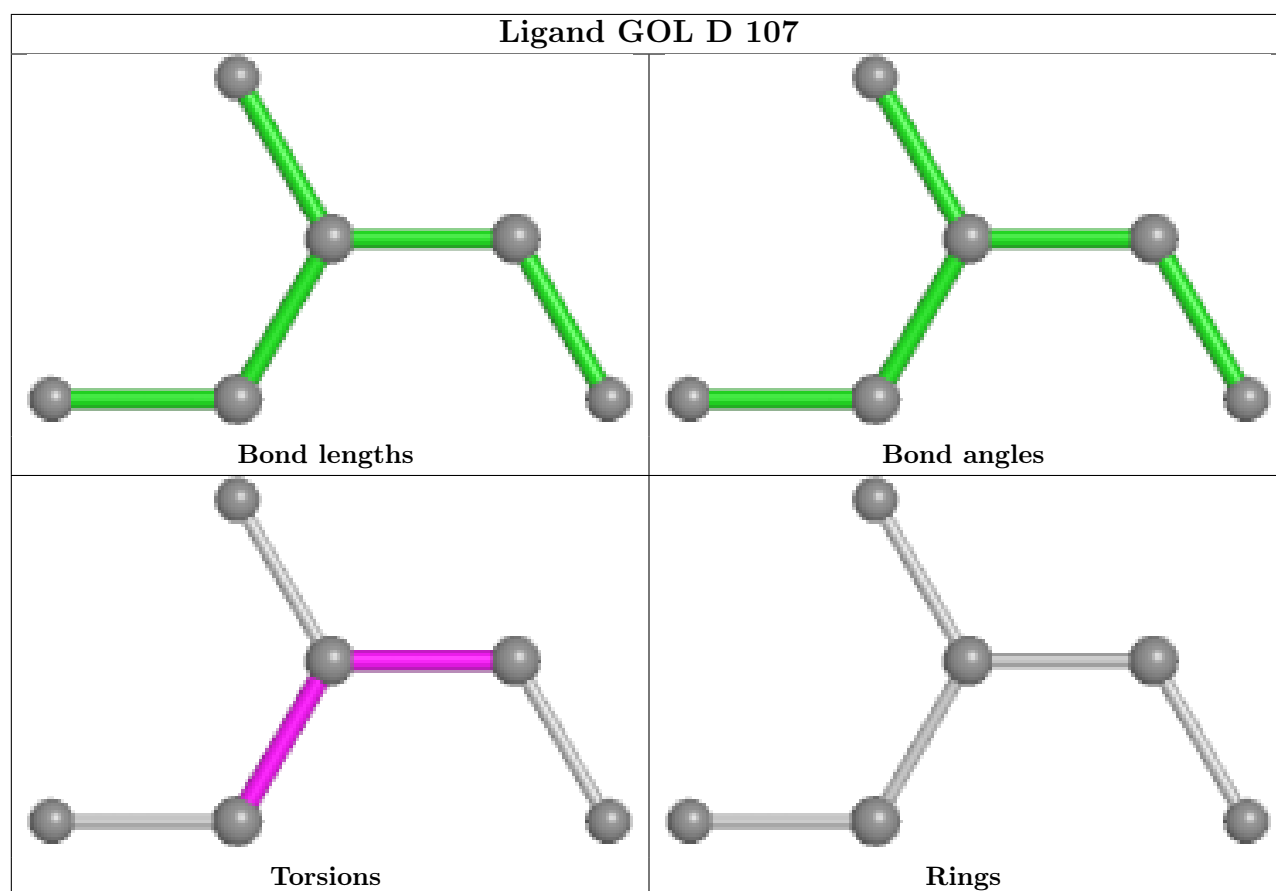
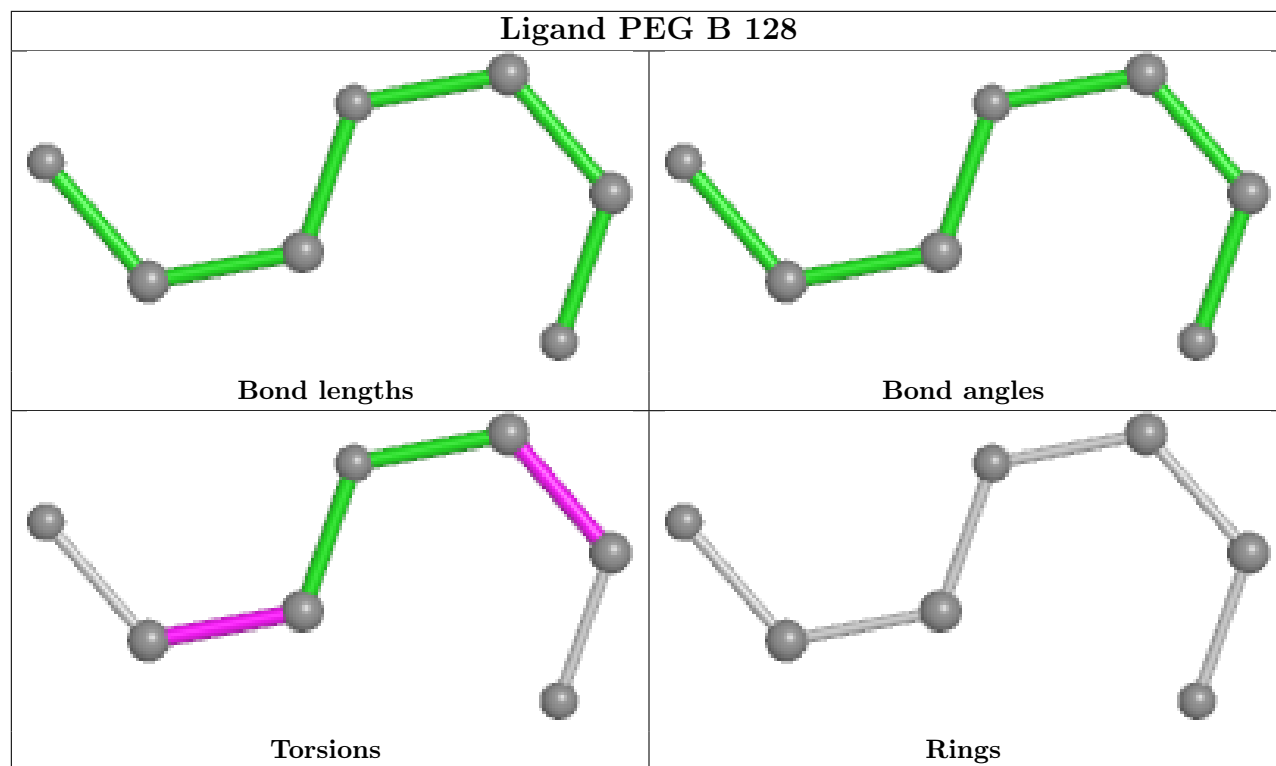


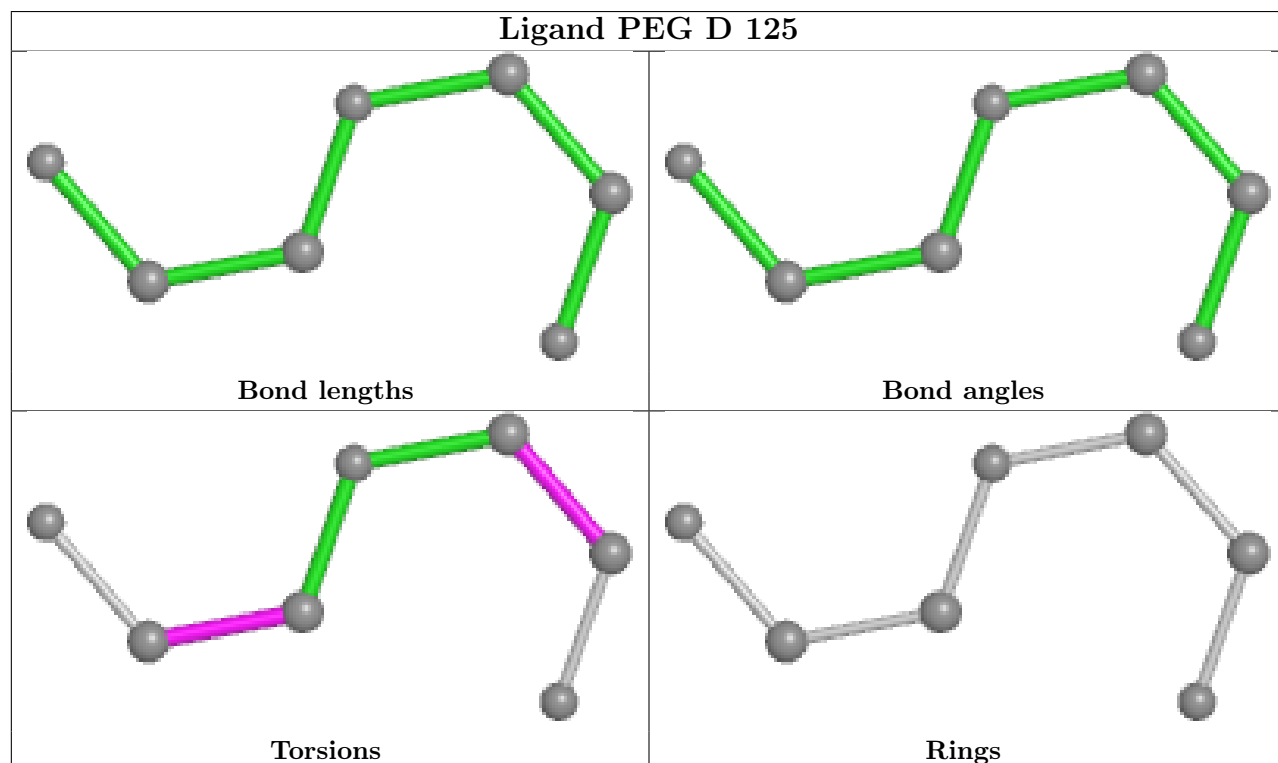
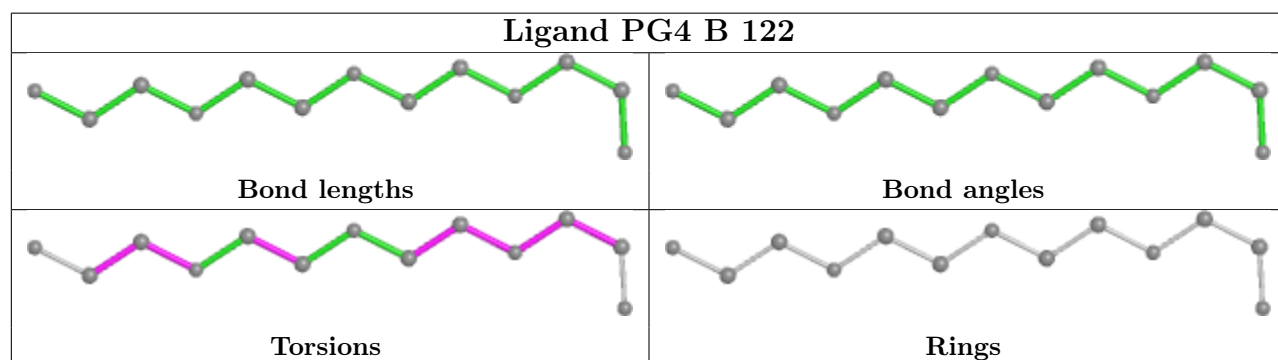
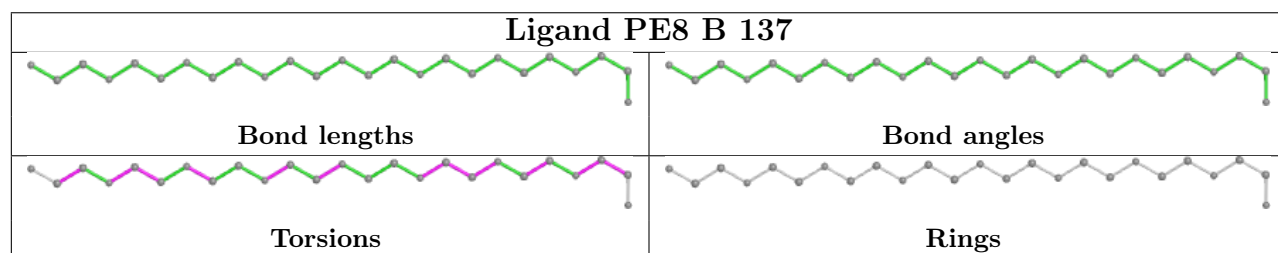
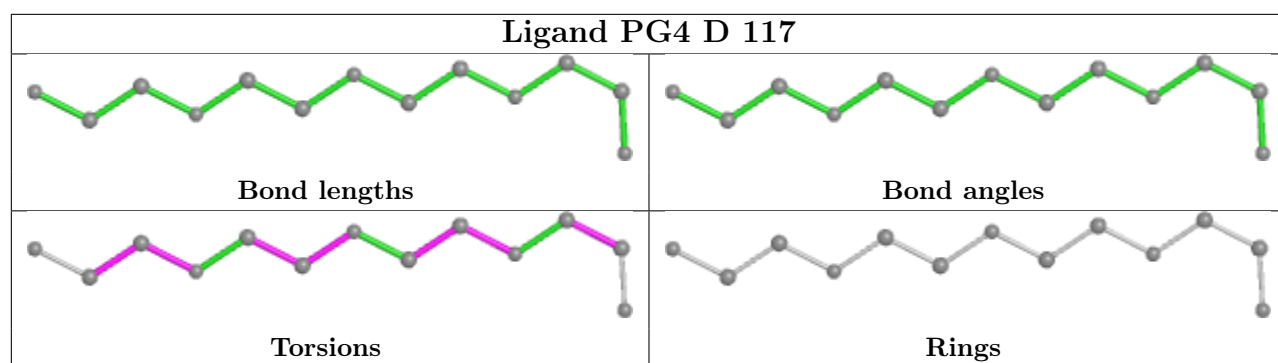


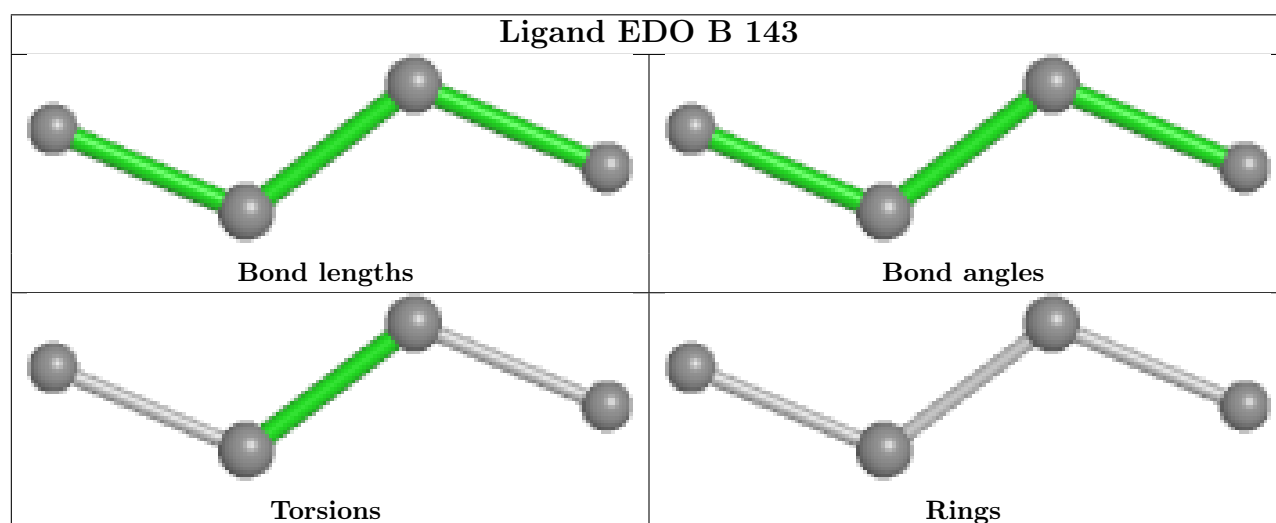
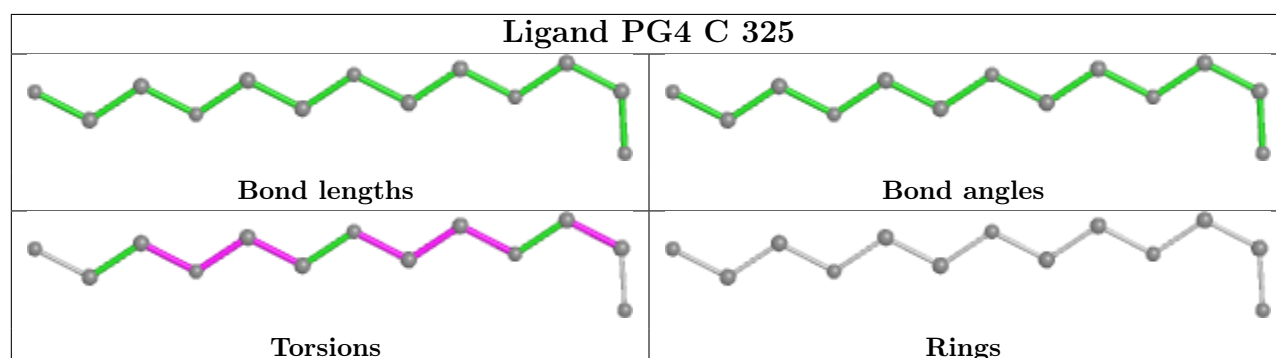
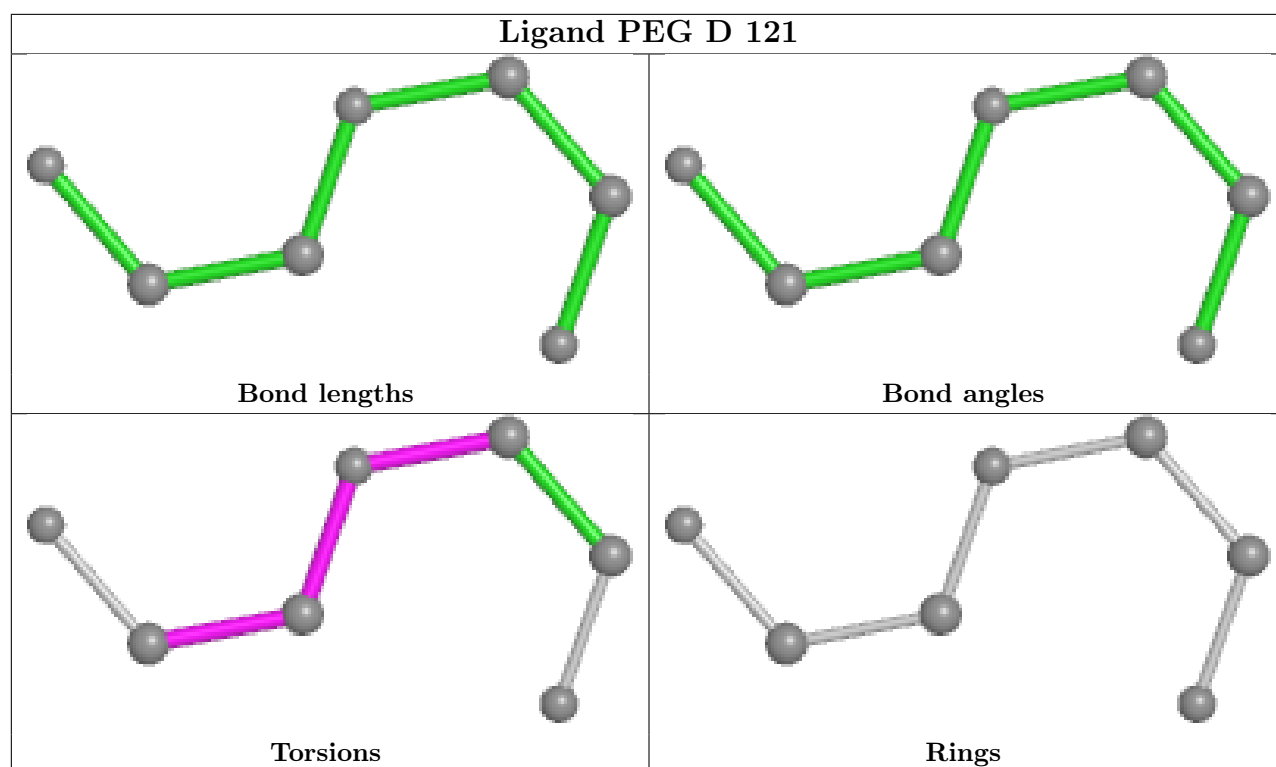


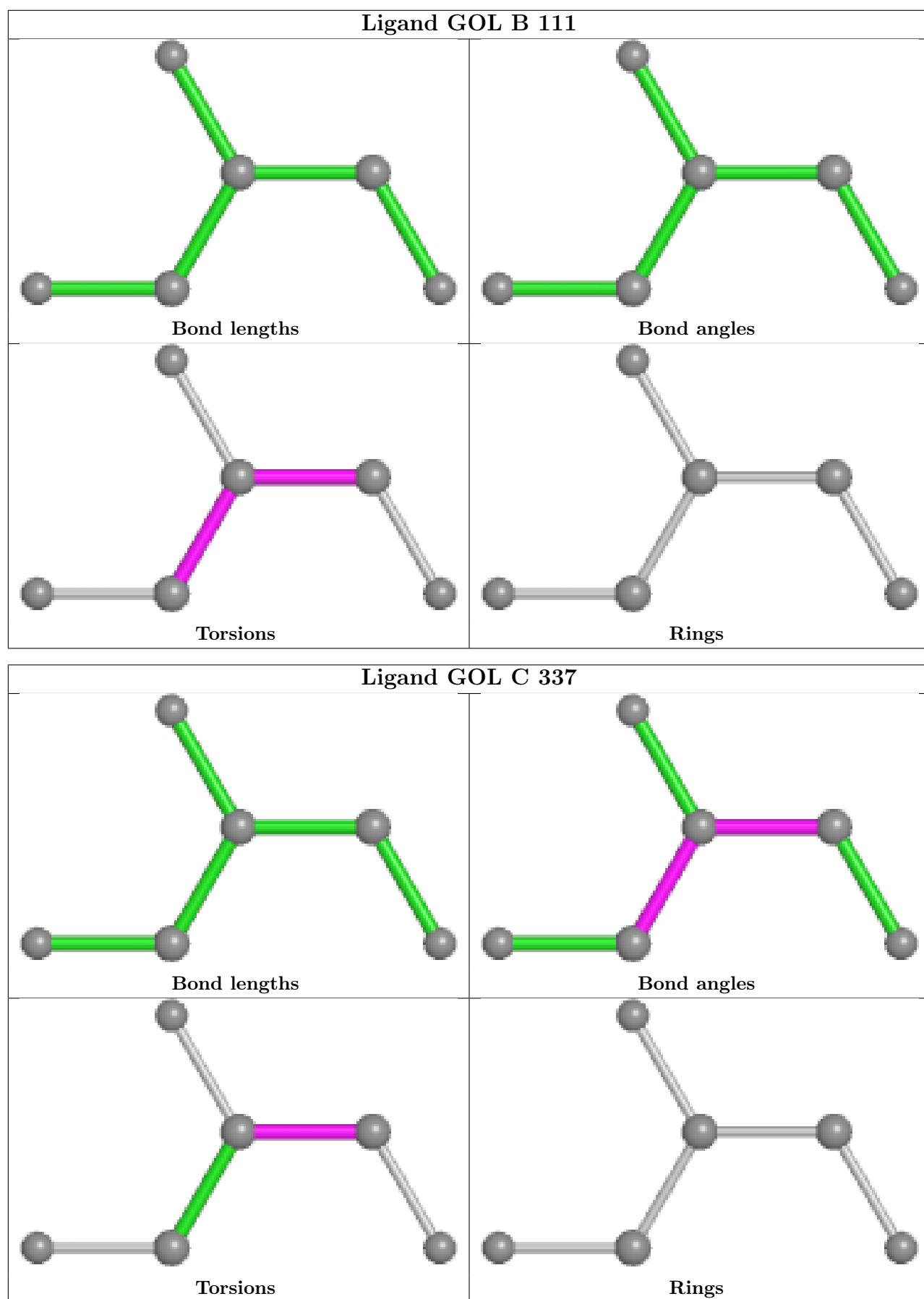


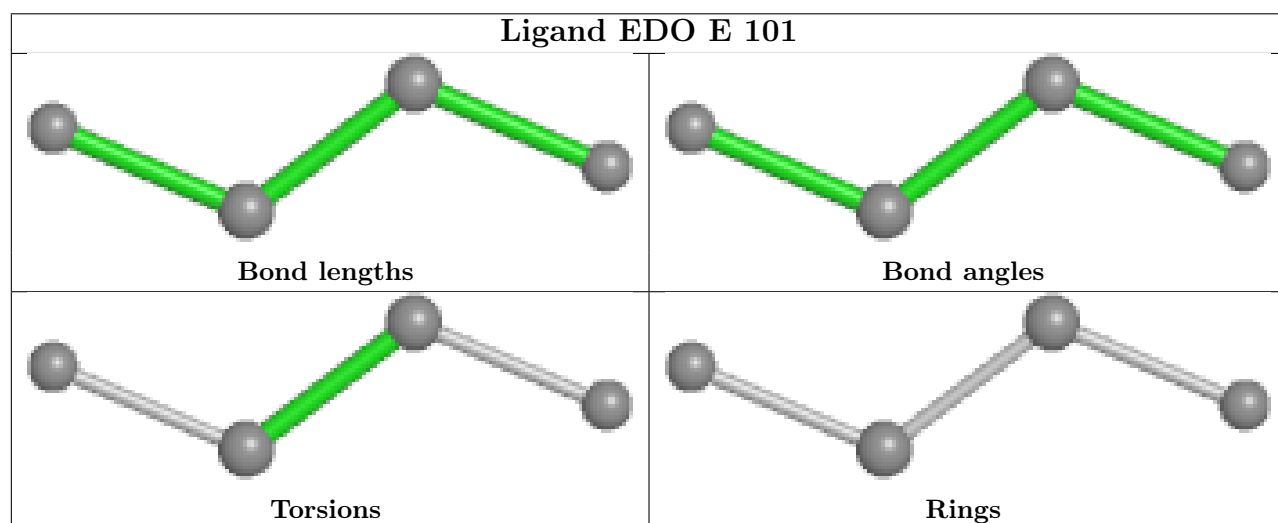
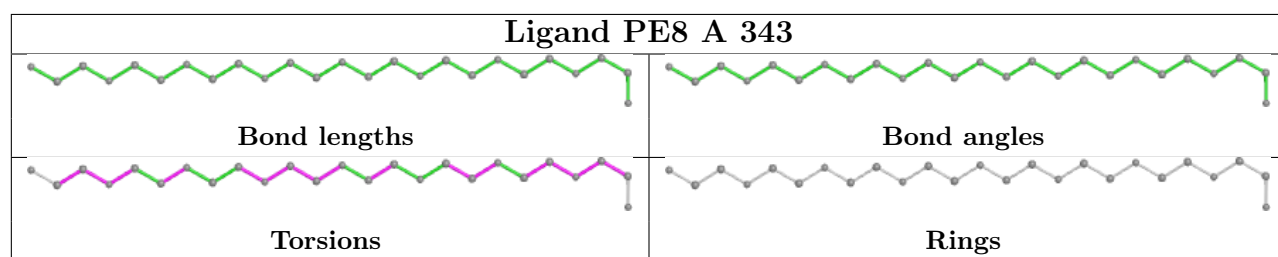
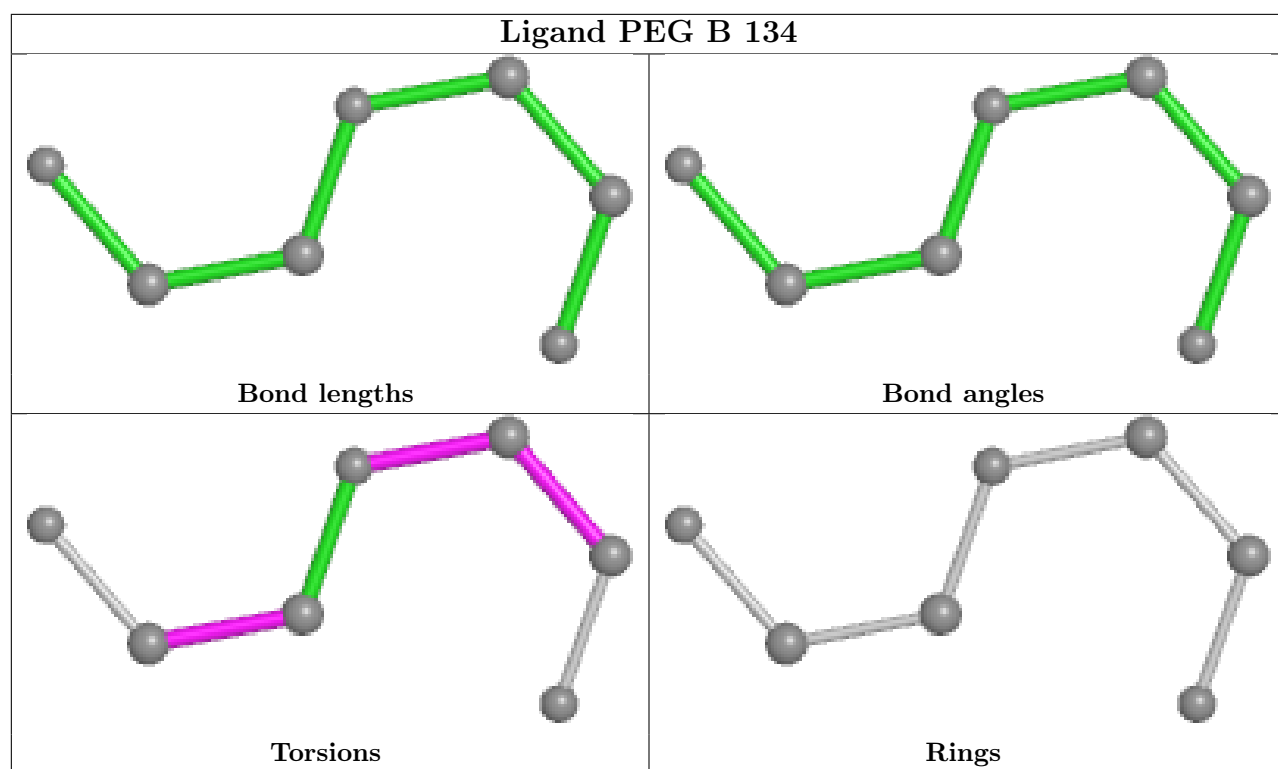


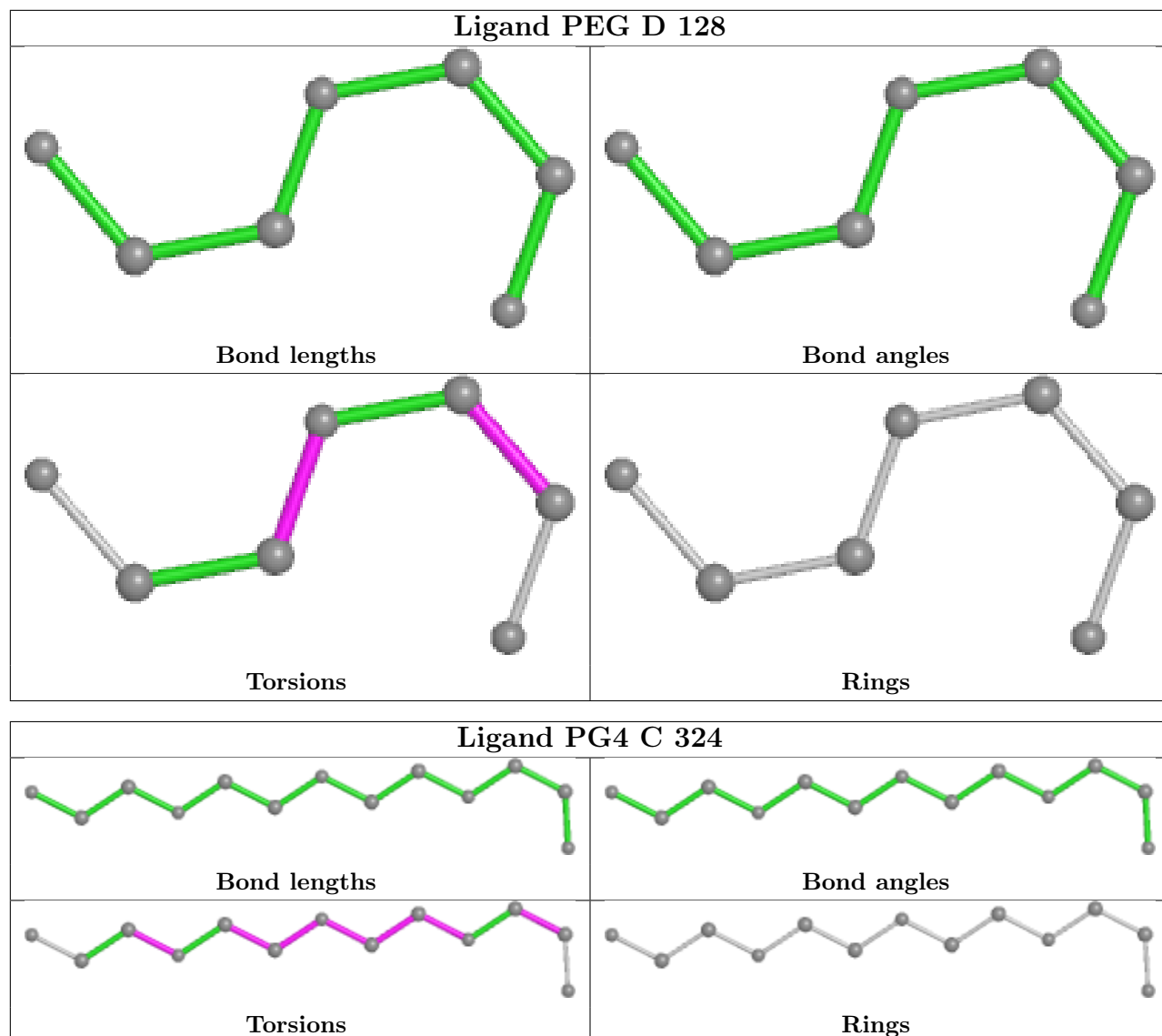


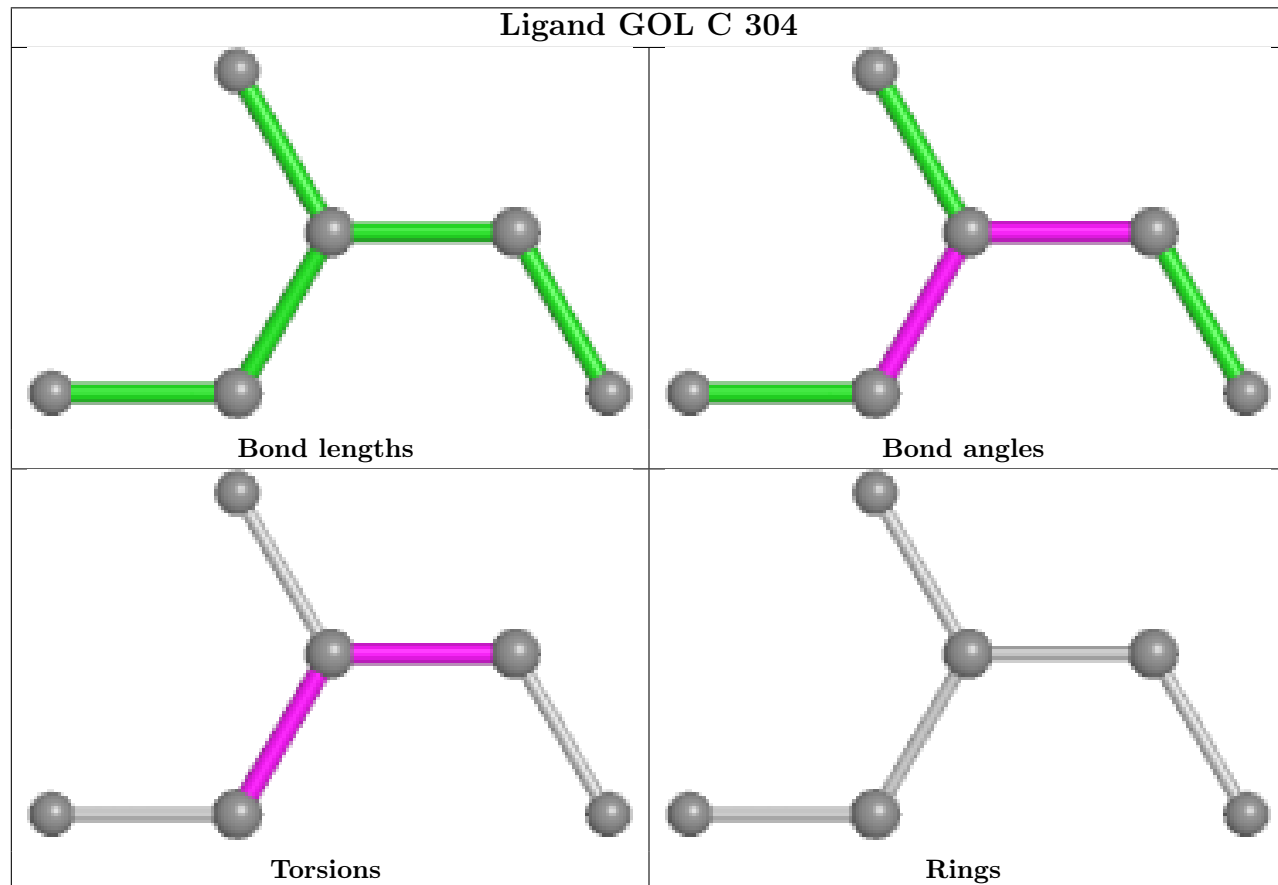
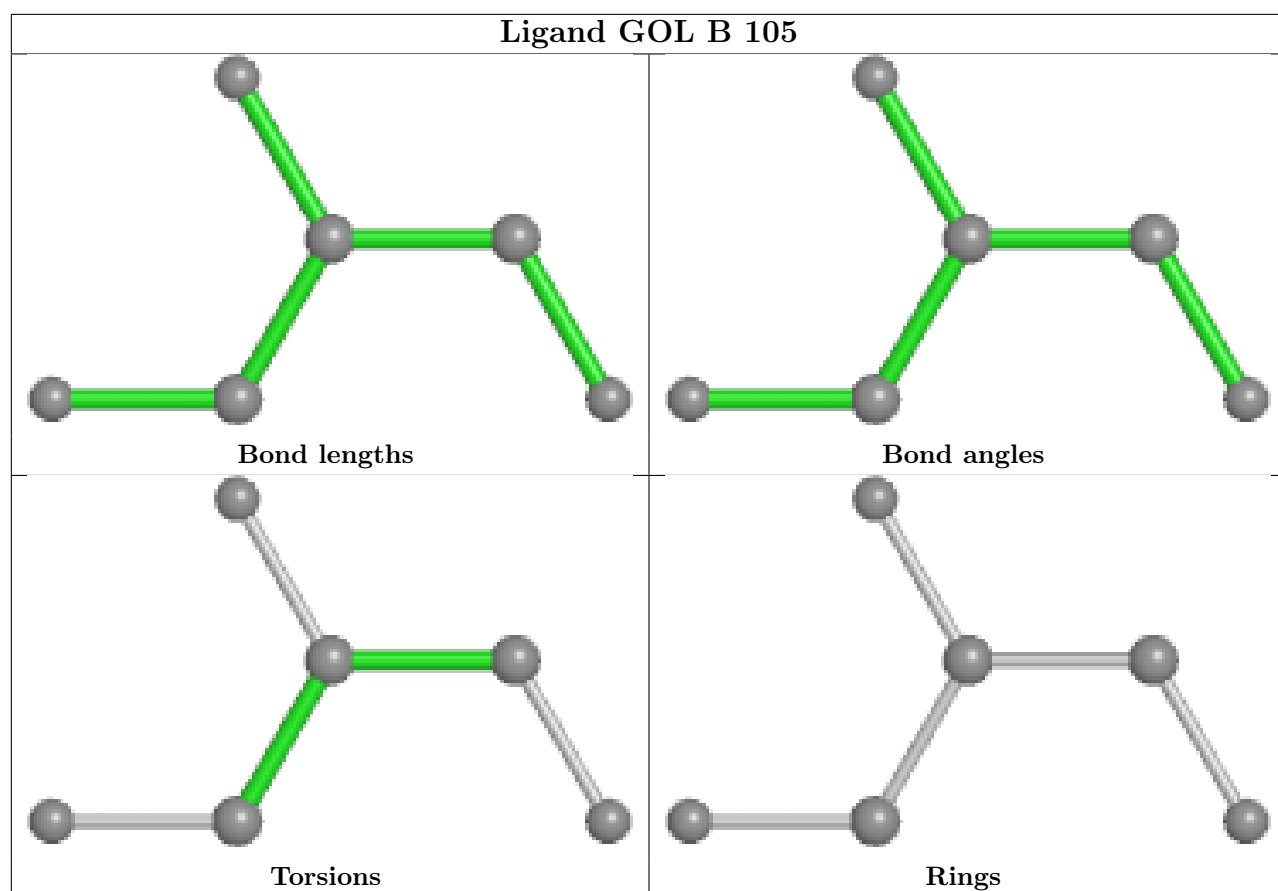


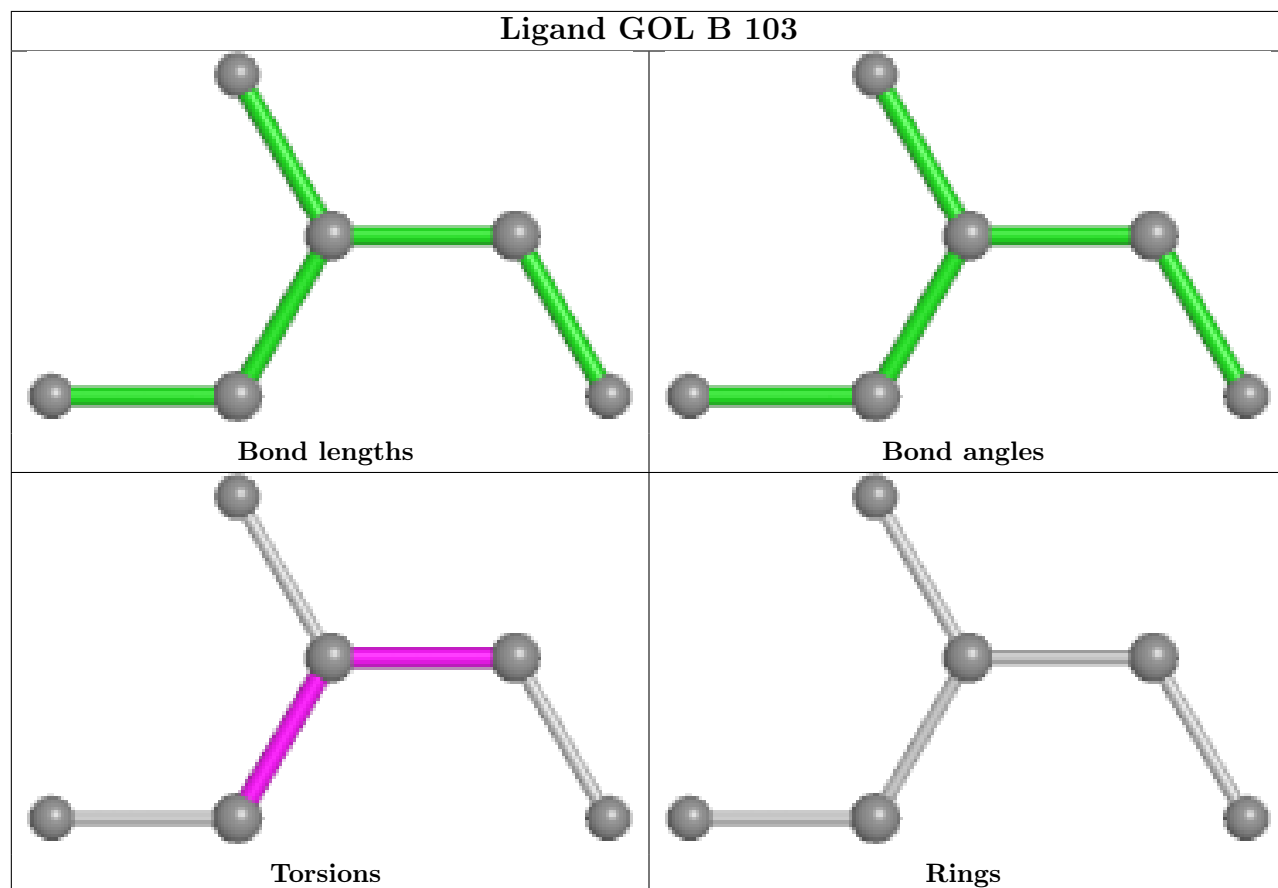
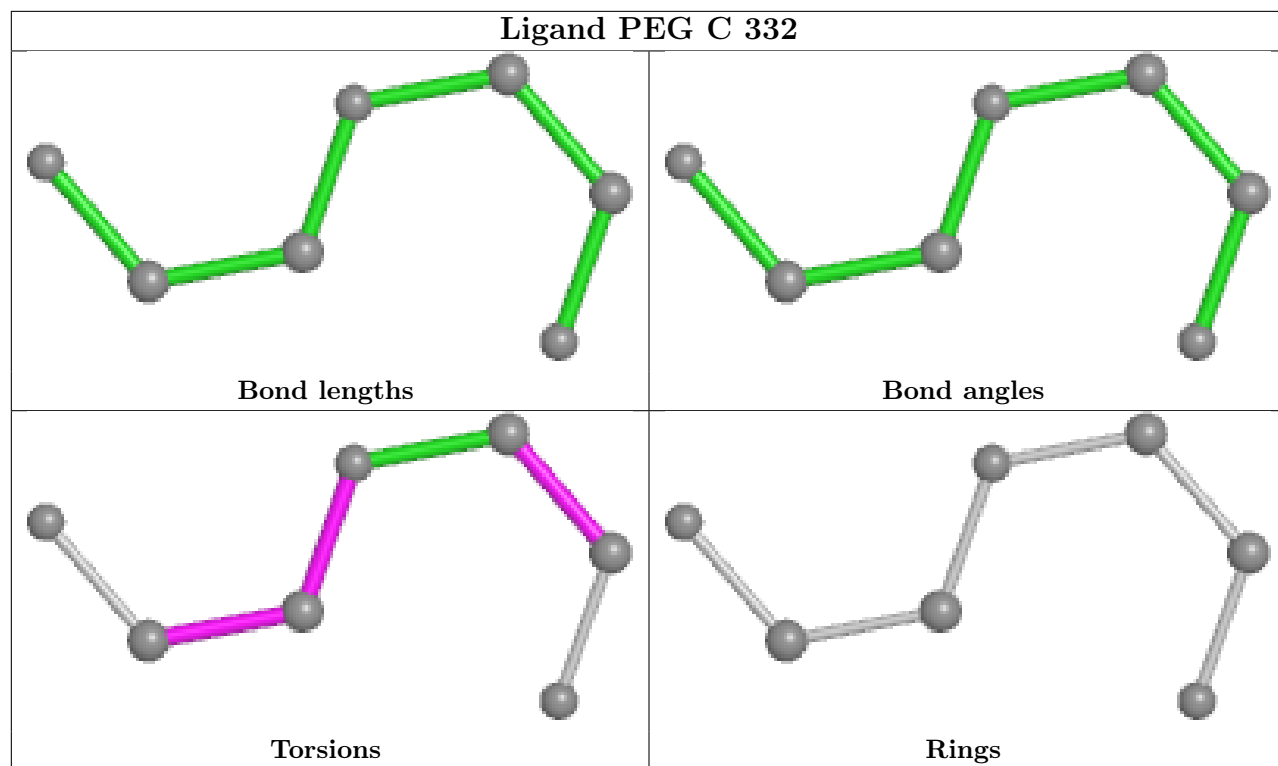


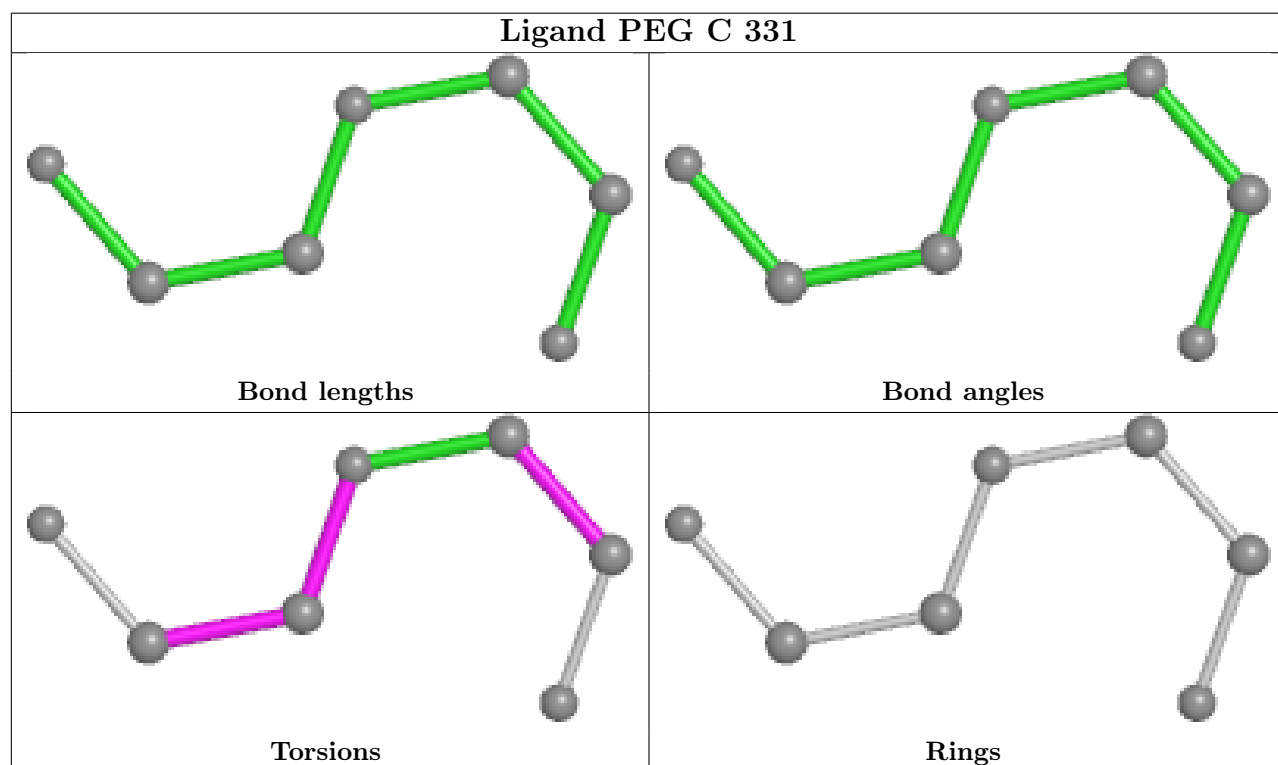
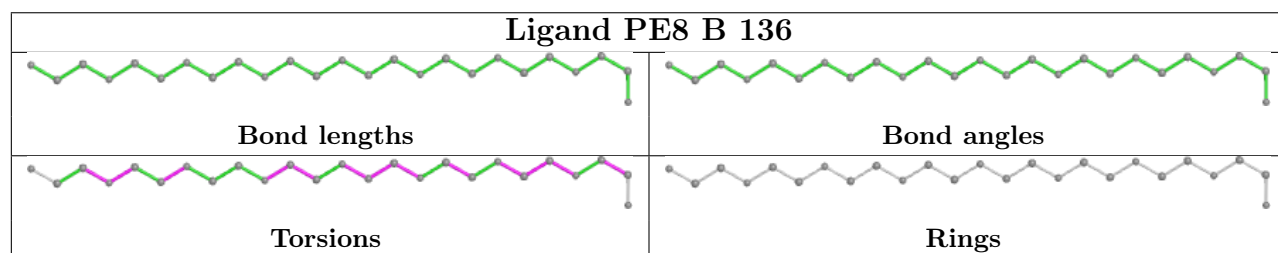
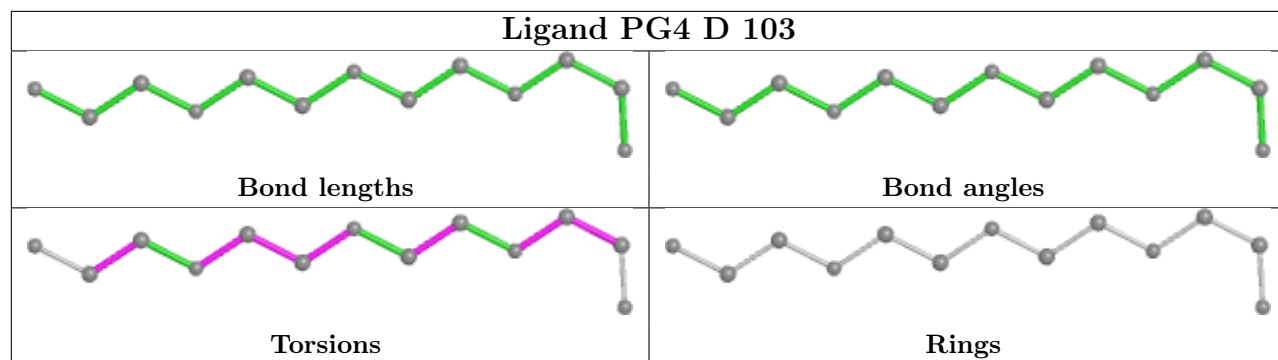


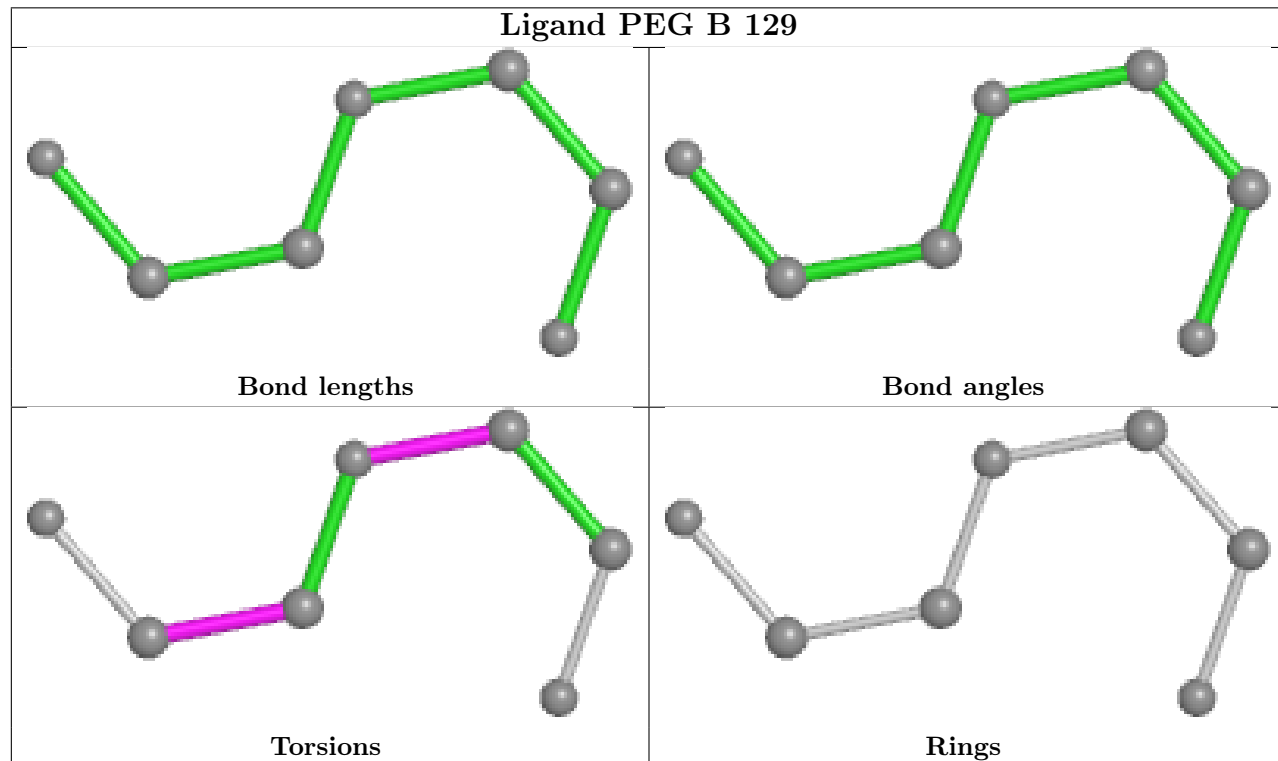
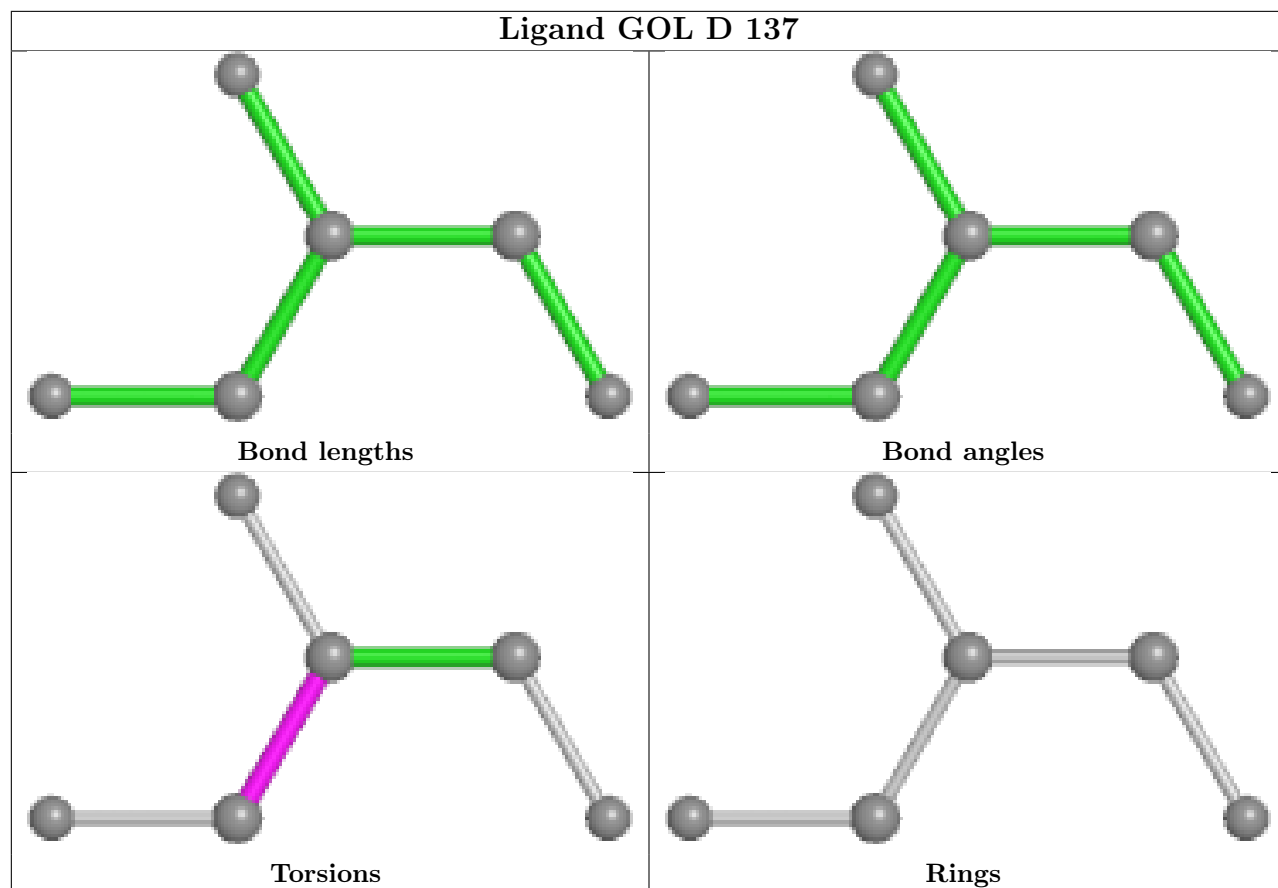


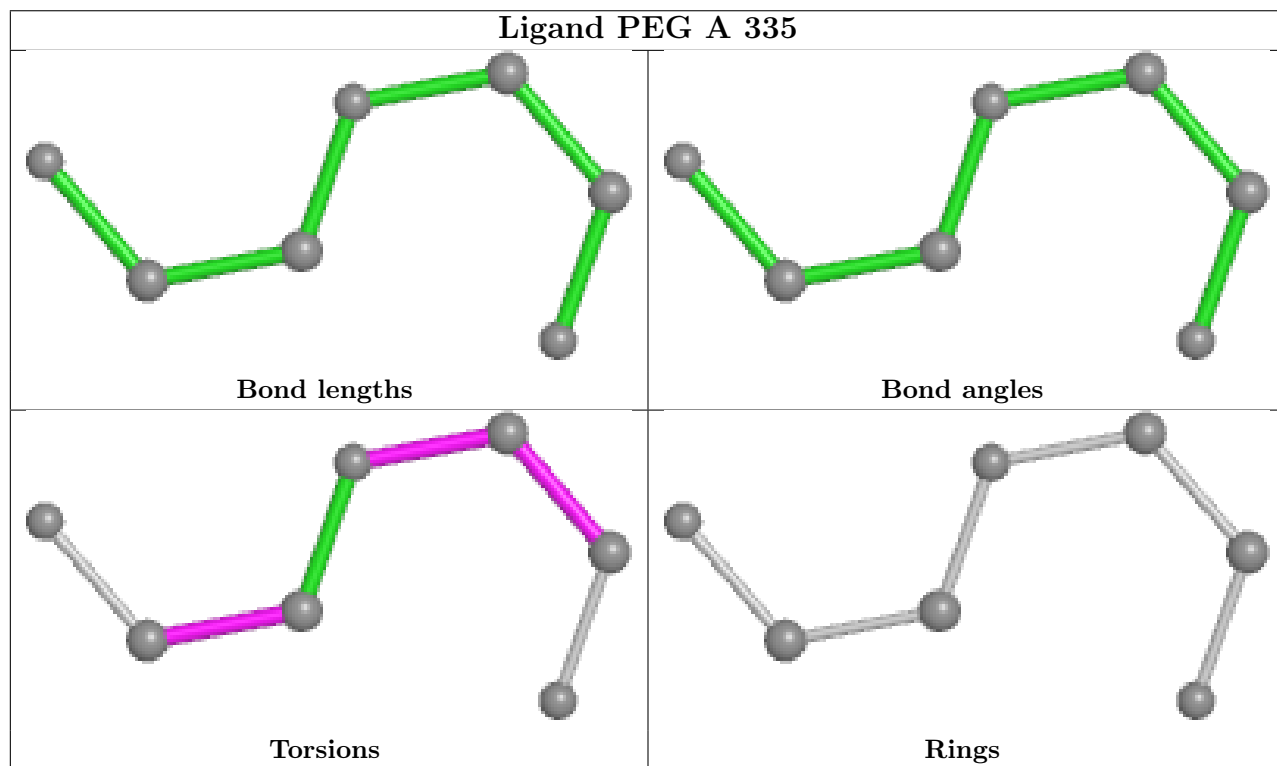
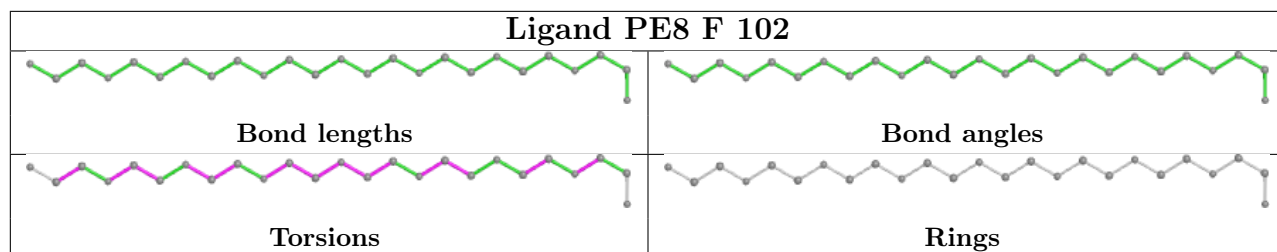


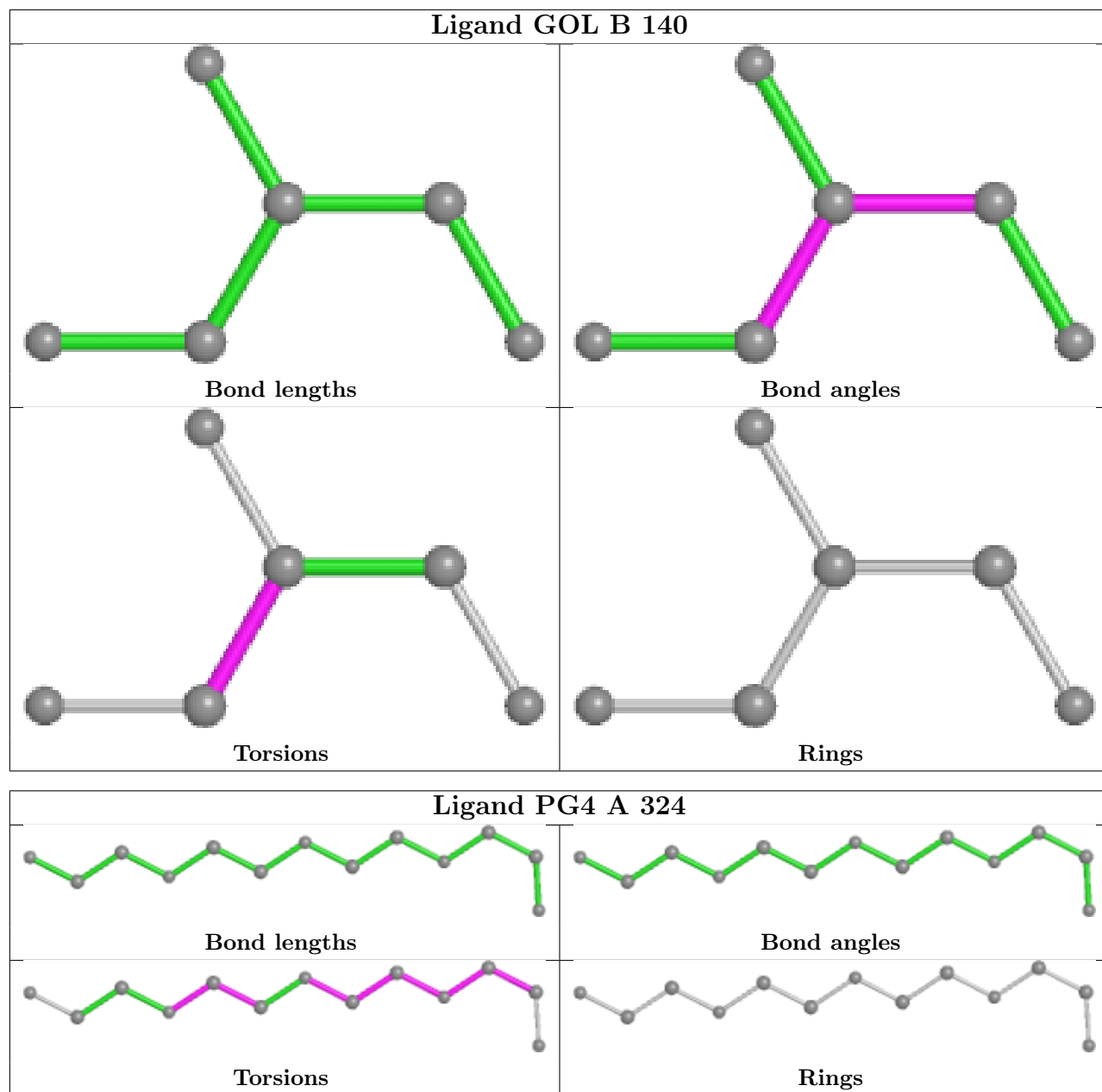


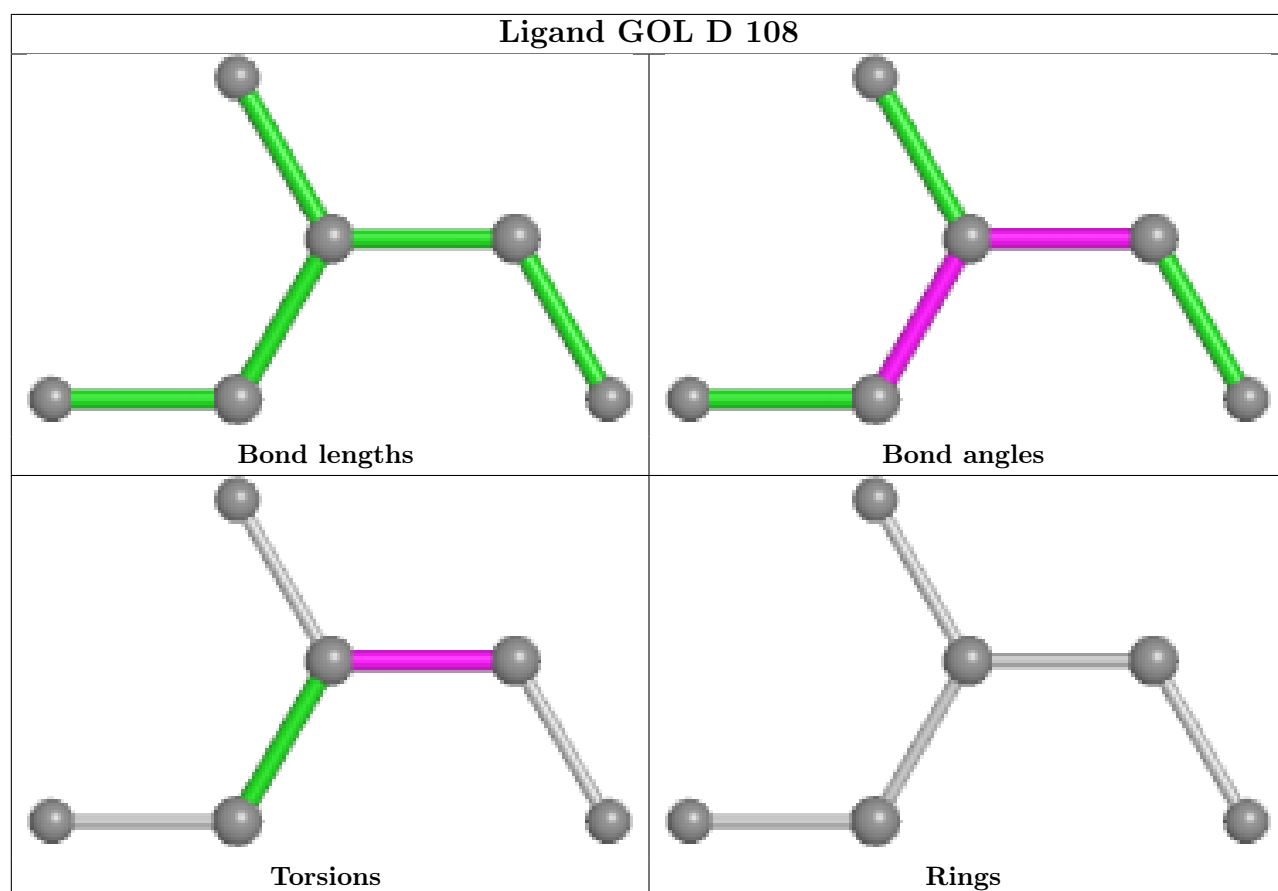
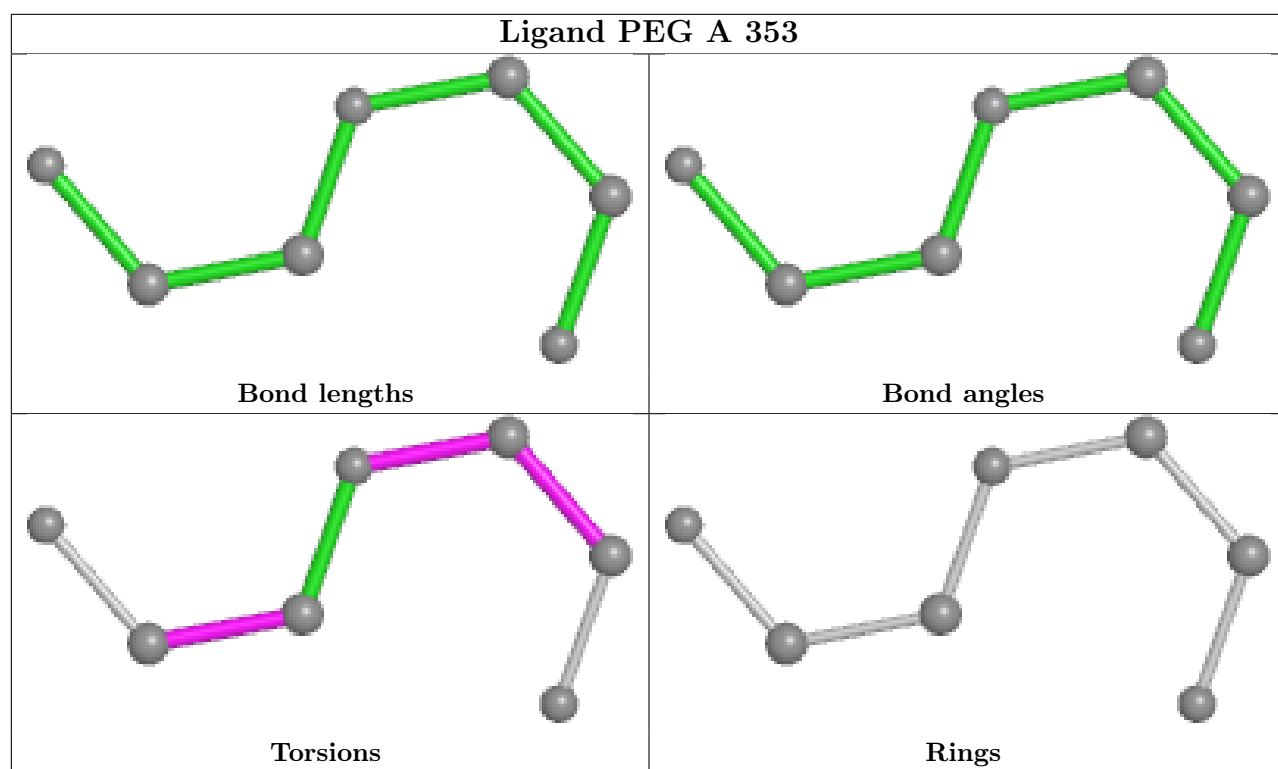


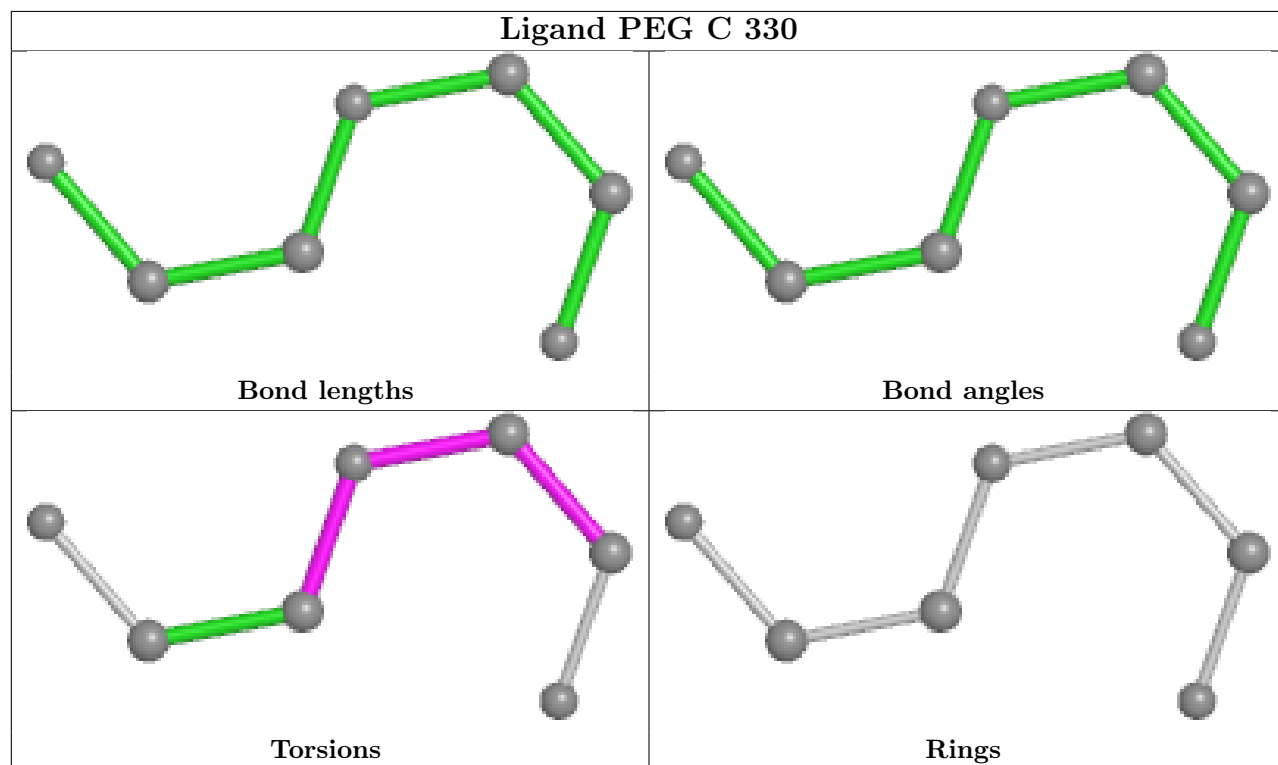
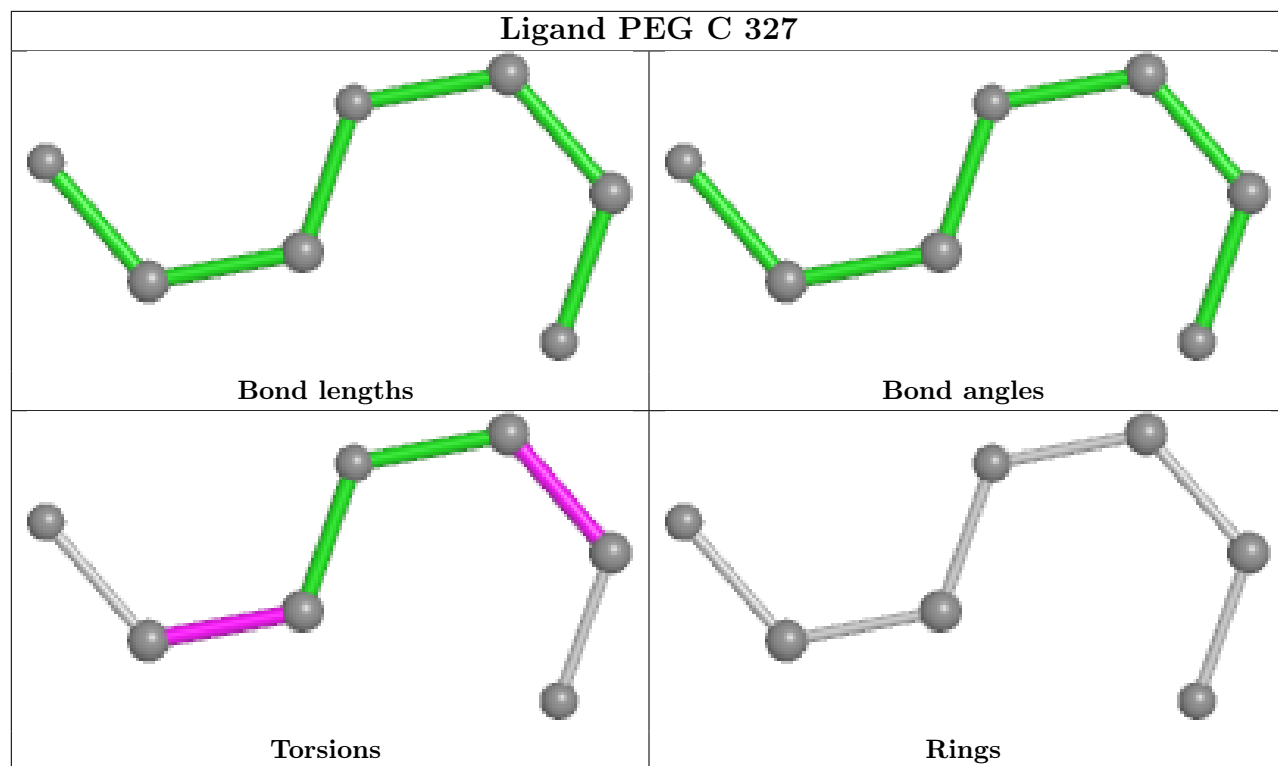


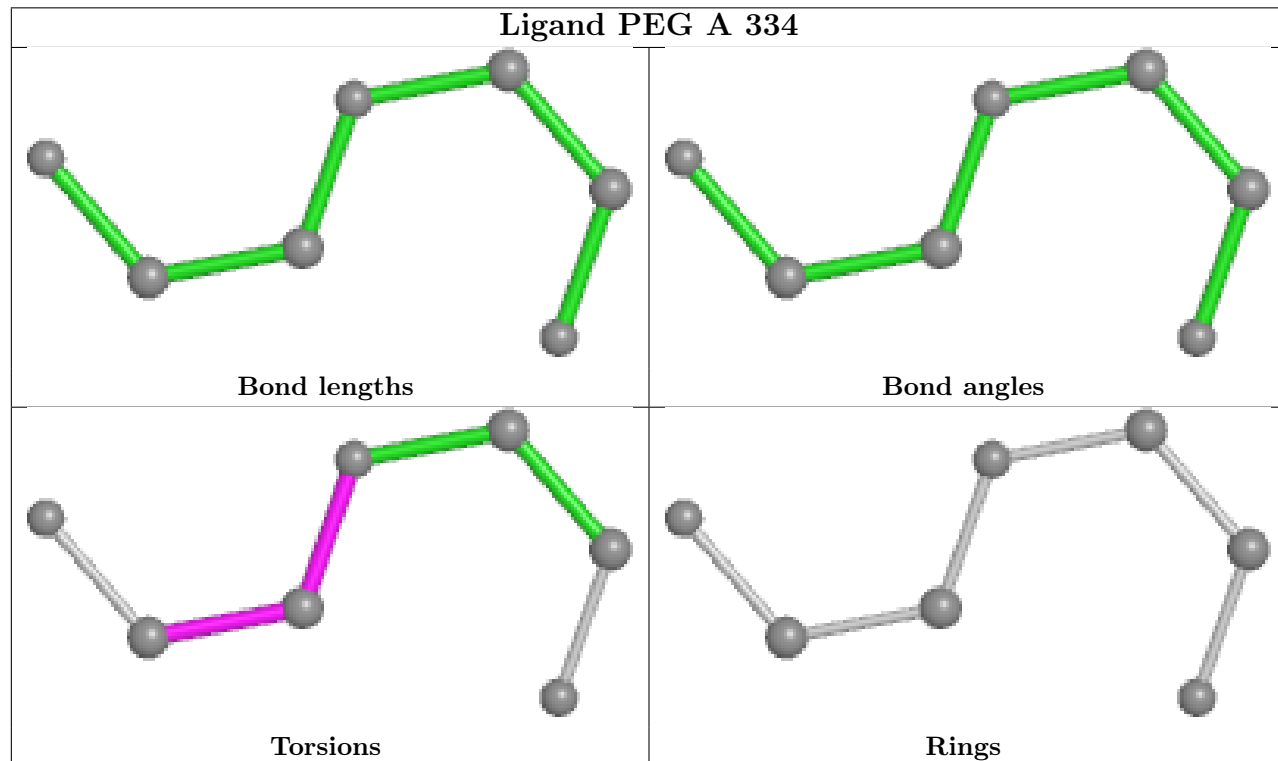
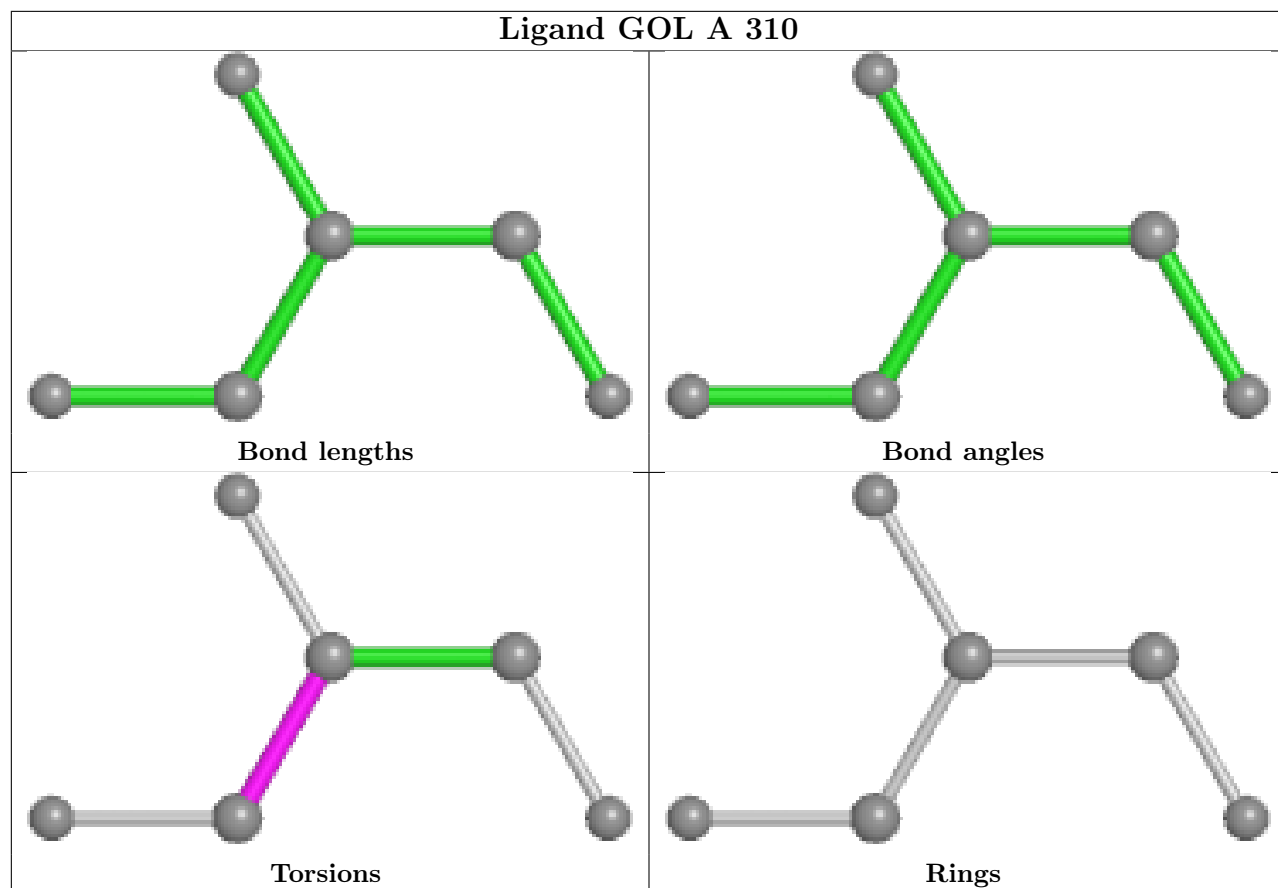


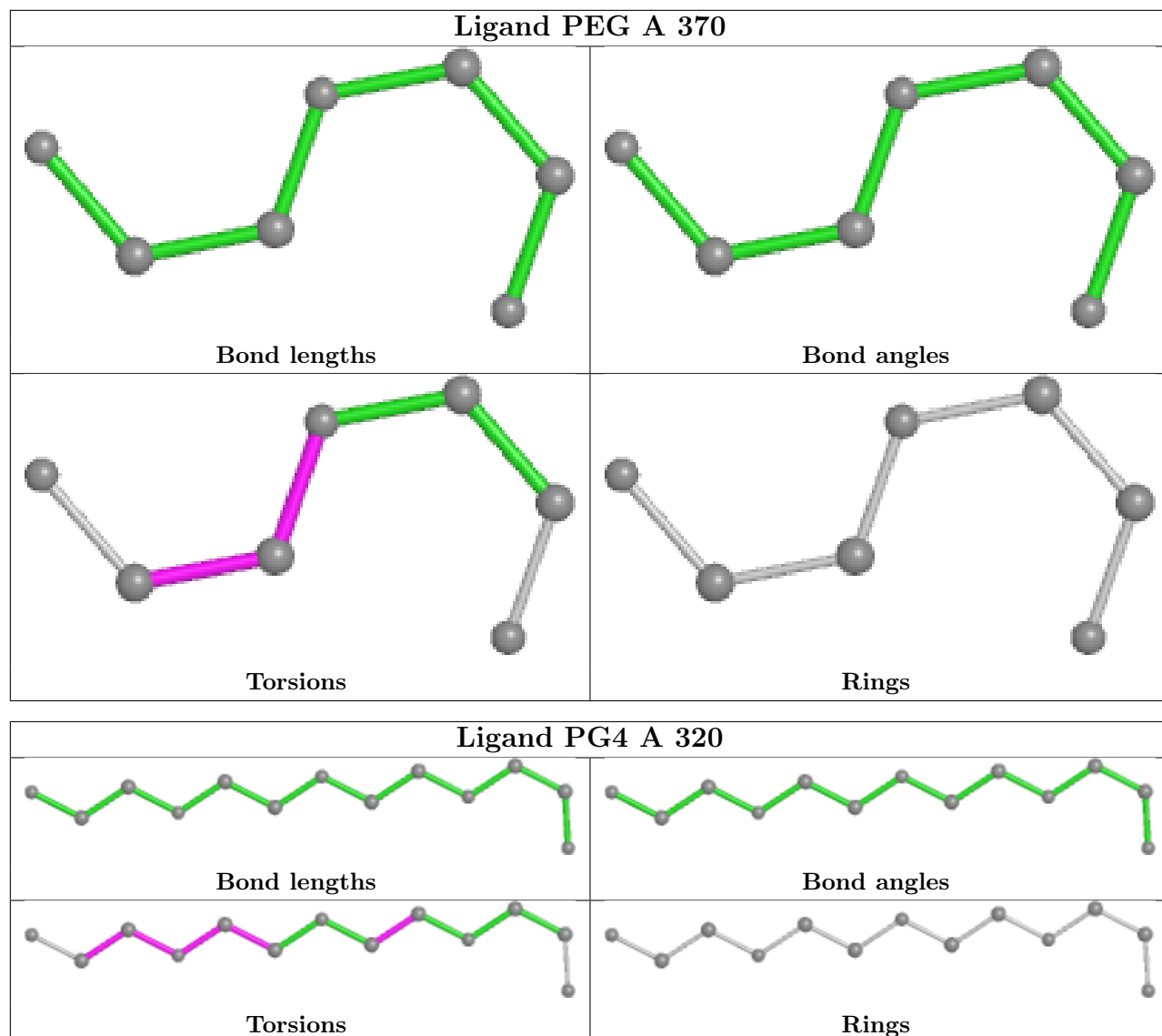


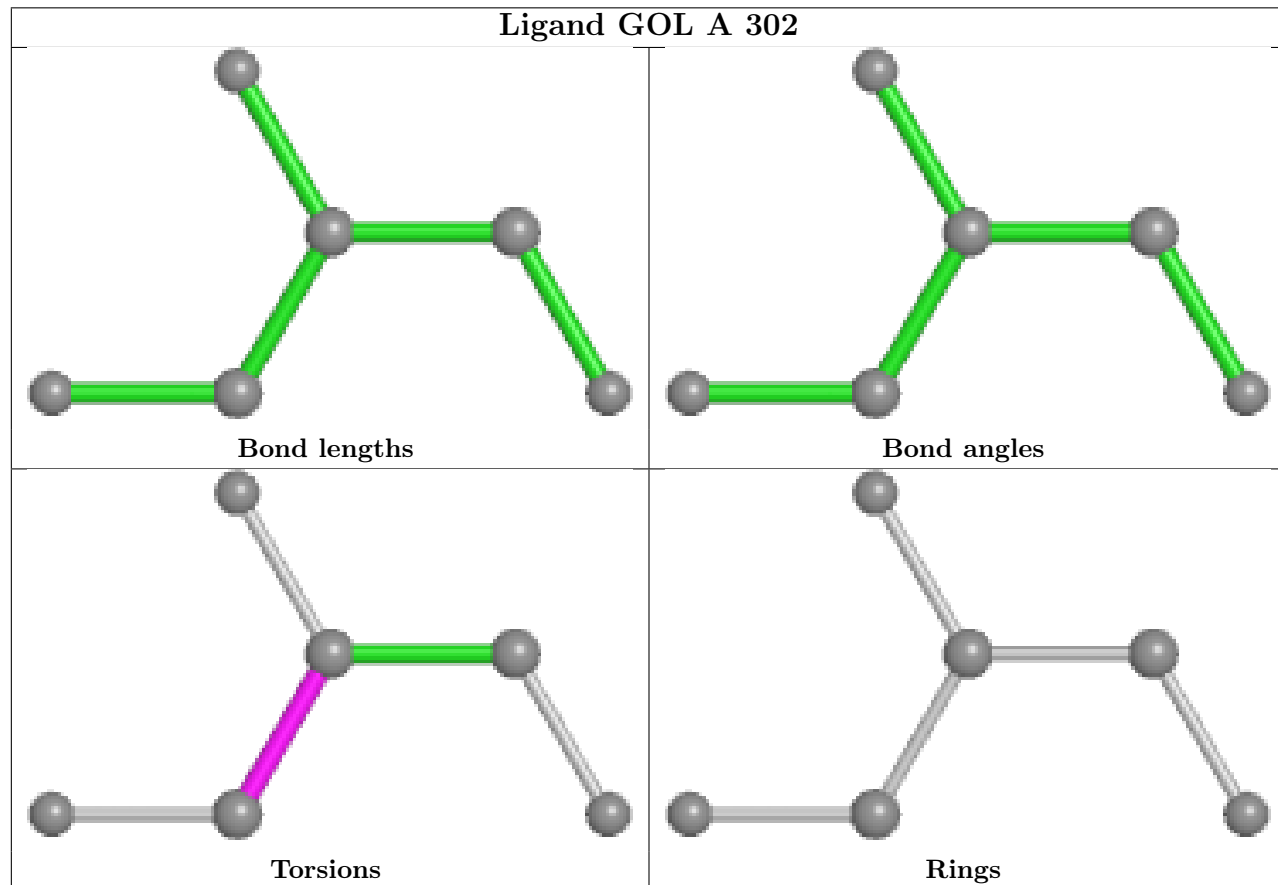
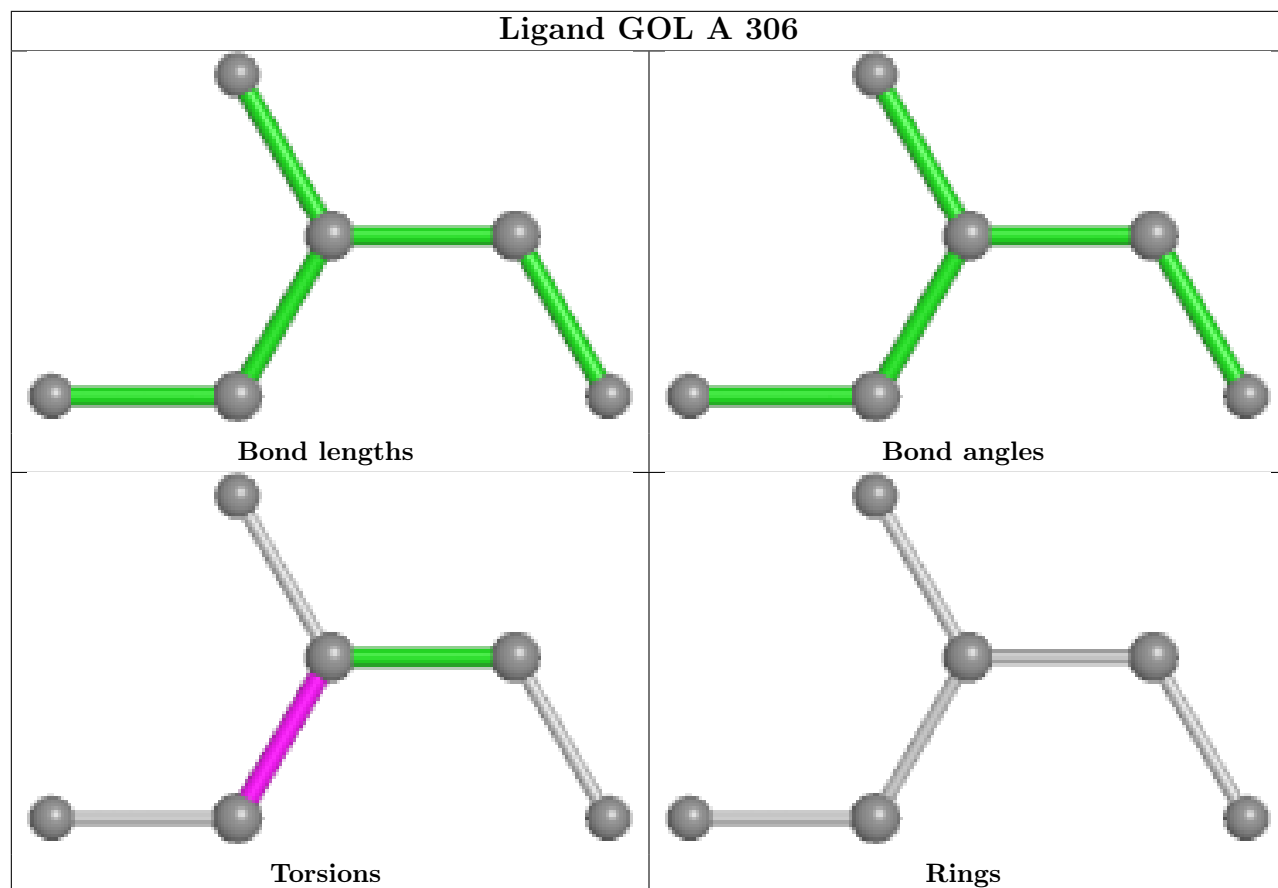


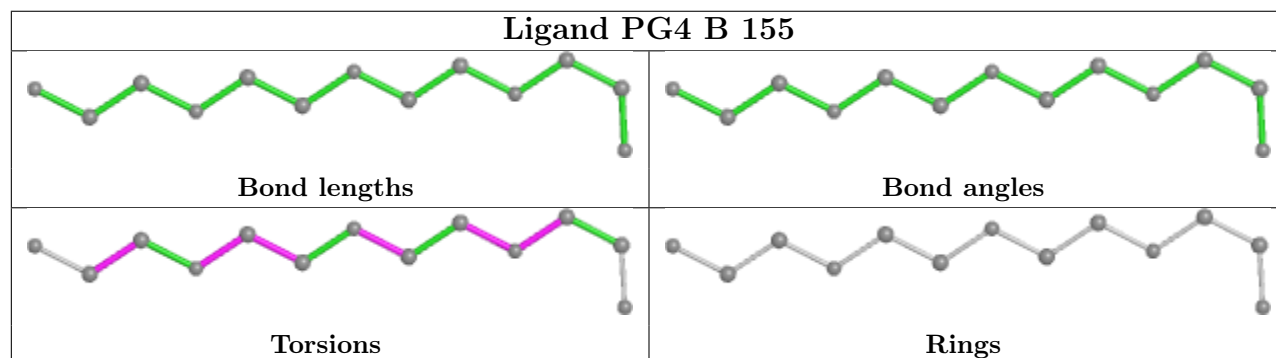
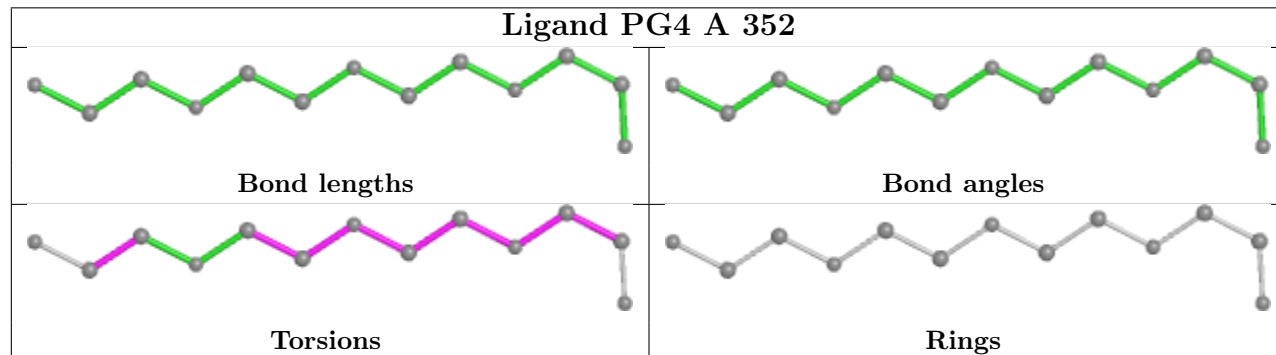
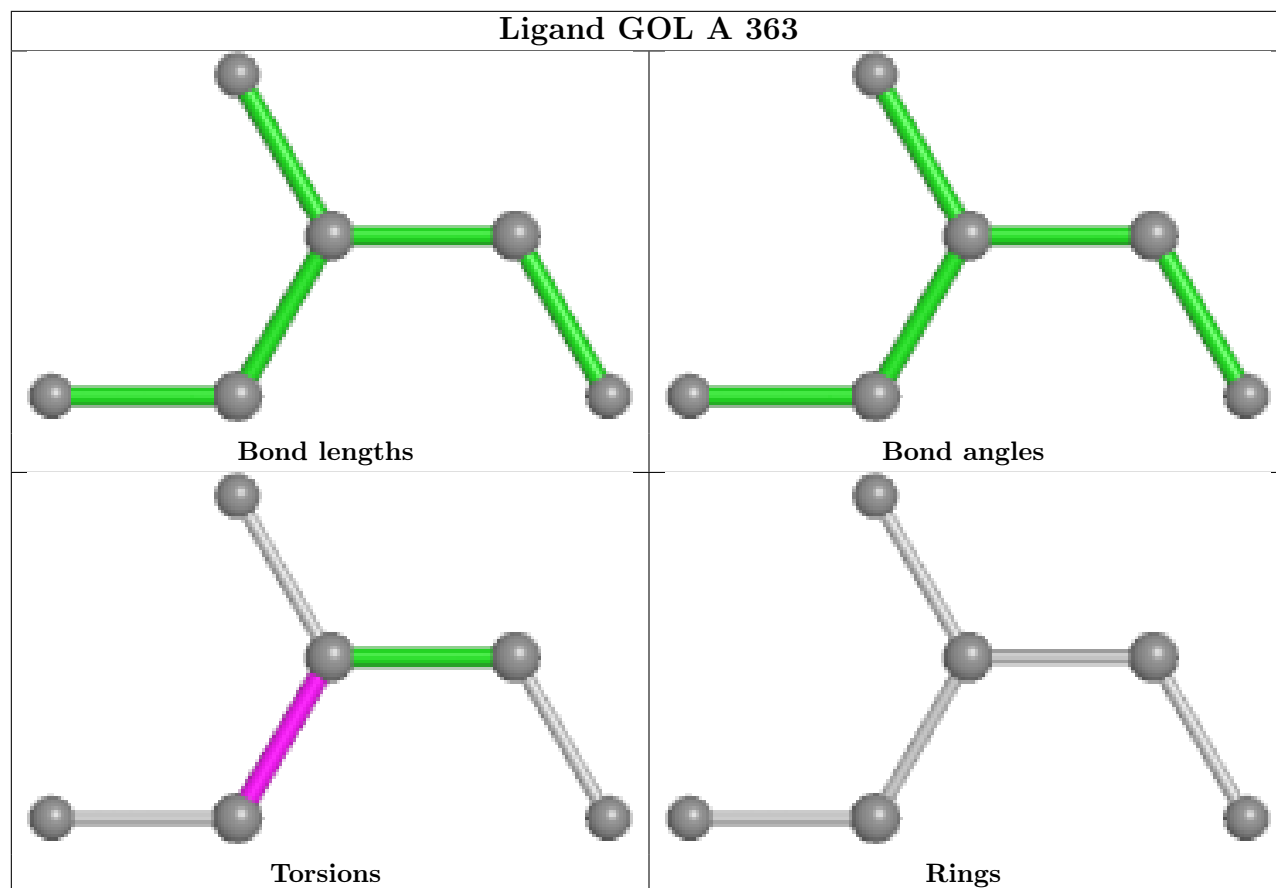


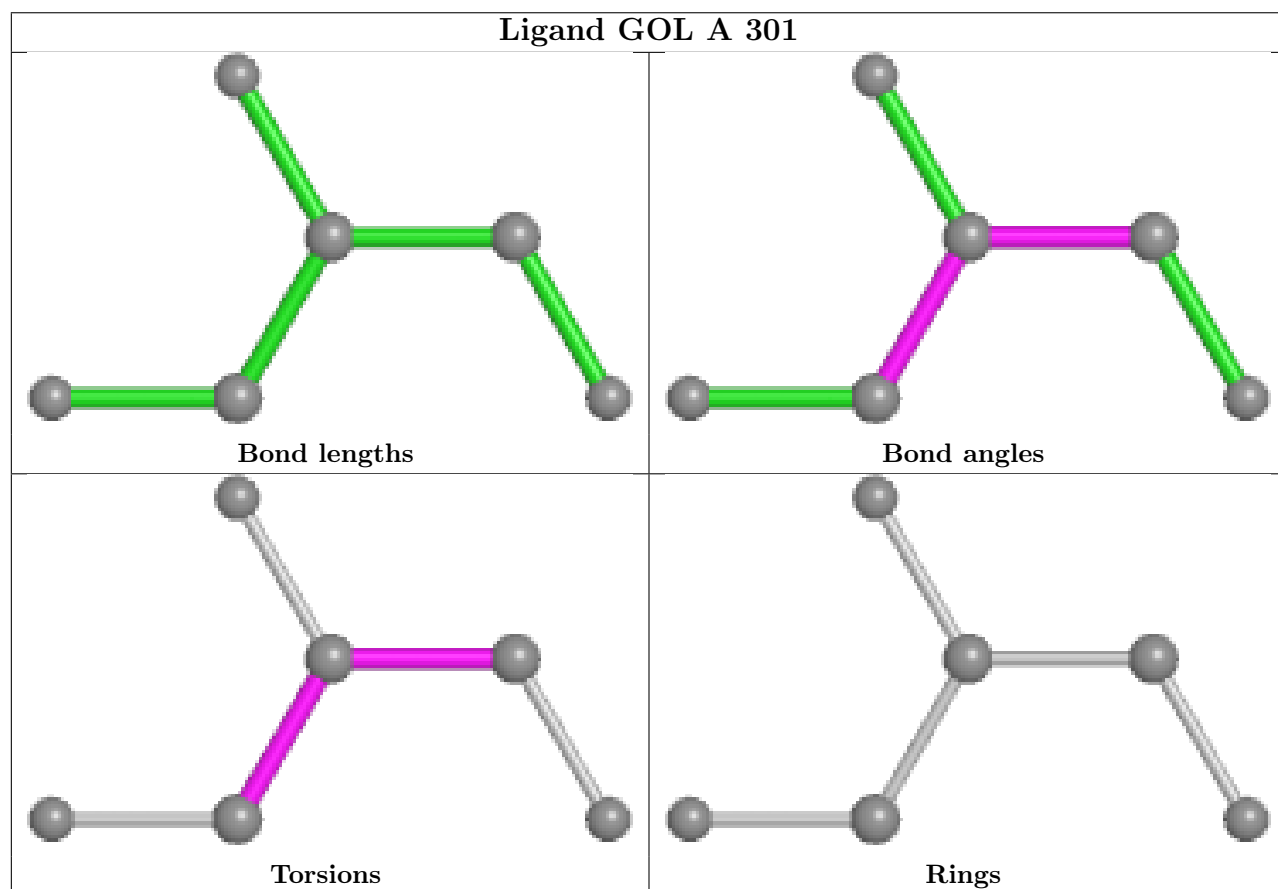
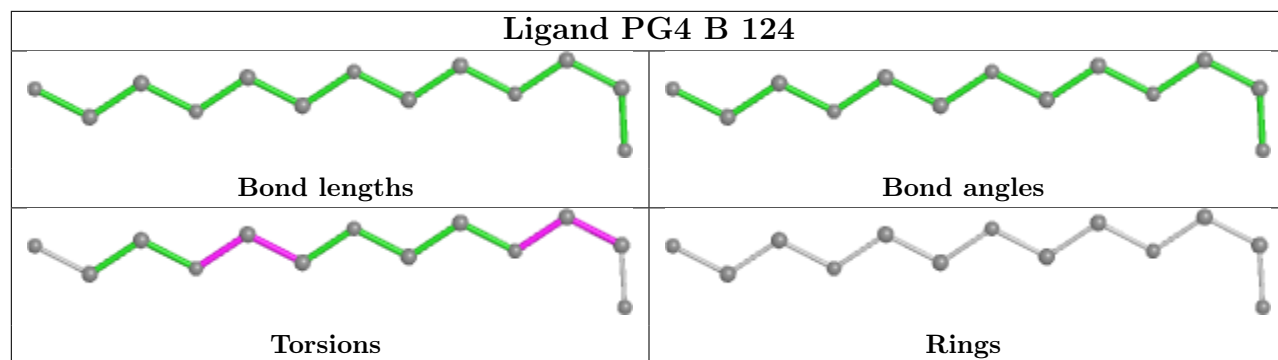


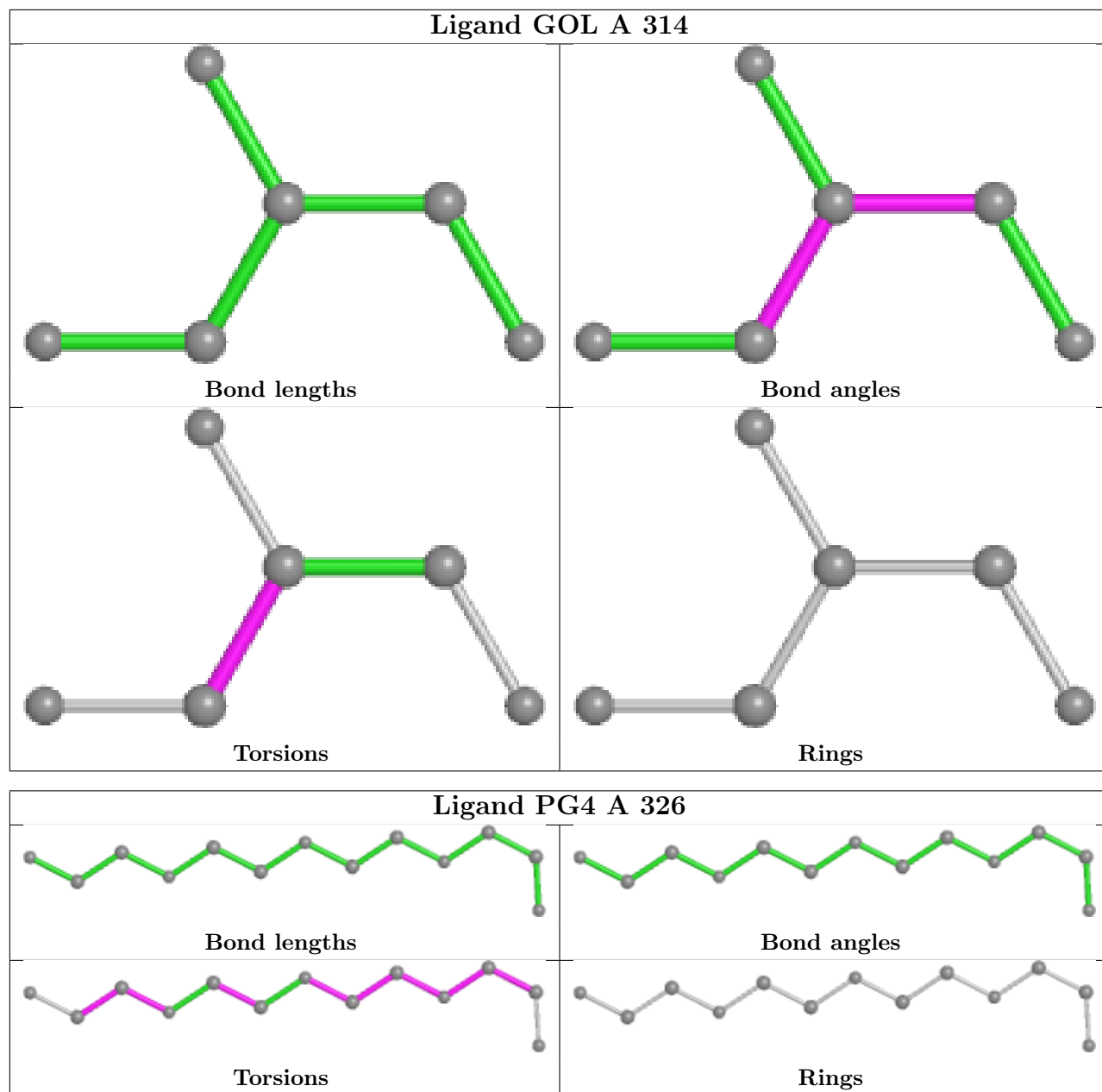


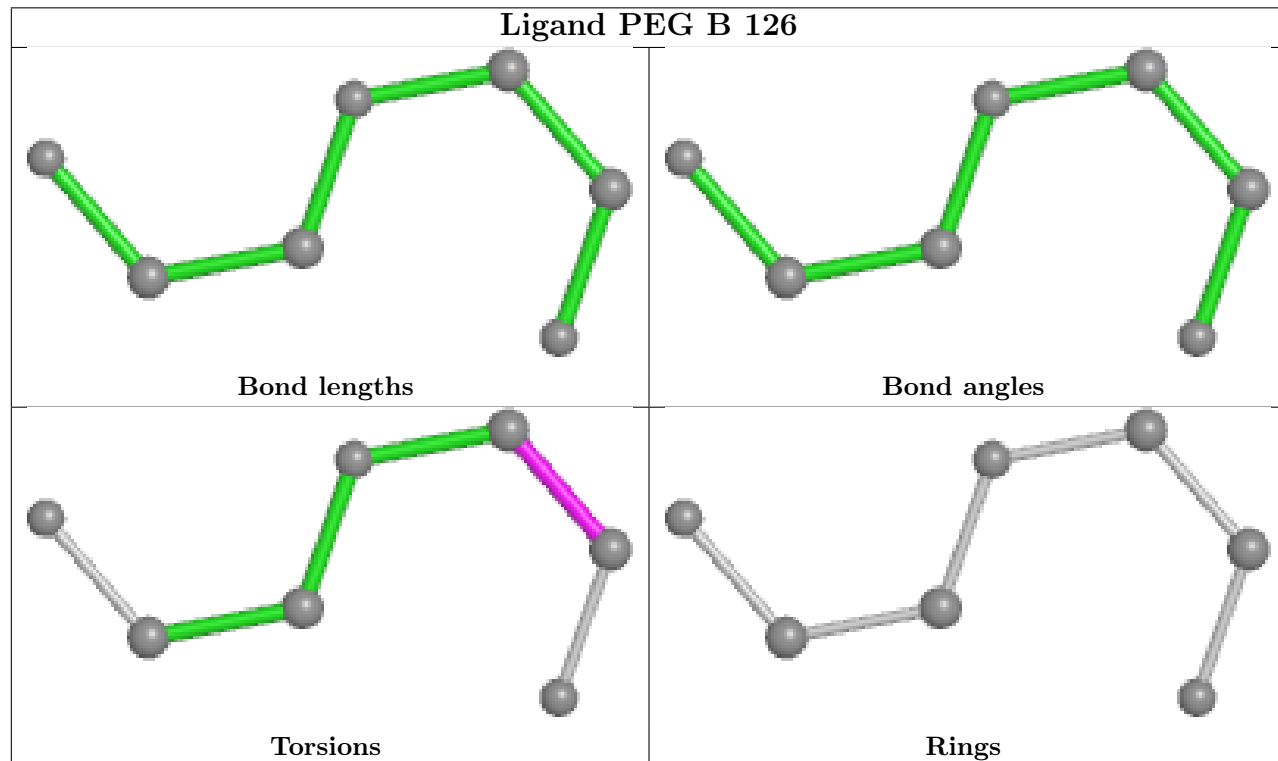
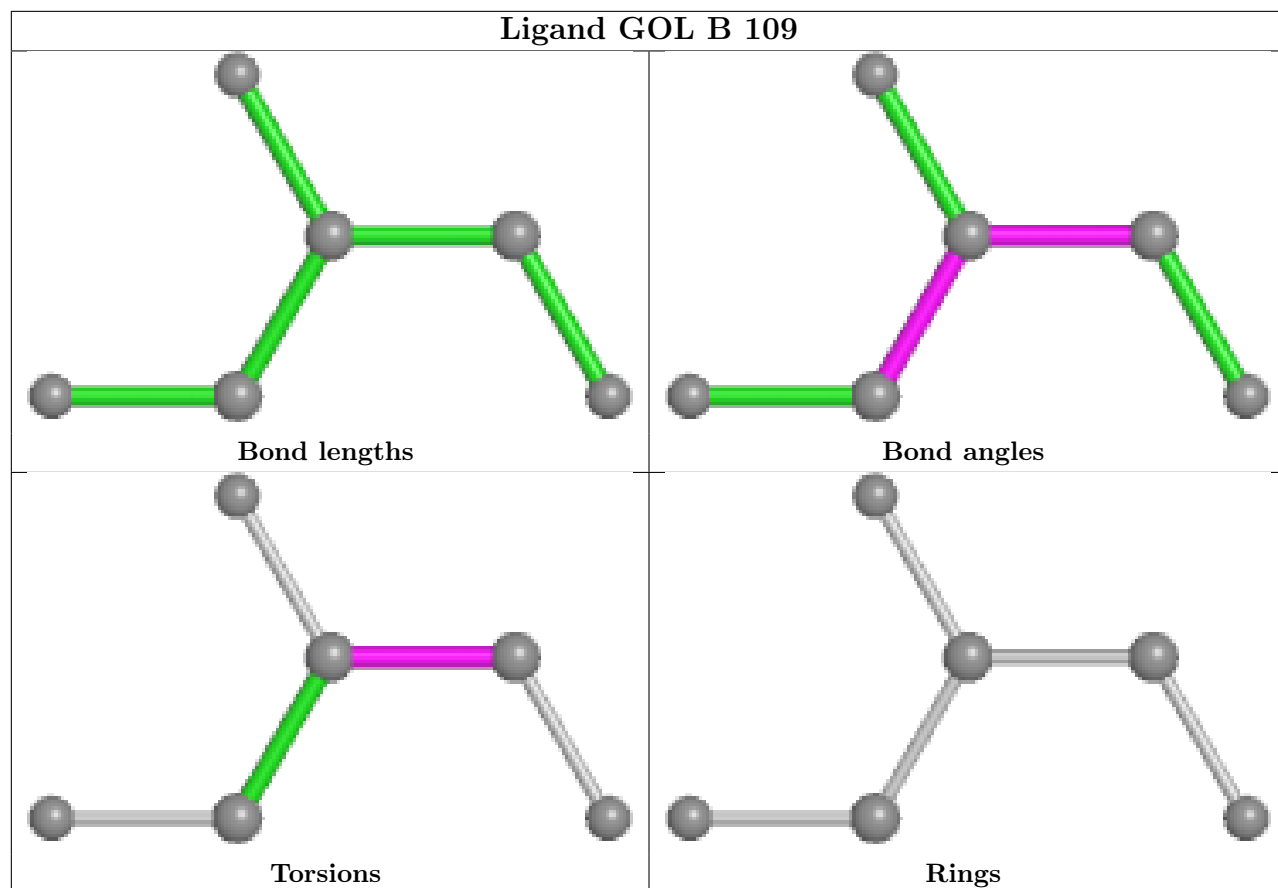


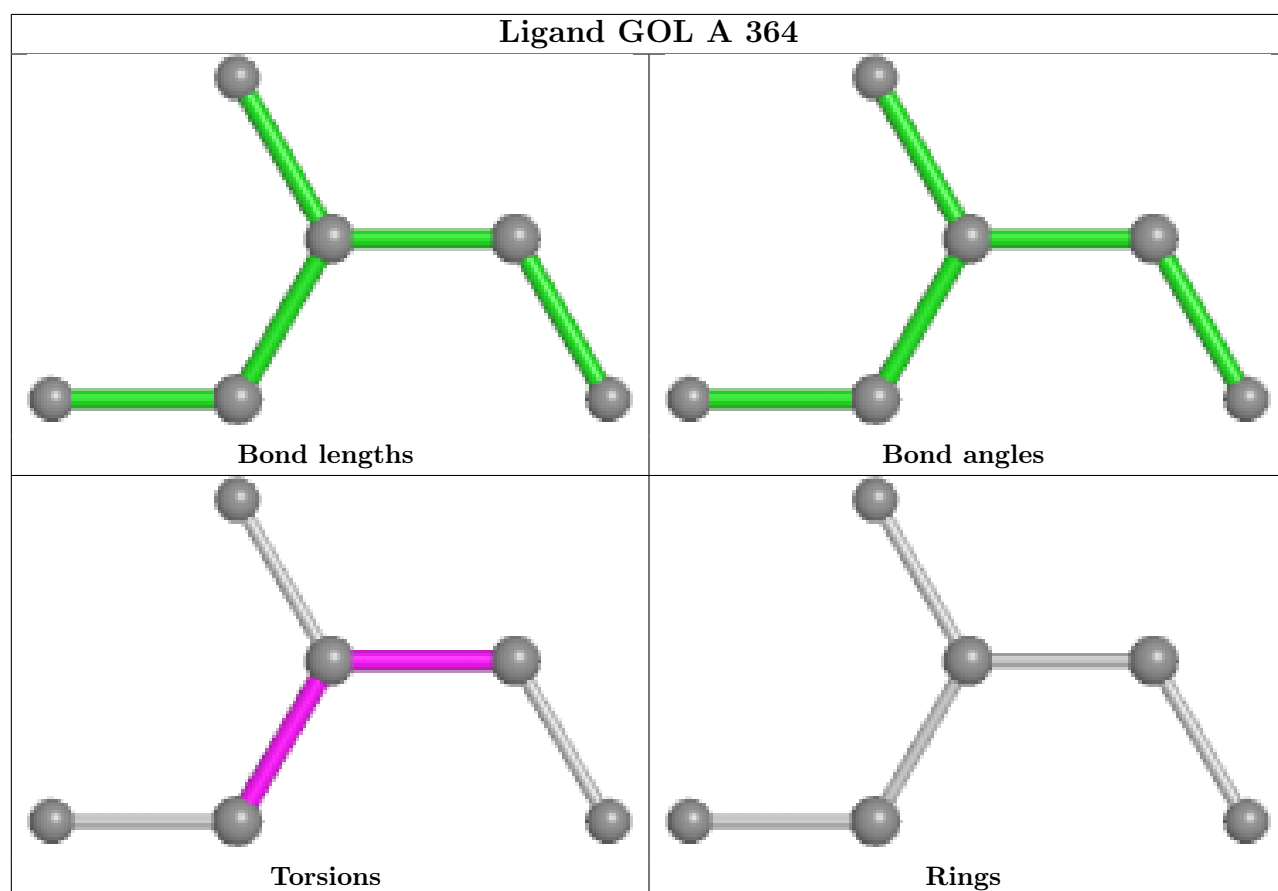
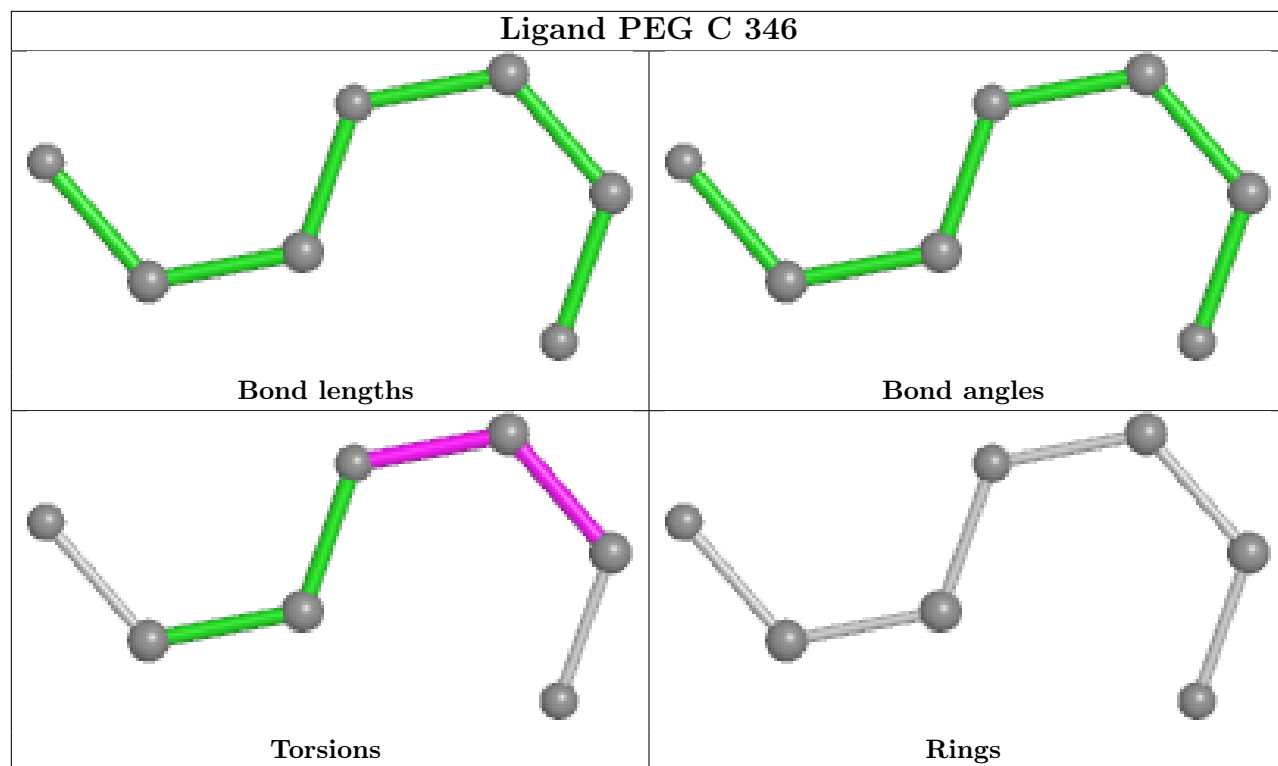


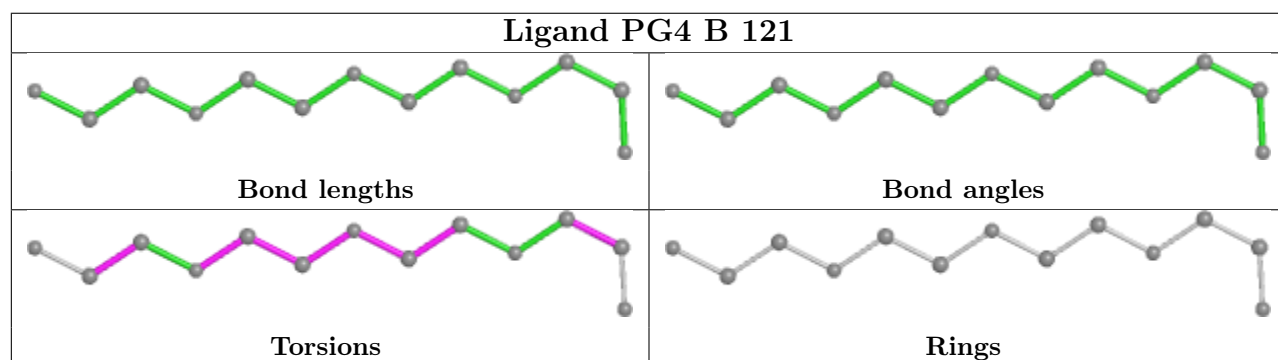
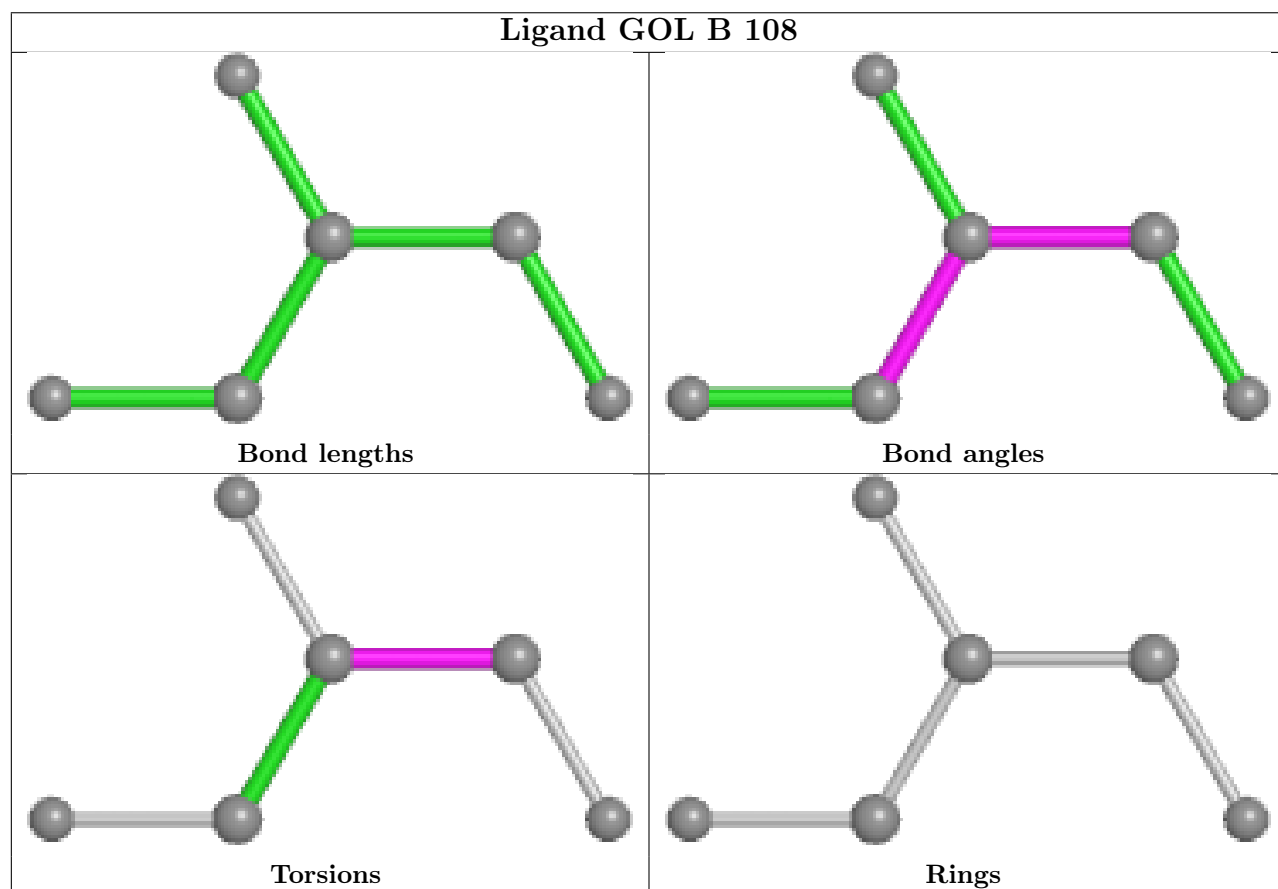
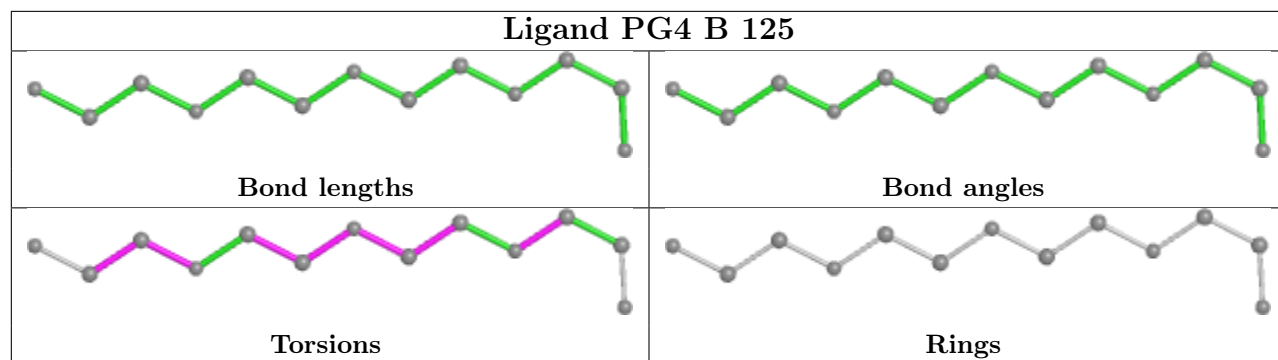


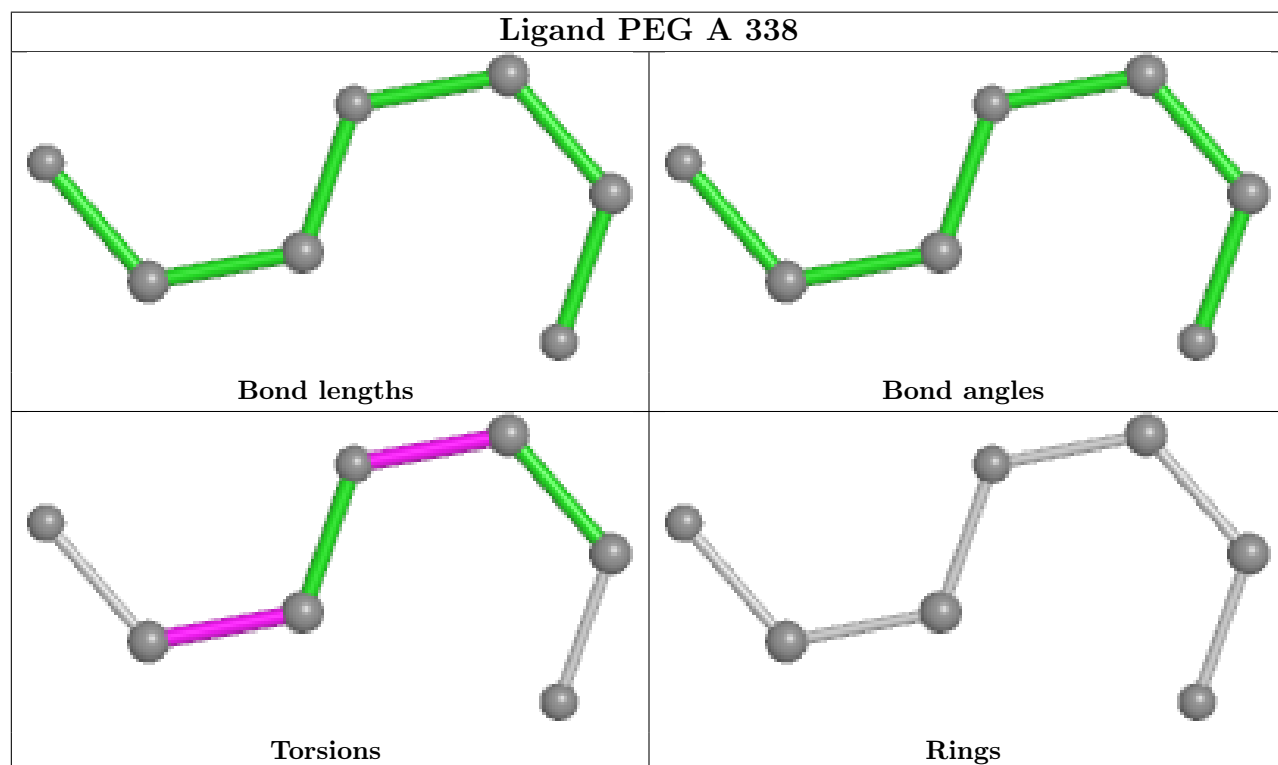
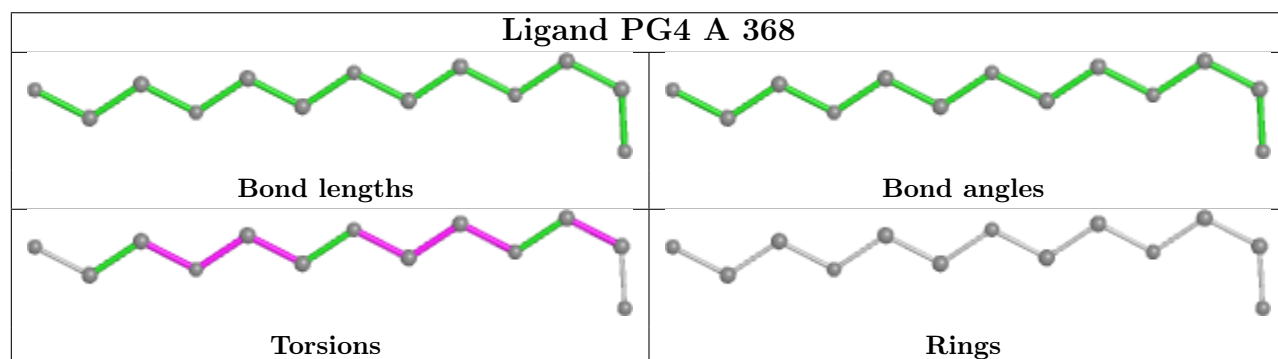
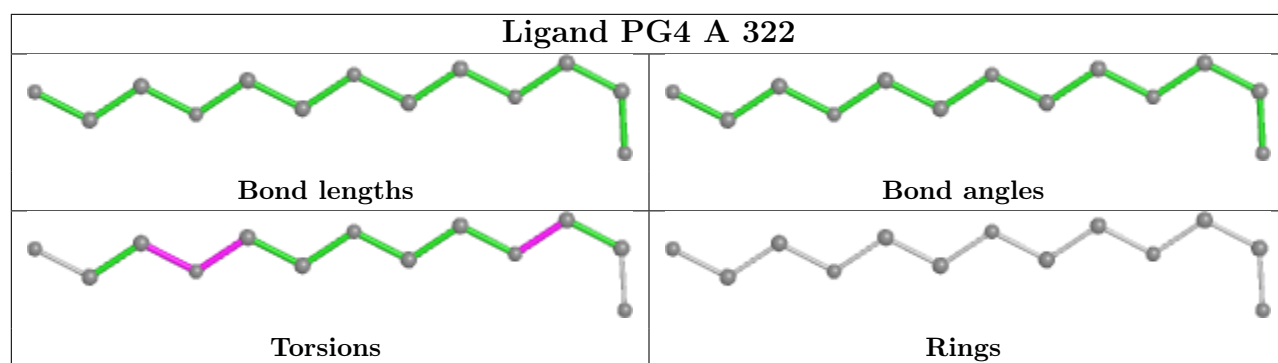


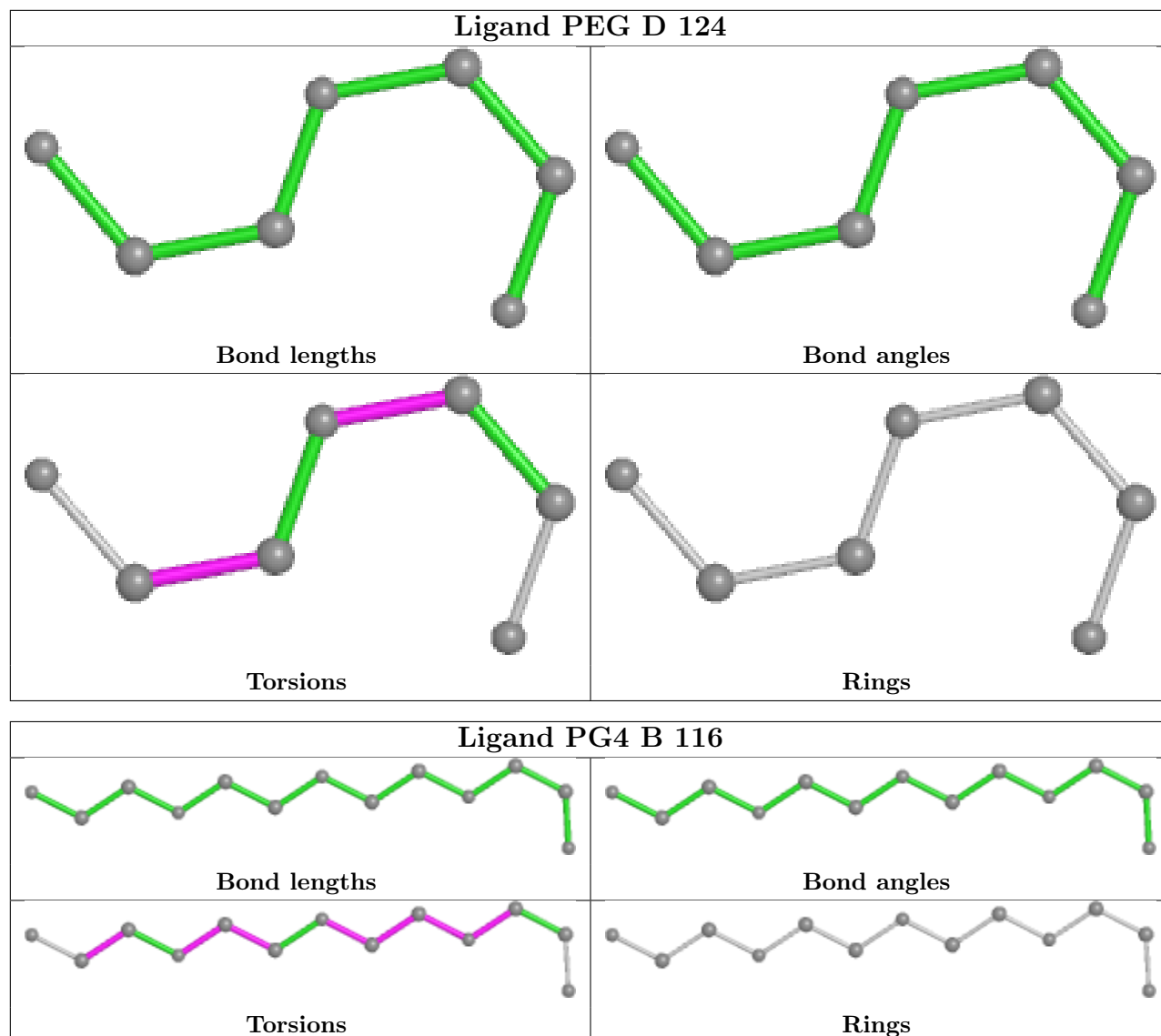


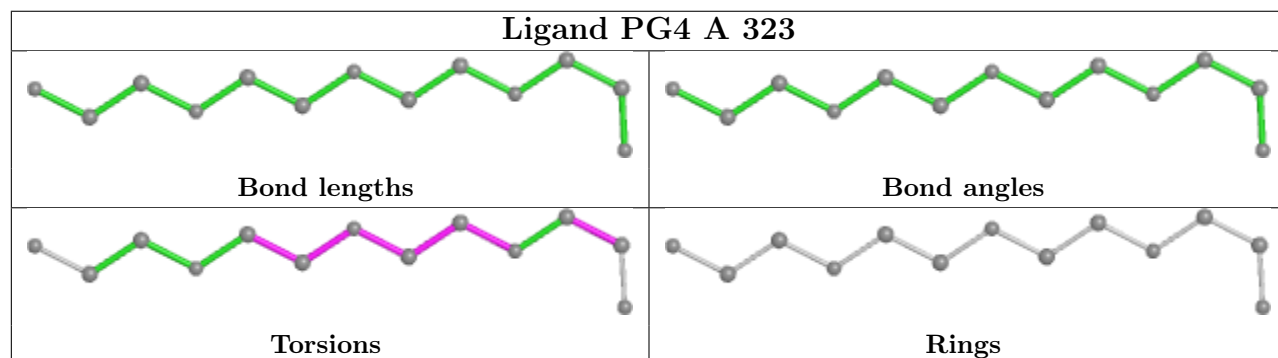
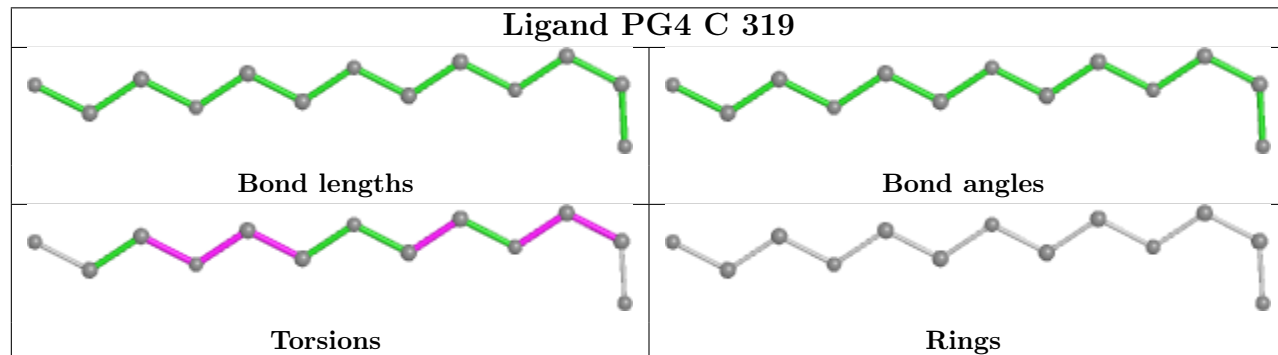
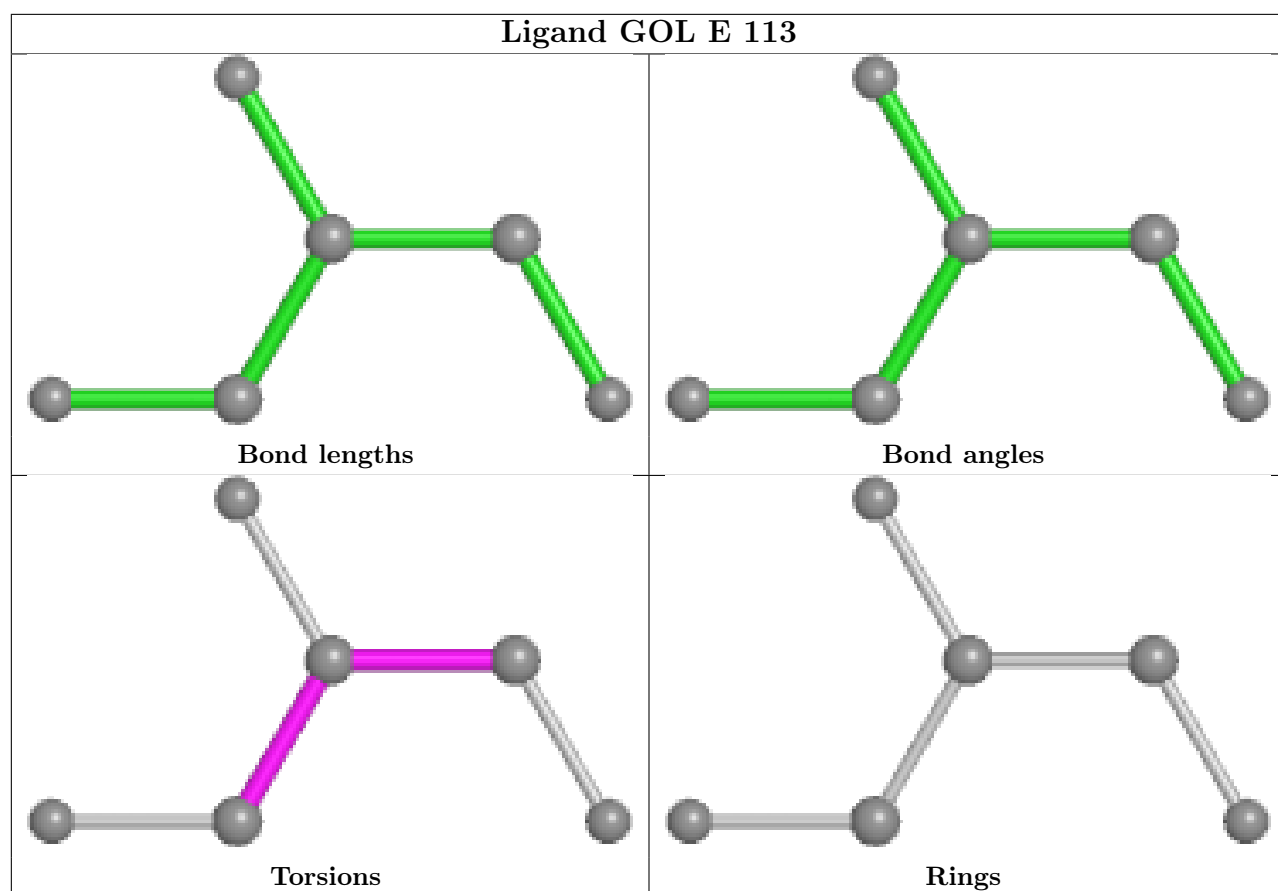


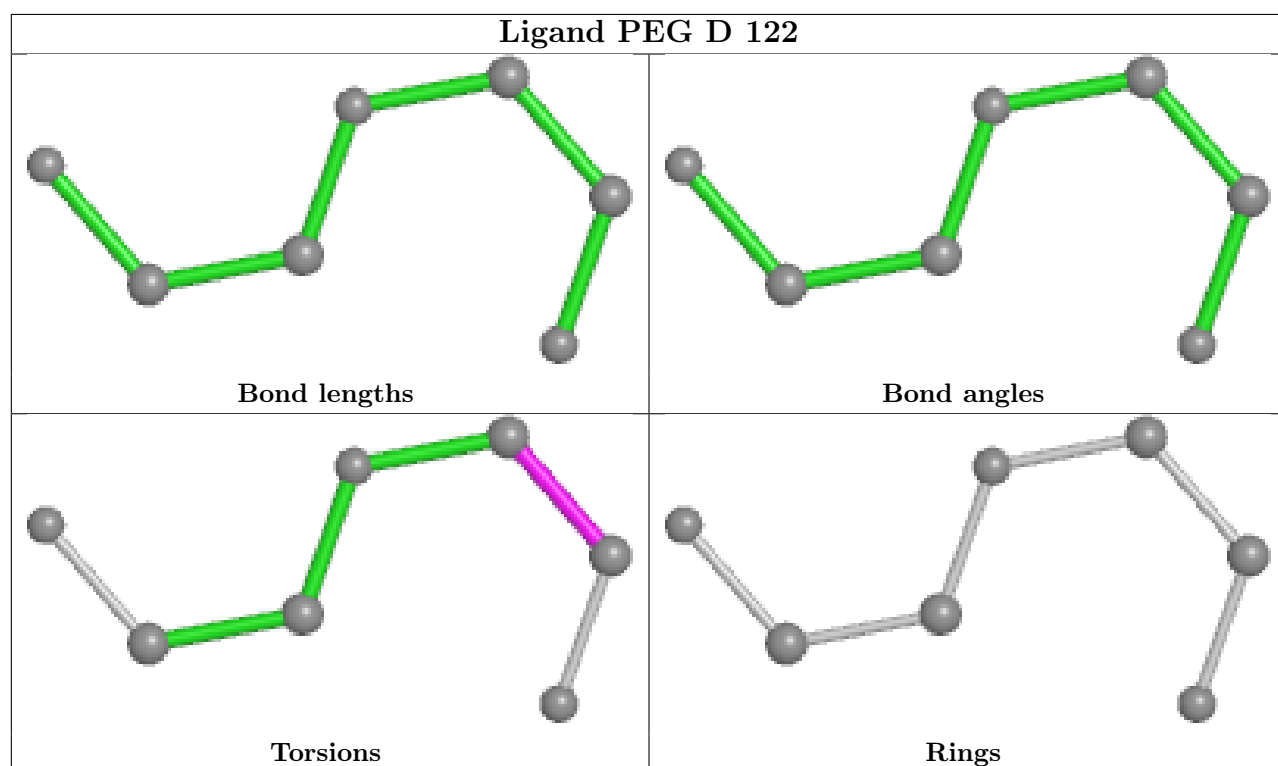
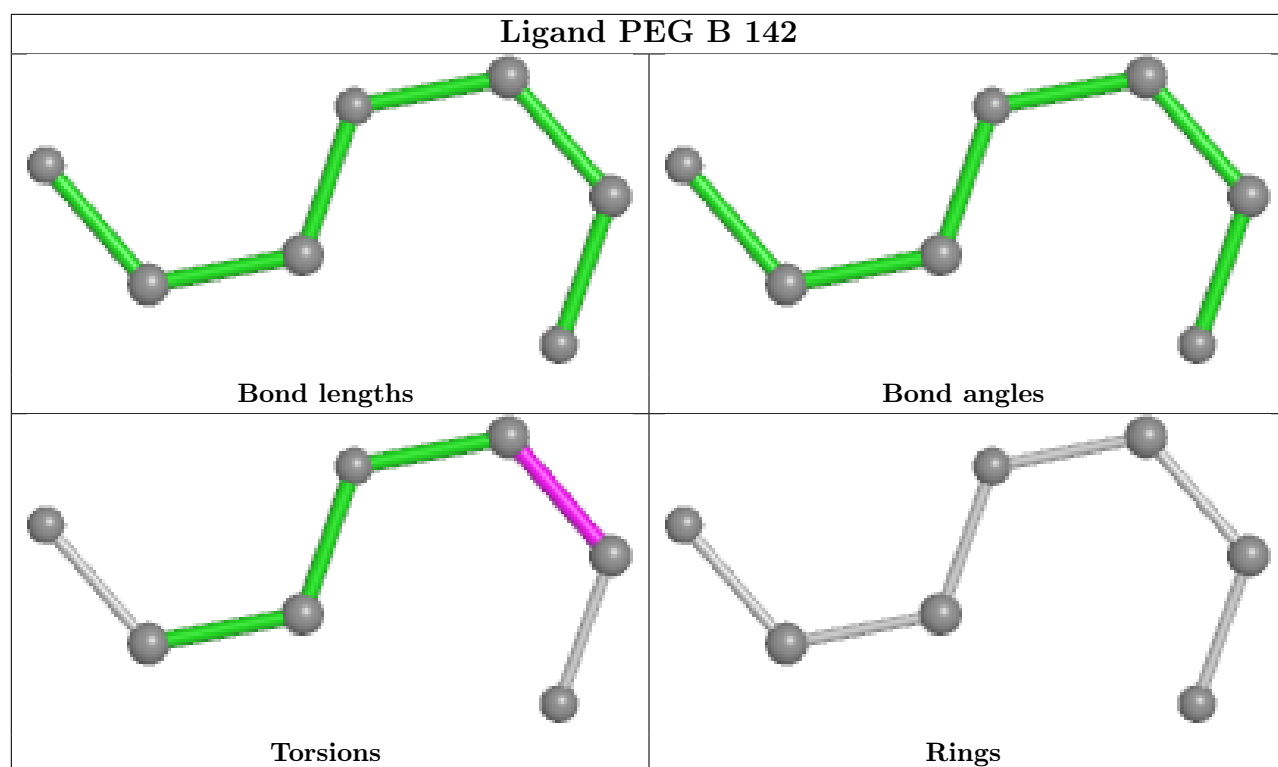


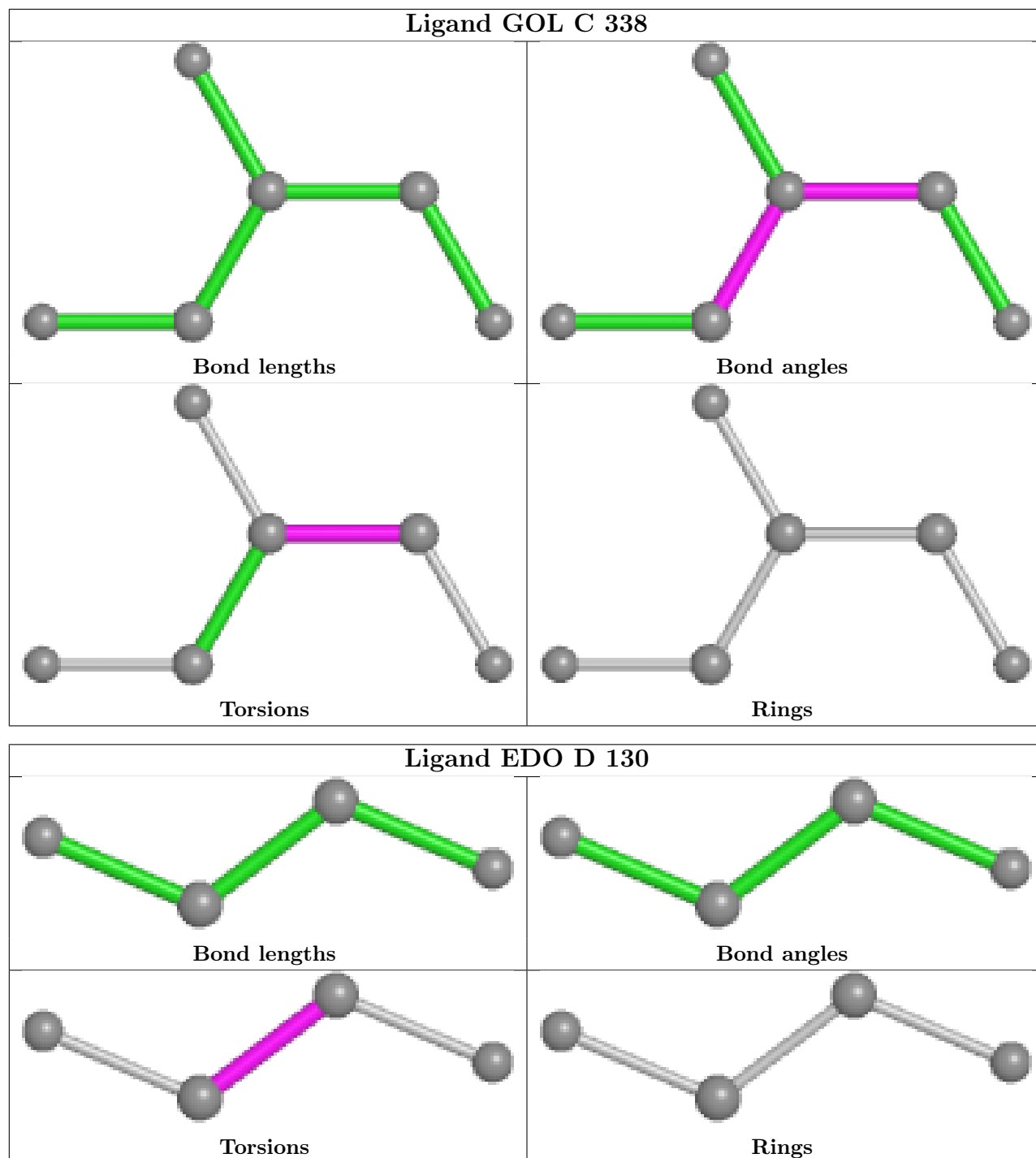


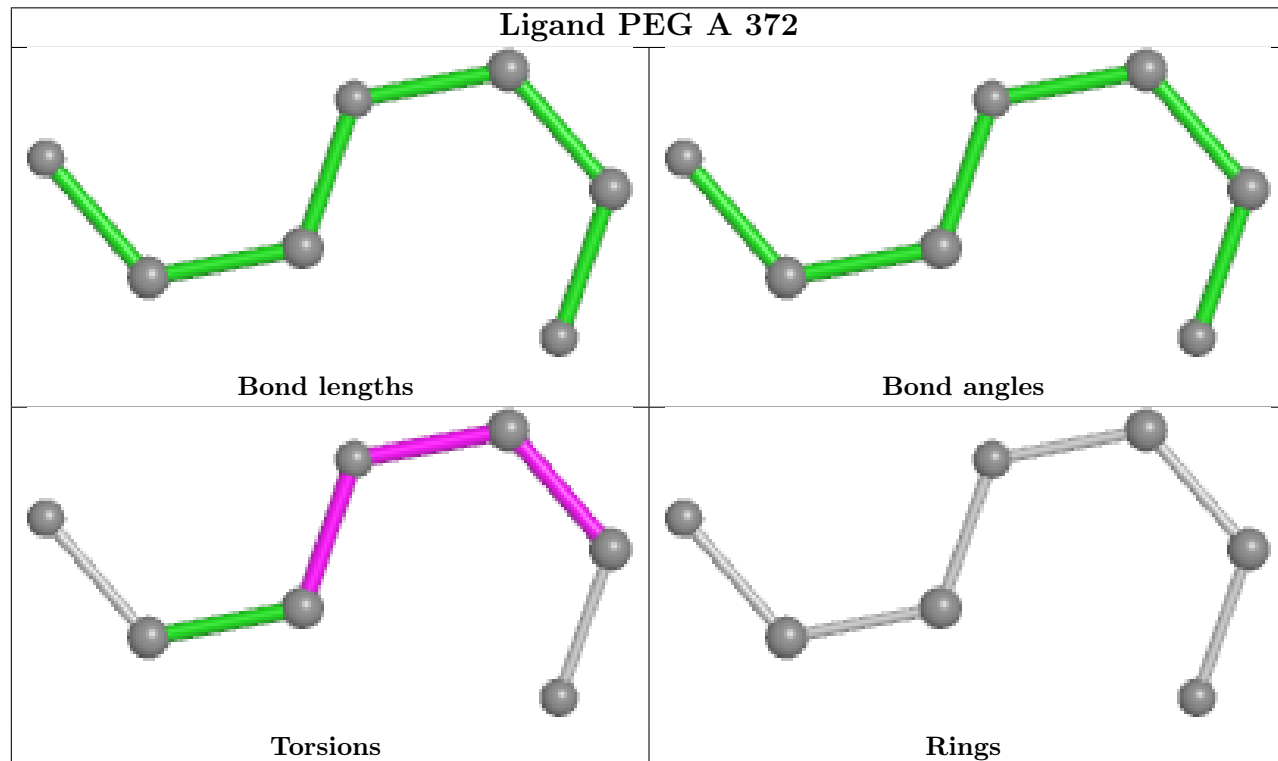
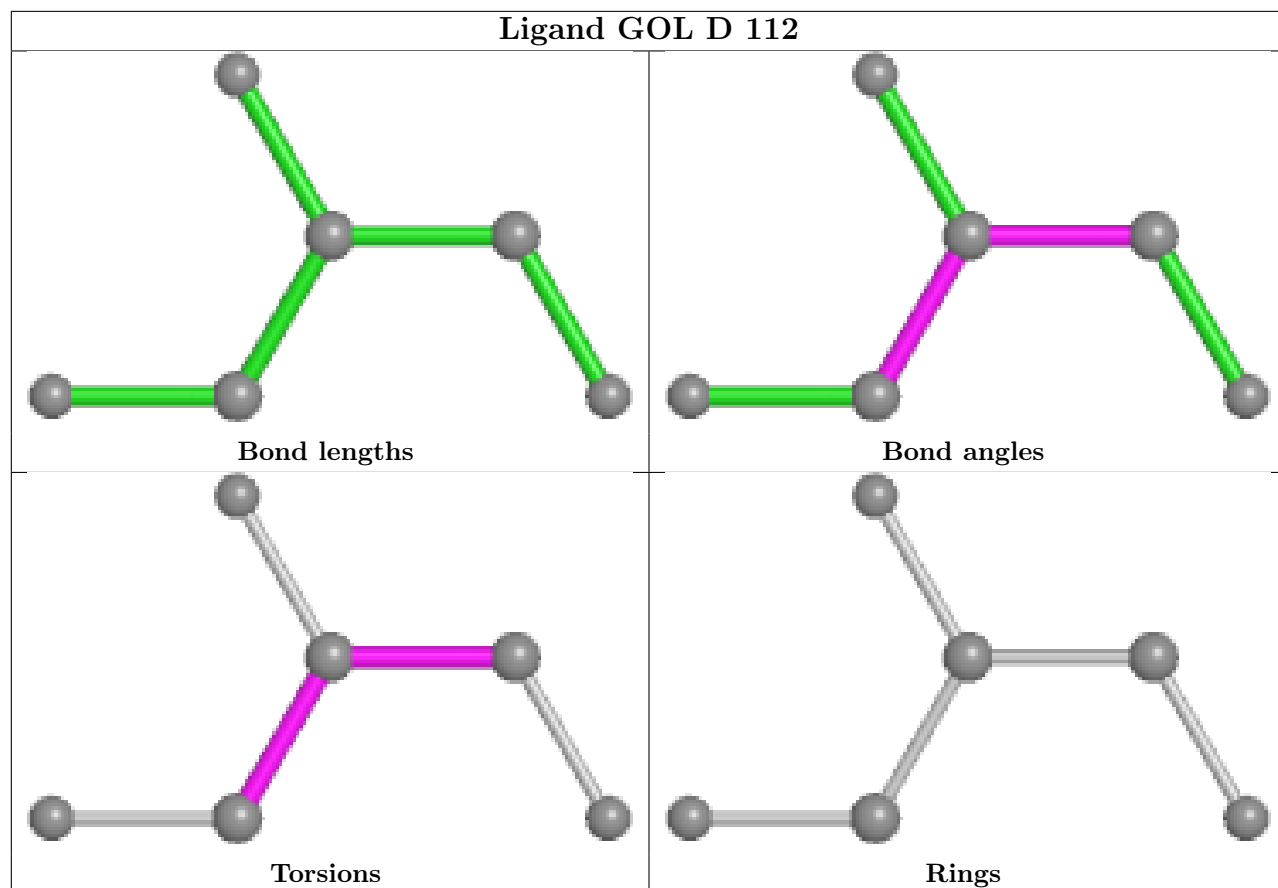


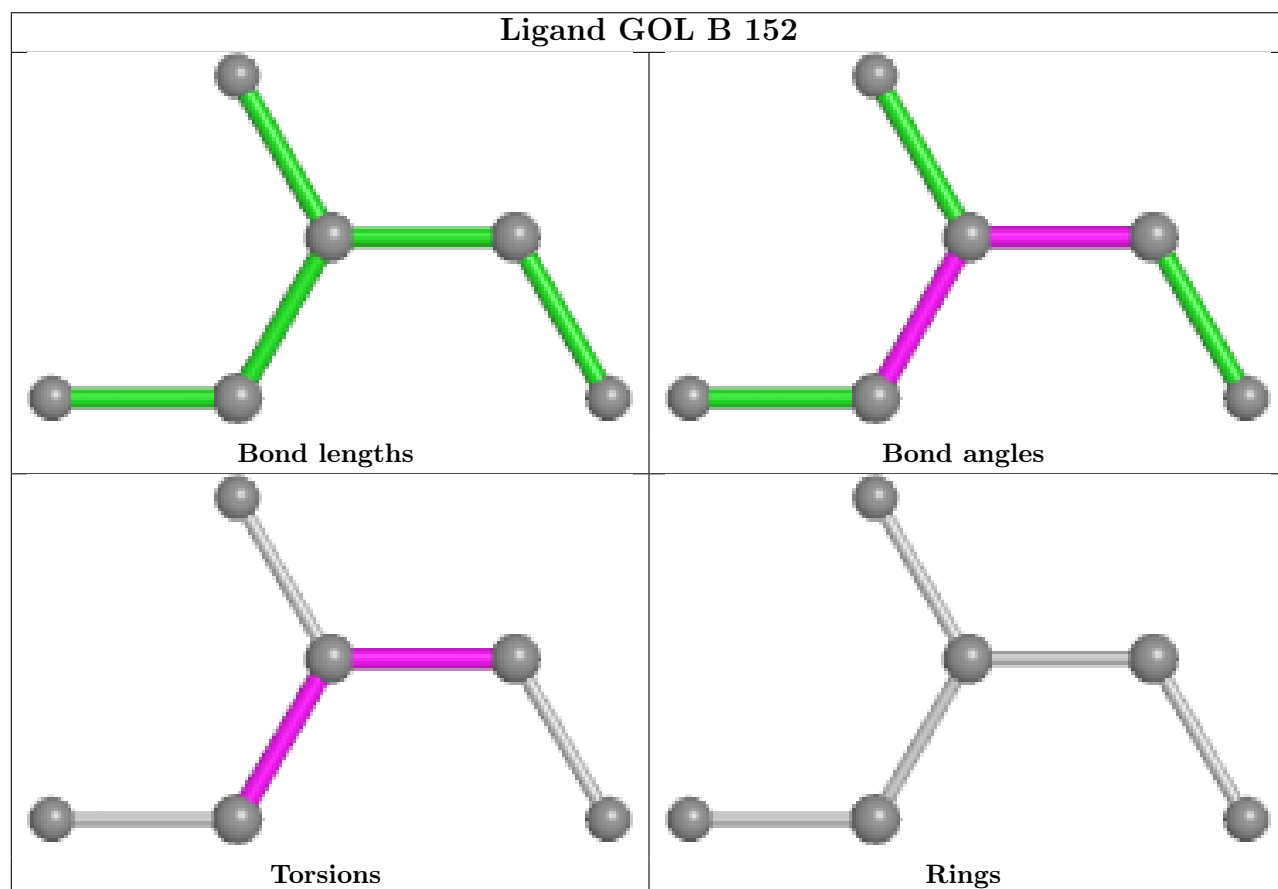
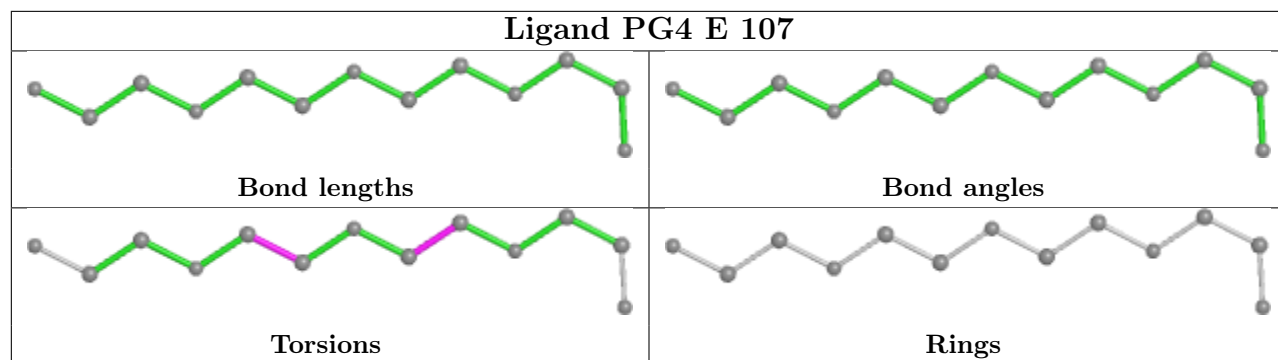


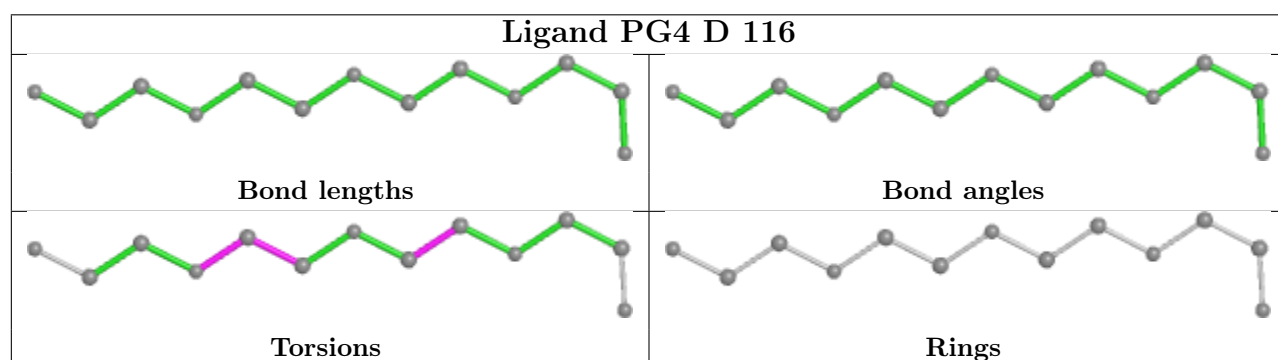
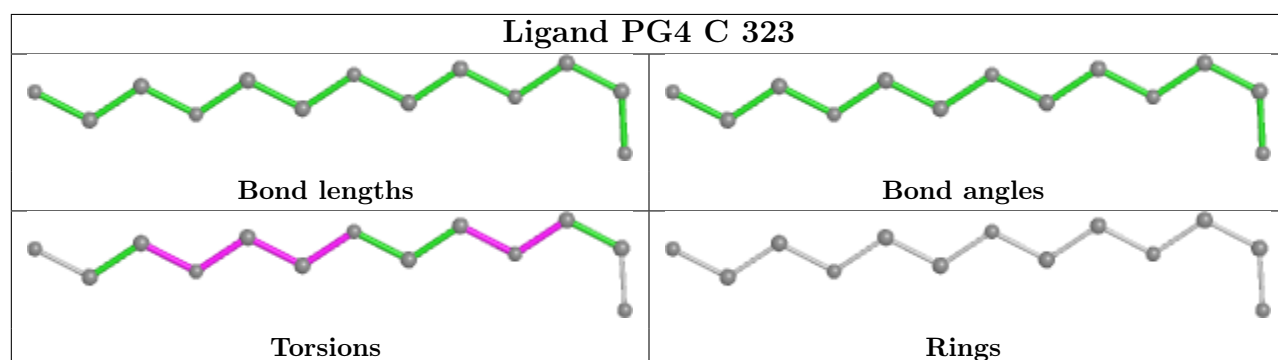
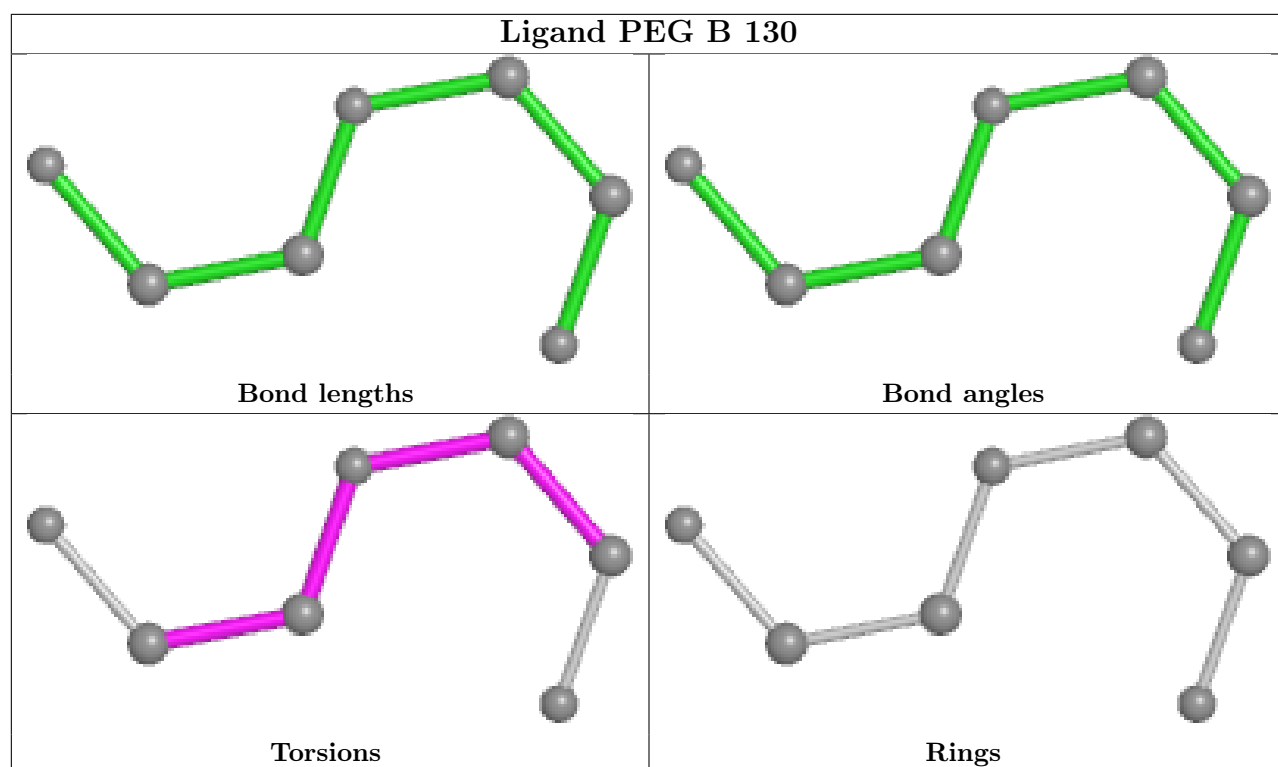


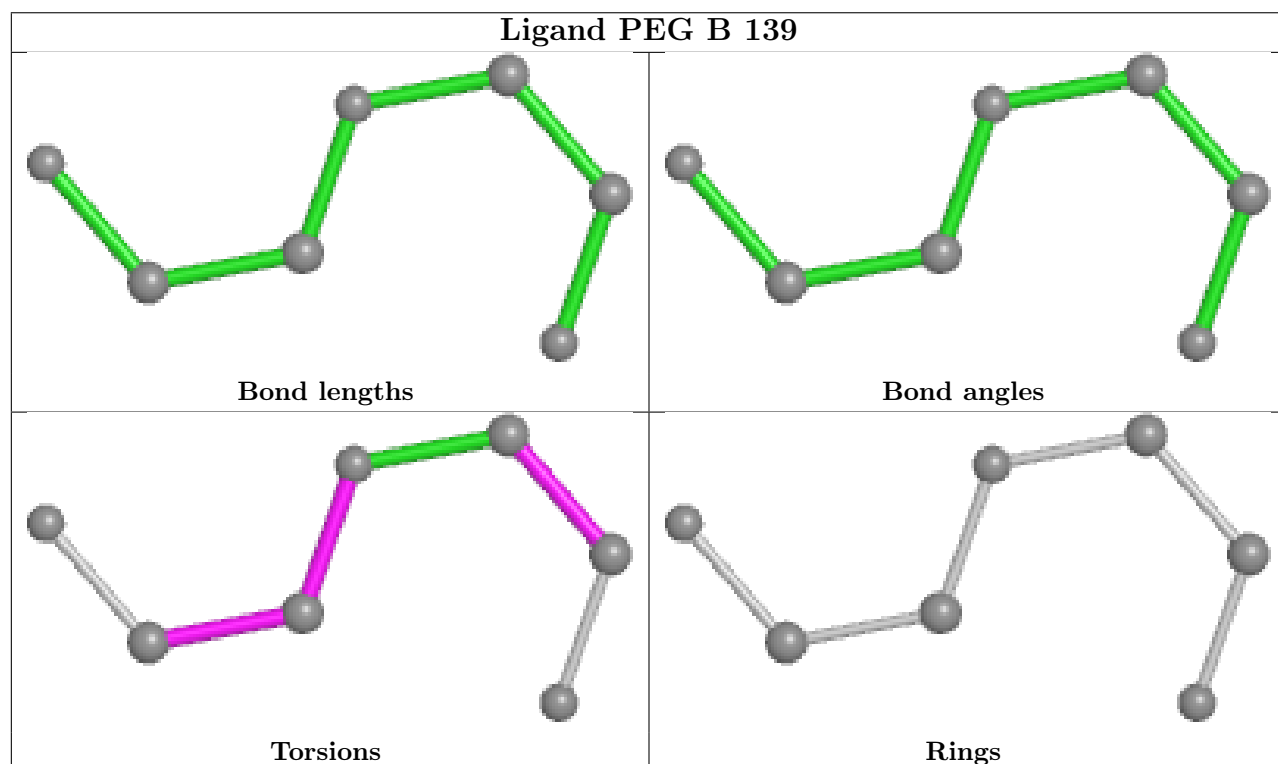
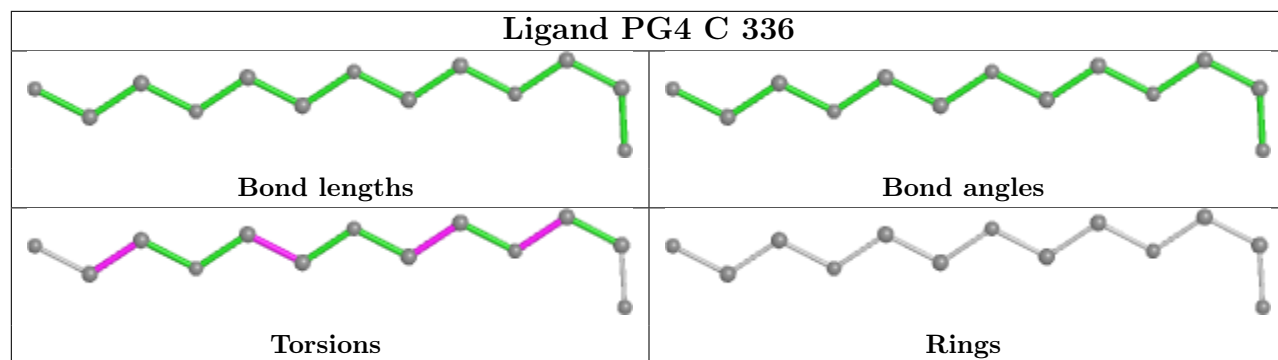


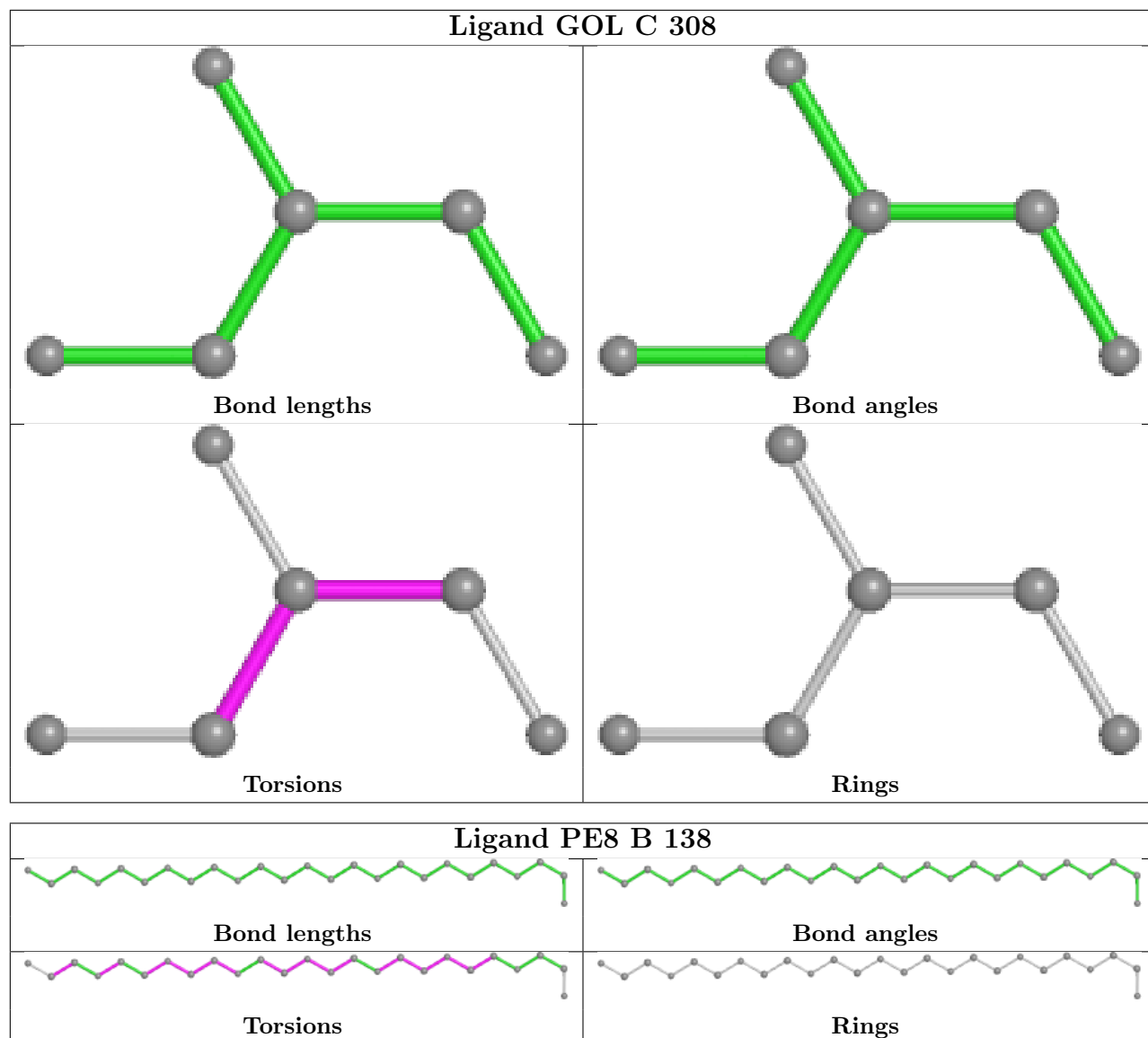


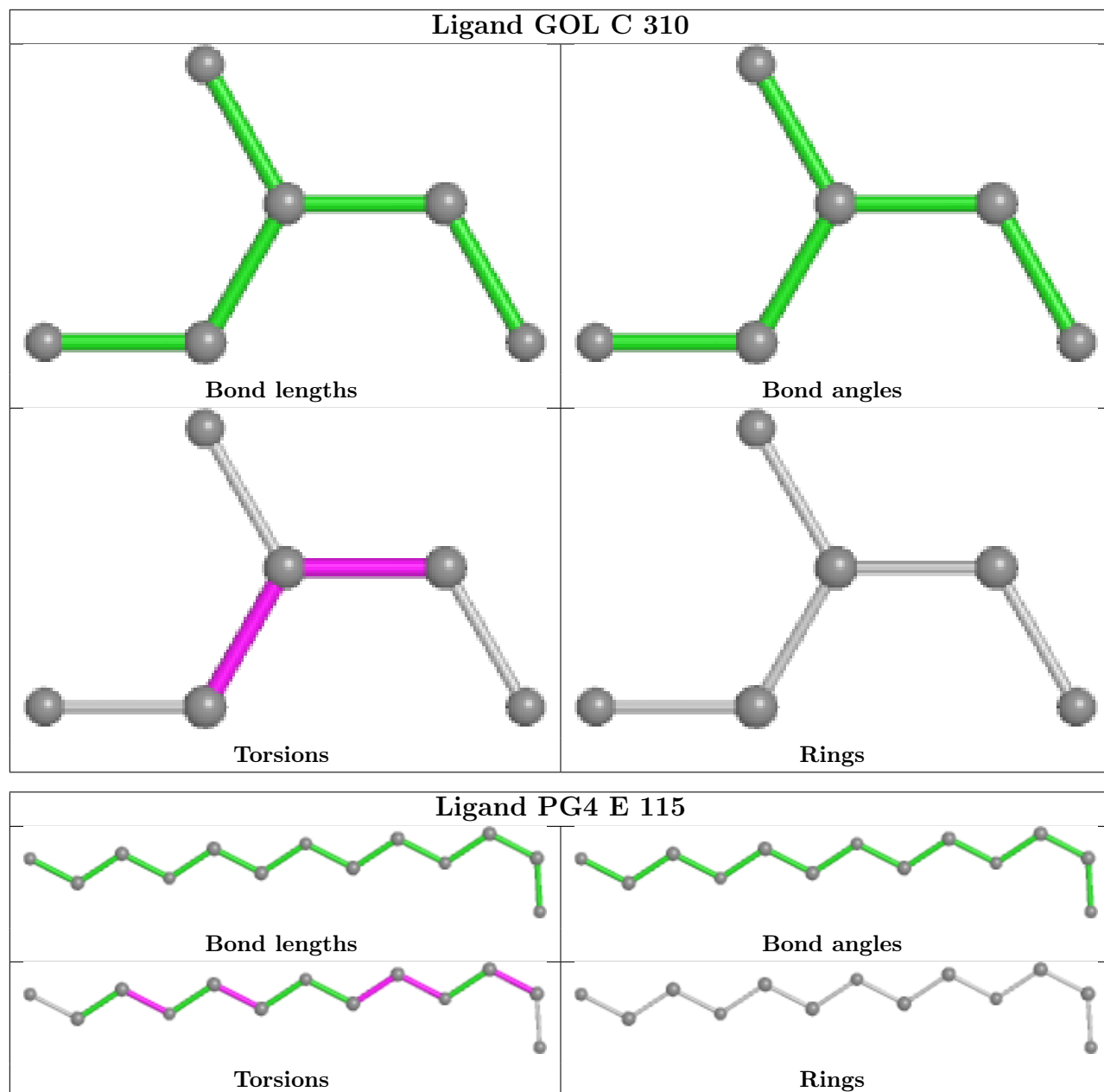


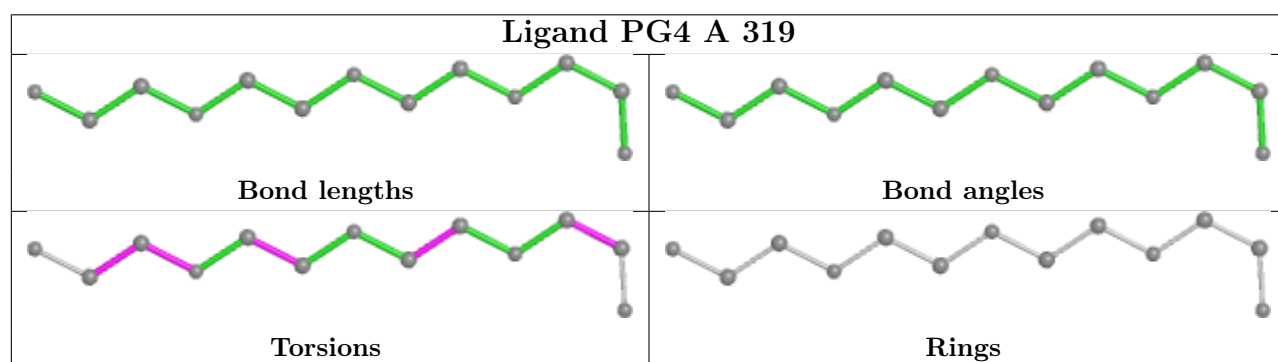
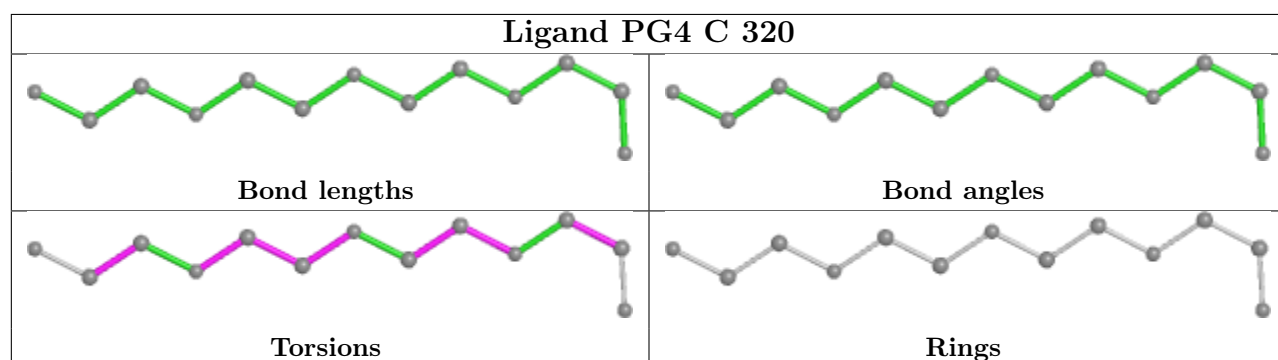
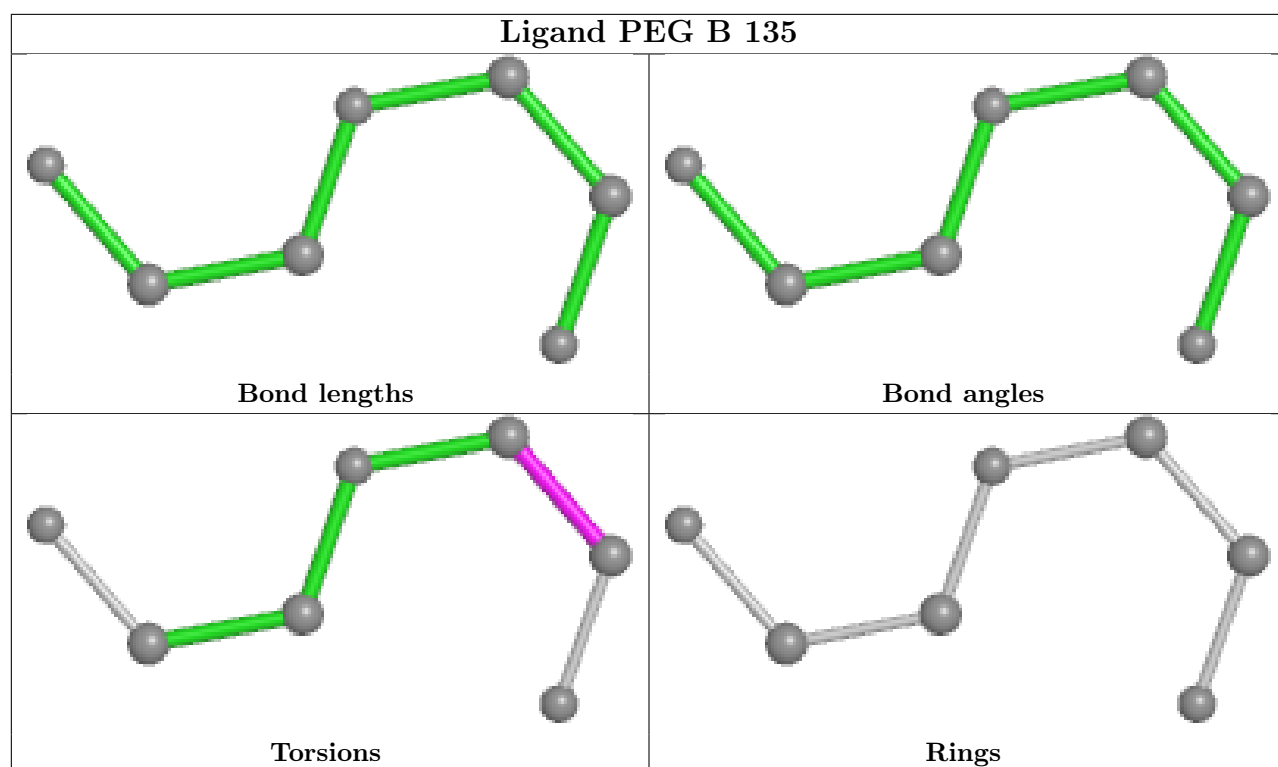


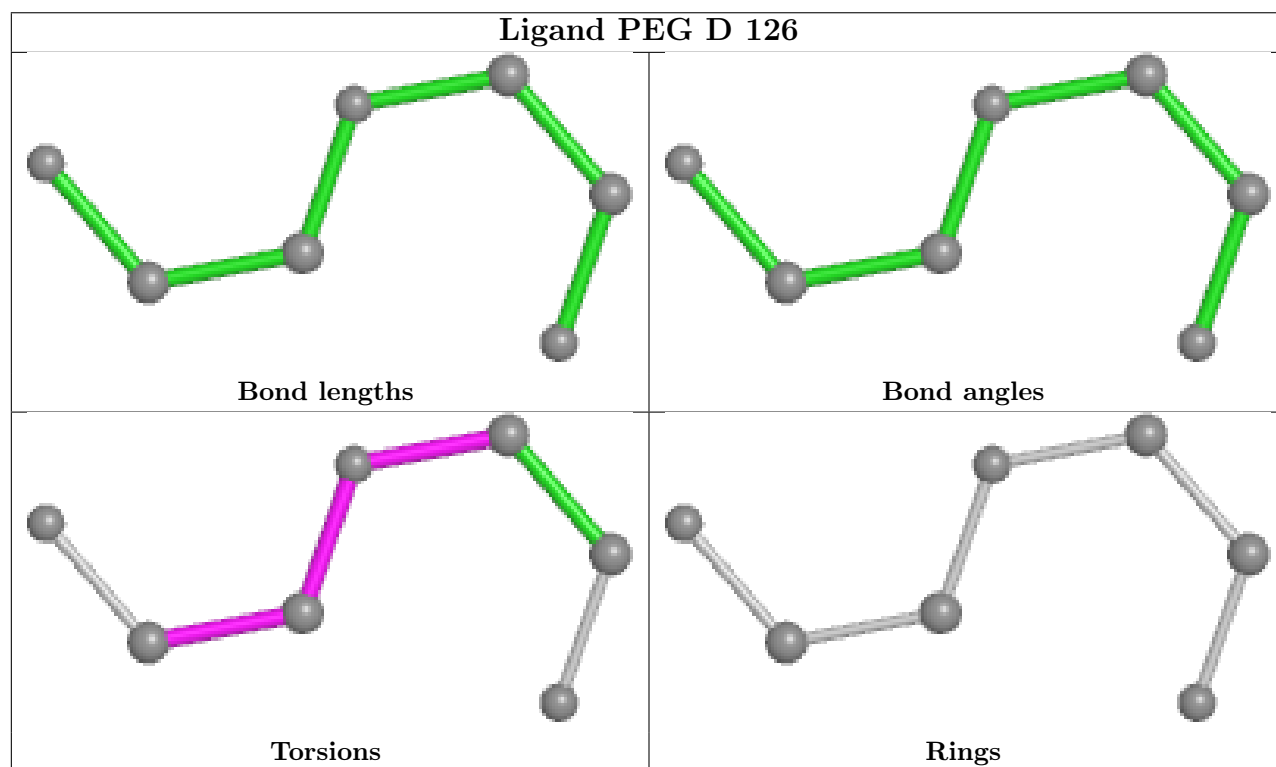
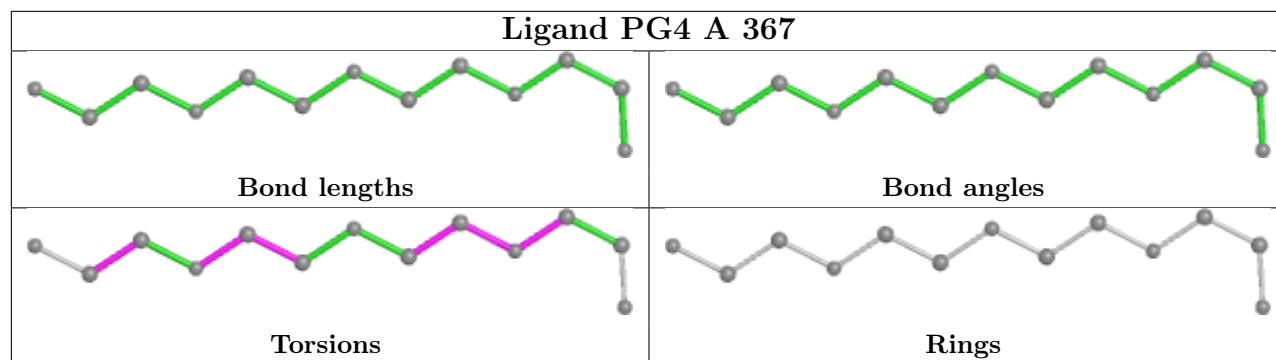


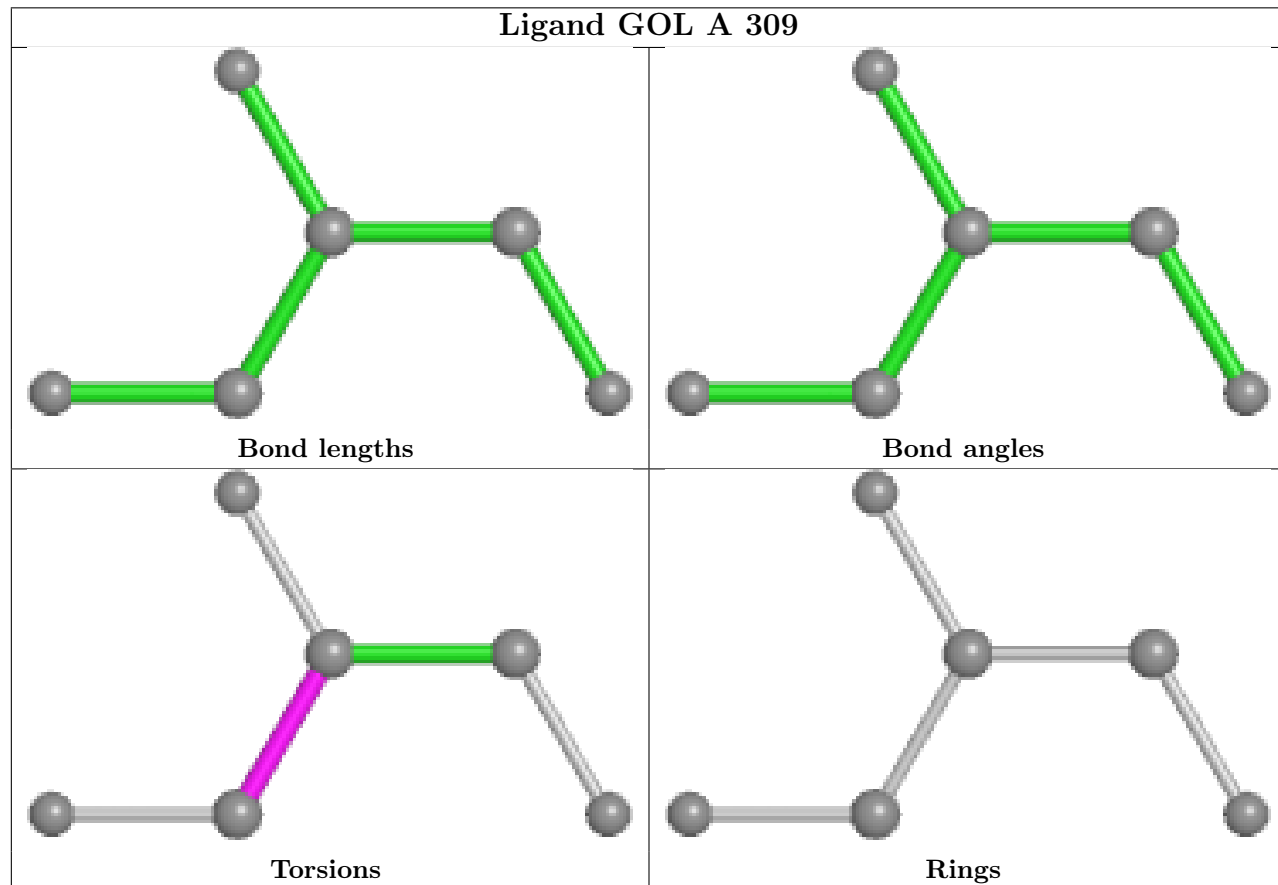
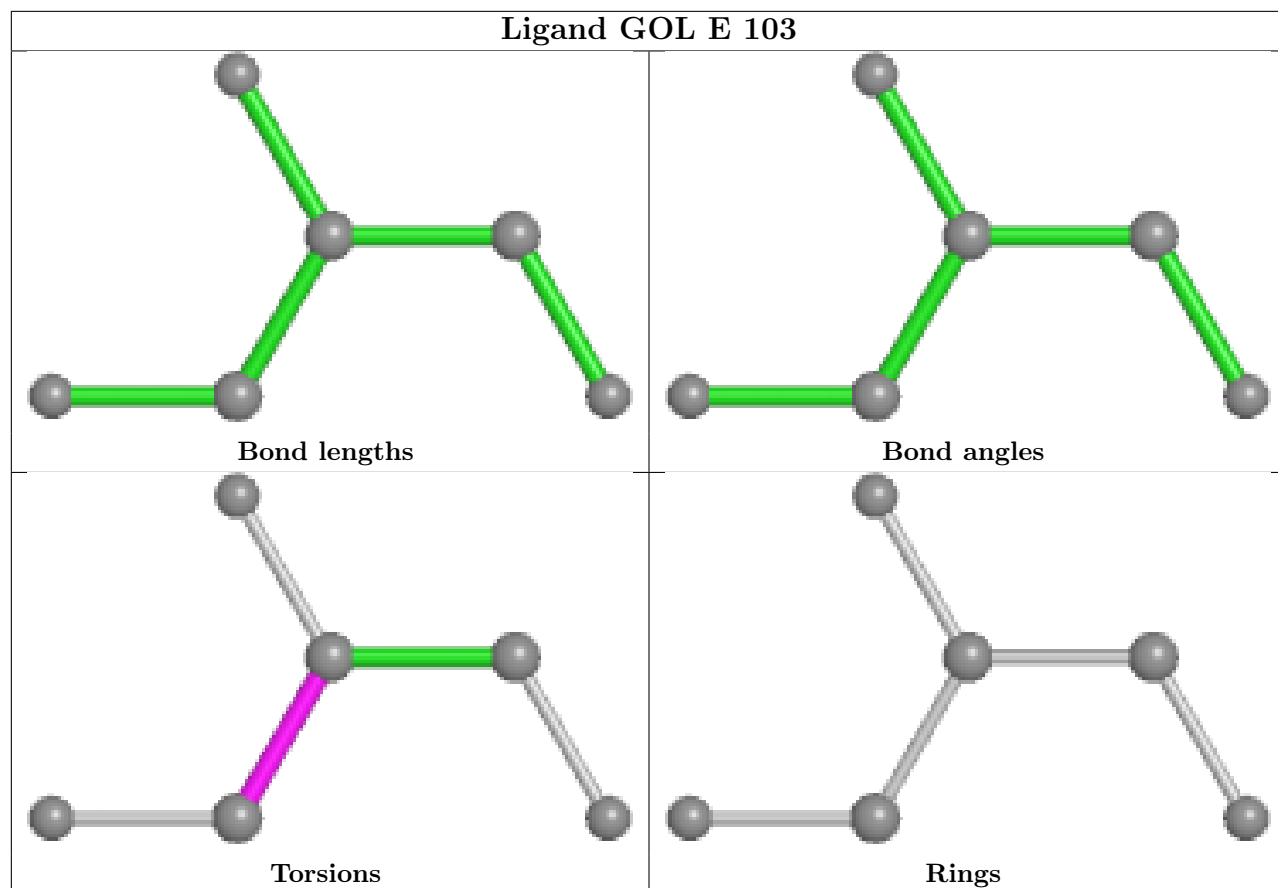












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	241/241 (100%)	0.48	18 (7%) 14 13	46, 74, 98, 128	0
1	C	241/241 (100%)	0.53	27 (11%) 5 5	48, 76, 94, 111	0
2	B	98/98 (100%)	0.98	19 (19%) 1 1	58, 86, 102, 107	0
2	D	98/98 (100%)	0.34	9 (9%) 9 9	53, 72, 96, 111	0
3	E	9/9 (100%)	-0.18	0 100 100	65, 80, 96, 97	0
4	F	9/9 (100%)	-0.15	0 100 100	54, 64, 70, 70	0
All	All	696/696 (100%)	0.53	73 (10%) 6 6	46, 76, 98, 128	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	45	THR	6.3
2	B	52	ASN	5.2
2	D	59	ALA	4.9
2	B	55	ILE	4.8
1	C	66	SER	4.8

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NA	A	360	1/1	0.58	0.34	48,48,48,48	0
9	PEG	B	134	7/7	0.61	0.32	46,61,76,88	0
5	GOL	C	305	6/6	0.63	0.42	60,80,82,90	0
6	NA	D	114	1/1	0.68	0.52	40,40,40,40	0
7	PG4	B	101	13/13	0.69	0.28	34,57,72,85	0
11	EDO	B	143	4/4	0.69	1.06	68,71,73,88	0
9	PEG	D	104	7/7	0.70	0.62	28,44,62,67	0
7	PG4	C	302	13/13	0.71	0.38	42,57,82,91	0
6	NA	D	135	1/1	0.72	0.25	50,50,50,50	0
6	NA	B	141	1/1	0.72	0.93	67,67,67,67	0
9	PEG	B	129	7/7	0.74	0.43	49,70,79,89	0
5	GOL	A	314	6/6	0.75	0.27	31,47,73,77	0
7	PG4	E	105	13/13	0.75	0.31	33,51,60,66	0
6	NA	D	136	1/1	0.76	0.28	69,69,69,69	0
5	GOL	C	307	6/6	0.76	0.34	67,72,78,86	0
5	GOL	D	110	6/6	0.76	0.36	48,64,67,74	0
5	GOL	B	152	6/6	0.76	0.31	65,76,91,96	0
6	NA	B	113	1/1	0.77	0.26	45,45,45,45	0
6	NA	B	115	1/1	0.77	1.02	55,55,55,55	0
7	PG4	A	326	13/13	0.77	0.45	42,55,77,85	0
9	PEG	B	135	7/7	0.77	0.28	38,42,62,67	0
6	NA	A	355	1/1	0.77	0.31	42,42,42,42	0
5	GOL	D	113	6/6	0.77	0.30	41,63,70,77	0
9	PEG	A	331	7/7	0.78	0.32	53,62,75,78	0
10	PE8	A	343	25/25	0.78	0.27	31,41,55,63	0
6	NA	A	356	1/1	0.78	0.40	49,49,49,49	0
7	PG4	D	120	13/13	0.79	0.26	49,58,75,75	0
9	PEG	D	105	7/7	0.79	0.51	55,68,82,83	0
6	NA	E	112	1/1	0.79	0.20	58,58,58,58	0
6	NA	B	114	1/1	0.79	0.48	66,66,66,66	0
6	NA	C	341	1/1	0.80	0.57	61,61,61,61	0
7	PG4	A	325	13/13	0.80	0.22	39,57,79,80	0
10	PE8	F	106	25/25	0.80	0.26	39,53,66,70	0
6	NA	B	146	1/1	0.80	0.36	45,45,45,45	0
9	PEG	A	337	7/7	0.81	0.32	62,71,78,88	0
5	GOL	E	104	6/6	0.81	0.28	74,76,79,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	PG4	A	324	13/13	0.81	0.22	43,55,70,80	0
5	GOL	F	103	6/6	0.81	0.43	37,42,55,62	0
9	PEG	C	328	7/7	0.81	0.28	39,43,55,60	0
9	PEG	B	128	7/7	0.82	0.28	51,60,69,69	0
7	PG4	D	118	13/13	0.82	0.20	32,51,72,73	0
7	PG4	A	321	13/13	0.82	0.24	47,57,71,81	0
7	PG4	B	118	13/13	0.82	0.24	53,57,67,73	0
7	PG4	F	105	13/13	0.82	0.23	38,54,62,63	0
9	PEG	C	331	7/7	0.82	0.23	53,70,81,89	0
9	PEG	A	329	7/7	0.82	0.41	42,58,66,72	0
7	PG4	A	368	13/13	0.82	0.31	37,45,64,68	0
10	PE8	A	342	25/25	0.82	0.20	40,65,79,86	0
9	PEG	A	333	7/7	0.82	0.23	43,50,70,80	0
7	PG4	D	103	13/13	0.82	0.24	53,66,75,78	0
9	PEG	A	341	7/7	0.82	0.36	42,51,64,67	0
11	EDO	D	101	4/4	0.82	0.32	56,57,57,59	0
7	PG4	C	325	13/13	0.83	0.39	46,56,70,75	0
5	GOL	E	103	6/6	0.83	0.23	64,69,72,90	0
5	GOL	B	105	6/6	0.83	0.23	34,44,54,69	0
5	GOL	C	344	6/6	0.83	0.20	27,53,58,61	0
7	PG4	C	320	13/13	0.83	0.27	35,52,63,72	0
7	PG4	C	324	13/13	0.83	0.29	57,68,77,81	0
9	PEG	C	333	7/7	0.84	0.44	50,53,54,71	0
6	NA	A	315	1/1	0.84	0.32	38,38,38,38	0
6	NA	B	151	1/1	0.84	0.21	34,34,34,34	0
9	PEG	D	127	7/7	0.84	0.22	46,60,68,71	0
7	PG4	C	336	13/13	0.84	0.29	36,58,72,73	0
7	PG4	A	365	13/13	0.84	0.20	34,39,52,57	0
10	PE8	B	102	25/25	0.84	0.19	31,48,62,80	0
5	GOL	B	140	6/6	0.84	0.26	61,68,73,80	0
11	EDO	A	351	4/4	0.84	0.54	51,58,60,70	0
9	PEG	A	335	7/7	0.84	0.23	34,48,58,62	0
7	PG4	C	322	13/13	0.84	0.23	51,57,66,73	0
5	GOL	A	345	6/6	0.85	0.39	41,53,53,56	0
7	PG4	A	323	13/13	0.85	0.26	67,76,84,87	0
5	GOL	C	306	6/6	0.85	0.27	48,60,77,81	0
5	GOL	B	107	6/6	0.85	0.20	48,51,54,59	0
6	NA	D	132	1/1	0.85	0.15	24,24,24,24	0
7	PG4	A	352	13/13	0.85	0.28	49,59,68,68	0
6	NA	A	348	1/1	0.85	0.38	51,51,51,51	0
7	PG4	A	366	13/13	0.85	0.20	35,47,70,80	0
9	PEG	A	371	7/7	0.85	0.36	40,44,55,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	PE8	E	110	25/25	0.85	0.19	40,51,63,64	0
10	PE8	F	102	25/25	0.85	0.20	40,52,65,82	0
7	PG4	D	116	13/13	0.85	0.26	19,41,61,79	0
7	PG4	D	117	13/13	0.85	0.21	30,52,68,73	0
5	GOL	D	131	6/6	0.85	0.27	58,64,84,96	0
5	GOL	C	312	6/6	0.85	0.24	40,68,71,72	0
11	EDO	D	102	4/4	0.85	0.25	62,66,73,90	0
11	EDO	D	130	4/4	0.85	0.24	44,57,58,61	0
7	PG4	E	106	13/13	0.86	0.18	26,50,62,68	0
7	PG4	F	101	13/13	0.86	0.18	43,56,74,75	0
7	PG4	B	120	13/13	0.86	0.27	36,48,53,59	0
10	PE8	A	344	25/25	0.86	0.25	31,56,73,77	0
5	GOL	D	107	6/6	0.86	0.26	57,61,61,62	0
7	PG4	C	319	13/13	0.86	0.23	31,50,66,67	0
5	GOL	B	109	6/6	0.86	0.24	48,50,58,62	0
9	PEG	C	329	7/7	0.86	0.23	50,53,59,63	0
9	PEG	C	330	7/7	0.86	0.26	37,45,51,61	0
6	NA	A	317	1/1	0.86	0.43	55,55,55,55	0
5	GOL	A	303	6/6	0.86	0.30	55,62,66,68	0
9	PEG	A	338	7/7	0.86	0.40	52,55,77,79	0
7	PG4	A	322	13/13	0.86	0.26	38,53,58,62	0
5	GOL	C	313	6/6	0.87	0.22	38,45,56,59	0
9	PEG	B	130	7/7	0.87	0.22	41,44,60,69	0
9	PEG	C	332	7/7	0.87	0.30	38,43,57,58	0
9	PEG	A	339	7/7	0.87	0.53	45,54,63,67	0
9	PEG	C	334	7/7	0.87	0.27	41,56,68,69	0
5	GOL	A	306	6/6	0.87	0.22	48,52,59,80	0
7	PG4	E	114	13/13	0.87	0.20	35,54,72,83	0
9	PEG	D	121	7/7	0.87	0.28	31,44,65,66	0
9	PEG	D	122	7/7	0.87	0.23	31,41,60,62	0
9	PEG	D	123	7/7	0.87	0.24	51,55,61,66	0
9	PEG	A	330	7/7	0.87	0.30	36,54,61,73	0
9	PEG	D	128	7/7	0.87	0.29	37,41,59,63	0
5	GOL	A	305	6/6	0.88	0.18	22,25,29,37	0
9	PEG	B	132	7/7	0.88	0.26	45,56,70,76	0
7	PG4	C	321	13/13	0.88	0.18	34,41,56,59	0
5	GOL	B	108	6/6	0.88	0.19	50,57,73,73	0
6	NA	D	134	1/1	0.88	0.21	37,37,37,37	0
5	GOL	C	314	6/6	0.88	0.21	37,58,65,69	0
5	GOL	C	309	6/6	0.88	0.28	29,43,50,74	0
10	PE8	B	136	25/25	0.88	0.24	34,62,80,86	0
5	GOL	C	310	6/6	0.88	0.27	47,62,77,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PG4	A	369	13/13	0.88	0.25	39,50,69,70	0
7	PG4	A	320	13/13	0.88	0.18	22,45,63,64	0
7	PG4	B	116	13/13	0.88	0.22	27,45,56,64	0
5	GOL	E	113	6/6	0.88	0.20	46,52,57,64	0
6	NA	A	358	1/1	0.88	0.23	47,47,47,47	0
6	NA	C	318	1/1	0.88	0.21	40,40,40,40	0
6	NA	A	359	1/1	0.88	0.25	58,58,58,58	0
5	GOL	A	347	6/6	0.89	0.24	60,71,75,79	0
9	PEG	D	126	7/7	0.89	0.35	47,57,74,79	0
5	GOL	C	304	6/6	0.89	0.27	44,54,59,71	0
5	GOL	C	311	6/6	0.89	0.26	54,73,88,92	0
5	GOL	B	103	6/6	0.89	0.42	55,59,70,86	0
6	NA	C	316	1/1	0.89	0.49	60,60,60,60	0
7	PG4	C	323	13/13	0.89	0.16	38,48,66,69	0
7	PG4	A	319	13/13	0.89	0.15	44,54,68,69	0
6	NA	C	317	1/1	0.89	0.19	36,36,36,36	0
10	PE8	C	335	25/25	0.89	0.15	36,49,61,76	0
6	NA	A	316	1/1	0.89	0.31	29,29,29,29	0
5	GOL	B	104	6/6	0.89	0.34	40,42,57,60	0
5	GOL	A	302	6/6	0.89	0.22	40,44,59,66	0
6	NA	D	129	1/1	0.89	0.27	82,82,82,82	0
7	PG4	B	121	13/13	0.89	0.17	46,55,78,83	0
9	PEG	A	353	7/7	0.89	0.19	39,52,64,65	0
7	PG4	B	123	13/13	0.89	0.15	29,41,58,62	0
7	PG4	B	125	13/13	0.89	0.19	49,57,66,79	0
7	PG4	B	117	13/13	0.90	0.15	39,51,59,61	0
7	PG4	A	367	13/13	0.90	0.16	27,42,62,62	0
9	PEG	A	332	7/7	0.90	0.21	54,56,65,69	0
7	PG4	B	119	13/13	0.90	0.19	36,54,64,64	0
9	PEG	A	334	7/7	0.90	0.19	36,45,65,78	0
9	PEG	C	303	7/7	0.90	0.19	32,44,66,69	0
9	PEG	C	327	7/7	0.90	0.21	45,52,64,80	0
6	NA	B	148	1/1	0.90	0.12	39,39,39,39	0
6	NA	C	342	1/1	0.90	0.34	24,24,24,24	0
7	PG4	B	122	13/13	0.90	0.14	41,53,65,74	0
7	PG4	E	107	13/13	0.90	0.24	50,58,68,69	0
6	NA	B	150	1/1	0.90	0.23	40,40,40,40	0
7	PG4	B	124	13/13	0.90	0.21	23,52,61,62	0
5	GOL	D	109	6/6	0.90	0.16	36,53,66,77	0
9	PEG	C	339	7/7	0.90	0.19	38,44,54,55	0
9	PEG	C	346	7/7	0.90	0.14	36,42,53,62	0
11	EDO	B	144	4/4	0.90	0.40	57,72,74,74	0

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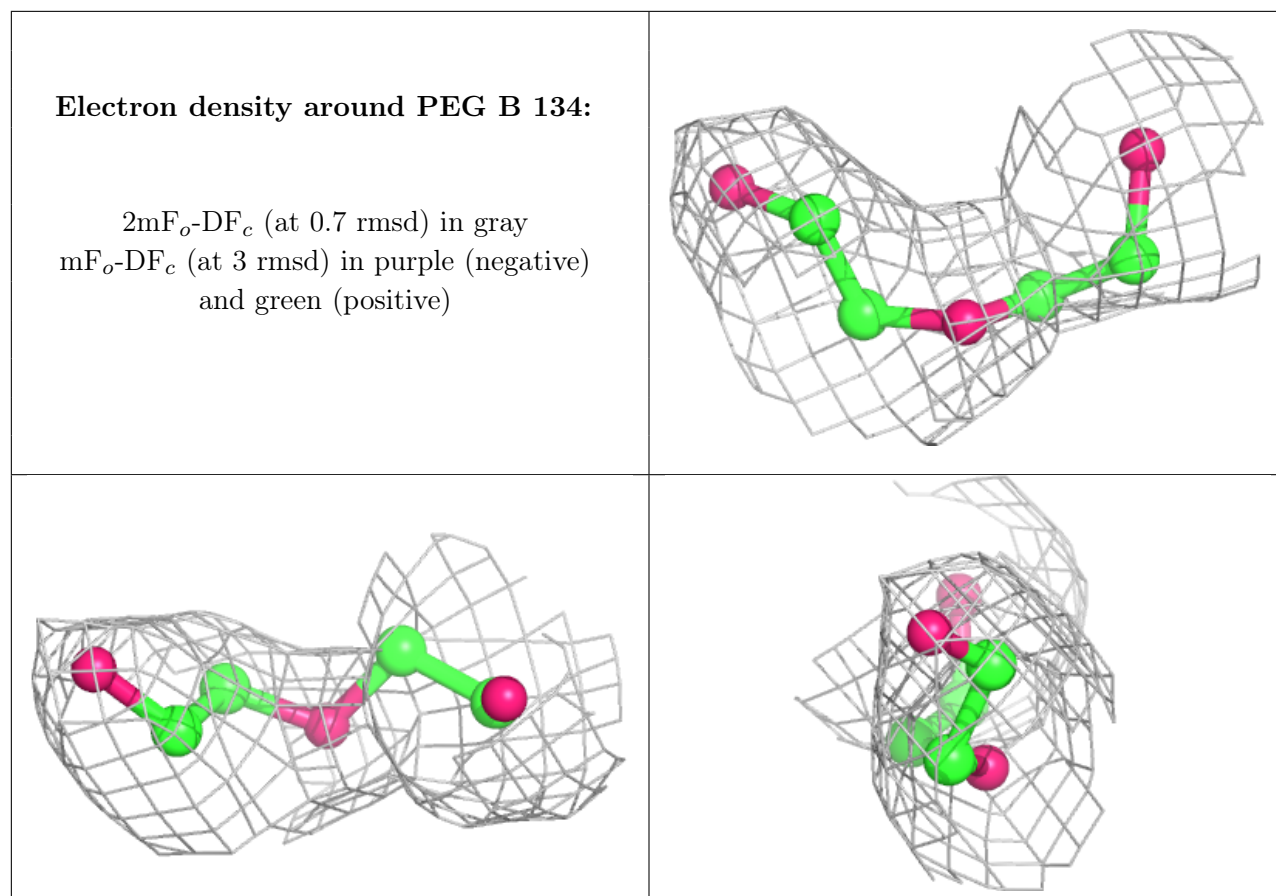
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	PEG	A	372	7/7	0.90	0.17	44,45,48,51	0
9	PEG	B	126	7/7	0.90	0.25	48,56,70,75	0
7	PG4	B	155	13/13	0.90	0.19	35,41,52,55	0
11	EDO	E	101	4/4	0.90	0.18	31,49,56,73	0
6	NA	C	315	1/1	0.91	0.38	33,33,33,33	0
5	GOL	D	112	6/6	0.91	0.16	25,44,46,47	0
9	PEG	A	336	7/7	0.91	0.18	44,50,69,70	0
10	PE8	B	137	25/25	0.91	0.17	20,49,64,72	0
5	GOL	A	309	6/6	0.91	0.17	22,32,34,47	0
5	GOL	B	111	6/6	0.91	0.15	57,72,83,87	0
9	PEG	B	139	7/7	0.91	0.17	34,38,45,46	0
9	PEG	B	142	7/7	0.91	0.24	33,37,41,49	0
5	GOL	A	310	6/6	0.91	0.24	38,49,51,68	0
5	GOL	A	313	6/6	0.91	0.27	31,40,43,47	0
6	NA	C	343	1/1	0.91	0.18	34,34,34,34	0
5	GOL	D	108	6/6	0.91	0.20	49,57,62,62	0
6	NA	D	115	1/1	0.91	0.16	31,31,31,31	0
5	GOL	A	362	6/6	0.91	0.31	23,36,45,55	0
5	GOL	A	373	6/6	0.91	0.20	47,54,60,71	0
5	GOL	B	112	6/6	0.92	0.20	38,51,58,61	0
9	PEG	B	127	7/7	0.92	0.34	23,29,56,59	0
9	PEG	B	156	7/7	0.92	0.14	25,42,51,56	0
9	PEG	B	157	7/7	0.92	0.16	42,49,65,73	0
5	GOL	A	308	6/6	0.92	0.15	29,32,36,52	0
6	NA	A	318	1/1	0.92	0.14	39,39,39,39	0
5	GOL	D	106	6/6	0.92	0.17	19,39,51,54	0
5	GOL	B	110	6/6	0.92	0.25	51,55,62,69	0
7	PG4	D	119	13/13	0.92	0.15	37,50,65,74	0
5	GOL	B	106	6/6	0.92	0.18	34,45,62,70	0
11	EDO	E	111	4/4	0.92	0.20	51,54,62,68	0
5	GOL	A	312	6/6	0.93	0.17	38,49,55,56	0
5	GOL	C	337	6/6	0.93	0.20	39,43,61,67	0
6	NA	A	349	1/1	0.93	0.20	32,32,32,32	0
10	PE8	B	138	25/25	0.93	0.17	32,49,67,70	0
5	GOL	A	307	6/6	0.93	0.34	56,64,75,84	0
10	PE8	E	109	25/25	0.93	0.12	27,46,67,71	0
6	NA	B	145	1/1	0.93	0.20	54,54,54,54	0
9	PEG	B	158	7/7	0.93	0.13	10,26,37,38	0
5	GOL	C	347	6/6	0.93	0.31	33,49,62,75	0
5	GOL	C	308	6/6	0.93	0.14	29,35,48,52	0
9	PEG	D	124	7/7	0.93	0.16	24,38,50,54	0
5	GOL	A	304	6/6	0.93	0.17	38,44,50,55	0

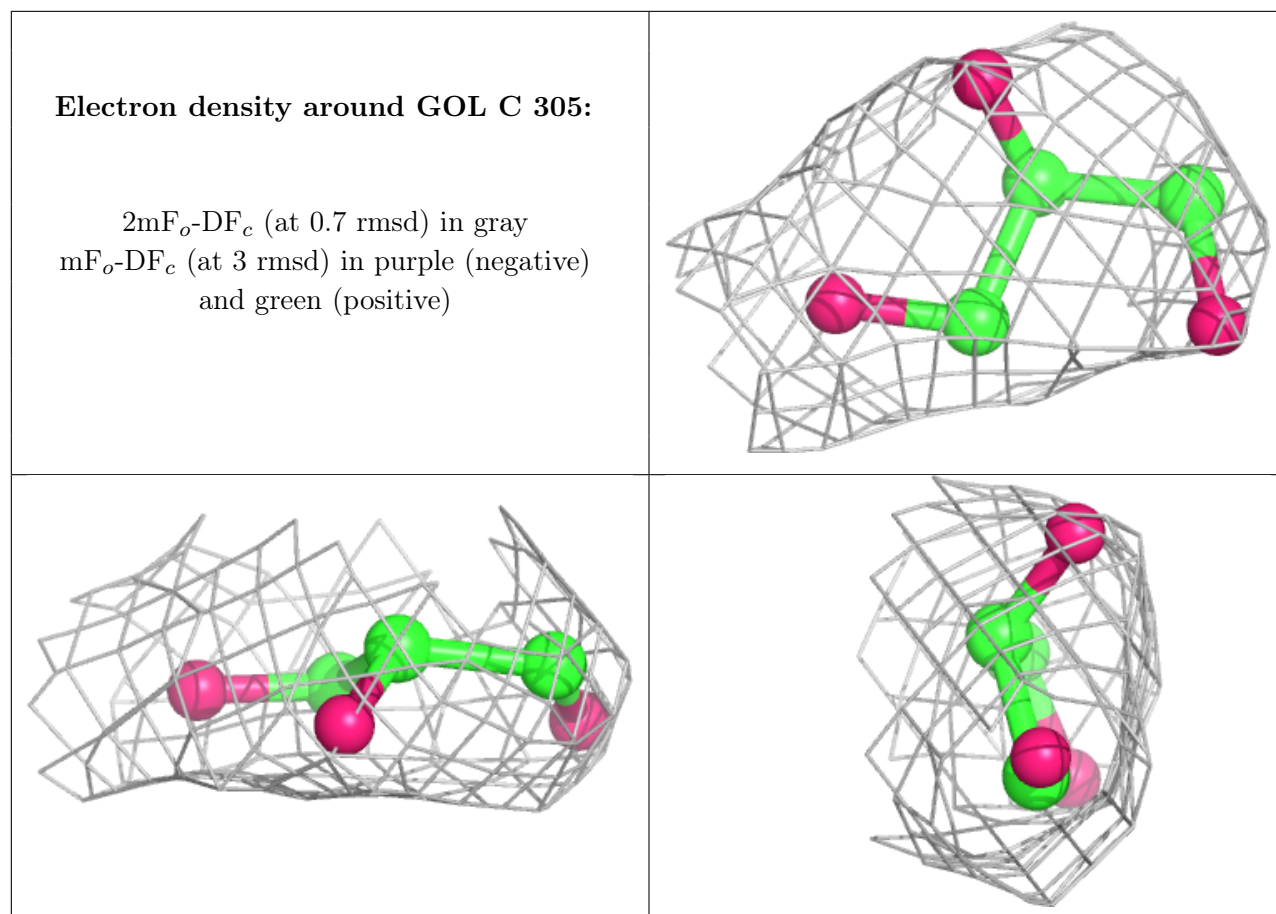
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	SO4	A	327	5/5	0.93	0.18	56,57,68,74	0
9	PEG	B	131	7/7	0.93	0.14	42,52,72,73	0
5	GOL	D	137	6/6	0.93	0.16	24,32,38,57	0
9	PEG	B	133	7/7	0.93	0.22	51,70,78,85	0
9	PEG	A	340	7/7	0.93	0.13	43,47,61,68	0
6	NA	A	350	1/1	0.94	0.16	30,30,30,30	0
6	NA	A	354	1/1	0.94	0.30	22,22,22,22	0
5	GOL	A	364	6/6	0.94	0.17	36,43,49,55	0
5	GOL	A	301	6/6	0.94	0.17	46,57,59,60	0
5	GOL	C	338	6/6	0.94	0.14	24,60,69,74	0
7	PG4	E	115	13/13	0.94	0.11	59,67,73,82	0
9	PEG	D	125	7/7	0.94	0.29	29,34,63,65	0
5	GOL	A	311	6/6	0.94	0.14	27,30,31,36	0
6	NA	C	340	1/1	0.94	0.17	34,34,34,34	0
5	GOL	C	345	6/6	0.94	0.22	37,44,54,61	0
8	SO4	C	326	5/5	0.94	0.13	60,62,71,98	0
6	NA	B	149	1/1	0.94	0.27	33,33,33,33	0
9	PEG	A	346	7/7	0.94	0.16	35,41,69,80	0
6	NA	F	107	1/1	0.94	0.28	35,35,35,35	0
9	PEG	A	370	7/7	0.94	0.33	28,33,54,57	0
8	SO4	A	328	5/5	0.95	0.16	43,55,61,65	0
8	SO4	C	301	5/5	0.95	0.18	71,72,72,92	0
5	GOL	B	154	6/6	0.95	0.39	23,26,27,31	0
5	GOL	B	153	6/6	0.95	0.11	44,45,46,53	0
5	GOL	D	111	6/6	0.95	0.17	42,47,54,60	0
6	NA	B	147	1/1	0.95	0.14	34,34,34,34	0
6	NA	F	104	1/1	0.95	0.37	36,36,36,36	0
5	GOL	A	363	6/6	0.96	0.12	34,45,54,54	0
8	SO4	E	108	5/5	0.96	0.17	41,52,66,72	0
6	NA	D	133	1/1	0.97	0.07	22,22,22,22	0
5	GOL	E	102	6/6	0.97	0.13	32,44,53,64	0
6	NA	A	357	1/1	0.98	0.11	21,21,21,21	0

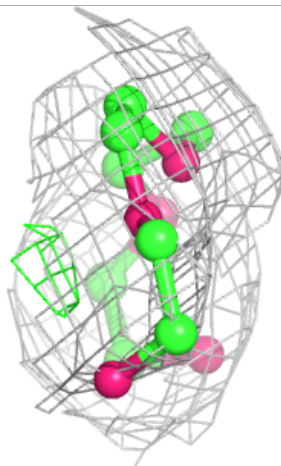
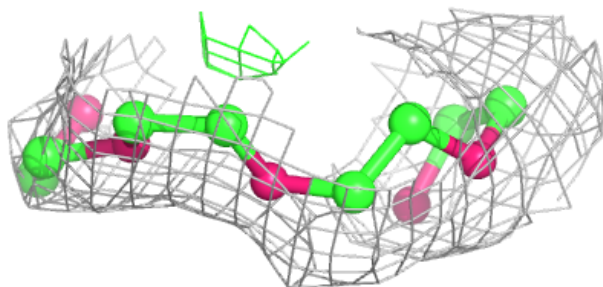
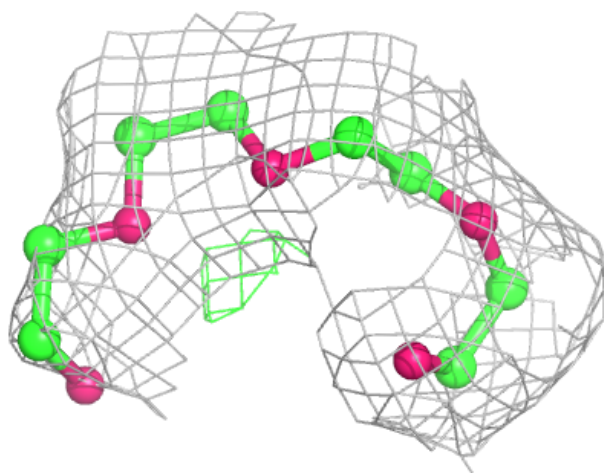
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

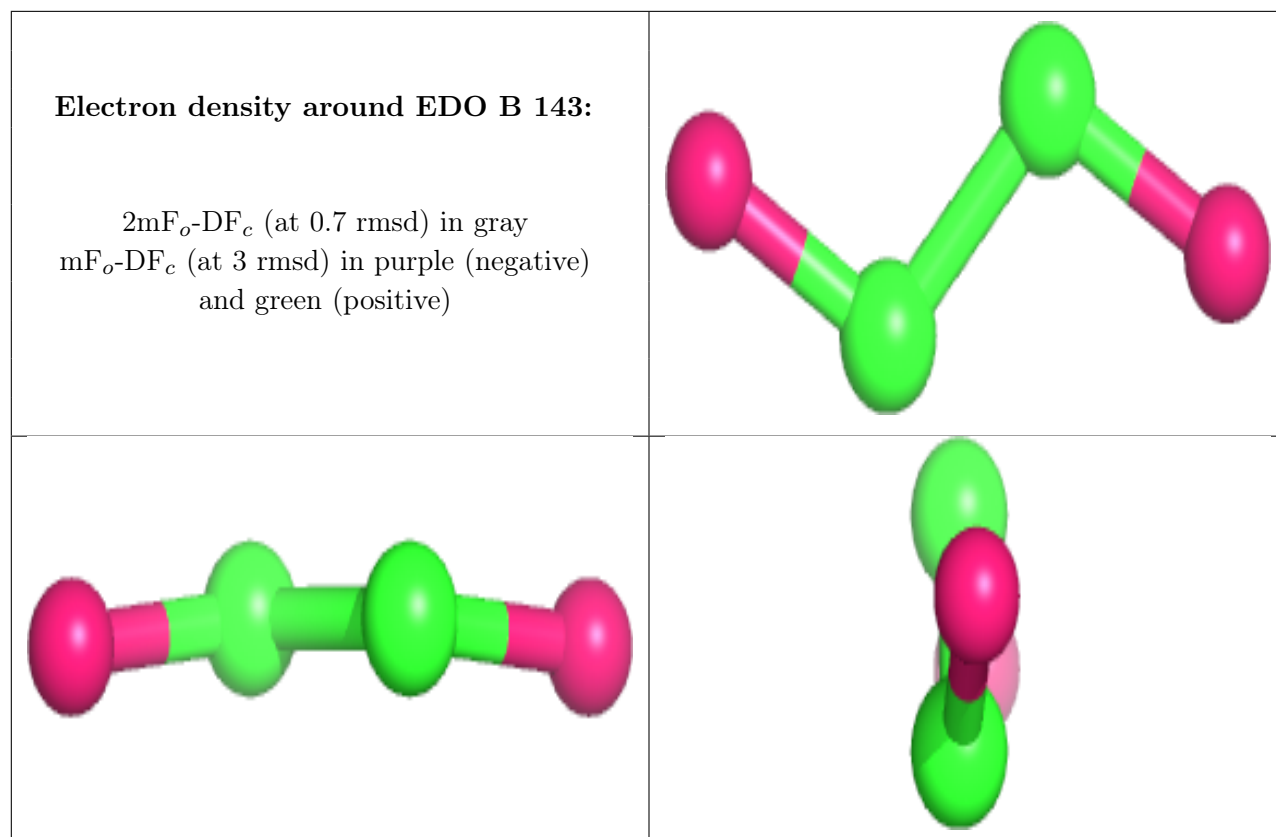


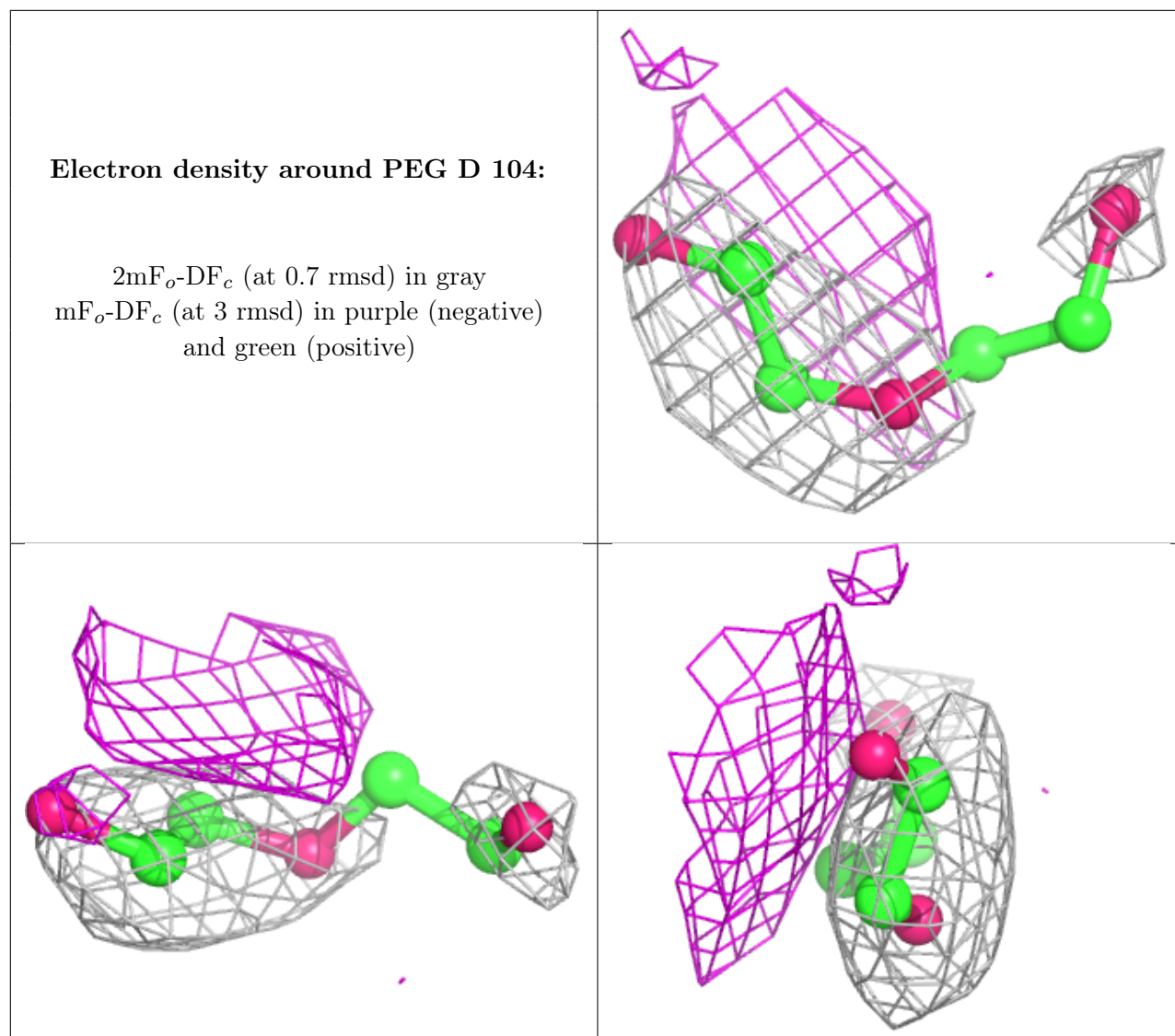


Electron density around PG4 B 101:

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

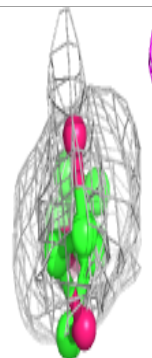
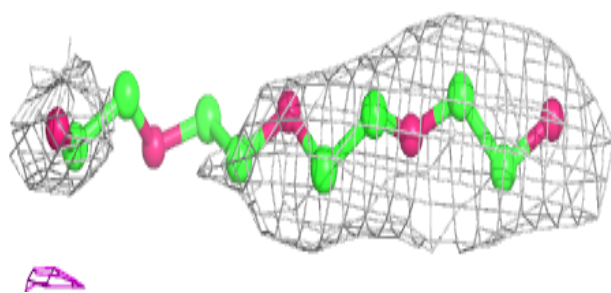
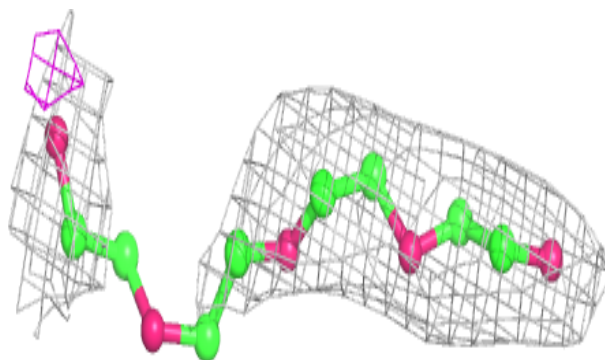




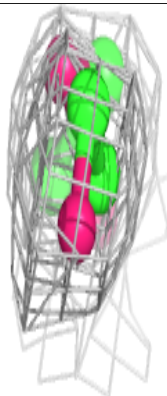
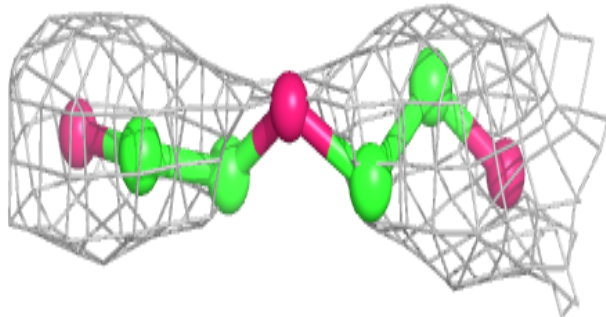
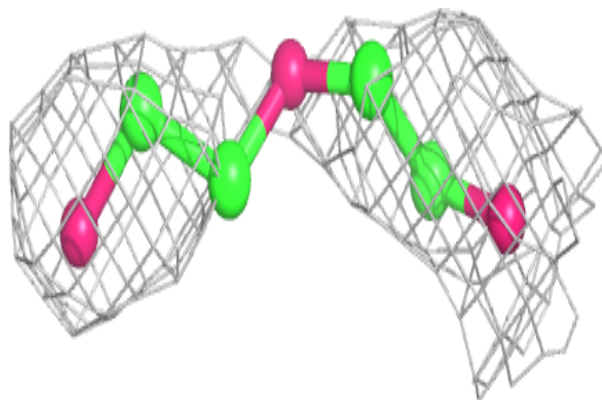


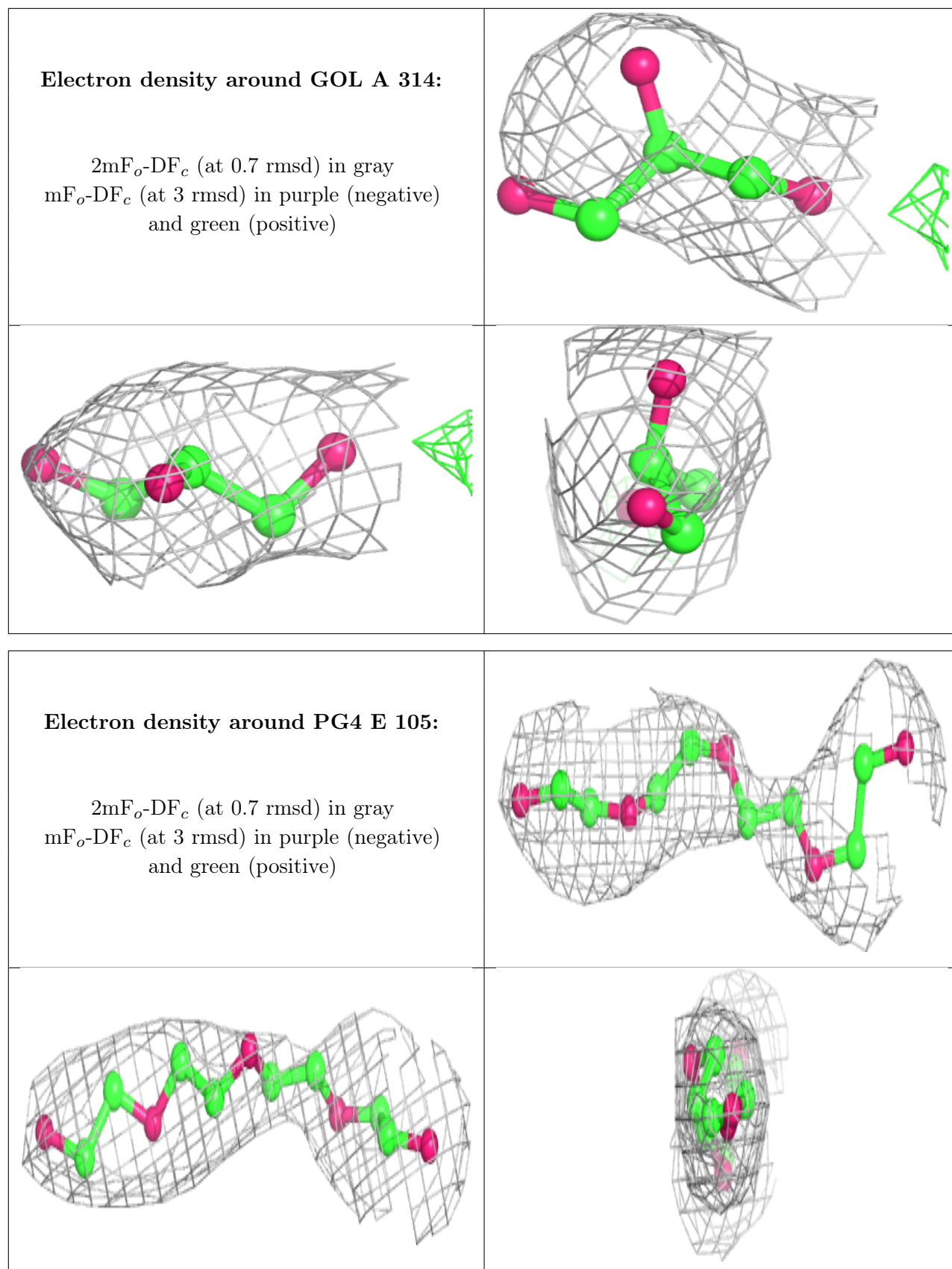
Electron density around PG4 C 302:

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

**Electron density around PEG B 129:**

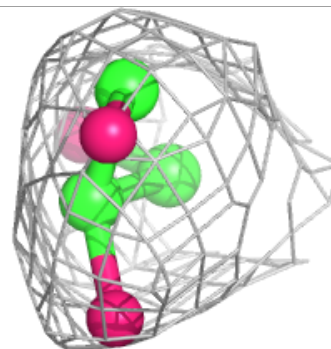
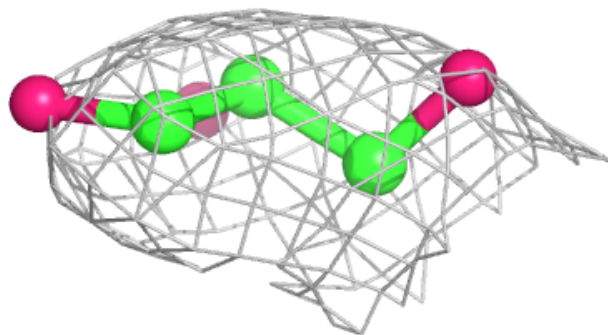
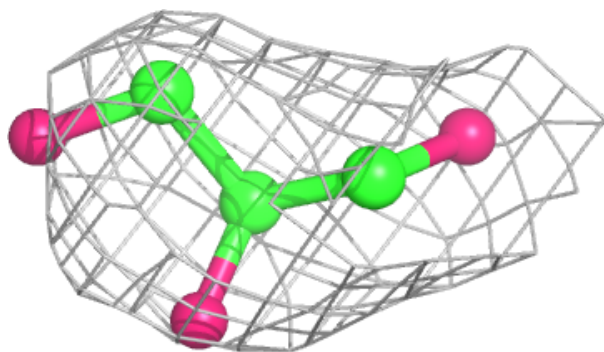
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



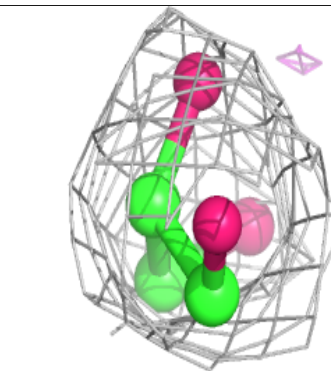
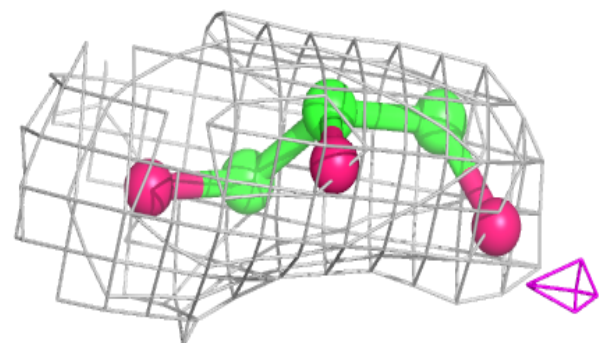
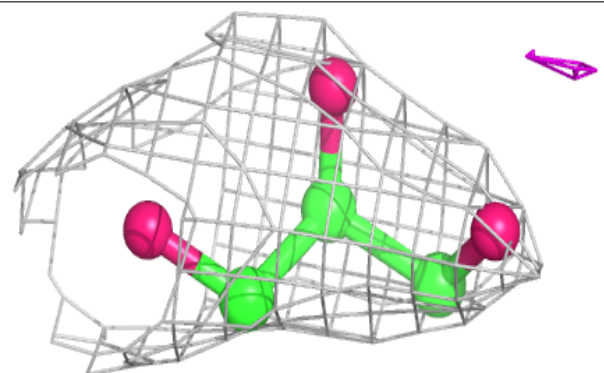


Electron density around GOL C 307:

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

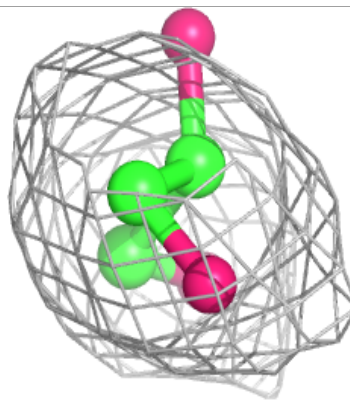
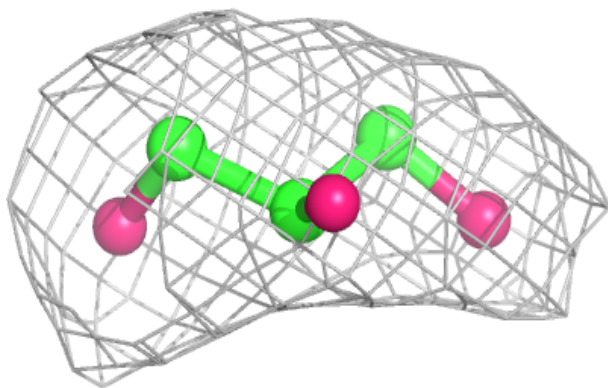
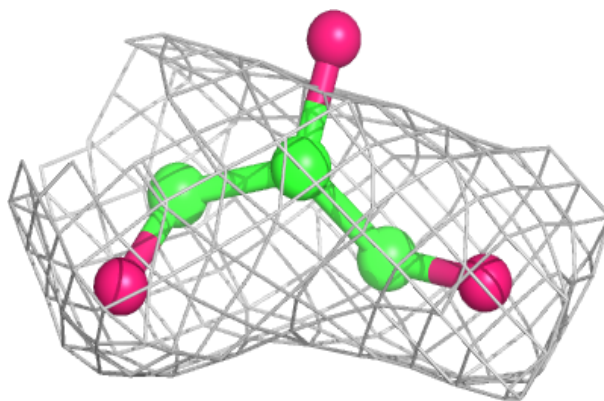
**Electron density around GOL D 110:**

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

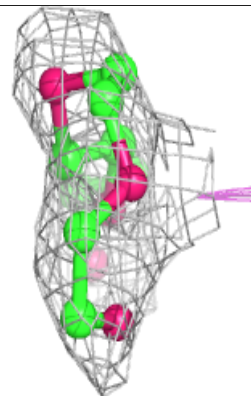
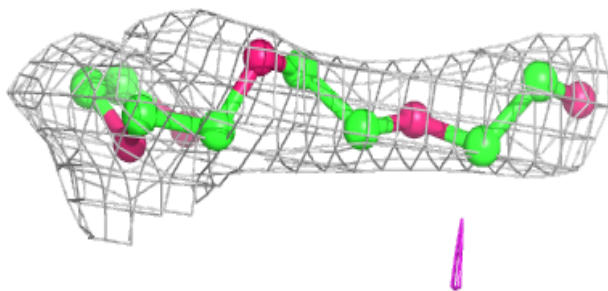
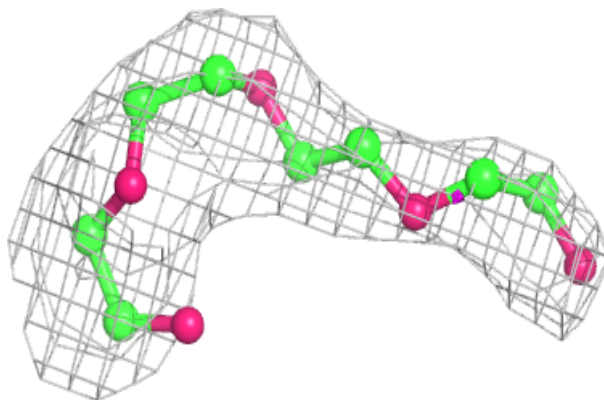


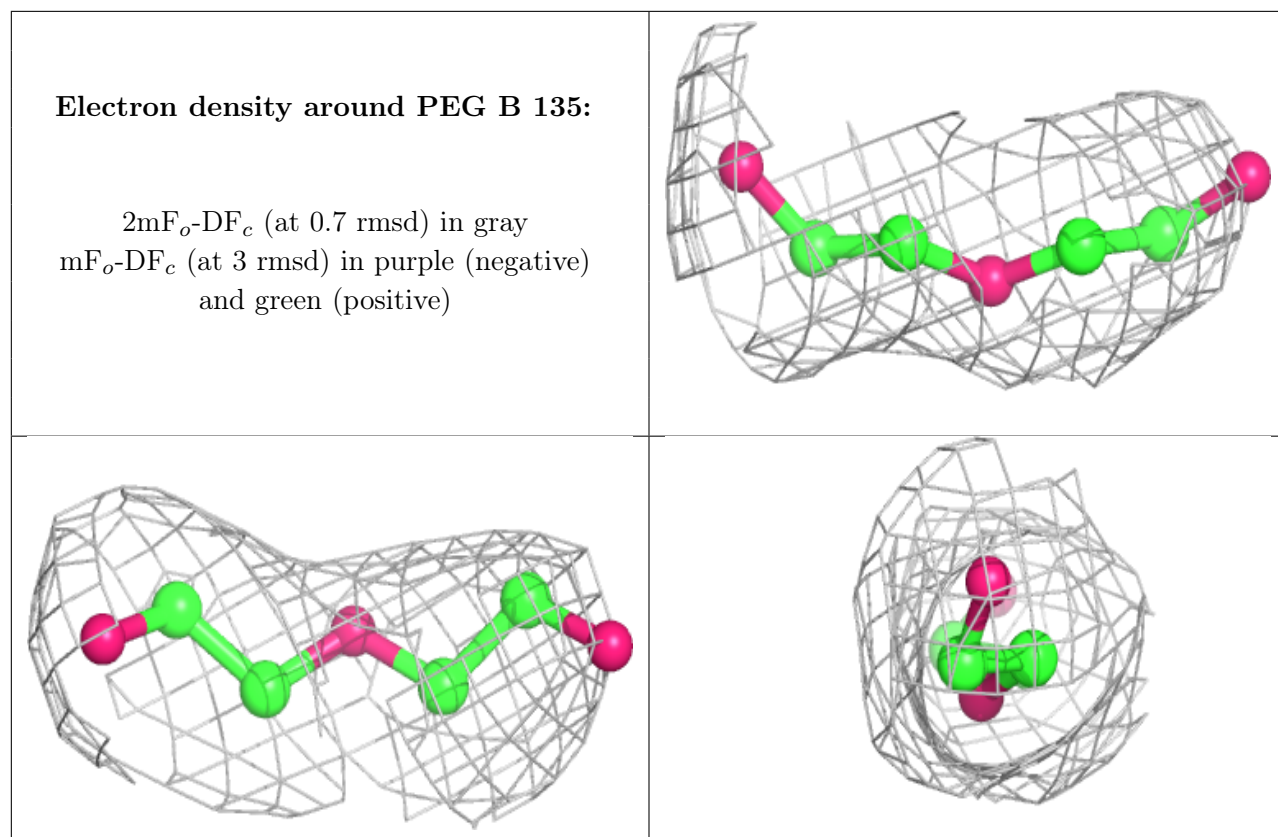
Electron density around GOL B 152:

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

**Electron density around PG4 A 326:**

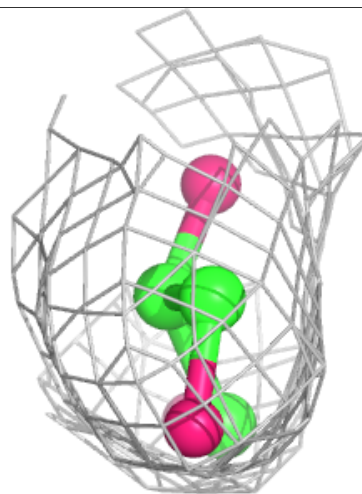
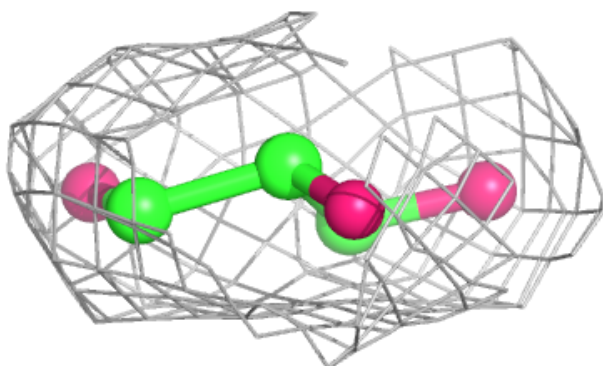
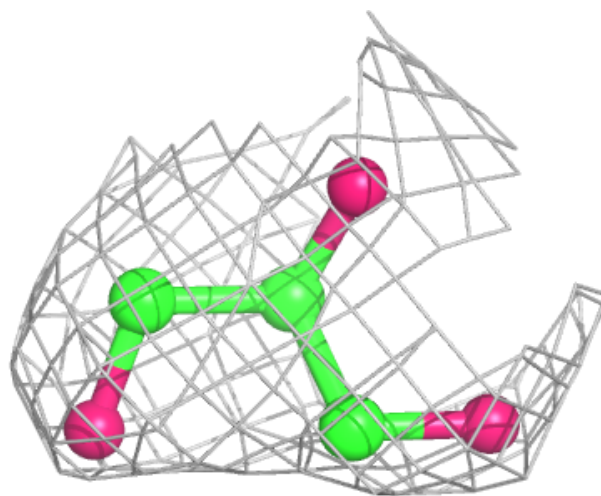
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

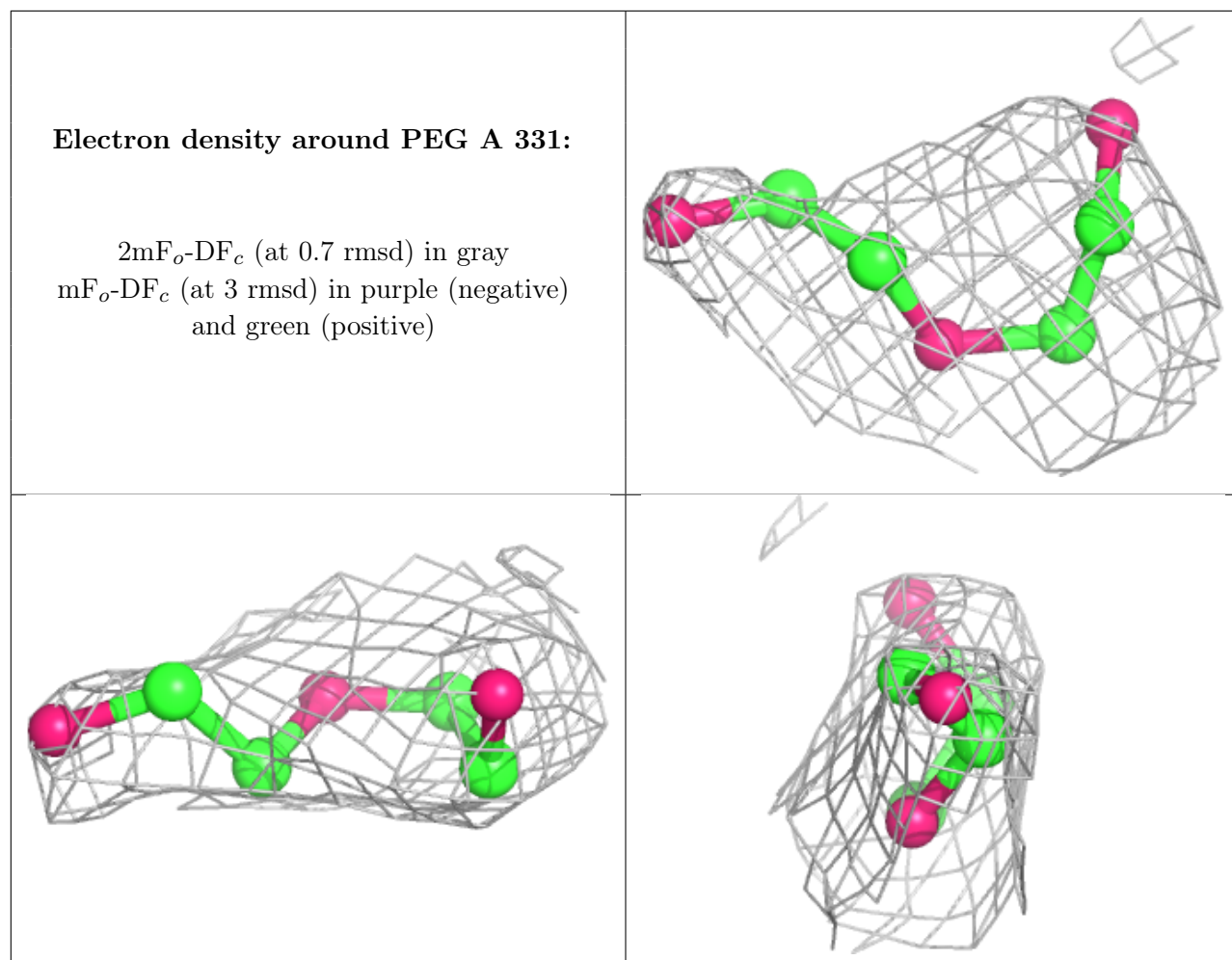




Electron density around GOL D 113:

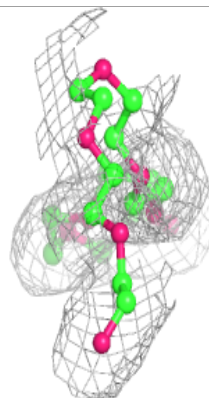
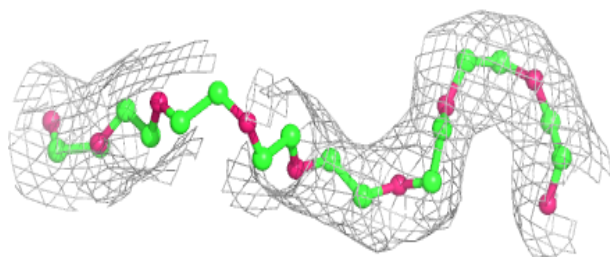
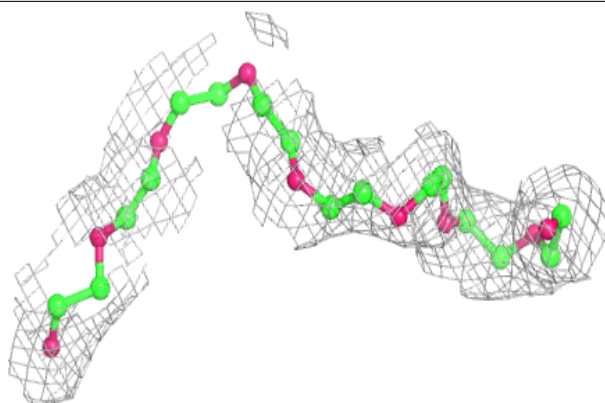
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



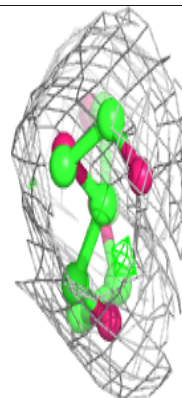
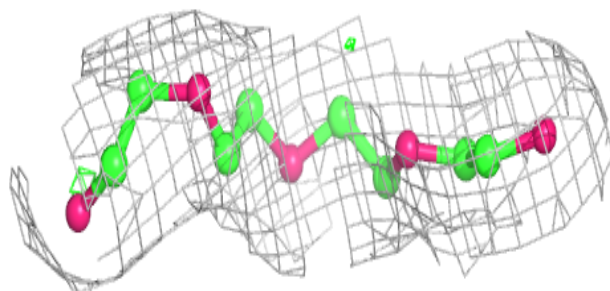
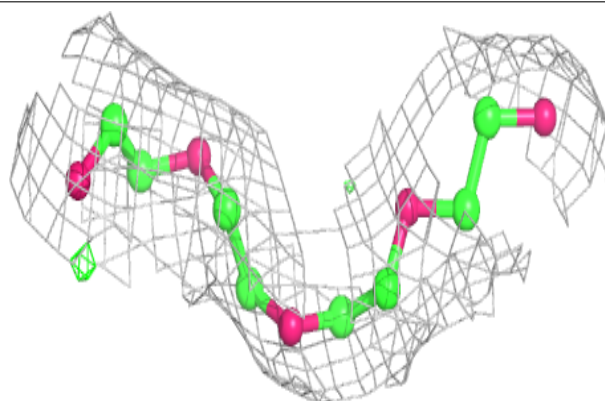


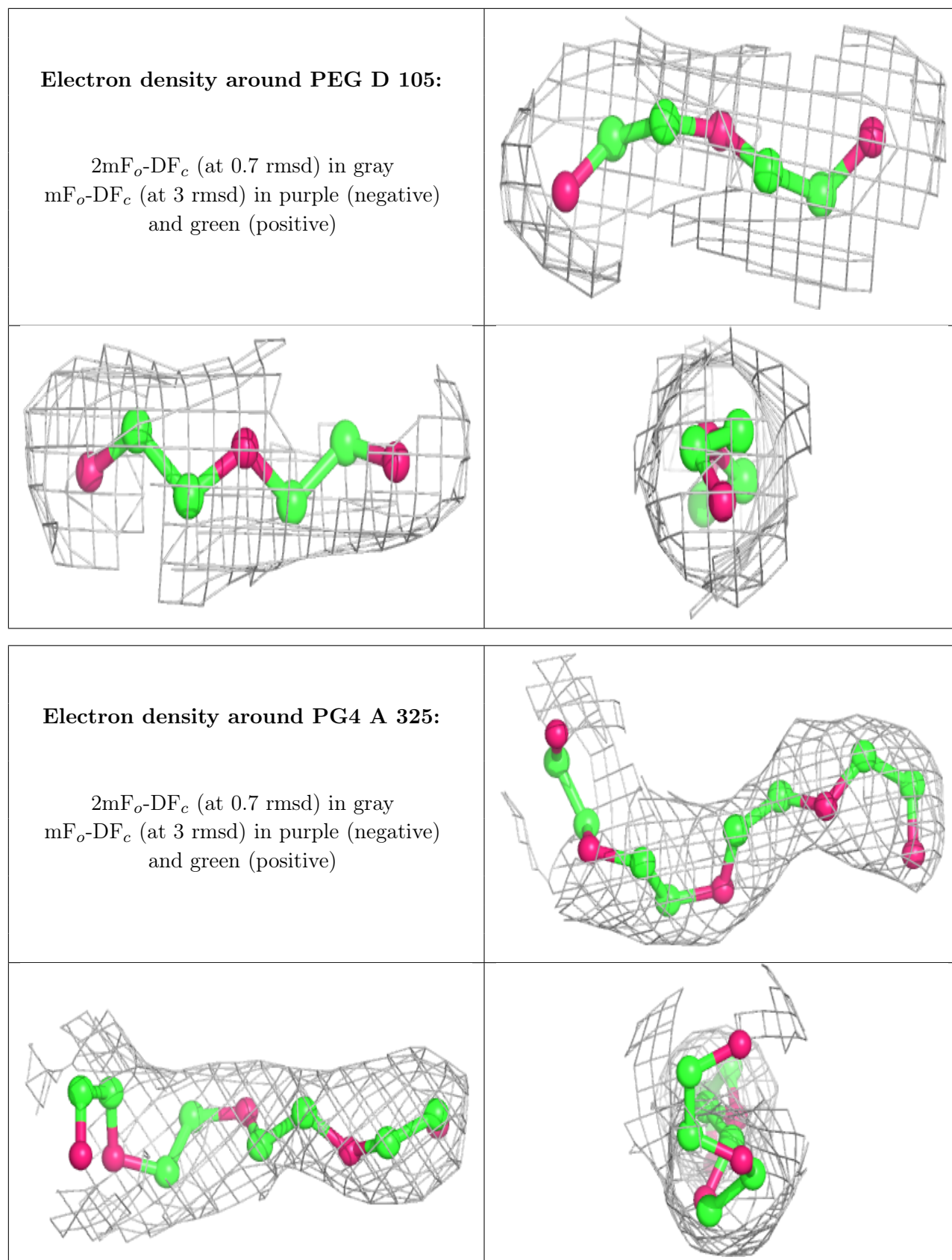
Electron density around PE8 A 343:

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

**Electron density around PG4 D 120:**

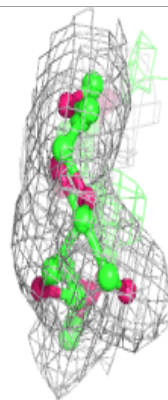
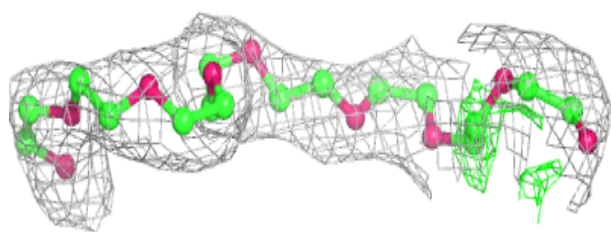
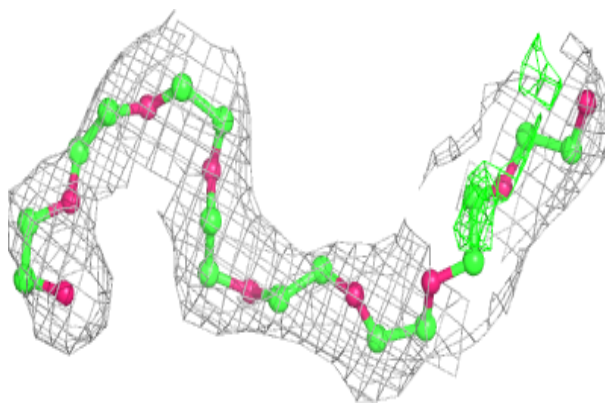
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



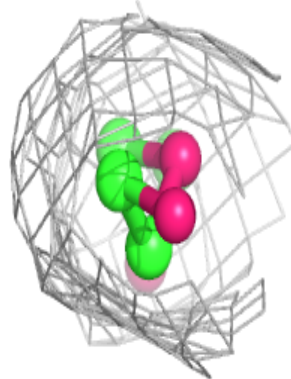
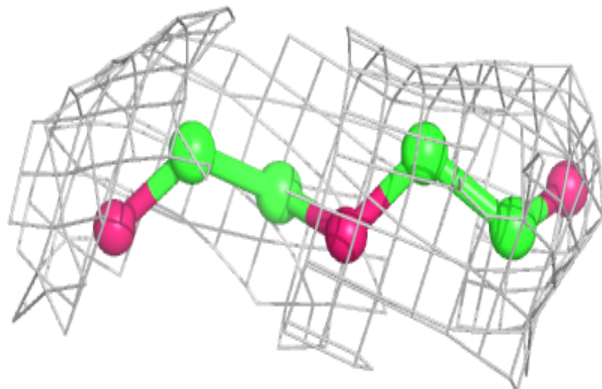
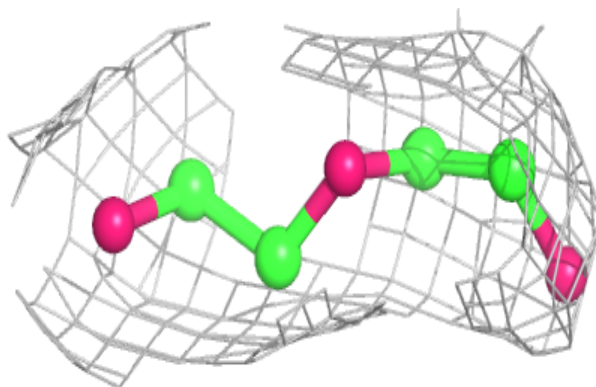


Electron density around PE8 F 106:

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

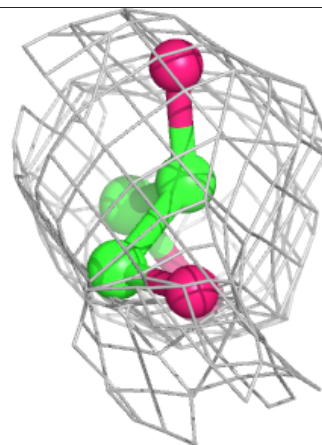
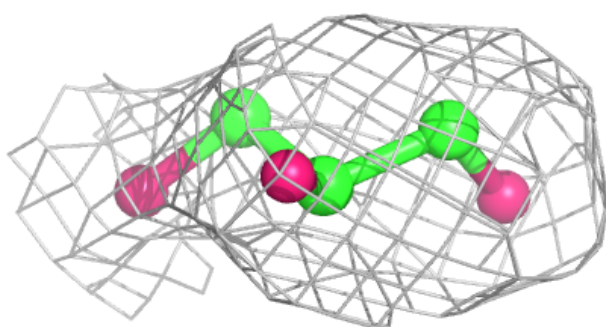
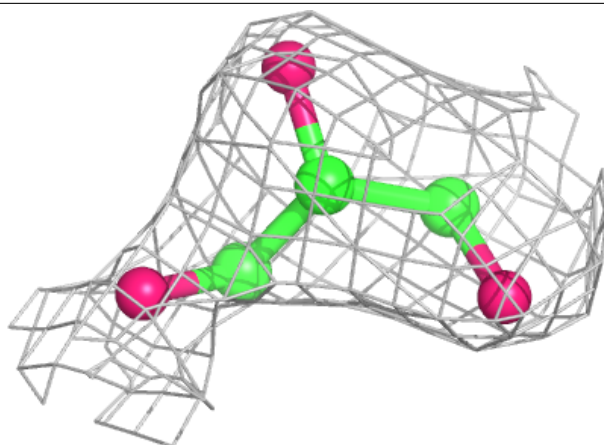
**Electron density around PEG A 337:**

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

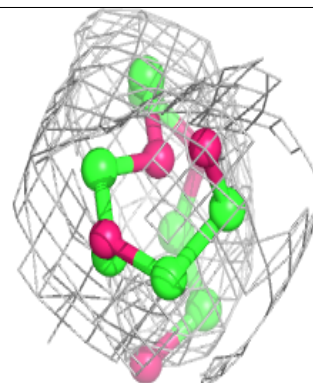
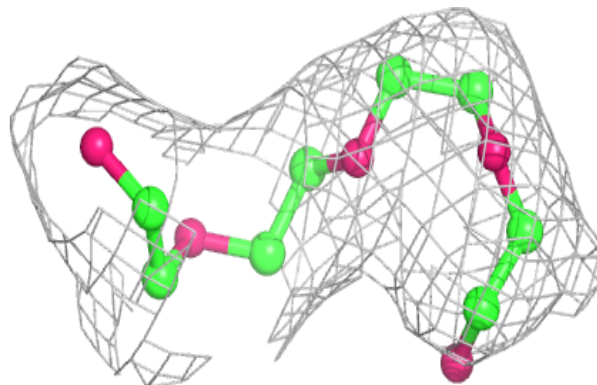


Electron density around GOL E 104:

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

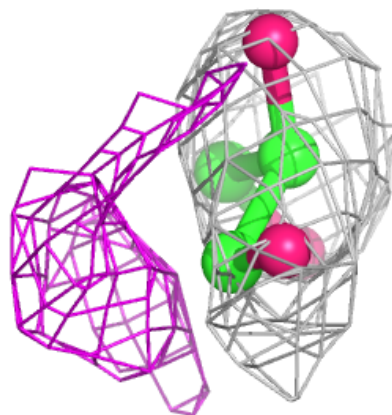
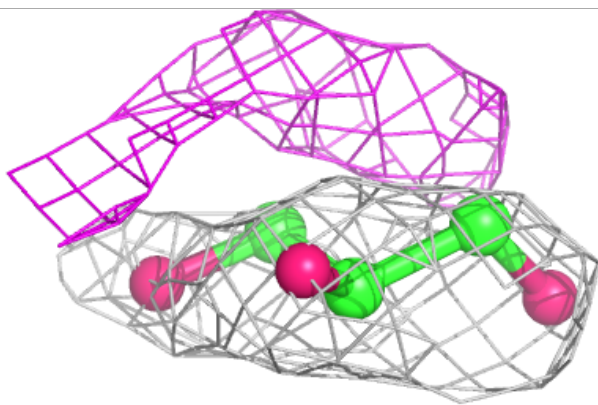
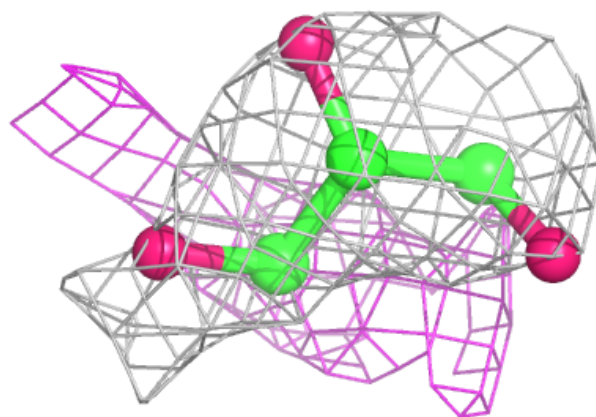
**Electron density around PG4 A 324:**

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



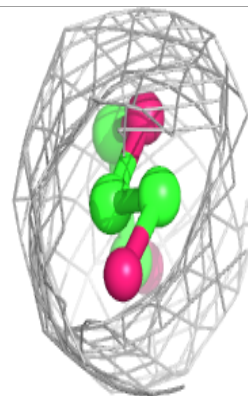
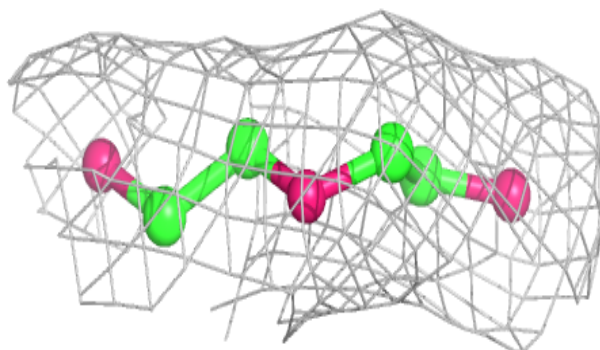
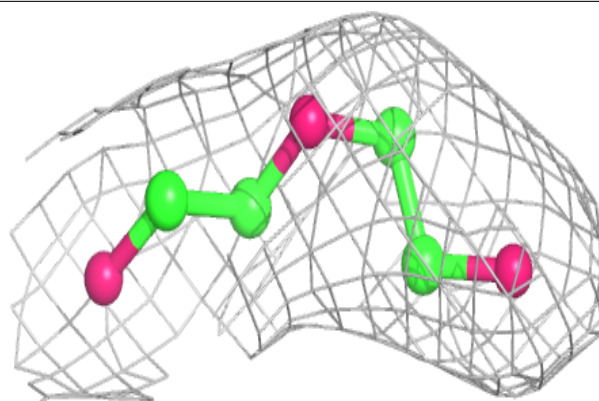
Electron density around GOL F 103:

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

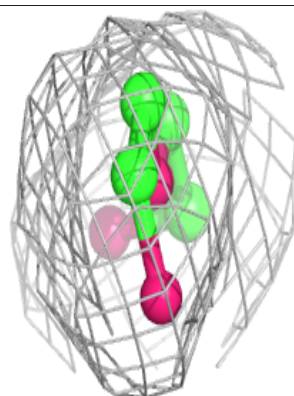
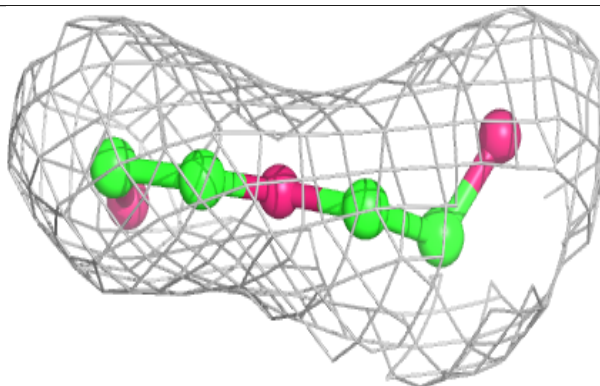
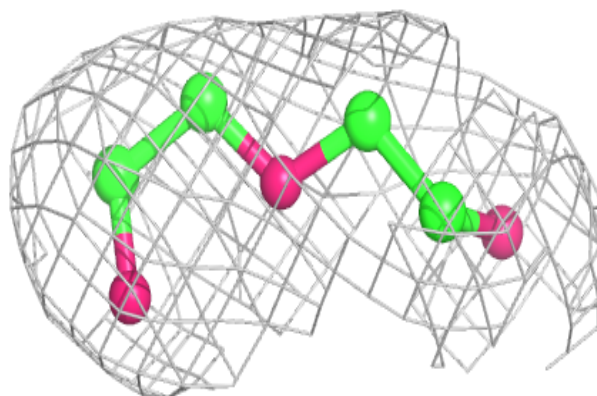


Electron density around PEG C 328:

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

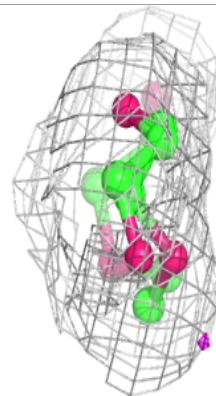
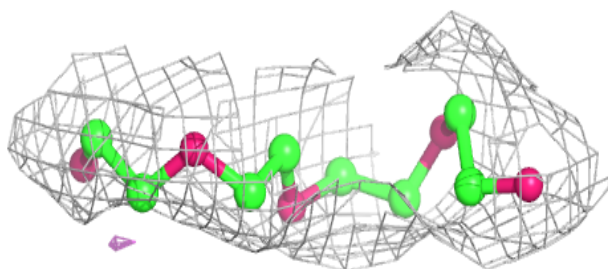
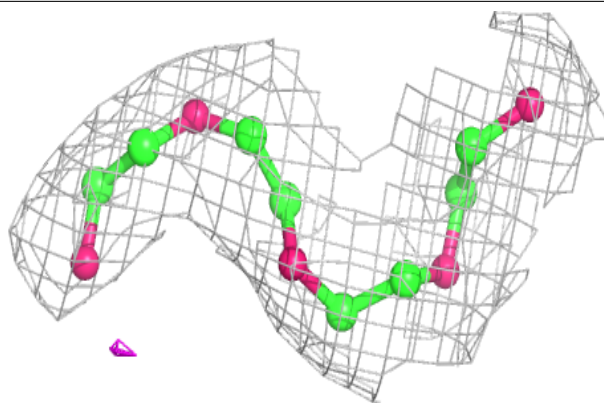
**Electron density around PEG B 128:**

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



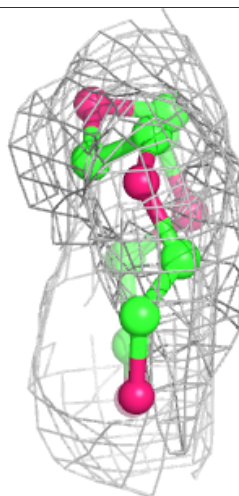
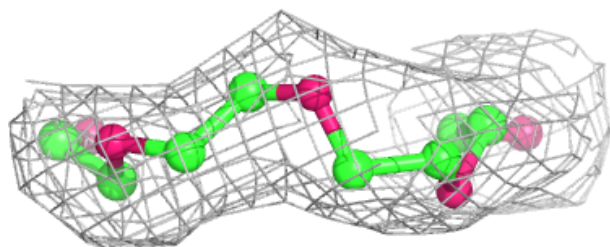
Electron density around PG4 D 118:

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



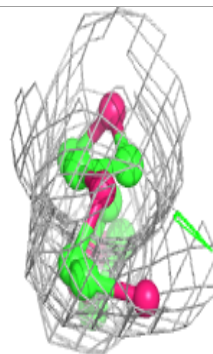
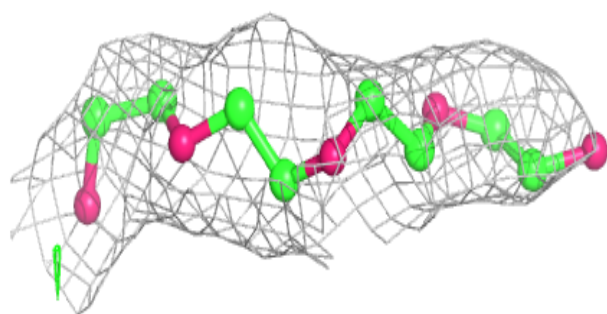
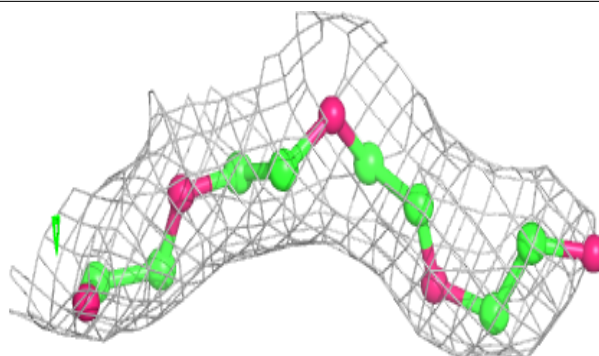
Electron density around PG4 A 321:

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

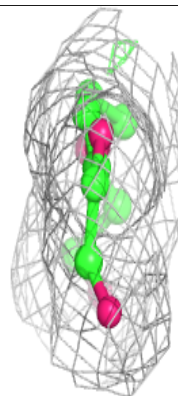
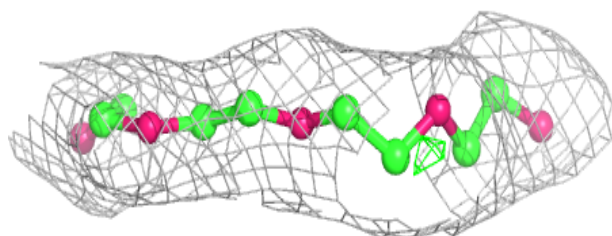
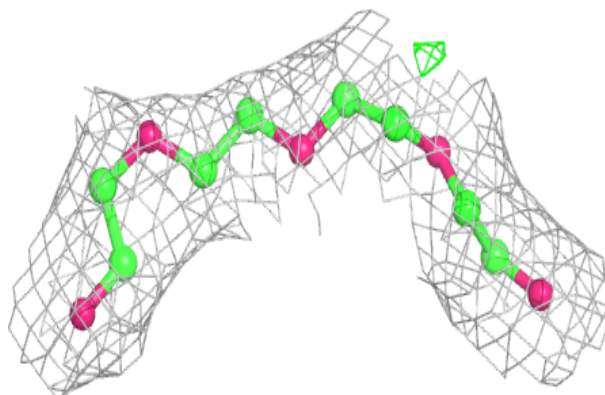


Electron density around PG4 B 118:

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

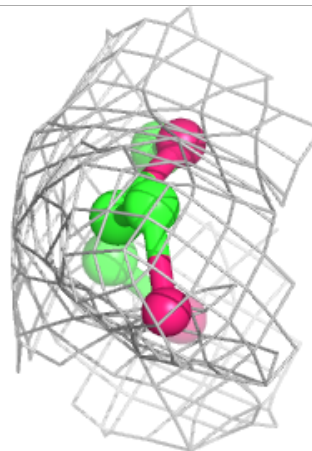
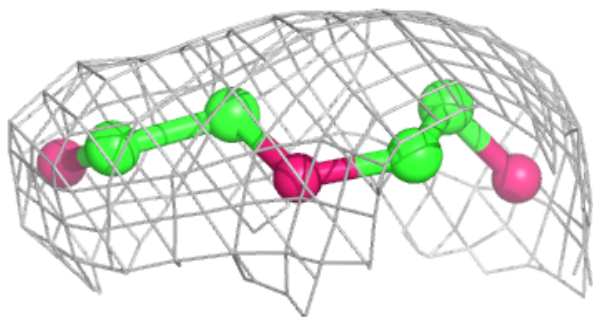
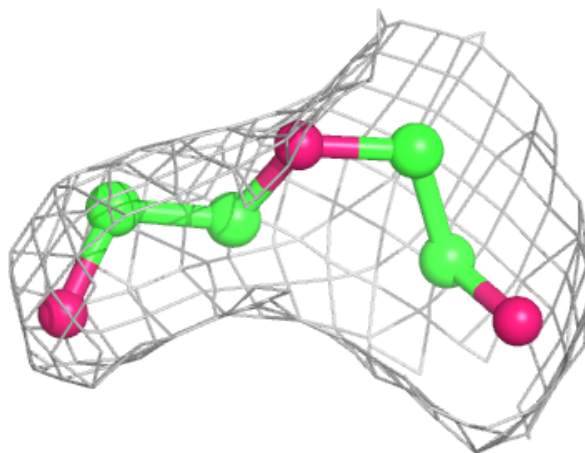
**Electron density around PG4 F 105:**

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



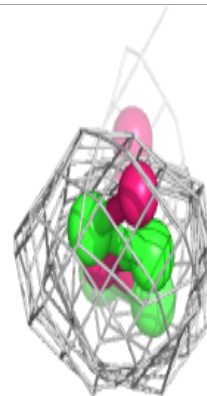
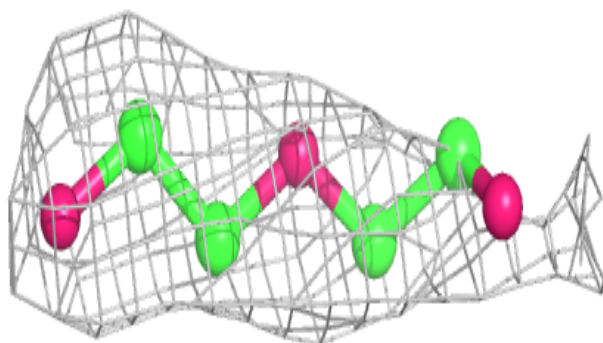
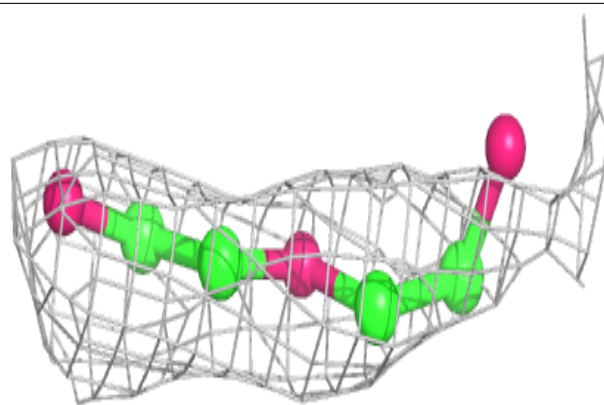
Electron density around PEG C 331:

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

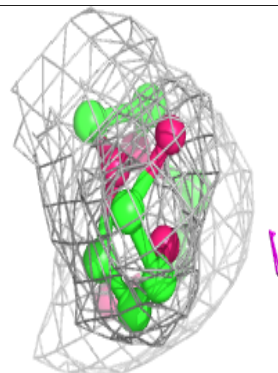
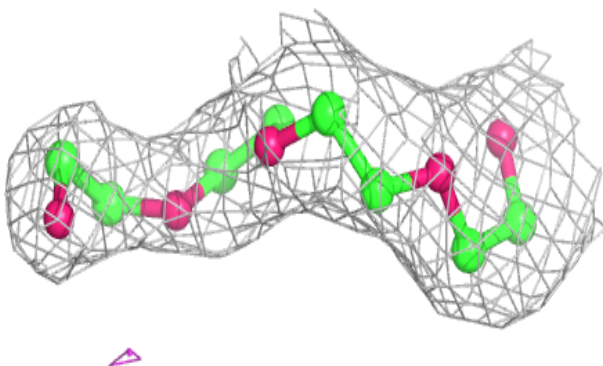
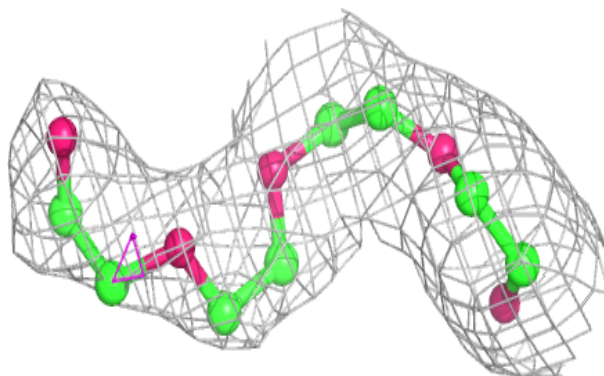


Electron density around PEG A 329:

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

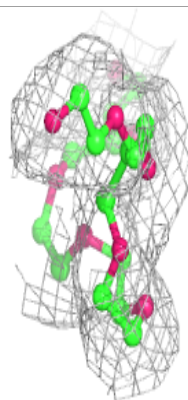
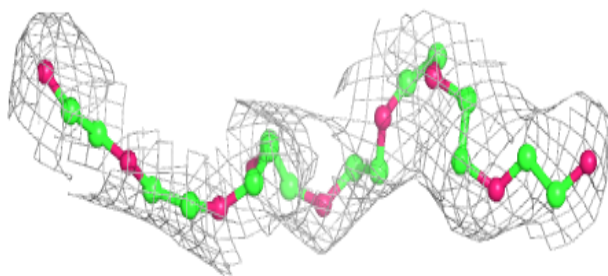
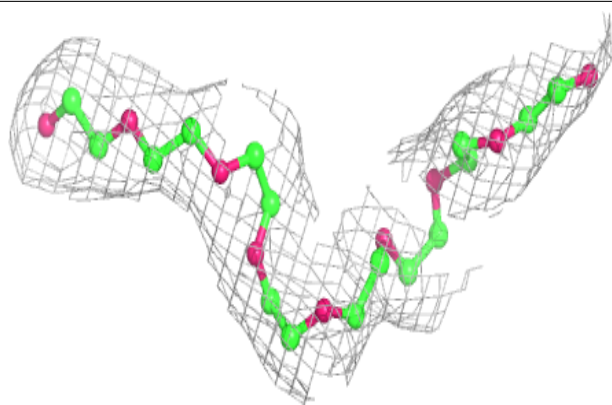
**Electron density around PG4 A 368:**

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



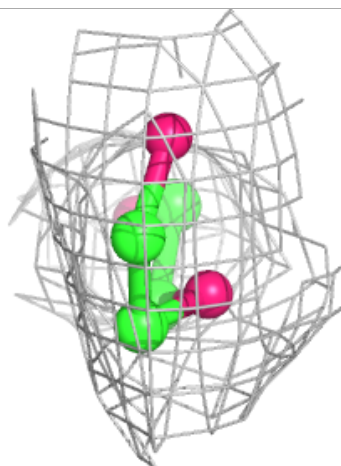
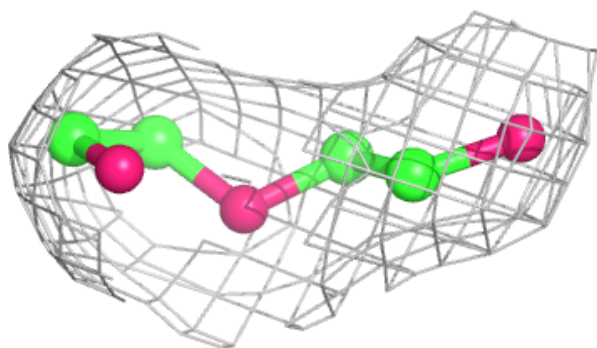
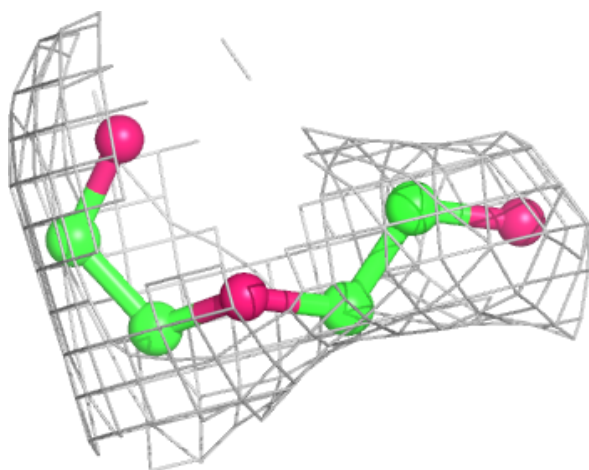
Electron density around PE8 A 342:

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



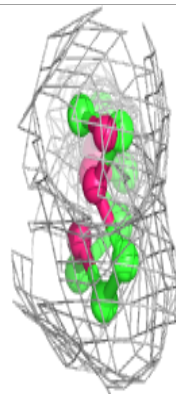
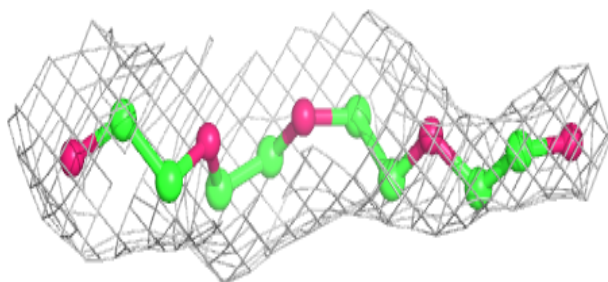
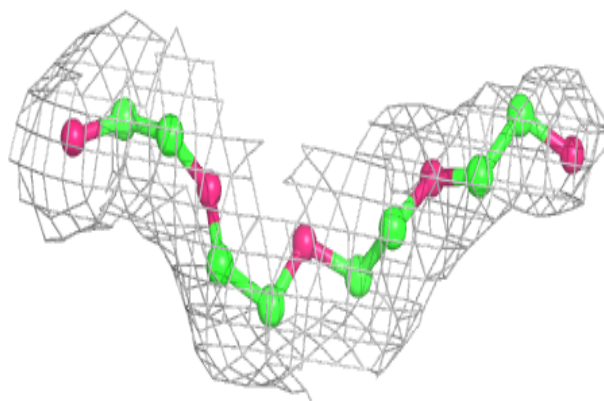
Electron density around PEG A 333:

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

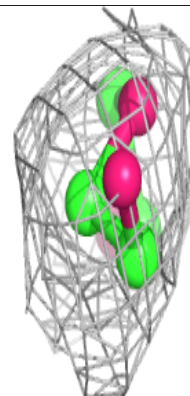
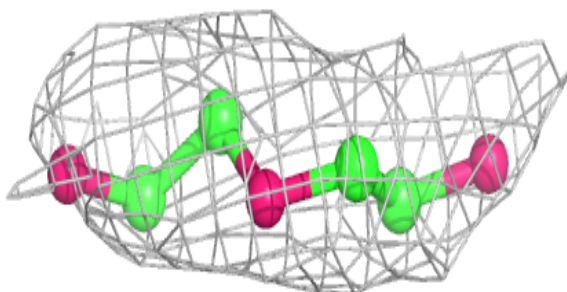
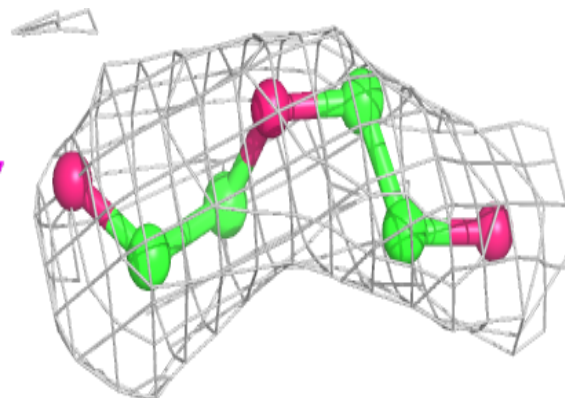


Electron density around PG4 D 103:

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

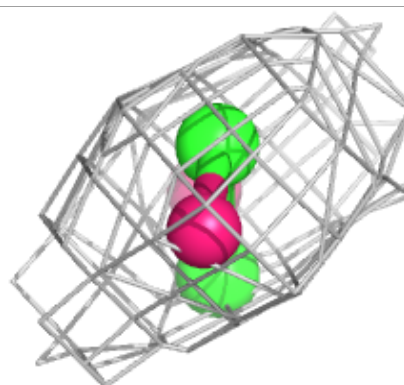
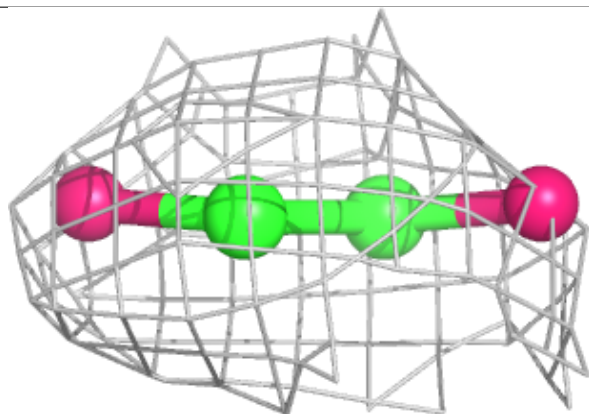
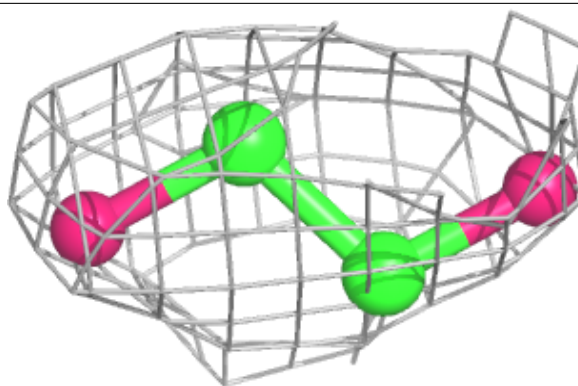
**Electron density around PEG A 341:**

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

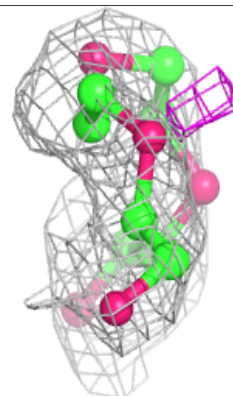
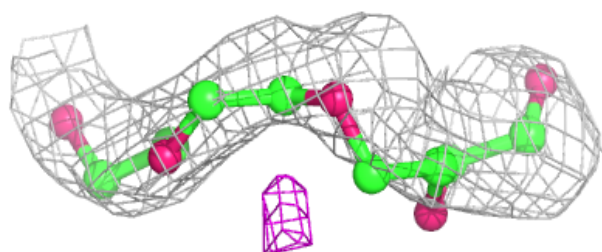
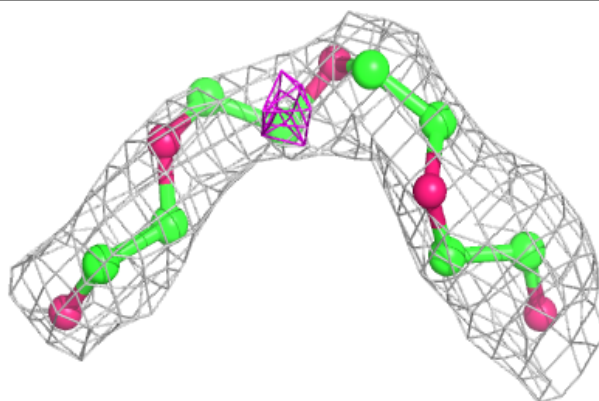


Electron density around EDO D 101:

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

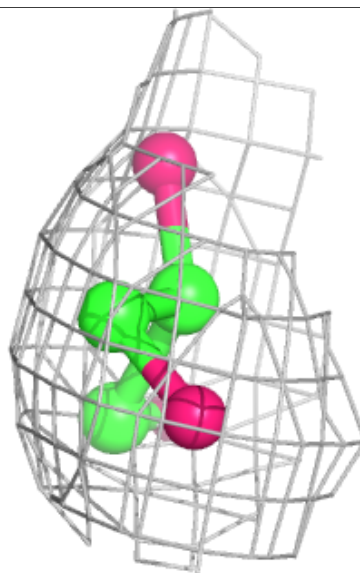
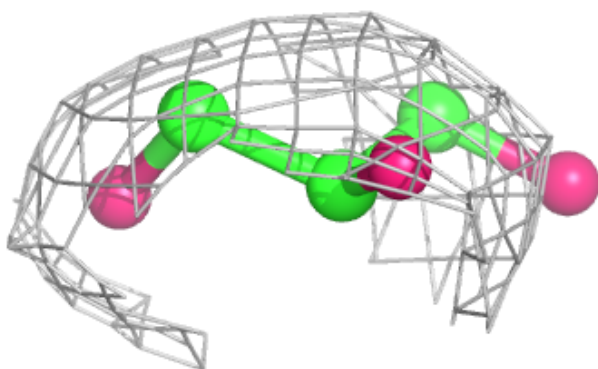
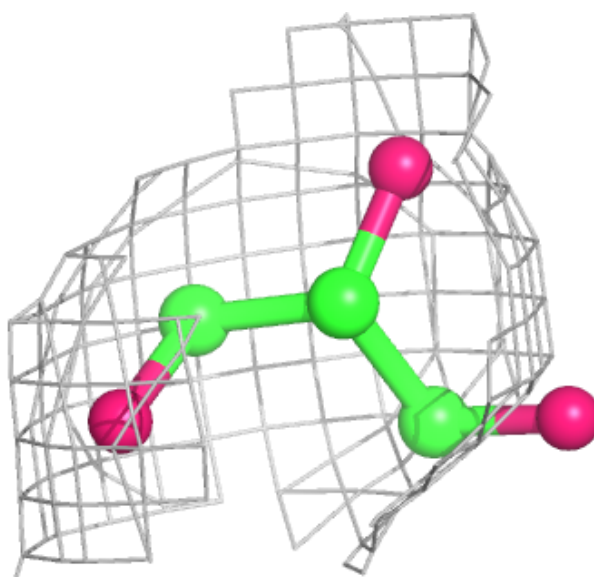
**Electron density around PG4 C 325:**

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



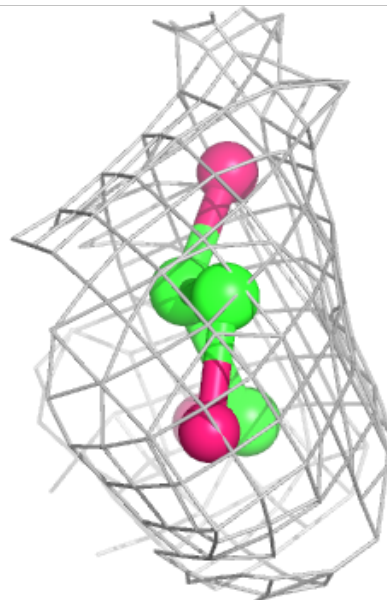
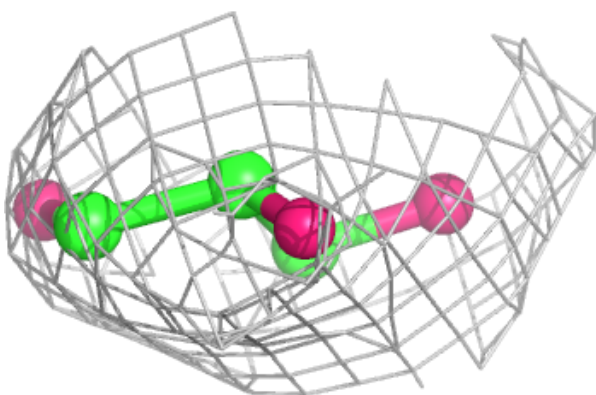
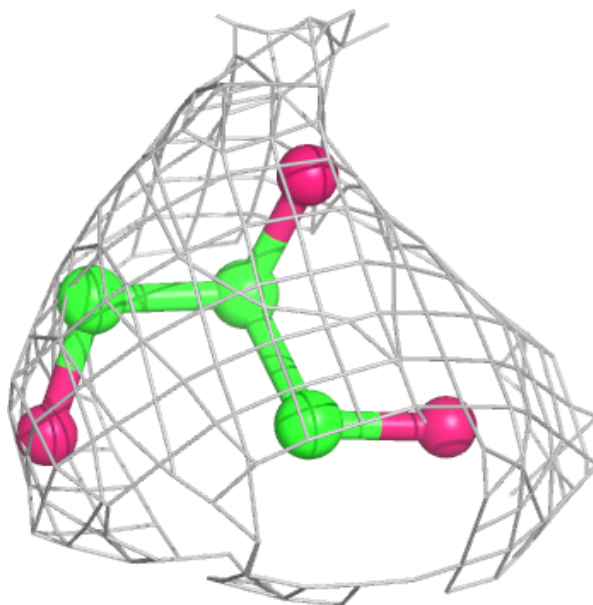
Electron density around GOL E 103:

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



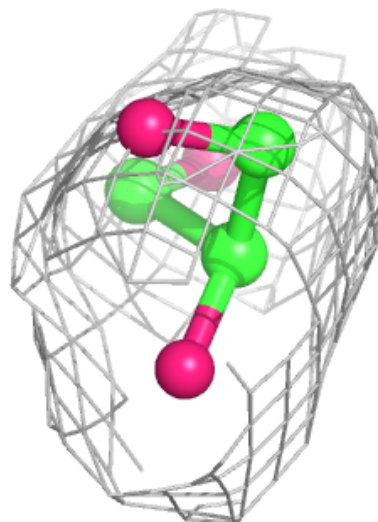
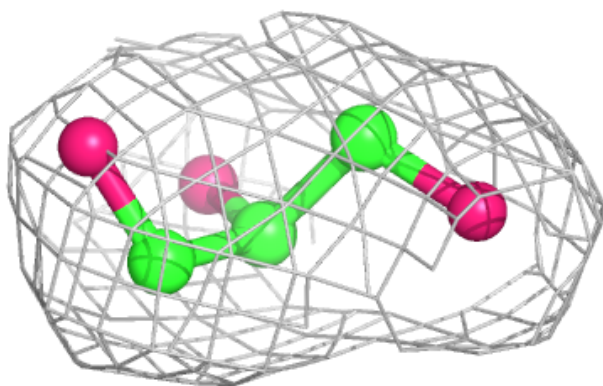
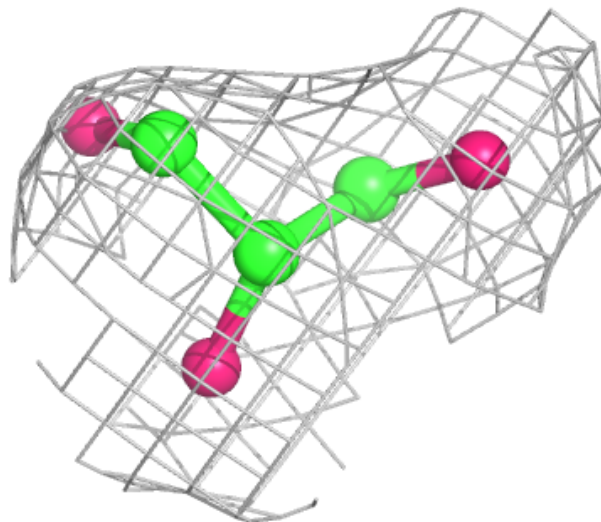
Electron density around GOL B 105:

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



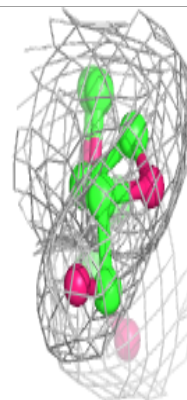
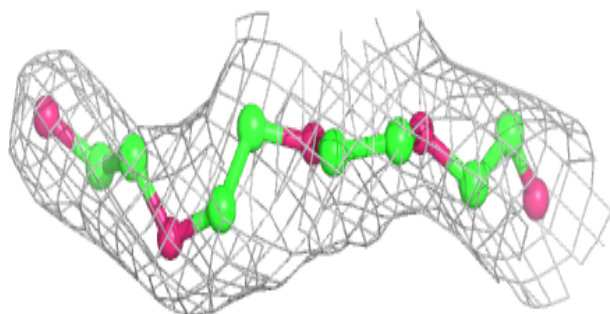
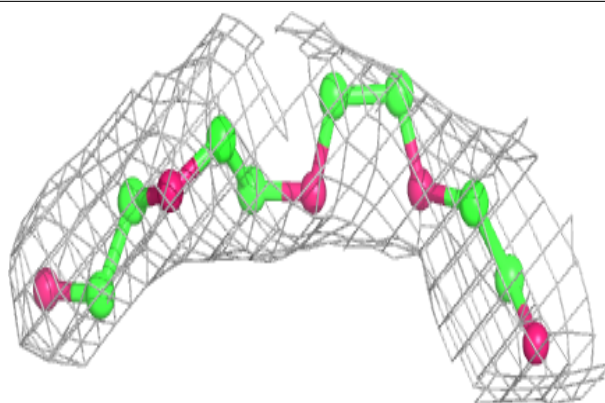
Electron density around GOL C 344:

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

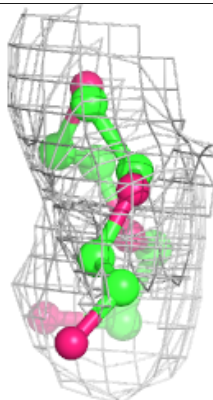
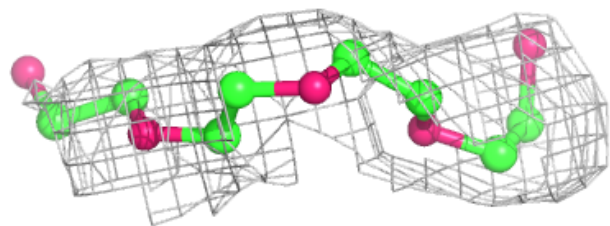
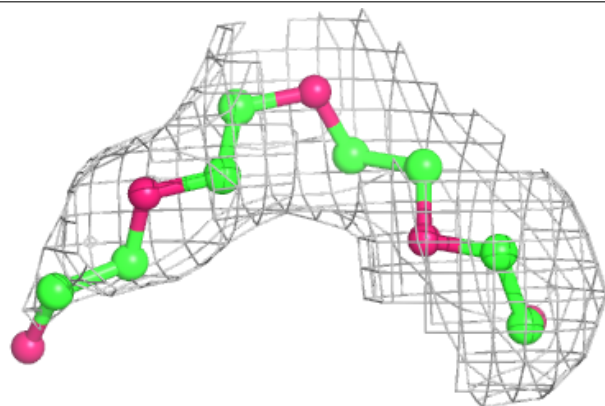


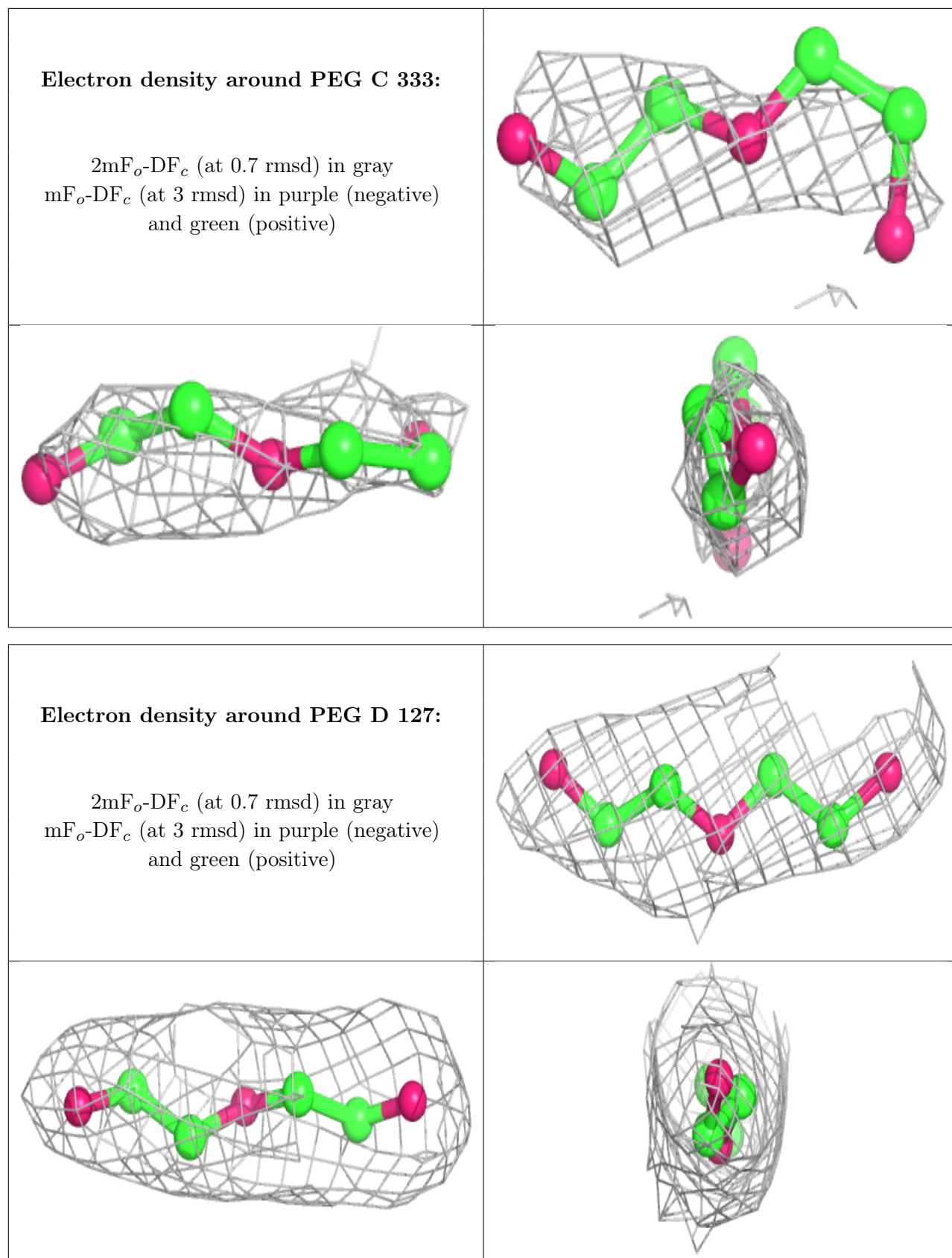
Electron density around PG4 C 320:

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

**Electron density around PG4 C 324:**

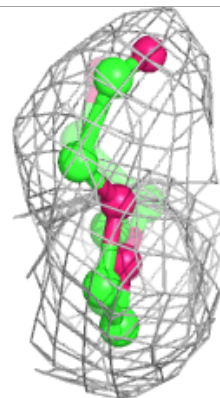
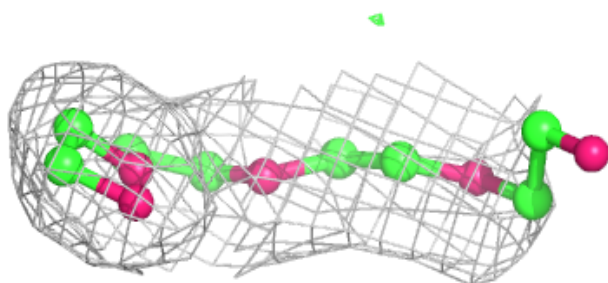
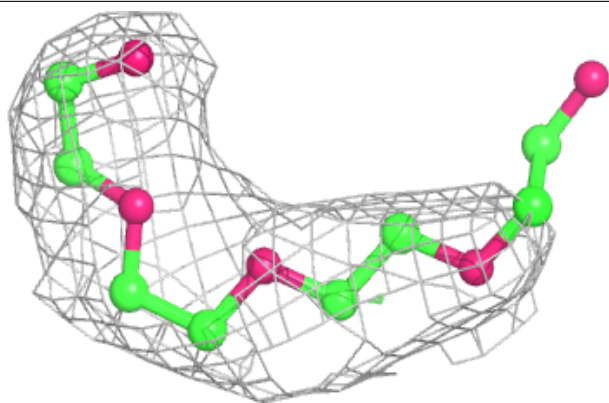
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



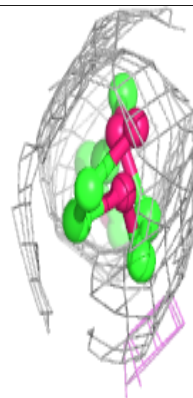
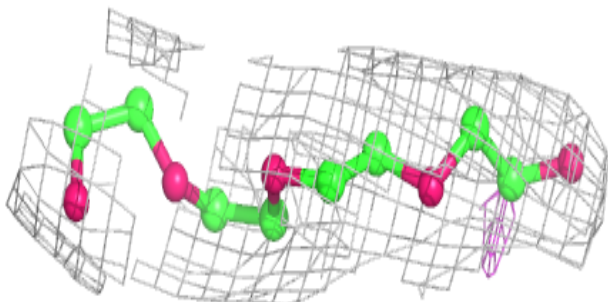
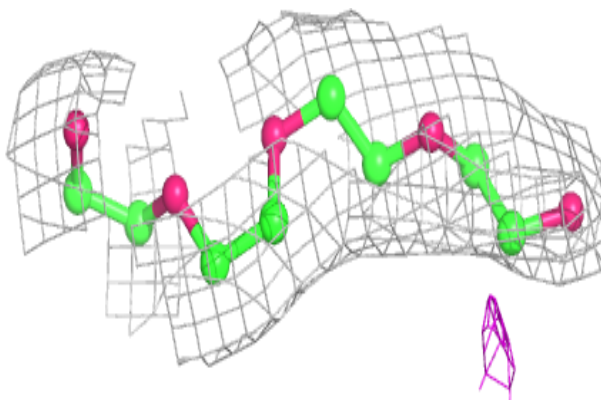


Electron density around PG4 C 336:

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

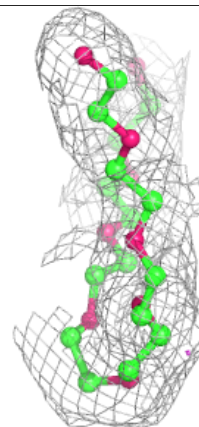
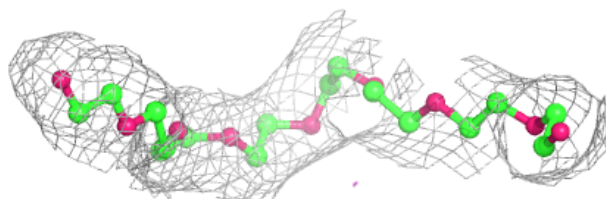
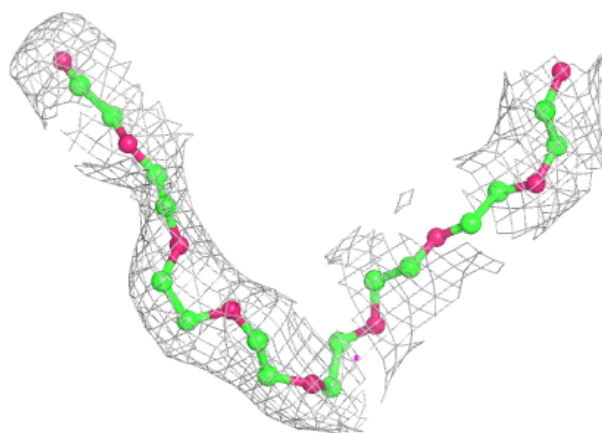
**Electron density around PG4 A 365:**

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

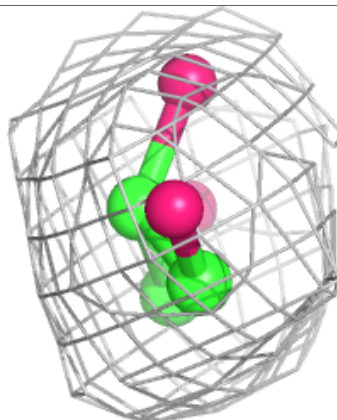
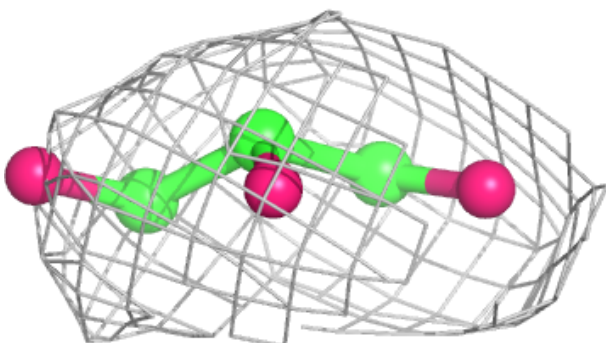
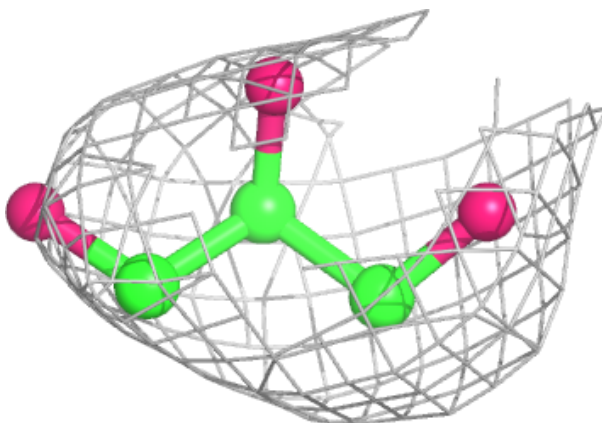


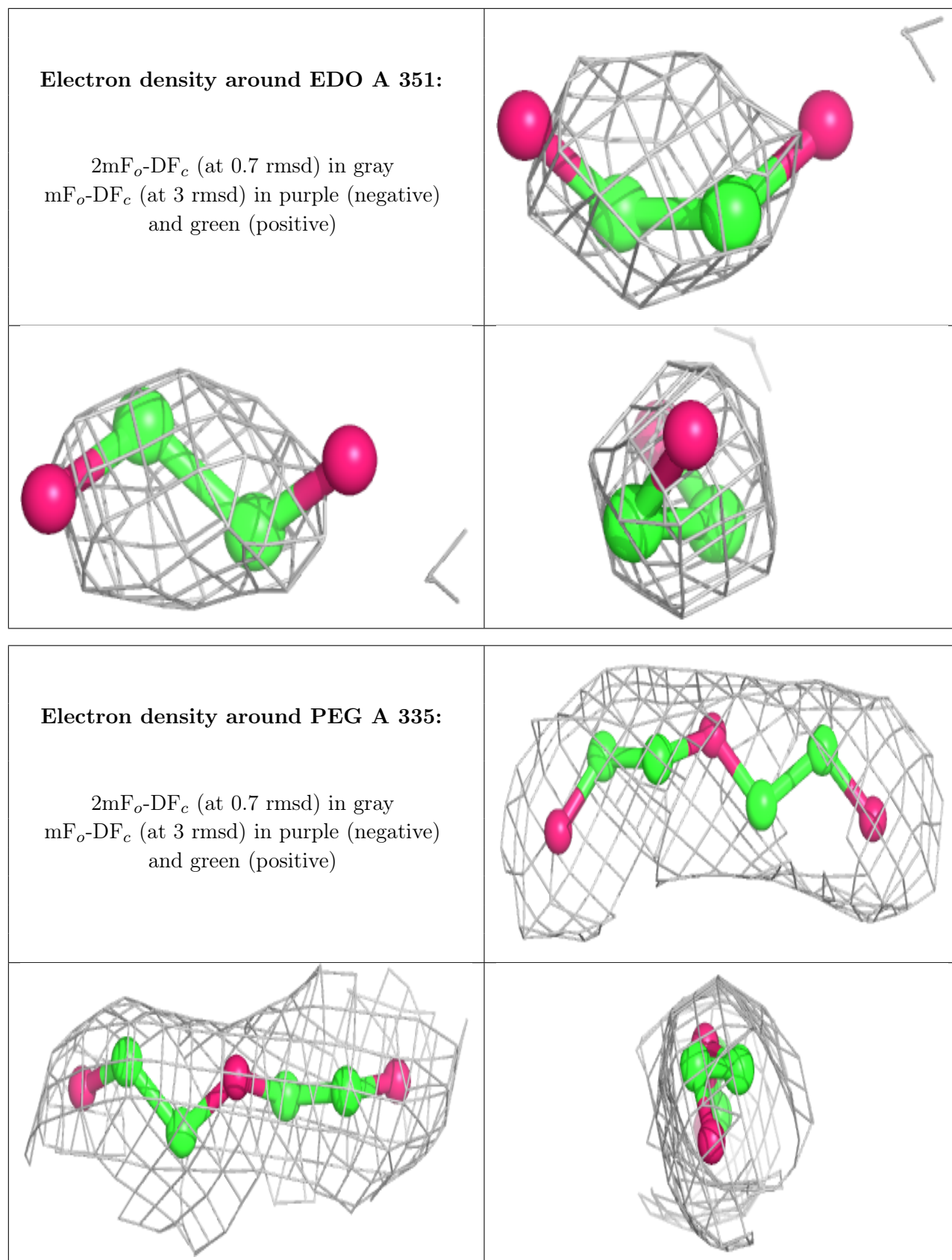
Electron density around PE8 B 102:

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

**Electron density around GOL B 140:**

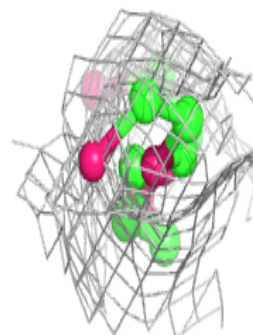
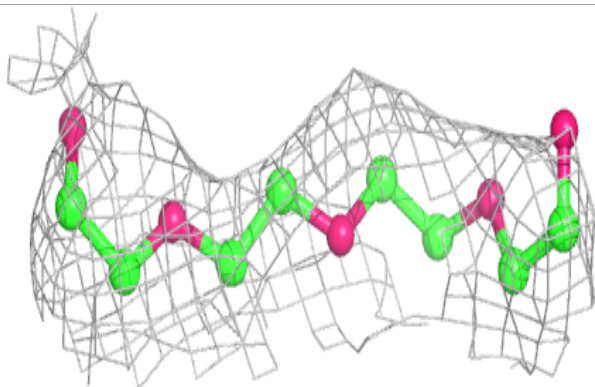
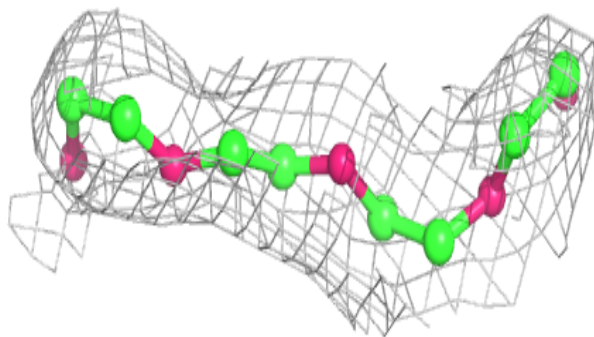
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



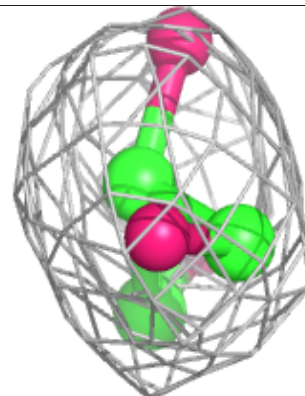
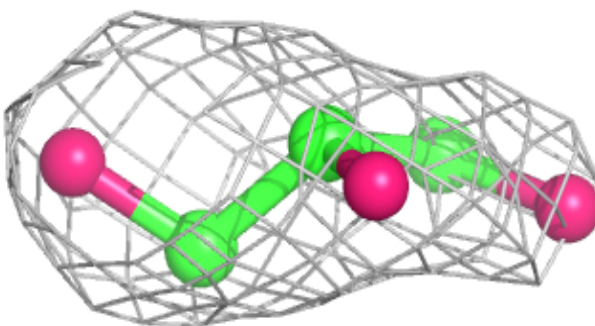
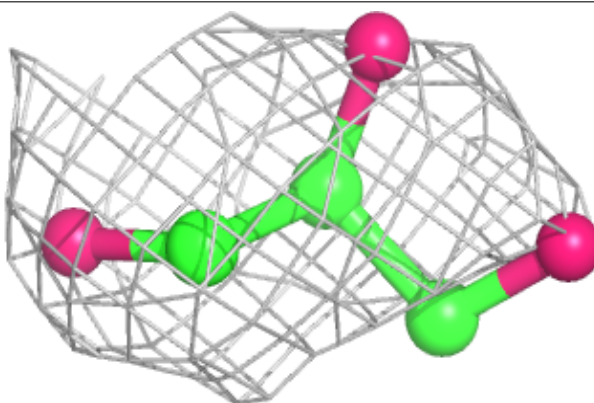


Electron density around PG4 C 322:

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

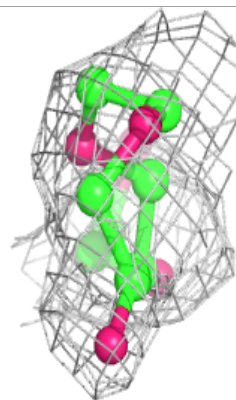
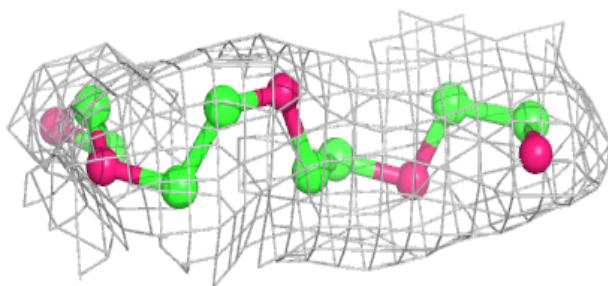
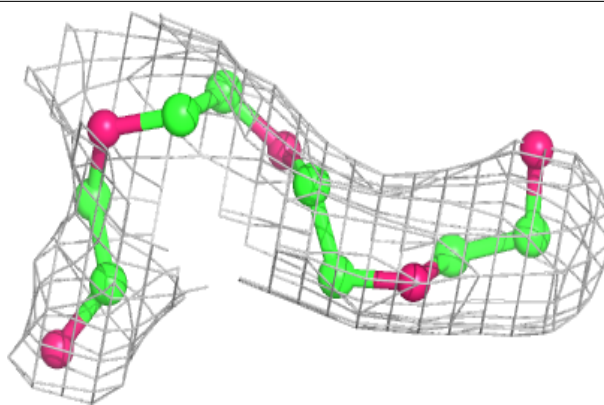
**Electron density around GOL A 345:**

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

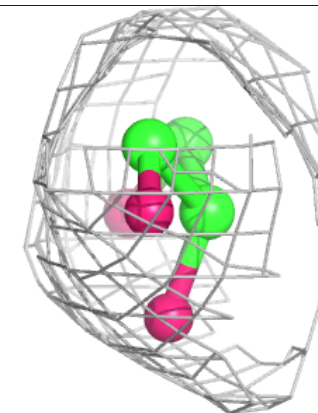
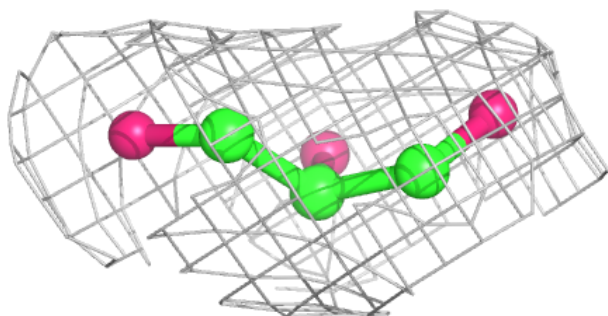
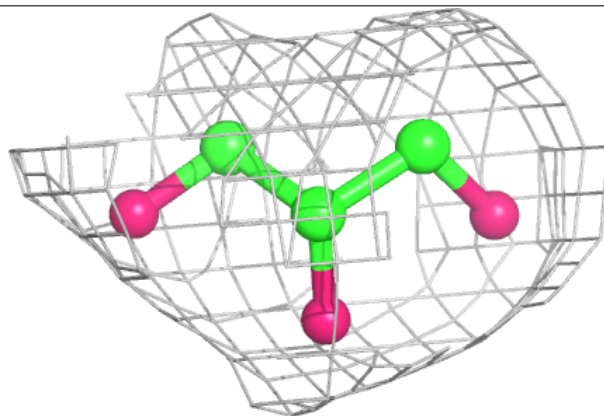


Electron density around PG4 A 323:

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

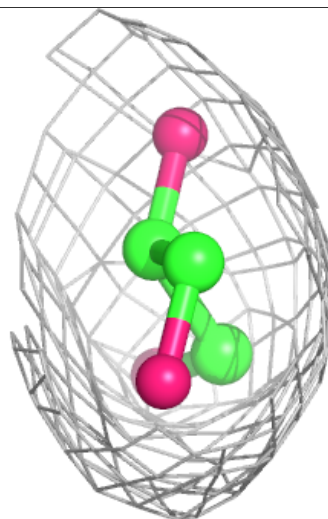
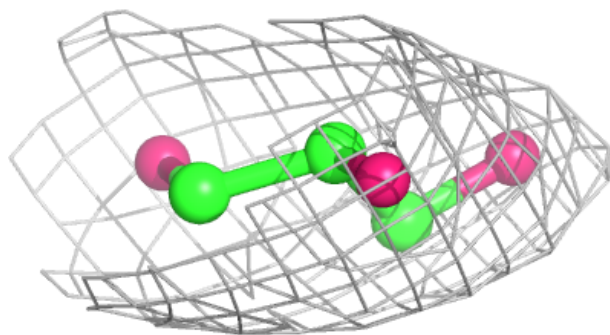
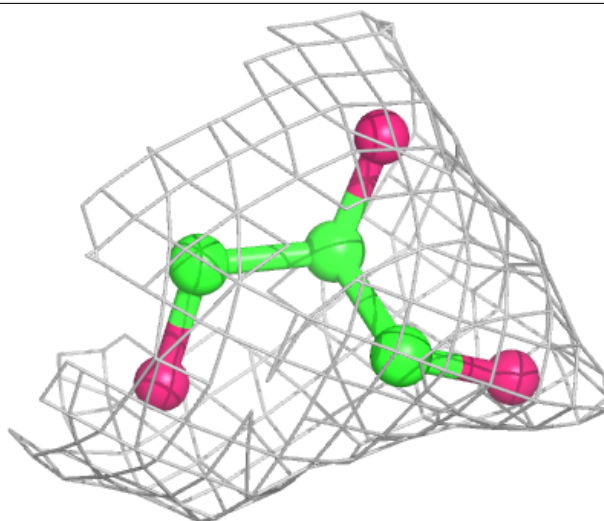
**Electron density around GOL C 306:**

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



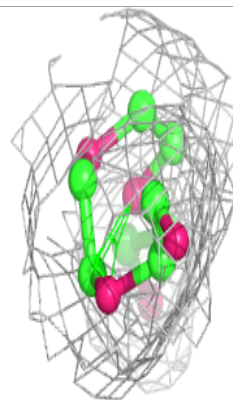
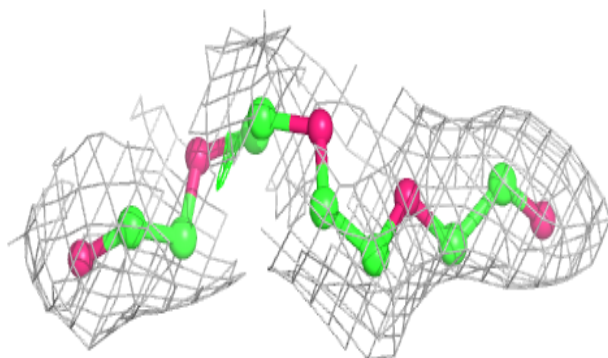
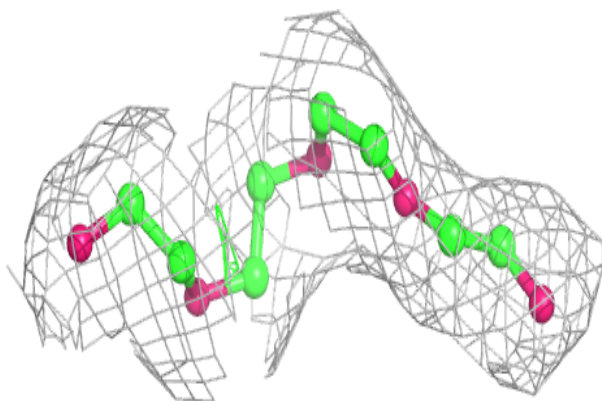
Electron density around GOL B 107:

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



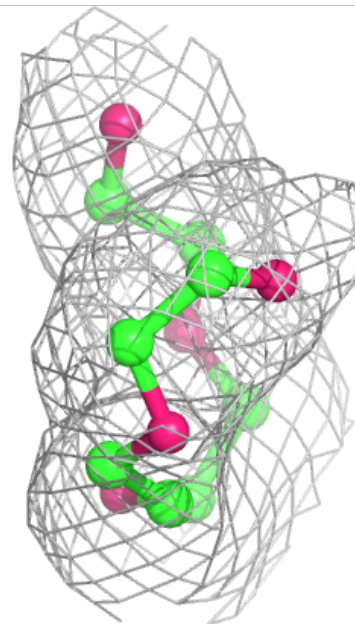
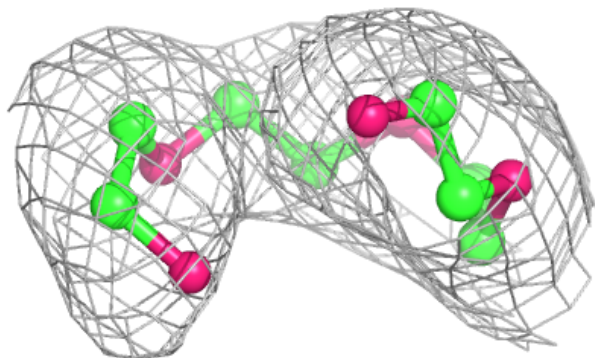
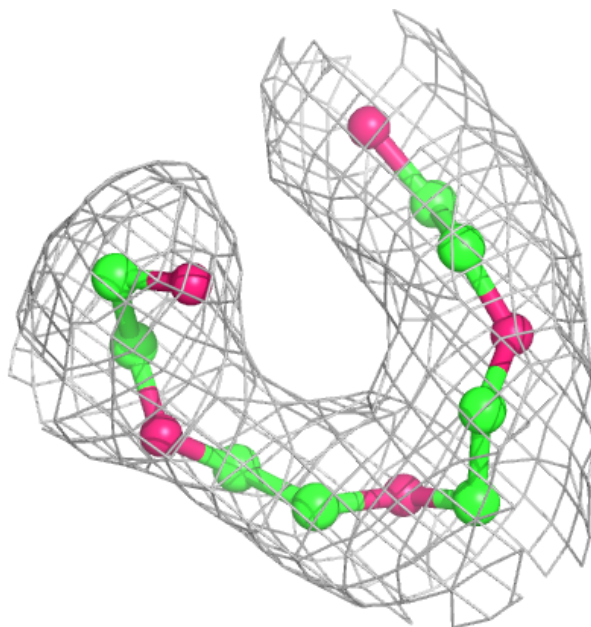
Electron density around PG4 A 352:

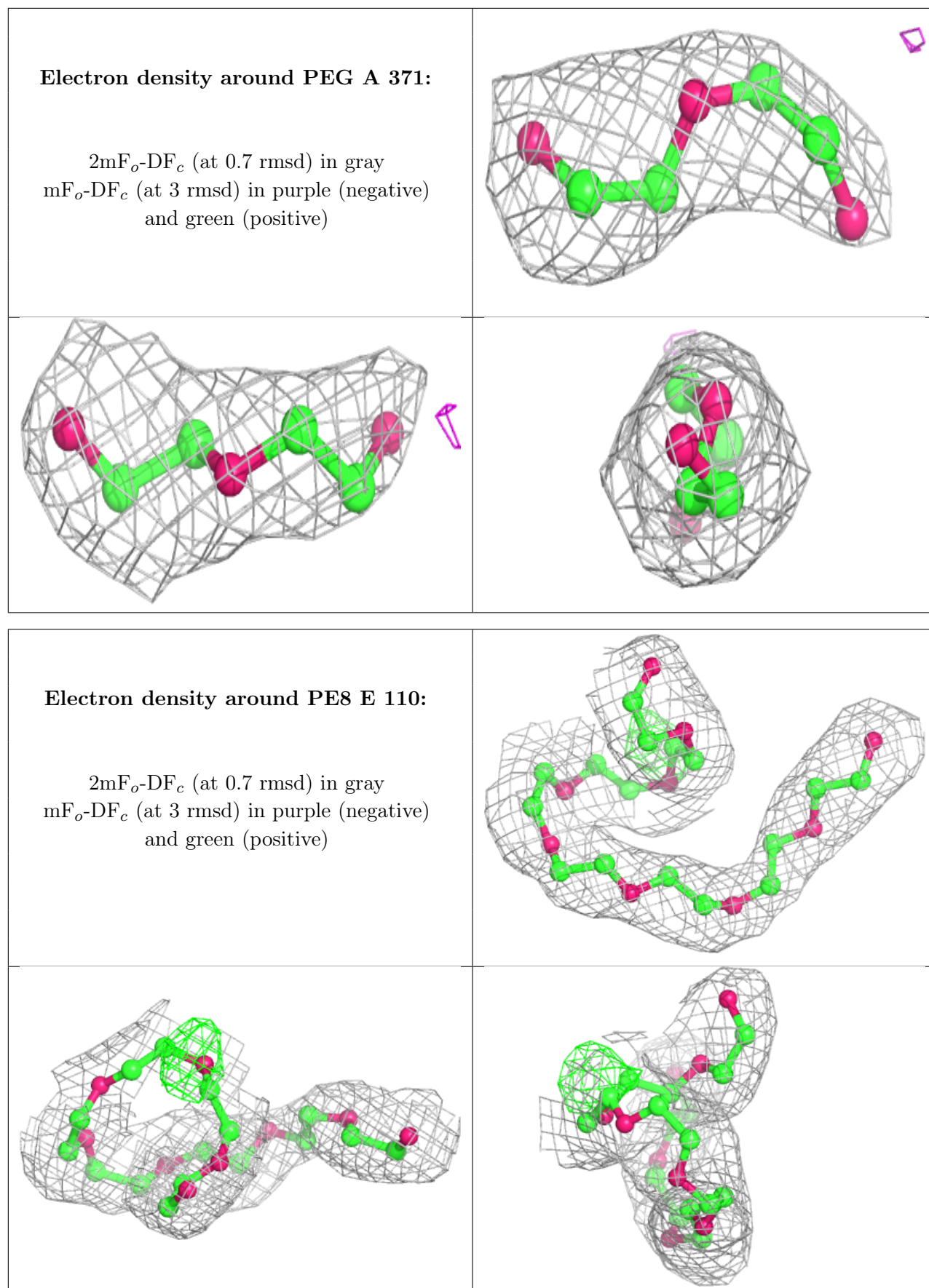
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PG4 A 366:

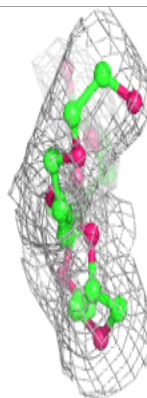
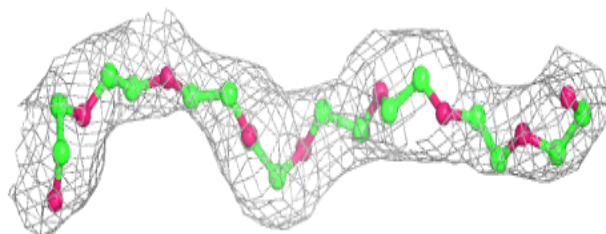
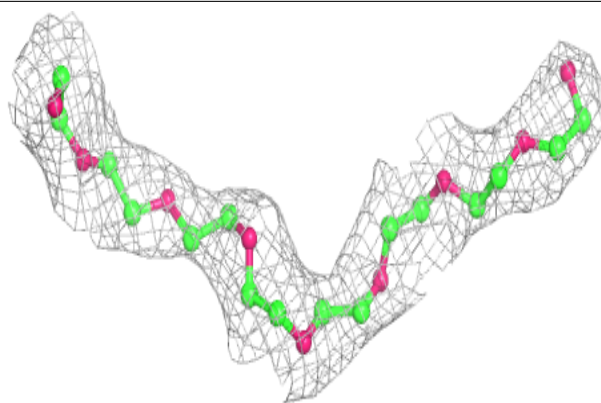
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



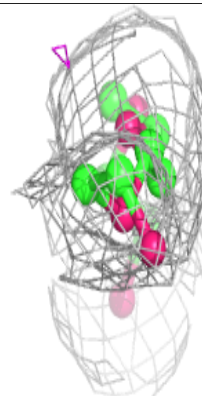
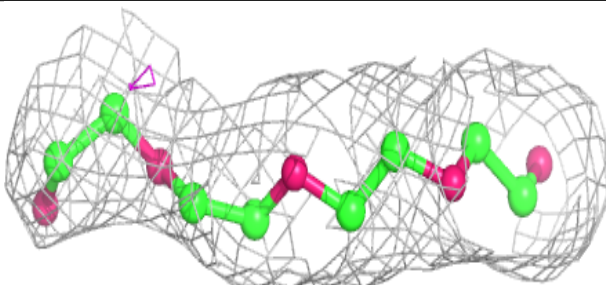
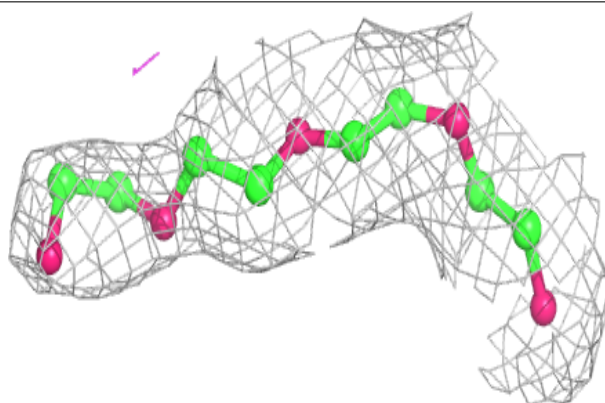


Electron density around PE8 F 102:

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

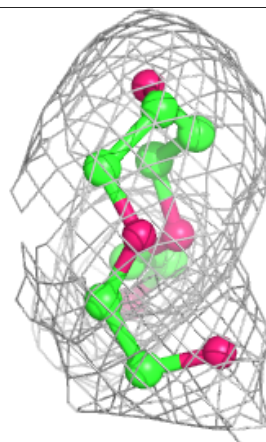
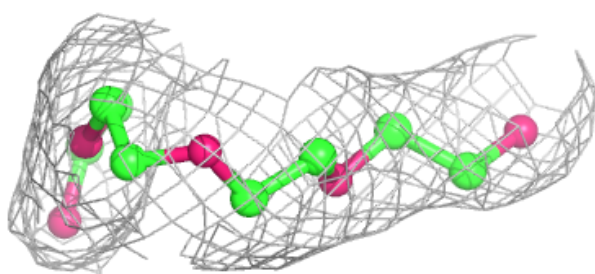
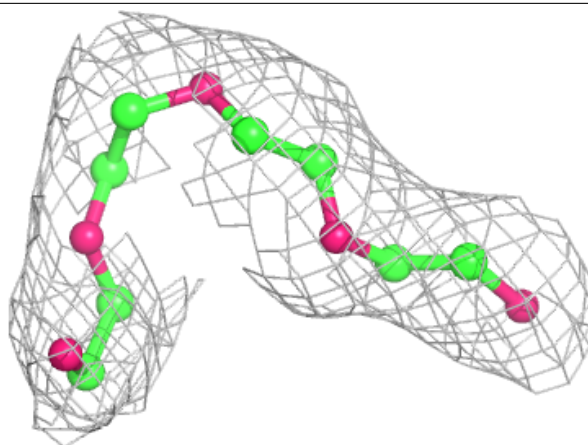
**Electron density around PG4 D 116:**

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

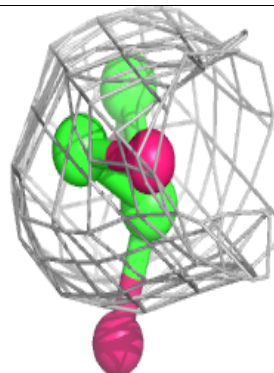
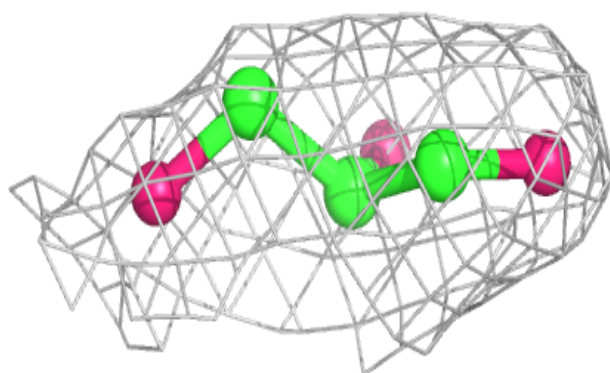
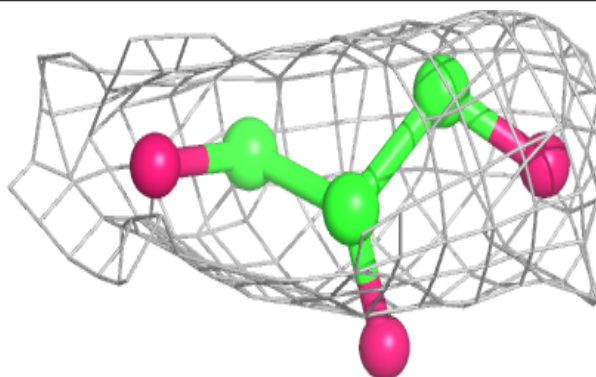


Electron density around PG4 D 117:

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

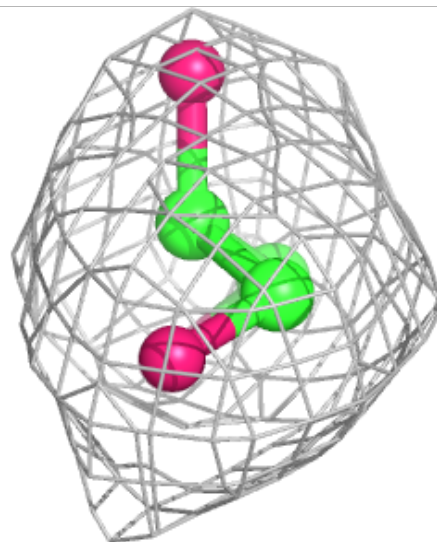
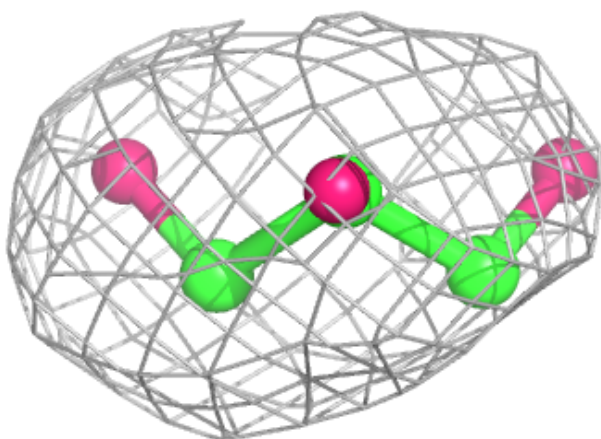
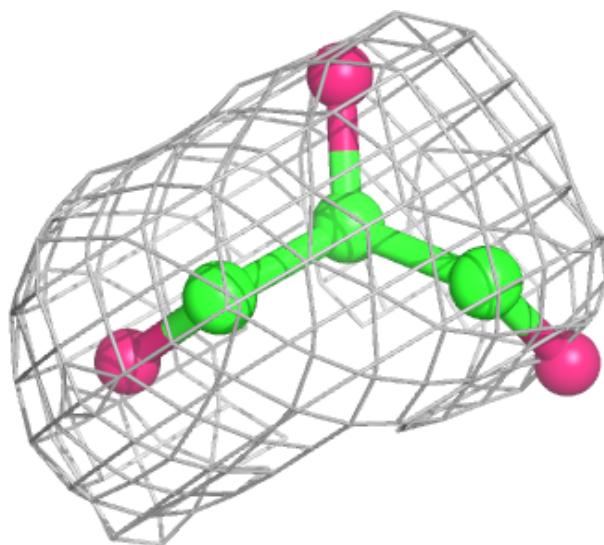
**Electron density around GOL D 131:**

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



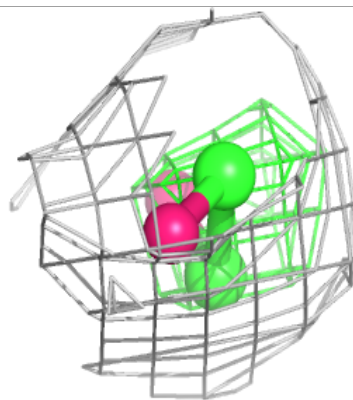
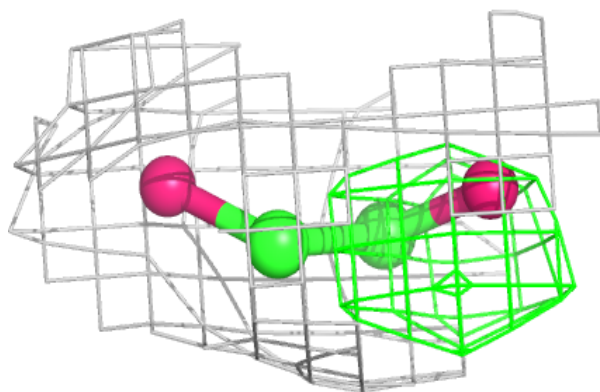
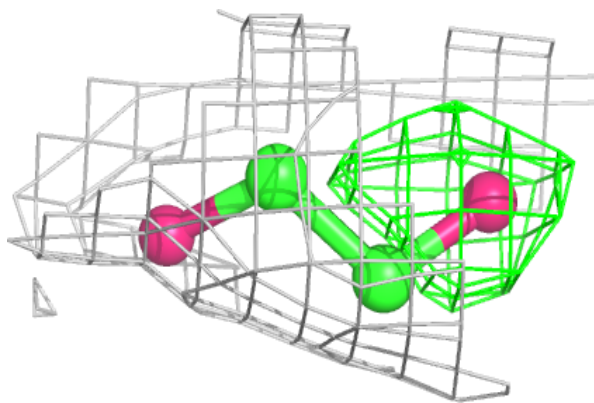
Electron density around GOL C 312:

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

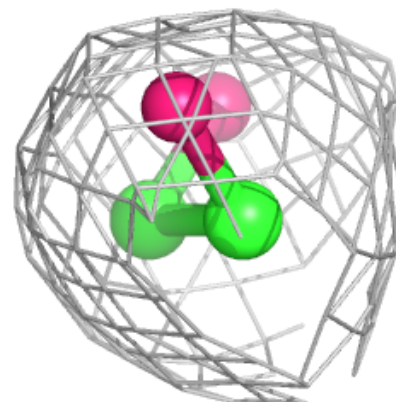
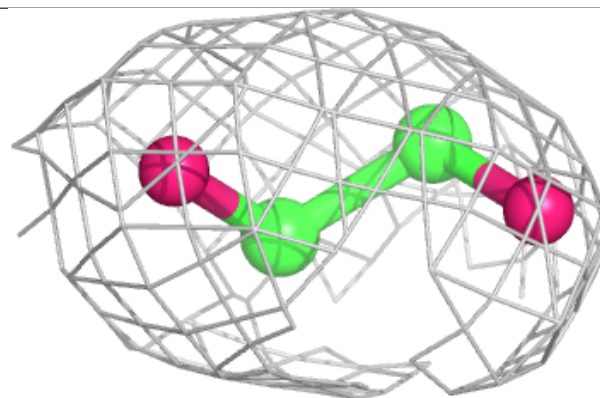
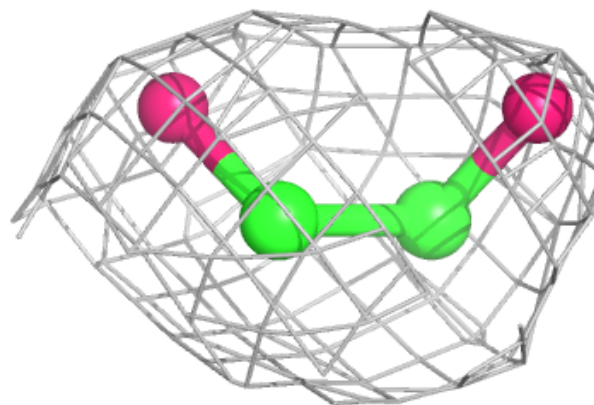


Electron density around EDO D 102:

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

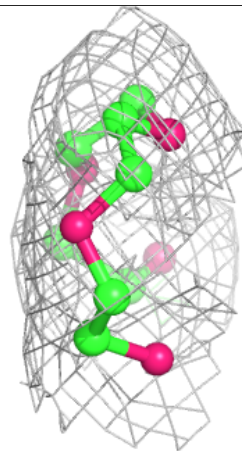
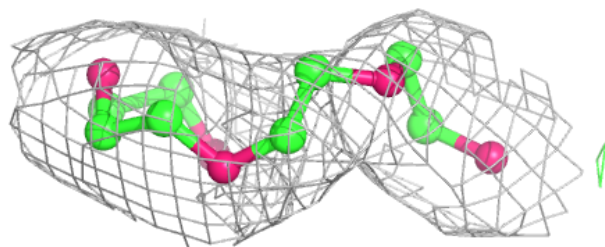
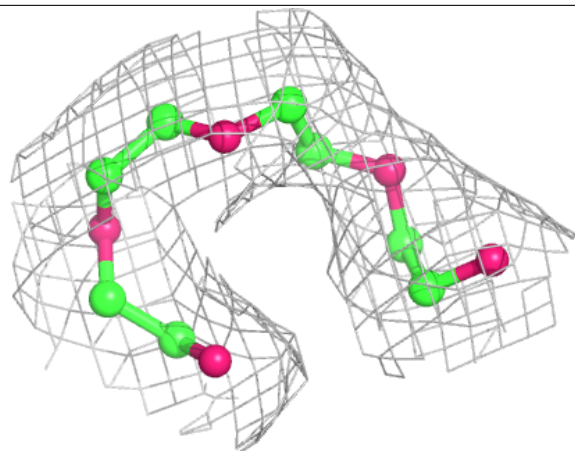
**Electron density around EDO D 130:**

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



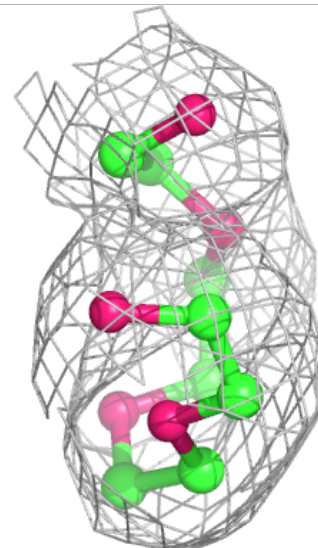
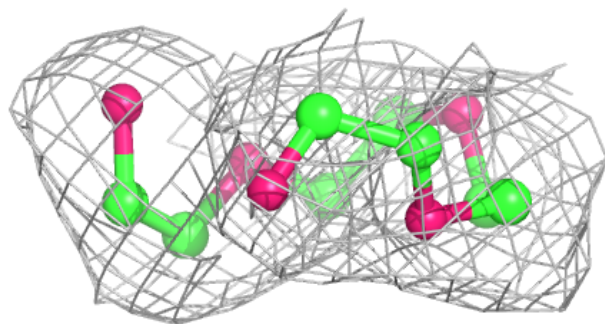
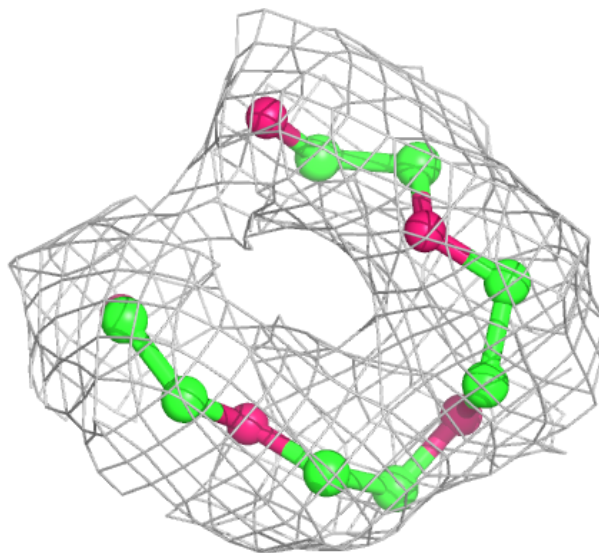
Electron density around PG4 E 106:

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



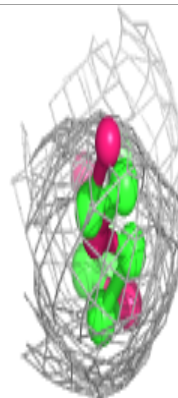
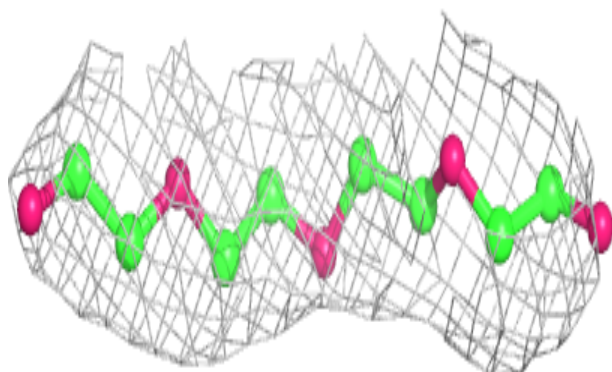
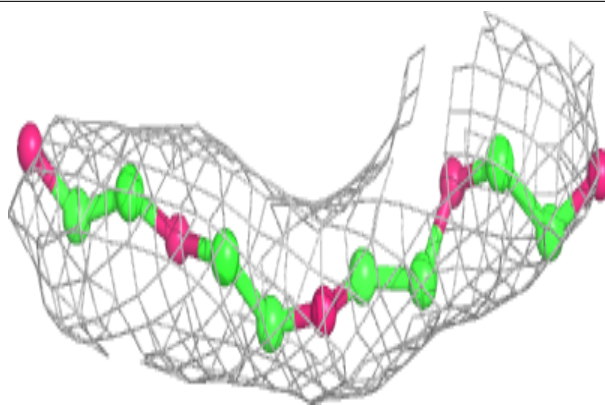
Electron density around PG4 F 101:

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



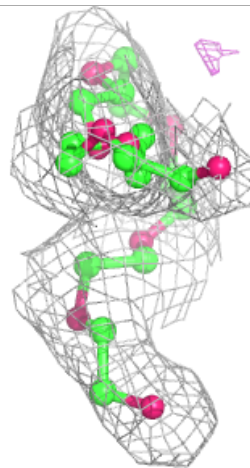
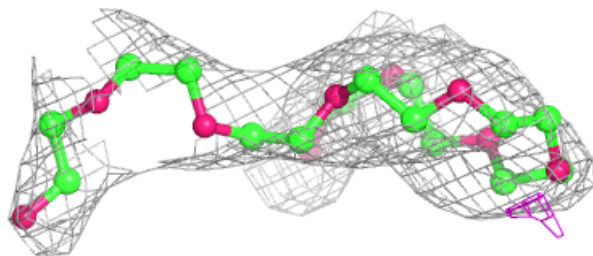
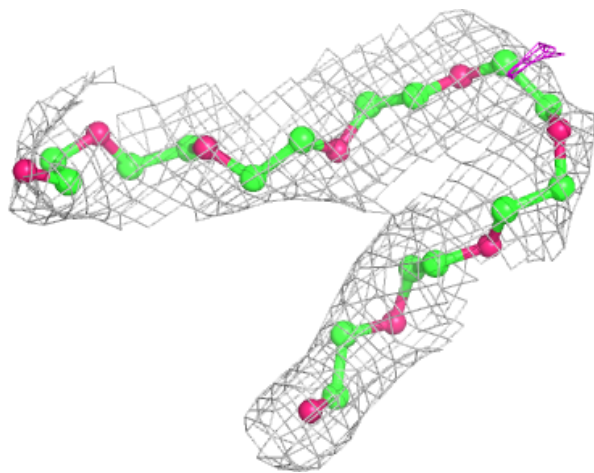
Electron density around PG4 B 120:

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



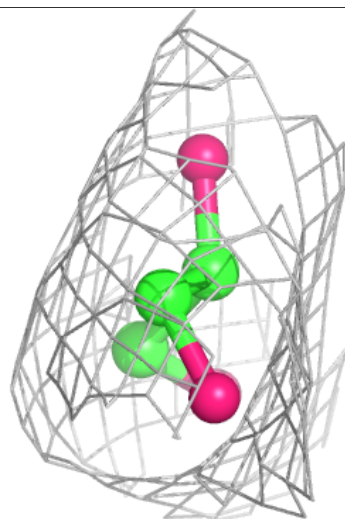
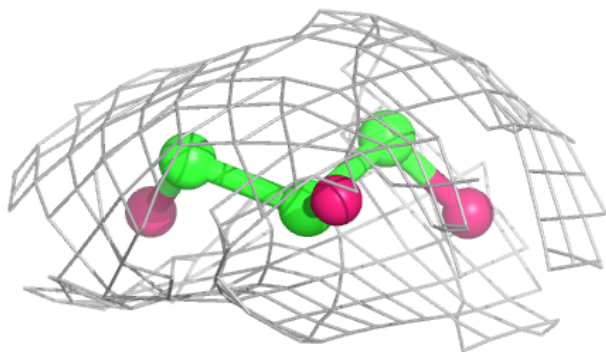
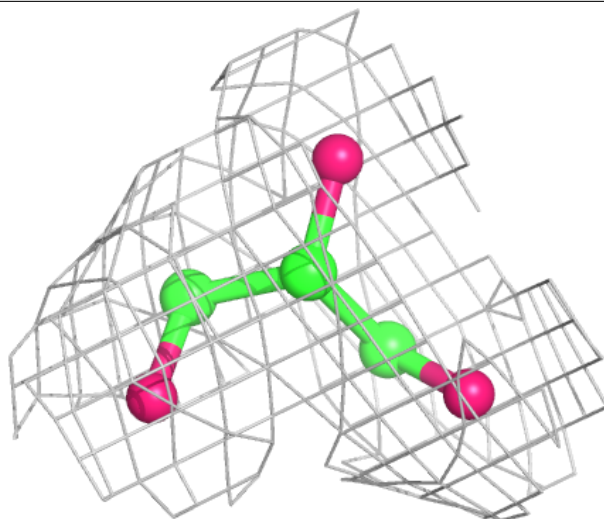
Electron density around PE8 A 344:

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



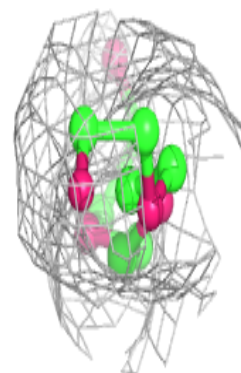
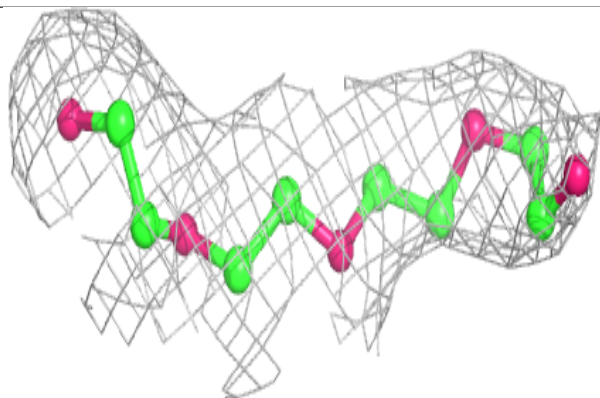
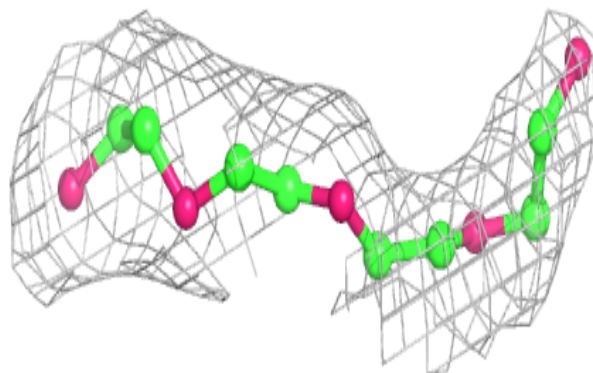
Electron density around GOL D 107:

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

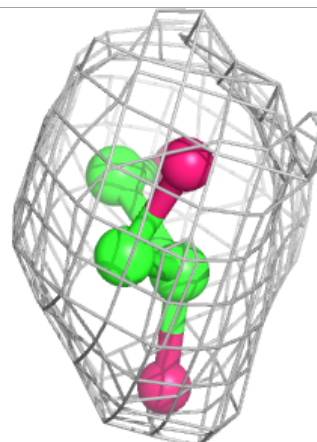
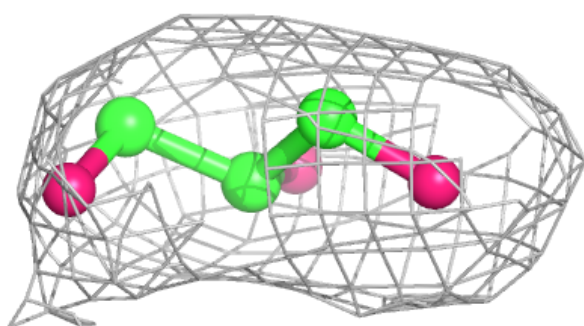
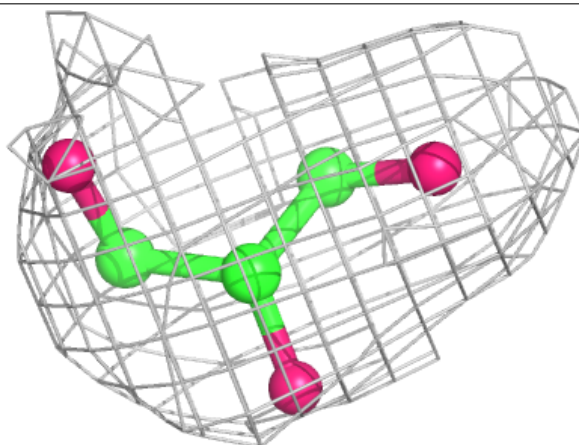


Electron density around PG4 C 319:

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

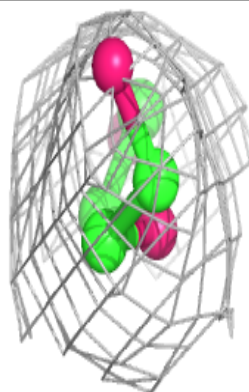
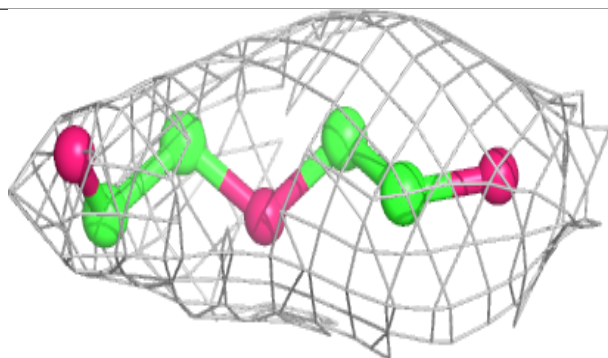
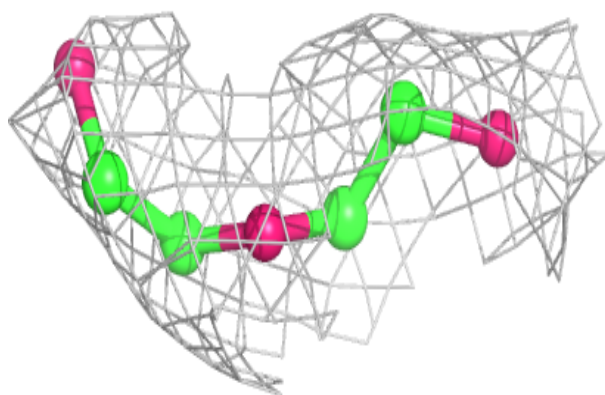
**Electron density around GOL B 109:**

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

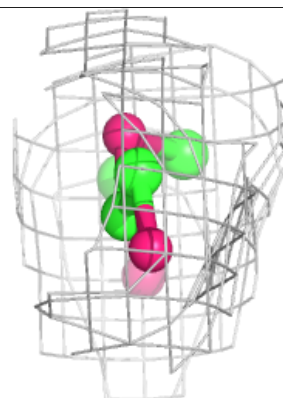
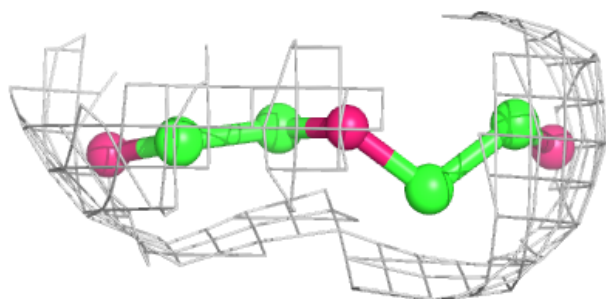
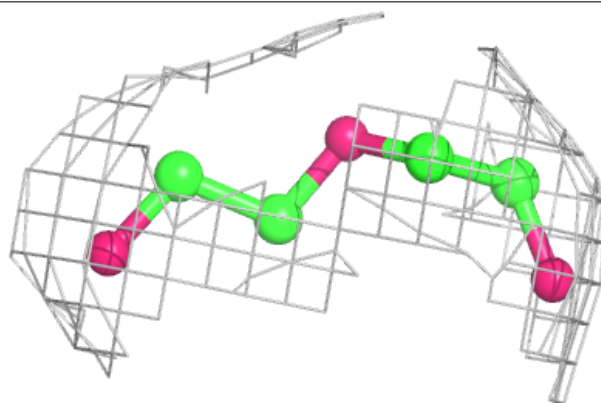


Electron density around PEG C 329:

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

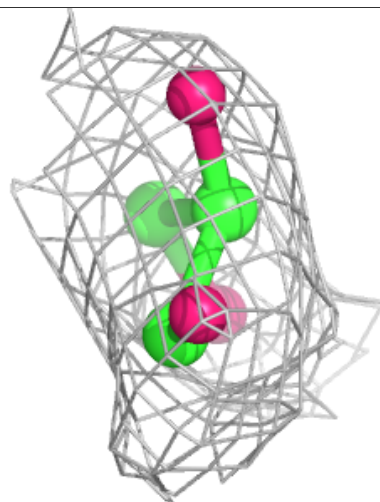
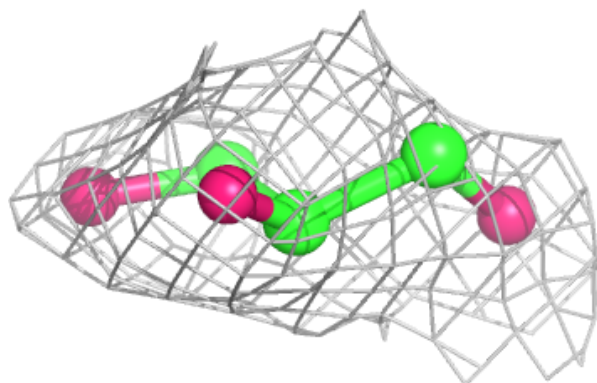
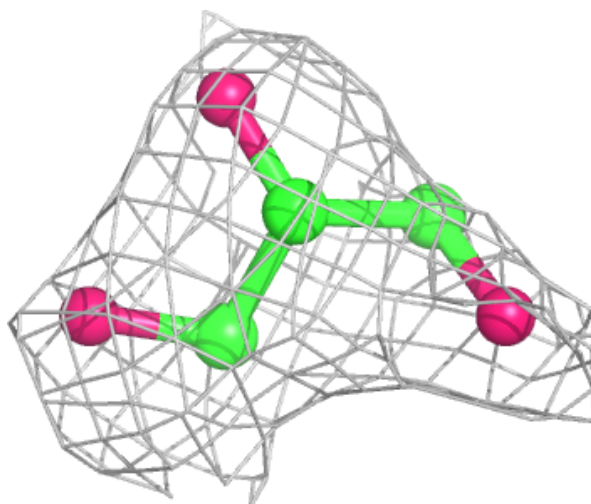
**Electron density around PEG C 330:**

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



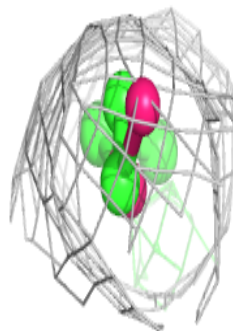
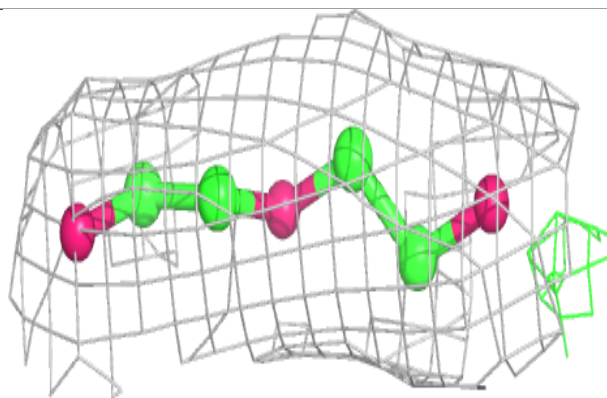
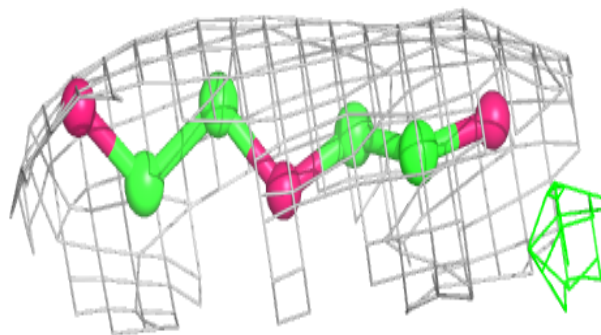
Electron density around GOL A 303:

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

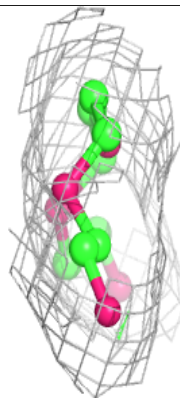
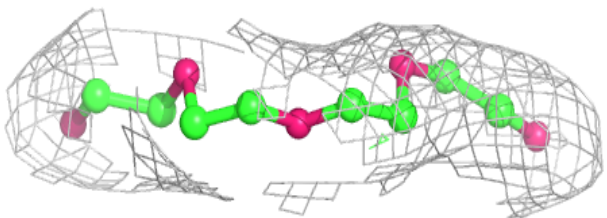
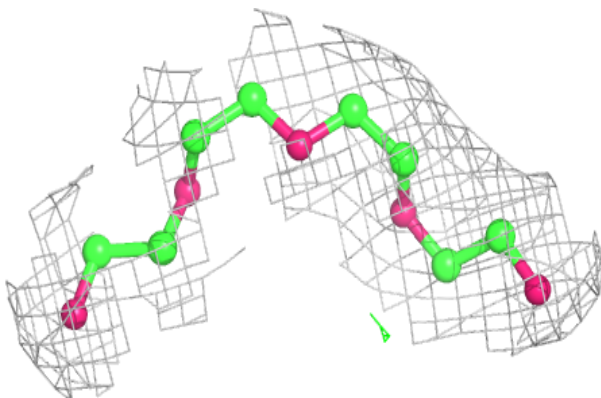


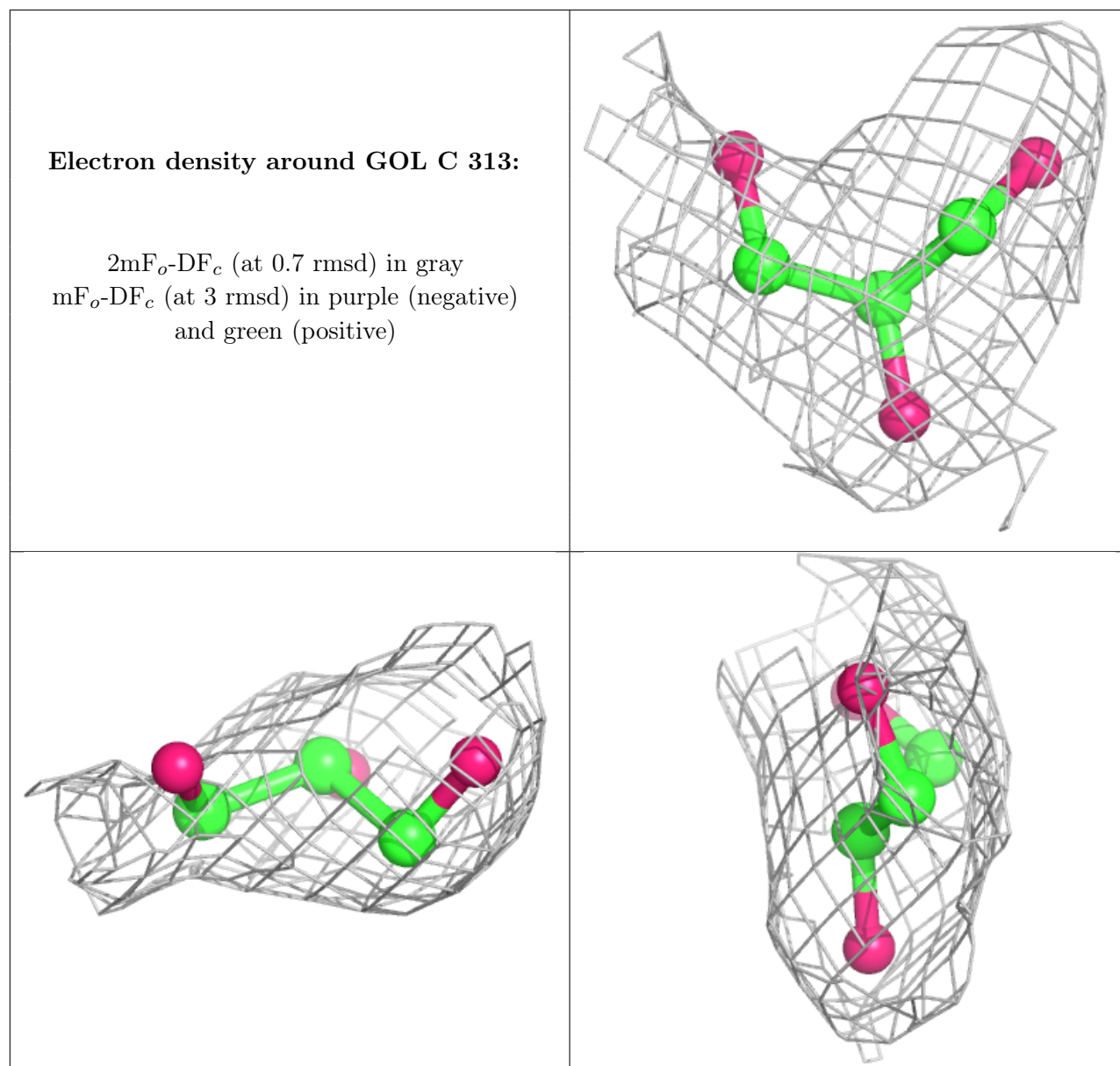
Electron density around PEG A 338:

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

**Electron density around PG4 A 322:**

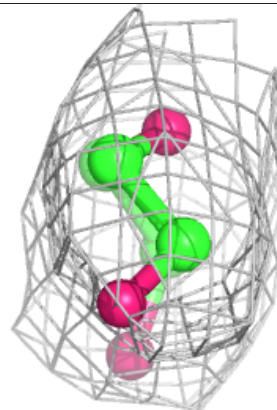
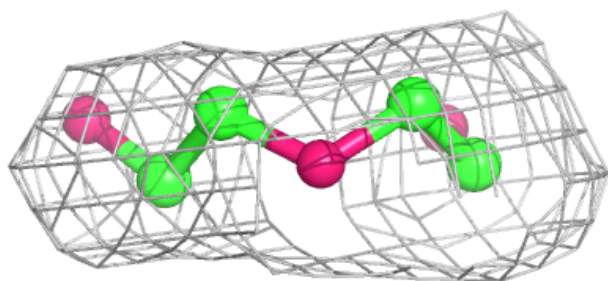
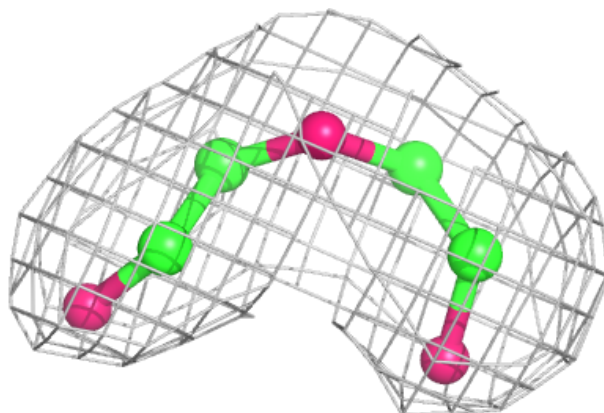
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



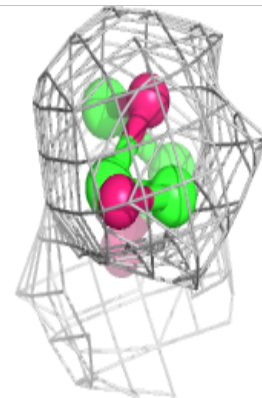
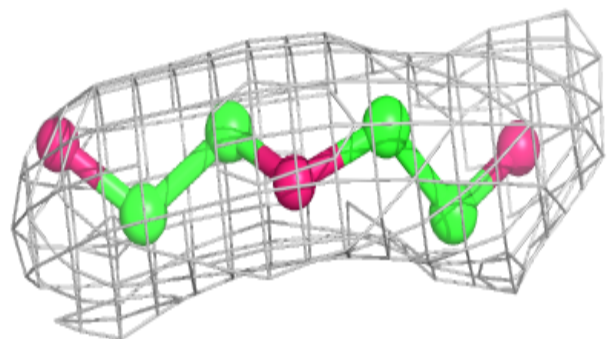
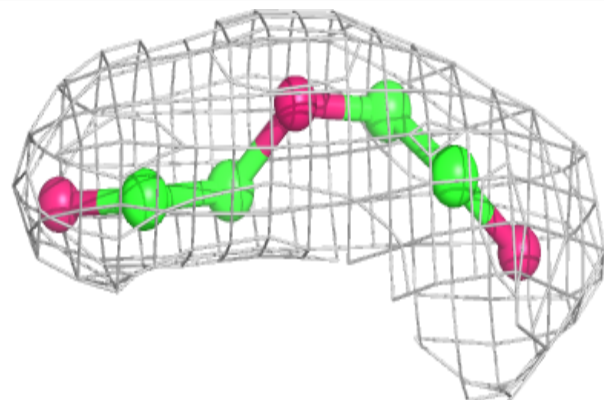


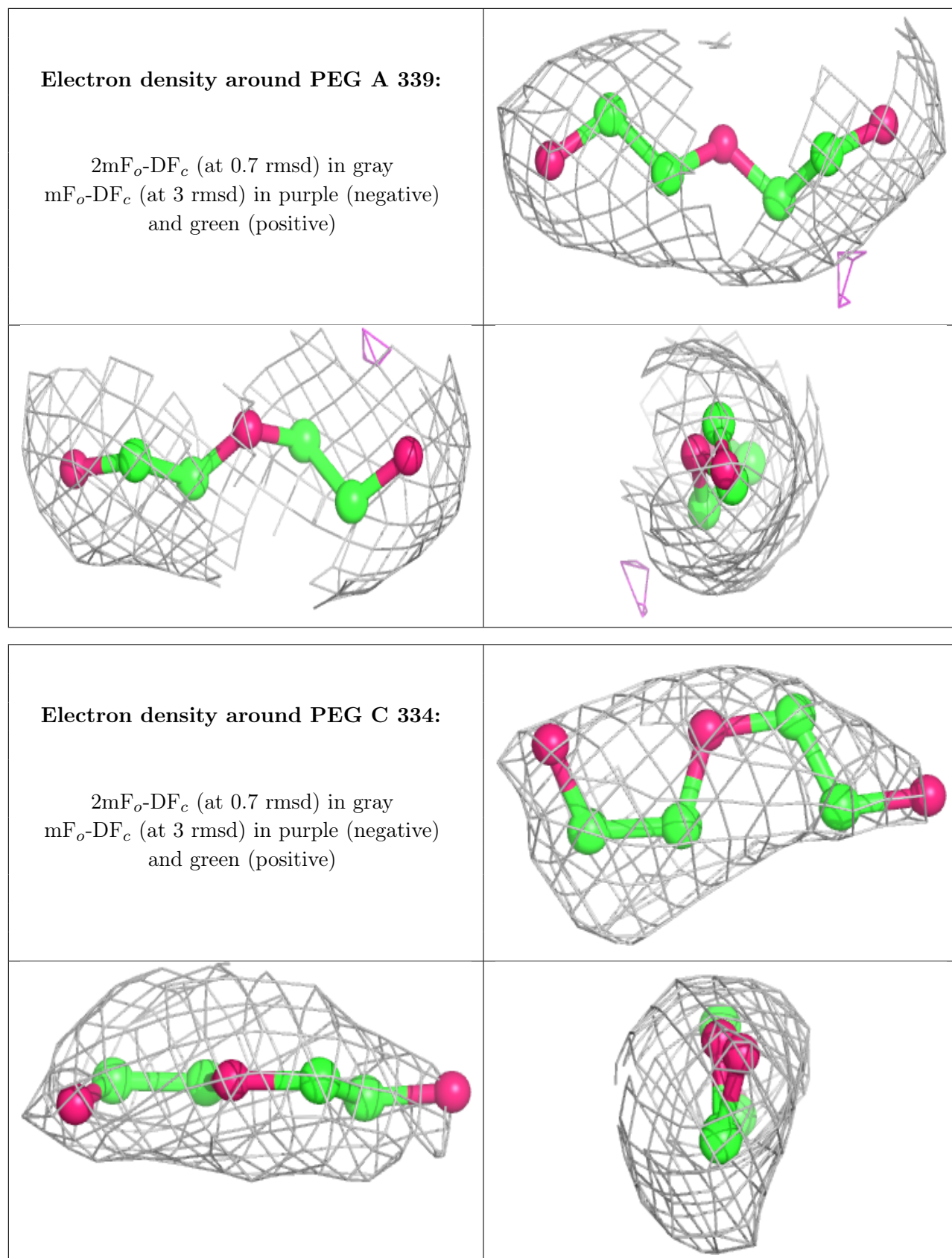
Electron density around PEG B 130:

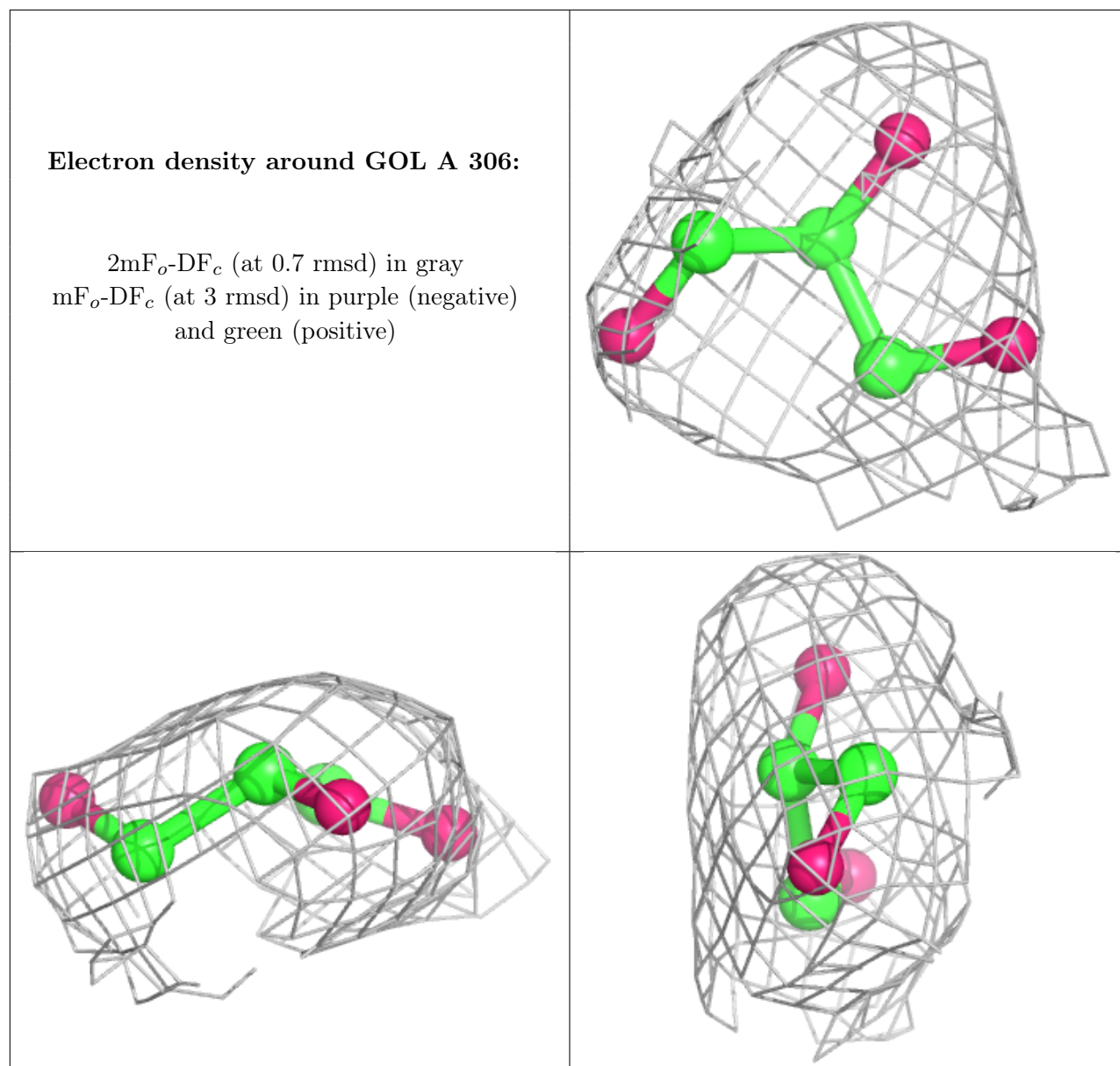
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PEG C 332:**

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

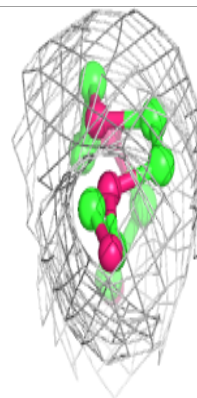
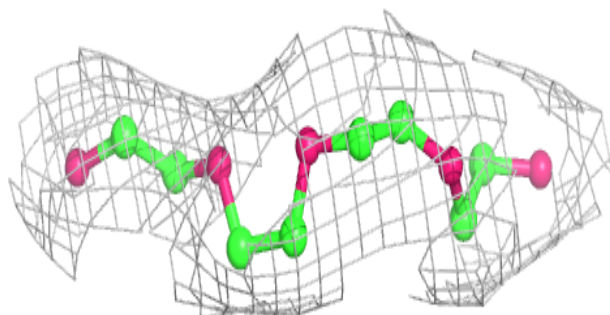
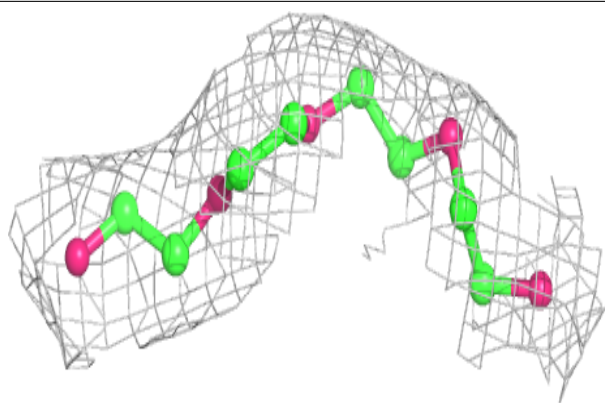




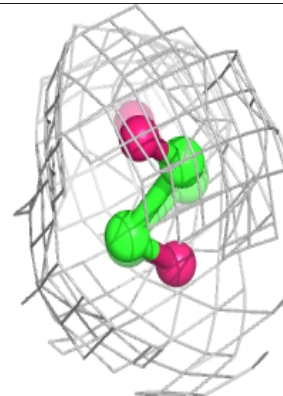
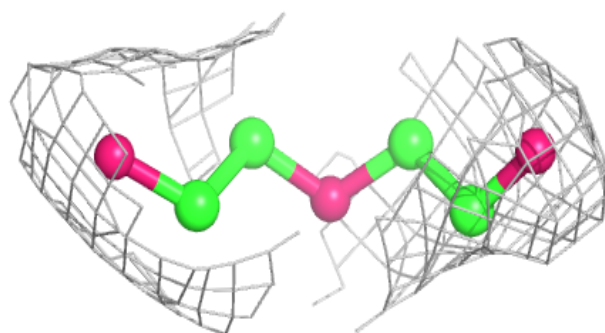
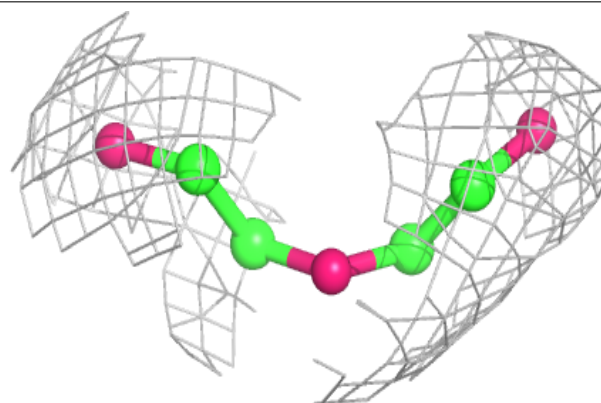


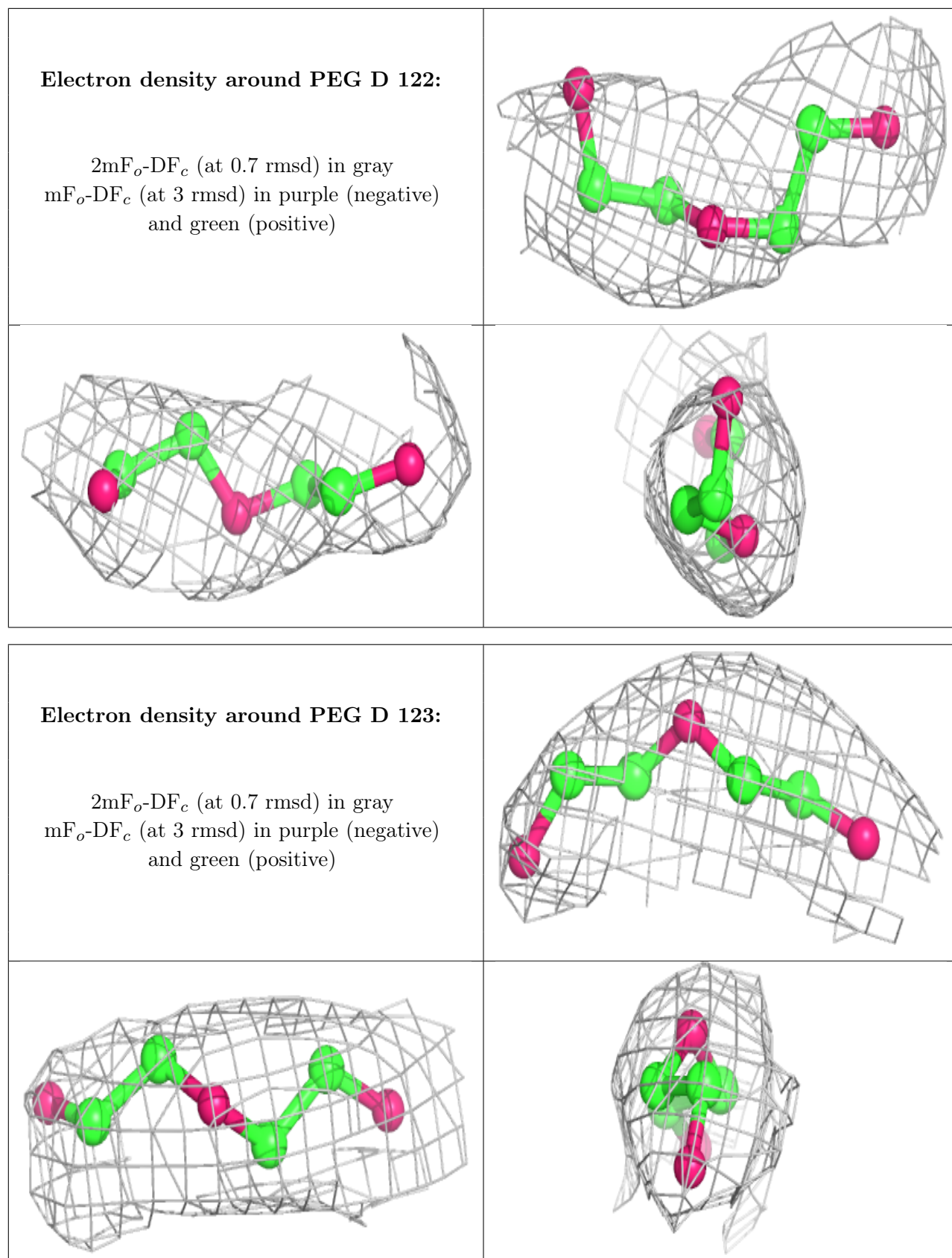
Electron density around PG4 E 114:

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

**Electron density around PEG D 121:**

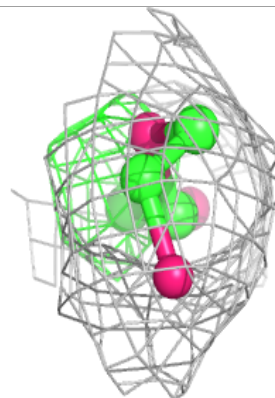
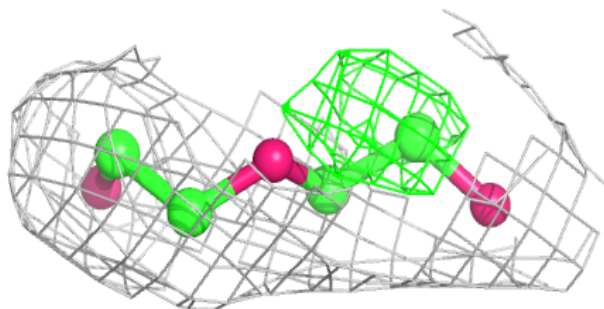
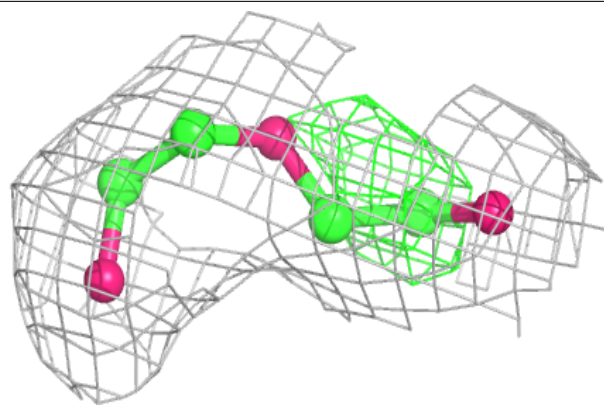
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



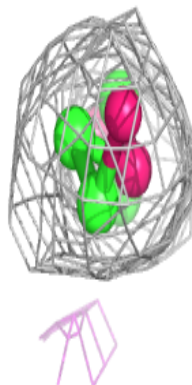
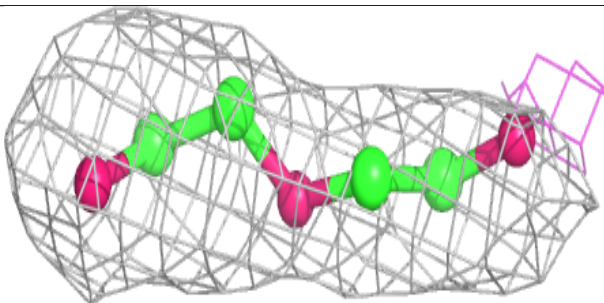
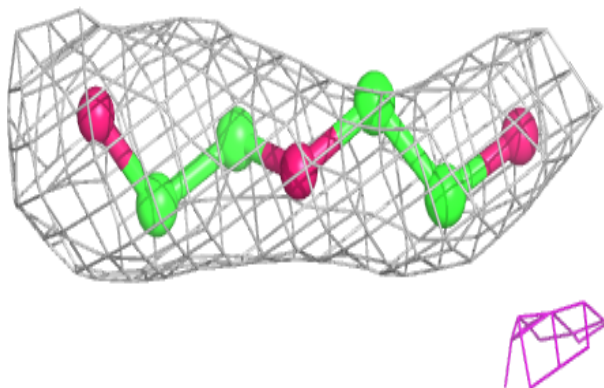


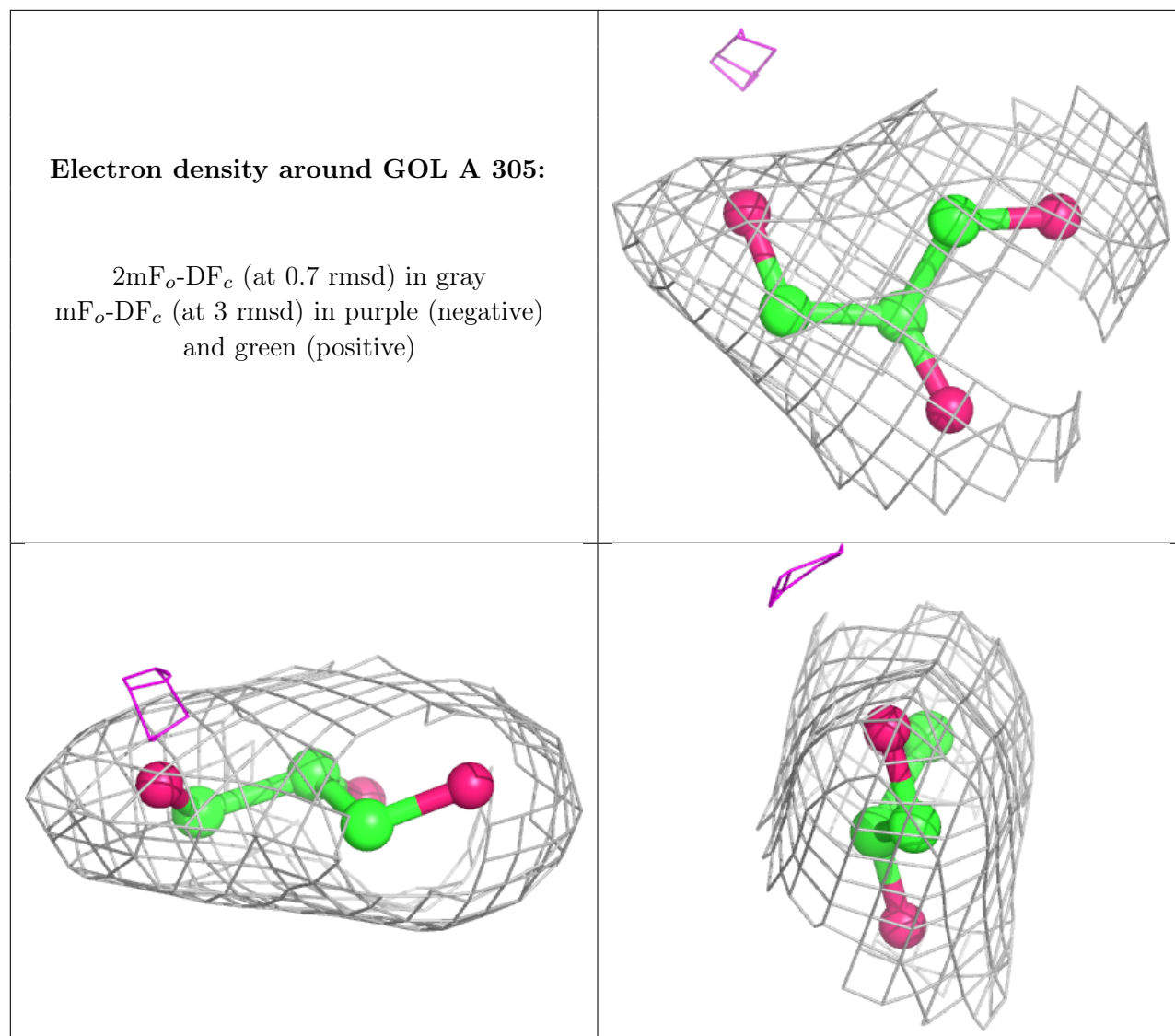
Electron density around PEG A 330:

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

**Electron density around PEG D 128:**

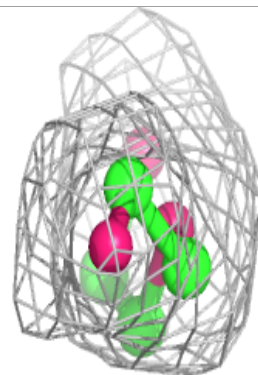
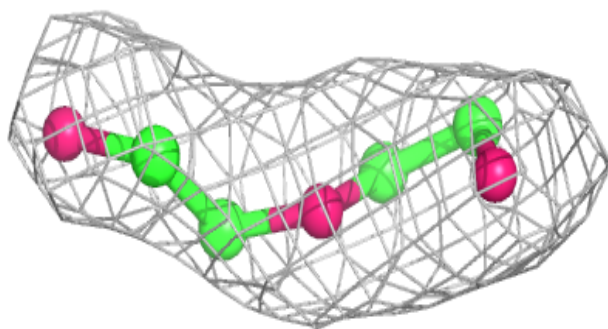
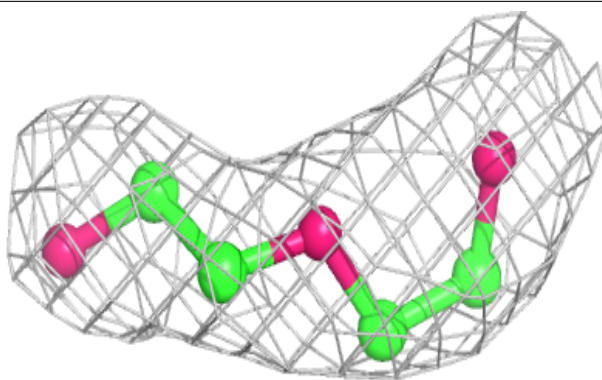
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



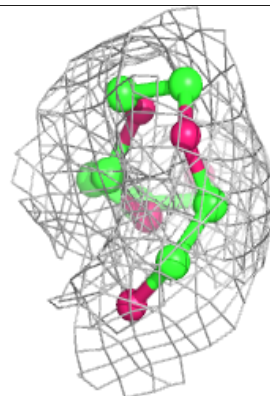
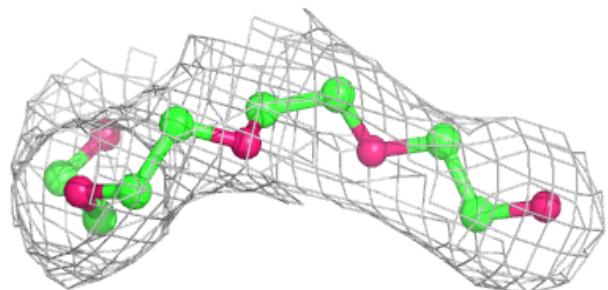
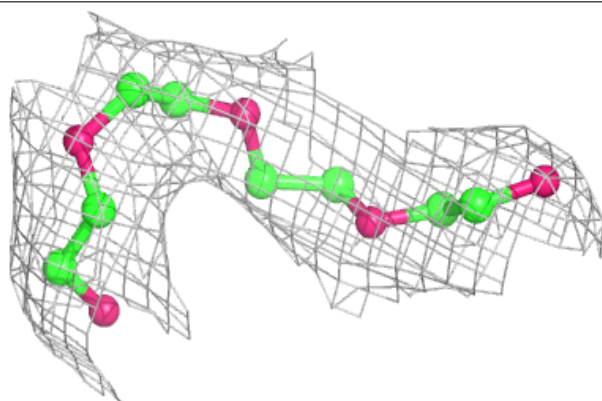


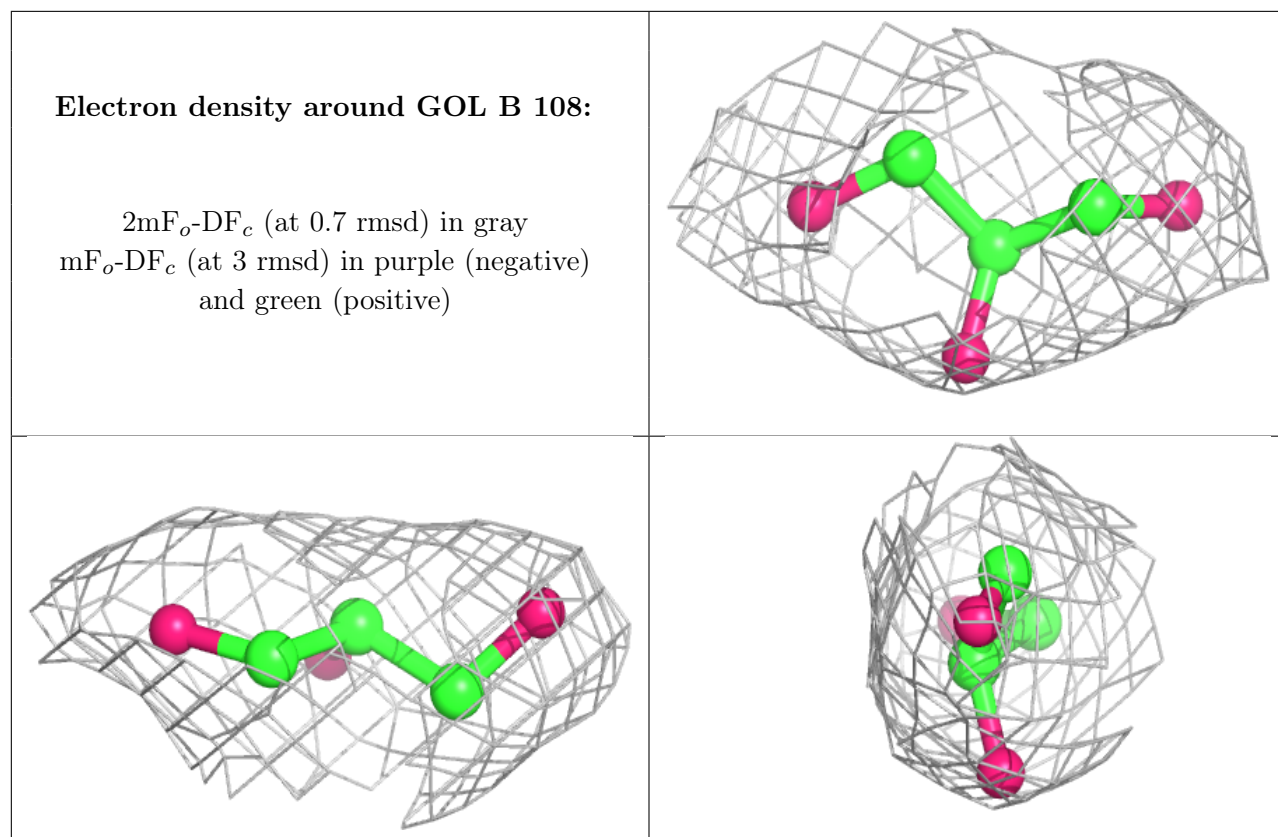
Electron density around PEG B 132:

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

**Electron density around PG4 C 321:**

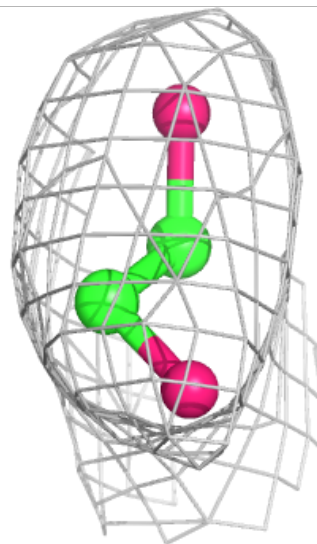
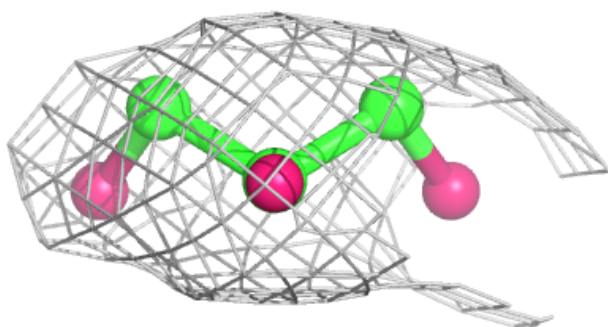
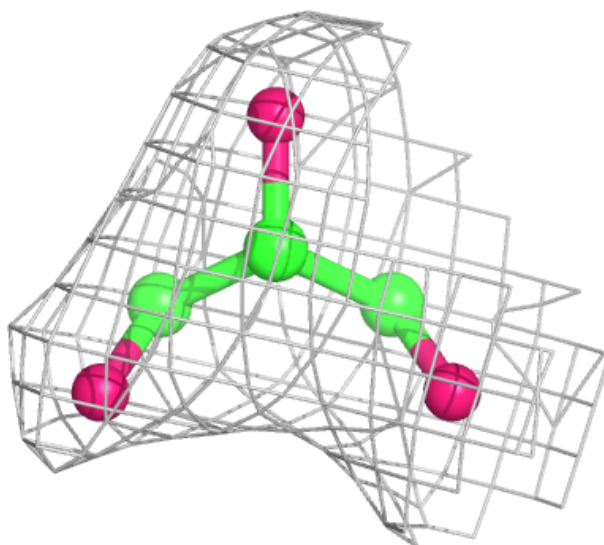
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

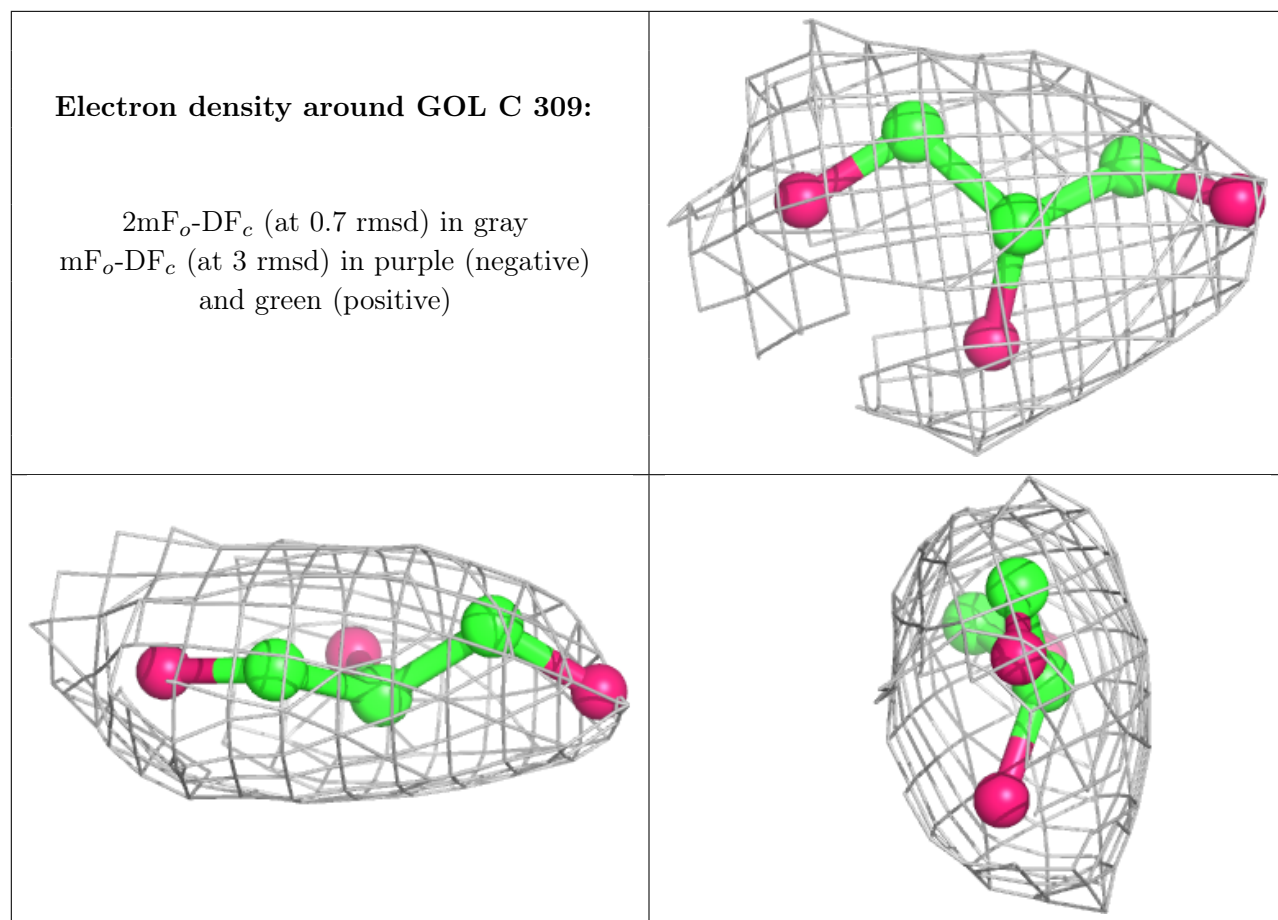




Electron density around GOL C 314:

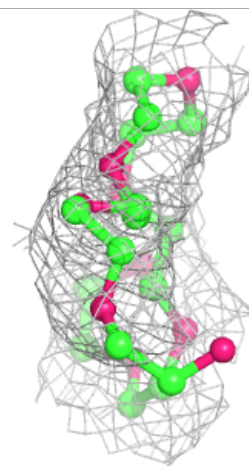
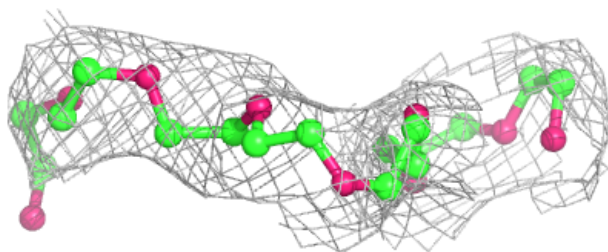
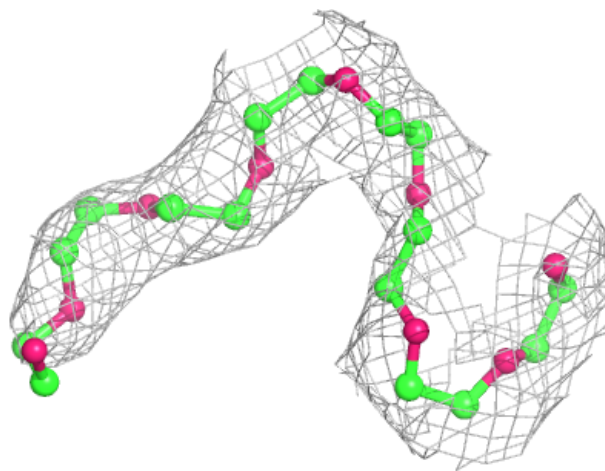
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





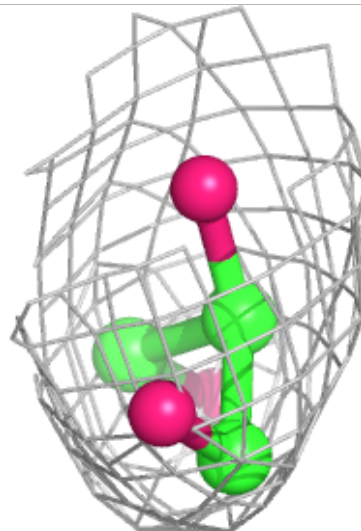
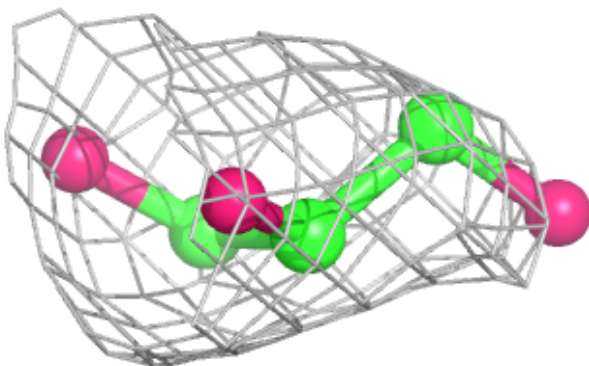
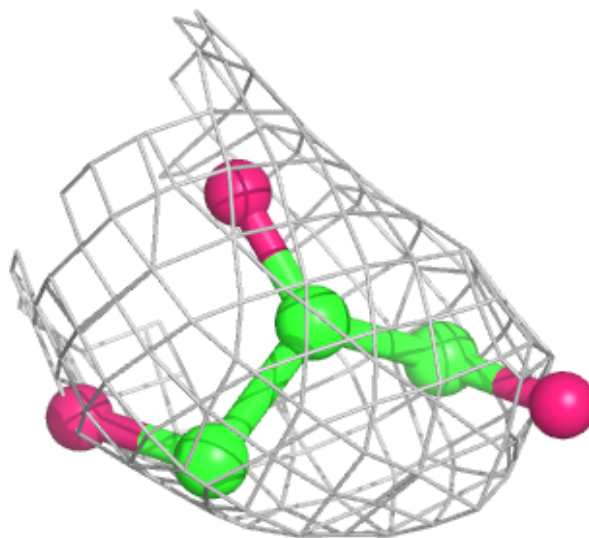
Electron density around PE8 B 136:

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



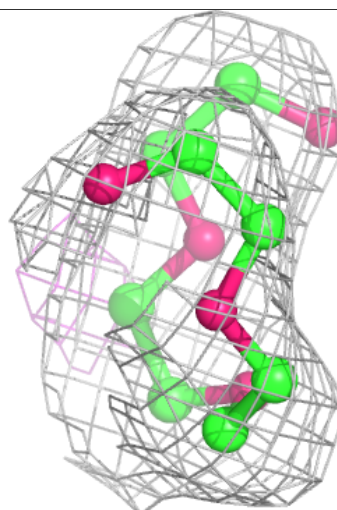
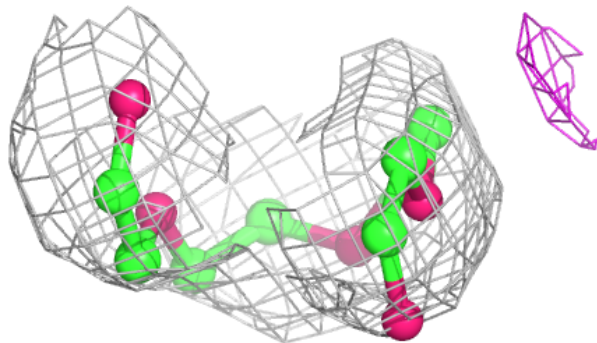
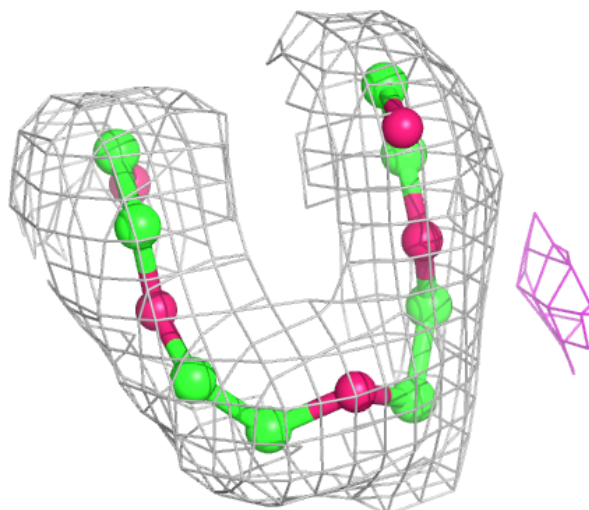
Electron density around GOL C 310:

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



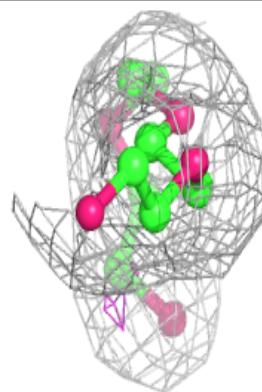
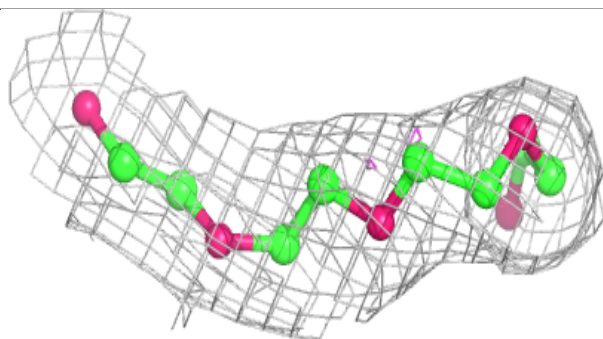
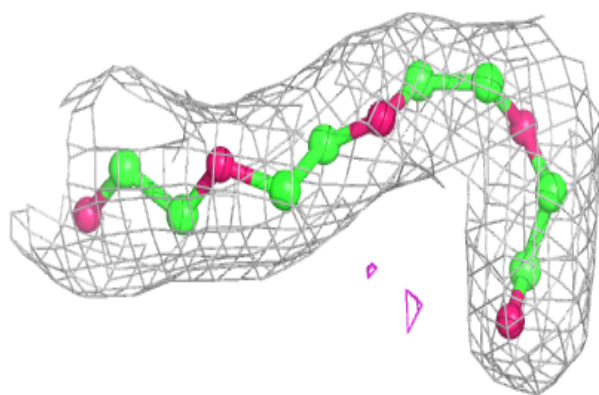
Electron density around PG4 A 369:

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

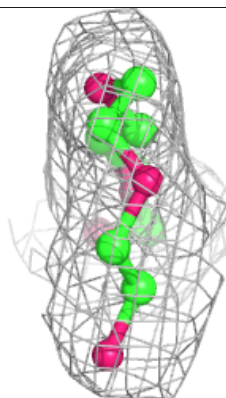
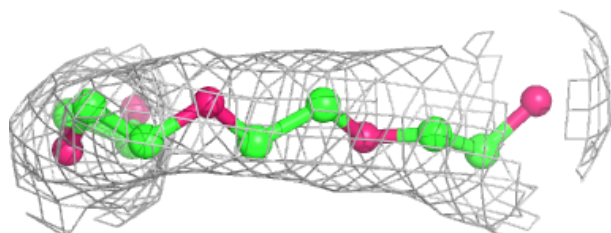
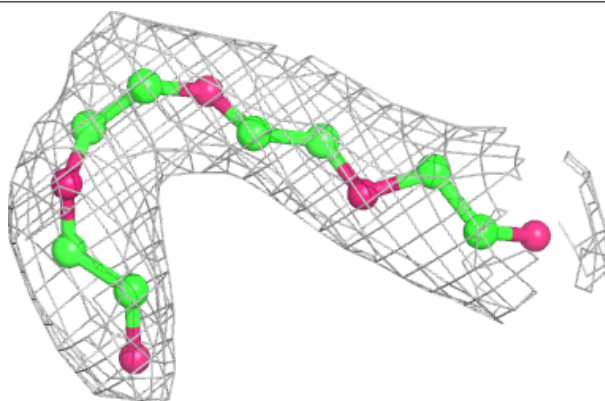


Electron density around PG4 A 320:

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

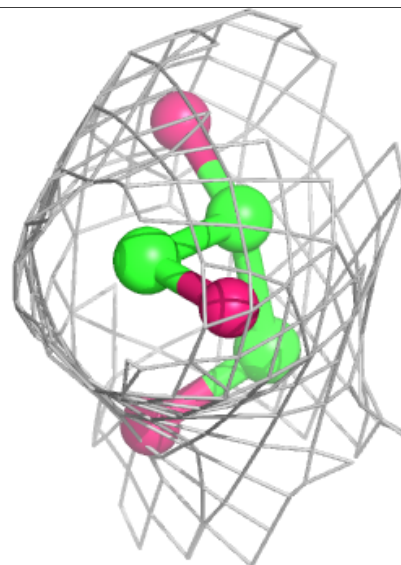
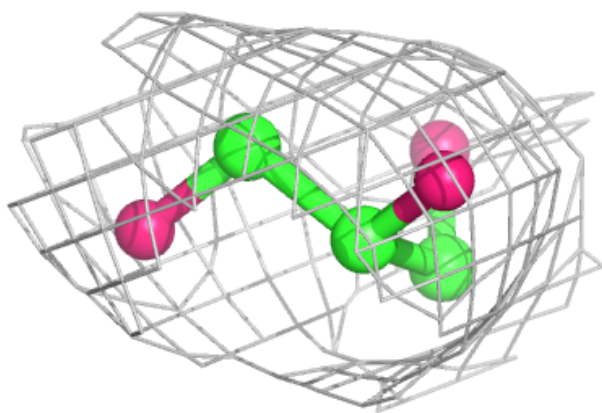
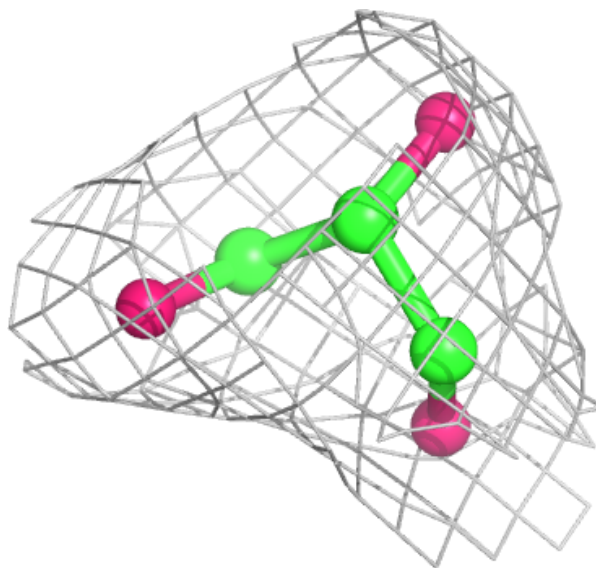
**Electron density around PG4 B 116:**

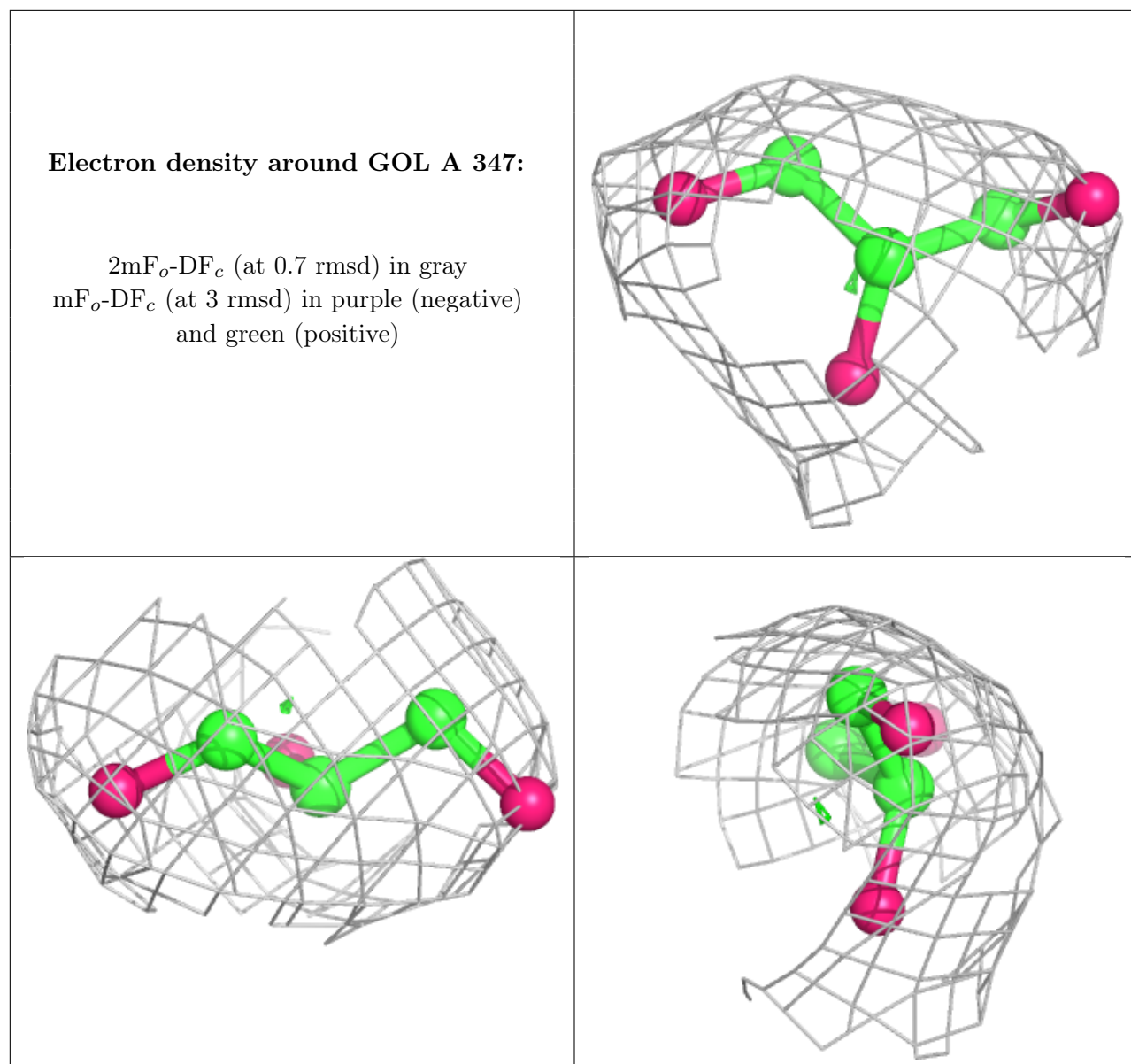
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GOL E 113:

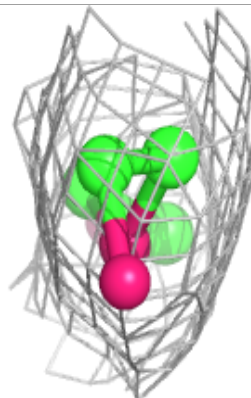
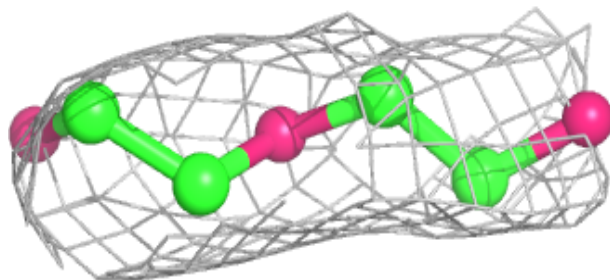
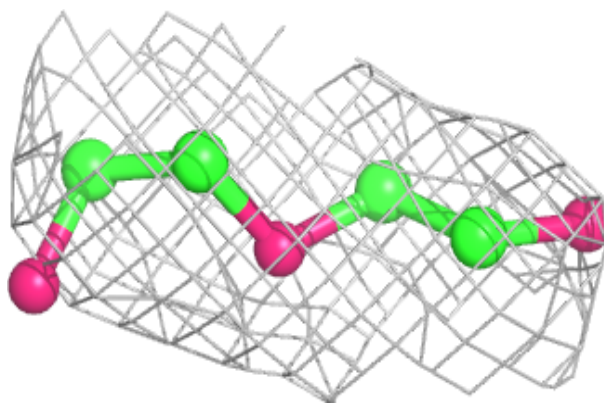
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



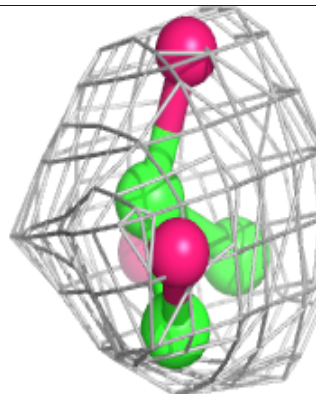
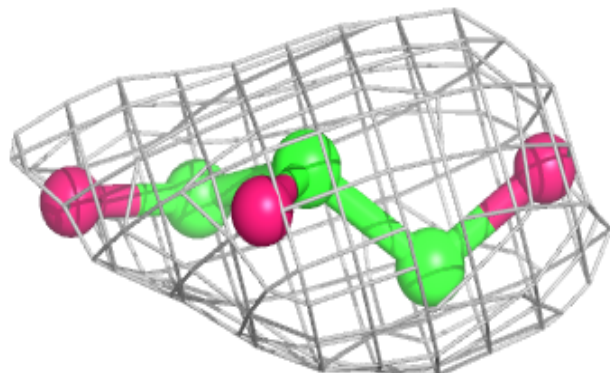
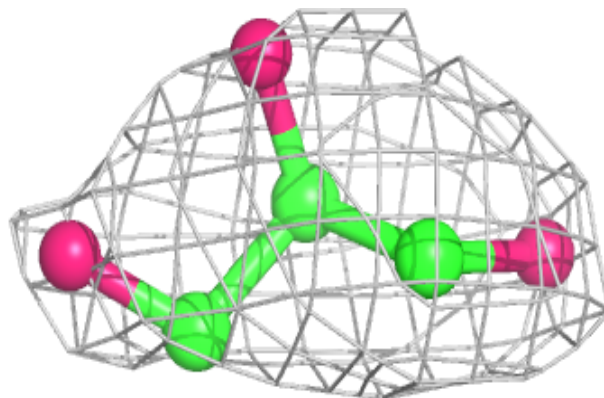


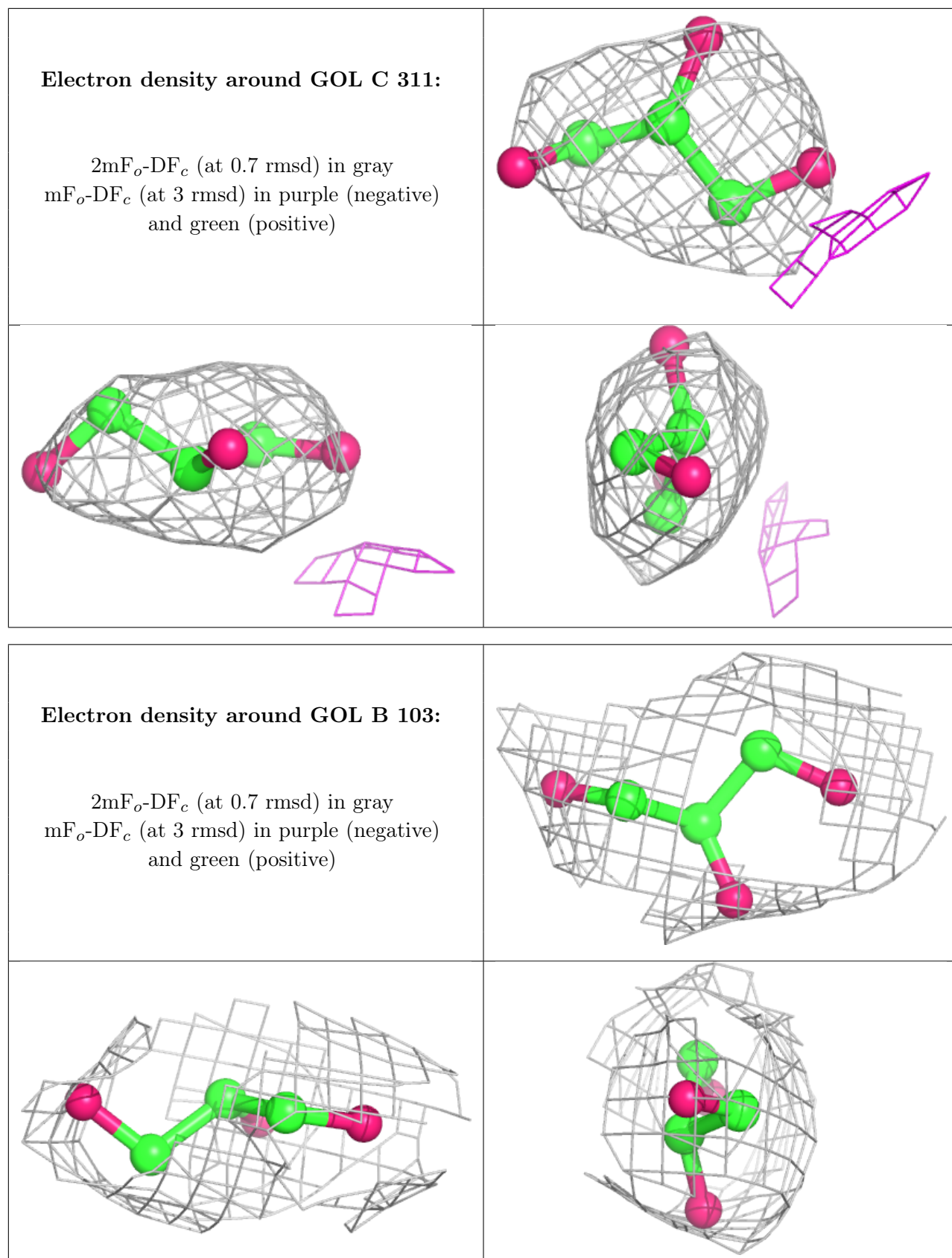
Electron density around PEG D 126:

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

**Electron density around GOL C 304:**

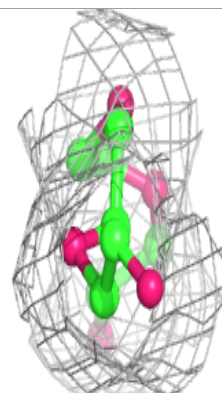
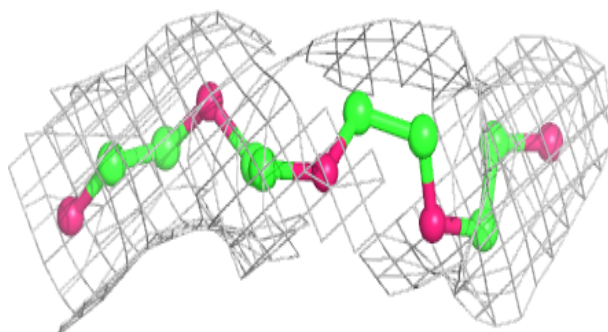
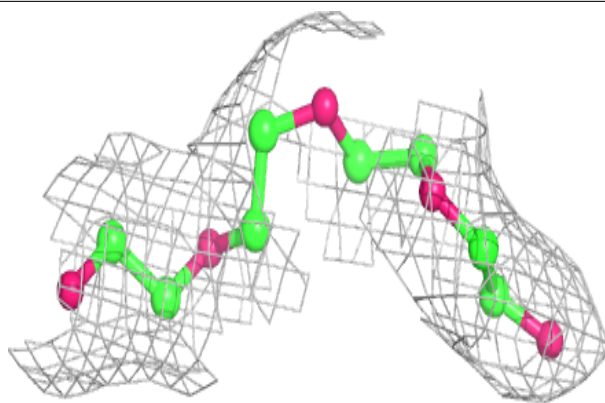
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



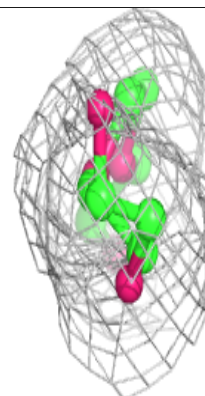
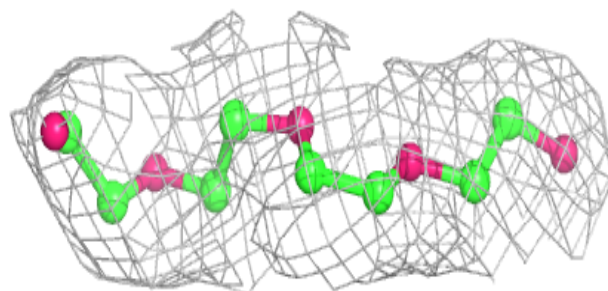
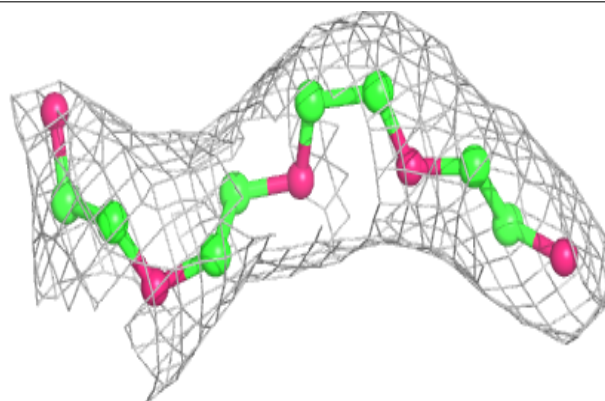


Electron density around PG4 C 323:

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

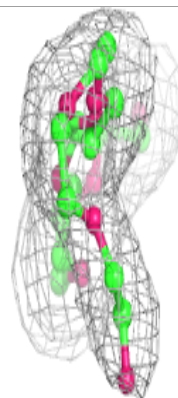
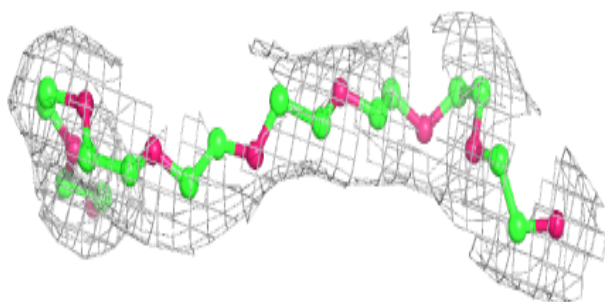
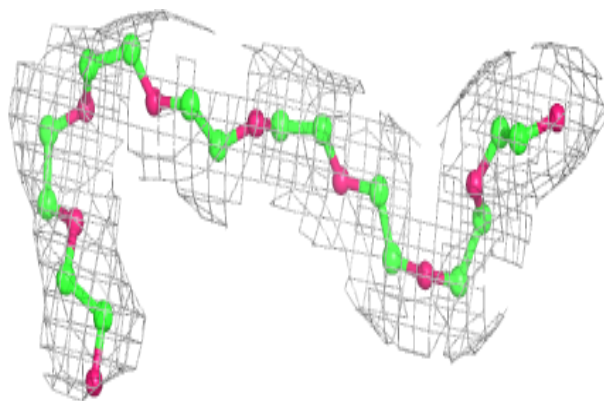
**Electron density around PG4 A 319:**

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

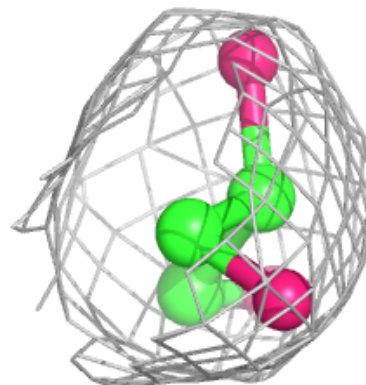
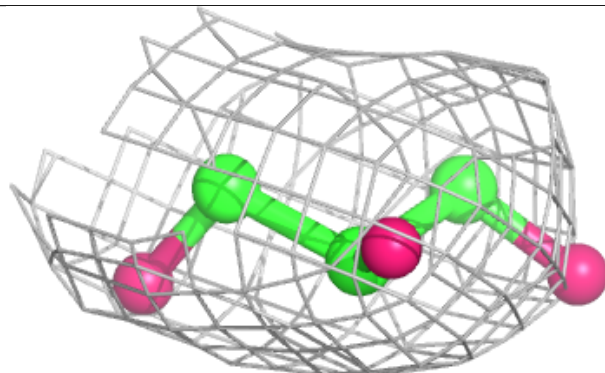
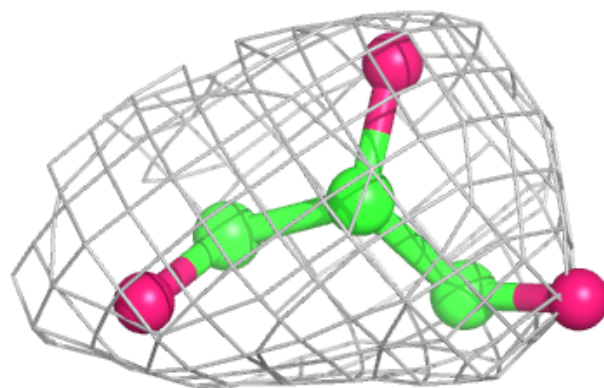


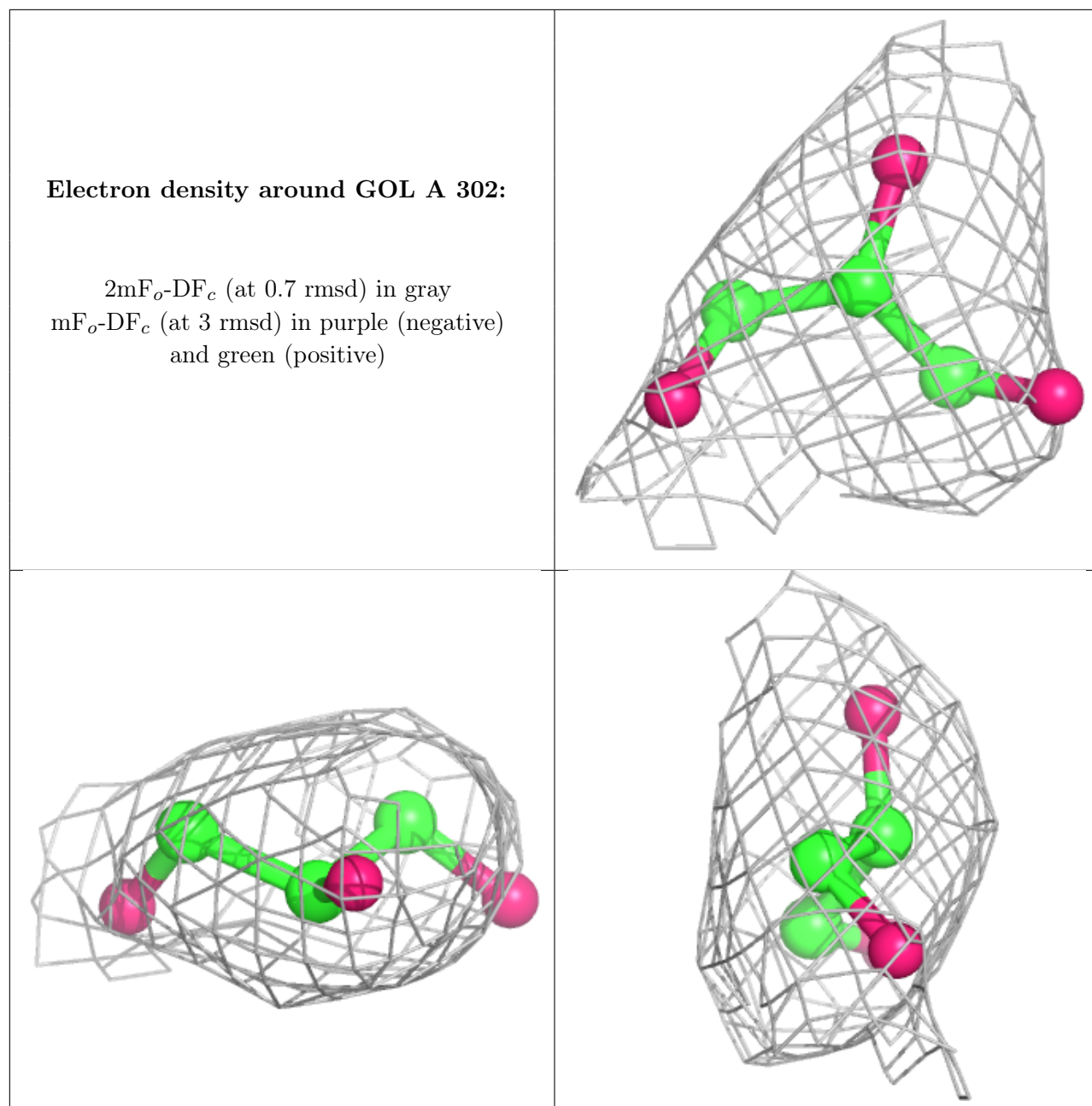
Electron density around PE8 C 335:

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

**Electron density around GOL B 104:**

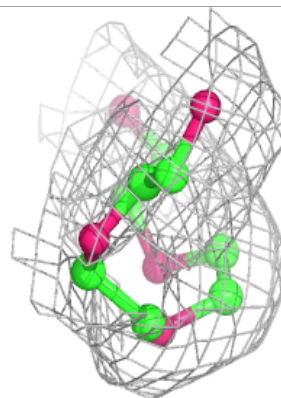
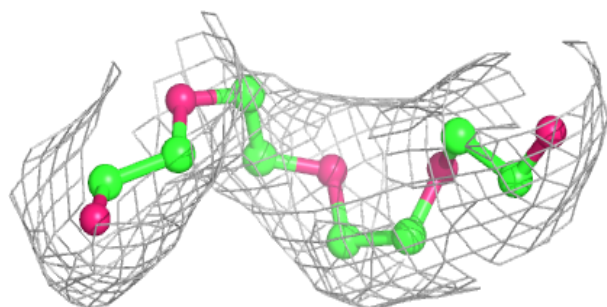
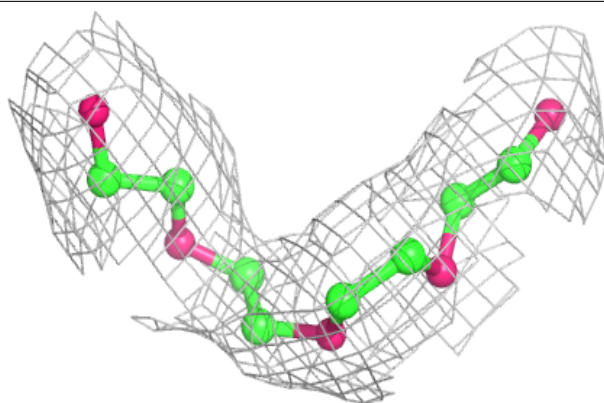
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



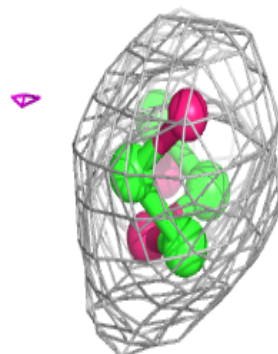
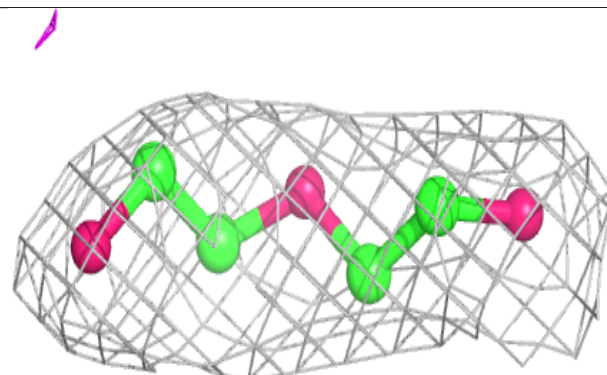
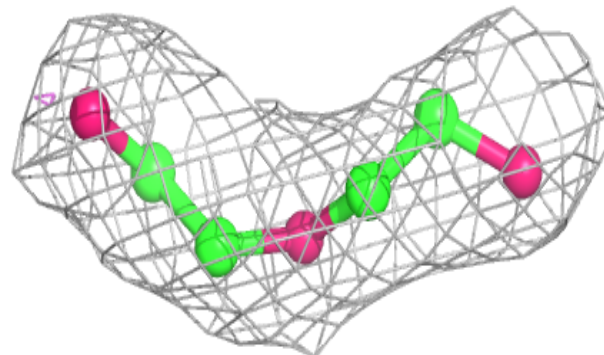


Electron density around PG4 B 121:

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

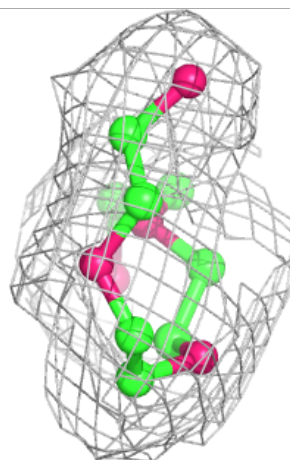
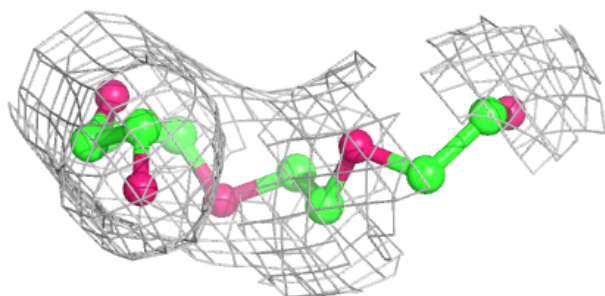
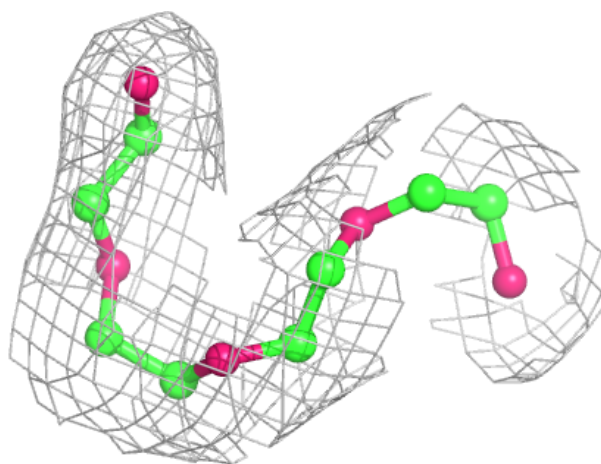
**Electron density around PEG A 353:**

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



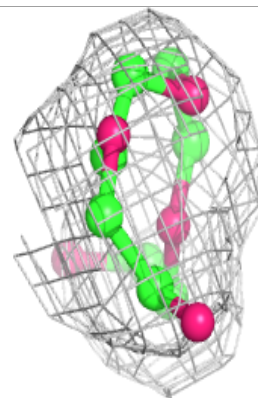
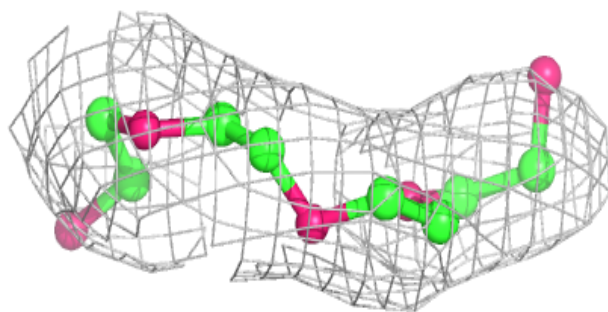
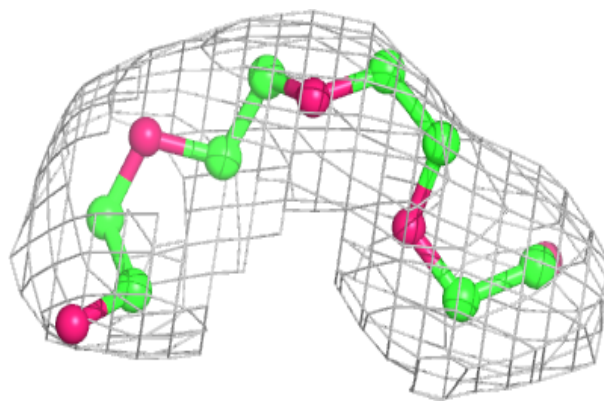
Electron density around PG4 B 123:

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

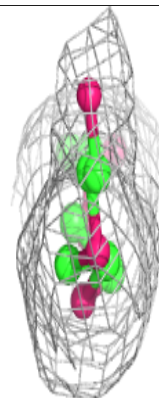
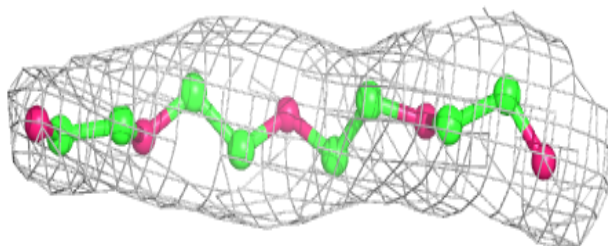
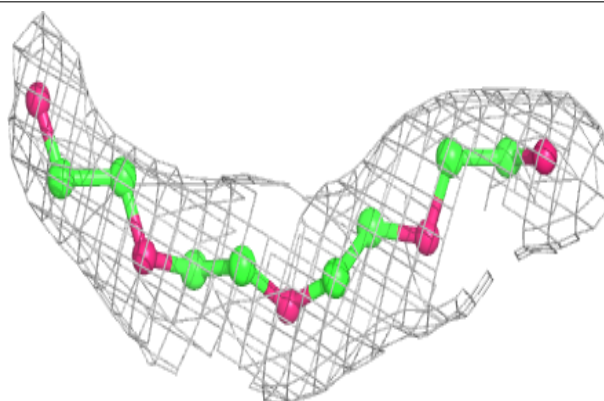


Electron density around PG4 B 125:

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

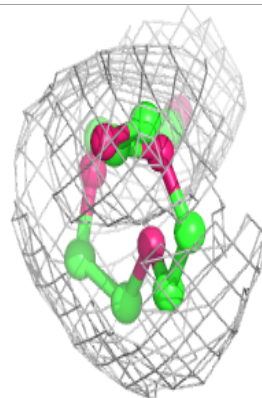
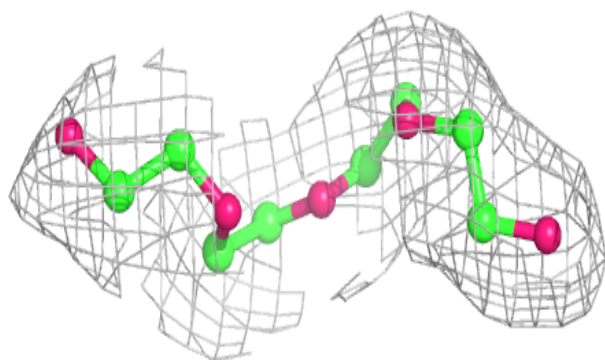
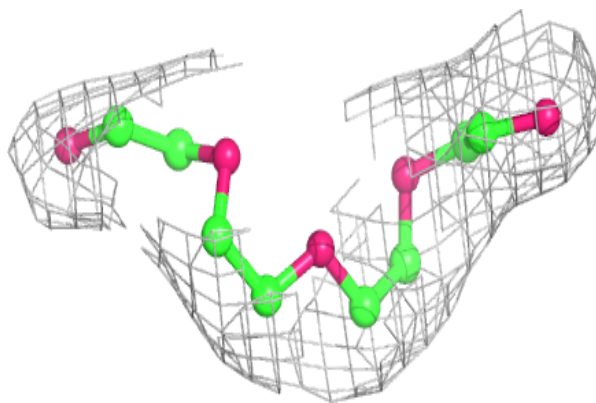
**Electron density around PG4 B 117:**

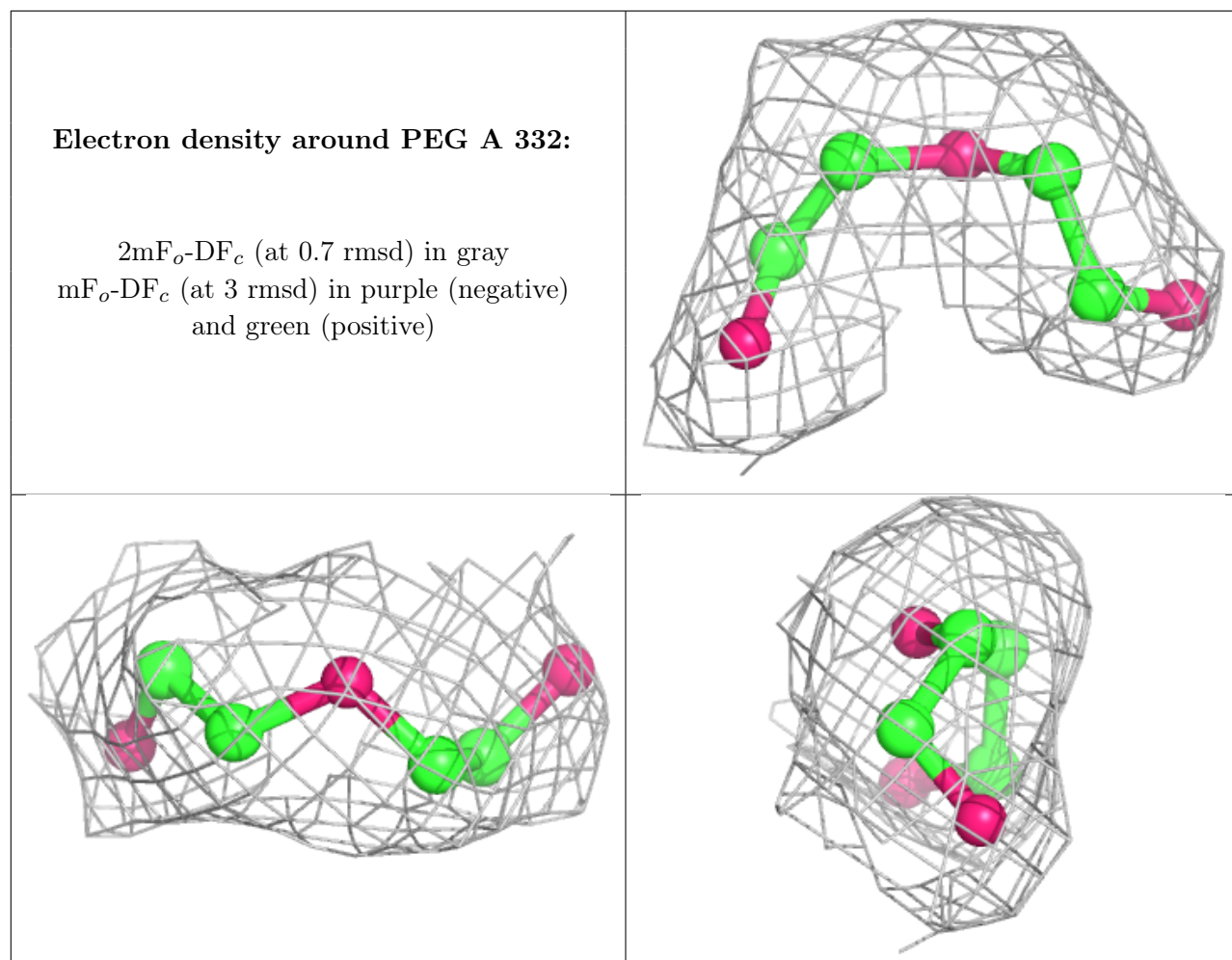
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PG4 A 367:

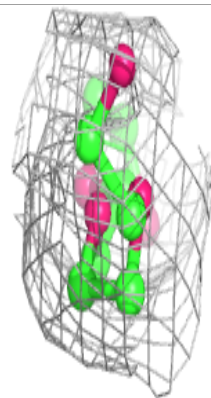
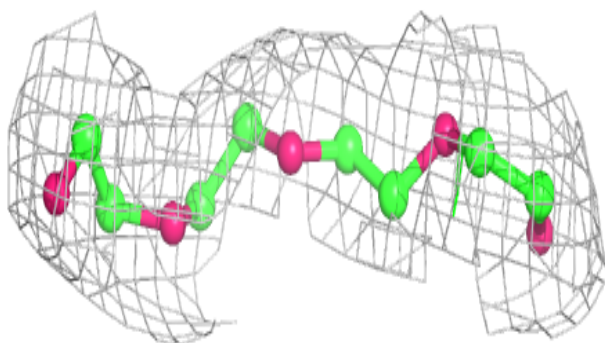
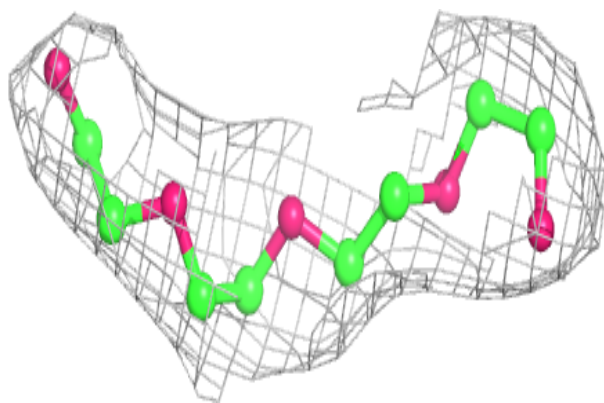
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



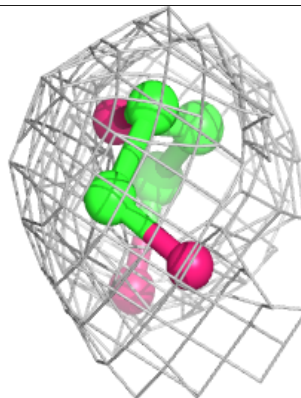
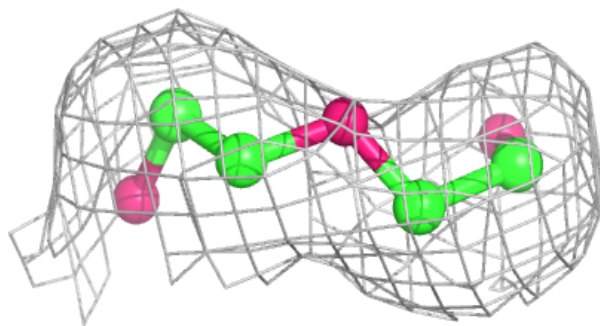
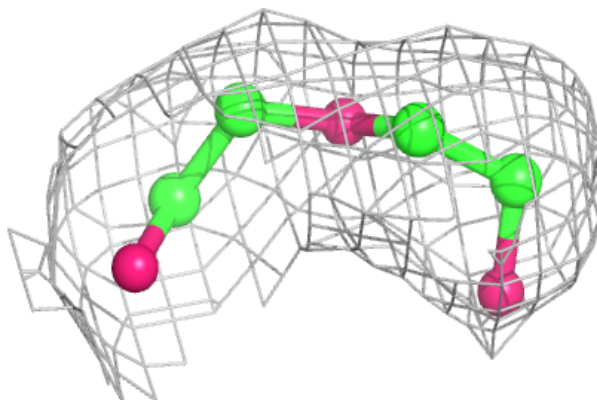


Electron density around PG4 B 119:

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

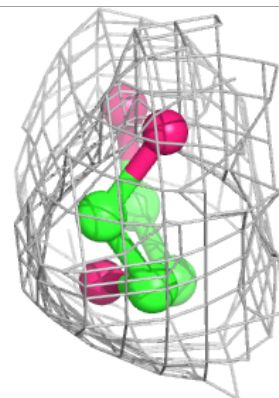
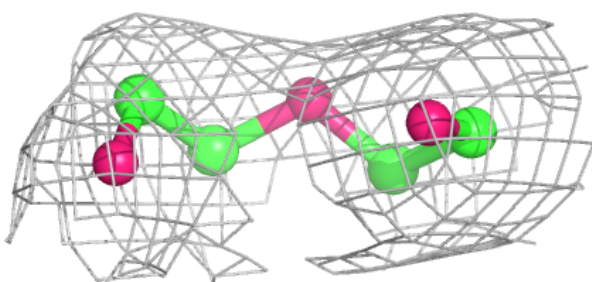
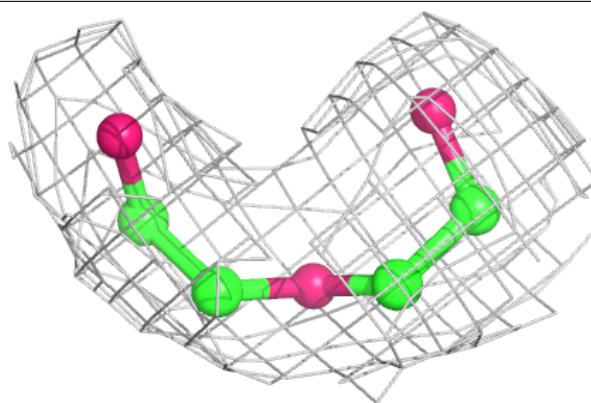
**Electron density around PEG A 334:**

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

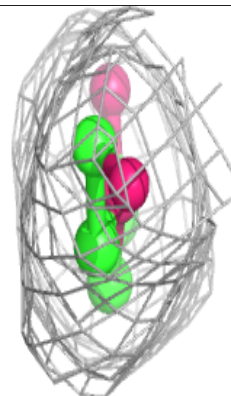
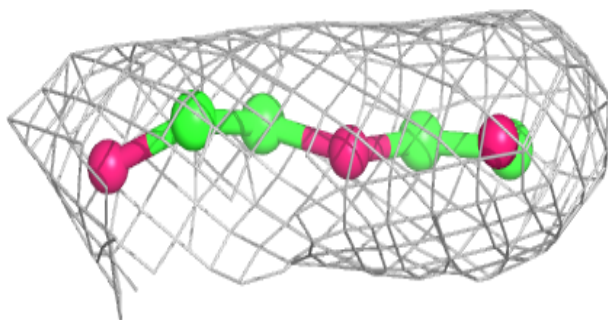
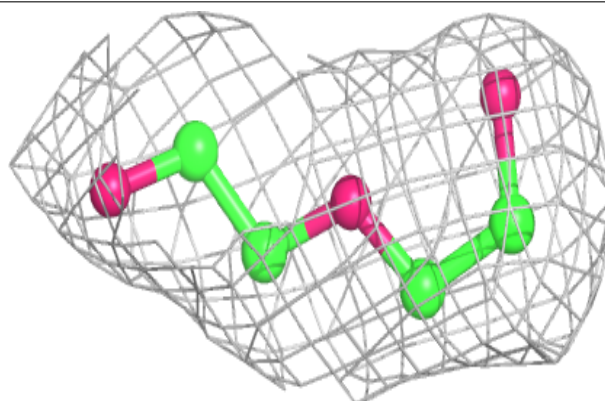


Electron density around PEG C 303:

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

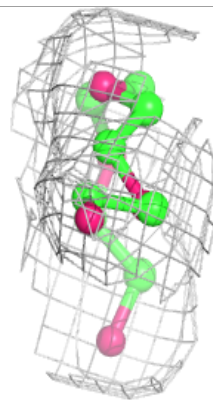
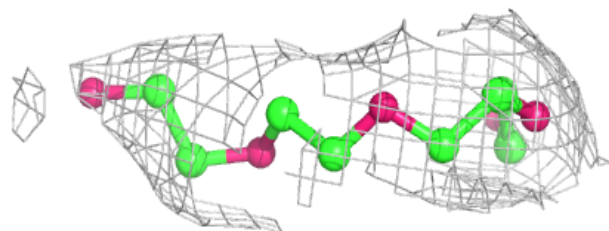
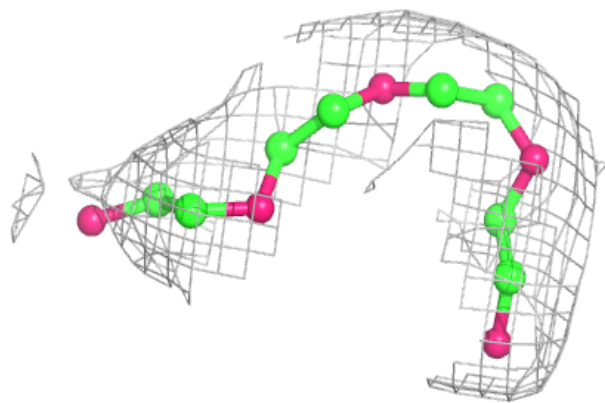
**Electron density around PEG C 327:**

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



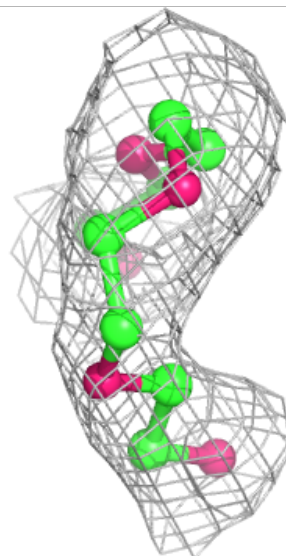
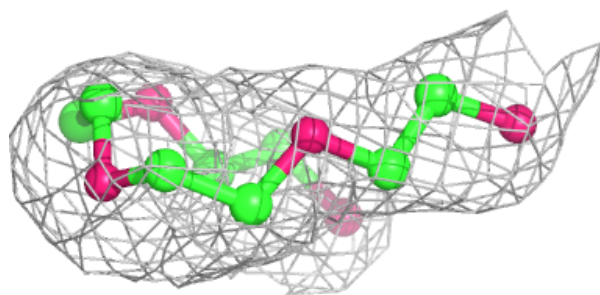
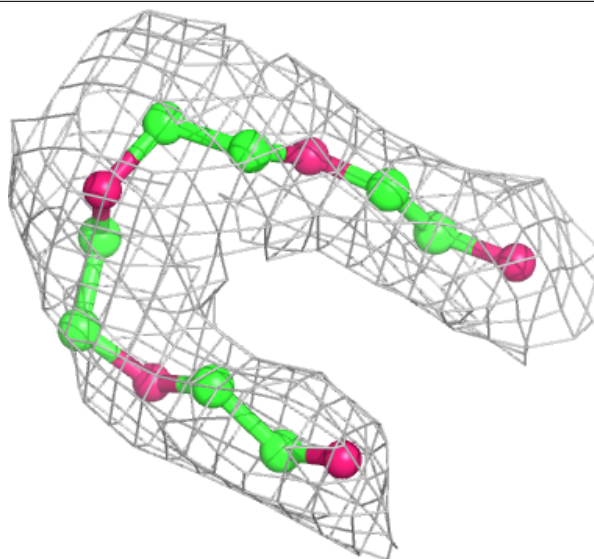
Electron density around PG4 B 122:

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



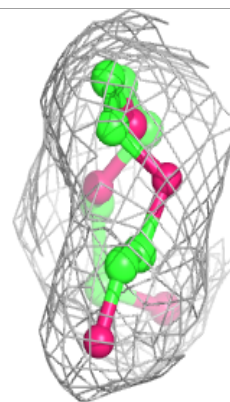
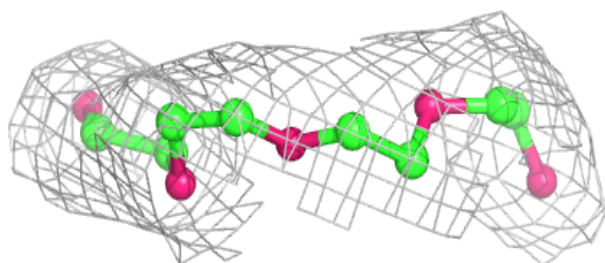
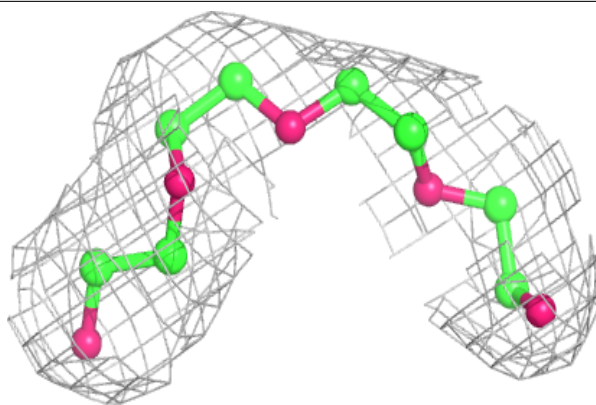
Electron density around PG4 E 107:

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

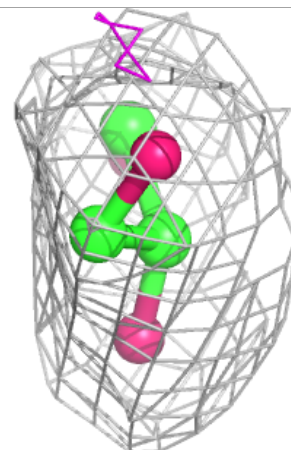
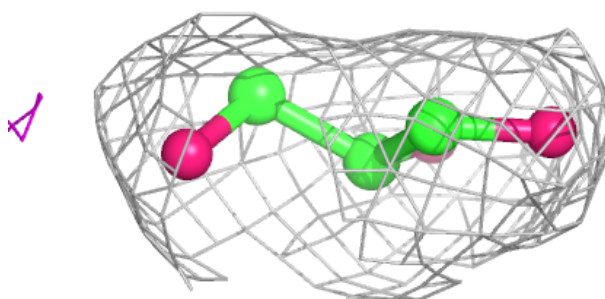
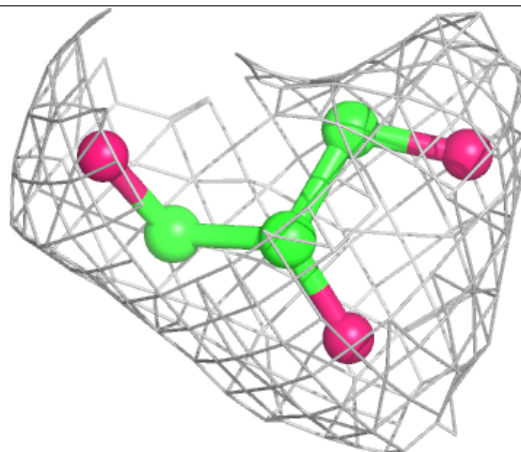


Electron density around PG4 B 124:

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

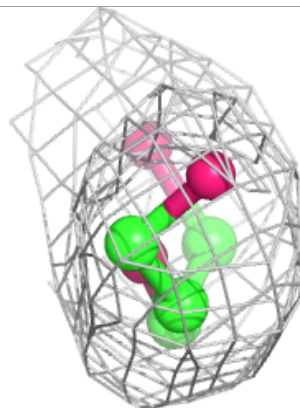
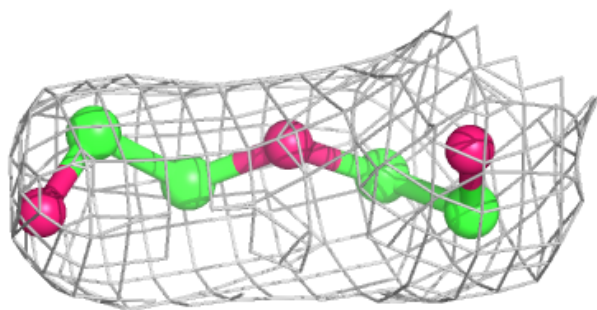
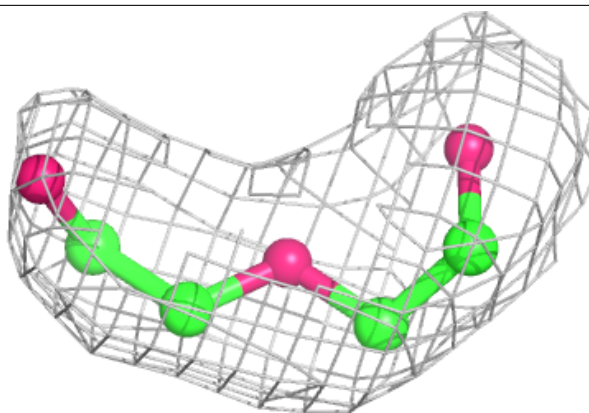
**Electron density around GOL D 109:**

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

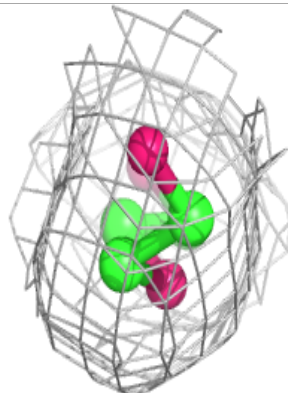
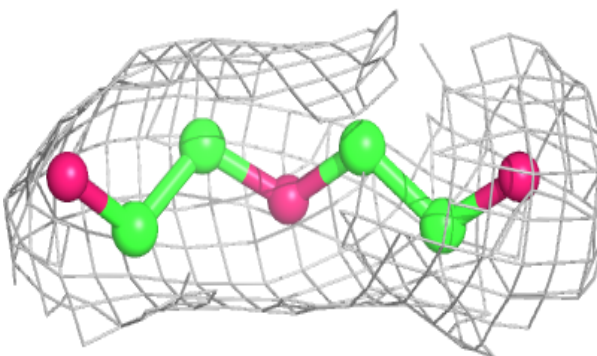
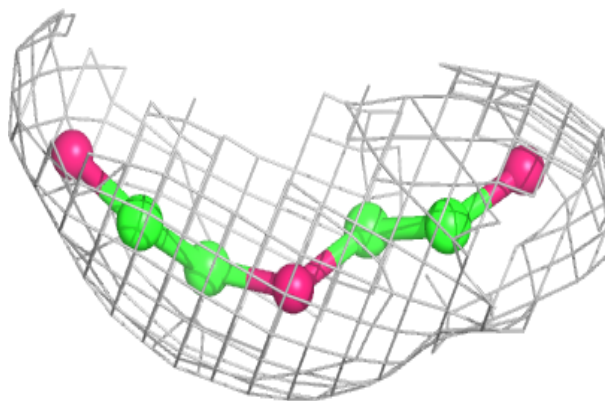


Electron density around PEG C 339:

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

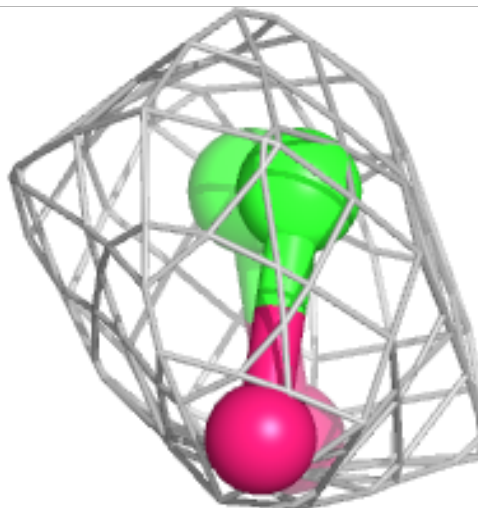
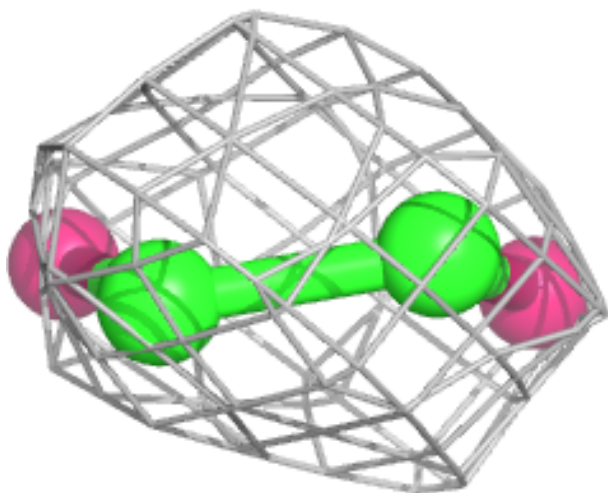
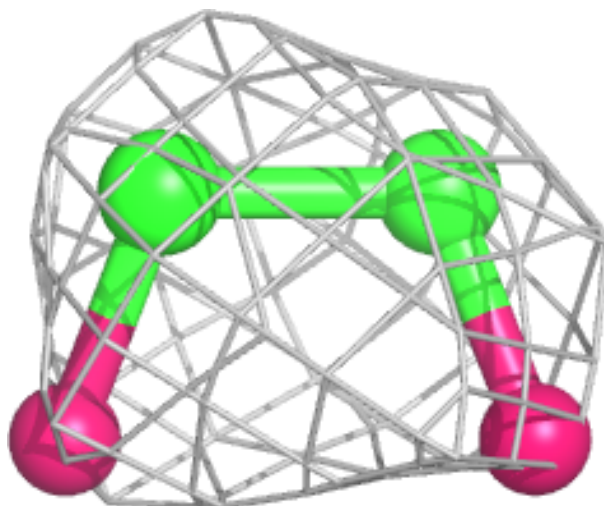
**Electron density around PEG C 346:**

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



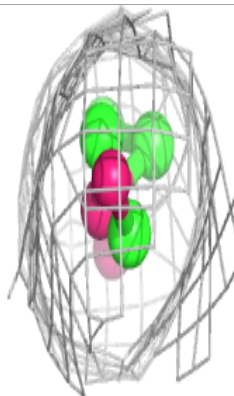
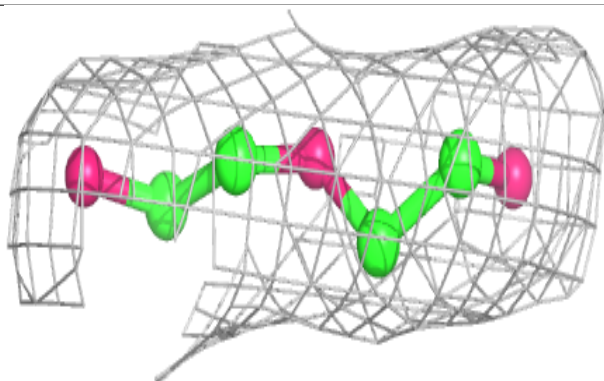
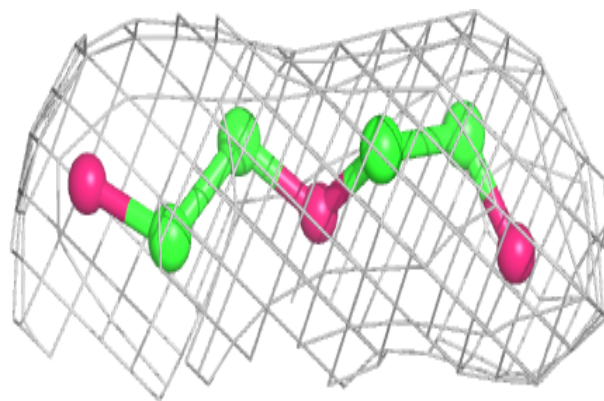
Electron density around EDO B 144:

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

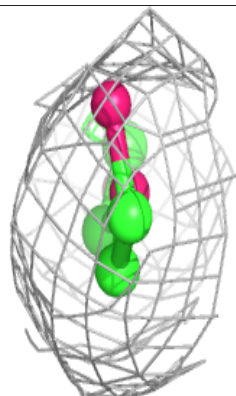
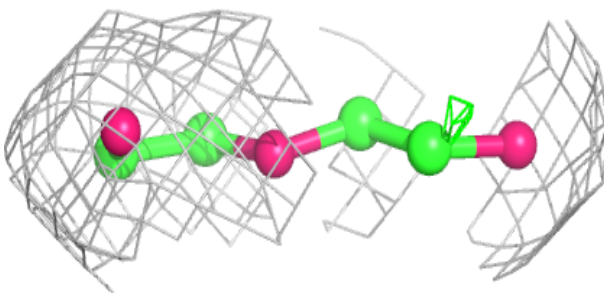
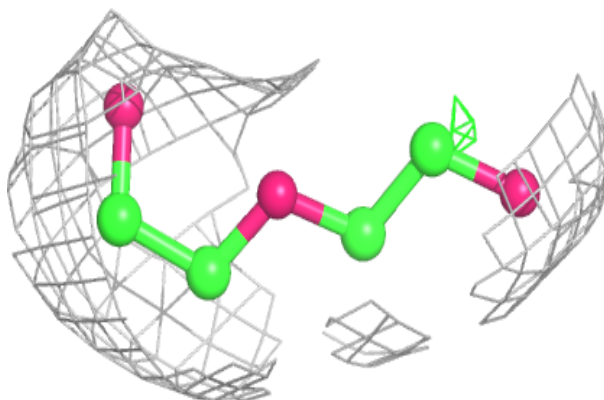


Electron density around PEG A 372:

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

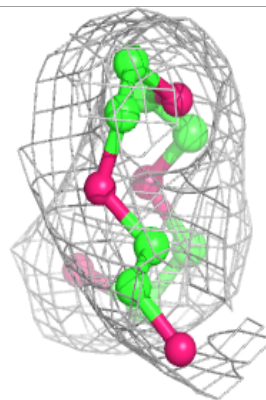
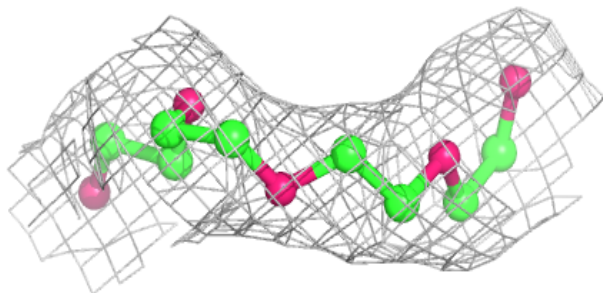
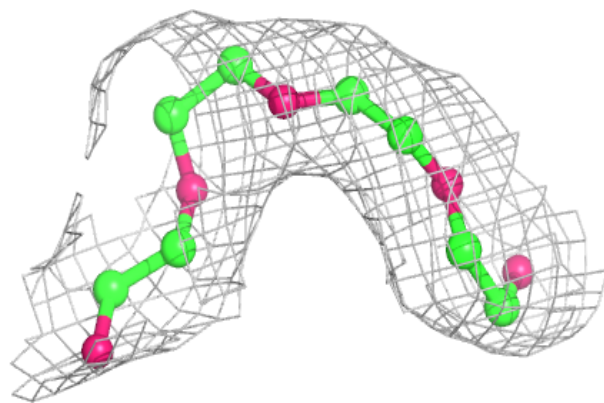
**Electron density around PEG B 126:**

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

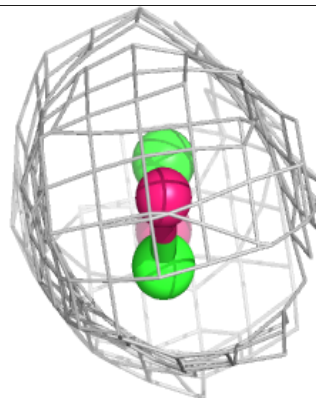
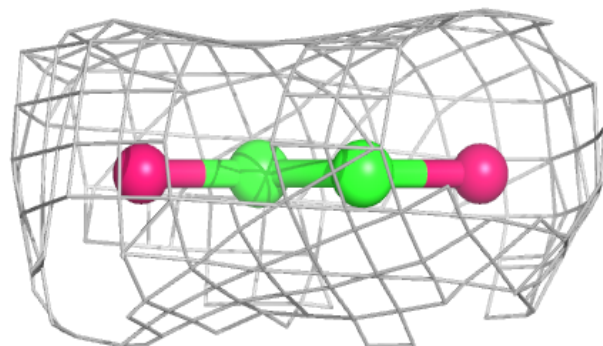
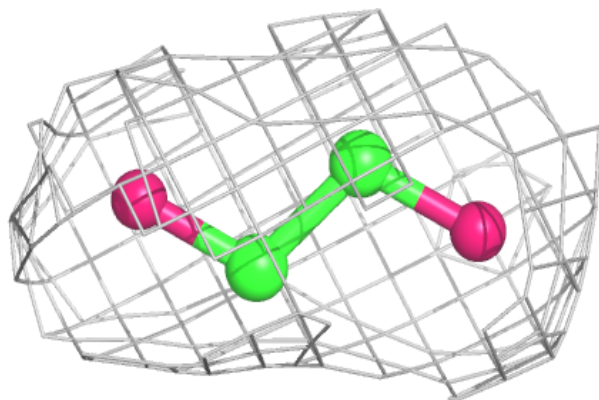


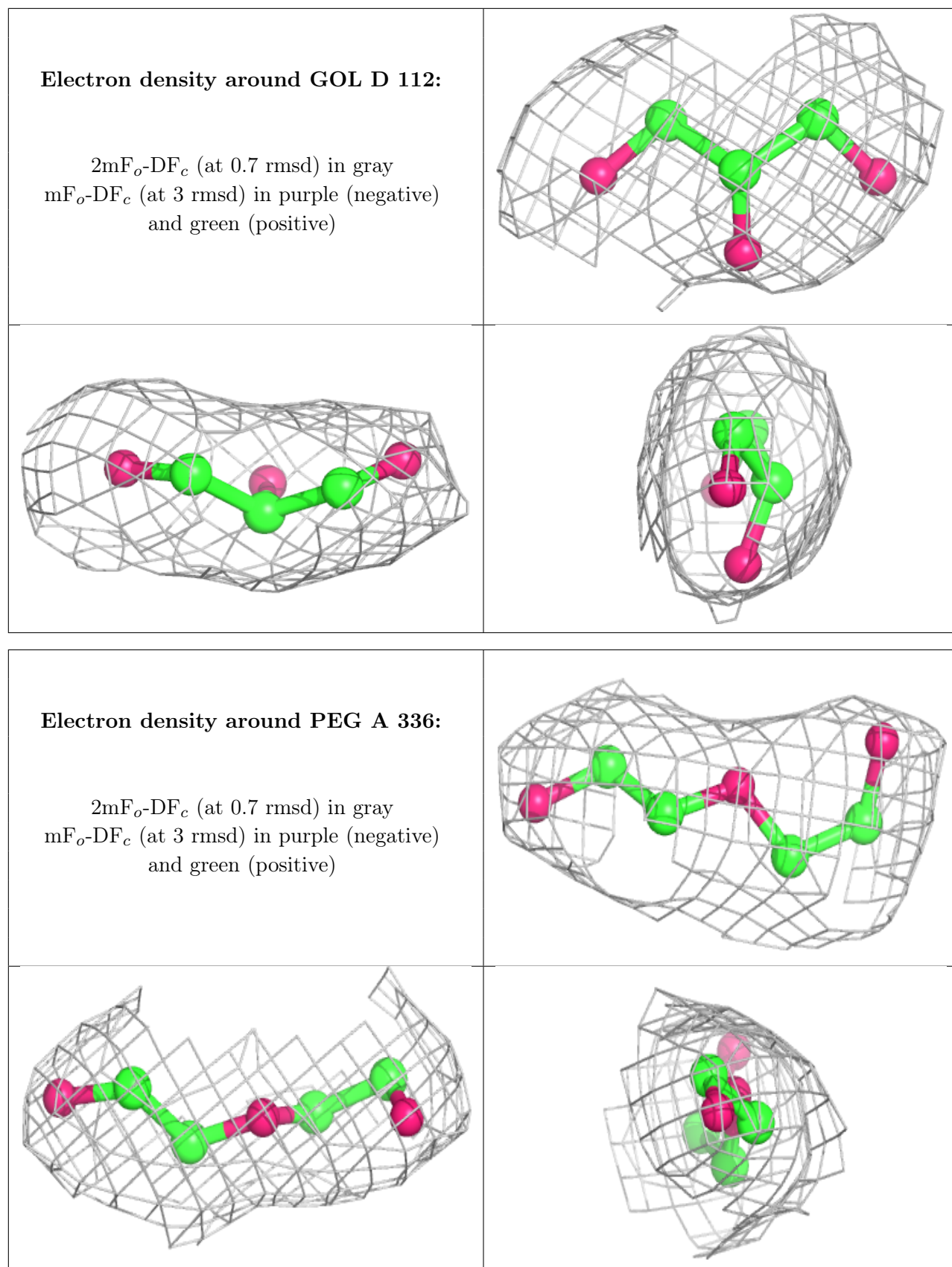
Electron density around PG4 B 155:

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

**Electron density around EDO E 101:**

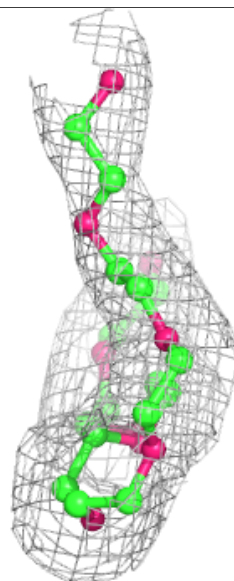
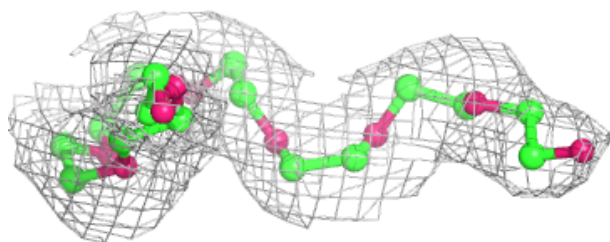
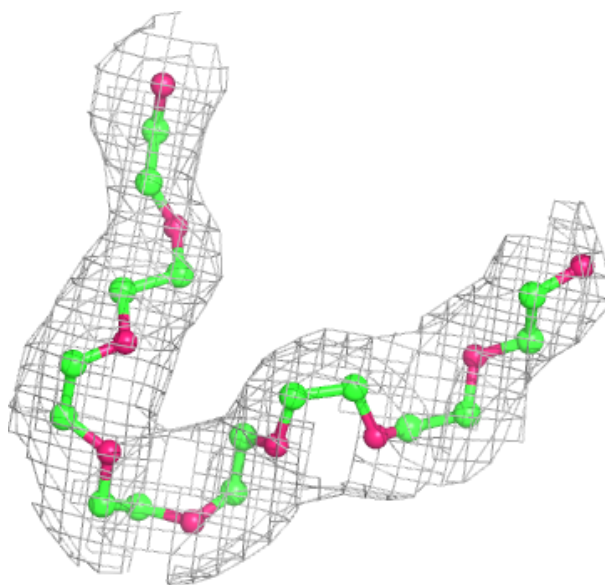
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





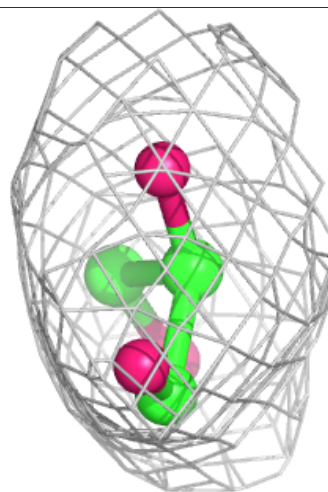
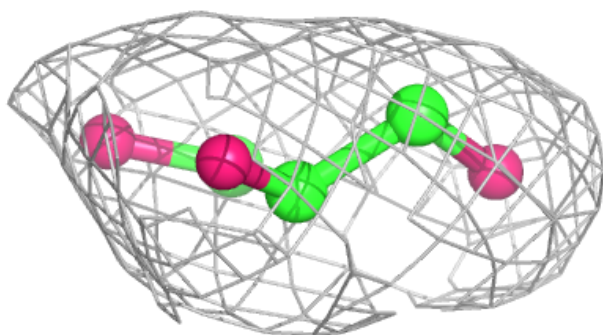
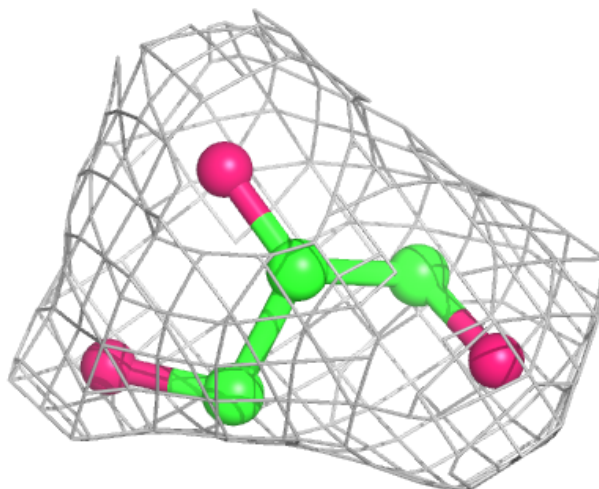
Electron density around PE8 B 137:

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



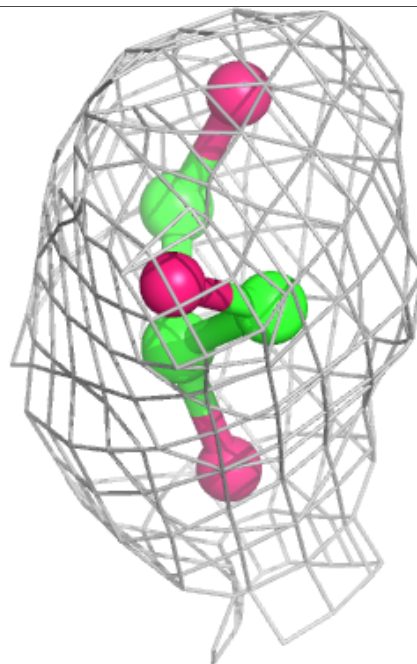
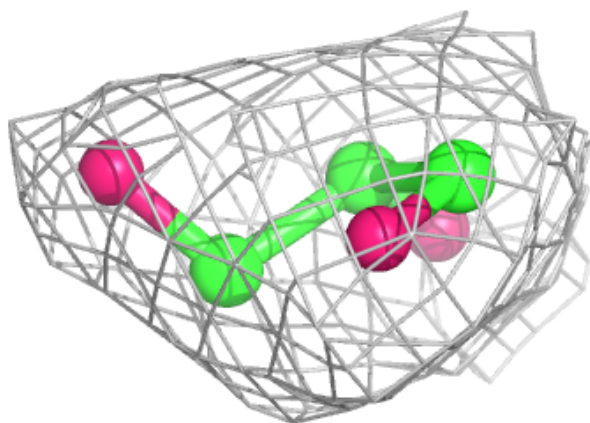
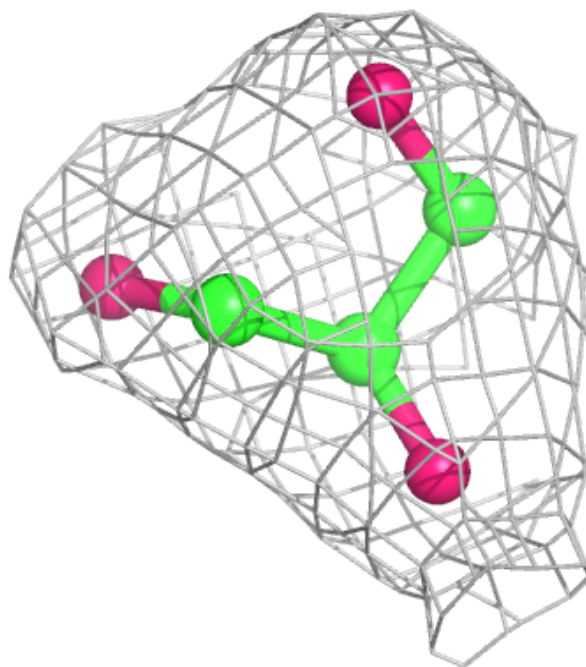
Electron density around GOL A 309:

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



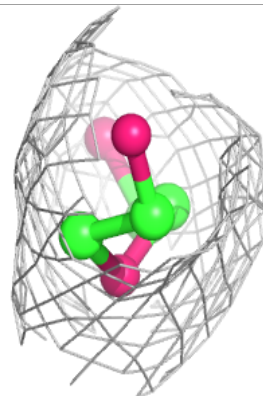
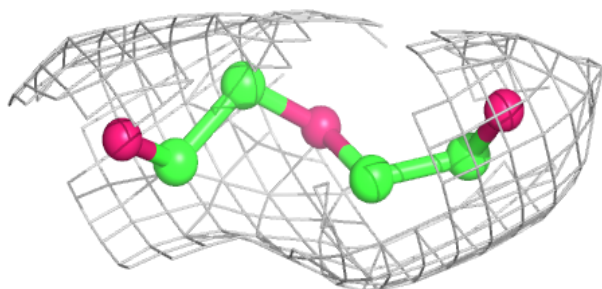
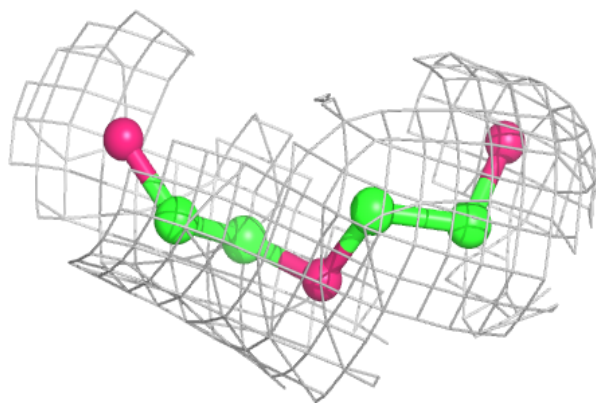
Electron density around GOL B 111:

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

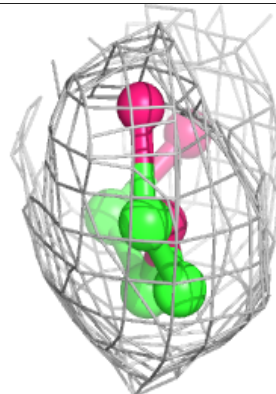
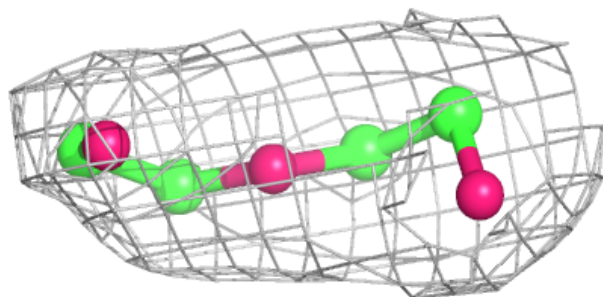
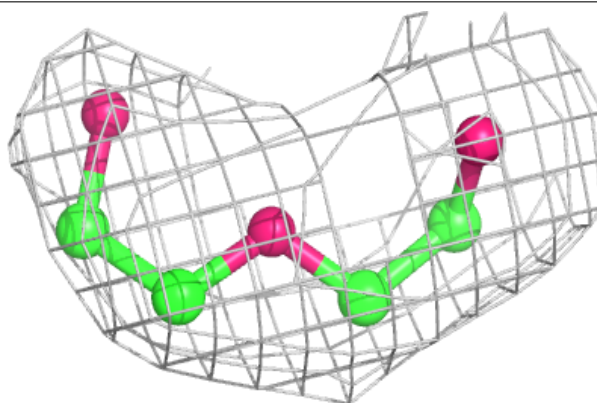


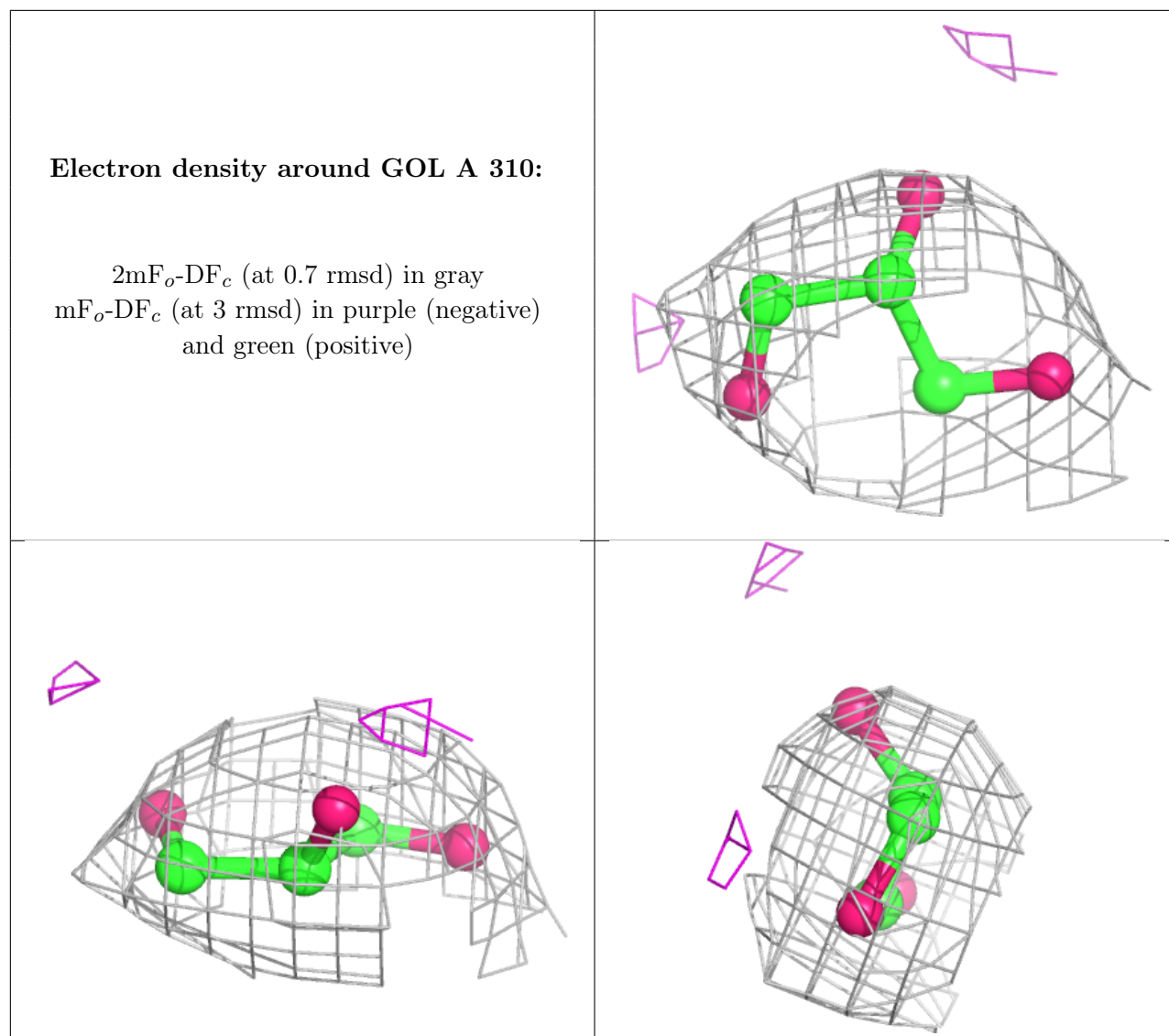
Electron density around PEG B 139:

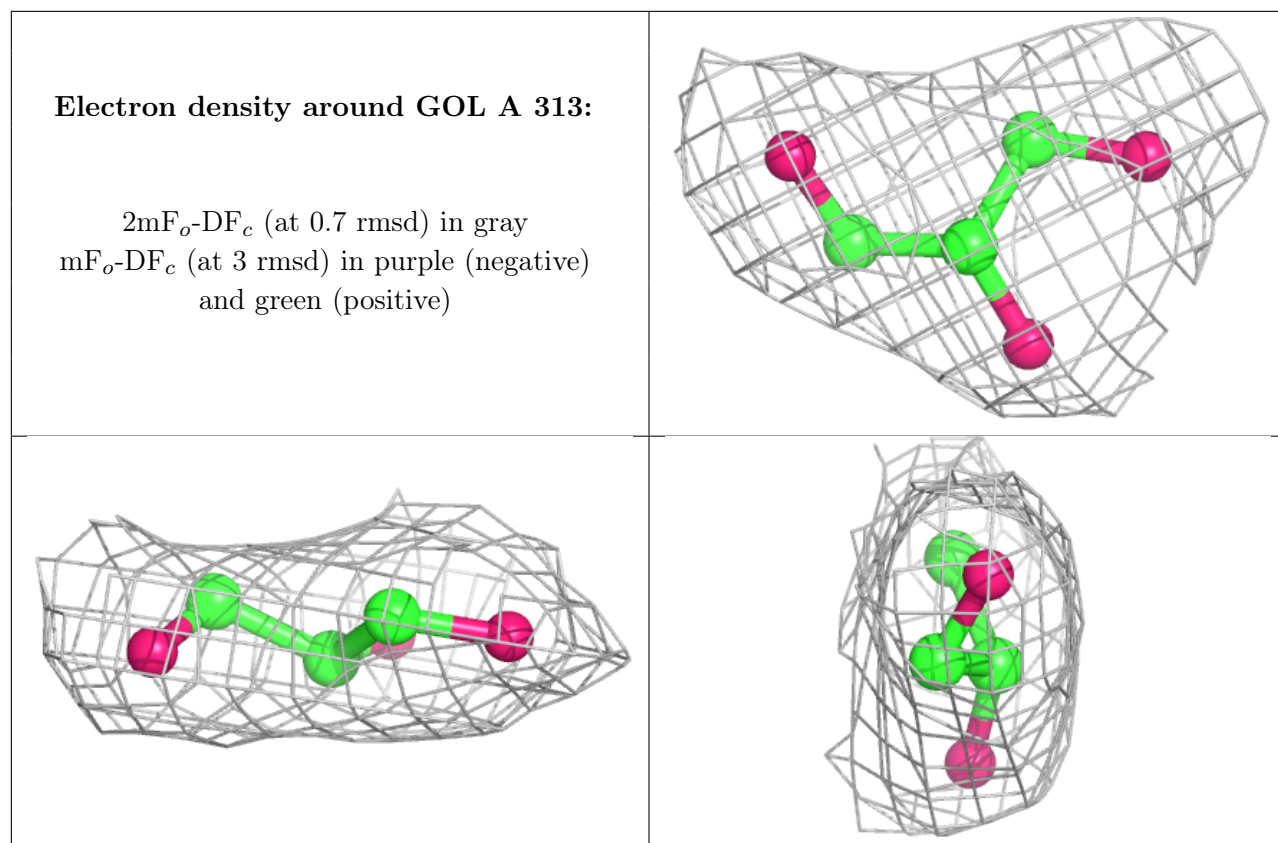
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PEG B 142:**

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

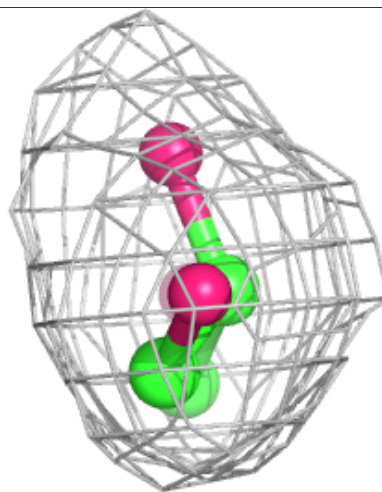
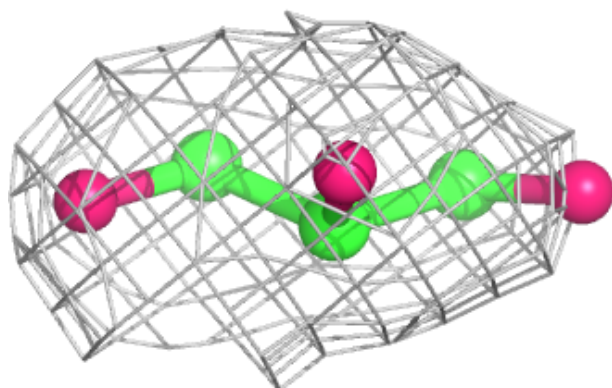
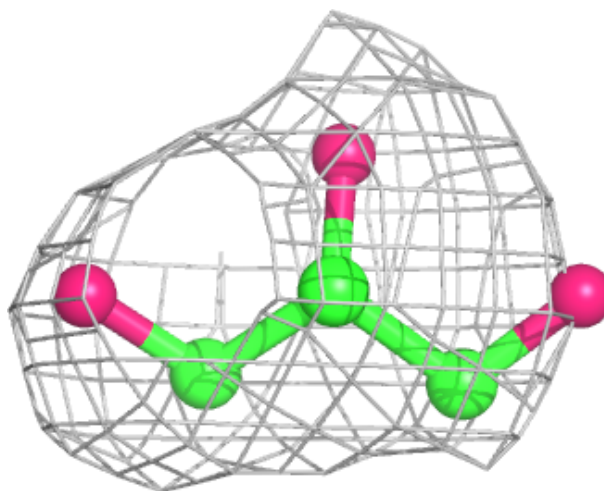


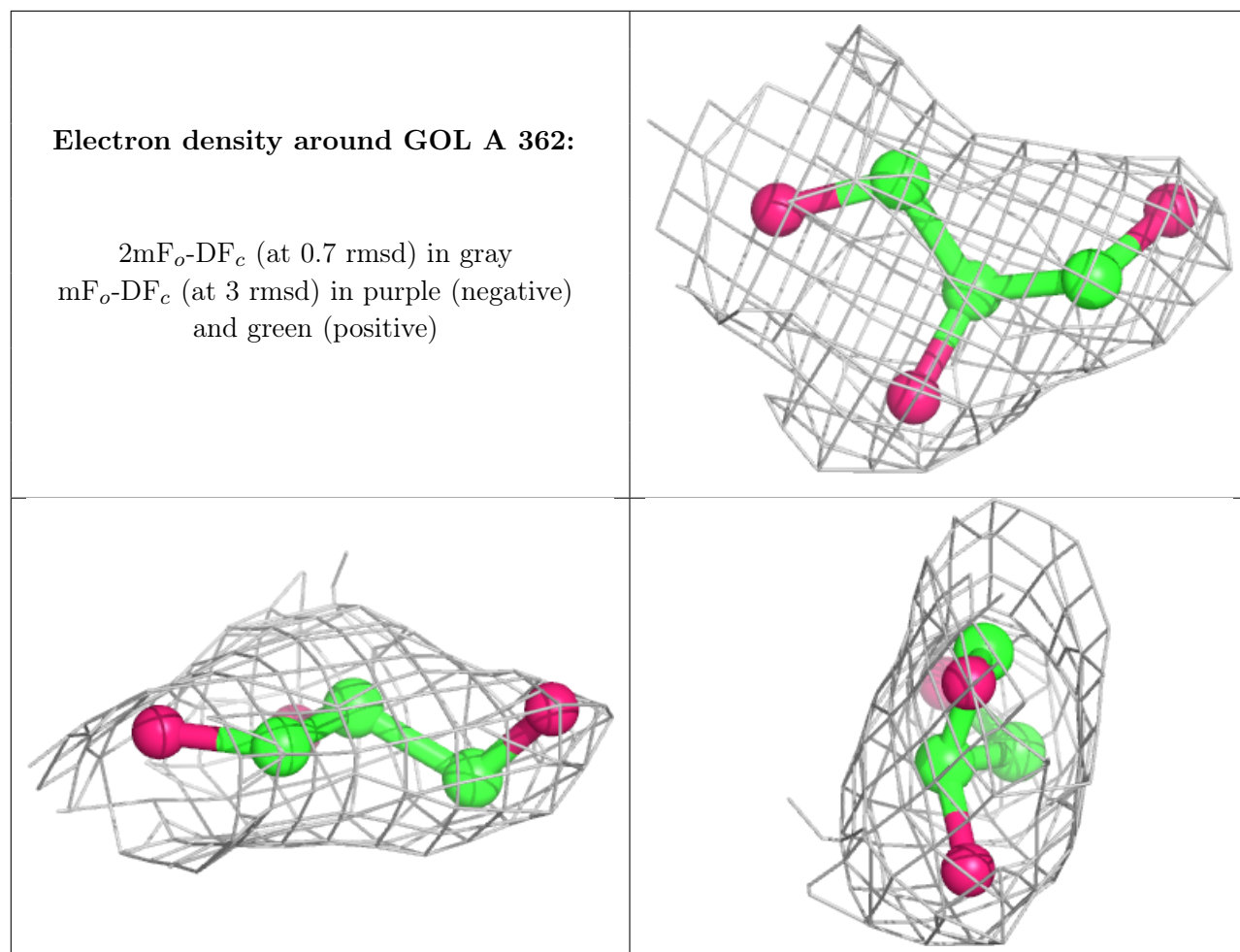


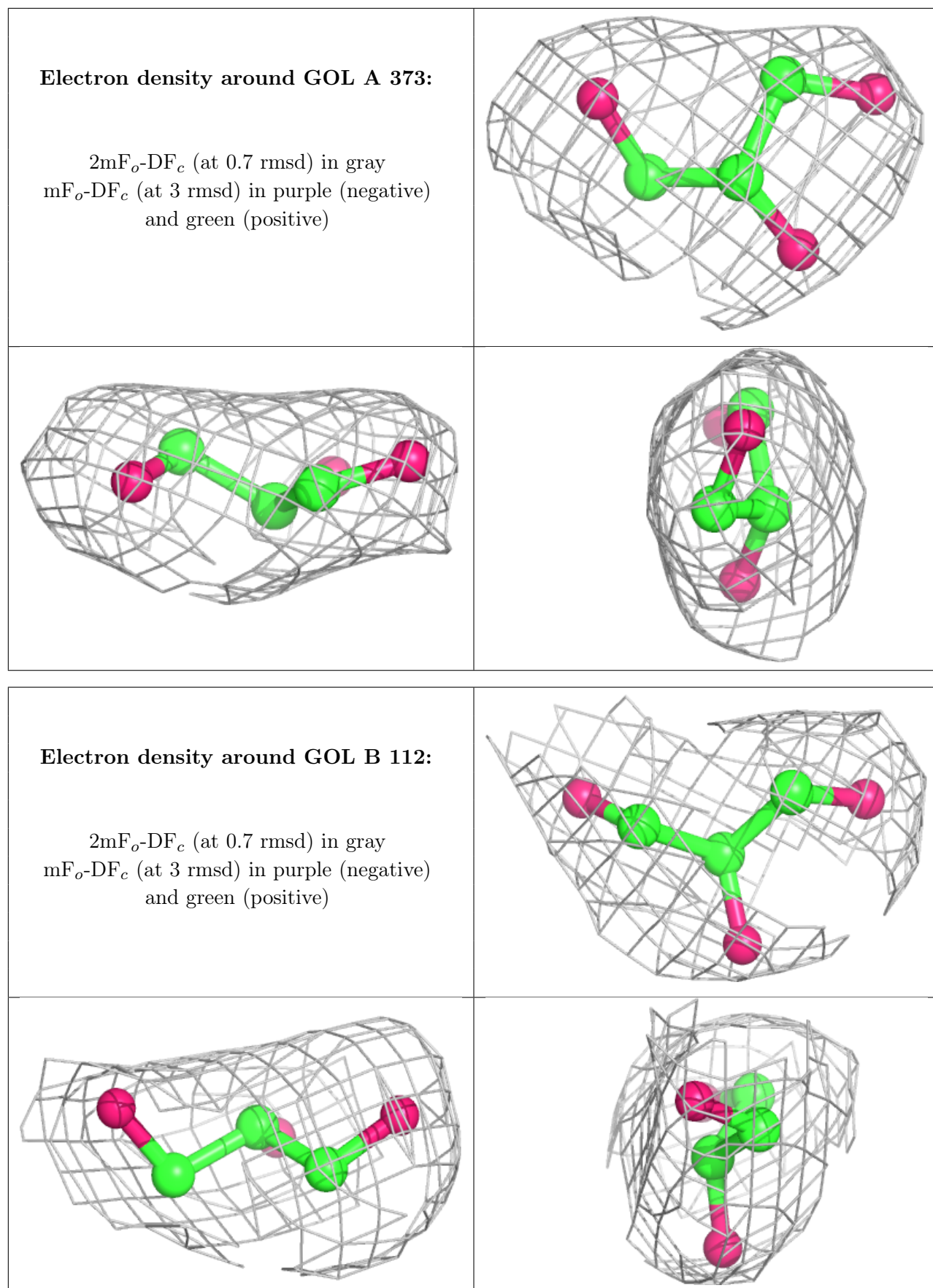


Electron density around GOL D 108:

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

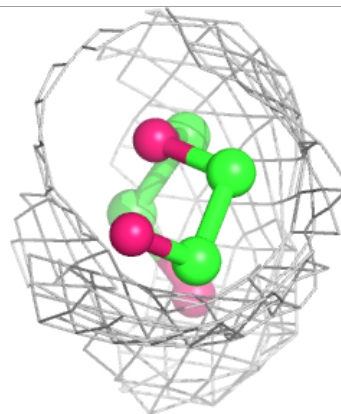
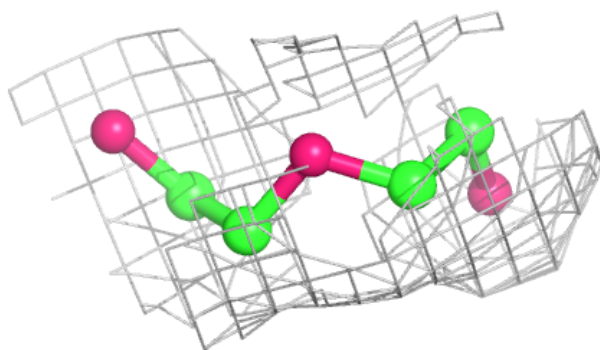
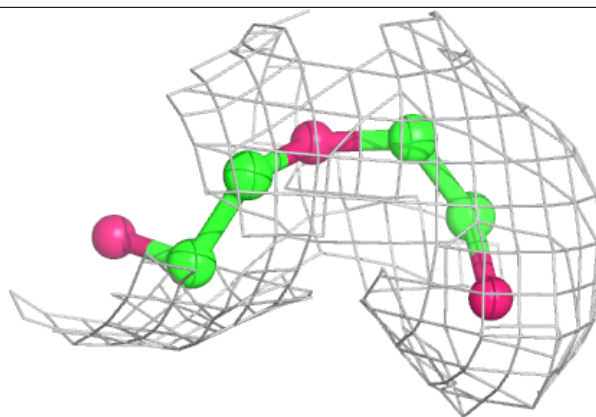




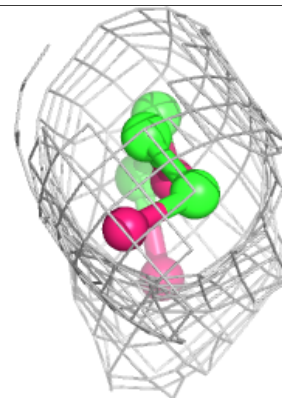
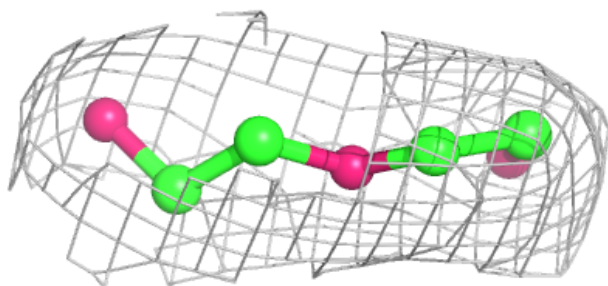
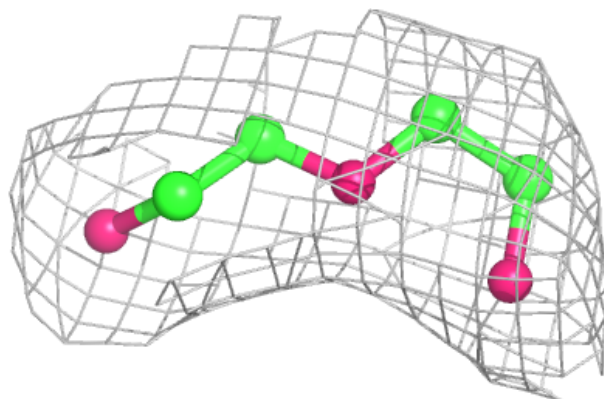


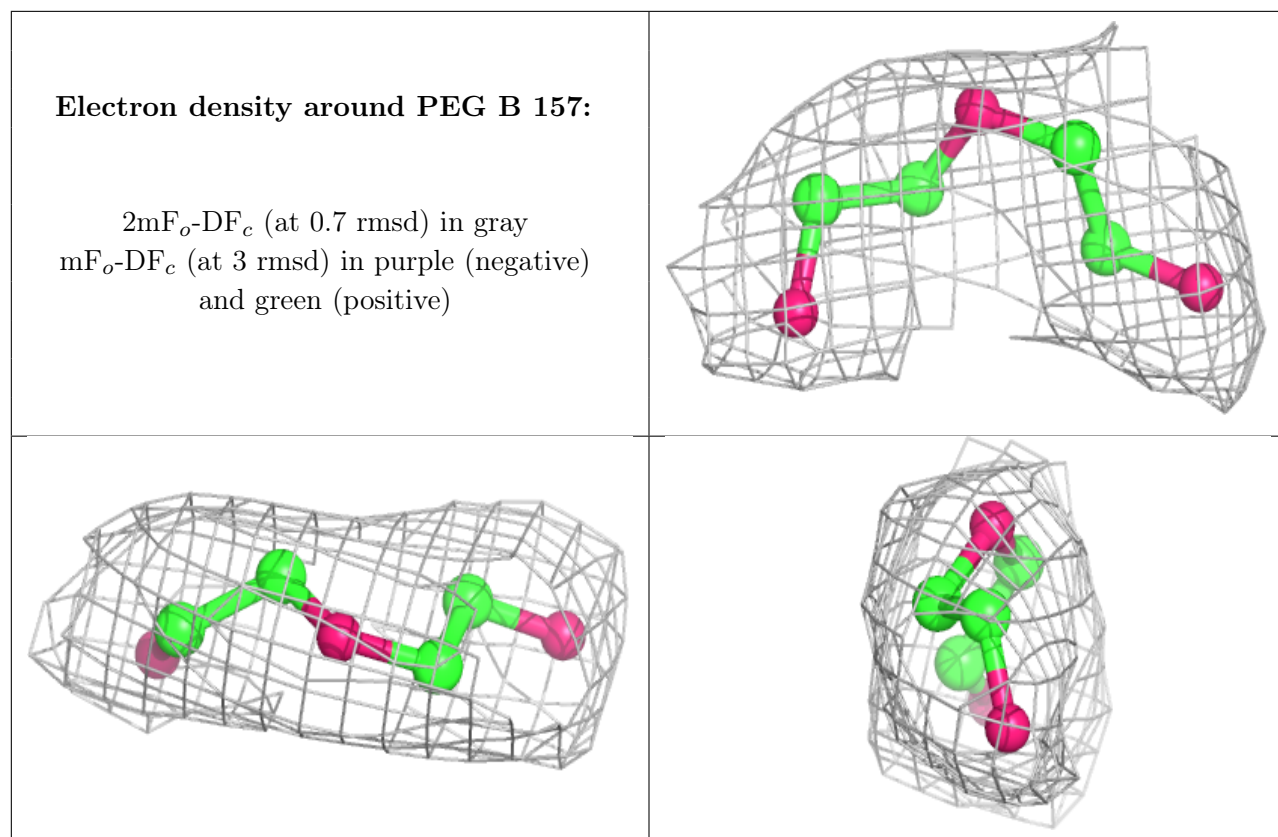
Electron density around PEG B 127:

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

**Electron density around PEG B 156:**

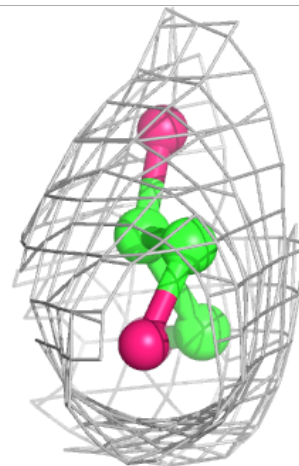
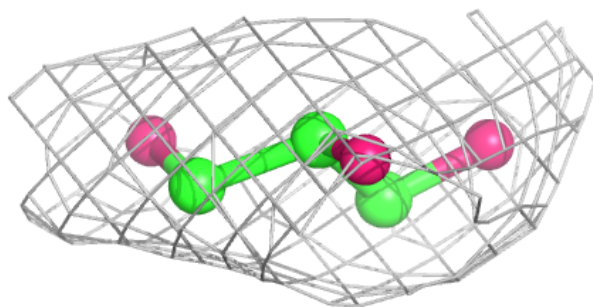
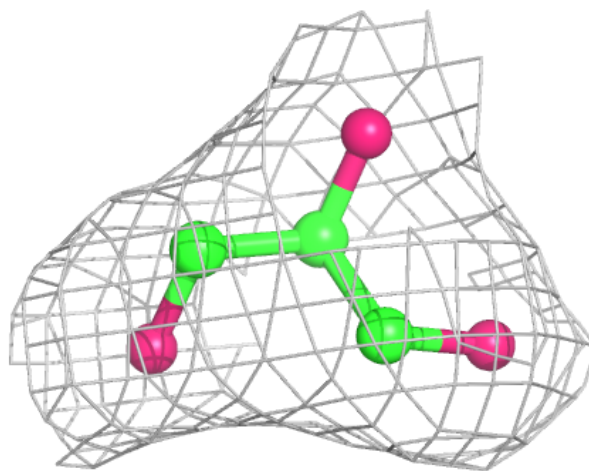
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





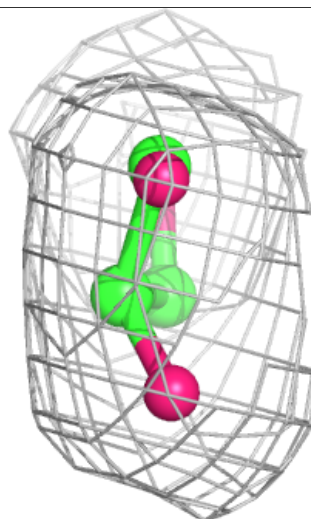
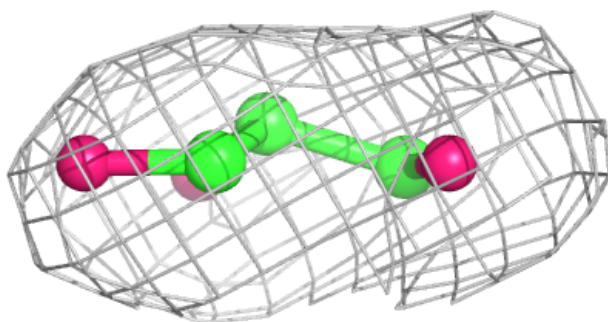
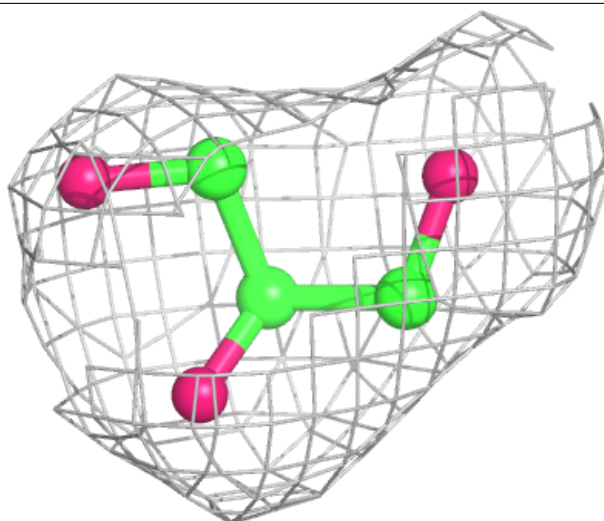
Electron density around GOL A 308:

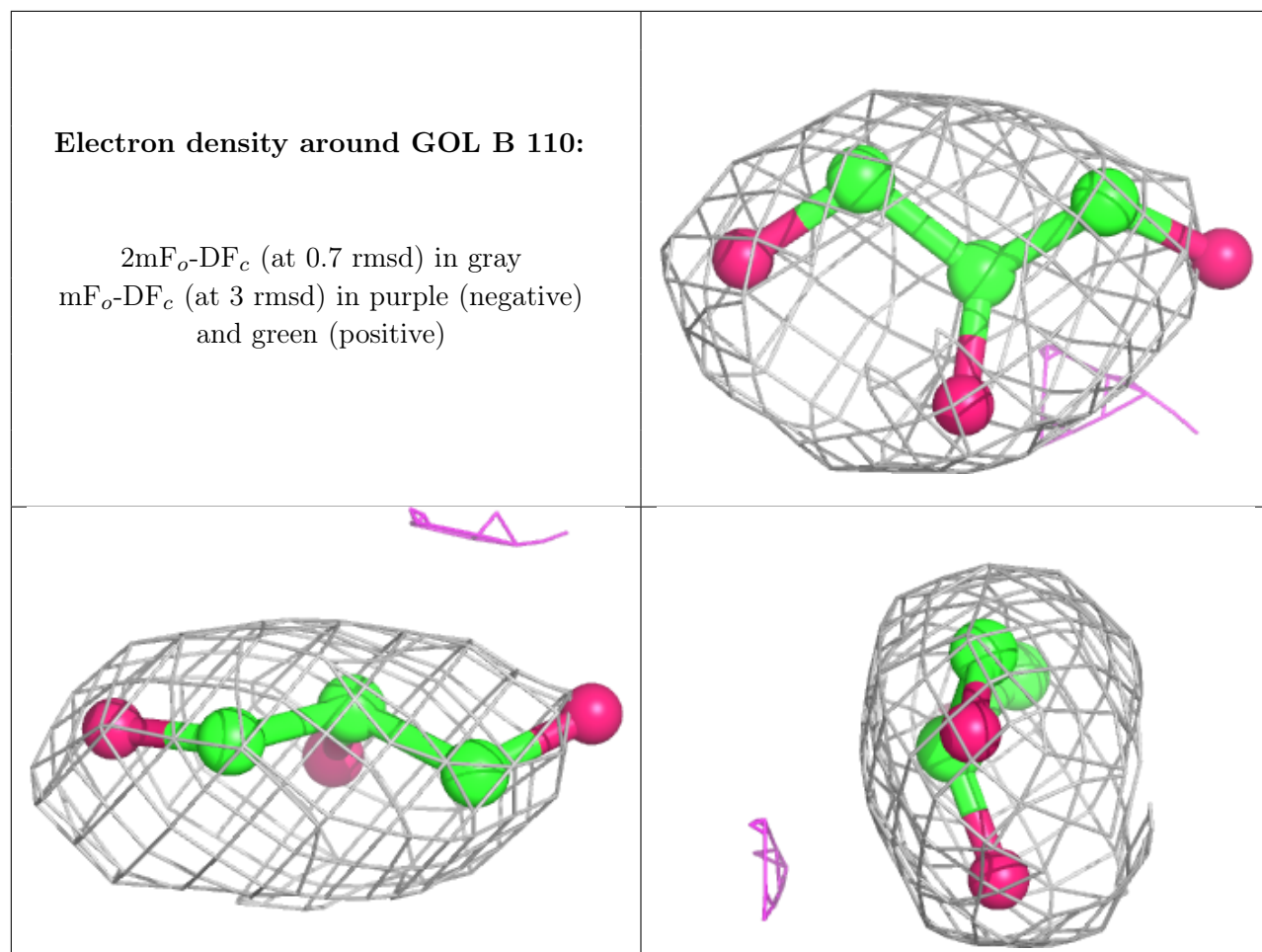
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GOL D 106:

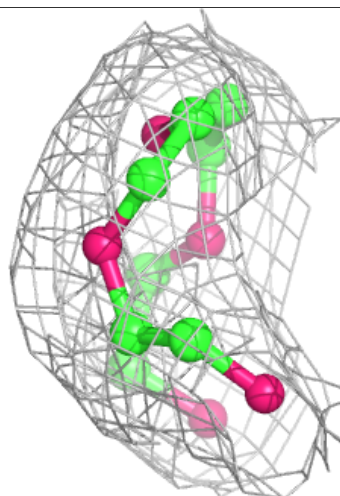
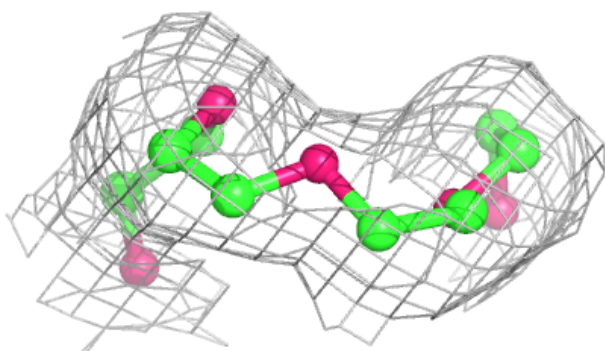
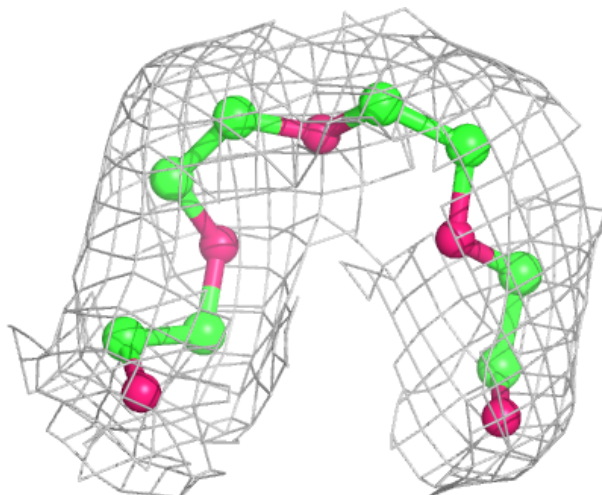
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

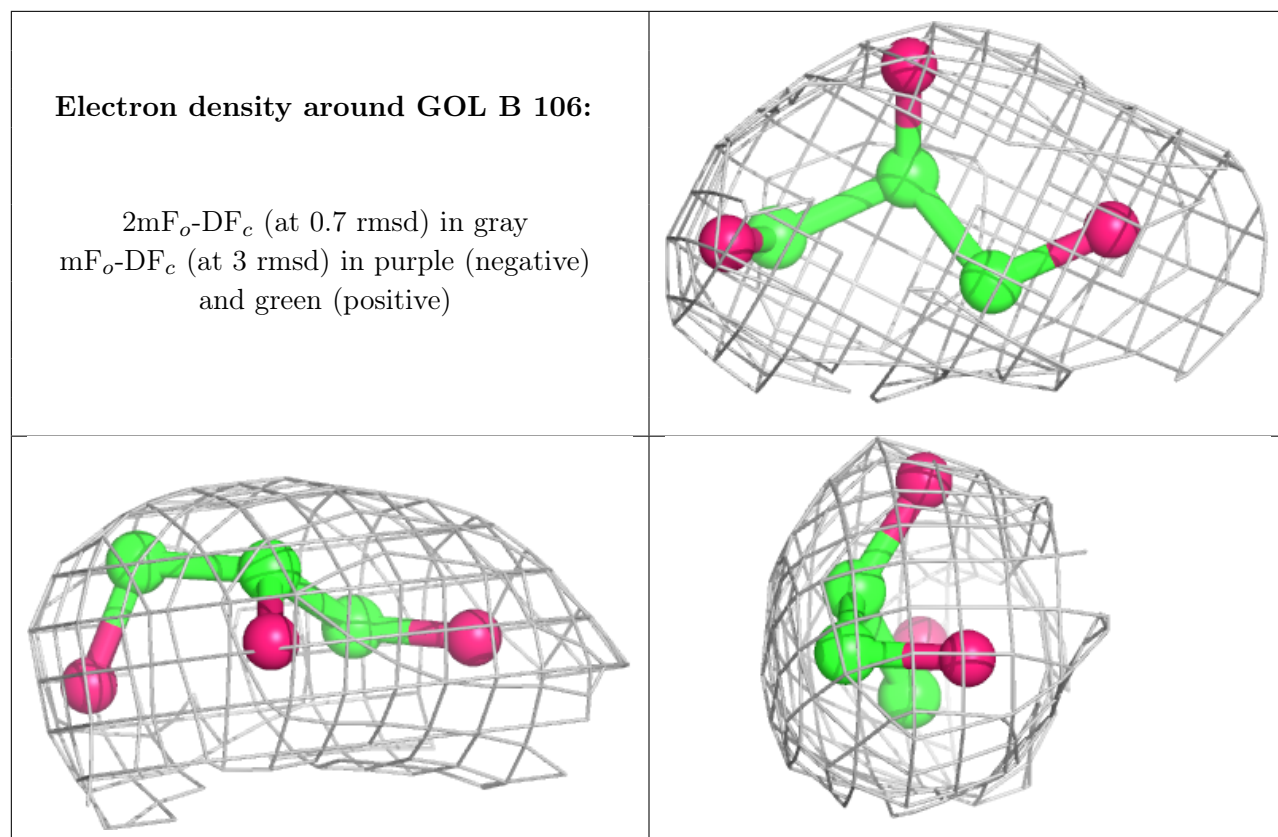




Electron density around PG4 D 119:

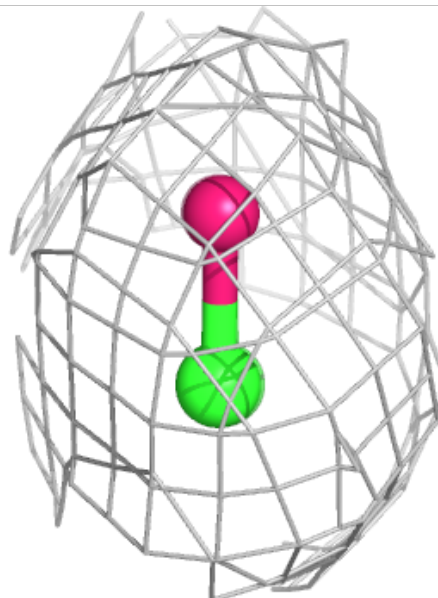
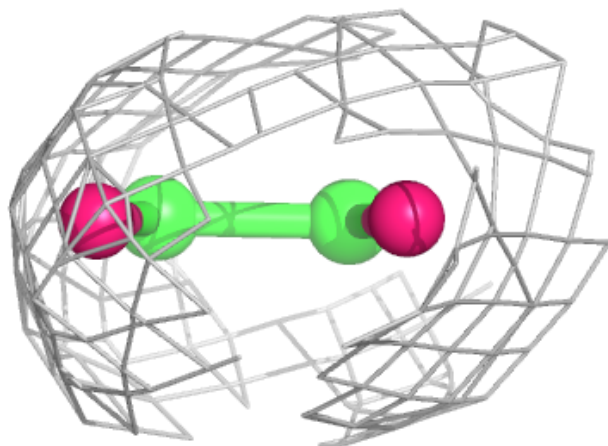
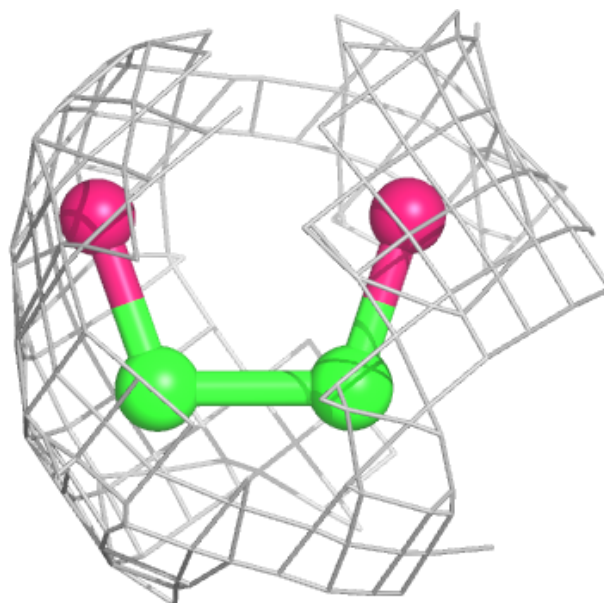
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

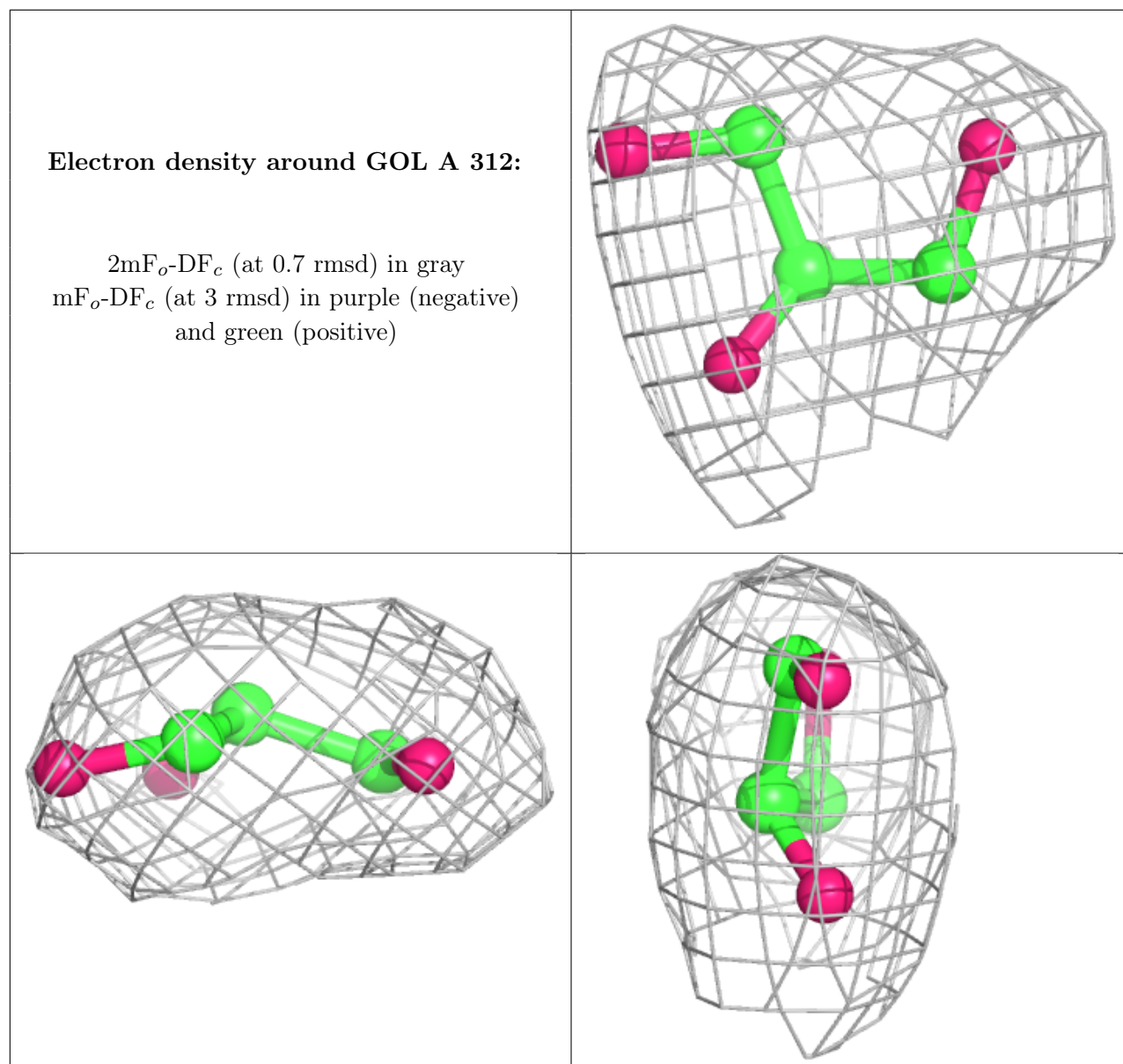


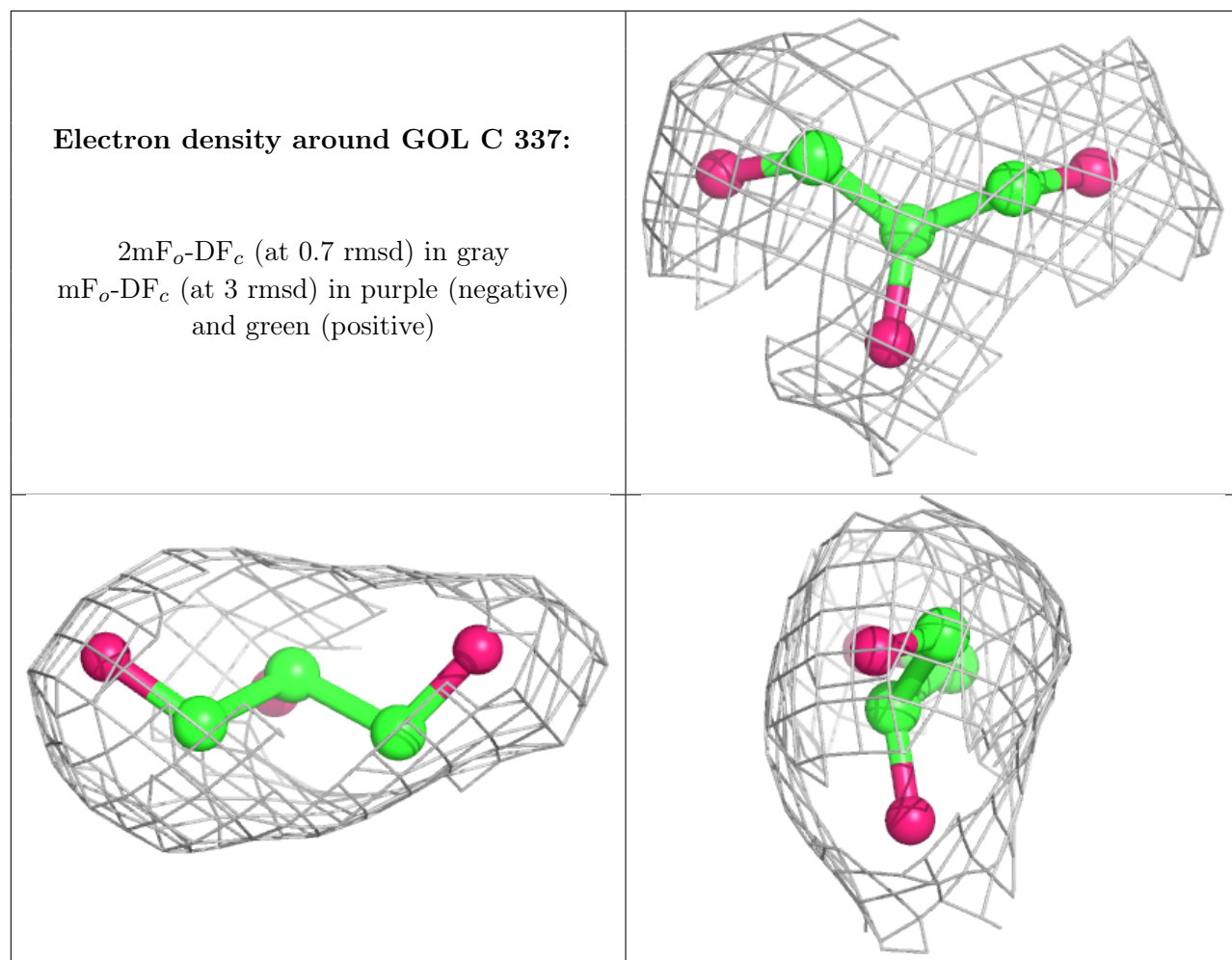


Electron density around EDO E 111:

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

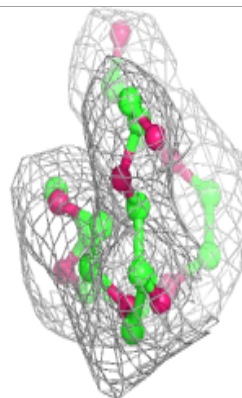
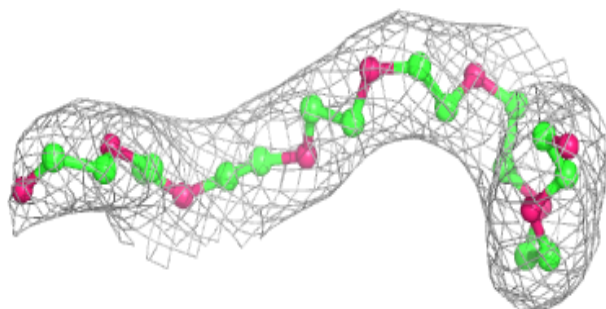
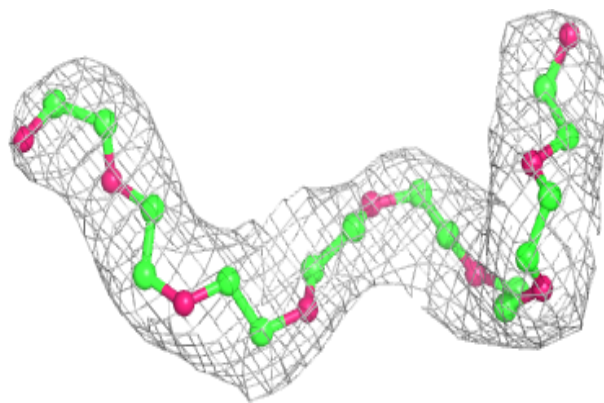






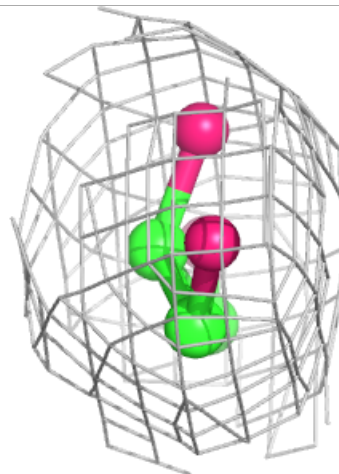
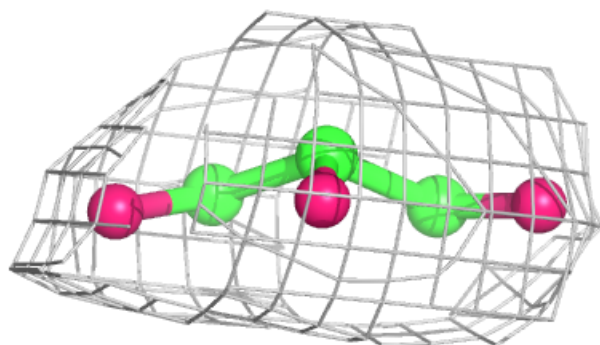
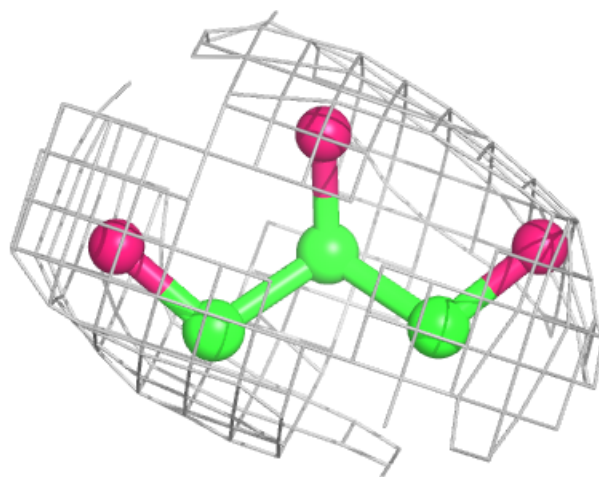
Electron density around PE8 B 138:

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



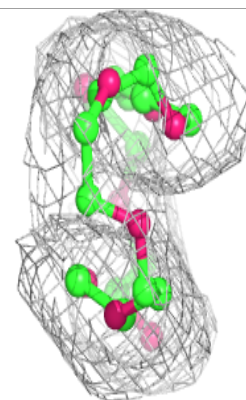
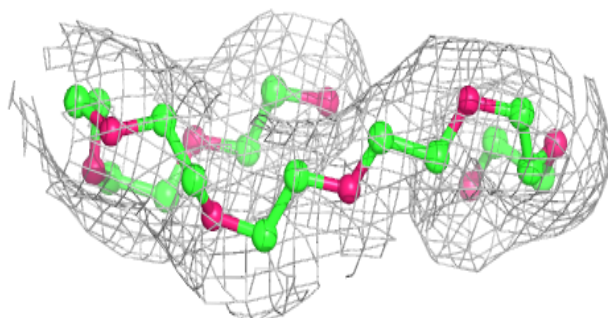
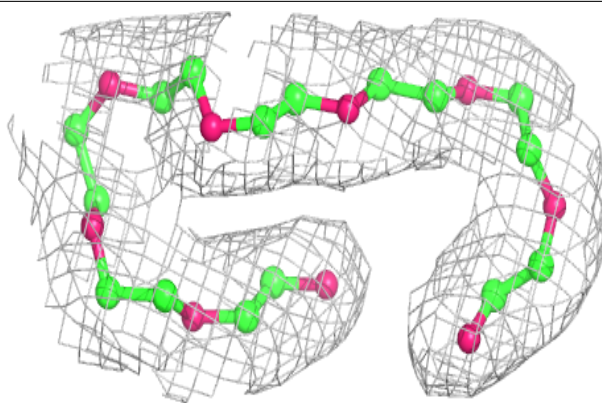
Electron density around GOL A 307:

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

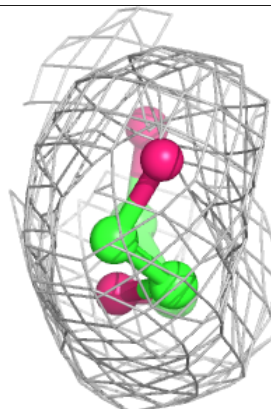
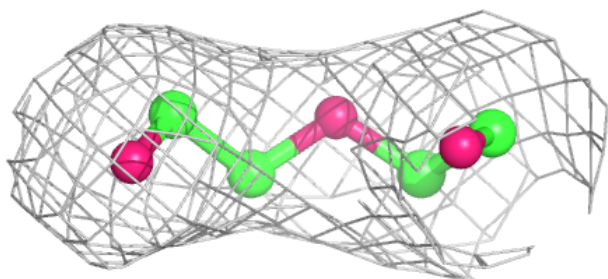
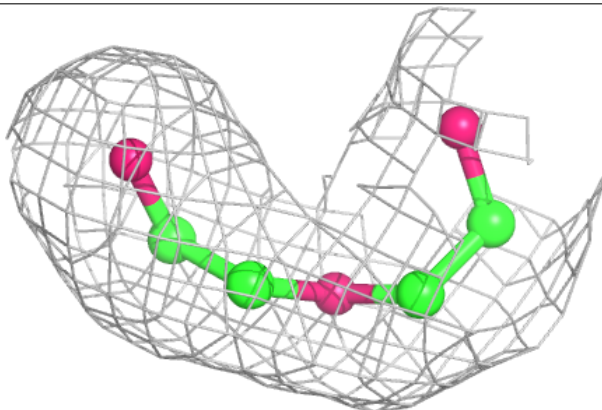


Electron density around PE8 E 109:

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

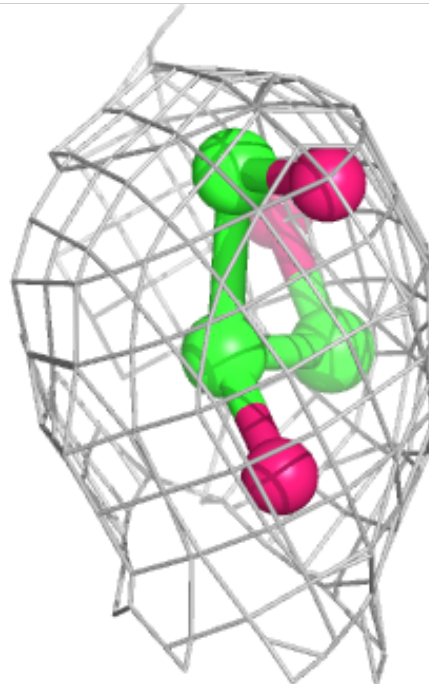
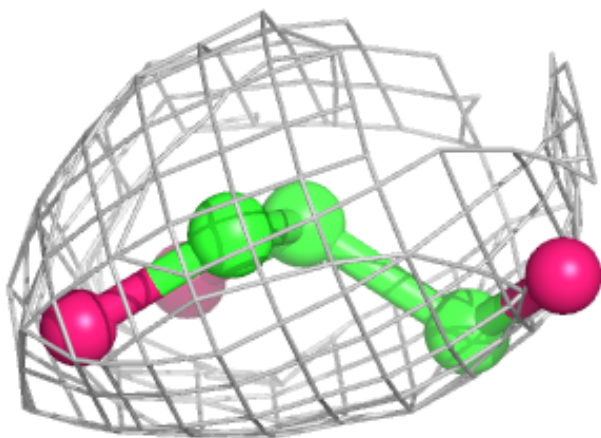
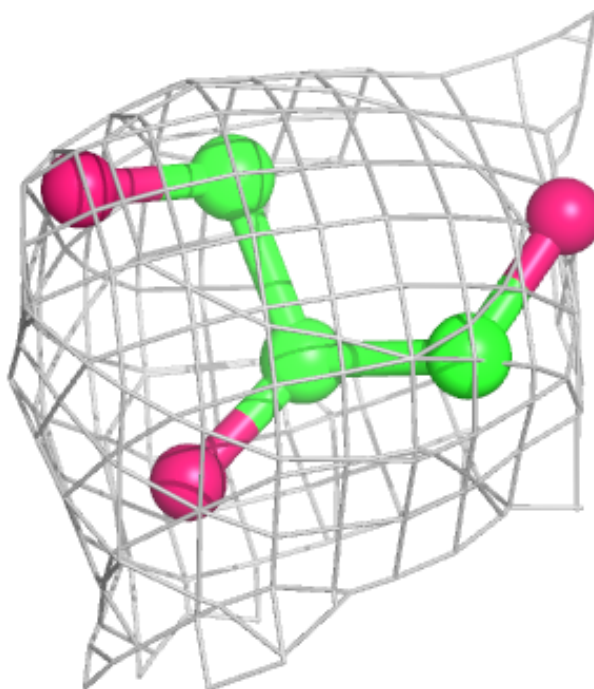
**Electron density around PEG B 158:**

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



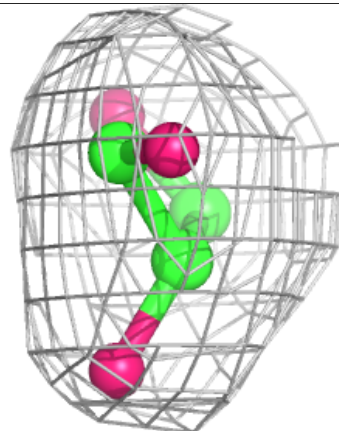
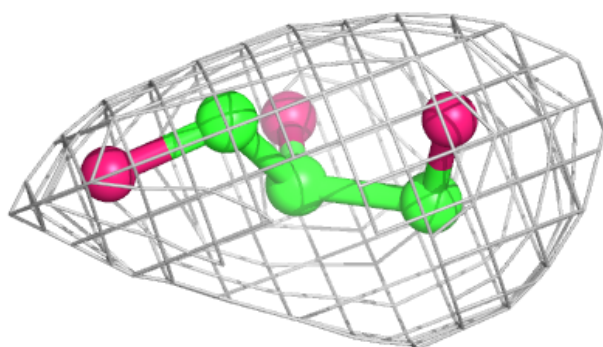
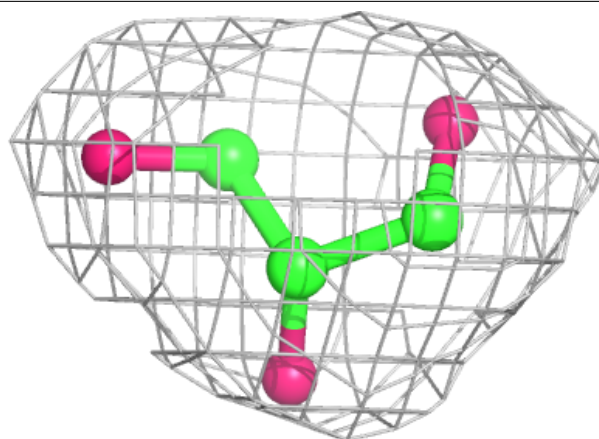
Electron density around GOL C 347:

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

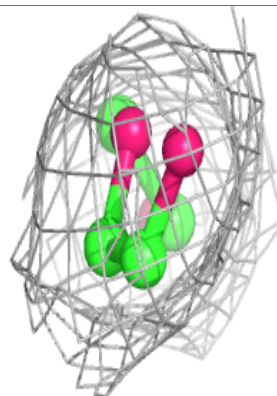
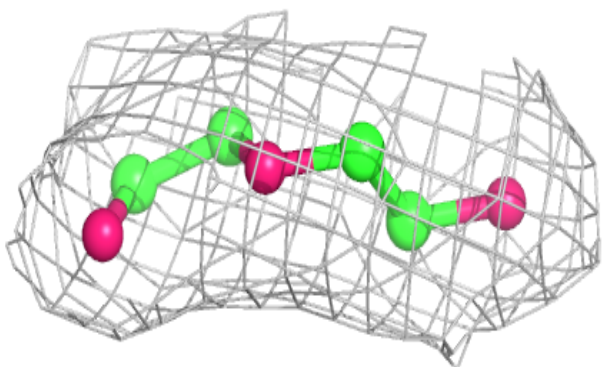
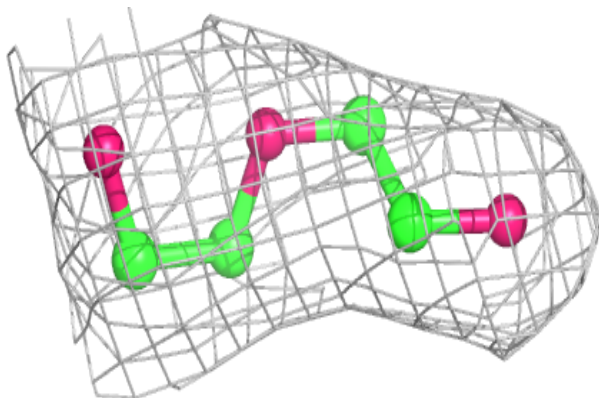


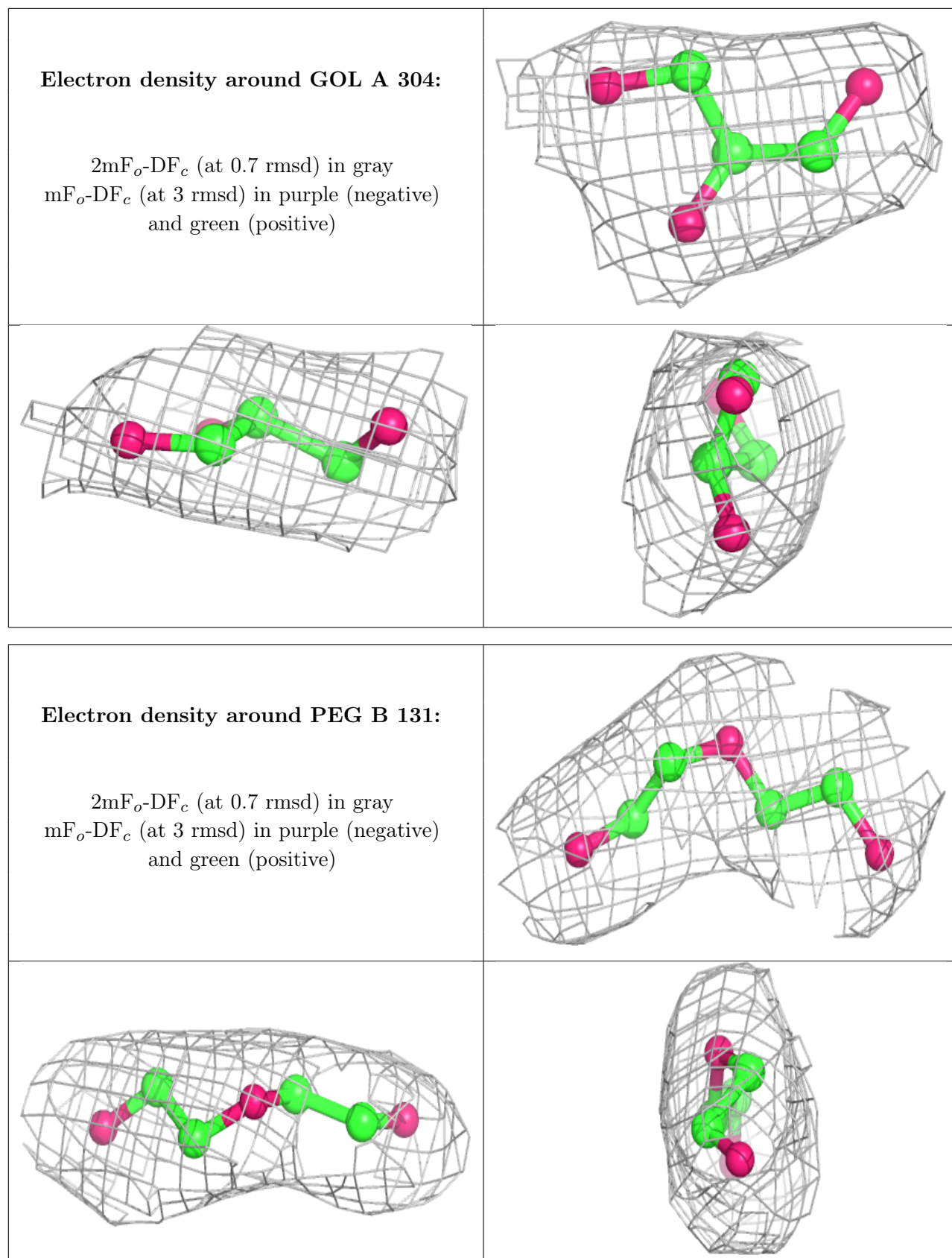
Electron density around GOL C 308:

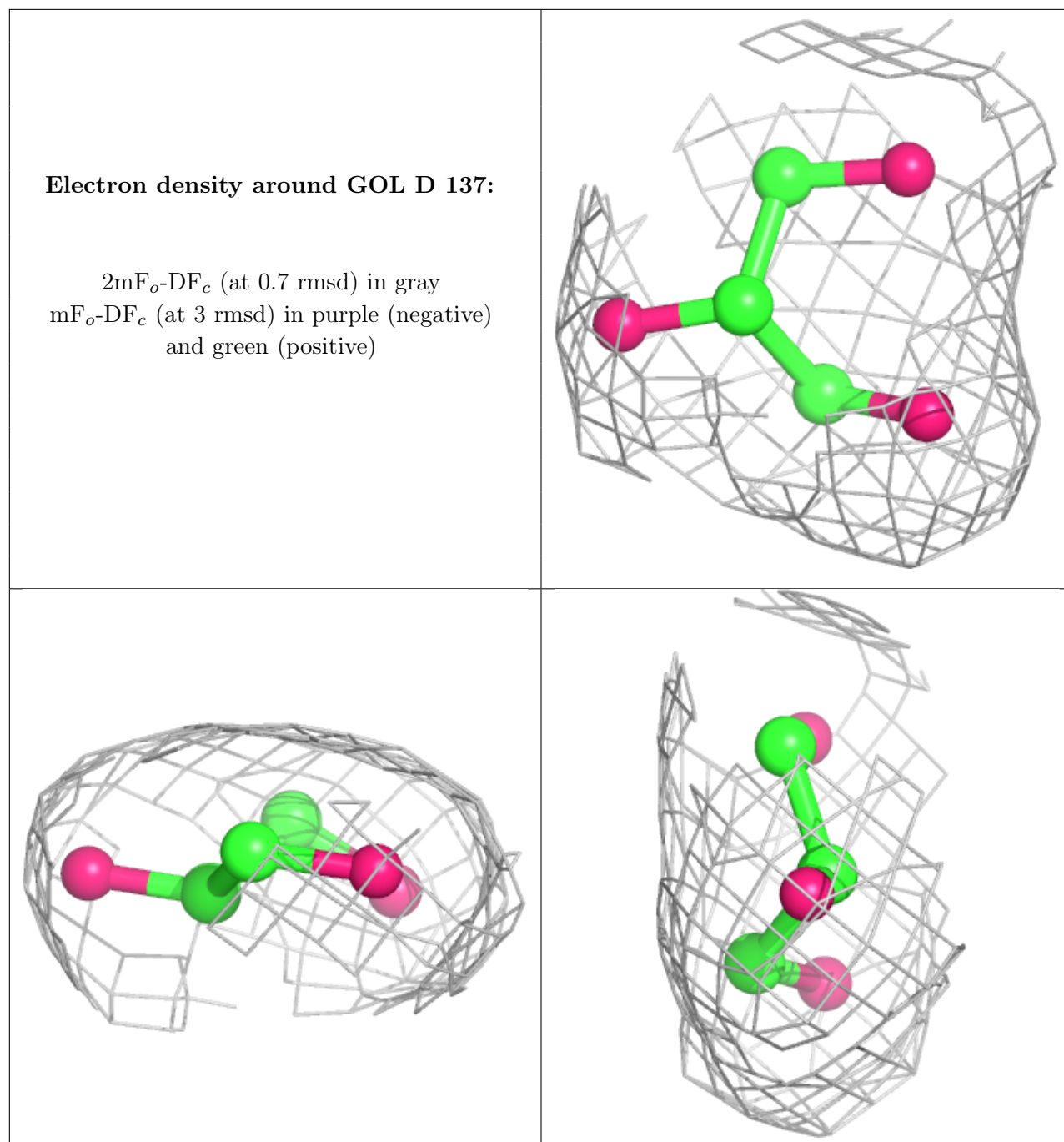
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PEG D 124:**

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

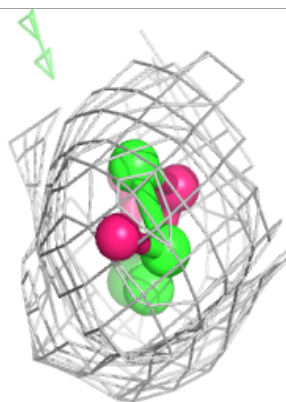
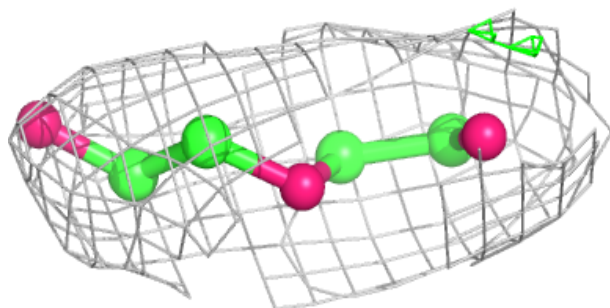
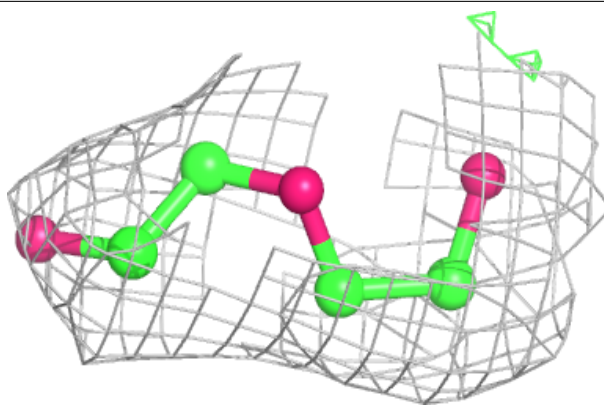




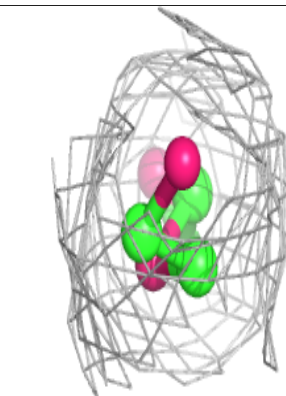
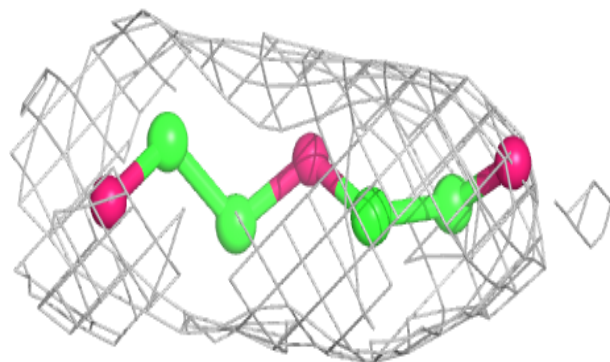
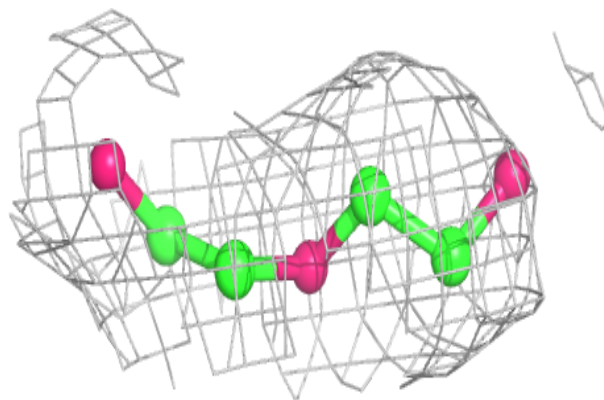


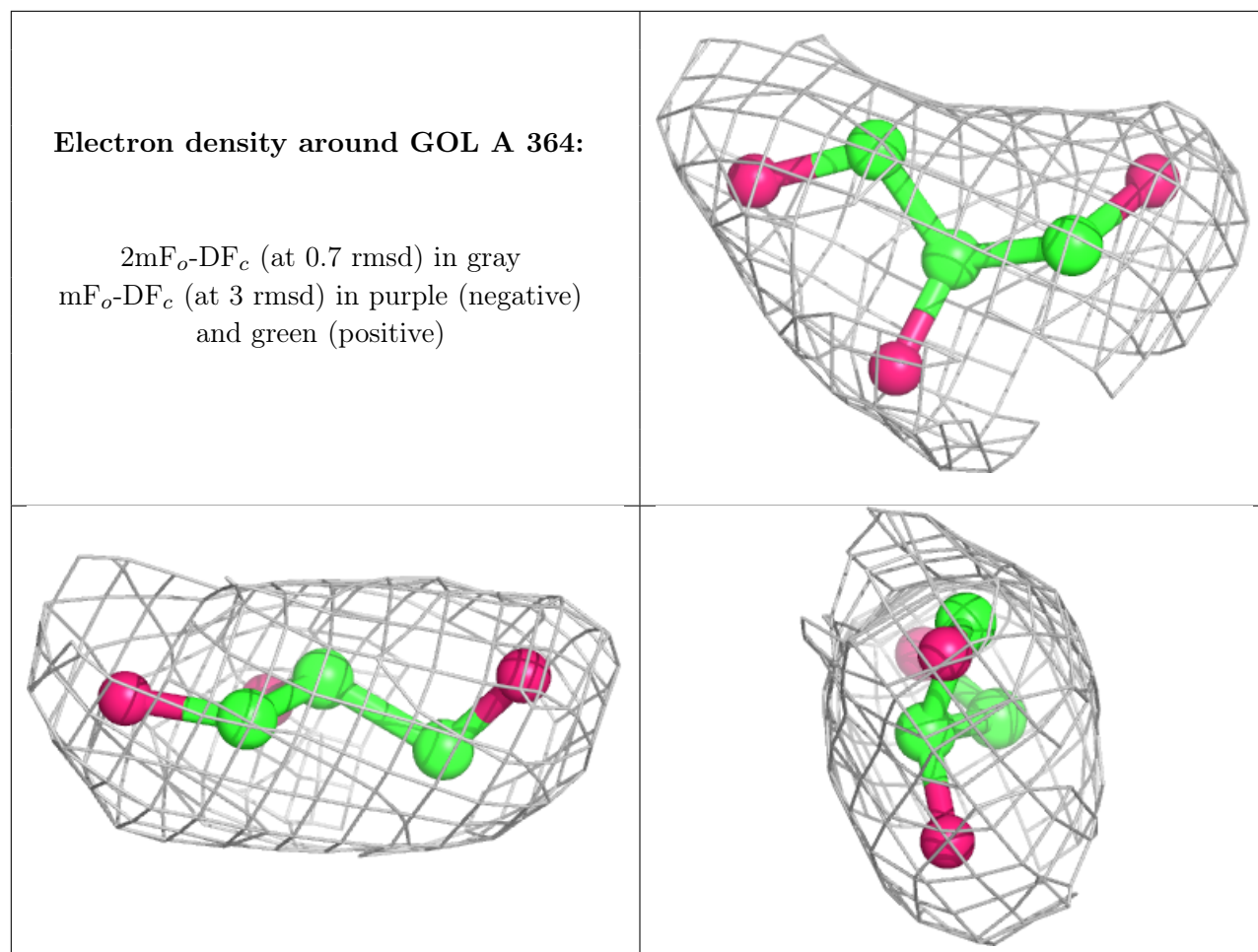
Electron density around PEG B 133:

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

**Electron density around PEG A 340:**

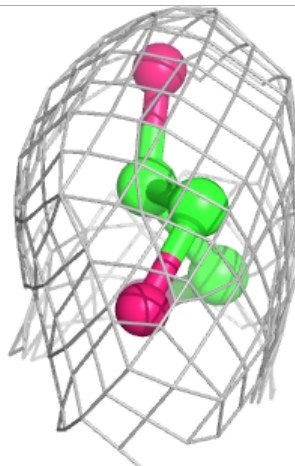
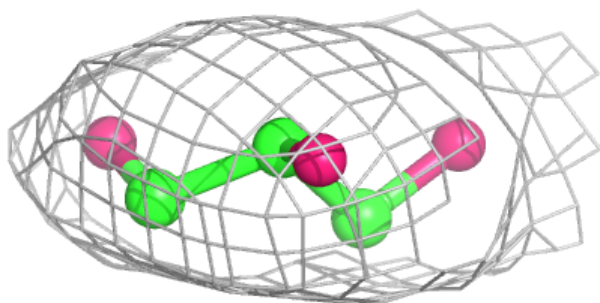
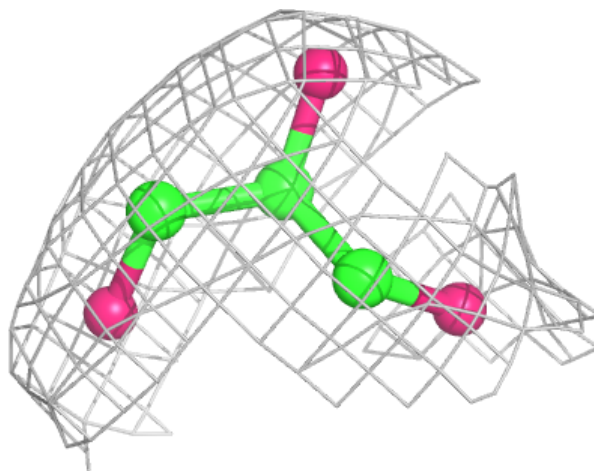
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

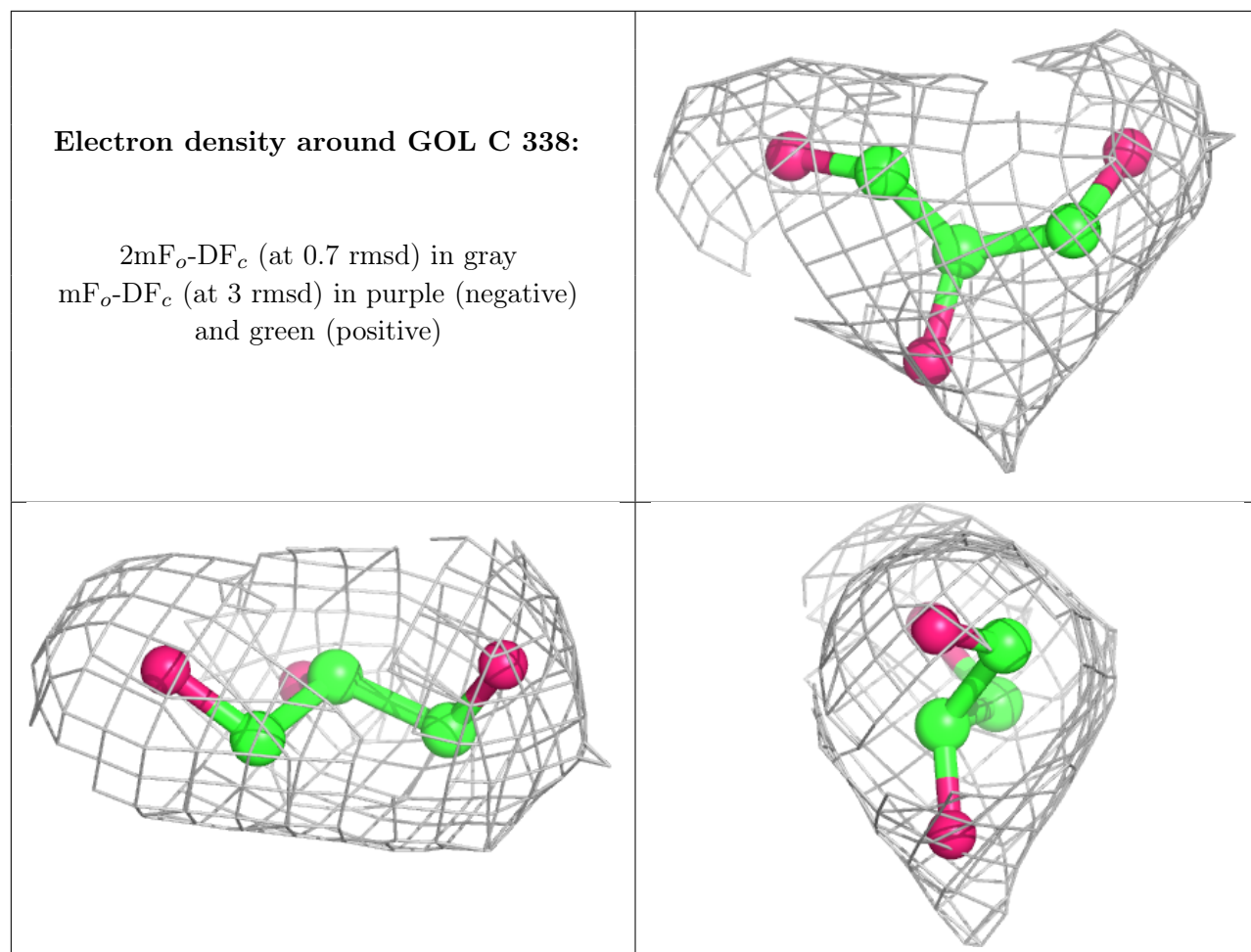




Electron density around GOL A 301:

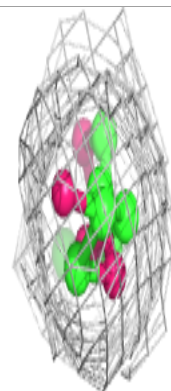
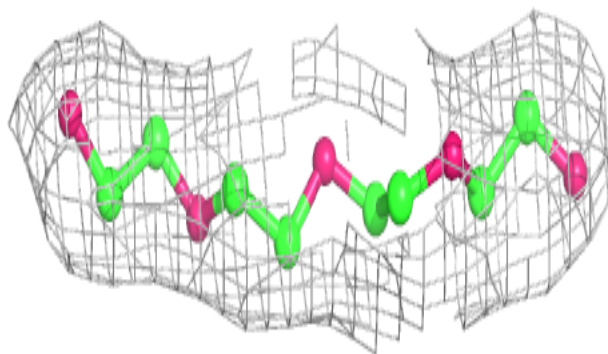
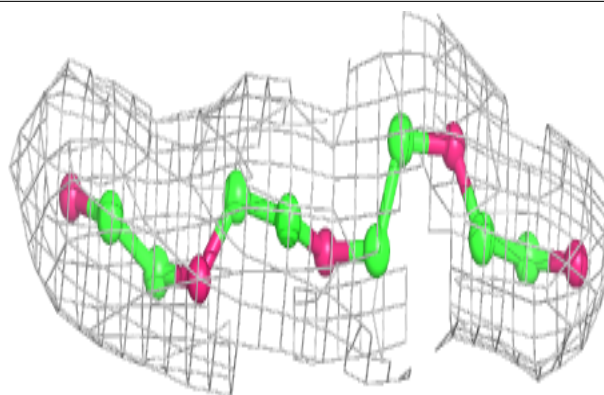
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



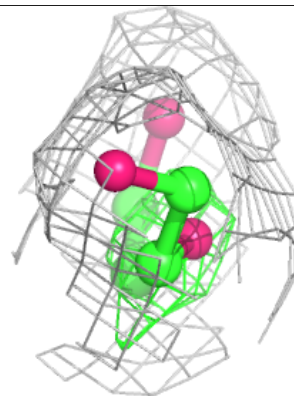
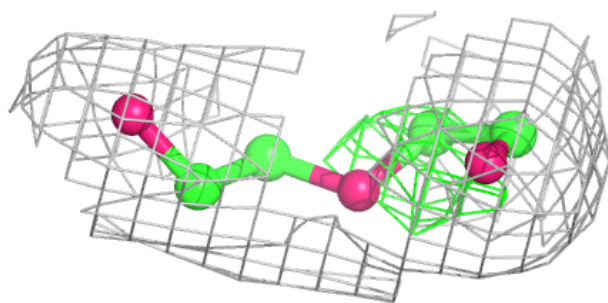
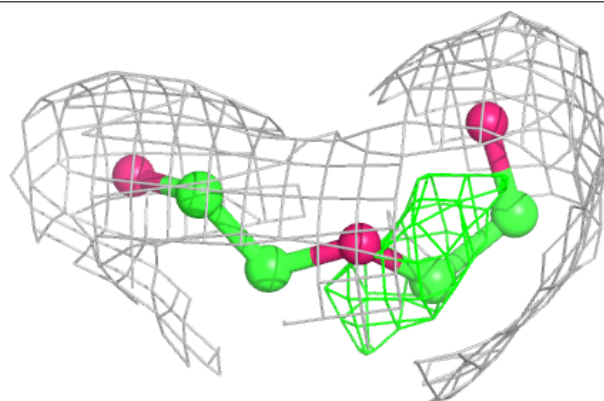


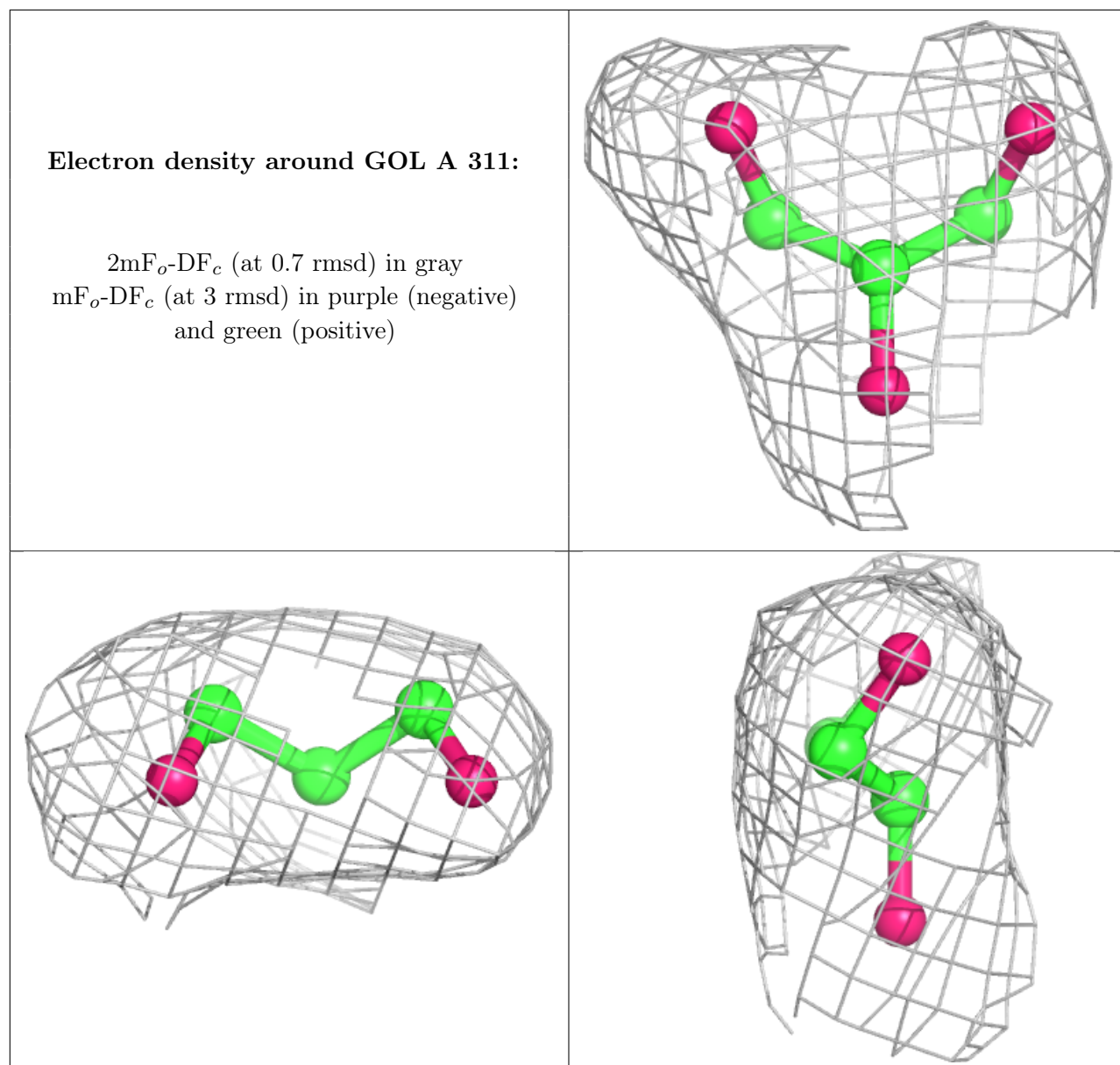
Electron density around PG4 E 115:

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

**Electron density around PEG D 125:**

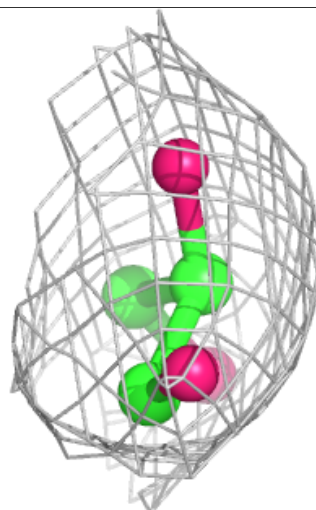
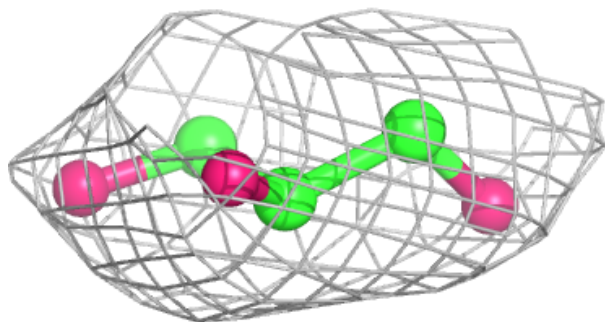
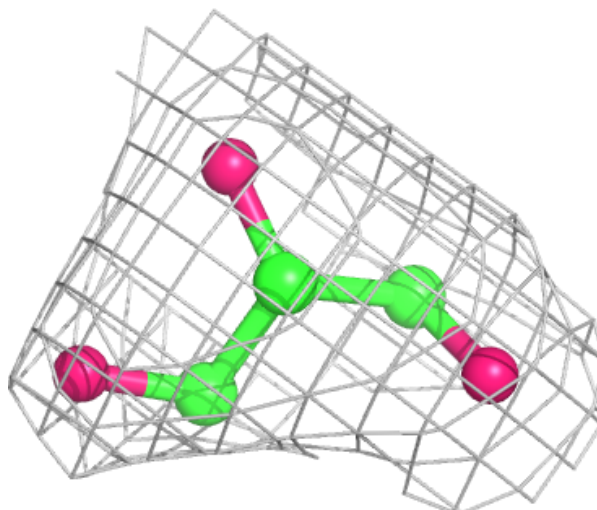
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





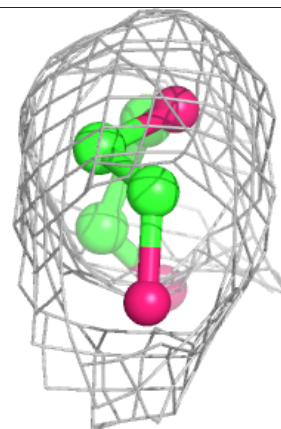
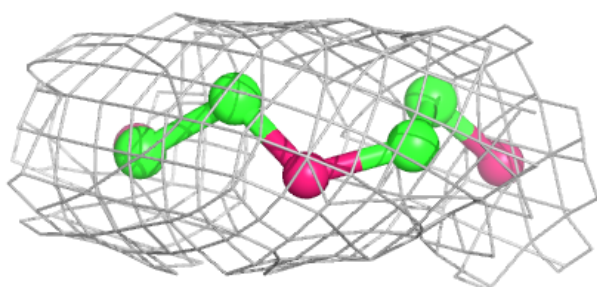
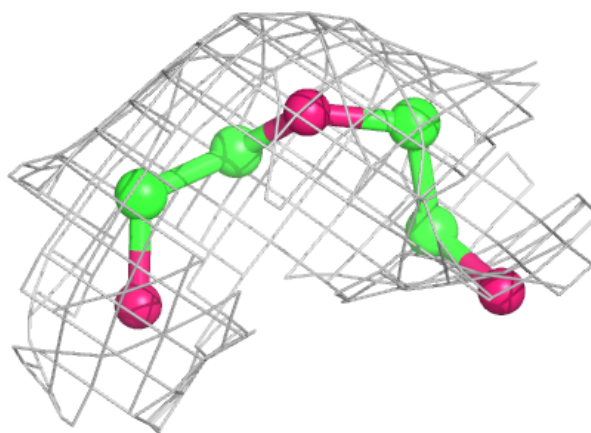
Electron density around GOL C 345:

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

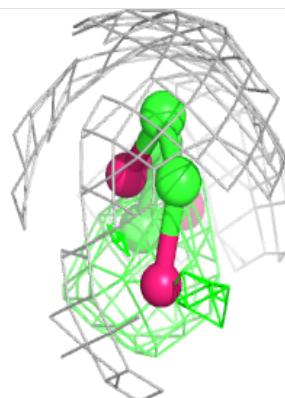
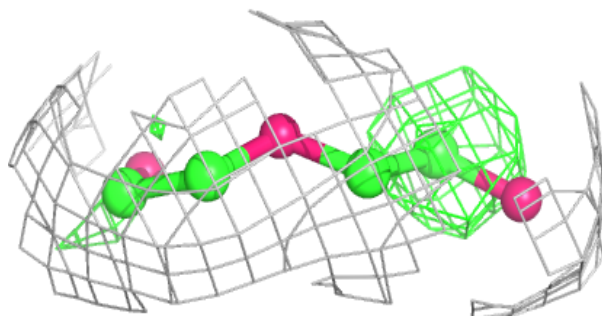
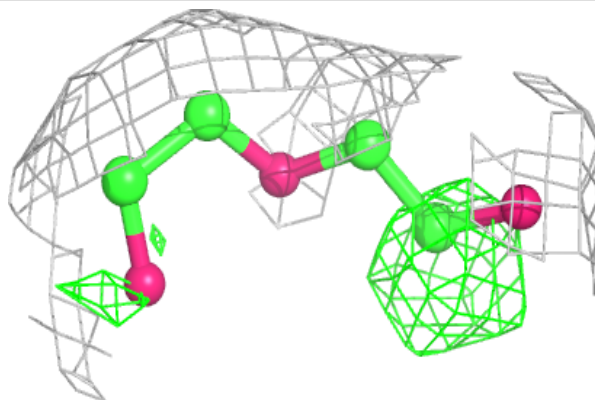


Electron density around PEG A 346:

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

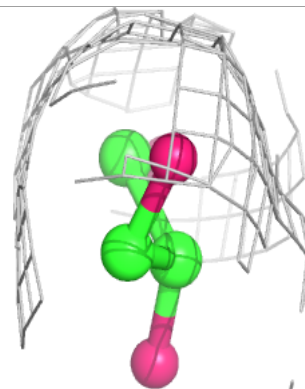
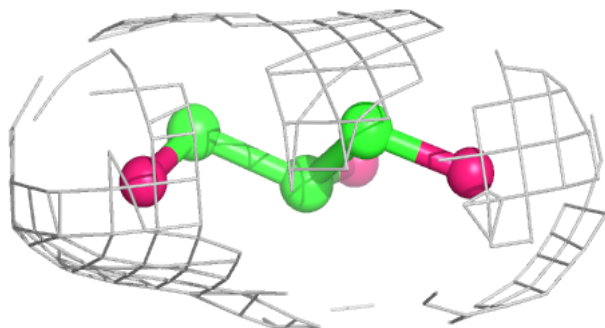
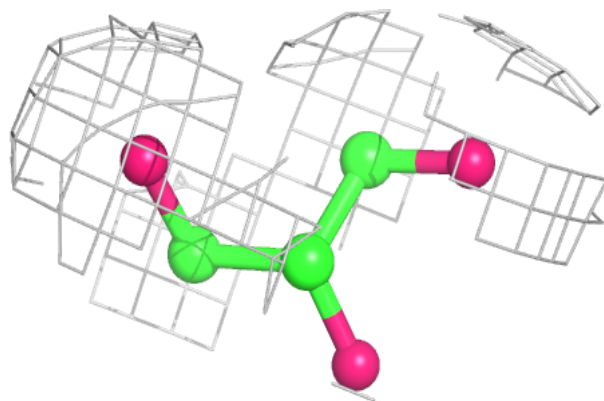
**Electron density around PEG A 370:**

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

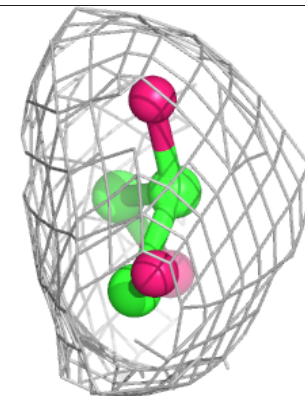
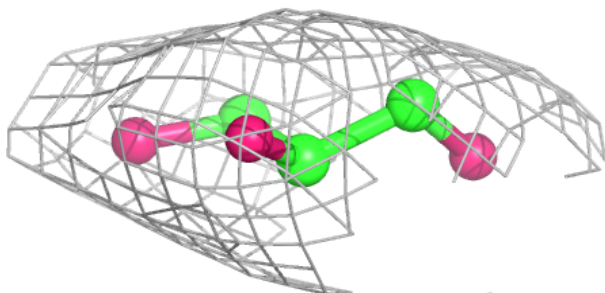
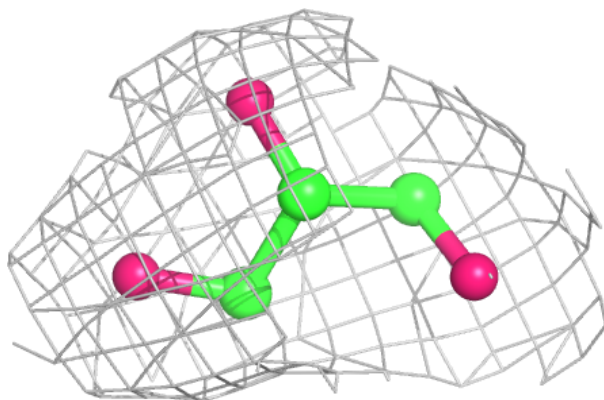


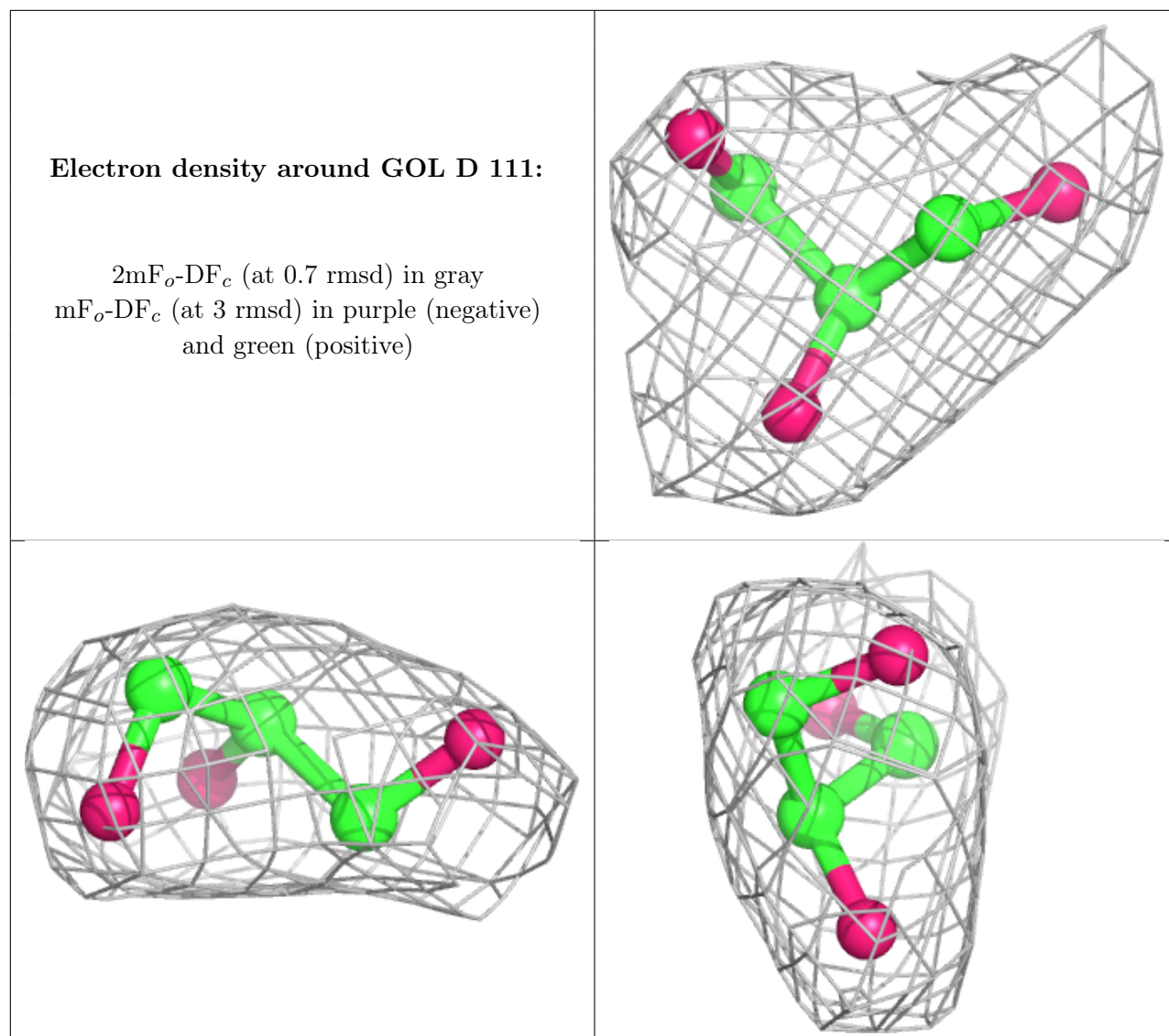
Electron density around GOL B 154:

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

**Electron density around GOL B 153:**

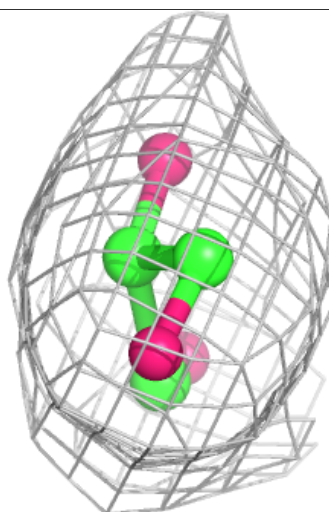
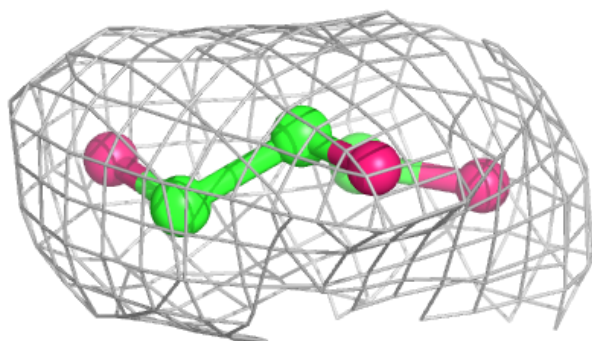
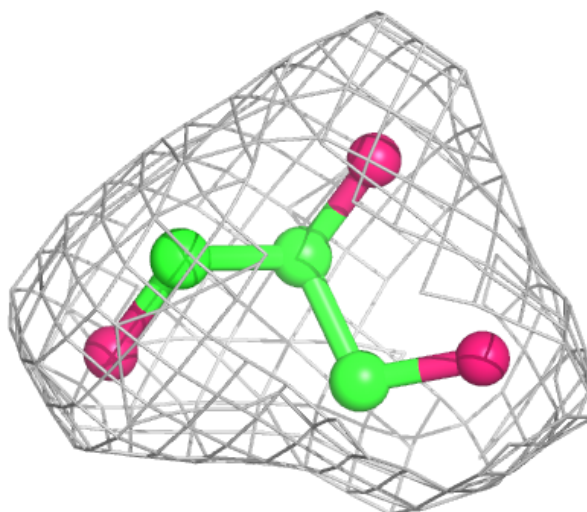
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

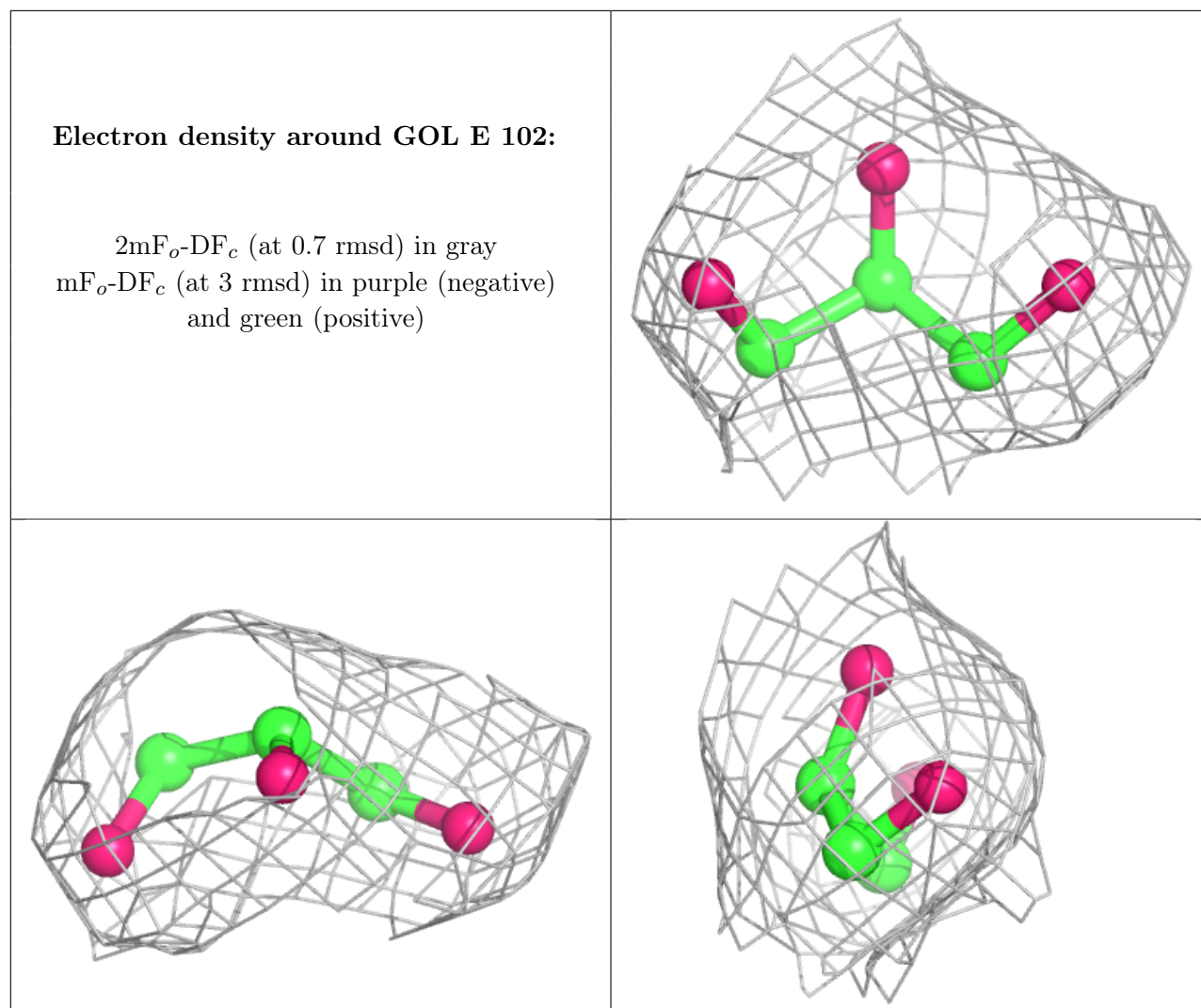




Electron density around GOL A 363:

$2mF_o-DF_c$ (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.