



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 08:34 AM UTC

PDB ID : 8GT7 / pdb_00008gt7
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

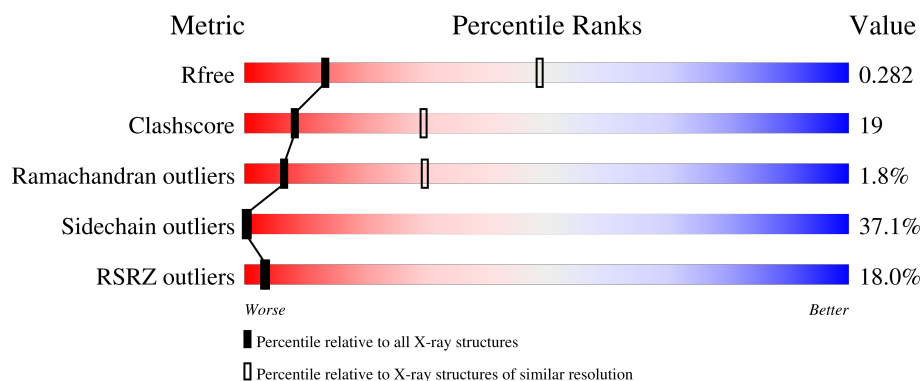
1 Overall quality at a glance

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}	180053	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	

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Mol	Chain	Length	Quality of chain
4	F	9	11% 22% 56% 22%

2 Entry composition

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
1	A	241	Total	C	N	O	S	0	1	0
			1914	1213	315	372	14			
1	C	241	Total	C	N	O	S	0	0	0
			1909	1210	314	371	14			

- Molecule 2 is a protein called Cystatin-A.

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

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.

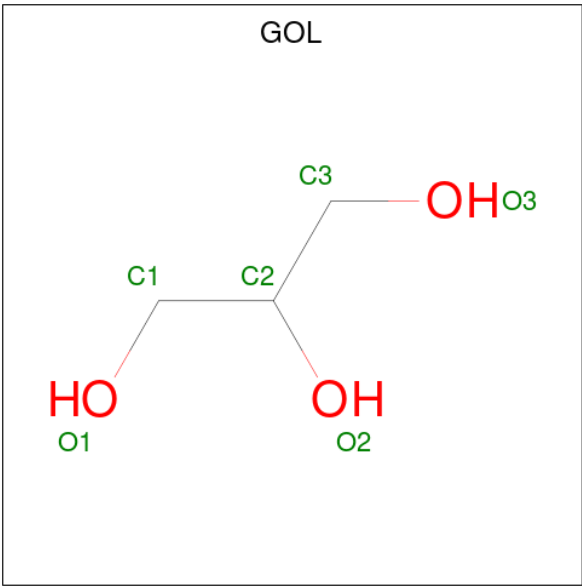
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	0	0	0
			73	47	12	14			

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

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of In-

terest" by depositor).



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

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

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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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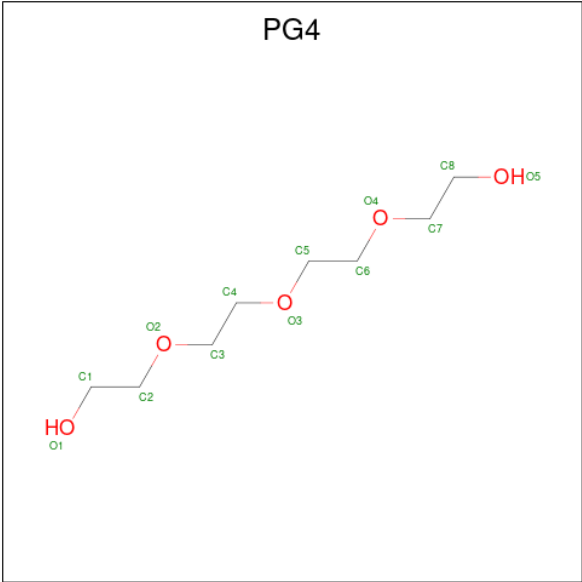
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
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 (CCD ID: 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 (CCD ID: PG4) (formula: C₈H₁₈O₅) (labeled as "Ligand of Interest" by depositor).



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

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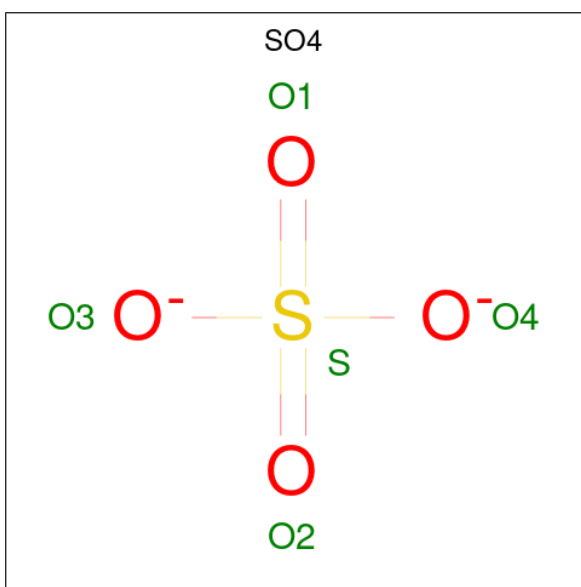
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	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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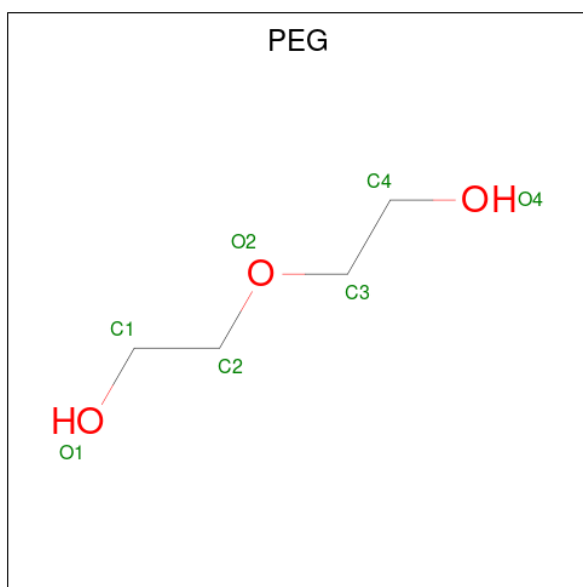
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		
7	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 (CCD ID: SO4) (formula: O₄S).



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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: 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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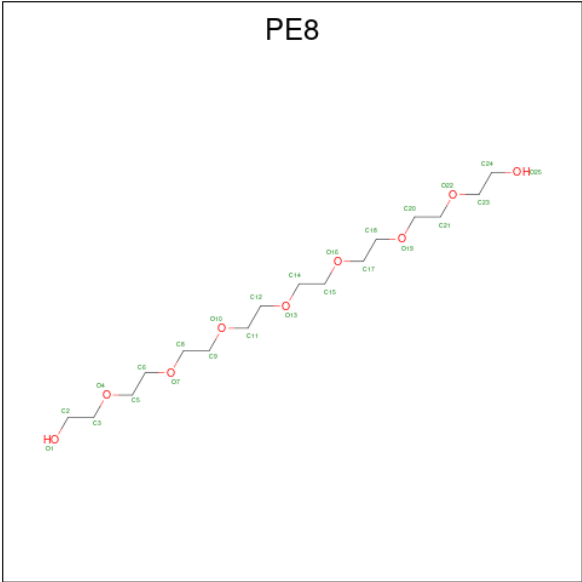
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	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	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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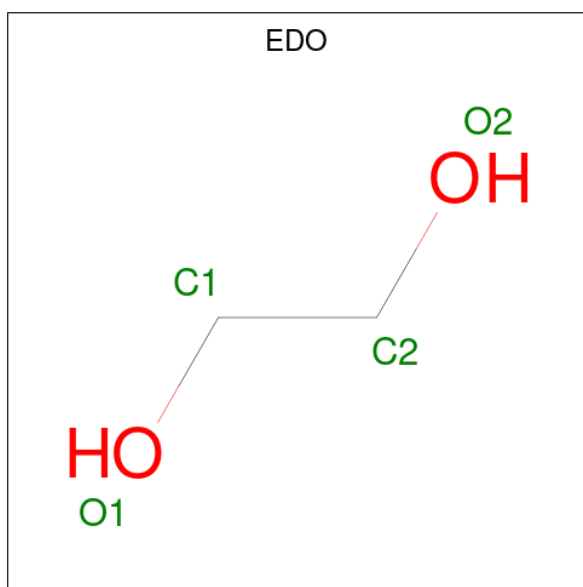
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0

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



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

- Molecule 11 is 1,2-ETHANEDIOL (CCD ID: 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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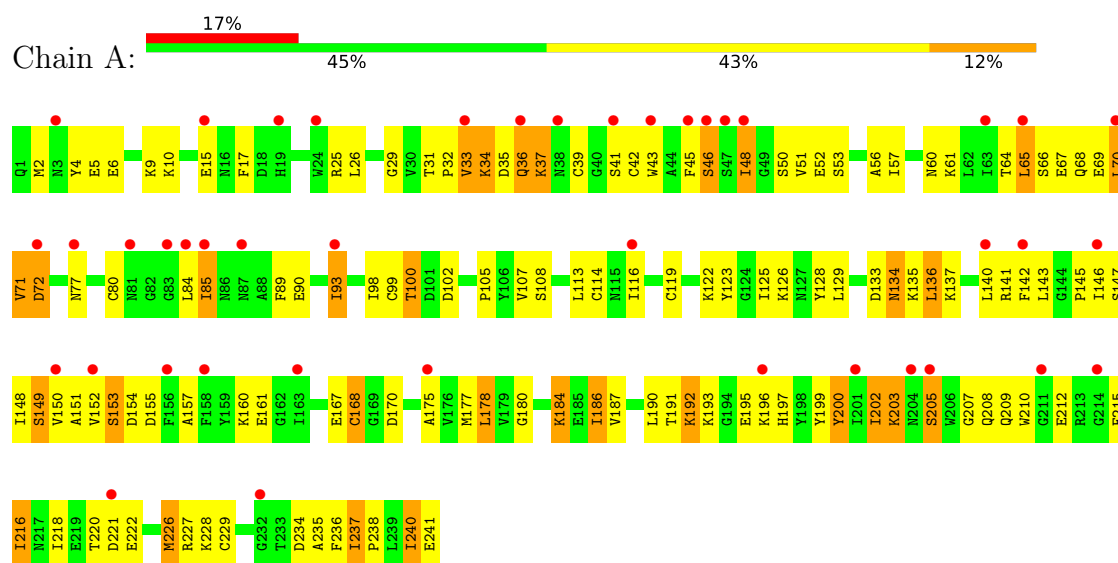
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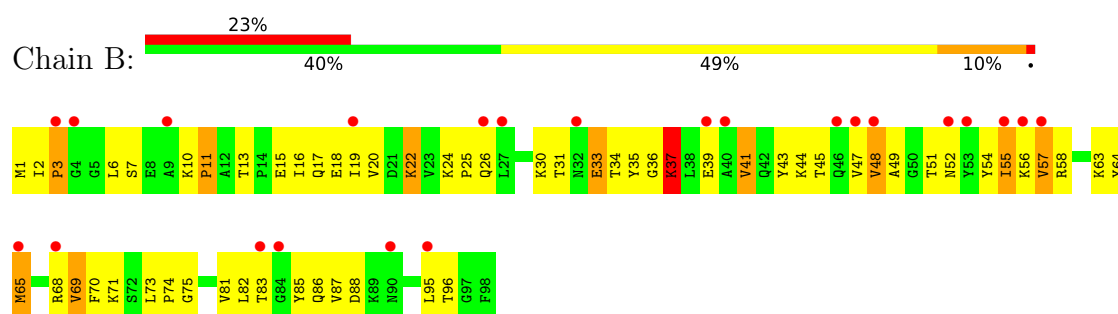
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	E	11	Total	O	0	0
			11	11		
12	F	7	Total	O	0	0
			7	7		

3 Residue-property plots [i](#)

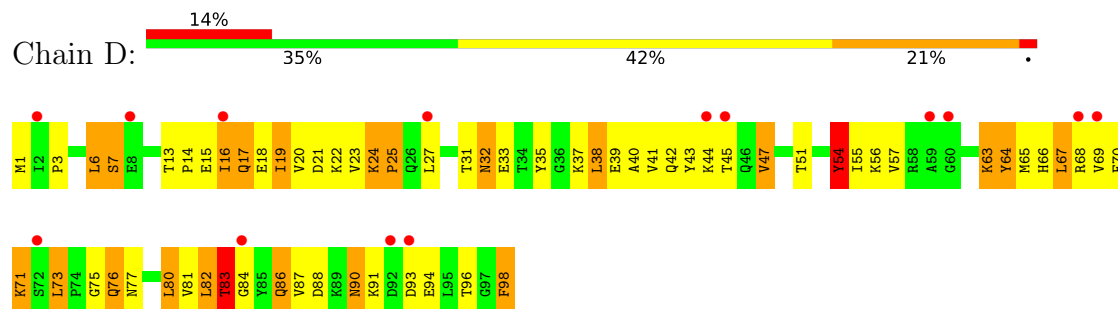
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Cysteine proteinase falcipain 2a





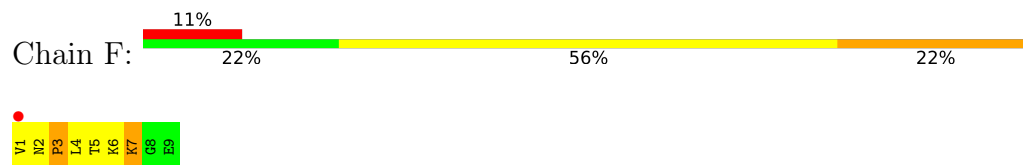
- Molecule 2: Cystatin-A



- 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

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 42.09 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.09-3.28) 99.6 (42.09-3.28)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.272 , 0.300 0.274 , 0.282	Depositor DCC
R_{free} test set	715 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	90.7	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.046 for k,h,-l	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

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	0.33	0/1959	0.79	2/2641 (0.1%)
1	C	0.41	2/1951 (0.1%)	0.92	5/2630 (0.2%)
2	B	0.50	2/790 (0.3%)	0.92	1/1065 (0.1%)
2	D	0.47	0/790	0.96	2/1065 (0.2%)
3	E	0.34	0/73	0.80	0/96
4	F	0.39	0/69	1.09	0/90
All	All	0.41	4/5632 (0.1%)	0.88	10/7587 (0.1%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	131	VAL	CA-C	6.09	1.58	1.53
1	C	131	VAL	N-CA	-5.76	1.42	1.46
2	B	3	PRO	C-O	-5.74	1.16	1.24
2	B	3	PRO	CA-C	5.66	1.60	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	18	GLU	N-CA-C	-6.68	105.75	114.04
1	A	4	TYR	CB-CA-C	-5.78	104.06	111.22
1	C	131	VAL	O-C-N	5.54	124.86	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	54	TYR	CA-CB-CG	5.50	123.80	113.90
1	C	10	LYS	N-CA-C	5.49	122.50	110.80

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 ⓘ

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	74	0
1	C	1909	0	1830	93	0
2	B	777	0	780	32	0
2	D	777	0	780	50	1
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	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
11	B	8	0	12	0	0
11	D	12	0	18	2	1
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	289	1

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 289 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

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:ASN:ND2	11:D:102:EDO:O2[4_555]	1.30	0.90

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%)	16	44
1	C	239/241 (99%)	180 (75%)	55 (23%)	4 (2%)	7	30
2	B	96/98 (98%)	63 (66%)	31 (32%)	2 (2%)	5	26
2	D	96/98 (98%)	63 (66%)	30 (31%)	3 (3%)	3	19
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%)	6	30

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%)	134 (64%)	74 (36%)	0	0
1	C	207/207 (100%)	127 (61%)	80 (39%)	0	0
2	B	85/85 (100%)	54 (64%)	31 (36%)	0	0
2	D	85/85 (100%)	50 (59%)	35 (41%)	0	0
3	E	9/9 (100%)	8 (89%)	1 (11%)	6	23
4	F	8/8 (100%)	5 (62%)	3 (38%)	0	0
All	All	602/601 (100%)	378 (63%)	224 (37%)	0	0

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	39	CYS
4	F	1	VAL
1	C	129	LEU
2	D	98	PHE
2	D	41	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	86	ASN
1	C	87	ASN
2	D	26	GLN
1	C	204	ASN
2	D	17	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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	A	306	-	5,5,5	0.97	0	5,5,5	1.14	0
9	PEG	A	333	-	6,6,6	0.10	0	5,5,5	0.10	0
9	PEG	A	339	-	6,6,6	0.11	0	5,5,5	0.08	0
5	GOL	B	107	-	5,5,5	0.99	0	5,5,5	1.15	1 (20%)
10	PE8	B	137	-	24,24,24	0.48	0	23,23,23	0.25	0
5	GOL	A	373	-	5,5,5	0.91	0	5,5,5	1.06	0
5	GOL	A	304	-	5,5,5	1.00	0	5,5,5	1.14	0
5	GOL	C	314	-	5,5,5	0.91	0	5,5,5	1.16	1 (20%)
7	PG4	D	103	-	12,12,12	0.10	0	11,11,11	0.64	0
10	PE8	A	344	-	24,24,24	0.49	0	23,23,23	0.23	0
9	PEG	D	126	-	6,6,6	0.10	0	5,5,5	0.09	0
7	PG4	C	325	-	12,12,12	0.11	0	11,11,11	0.72	0
5	GOL	A	302	-	5,5,5	0.93	0	5,5,5	1.24	1 (20%)
7	PG4	A	368	-	12,12,12	0.08	0	11,11,11	0.69	0
5	GOL	D	106	-	5,5,5	1.05	0	5,5,5	1.03	0
5	GOL	A	308	-	5,5,5	0.97	0	5,5,5	1.18	1 (20%)
5	GOL	C	338	-	5,5,5	0.95	0	5,5,5	1.20	1 (20%)
7	PG4	D	116	-	12,12,12	0.12	0	11,11,11	0.61	0
9	PEG	D	105	-	6,6,6	0.11	0	5,5,5	0.10	0
7	PG4	B	155	-	12,12,12	0.09	0	11,11,11	0.68	0
7	PG4	A	366	-	12,12,12	0.10	0	11,11,11	0.72	0
9	PEG	B	158	-	6,6,6	0.11	0	5,5,5	0.10	0
9	PEG	A	332	-	6,6,6	0.10	0	5,5,5	0.08	0
5	GOL	A	311	-	5,5,5	0.91	0	5,5,5	1.12	1 (20%)
7	PG4	A	320	-	12,12,12	0.10	0	11,11,11	0.68	0
9	PEG	A	335	-	6,6,6	0.10	0	5,5,5	0.11	0
7	PG4	C	319	-	12,12,12	0.12	0	11,11,11	0.70	0
10	PE8	E	109	-	24,24,24	0.50	0	23,23,23	0.27	0
5	GOL	C	310	-	5,5,5	0.95	0	5,5,5	1.18	0
7	PG4	C	336	-	12,12,12	0.10	0	11,11,11	0.64	0
7	PG4	D	120	-	12,12,12	0.11	0	11,11,11	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PEG	A	346	-	6,6,6	0.12	0	5,5,5	0.08	0
9	PEG	C	328	-	6,6,6	0.11	0	5,5,5	0.07	0
5	GOL	C	307	-	5,5,5	0.97	0	5,5,5	1.20	1 (20%)
7	PG4	A	365	-	12,12,12	0.10	0	11,11,11	0.59	0
9	PEG	B	131	-	6,6,6	0.12	0	5,5,5	0.06	0
7	PG4	F	105	-	12,12,12	0.15	0	11,11,11	0.57	0
9	PEG	B	157	-	6,6,6	0.15	0	5,5,5	0.24	0
7	PG4	C	321	-	12,12,12	0.10	0	11,11,11	0.69	0
7	PG4	B	124	-	12,12,12	0.10	0	11,11,11	0.64	0
5	GOL	E	104	-	5,5,5	0.96	0	5,5,5	1.21	1 (20%)
7	PG4	E	115	-	12,12,12	0.12	0	11,11,11	0.57	0
9	PEG	C	330	-	6,6,6	0.10	0	5,5,5	0.11	0
7	PG4	A	352	-	12,12,12	0.10	0	11,11,11	0.68	0
9	PEG	B	156	-	6,6,6	0.09	0	5,5,5	0.14	0
5	GOL	D	107	-	5,5,5	0.94	0	5,5,5	1.17	1 (20%)
7	PG4	A	324	-	12,12,12	0.10	0	11,11,11	0.67	0
9	PEG	B	129	-	6,6,6	0.12	0	5,5,5	0.08	0
7	PG4	E	114	-	12,12,12	0.10	0	11,11,11	0.64	0
5	GOL	A	363	-	5,5,5	0.98	0	5,5,5	1.14	0
5	GOL	A	303	-	5,5,5	0.98	0	5,5,5	1.15	0
5	GOL	A	310	-	5,5,5	1.04	0	5,5,5	1.06	0
5	GOL	D	113	-	5,5,5	1.03	0	5,5,5	1.07	0
10	PE8	A	343	-	24,24,24	0.50	0	23,23,23	0.26	0
9	PEG	B	134	-	6,6,6	0.11	0	5,5,5	0.11	0
5	GOL	D	108	-	5,5,5	0.97	0	5,5,5	1.28	1 (20%)
5	GOL	C	304	-	5,5,5	0.97	0	5,5,5	1.25	1 (20%)
7	PG4	A	321	-	12,12,12	0.11	0	11,11,11	0.65	0
11	EDO	D	101	-	3,3,3	0.38	0	2,2,2	0.44	0
9	PEG	A	334	-	6,6,6	0.10	0	5,5,5	0.09	0
9	PEG	B	127	-	6,6,6	0.11	0	5,5,5	0.07	0
7	PG4	B	101	-	12,12,12	0.10	0	11,11,11	0.66	0
5	GOL	A	345	-	5,5,5	0.98	0	5,5,5	1.24	1 (20%)
5	GOL	D	111	-	5,5,5	0.99	0	5,5,5	1.16	0
7	PG4	C	324	-	12,12,12	0.11	0	11,11,11	0.64	0
10	PE8	B	102	-	24,24,24	0.49	0	23,23,23	0.26	0
9	PEG	C	303	-	6,6,6	0.10	0	5,5,5	0.11	0
11	EDO	A	351	-	3,3,3	0.43	0	2,2,2	0.40	0
7	PG4	E	106	-	12,12,12	0.10	0	11,11,11	0.69	0
11	EDO	D	102	-	3,3,3	0.32	0	2,2,2	0.63	0
5	GOL	B	153	-	5,5,5	0.99	0	5,5,5	1.15	1 (20%)
9	PEG	C	331	-	6,6,6	0.17	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PEG	C	339	-	6,6,6	0.09	0	5,5,5	0.12	0
5	GOL	A	301	-	5,5,5	0.95	0	5,5,5	1.20	1 (20%)
5	GOL	C	344	-	5,5,5	0.99	0	5,5,5	1.14	0
5	GOL	D	131	-	5,5,5	0.97	0	5,5,5	1.26	1 (20%)
7	PG4	A	325	-	12,12,12	0.15	0	11,11,11	0.53	0
7	PG4	A	367	-	12,12,12	0.10	0	11,11,11	0.68	0
9	PEG	C	346	-	6,6,6	0.10	0	5,5,5	0.11	0
9	PEG	D	124	-	6,6,6	0.11	0	5,5,5	0.09	0
5	GOL	E	103	-	5,5,5	0.95	0	5,5,5	1.20	1 (20%)
5	GOL	A	305	-	5,5,5	0.99	0	5,5,5	1.13	0
5	GOL	B	112	-	5,5,5	0.94	0	5,5,5	1.26	1 (20%)
5	GOL	B	106	-	5,5,5	1.02	0	5,5,5	1.22	1 (20%)
5	GOL	C	311	-	5,5,5	0.98	0	5,5,5	1.22	1 (20%)
7	PG4	B	121	-	12,12,12	0.09	0	11,11,11	0.73	0
7	PG4	D	119	-	12,12,12	0.13	0	11,11,11	0.68	0
9	PEG	B	142	-	6,6,6	0.11	0	5,5,5	0.11	0
7	PG4	E	105	-	12,12,12	0.12	0	11,11,11	0.61	0
5	GOL	B	108	-	5,5,5	0.98	0	5,5,5	1.25	1 (20%)
7	PG4	A	323	-	12,12,12	0.14	0	11,11,11	0.65	0
5	GOL	B	111	-	5,5,5	0.99	0	5,5,5	1.04	0
9	PEG	D	123	-	6,6,6	0.10	0	5,5,5	0.08	0
9	PEG	A	372	-	6,6,6	0.10	0	5,5,5	0.10	0
9	PEG	C	327	-	6,6,6	0.10	0	5,5,5	0.13	0
7	PG4	C	323	-	12,12,12	0.13	0	11,11,11	0.59	0
9	PEG	A	330	-	6,6,6	0.12	0	5,5,5	0.08	0
7	PG4	C	322	-	12,12,12	0.09	0	11,11,11	0.65	0
9	PEG	B	135	-	6,6,6	0.12	0	5,5,5	0.08	0
10	PE8	B	136	-	24,24,24	0.49	0	23,23,23	0.32	0
5	GOL	E	102	-	5,5,5	0.99	0	5,5,5	1.27	1 (20%)
9	PEG	D	125	-	6,6,6	0.11	0	5,5,5	0.10	0
5	GOL	D	110	-	5,5,5	1.02	0	5,5,5	1.22	1 (20%)
7	PG4	A	326	-	12,12,12	0.11	0	11,11,11	0.62	0
9	PEG	B	132	-	6,6,6	0.10	0	5,5,5	0.10	0
5	GOL	A	364	-	5,5,5	0.98	0	5,5,5	1.19	1 (20%)
10	PE8	F	102	-	24,24,24	0.49	0	23,23,23	0.22	0
5	GOL	E	113	-	5,5,5	0.96	0	5,5,5	1.00	0
5	GOL	B	103	-	5,5,5	0.99	0	5,5,5	1.23	1 (20%)
9	PEG	A	341	-	6,6,6	0.12	0	5,5,5	0.06	0
5	GOL	C	306	-	5,5,5	1.00	0	5,5,5	1.27	1 (20%)
7	PG4	B	117	-	12,12,12	0.13	0	11,11,11	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	C	301	-	4,4,4	0.24	0	6,6,6	0.07	0
9	PEG	B	126	-	6,6,6	0.11	0	5,5,5	0.09	0
9	PEG	C	334	-	6,6,6	0.16	0	5,5,5	0.19	0
11	EDO	B	144	-	3,3,3	0.47	0	2,2,2	0.41	0
5	GOL	B	140	-	5,5,5	0.98	0	5,5,5	1.26	1 (20%)
9	PEG	A	338	-	6,6,6	0.11	0	5,5,5	0.09	0
7	PG4	C	320	-	12,12,12	0.11	0	11,11,11	0.49	0
9	PEG	D	121	-	6,6,6	0.11	0	5,5,5	0.10	0
9	PEG	B	128	-	6,6,6	0.11	0	5,5,5	0.11	0
5	GOL	C	309	-	5,5,5	0.96	0	5,5,5	1.29	1 (20%)
8	SO4	A	327	-	4,4,4	0.24	0	6,6,6	0.06	0
9	PEG	B	130	-	6,6,6	0.11	0	5,5,5	0.09	0
5	GOL	A	309	-	5,5,5	0.99	0	5,5,5	1.15	0
5	GOL	C	337	-	5,5,5	0.96	0	5,5,5	1.27	1 (20%)
10	PE8	A	342	-	24,24,24	0.50	0	23,23,23	0.24	0
8	SO4	A	328	-	4,4,4	0.24	0	6,6,6	0.07	0
9	PEG	D	122	-	6,6,6	0.08	0	5,5,5	0.14	0
5	GOL	D	112	-	5,5,5	0.99	0	5,5,5	1.26	1 (20%)
8	SO4	E	108	-	4,4,4	0.25	0	6,6,6	0.07	0
5	GOL	A	314	-	5,5,5	0.97	0	5,5,5	1.25	1 (20%)
5	GOL	C	345	-	5,5,5	0.99	0	5,5,5	1.18	1 (20%)
9	PEG	A	337	-	6,6,6	0.10	0	5,5,5	0.10	0
9	PEG	B	133	-	6,6,6	0.11	0	5,5,5	0.08	0
10	PE8	F	106	-	24,24,24	0.49	0	23,23,23	0.26	0
9	PEG	C	332	-	6,6,6	0.11	0	5,5,5	0.09	0
11	EDO	E	111	-	3,3,3	0.43	0	2,2,2	0.46	0
5	GOL	D	137	-	5,5,5	0.91	0	5,5,5	1.05	0
10	PE8	C	335	-	24,24,24	0.49	0	23,23,23	0.23	0
5	GOL	B	105	-	5,5,5	1.02	0	5,5,5	1.08	0
5	GOL	B	152	-	5,5,5	0.95	0	5,5,5	1.22	1 (20%)
9	PEG	A	329	-	6,6,6	0.11	0	5,5,5	0.09	0
5	GOL	A	313	-	5,5,5	0.99	0	5,5,5	1.14	0
8	SO4	C	326	-	4,4,4	0.24	0	6,6,6	0.08	0
7	PG4	D	118	-	12,12,12	0.12	0	11,11,11	0.72	0
5	GOL	B	110	-	5,5,5	0.97	0	5,5,5	1.27	1 (20%)
9	PEG	D	128	-	6,6,6	0.11	0	5,5,5	0.08	0
9	PEG	B	139	-	6,6,6	0.10	0	5,5,5	0.09	0
5	GOL	A	362	-	5,5,5	0.97	0	5,5,5	1.18	1 (20%)
7	PG4	B	118	-	12,12,12	0.14	0	11,11,11	0.70	0
7	PG4	A	319	-	12,12,12	0.10	0	11,11,11	0.66	0
9	PEG	D	127	-	6,6,6	0.11	0	5,5,5	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PG4	B	122	-	12,12,12	0.10	0	11,11,11	0.66	0
5	GOL	B	104	-	5,5,5	0.96	0	5,5,5	1.19	1 (20%)
7	PG4	F	101	-	12,12,12	0.13	0	11,11,11	0.58	0
5	GOL	C	347	-	5,5,5	0.97	0	5,5,5	1.15	0
5	GOL	F	103	-	5,5,5	0.98	0	5,5,5	1.20	1 (20%)
9	PEG	A	340	-	6,6,6	0.12	0	5,5,5	0.09	0
5	GOL	A	312	-	5,5,5	1.04	0	5,5,5	1.03	0
5	GOL	C	312	-	5,5,5	0.93	0	5,5,5	1.22	1 (20%)
7	PG4	A	369	-	12,12,12	0.09	0	11,11,11	0.69	0
11	EDO	B	143	-	3,3,3	0.40	0	2,2,2	0.40	0
7	PG4	D	117	-	12,12,12	0.10	0	11,11,11	0.69	0
7	PG4	B	116	-	12,12,12	0.11	0	11,11,11	0.67	0
10	PE8	E	110	-	24,24,24	0.49	0	23,23,23	0.31	0
9	PEG	C	329	-	6,6,6	0.12	0	5,5,5	0.09	0
10	PE8	B	138	-	24,24,24	0.48	0	23,23,23	0.27	0
5	GOL	D	109	-	5,5,5	0.99	0	5,5,5	1.16	0
5	GOL	A	347	-	5,5,5	0.80	0	5,5,5	1.31	1 (20%)
11	EDO	E	101	-	3,3,3	0.38	0	2,2,2	0.44	0
5	GOL	C	313	-	5,5,5	0.92	0	5,5,5	1.14	1 (20%)
7	PG4	B	120	-	12,12,12	0.11	0	11,11,11	0.76	0
7	PG4	C	302	-	12,12,12	0.13	0	11,11,11	0.52	0
9	PEG	A	371	-	6,6,6	0.11	0	5,5,5	0.08	0
9	PEG	A	370	-	6,6,6	0.12	0	5,5,5	0.09	0
5	GOL	A	307	-	5,5,5	1.01	0	5,5,5	1.26	1 (20%)
5	GOL	B	154	-	5,5,5	1.00	0	5,5,5	1.16	1 (20%)
7	PG4	B	123	-	12,12,12	0.10	0	11,11,11	0.72	0
7	PG4	E	107	-	12,12,12	0.11	0	11,11,11	0.63	0
7	PG4	A	322	-	12,12,12	0.12	0	11,11,11	0.63	0
9	PEG	A	331	-	6,6,6	0.16	0	5,5,5	0.26	0
5	GOL	C	305	-	5,5,5	1.06	0	5,5,5	1.02	0
9	PEG	D	104	-	6,6,6	0.11	0	5,5,5	0.09	0
5	GOL	C	308	-	5,5,5	1.01	0	5,5,5	1.13	0
9	PEG	A	336	-	6,6,6	0.11	0	5,5,5	0.12	0
5	GOL	B	109	-	5,5,5	0.97	0	5,5,5	1.20	1 (20%)
11	EDO	D	130	-	3,3,3	0.44	0	2,2,2	0.40	0
9	PEG	A	353	-	6,6,6	0.11	0	5,5,5	0.10	0
7	PG4	B	125	-	12,12,12	0.12	0	11,11,11	0.74	0
9	PEG	C	333	-	6,6,6	0.09	0	5,5,5	0.14	0
7	PG4	B	119	-	12,12,12	0.12	0	11,11,11	0.70	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	A	306	-	-	2/4/4/4	-
9	PEG	A	333	-	-	3/4/4/4	-
9	PEG	A	339	-	-	3/4/4/4	-
5	GOL	B	107	-	-	0/4/4/4	-
10	PE8	B	137	-	-	11/22/22/22	-
5	GOL	A	373	-	-	2/4/4/4	-
5	GOL	A	304	-	-	1/4/4/4	-
5	GOL	C	314	-	-	4/4/4/4	-
7	PG4	D	103	-	-	7/10/10/10	-
10	PE8	A	344	-	-	12/22/22/22	-
9	PEG	D	126	-	-	3/4/4/4	-
7	PG4	C	325	-	-	7/10/10/10	-
5	GOL	A	302	-	-	2/4/4/4	-
7	PG4	A	368	-	-	7/10/10/10	-
5	GOL	D	106	-	-	3/4/4/4	-
5	GOL	A	308	-	-	0/4/4/4	-
5	GOL	C	338	-	-	2/4/4/4	-
7	PG4	D	116	-	-	3/10/10/10	-
9	PEG	D	105	-	-	3/4/4/4	-
7	PG4	B	155	-	-	6/10/10/10	-
7	PG4	A	366	-	-	5/10/10/10	-
9	PEG	B	158	-	-	2/4/4/4	-
9	PEG	A	332	-	-	3/4/4/4	-
5	GOL	A	311	-	-	4/4/4/4	-
7	PG4	A	320	-	-	5/10/10/10	-
9	PEG	A	335	-	-	3/4/4/4	-
7	PG4	C	319	-	-	6/10/10/10	-
10	PE8	E	109	-	-	11/22/22/22	-
5	GOL	C	310	-	-	4/4/4/4	-
7	PG4	C	336	-	-	4/10/10/10	-
7	PG4	D	120	-	-	7/10/10/10	-
9	PEG	A	346	-	-	3/4/4/4	-
9	PEG	C	328	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	307	-	-	3/4/4/4	-
7	PG4	A	365	-	-	8/10/10/10	-
9	PEG	B	131	-	-	2/4/4/4	-
7	PG4	F	105	-	-	5/10/10/10	-
9	PEG	B	157	-	-	3/4/4/4	-
7	PG4	C	321	-	-	6/10/10/10	-
7	PG4	B	124	-	-	4/10/10/10	-
5	GOL	E	104	-	-	2/4/4/4	-
7	PG4	E	115	-	-	5/10/10/10	-
9	PEG	C	330	-	-	3/4/4/4	-
7	PG4	A	352	-	-	8/10/10/10	-
9	PEG	B	156	-	-	2/4/4/4	-
5	GOL	D	107	-	-	4/4/4/4	-
7	PG4	A	324	-	-	7/10/10/10	-
9	PEG	B	129	-	-	2/4/4/4	-
7	PG4	E	114	-	-	7/10/10/10	-
5	GOL	A	363	-	-	2/4/4/4	-
5	GOL	A	303	-	-	1/4/4/4	-
5	GOL	A	310	-	-	2/4/4/4	-
5	GOL	D	113	-	-	0/4/4/4	-
10	PE8	A	343	-	-	15/22/22/22	-
9	PEG	B	134	-	-	3/4/4/4	-
5	GOL	D	108	-	-	1/4/4/4	-
5	GOL	C	304	-	-	4/4/4/4	-
7	PG4	A	321	-	-	8/10/10/10	-
11	EDO	D	101	-	-	0/1/1/1	-
9	PEG	A	334	-	-	2/4/4/4	-
9	PEG	B	127	-	-	3/4/4/4	-
7	PG4	B	101	-	-	3/10/10/10	-
5	GOL	A	345	-	-	4/4/4/4	-
5	GOL	D	111	-	-	2/4/4/4	-
7	PG4	C	324	-	-	7/10/10/10	-
10	PE8	B	102	-	-	9/22/22/22	-
9	PEG	C	303	-	-	3/4/4/4	-
11	EDO	A	351	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	E	106	-	-	7/10/10/10	-
11	EDO	D	102	-	-	1/1/1/1	-
5	GOL	B	153	-	-	0/4/4/4	-
9	PEG	C	331	-	-	3/4/4/4	-
9	PEG	C	339	-	-	3/4/4/4	-
5	GOL	A	301	-	-	4/4/4/4	-
5	GOL	C	344	-	-	2/4/4/4	-
5	GOL	D	131	-	-	4/4/4/4	-
7	PG4	A	325	-	-	8/10/10/10	-
7	PG4	A	367	-	-	6/10/10/10	-
9	PEG	C	346	-	-	2/4/4/4	-
9	PEG	D	124	-	-	2/4/4/4	-
5	GOL	E	103	-	-	2/4/4/4	-
5	GOL	A	305	-	-	0/4/4/4	-
5	GOL	B	112	-	-	2/4/4/4	-
5	GOL	B	106	-	-	0/4/4/4	-
5	GOL	C	311	-	-	4/4/4/4	-
7	PG4	B	121	-	-	7/10/10/10	-
7	PG4	D	119	-	-	4/10/10/10	-
9	PEG	B	142	-	-	1/4/4/4	-
7	PG4	E	105	-	-	4/10/10/10	-
5	GOL	B	108	-	-	2/4/4/4	-
7	PG4	A	323	-	-	6/10/10/10	-
5	GOL	B	111	-	-	4/4/4/4	-
9	PEG	D	123	-	-	2/4/4/4	-
9	PEG	A	372	-	-	4/4/4/4	-
9	PEG	C	327	-	-	2/4/4/4	-
7	PG4	C	323	-	-	6/10/10/10	-
9	PEG	A	330	-	-	2/4/4/4	-
7	PG4	C	322	-	-	5/10/10/10	-
9	PEG	B	135	-	-	1/4/4/4	-
10	PE8	B	136	-	-	13/22/22/22	-
5	GOL	E	102	-	-	4/4/4/4	-
9	PEG	D	125	-	-	2/4/4/4	-
5	GOL	D	110	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	A	326	-	-	8/10/10/10	-
9	PEG	B	132	-	-	3/4/4/4	-
5	GOL	A	364	-	-	3/4/4/4	-
10	PE8	F	102	-	-	14/22/22/22	-
5	GOL	E	113	-	-	4/4/4/4	-
5	GOL	B	103	-	-	4/4/4/4	-
9	PEG	A	341	-	-	2/4/4/4	-
5	GOL	C	306	-	-	2/4/4/4	-
7	PG4	B	117	-	-	7/10/10/10	-
9	PEG	B	126	-	-	1/4/4/4	-
9	PEG	C	334	-	-	2/4/4/4	-
11	EDO	B	144	-	-	1/1/1/1	-
5	GOL	B	140	-	-	2/4/4/4	-
9	PEG	A	338	-	-	2/4/4/4	-
7	PG4	C	320	-	-	7/10/10/10	-
9	PEG	D	121	-	-	3/4/4/4	-
9	PEG	B	128	-	-	2/4/4/4	-
5	GOL	C	309	-	-	4/4/4/4	-
9	PEG	B	130	-	-	4/4/4/4	-
5	GOL	A	309	-	-	2/4/4/4	-
5	GOL	C	337	-	-	2/4/4/4	-
10	PE8	A	342	-	-	13/22/22/22	-
9	PEG	D	122	-	-	1/4/4/4	-
5	GOL	D	112	-	-	3/4/4/4	-
5	GOL	A	314	-	-	2/4/4/4	-
5	GOL	C	345	-	-	2/4/4/4	-
9	PEG	A	337	-	-	4/4/4/4	-
9	PEG	B	133	-	-	3/4/4/4	-
10	PE8	F	106	-	-	16/22/22/22	-
9	PEG	C	332	-	-	3/4/4/4	-
11	EDO	E	111	-	-	1/1/1/1	-
5	GOL	D	137	-	-	2/4/4/4	-
10	PE8	C	335	-	-	13/22/22/22	-
5	GOL	B	105	-	-	0/4/4/4	-
5	GOL	B	152	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PEG	A	329	-	-	1/4/4/4	-
5	GOL	A	313	-	-	0/4/4/4	-
7	PG4	D	118	-	-	8/10/10/10	-
5	GOL	B	110	-	-	1/4/4/4	-
9	PEG	D	128	-	-	2/4/4/4	-
9	PEG	B	139	-	-	3/4/4/4	-
5	GOL	A	362	-	-	3/4/4/4	-
7	PG4	B	118	-	-	5/10/10/10	-
7	PG4	A	319	-	-	6/10/10/10	-
9	PEG	D	127	-	-	2/4/4/4	-
7	PG4	B	122	-	-	7/10/10/10	-
5	GOL	B	104	-	-	2/4/4/4	-
7	PG4	F	101	-	-	6/10/10/10	-
5	GOL	C	347	-	-	2/4/4/4	-
5	GOL	F	103	-	-	2/4/4/4	-
9	PEG	A	340	-	-	4/4/4/4	-
5	GOL	A	312	-	-	4/4/4/4	-
5	GOL	C	312	-	-	4/4/4/4	-
7	PG4	A	369	-	-	6/10/10/10	-
11	EDO	B	143	-	-	0/1/1/1	-
7	PG4	D	117	-	-	7/10/10/10	-
7	PG4	B	116	-	-	7/10/10/10	-
10	PE8	E	110	-	-	16/22/22/22	-
9	PEG	C	329	-	-	3/4/4/4	-
10	PE8	B	138	-	-	15/22/22/22	-
5	GOL	D	109	-	-	4/4/4/4	-
5	GOL	A	347	-	-	2/4/4/4	-
11	EDO	E	101	-	-	0/1/1/1	-
5	GOL	C	313	-	-	2/4/4/4	-
7	PG4	B	120	-	-	4/10/10/10	-
7	PG4	C	302	-	-	5/10/10/10	-
9	PEG	A	371	-	-	1/4/4/4	-
9	PEG	A	370	-	-	2/4/4/4	-
5	GOL	A	307	-	-	2/4/4/4	-
5	GOL	B	154	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	B	123	-	-	8/10/10/10	-
7	PG4	E	107	-	-	2/10/10/10	-
7	PG4	A	322	-	-	3/10/10/10	-
9	PEG	A	331	-	-	3/4/4/4	-
5	GOL	C	305	-	-	2/4/4/4	-
9	PEG	D	104	-	-	1/4/4/4	-
5	GOL	C	308	-	-	4/4/4/4	-
9	PEG	A	336	-	-	2/4/4/4	-
5	GOL	B	109	-	-	2/4/4/4	-
11	EDO	D	130	-	-	1/1/1/1	-
9	PEG	A	353	-	-	3/4/4/4	-
7	PG4	B	125	-	-	7/10/10/10	-
9	PEG	C	333	-	-	2/4/4/4	-
7	PG4	B	119	-	-	7/10/10/10	-

There are no bond length outliers.

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	347	GOL	C3-C2-C1	-2.58	102.34	111.80
5	C	309	GOL	C3-C2-C1	-2.36	103.15	111.80
5	B	104	GOL	C3-C2-C1	-2.26	103.51	111.80
5	C	304	GOL	C3-C2-C1	-2.26	103.51	111.80
5	C	337	GOL	C3-C2-C1	-2.25	103.55	111.80

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.

55 monomers are involved in 66 short contacts:

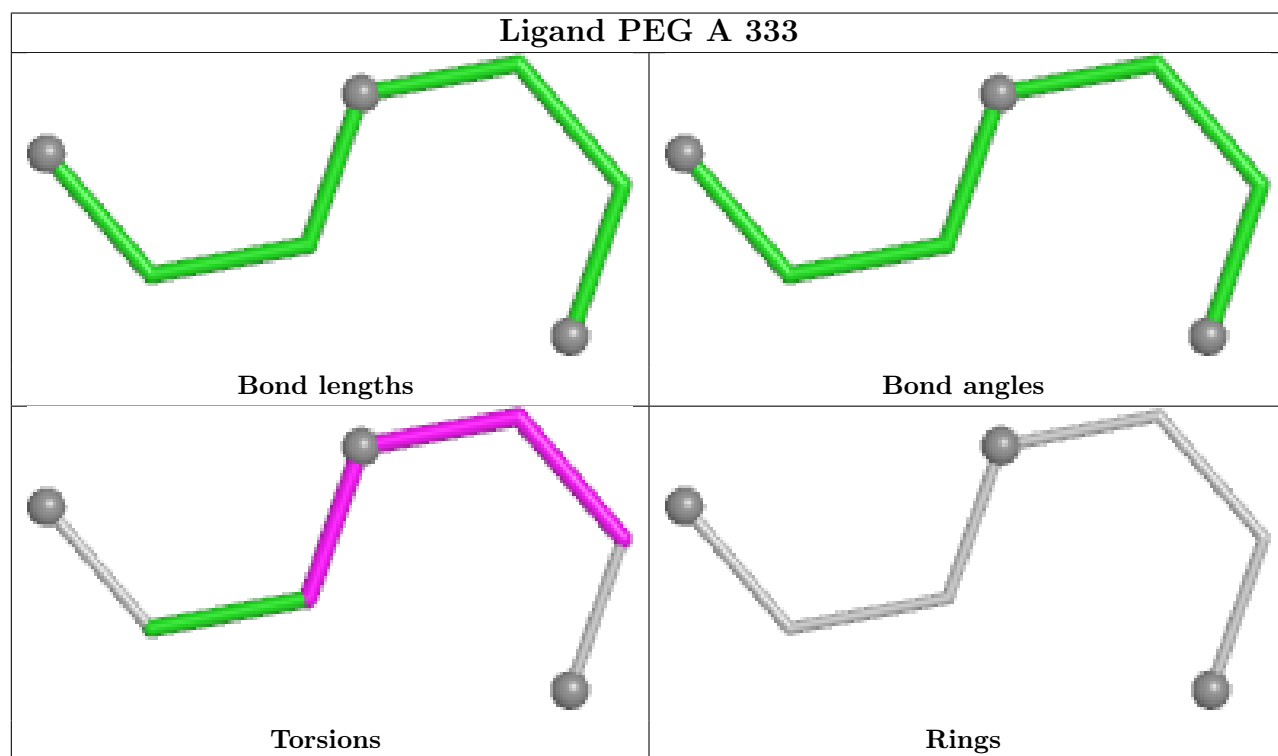
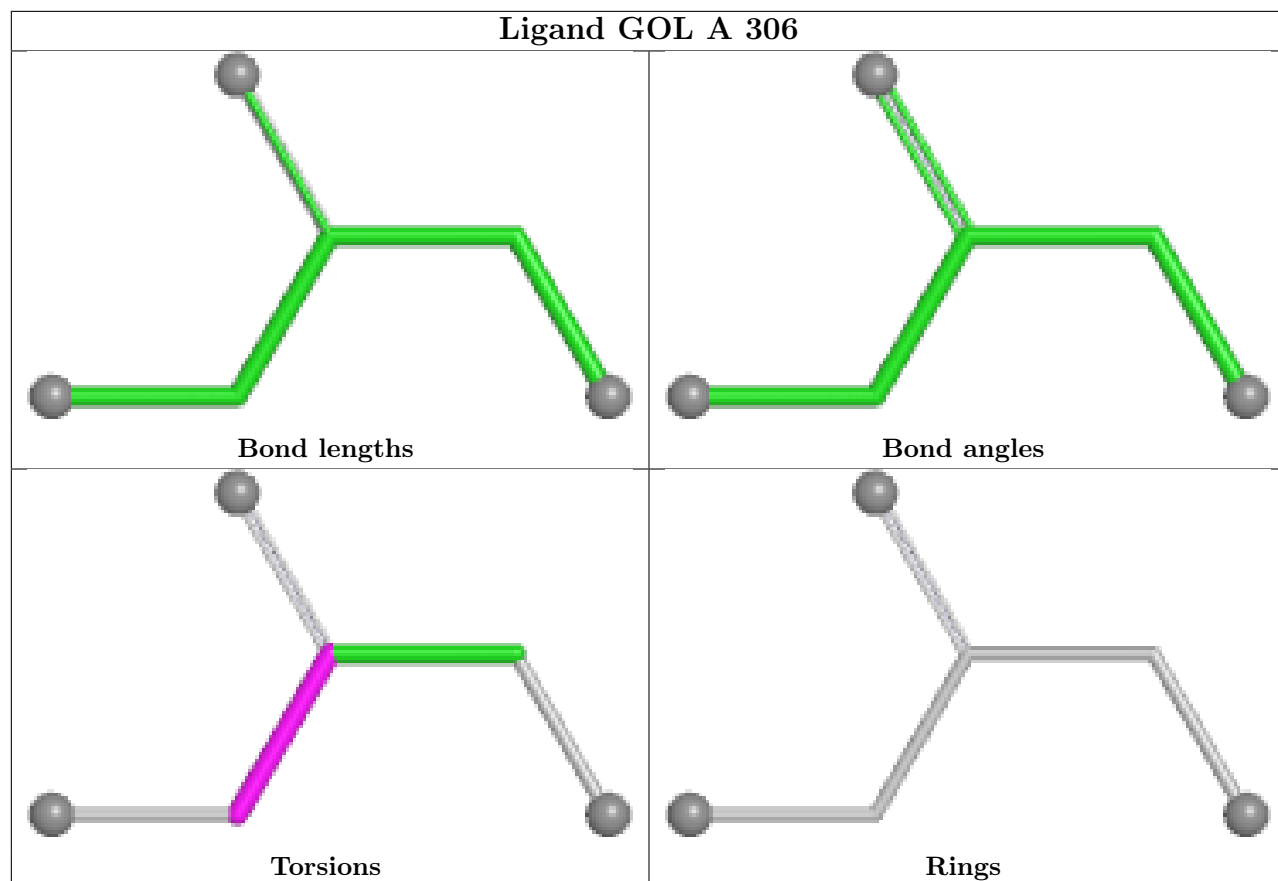
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	137	PE8	1	0
7	D	103	PG4	2	0
7	C	325	PG4	3	0
5	D	106	GOL	2	0
5	C	338	GOL	1	0
7	B	155	PG4	1	0
7	A	366	PG4	1	0
10	E	109	PE8	2	0
7	A	365	PG4	1	0
7	F	105	PG4	1	0
9	B	157	PEG	1	0
7	C	321	PG4	2	0
7	E	115	PG4	1	0
5	A	363	GOL	1	0
5	A	303	GOL	1	0
5	A	310	GOL	1	0
5	D	108	GOL	1	0
7	B	101	PG4	1	0
7	C	324	PG4	1	0
7	E	106	PG4	1	0
11	D	102	EDO	2	1
9	C	331	PEG	1	0
5	C	344	GOL	1	0
7	A	325	PG4	2	0
5	E	103	GOL	1	0
7	D	119	PG4	1	0
7	A	323	PG4	1	0
7	C	323	PG4	2	0
7	C	322	PG4	3	0
10	B	136	PE8	3	0
10	F	102	PE8	2	0
5	E	113	GOL	1	0
9	A	341	PEG	1	0
7	B	117	PG4	1	0
5	B	140	GOL	2	0
7	C	320	PG4	2	0
5	C	309	GOL	1	0
9	B	130	PEG	1	0
10	A	342	PE8	2	0
5	C	345	GOL	2	0
10	F	106	PE8	2	0
9	C	332	PEG	1	0
10	C	335	PE8	2	0

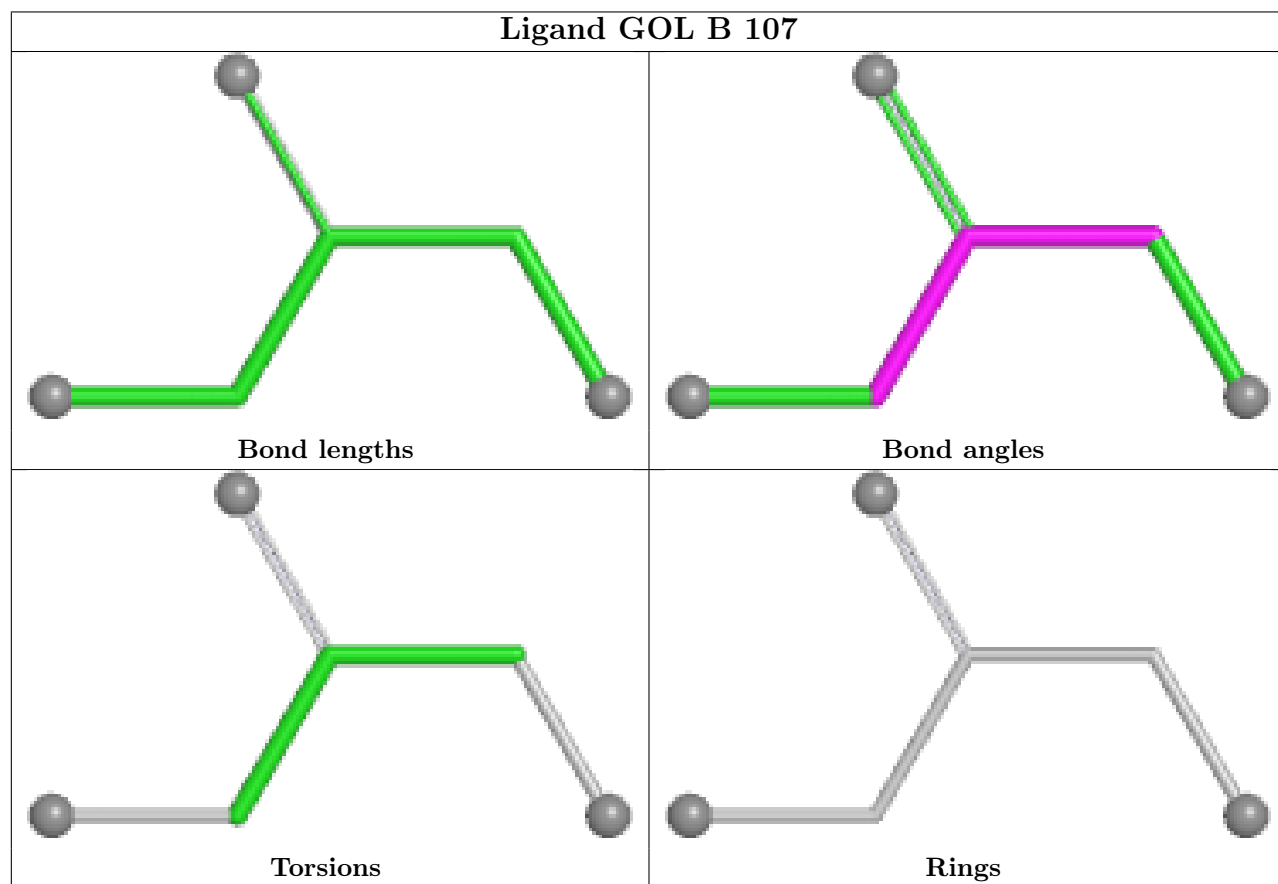
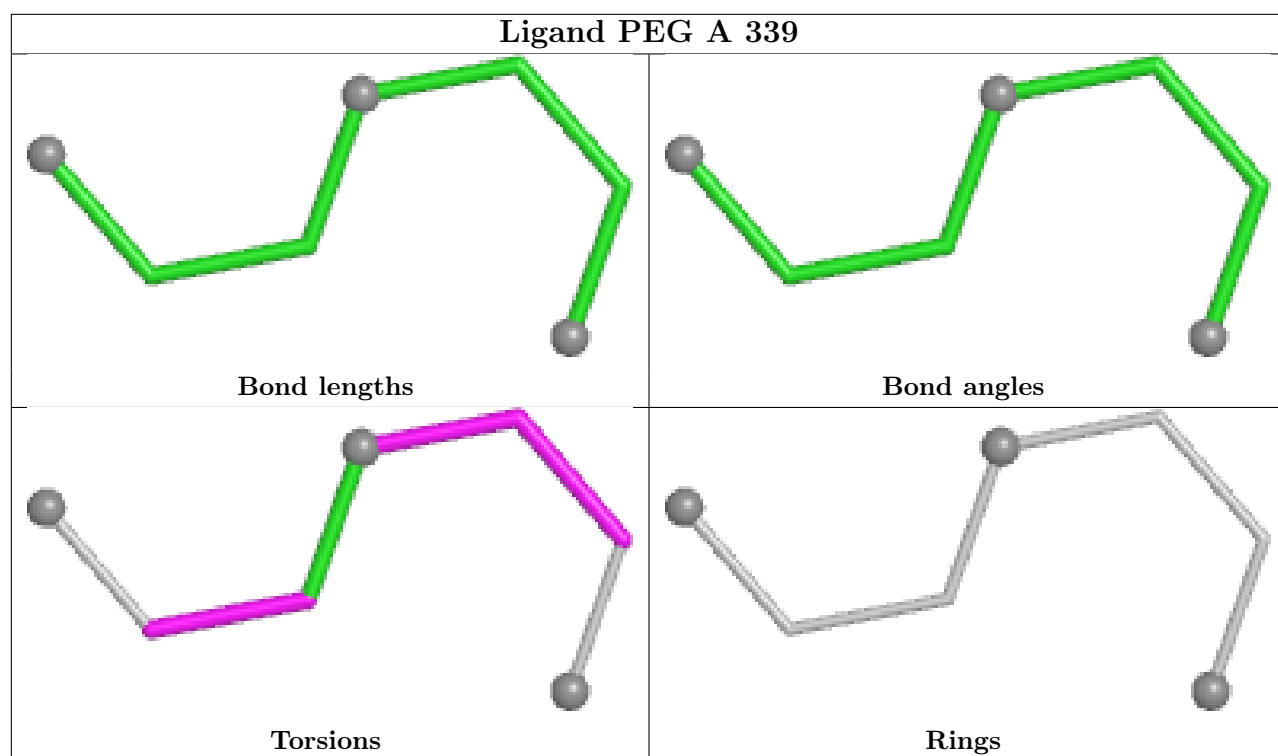
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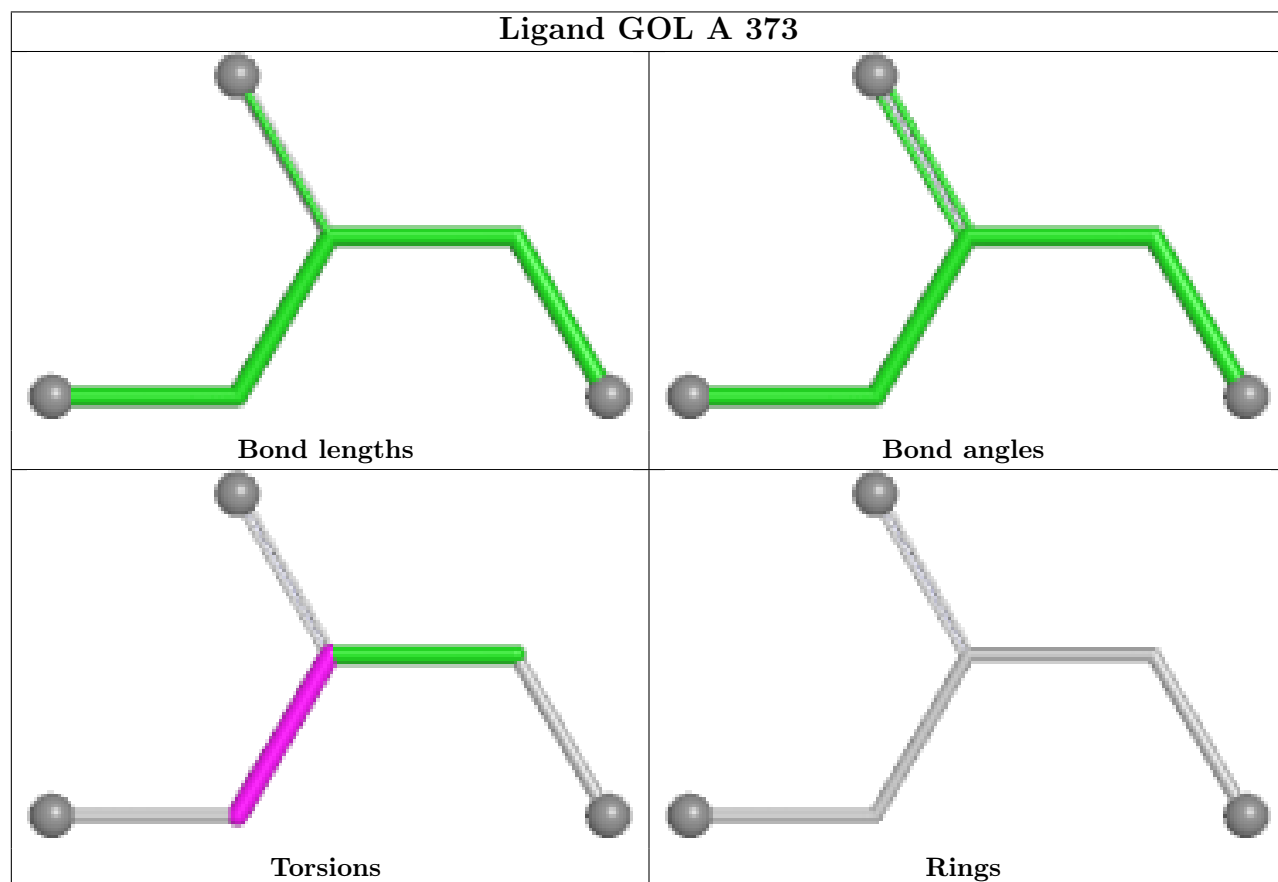
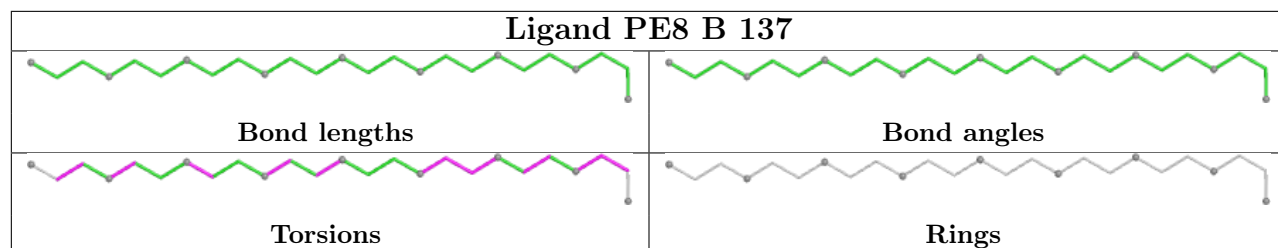
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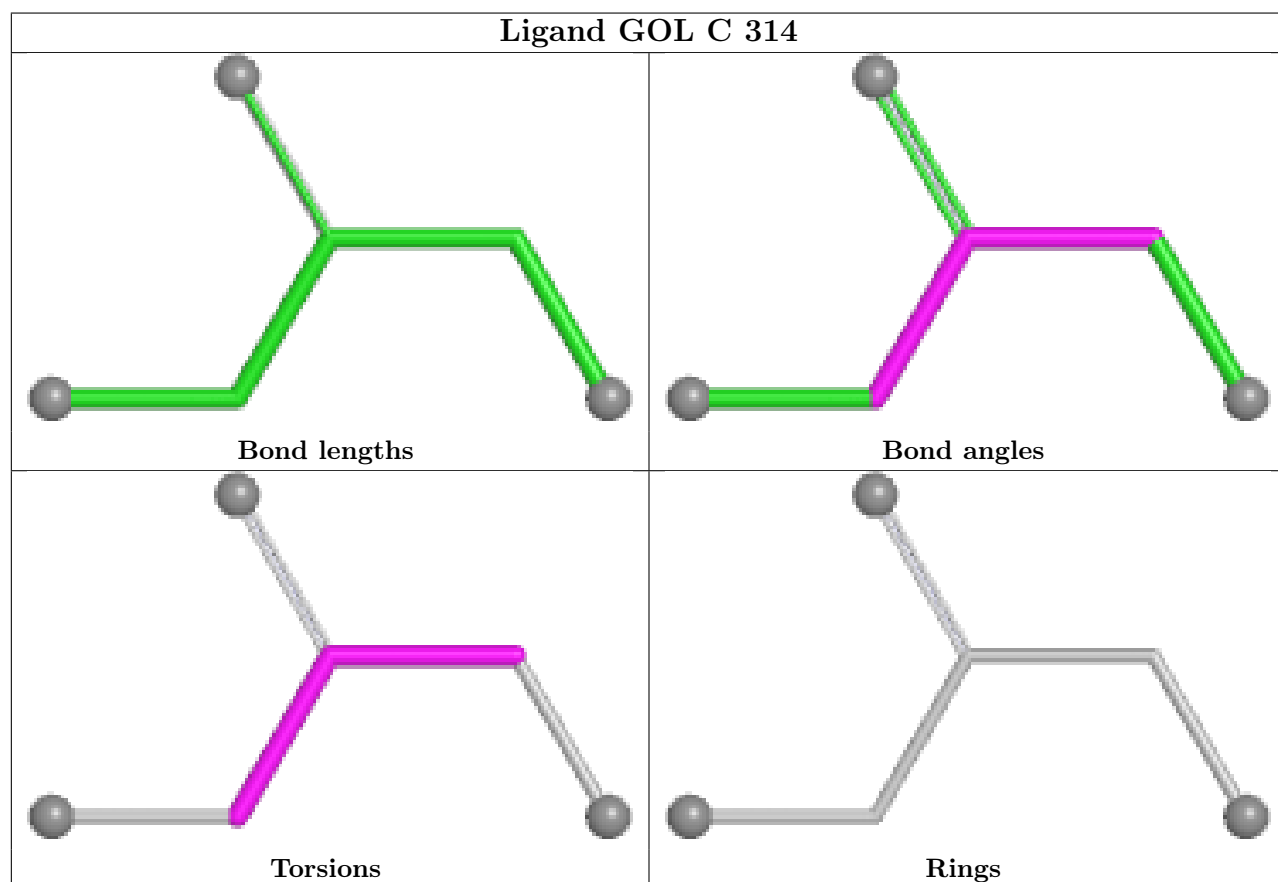
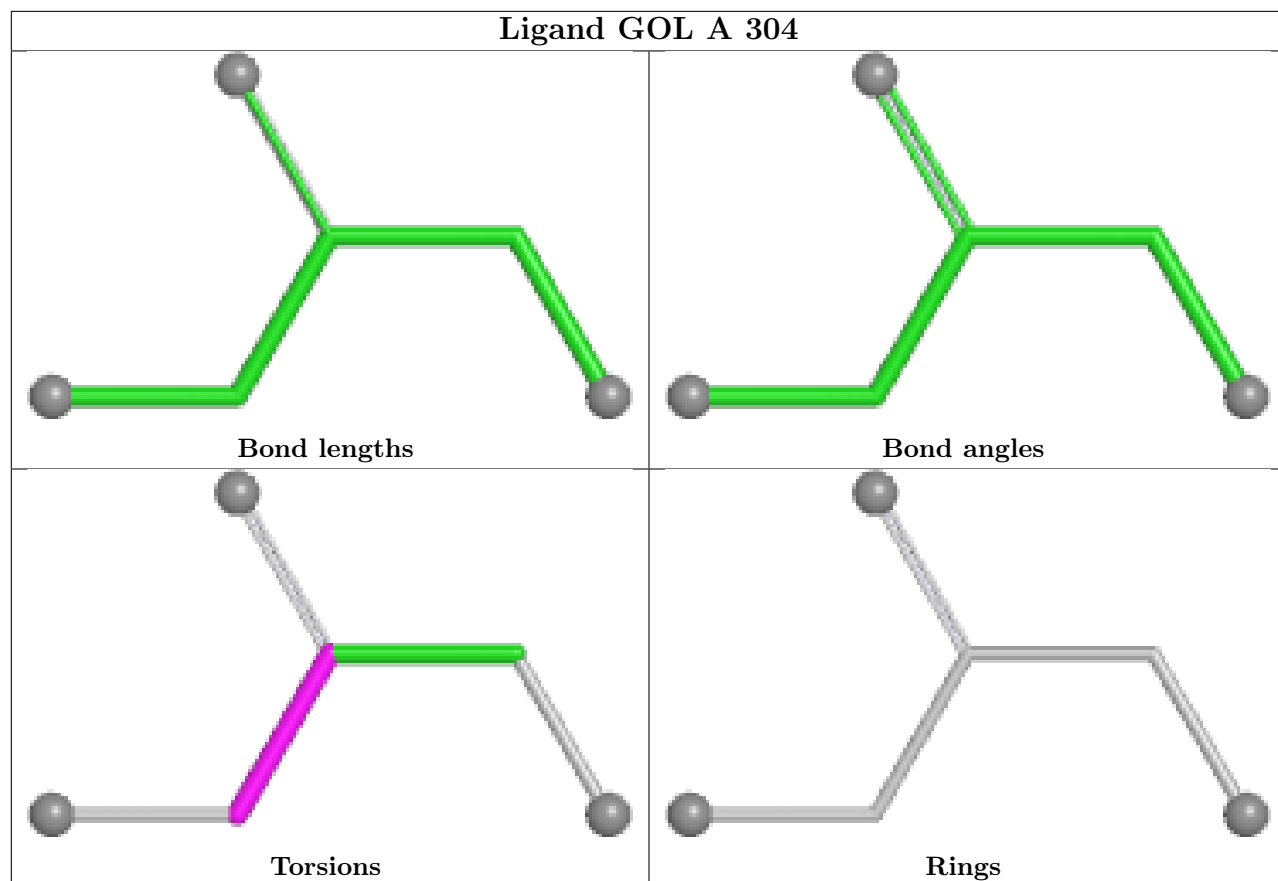
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	329	PEG	1	0
7	B	118	PG4	2	0
7	B	122	PG4	2	0
7	F	101	PG4	1	0
10	E	110	PE8	2	0
10	B	138	PE8	2	0
5	A	347	GOL	1	0
7	C	302	PG4	2	0
9	A	331	PEG	2	0
9	A	336	PEG	1	0
7	B	125	PG4	1	0
9	C	333	PEG	1	0

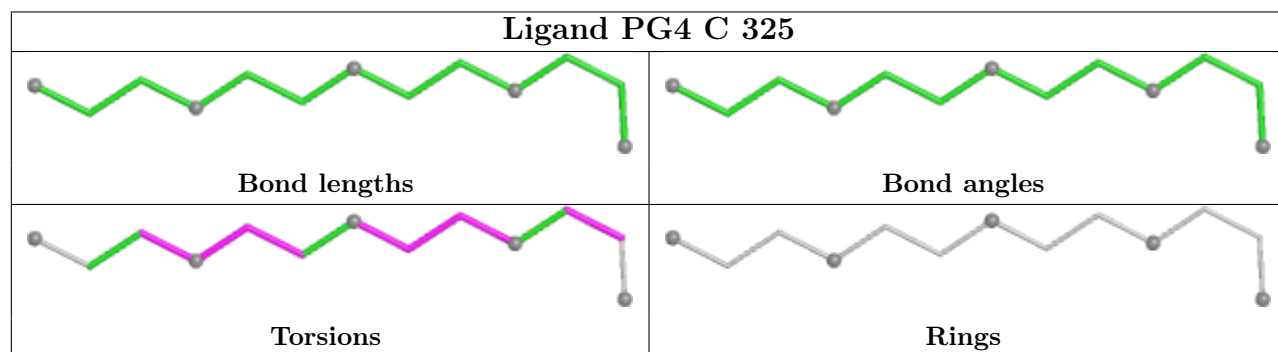
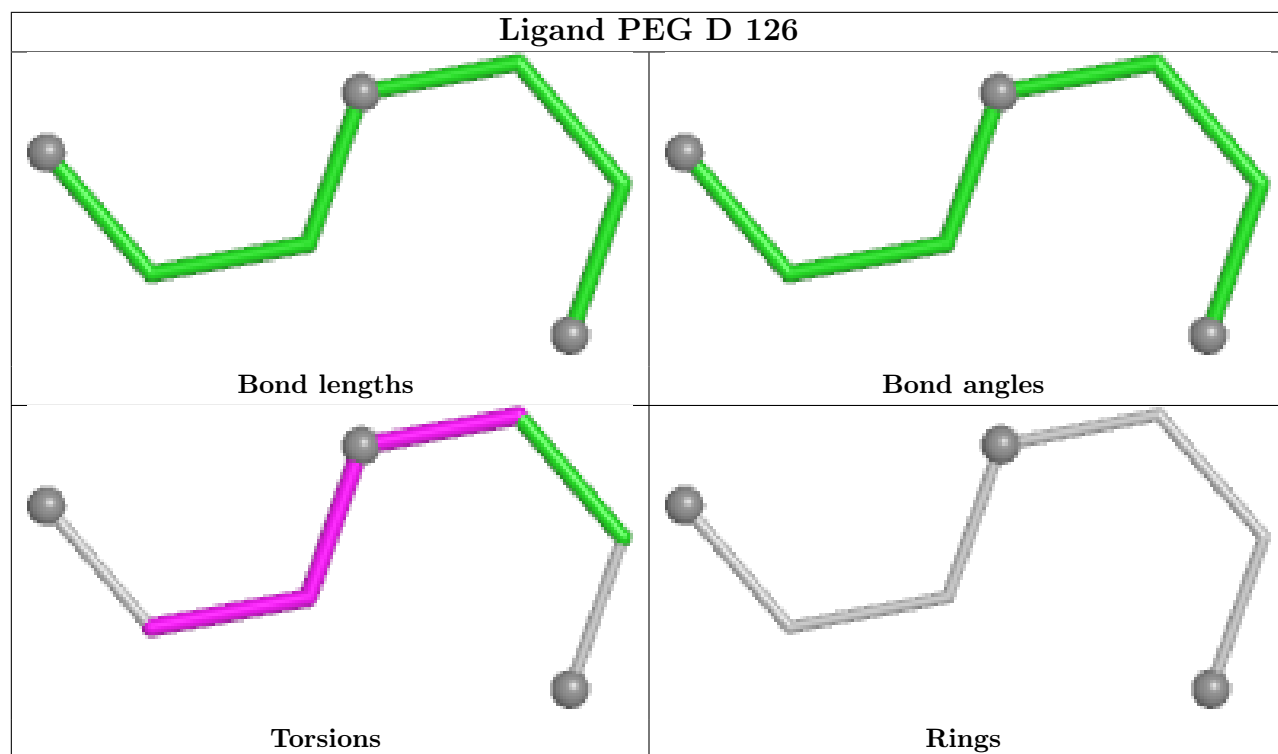
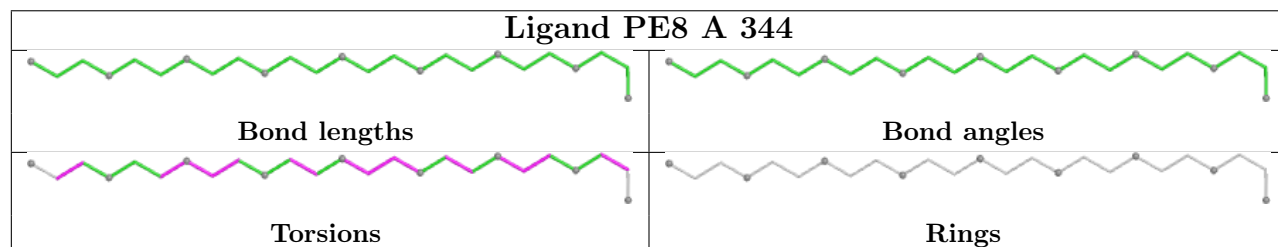
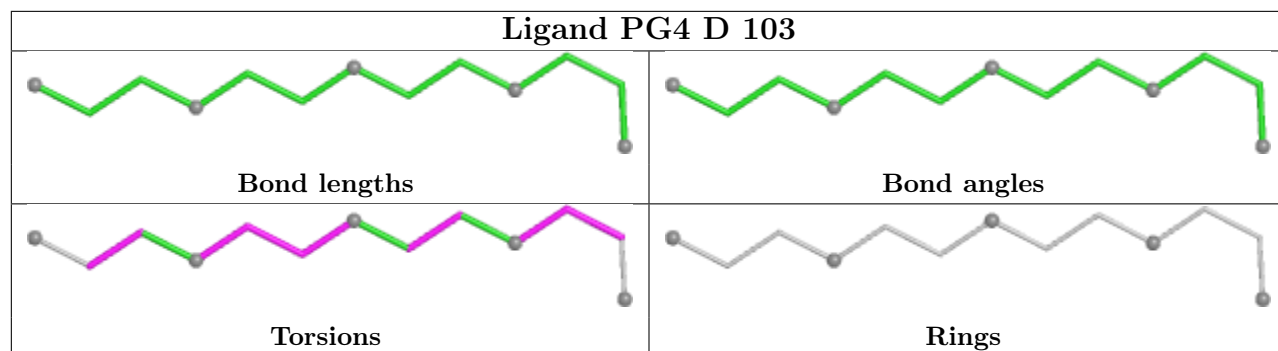
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

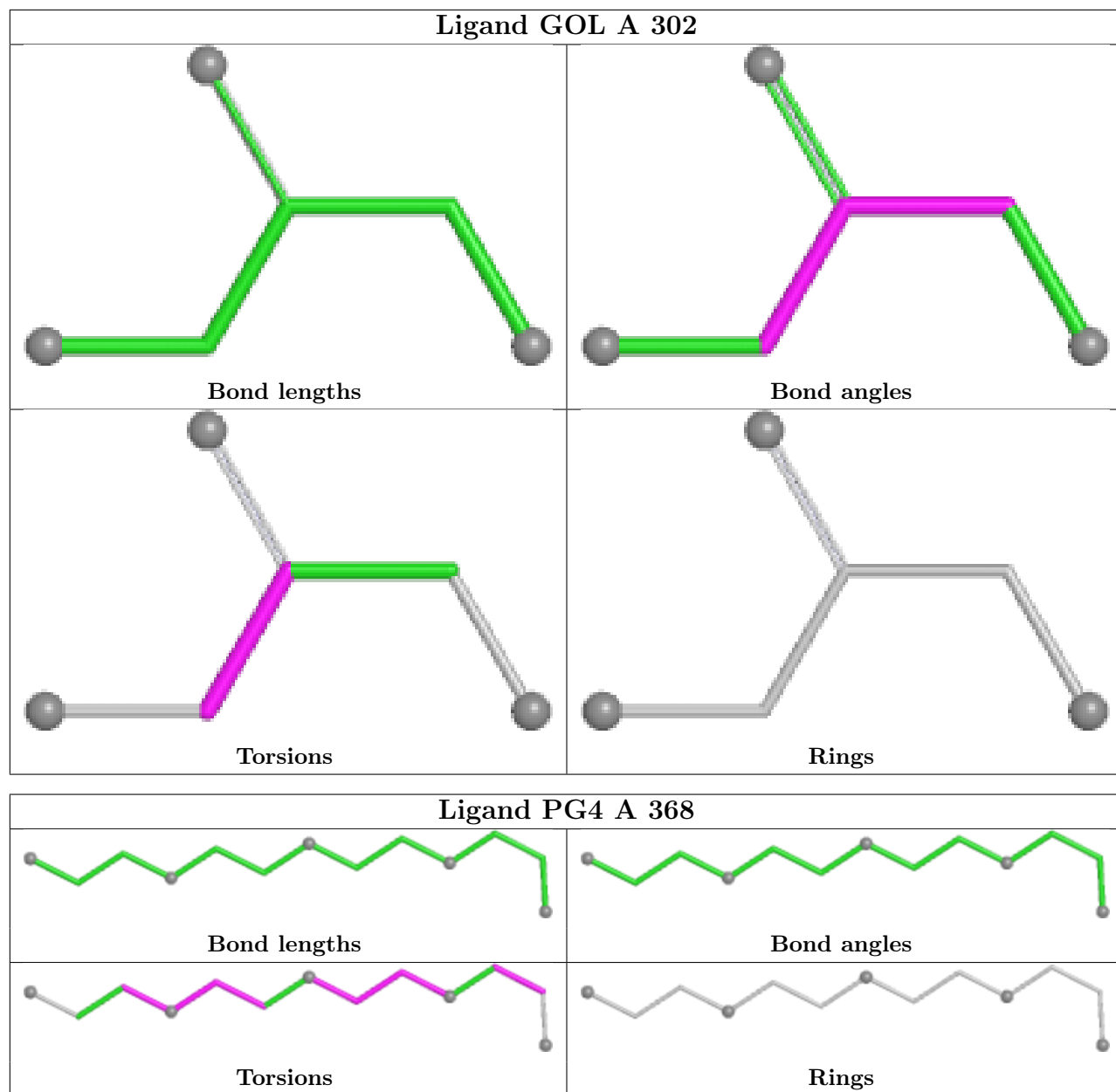


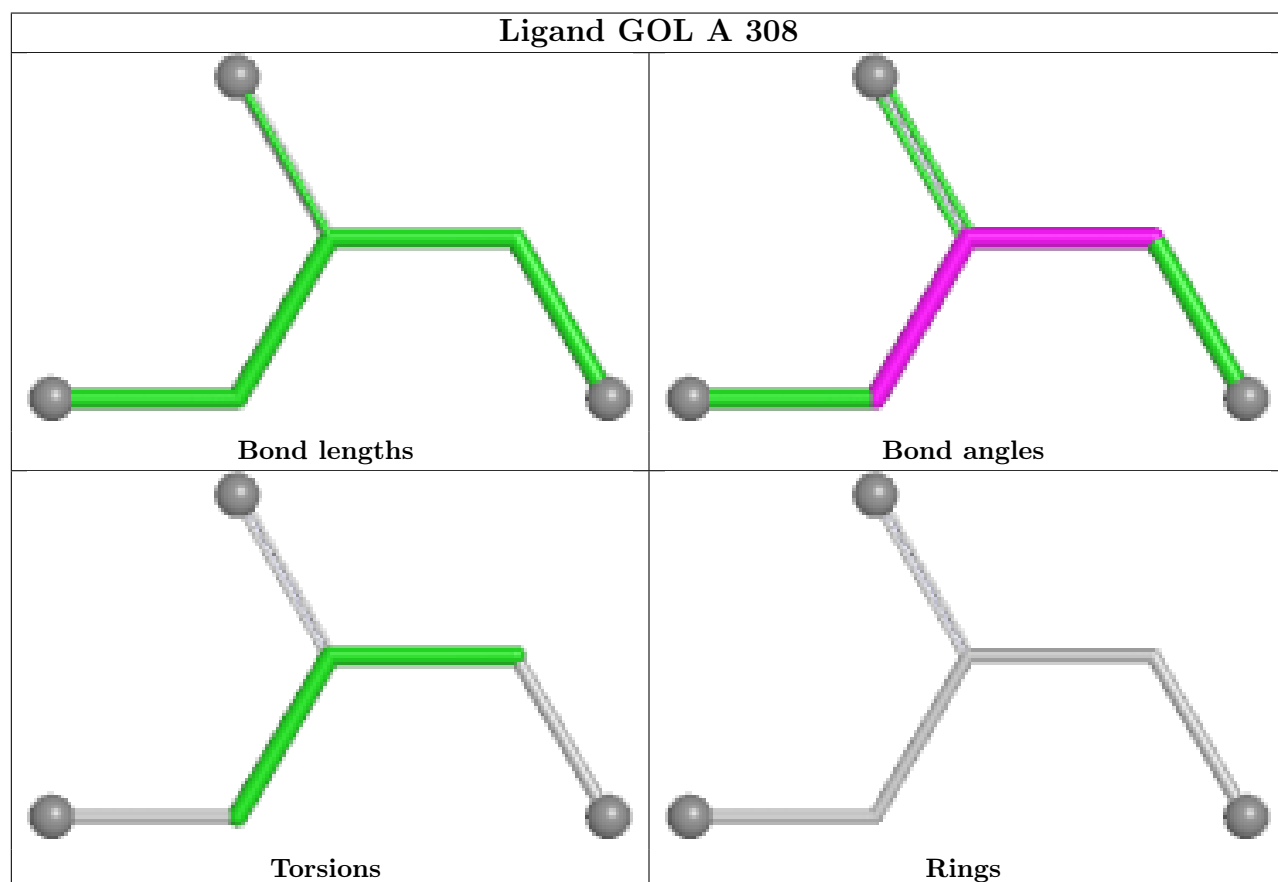
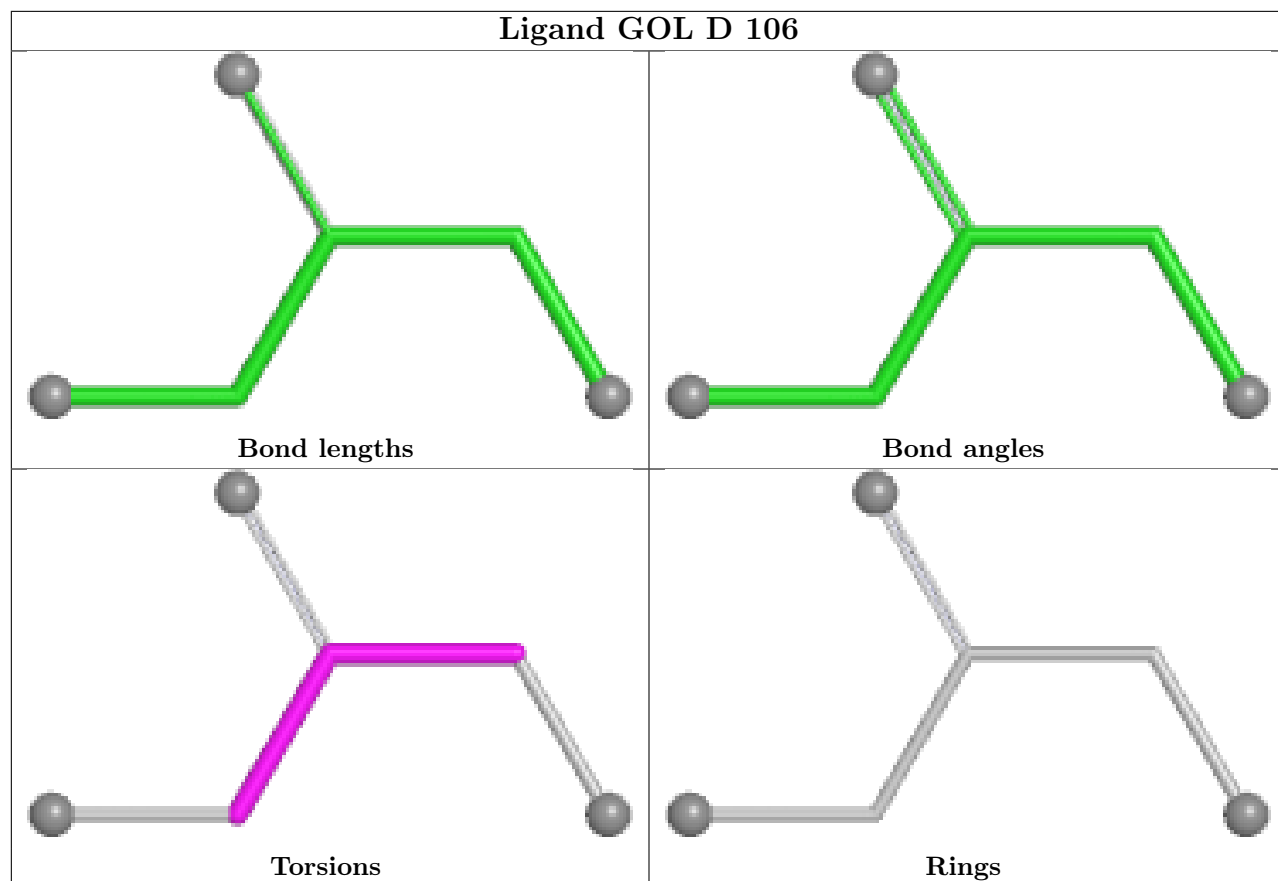


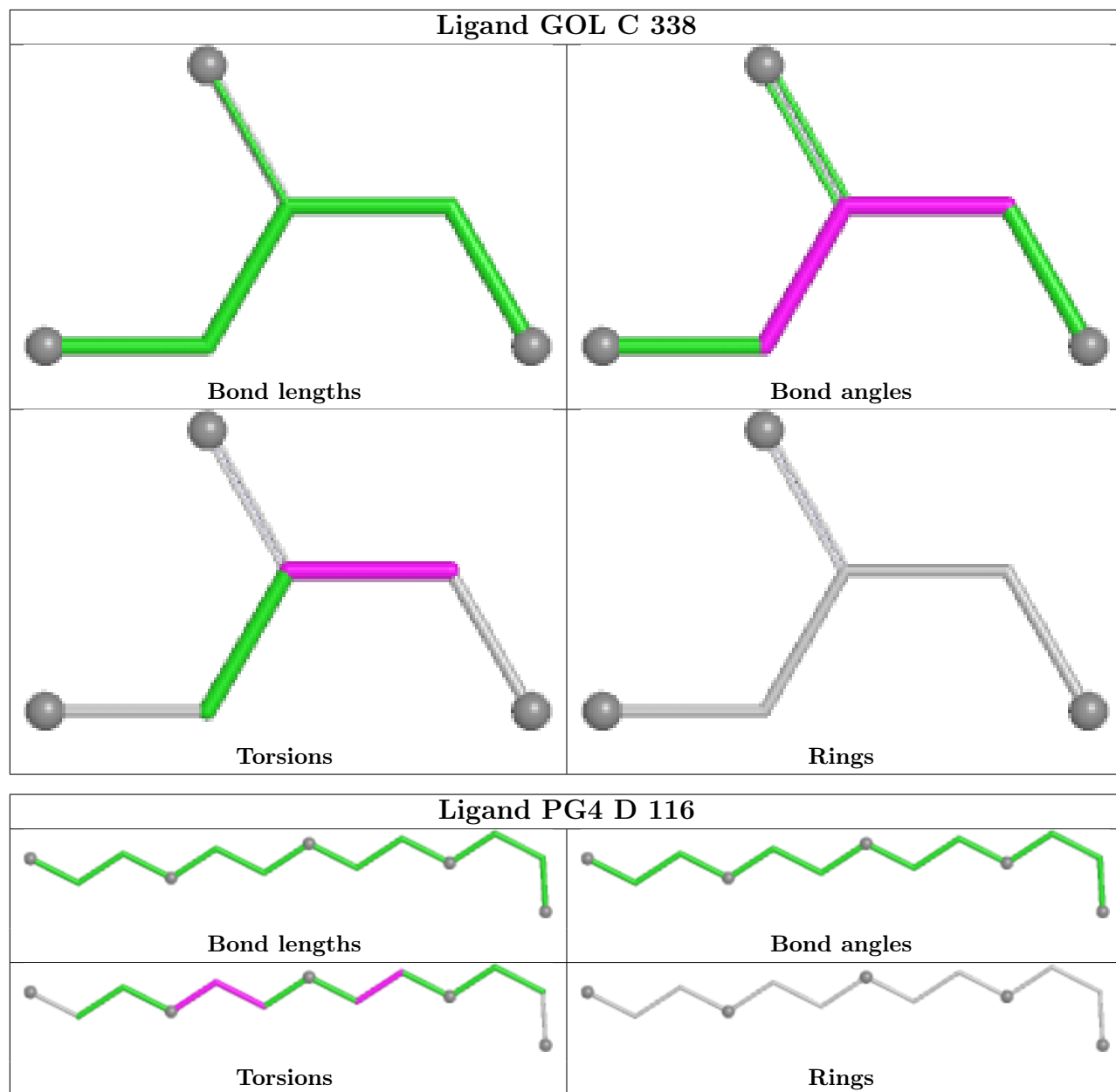


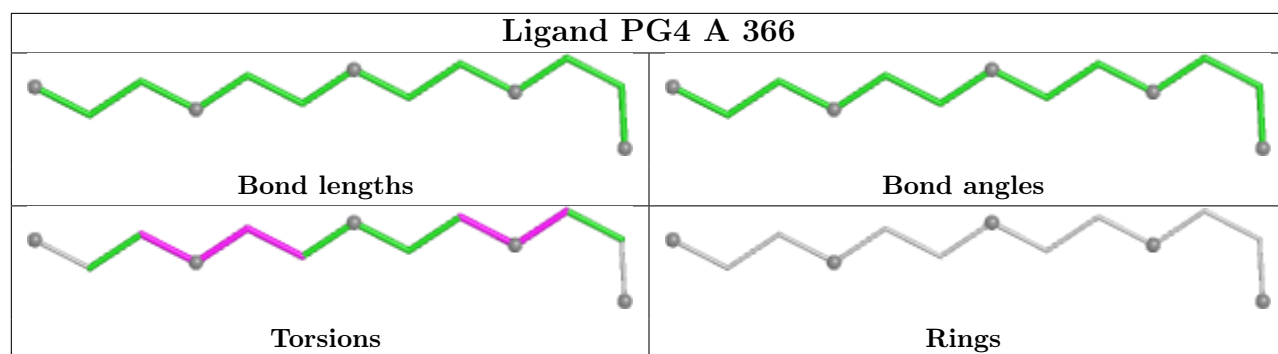
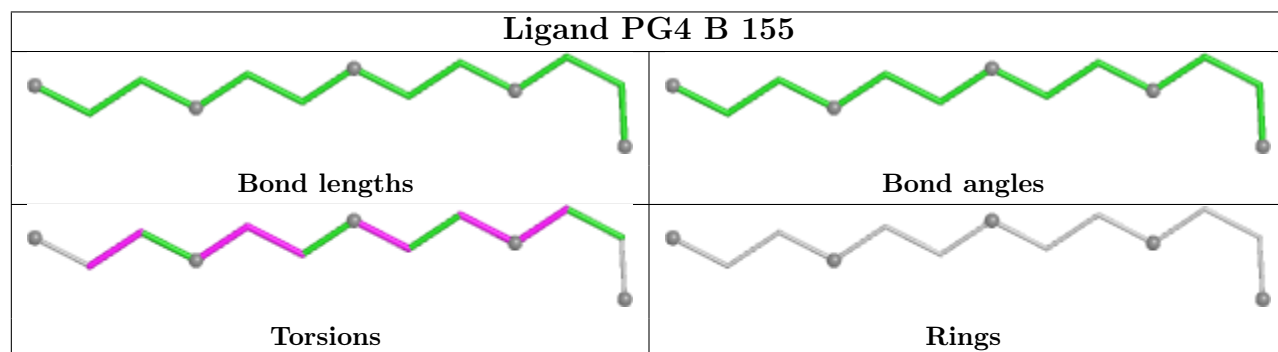
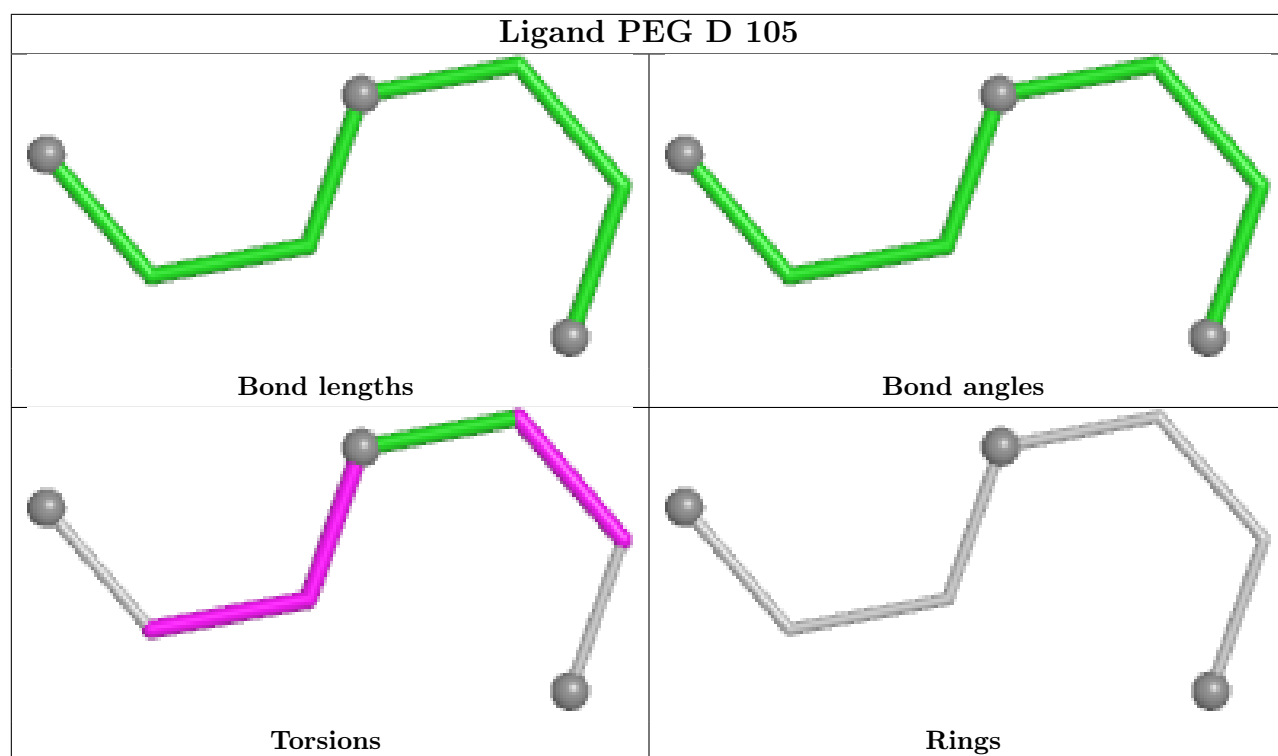


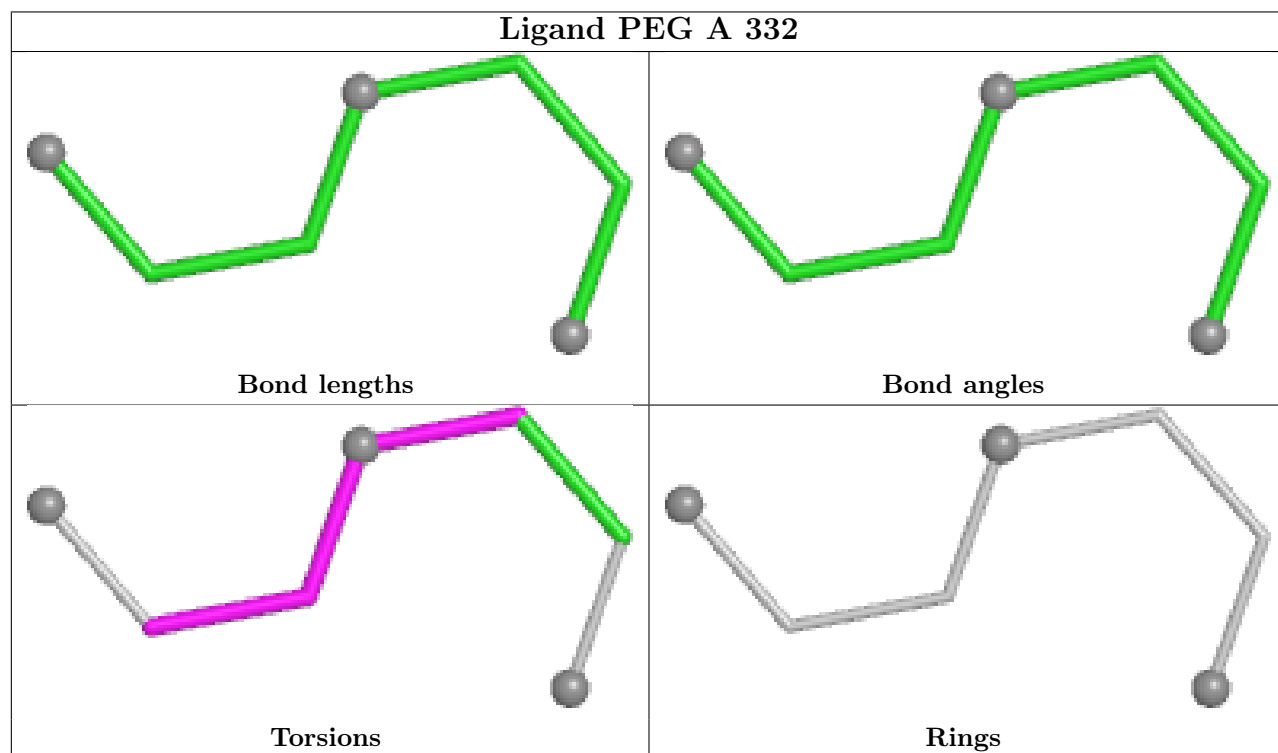
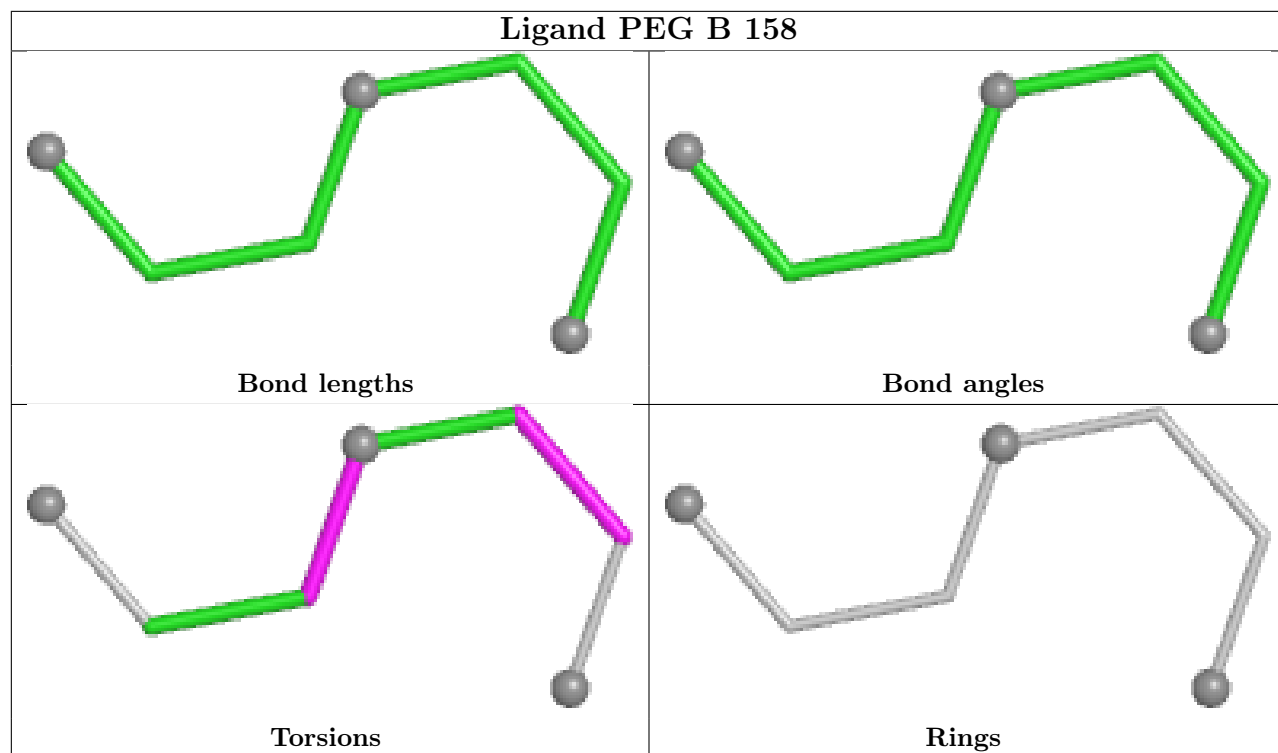


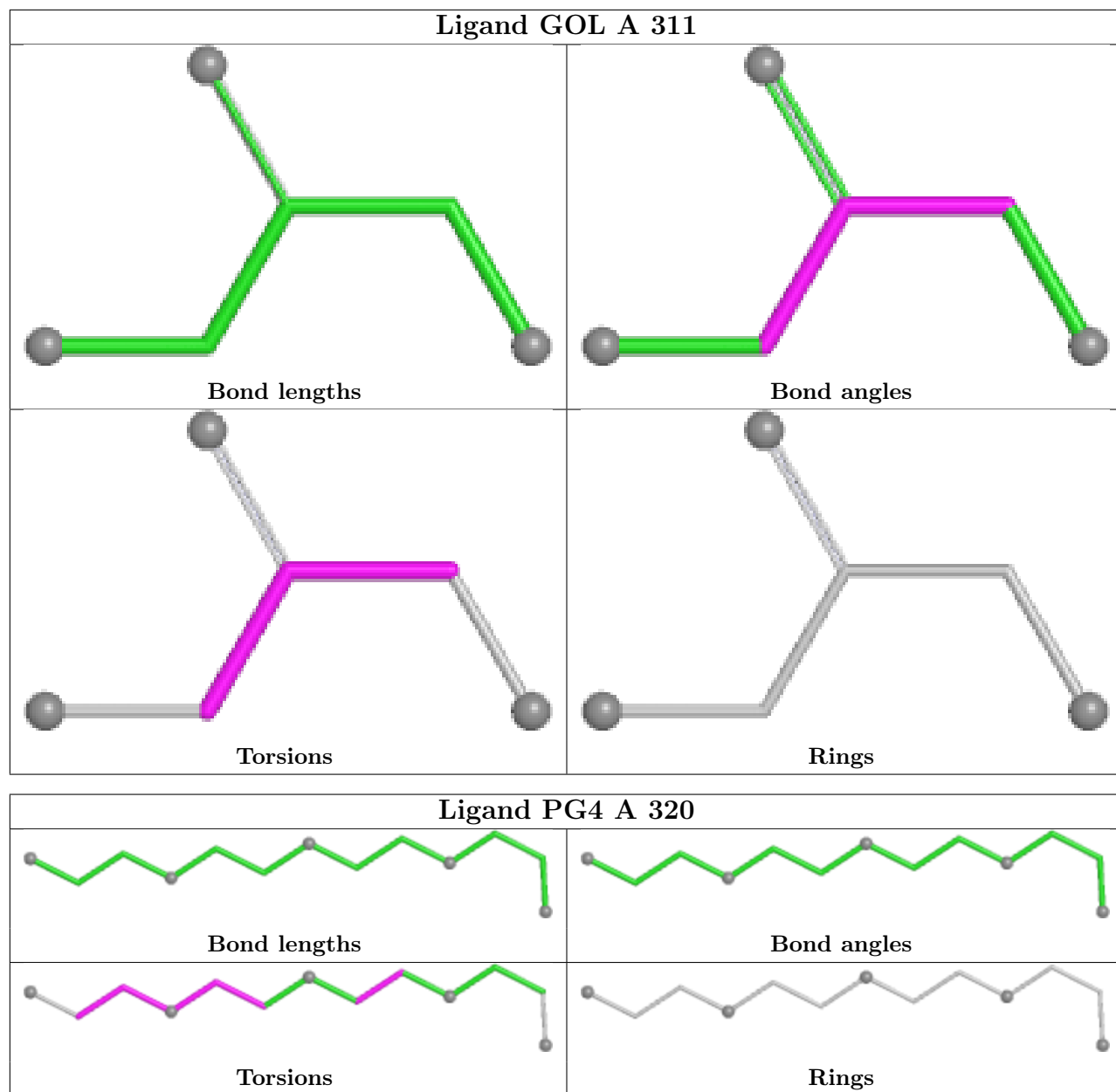


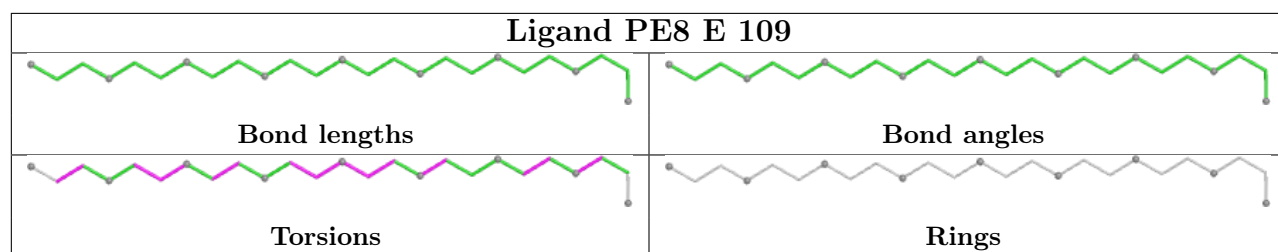
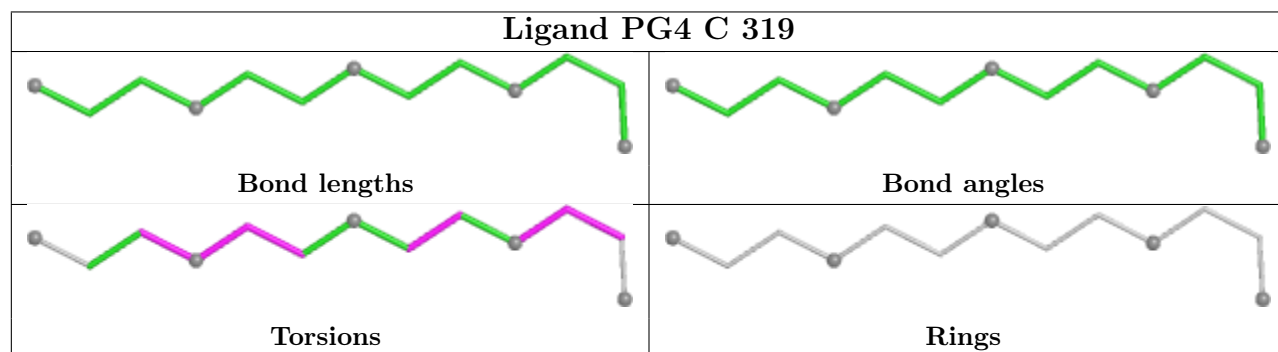
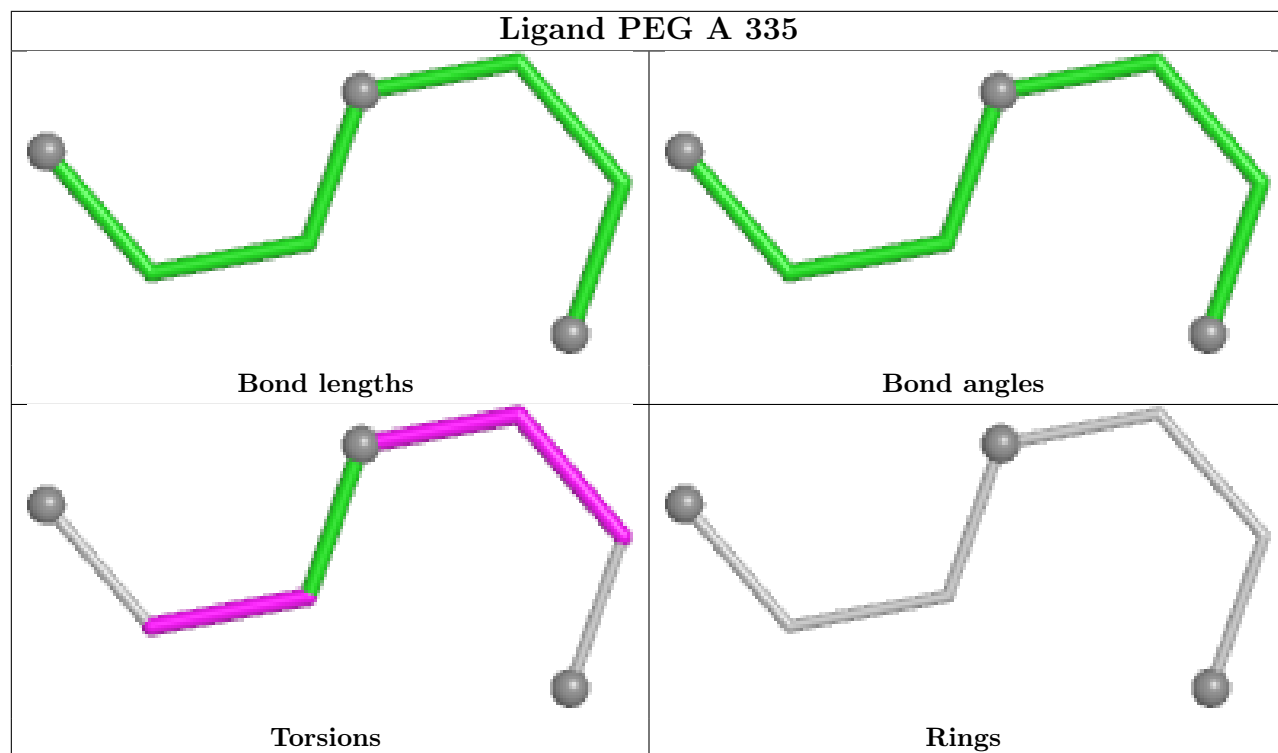


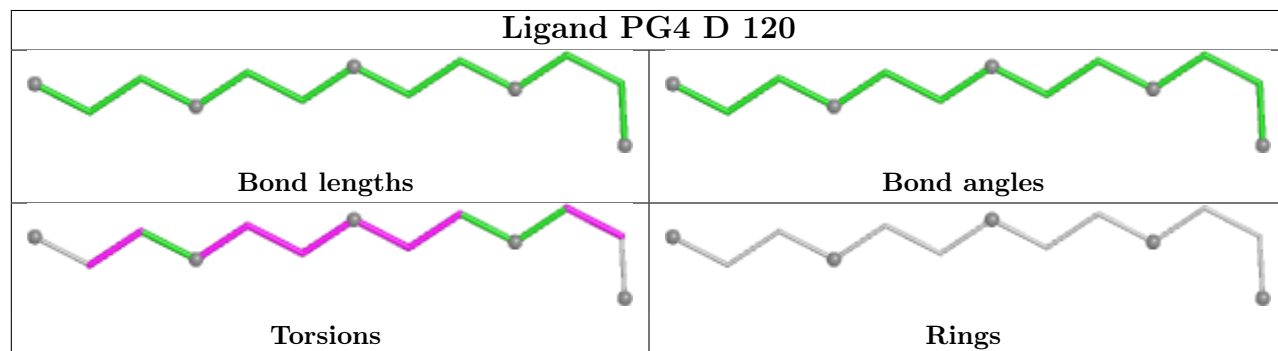
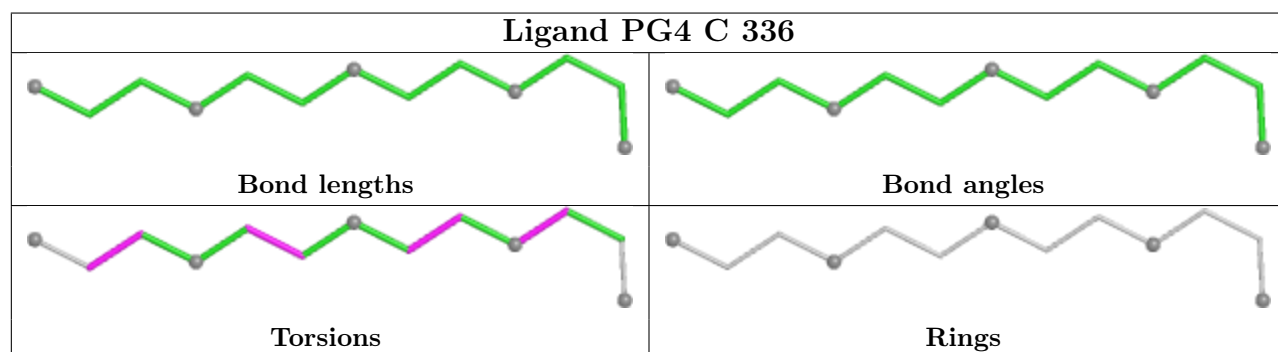
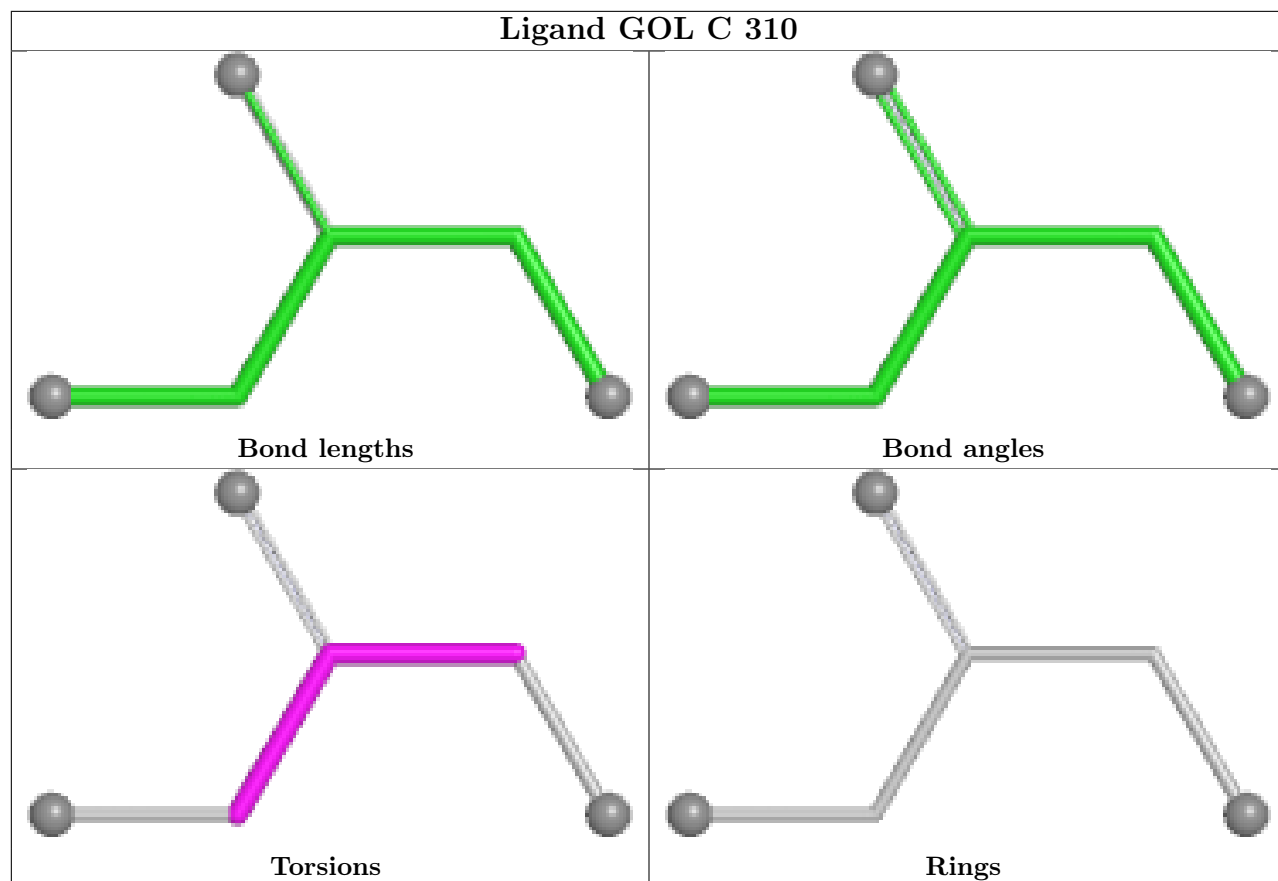


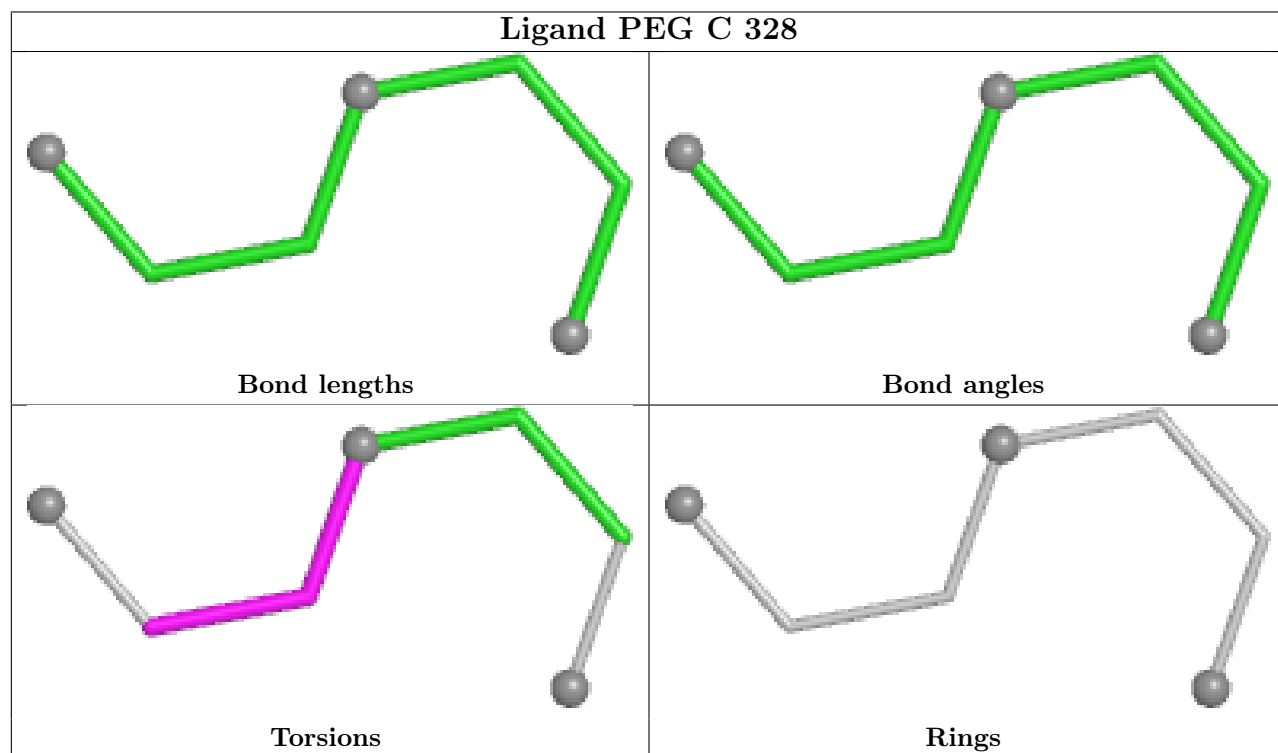
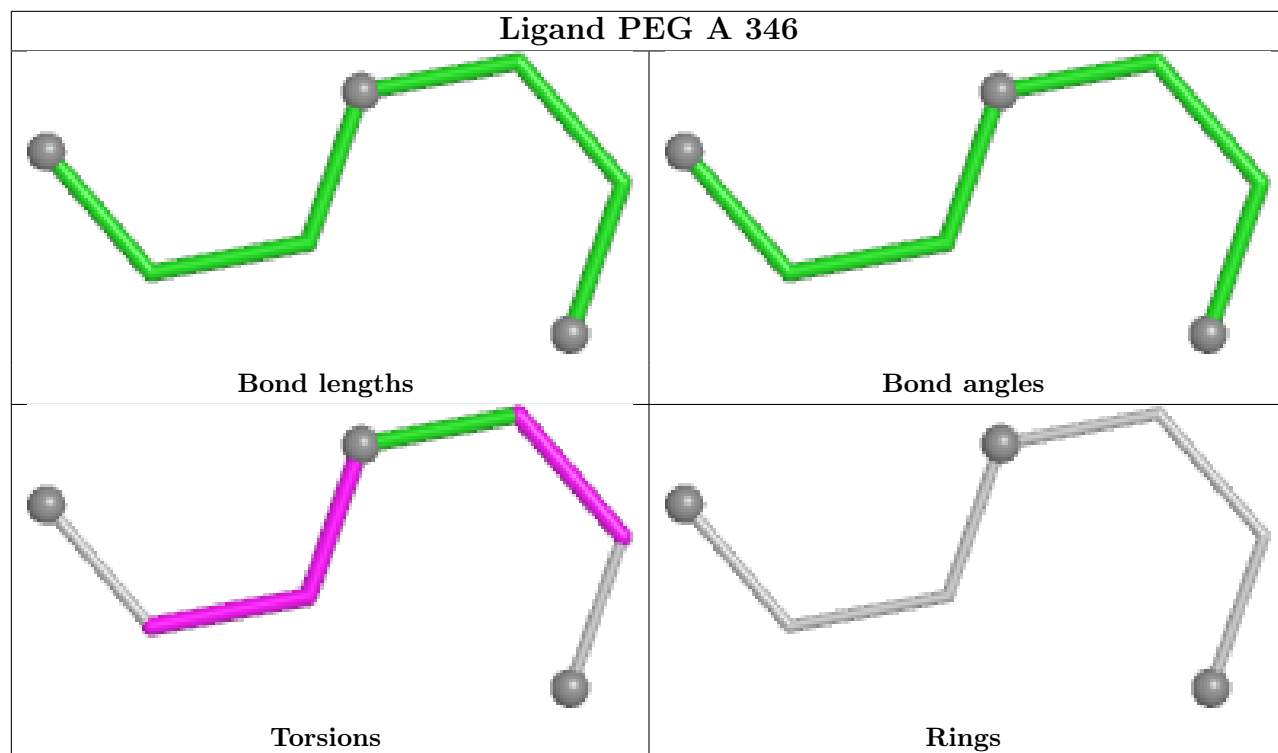


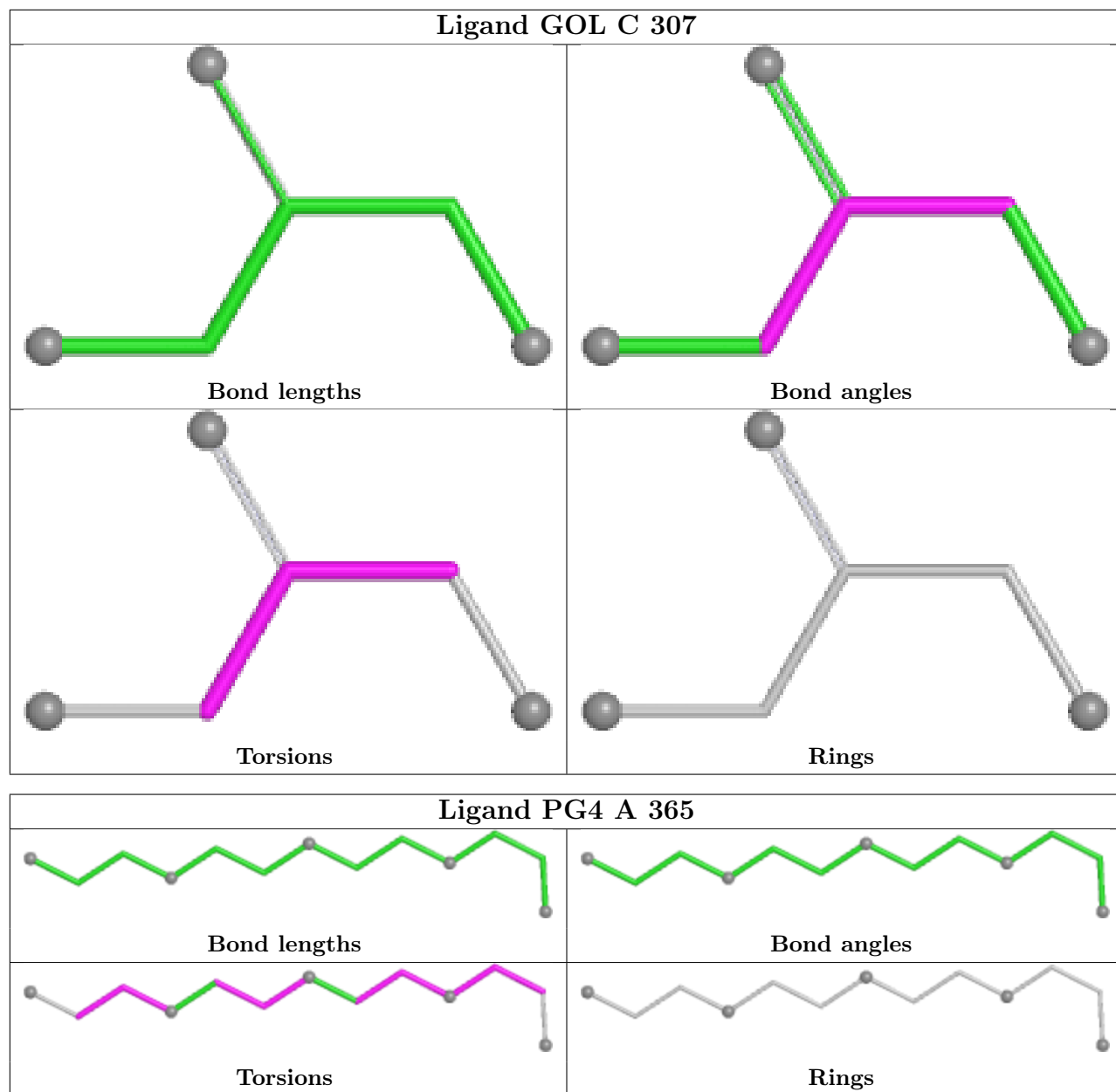


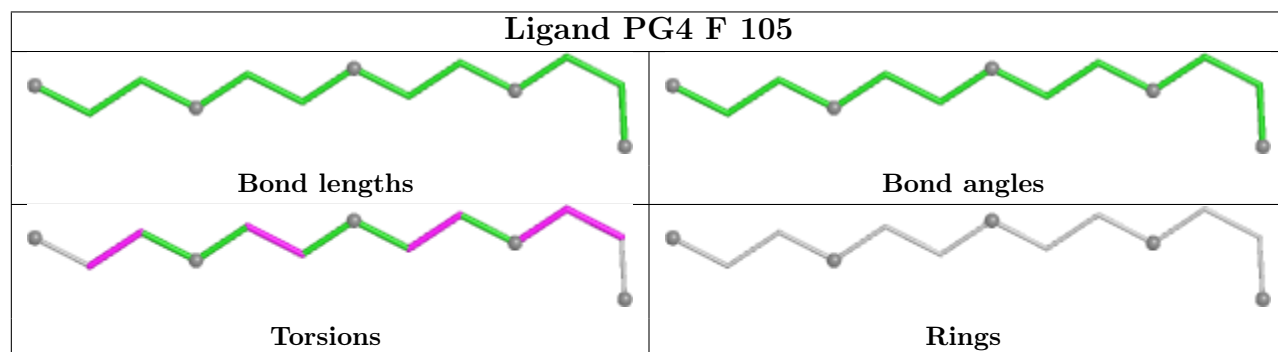
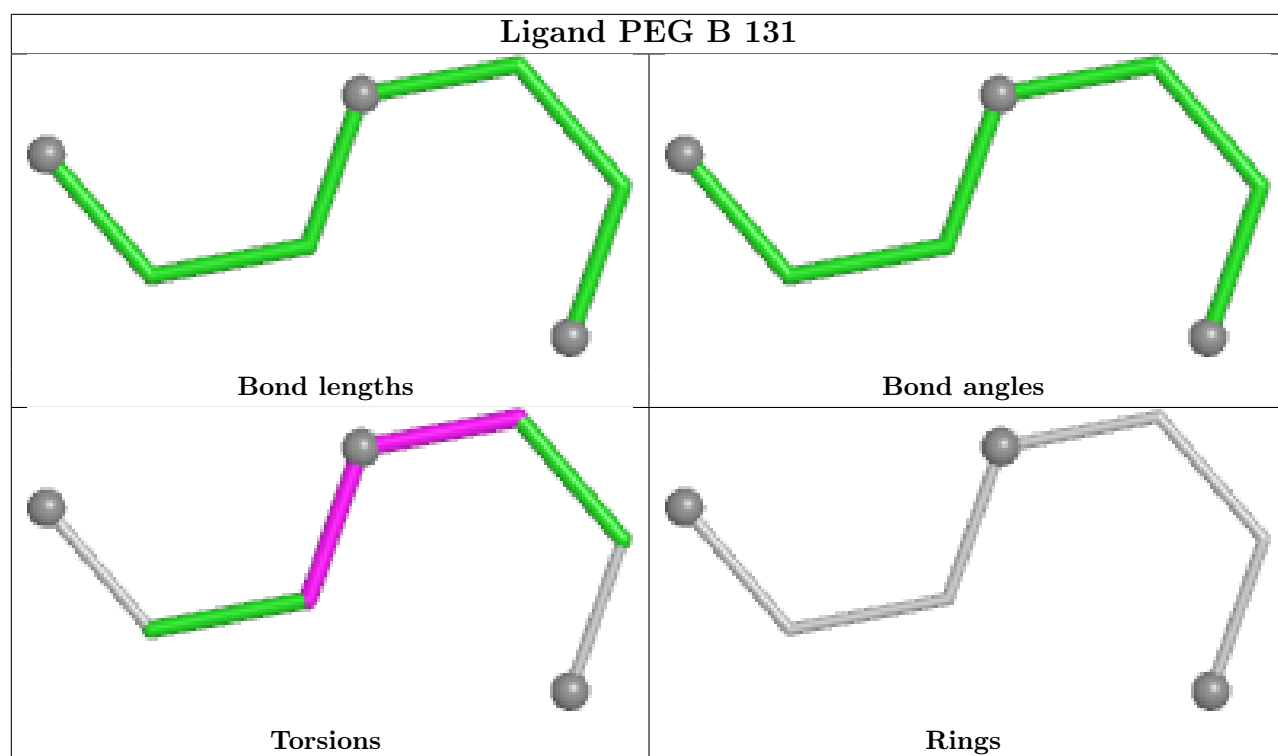


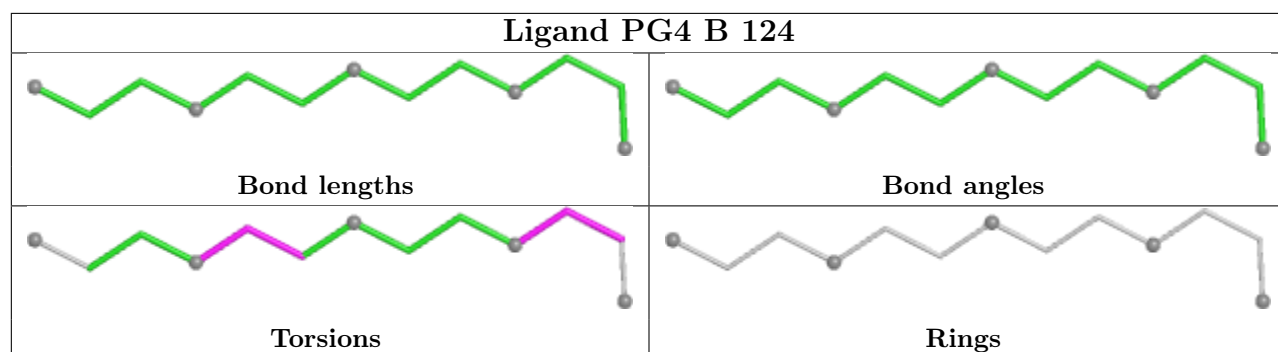
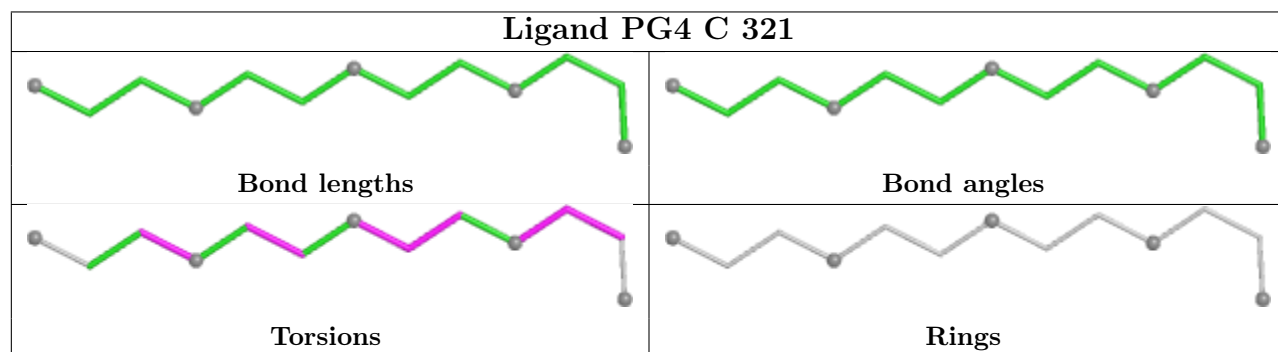
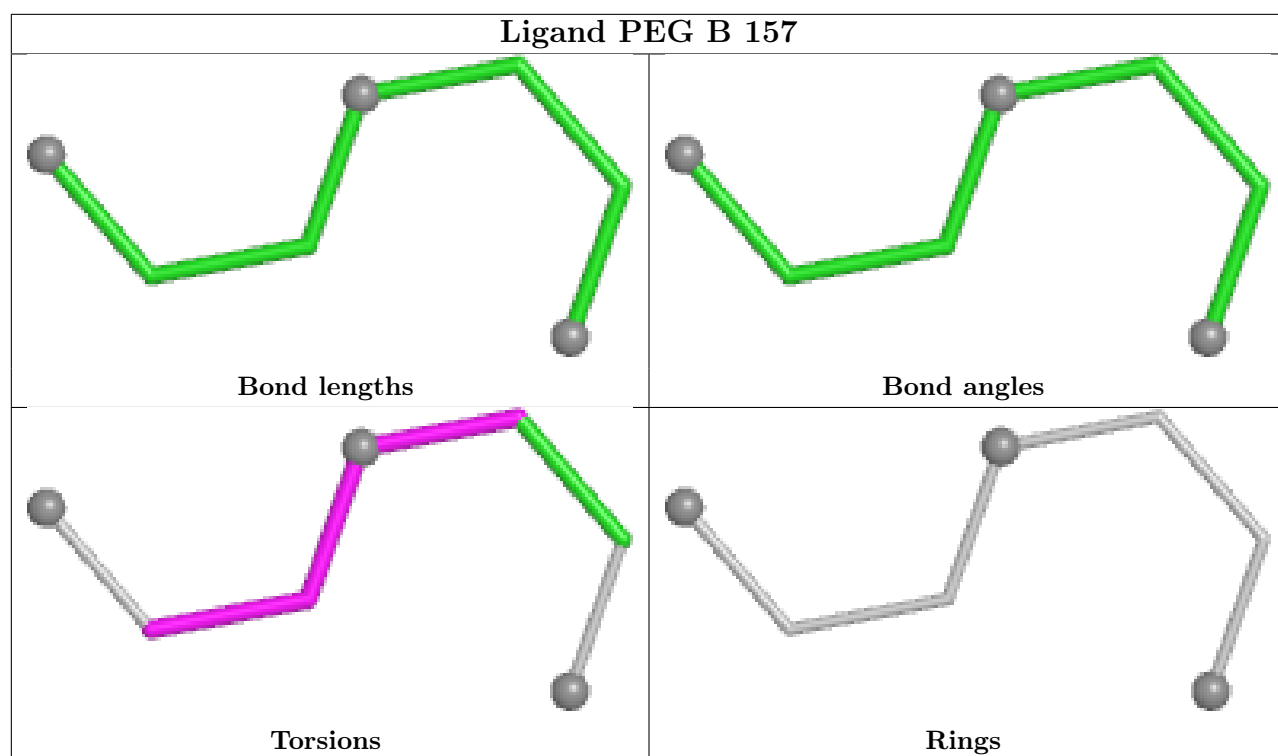


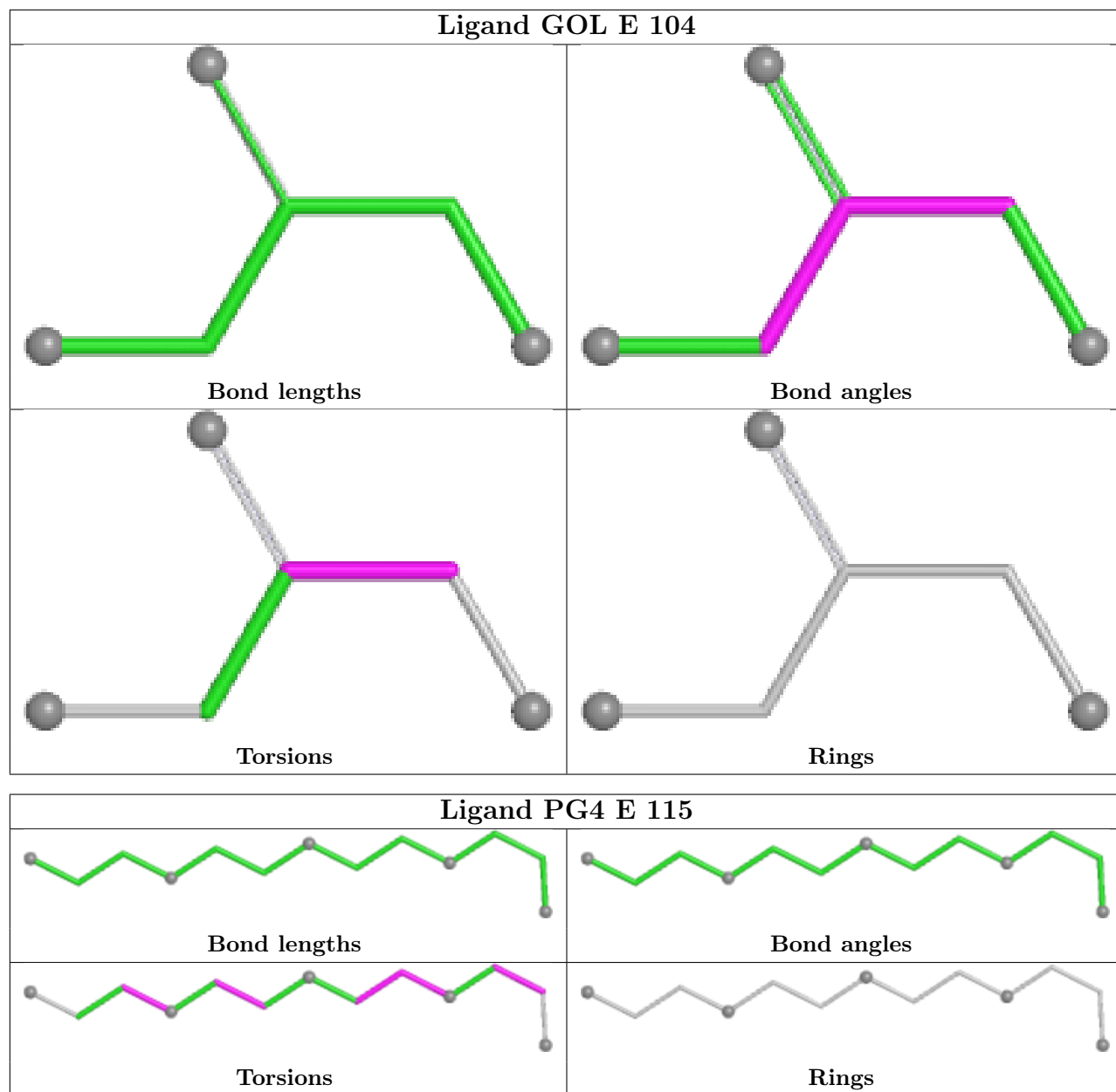


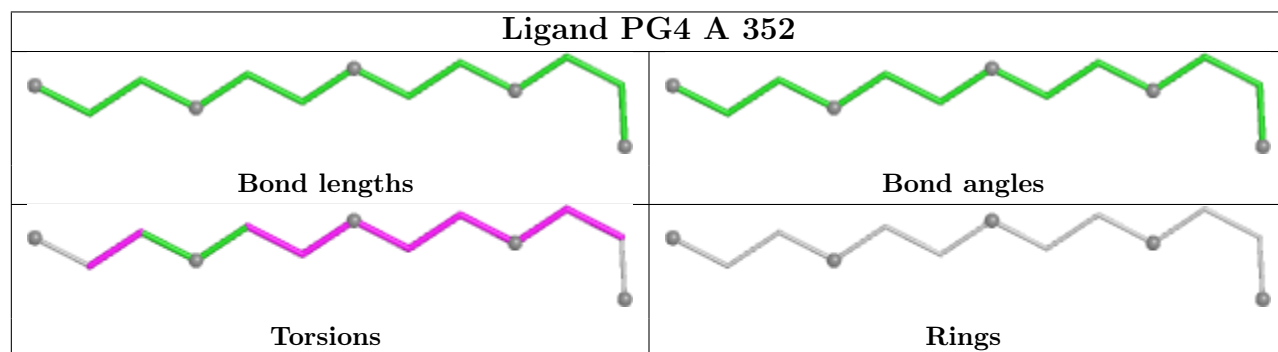
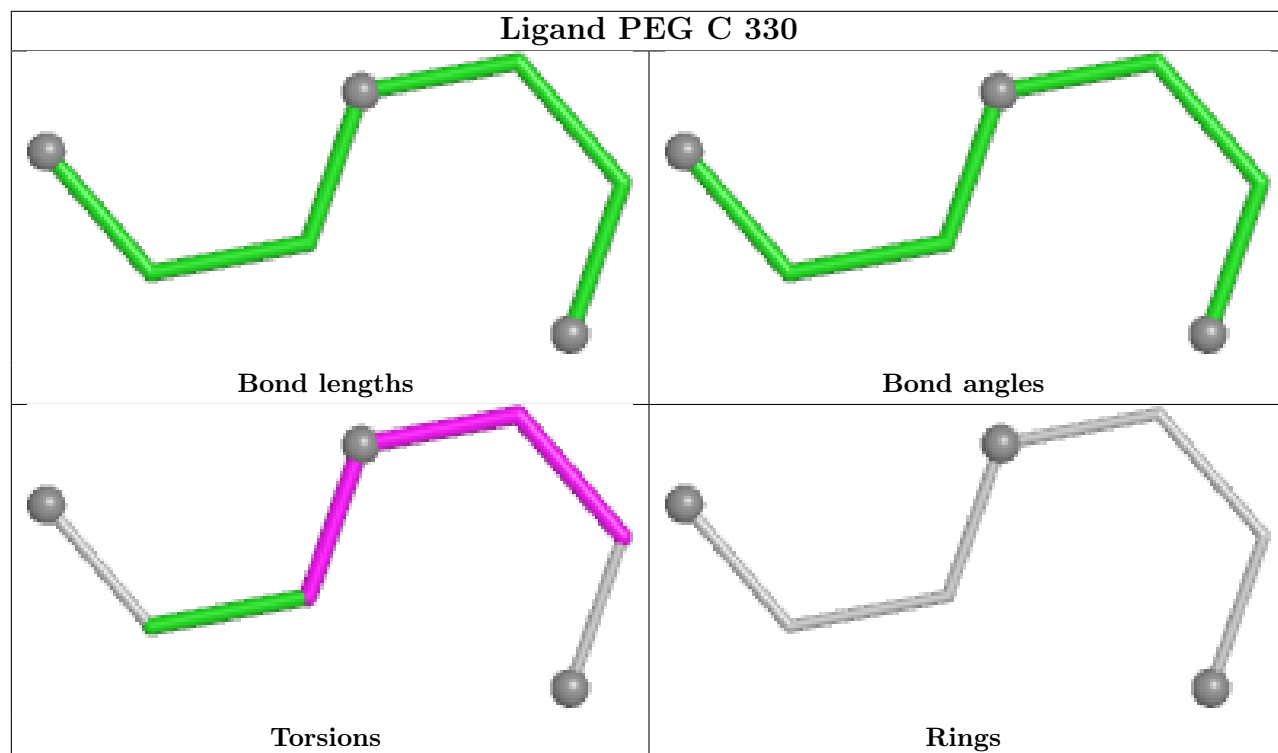


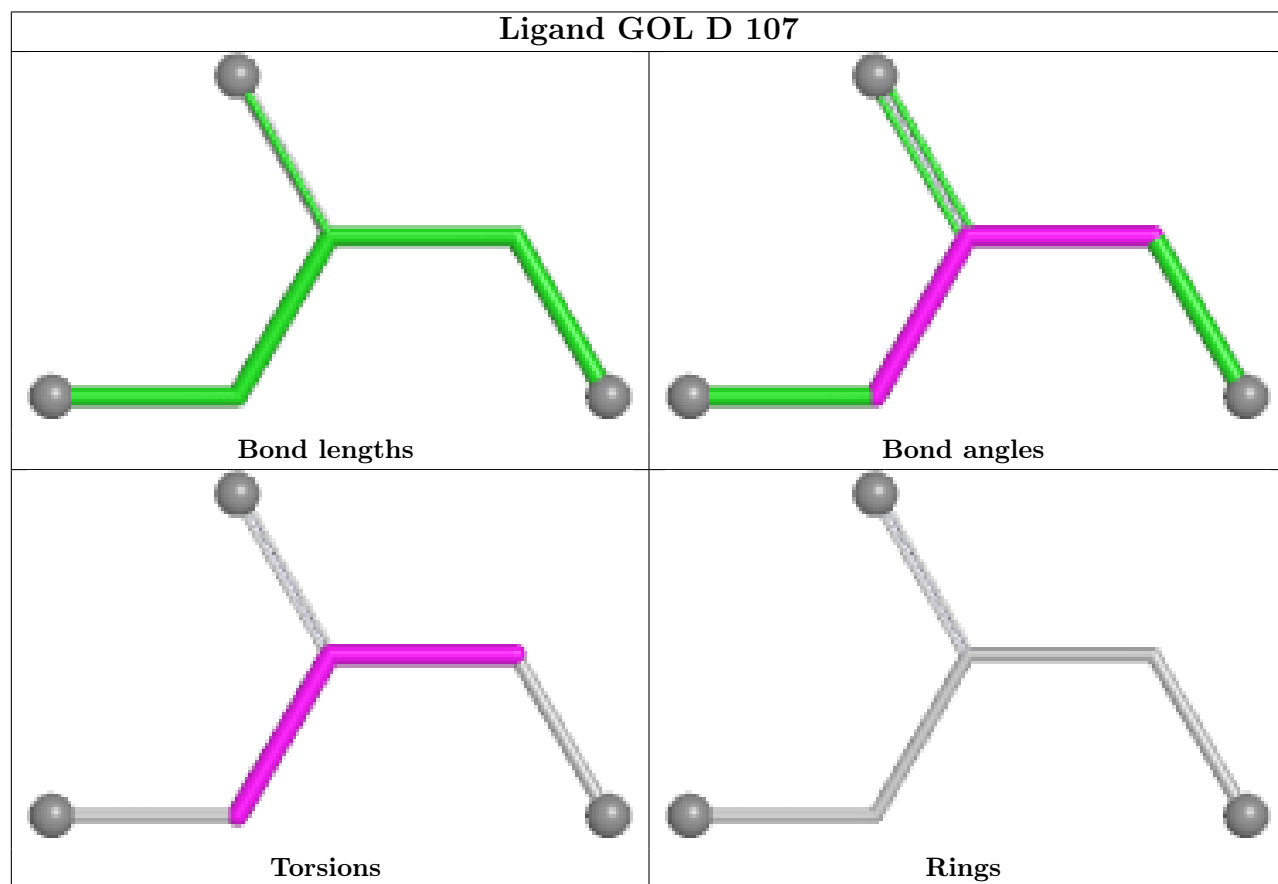
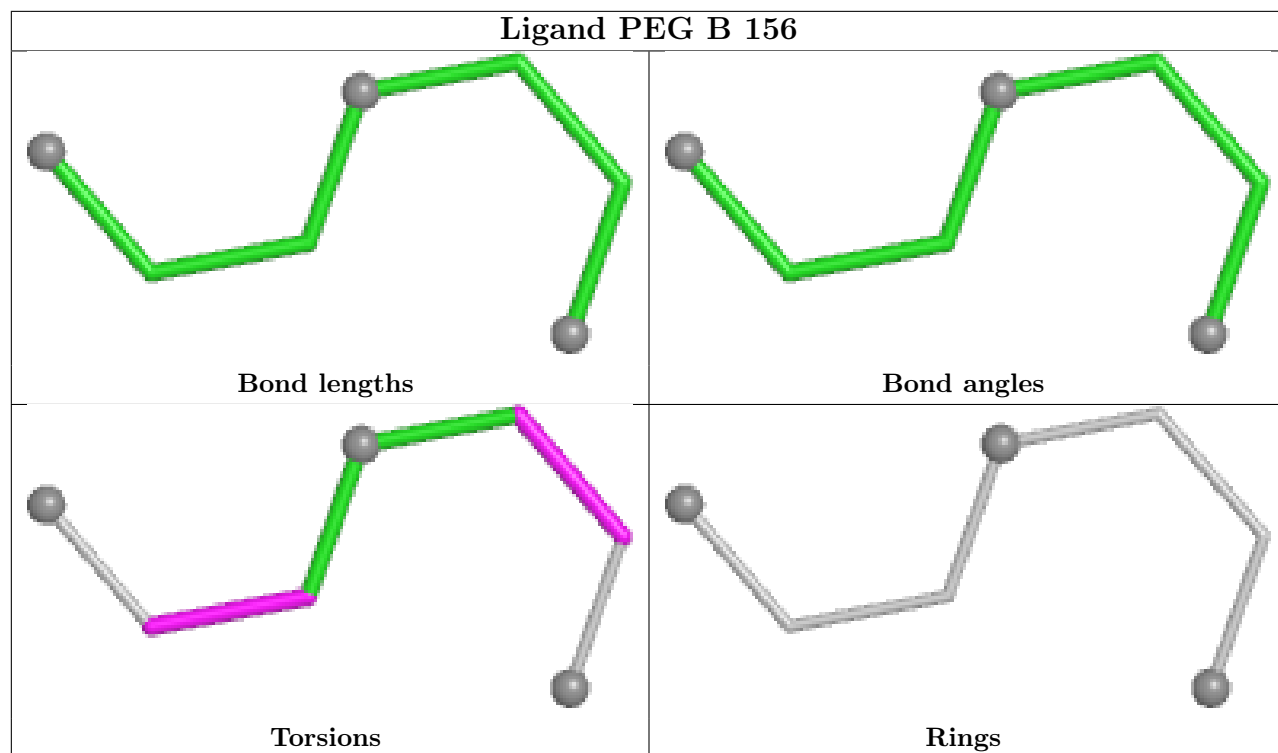


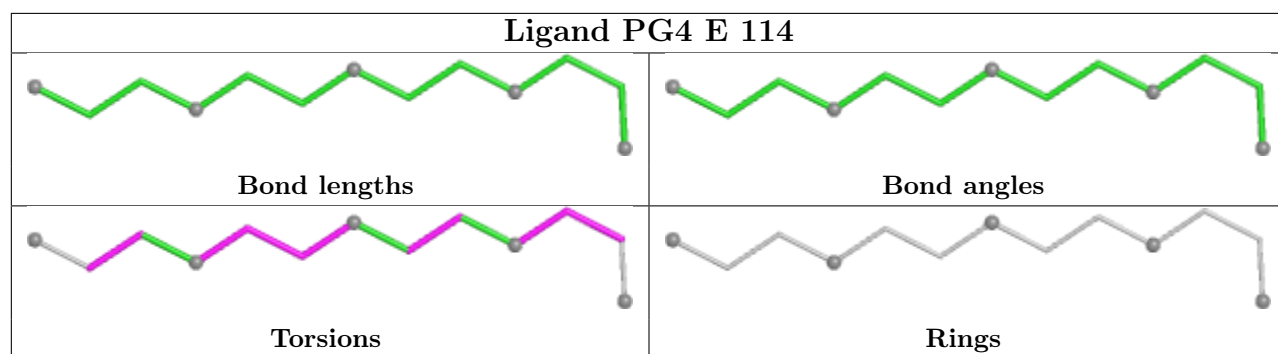
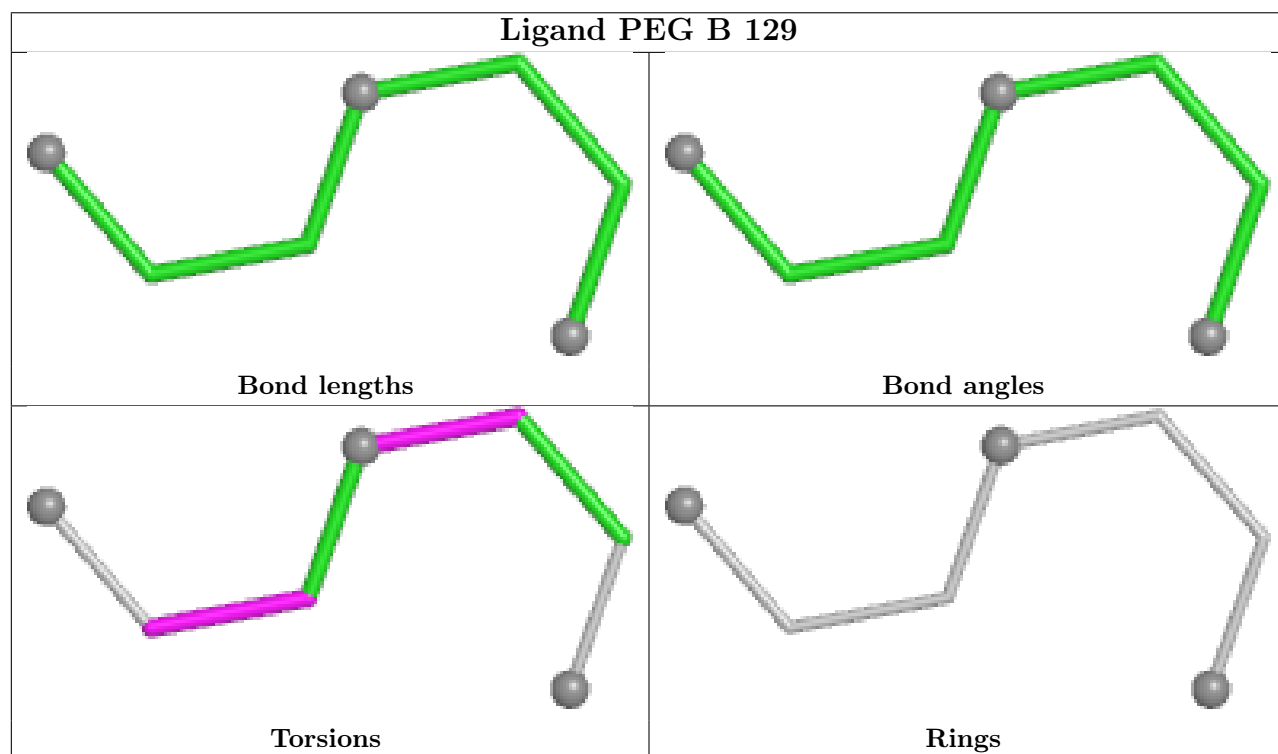
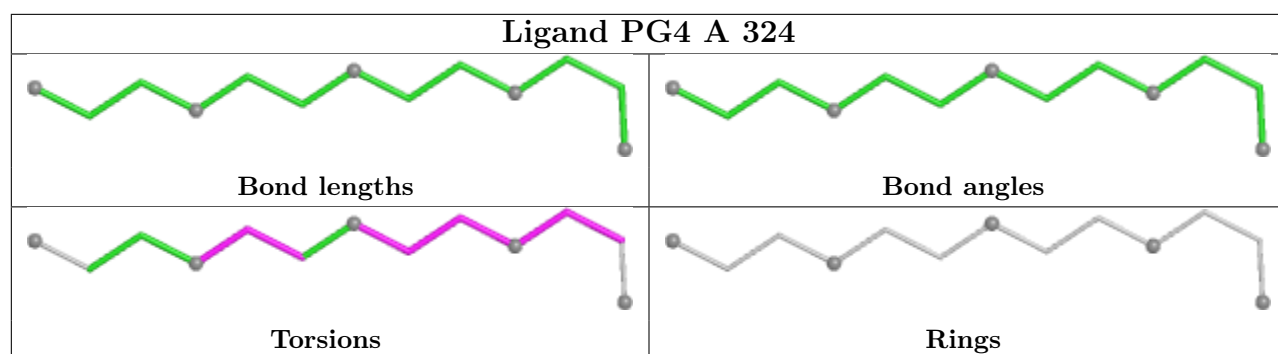


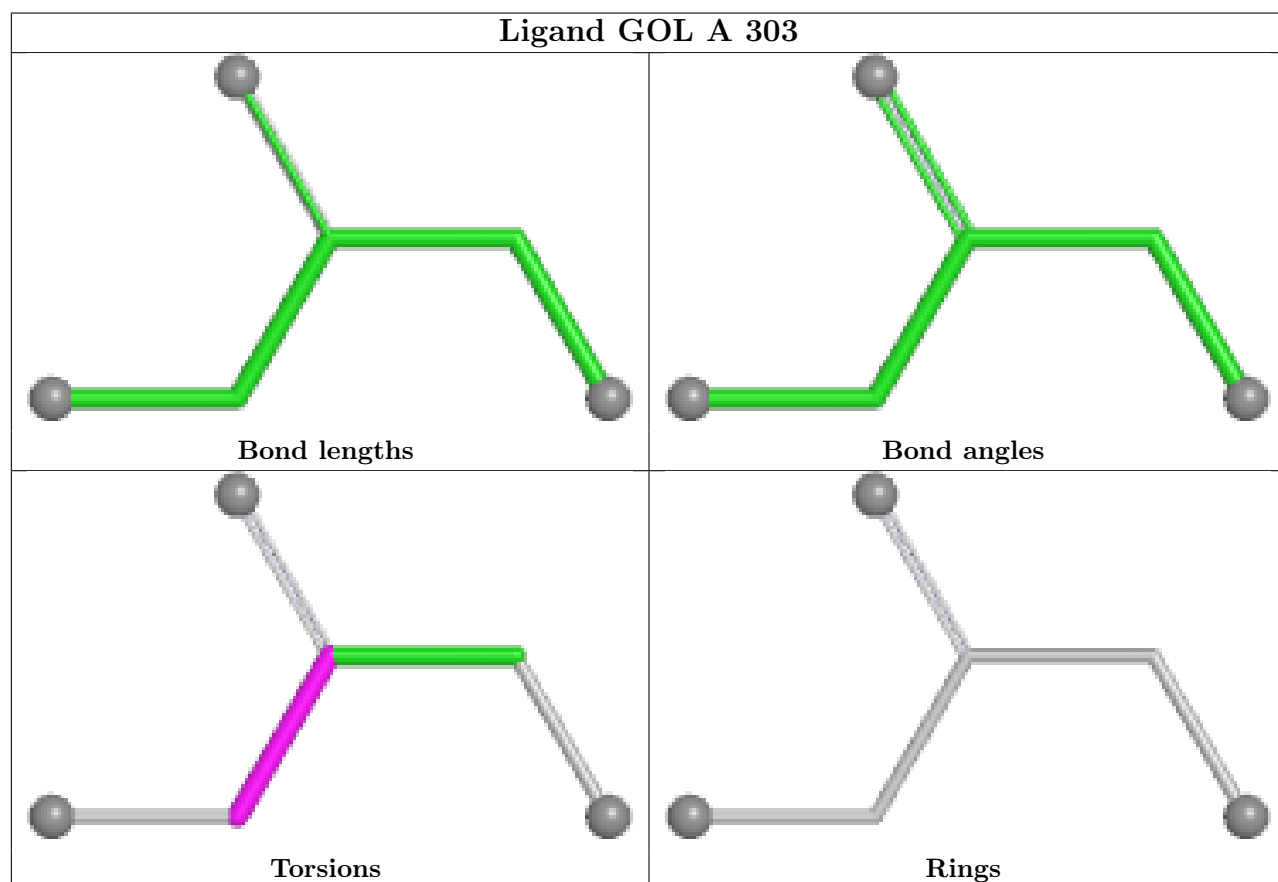
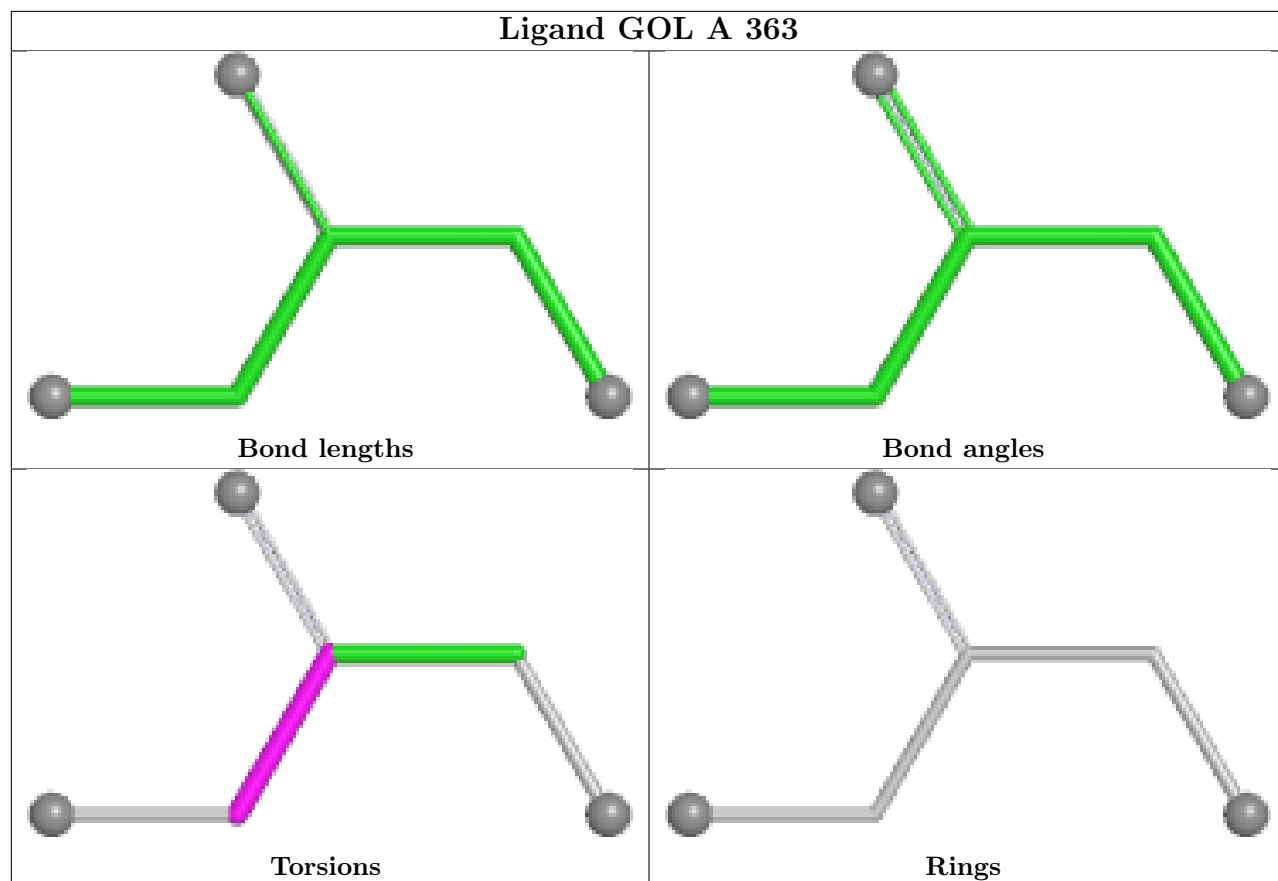


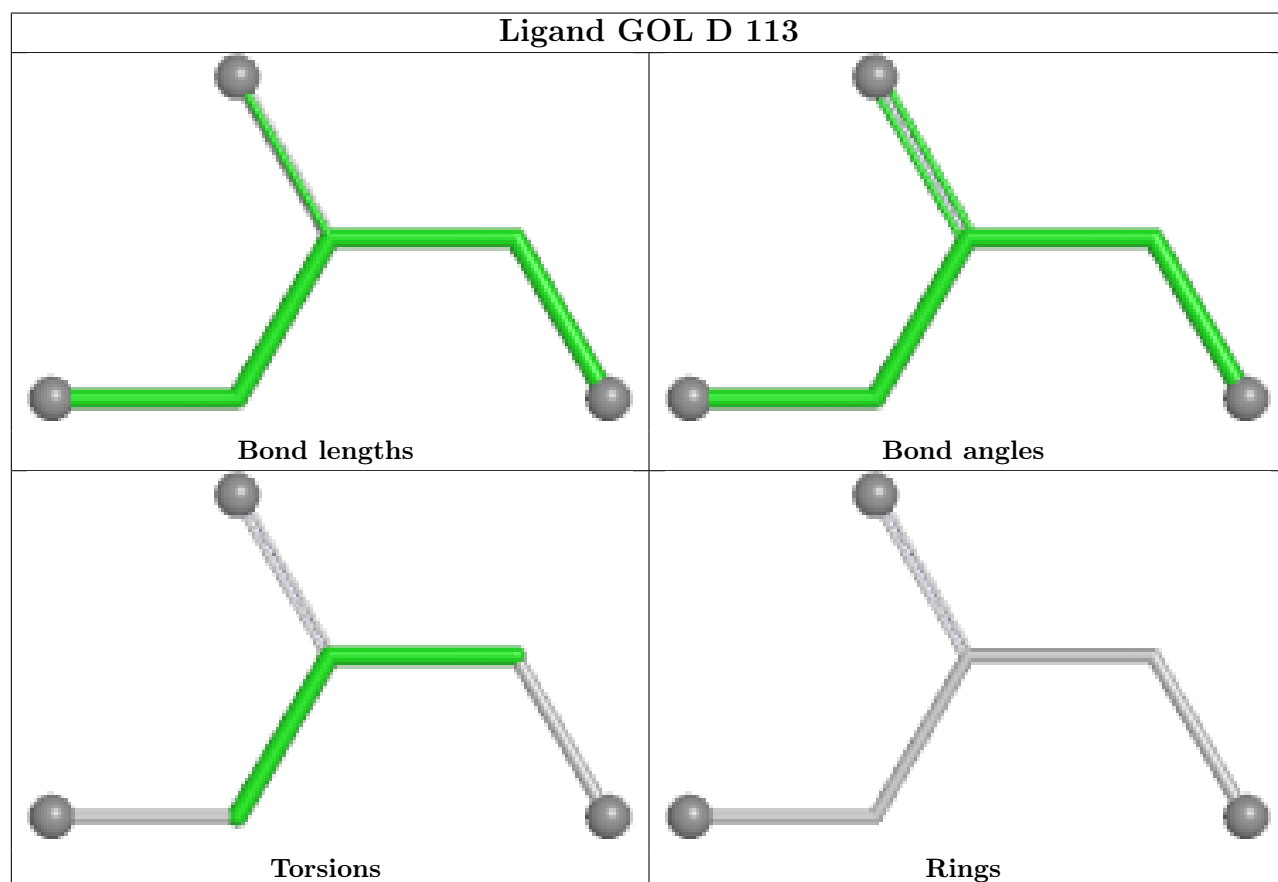
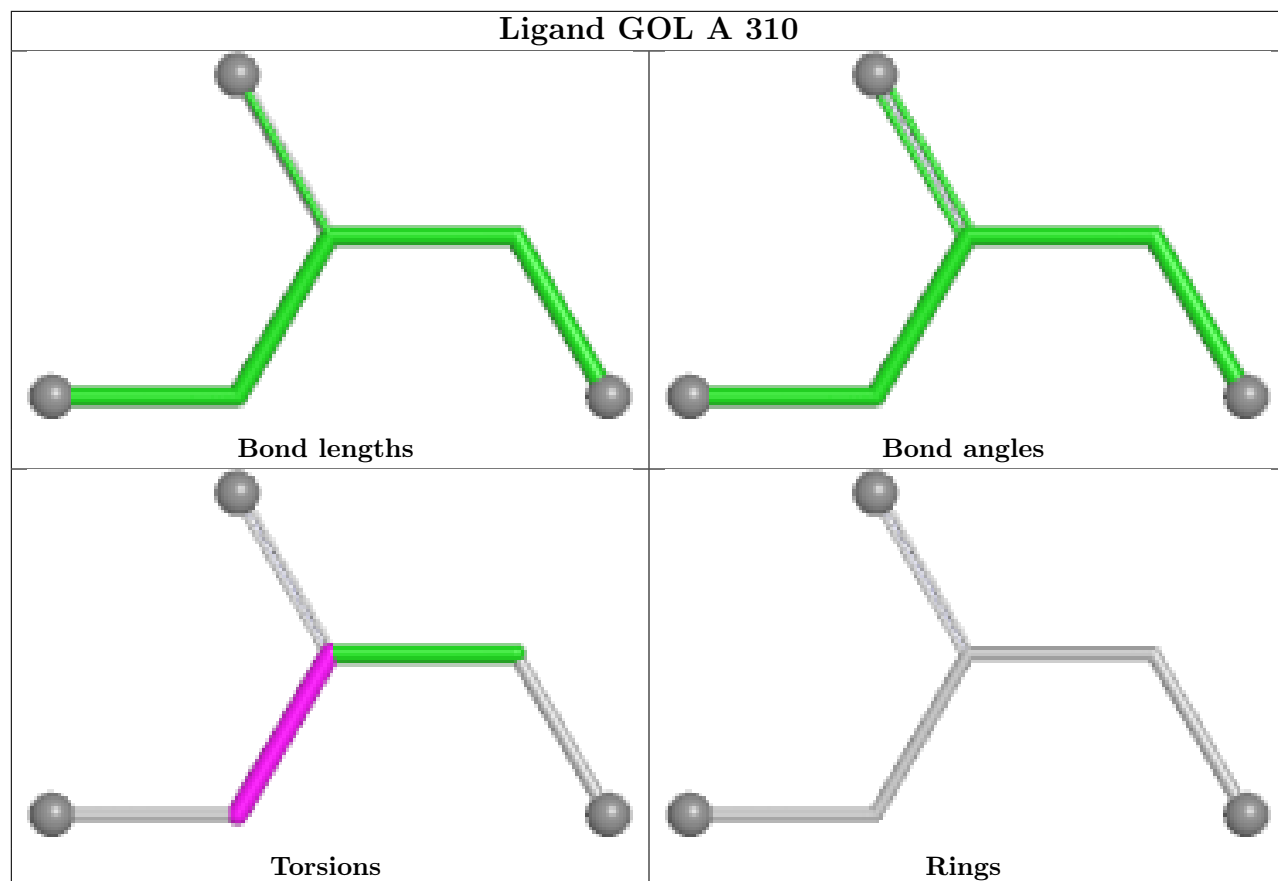


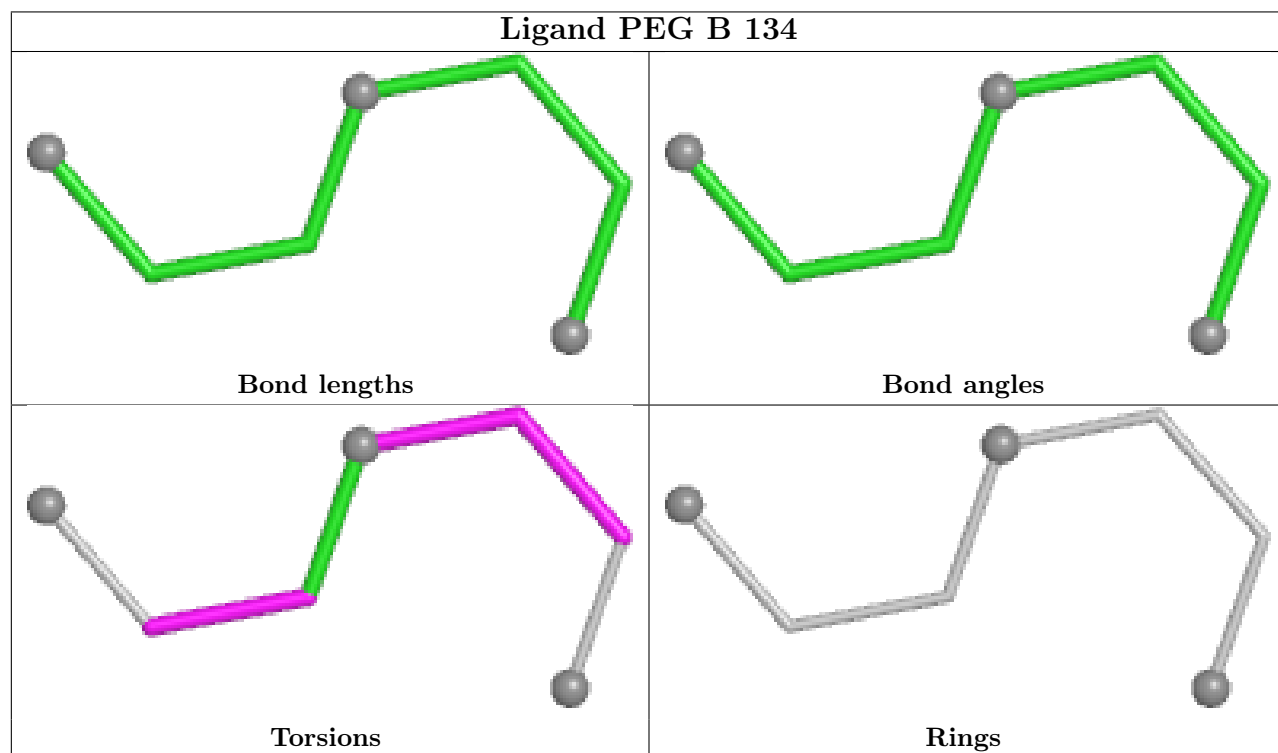
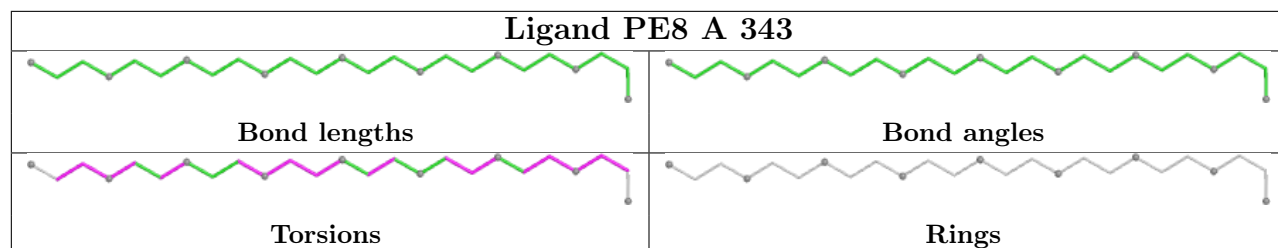


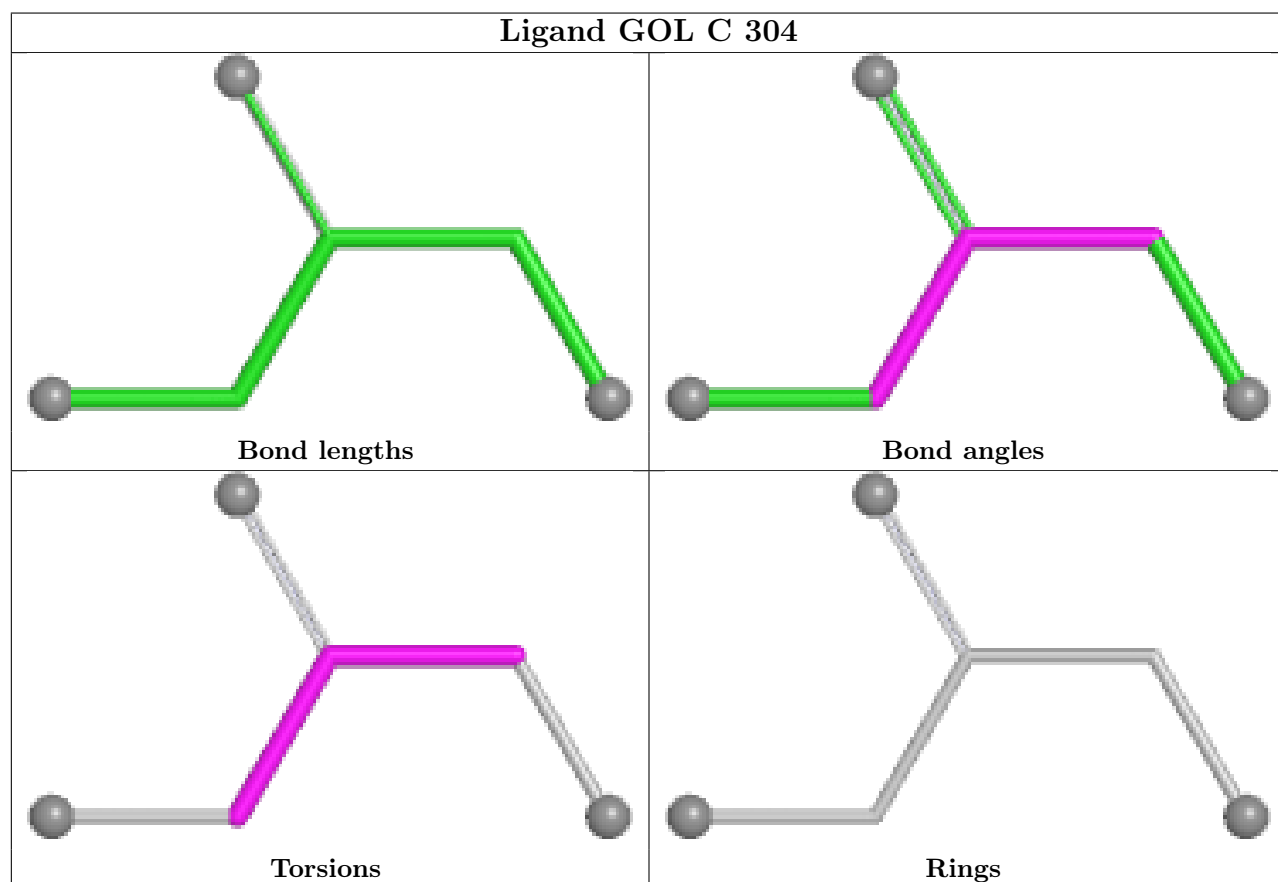
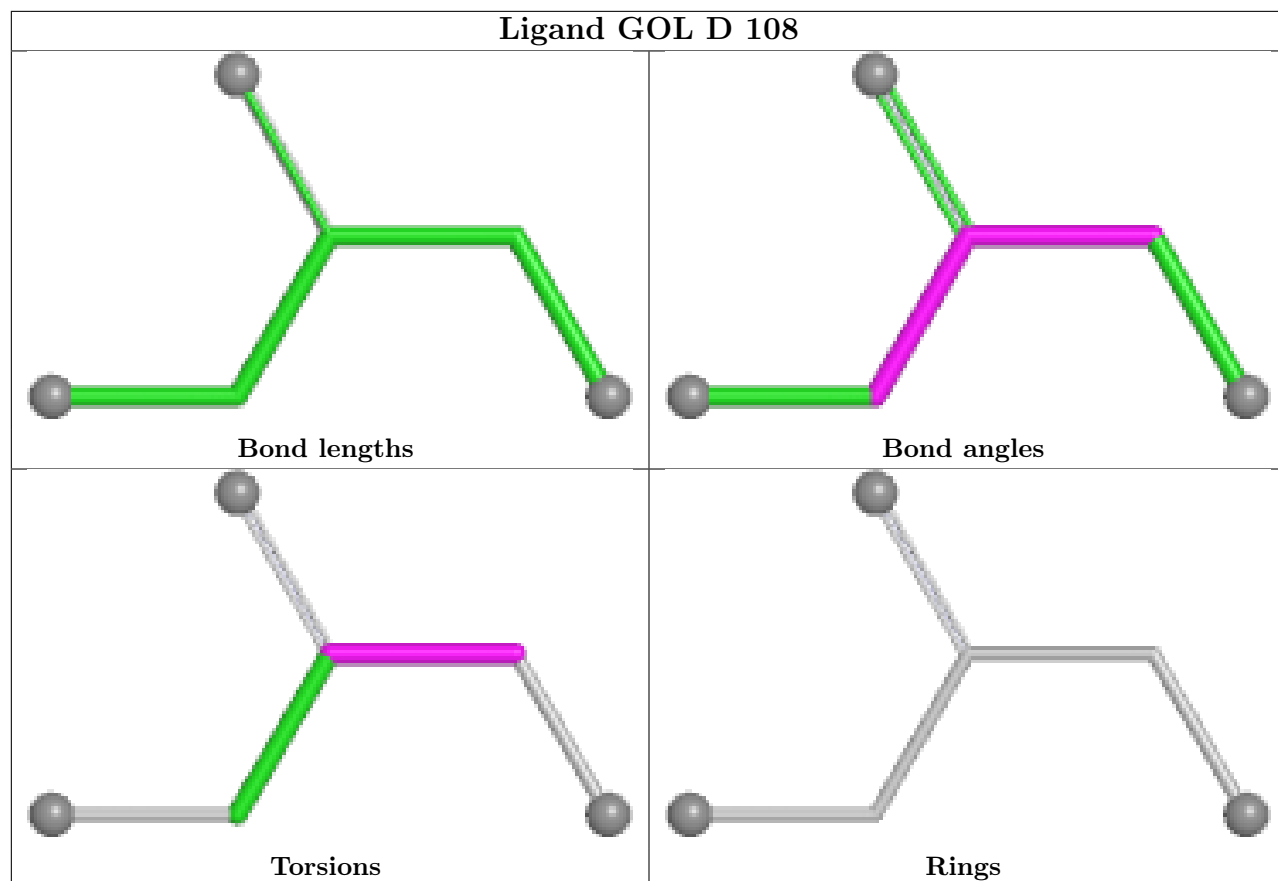


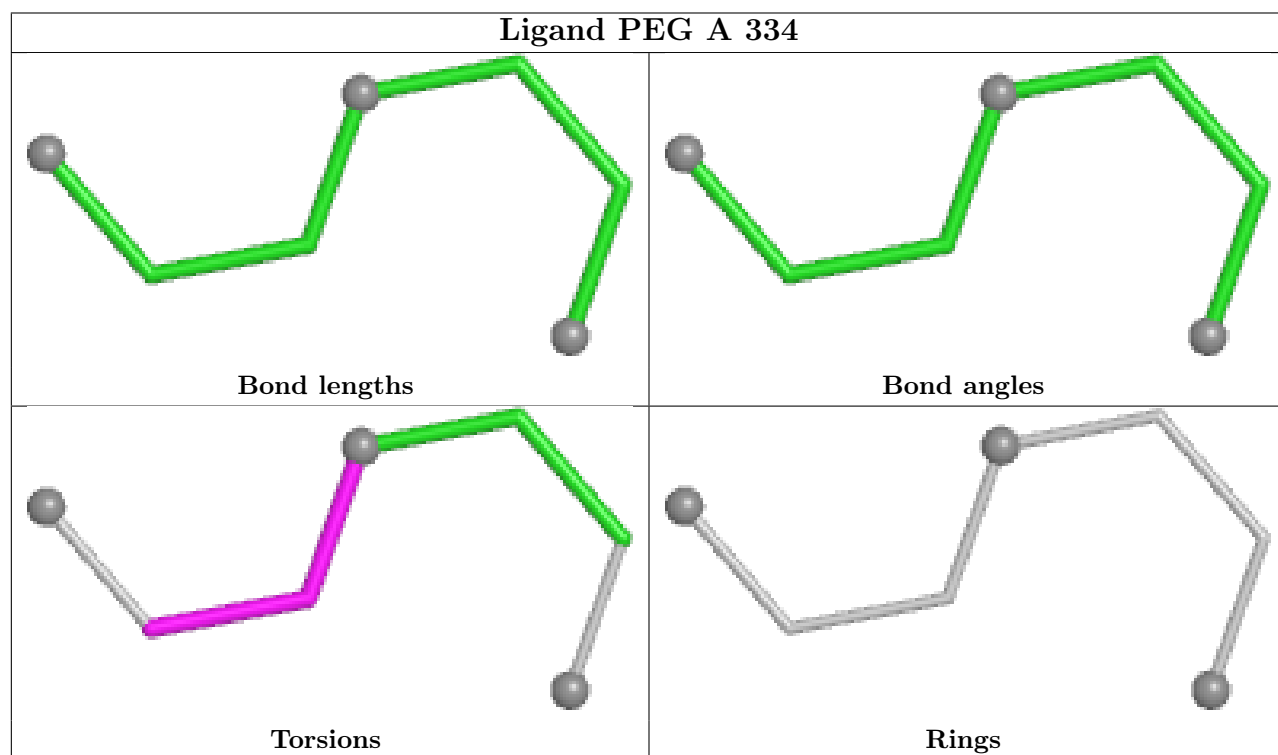
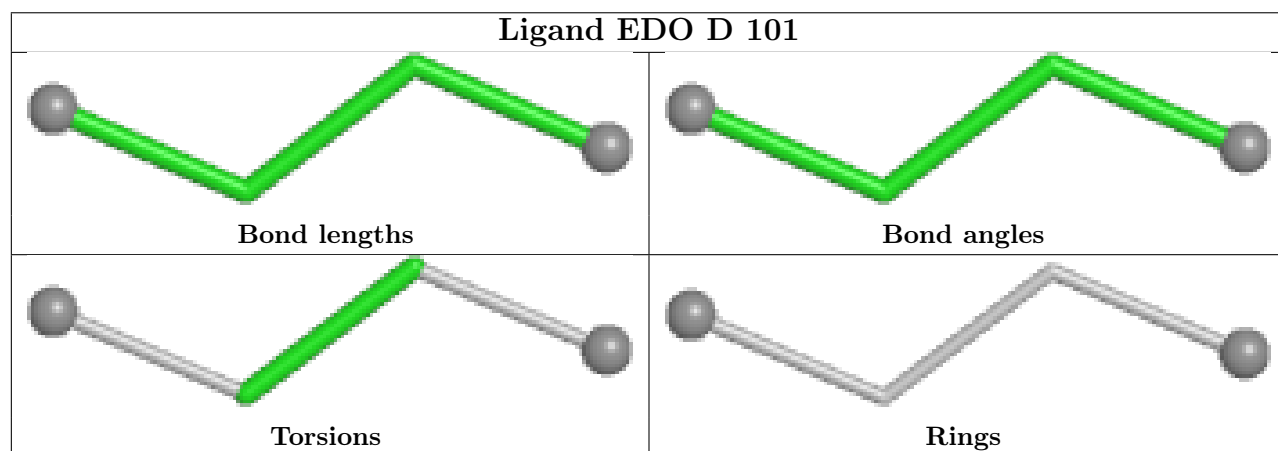
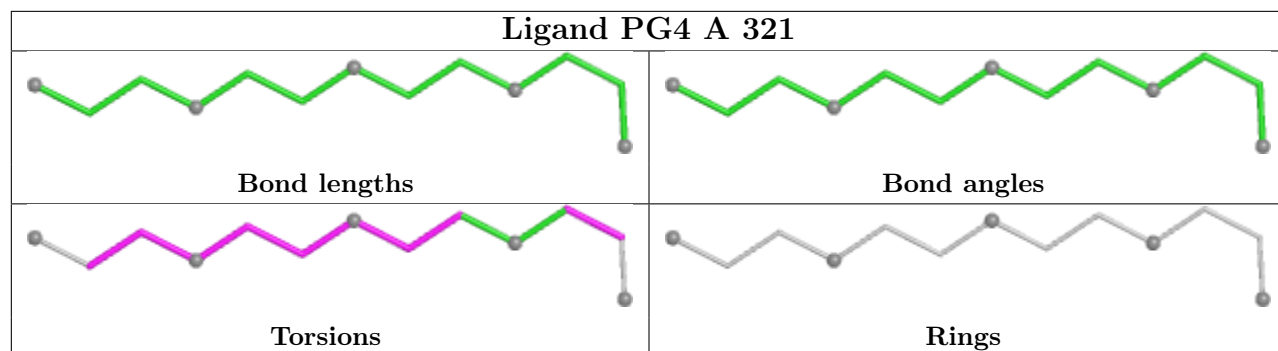


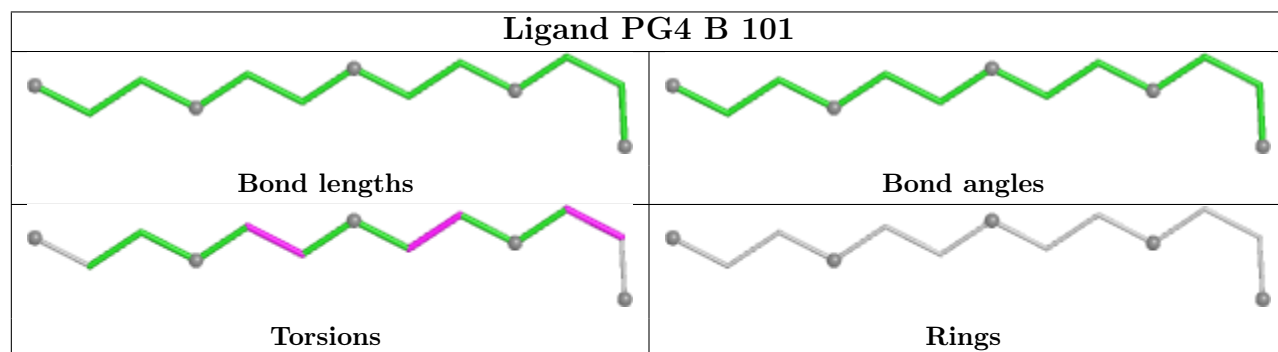
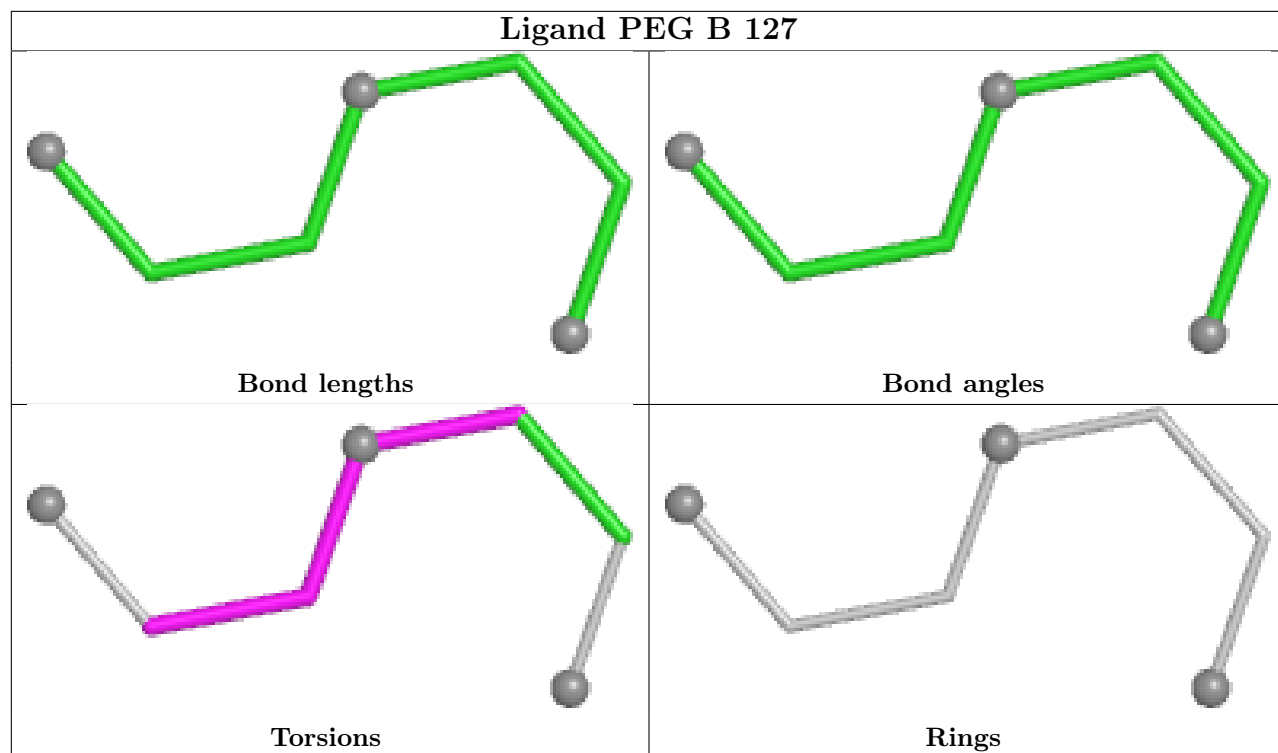


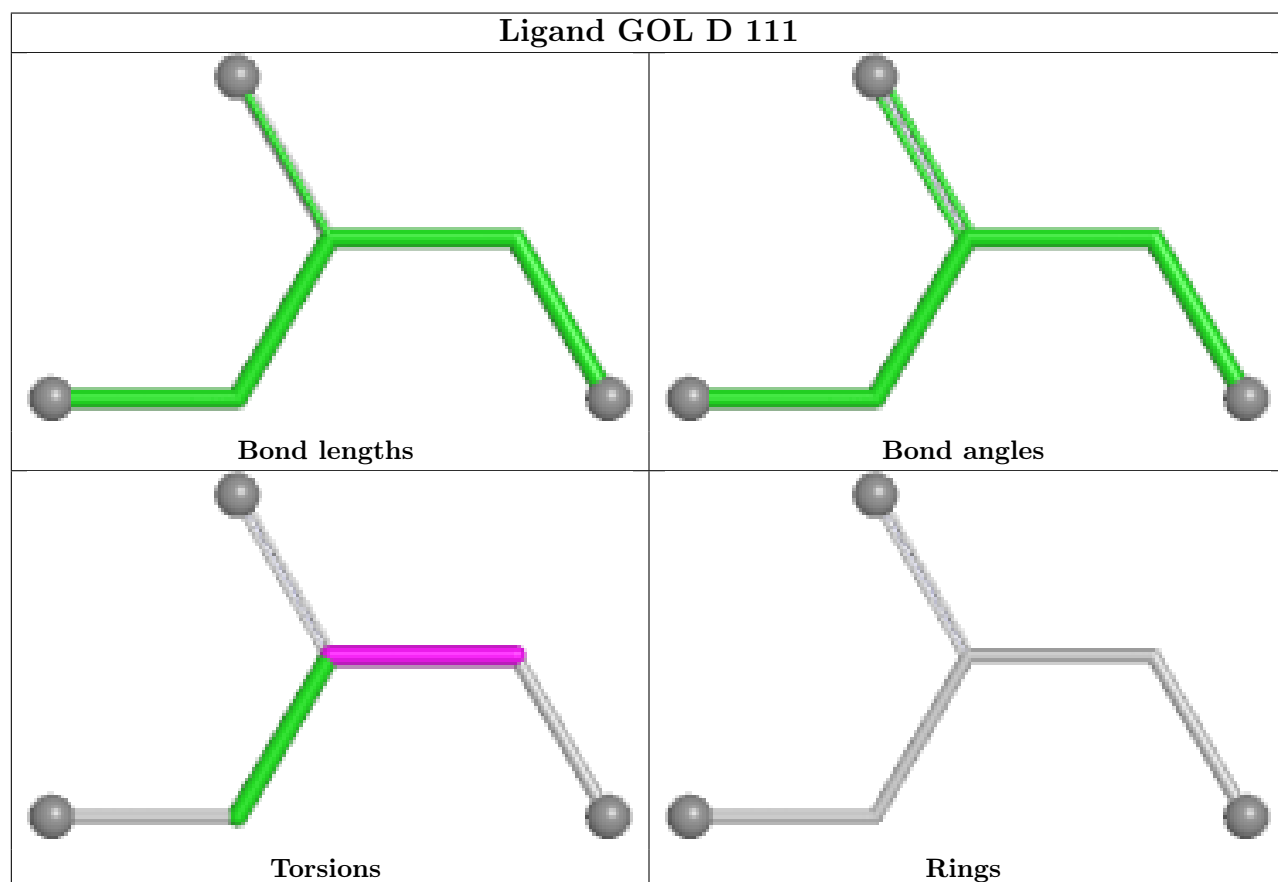
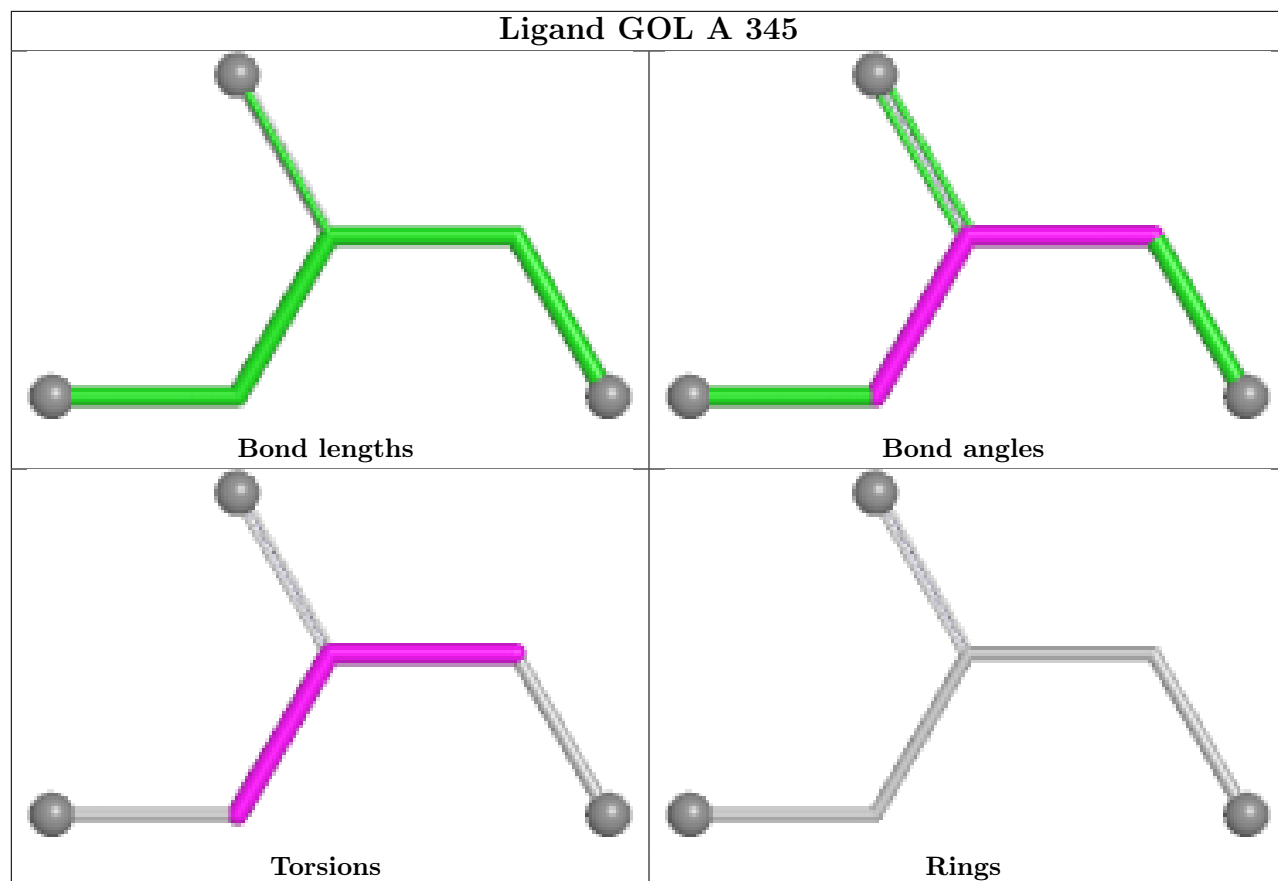


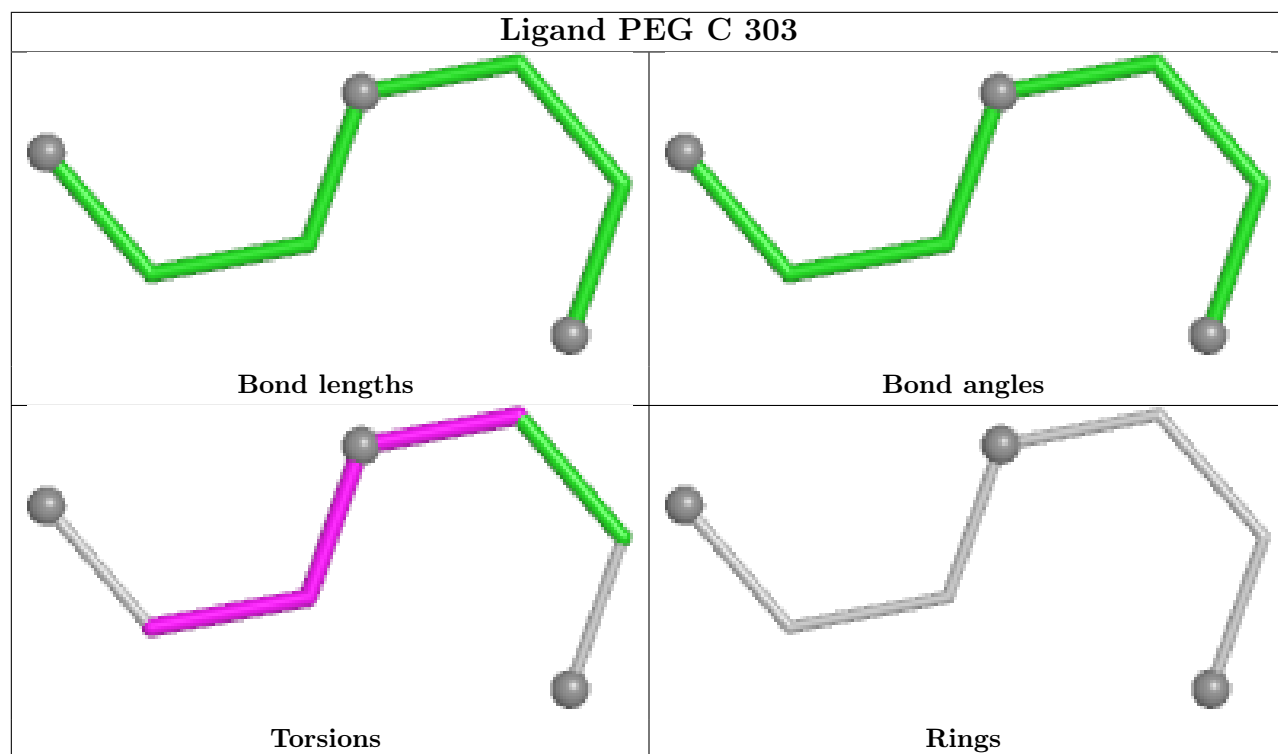
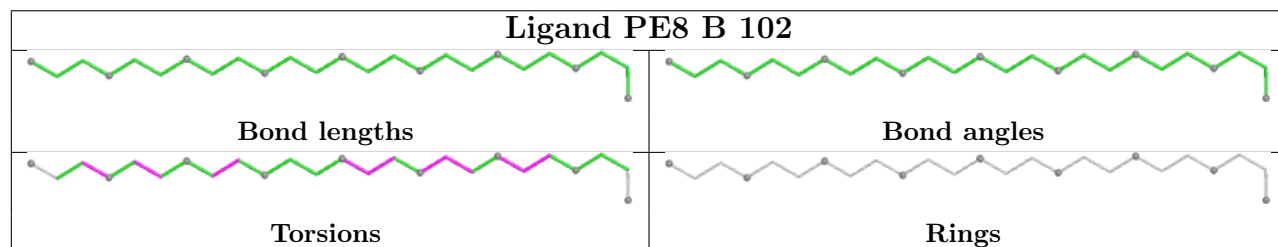
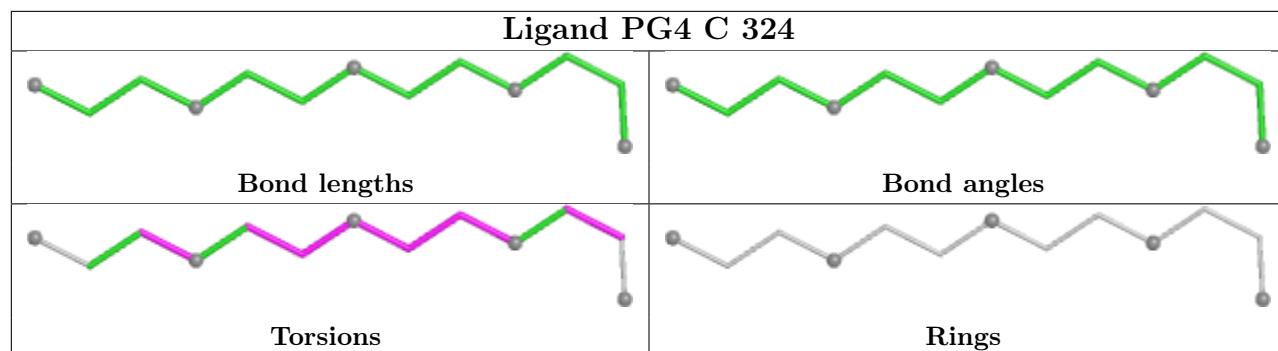


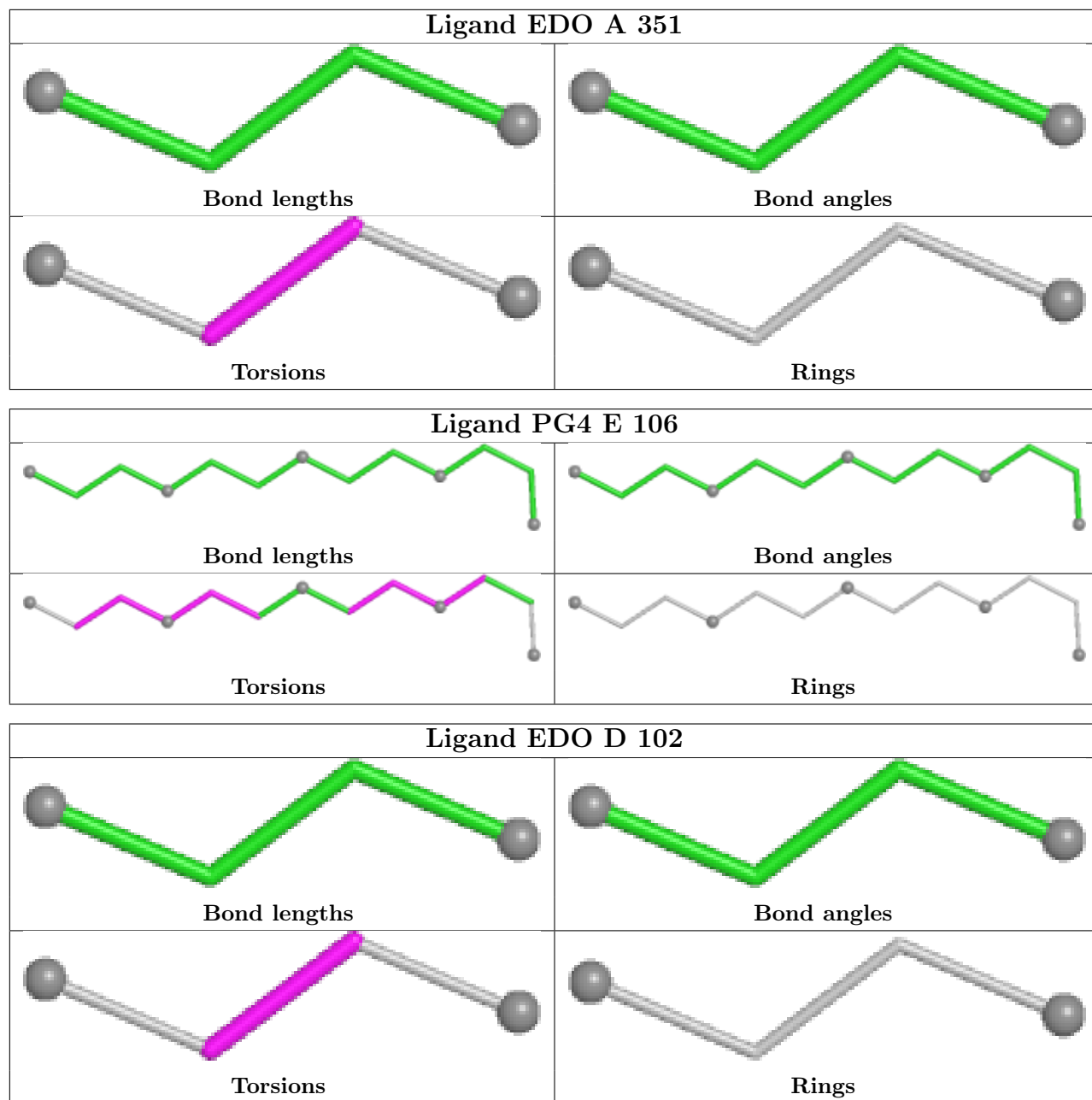


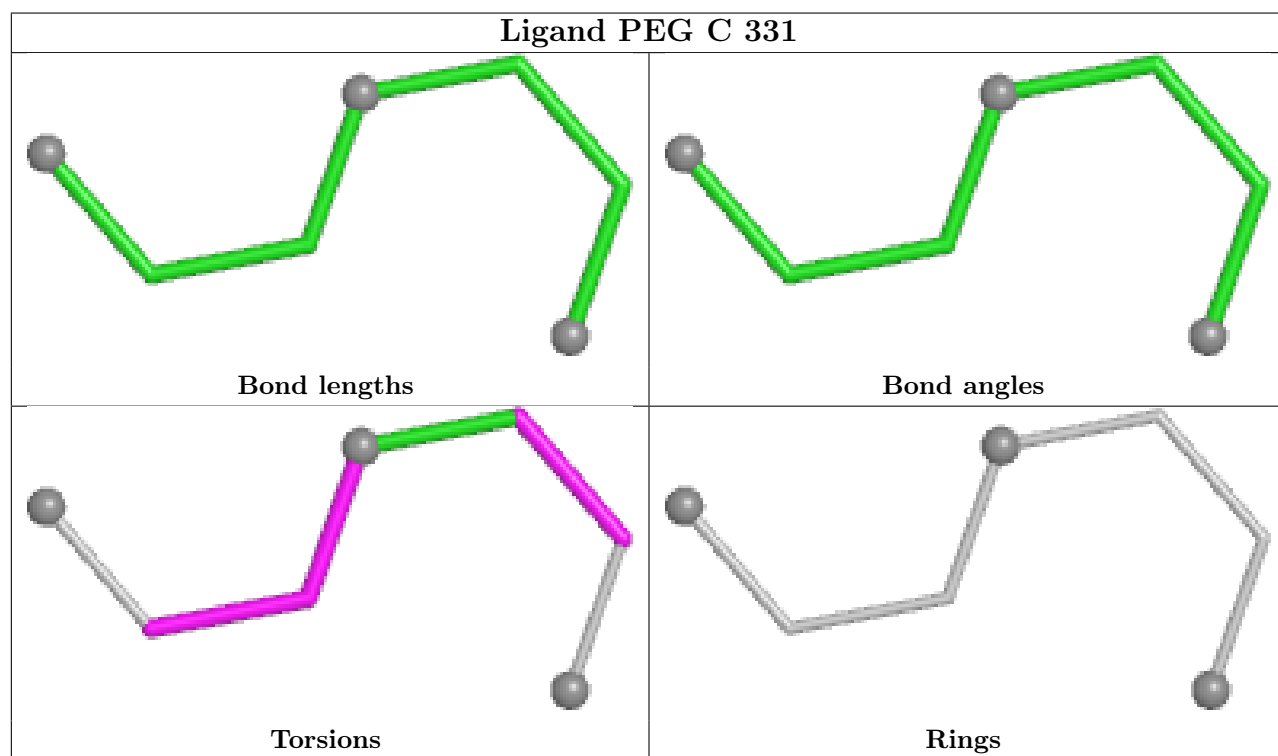
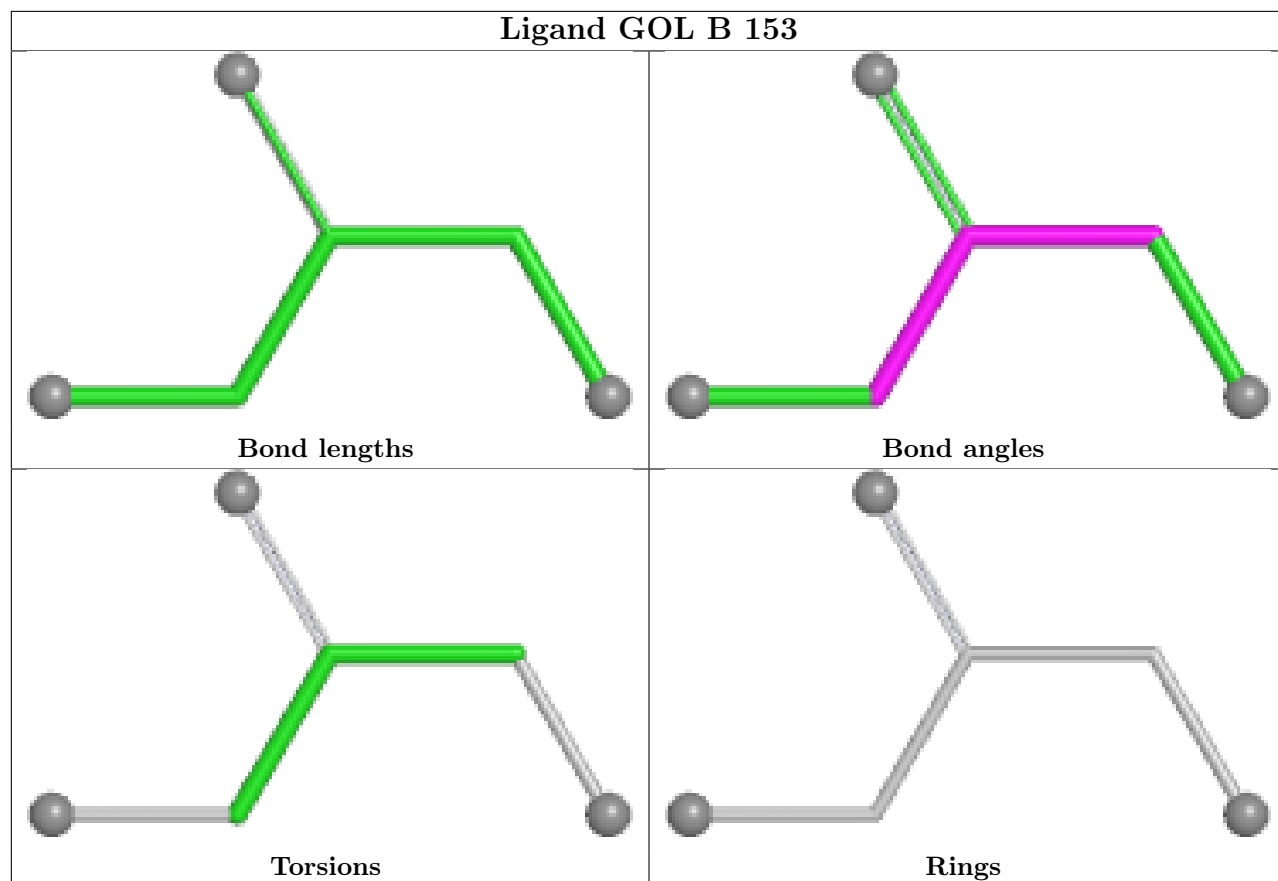


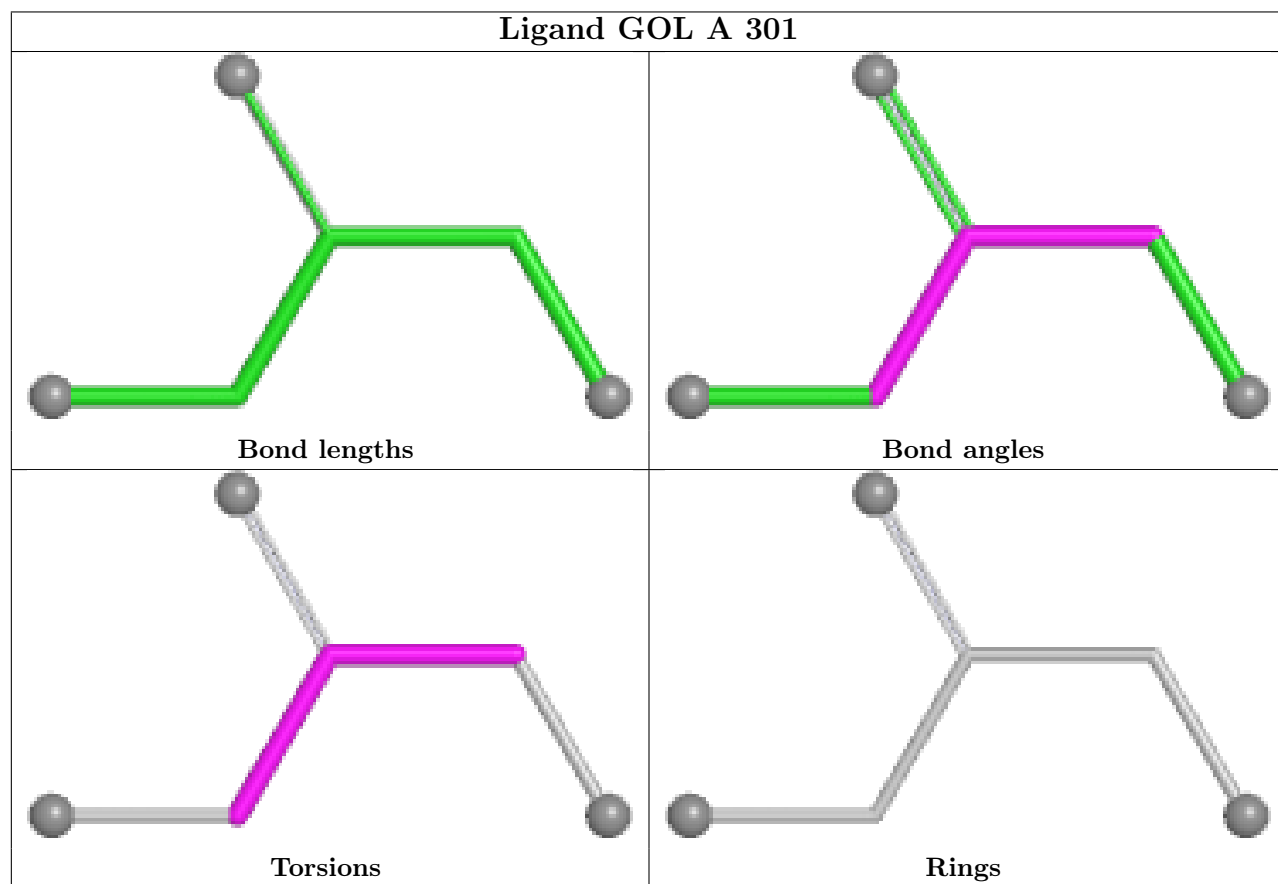
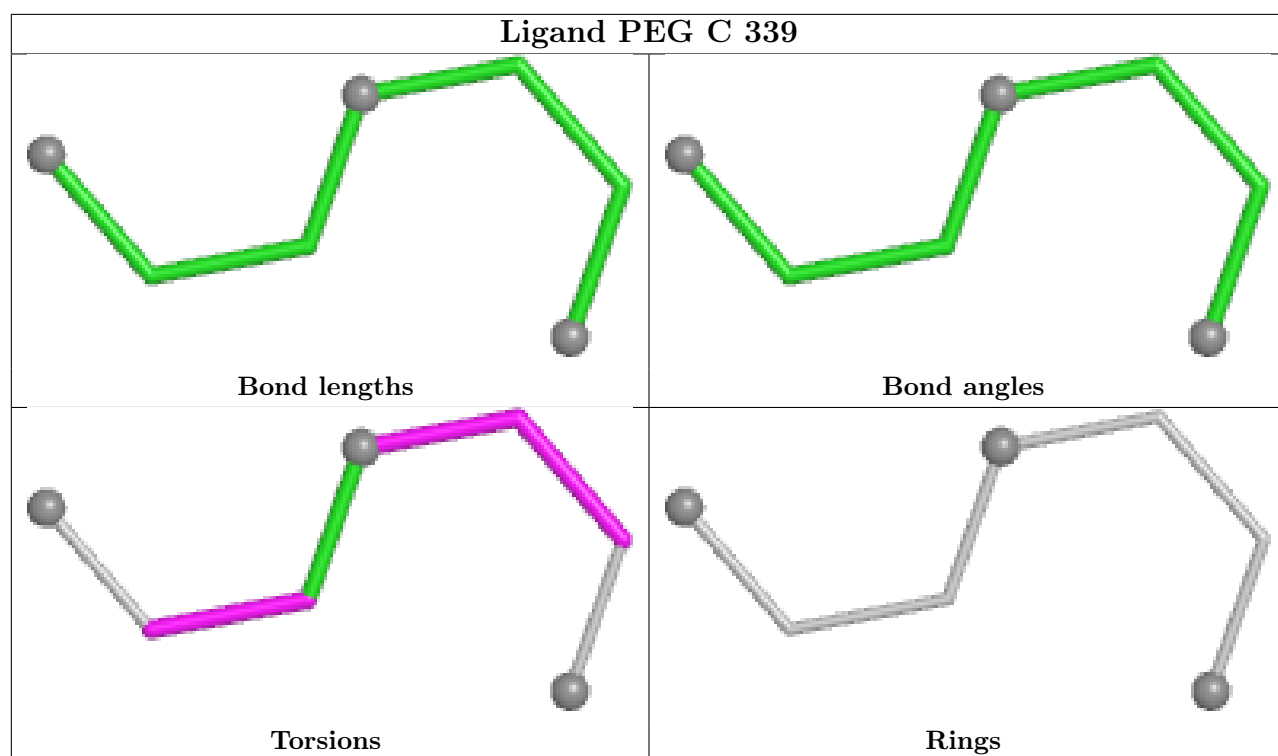


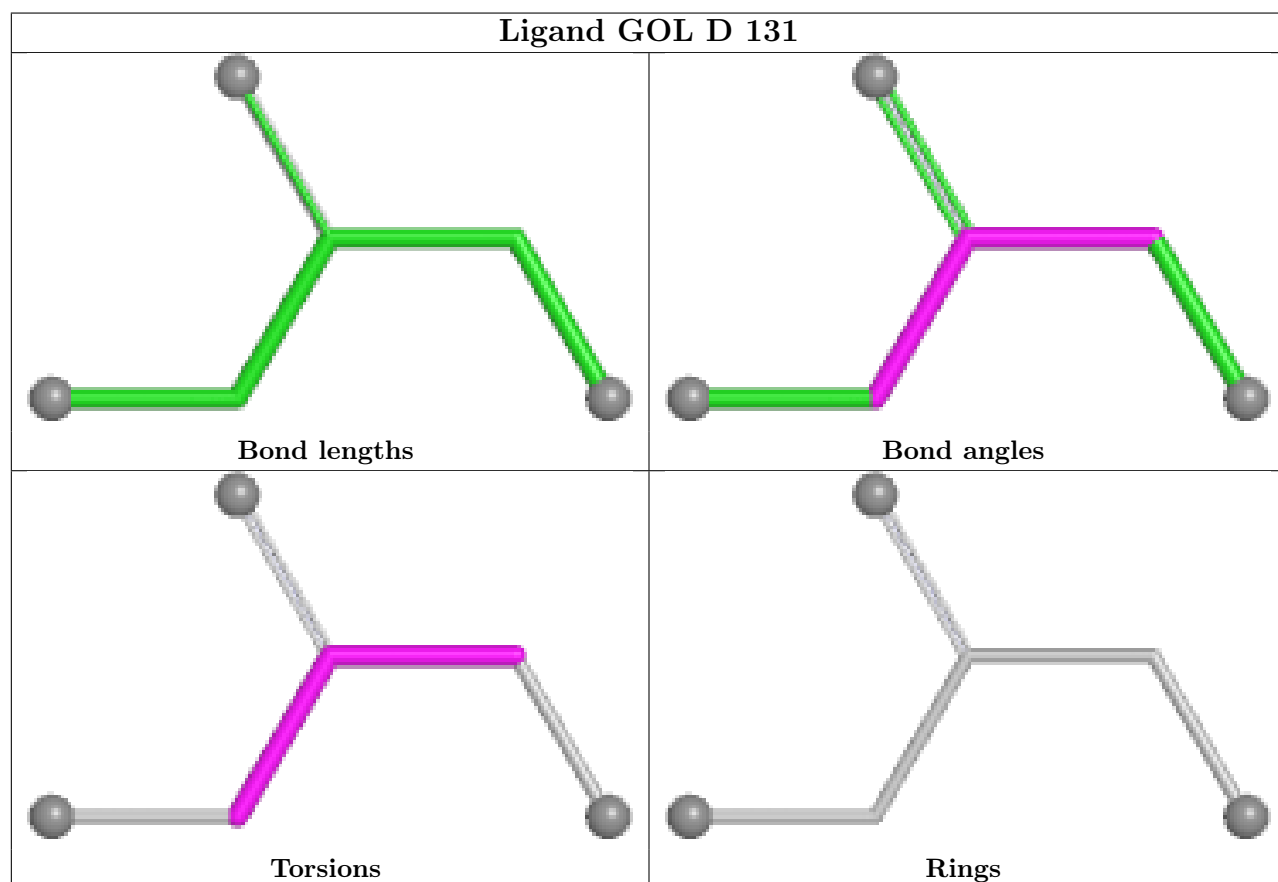
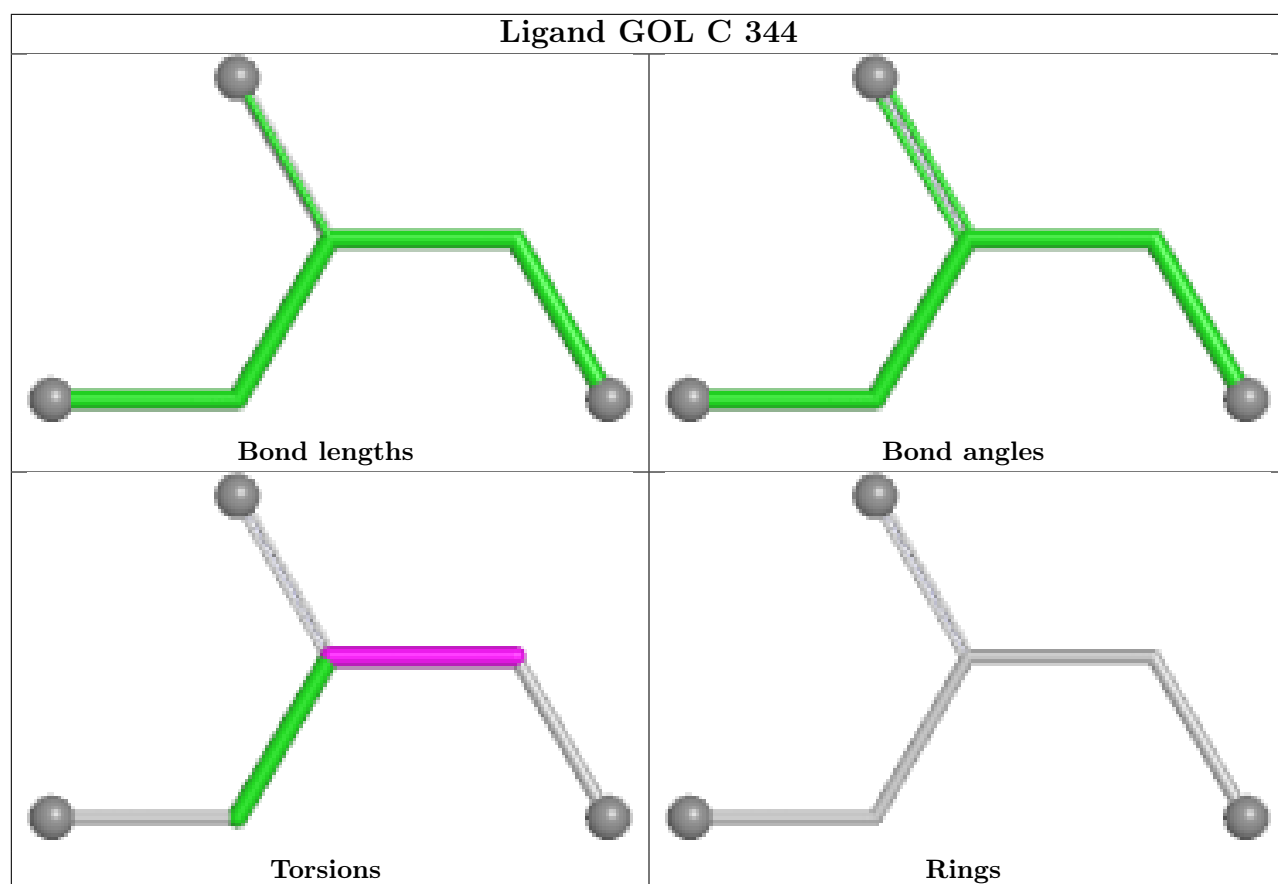


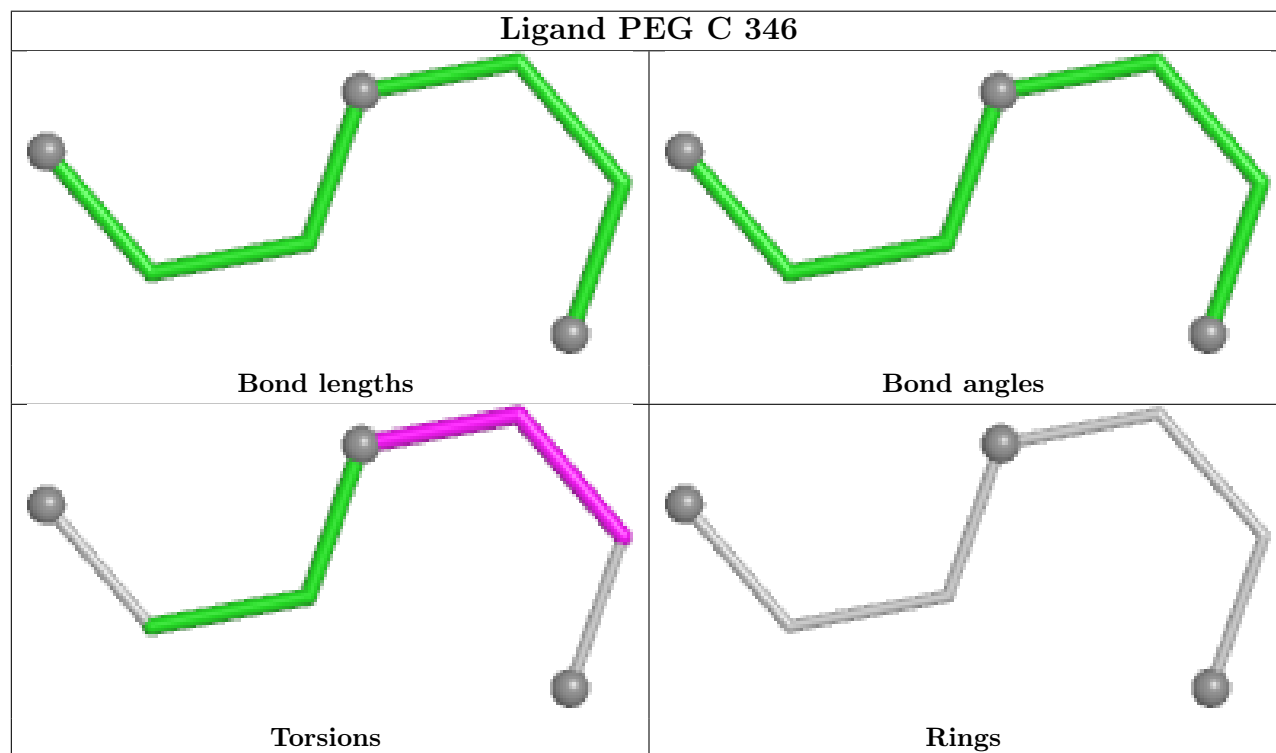
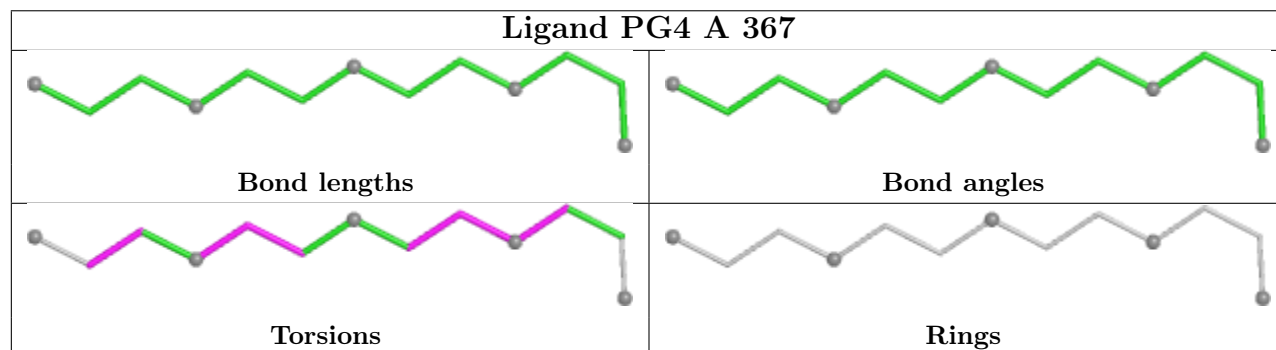
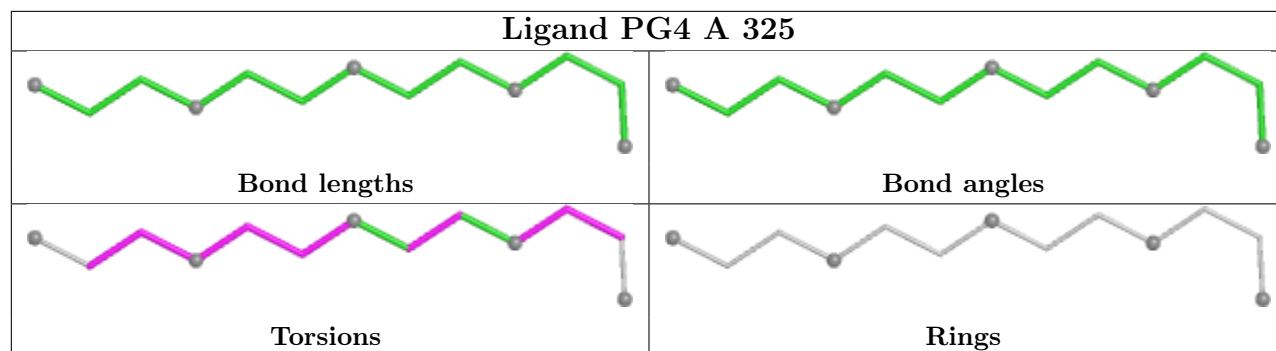


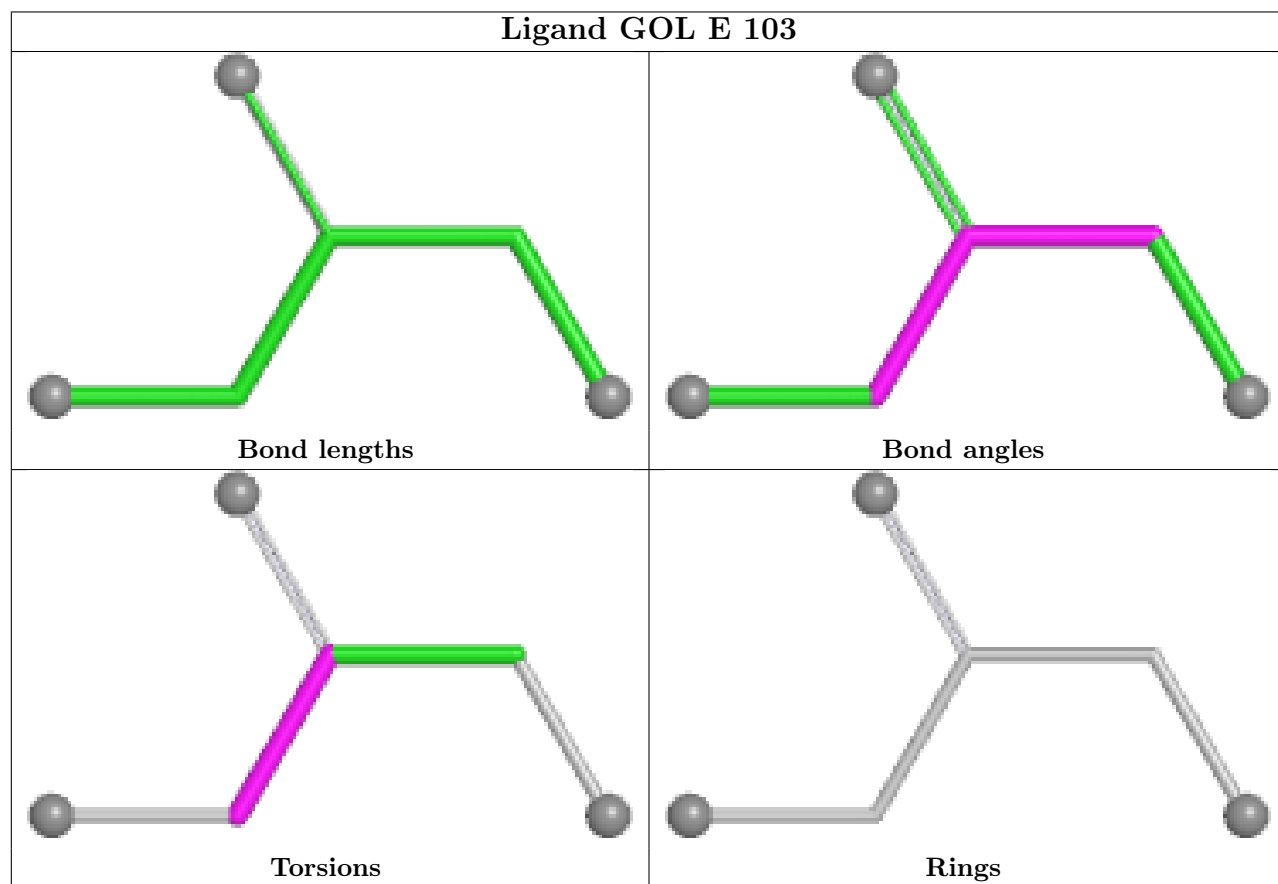
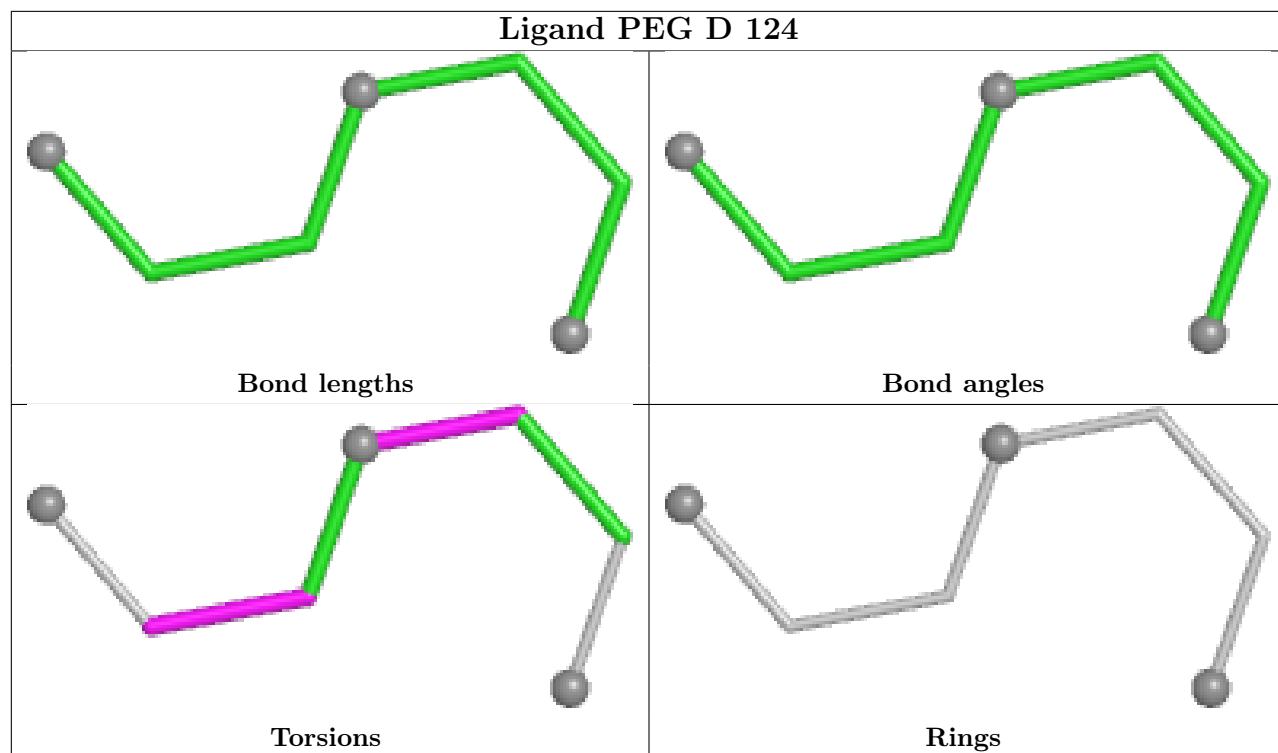


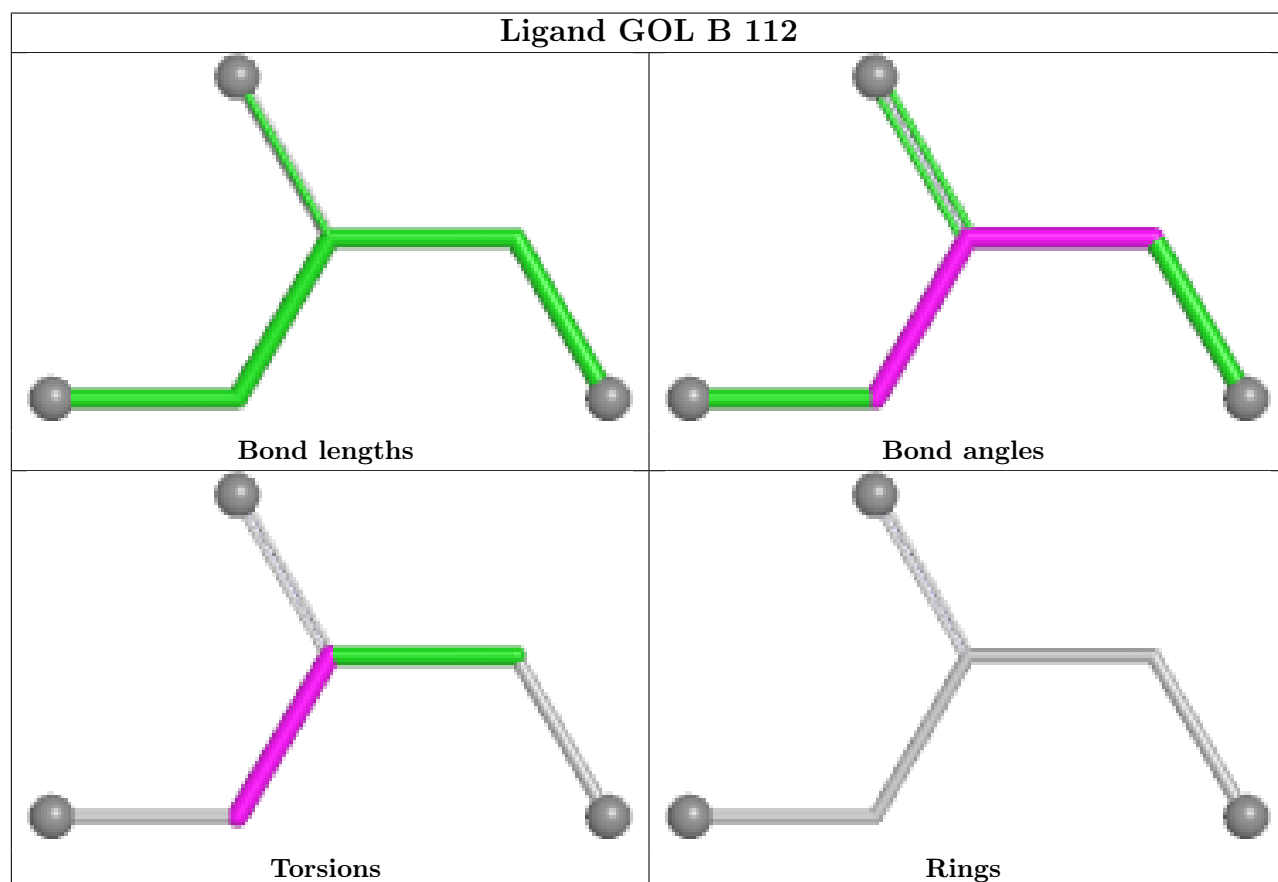
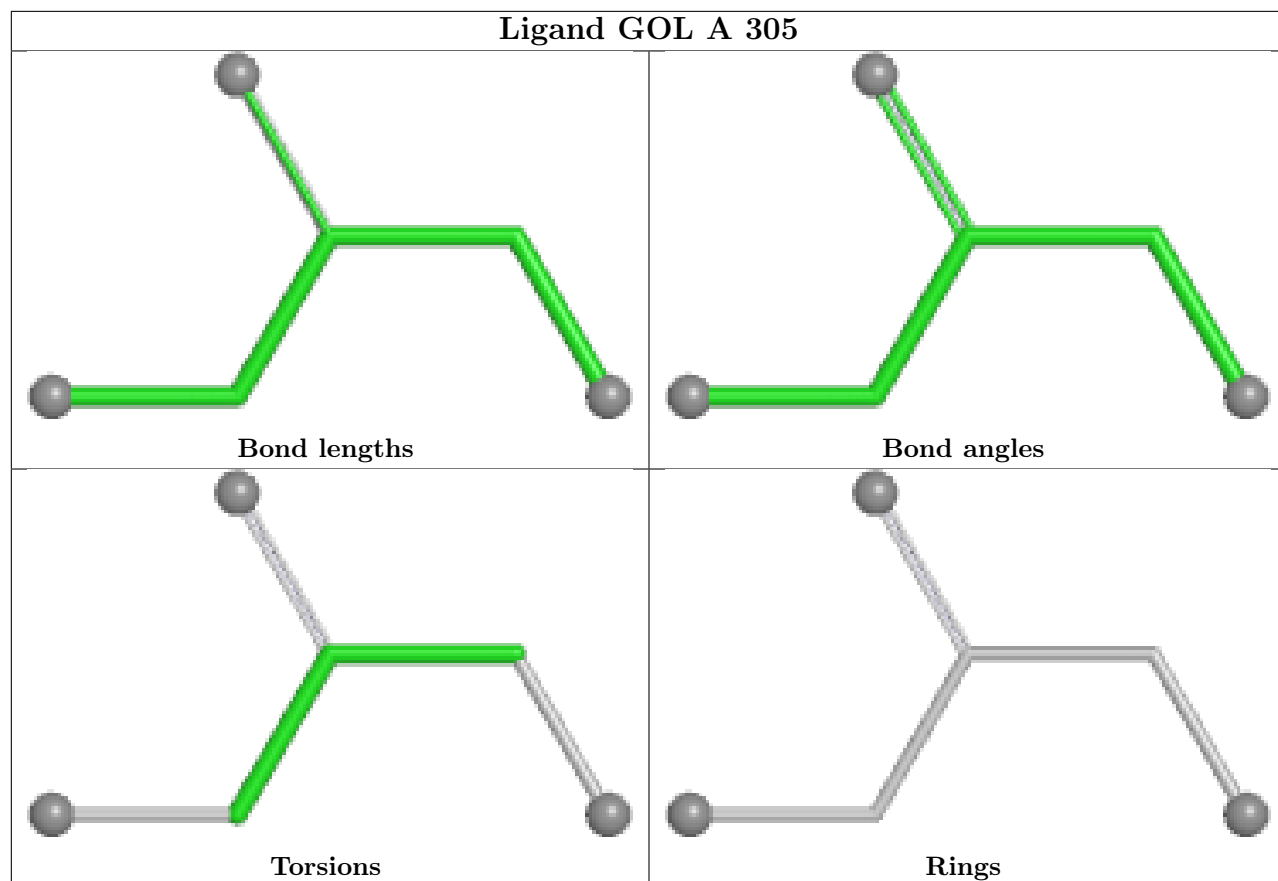


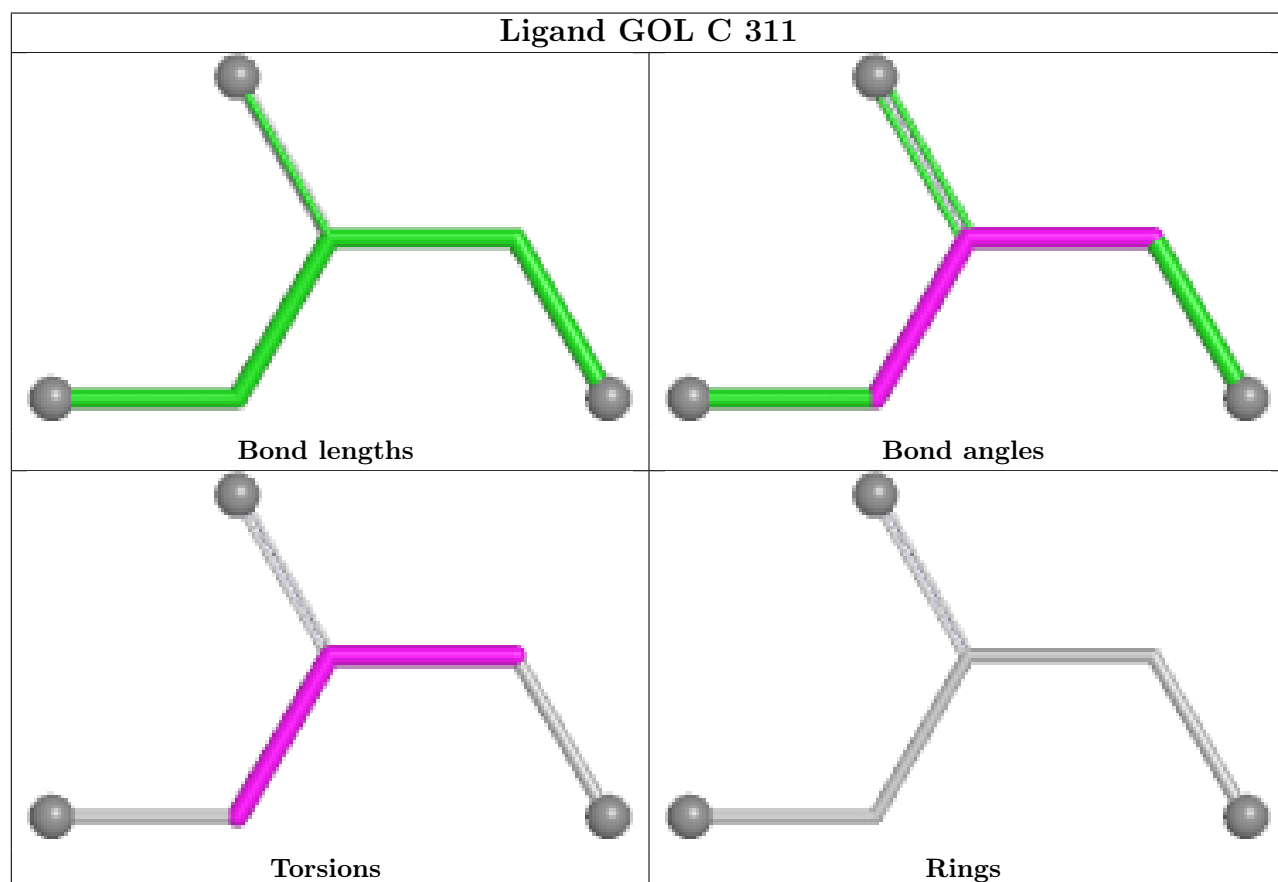
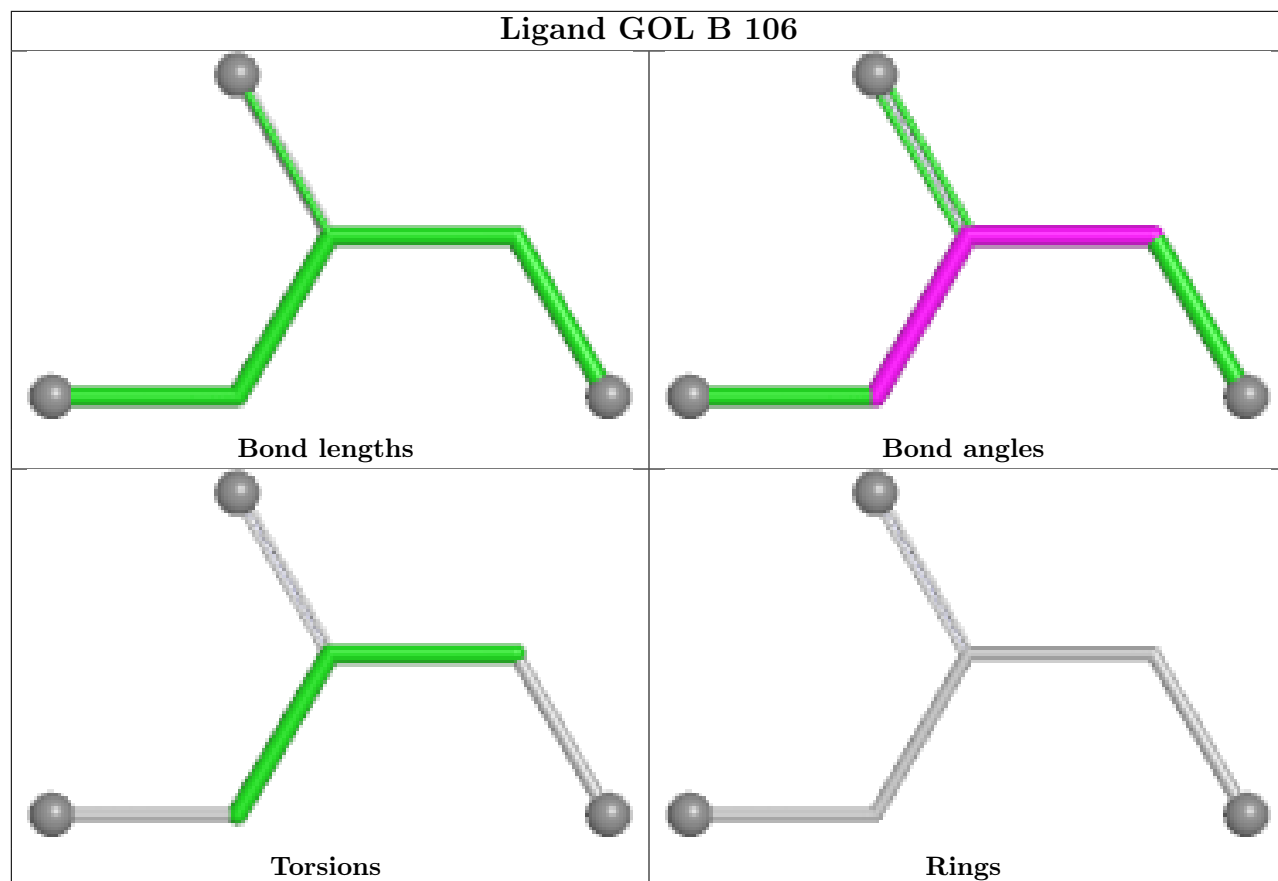


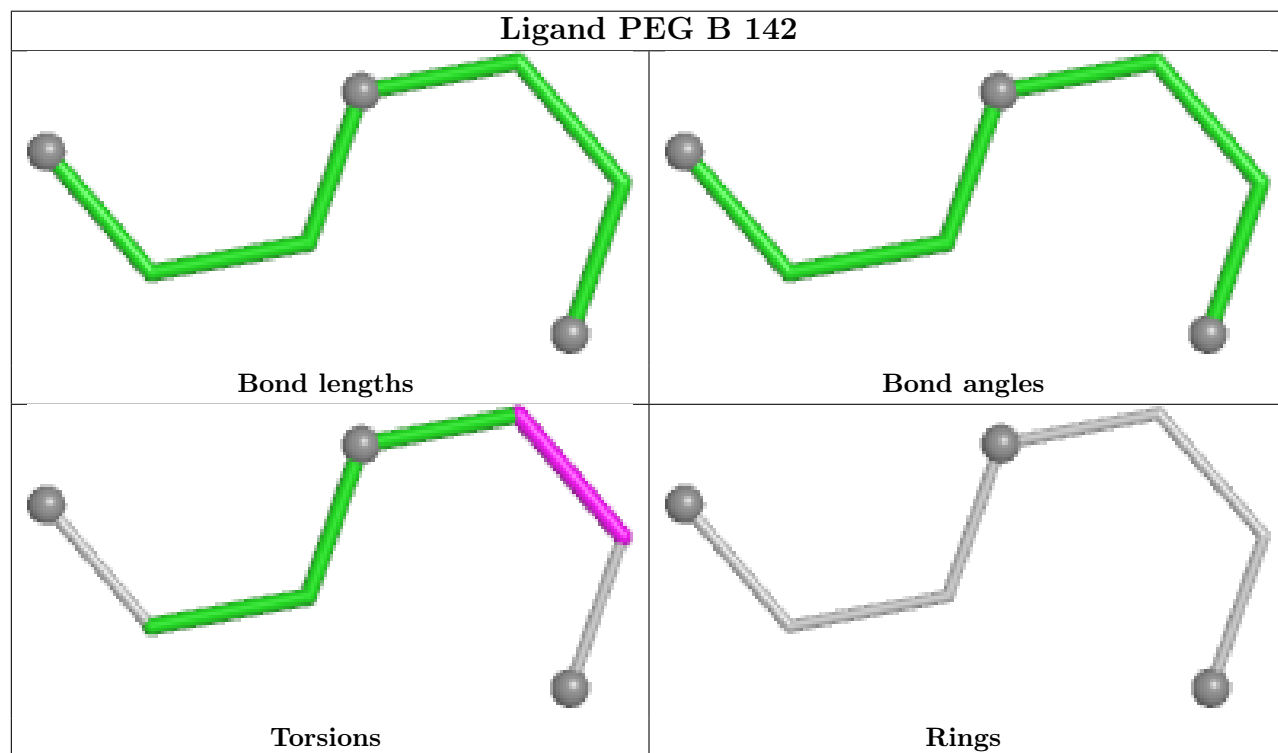
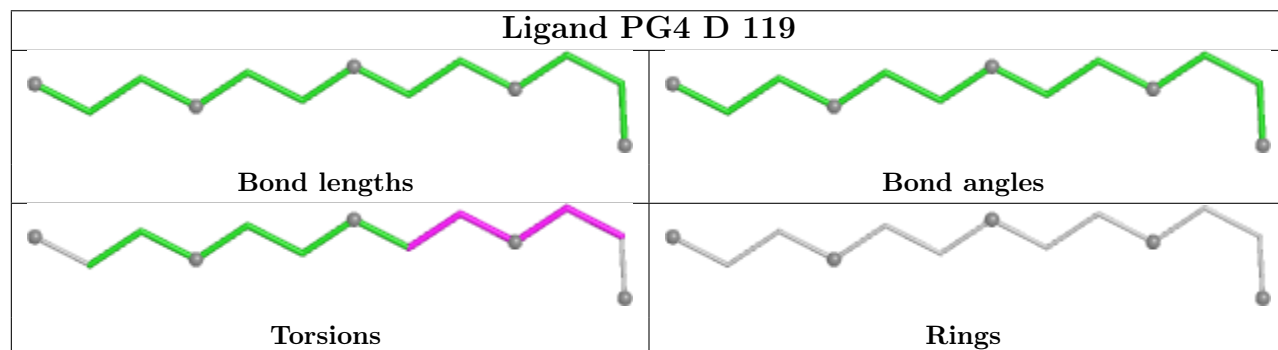
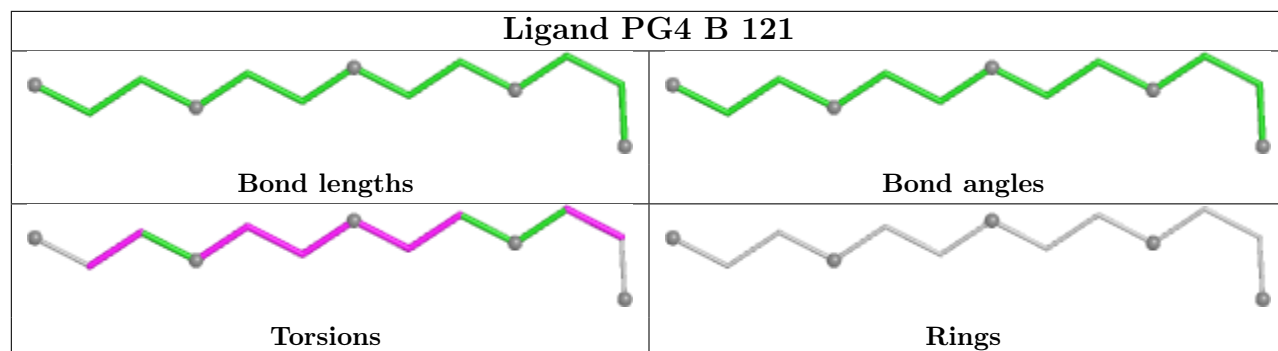


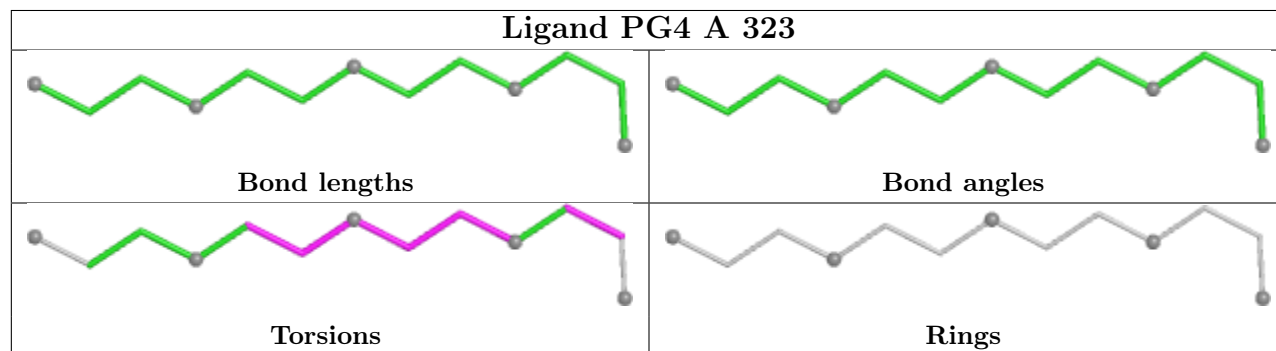
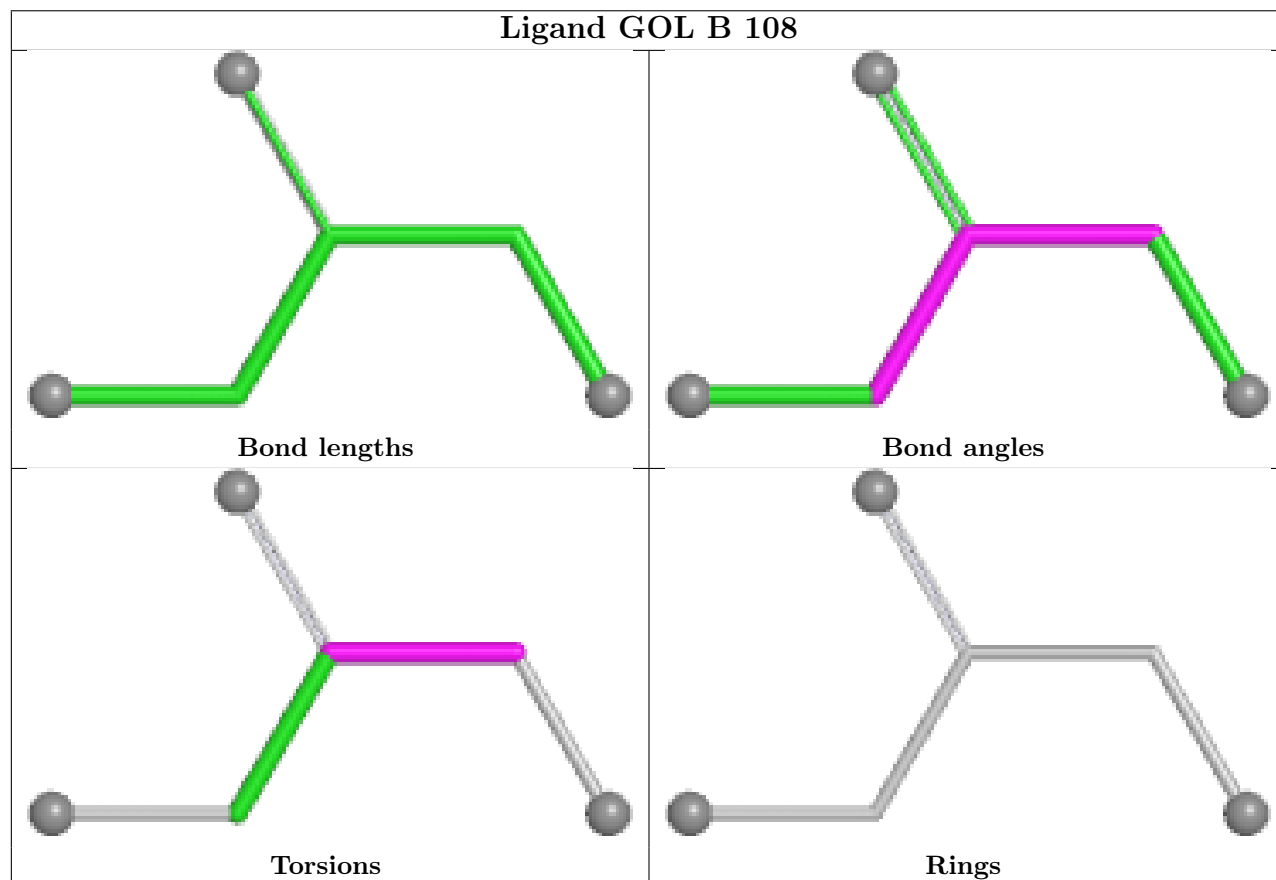
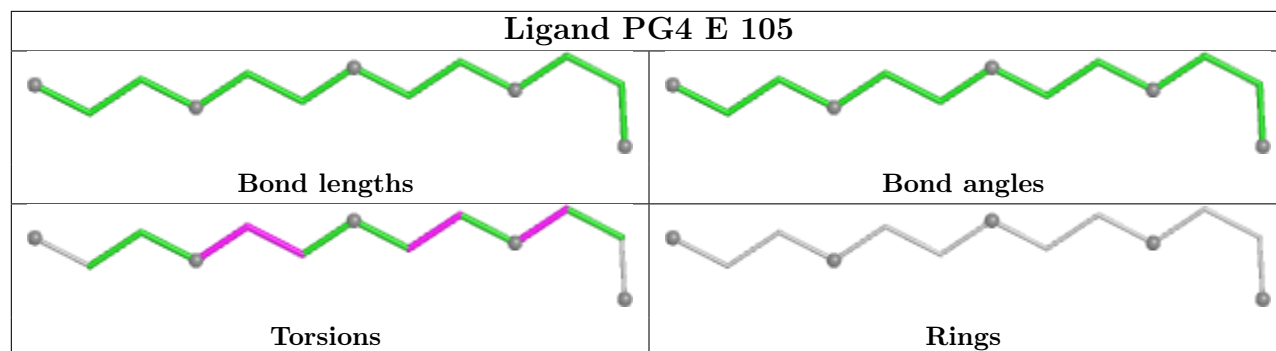


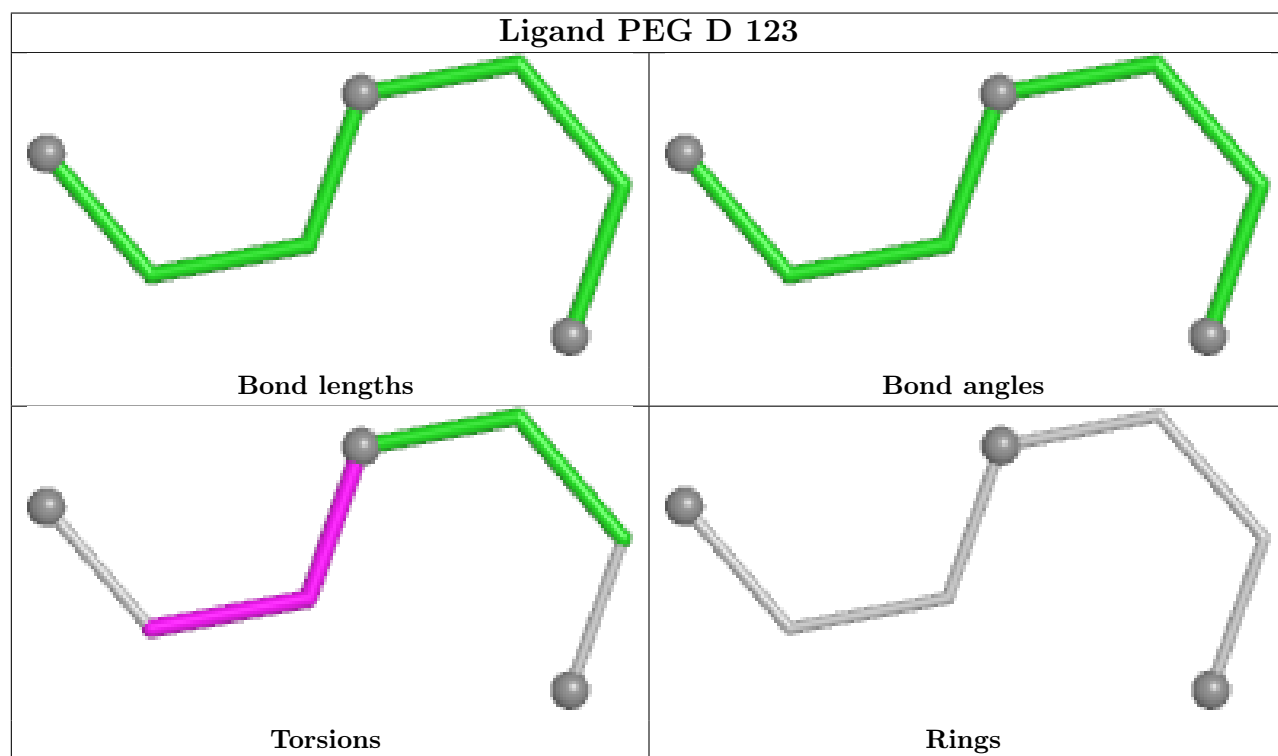
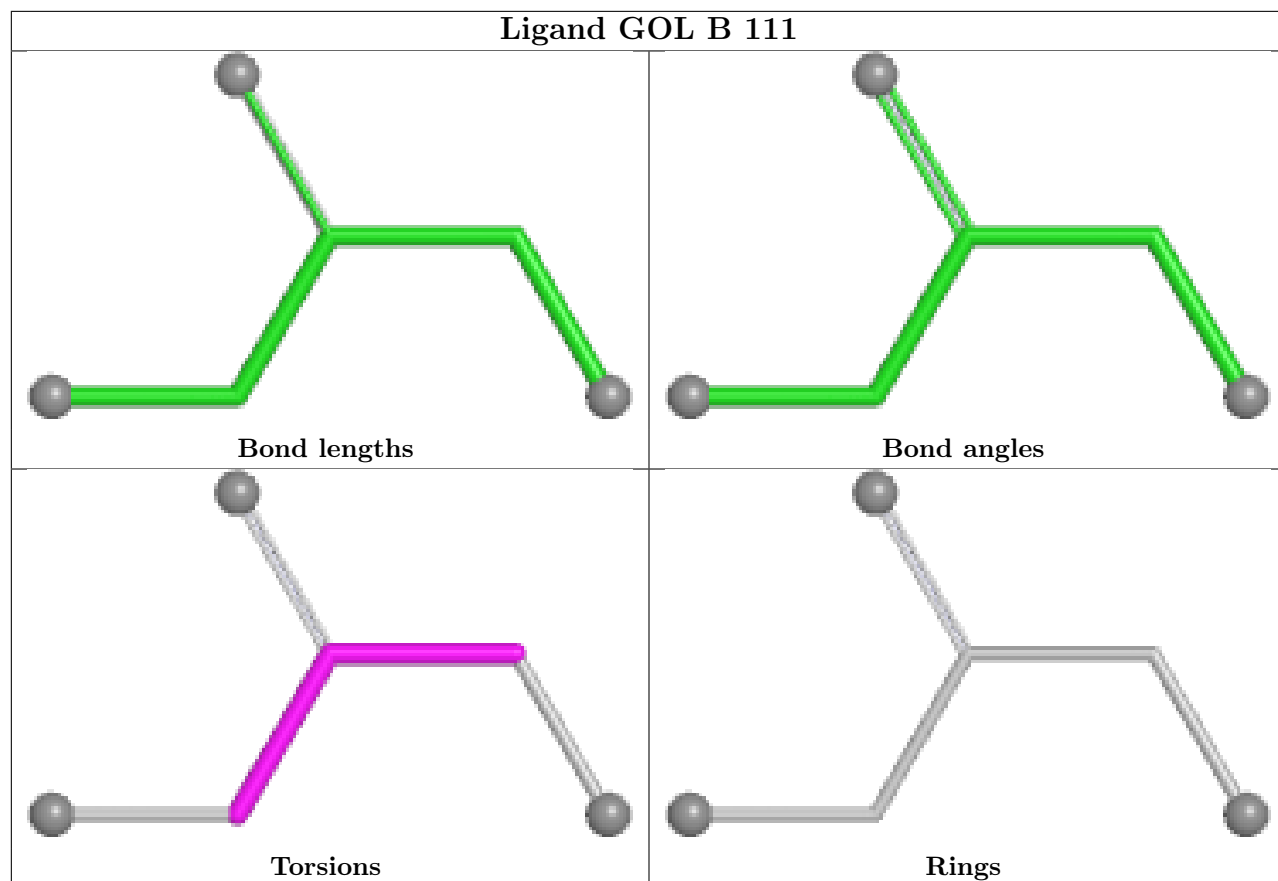


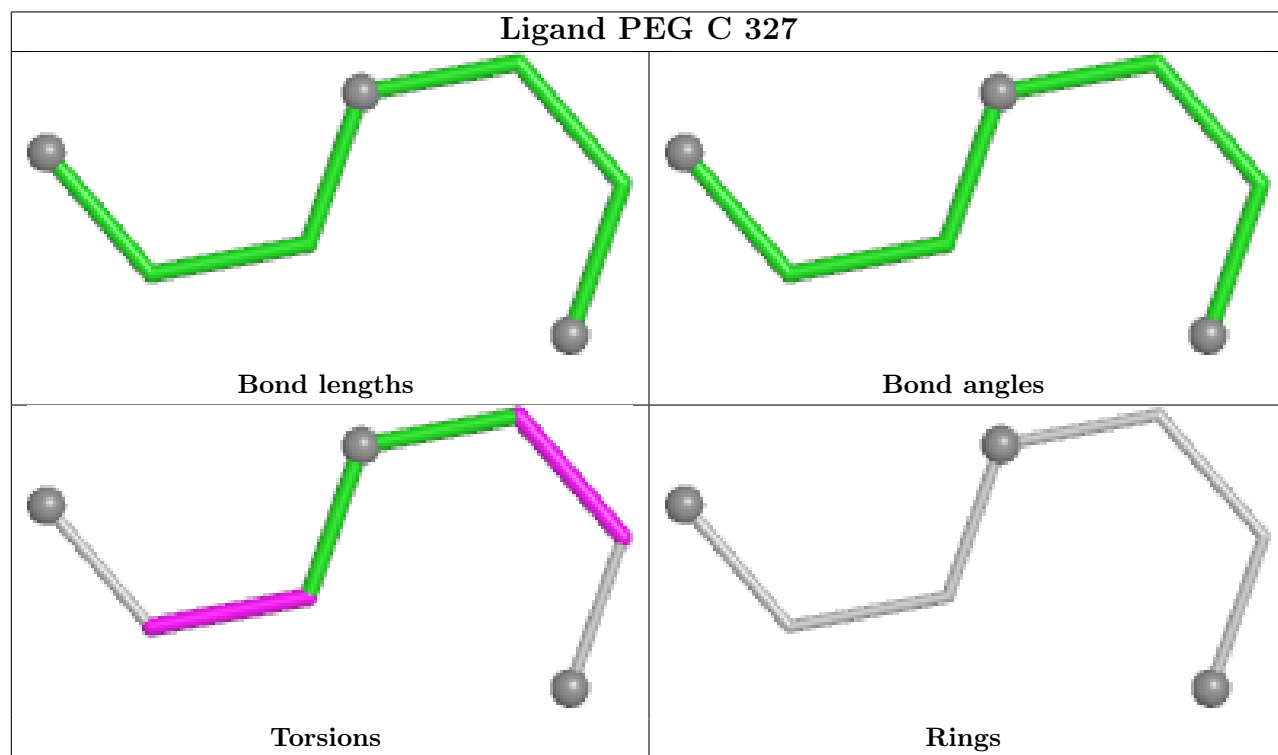
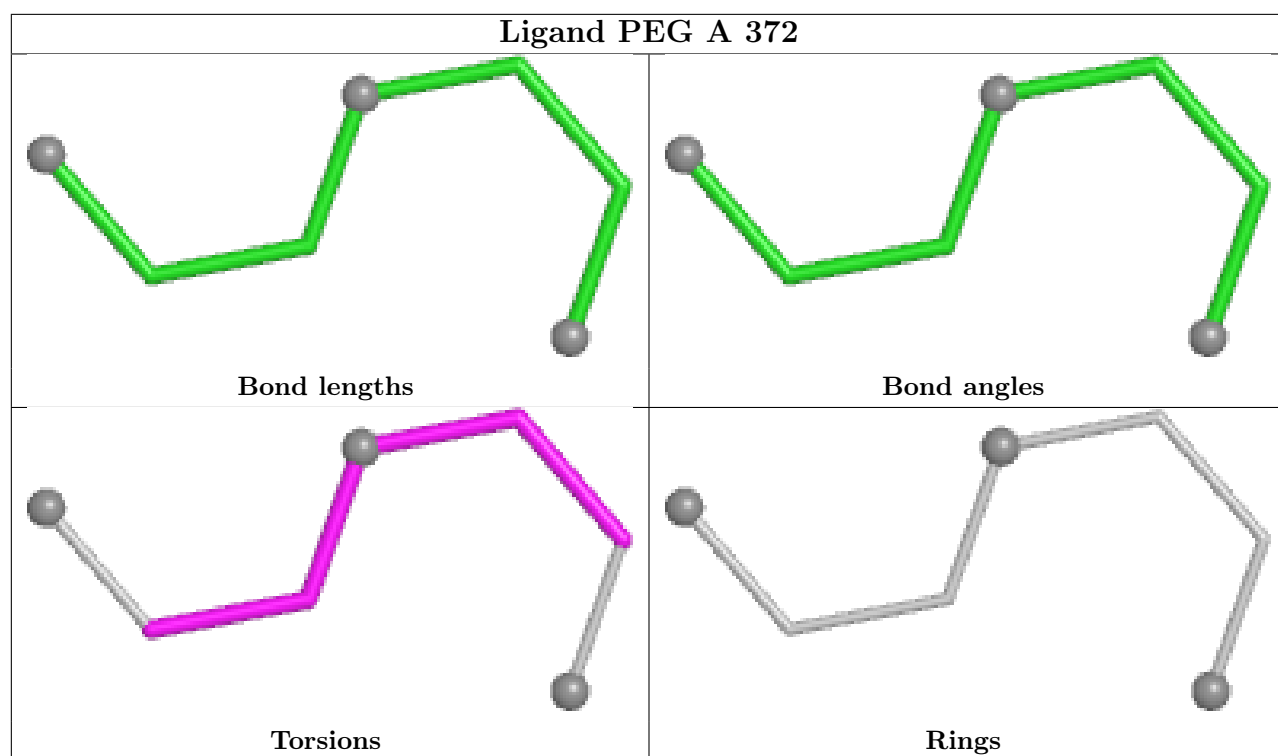


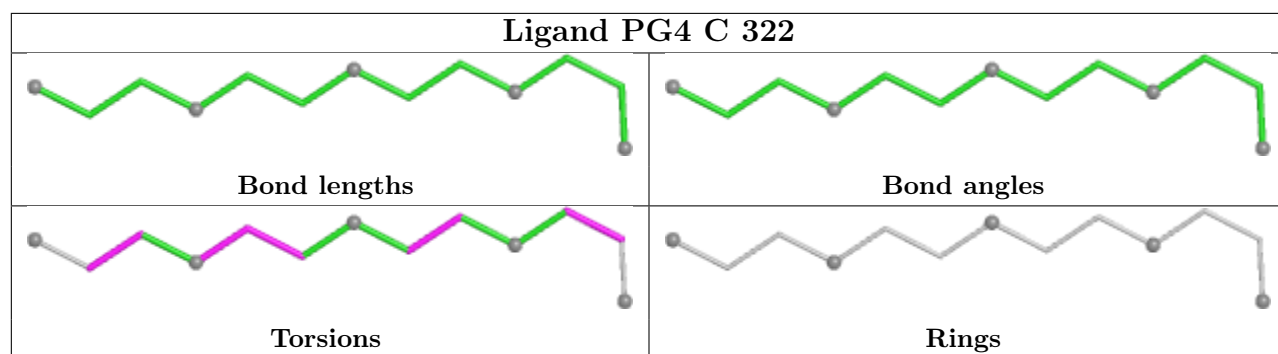
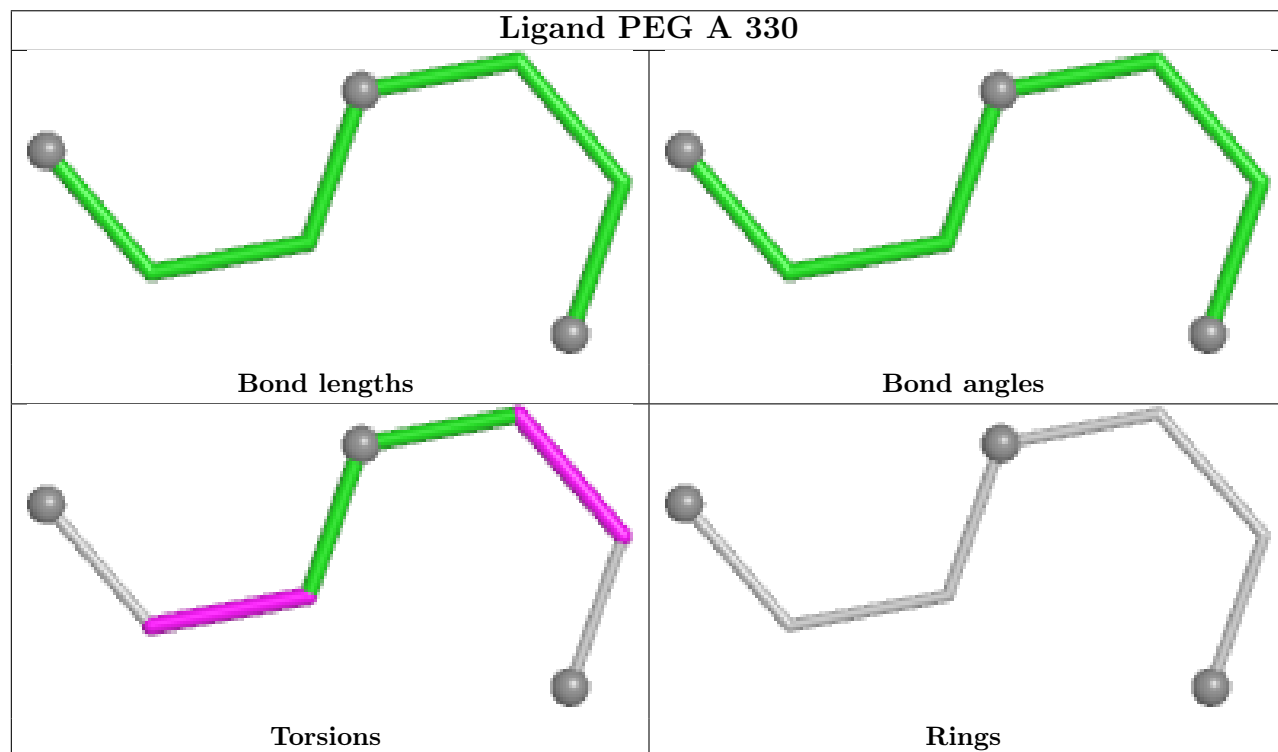
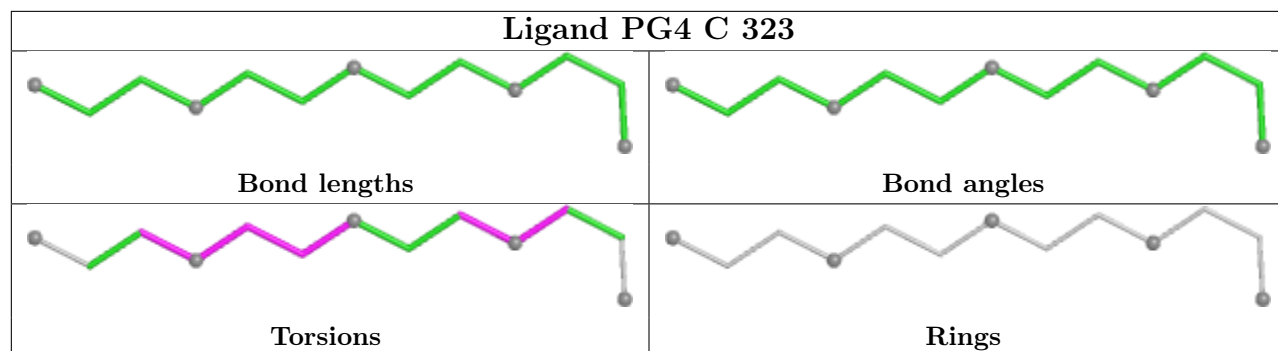


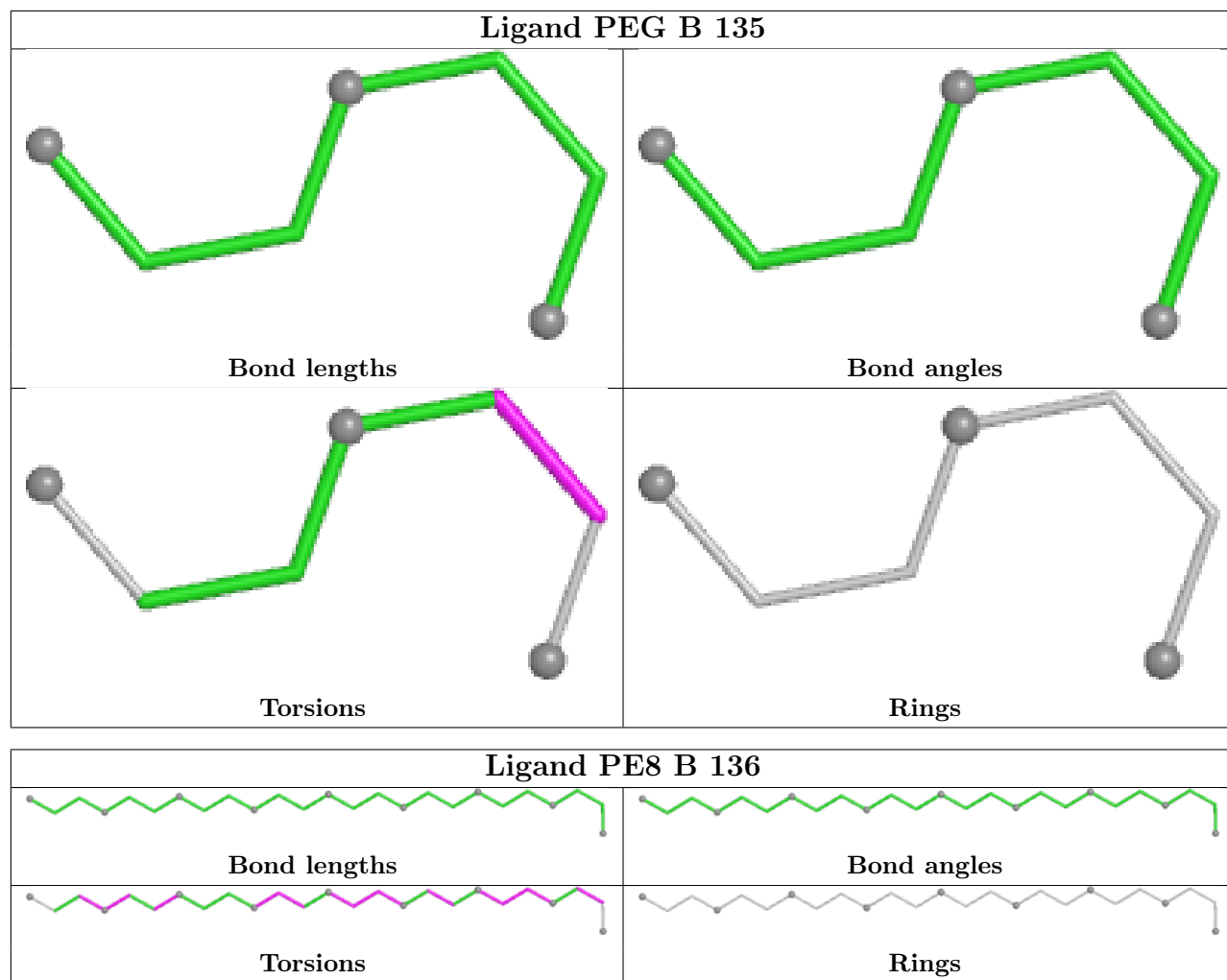


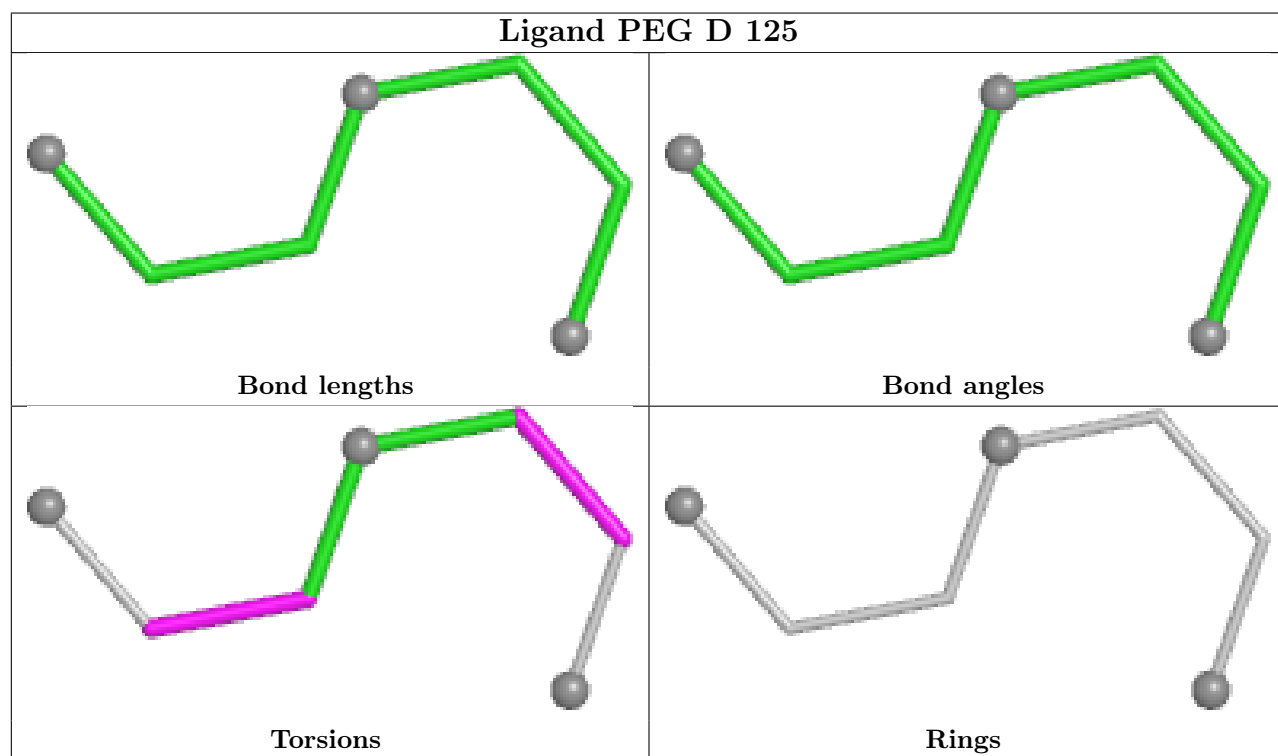
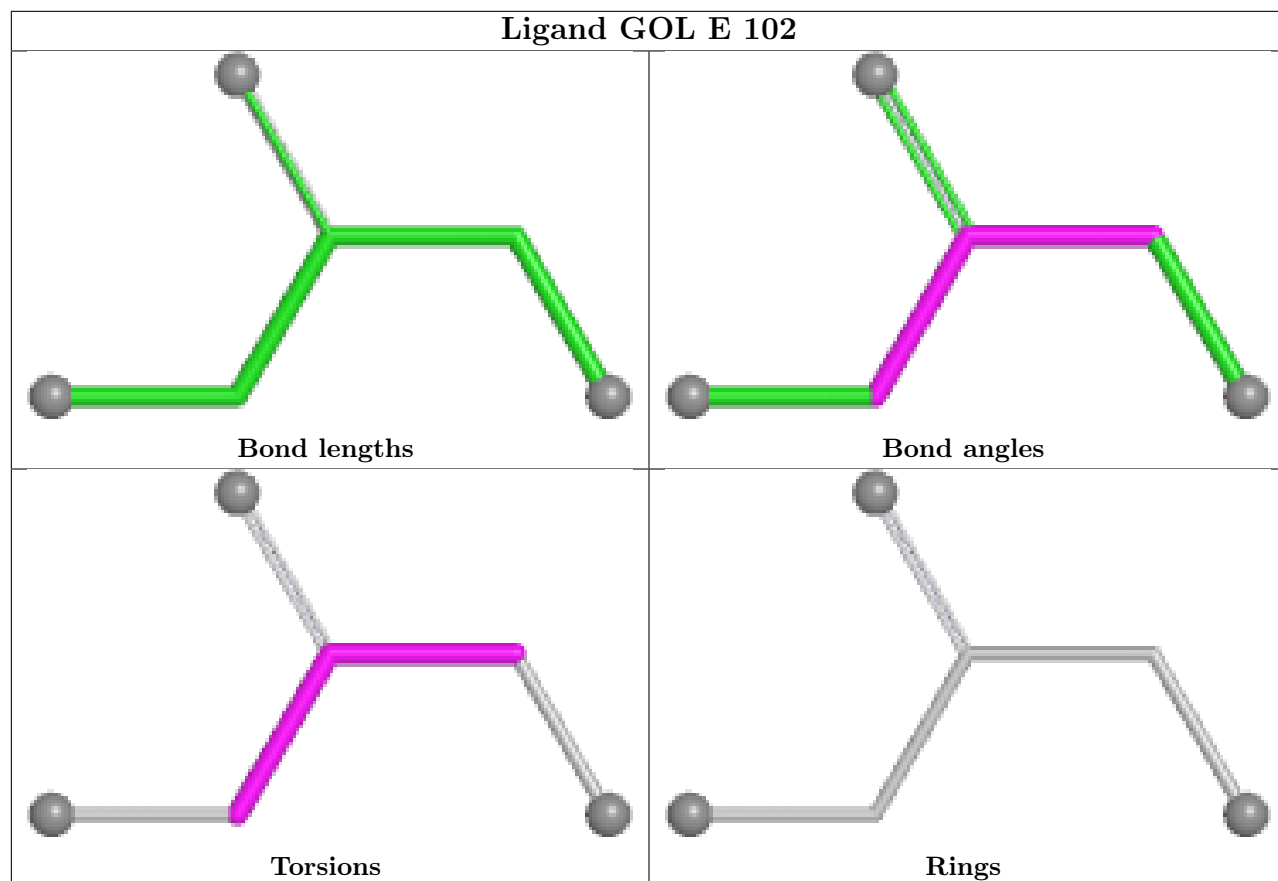


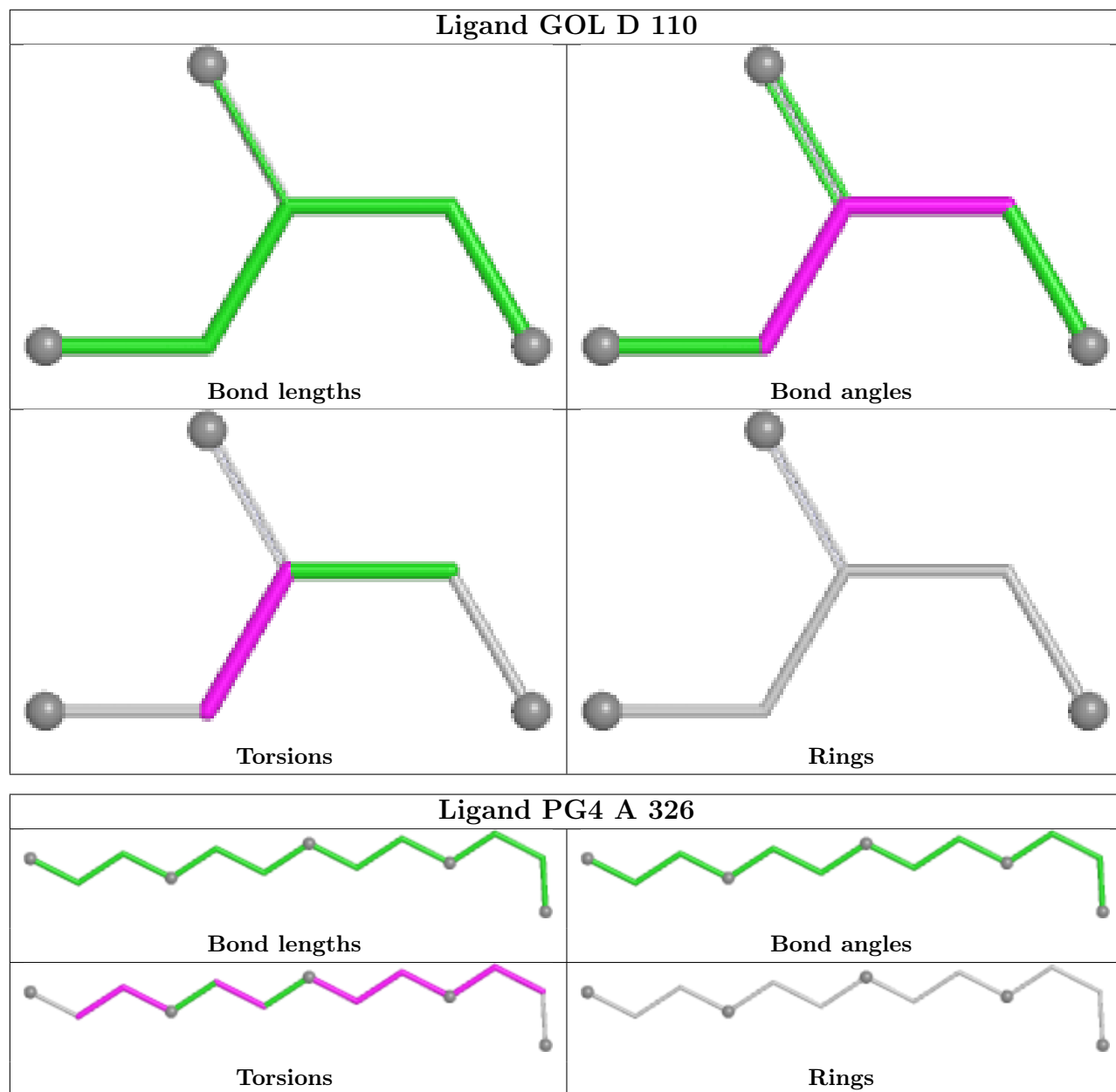


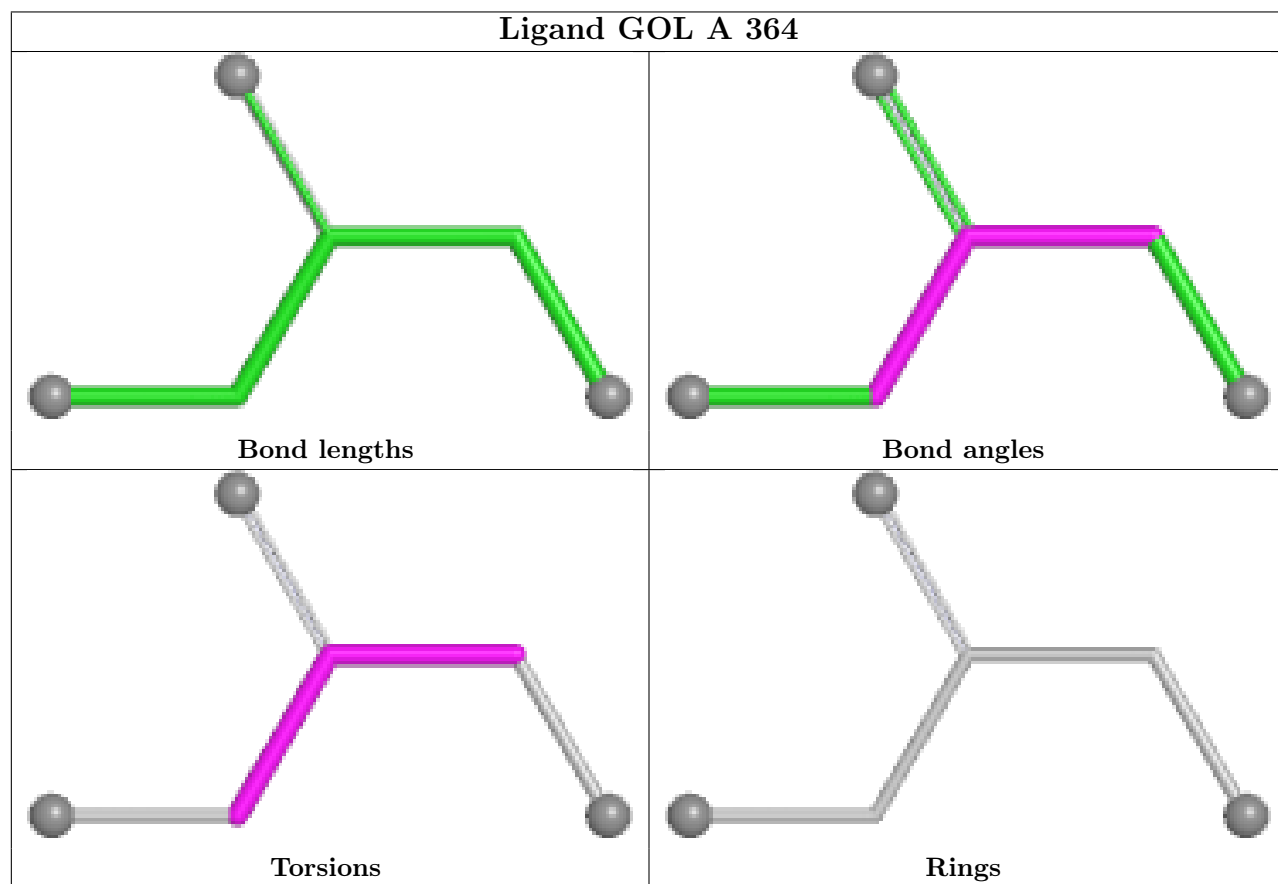
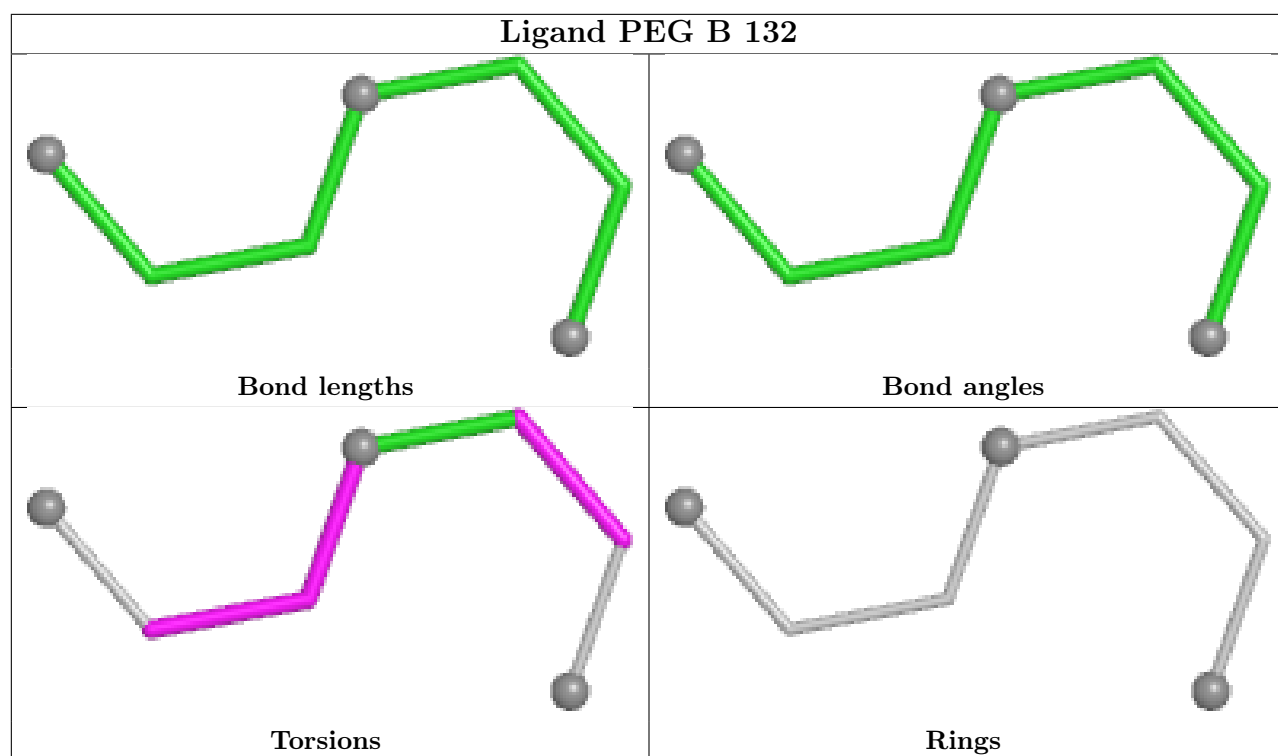


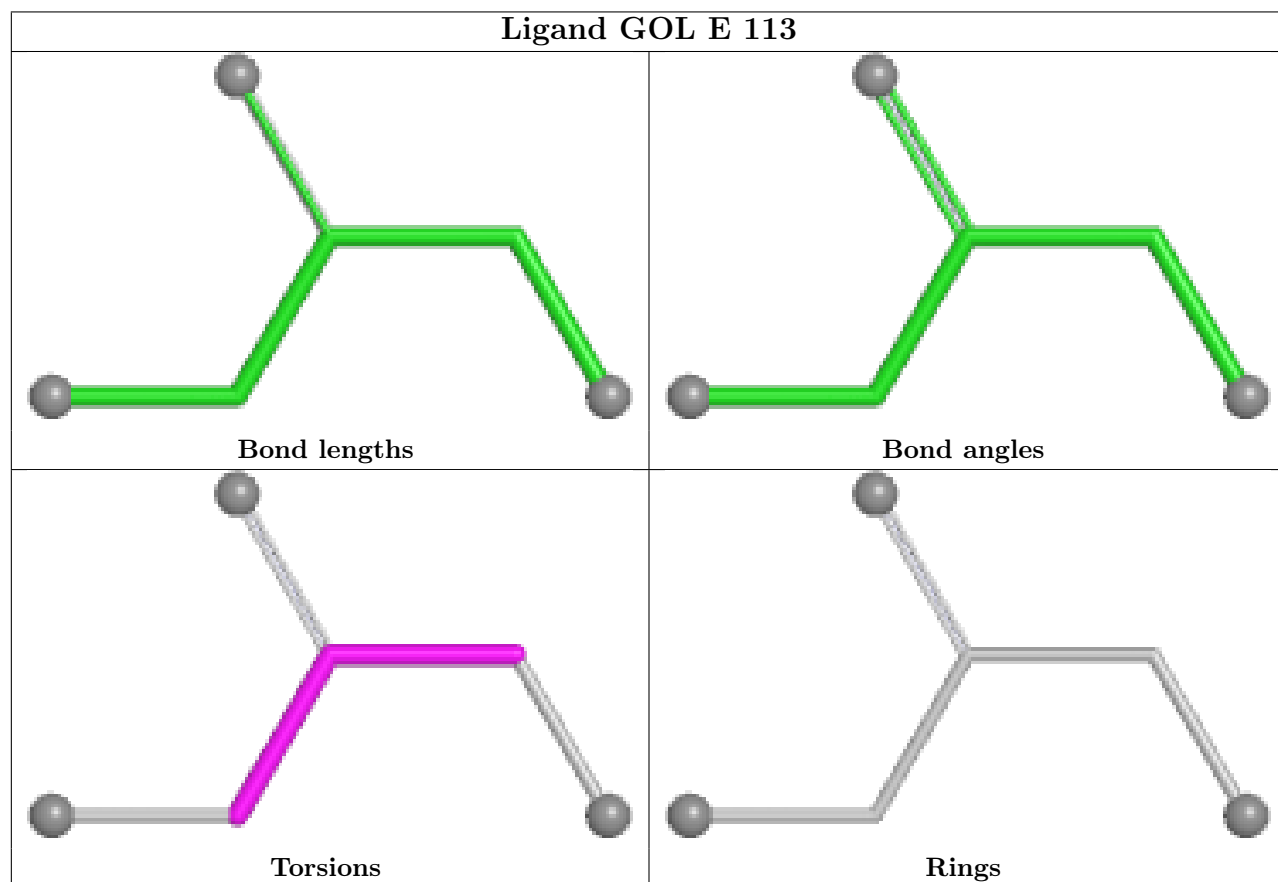
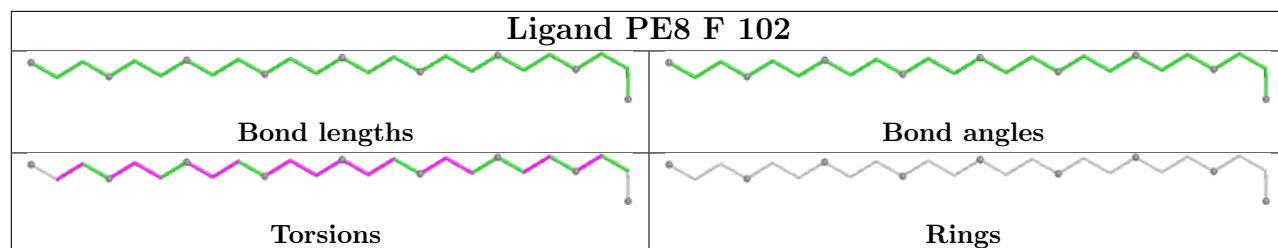


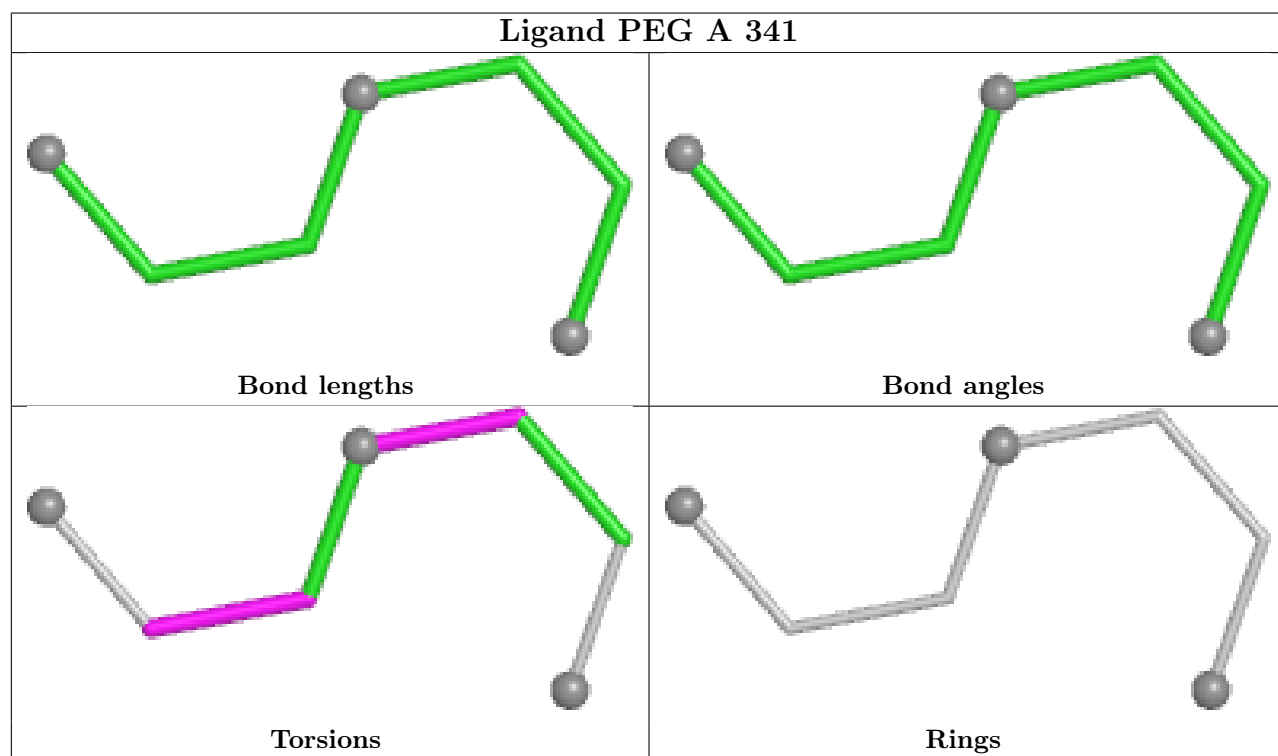
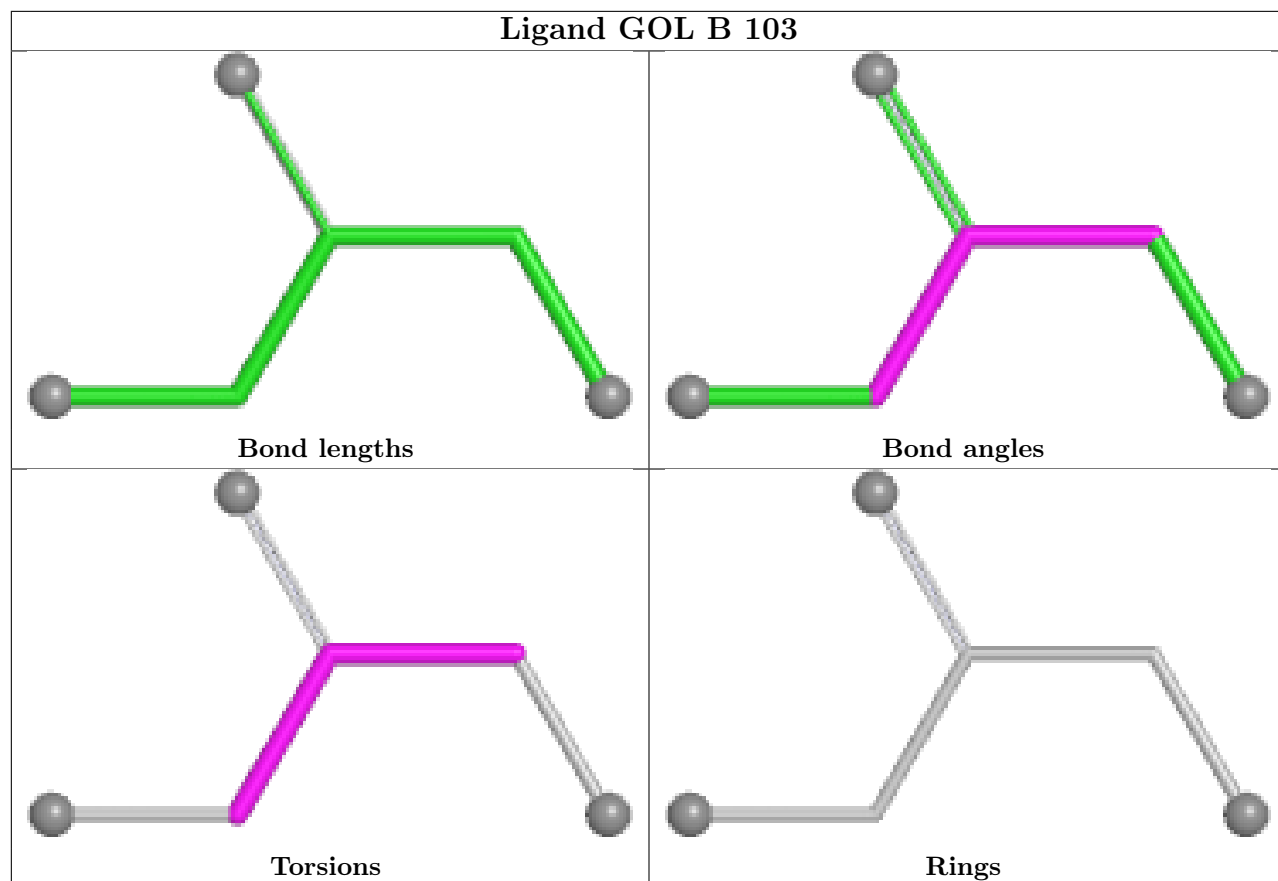


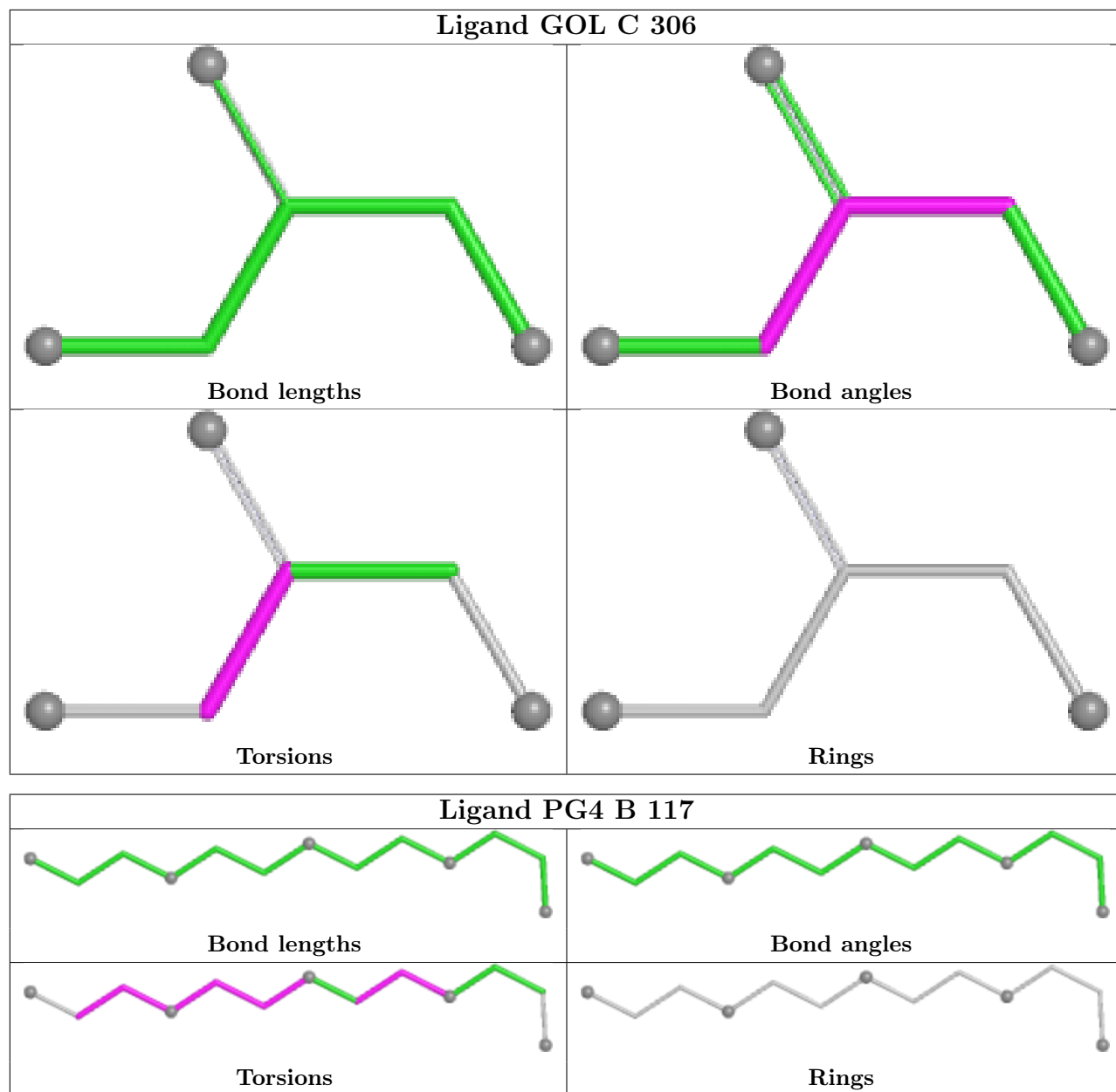


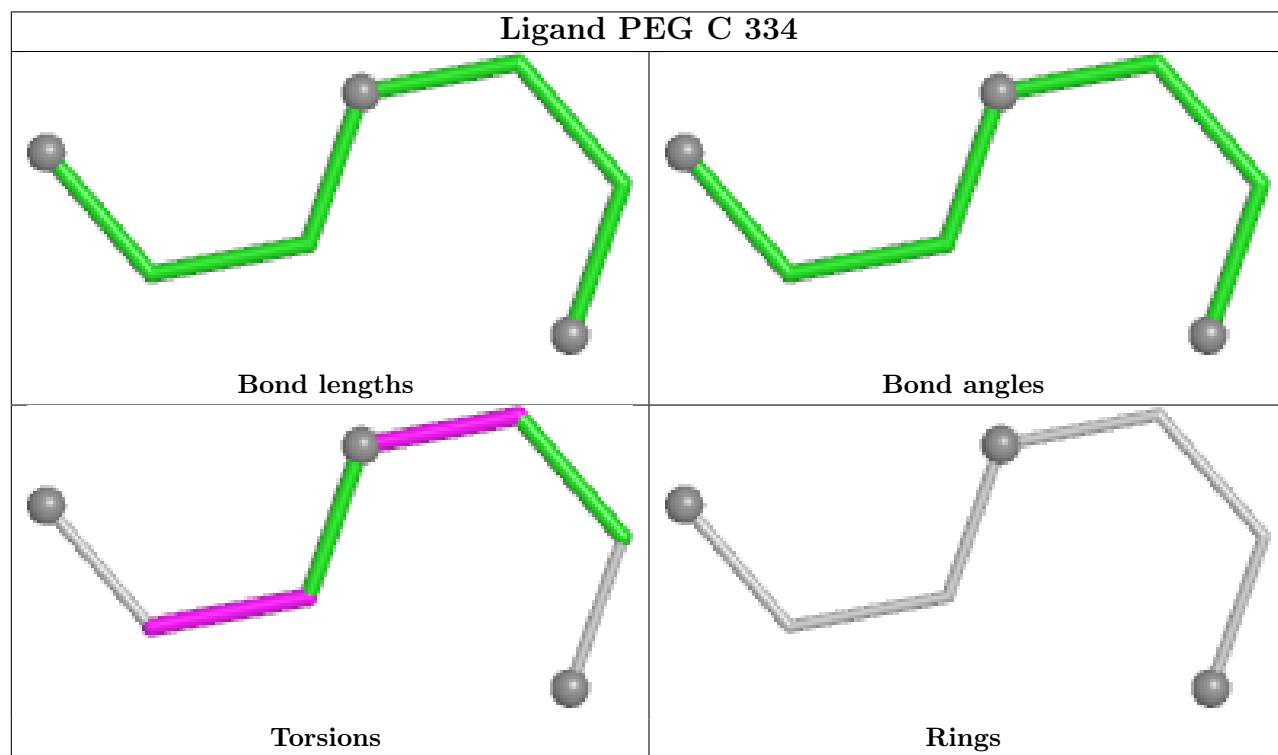
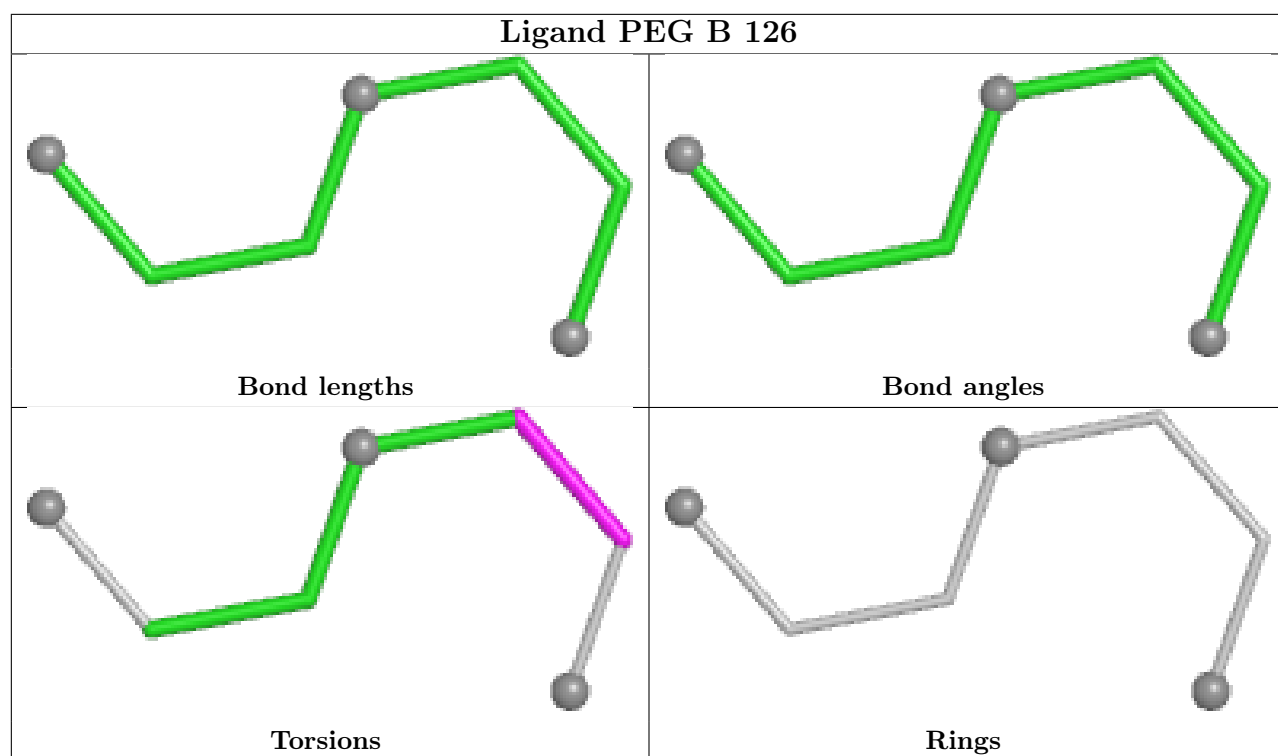


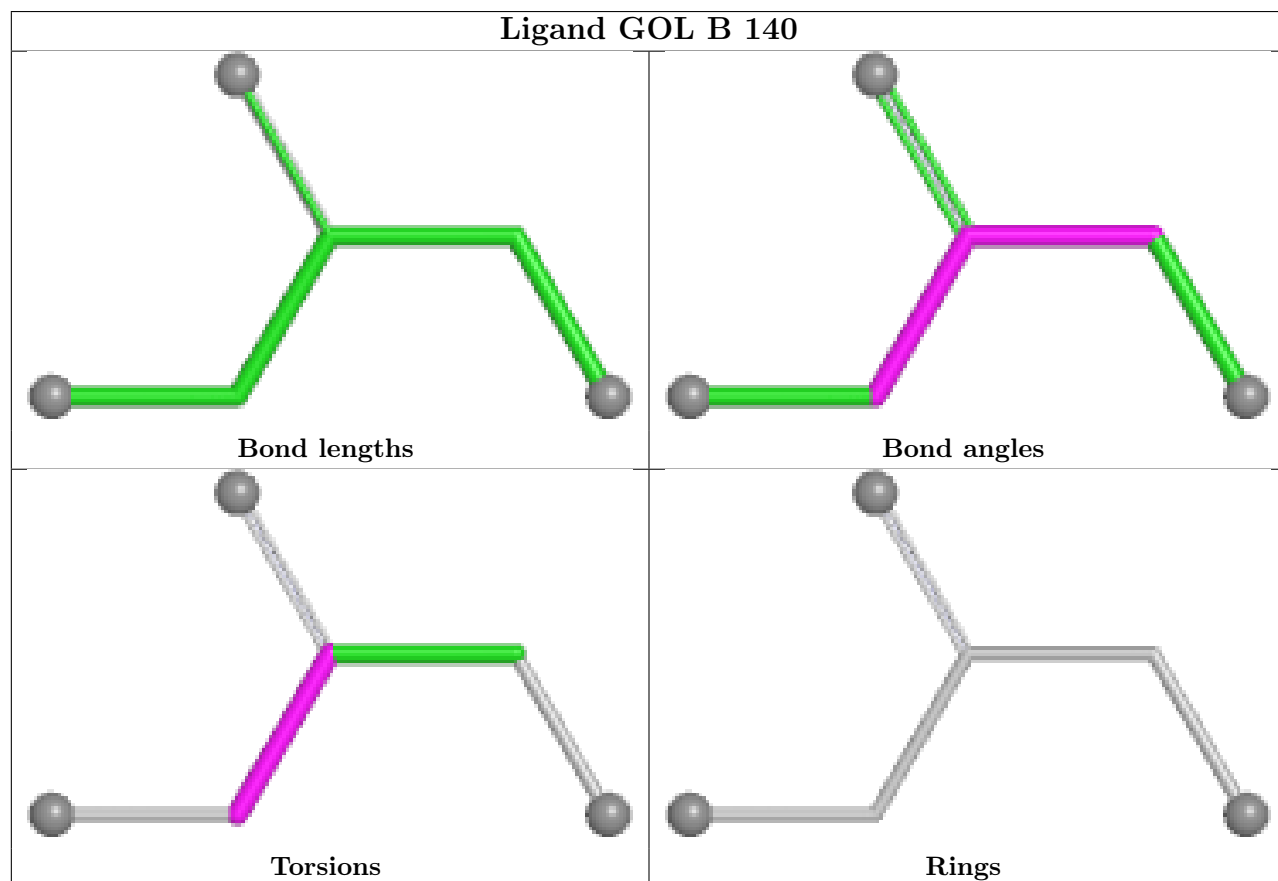
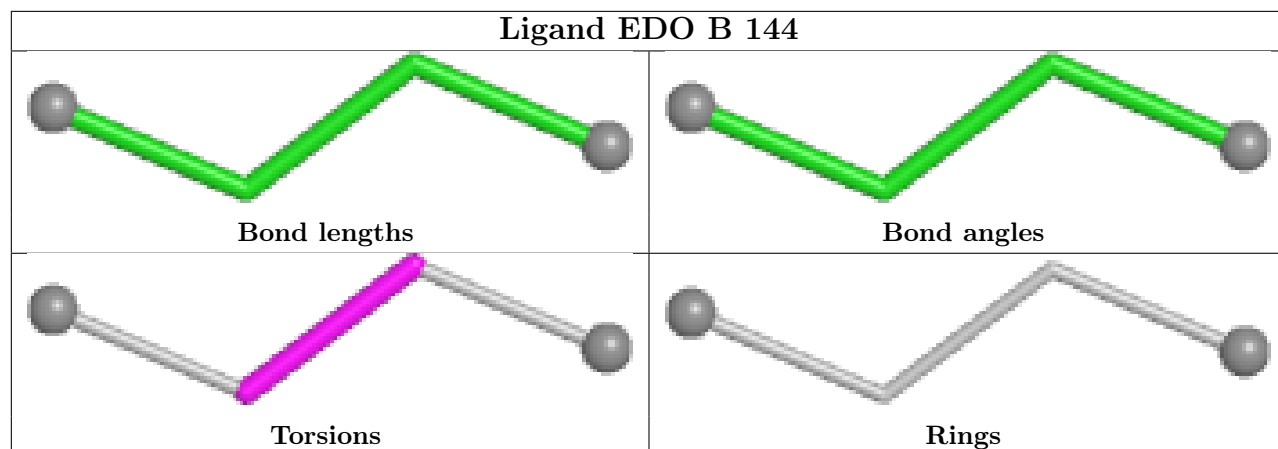


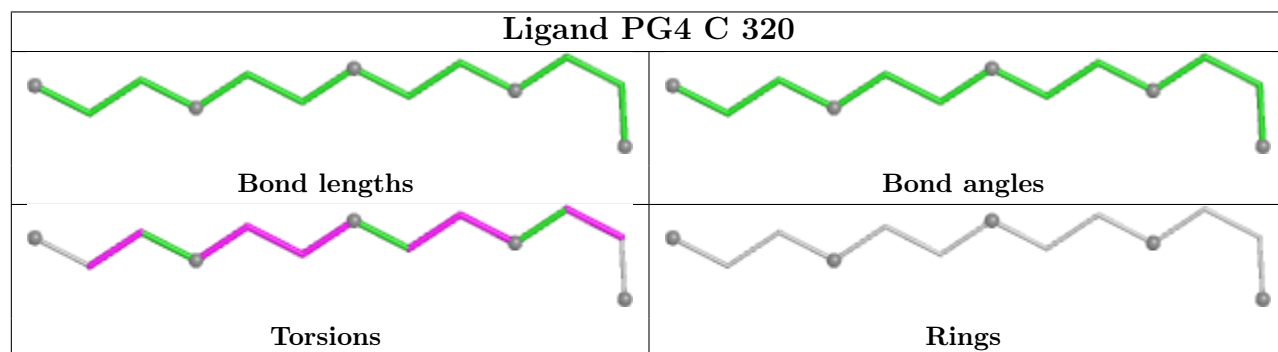
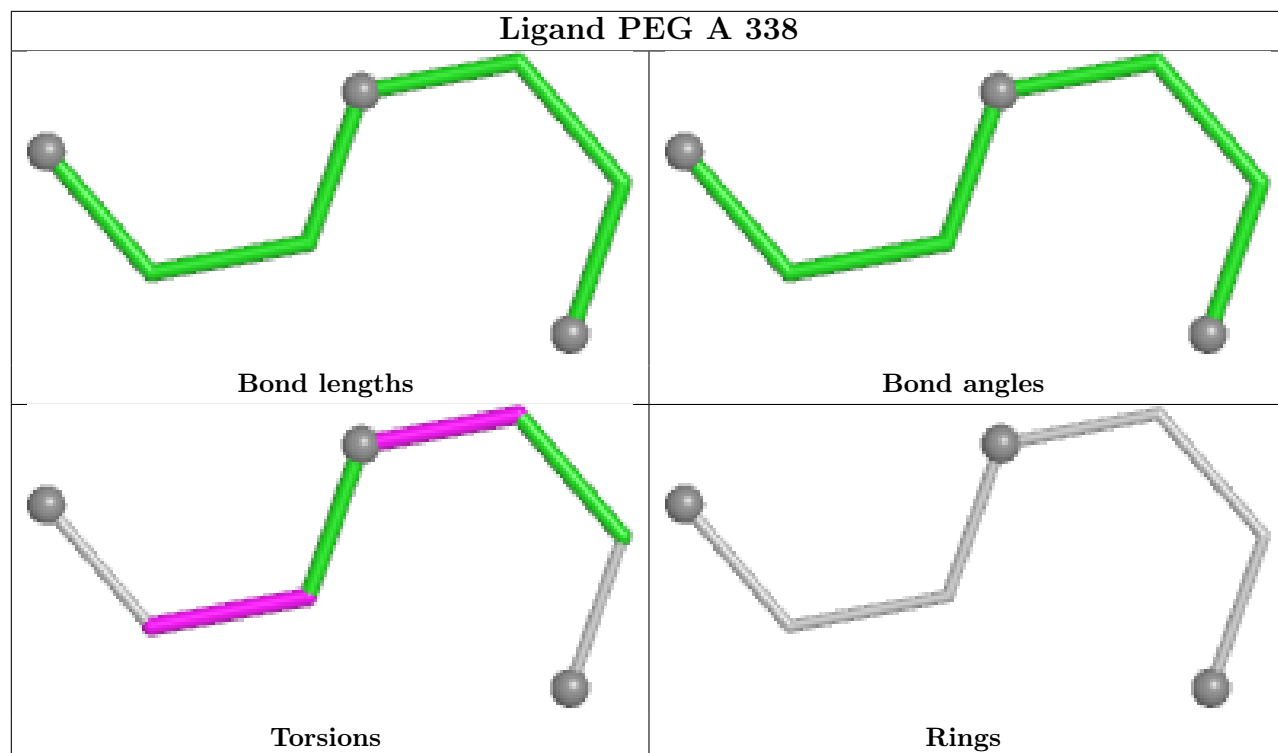


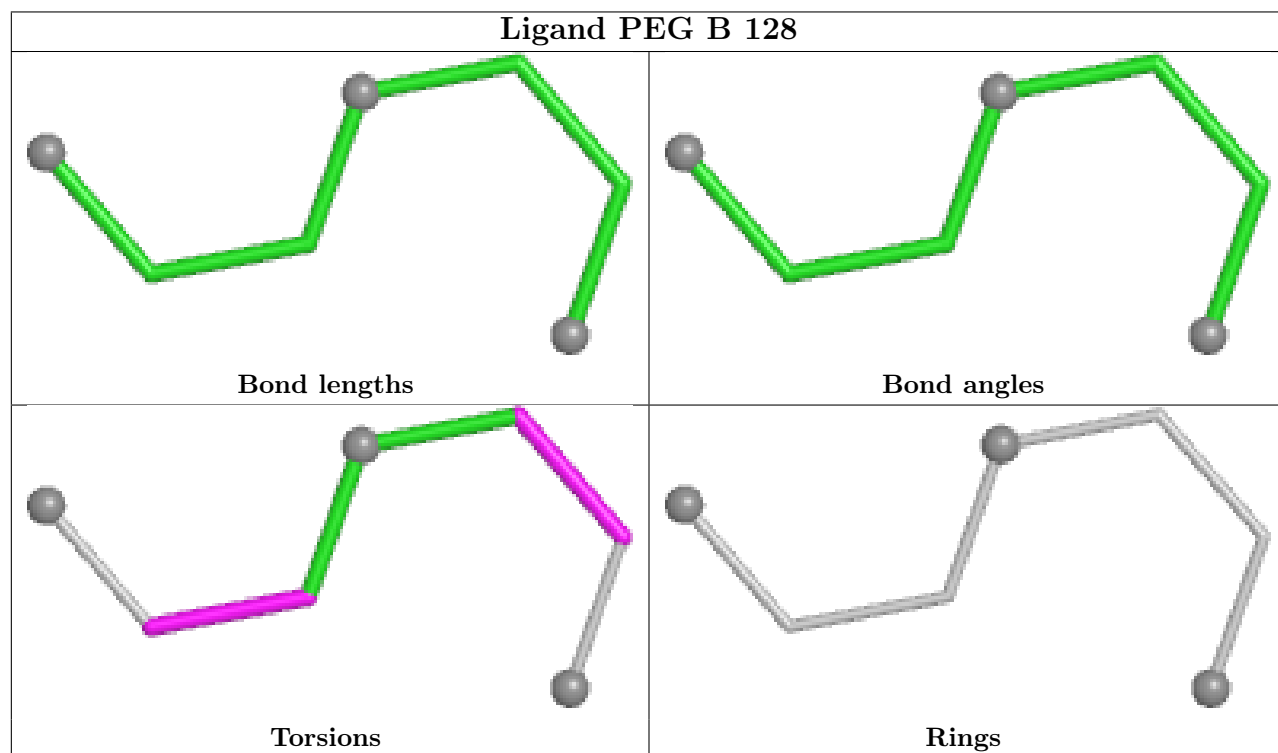
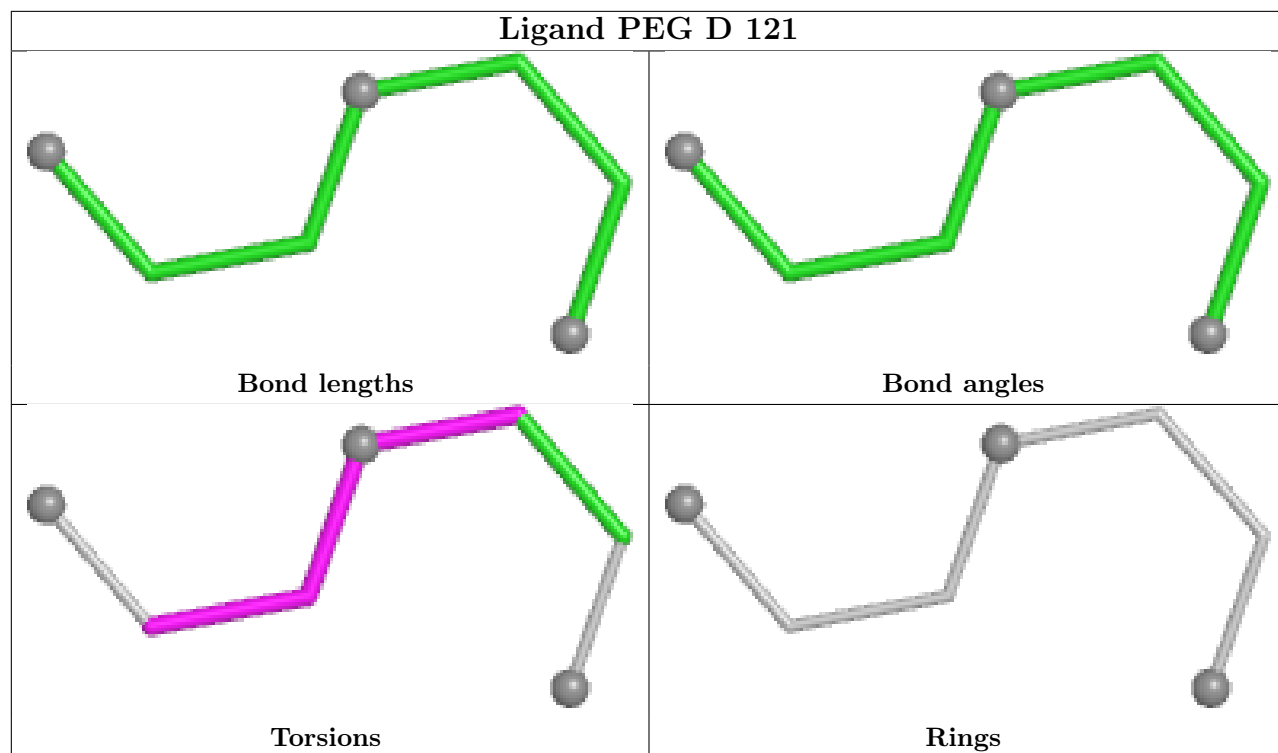


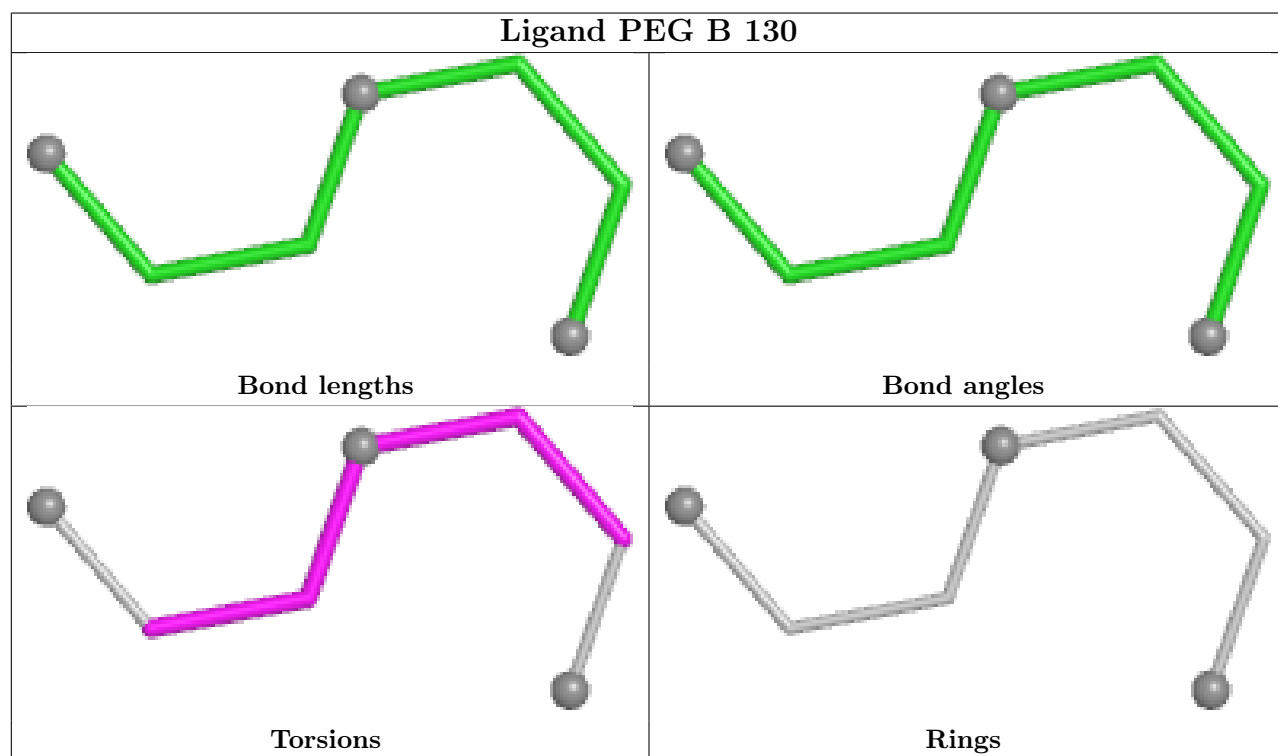
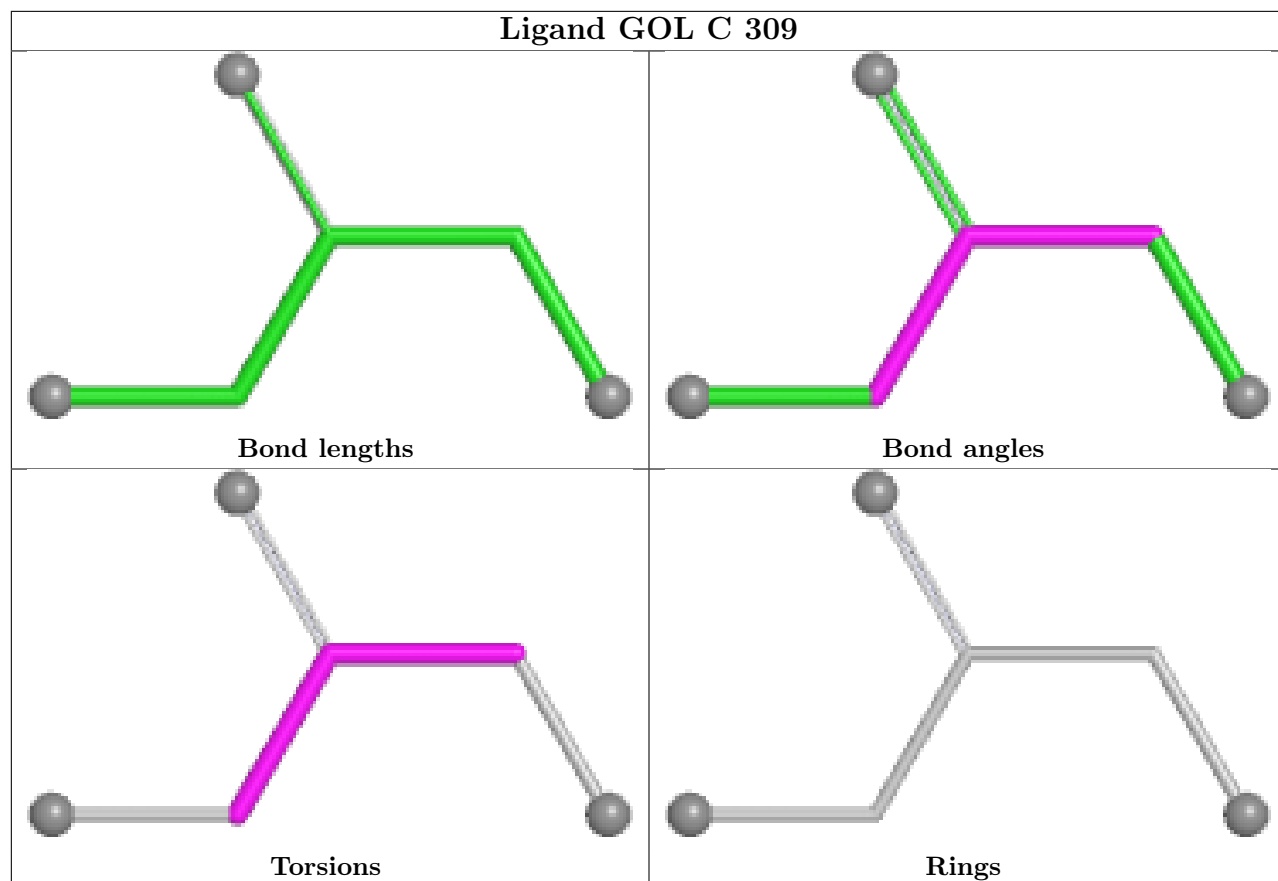


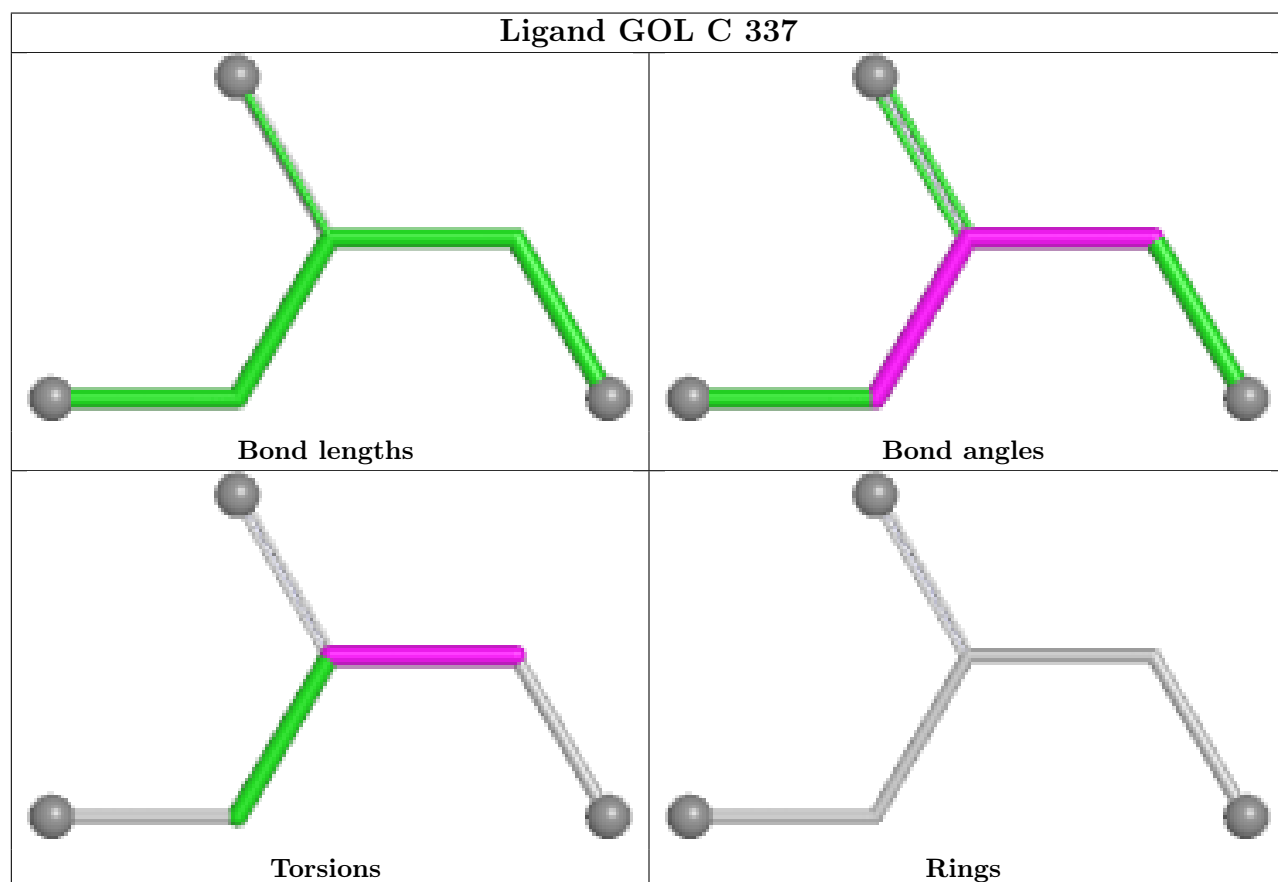
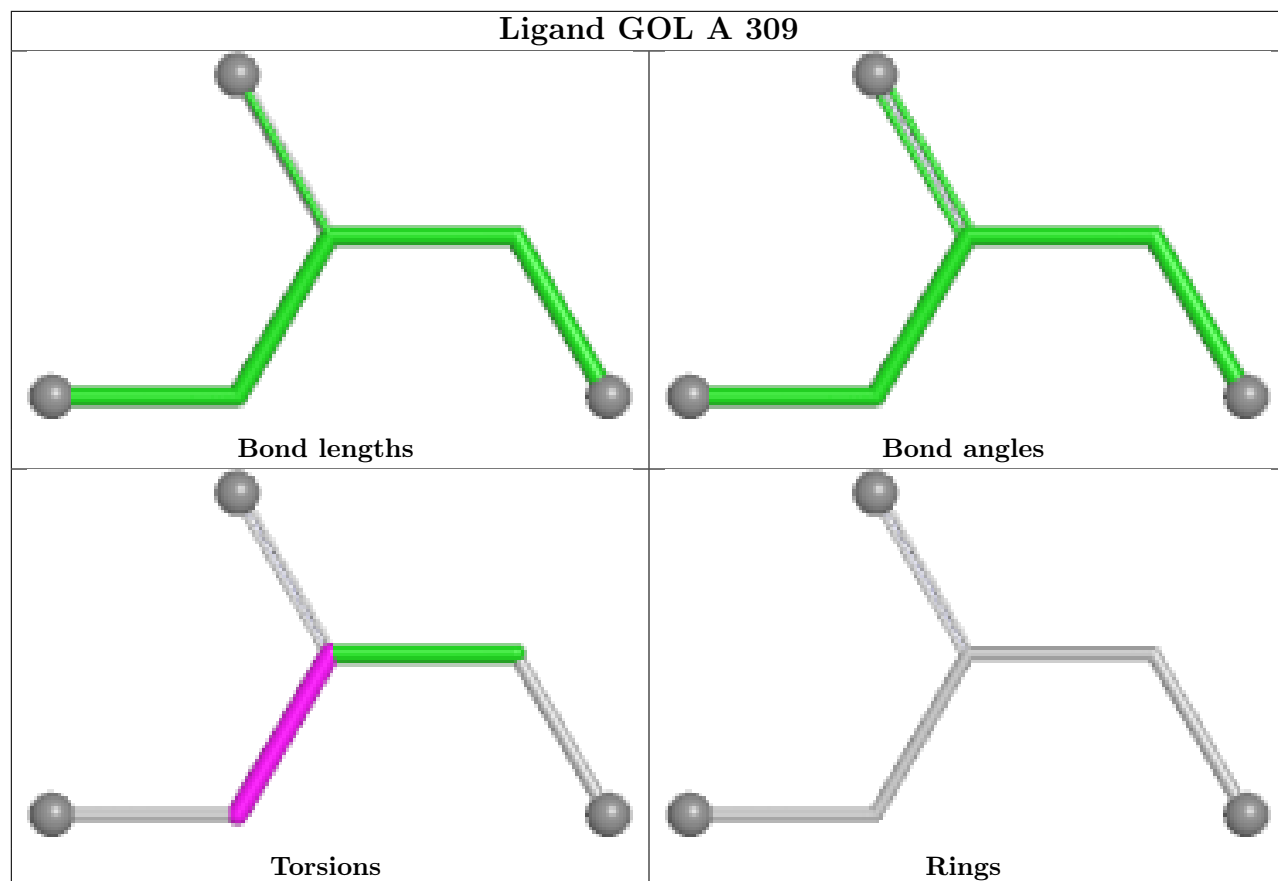


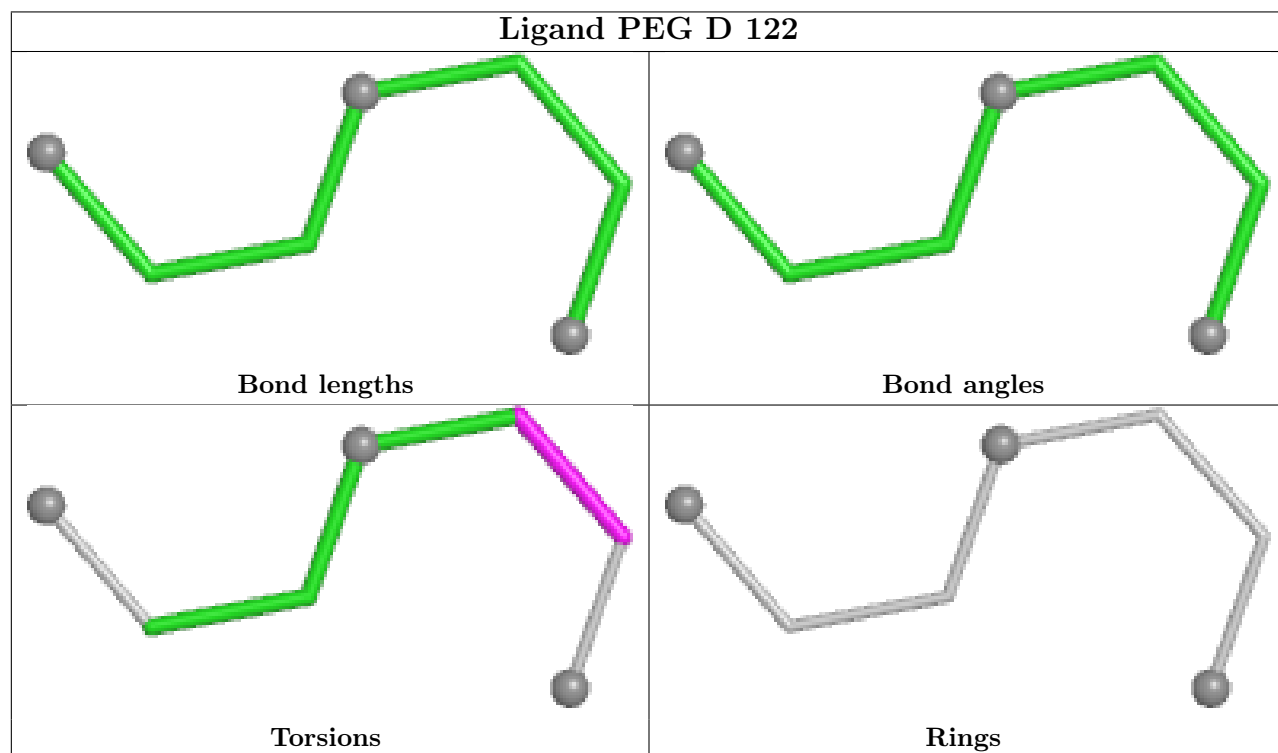
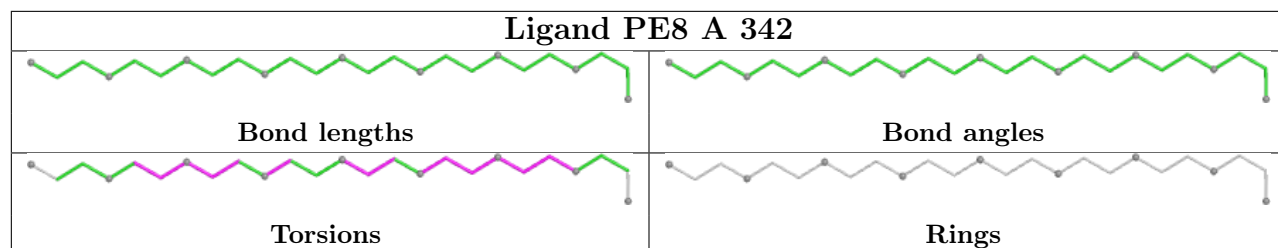


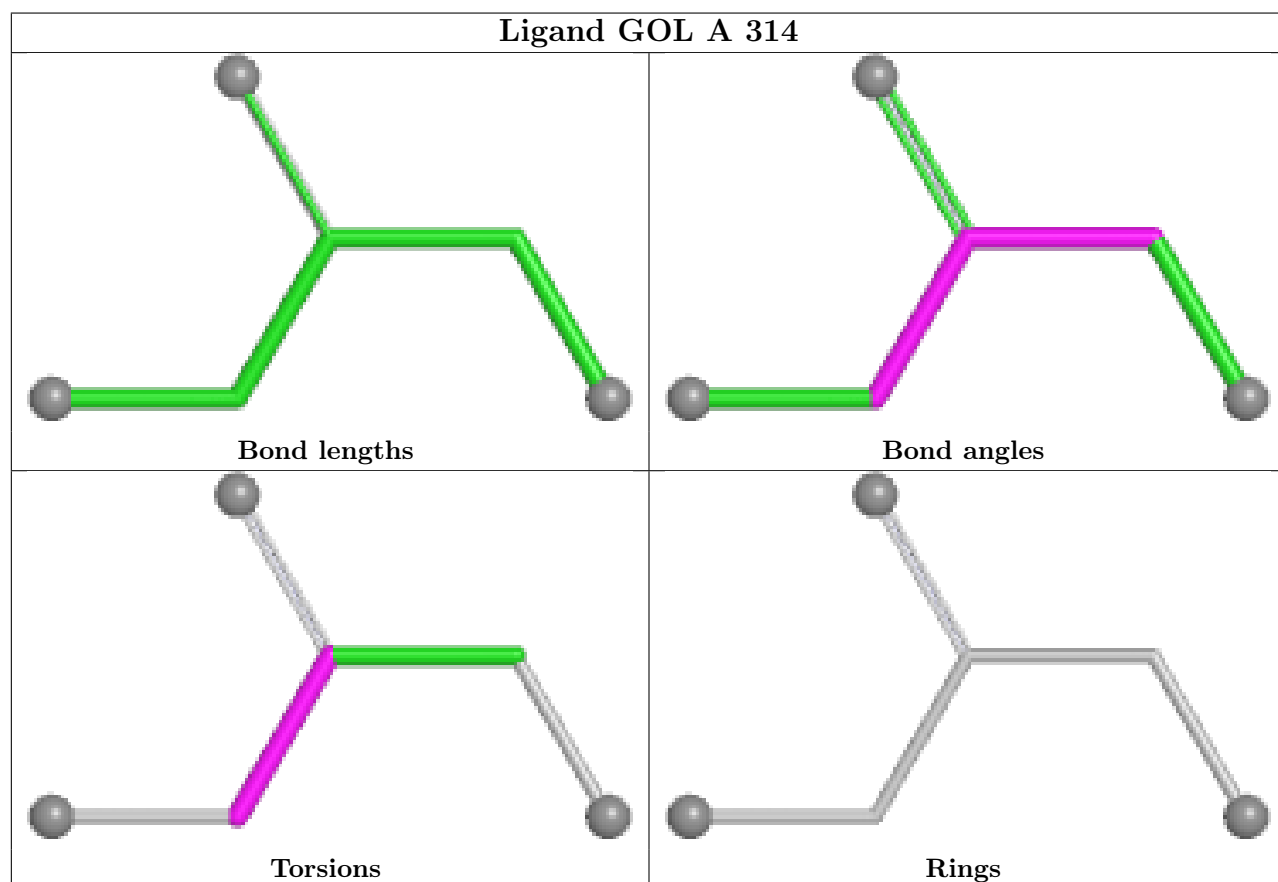
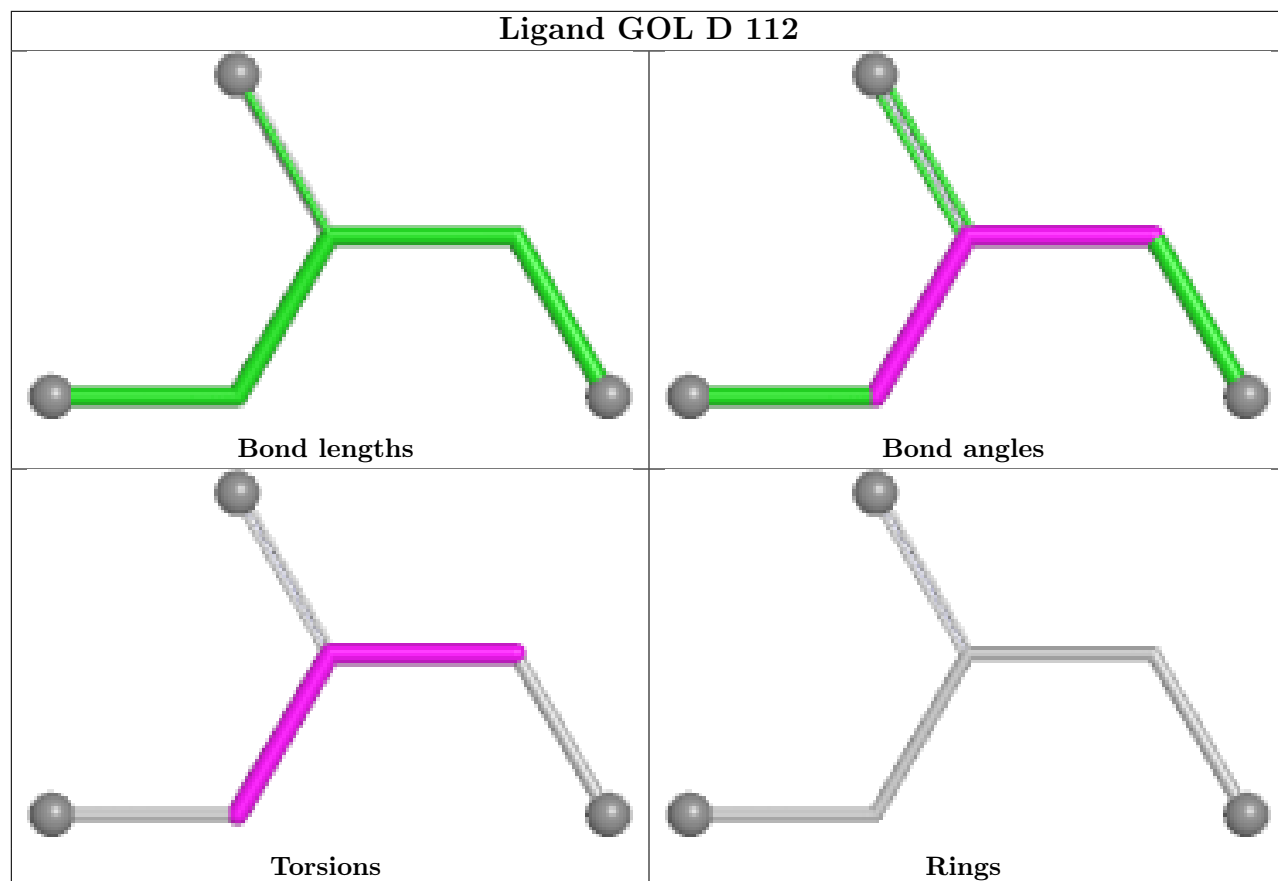


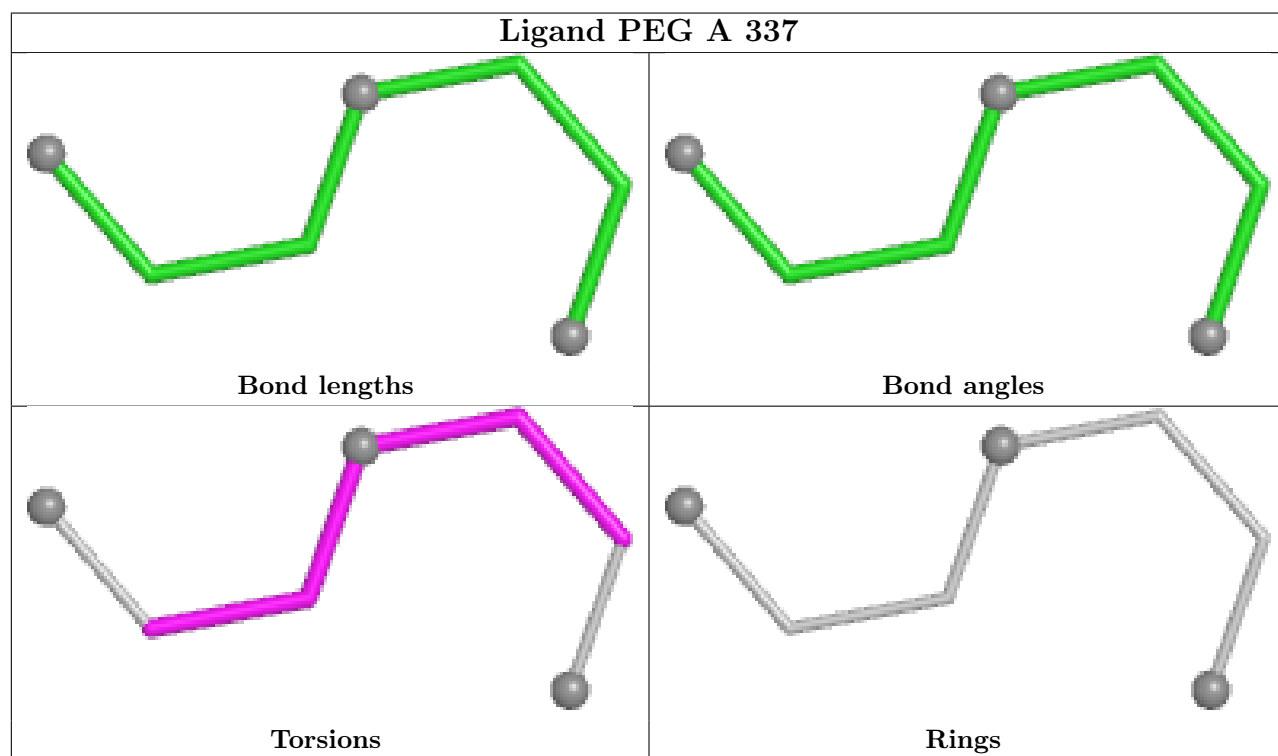
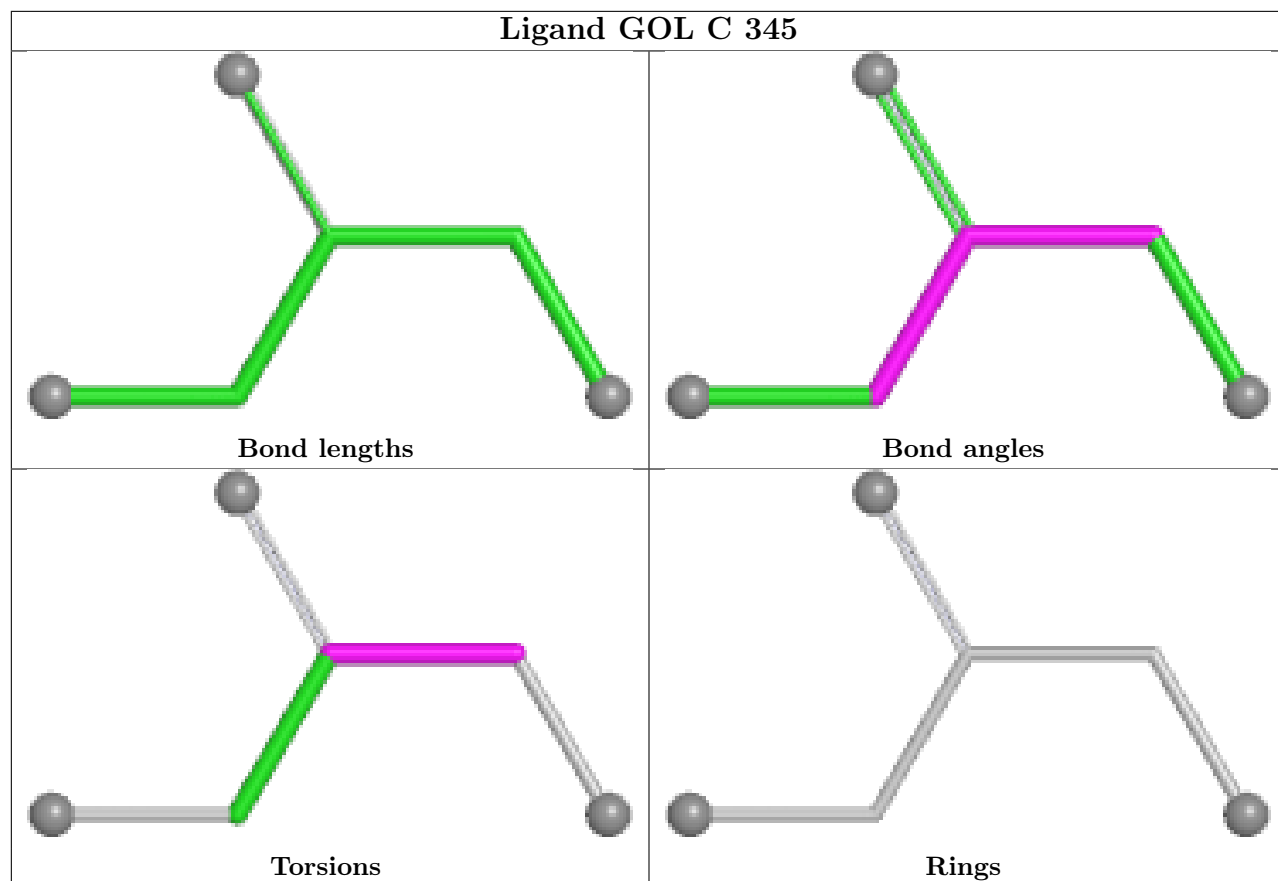


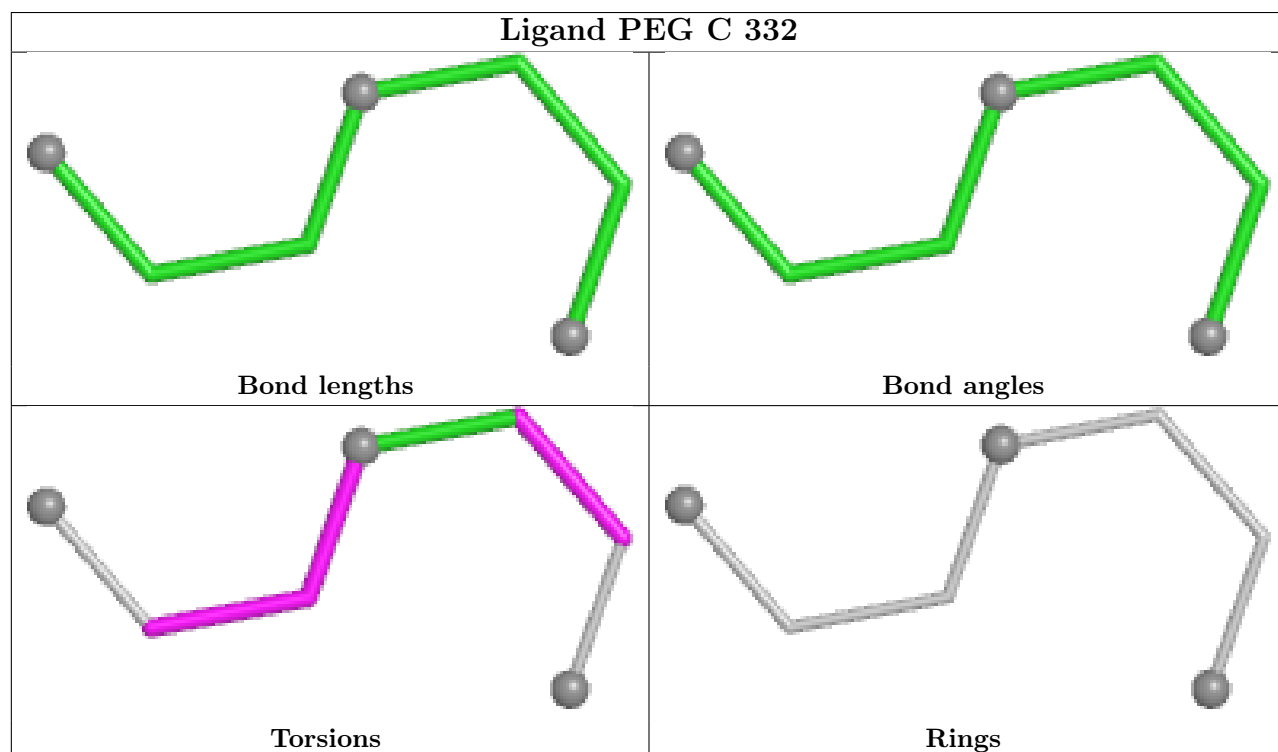
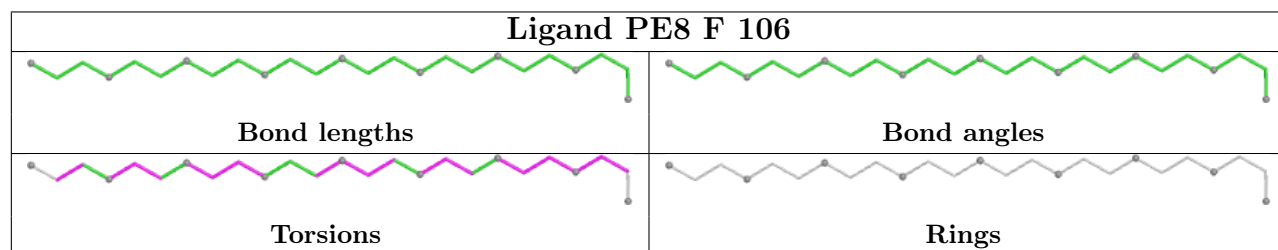
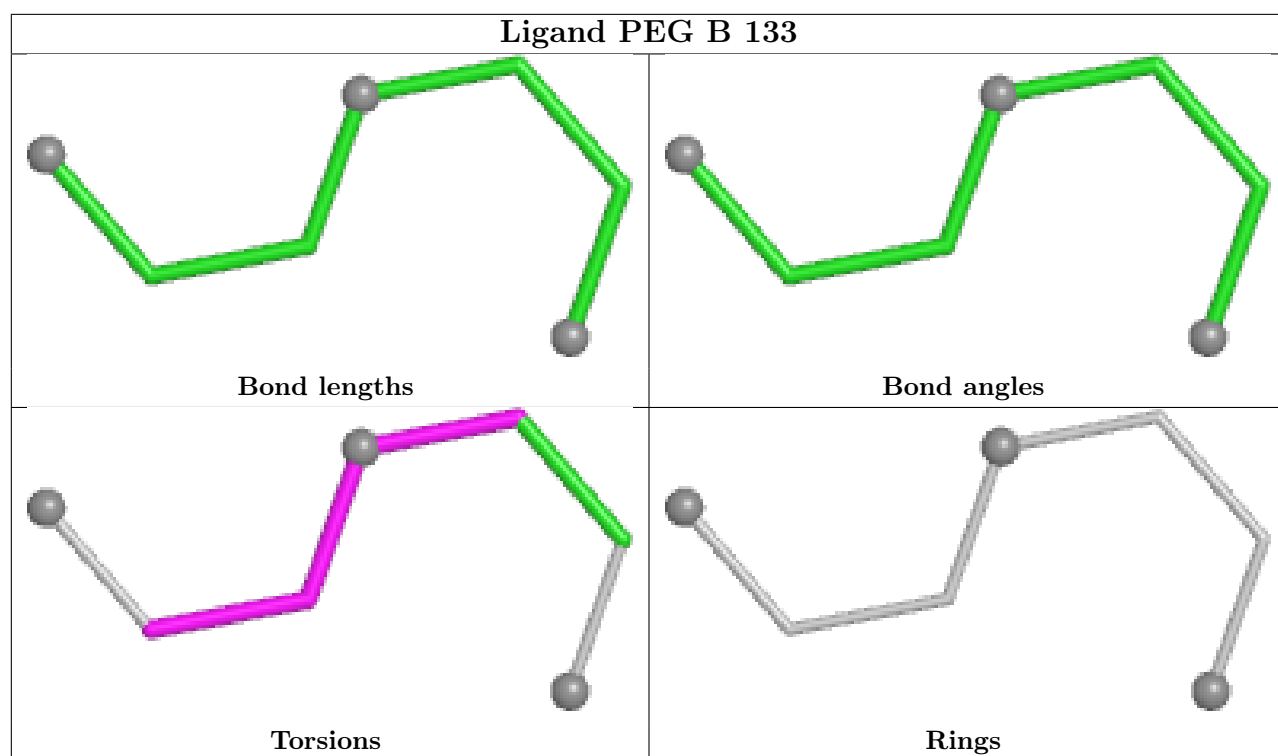


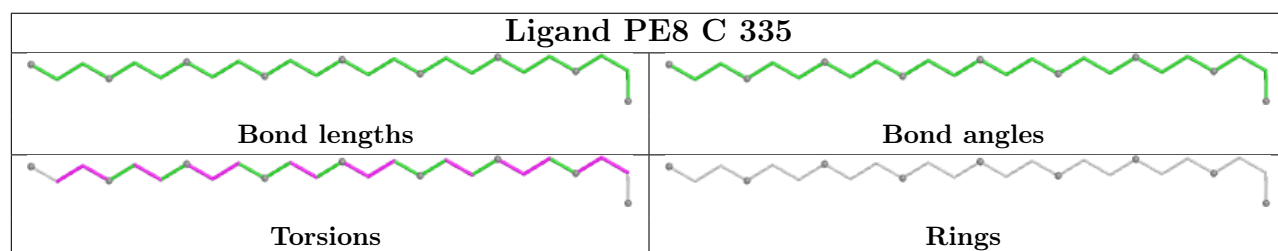
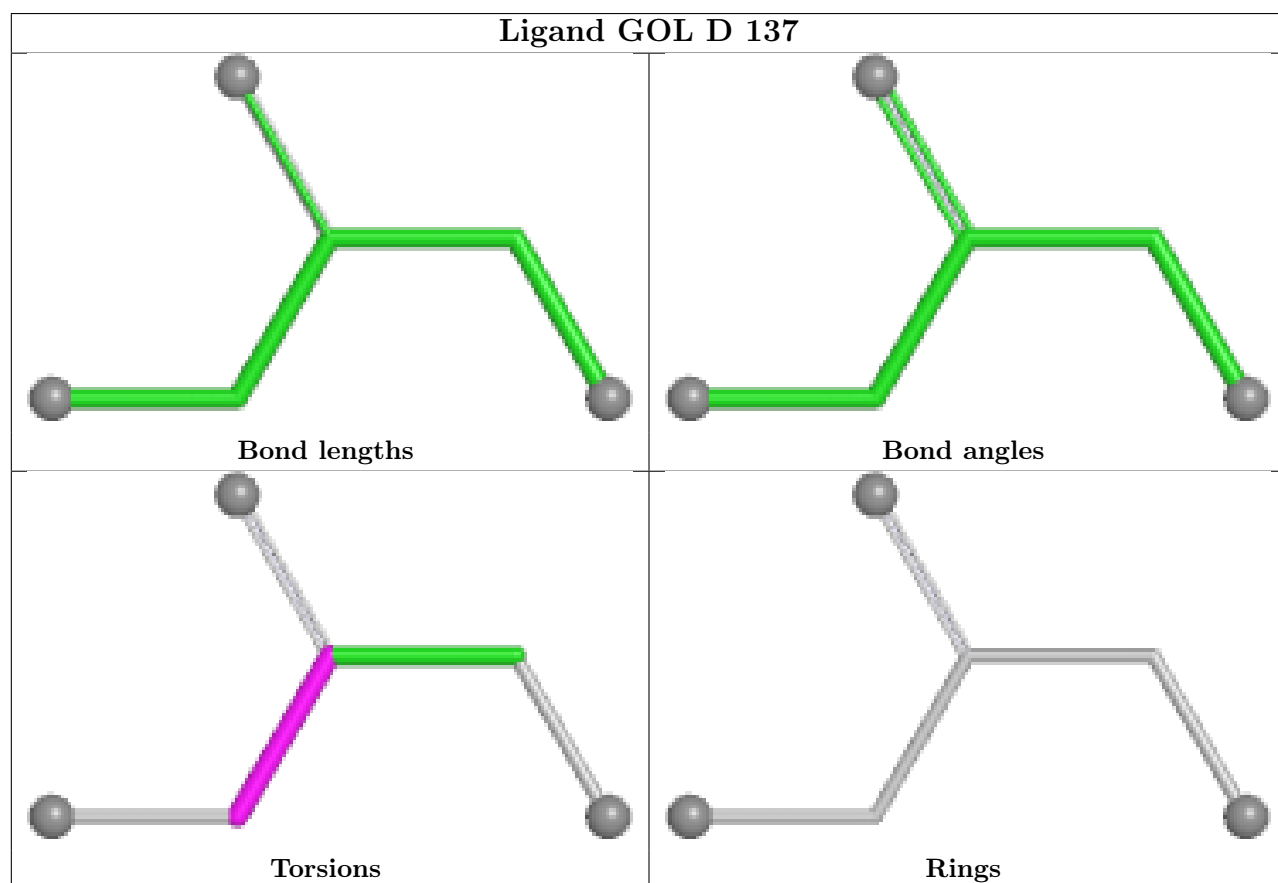
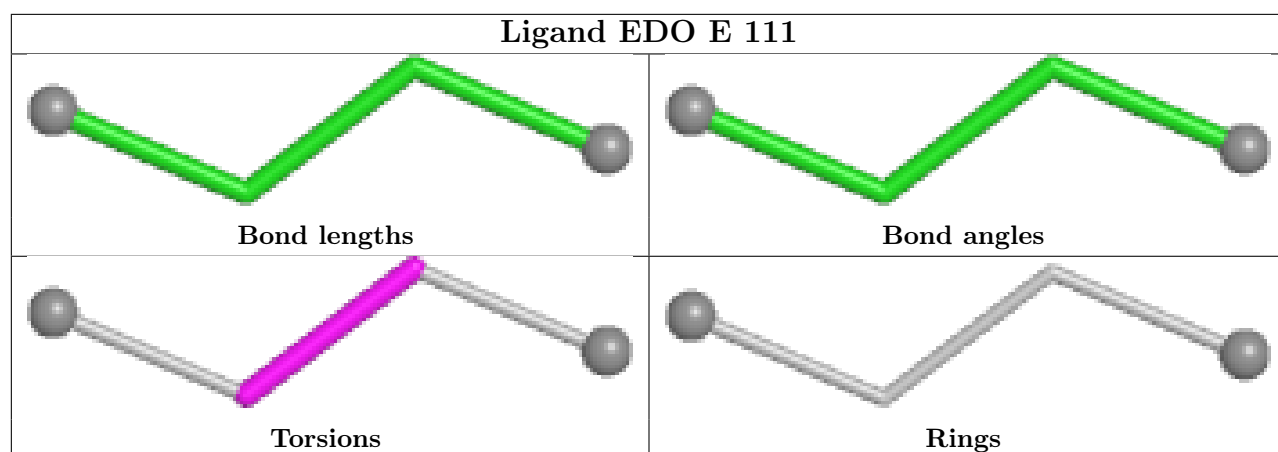


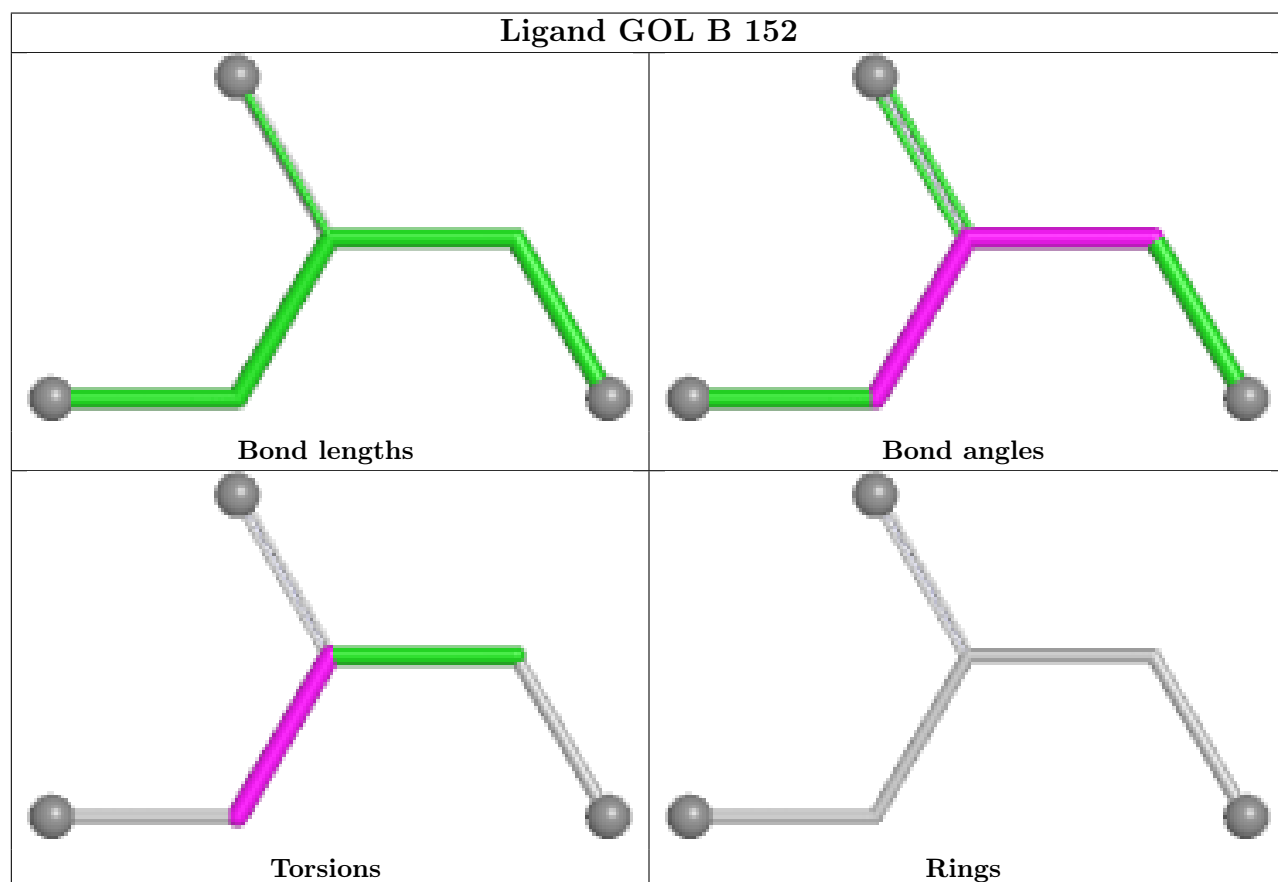
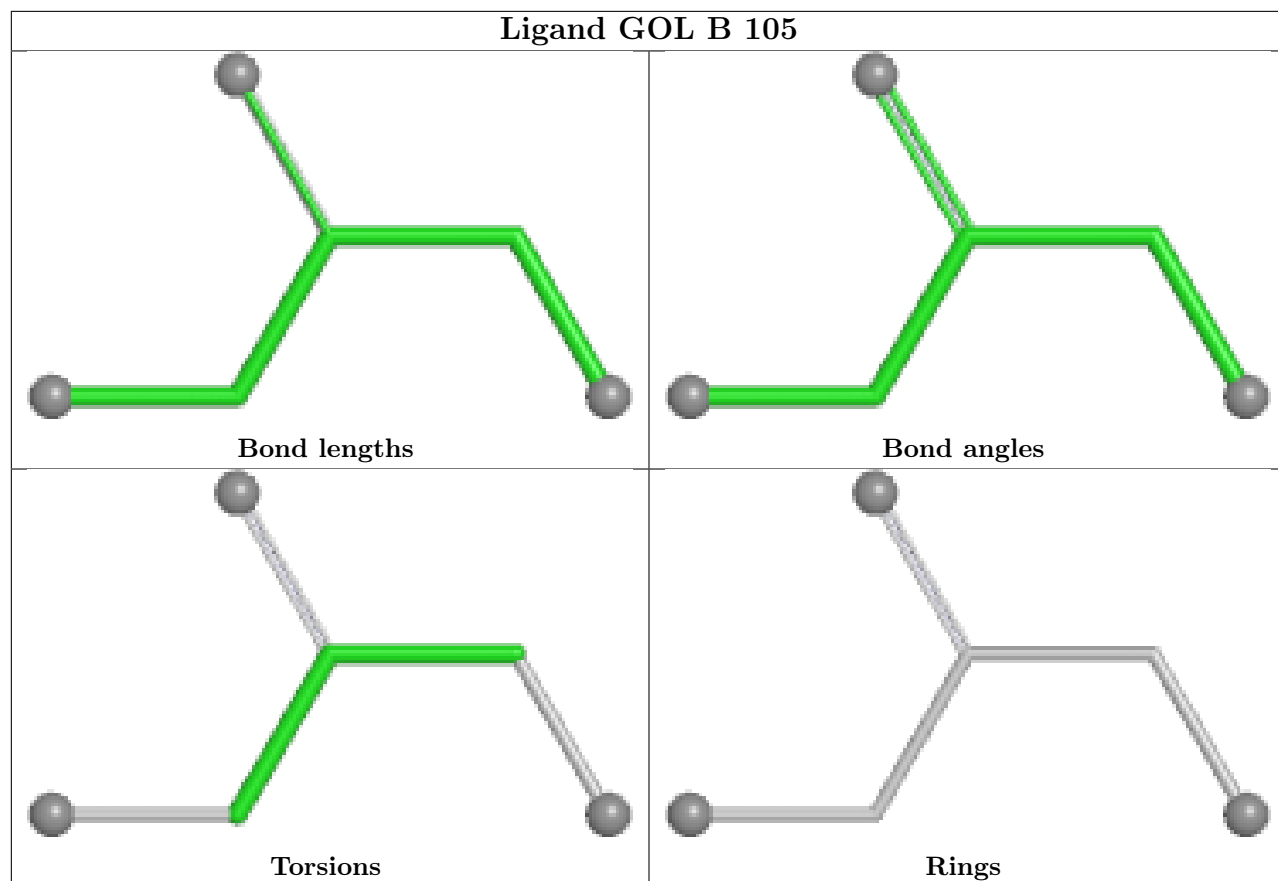


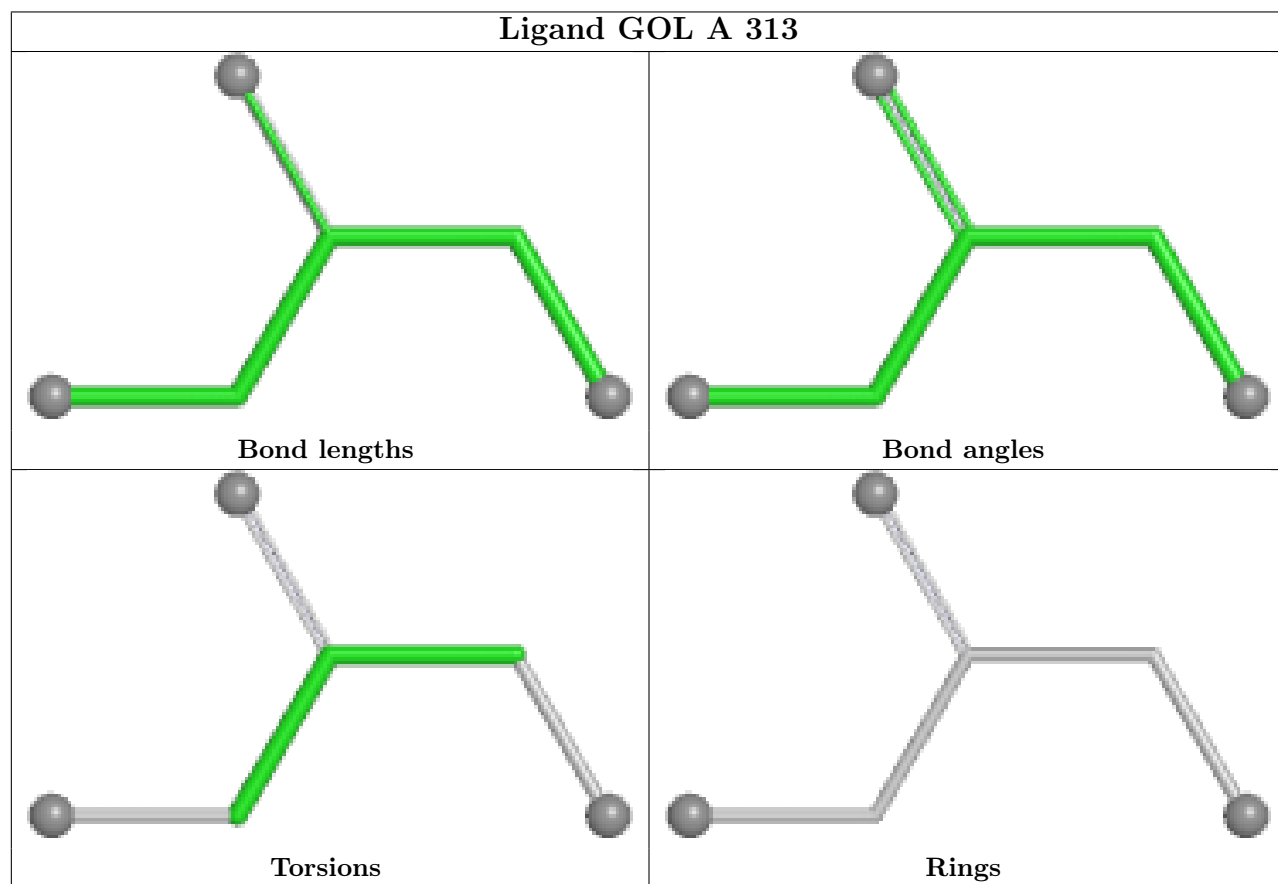
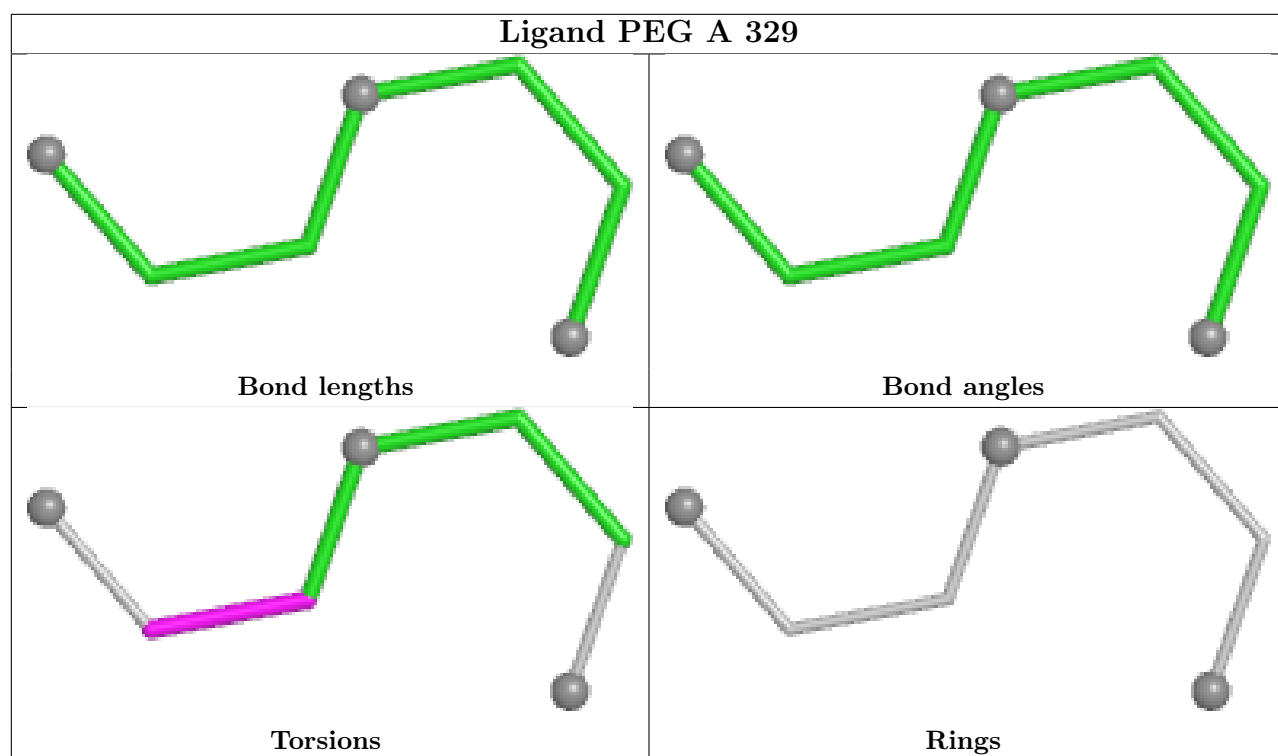


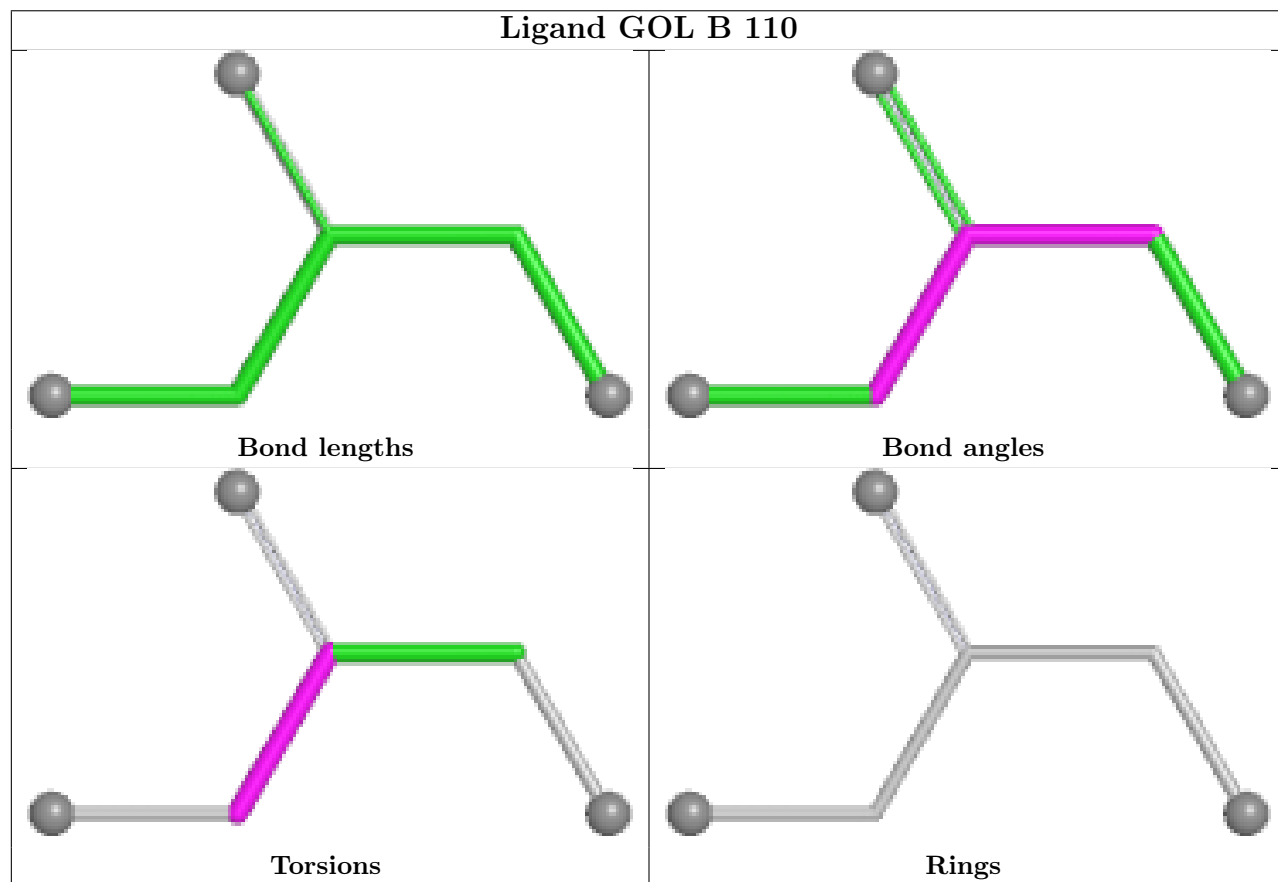
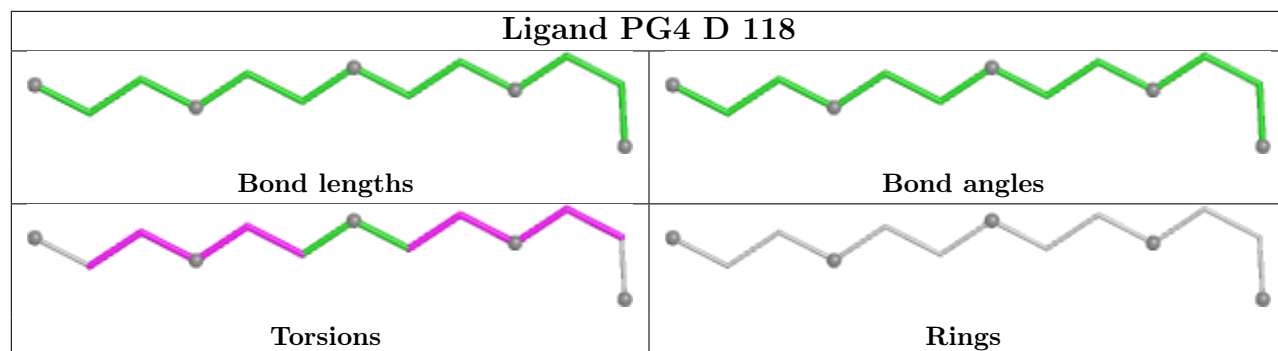


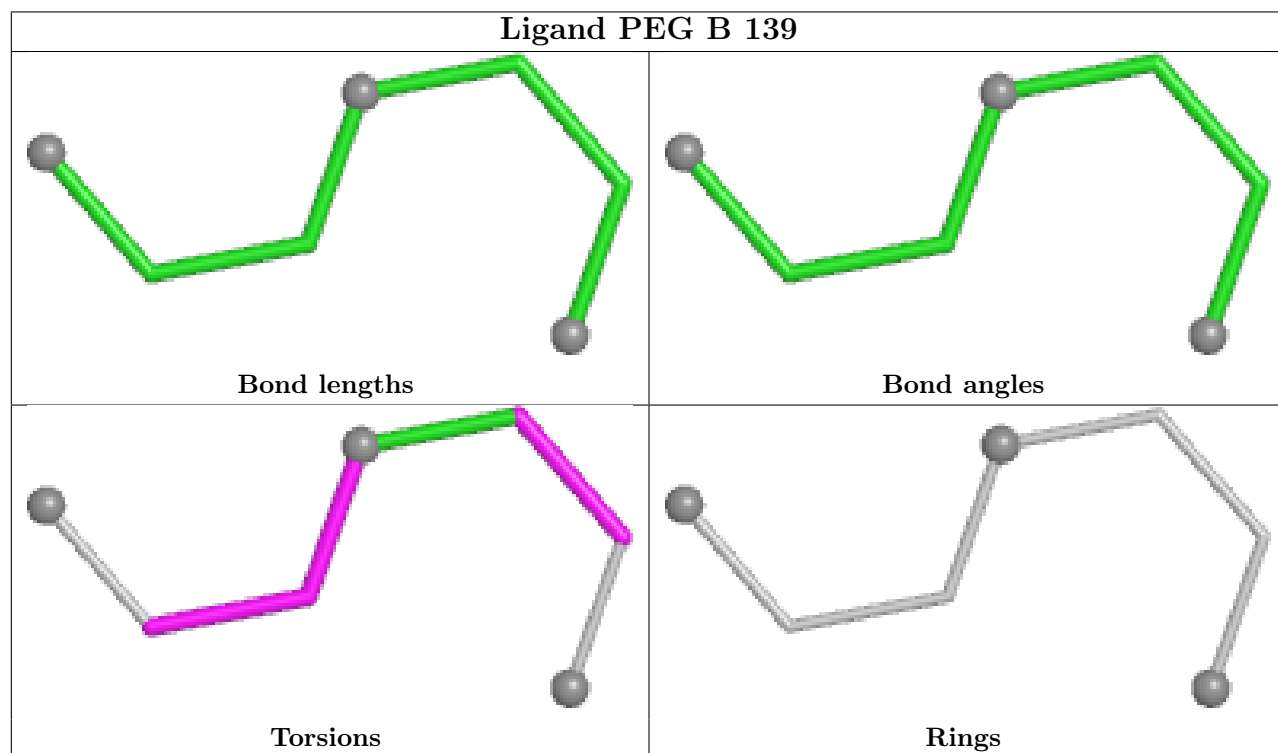
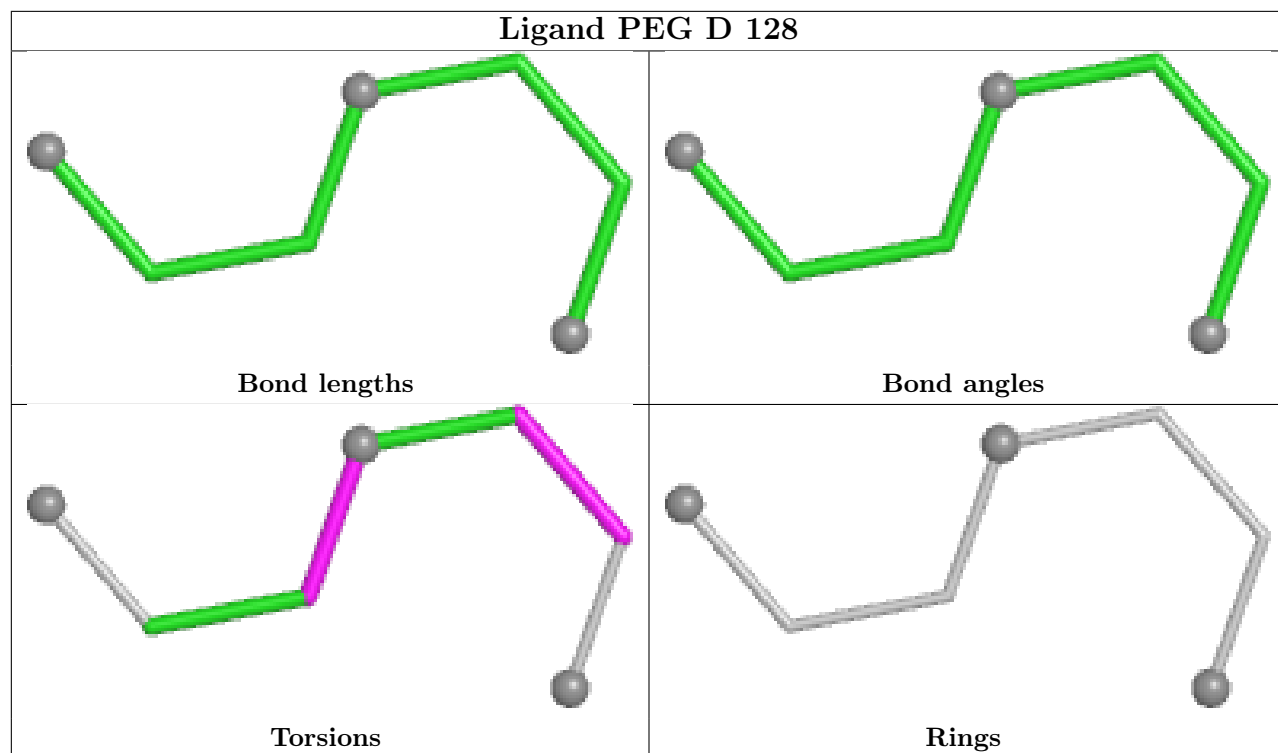


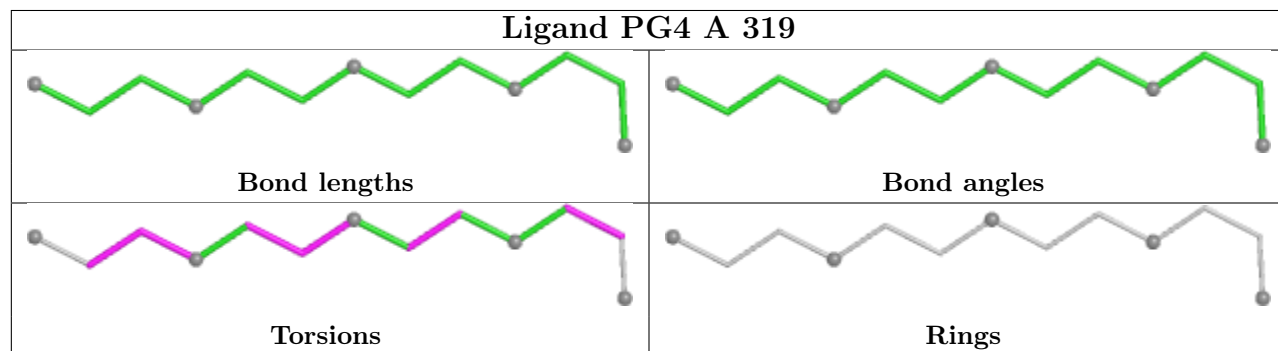
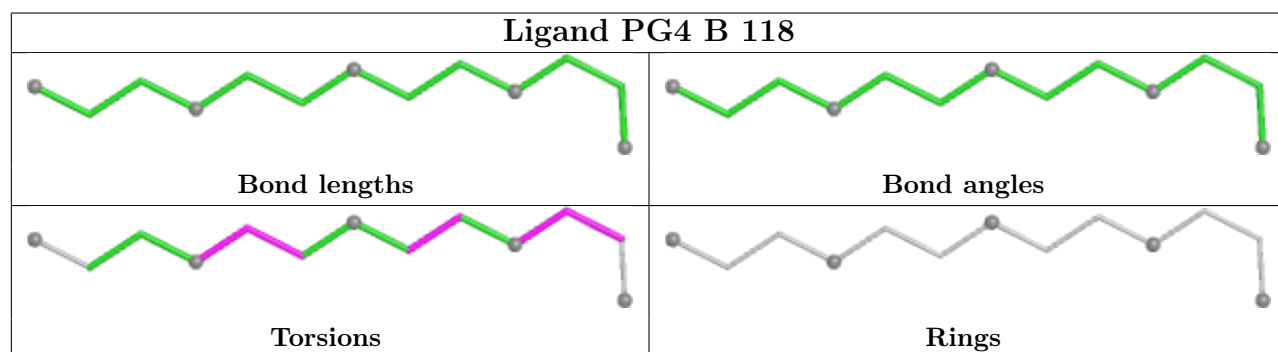
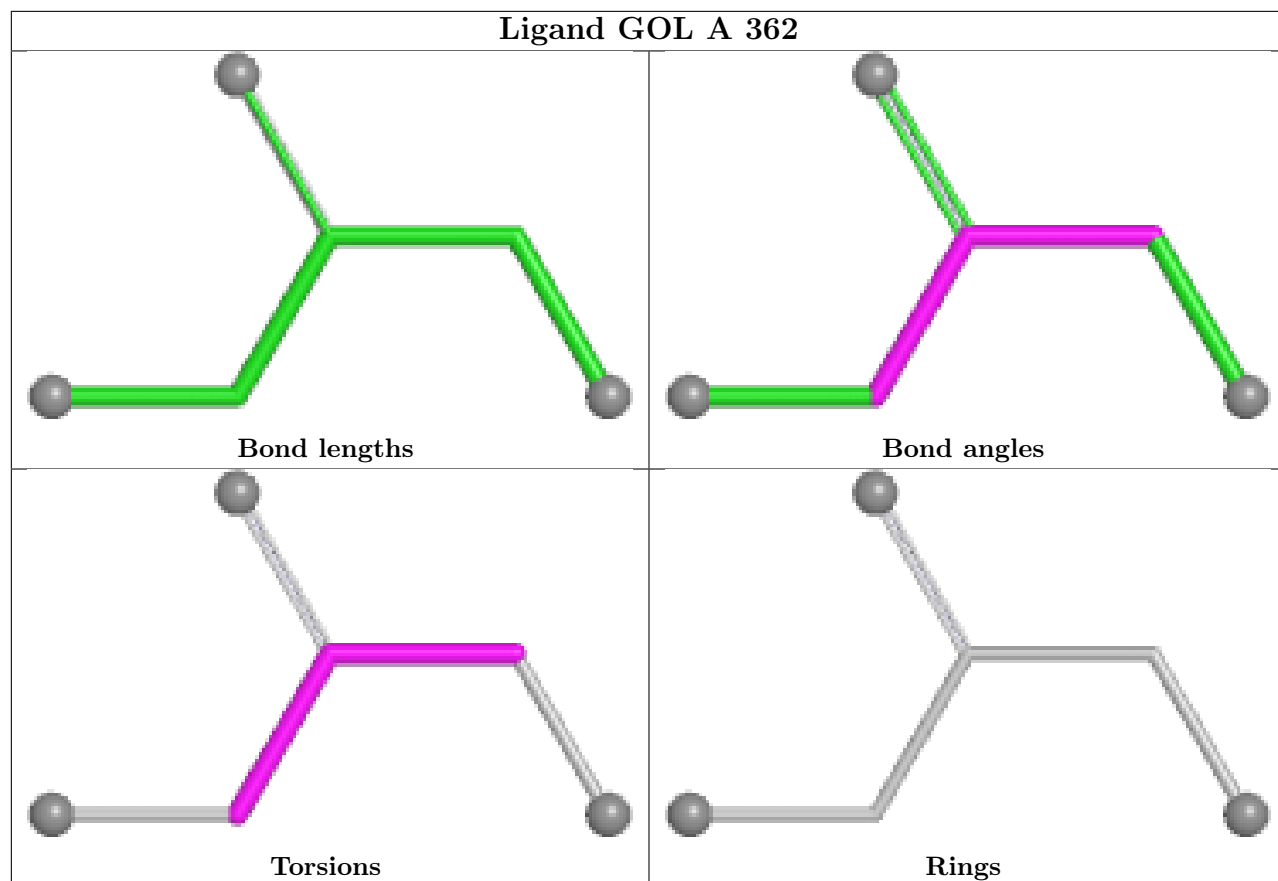


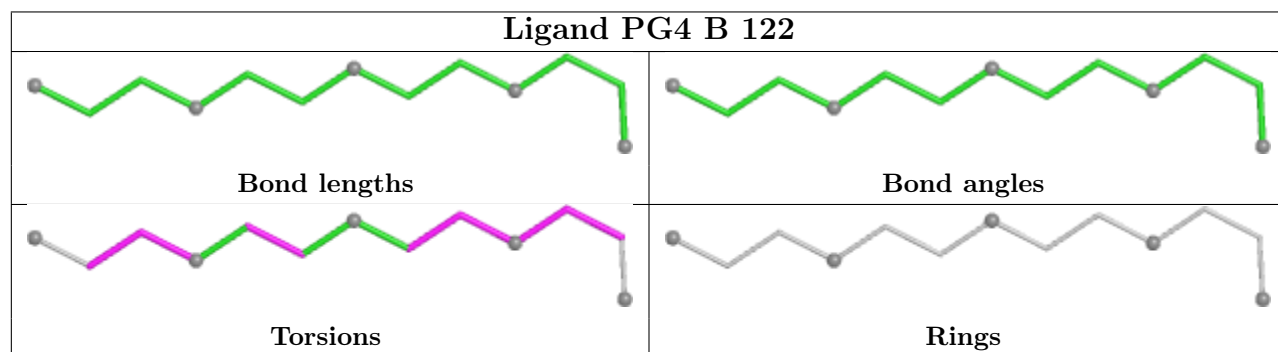
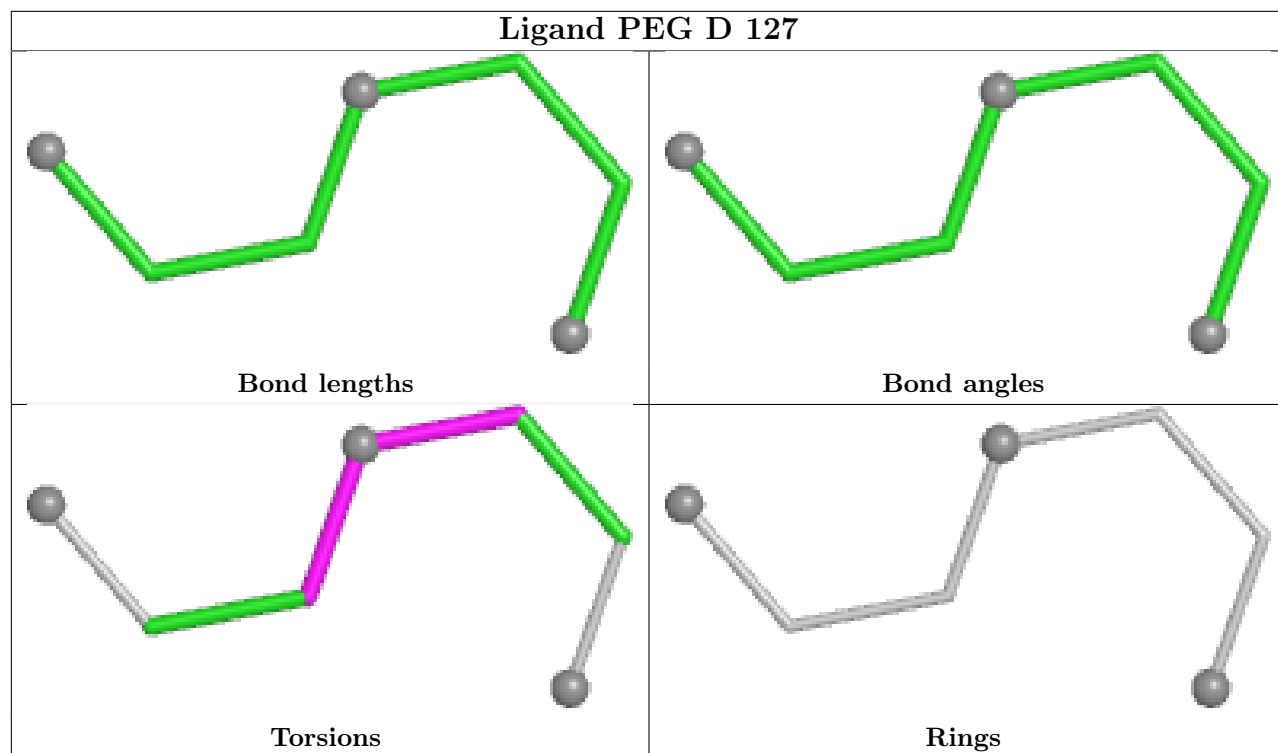


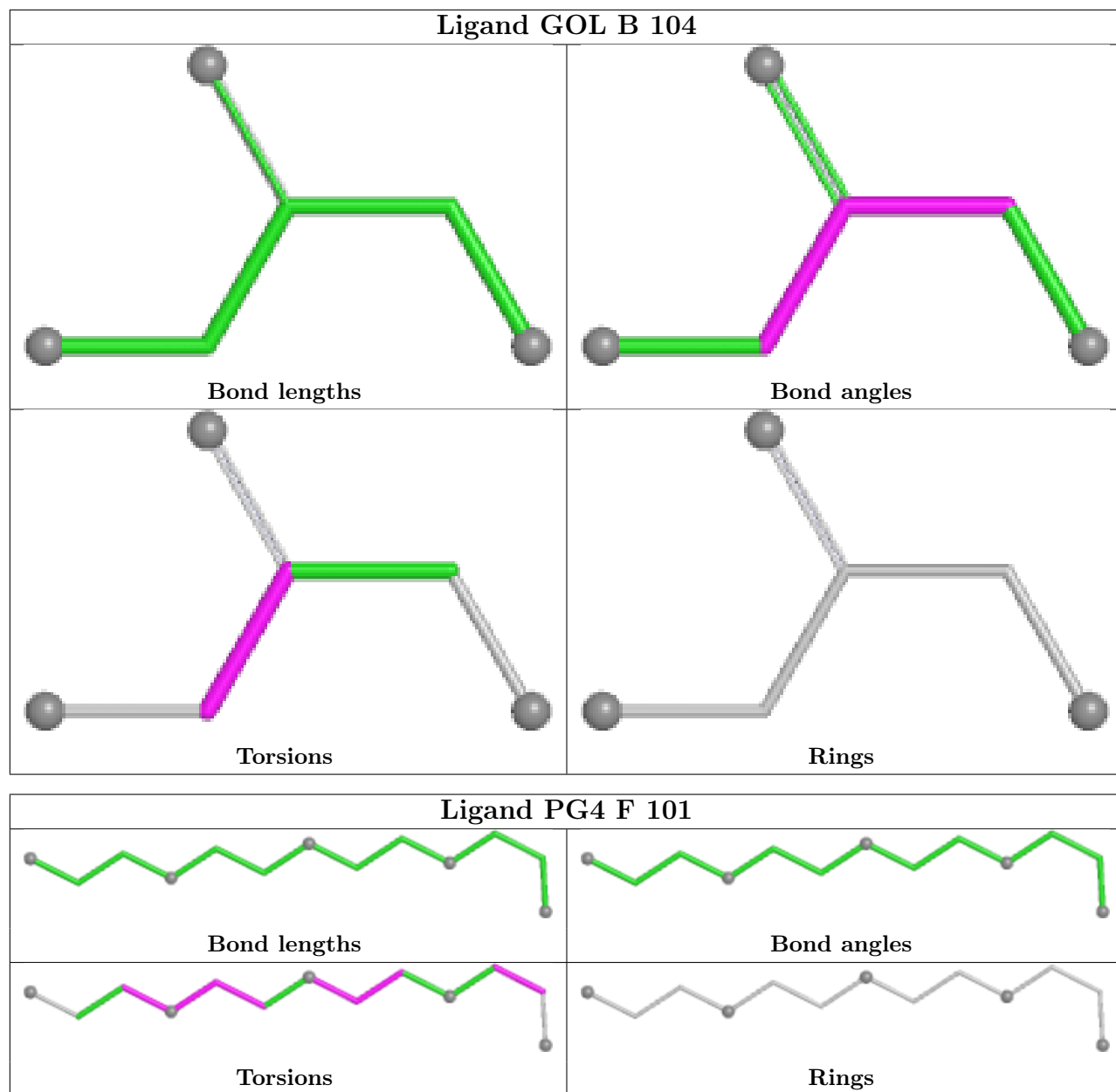


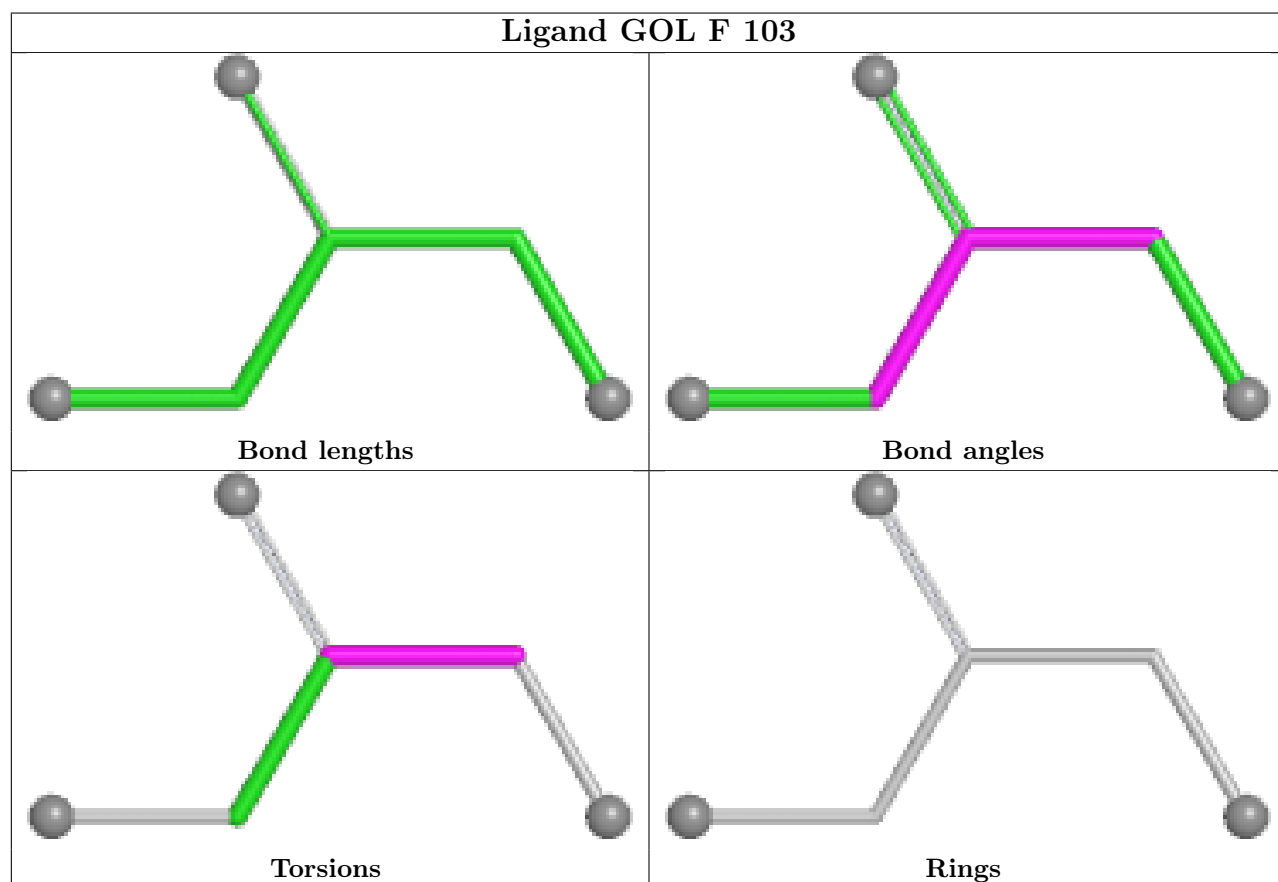
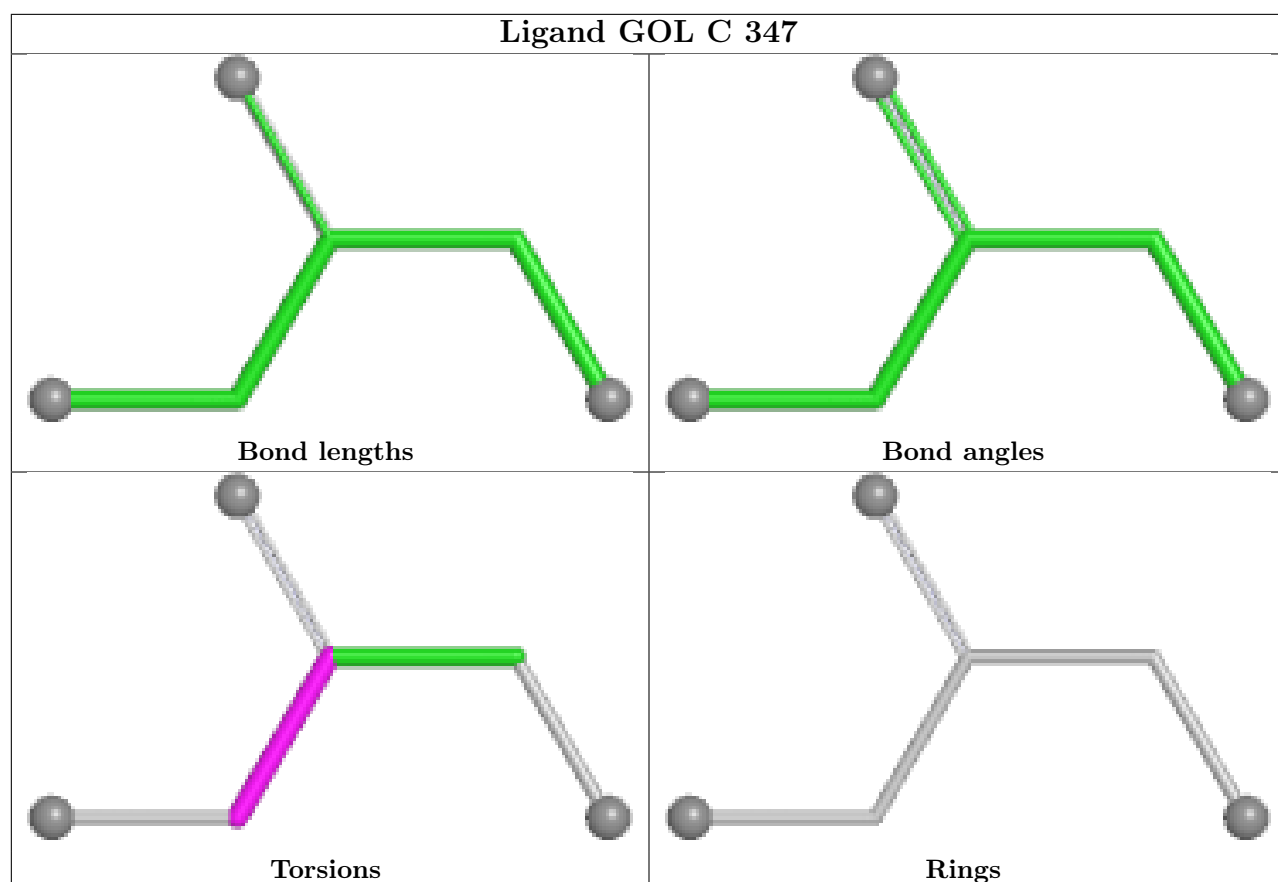


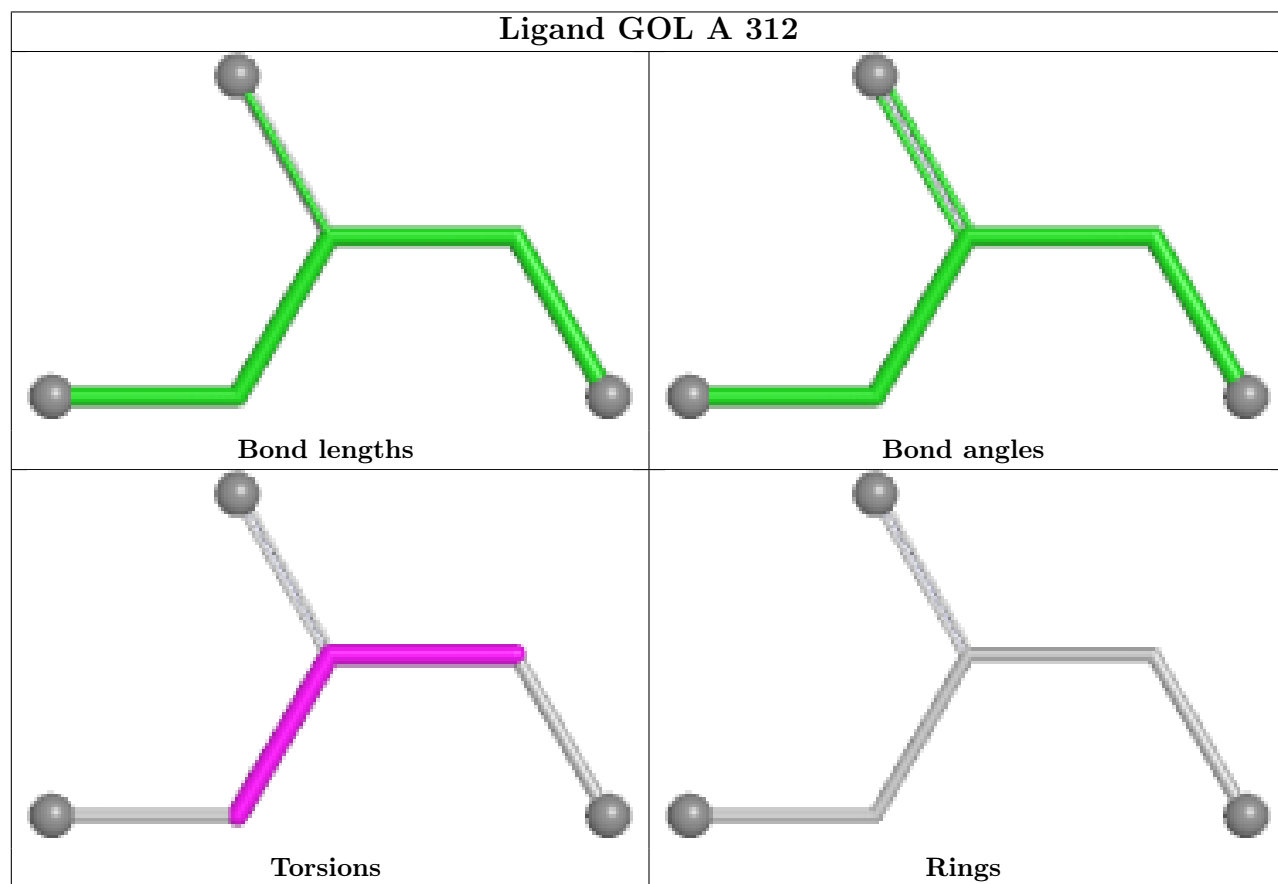
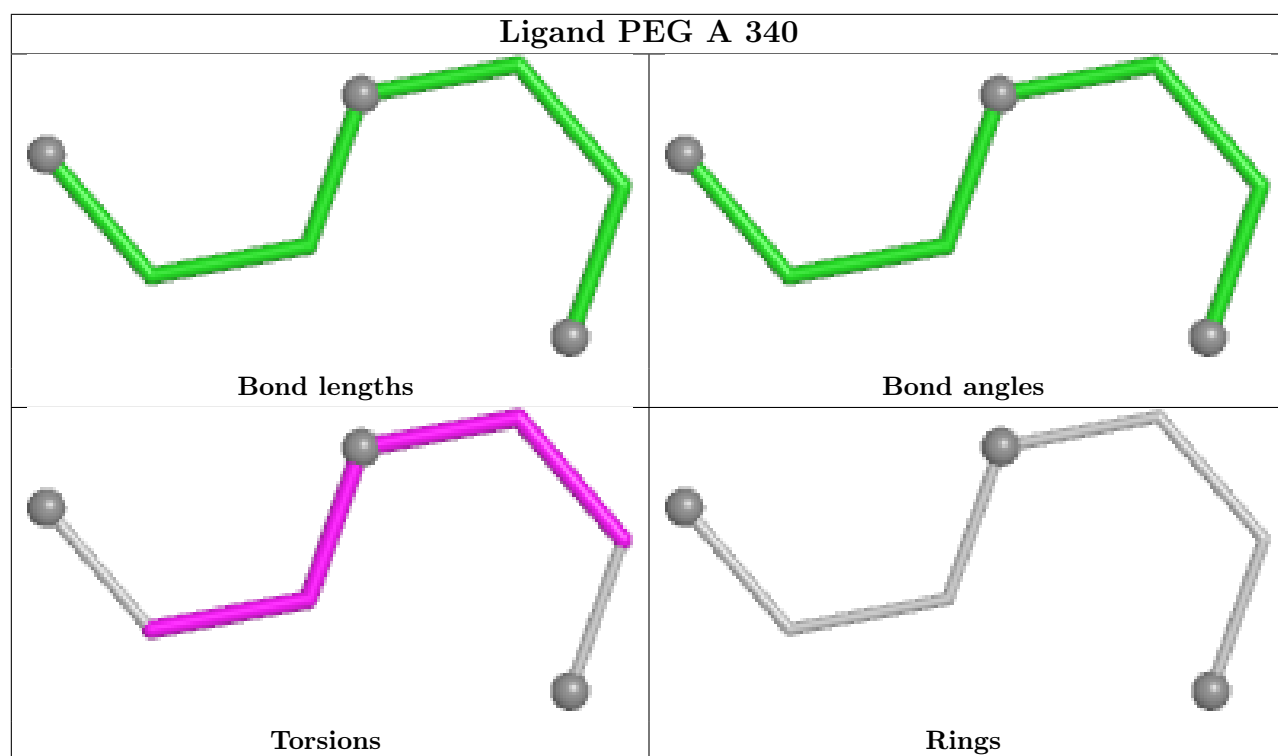


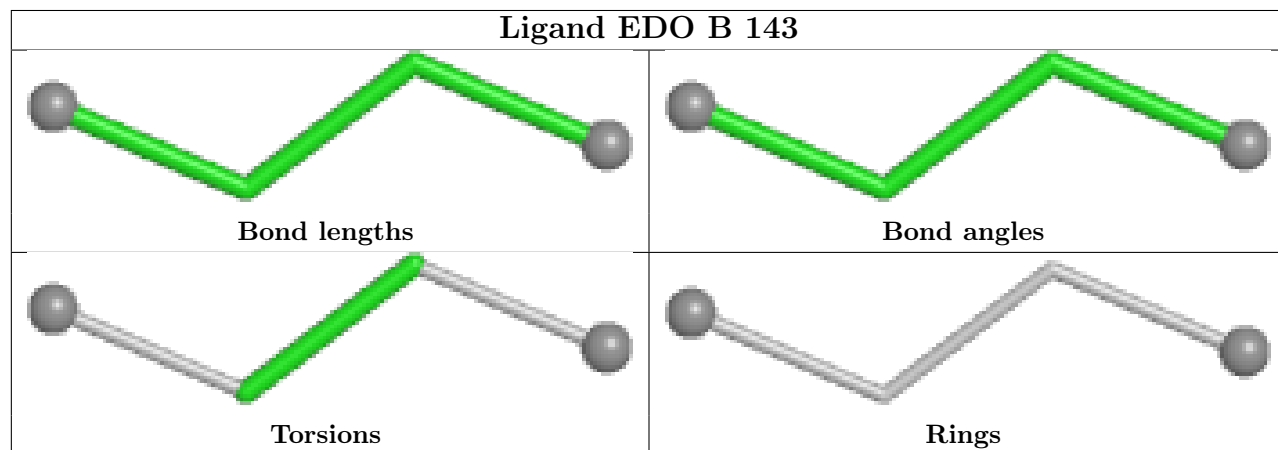
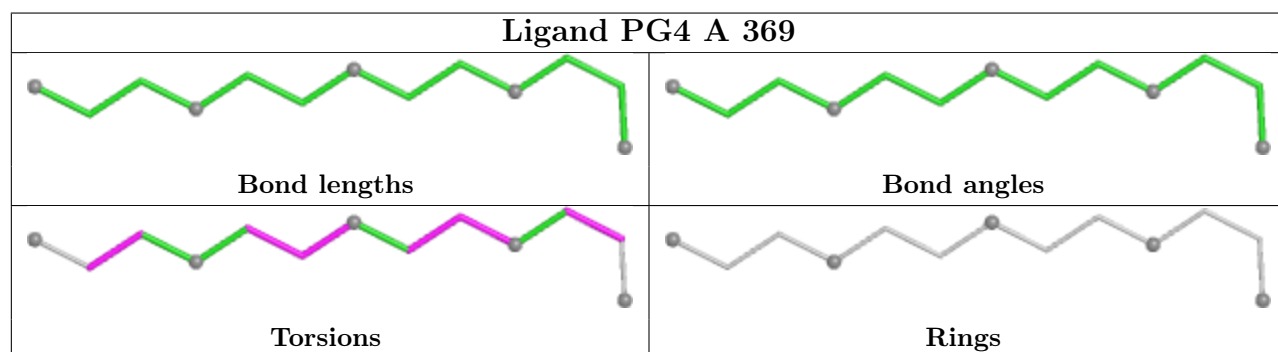
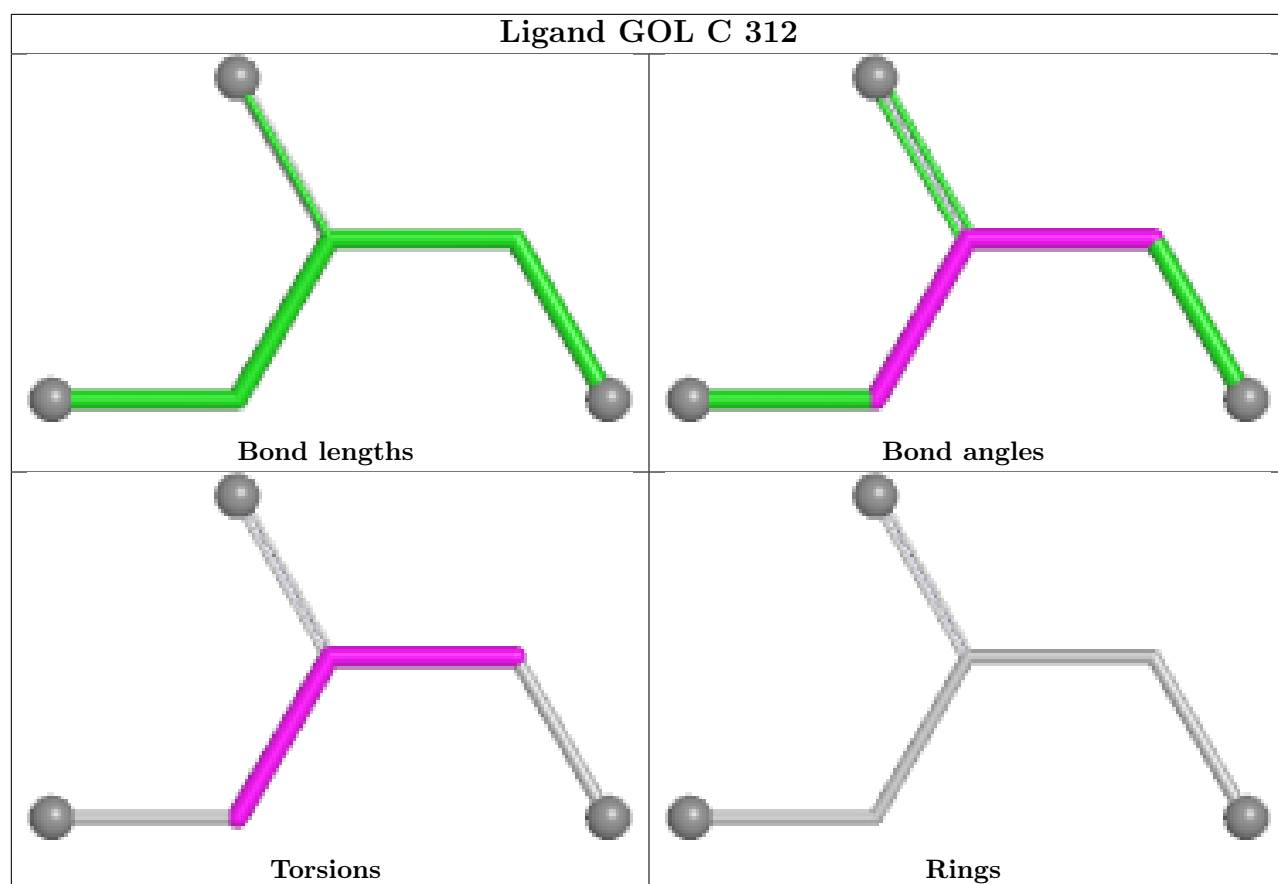


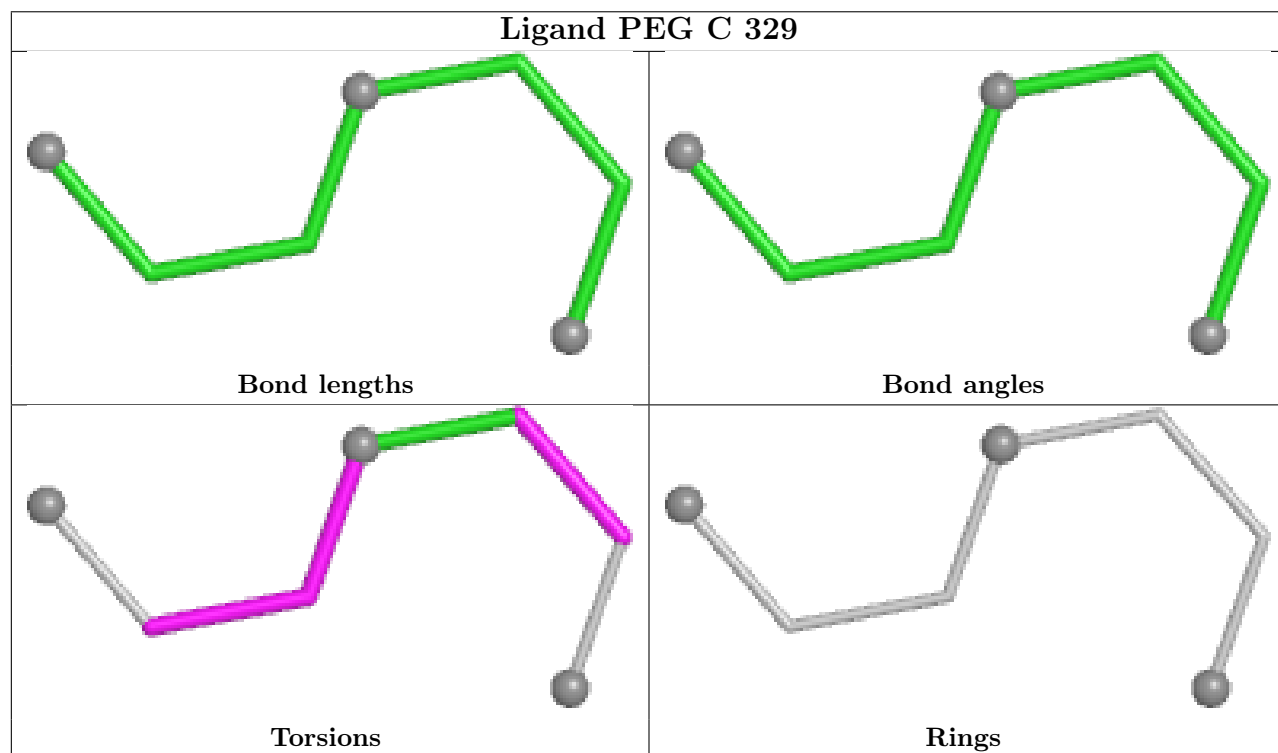
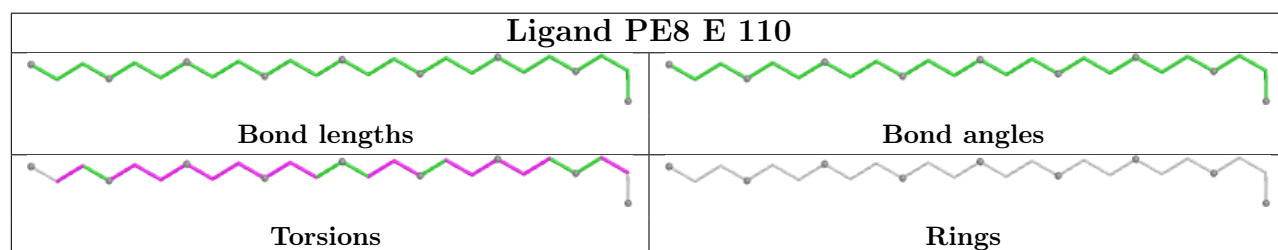
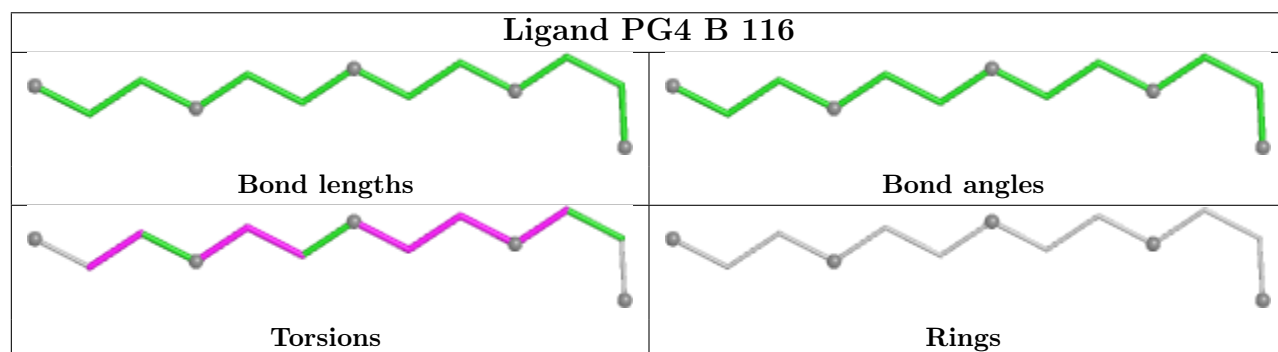
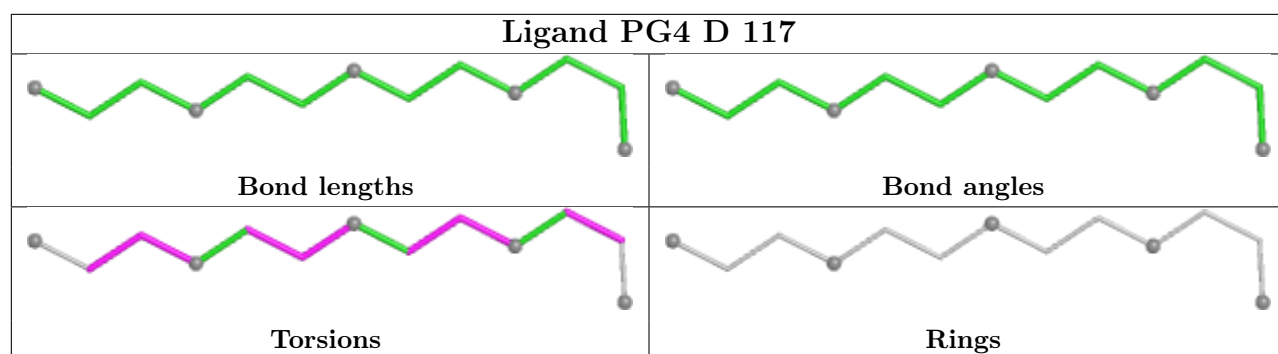


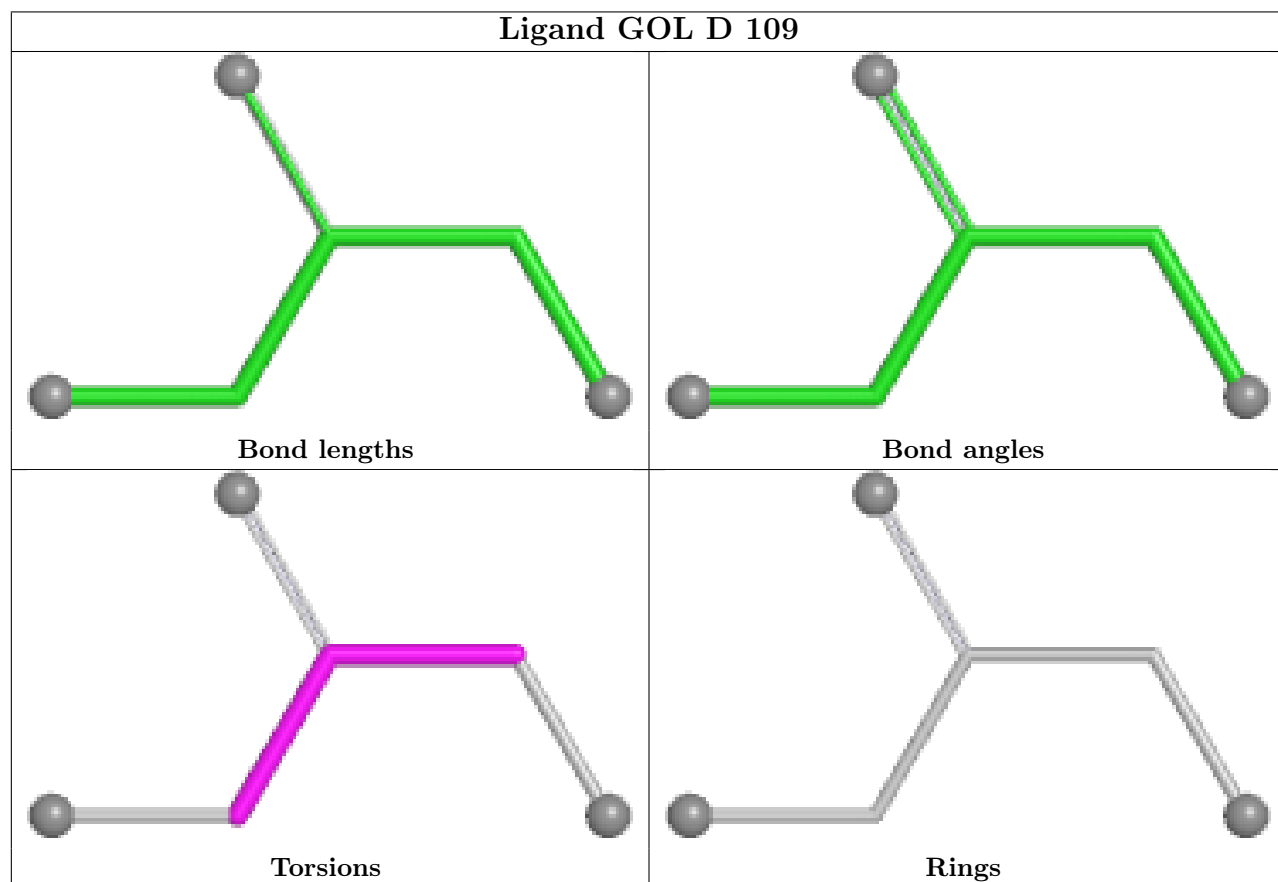
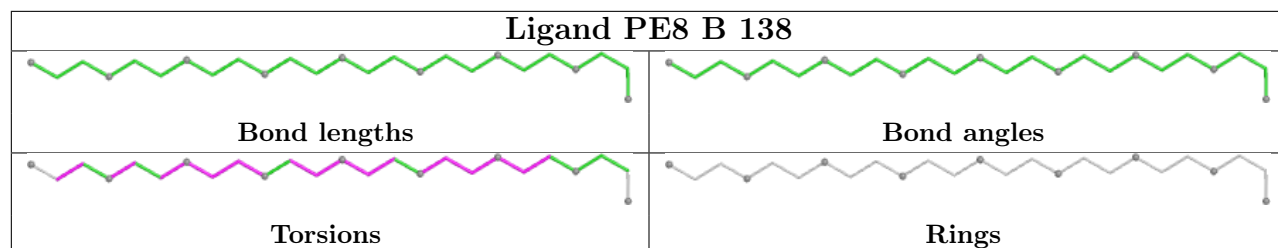


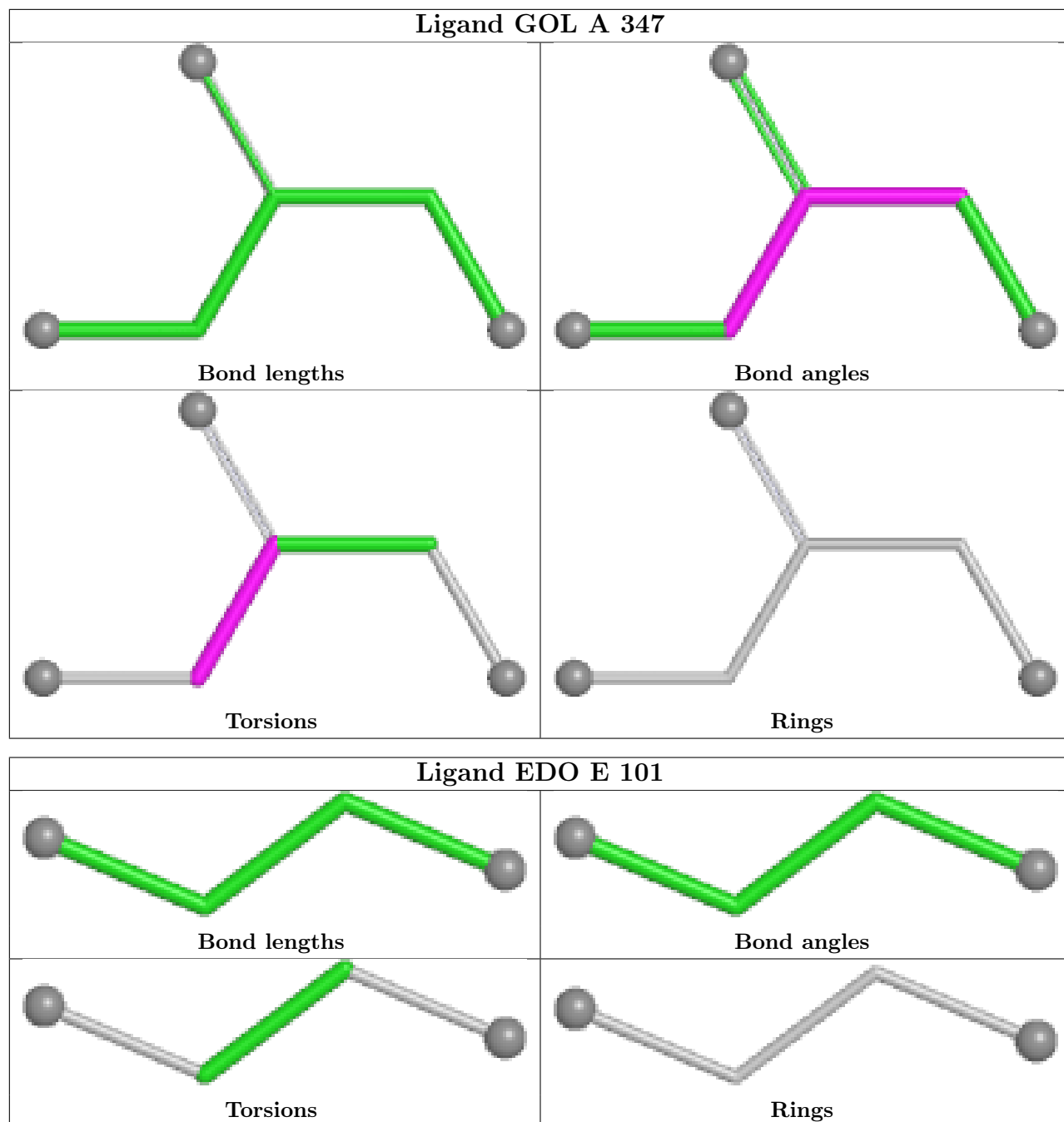


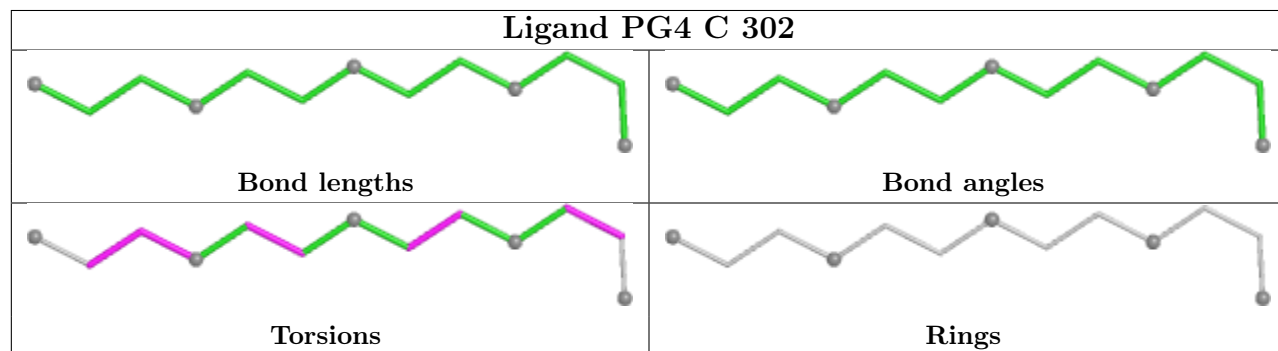
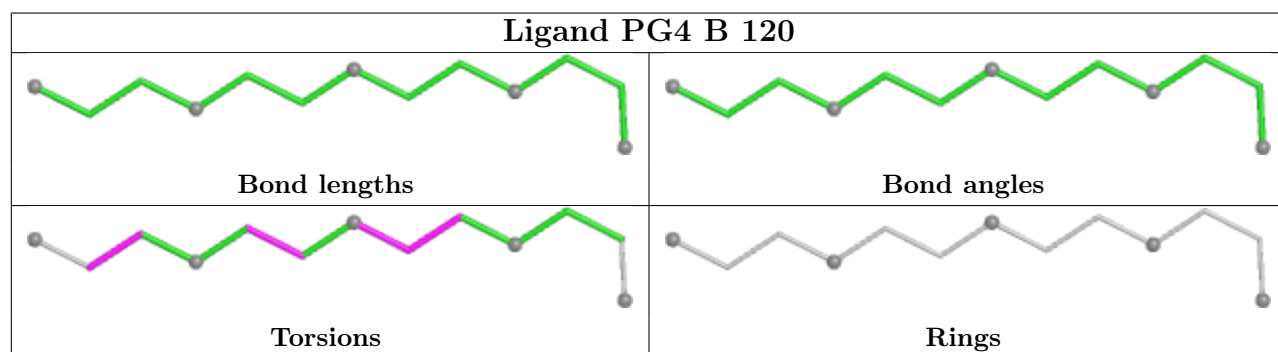
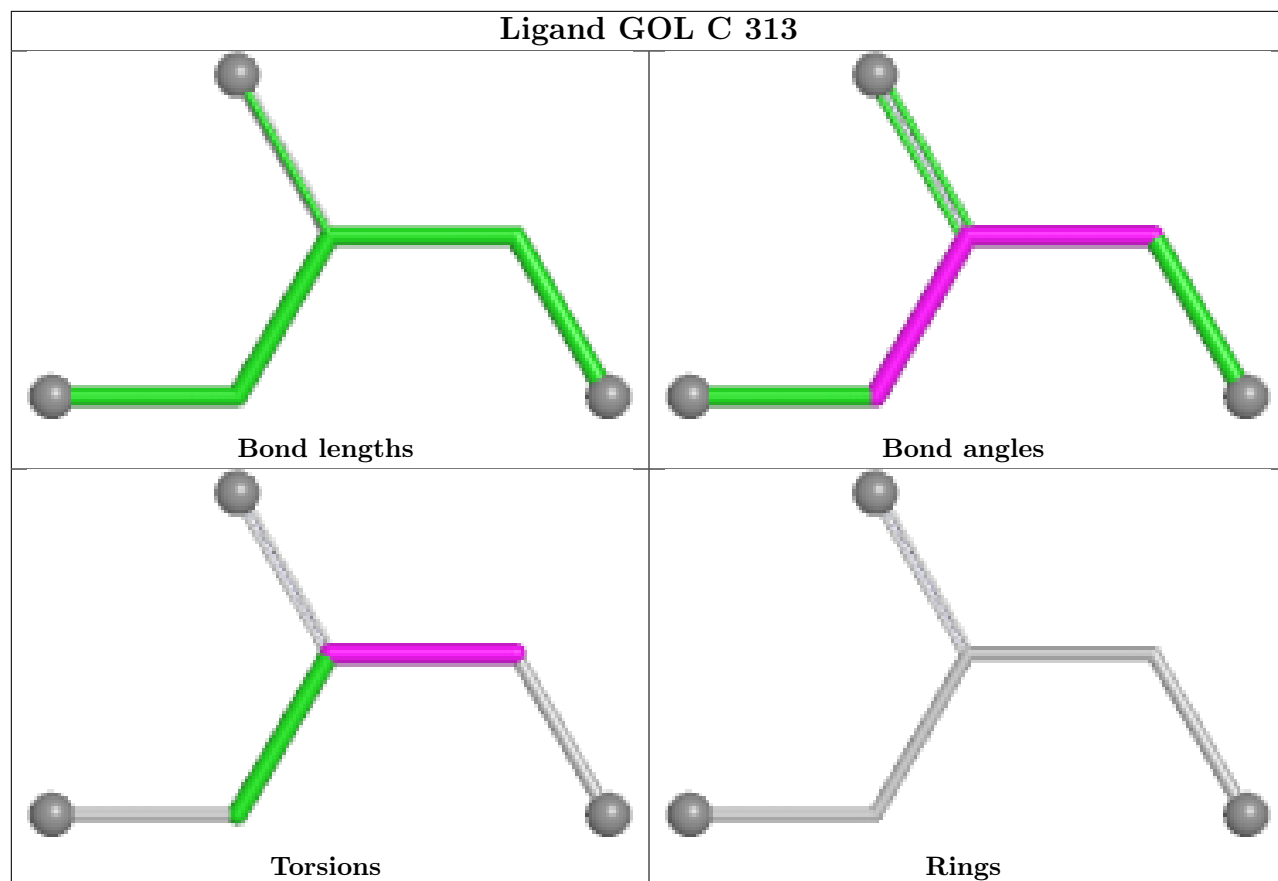


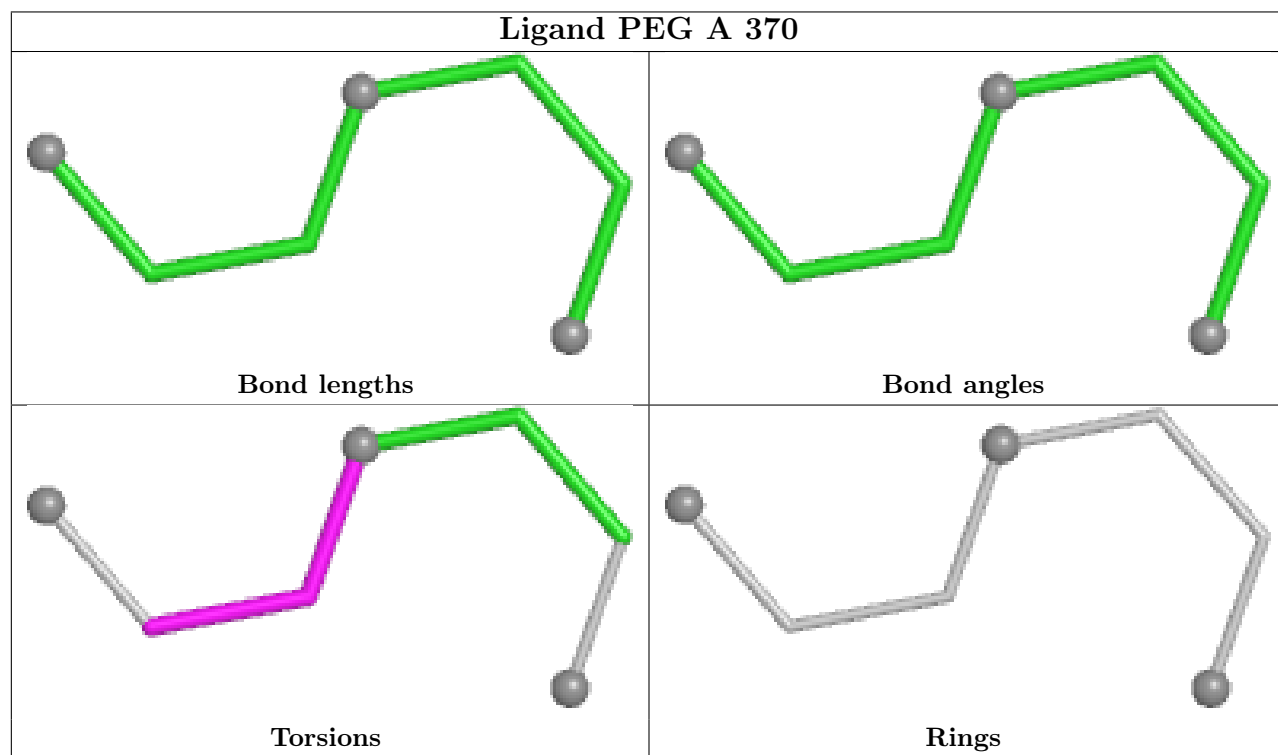
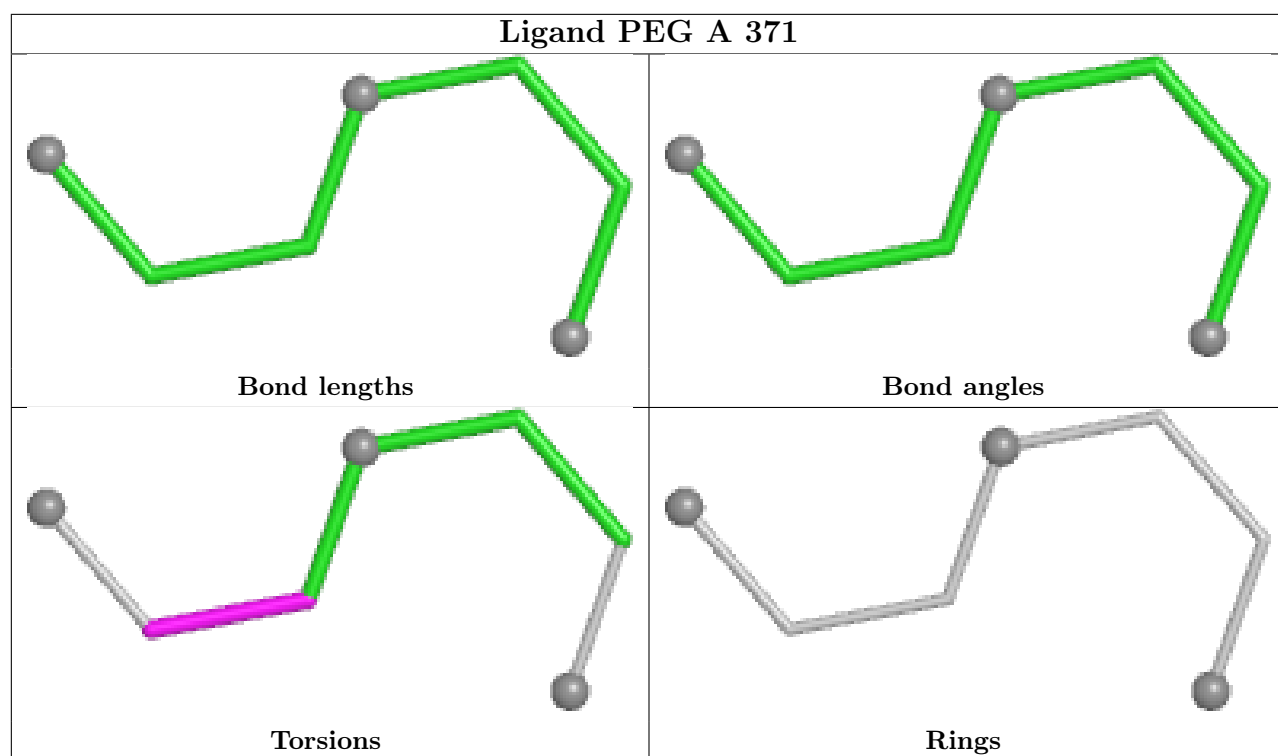


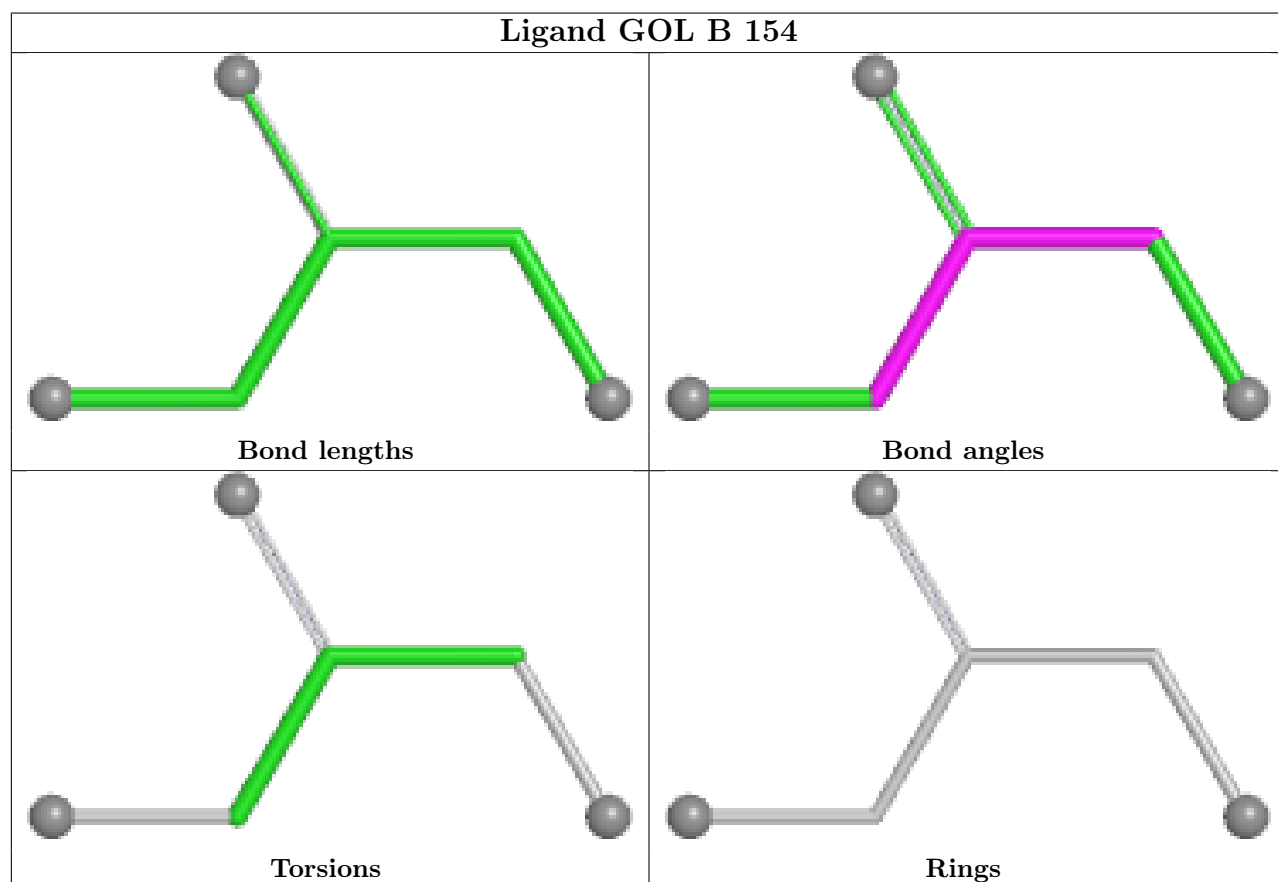
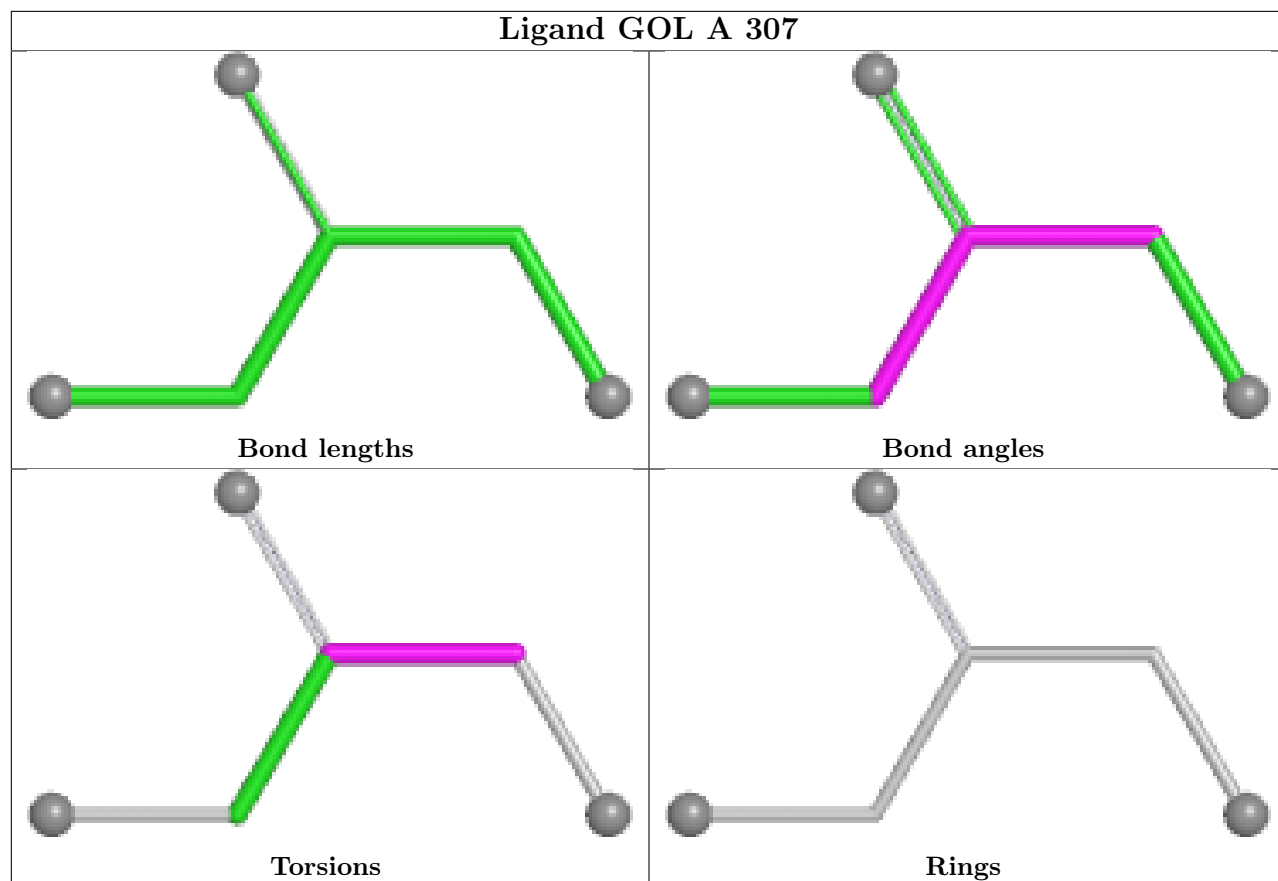


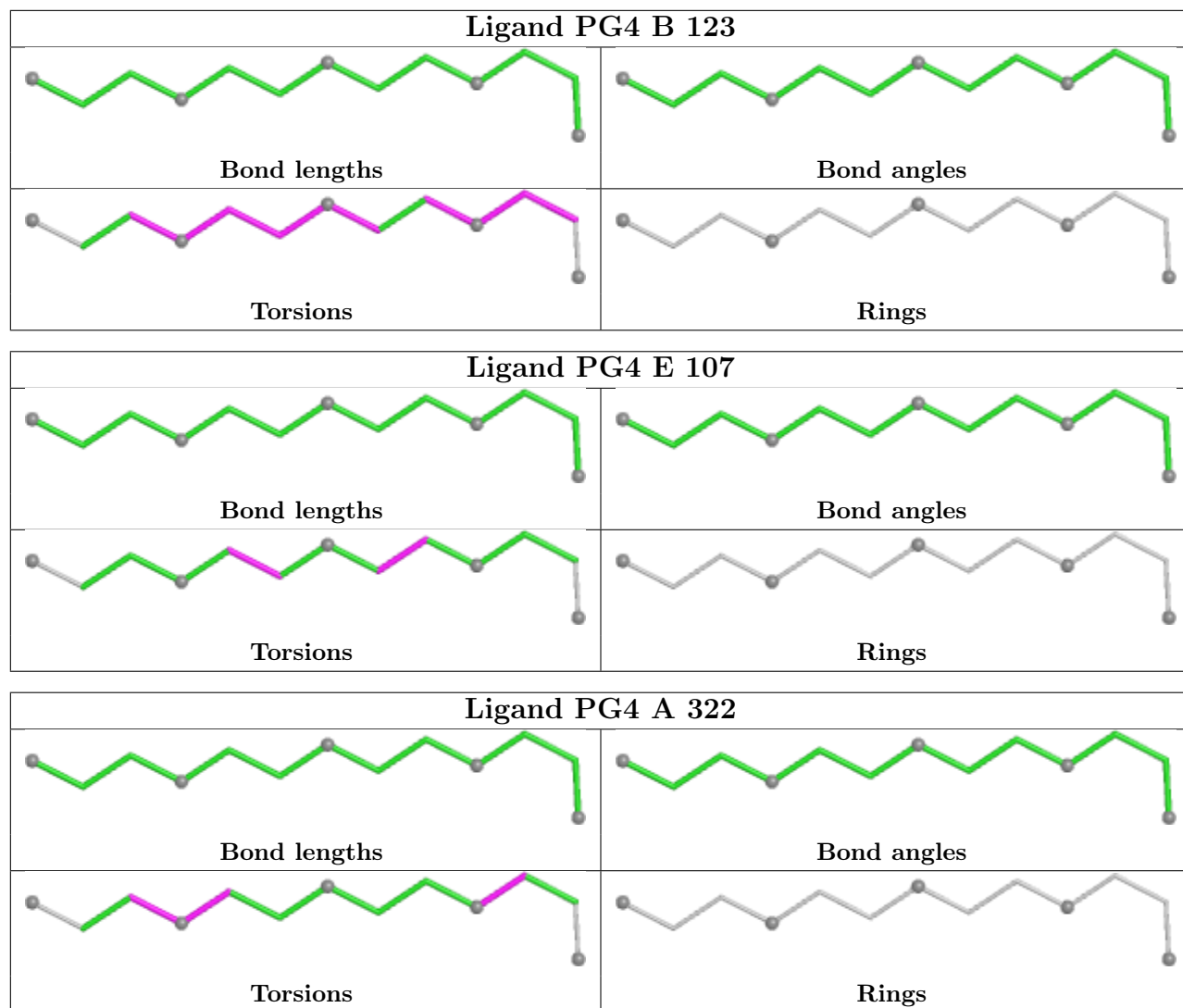


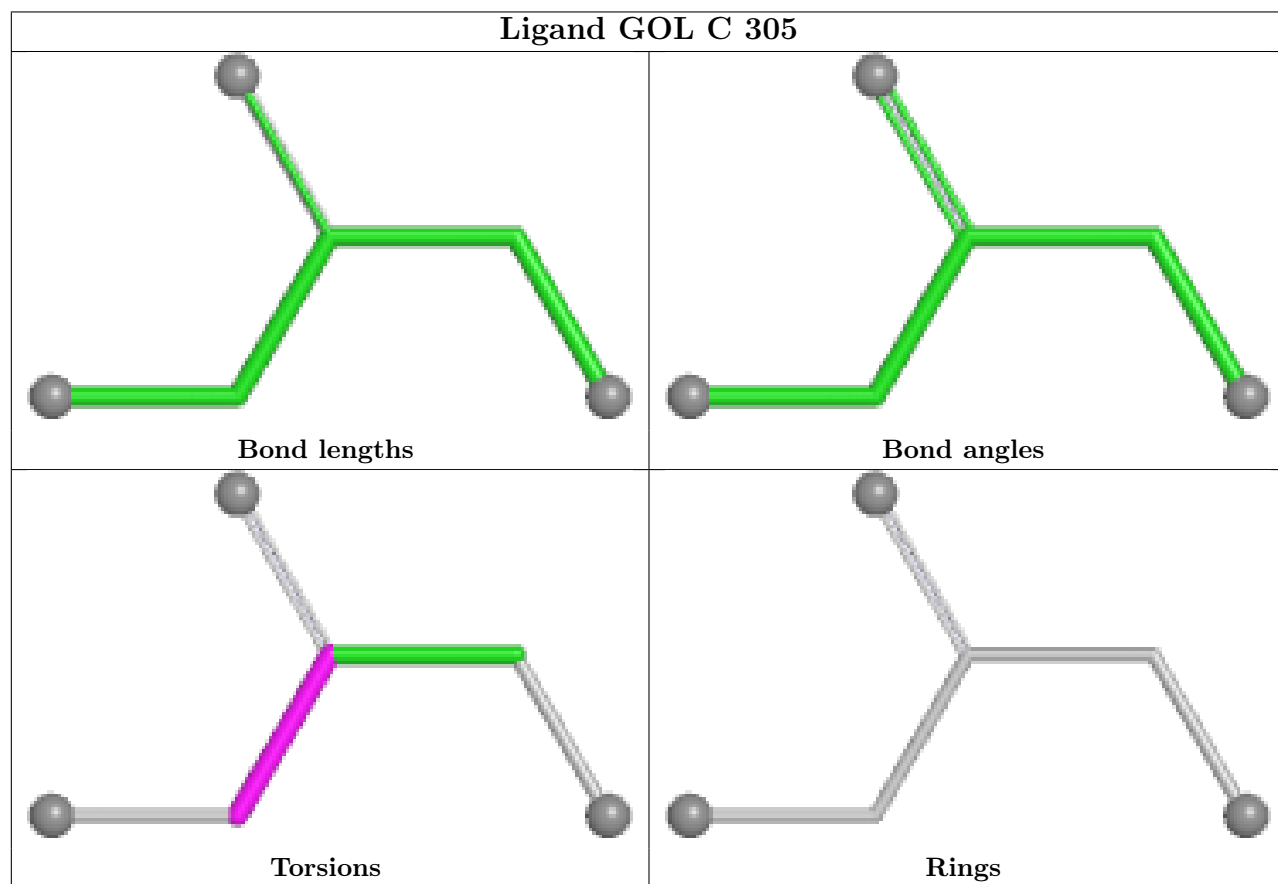
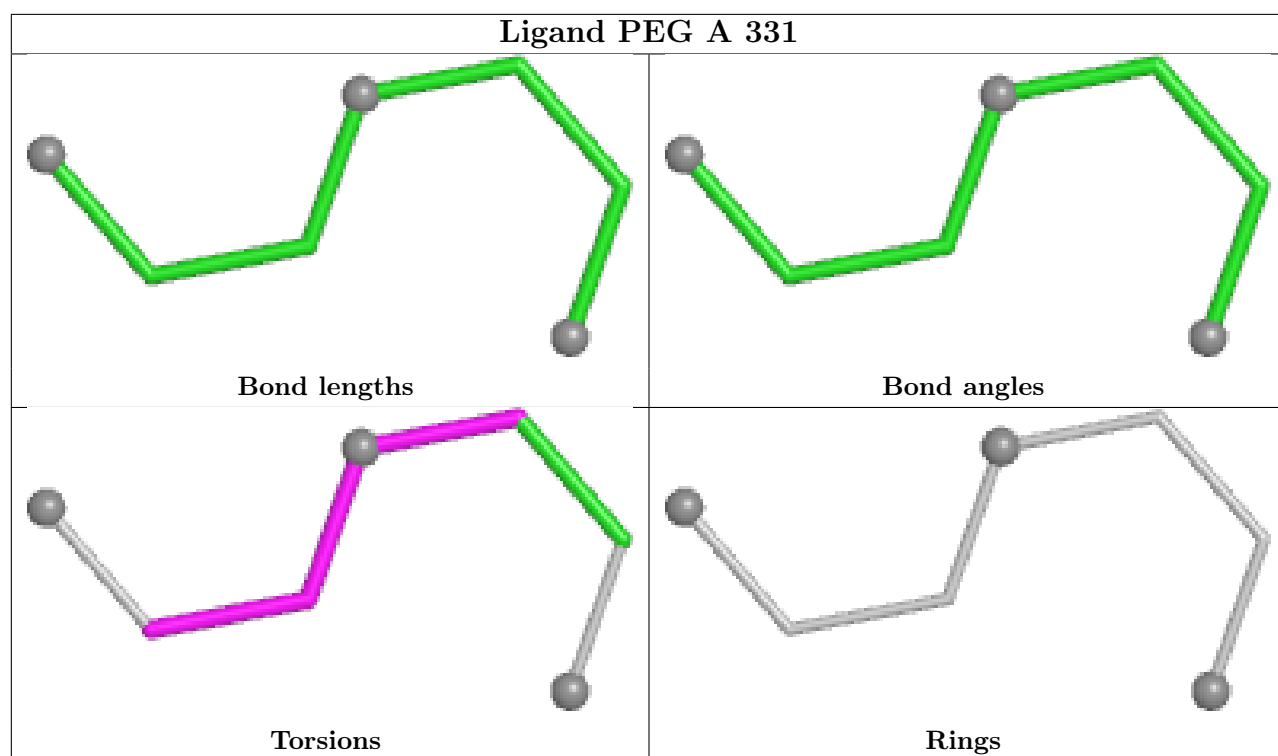


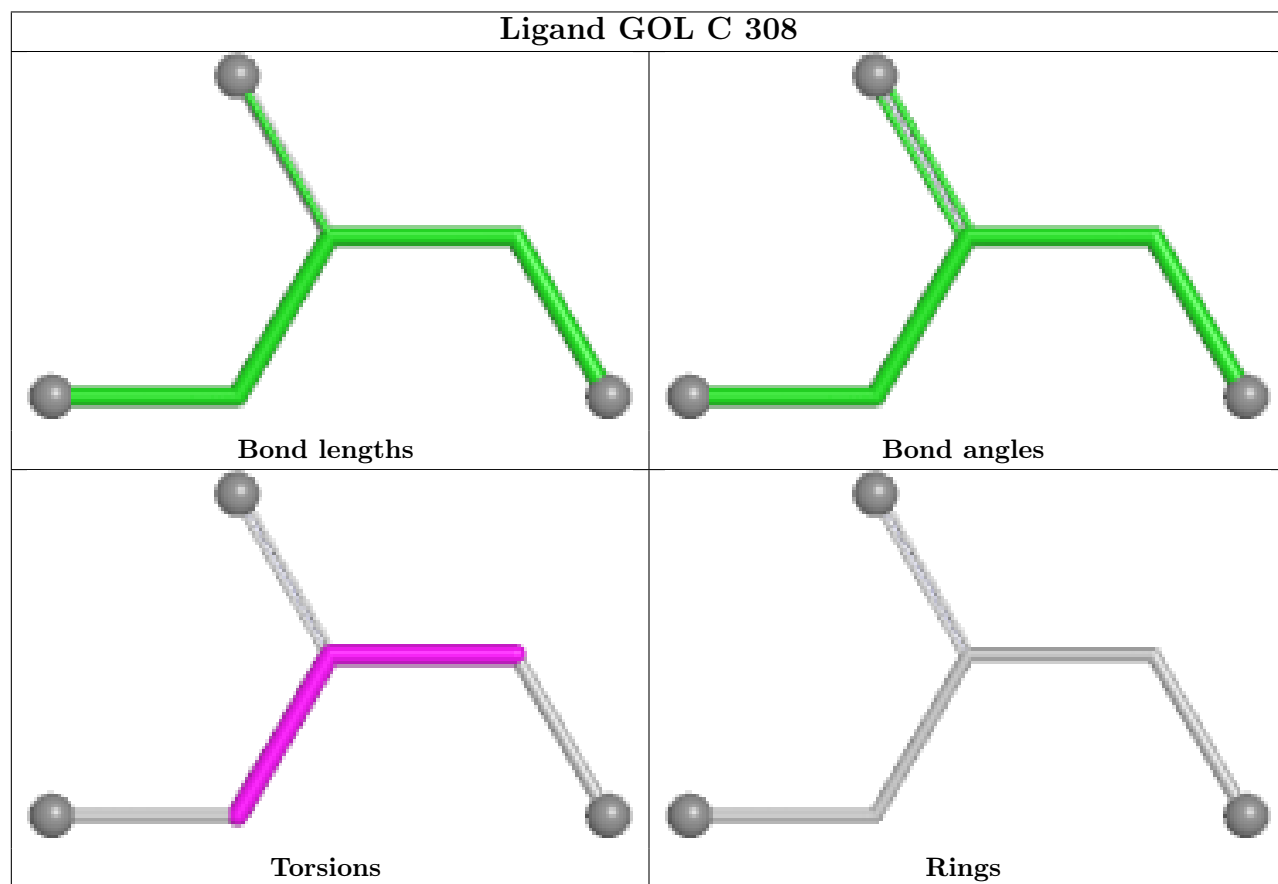
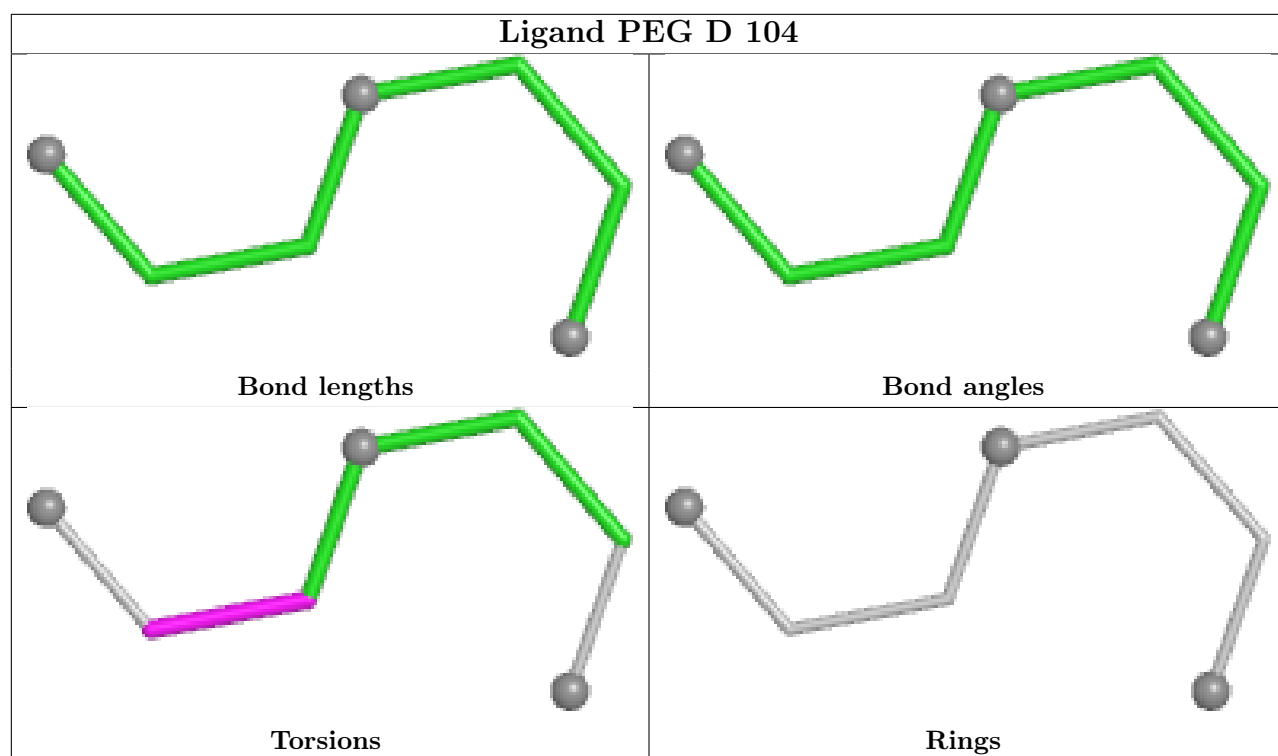


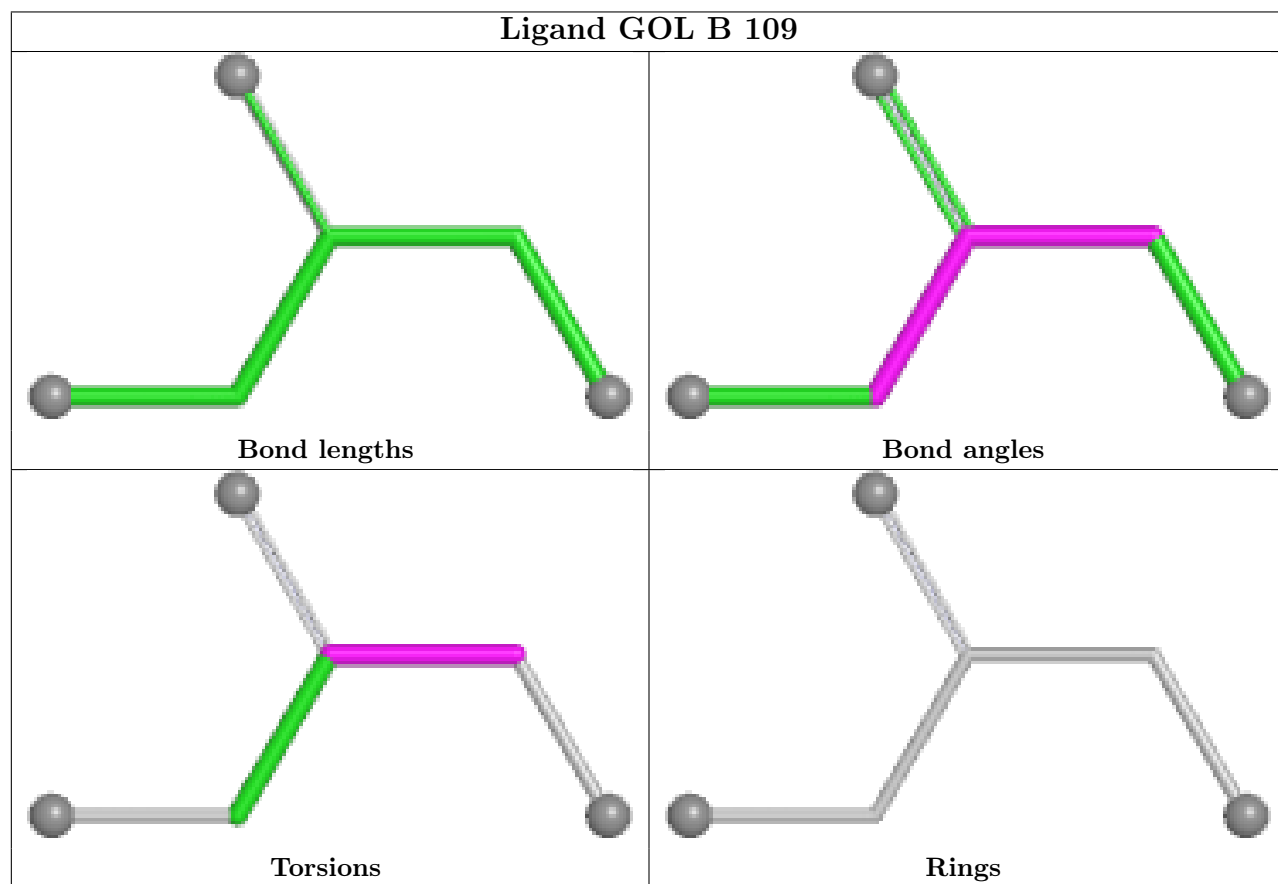
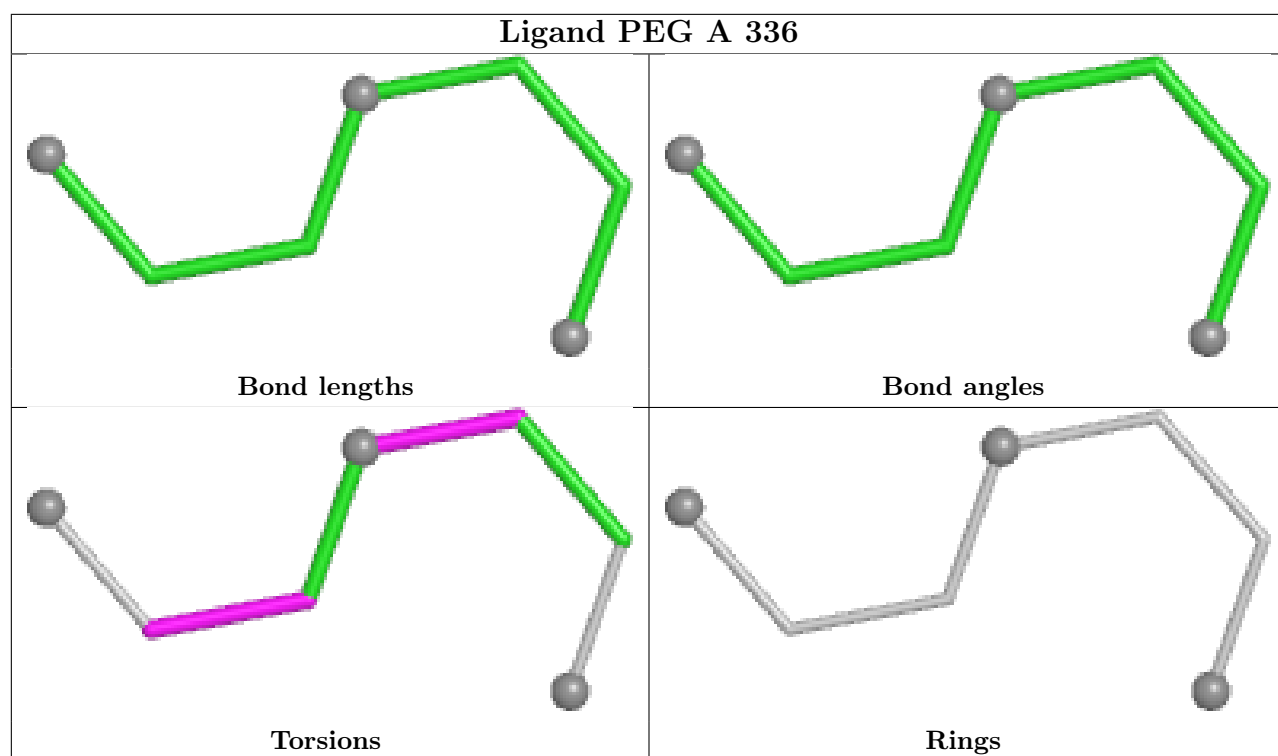


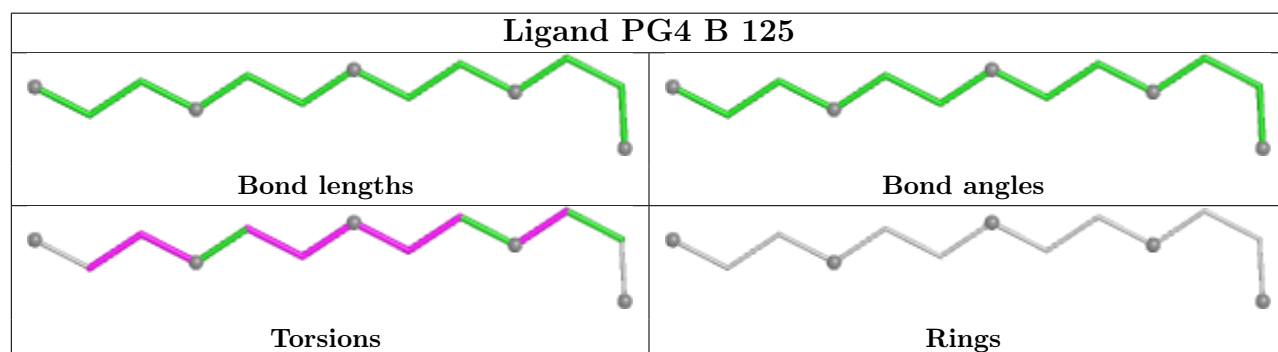
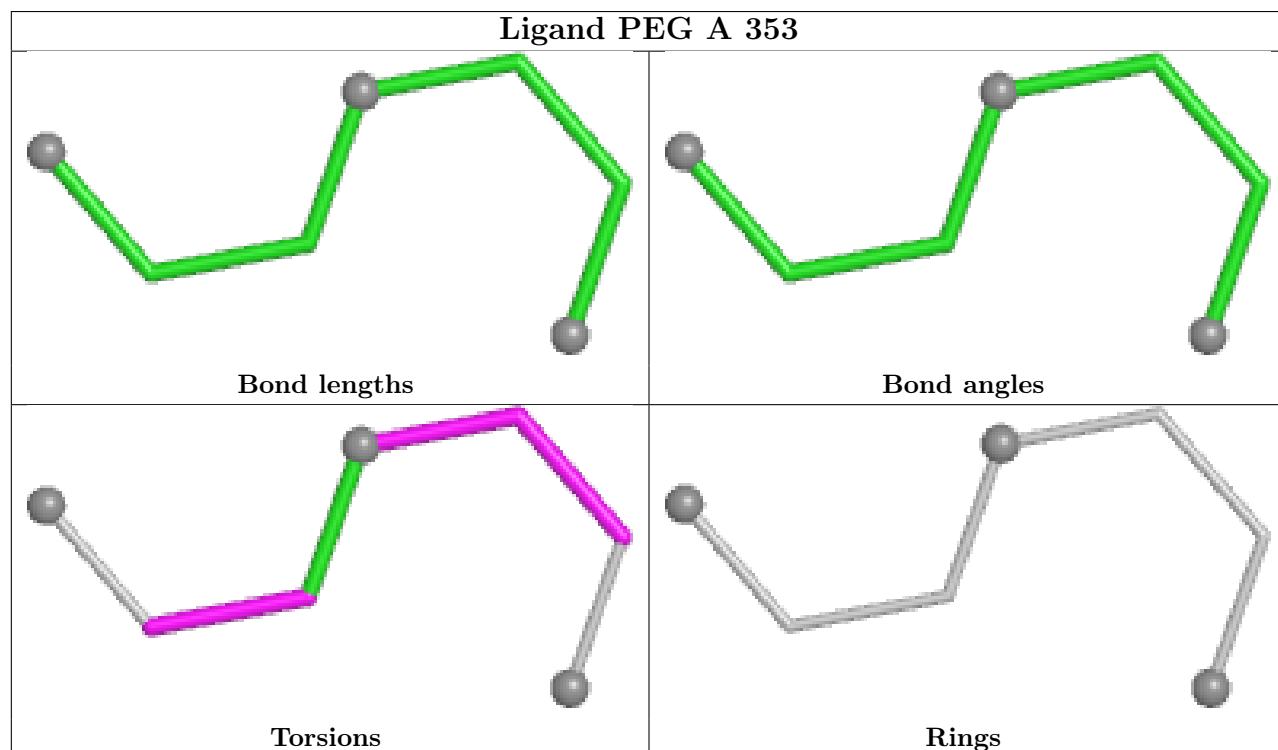
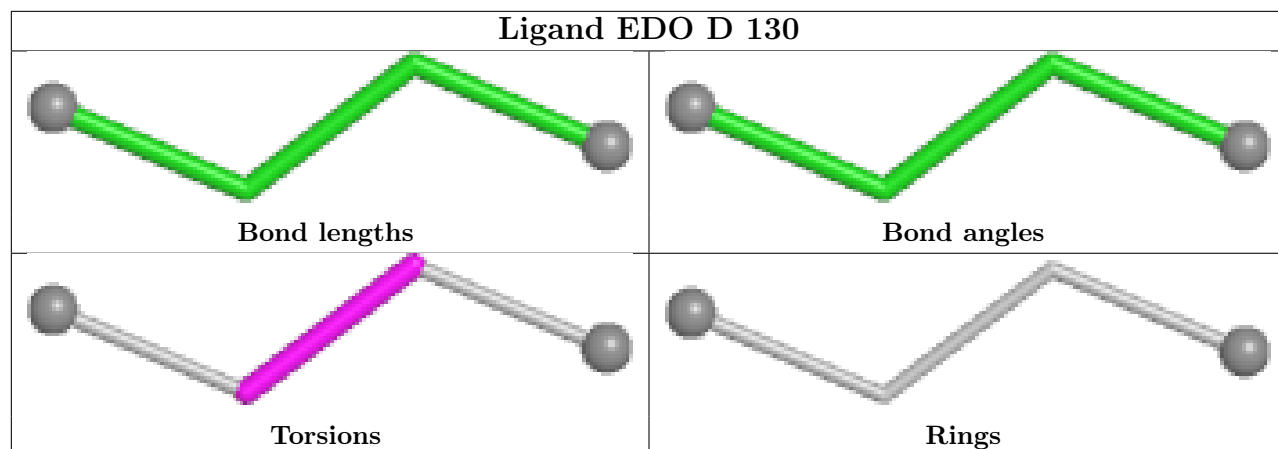


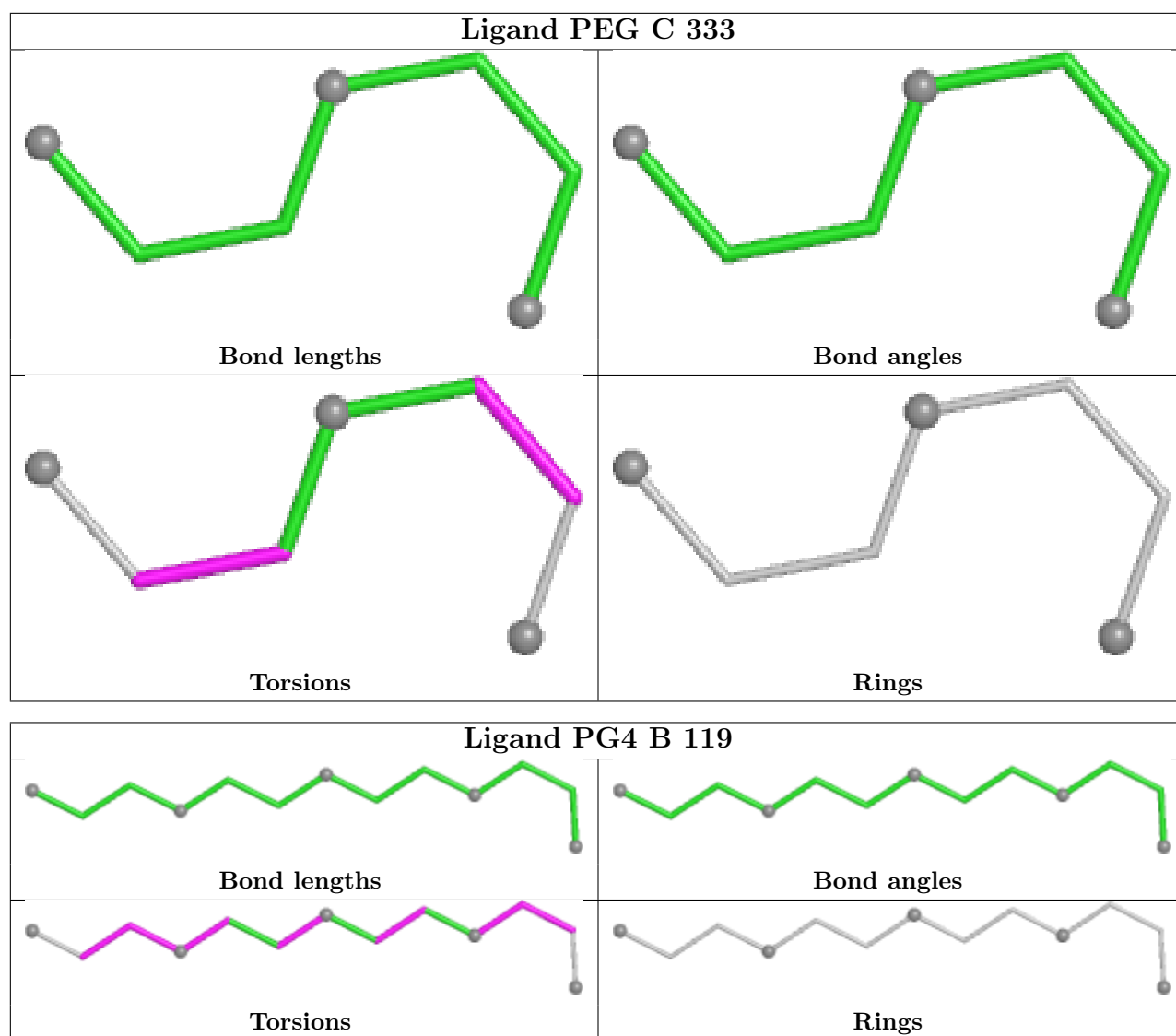












5.7 Other polymers [i](#)

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%)	1.16	42 (17%)	4 4	46, 74, 98, 128	1 (0%)
1	C	241/241 (100%)	1.18	45 (18%)	3 3	48, 76, 94, 111	0
2	B	98/98 (100%)	1.47	23 (23%)	2 2	58, 86, 102, 107	0
2	D	98/98 (100%)	1.19	14 (14%)	6 5	53, 72, 96, 111	0
3	E	9/9 (100%)	0.45	0 100	100	65, 80, 96, 97	0
4	F	9/9 (100%)	0.75	1 (11%)	10 9	54, 64, 70, 70	0
All	All	696/696 (100%)	1.20	125 (17%)	3 3	46, 76, 98, 128	1 (0%)

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	59	ALA	8.1
2	B	47	VAL	6.5
2	D	45	THR	5.6
2	B	95	LEU	5.5
2	B	52	ASN	5.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	0.50	0.12	48,48,48,48	0
9	PEG	B	129	7/7	0.56	0.16	49,70,79,89	0
11	EDO	B	143	4/4	0.58	0.38	68,71,73,88	0
5	GOL	C	305	6/6	0.59	0.16	60,80,82,90	0
5	GOL	D	113	6/6	0.60	0.14	41,63,70,77	0
9	PEG	A	338	7/7	0.60	0.18	52,55,77,79	0
5	GOL	F	103	6/6	0.62	0.24	37,42,55,62	0
9	PEG	B	128	7/7	0.63	0.13	51,60,69,69	0
7	PG4	E	105	13/13	0.63	0.17	33,51,60,66	0
9	PEG	B	133	7/7	0.63	0.21	51,70,78,85	0
5	GOL	D	107	6/6	0.63	0.12	57,61,61,62	0
9	PEG	A	337	7/7	0.65	0.16	62,71,78,88	0
7	PG4	B	101	13/13	0.65	0.16	34,57,72,85	0
7	PG4	A	325	13/13	0.65	0.12	39,57,79,80	0
6	NA	A	355	1/1	0.66	0.11	42,42,42,42	0
5	GOL	E	103	6/6	0.66	0.14	64,69,72,90	0
6	NA	D	114	1/1	0.66	0.14	40,40,40,40	0
11	EDO	A	351	4/4	0.66	0.24	51,58,60,70	0
5	GOL	B	105	6/6	0.66	0.15	34,44,54,69	0
7	PG4	C	322	13/13	0.67	0.13	51,57,66,73	0
7	PG4	A	326	13/13	0.67	0.17	42,55,77,85	0
5	GOL	C	311	6/6	0.67	0.15	54,73,88,92	0
9	PEG	B	134	7/7	0.68	0.15	46,61,76,88	0
9	PEG	A	341	7/7	0.68	0.20	42,51,64,67	0
6	NA	B	141	1/1	0.68	0.16	67,67,67,67	0
9	PEG	D	104	7/7	0.69	0.35	28,44,62,67	0
6	NA	A	356	1/1	0.69	0.12	49,49,49,49	0
7	PG4	A	323	13/13	0.69	0.12	67,76,84,87	0
5	GOL	B	104	6/6	0.70	0.14	40,42,57,60	0
9	PEG	A	335	7/7	0.70	0.15	34,48,58,62	0
7	PG4	A	324	13/13	0.70	0.12	43,55,70,80	0
7	PG4	C	324	13/13	0.70	0.13	57,68,77,81	0
6	NA	A	318	1/1	0.71	0.10	39,39,39,39	0
7	PG4	D	120	13/13	0.71	0.17	49,58,75,75	0
7	PG4	B	118	13/13	0.71	0.15	53,57,67,73	0
9	PEG	A	330	7/7	0.71	0.16	36,54,61,73	0
5	GOL	B	140	6/6	0.71	0.14	61,68,73,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	306	6/6	0.72	0.14	48,52,59,80	0
5	GOL	B	152	6/6	0.72	0.12	65,76,91,96	0
9	PEG	D	105	7/7	0.72	0.17	55,68,82,83	0
9	PEG	B	132	7/7	0.72	0.12	45,56,70,76	0
7	PG4	C	320	13/13	0.72	0.14	35,52,63,72	0
11	EDO	D	101	4/4	0.72	0.14	56,57,57,59	0
6	NA	B	150	1/1	0.73	0.13	40,40,40,40	0
7	PG4	D	117	13/13	0.73	0.13	30,52,68,73	0
6	NA	B	151	1/1	0.73	0.10	34,34,34,34	0
7	PG4	A	368	13/13	0.73	0.15	37,45,64,68	0
5	GOL	B	108	6/6	0.73	0.11	50,57,73,73	0
6	NA	E	112	1/1	0.73	0.15	58,58,58,58	0
7	PG4	C	302	13/13	0.73	0.17	42,57,82,91	0
5	GOL	C	309	6/6	0.73	0.13	29,43,50,74	0
9	PEG	A	339	7/7	0.73	0.16	45,54,63,67	0
5	GOL	E	104	6/6	0.73	0.13	74,76,79,82	0
5	GOL	D	110	6/6	0.74	0.17	48,64,67,74	0
7	PG4	E	106	13/13	0.74	0.14	26,50,62,68	0
6	NA	D	136	1/1	0.74	0.18	69,69,69,69	0
7	PG4	C	336	13/13	0.74	0.20	36,58,72,73	0
5	GOL	B	109	6/6	0.74	0.12	48,50,58,62	0
6	NA	C	343	1/1	0.74	0.09	34,34,34,34	0
5	GOL	A	362	6/6	0.75	0.18	23,36,45,55	0
9	PEG	D	127	7/7	0.75	0.15	46,60,68,71	0
10	PE8	A	342	25/25	0.75	0.11	40,65,79,86	0
9	PEG	A	336	7/7	0.75	0.10	44,50,69,70	0
5	GOL	A	345	6/6	0.75	0.19	41,53,53,56	0
9	PEG	A	332	7/7	0.75	0.11	54,56,65,69	0
9	PEG	A	333	7/7	0.76	0.13	43,50,70,80	0
7	PG4	B	125	13/13	0.76	0.12	49,57,66,79	0
6	NA	B	114	1/1	0.76	0.20	66,66,66,66	0
7	PG4	A	369	13/13	0.76	0.13	39,50,69,70	0
10	PE8	F	106	25/25	0.76	0.14	39,53,66,70	0
9	PEG	C	330	7/7	0.76	0.17	37,45,51,61	0
9	PEG	C	331	7/7	0.76	0.12	53,70,81,89	0
9	PEG	C	332	7/7	0.76	0.16	38,43,57,58	0
9	PEG	B	135	7/7	0.77	0.11	38,42,62,67	0
7	PG4	B	124	13/13	0.77	0.10	23,52,61,62	0
6	NA	C	341	1/1	0.77	0.13	61,61,61,61	0
5	GOL	B	103	6/6	0.77	0.15	55,59,70,86	0
9	PEG	A	329	7/7	0.77	0.18	42,58,66,72	0
9	PEG	A	371	7/7	0.77	0.17	40,44,55,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	PEG	D	121	7/7	0.77	0.14	31,44,65,66	0
5	GOL	C	307	6/6	0.77	0.16	67,72,78,86	0
9	PEG	D	128	7/7	0.77	0.19	37,41,59,63	0
6	NA	D	135	1/1	0.77	0.07	50,50,50,50	0
10	PE8	A	344	25/25	0.77	0.12	31,56,73,77	0
10	PE8	B	102	25/25	0.77	0.11	31,48,62,80	0
9	PEG	B	130	7/7	0.77	0.12	41,44,60,69	0
5	GOL	C	314	6/6	0.77	0.09	37,58,65,69	0
5	GOL	D	131	6/6	0.77	0.14	58,64,84,96	0
11	EDO	B	144	4/4	0.77	0.21	57,72,74,74	0
5	GOL	C	338	6/6	0.77	0.11	24,60,69,74	0
11	EDO	E	111	4/4	0.77	0.13	51,54,62,68	0
7	PG4	D	118	13/13	0.78	0.11	32,51,72,73	0
9	PEG	C	333	7/7	0.78	0.33	50,53,54,71	0
9	PEG	C	327	7/7	0.78	0.11	45,52,64,80	0
10	PE8	A	343	25/25	0.78	0.11	31,41,55,63	0
7	PG4	D	103	13/13	0.78	0.13	53,66,75,78	0
5	GOL	A	303	6/6	0.78	0.14	55,62,66,68	0
9	PEG	D	126	7/7	0.79	0.16	47,57,74,79	0
7	PG4	B	155	13/13	0.79	0.12	35,41,52,55	0
5	GOL	B	107	6/6	0.79	0.12	48,51,54,59	0
6	NA	C	340	1/1	0.79	0.09	34,34,34,34	0
5	GOL	A	301	6/6	0.79	0.09	46,57,59,60	0
9	PEG	C	329	7/7	0.79	0.15	50,53,59,63	0
7	PG4	B	119	13/13	0.79	0.15	36,54,64,64	0
10	PE8	F	102	25/25	0.79	0.11	40,52,65,82	0
7	PG4	E	114	13/13	0.79	0.13	35,54,72,83	0
7	PG4	C	325	13/13	0.79	0.21	46,56,70,75	0
6	NA	B	113	1/1	0.79	0.10	45,45,45,45	0
9	PEG	A	331	7/7	0.79	0.16	53,62,75,78	0
7	PG4	A	322	13/13	0.79	0.15	38,53,58,62	0
7	PG4	D	116	13/13	0.79	0.14	19,41,61,79	0
6	NA	C	318	1/1	0.80	0.09	40,40,40,40	0
8	SO4	A	327	5/5	0.80	0.10	56,57,68,74	0
9	PEG	C	339	7/7	0.80	0.12	38,44,54,55	0
10	PE8	B	136	25/25	0.80	0.11	34,62,80,86	0
10	PE8	E	110	25/25	0.80	0.11	40,51,63,64	0
6	NA	D	132	1/1	0.80	0.06	24,24,24,24	0
5	GOL	C	312	6/6	0.80	0.12	40,68,71,72	0
5	GOL	A	305	6/6	0.80	0.11	22,25,29,37	0
9	PEG	A	353	7/7	0.80	0.11	39,52,64,65	0
7	PG4	B	120	13/13	0.80	0.12	36,48,53,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NA	A	317	1/1	0.80	0.17	55,55,55,55	0
7	PG4	A	320	13/13	0.80	0.08	22,45,63,64	0
7	PG4	C	319	13/13	0.81	0.14	31,50,66,67	0
7	PG4	A	321	13/13	0.81	0.12	47,57,71,81	0
7	PG4	A	352	13/13	0.81	0.11	49,59,68,68	0
7	PG4	D	119	13/13	0.81	0.10	37,50,65,74	0
5	GOL	C	310	6/6	0.81	0.16	47,62,77,95	0
5	GOL	C	306	6/6	0.81	0.14	48,60,77,81	0
5	GOL	A	314	6/6	0.81	0.11	31,47,73,77	0
5	GOL	A	302	6/6	0.81	0.14	40,44,59,66	0
7	PG4	F	105	13/13	0.81	0.12	38,54,62,63	0
11	EDO	D	130	4/4	0.81	0.10	44,57,58,61	0
9	PEG	C	334	7/7	0.81	0.15	41,56,68,69	0
5	GOL	B	153	6/6	0.82	0.09	44,45,46,53	0
7	PG4	B	122	13/13	0.82	0.10	41,53,65,74	0
6	NA	C	317	1/1	0.82	0.07	36,36,36,36	0
6	NA	B	146	1/1	0.82	0.12	45,45,45,45	0
7	PG4	C	323	13/13	0.82	0.11	38,48,66,69	0
7	PG4	E	115	13/13	0.82	0.09	59,67,73,82	0
9	PEG	A	370	7/7	0.82	0.18	28,33,54,57	0
9	PEG	B	157	7/7	0.82	0.09	42,49,65,73	0
5	GOL	E	113	6/6	0.82	0.09	46,52,57,64	0
9	PEG	A	334	7/7	0.83	0.09	36,45,65,78	0
5	GOL	C	344	6/6	0.83	0.10	27,53,58,61	0
7	PG4	A	319	13/13	0.83	0.09	44,54,68,69	0
7	PG4	B	121	13/13	0.83	0.11	46,55,78,83	0
8	SO4	C	326	5/5	0.83	0.08	60,62,71,98	0
9	PEG	C	346	7/7	0.83	0.10	36,42,53,62	0
5	GOL	C	347	6/6	0.83	0.13	33,49,62,75	0
5	GOL	A	307	6/6	0.83	0.14	56,64,75,84	0
5	GOL	B	111	6/6	0.83	0.07	57,72,83,87	0
9	PEG	C	303	7/7	0.83	0.10	32,44,66,69	0
5	GOL	C	304	6/6	0.83	0.14	44,54,59,71	0
11	EDO	D	102	4/4	0.83	0.21	62,66,73,90	0
5	GOL	A	308	6/6	0.83	0.10	29,32,36,52	0
9	PEG	A	372	7/7	0.83	0.09	44,45,48,51	0
5	GOL	D	109	6/6	0.84	0.08	36,53,66,77	0
5	GOL	A	310	6/6	0.84	0.15	38,49,51,68	0
7	PG4	B	116	13/13	0.84	0.11	27,45,56,64	0
9	PEG	B	139	7/7	0.84	0.10	34,38,45,46	0
9	PEG	B	142	7/7	0.84	0.09	33,37,41,49	0
5	GOL	D	112	6/6	0.84	0.11	25,44,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NA	A	315	1/1	0.84	0.11	38,38,38,38	0
9	PEG	D	123	7/7	0.84	0.09	51,55,61,66	0
7	PG4	F	101	13/13	0.84	0.10	43,56,74,75	0
5	GOL	A	363	6/6	0.84	0.07	34,45,54,54	0
5	GOL	C	313	6/6	0.84	0.10	38,45,56,59	0
5	GOL	A	347	6/6	0.84	0.14	60,71,75,79	0
8	SO4	E	108	5/5	0.84	0.09	41,52,66,72	0
5	GOL	B	110	6/6	0.85	0.15	51,55,62,69	0
7	PG4	E	107	13/13	0.85	0.10	50,58,68,69	0
6	NA	A	348	1/1	0.85	0.10	51,51,51,51	0
7	PG4	A	367	13/13	0.85	0.10	27,42,62,62	0
7	PG4	B	117	13/13	0.85	0.09	39,51,59,61	0
6	NA	A	359	1/1	0.85	0.10	58,58,58,58	0
7	PG4	C	321	13/13	0.85	0.10	34,41,56,59	0
9	PEG	D	124	7/7	0.85	0.09	24,38,50,54	0
9	PEG	D	125	7/7	0.85	0.15	29,34,63,65	0
9	PEG	C	328	7/7	0.86	0.10	39,43,55,60	0
6	NA	D	134	1/1	0.86	0.08	37,37,37,37	0
7	PG4	A	366	13/13	0.86	0.08	35,47,70,80	0
6	NA	B	115	1/1	0.86	0.25	55,55,55,55	0
9	PEG	B	156	7/7	0.86	0.09	25,42,51,56	0
7	PG4	B	123	13/13	0.86	0.10	29,41,58,62	0
5	GOL	C	337	6/6	0.86	0.15	39,43,61,67	0
10	PE8	C	335	25/25	0.86	0.10	36,49,61,76	0
5	GOL	B	106	6/6	0.86	0.09	34,45,62,70	0
6	NA	A	349	1/1	0.87	0.12	32,32,32,32	0
7	PG4	A	365	13/13	0.87	0.10	34,39,52,57	0
6	NA	B	148	1/1	0.87	0.08	39,39,39,39	0
9	PEG	B	127	7/7	0.87	0.12	23,29,56,59	0
5	GOL	A	312	6/6	0.87	0.09	38,49,55,56	0
5	GOL	A	311	6/6	0.87	0.10	27,30,31,36	0
9	PEG	A	340	7/7	0.87	0.12	43,47,61,68	0
9	PEG	B	131	7/7	0.87	0.11	42,52,72,73	0
8	SO4	C	301	5/5	0.87	0.12	71,72,72,92	0
6	NA	C	342	1/1	0.87	0.12	24,24,24,24	0
11	EDO	E	101	4/4	0.87	0.07	31,49,56,73	0
9	PEG	D	122	7/7	0.87	0.13	31,41,60,62	0
6	NA	F	107	1/1	0.88	0.07	35,35,35,35	0
6	NA	A	358	1/1	0.88	0.07	47,47,47,47	0
5	GOL	E	102	6/6	0.88	0.10	32,44,53,64	0
5	GOL	D	106	6/6	0.88	0.08	19,39,51,54	0
5	GOL	C	345	6/6	0.88	0.09	37,44,54,61	0

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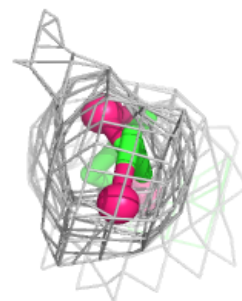
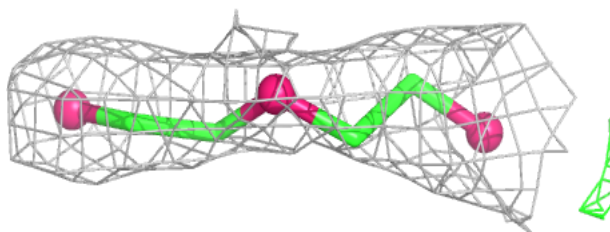
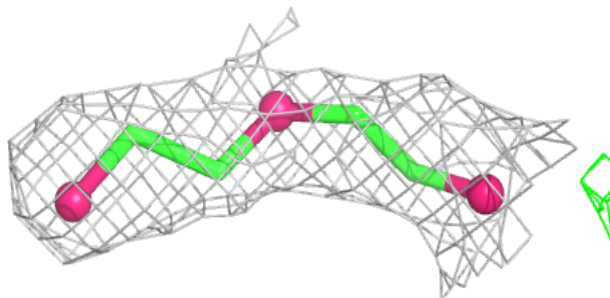
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NA	C	315	1/1	0.88	0.07	33,33,33,33	0
6	NA	C	316	1/1	0.88	0.12	60,60,60,60	0
5	GOL	D	108	6/6	0.88	0.13	49,57,62,62	0
5	GOL	A	373	6/6	0.88	0.09	47,54,60,71	0
5	GOL	D	137	6/6	0.88	0.08	24,32,38,57	0
10	PE8	E	109	25/25	0.88	0.08	27,46,67,71	0
5	GOL	A	364	6/6	0.89	0.09	36,43,49,55	0
5	GOL	A	304	6/6	0.89	0.08	38,44,50,55	0
6	NA	D	129	1/1	0.89	0.20	82,82,82,82	0
10	PE8	B	137	25/25	0.89	0.08	20,49,64,72	0
10	PE8	B	138	25/25	0.89	0.08	32,49,67,70	0
6	NA	F	104	1/1	0.89	0.12	36,36,36,36	0
5	GOL	B	112	6/6	0.89	0.08	38,51,58,61	0
5	GOL	A	309	6/6	0.89	0.09	22,32,34,47	0
8	SO4	A	328	5/5	0.89	0.09	43,55,61,65	0
5	GOL	A	313	6/6	0.90	0.07	31,40,43,47	0
9	PEG	B	126	7/7	0.90	0.10	48,56,70,75	0
6	NA	B	147	1/1	0.90	0.07	34,34,34,34	0
9	PEG	A	346	7/7	0.90	0.10	35,41,69,80	0
5	GOL	D	111	6/6	0.91	0.10	42,47,54,60	0
6	NA	A	316	1/1	0.91	0.14	29,29,29,29	0
5	GOL	C	308	6/6	0.91	0.08	29,35,48,52	0
9	PEG	B	158	7/7	0.91	0.07	10,26,37,38	0
6	NA	B	145	1/1	0.91	0.06	54,54,54,54	0
6	NA	A	357	1/1	0.92	0.05	21,21,21,21	0
5	GOL	B	154	6/6	0.92	0.11	23,26,27,31	0
6	NA	D	133	1/1	0.93	0.04	22,22,22,22	0
6	NA	D	115	1/1	0.93	0.07	31,31,31,31	0
6	NA	A	350	1/1	0.94	0.06	30,30,30,30	0
6	NA	B	149	1/1	0.94	0.06	33,33,33,33	0
6	NA	A	354	1/1	0.97	0.10	22,22,22,22	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 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)

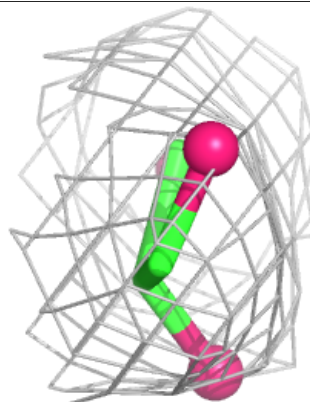
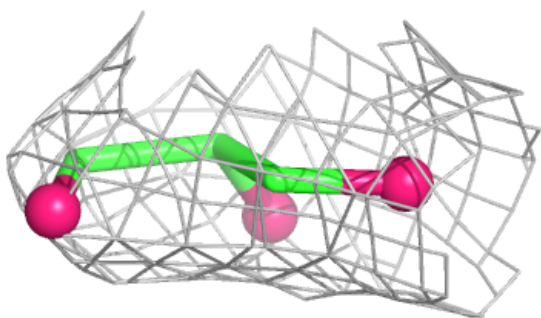
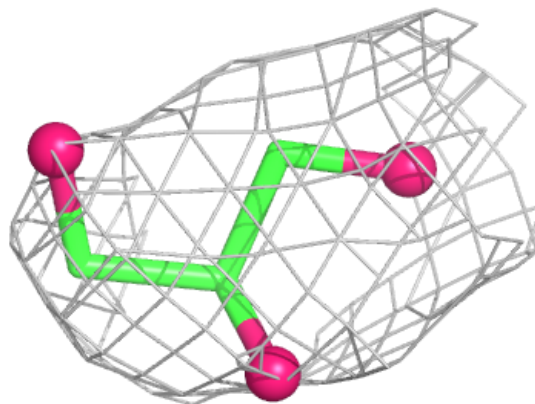
**Electron density around EDO B 143:**

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



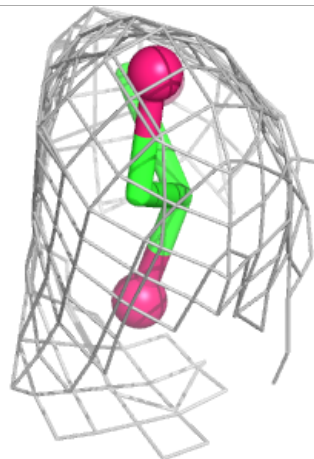
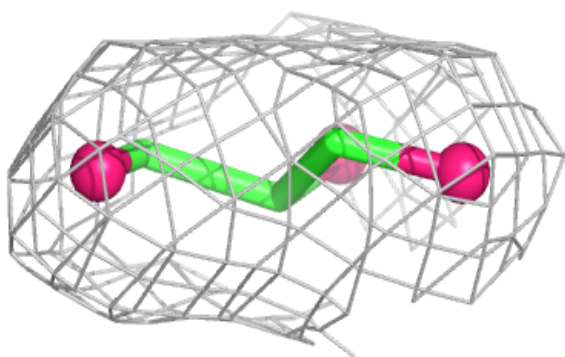
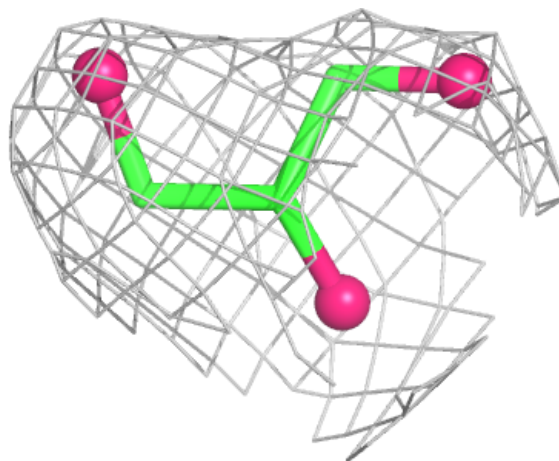
Electron density around GOL C 305:

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



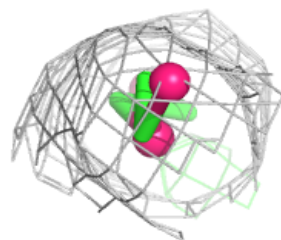
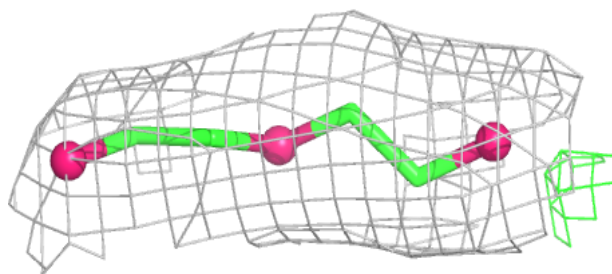
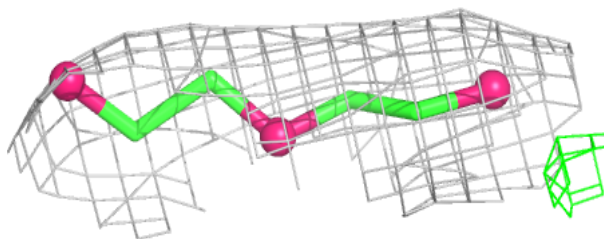
Electron density around GOL D 113:

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

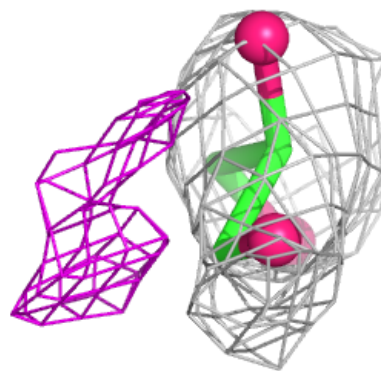
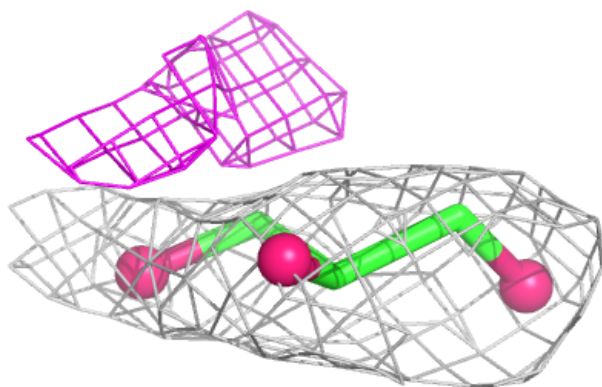
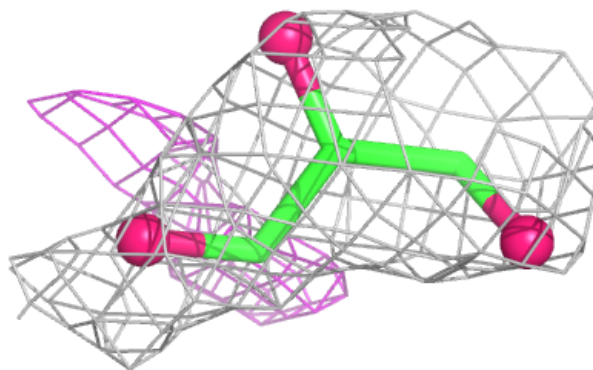


Electron density around PEG A 338:

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

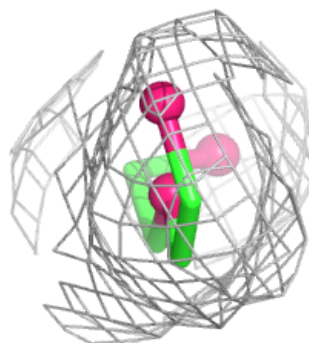
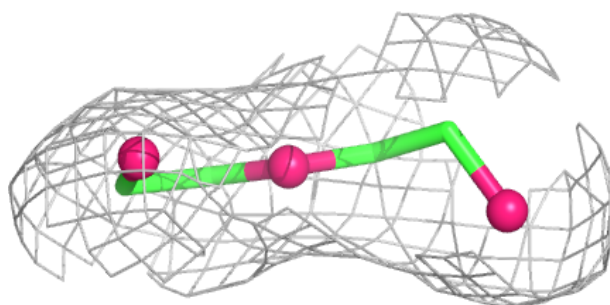
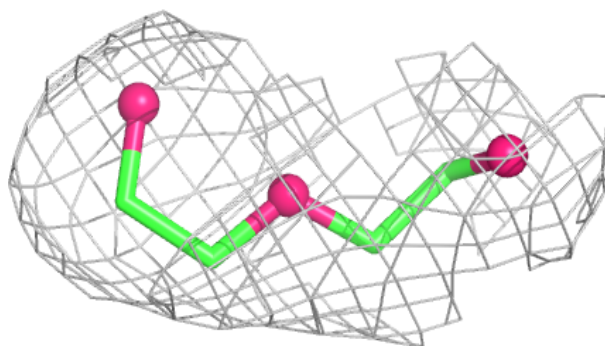
**Electron density around GOL F 103:**

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

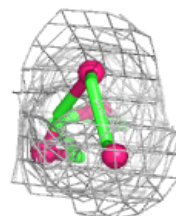
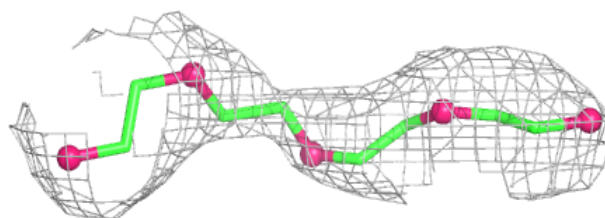


Electron density around PEG B 128:

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

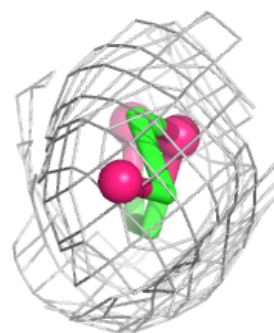
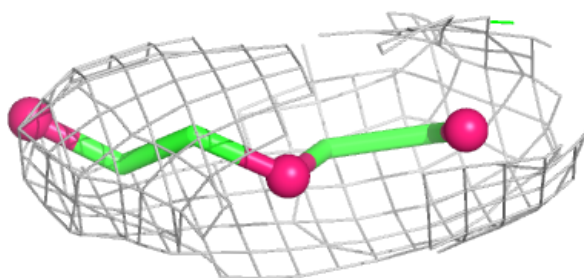
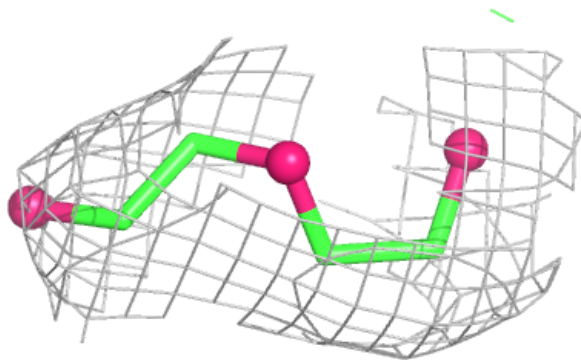
**Electron density around PG4 E 105:**

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



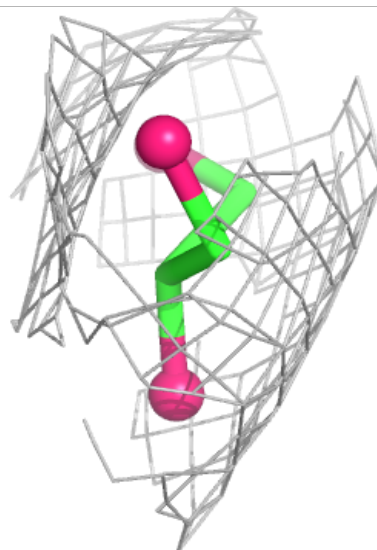
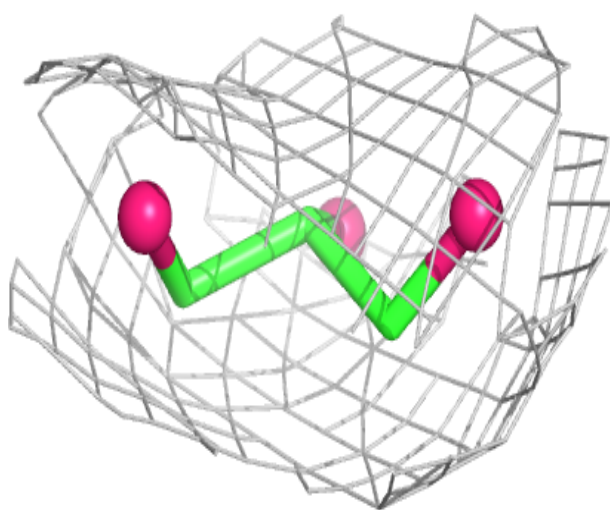
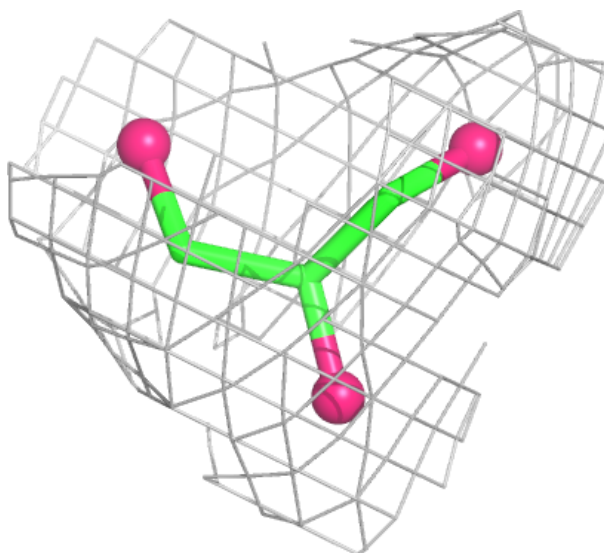
Electron density around PEG B 133:

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



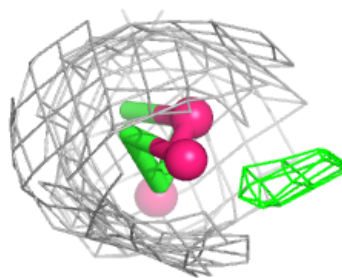
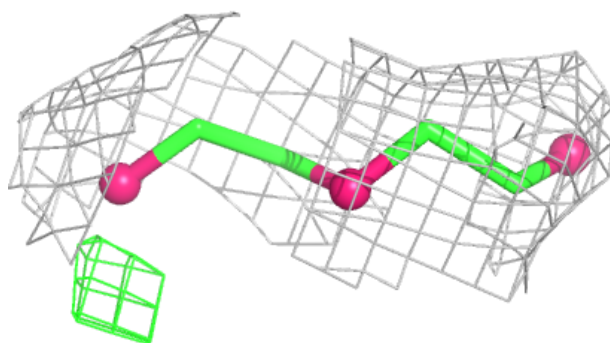
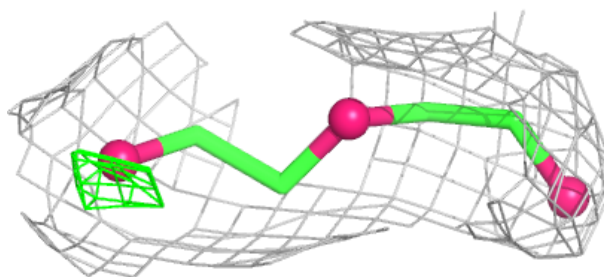
Electron density around GOL D 107:

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



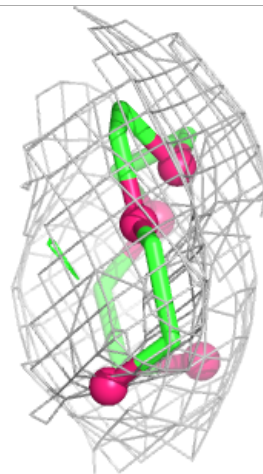
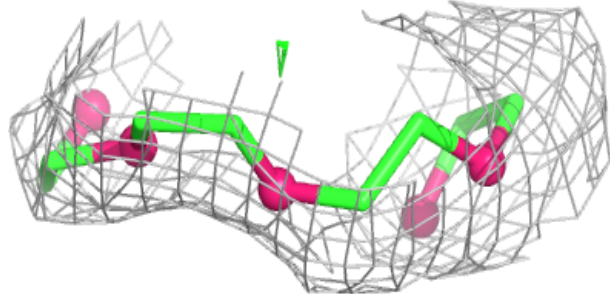
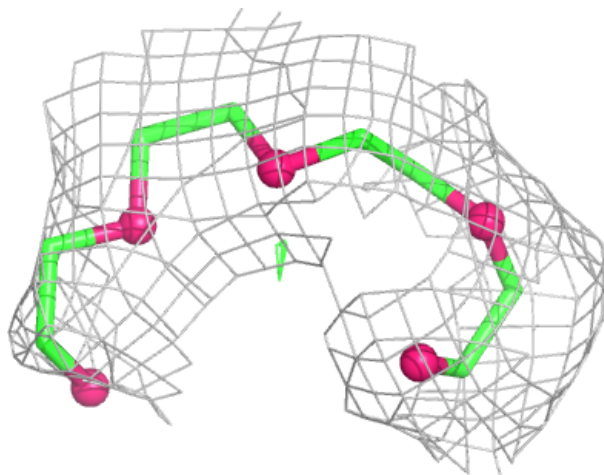
Electron density around PEG A 337:

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



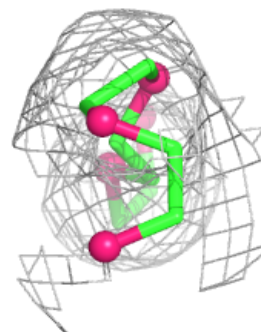
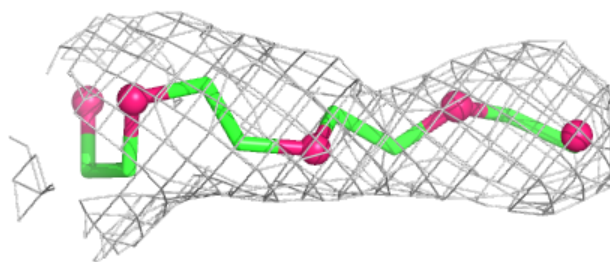
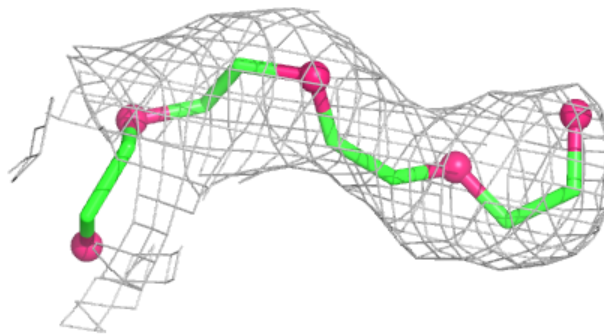
Electron density around PG4 B 101:

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



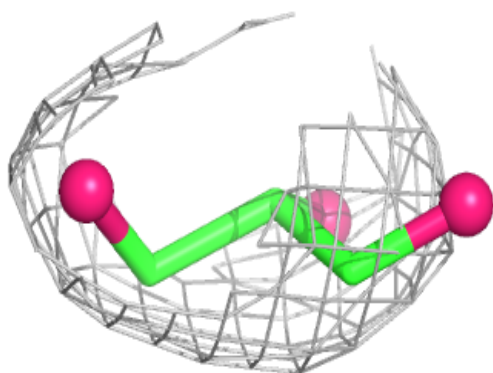
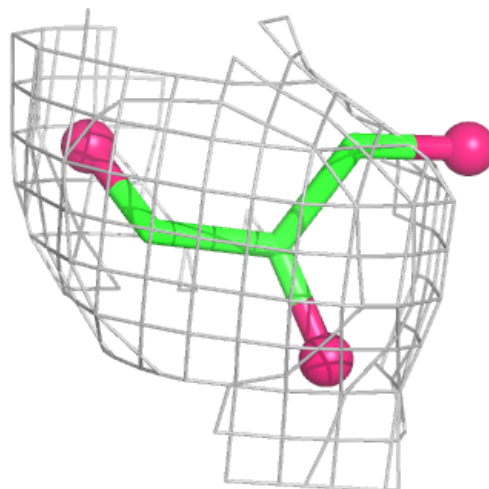
Electron density around PG4 A 325:

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



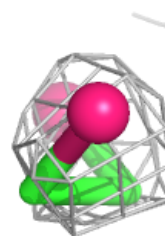
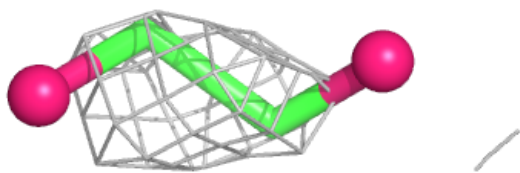
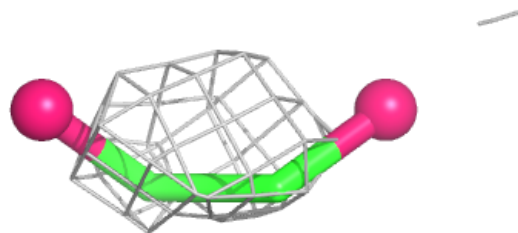
Electron density around GOL E 103:

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



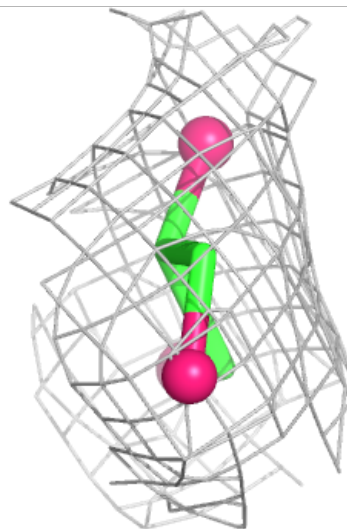
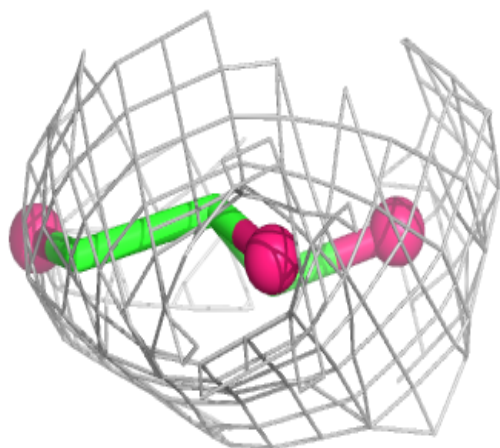
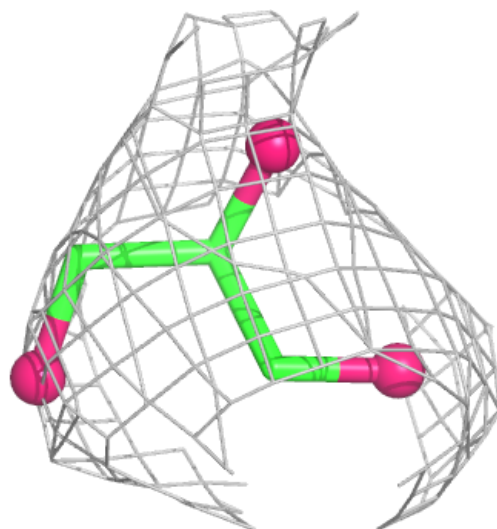
Electron density around EDO A 351:

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



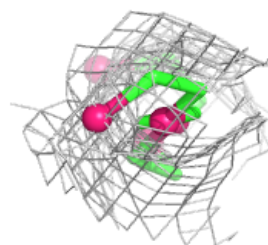
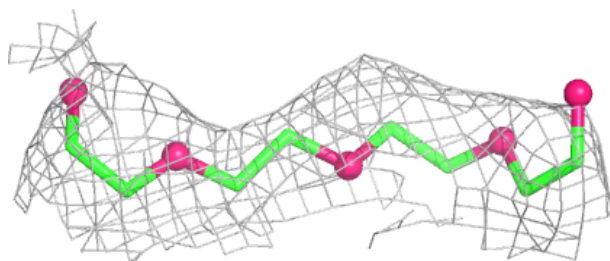
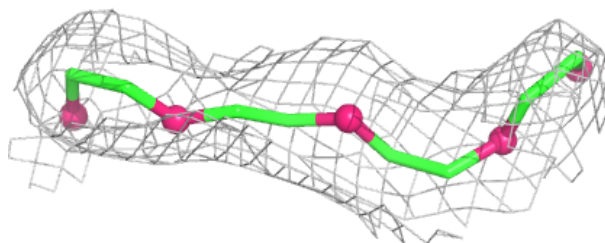
Electron density around GOL B 105:

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

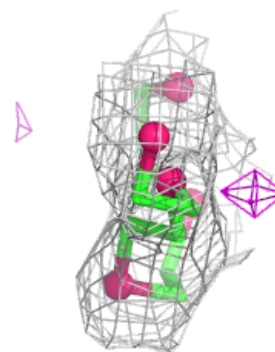
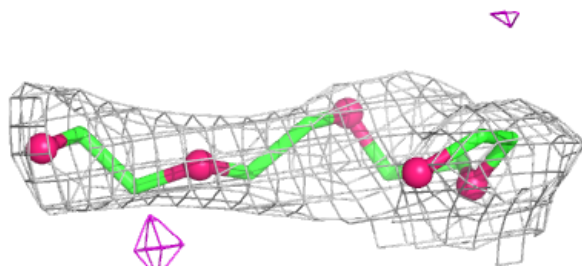
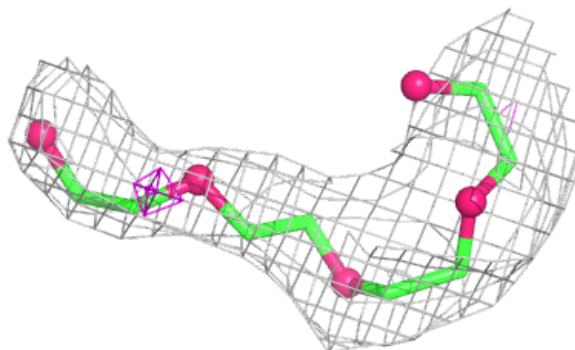


Electron density around PG4 C 322:

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

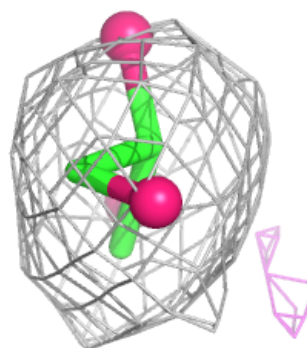
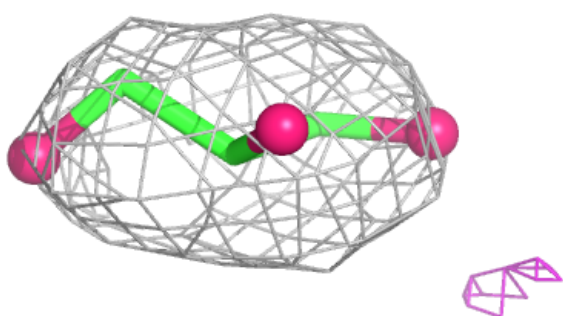
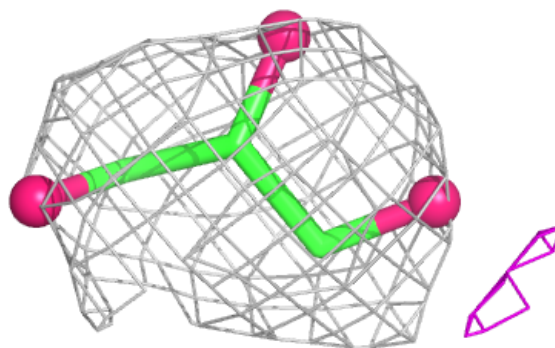
**Electron density around PG4 A 326:**

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

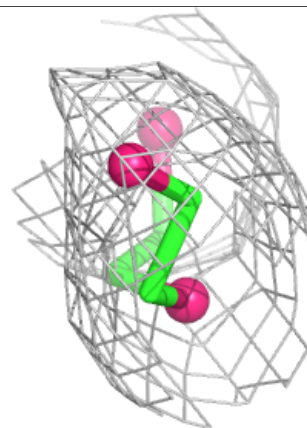
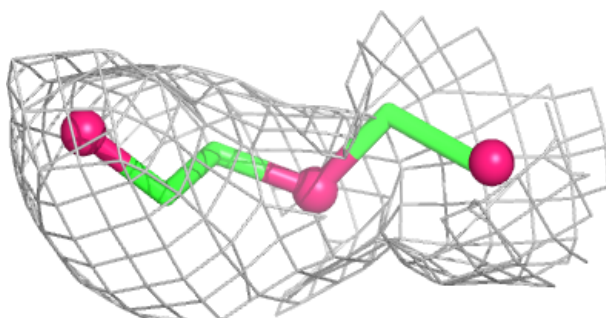
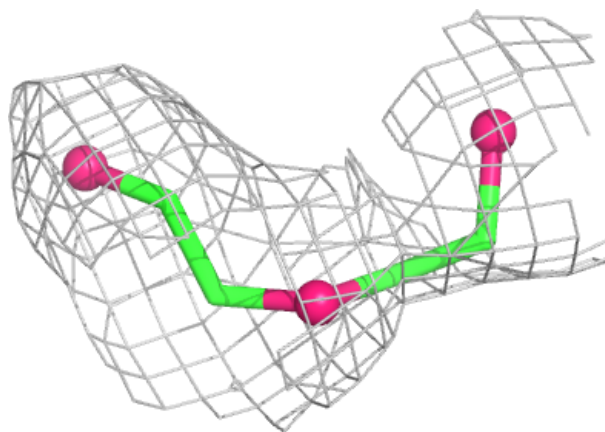


Electron density around GOL C 311:

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

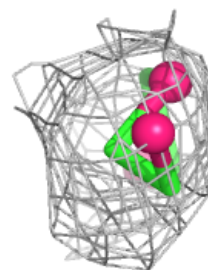
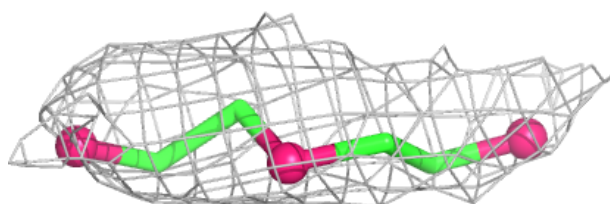
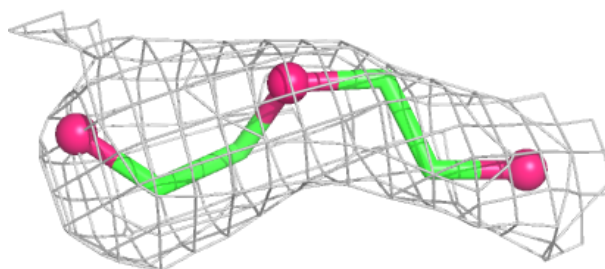
**Electron density around PEG B 134:**

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

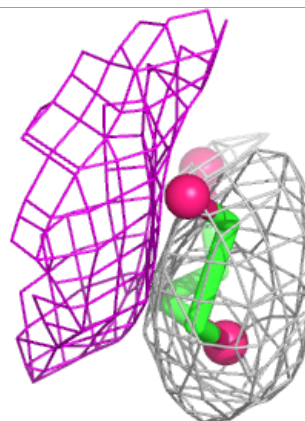
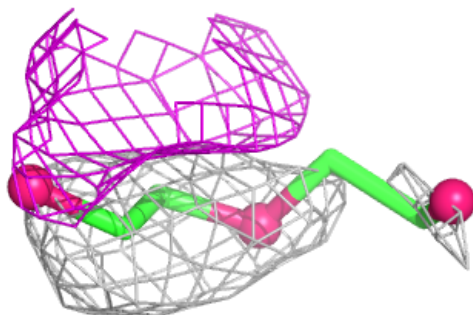
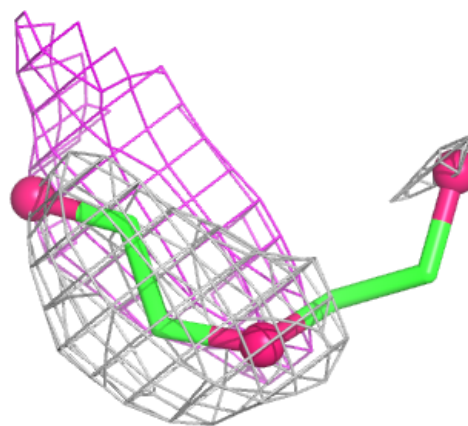


Electron density around PEG A 341:

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

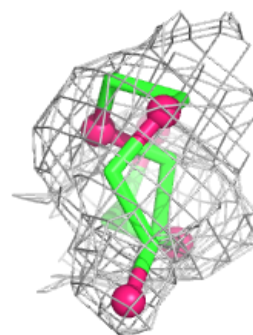
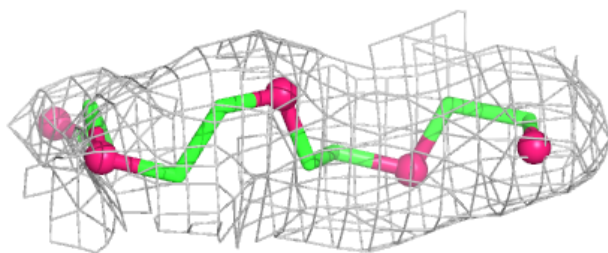
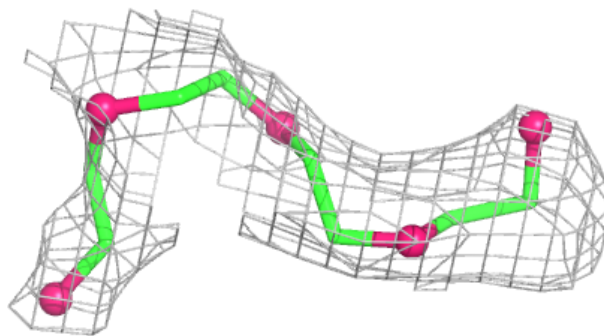
**Electron density around PEG D 104:**

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

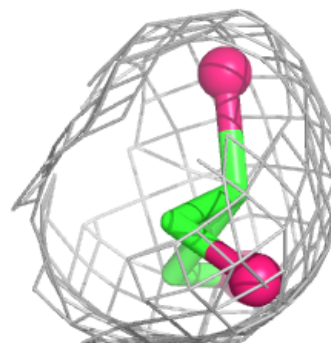
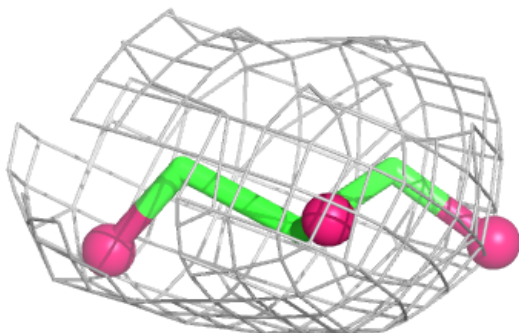
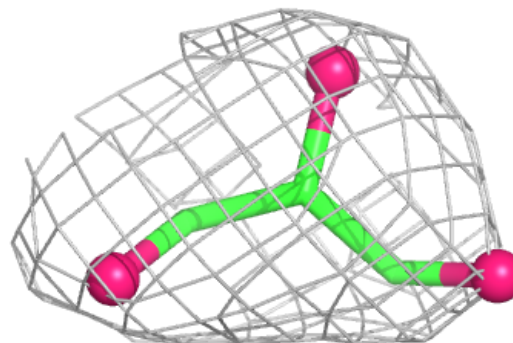


Electron density around PG4 A 323:

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

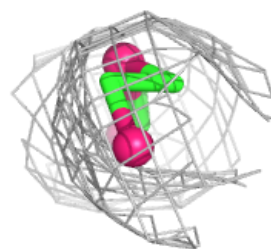
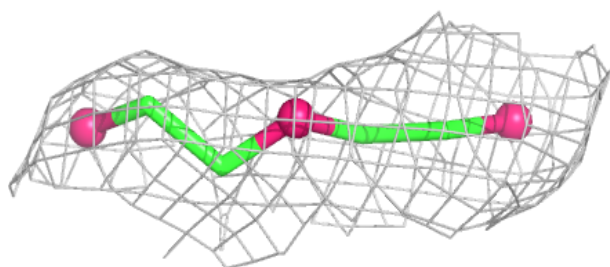
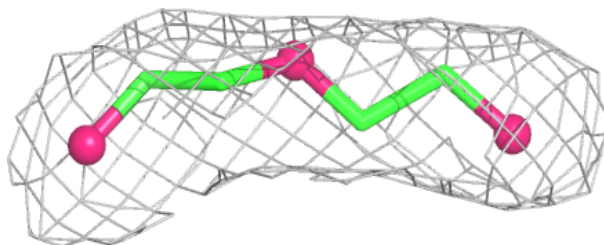
**Electron density around GOL B 104:**

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

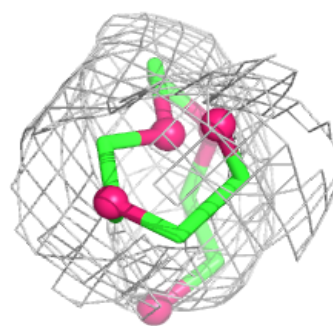
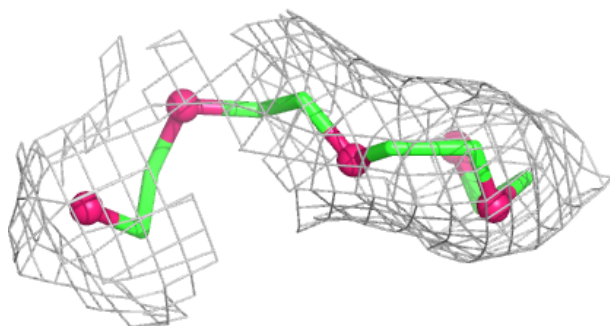
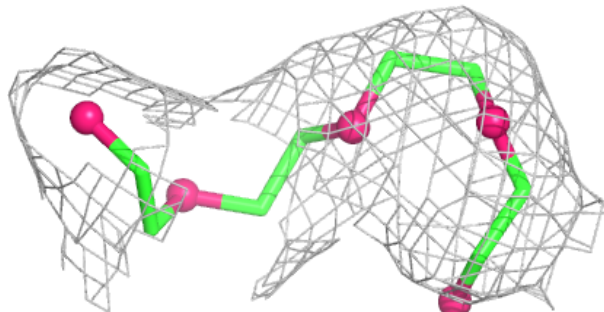


Electron density around PEG A 335:

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

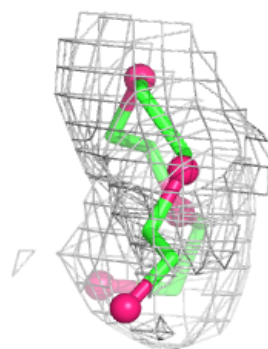
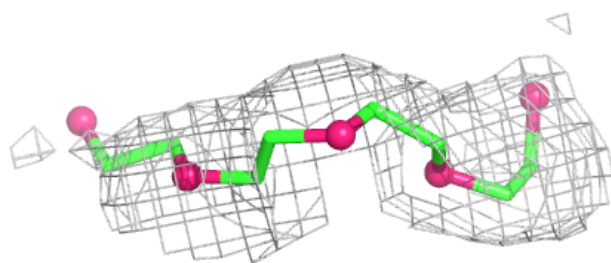
**Electron density around PG4 A 324:**

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

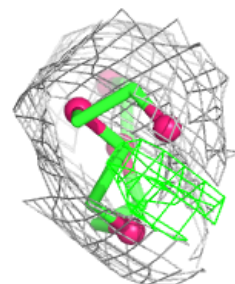
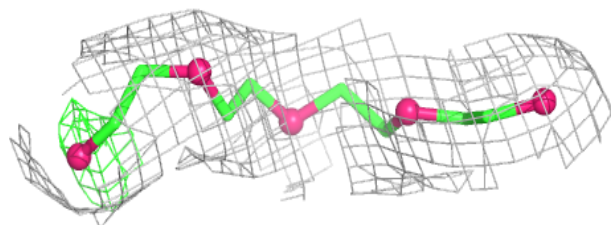
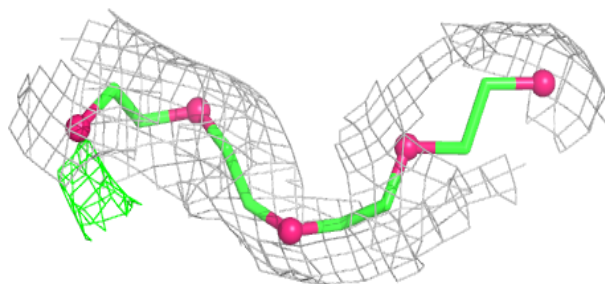


Electron density around PG4 C 324:

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

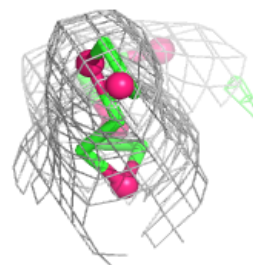
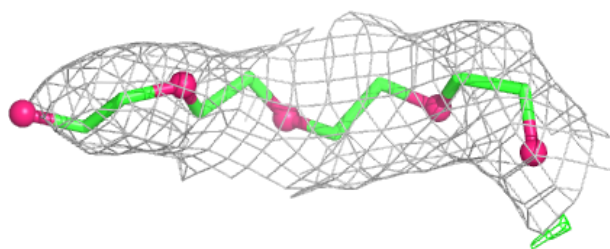
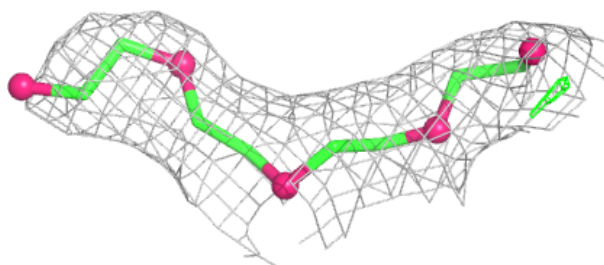
**Electron density around PG4 D 120:**

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

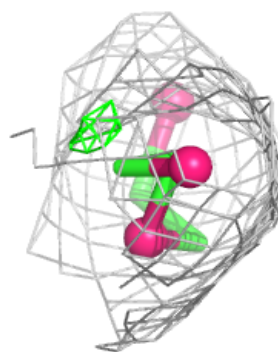
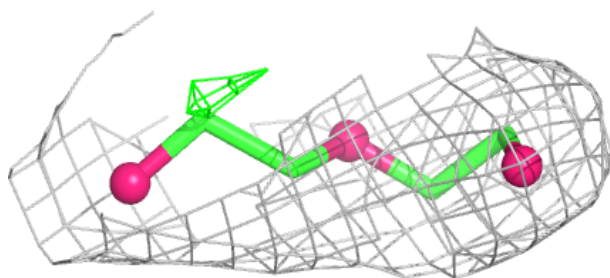
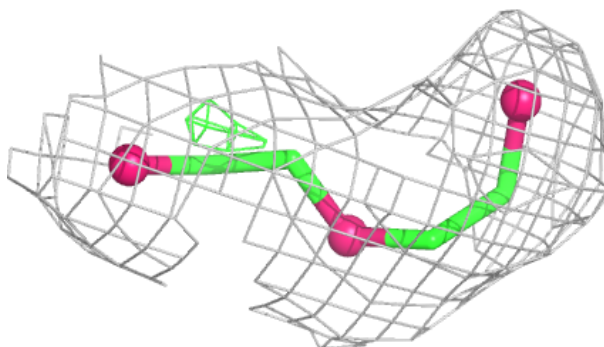


Electron density around PG4 B 118:

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

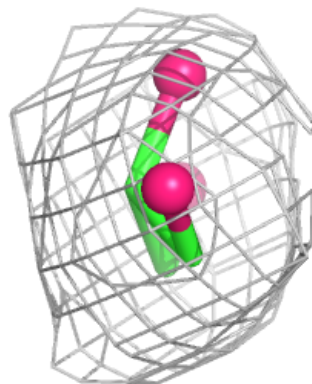
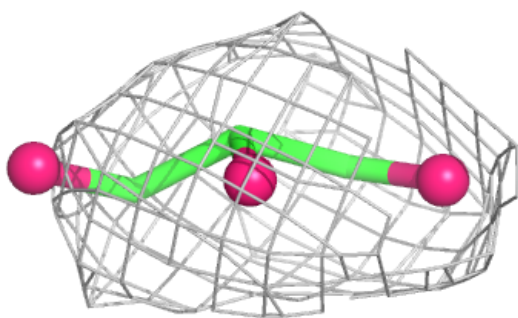
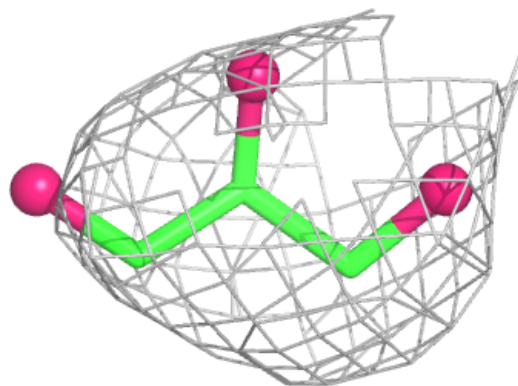
**Electron density around PEG A 330:**

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



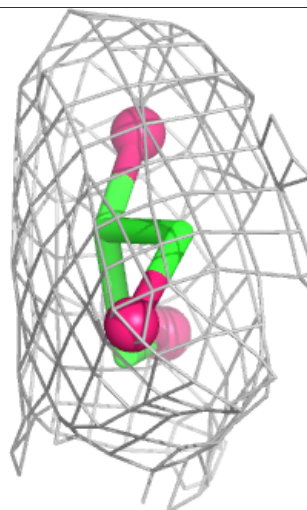
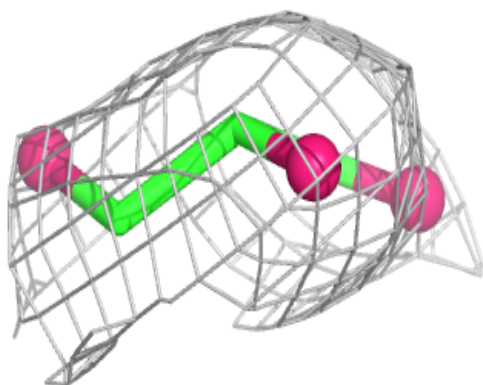
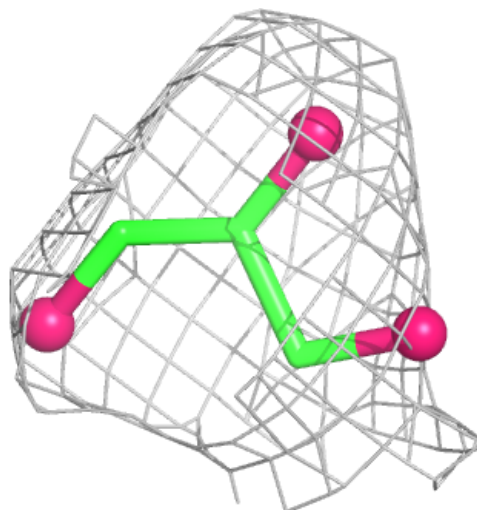
Electron density around GOL B 140:

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



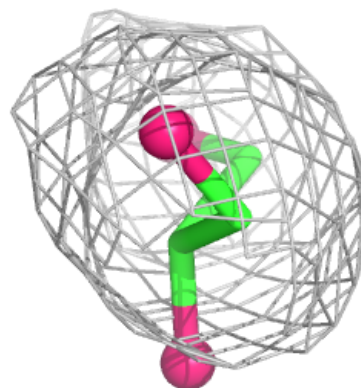
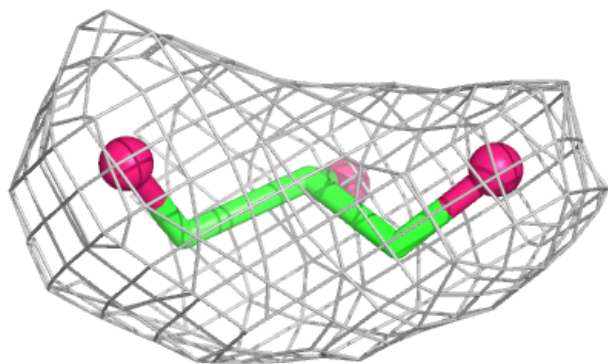
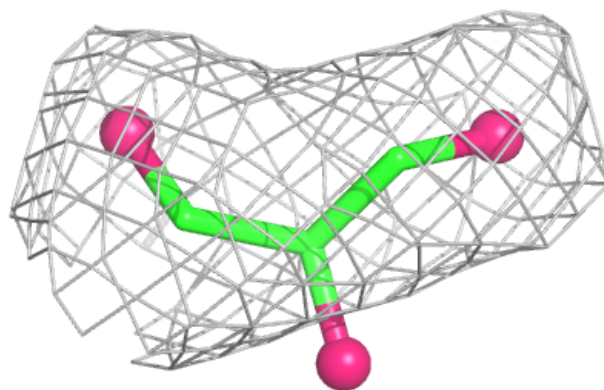
Electron density around GOL A 306:

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

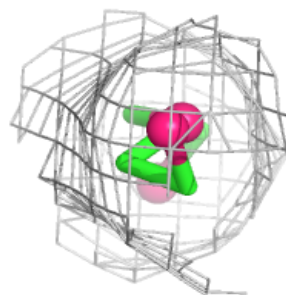
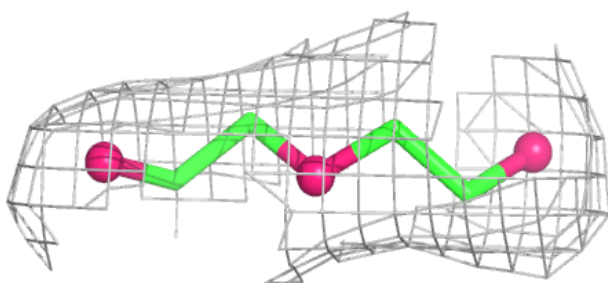
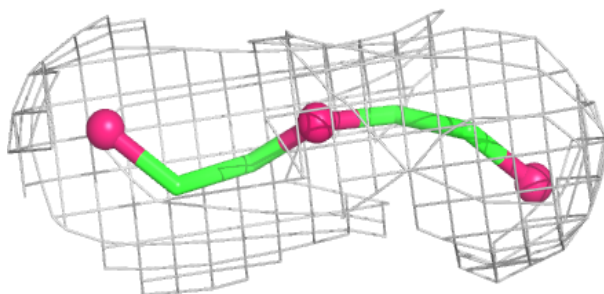


Electron density around GOL B 152:

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

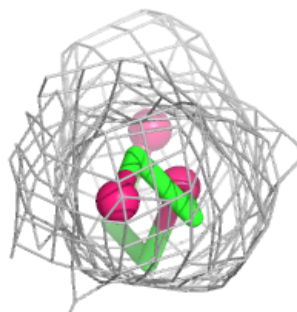
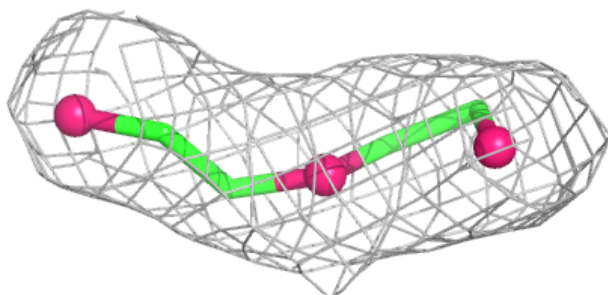
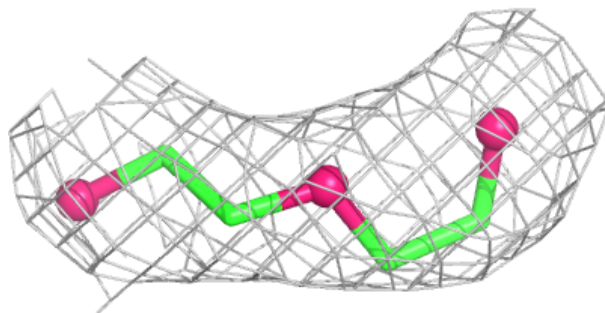
**Electron density around PEG D 105:**

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

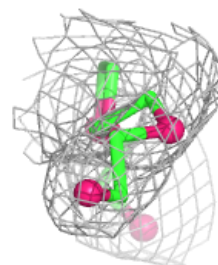
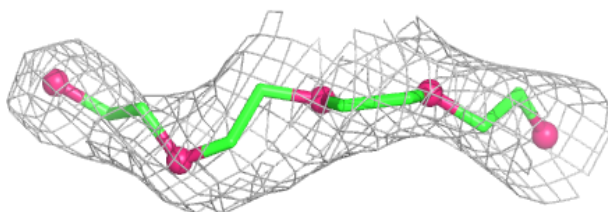
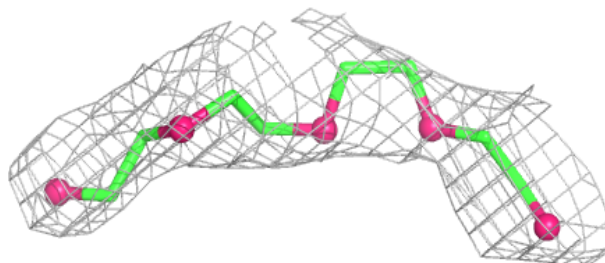


Electron density around PEG B 132:

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

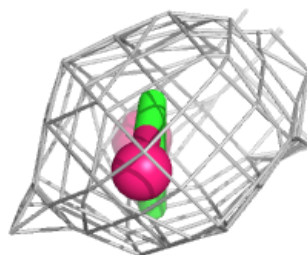
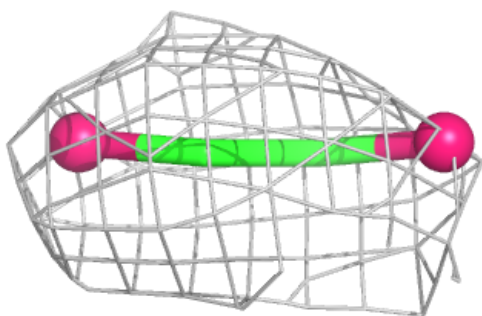
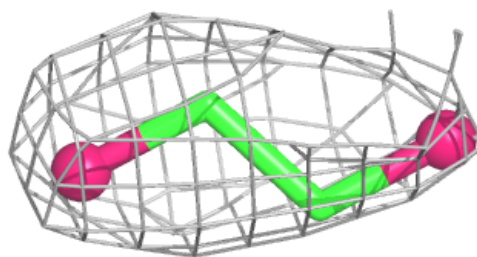
**Electron density around PG4 C 320:**

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

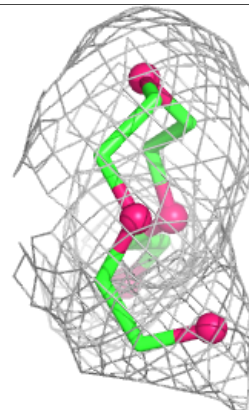
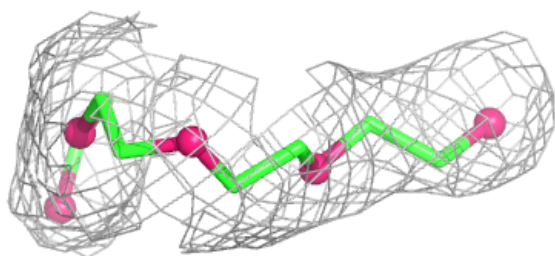
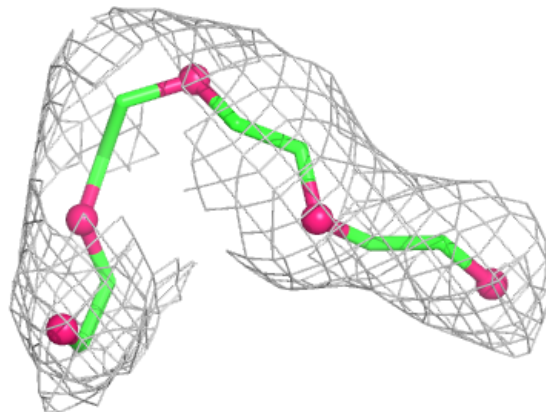


Electron density around EDO D 101:

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

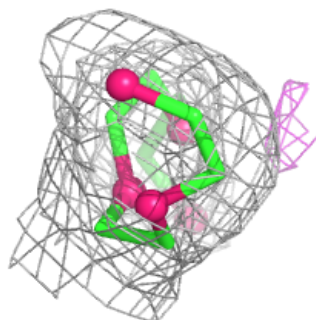
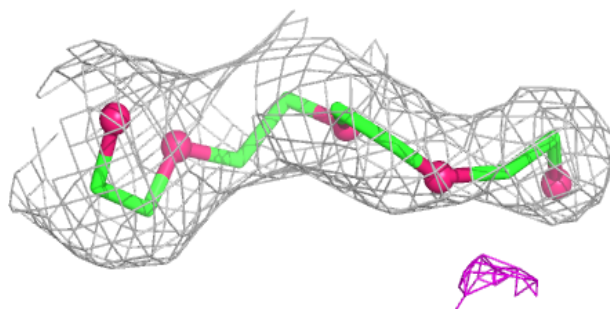
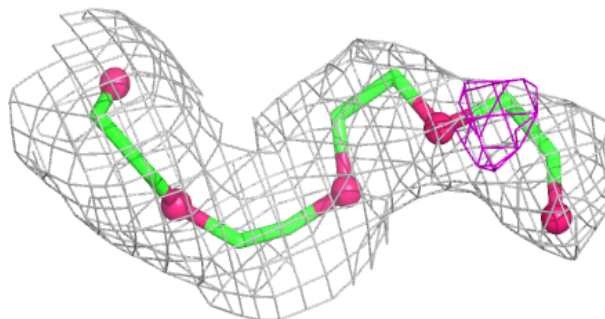
**Electron density around PG4 D 117:**

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

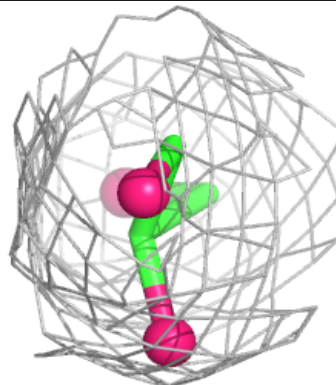
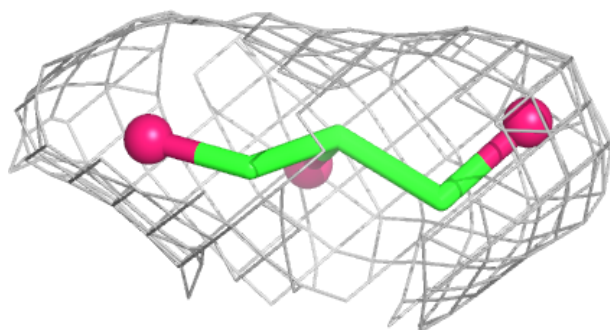
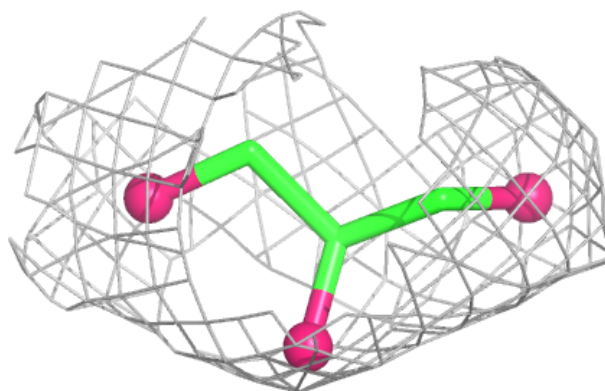


Electron density around PG4 A 368:

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

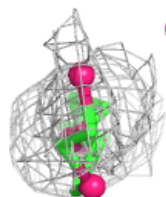
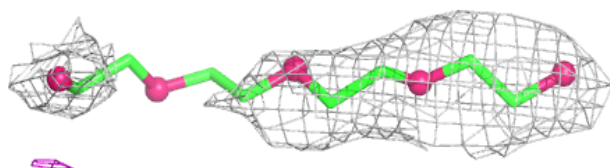
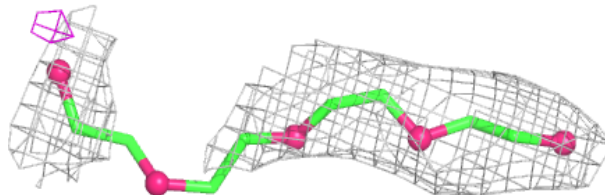
**Electron density around GOL B 108:**

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

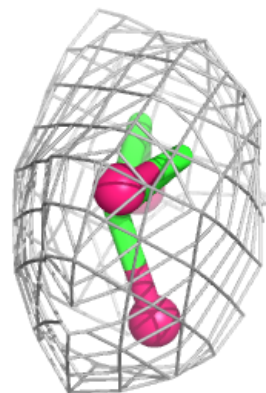
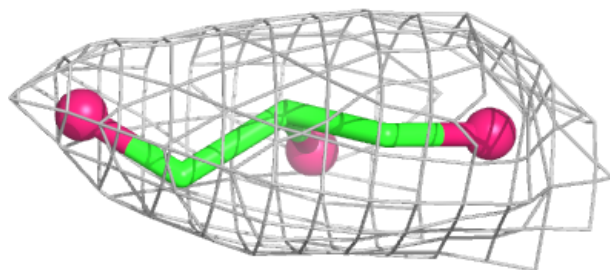
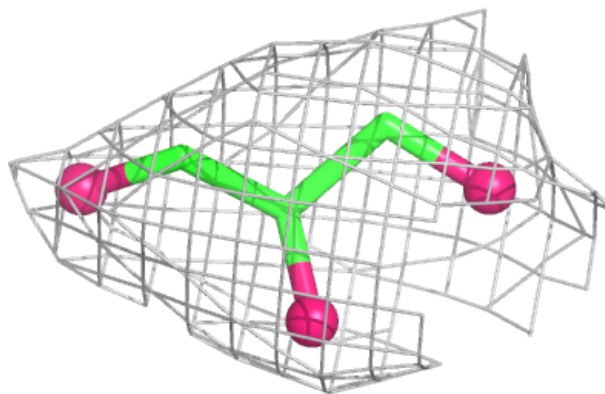


Electron density around PG4 C 302:

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

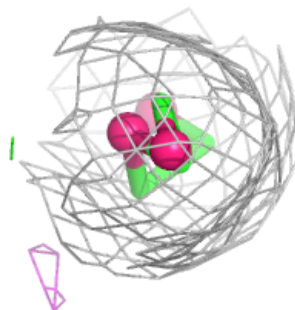
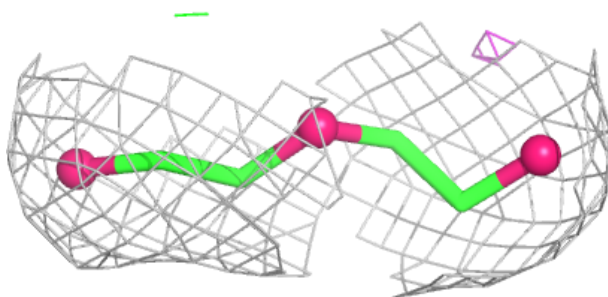
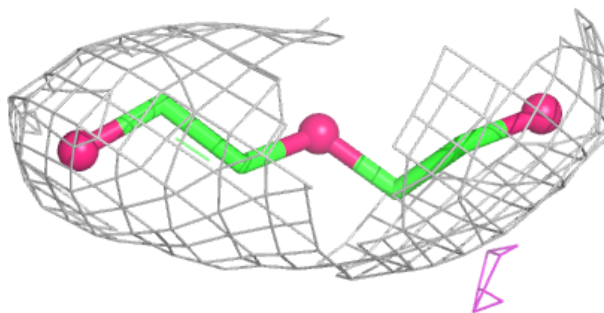
**Electron density around GOL C 309:**

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



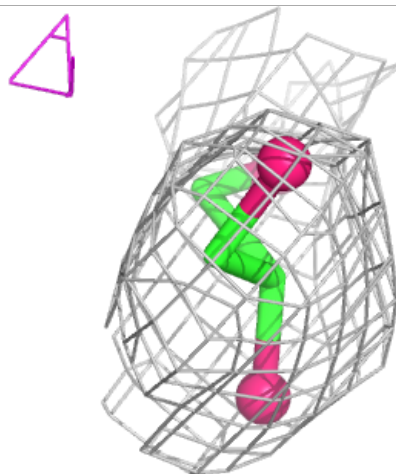
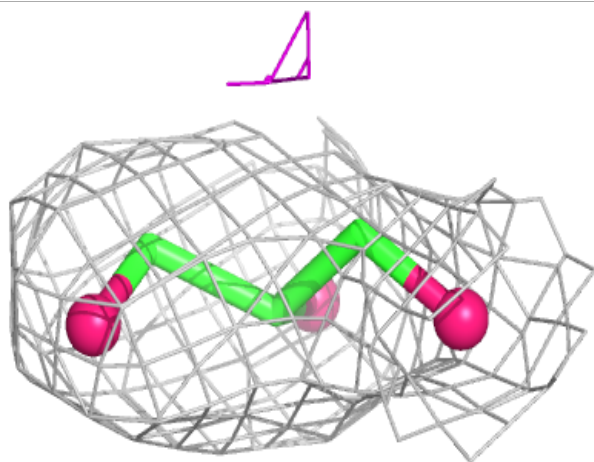
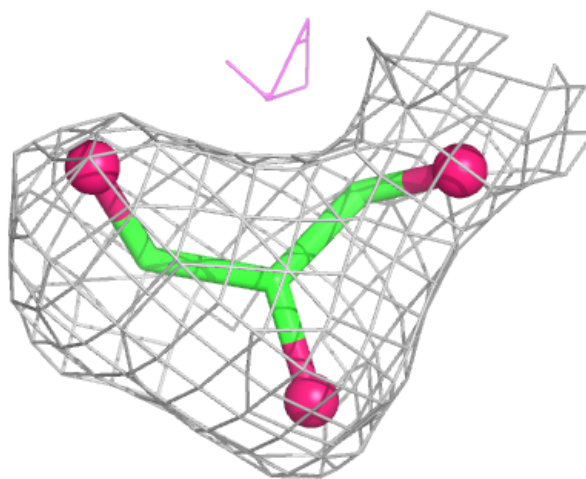
Electron density around PEG A 339:

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



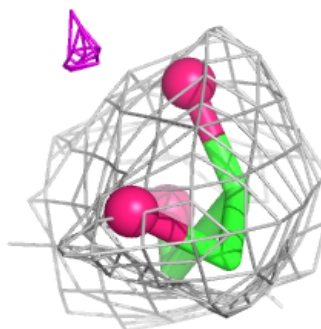
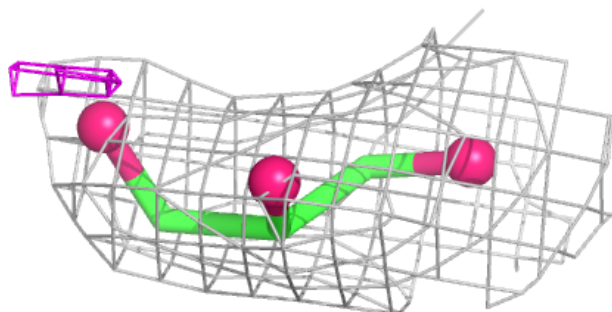
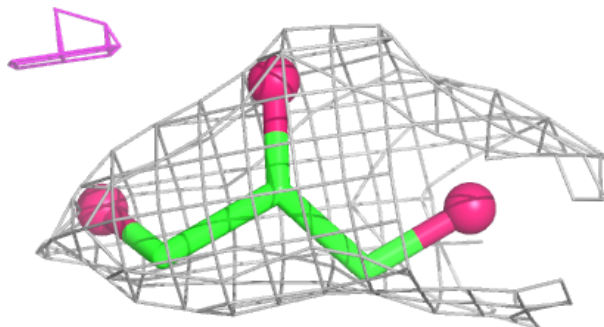
Electron density around GOL E 104:

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

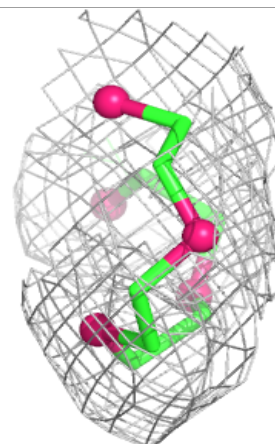
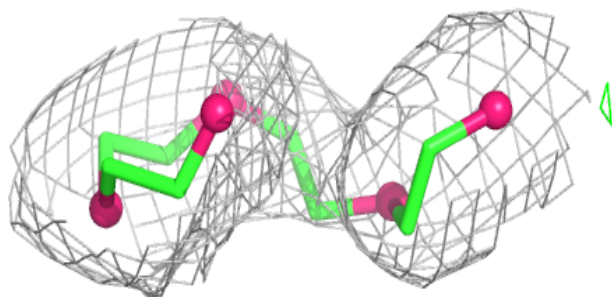
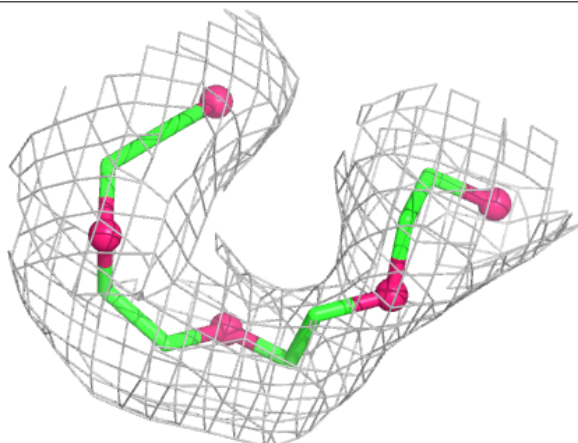


Electron density around GOL D 110:

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

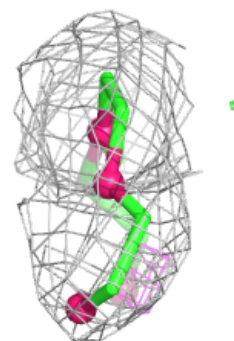
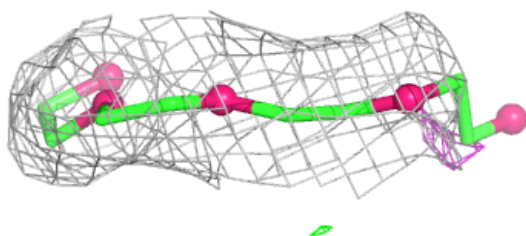
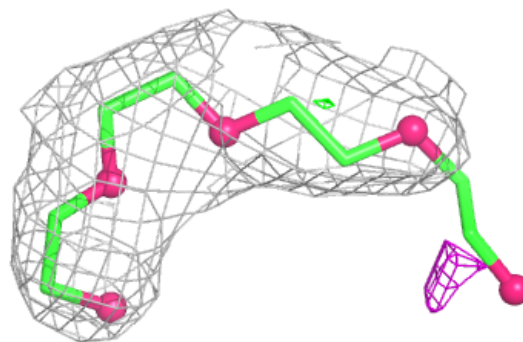
**Electron density around PG4 E 106:**

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



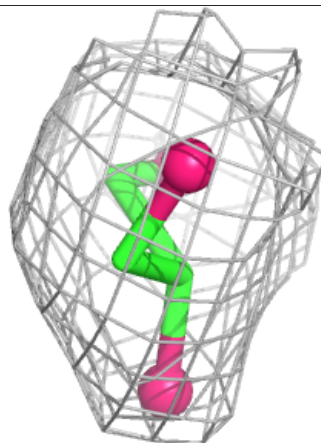
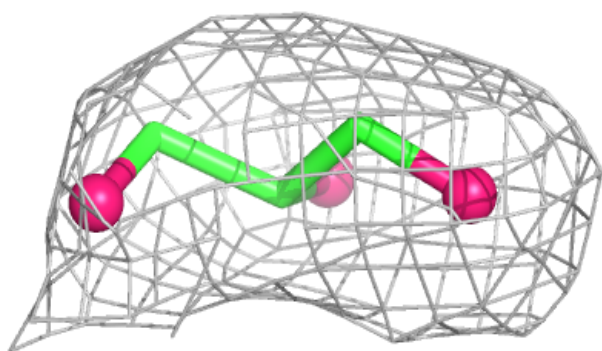
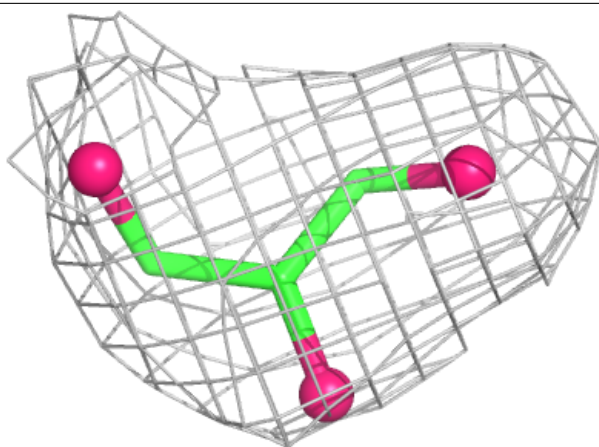
Electron density around PG4 C 336:

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



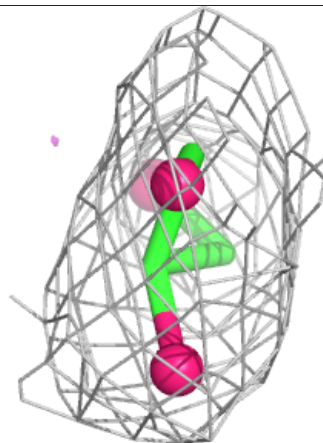
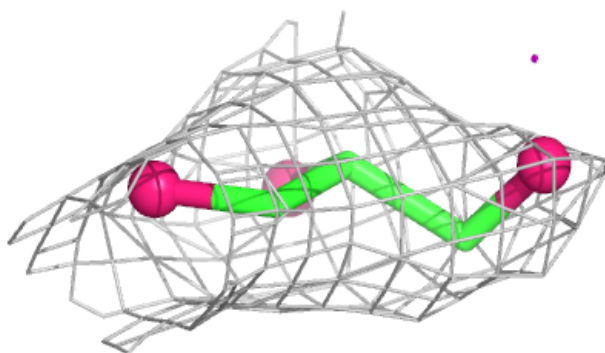
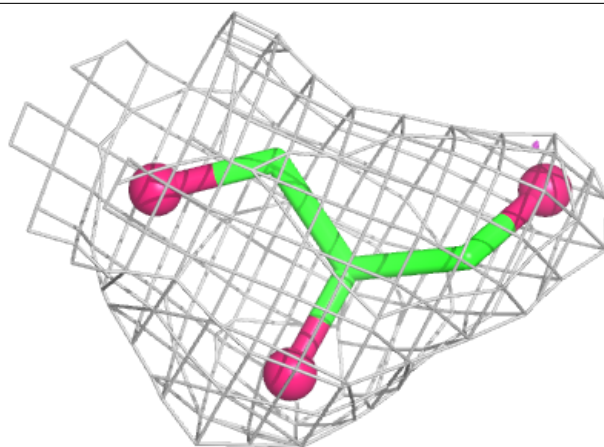
Electron density around GOL B 109:

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

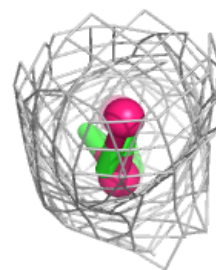
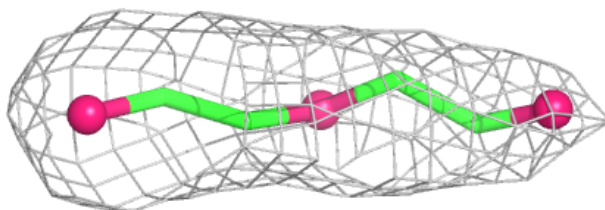
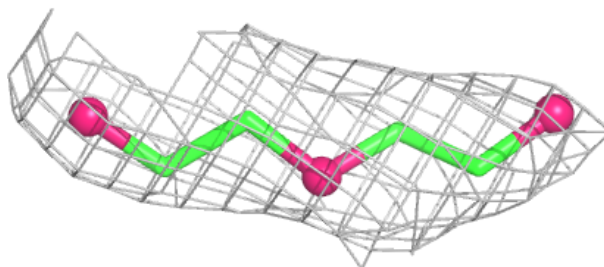


Electron density around GOL A 362:

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

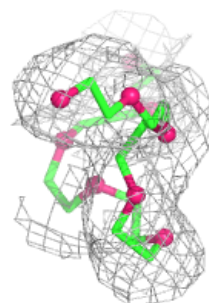
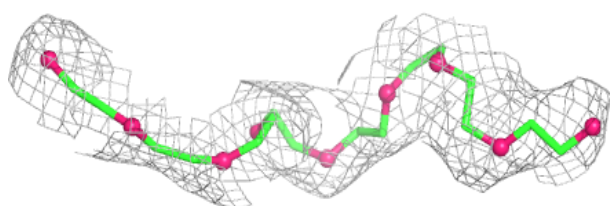
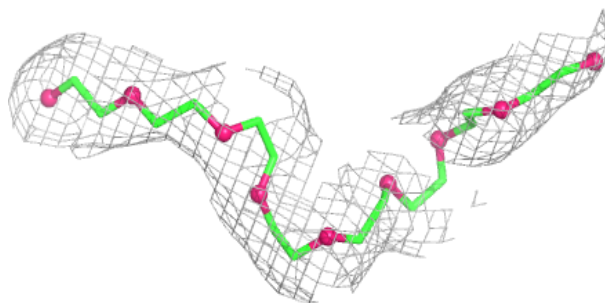
**Electron density around PEG D 127:**

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

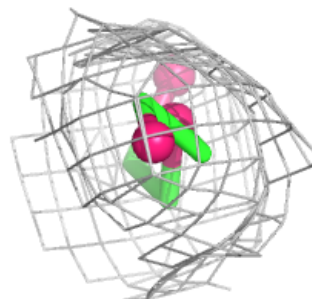
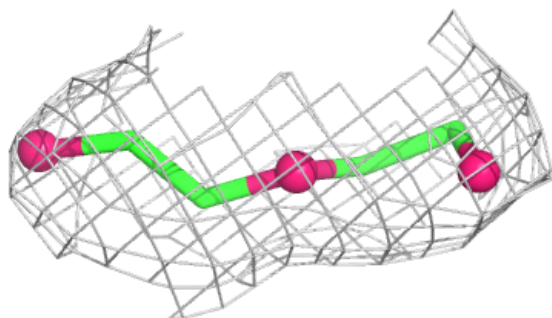
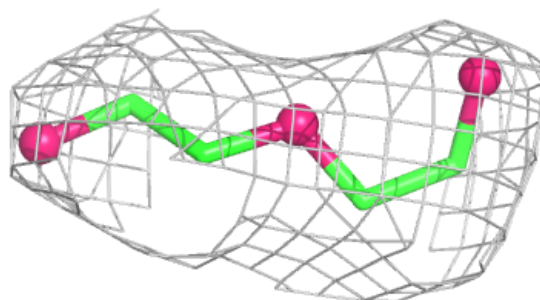


Electron density around PE8 A 342:

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

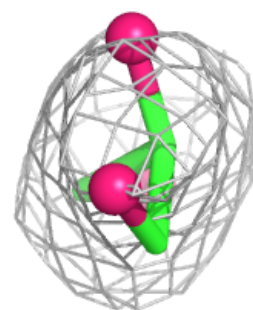
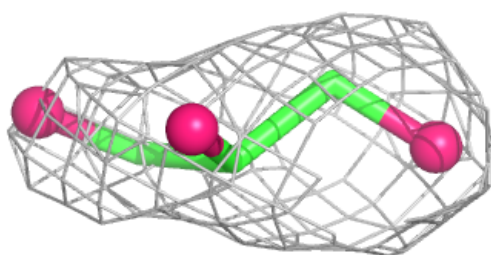
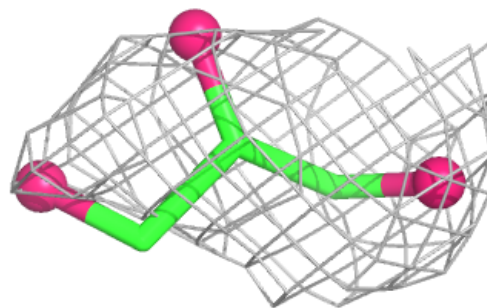
**Electron density around PEG A 336:**

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



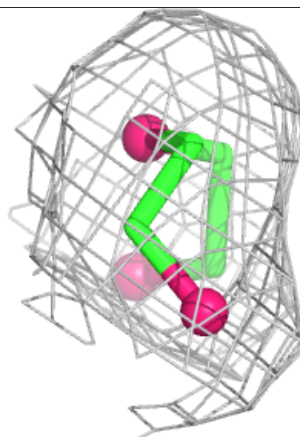
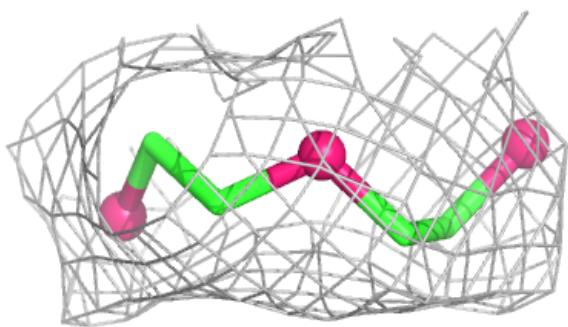
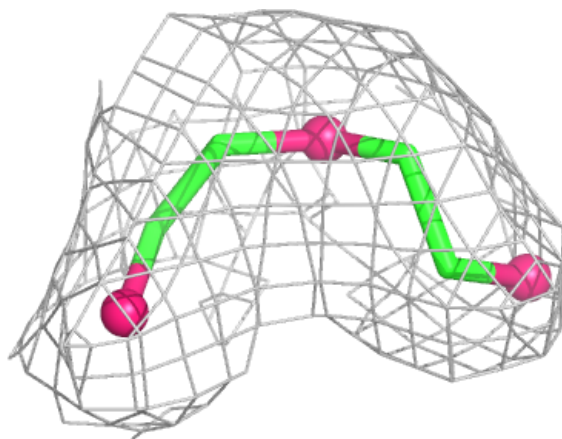
Electron density around GOL A 345:

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



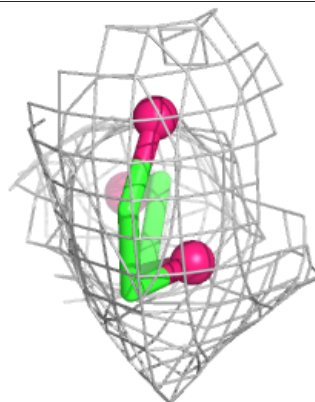
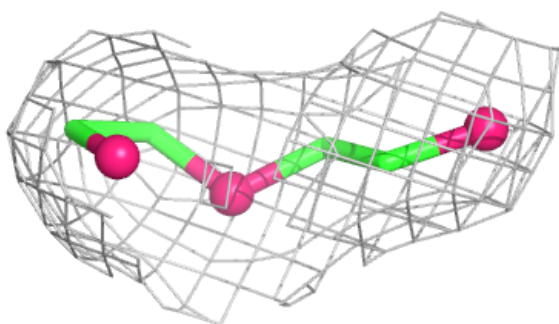
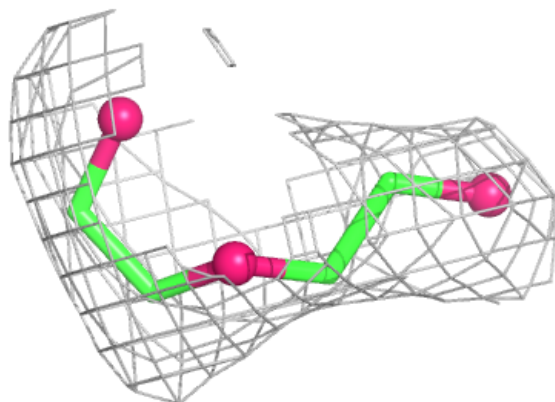
Electron density around PEG A 332:

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

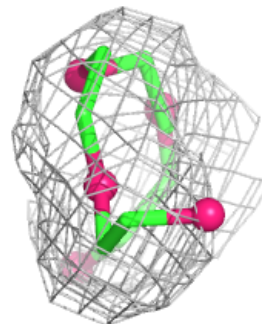
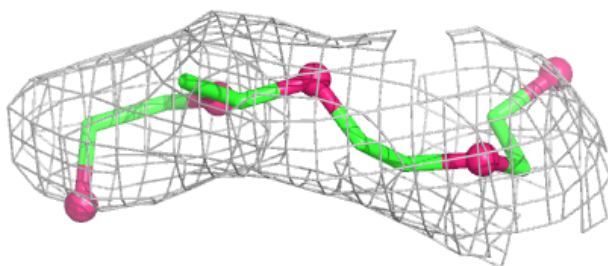
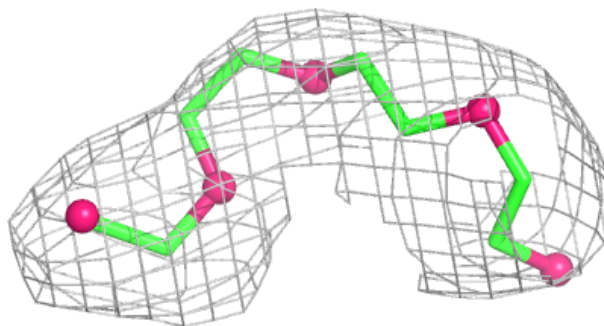


Electron density around PEG A 333:

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

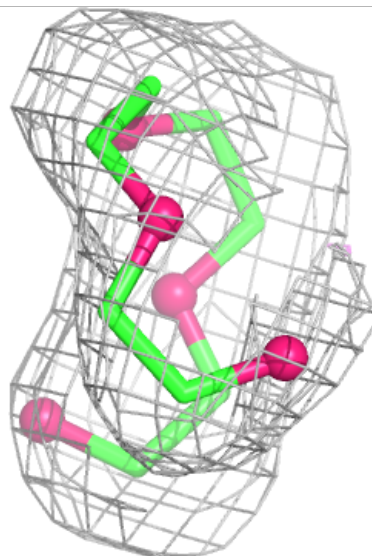
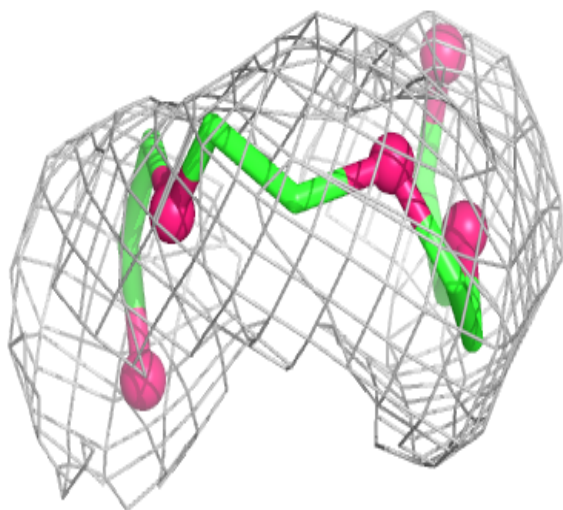
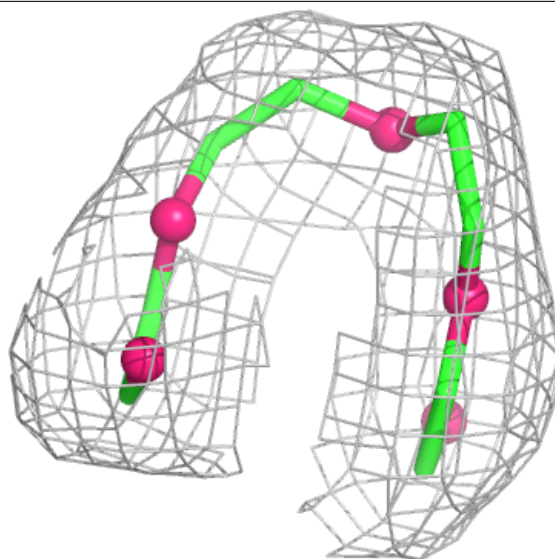
**Electron density around PG4 B 125:**

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



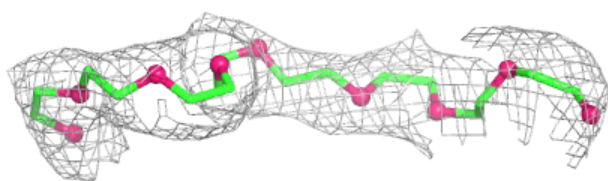
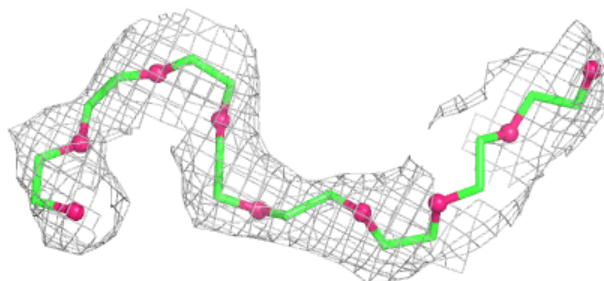
Electron density around PG4 A 369:

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

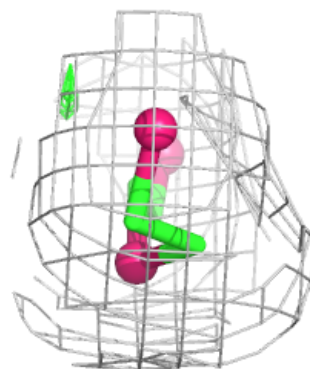
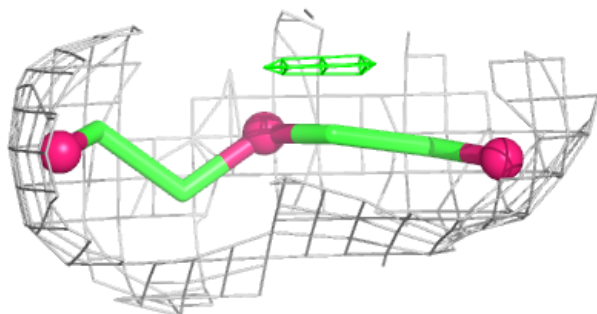
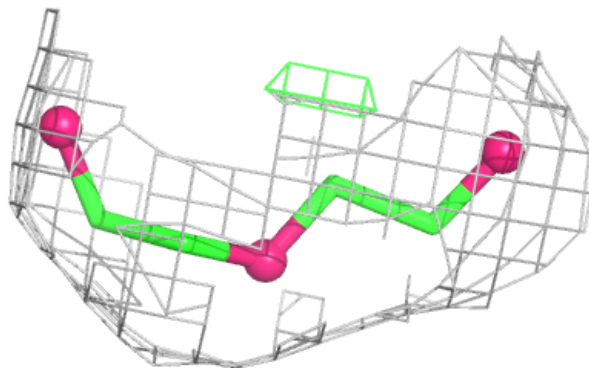


Electron density around PE8 F 106:

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

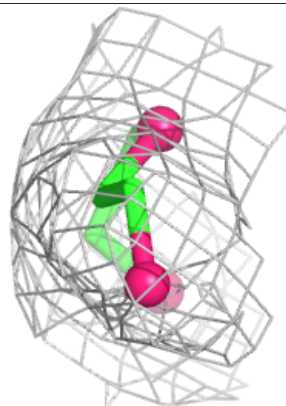
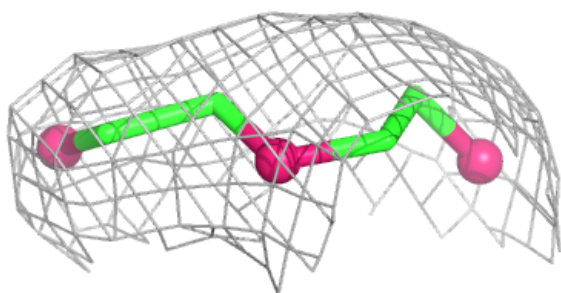
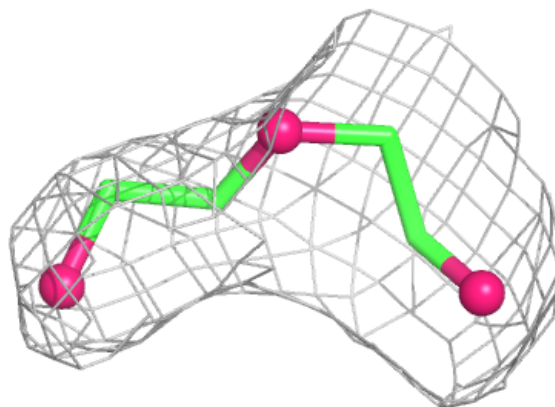
**Electron density around PEG C 330:**

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

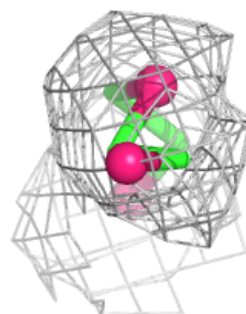
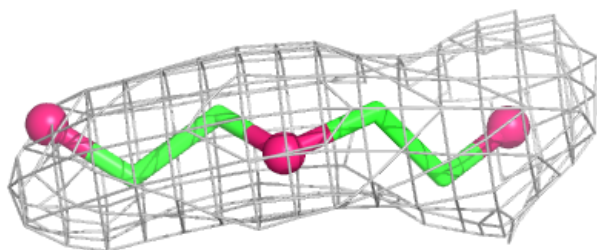
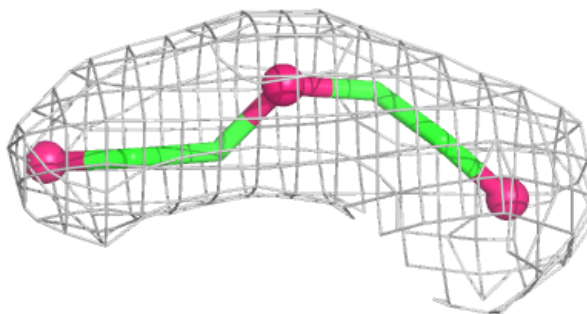


Electron density around PEG C 331:

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

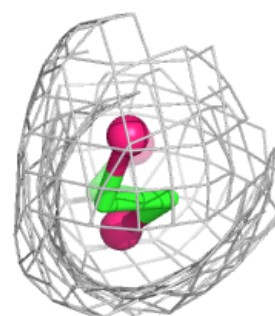
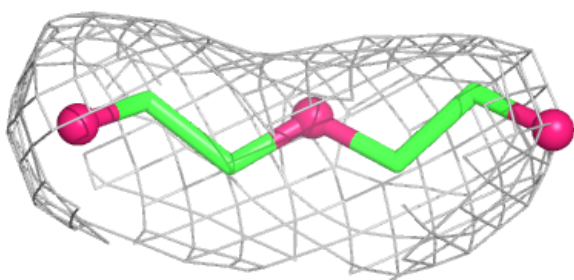
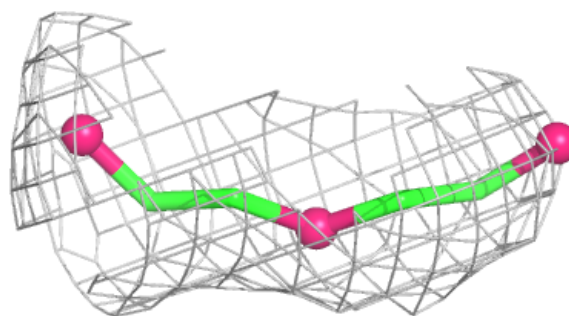
**Electron density around PEG C 332:**

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

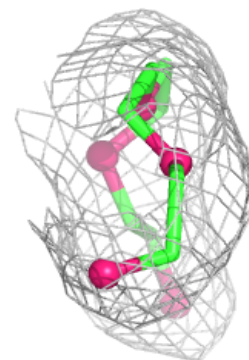
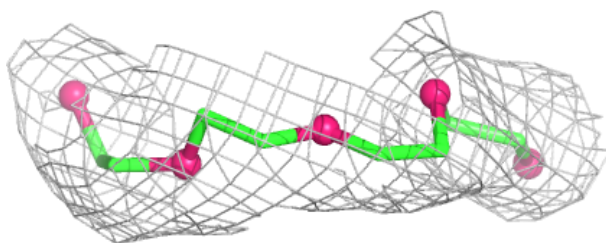
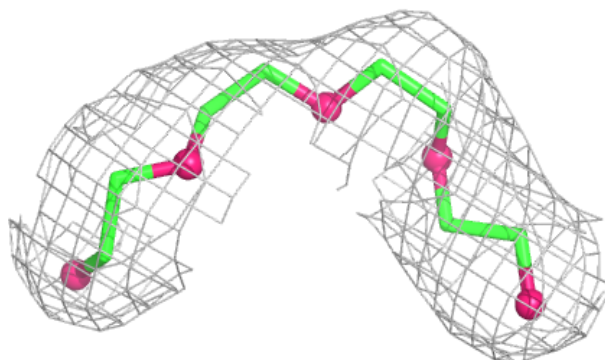


Electron density around PEG B 135:

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

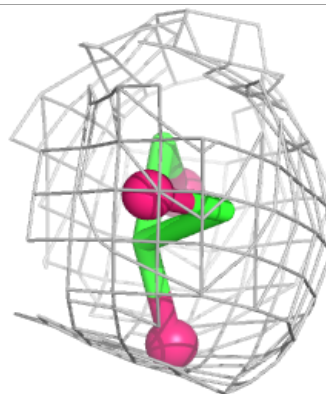
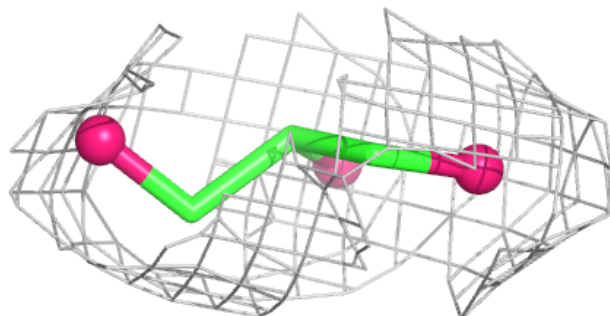
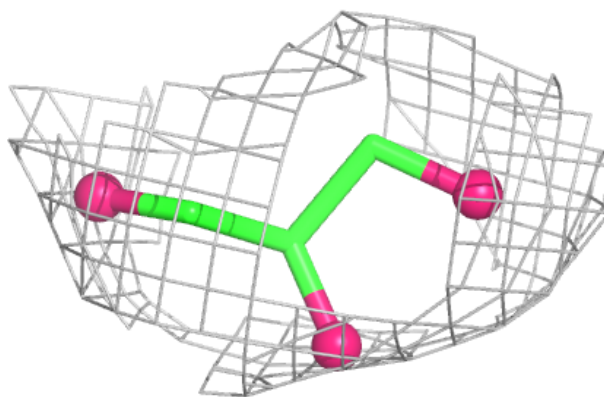
**Electron density around PG4 B 124:**

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

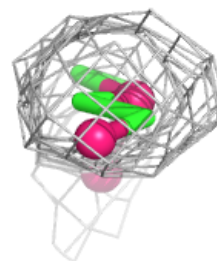
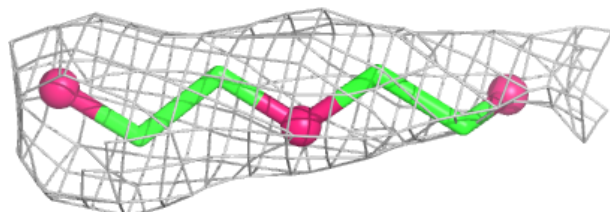
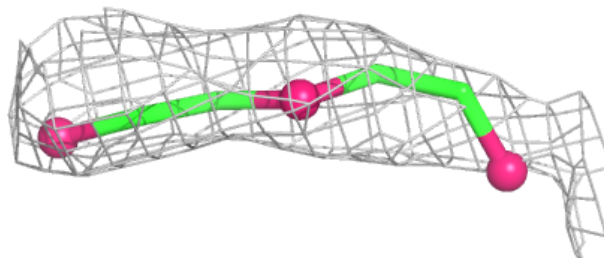


Electron density around GOL B 103:

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

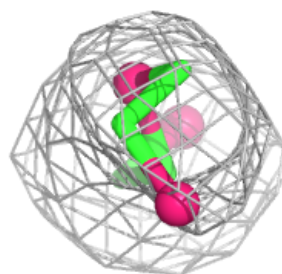
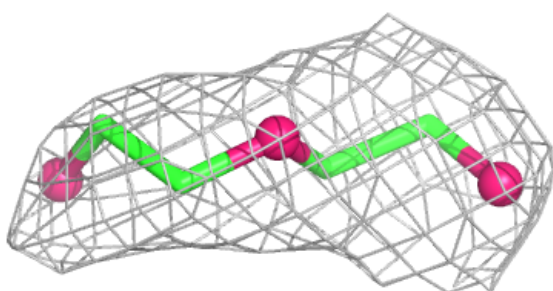
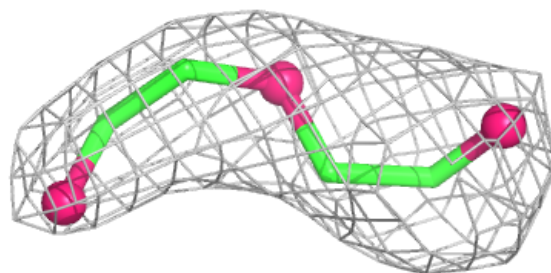
**Electron density around PEG A 329:**

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

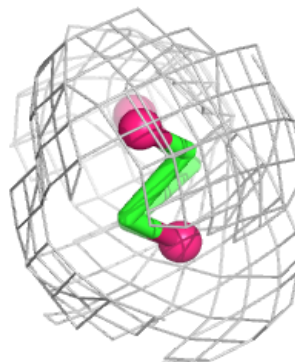
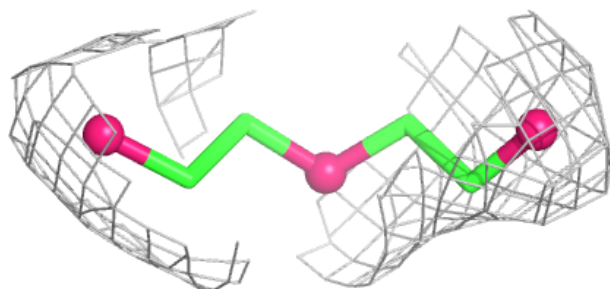
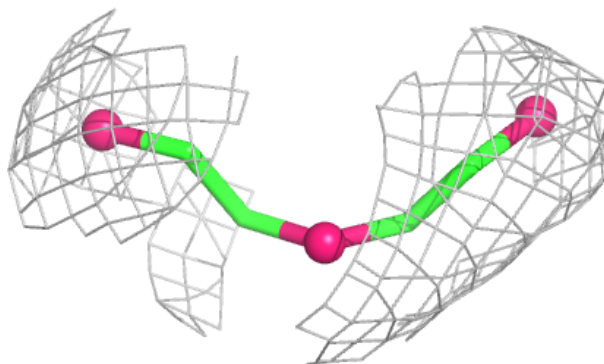


Electron density around PEG A 371:

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

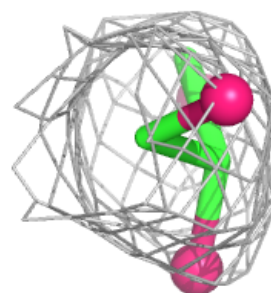
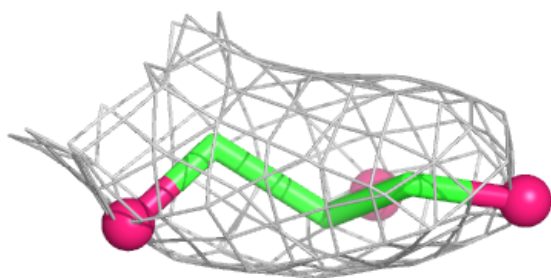
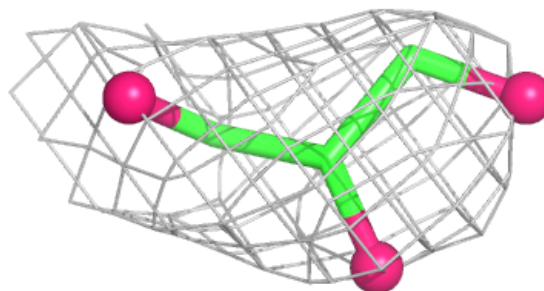
**Electron density around PEG D 121:**

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

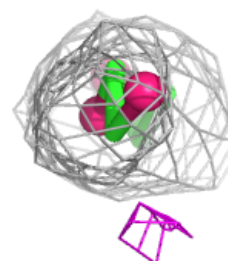
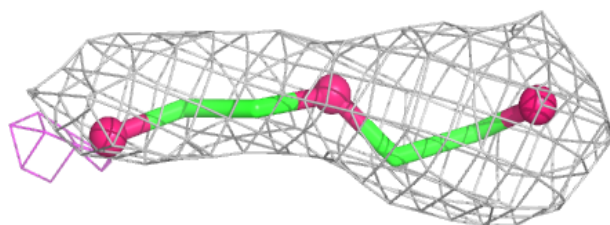
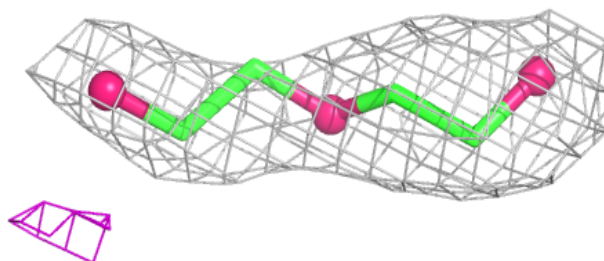


Electron density around GOL C 307:

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

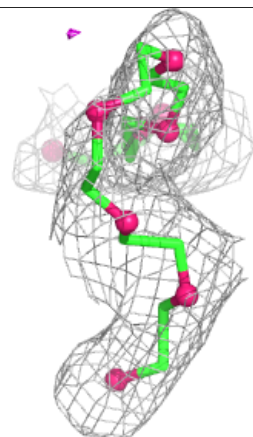
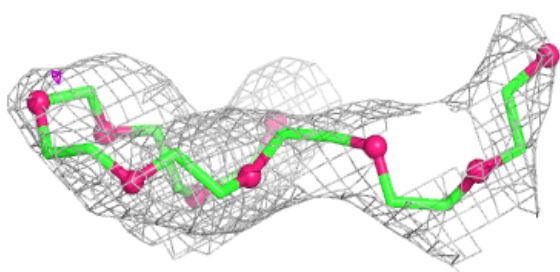
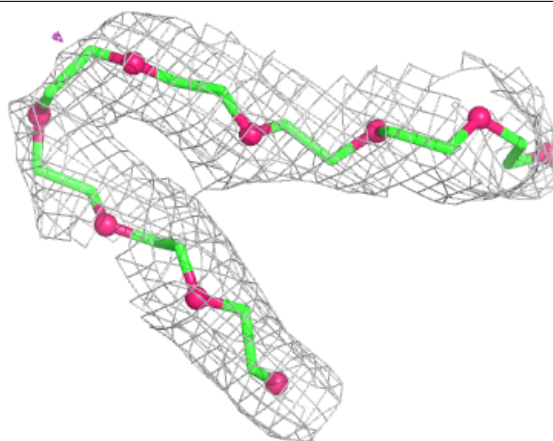
**Electron density around PEG D 128:**

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



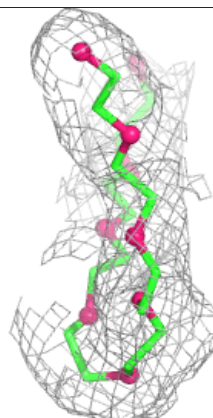
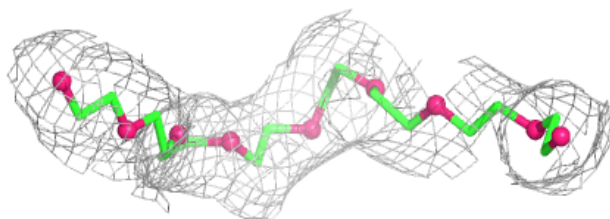
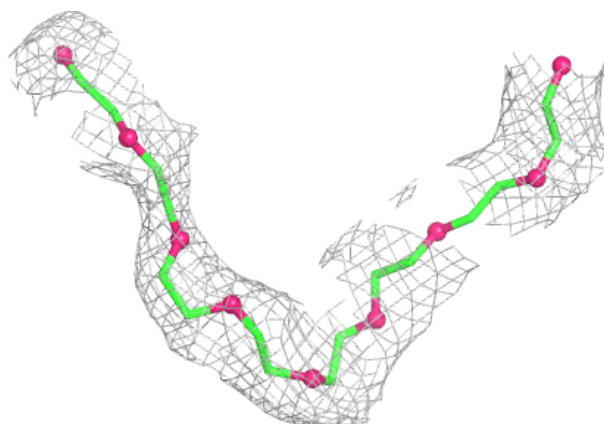
Electron density around PE8 A 344:

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

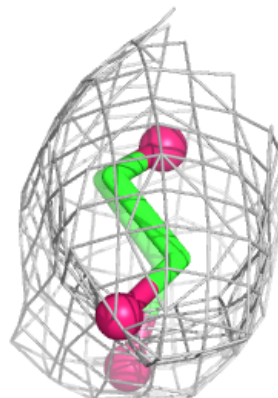
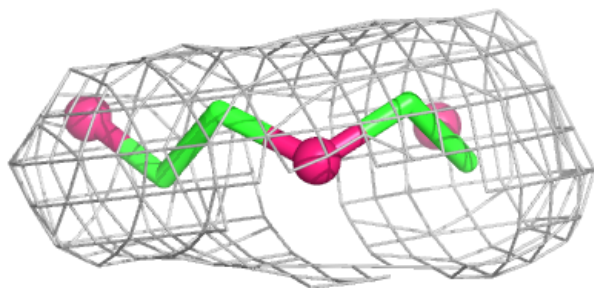
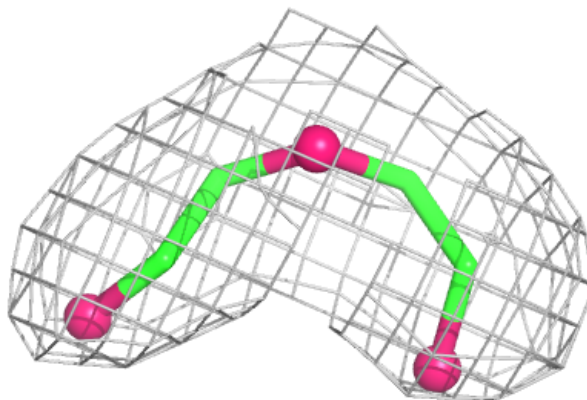


Electron density around PE8 B 102:

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

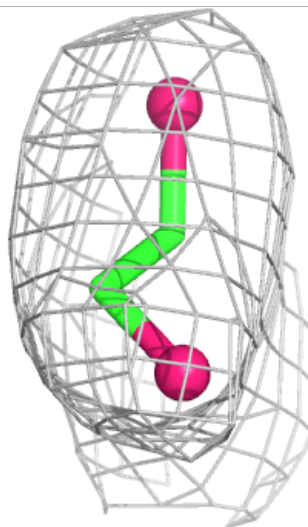
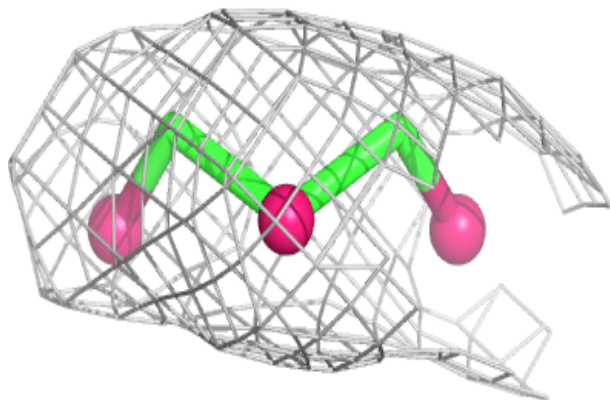
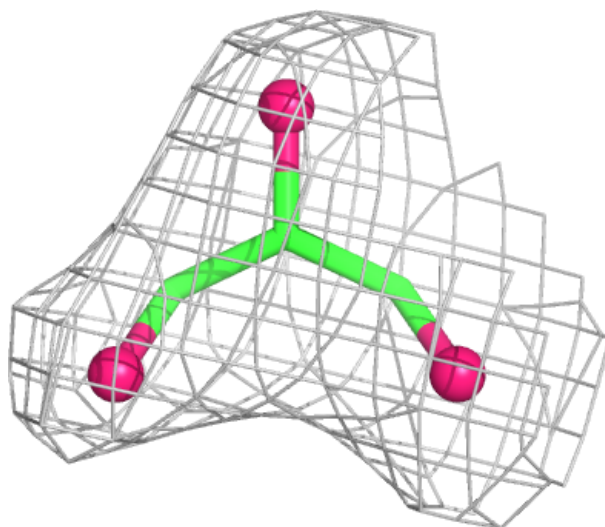
**Electron density around PEG B 130:**

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



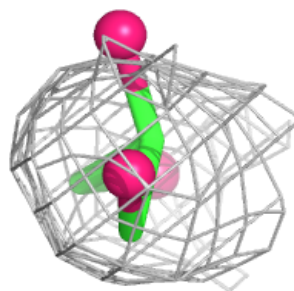
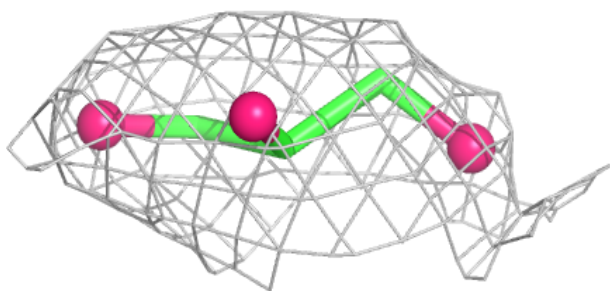
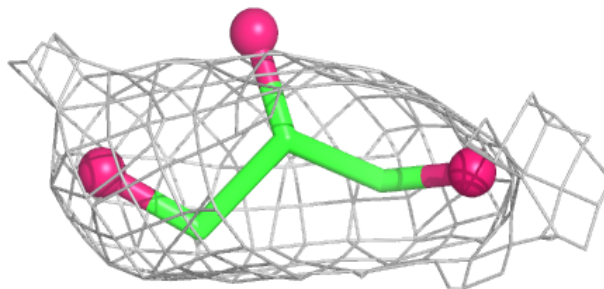
Electron density around GOL C 314:

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

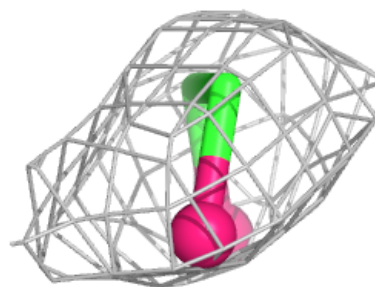
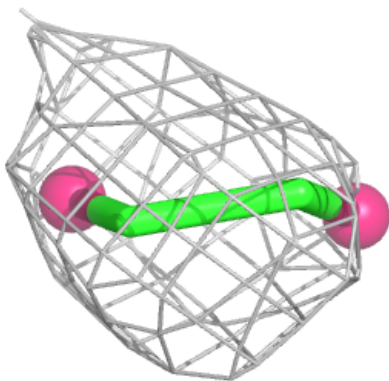
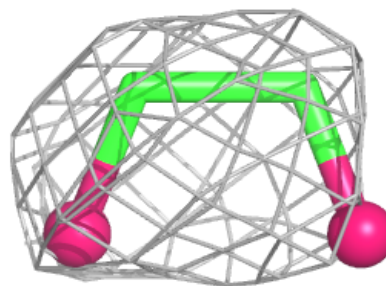


Electron density around GOL D 131:

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

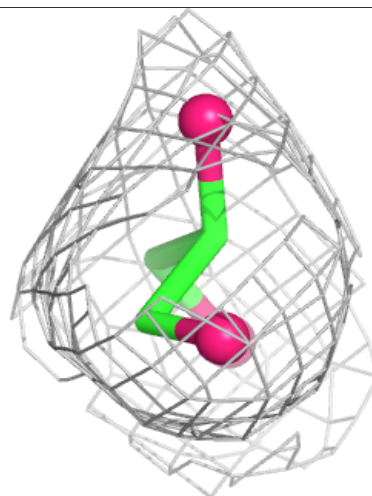
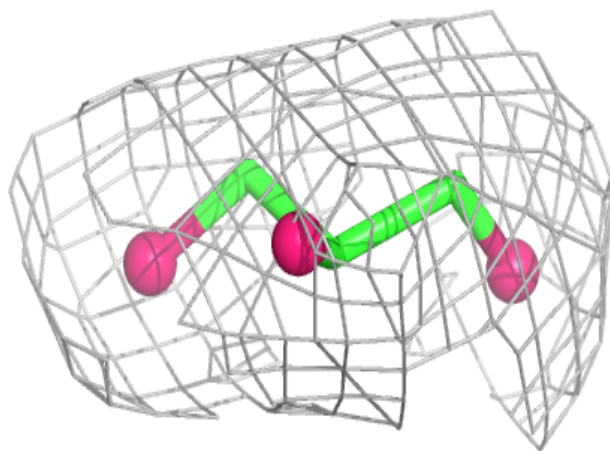
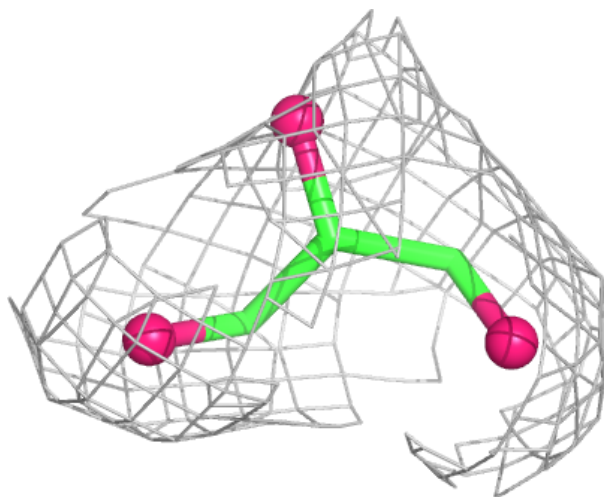
**Electron density around EDO B 144:**

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



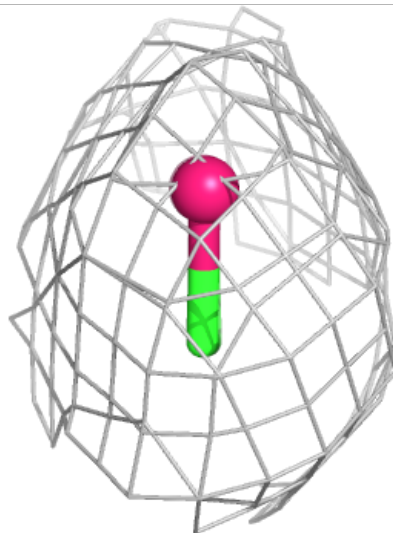
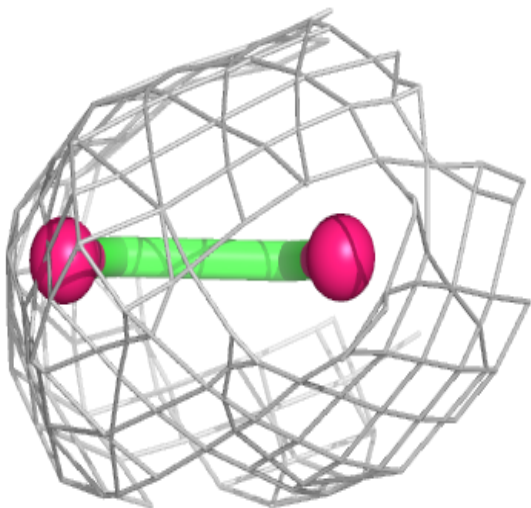
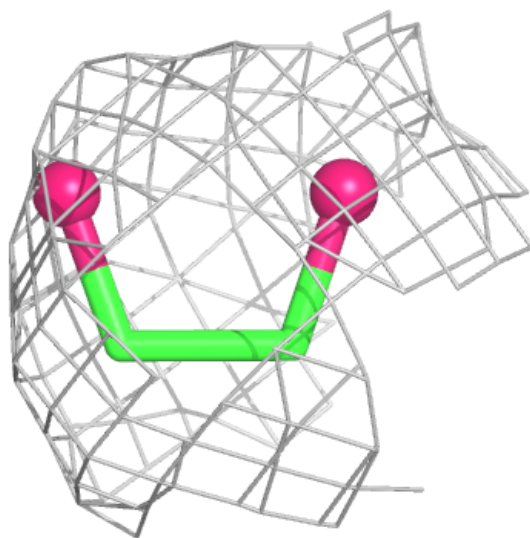
Electron density around GOL C 338:

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



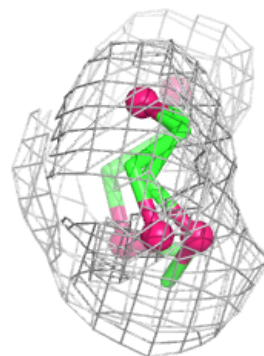
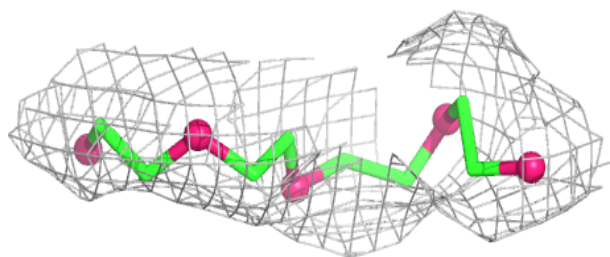
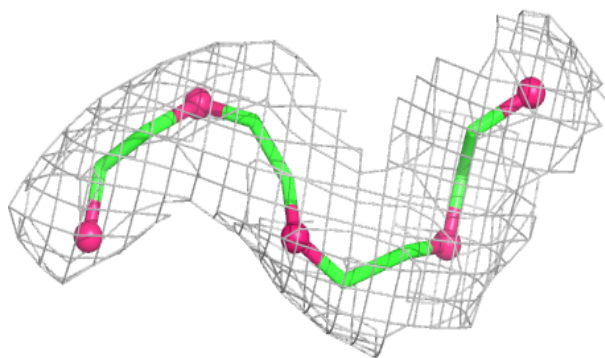
Electron density around EDO E 111:

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

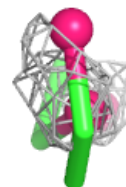
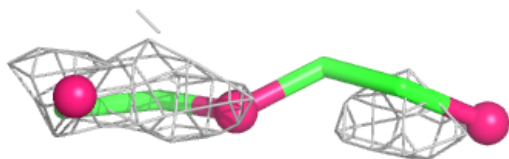
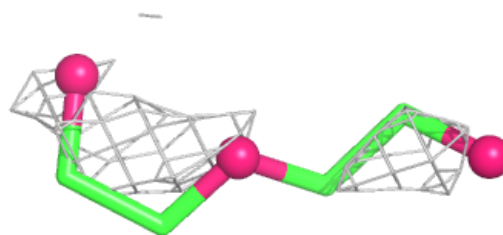


Electron density around PG4 D 118:

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

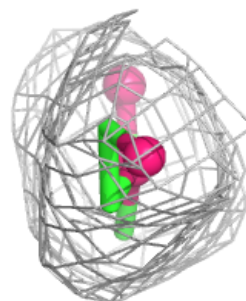
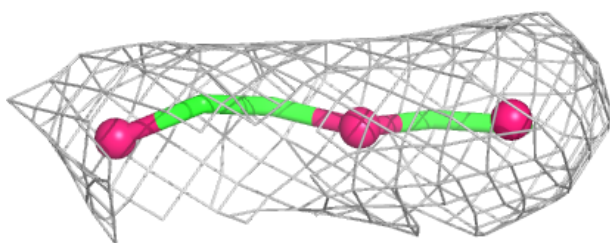
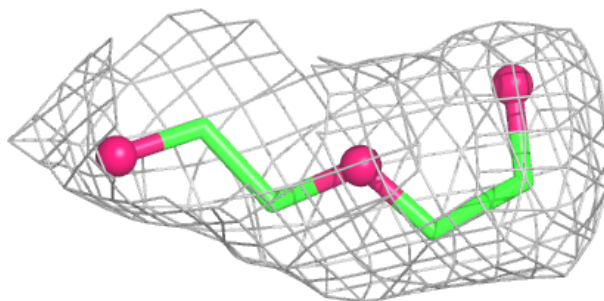
**Electron density around PEG C 333:**

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

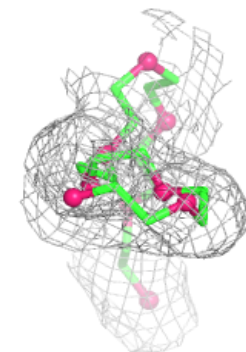
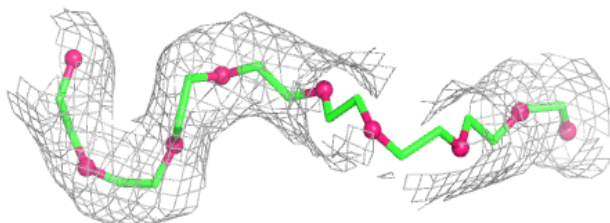
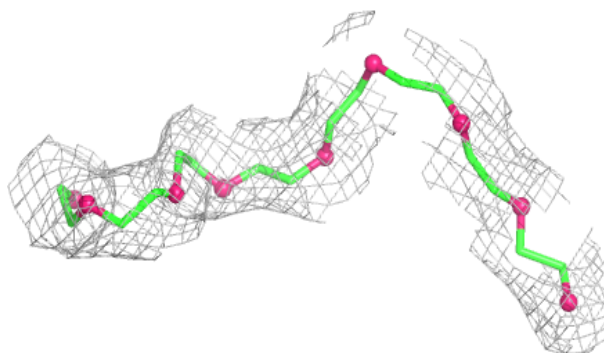


Electron density around PEG C 327:

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

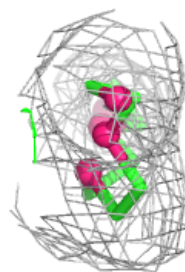
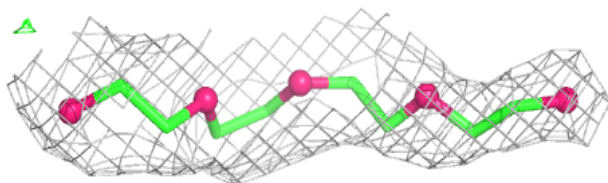
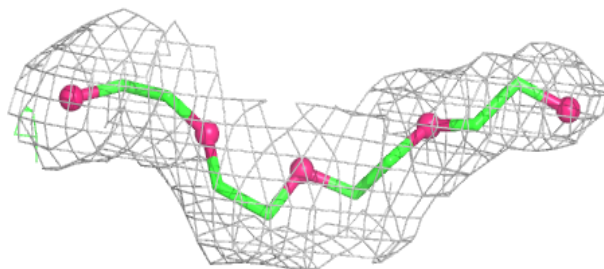
**Electron density around PE8 A 343:**

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

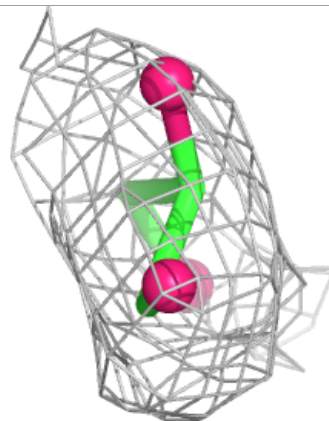
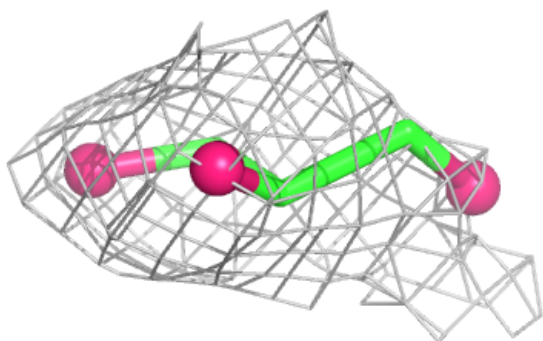
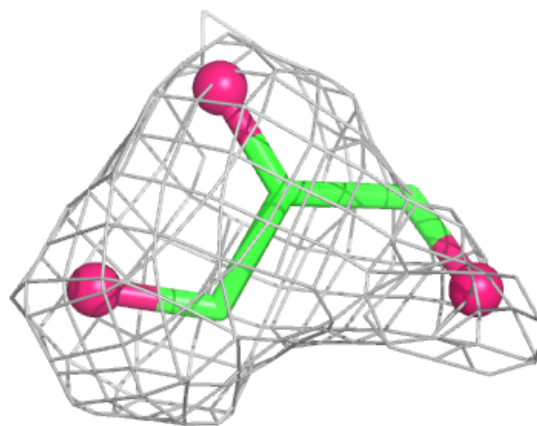


Electron density around PG4 D 103:

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

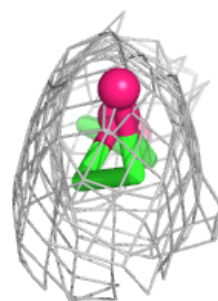
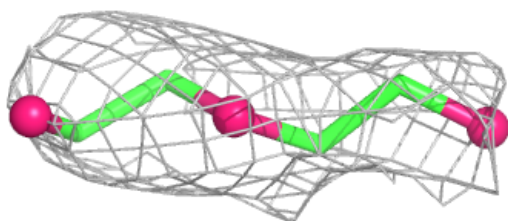
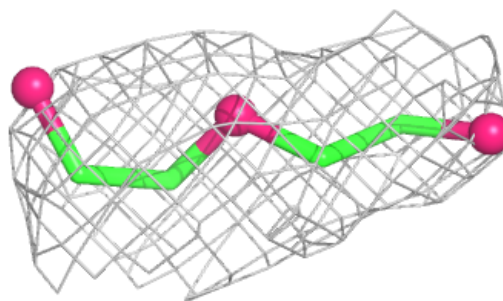
**Electron density around GOL A 303:**

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

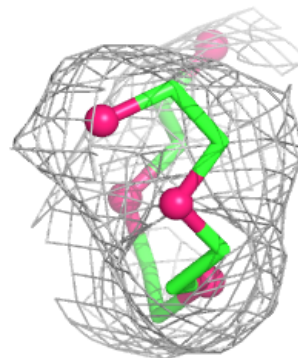
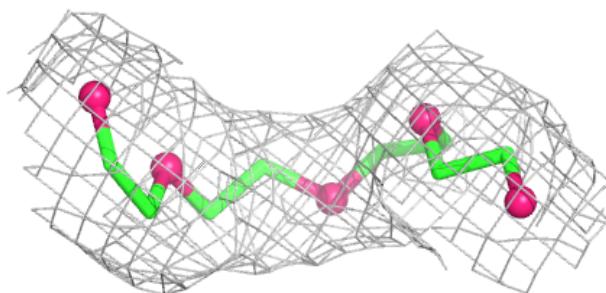
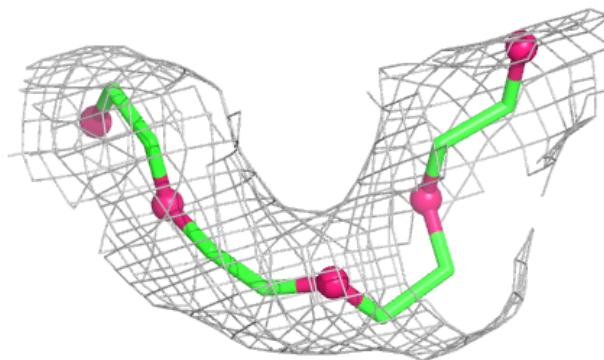


Electron density around PEG D 126:

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

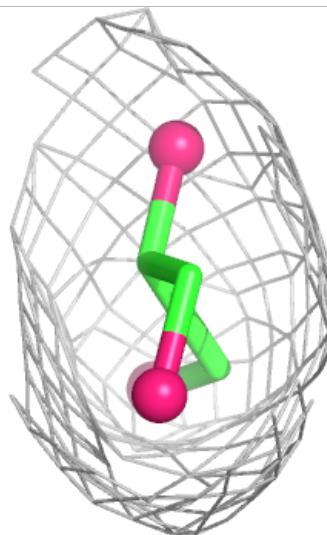
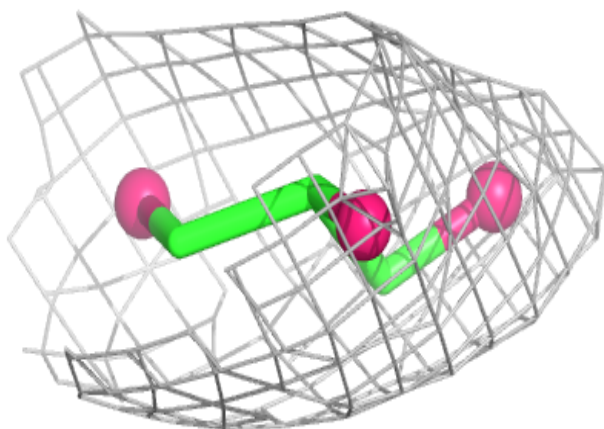
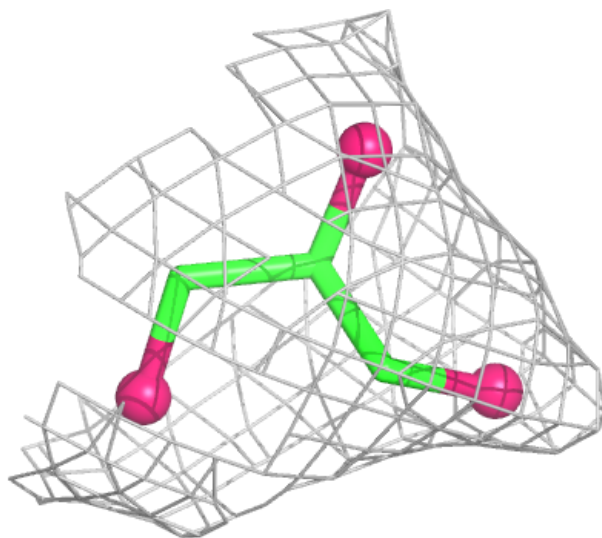
**Electron density around PG4 B 155:**

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



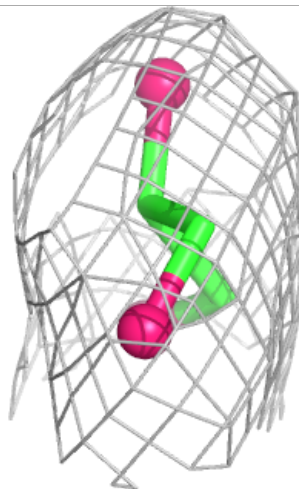
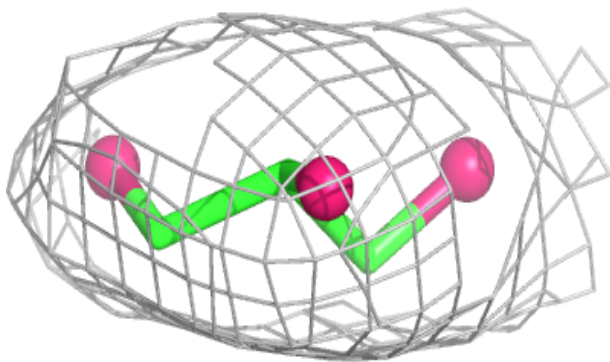
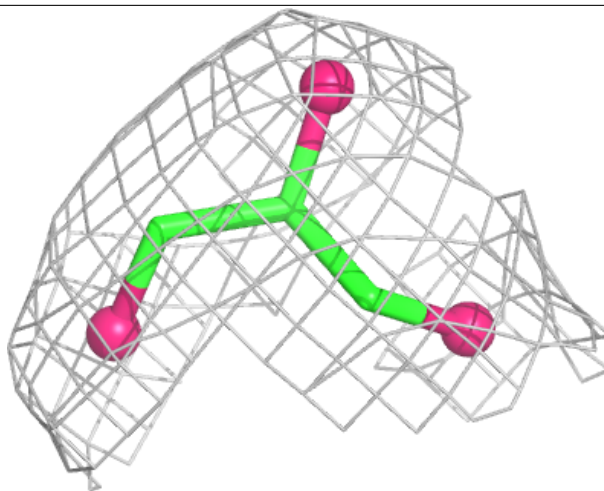
Electron density around GOL B 107:

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



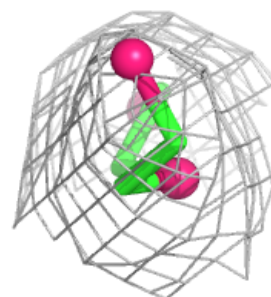
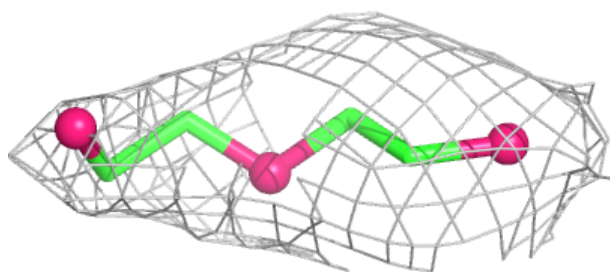
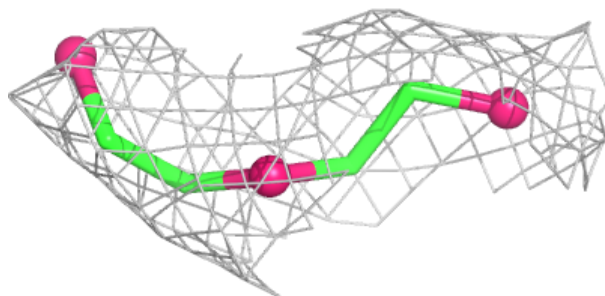
Electron density around GOL A 301:

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

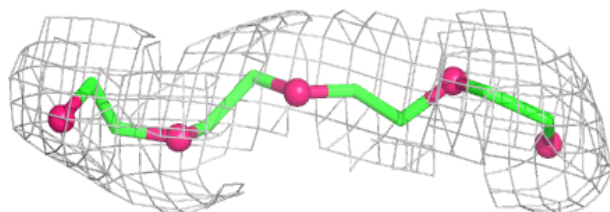
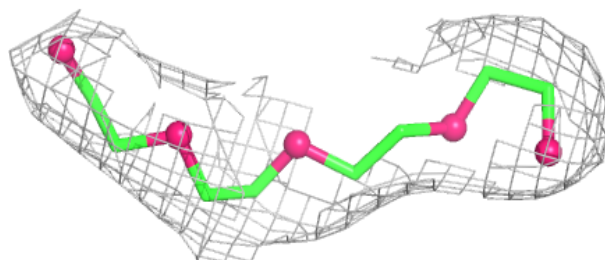


Electron density around PEG C 329:

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

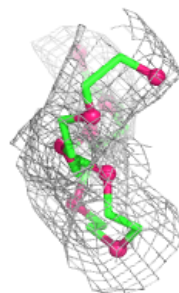
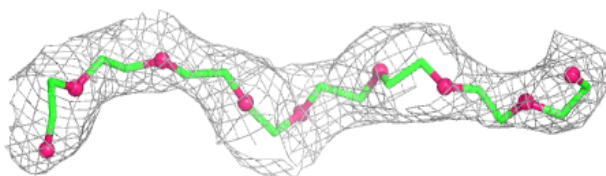
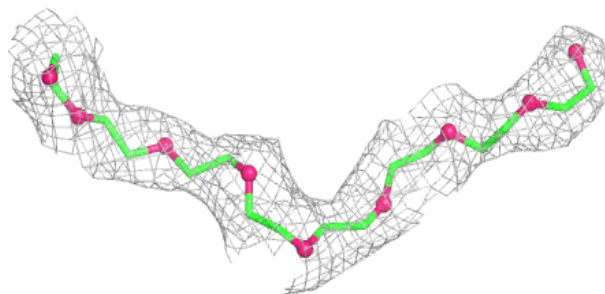
**Electron density around PG4 B 119:**

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

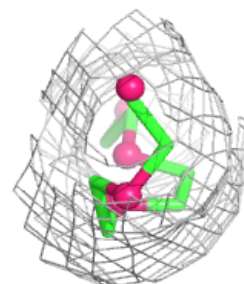
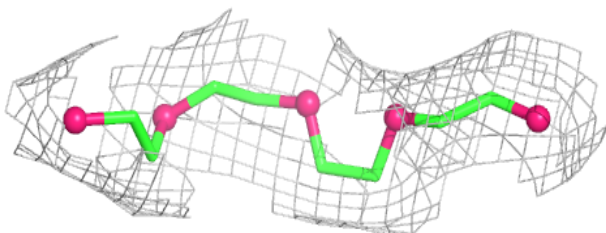
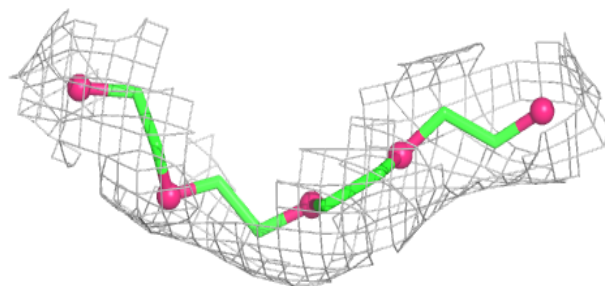


Electron density around PE8 F 102:

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

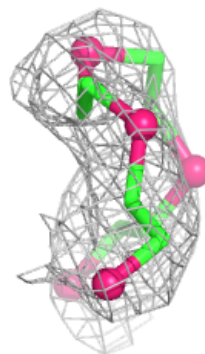
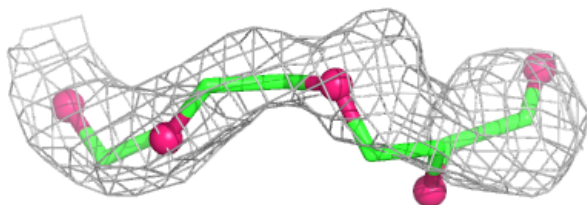
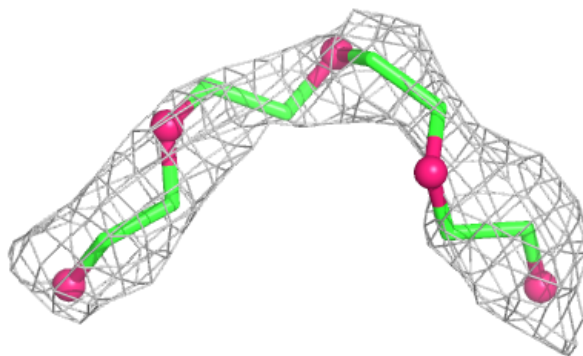
**Electron density around PG4 E 114:**

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

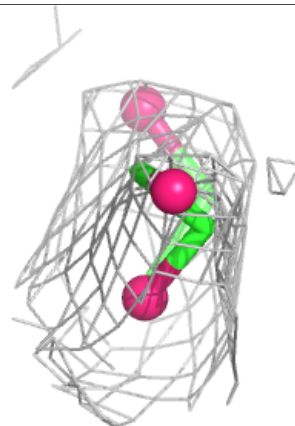
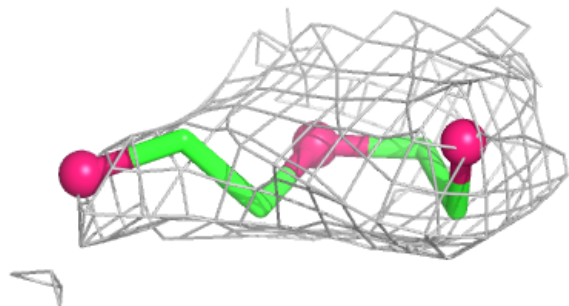
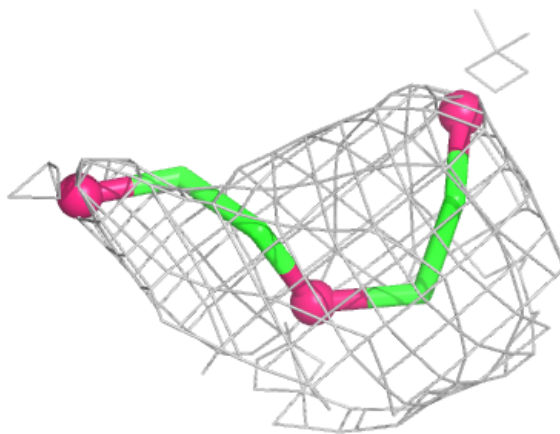


Electron density around PG4 C 325:

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

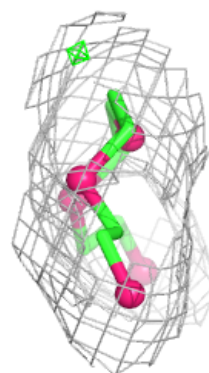
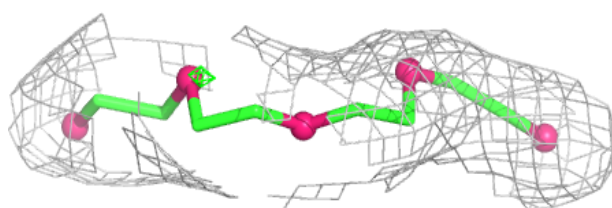
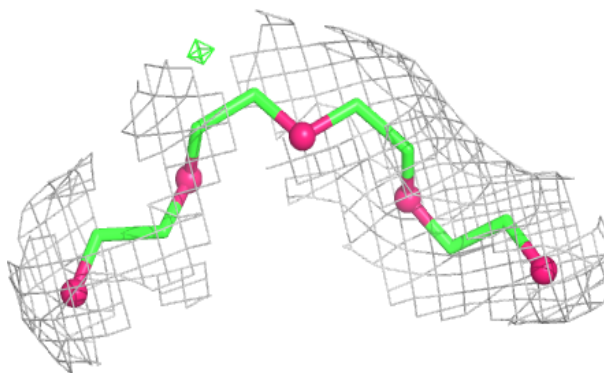
**Electron density around PEG A 331:**

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

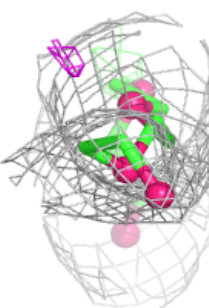
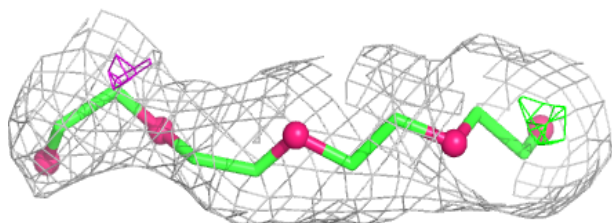
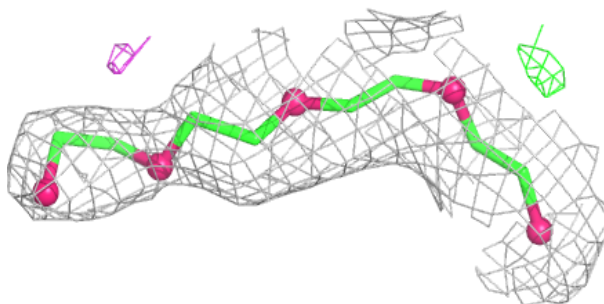


Electron density around PG4 A 322:

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

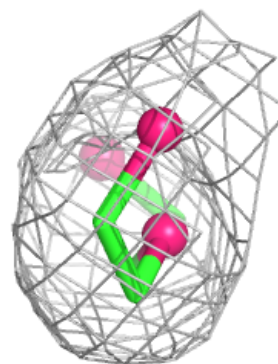
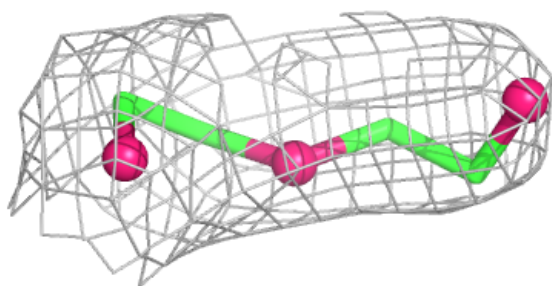
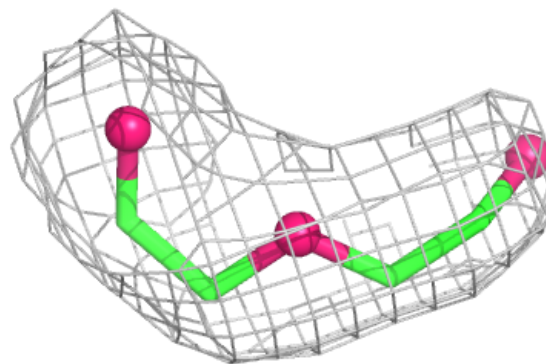
**Electron density around PG4 D 116:**

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



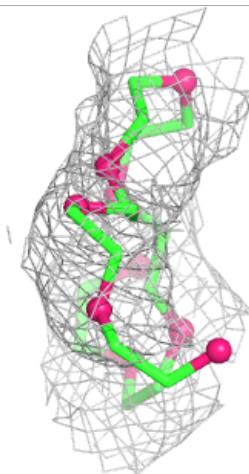
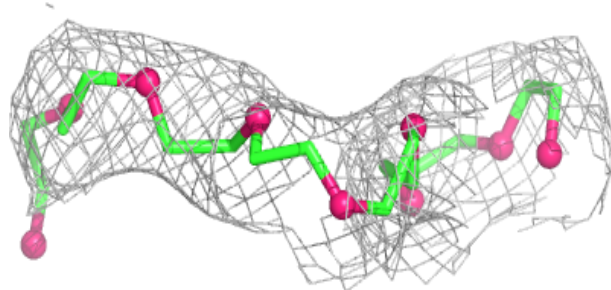
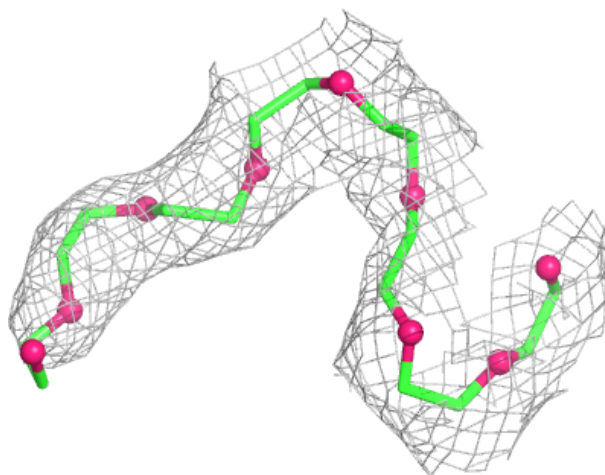
Electron density around PEG C 339:

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



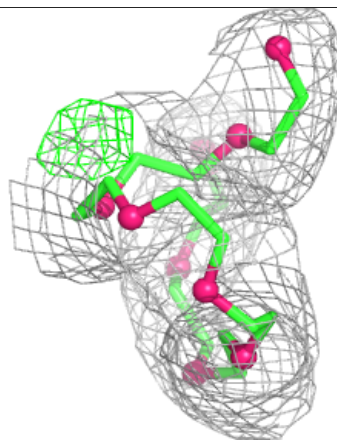
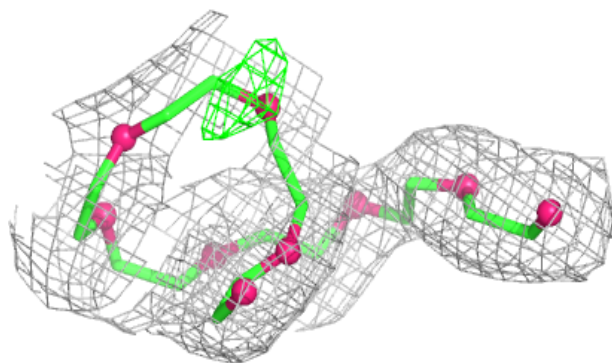
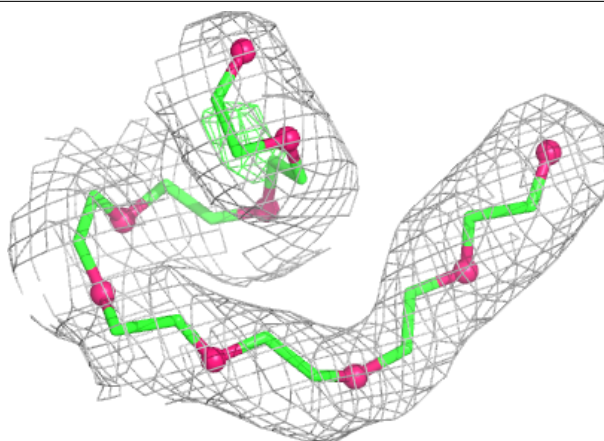
Electron density around PE8 B 136:

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



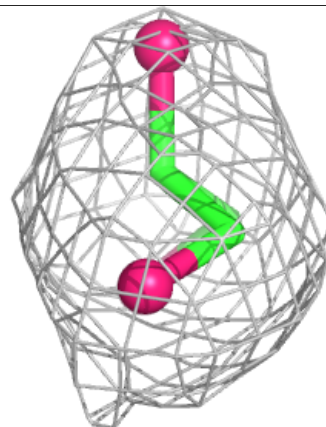
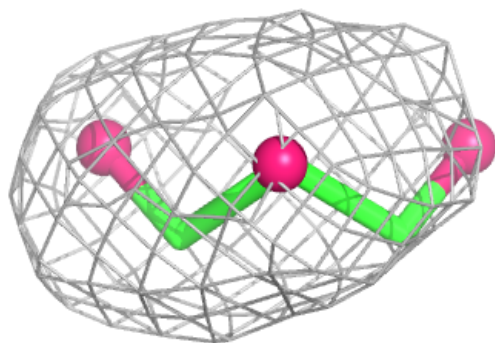
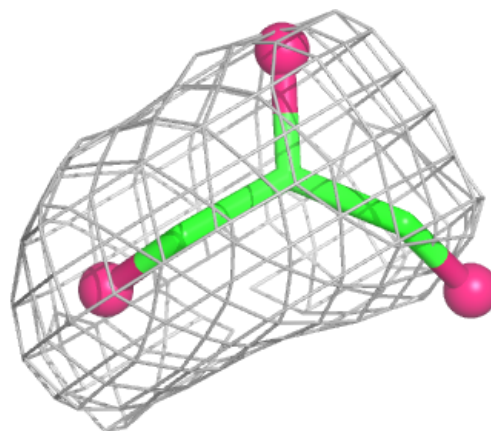
Electron density around PE8 E 110:

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



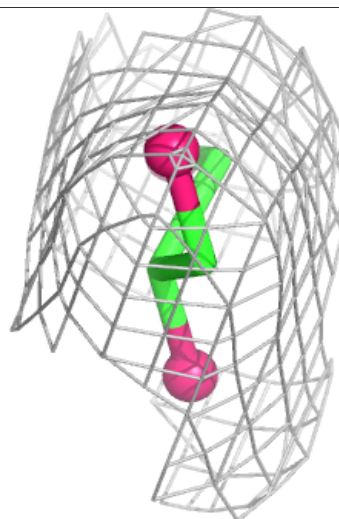
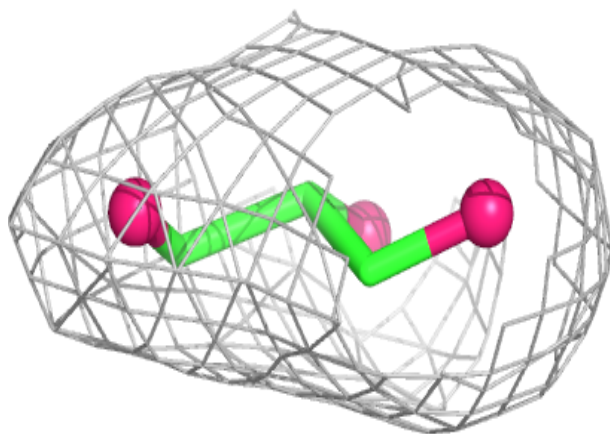
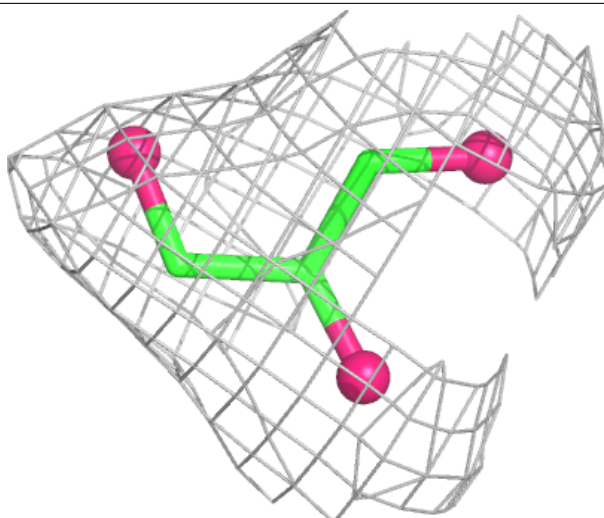
Electron density around GOL C 312:

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



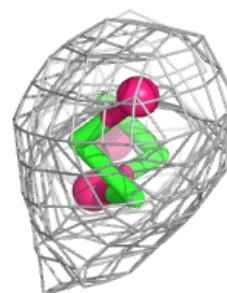
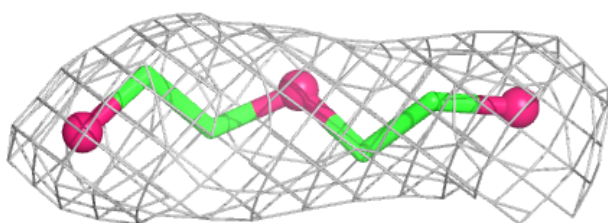
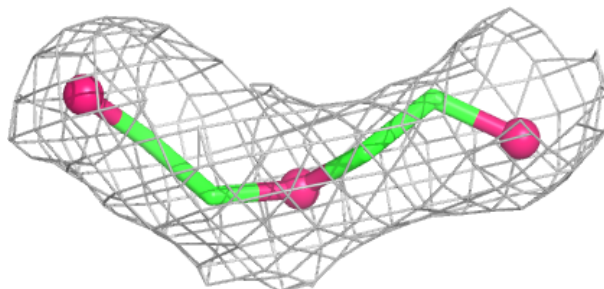
Electron density around GOL A 305:

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

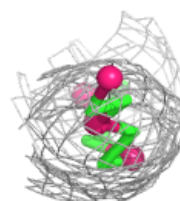
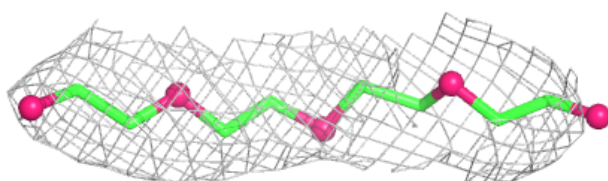
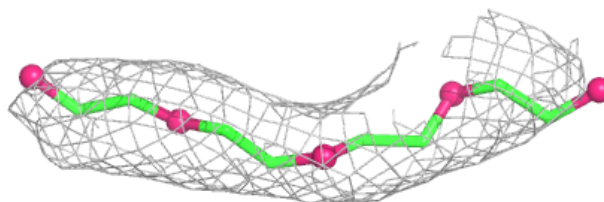


Electron density around PEG A 353:

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

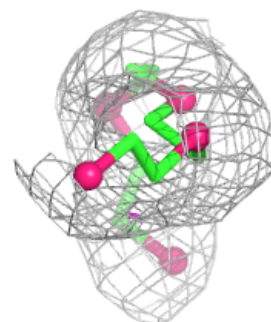
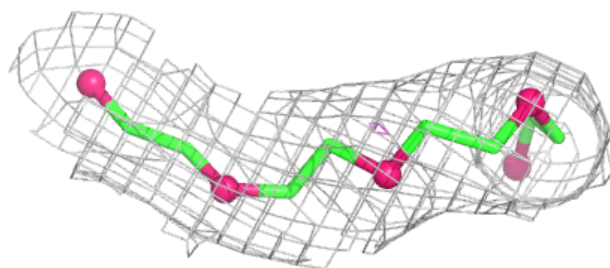
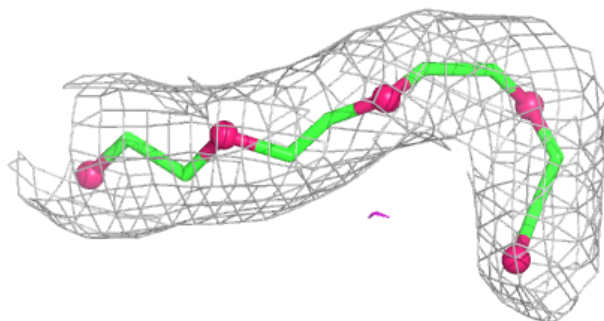
**Electron density around PG4 B 120:**

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

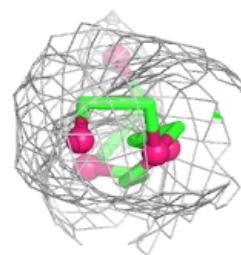
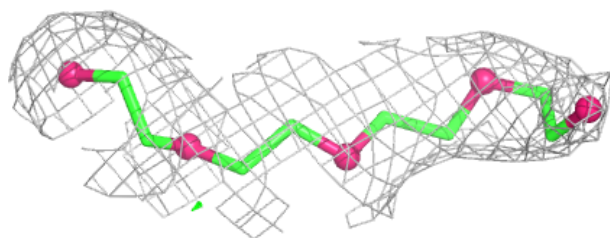
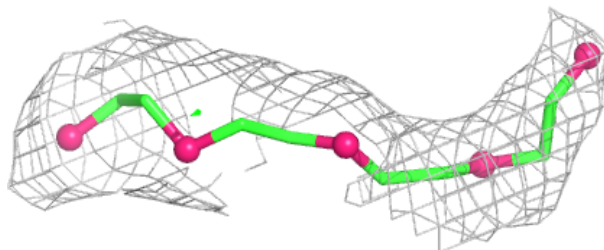


Electron density around PG4 A 320:

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

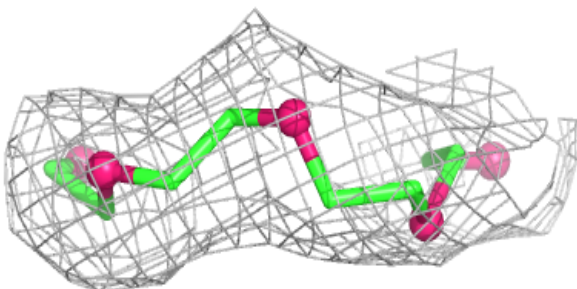
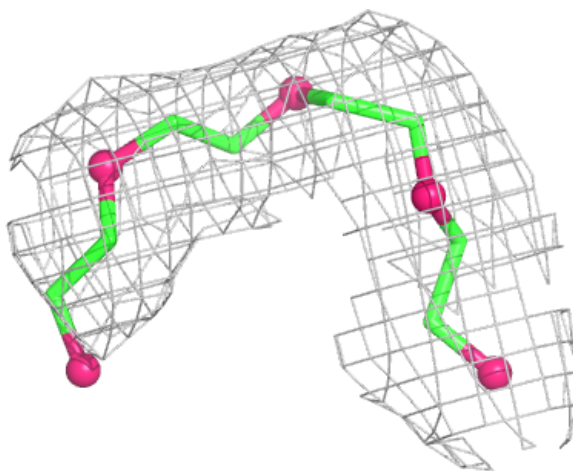
**Electron density around PG4 C 319:**

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



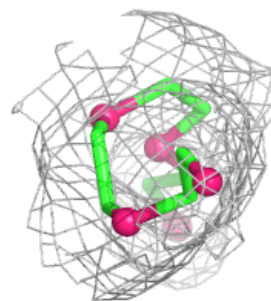
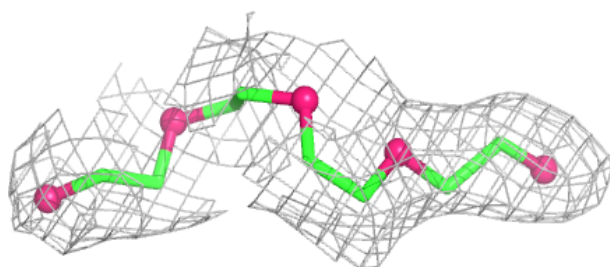
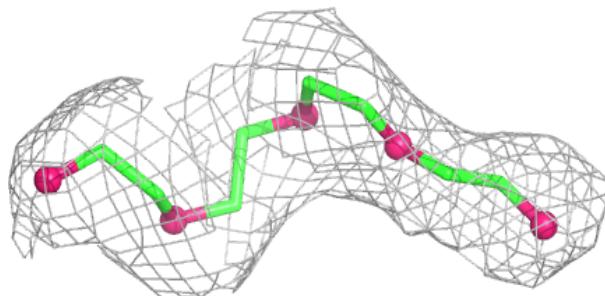
Electron density around PG4 A 321:

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



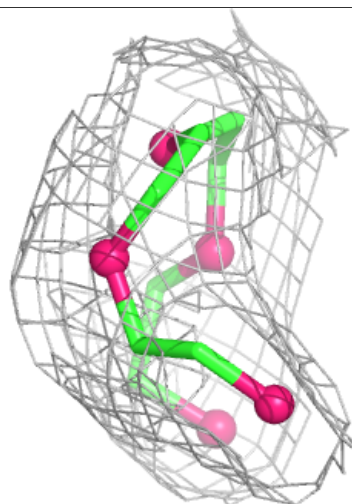
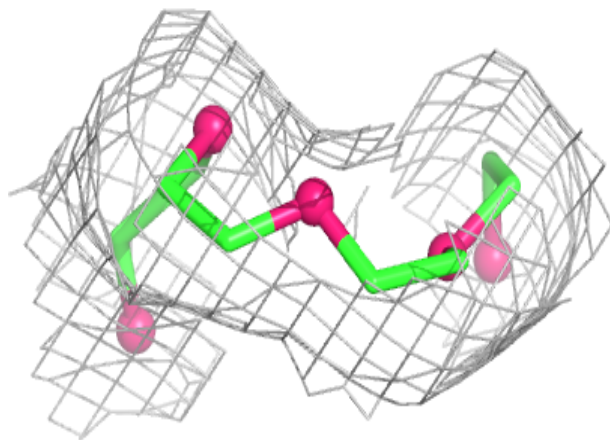
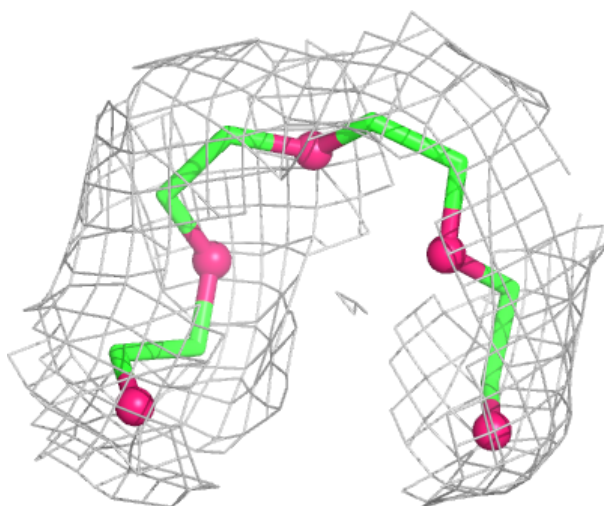
Electron density around PG4 A 352:

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



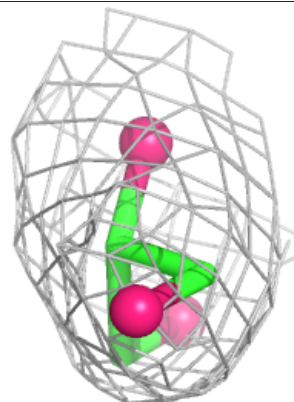
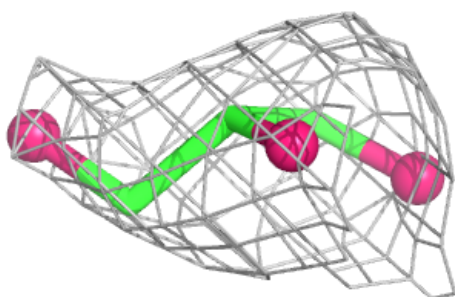
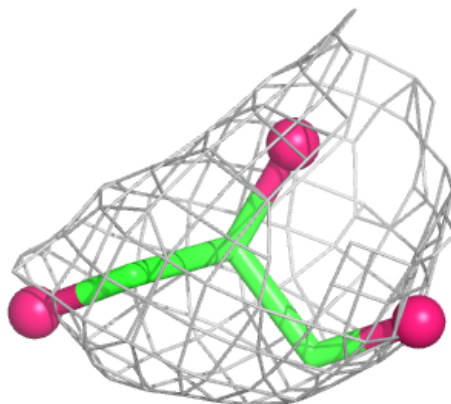
Electron density around PG4 D 119:

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

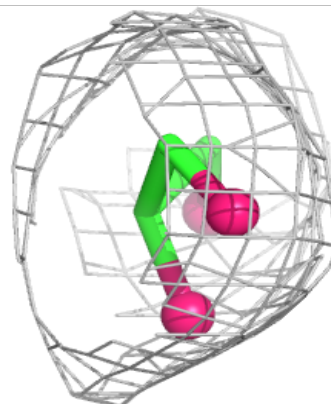
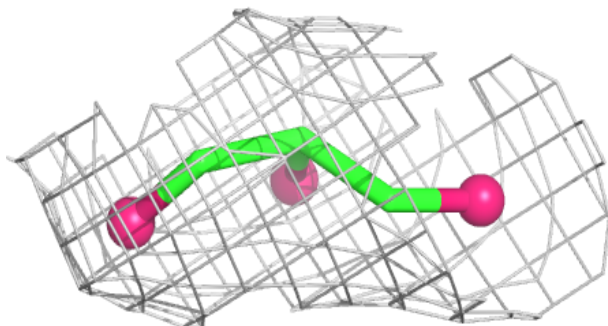
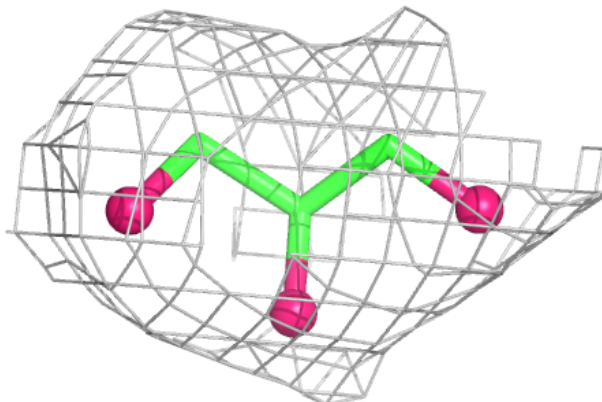


Electron density around GOL C 310:

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

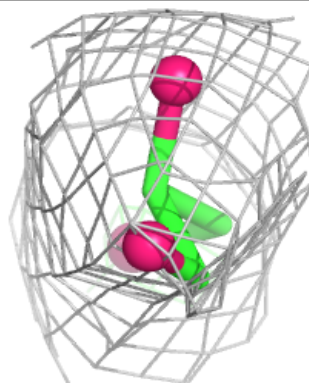
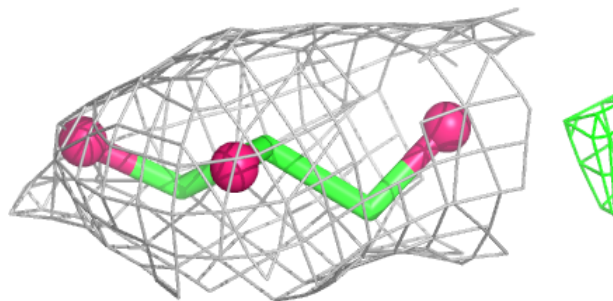
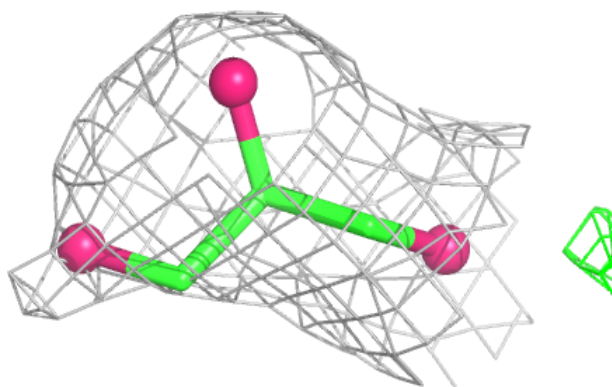
**Electron density around GOL C 306:**

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



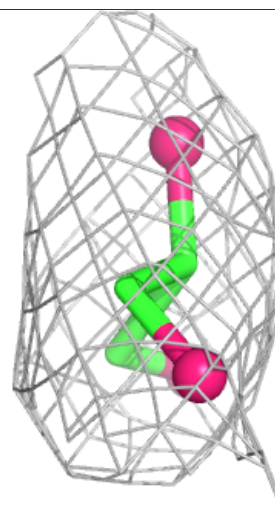
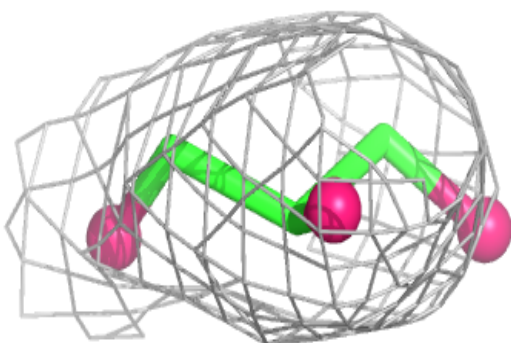
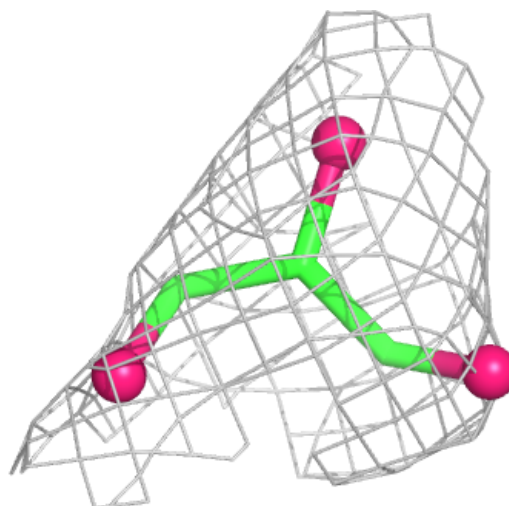
Electron density around GOL A 314:

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



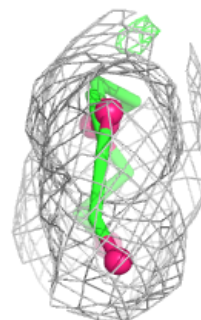
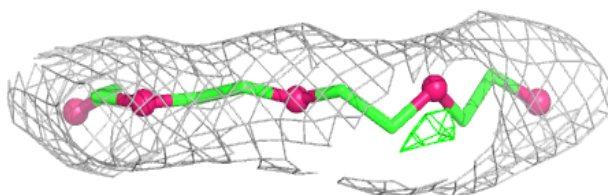
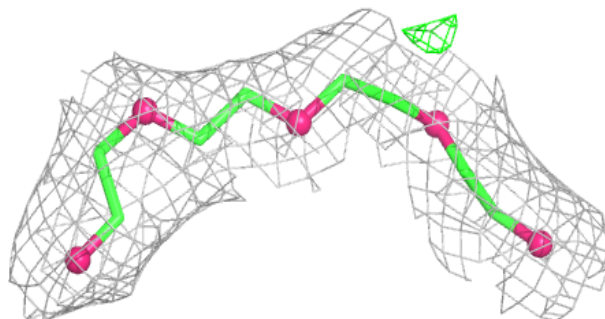
Electron density around GOL A 302:

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

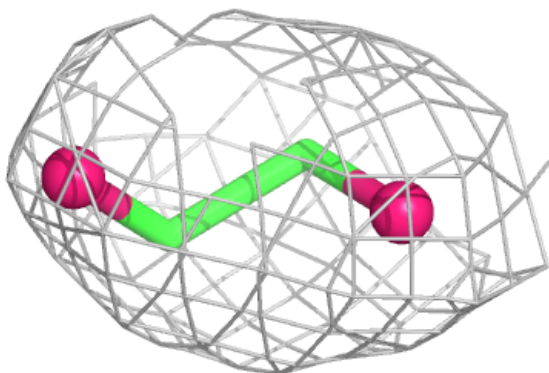
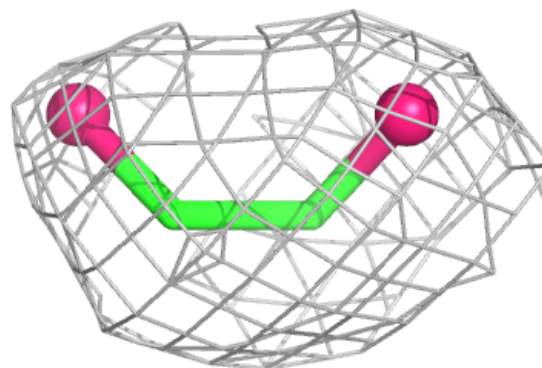


Electron density around PG4 F 105:

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

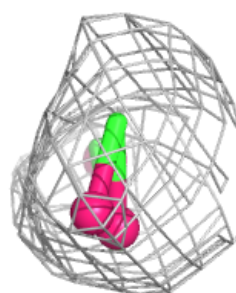
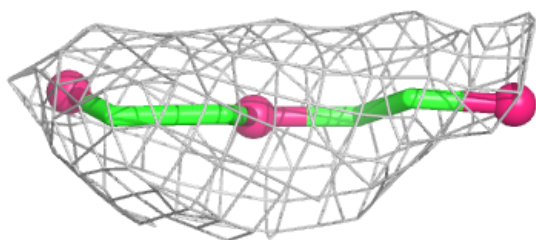
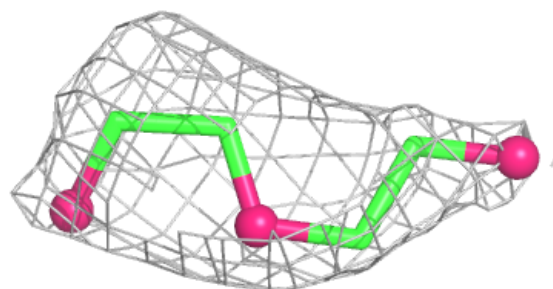
**Electron density around EDO D 130:**

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

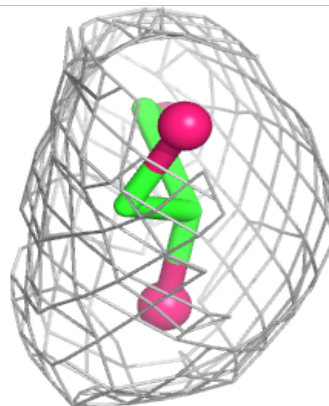
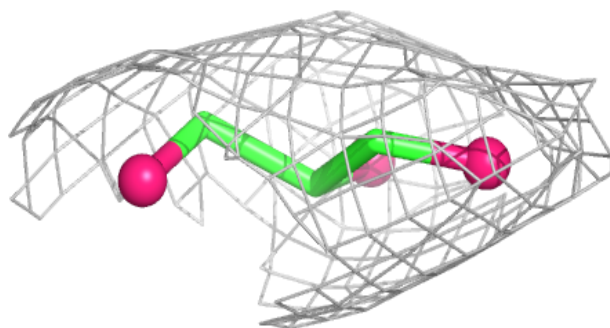
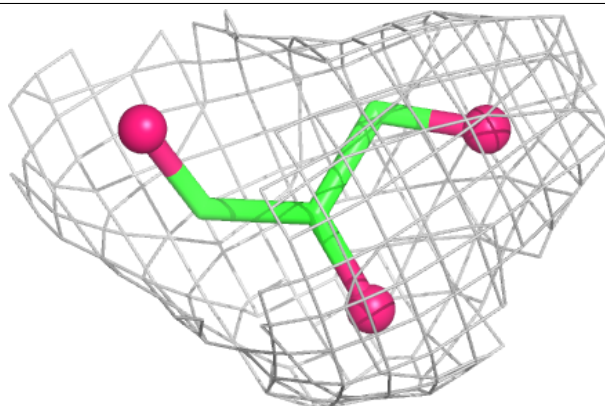


Electron density around PEG C 334:

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

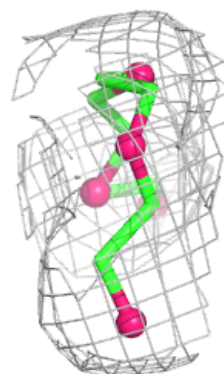
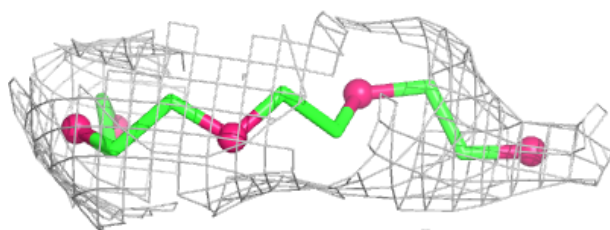
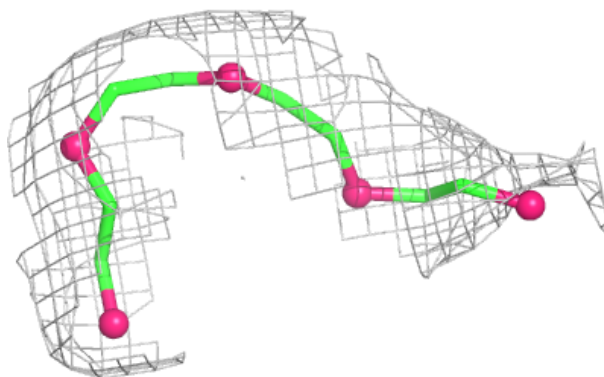
**Electron density around GOL B 153:**

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

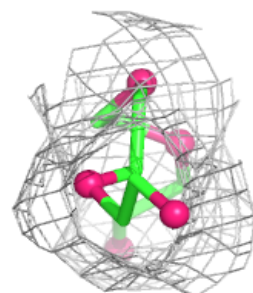
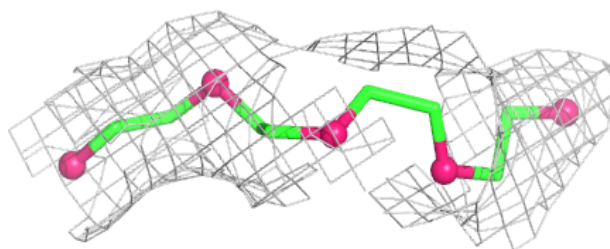
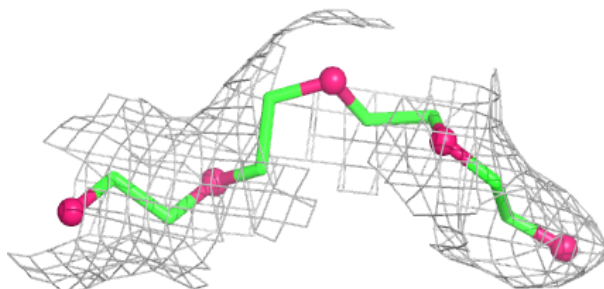


Electron density around PG4 B 122:

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

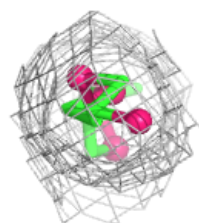
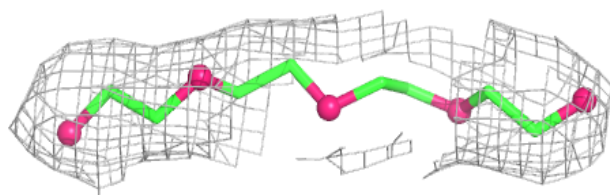
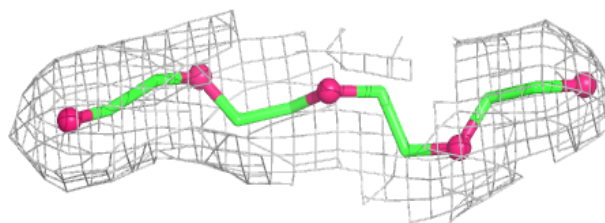
**Electron density around PG4 C 323:**

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

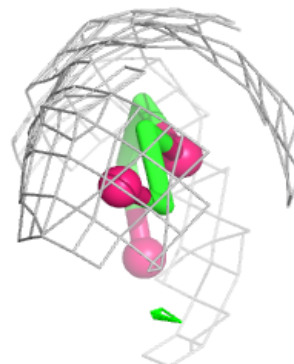
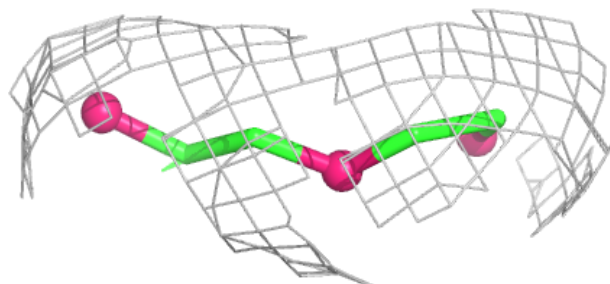
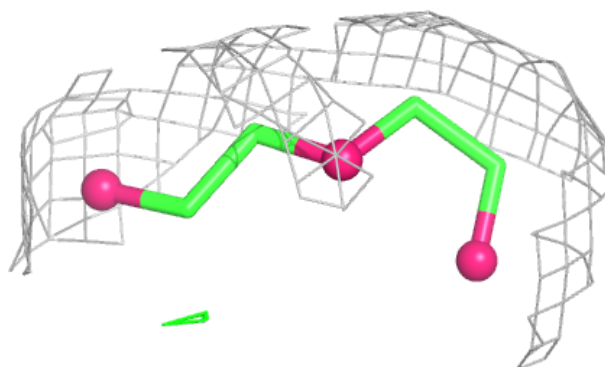


Electron density around PG4 E 115:

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

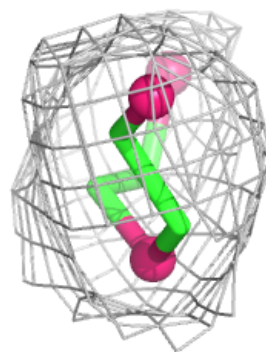
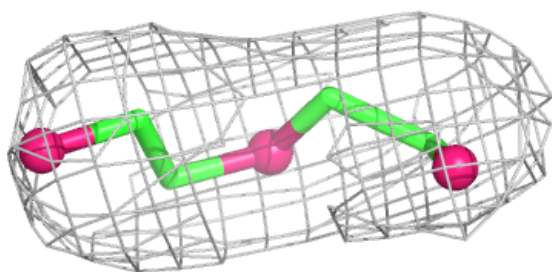
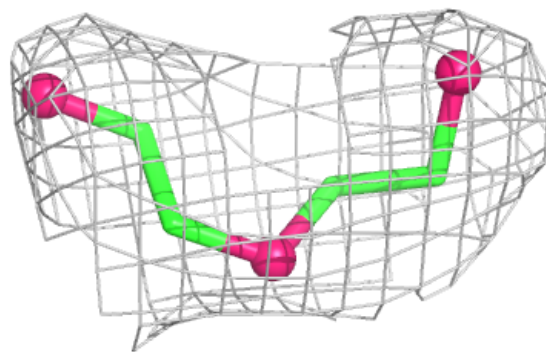
**Electron density around PEG A 370:**

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



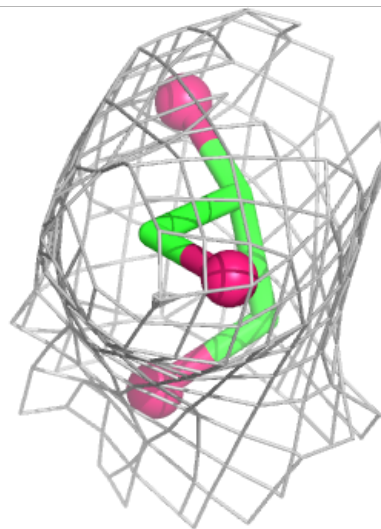
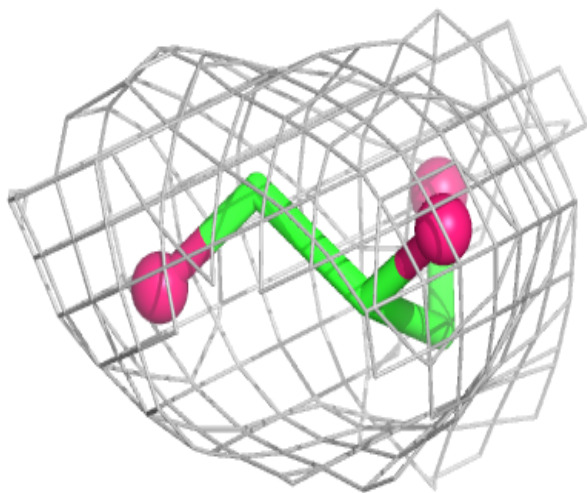
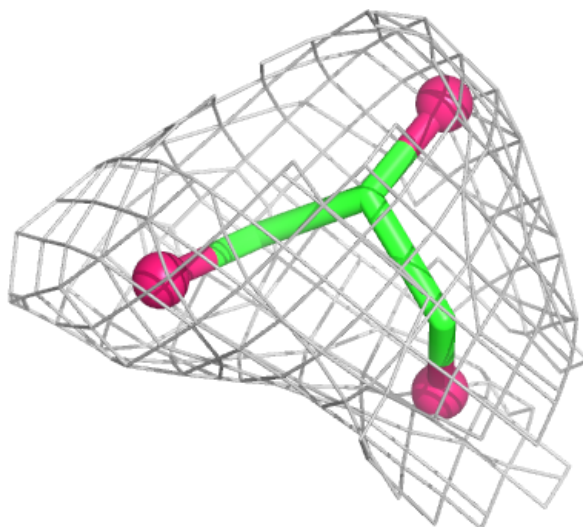
Electron density around PEG B 157:

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



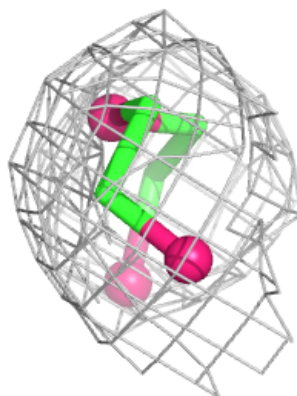
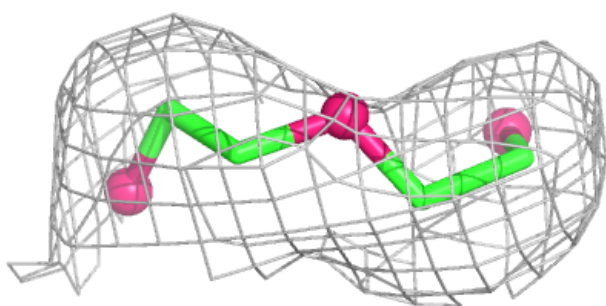
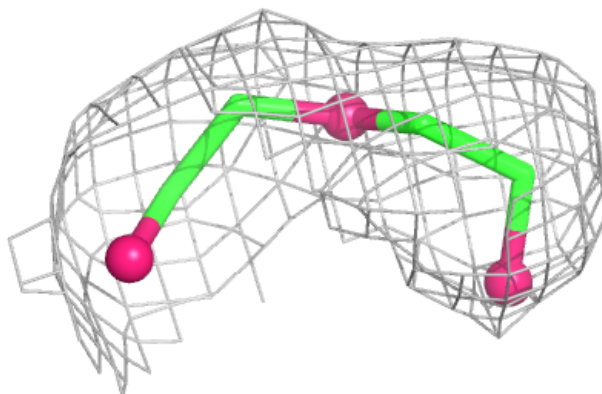
Electron density around GOL E 113:

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



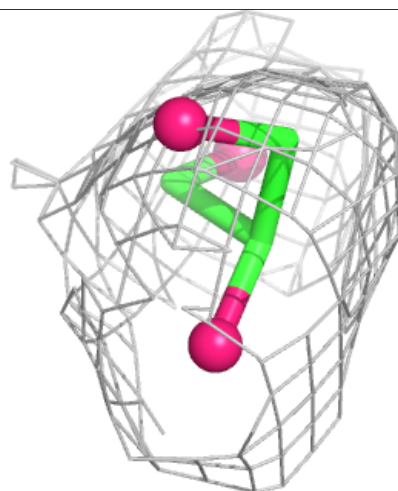
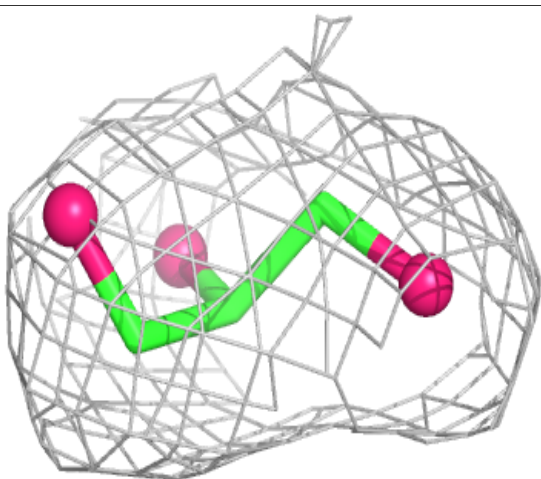
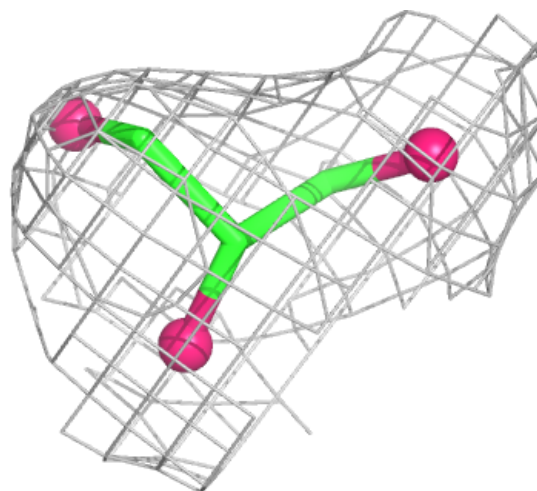
Electron density around PEG A 334:

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



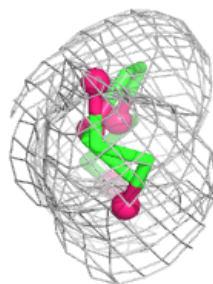
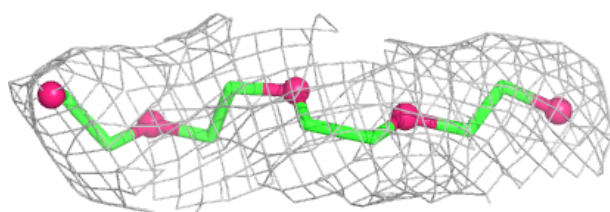
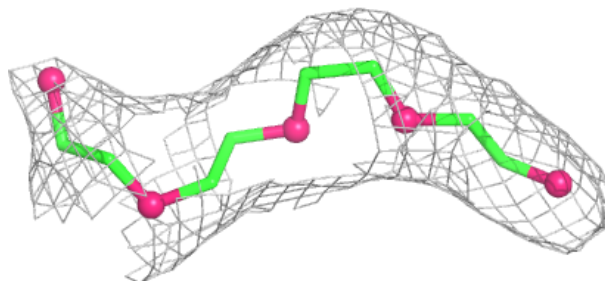
Electron density around GOL C 344:

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

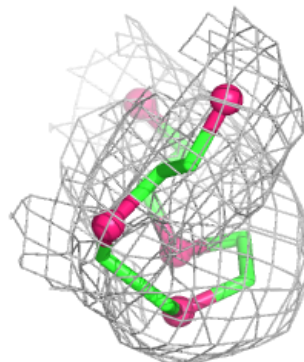
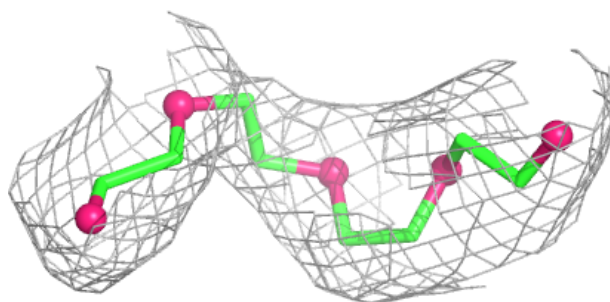
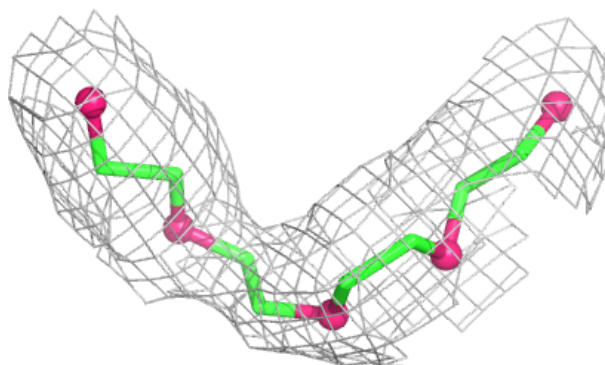


Electron density around PG4 A 319:

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

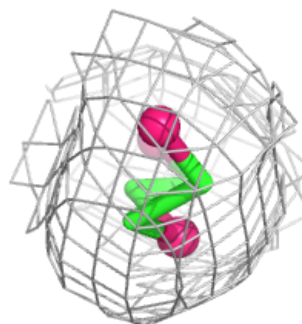
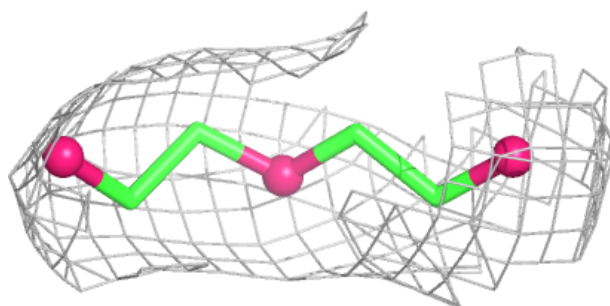
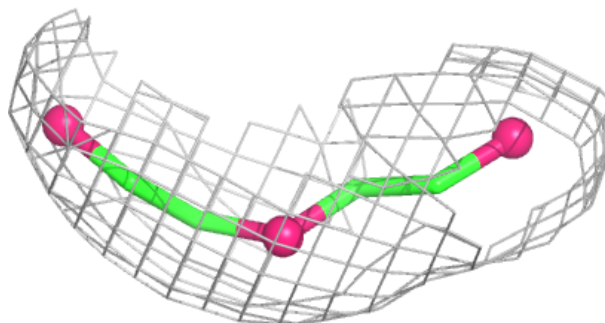
**Electron density around PG4 B 121:**

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



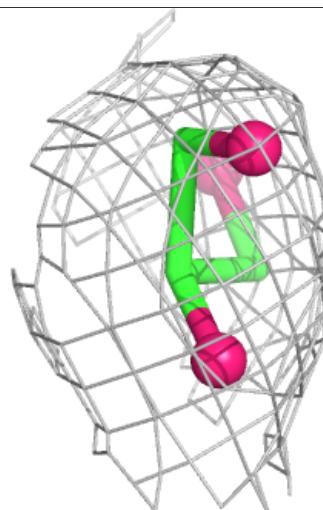
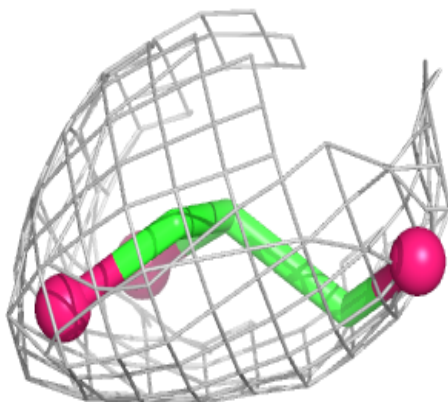
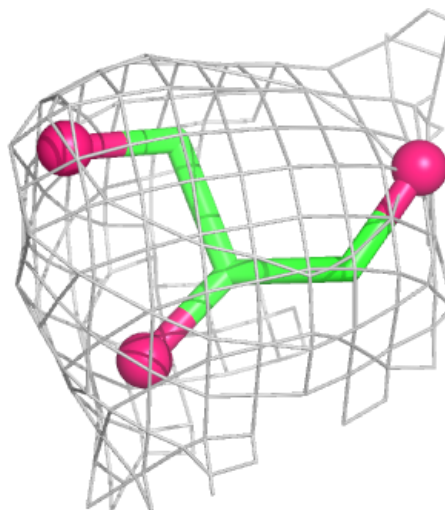
Electron density around PEG C 346:

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



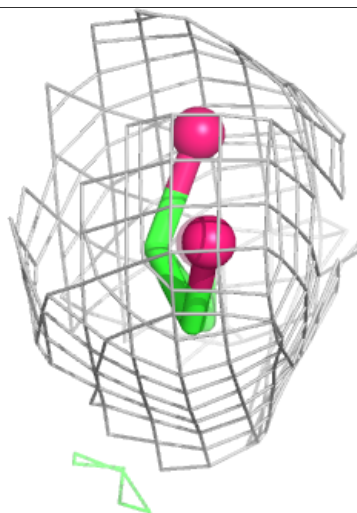
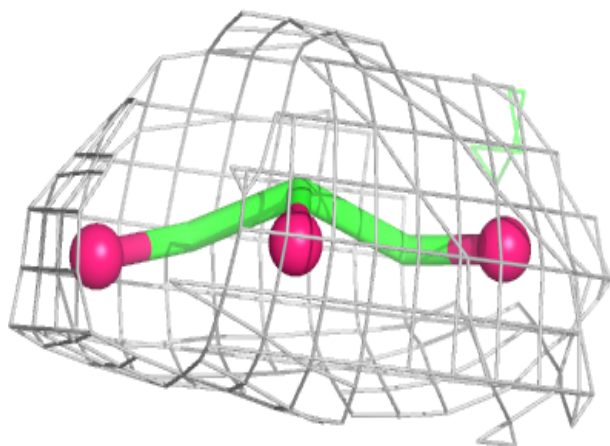
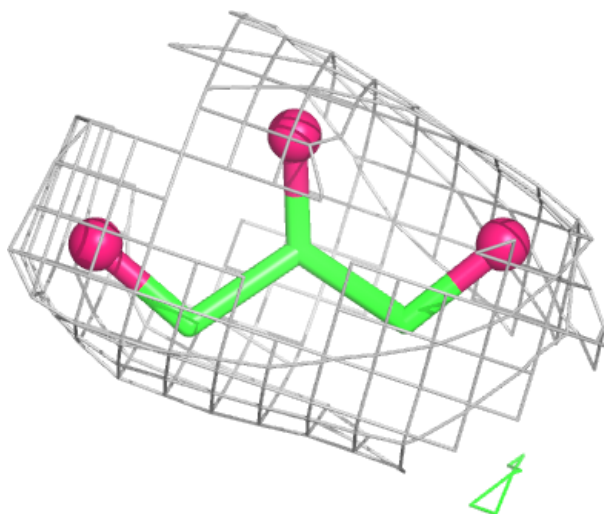
Electron density around GOL C 347:

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



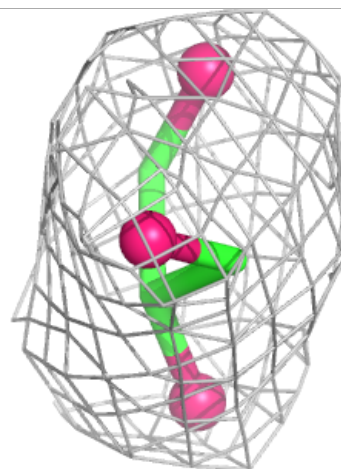
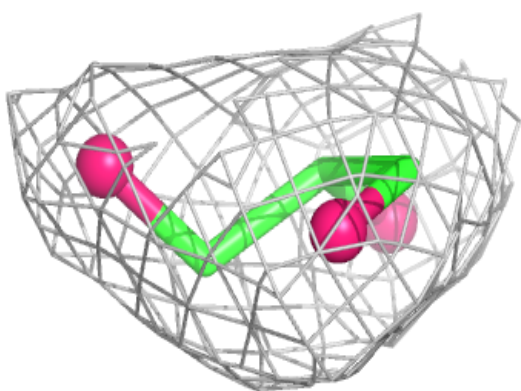
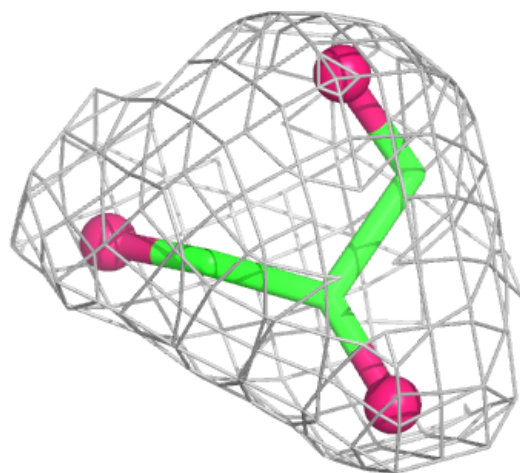
Electron density around GOL A 307:

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



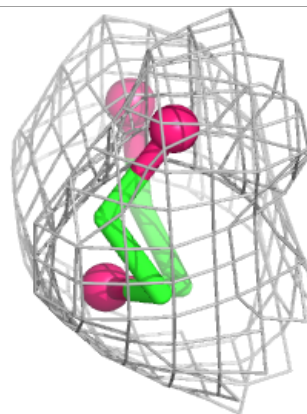
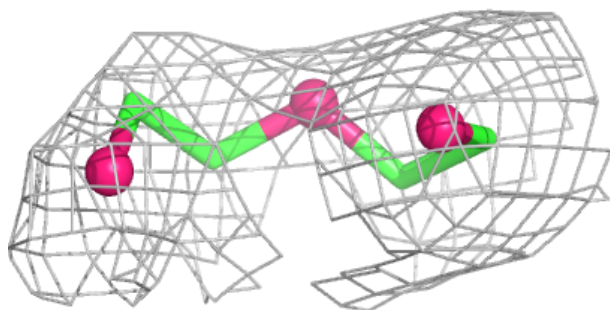
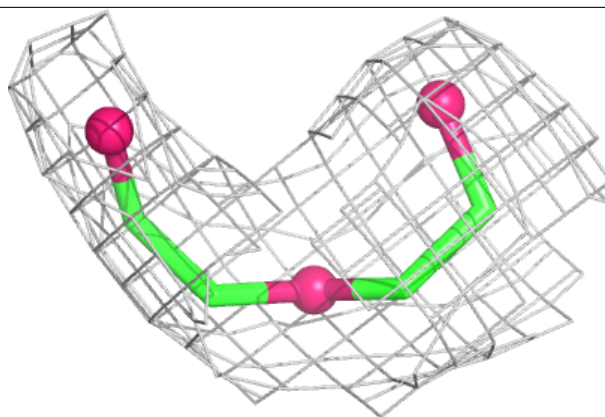
Electron density around GOL B 111:

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

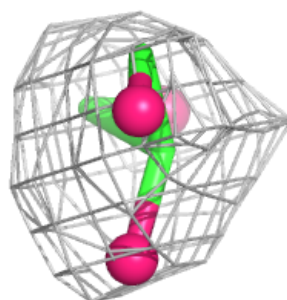
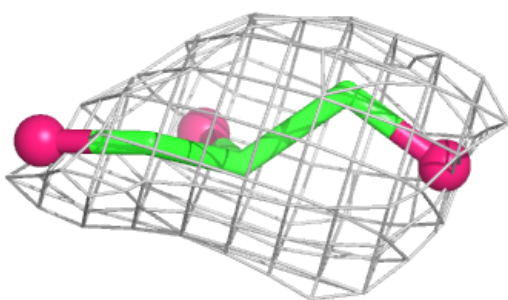
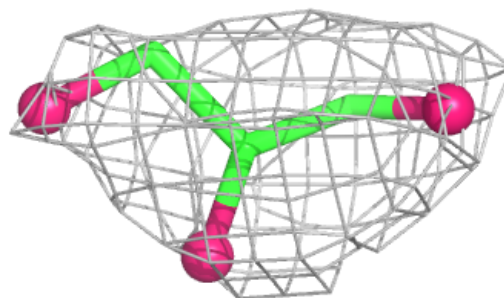


Electron density around PEG C 303:

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

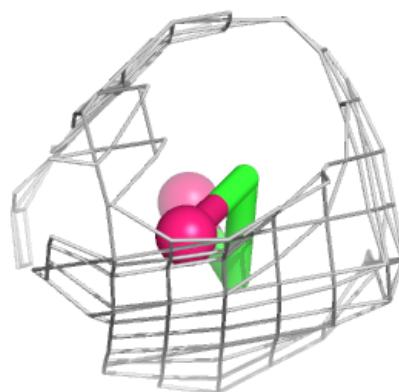
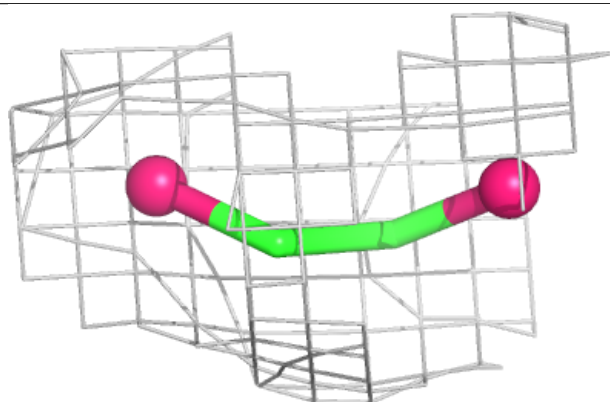
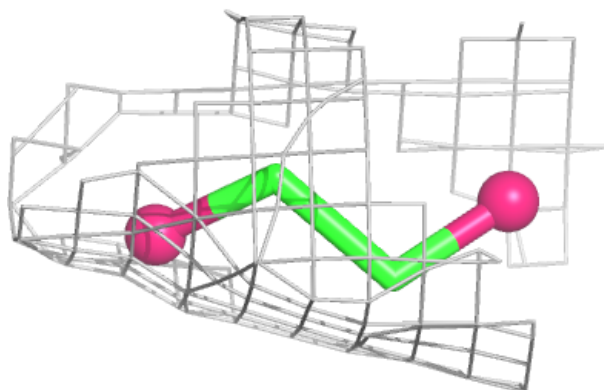
**Electron density around GOL C 304:**

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



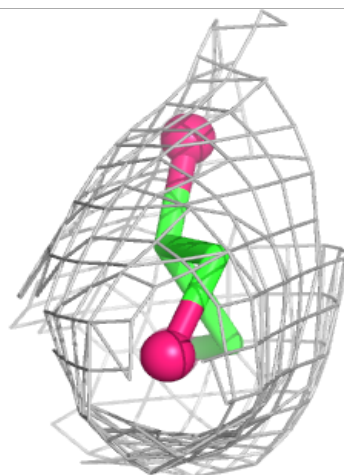
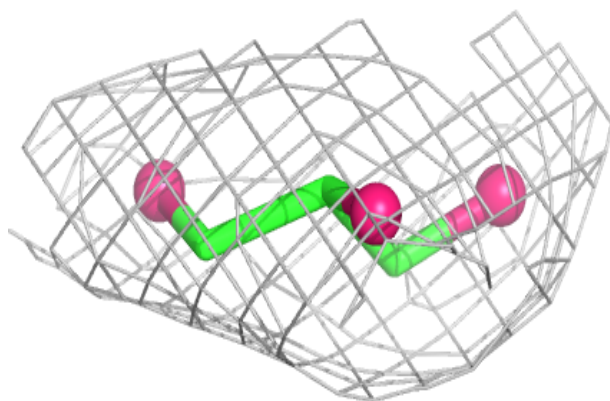
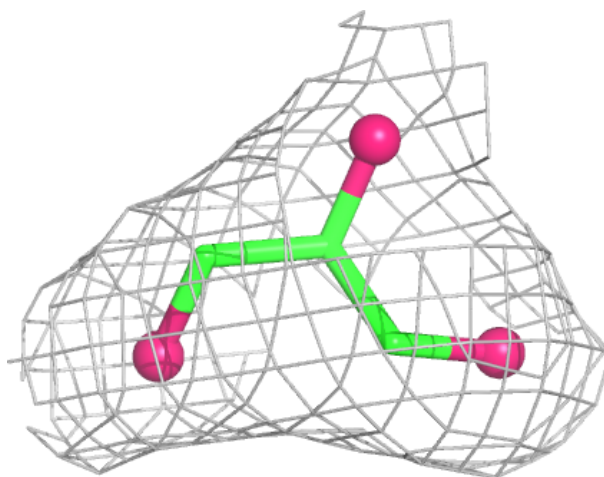
Electron density around EDO D 102:

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



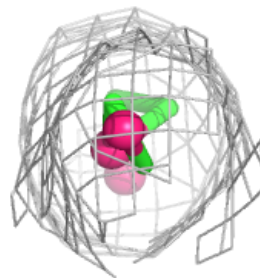
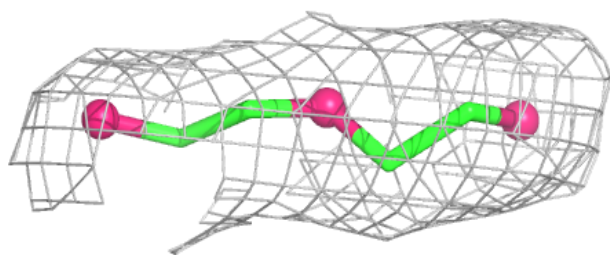
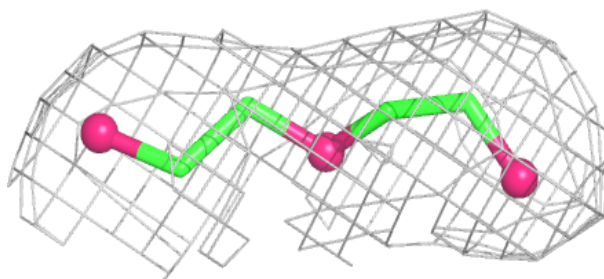
Electron density around GOL A 308:

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

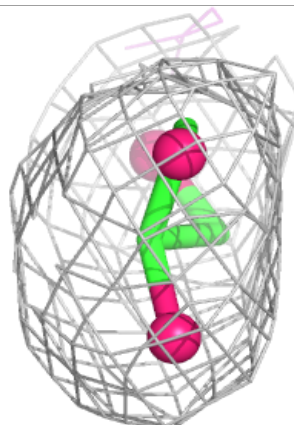
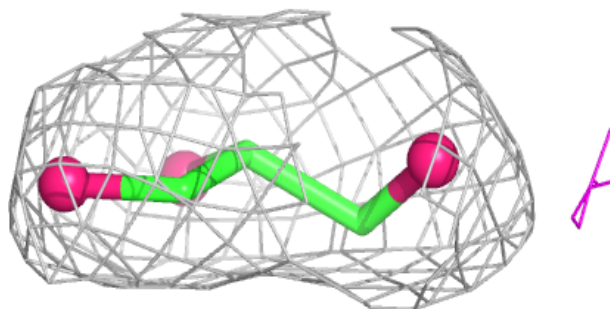
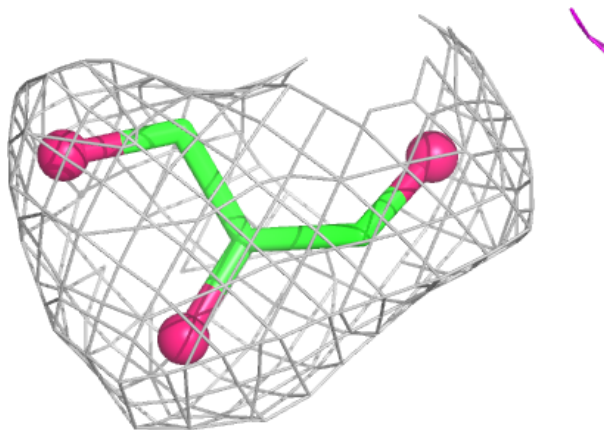


Electron density around PEG A 372:

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

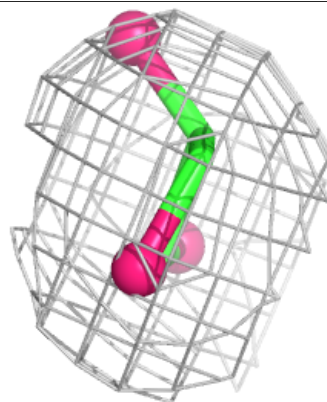
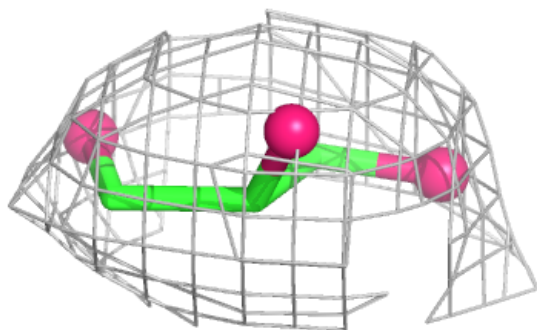
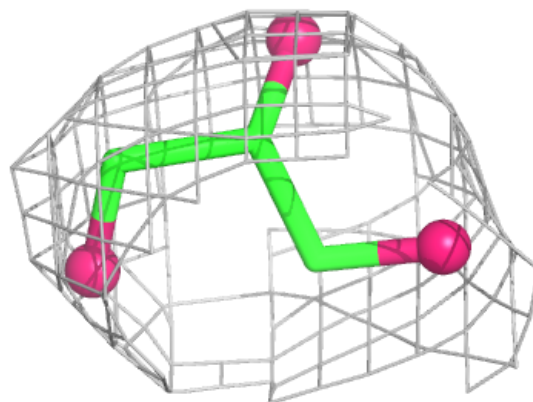
**Electron density around GOL D 109:**

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

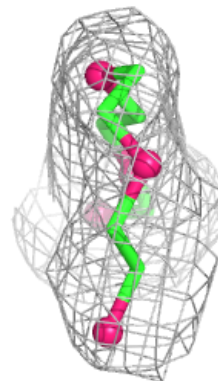
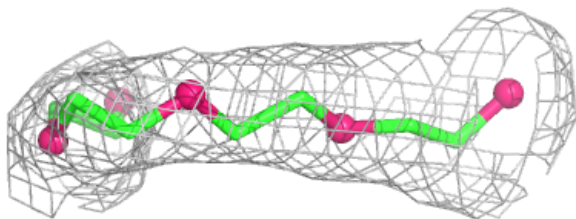
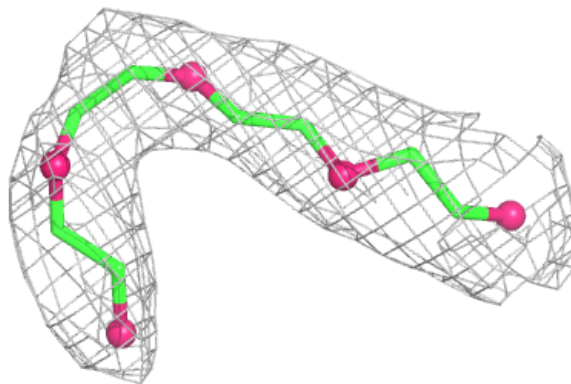


Electron density around GOL A 310:

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

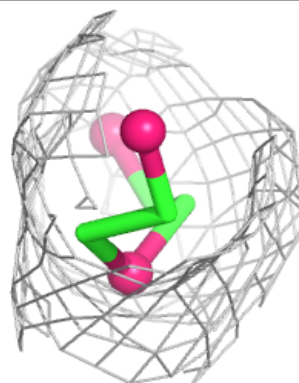
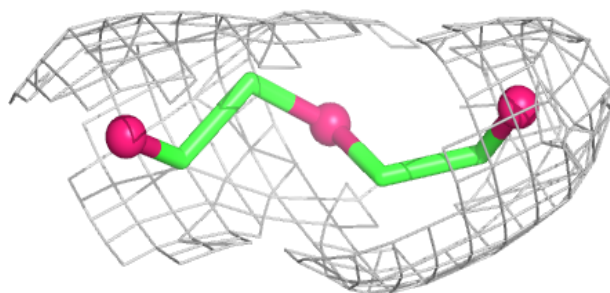
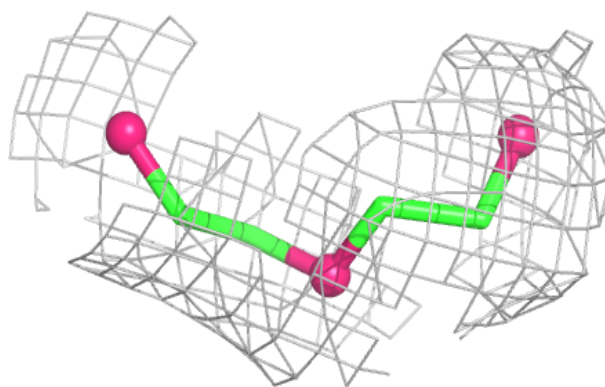
**Electron density around PG4 B 116:**

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

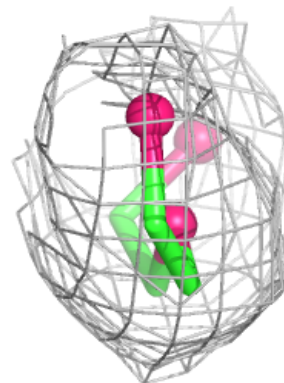
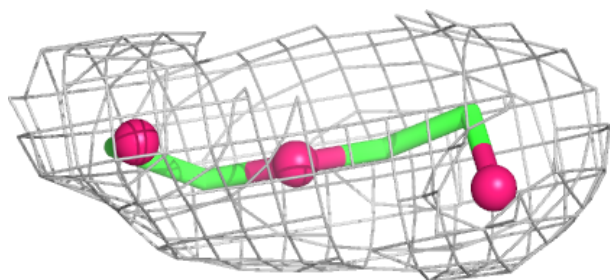
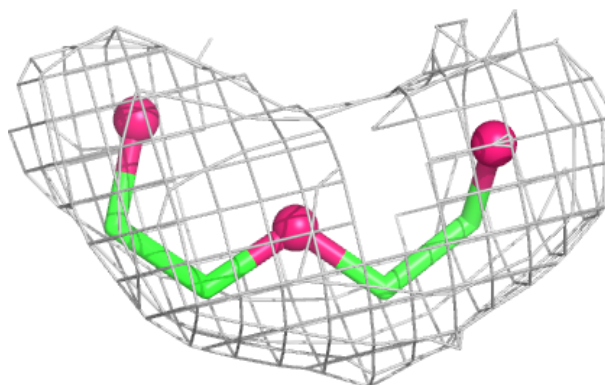


Electron density around PEG B 139:

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

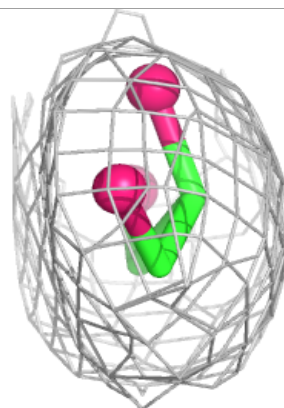
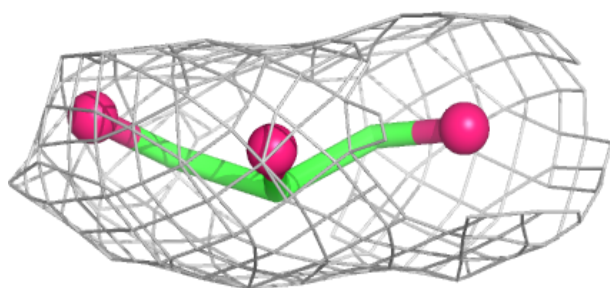
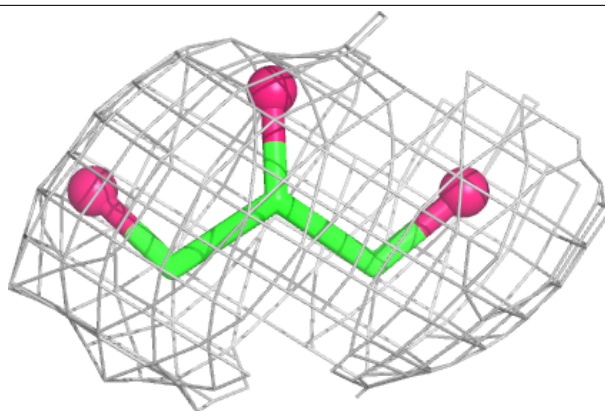
**Electron density around PEG B 142:**

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

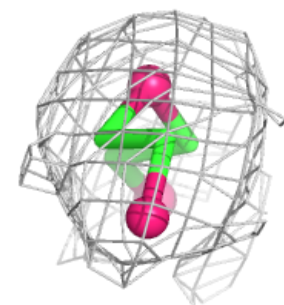
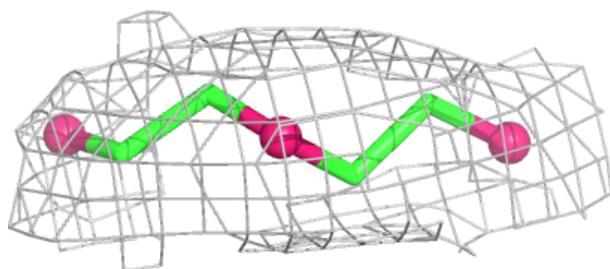
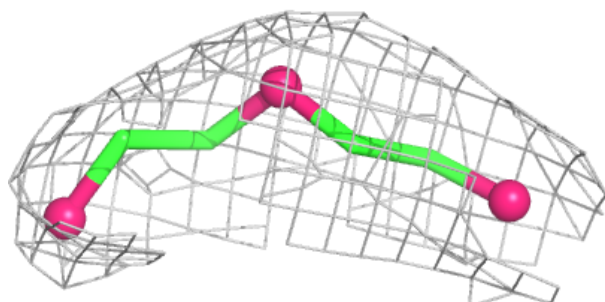


Electron density around GOL D 112:

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

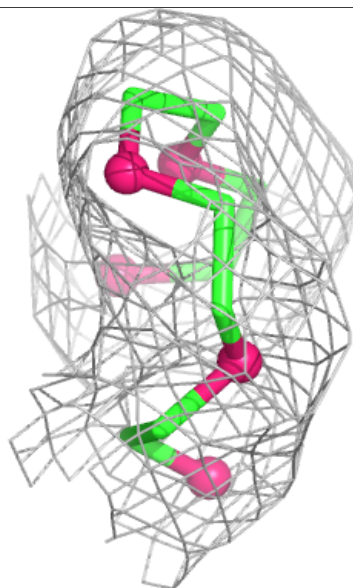
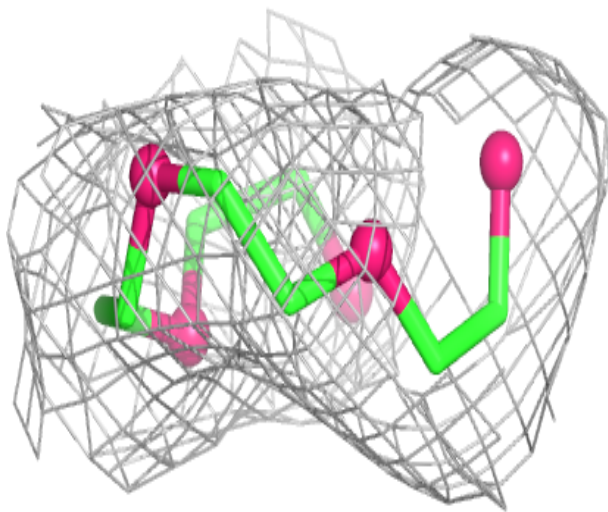
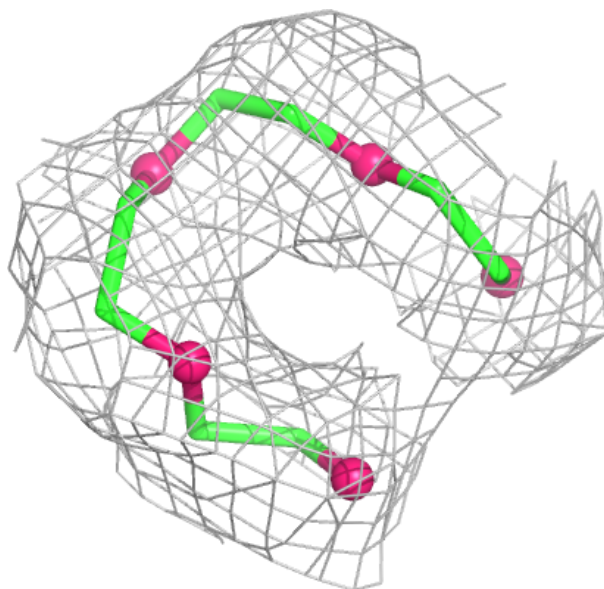
**Electron density around PEG D 123:**

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



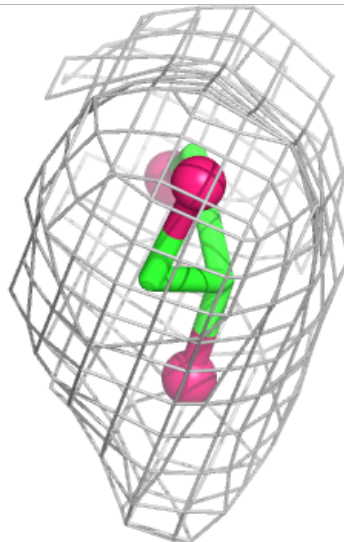
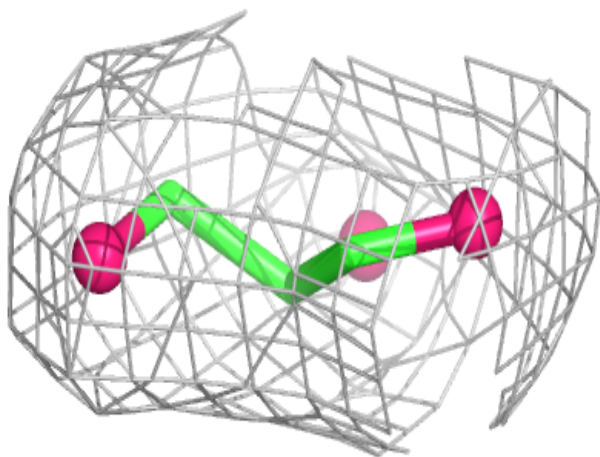
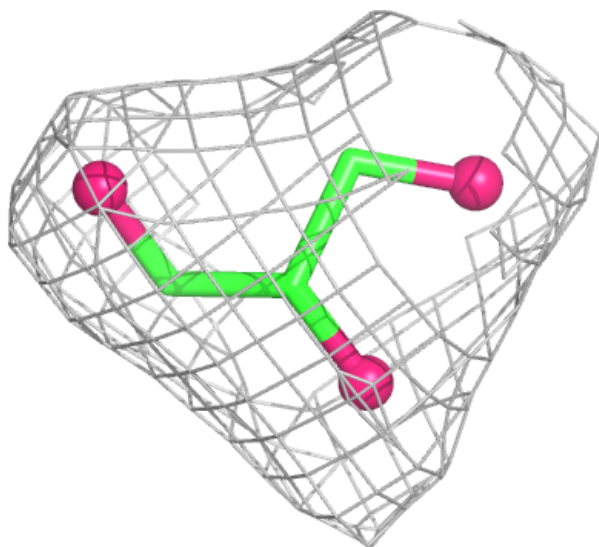
Electron density around PG4 F 101:

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



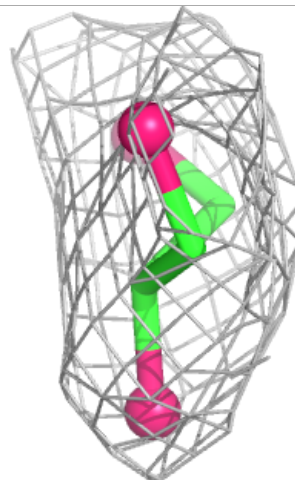
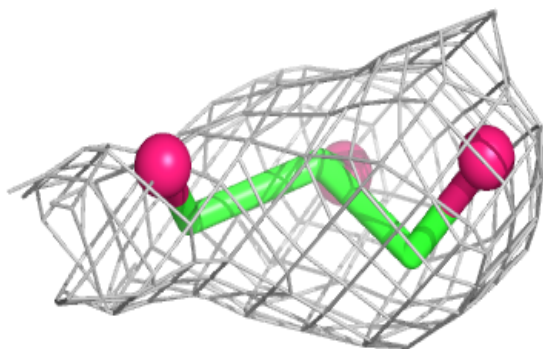
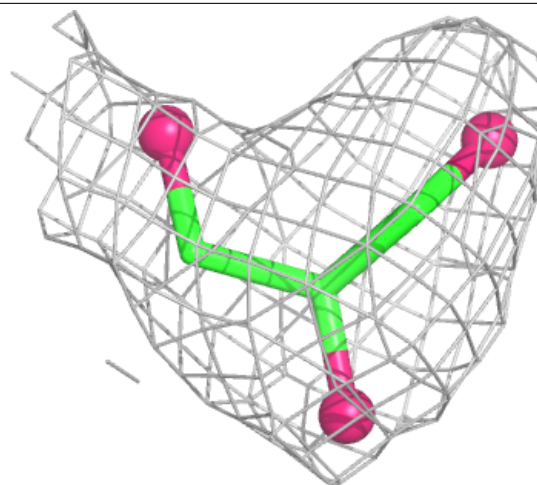
Electron density around GOL A 363:

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



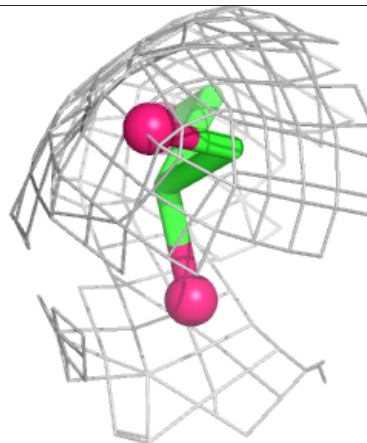
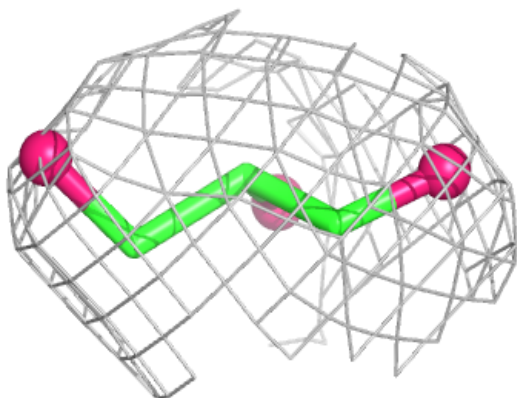
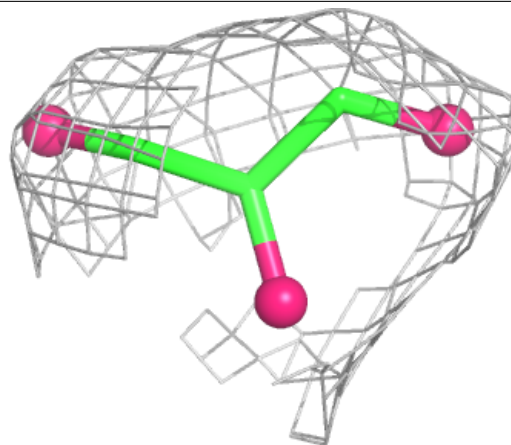
Electron density around GOL C 313:

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



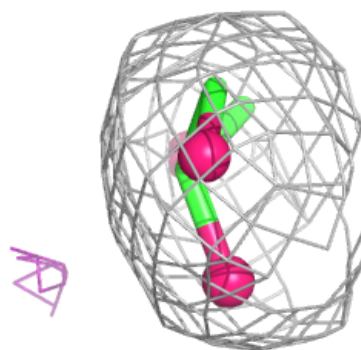
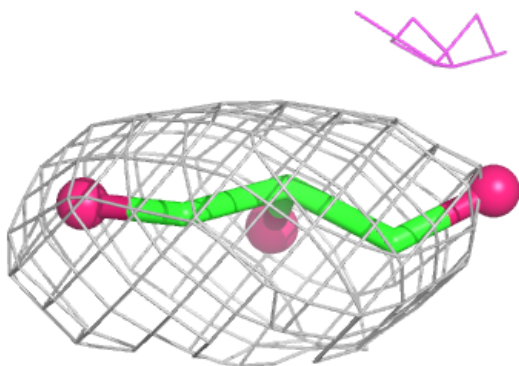
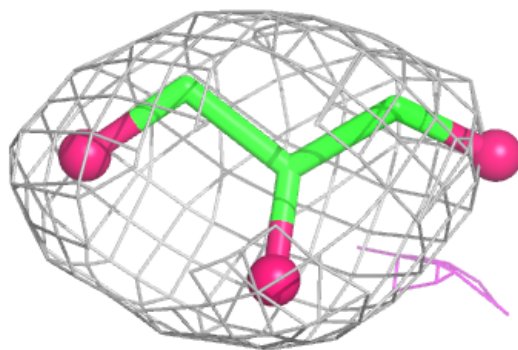
Electron density around GOL A 347:

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



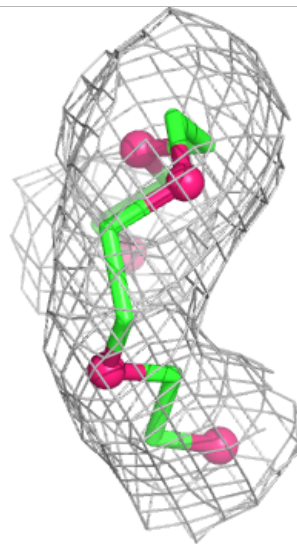
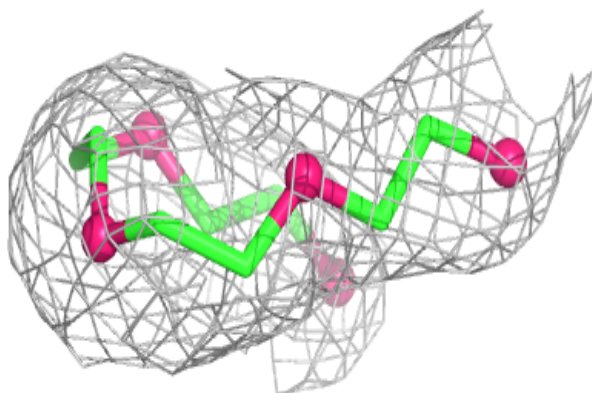
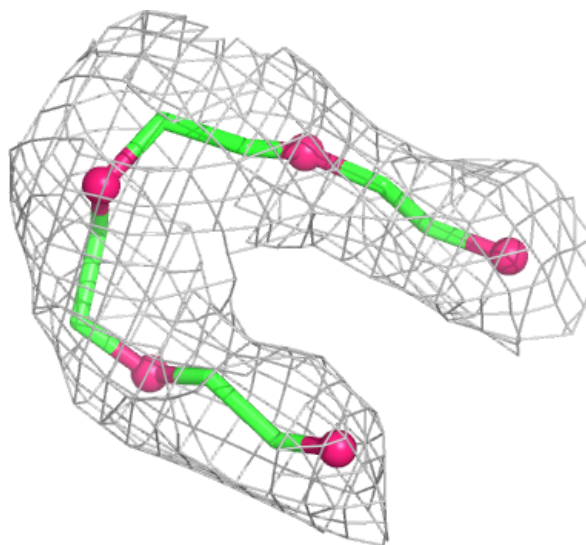
Electron density around GOL B 110:

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



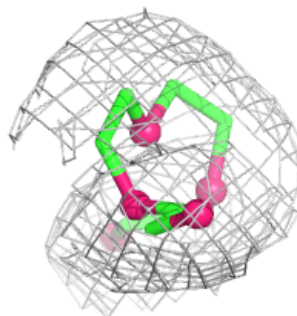
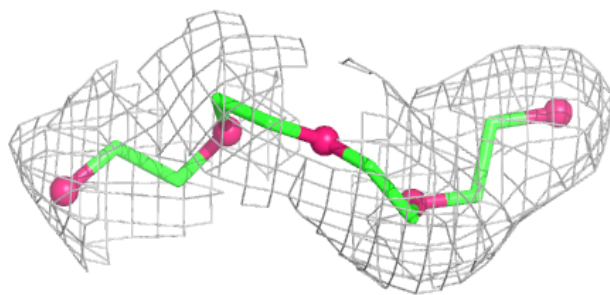
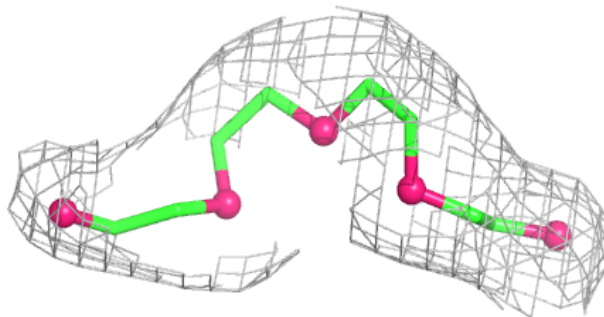
Electron density around PG4 E 107:

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

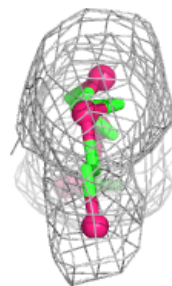
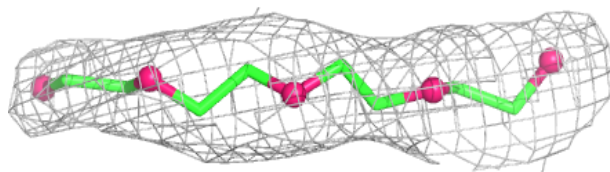
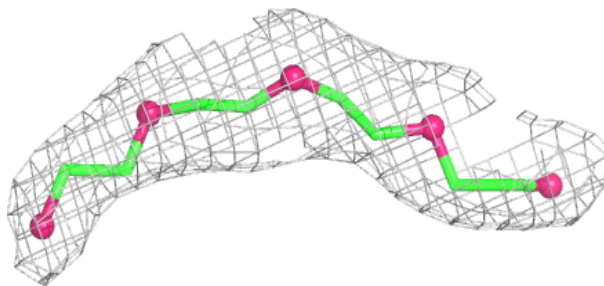


Electron density around PG4 A 367:

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

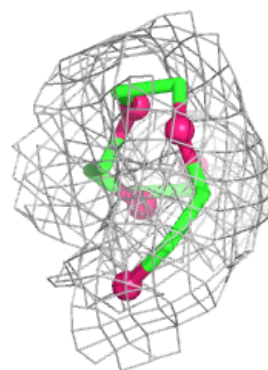
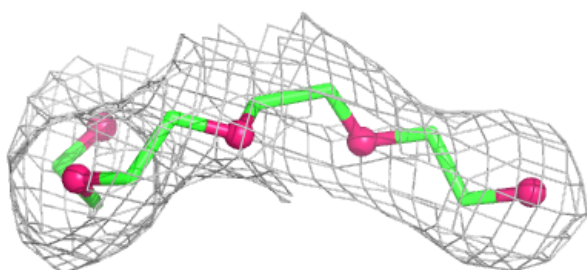
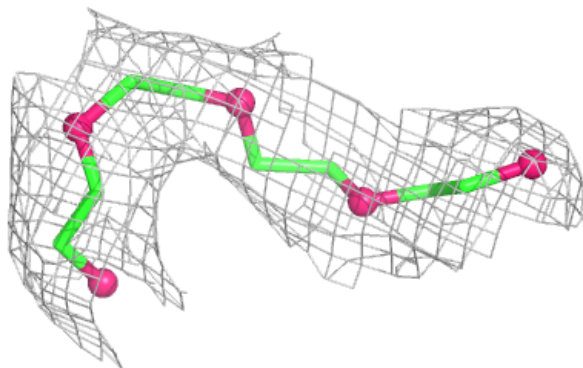
**Electron density around PG4 B 117:**

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

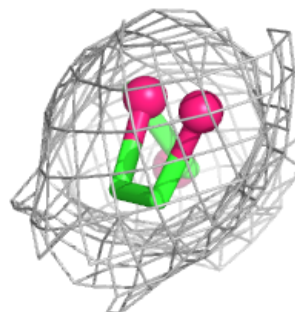
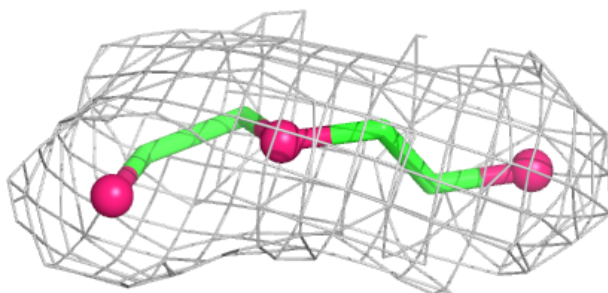
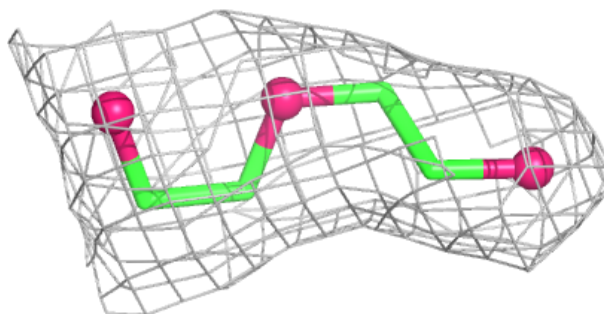


Electron density around PG4 C 321:

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

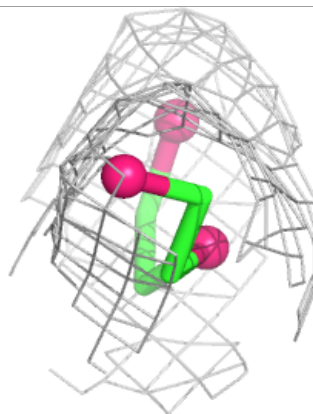
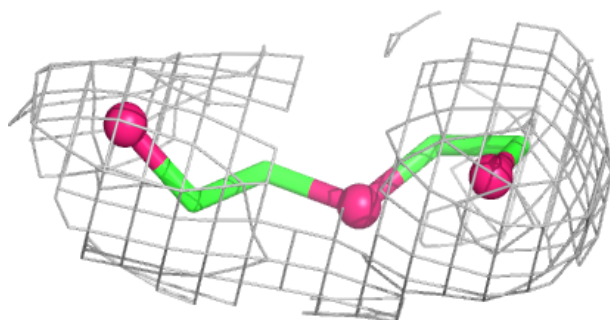
**Electron density around PEG D 124:**

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

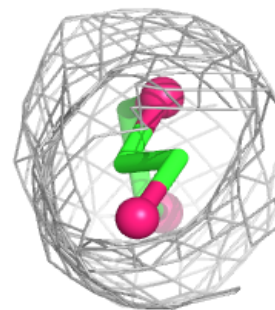
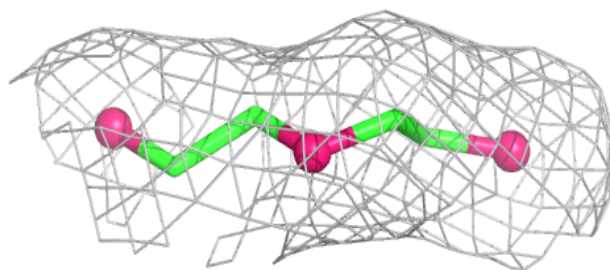
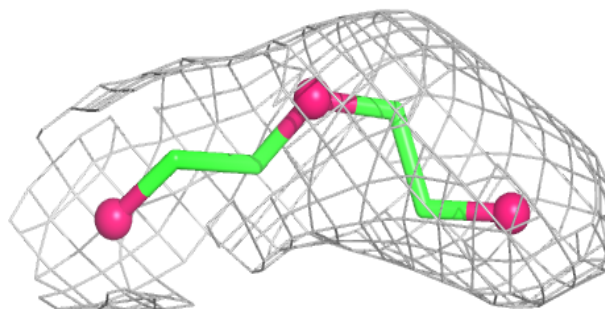


Electron density around PEG D 125:

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

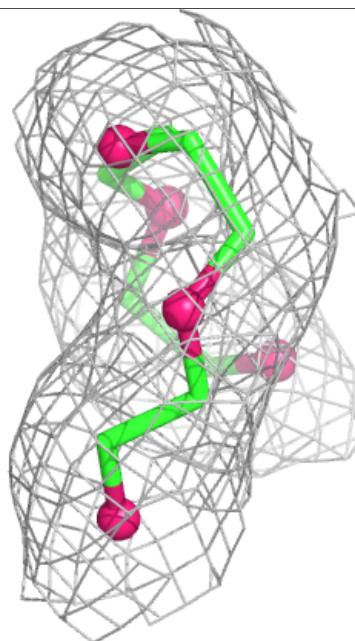
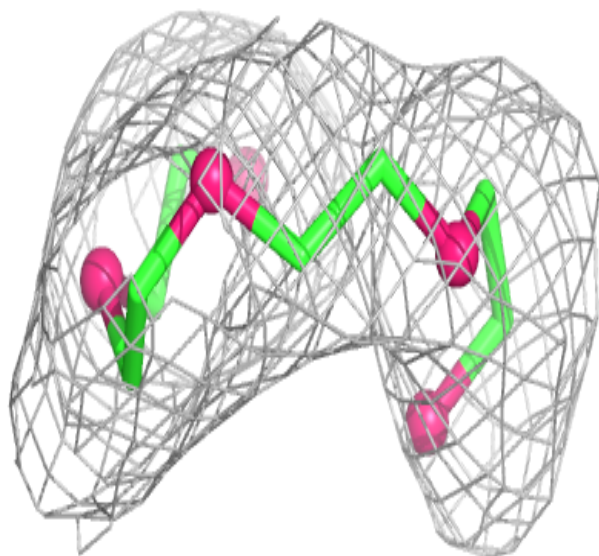
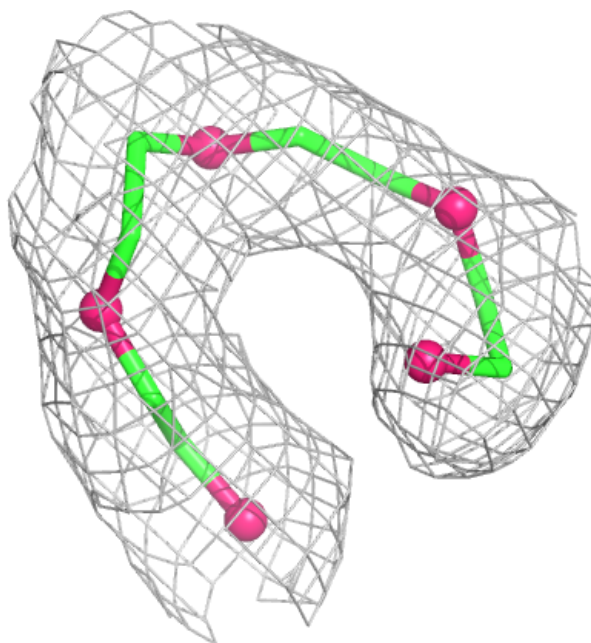
**Electron density around PEG C 328:**

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



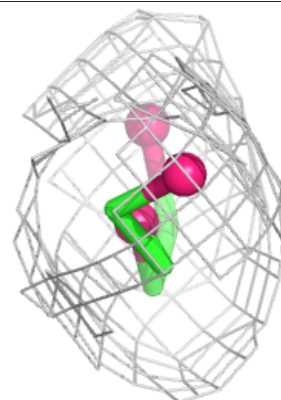
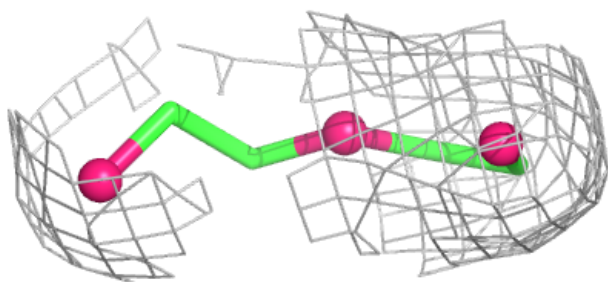
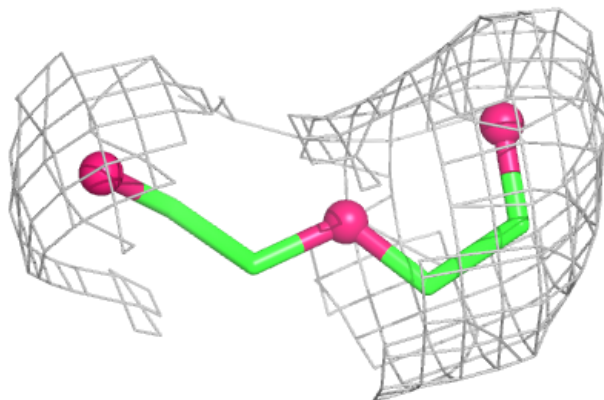
Electron density around PG4 A 366:

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



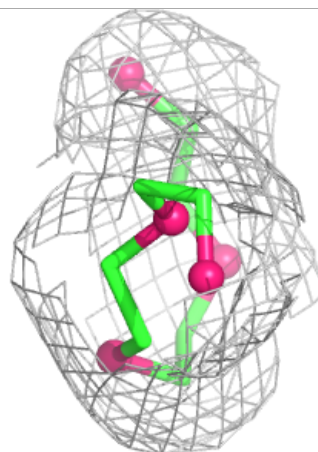
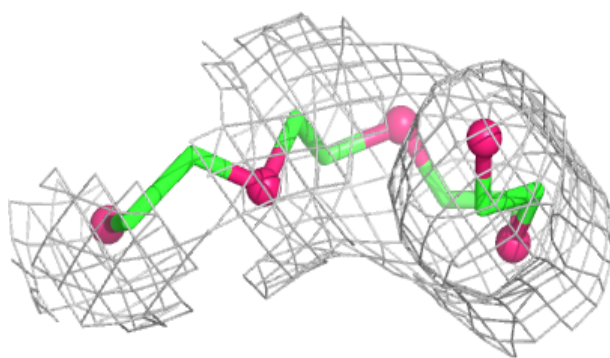
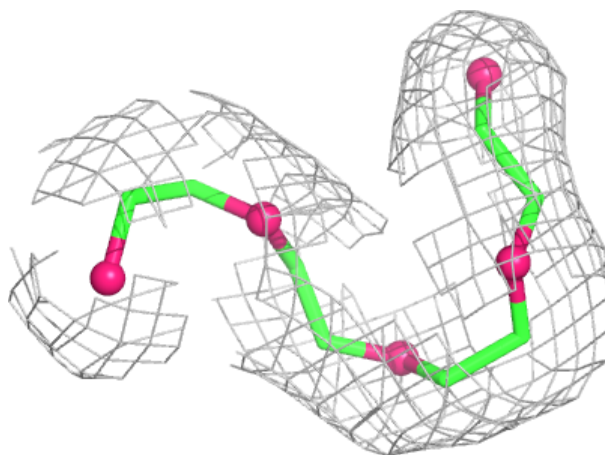
Electron density around PEG B 156:

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



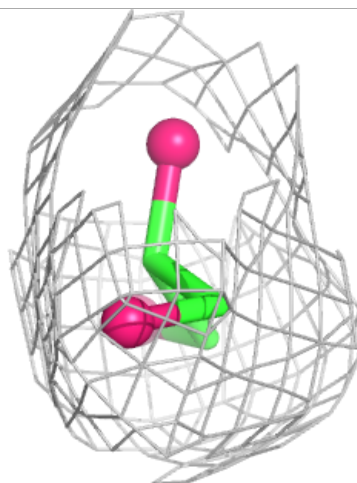
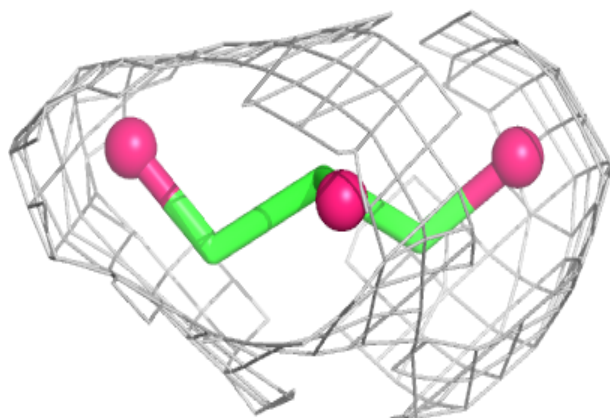
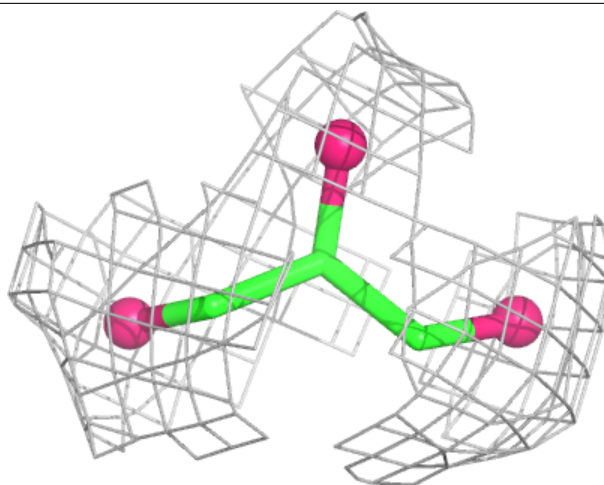
Electron density around PG4 B 123:

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



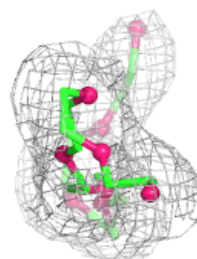
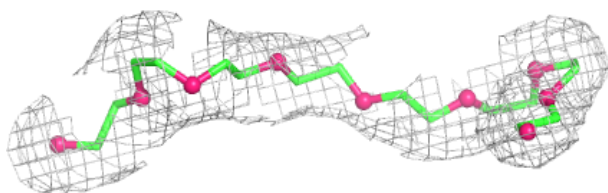
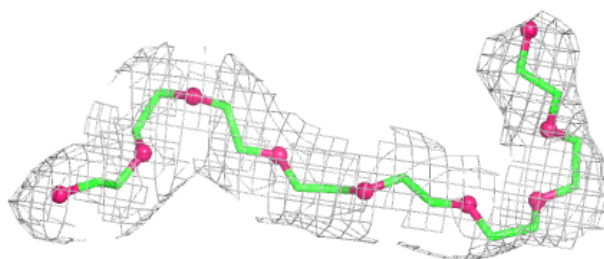
Electron density around GOL C 337:

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

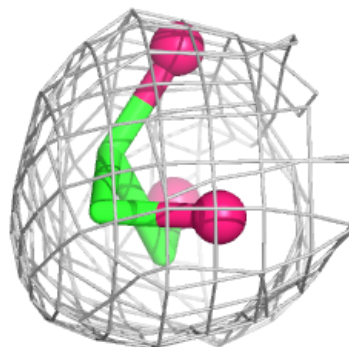
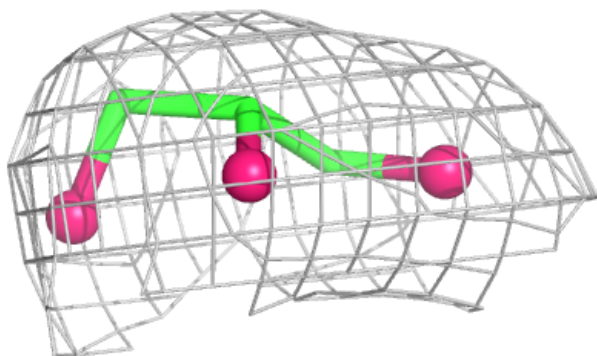
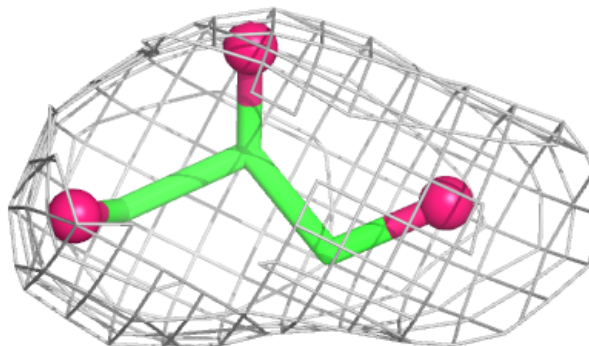


Electron density around PE8 C 335:

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

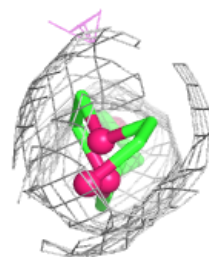
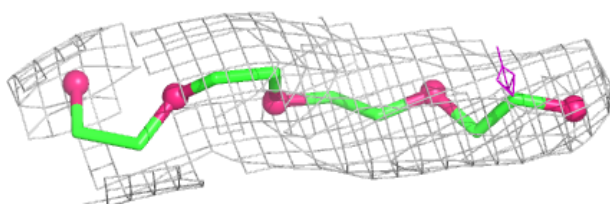
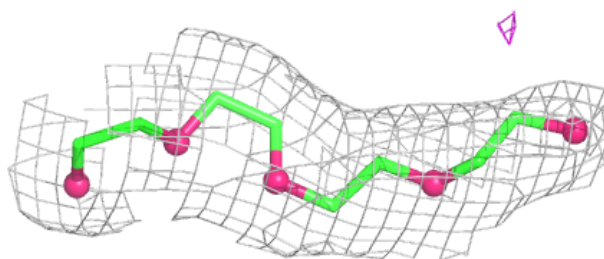
**Electron density around GOL B 106:**

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

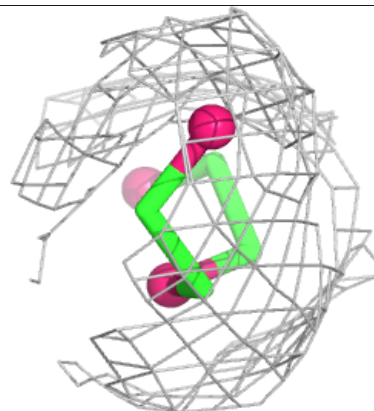
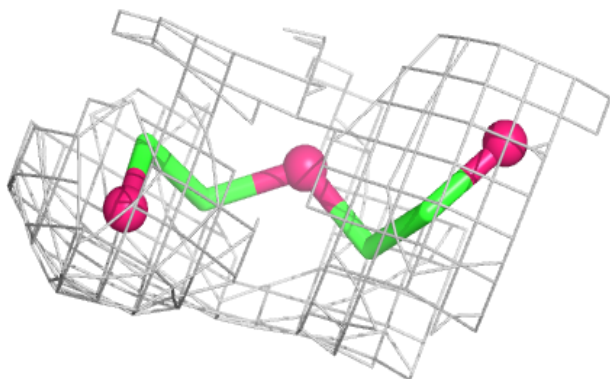
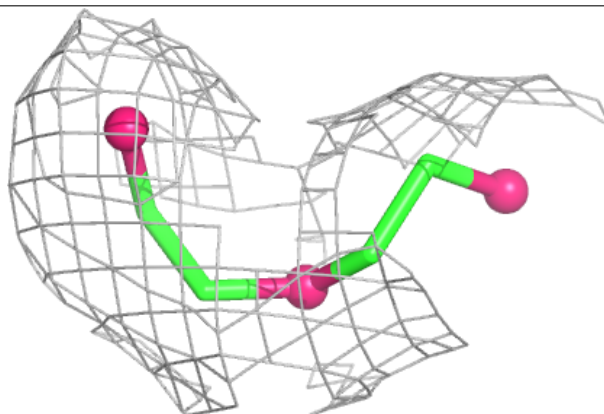


Electron density around PG4 A 365:

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

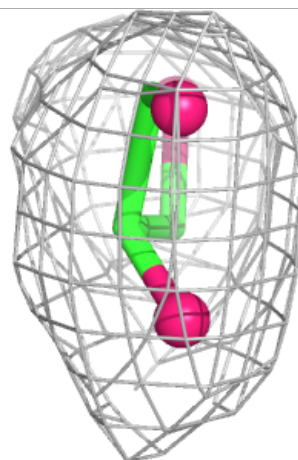
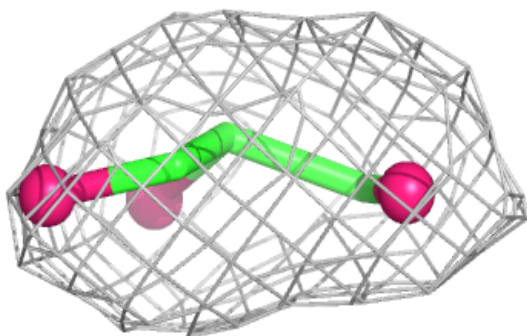
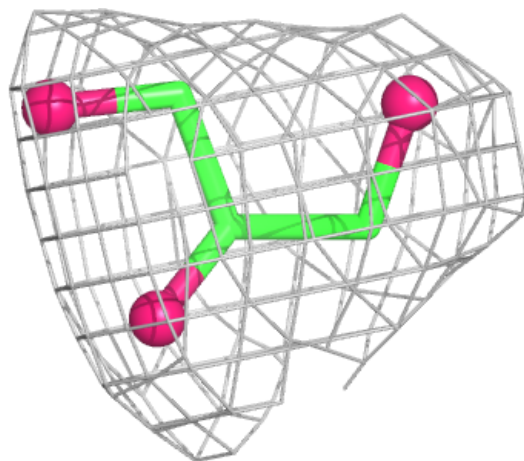
**Electron density around PEG B 127:**

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



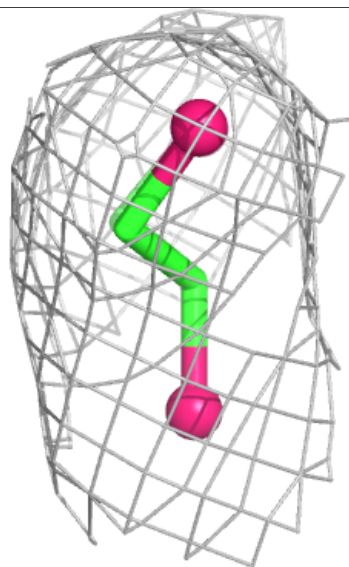
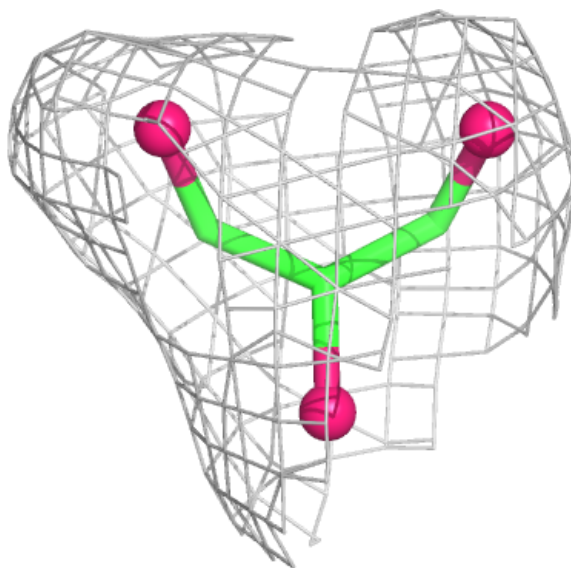
Electron density around GOL A 312:

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



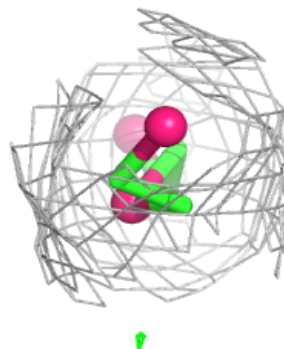
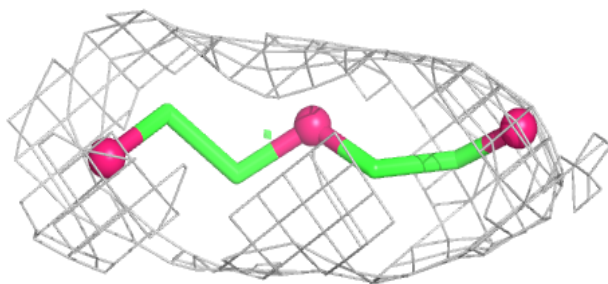
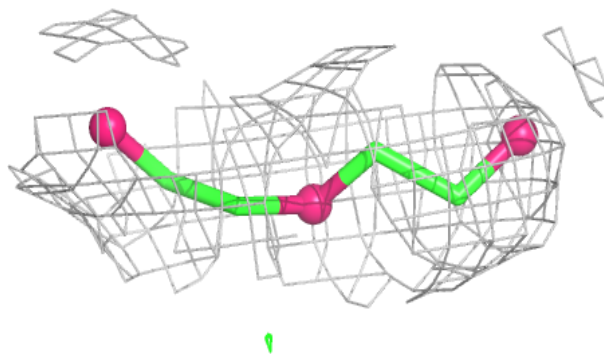
Electron density around GOL A 311:

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

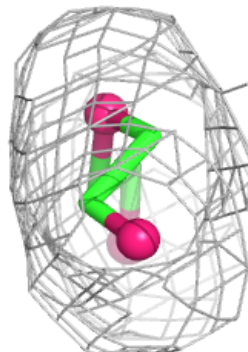
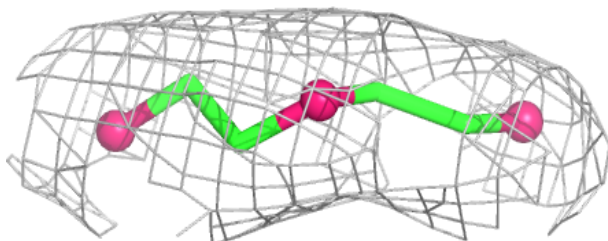
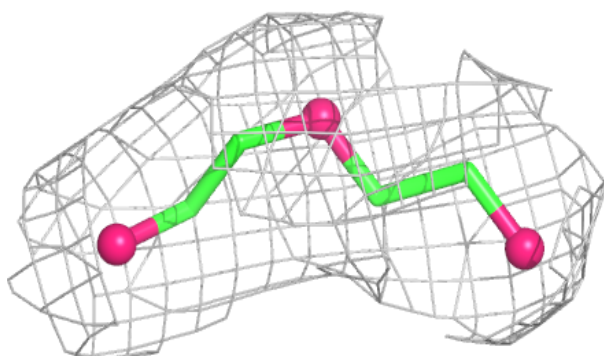


Electron density around PEG A 340:

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

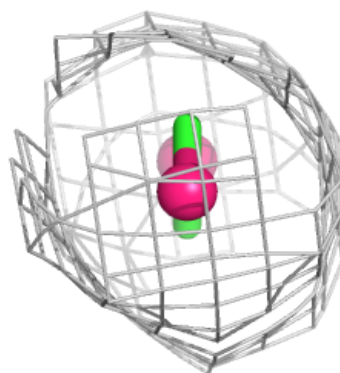
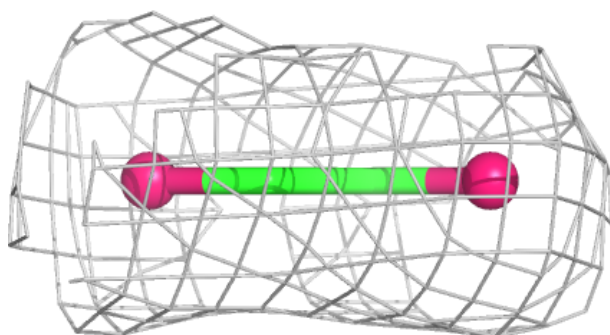
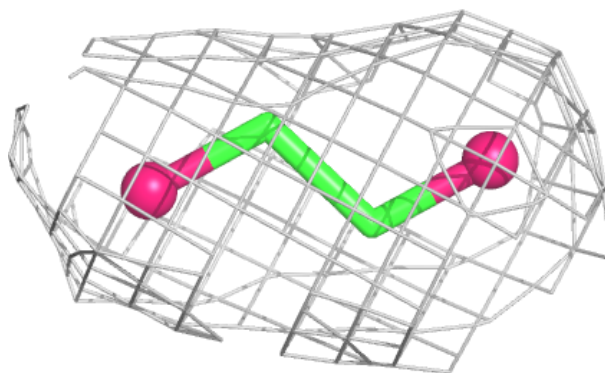
**Electron density around PEG B 131:**

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

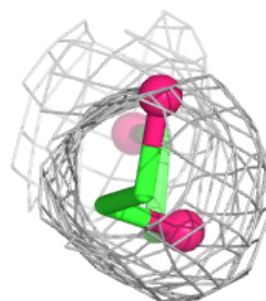
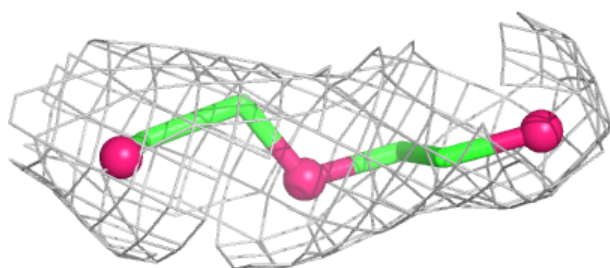
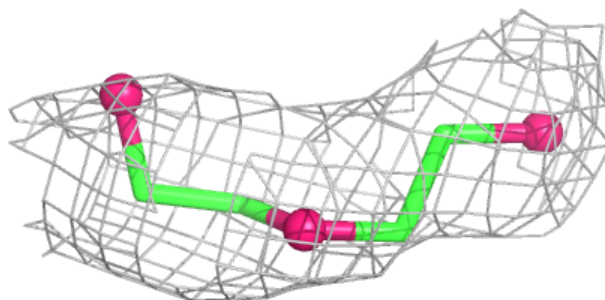


Electron density around EDO E 101:

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

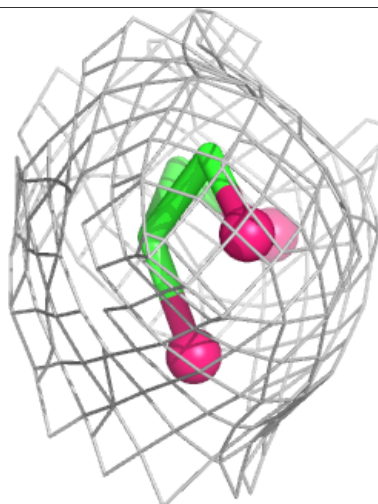
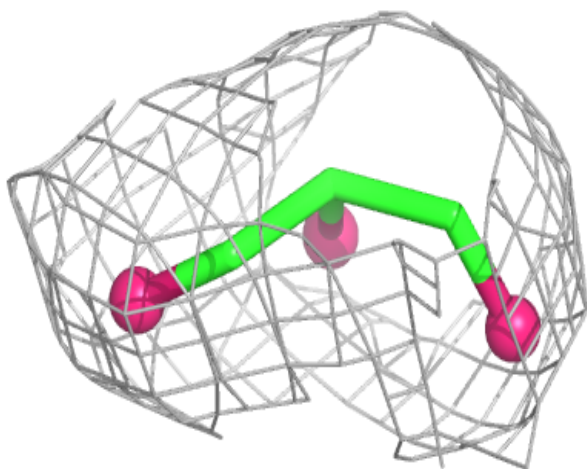
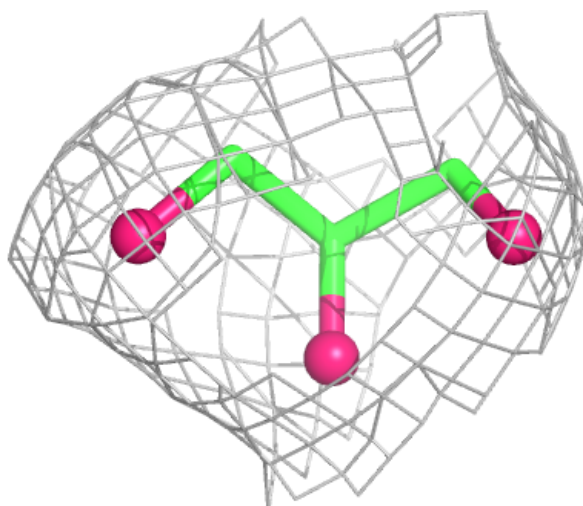
**Electron density around PEG D 122:**

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



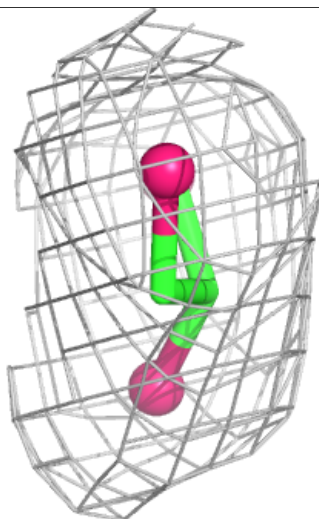
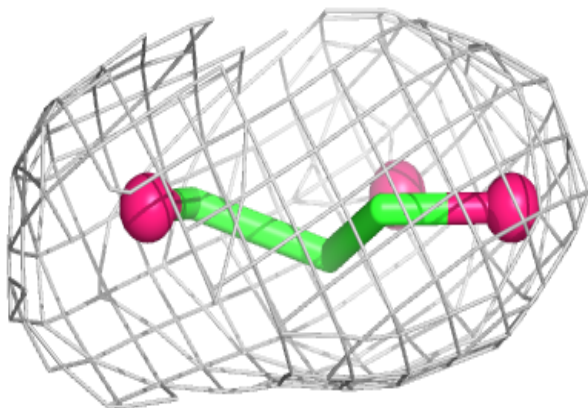
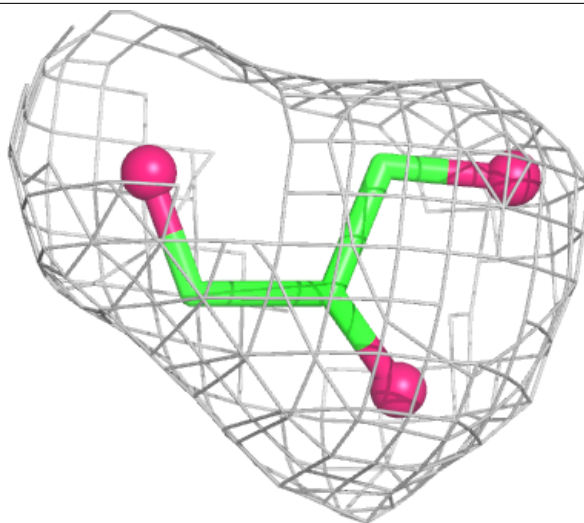
Electron density around GOL E 102:

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



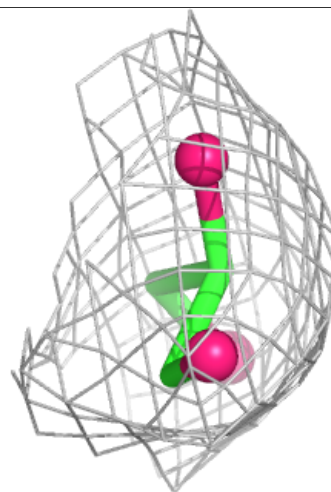
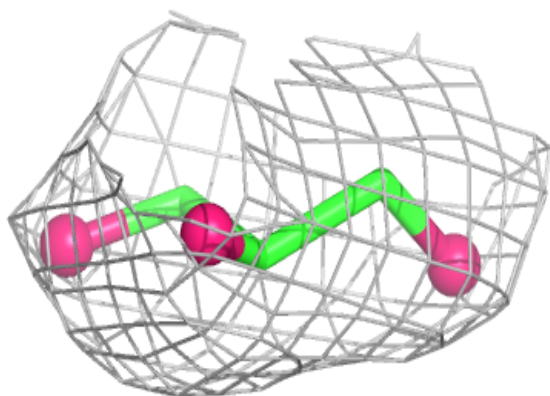
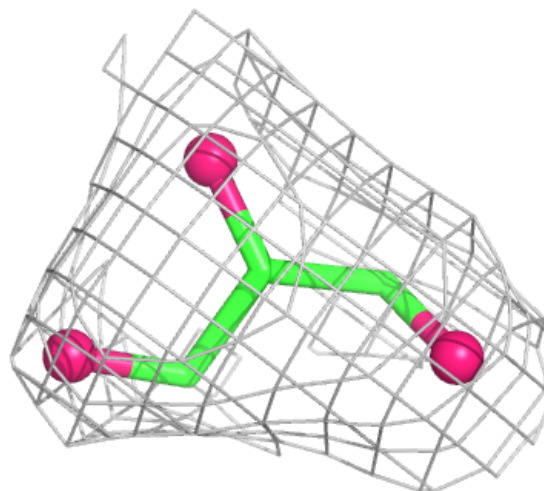
Electron density around GOL D 106:

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



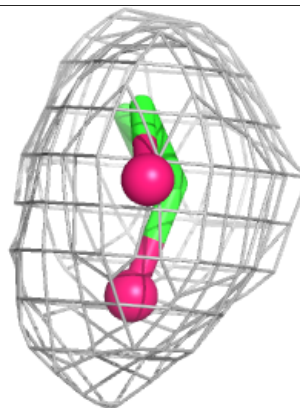
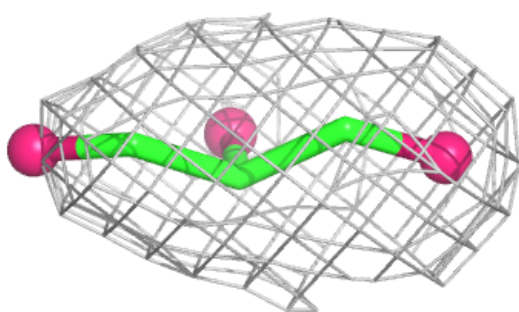
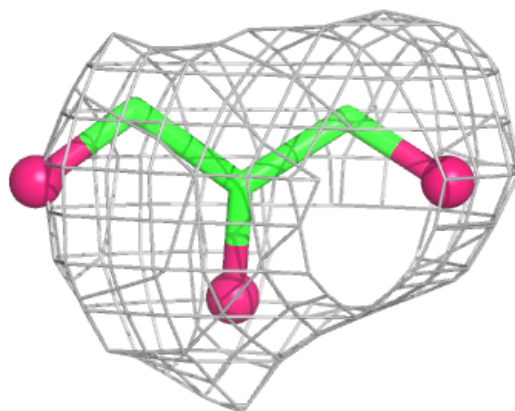
Electron density around GOL C 345:

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

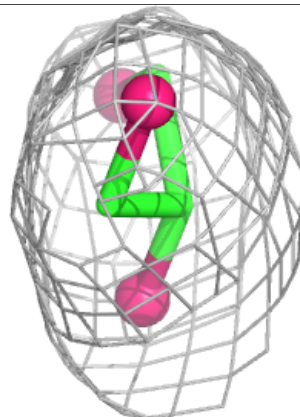
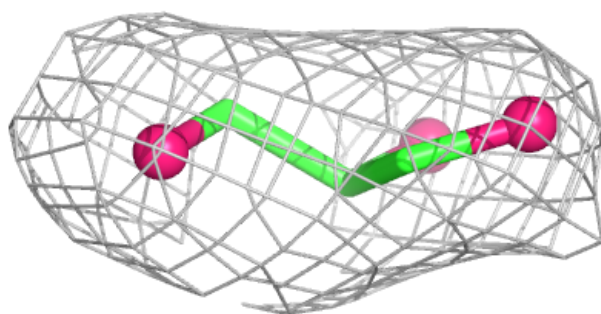
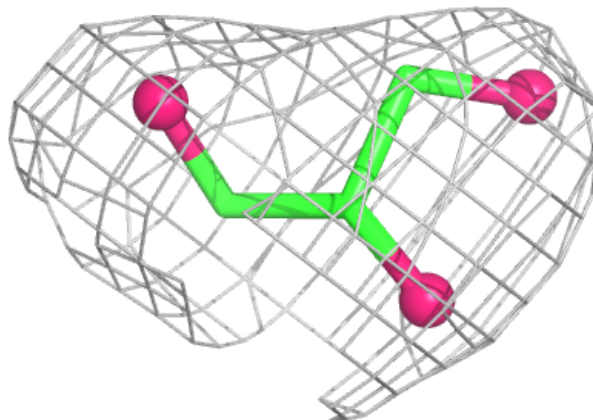


Electron density around GOL D 108:

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

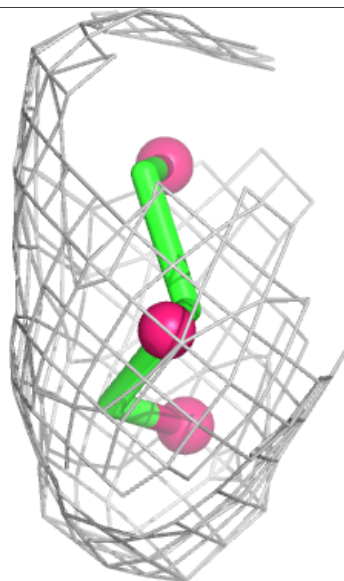
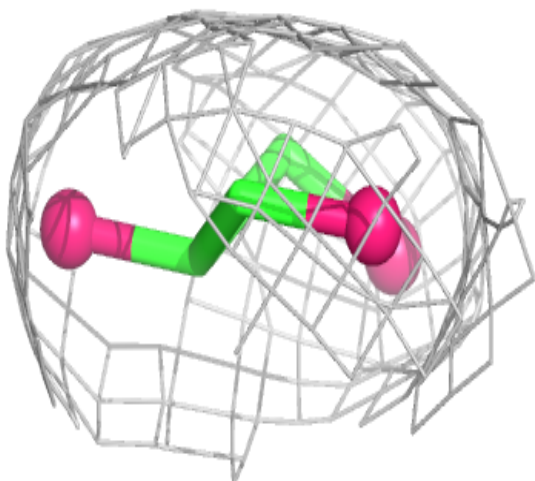
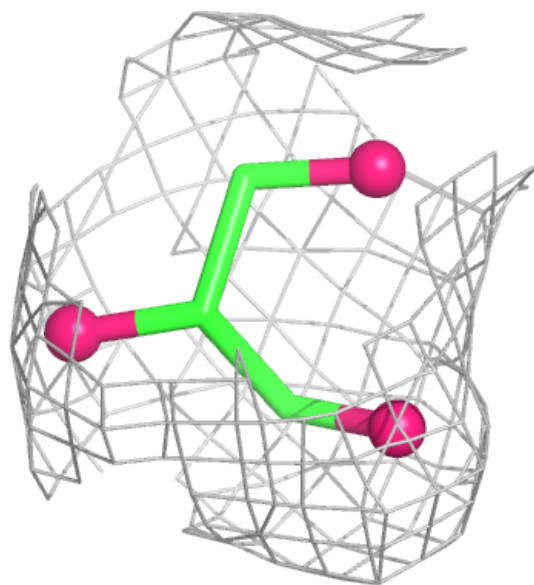
**Electron density around GOL A 373:**

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



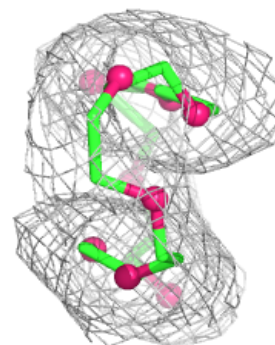
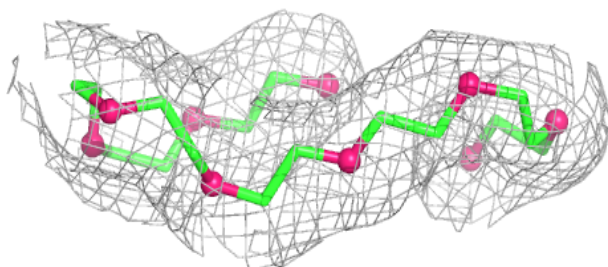
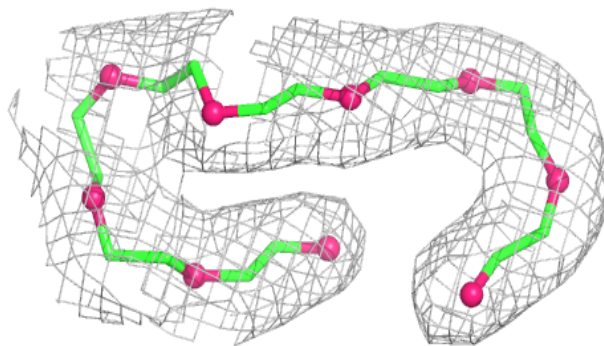
Electron density around GOL D 137:

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

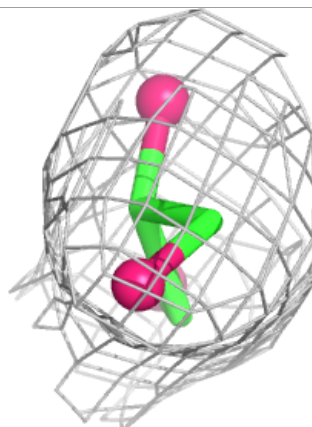
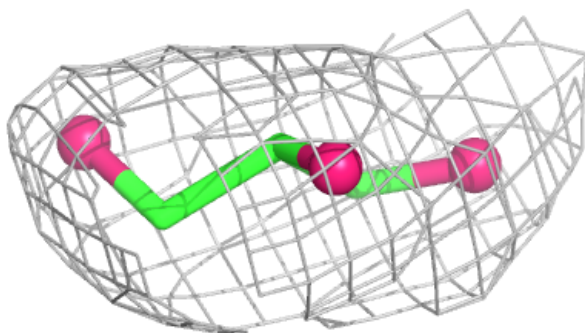
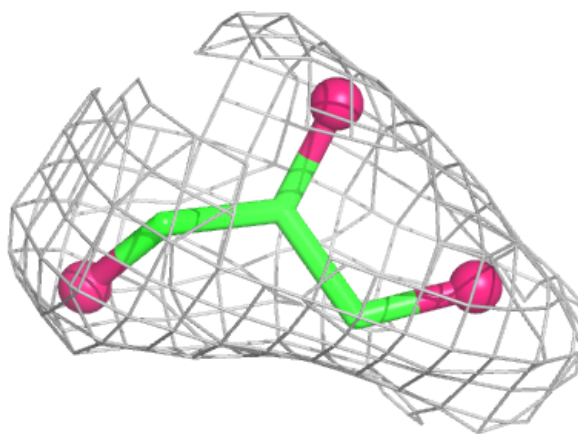


Electron density around PE8 E 109:

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

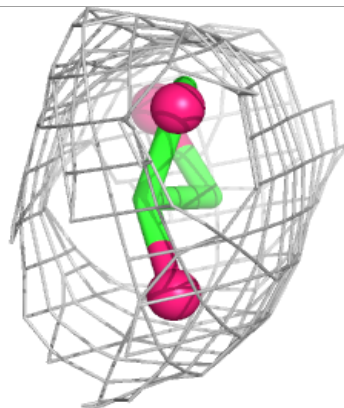
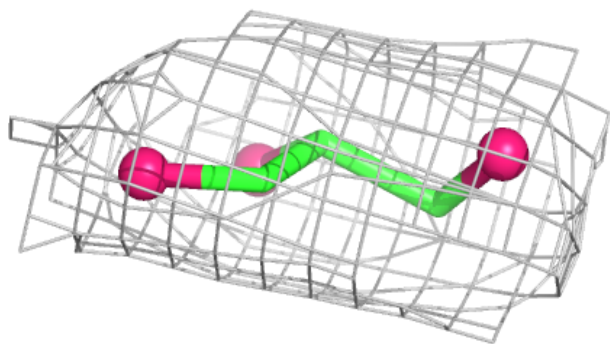
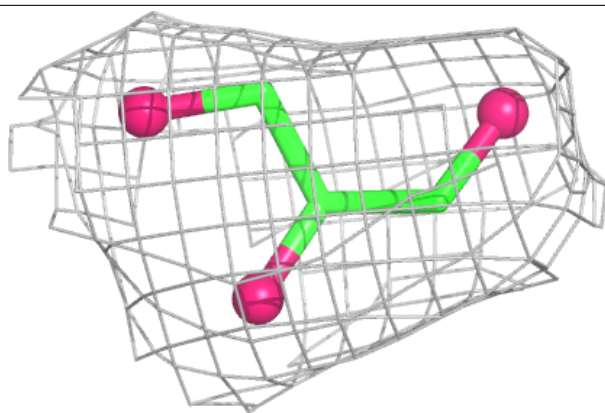
**Electron density around GOL A 364:**

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



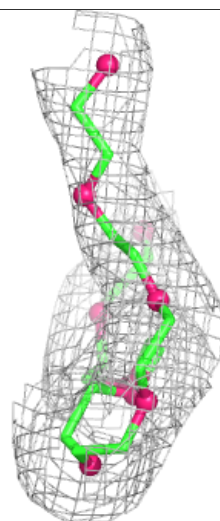
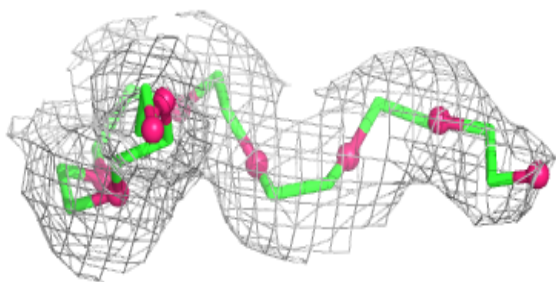
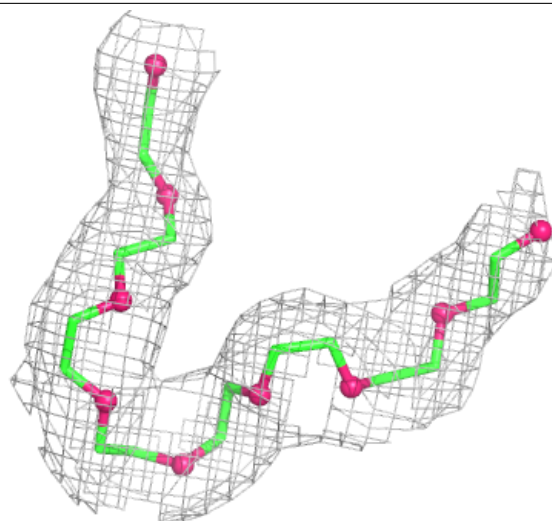
Electron density around GOL A 304:

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



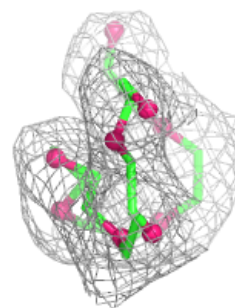
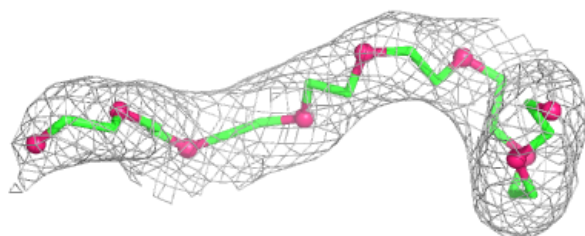
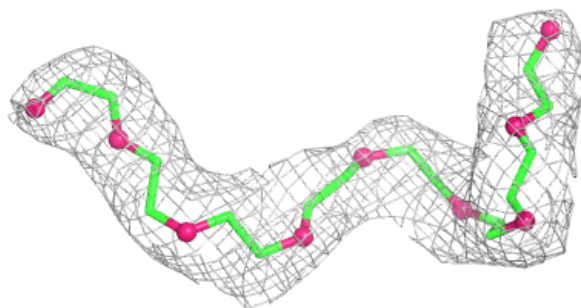
Electron density around PE8 B 137:

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

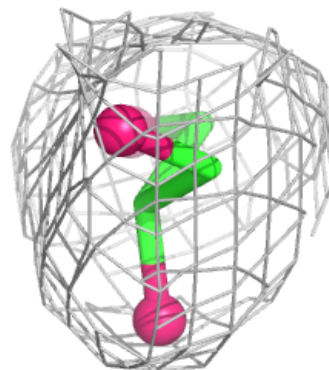
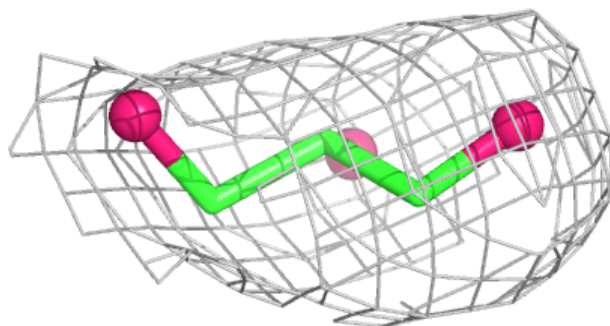
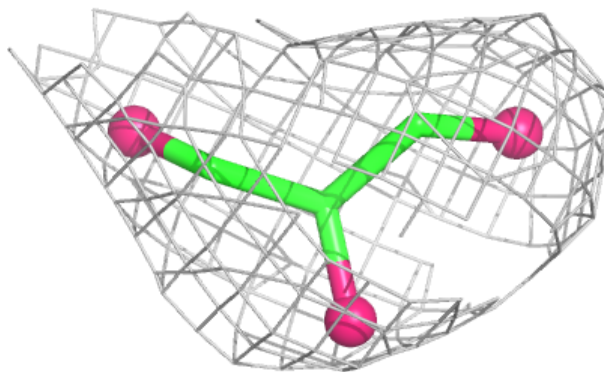


Electron density around PE8 B 138:

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

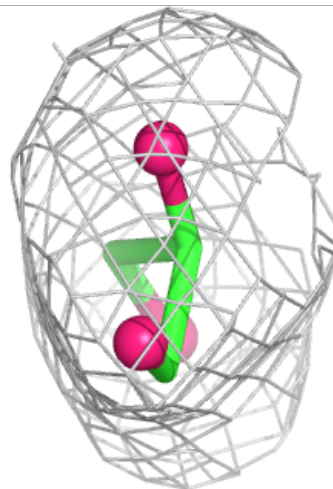
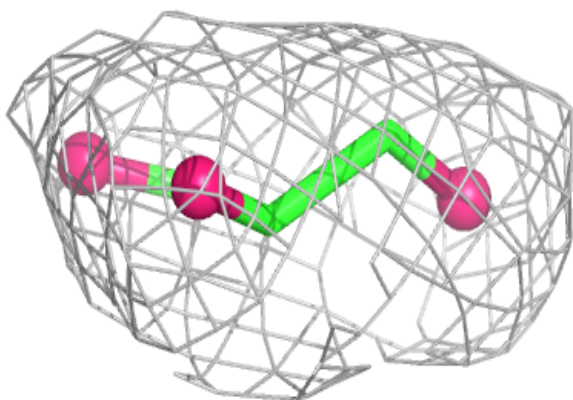
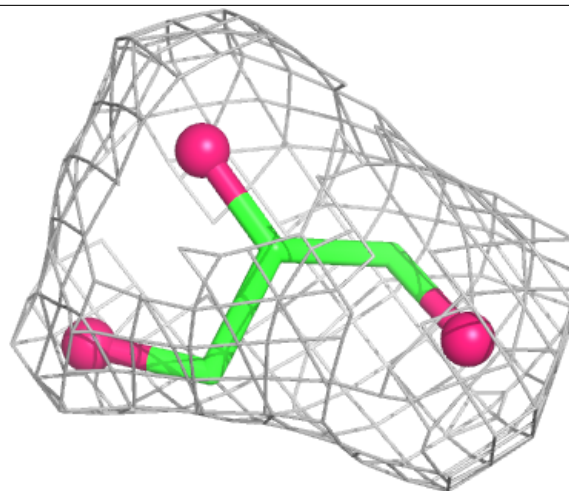
**Electron density around GOL B 112:**

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



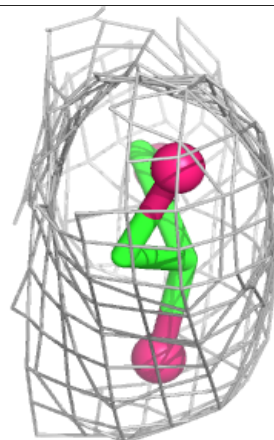
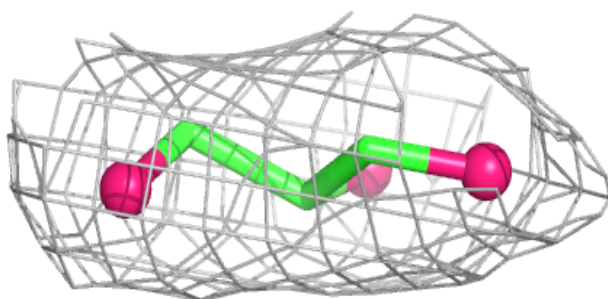
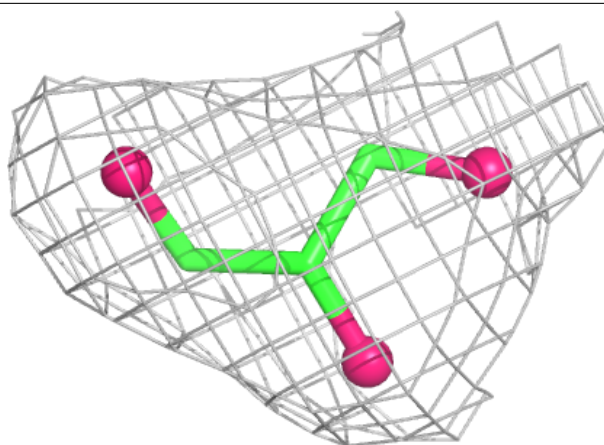
Electron density around GOL A 309:

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

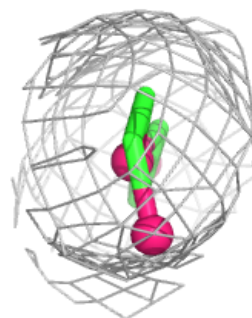
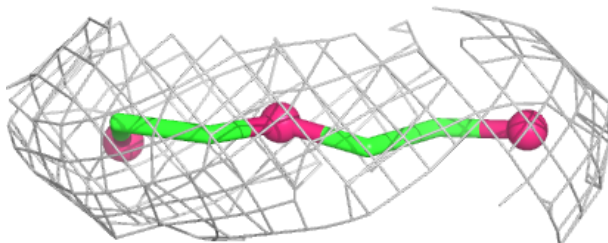
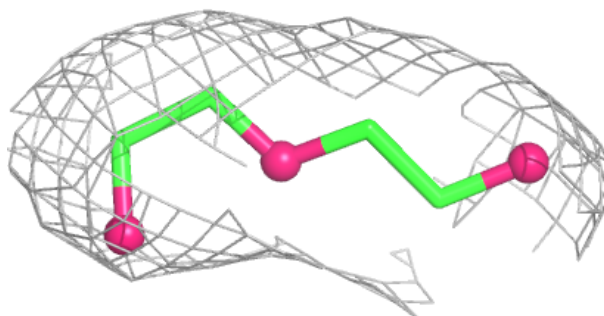


Electron density around GOL A 313:

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

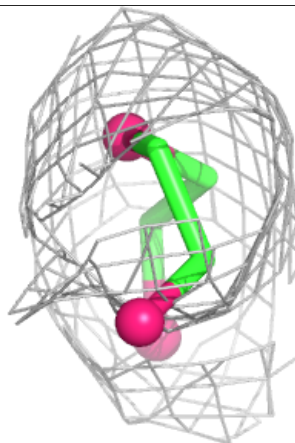
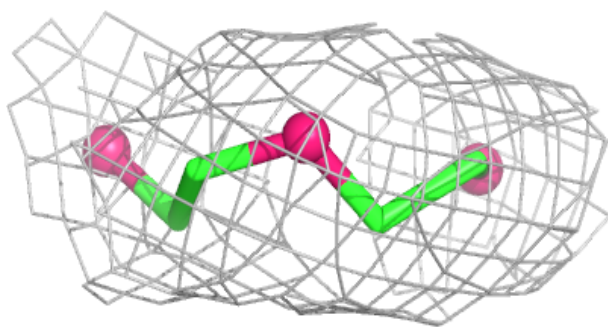
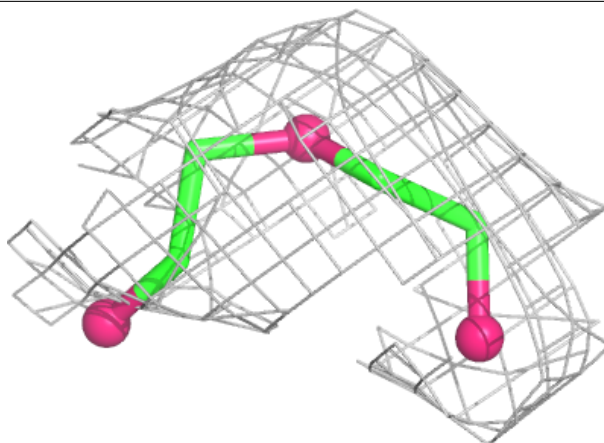
**Electron density around PEG B 126:**

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



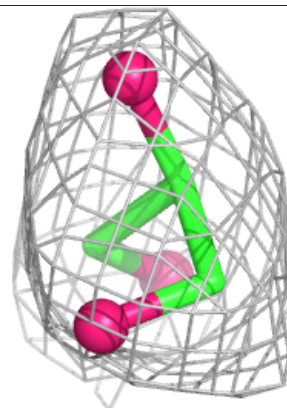
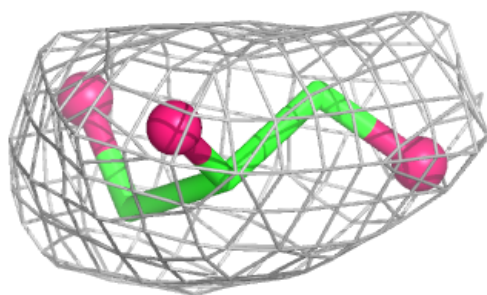
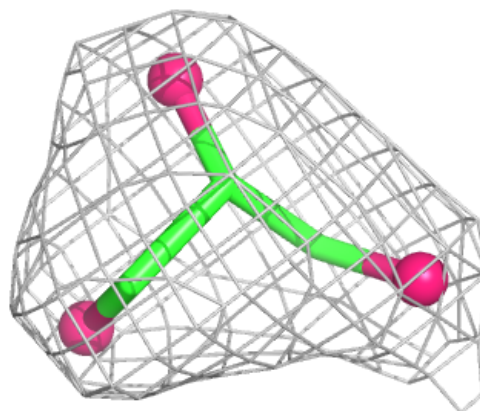
Electron density around PEG A 346:

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



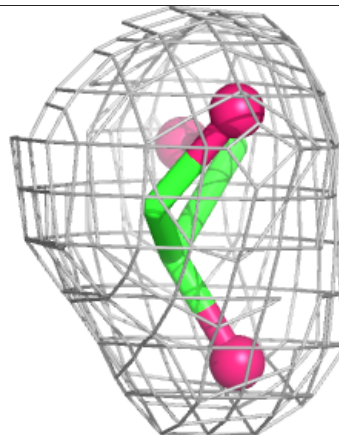
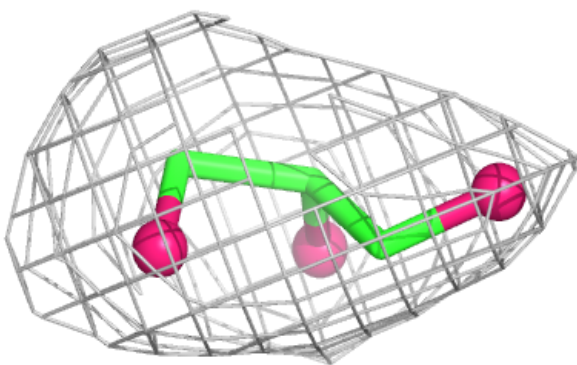
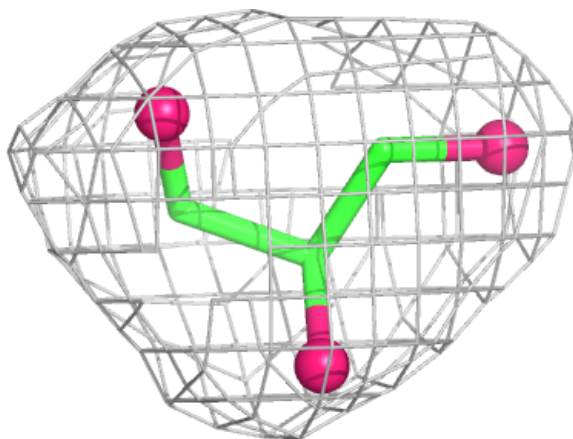
Electron density around GOL D 111:

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



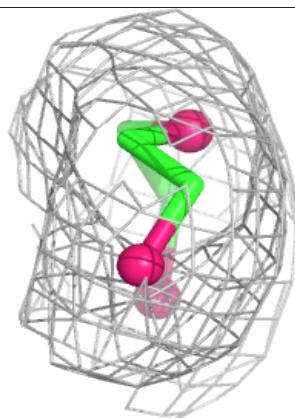
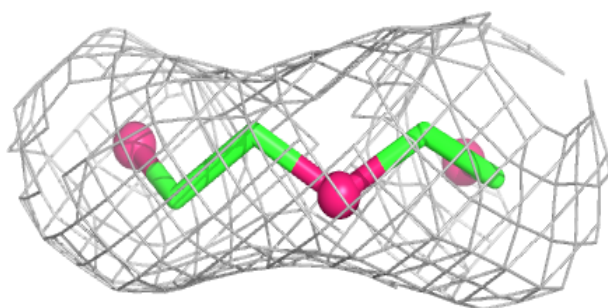
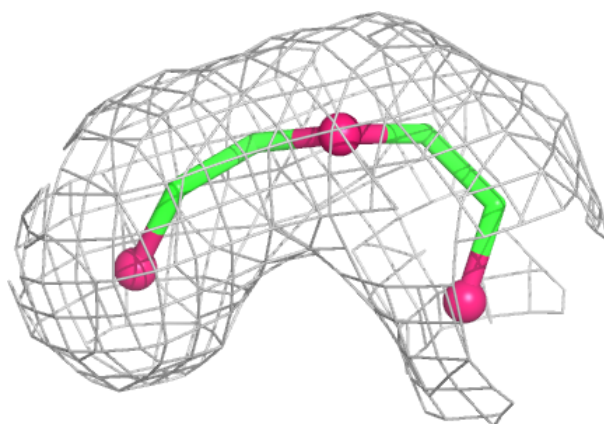
Electron density around GOL C 308:

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

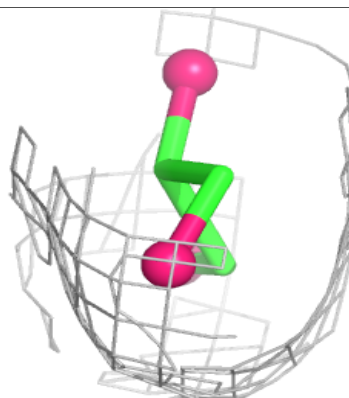
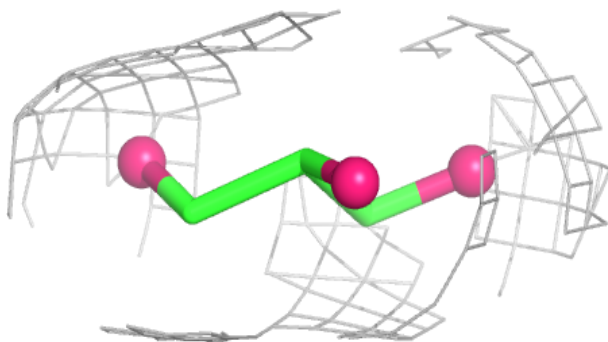


Electron density around PEG B 158:

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

**Electron density around GOL 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.