



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:40 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
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

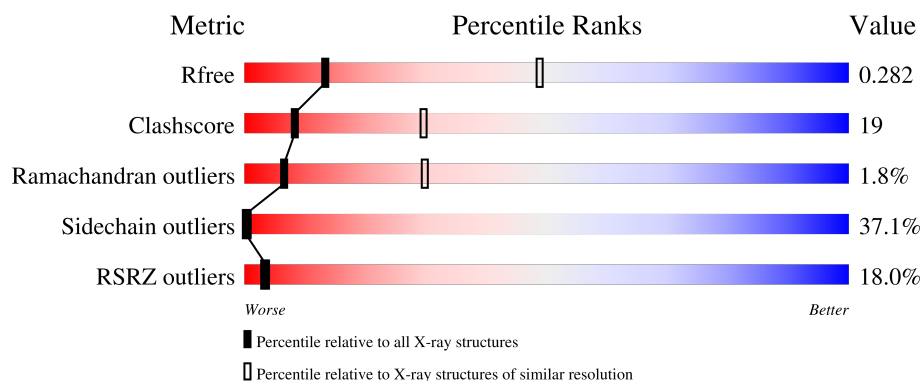
1 Overall quality at a glance

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.



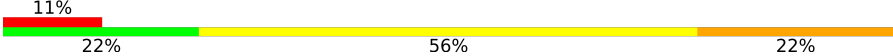
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	17% 45% 43% 12%
1	C	241	19% 36% 46% 17% .
2	B	98	23% 40% 49% 10% .
2	D	98	14% 35% 42% 21% .
3	E	9	56% 44%

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Mol	Chain	Length	Quality of chain
4	F	9	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (11%), green (22%), yellow (56%), and orange (22%). The percentages are labeled below the bar.

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.

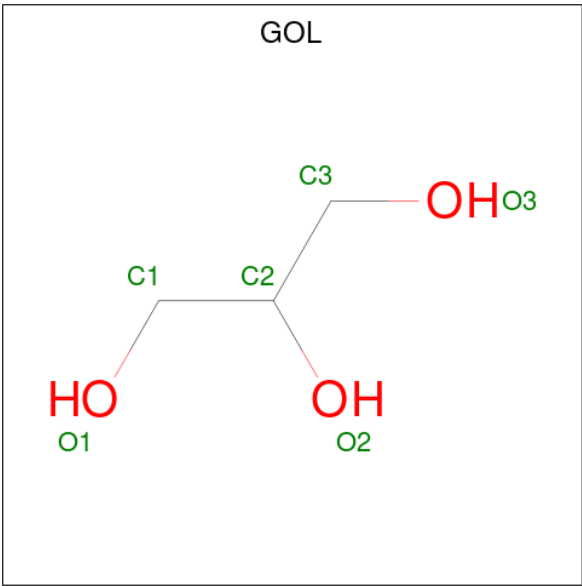
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	0	0	0
			73	47	12	14			

- 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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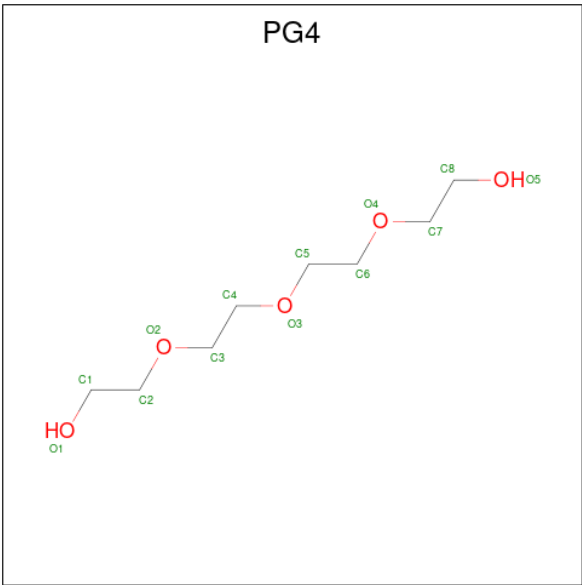
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
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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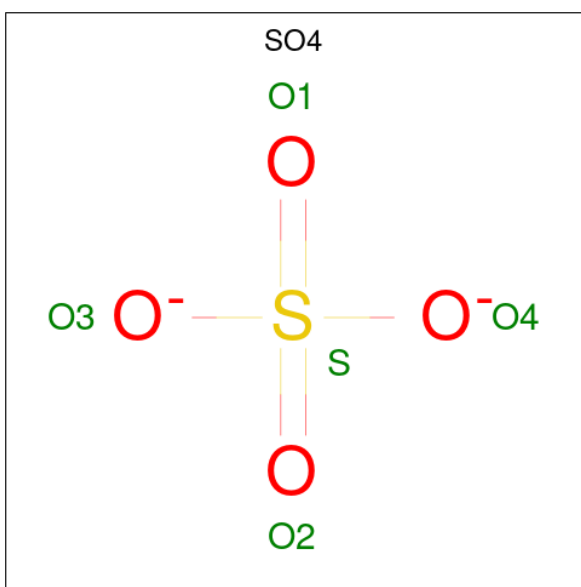
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	B	1	Total	C	O	0	0
			13	8	5		
7	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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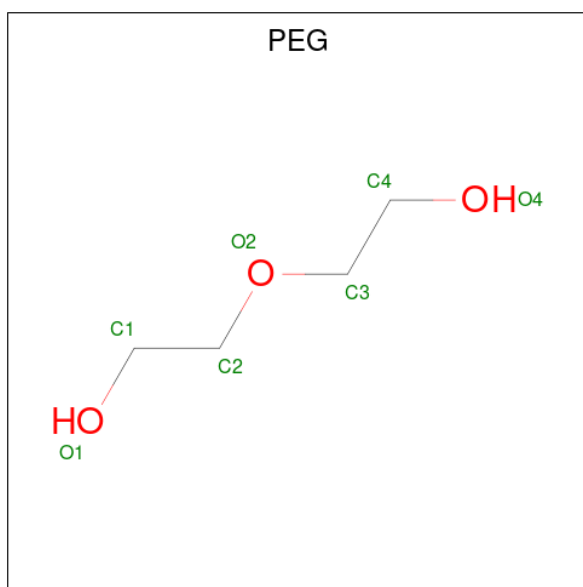
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		
7	D	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		
7	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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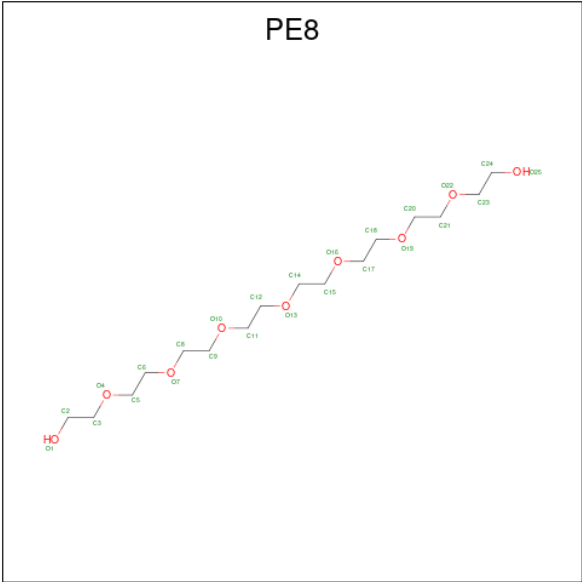
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	A	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	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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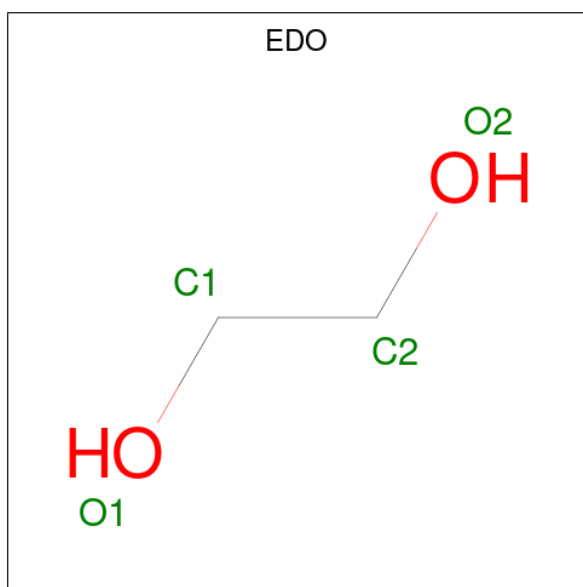
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0
9	D	1	Total C O 7 4 3	0	0
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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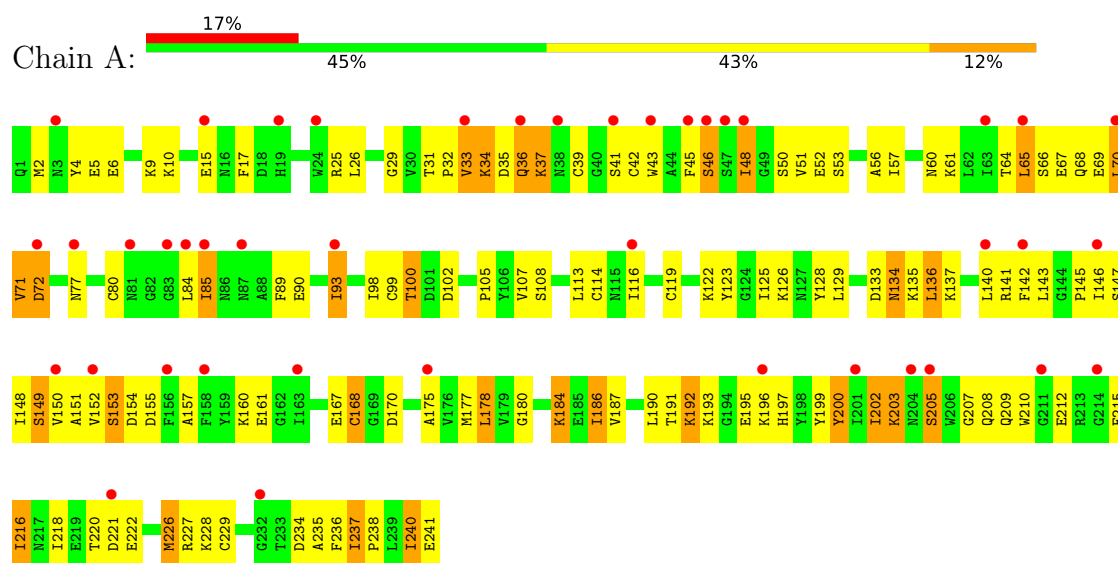
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	E	11	Total	O	0	0
			11	11		
12	F	7	Total	O	0	0
			7	7		

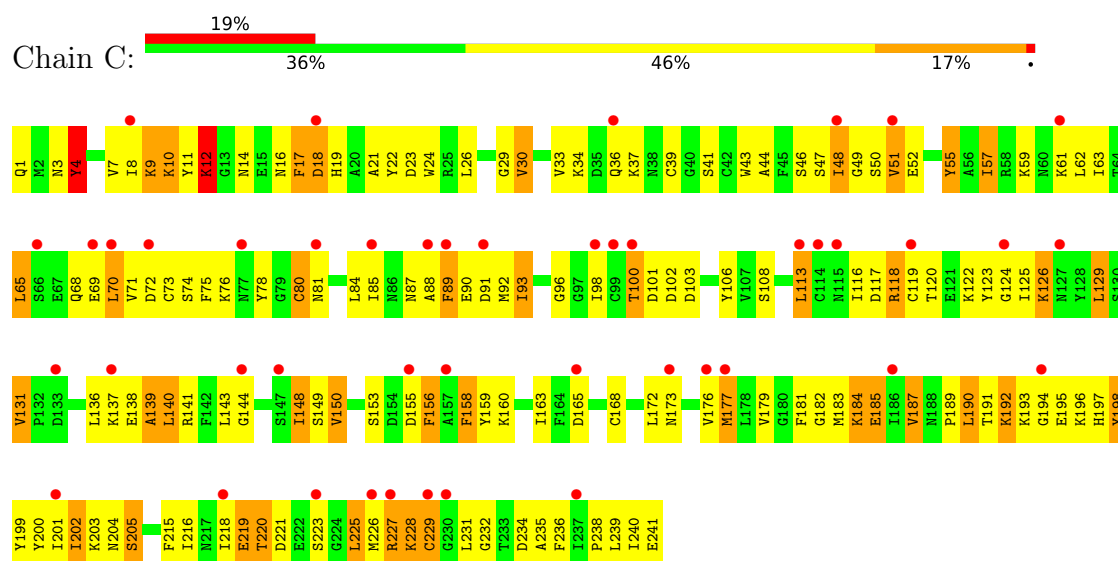
3 Residue-property plots [i](#)

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.

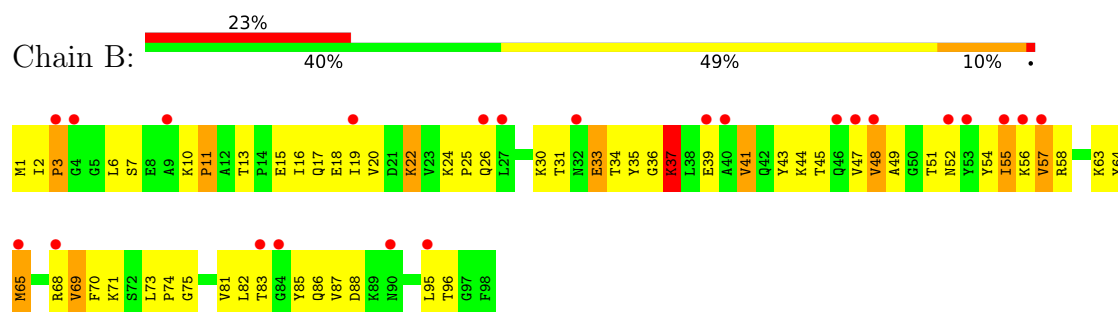
• Molecule 1: Cysteine proteinase falcipain 2a



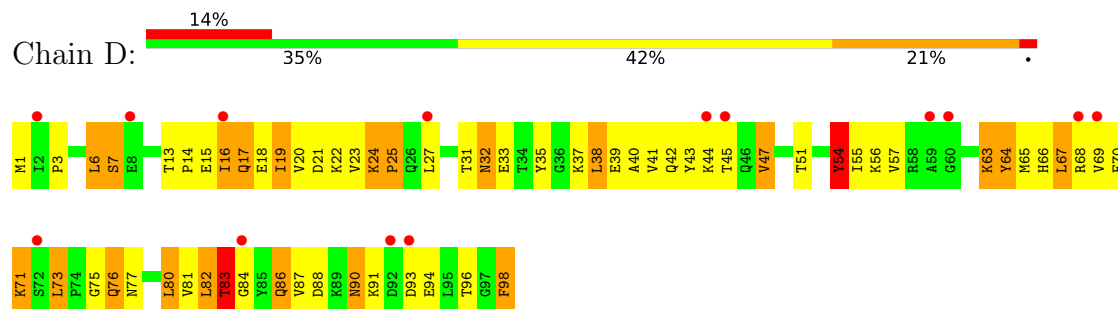
• Molecule 1: Cysteine proteinase falcipain 2a



• Molecule 2: Cystatin-A



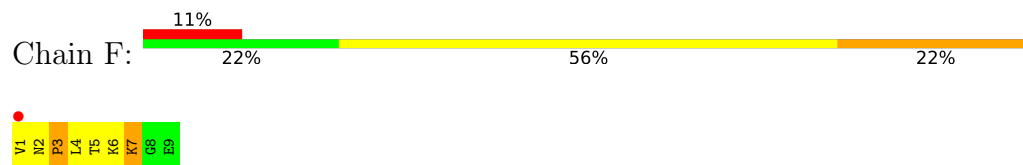
• Molecule 2: Cystatin-A



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



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



4 Data and refinement statistics

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

All (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
1	A	37	LYS	N-CA-C	5.46	117.30	110.91
1	C	17	PHE	CA-C-N	-5.45	113.78	122.17
1	C	17	PHE	C-N-CA	-5.45	113.78	122.17
2	D	25	PRO	CA-N-CD	-5.25	104.65	112.00
1	C	228	LYS	N-CA-C	-5.15	100.96	108.07

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	156	0	216	7	0
7	C	117	0	162	13	0
7	D	78	0	108	3	0
7	E	65	0	90	2	0
7	F	26	0	36	2	0
8	A	10	0	0	0	0
8	C	10	0	0	0	0
8	E	5	0	0	0	0
9	A	126	0	180	5	0
9	B	105	0	150	2	0
9	C	77	0	110	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.

All (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
1:A:125:ILE:HG22	1:A:240:ILE:HG22	1.63	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:GLN:HE21	1:C:205:SER:HB2	1.50	0.76
1:C:21:ALA:HB3	1:C:183:MET:HB2	1.67	0.75
1:C:129:LEU:HB2	1:C:236:PHE:HB3	1.69	0.73
1:C:69:GLU:HB2	1:C:98:ILE:HG23	1.71	0.72
1:C:190:LEU:HB2	1:C:194:GLY:HA2	1.71	0.72
2:D:38:LEU:HD12	2:D:57:VAL:HG11	1.72	0.72
3:E:5:ASN:HA	7:E:106:PG4:H72	1.70	0.72
1:C:9:LYS:HD2	1:C:10:LYS:HG2	1.73	0.71
2:D:24:LYS:HG3	2:D:25:PRO:HD2	1.74	0.70
7:C:320:PG4:H52	10:C:335:PE8:H142	1.72	0.70
2:D:20:VAL:O	2:D:23:VAL:HG22	1.93	0.69
2:B:87:VAL:HG22	2:B:88:ASP:H	1.58	0.67
1:C:84:LEU:O	1:C:88:ALA:HB2	1.95	0.67
2:D:65:MET:HG3	2:D:88:ASP:H	1.60	0.67
4:F:2:ASN:HA	4:F:5:THR:OG1	1.95	0.67
1:C:96:GLY:HA2	7:C:325:PG4:H62	1.75	0.67
1:C:125:ILE:HA	1:C:240:ILE:HG12	1.77	0.66
1:C:34:LYS:HB2	9:C:333:PEG:H31	1.77	0.66
1:C:1:GLN:N	12:C:401:HOH:O	2.27	0.65
2:D:68:ARG:HB2	2:D:98:PHE:CD1	2.32	0.65
1:A:50:SER:HA	1:A:177:MET:HE1	1.79	0.64
1:A:145:PRO:HB2	1:A:177:MET:HE2	1.79	0.64
7:B:122:PG4:H82	7:B:155:PG4:H31	1.80	0.63
1:A:36:GLN:HB3	1:A:41:SER:O	1.99	0.62
1:A:240:ILE:HG13	1:A:241:GLU:N	2.15	0.62
2:D:15:GLU:O	2:D:18:GLU:HG2	2.01	0.61
1:A:43:TRP:H	1:A:43:TRP:CD1	2.17	0.61
1:A:209:GLN:HE21	1:A:210:TRP:CD1	2.18	0.61
1:A:191:THR:HG22	1:A:192:LYS:H	1.65	0.60
1:C:227:ARG:HD2	1:C:228:LYS:N	2.12	0.60
1:C:122:LYS:HB2	7:C:325:PG4:H32	1.83	0.60
1:C:55:TYR:O	1:C:59:LYS:O	2.20	0.60
2:D:19:ILE:HD11	7:D:103:PG4:H72	1.84	0.59
2:D:19:ILE:O	2:D:23:VAL:HG13	2.02	0.59
2:D:73:LEU:O	2:D:75:GLY:N	2.33	0.59
1:A:212:GLU:HB2	1:A:215:PHE:O	2.02	0.59
5:A:303:GOL:H2	9:A:331:PEG:H12	1.83	0.59
1:C:192:LYS:HG2	11:D:102:EDO:H21	1.83	0.59
1:A:35:ASP:HA	1:A:205:SER:O	2.03	0.58
1:C:93:ILE:HG23	1:C:125:ILE:HG13	1.85	0.58
2:D:64:TYR:O	2:D:88:ASP:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:HA	1:A:235:ALA:HA	1.84	0.58
1:C:3:ASN:O	1:C:4:TYR:HB2	2.04	0.58
2:D:17:GLN:HG3	2:D:40:ALA:HB3	1.85	0.58
1:A:29:GLY:HA3	1:A:57:ILE:HG12	1.86	0.58
7:C:320:PG4:H41	10:C:335:PE8:H121	1.85	0.58
10:F:102:PE8:H91	7:F:105:PG4:H11	1.86	0.57
2:D:86:GLN:HB2	2:D:98:PHE:HD2	1.67	0.57
1:A:202:ILE:O	1:A:215:PHE:HA	2.04	0.57
1:A:202:ILE:HG13	1:A:203:LYS:O	2.03	0.57
2:B:17:GLN:HA	2:B:20:VAL:HG22	1.86	0.57
7:C:321:PG4:H11	7:C:322:PG4:H72	1.86	0.57
1:A:31:THR:HB	1:A:32:PRO:CD	2.34	0.57
2:D:86:GLN:HB2	2:D:98:PHE:CD2	2.40	0.57
2:B:10:LYS:HG2	2:B:43:TYR:CD2	2.40	0.56
2:B:48:VAL:HG12	2:B:49:ALA:H	1.70	0.56
4:F:5:THR:HG22	4:F:7:LYS:HG2	1.86	0.56
1:C:49:GLY:O	1:C:52:GLU:HG2	2.06	0.56
1:A:70:LEU:O	1:A:71:VAL:HB	2.04	0.56
1:A:43:TRP:CZ2	1:A:71:VAL:HA	2.40	0.56
1:C:55:TYR:HE2	1:C:123:TYR:HD2	1.53	0.56
2:D:23:VAL:HG21	2:D:55:ILE:HD11	1.87	0.55
2:D:19:ILE:HG23	2:D:80:LEU:HD13	1.88	0.55
2:D:42:GLN:HB2	2:D:56:LYS:HD3	1.88	0.55
2:B:41:VAL:HG13	2:B:56:LYS:HG3	1.89	0.55
1:C:72:ASP:OD1	1:C:73:CYS:N	2.40	0.55
1:C:72:ASP:HB2	1:C:113:LEU:O	2.07	0.55
2:D:15:GLU:HB3	7:D:103:PG4:H82	1.89	0.55
2:B:16:ILE:O	2:B:20:VAL:HG13	2.07	0.54
1:C:89:PHE:CD1	1:C:89:PHE:N	2.75	0.54
1:C:182:GLY:HA3	1:C:199:TYR:CE2	2.43	0.54
2:D:68:ARG:HB2	2:D:98:PHE:HD1	1.72	0.54
1:C:153:SER:C	1:C:155:ASP:H	2.16	0.54
1:C:8:ILE:HG13	1:C:9:LYS:HG3	1.90	0.53
1:C:226:MET:HE3	9:C:332:PEG:H41	1.90	0.53
1:A:90:GLU:HB3	9:A:329:PEG:H11	1.91	0.53
2:D:21:ASP:O	2:D:24:LYS:HG3	2.07	0.53
2:D:65:MET:HE3	2:D:87:VAL:HG13	1.90	0.53
1:C:55:TYR:CE2	1:C:123:TYR:HD2	2.27	0.53
2:D:16:ILE:HA	2:D:19:ILE:HG13	1.89	0.53
1:A:65:LEU:HD21	1:A:123:TYR:HD2	1.73	0.53
2:B:54:TYR:C	2:B:55:ILE:HG13	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:SER:HB3	1:C:238:PRO:HG2	1.91	0.52
1:A:53:SER:O	1:A:57:ILE:HG13	2.09	0.52
1:A:72:ASP:HB2	1:A:114:CYS:HB2	1.92	0.52
1:C:36:GLN:NE2	1:C:205:SER:HB2	2.20	0.52
2:D:19:ILE:HG22	2:D:69:VAL:HG11	1.92	0.52
1:A:150:VAL:HG22	1:A:151:ALA:H	1.75	0.52
1:A:128:TYR:HB2	1:A:238:PRO:HA	1.90	0.52
2:D:17:GLN:O	2:D:20:VAL:HB	2.09	0.52
1:A:140:LEU:HD13	1:A:180:GLY:HA2	1.92	0.52
2:B:36:GLY:O	2:B:37:LYS:HB2	2.10	0.51
2:B:10:LYS:HD3	7:B:118:PG4:H61	1.92	0.51
1:C:124:GLY:O	1:C:240:ILE:HG12	2.10	0.51
2:D:84:GLY:HA3	2:D:98:PHE:HB2	1.93	0.51
1:C:219:GLU:O	1:C:227:ARG:HG2	2.11	0.51
2:B:22:LYS:C	2:B:25:PRO:HD2	2.36	0.50
10:A:342:PE8:H231	5:A:363:GOL:H11	1.92	0.50
1:C:43:TRP:O	1:C:47:SER:OG	2.25	0.50
1:A:186:ILE:HG22	1:A:195:GLU:O	2.12	0.50
1:C:43:TRP:HZ3	1:C:70:LEU:HD23	1.77	0.50
1:A:237:ILE:HG12	1:A:238:PRO:CD	2.42	0.50
2:D:16:ILE:HD13	2:D:43:TYR:HB3	1.94	0.50
1:A:39:CYS:C	1:A:41:SER:H	2.19	0.50
2:B:26:GLN:O	2:B:82:LEU:HD12	2.11	0.50
1:A:126:LYS:HD3	7:A:325:PG4:H71	1.93	0.50
1:C:68:GLN:HB2	1:C:106:TYR:HA	1.93	0.50
2:D:76:GLN:NE2	12:D:203:HOH:O	2.45	0.50
1:A:184:LYS:HB2	1:A:199:TYR:HE1	1.75	0.49
1:C:41:SER:OG	1:C:80:CYS:SG	2.70	0.49
4:F:6:LYS:HB2	10:F:102:PE8:H212	1.94	0.49
1:C:65:LEU:HD13	1:C:100:THR:HA	1.93	0.49
1:C:140:LEU:HD12	1:C:144:GLY:O	2.13	0.49
1:A:65:LEU:HD21	1:A:123:TYR:CD2	2.46	0.49
7:C:302:PG4:H22	11:D:102:EDO:H12	1.94	0.49
2:D:77:ASN:H	5:D:106:GOL:H32	1.77	0.49
2:B:41:VAL:O	9:B:130:PEG:H12	2.12	0.49
1:C:14:ASN:O	1:C:14:ASN:ND2	2.45	0.49
1:A:137:LYS:HG2	1:A:200:TYR:CE1	2.47	0.49
2:D:63:LYS:O	2:D:64:TYR:HB2	2.13	0.49
1:A:153:SER:HB3	1:A:168:CYS:C	2.37	0.48
1:C:136:LEU:HD13	1:C:232:GLY:HA2	1.95	0.48
2:B:25:PRO:HA	5:B:140:GOL:H11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HA	1:A:93:ILE:HG13	1.94	0.48
1:C:153:SER:HB2	1:C:168:CYS:HA	1.94	0.48
1:A:177:MET:O	1:A:202:ILE:HB	2.12	0.48
2:D:57:VAL:HG23	2:D:65:MET:HB3	1.94	0.48
2:D:65:MET:HG3	2:D:88:ASP:N	2.28	0.48
1:C:187:VAL:O	1:C:189:PRO:HD3	2.14	0.48
7:E:115:PG4:H22	7:E:115:PG4:H42	1.54	0.48
1:C:36:GLN:HB2	1:C:205:SER:O	2.14	0.48
1:C:136:LEU:HA	1:C:139:ALA:HA	1.95	0.48
7:C:322:PG4:H62	5:C:345:GOL:H11	1.95	0.47
5:E:103:GOL:H11	5:E:113:GOL:H11	1.95	0.47
1:C:193:LYS:HE2	5:C:309:GOL:H12	1.97	0.47
1:A:149:SER:HB3	1:A:234:ASP:HB3	1.96	0.47
1:A:34:LYS:HB2	1:A:34:LYS:HE2	1.53	0.47
1:A:135:LYS:O	1:A:136:LEU:HD23	2.14	0.47
7:A:323:PG4:H12	7:B:101:PG4:H32	1.96	0.47
1:C:43:TRP:H	1:C:43:TRP:CD1	2.32	0.47
1:C:220:THR:OG1	1:C:221:ASP:N	2.47	0.47
1:A:65:LEU:HD13	1:A:98:ILE:HB	1.97	0.47
1:A:84:LEU:HG	2:B:3:PRO:HD2	1.96	0.47
1:C:126:LYS:H	1:C:240:ILE:HA	1.80	0.47
2:D:16:ILE:HD12	2:D:55:ILE:HG22	1.95	0.47
1:A:68:GLN:C	1:A:70:LEU:H	2.22	0.47
1:C:73:CYS:HB2	1:C:75:PHE:CE2	2.50	0.47
1:C:184:LYS:HZ3	1:C:184:LYS:HG3	1.59	0.47
1:A:36:GLN:OE1	2:B:49:ALA:HB2	2.15	0.47
1:A:197:HIS:HB2	12:A:447:HOH:O	2.15	0.47
2:D:90:ASN:OD1	2:D:90:ASN:N	2.41	0.47
1:C:51:VAL:HG11	1:C:92:MET:SD	2.55	0.46
7:C:322:PG4:H31	5:C:345:GOL:H32	1.97	0.46
1:A:202:ILE:HG12	1:A:216:ILE:O	2.15	0.46
1:C:89:PHE:O	1:C:92:MET:HG2	2.15	0.46
1:C:71:VAL:HG13	1:C:71:VAL:O	2.16	0.46
1:C:52:GLU:HB2	1:C:63:ILE:O	2.15	0.46
7:A:325:PG4:H41	7:A:325:PG4:H61	1.40	0.46
1:C:48:ILE:O	1:C:51:VAL:HG22	2.15	0.46
2:B:39:GLU:O	2:B:58:ARG:HG3	2.15	0.46
2:D:27:LEU:O	2:D:31:THR:OG1	2.20	0.46
2:D:63:LYS:HB2	2:D:63:LYS:HE3	1.46	0.46
2:D:83:THR:O	2:D:83:THR:HG23	2.15	0.46
1:C:101:ASP:C	1:C:103:ASP:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:THR:HG21	1:A:52:GLU:HB3	1.98	0.45
2:D:7:SER:O	2:D:44:LYS:HD3	2.15	0.45
1:A:51:VAL:HG11	1:A:65:LEU:HD12	1.99	0.45
1:A:137:LYS:HE2	1:A:200:TYR:CE1	2.51	0.45
10:E:110:PE8:H62	10:E:110:PE8:H92	1.35	0.45
1:A:33:VAL:HA	1:A:45:PHE:CZ	2.52	0.45
1:A:35:ASP:HB3	1:A:37:LYS:HG3	1.98	0.45
2:D:55:ILE:HG13	2:D:67:LEU:HB2	1.98	0.45
1:A:48:ILE:O	1:A:52:GLU:HG3	2.16	0.45
1:C:148:ILE:HA	1:C:234:ASP:O	2.16	0.45
1:C:184:LYS:HB2	1:C:199:TYR:CD1	2.52	0.45
1:A:37:LYS:HE3	1:A:37:LYS:HB2	1.63	0.45
1:A:170:ASP:H	5:A:310:GOL:H11	1.81	0.45
1:C:156:PHE:C	1:C:158:PHE:H	2.25	0.45
10:F:106:PE8:H121	10:F:106:PE8:H151	1.67	0.45
1:A:31:THR:HB	1:A:32:PRO:HD2	1.99	0.45
3:E:2:GLU:HA	3:E:6:PRO:HG2	1.97	0.45
1:A:85:ILE:HD11	1:A:175:ALA:HB1	1.98	0.44
1:C:177:MET:O	1:C:202:ILE:HG23	2.17	0.44
2:B:10:LYS:HG2	2:B:43:TYR:CE2	2.52	0.44
2:B:58:ARG:HG2	2:B:64:TYR:CE2	2.53	0.44
1:C:7:VAL:CG2	1:C:12:LYS:HA	2.47	0.44
1:C:24:TRP:O	1:C:29:GLY:HA3	2.16	0.44
2:B:10:LYS:HG3	2:B:11:PRO:N	2.32	0.44
1:C:185:GLU:O	1:C:198:TYR:HD1	2.01	0.44
1:A:237:ILE:HG12	1:A:238:PRO:HD2	1.99	0.44
1:C:48:ILE:H	1:C:48:ILE:HG13	1.63	0.44
1:A:221:ASP:OD1	1:A:226:MET:HB2	2.18	0.44
2:B:57:VAL:HG23	2:B:65:MET:SD	2.58	0.44
1:C:18:ASP:O	1:C:19:HIS:HB2	2.18	0.44
1:C:173:ASN:HB3	2:D:47:VAL:HG11	2.00	0.44
2:D:6:LEU:HD21	2:D:54:TYR:OH	2.18	0.44
1:A:209:GLN:HE21	1:A:210:TRP:HD1	1.64	0.44
2:B:82:LEU:HG	2:B:85:TYR:CE1	2.53	0.44
7:B:125:PG4:H31	7:B:125:PG4:H11	1.53	0.44
1:C:23:ASP:HB3	1:C:26:LEU:HD12	1.99	0.44
7:C:323:PG4:H31	7:C:323:PG4:H12	1.41	0.44
9:C:331:PEG:H31	9:C:331:PEG:H11	1.53	0.44
2:D:71:LYS:HE3	2:D:71:LYS:HB3	1.68	0.43
7:B:118:PG4:H11	7:B:118:PG4:H31	1.47	0.43
1:C:21:ALA:HB1	1:C:181:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LEU:HG	1:C:74:SER:HB2	2.01	0.43
1:C:228:LYS:HD3	1:C:229:CYS:H	1.83	0.43
2:D:77:ASN:N	5:D:106:GOL:H32	2.32	0.43
7:C:324:PG4:H31	7:C:324:PG4:H52	1.58	0.43
1:A:26:LEU:HD23	1:C:73:CYS:SG	2.59	0.43
10:B:137:PE8:H51	10:B:138:PE8:H51	2.00	0.43
1:C:89:PHE:CD2	1:C:238:PRO:HG3	2.53	0.43
1:C:168:CYS:HB2	1:C:229:CYS:HA	2.00	0.43
1:A:84:LEU:HD11	2:B:2:ILE:HG22	2.01	0.43
1:C:96:GLY:O	7:C:325:PG4:H41	2.19	0.43
1:A:207:GLY:C	1:A:209:GLN:H	2.26	0.43
1:A:157:ALA:O	2:B:74:PRO:HG3	2.19	0.42
10:B:138:PE8:H121	10:B:138:PE8:H151	1.34	0.42
10:E:109:PE8:H211	10:E:109:PE8:H181	1.56	0.42
1:A:39:CYS:O	1:A:41:SER:N	2.47	0.42
1:C:158:PHE:O	1:C:159:TYR:C	2.61	0.42
7:D:119:PG4:H31	7:D:119:PG4:H11	1.23	0.42
1:C:7:VAL:HG21	1:C:12:LYS:HA	2.00	0.42
1:A:149:SER:HA	1:A:175:ALA:HA	2.01	0.42
1:A:43:TRP:HZ2	1:A:71:VAL:HA	1.81	0.42
1:C:189:PRO:HA	1:C:194:GLY:HA3	2.02	0.42
10:E:109:PE8:H82	10:E:109:PE8:H112	1.55	0.42
1:A:136:LEU:HD13	1:A:178:LEU:HD12	2.01	0.42
2:B:25:PRO:HG3	5:B:140:GOL:H31	2.02	0.42
10:B:136:PE8:H182	10:B:136:PE8:H212	1.61	0.42
4:F:7:LYS:HB3	4:F:7:LYS:HE3	1.74	0.42
1:C:137:LYS:HB3	1:C:137:LYS:HE3	1.85	0.42
1:C:225:LEU:HD12	1:C:226:MET:HG2	2.01	0.42
1:A:153:SER:O	1:A:154:ASP:HB2	2.20	0.42
2:B:73:LEU:HB2	2:B:74:PRO:HD2	2.00	0.42
1:C:74:SER:C	1:C:76:LYS:H	2.27	0.42
2:D:14:PRO:HA	2:D:17:GLN:NE2	2.35	0.42
1:C:156:PHE:HA	12:C:403:HOH:O	2.20	0.41
4:F:2:ASN:N	4:F:3:PRO:HD3	2.35	0.41
1:A:64:THR:O	1:A:100:THR:HG22	2.20	0.41
7:C:302:PG4:H11	7:C:323:PG4:H32	2.02	0.41
1:A:56:ALA:O	1:A:60:ASN:HA	2.20	0.41
1:A:105:PRO:HB3	5:D:108:GOL:H31	2.02	0.41
9:A:331:PEG:H22	9:A:331:PEG:H42	1.37	0.41
2:D:19:ILE:CG2	2:D:69:VAL:HG11	2.51	0.41
9:A:336:PEG:H32	10:A:342:PE8:H232	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:GLU:HG3	7:B:117:PG4:H42	2.02	0.41
1:C:131:VAL:O	1:C:235:ALA:HB3	2.20	0.41
1:A:89:PHE:CE1	1:A:238:PRO:HG3	2.56	0.41
1:A:153:SER:HB2	1:A:155:ASP:H	1.86	0.41
2:B:65:MET:HE3	2:B:65:MET:HB3	1.83	0.41
2:B:68:ARG:O	2:B:83:THR:HB	2.20	0.41
2:B:73:LEU:O	2:B:75:GLY:N	2.48	0.41
10:B:136:PE8:H141	10:B:136:PE8:H111	1.50	0.41
2:D:64:TYR:CD2	2:D:91:LYS:HB3	2.56	0.41
10:E:110:PE8:H111	12:E:206:HOH:O	2.19	0.41
7:A:365:PG4:H62	7:A:365:PG4:H41	1.61	0.41
2:B:69:VAL:HG12	2:B:70:PHE:H	1.85	0.41
1:C:179:VAL:HG11	1:C:215:PHE:HE2	1.85	0.41
2:D:16:ILE:O	2:D:20:VAL:HG23	2.21	0.41
1:A:39:CYS:O	2:B:48:VAL:HG11	2.21	0.41
1:A:46:SER:O	1:A:50:SER:OG	2.29	0.41
1:A:140:LEU:HD23	1:A:178:LEU:HD13	2.02	0.41
10:B:136:PE8:H122	10:B:136:PE8:H92	1.38	0.41
1:C:225:LEU:HD21	10:F:106:PE8:H141	2.03	0.41
7:F:101:PG4:H52	7:F:101:PG4:H32	1.29	0.41
7:C:321:PG4:H31	5:C:344:GOL:H12	2.02	0.41
2:D:55:ILE:HG13	2:D:55:ILE:O	2.21	0.41
1:C:50:SER:HB3	1:C:238:PRO:CG	2.50	0.40
3:E:5:ASN:N	3:E:6:PRO:CD	2.84	0.40
7:A:366:PG4:H31	7:A:366:PG4:H51	1.92	0.40
2:B:37:LYS:HB3	2:B:37:LYS:HE3	1.42	0.40
1:C:118:ARG:O	5:C:338:GOL:H11	2.22	0.40
1:C:173:ASN:O	2:D:3:PRO:HA	2.20	0.40
9:A:341:PEG:H41	9:A:341:PEG:H22	1.78	0.40
9:B:157:PEG:H22	9:B:157:PEG:H42	1.55	0.40
1:A:134[B]:ASN:HB3	5:A:347:GOL:H11	2.02	0.40
1:C:90:GLU:HA	1:C:93:ILE:HG13	2.03	0.40
1:C:193:LYS:HE2	1:C:193:LYS:HB2	1.67	0.40
7:B:122:PG4:H11	7:B:122:PG4:H31	1.90	0.40
1:C:44:ALA:O	1:C:48:ILE:HG13	2.21	0.40
1:C:150:VAL:HB	1:C:176:VAL:HG21	2.04	0.40
2:D:82:LEU:HB3	2:D:83:THR:H	1.58	0.40

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

All (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
2	D	82	LEU
2	D	83	THR
1	A	108	SER
1	C	30	VAL
2	B	11	PRO
1	C	12	LYS
4	F	3	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	5	GLU
1	A	6	GLU
1	A	9	LYS
1	A	10	LYS
1	A	15	GLU
1	A	17	PHE
1	A	25	ARG
1	A	33	VAL
1	A	34	LYS
1	A	36	GLN
1	A	42	CYS
1	A	46	SER
1	A	48	ILE
1	A	61	LYS
1	A	65	LEU
1	A	66	SER
1	A	67	GLU
1	A	69	GLU
1	A	70	LEU
1	A	72	ASP
1	A	77	ASN

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Mol	Chain	Res	Type
1	A	80	CYS
1	A	85	ILE
1	A	93	ILE
1	A	99	CYS
1	A	100	THR
1	A	102	ASP
1	A	107	VAL
1	A	113	LEU
1	A	116	ILE
1	A	119	CYS
1	A	122	LYS
1	A	129	LEU
1	A	133	ASP
1	A	134[A]	ASN
1	A	134[B]	ASN
1	A	136	LEU
1	A	141	ARG
1	A	142	PHE
1	A	143	LEU
1	A	146	ILE
1	A	147	SER
1	A	149	SER
1	A	152	VAL
1	A	153	SER
1	A	160	LYS
1	A	161	GLU
1	A	167	GLU
1	A	168	CYS
1	A	178	LEU
1	A	184	LYS
1	A	186	ILE
1	A	187	VAL
1	A	190	LEU
1	A	192	LYS
1	A	193	LYS
1	A	196	LYS
1	A	200	TYR
1	A	202	ILE
1	A	203	LYS
1	A	205	SER
1	A	208	GLN
1	A	216	ILE

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Mol	Chain	Res	Type
1	A	218	ILE
1	A	220	THR
1	A	222	GLU
1	A	226	MET
1	A	227	ARG
1	A	228	LYS
1	A	229	CYS
1	A	236	PHE
1	A	237	ILE
1	A	240	ILE
2	B	1	MET
2	B	6	LEU
2	B	7	SER
2	B	13	THR
2	B	15	GLU
2	B	19	ILE
2	B	22	LYS
2	B	24	LYS
2	B	30	LYS
2	B	31	THR
2	B	33	GLU
2	B	34	THR
2	B	35	TYR
2	B	37	LYS
2	B	41	VAL
2	B	44	LYS
2	B	45	THR
2	B	47	VAL
2	B	48	VAL
2	B	51	THR
2	B	52	ASN
2	B	55	ILE
2	B	57	VAL
2	B	63	LYS
2	B	65	MET
2	B	69	VAL
2	B	71	LYS
2	B	81	VAL
2	B	86	GLN
2	B	95	LEU
2	B	96	THR
1	C	4	TYR

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Mol	Chain	Res	Type
1	C	9	LYS
1	C	11	TYR
1	C	12	LYS
1	C	17	PHE
1	C	18	ASP
1	C	22	TYR
1	C	30	VAL
1	C	33	VAL
1	C	37	LYS
1	C	39	CYS
1	C	46	SER
1	C	48	ILE
1	C	51	VAL
1	C	55	TYR
1	C	57	ILE
1	C	61	LYS
1	C	62	LEU
1	C	65	LEU
1	C	70	LEU
1	C	78	TYR
1	C	80	CYS
1	C	81	ASN
1	C	85	ILE
1	C	87	ASN
1	C	89	PHE
1	C	91	ASP
1	C	93	ILE
1	C	100	THR
1	C	102	ASP
1	C	108	SER
1	C	113	LEU
1	C	116	ILE
1	C	117	ASP
1	C	118	ARG
1	C	119	CYS
1	C	120	THR
1	C	126	LYS
1	C	129	LEU
1	C	138	GLU
1	C	140	LEU
1	C	141	ARG
1	C	143	LEU

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Mol	Chain	Res	Type
1	C	148	ILE
1	C	149	SER
1	C	150	VAL
1	C	156	PHE
1	C	158	PHE
1	C	160	LYS
1	C	163	ILE
1	C	165	ASP
1	C	172	LEU
1	C	177	MET
1	C	184	LYS
1	C	185	GLU
1	C	187	VAL
1	C	190	LEU
1	C	191	THR
1	C	192	LYS
1	C	195	GLU
1	C	196	LYS
1	C	197	HIS
1	C	198	TYR
1	C	200	TYR
1	C	201	ILE
1	C	202	ILE
1	C	203	LYS
1	C	204	ASN
1	C	205	SER
1	C	216	ILE
1	C	218	ILE
1	C	219	GLU
1	C	220	THR
1	C	223	SER
1	C	225	LEU
1	C	227	ARG
1	C	229	CYS
1	C	231	LEU
1	C	239	LEU
1	C	241	GLU
2	D	1	MET
2	D	6	LEU
2	D	7	SER
2	D	13	THR
2	D	16	ILE

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Mol	Chain	Res	Type
2	D	17	GLN
2	D	19	ILE
2	D	24	LYS
2	D	32	ASN
2	D	33	GLU
2	D	35	TYR
2	D	37	LYS
2	D	38	LEU
2	D	39	GLU
2	D	41	VAL
2	D	45	THR
2	D	47	VAL
2	D	51	THR
2	D	54	TYR
2	D	63	LYS
2	D	66	HIS
2	D	67	LEU
2	D	70	PHE
2	D	71	LYS
2	D	73	LEU
2	D	76	GLN
2	D	80	LEU
2	D	81	VAL
2	D	83	THR
2	D	86	GLN
2	D	90	ASN
2	D	93	ASP
2	D	94	GLU
2	D	96	THR
2	D	98	PHE
3	E	7	LEU
4	F	1	VAL
4	F	4	LEU
4	F	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	60	ASN
1	A	174	HIS
1	A	188	ASN

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Mol	Chain	Res	Type
2	B	32	ASN
1	C	36	GLN
1	C	38	ASN
1	C	86	ASN
1	C	87	ASN
1	C	134	ASN
1	C	204	ASN
2	D	17	GLN
2	D	26	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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.

All (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
5	B	112	GOL	C3-C2-C1	-2.24	103.58	111.80
5	D	108	GOL	C3-C2-C1	-2.23	103.63	111.80
5	C	306	GOL	C3-C2-C1	-2.22	103.64	111.80
5	C	312	GOL	C3-C2-C1	-2.22	103.64	111.80
5	D	112	GOL	C3-C2-C1	-2.21	103.70	111.80
5	A	314	GOL	C3-C2-C1	-2.21	103.70	111.80
5	B	108	GOL	C3-C2-C1	-2.21	103.71	111.80
5	D	131	GOL	C3-C2-C1	-2.20	103.72	111.80
5	B	110	GOL	C3-C2-C1	-2.18	103.79	111.80
5	E	104	GOL	C3-C2-C1	-2.18	103.80	111.80
5	C	338	GOL	C3-C2-C1	-2.18	103.80	111.80
5	B	140	GOL	C3-C2-C1	-2.18	103.81	111.80
5	A	345	GOL	C3-C2-C1	-2.17	103.86	111.80
5	A	301	GOL	C3-C2-C1	-2.16	103.87	111.80
5	C	311	GOL	C3-C2-C1	-2.16	103.87	111.80
5	B	109	GOL	C3-C2-C1	-2.16	103.88	111.80
5	B	152	GOL	C3-C2-C1	-2.15	103.90	111.80
5	E	102	GOL	C3-C2-C1	-2.14	103.94	111.80
5	A	302	GOL	C3-C2-C1	-2.13	103.97	111.80
5	B	103	GOL	C3-C2-C1	-2.12	104.00	111.80
5	F	103	GOL	C3-C2-C1	-2.12	104.01	111.80
5	D	110	GOL	C3-C2-C1	-2.11	104.06	111.80
5	A	362	GOL	C3-C2-C1	-2.11	104.07	111.80
5	A	307	GOL	C3-C2-C1	-2.10	104.11	111.80
5	A	308	GOL	C3-C2-C1	-2.09	104.14	111.80
5	A	364	GOL	C3-C2-C1	-2.09	104.14	111.80
5	C	345	GOL	C3-C2-C1	-2.08	104.17	111.80
5	C	314	GOL	C3-C2-C1	-2.07	104.21	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	107	GOL	C3-C2-C1	-2.07	104.21	111.80
5	B	106	GOL	C3-C2-C1	-2.05	104.26	111.80
5	E	103	GOL	C3-C2-C1	-2.05	104.27	111.80
5	B	154	GOL	C3-C2-C1	-2.05	104.28	111.80
5	B	107	GOL	C3-C2-C1	-2.05	104.28	111.80
5	C	313	GOL	C3-C2-C1	-2.02	104.39	111.80
5	A	311	GOL	C3-C2-C1	-2.02	104.39	111.80
5	B	153	GOL	C3-C2-C1	-2.02	104.39	111.80
5	C	307	GOL	C3-C2-C1	-2.01	104.44	111.80

There are no chirality outliers.

All (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
5	A	312	GOL	C1-C2-C3-O3
5	A	314	GOL	C1-C2-C3-O3
5	A	314	GOL	O2-C2-C3-O3
5	A	345	GOL	O1-C1-C2-O2
5	A	345	GOL	O1-C1-C2-C3
5	A	345	GOL	C1-C2-C3-O3
5	A	347	GOL	C1-C2-C3-O3
5	A	347	GOL	O2-C2-C3-O3
5	A	363	GOL	C1-C2-C3-O3
5	A	373	GOL	C1-C2-C3-O3
5	B	103	GOL	O1-C1-C2-C3
5	B	103	GOL	C1-C2-C3-O3
5	B	104	GOL	C1-C2-C3-O3
5	B	108	GOL	O1-C1-C2-O2
5	B	108	GOL	O1-C1-C2-C3
5	B	111	GOL	O1-C1-C2-C3
5	B	112	GOL	C1-C2-C3-O3
5	B	112	GOL	O2-C2-C3-O3
5	B	152	GOL	O2-C2-C3-O3
5	C	304	GOL	O1-C1-C2-C3
5	C	304	GOL	C1-C2-C3-O3
5	C	304	GOL	O2-C2-C3-O3
5	C	305	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	C	306	GOL	C1-C2-C3-O3
5	C	307	GOL	O1-C1-C2-C3
5	C	308	GOL	O1-C1-C2-C3
5	C	308	GOL	C1-C2-C3-O3
5	C	310	GOL	O1-C1-C2-C3
5	C	311	GOL	O1-C1-C2-C3
5	C	312	GOL	O1-C1-C2-C3
5	C	312	GOL	C1-C2-C3-O3
5	C	312	GOL	O2-C2-C3-O3
5	C	313	GOL	O1-C1-C2-O2
5	C	313	GOL	O1-C1-C2-C3
5	C	314	GOL	O1-C1-C2-C3
5	C	314	GOL	C1-C2-C3-O3
5	C	337	GOL	O1-C1-C2-O2
5	C	337	GOL	O1-C1-C2-C3
5	C	347	GOL	C1-C2-C3-O3
5	D	107	GOL	O1-C1-C2-C3
5	D	112	GOL	C1-C2-C3-O3
5	D	131	GOL	O1-C1-C2-C3
5	D	131	GOL	C1-C2-C3-O3
7	F	105	PG4	C1-C2-O2-C3
7	B	118	PG4	C1-C2-O2-C3
7	D	119	PG4	C1-C2-O2-C3
9	B	157	PEG	C4-C3-O2-C2
10	E	110	PE8	C9-C8-O7-C6
7	A	325	PG4	C6-C5-O3-C4
9	A	331	PEG	C4-C3-O2-C2
9	C	334	PEG	C4-C3-O2-C2
9	C	331	PEG	C1-C2-O2-C3
7	B	125	PG4	C1-C2-O2-C3
10	B	136	PE8	C12-C11-O10-C9
10	B	138	PE8	C15-C14-O13-C12
7	C	323	PG4	C1-C2-O2-C3
7	A	322	PG4	C1-C2-O2-C3
7	A	323	PG4	C3-C4-O3-C5
10	A	342	PE8	C6-C5-O4-C3
10	E	109	PE8	C21-C20-O19-C18
7	E	115	PG4	C4-C3-O2-C2
10	B	136	PE8	C11-C12-O13-C14
7	D	118	PG4	C1-C2-O2-C3
7	F	101	PG4	C3-C4-O3-C5
10	B	136	PE8	C21-C20-O19-C18

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Mol	Chain	Res	Type	Atoms
10	E	109	PE8	C8-C9-O10-C11
7	C	323	PG4	C6-C5-O3-C4
7	A	320	PG4	O2-C3-C4-O3
7	A	324	PG4	O3-C5-C6-O4
7	C	325	PG4	O2-C3-C4-O3
7	E	106	PG4	O2-C3-C4-O3
7	E	115	PG4	O2-C3-C4-O3
10	B	102	PE8	O10-C11-C12-O13
10	B	136	PE8	O10-C11-C12-O13
10	C	335	PE8	O13-C14-C15-O16
7	B	119	PG4	O2-C3-C4-O3
7	B	122	PG4	O3-C5-C6-O4
7	B	123	PG4	O3-C5-C6-O4
7	B	155	PG4	O3-C5-C6-O4
7	D	118	PG4	O2-C3-C4-O3
10	A	342	PE8	O10-C11-C12-O13
10	A	344	PE8	O7-C8-C9-O10
10	B	138	PE8	C5-C6-O7-C8
7	C	320	PG4	O3-C5-C6-O4
10	B	102	PE8	O16-C17-C18-O19
10	F	106	PE8	O4-C5-C6-O7
7	C	319	PG4	O2-C3-C4-O3
7	C	323	PG4	O3-C5-C6-O4
7	C	324	PG4	O3-C5-C6-O4
7	D	118	PG4	O3-C5-C6-O4
10	E	110	PE8	O7-C8-C9-O10
7	A	323	PG4	O2-C3-C4-O3
7	C	321	PG4	O2-C3-C4-O3
10	A	344	PE8	O4-C5-C6-O7
7	D	118	PG4	O1-C1-C2-O2
7	D	120	PG4	O1-C1-C2-O2
9	A	340	PEG	O1-C1-C2-O2
9	C	333	PEG	O1-C1-C2-O2
7	B	122	PG4	O2-C3-C4-O3
10	A	344	PE8	O10-C11-C12-O13
7	B	120	PG4	O3-C5-C6-O4
7	B	125	PG4	O3-C5-C6-O4
7	D	117	PG4	O2-C3-C4-O3
10	F	102	PE8	O4-C5-C6-O7
10	F	102	PE8	O16-C17-C18-O19
9	A	346	PEG	C1-C2-O2-C3
7	A	323	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
7	B	101	PG4	O2-C3-C4-O3
7	D	120	PG4	O3-C5-C6-O4
7	A	368	PG4	O2-C3-C4-O3
7	D	116	PG4	O2-C3-C4-O3
7	A	320	PG4	O3-C5-C6-O4
10	B	138	PE8	O16-C17-C18-O19
10	E	110	PE8	O16-C17-C18-O19
7	C	325	PG4	O3-C5-C6-O4
7	B	116	PG4	O2-C3-C4-O3
7	E	107	PG4	O3-C5-C6-O4
10	F	102	PE8	O10-C11-C12-O13
7	A	321	PG4	O3-C5-C6-O4
10	A	344	PE8	O16-C17-C18-O19
10	B	138	PE8	O13-C14-C15-O16
10	F	106	PE8	O19-C20-C21-O22
10	B	136	PE8	O13-C14-C15-O16
10	E	109	PE8	O19-C20-C21-O22
7	C	322	PG4	O3-C5-C6-O4
10	B	138	PE8	C18-C17-O16-C15
5	A	302	GOL	O2-C2-C3-O3
5	A	311	GOL	O1-C1-C2-O2
5	A	345	GOL	O2-C2-C3-O3
5	C	305	GOL	O2-C2-C3-O3
5	C	306	GOL	O2-C2-C3-O3
5	C	312	GOL	O1-C1-C2-O2
5	C	338	GOL	O1-C1-C2-O2
5	D	131	GOL	O1-C1-C2-O2
7	E	114	PG4	O3-C5-C6-O4
7	D	117	PG4	O3-C5-C6-O4
7	E	107	PG4	O2-C3-C4-O3
10	A	344	PE8	O13-C14-C15-O16
10	A	343	PE8	O4-C5-C6-O7
7	A	325	PG4	O4-C7-C8-O5
7	A	326	PG4	O1-C1-C2-O2
7	A	365	PG4	O1-C1-C2-O2
7	A	369	PG4	O1-C1-C2-O2
7	A	369	PG4	O4-C7-C8-O5
7	B	124	PG4	O1-C1-C2-O2
7	B	155	PG4	O4-C7-C8-O5
7	C	321	PG4	O1-C1-C2-O2
7	C	322	PG4	O1-C1-C2-O2
7	C	322	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
7	D	103	PG4	O1-C1-C2-O2
7	D	103	PG4	O4-C7-C8-O5
7	D	118	PG4	O4-C7-C8-O5
9	A	333	PEG	O2-C3-C4-O4
9	A	346	PEG	O2-C3-C4-O4
9	A	370	PEG	O1-C1-C2-O2
9	A	371	PEG	O1-C1-C2-O2
9	B	133	PEG	O1-C1-C2-O2
9	B	156	PEG	O2-C3-C4-O4
9	B	158	PEG	O2-C3-C4-O4
9	C	327	PEG	O2-C3-C4-O4
9	C	329	PEG	O2-C3-C4-O4
9	D	104	PEG	O1-C1-C2-O2
9	D	105	PEG	O2-C3-C4-O4
9	D	124	PEG	O1-C1-C2-O2
9	D	128	PEG	O2-C3-C4-O4
10	B	136	PE8	O1-C2-C3-O4
10	F	106	PE8	O22-C23-C24-O25
7	D	103	PG4	O3-C5-C6-O4
7	E	115	PG4	O3-C5-C6-O4
10	B	136	PE8	O7-C8-C9-O10
7	A	325	PG4	C5-C6-O4-C7
10	E	109	PE8	C15-C14-O13-C12
10	E	109	PE8	O10-C11-C12-O13
7	B	117	PG4	O3-C5-C6-O4
7	C	319	PG4	O3-C5-C6-O4
7	F	105	PG4	O3-C5-C6-O4
7	B	118	PG4	O2-C3-C4-O3
10	F	102	PE8	O7-C8-C9-O10
7	E	105	PG4	C1-C2-O2-C3
10	C	335	PE8	O10-C11-C12-O13
7	A	320	PG4	O4-C7-C8-O5
7	A	321	PG4	O4-C7-C8-O5
7	A	324	PG4	O1-C1-C2-O2
7	A	365	PG4	O4-C7-C8-O5
7	B	116	PG4	O4-C7-C8-O5
7	B	125	PG4	O4-C7-C8-O5
7	C	325	PG4	O1-C1-C2-O2
7	D	119	PG4	O1-C1-C2-O2
7	E	106	PG4	O4-C7-C8-O5
7	E	115	PG4	O1-C1-C2-O2
9	A	330	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
9	A	331	PEG	O1-C1-C2-O2
9	A	332	PEG	O1-C1-C2-O2
9	A	334	PEG	O1-C1-C2-O2
9	A	337	PEG	O1-C1-C2-O2
9	A	337	PEG	O2-C3-C4-O4
9	A	339	PEG	O2-C3-C4-O4
9	A	346	PEG	O1-C1-C2-O2
9	A	353	PEG	O1-C1-C2-O2
9	B	139	PEG	O1-C1-C2-O2
9	B	157	PEG	O1-C1-C2-O2
9	C	303	PEG	O1-C1-C2-O2
9	C	331	PEG	O1-C1-C2-O2
9	C	331	PEG	O2-C3-C4-O4
9	C	339	PEG	O1-C1-C2-O2
10	A	343	PE8	O22-C23-C24-O25
10	A	344	PE8	O22-C23-C24-O25
10	B	138	PE8	O22-C23-C24-O25
10	E	110	PE8	O22-C23-C24-O25
10	E	109	PE8	O4-C5-C6-O7
7	A	325	PG4	O2-C3-C4-O3
7	B	122	PG4	C1-C2-O2-C3
7	A	366	PG4	O3-C5-C6-O4
7	A	365	PG4	C6-C5-O3-C4
7	A	325	PG4	O3-C5-C6-O4
10	A	343	PE8	O7-C8-C9-O10
10	A	342	PE8	O19-C20-C21-O22
7	E	106	PG4	O3-C5-C6-O4
5	A	301	GOL	O1-C1-C2-C3
5	A	302	GOL	C1-C2-C3-O3
5	A	311	GOL	O1-C1-C2-C3
5	A	311	GOL	C1-C2-C3-O3
5	A	362	GOL	O1-C1-C2-C3
5	A	364	GOL	O1-C1-C2-C3
5	B	109	GOL	O1-C1-C2-C3
5	B	111	GOL	C1-C2-C3-O3
5	B	140	GOL	C1-C2-C3-O3
5	B	152	GOL	C1-C2-C3-O3
5	C	309	GOL	C1-C2-C3-O3
5	C	310	GOL	C1-C2-C3-O3
5	C	311	GOL	C1-C2-C3-O3
5	C	338	GOL	O1-C1-C2-C3
5	C	344	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	C	345	GOL	O1-C1-C2-C3
5	D	106	GOL	O1-C1-C2-C3
5	D	107	GOL	C1-C2-C3-O3
5	D	110	GOL	C1-C2-C3-O3
5	D	111	GOL	O1-C1-C2-C3
5	D	137	GOL	C1-C2-C3-O3
5	E	102	GOL	O1-C1-C2-C3
5	E	102	GOL	C1-C2-C3-O3
5	E	103	GOL	C1-C2-C3-O3
5	E	104	GOL	O1-C1-C2-C3
5	E	113	GOL	O1-C1-C2-C3
5	E	113	GOL	C1-C2-C3-O3
5	F	103	GOL	O1-C1-C2-C3
10	B	136	PE8	O4-C5-C6-O7
7	A	325	PG4	O1-C1-C2-O2
7	A	352	PG4	O1-C1-C2-O2
7	B	101	PG4	O1-C1-C2-O2
7	B	119	PG4	O1-C1-C2-O2
7	C	319	PG4	O1-C1-C2-O2
7	C	320	PG4	O1-C1-C2-O2
9	B	127	PEG	O1-C1-C2-O2
9	B	128	PEG	O1-C1-C2-O2
9	B	128	PEG	O2-C3-C4-O4
9	B	142	PEG	O2-C3-C4-O4
9	B	156	PEG	O1-C1-C2-O2
9	C	330	PEG	O2-C3-C4-O4
9	C	332	PEG	O2-C3-C4-O4
9	C	333	PEG	O2-C3-C4-O4
9	C	334	PEG	O1-C1-C2-O2
9	D	125	PEG	O1-C1-C2-O2
10	A	343	PE8	O1-C2-C3-O4
10	E	110	PE8	O1-C2-C3-O4
7	B	125	PG4	C8-C7-O4-C6
7	A	319	PG4	O2-C3-C4-O3
10	A	342	PE8	O7-C8-C9-O10
10	F	106	PE8	C15-C14-O13-C12
7	E	114	PG4	O2-C3-C4-O3
5	A	306	GOL	O2-C2-C3-O3
5	A	309	GOL	O2-C2-C3-O3
5	A	311	GOL	O2-C2-C3-O3
5	A	312	GOL	O1-C1-C2-O2
5	A	312	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	364	GOL	O1-C1-C2-O2
5	A	373	GOL	O2-C2-C3-O3
5	B	103	GOL	O1-C1-C2-O2
5	B	103	GOL	O2-C2-C3-O3
5	B	104	GOL	O2-C2-C3-O3
5	B	111	GOL	O1-C1-C2-O2
5	B	111	GOL	O2-C2-C3-O3
5	C	307	GOL	O1-C1-C2-O2
5	C	308	GOL	O2-C2-C3-O3
5	C	310	GOL	O2-C2-C3-O3
5	C	311	GOL	O1-C1-C2-O2
5	C	314	GOL	O1-C1-C2-O2
5	C	314	GOL	O2-C2-C3-O3
5	C	344	GOL	O1-C1-C2-O2
5	C	345	GOL	O1-C1-C2-O2
5	C	347	GOL	O2-C2-C3-O3
5	D	107	GOL	O1-C1-C2-O2
5	D	110	GOL	O2-C2-C3-O3
5	D	111	GOL	O1-C1-C2-O2
5	D	137	GOL	O2-C2-C3-O3
5	E	104	GOL	O1-C1-C2-O2
7	C	325	PG4	C4-C3-O2-C2
10	F	102	PE8	O19-C20-C21-O22
7	B	118	PG4	O3-C5-C6-O4
7	A	319	PG4	O4-C7-C8-O5
7	A	323	PG4	O1-C1-C2-O2
7	B	117	PG4	O4-C7-C8-O5
7	B	119	PG4	O4-C7-C8-O5
7	E	114	PG4	O4-C7-C8-O5
7	F	105	PG4	O1-C1-C2-O2
9	A	329	PEG	O1-C1-C2-O2
9	A	340	PEG	O2-C3-C4-O4
9	A	353	PEG	O2-C3-C4-O4
9	B	134	PEG	O1-C1-C2-O2
9	B	135	PEG	O2-C3-C4-O4
9	D	105	PEG	O1-C1-C2-O2
10	A	344	PE8	O1-C2-C3-O4
10	B	137	PE8	O22-C23-C24-O25
7	A	368	PG4	O3-C5-C6-O4
7	B	121	PG4	O2-C3-C4-O3
11	A	351	EDO	O1-C1-C2-O2
11	E	111	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
10	B	102	PE8	O4-C5-C6-O7
10	E	110	PE8	O4-C5-C6-O7
7	C	320	PG4	O2-C3-C4-O3
7	E	105	PG4	O3-C5-C6-O4
10	E	110	PE8	O10-C11-C12-O13
7	B	120	PG4	O4-C7-C8-O5
7	C	302	PG4	O1-C1-C2-O2
7	C	320	PG4	O4-C7-C8-O5
7	F	101	PG4	O1-C1-C2-O2
9	C	346	PEG	O2-C3-C4-O4
9	D	125	PEG	O2-C3-C4-O4
10	F	106	PE8	O1-C2-C3-O4
7	A	352	PG4	O3-C5-C6-O4
7	C	336	PG4	O2-C3-C4-O3
10	B	137	PE8	O7-C8-C9-O10
7	D	119	PG4	O2-C3-C4-O3
10	F	106	PE8	O7-C8-C9-O10
10	B	137	PE8	O4-C5-C6-O7
7	B	121	PG4	O3-C5-C6-O4
10	B	138	PE8	O10-C11-C12-O13
7	A	365	PG4	O2-C3-C4-O3
7	C	336	PG4	O3-C5-C6-O4
7	A	352	PG4	O2-C3-C4-O3
7	A	321	PG4	O1-C1-C2-O2
7	B	118	PG4	O1-C1-C2-O2
9	A	335	PEG	O2-C3-C4-O4
9	A	339	PEG	O1-C1-C2-O2
9	B	129	PEG	O1-C1-C2-O2
9	B	139	PEG	O2-C3-C4-O4
9	C	327	PEG	O1-C1-C2-O2
9	C	328	PEG	O1-C1-C2-O2
9	C	329	PEG	O1-C1-C2-O2
9	C	332	PEG	O1-C1-C2-O2
10	C	335	PE8	O22-C23-C24-O25
10	F	106	PE8	O16-C17-C18-O19
5	A	362	GOL	O1-C1-C2-O2
5	A	363	GOL	O2-C2-C3-O3
5	B	140	GOL	O2-C2-C3-O3
5	C	304	GOL	O1-C1-C2-O2
5	C	308	GOL	O1-C1-C2-O2
5	C	310	GOL	O1-C1-C2-O2
5	D	112	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	D	131	GOL	O2-C2-C3-O3
5	E	102	GOL	O1-C1-C2-O2
5	E	102	GOL	O2-C2-C3-O3
5	F	103	GOL	O1-C1-C2-O2
10	F	106	PE8	O10-C11-C12-O13
10	A	342	PE8	O16-C17-C18-O19
7	A	319	PG4	O1-C1-C2-O2
7	B	121	PG4	O4-C7-C8-O5
7	C	302	PG4	O4-C7-C8-O5
10	C	335	PE8	O1-C2-C3-O4
7	A	367	PG4	O2-C3-C4-O3
7	B	101	PG4	O3-C5-C6-O4
11	D	102	EDO	O1-C1-C2-O2
7	D	103	PG4	O2-C3-C4-O3
9	C	328	PEG	C1-C2-O2-C3
10	F	102	PE8	C8-C9-O10-C11
7	F	105	PG4	O4-C7-C8-O5
9	A	330	PEG	O2-C3-C4-O4
9	B	132	PEG	O2-C3-C4-O4
9	D	122	PEG	O2-C3-C4-O4
9	D	123	PEG	O1-C1-C2-O2
10	B	137	PE8	C20-C21-O22-C23
7	A	367	PG4	O3-C5-C6-O4
7	A	369	PG4	O3-C5-C6-O4
10	C	335	PE8	O7-C8-C9-O10
10	C	335	PE8	O19-C20-C21-O22
9	D	124	PEG	C4-C3-O2-C2
7	B	117	PG4	O2-C3-C4-O3
10	C	335	PE8	O4-C5-C6-O7
7	D	117	PG4	O1-C1-C2-O2
5	A	307	GOL	O1-C1-C2-O2
5	A	364	GOL	O2-C2-C3-O3
5	C	311	GOL	O2-C2-C3-O3
5	D	109	GOL	O2-C2-C3-O3
5	E	103	GOL	O2-C2-C3-O3
10	E	110	PE8	O13-C14-C15-O16
7	B	124	PG4	O3-C5-C6-O4
7	C	319	PG4	C1-C2-O2-C3
7	C	336	PG4	O4-C7-C8-O5
7	A	326	PG4	O2-C3-C4-O3
7	C	321	PG4	O3-C5-C6-O4
9	B	126	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
9	D	126	PEG	O1-C1-C2-O2
7	A	369	PG4	O2-C3-C4-O3
10	A	342	PE8	O4-C5-C6-O7
7	A	326	PG4	O3-C5-C6-O4
7	C	320	PG4	C5-C6-O4-C7
7	B	120	PG4	O2-C3-C4-O3
7	C	324	PG4	C3-C4-O3-C5
5	A	304	GOL	O2-C2-C3-O3
5	A	362	GOL	O2-C2-C3-O3
5	C	307	GOL	O2-C2-C3-O3
5	C	309	GOL	O1-C1-C2-O2
10	A	343	PE8	C20-C21-O22-C23
10	E	110	PE8	C20-C21-O22-C23
7	A	320	PG4	C5-C6-O4-C7
7	C	319	PG4	C5-C6-O4-C7
9	A	353	PEG	C4-C3-O2-C2
7	A	326	PG4	O4-C7-C8-O5
9	B	130	PEG	O2-C3-C4-O4
7	B	118	PG4	C5-C6-O4-C7
9	D	121	PEG	C4-C3-O2-C2
10	B	138	PE8	C21-C20-O19-C18
7	A	321	PG4	C5-C6-O4-C7
7	C	323	PG4	C5-C6-O4-C7
9	A	334	PEG	C1-C2-O2-C3
9	B	127	PEG	C4-C3-O2-C2
10	F	106	PE8	C5-C6-O7-C8
7	A	321	PG4	C6-C5-O3-C4
7	C	321	PG4	C3-C4-O3-C5
9	A	372	PEG	C1-C2-O2-C3
7	A	324	PG4	C1-C2-O2-C3
7	A	352	PG4	C1-C2-O2-C3
9	C	346	PEG	C4-C3-O2-C2
7	B	119	PG4	C5-C6-O4-C7
7	B	124	PG4	C5-C6-O4-C7
7	D	103	PG4	C1-C2-O2-C3
10	A	342	PE8	C14-C15-O16-C17
7	B	123	PG4	C4-C3-O2-C2
7	E	114	PG4	C5-C6-O4-C7
9	B	133	PEG	C4-C3-O2-C2
9	D	126	PEG	C4-C3-O2-C2
10	F	102	PE8	C17-C18-O19-C20
9	A	332	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
10	A	342	PE8	C5-C6-O7-C8
10	A	343	PE8	C9-C8-O7-C6
7	C	322	PG4	C5-C6-O4-C7
10	F	102	PE8	C2-C3-O4-C5
7	A	325	PG4	C1-C2-O2-C3
7	D	119	PG4	C4-C3-O2-C2
7	E	106	PG4	C8-C7-O4-C6
10	F	102	PE8	C15-C14-O13-C12
5	A	307	GOL	O1-C1-C2-C3
7	A	324	PG4	C3-C4-O3-C5
10	A	342	PE8	C9-C8-O7-C6
10	A	343	PE8	C21-C20-O19-C18
7	B	119	PG4	C6-C5-O3-C4
7	C	320	PG4	C6-C5-O3-C4
7	E	106	PG4	C5-C6-O4-C7
10	A	344	PE8	C21-C20-O19-C18
10	C	335	PE8	C24-C23-O22-C21
7	A	324	PG4	C4-C3-O2-C2
7	A	367	PG4	C4-C3-O2-C2
7	C	319	PG4	C8-C7-O4-C6
9	B	132	PEG	C1-C2-O2-C3
7	A	326	PG4	C8-C7-O4-C6
7	B	116	PG4	C4-C3-O2-C2
7	A	325	PG4	C8-C7-O4-C6
7	B	120	PG4	C3-C4-O3-C5
7	F	101	PG4	C5-C6-O4-C7
9	A	331	PEG	C1-C2-O2-C3
9	A	333	PEG	C4-C3-O2-C2
9	A	340	PEG	C4-C3-O2-C2
10	A	343	PE8	C6-C5-O4-C3
10	B	137	PE8	C2-C3-O4-C5
10	B	138	PE8	C20-C21-O22-C23
7	A	324	PG4	C5-C6-O4-C7
7	B	122	PG4	C4-C3-O2-C2
7	B	125	PG4	C6-C5-O3-C4
9	D	121	PEG	C1-C2-O2-C3
10	C	335	PE8	C5-C6-O7-C8
10	F	102	PE8	C20-C21-O22-C23
7	A	368	PG4	C8-C7-O4-C6
7	C	324	PG4	C8-C7-O4-C6
10	A	342	PE8	C8-C9-O10-C11
10	A	343	PE8	C14-C15-O16-C17

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Mol	Chain	Res	Type	Atoms
10	E	110	PE8	C5-C6-O7-C8
7	A	368	PG4	O1-C1-C2-O2
9	A	338	PEG	O1-C1-C2-O2
9	B	132	PEG	O1-C1-C2-O2
9	B	134	PEG	O2-C3-C4-O4
10	E	109	PE8	O22-C23-C24-O25
7	B	119	PG4	C8-C7-O4-C6
7	C	325	PG4	C5-C6-O4-C7
9	A	337	PEG	C4-C3-O2-C2
9	B	157	PEG	C1-C2-O2-C3
7	A	319	PG4	C8-C7-O4-C6
9	B	158	PEG	C1-C2-O2-C3
7	B	121	PG4	C5-C6-O4-C7
10	F	106	PE8	C8-C9-O10-C11
7	B	124	PG4	C1-C2-O2-C3
7	A	320	PG4	C8-C7-O4-C6
7	E	114	PG4	C1-C2-O2-C3
9	D	128	PEG	C1-C2-O2-C3
7	B	121	PG4	C3-C4-O3-C5
7	D	118	PG4	C4-C3-O2-C2
7	D	120	PG4	C3-C4-O3-C5
7	B	119	PG4	C1-C2-O2-C3
7	B	155	PG4	C4-C3-O2-C2
7	E	106	PG4	C1-C2-O2-C3
9	A	338	PEG	C4-C3-O2-C2
10	C	335	PE8	C17-C18-O19-C20
7	A	365	PG4	C8-C7-O4-C6
7	C	324	PG4	C4-C3-O2-C2
9	B	130	PEG	C1-C2-O2-C3
10	B	137	PE8	C17-C18-O19-C20
7	D	120	PG4	O2-C3-C4-O3
9	D	126	PEG	C1-C2-O2-C3
9	A	335	PEG	C4-C3-O2-C2
9	A	372	PEG	C4-C3-O2-C2
10	B	137	PE8	C9-C8-O7-C6
7	B	122	PG4	O4-C7-C8-O5
7	D	120	PG4	O4-C7-C8-O5
9	C	339	PEG	O2-C3-C4-O4
9	D	121	PEG	O1-C1-C2-O2
10	B	137	PE8	O1-C2-C3-O4
7	B	123	PG4	C3-C4-O3-C5
7	A	365	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
7	B	117	PG4	C5-C6-O4-C7
9	B	130	PEG	C4-C3-O2-C2
10	B	138	PE8	C17-C18-O19-C20
5	D	106	GOL	O1-C1-C2-O2
9	B	131	PEG	C1-C2-O2-C3
7	B	117	PG4	C6-C5-O3-C4
9	B	127	PEG	C1-C2-O2-C3
10	E	109	PE8	C2-C3-O4-C5
7	B	123	PG4	C6-C5-O3-C4
7	A	365	PG4	C4-C3-O2-C2
7	B	123	PG4	C8-C7-O4-C6
9	A	333	PEG	C1-C2-O2-C3
9	A	337	PEG	C1-C2-O2-C3
7	B	123	PG4	O1-C1-C2-O2
9	B	130	PEG	O1-C1-C2-O2
10	F	106	PE8	C11-C12-O13-C14
10	B	102	PE8	C11-C12-O13-C14
10	B	138	PE8	C9-C8-O7-C6
10	A	343	PE8	O10-C11-C12-O13
9	C	330	PEG	C1-C2-O2-C3
7	B	125	PG4	C3-C4-O3-C5
7	B	155	PG4	C3-C4-O3-C5
10	B	102	PE8	C8-C9-O10-C11
9	C	329	PEG	C1-C2-O2-C3
10	A	344	PE8	C12-C11-O10-C9
10	B	136	PE8	C6-C5-O4-C3
10	E	110	PE8	C18-C17-O16-C15
10	E	109	PE8	C11-C12-O13-C14
7	C	325	PG4	C3-C4-O3-C5
7	A	352	PG4	C6-C5-O3-C4
7	E	114	PG4	O1-C1-C2-O2
7	A	369	PG4	C6-C5-O3-C4
10	E	109	PE8	O16-C17-C18-O19
10	A	342	PE8	C21-C20-O19-C18
7	A	366	PG4	C5-C6-O4-C7
10	E	110	PE8	C17-C18-O19-C20
7	C	336	PG4	C1-C2-O2-C3
7	B	123	PG4	C5-C6-O4-C7
7	B	116	PG4	C3-C4-O3-C5
10	B	137	PE8	C8-C9-O10-C11
10	A	343	PE8	C24-C23-O22-C21
7	D	117	PG4	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
7	A	367	PG4	O4-C7-C8-O5
10	F	102	PE8	O22-C23-C24-O25
7	A	319	PG4	O3-C5-C6-O4
7	A	366	PG4	C1-C2-O2-C3
7	D	103	PG4	C6-C5-O3-C4
10	A	342	PE8	C17-C18-O19-C20
5	B	109	GOL	O1-C1-C2-O2
5	D	106	GOL	O2-C2-C3-O3
5	E	113	GOL	O2-C2-C3-O3
7	D	118	PG4	C8-C7-O4-C6
9	B	139	PEG	C1-C2-O2-C3
7	C	323	PG4	C4-C3-O2-C2
7	D	120	PG4	C6-C5-O3-C4
7	F	105	PG4	O2-C3-C4-O3
7	A	326	PG4	C4-C3-O2-C2
7	A	365	PG4	C1-C2-O2-C3
7	C	323	PG4	C8-C7-O4-C6
10	E	110	PE8	C21-C20-O19-C18
9	D	123	PEG	C1-C2-O2-C3
9	C	303	PEG	C1-C2-O2-C3
9	A	336	PEG	C4-C3-O2-C2
10	B	137	PE8	C15-C14-O13-C12
7	A	352	PG4	C3-C4-O3-C5
10	C	335	PE8	O16-C17-C18-O19
7	B	121	PG4	C6-C5-O3-C4
9	A	336	PEG	O1-C1-C2-O2
7	A	366	PG4	C4-C3-O2-C2
7	A	367	PG4	C5-C6-O4-C7
7	C	302	PG4	C8-C7-O4-C6
10	B	137	PE8	C14-C15-O16-C17
7	A	366	PG4	C8-C7-O4-C6
9	C	339	PEG	C4-C3-O2-C2
7	A	369	PG4	C4-C3-O2-C2
10	B	102	PE8	C5-C6-O7-C8
7	A	323	PG4	C4-C3-O2-C2
9	C	303	PEG	C4-C3-O2-C2
7	D	117	PG4	C4-C3-O2-C2
10	E	110	PE8	C14-C15-O16-C17
7	B	121	PG4	O1-C1-C2-O2
5	B	110	GOL	O2-C2-C3-O3
5	C	309	GOL	O2-C2-C3-O3
10	E	109	PE8	O13-C14-C15-O16

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Mol	Chain	Res	Type	Atoms
7	C	320	PG4	C4-C3-O2-C2
7	C	325	PG4	C8-C7-O4-C6
7	E	106	PG4	C4-C3-O2-C2
9	A	341	PEG	C4-C3-O2-C2
9	C	330	PEG	C4-C3-O2-C2
7	E	114	PG4	C6-C5-O3-C4
7	D	120	PG4	C5-C6-O4-C7
7	A	368	PG4	C4-C3-O2-C2
10	A	344	PE8	C11-C12-O13-C14
7	C	302	PG4	O2-C3-C4-O3
7	A	326	PG4	C1-C2-O2-C3
7	B	125	PG4	O2-C3-C4-O3
10	F	106	PE8	C17-C18-O19-C20
7	D	118	PG4	C5-C6-O4-C7
7	A	324	PG4	O2-C3-C4-O3
7	F	101	PG4	C8-C7-O4-C6
10	A	343	PE8	C2-C3-O4-C5
5	C	309	GOL	O1-C1-C2-C3
5	D	109	GOL	C1-C2-C3-O3
7	B	116	PG4	C1-C2-O2-C3
9	B	134	PEG	C4-C3-O2-C2
9	A	340	PEG	C1-C2-O2-C3
11	D	130	EDO	O1-C1-C2-O2
5	D	107	GOL	O2-C2-C3-O3
10	A	343	PE8	C18-C17-O16-C15
10	F	106	PE8	C6-C5-O4-C3
7	D	117	PG4	C8-C7-O4-C6
10	B	102	PE8	O7-C8-C9-O10
10	F	106	PE8	C20-C21-O22-C23
10	F	102	PE8	C14-C15-O16-C17
9	D	127	PEG	C4-C3-O2-C2
10	B	138	PE8	O7-C8-C9-O10
10	F	102	PE8	C11-C12-O13-C14
9	A	339	PEG	C4-C3-O2-C2
7	B	117	PG4	C4-C3-O2-C2
9	C	332	PEG	C1-C2-O2-C3
10	B	138	PE8	C8-C9-O10-C11
7	E	105	PG4	C5-C6-O4-C7
7	C	324	PG4	C6-C5-O3-C4
7	A	322	PG4	C5-C6-O4-C7
7	E	115	PG4	C8-C7-O4-C6
9	B	133	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
10	B	136	PE8	C5-C6-O7-C8
7	C	324	PG4	O1-C1-C2-O2
7	F	101	PG4	O2-C3-C4-O3
9	B	131	PEG	C4-C3-O2-C2
10	B	136	PE8	C24-C23-O22-C21
5	A	301	GOL	O1-C1-C2-O2
5	D	108	GOL	O1-C1-C2-O2
5	D	112	GOL	O1-C1-C2-O2
10	A	343	PE8	C15-C14-O13-C12
11	B	144	EDO	O1-C1-C2-O2
9	A	335	PEG	O1-C1-C2-O2
7	B	116	PG4	O3-C5-C6-O4
7	A	322	PG4	C8-C7-O4-C6
10	E	110	PE8	O19-C20-C21-O22
7	B	123	PG4	C1-C2-O2-C3
7	A	326	PG4	C3-C4-O3-C5
7	B	116	PG4	C5-C6-O4-C7
9	A	370	PEG	C1-C2-O2-C3
7	C	302	PG4	O3-C5-C6-O4
10	C	335	PE8	C11-C12-O13-C14
10	A	344	PE8	C5-C6-O7-C8
9	D	105	PEG	C1-C2-O2-C3
5	A	303	GOL	O2-C2-C3-O3
10	E	110	PE8	C12-C11-O10-C9
7	D	116	PG4	C5-C6-O4-C7
9	D	127	PEG	C1-C2-O2-C3
9	A	332	PEG	C4-C3-O2-C2
7	A	352	PG4	C4-C3-O2-C2
10	F	102	PE8	O13-C14-C15-O16
10	A	344	PE8	C17-C18-O19-C20
7	A	367	PG4	C1-C2-O2-C3
9	B	129	PEG	C4-C3-O2-C2
7	E	105	PG4	O2-C3-C4-O3
10	B	136	PE8	C20-C21-O22-C23
7	A	352	PG4	O4-C7-C8-O5
7	B	122	PG4	O1-C1-C2-O2
7	D	117	PG4	O4-C7-C8-O5
7	B	117	PG4	C8-C7-O4-C6
7	A	321	PG4	C3-C4-O3-C5
7	B	122	PG4	C8-C7-O4-C6
10	F	106	PE8	C2-C3-O4-C5
9	A	341	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	301	GOL	O2-C2-C3-O3
7	A	321	PG4	O2-C3-C4-O3
10	B	102	PE8	O19-C20-C21-O22
10	F	106	PE8	C18-C17-O16-C15
7	B	155	PG4	C5-C6-O4-C7
7	F	101	PG4	O3-C5-C6-O4
7	A	323	PG4	C6-C5-O3-C4
7	B	155	PG4	C1-C2-O2-C3
9	A	372	PEG	O2-C3-C4-O4
5	A	301	GOL	C1-C2-C3-O3
5	D	109	GOL	O1-C1-C2-C3
7	C	321	PG4	C8-C7-O4-C6
7	C	321	PG4	C1-C2-O2-C3
10	B	138	PE8	C11-C12-O13-C14
10	C	335	PE8	C2-C3-O4-C5
7	A	368	PG4	C3-C4-O3-C5
10	B	102	PE8	C24-C23-O22-C21
7	A	321	PG4	C8-C7-O4-C6
7	C	324	PG4	O2-C3-C4-O3
5	D	109	GOL	O1-C1-C2-O2
5	E	113	GOL	O1-C1-C2-O2
7	A	368	PG4	C5-C6-O4-C7
10	B	136	PE8	C14-C15-O16-C17
10	B	138	PE8	O4-C5-C6-O7
7	A	319	PG4	C6-C5-O3-C4
7	D	103	PG4	C5-C6-O4-C7
10	A	342	PE8	C11-C12-O13-C14
9	A	372	PEG	O1-C1-C2-O2
7	C	322	PG4	O2-C3-C4-O3
7	D	116	PG4	O3-C5-C6-O4
10	A	343	PE8	O13-C14-C15-O16

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

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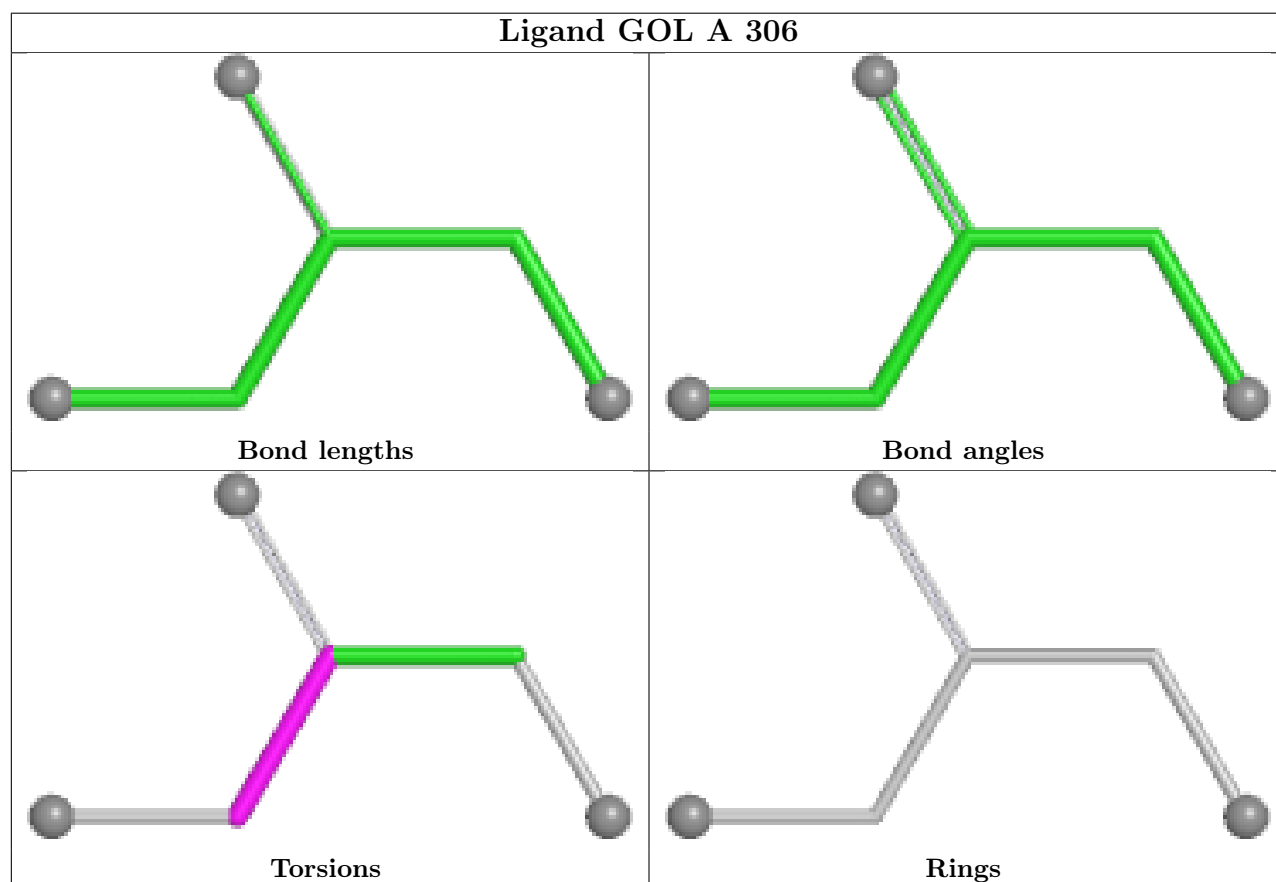
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	366	PG4	1	0
10	E	109	PE8	2	0
7	A	365	PG4	1	0
7	F	105	PG4	1	0
9	B	157	PEG	1	0
7	C	321	PG4	2	0
7	E	115	PG4	1	0
5	A	363	GOL	1	0
5	A	303	GOL	1	0
5	A	310	GOL	1	0
5	D	108	GOL	1	0
7	B	101	PG4	1	0
7	C	324	PG4	1	0
7	E	106	PG4	1	0
11	D	102	EDO	2	1
9	C	331	PEG	1	0
5	C	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
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

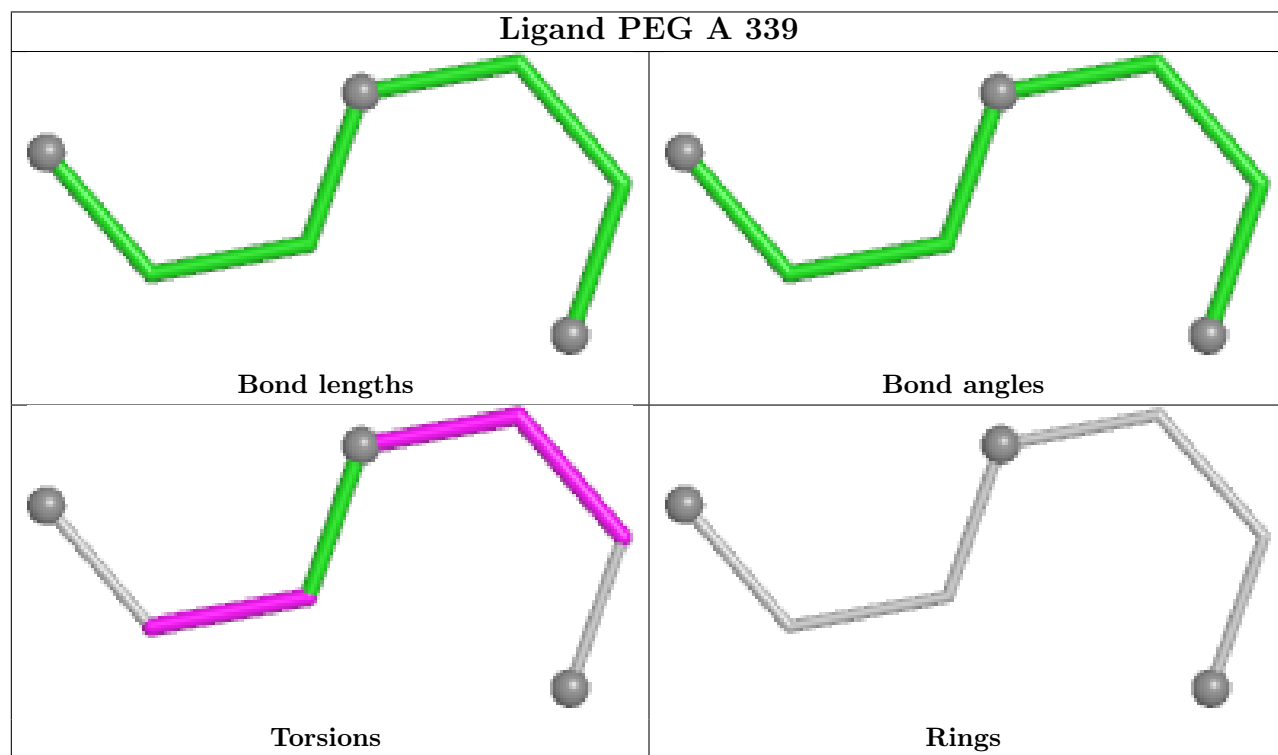
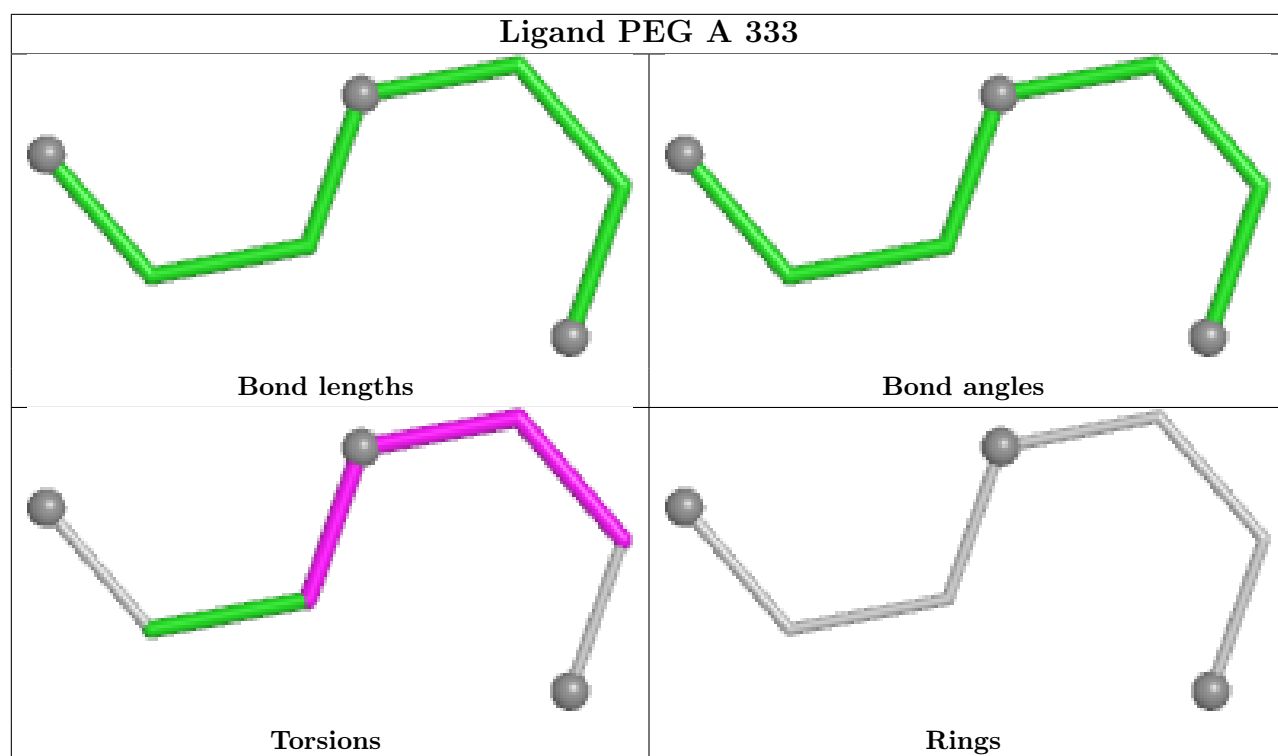
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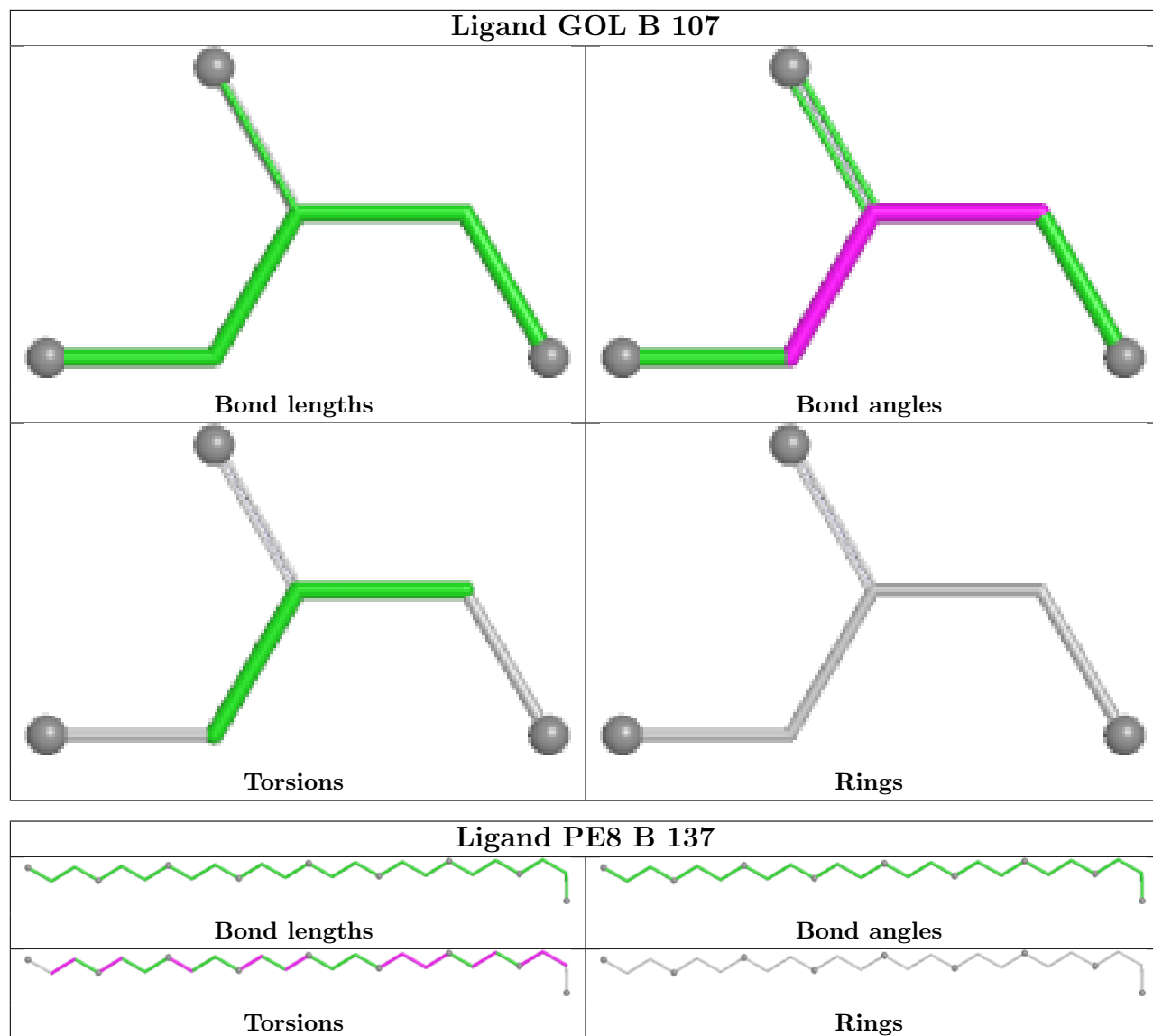
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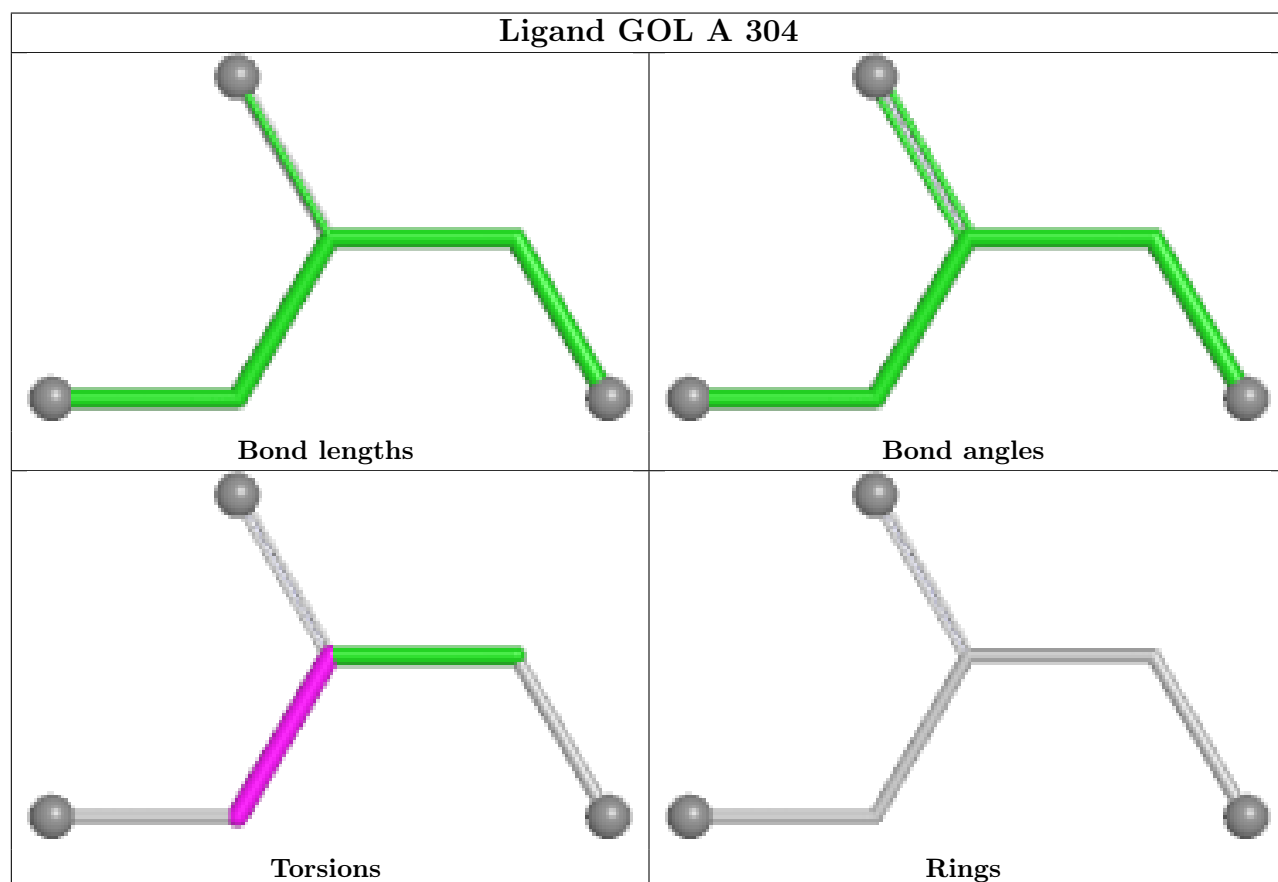
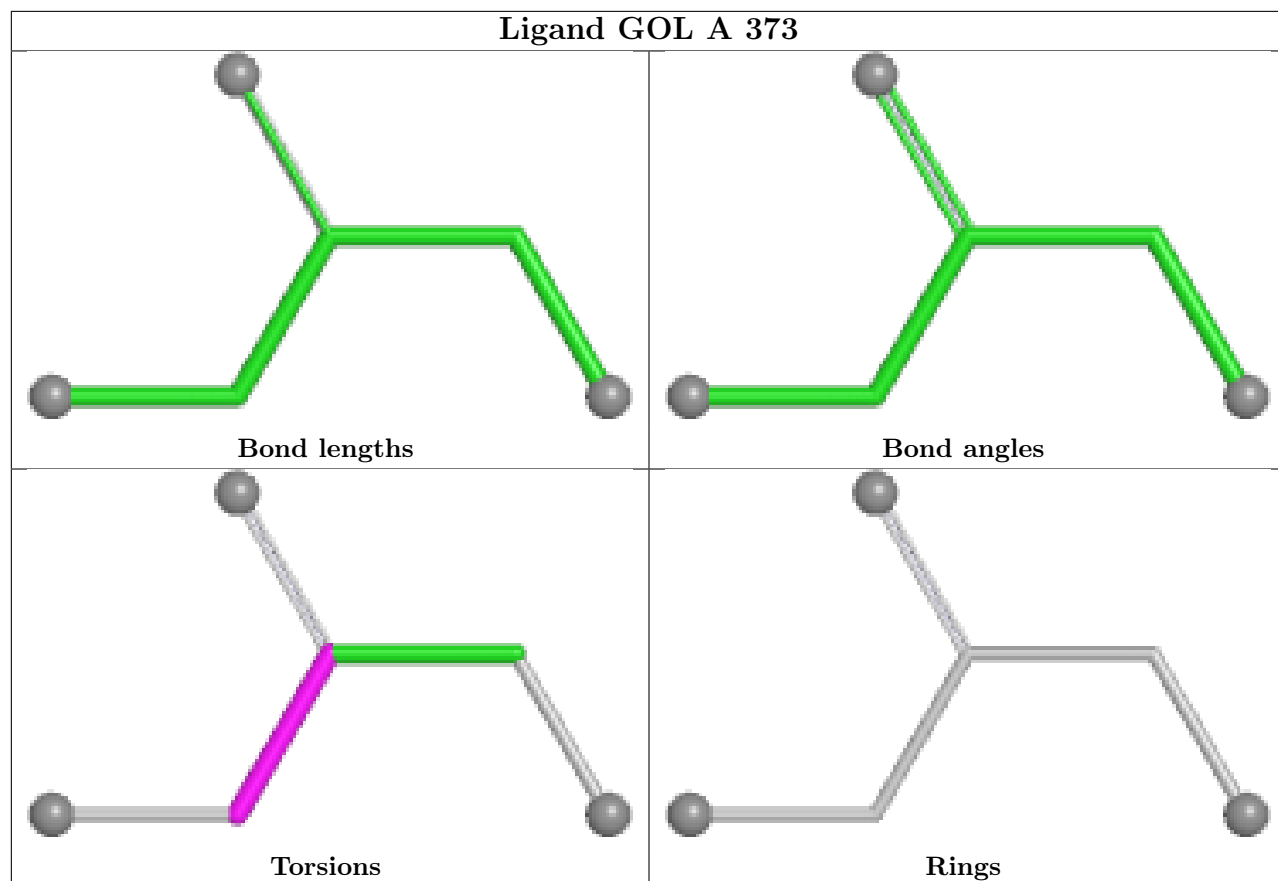
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	138	PE8	2	0
5	A	347	GOL	1	0
7	C	302	PG4	2	0
9	A	331	PEG	2	0
9	A	336	PEG	1	0
7	B	125	PG4	1	0
9	C	333	PEG	1	0

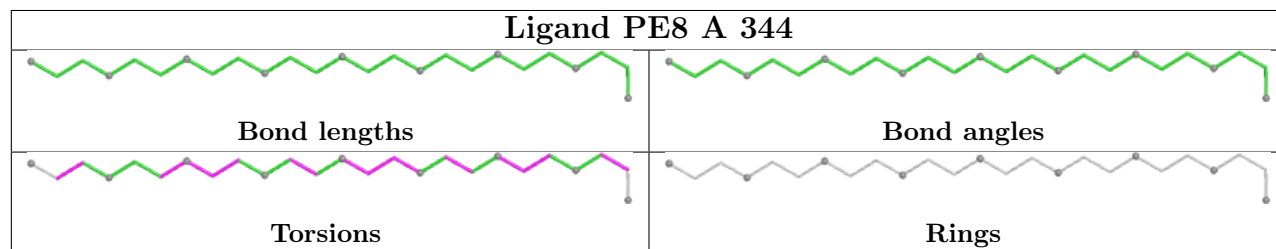
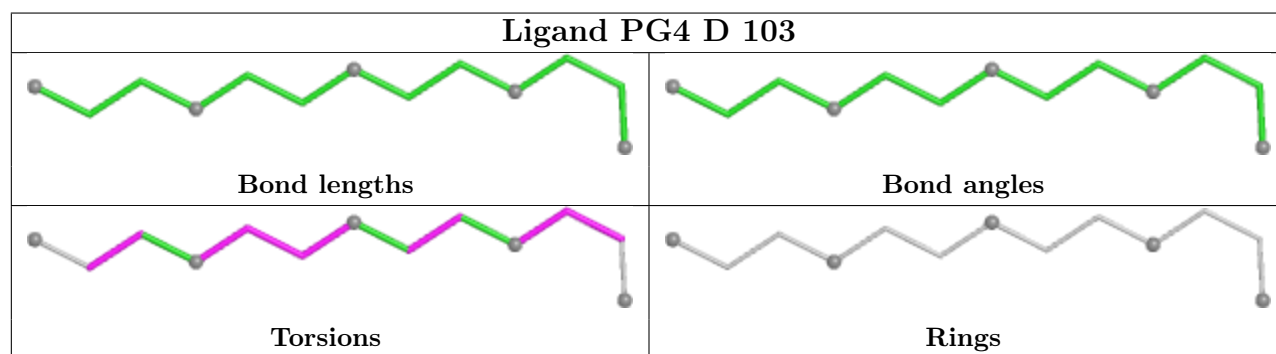
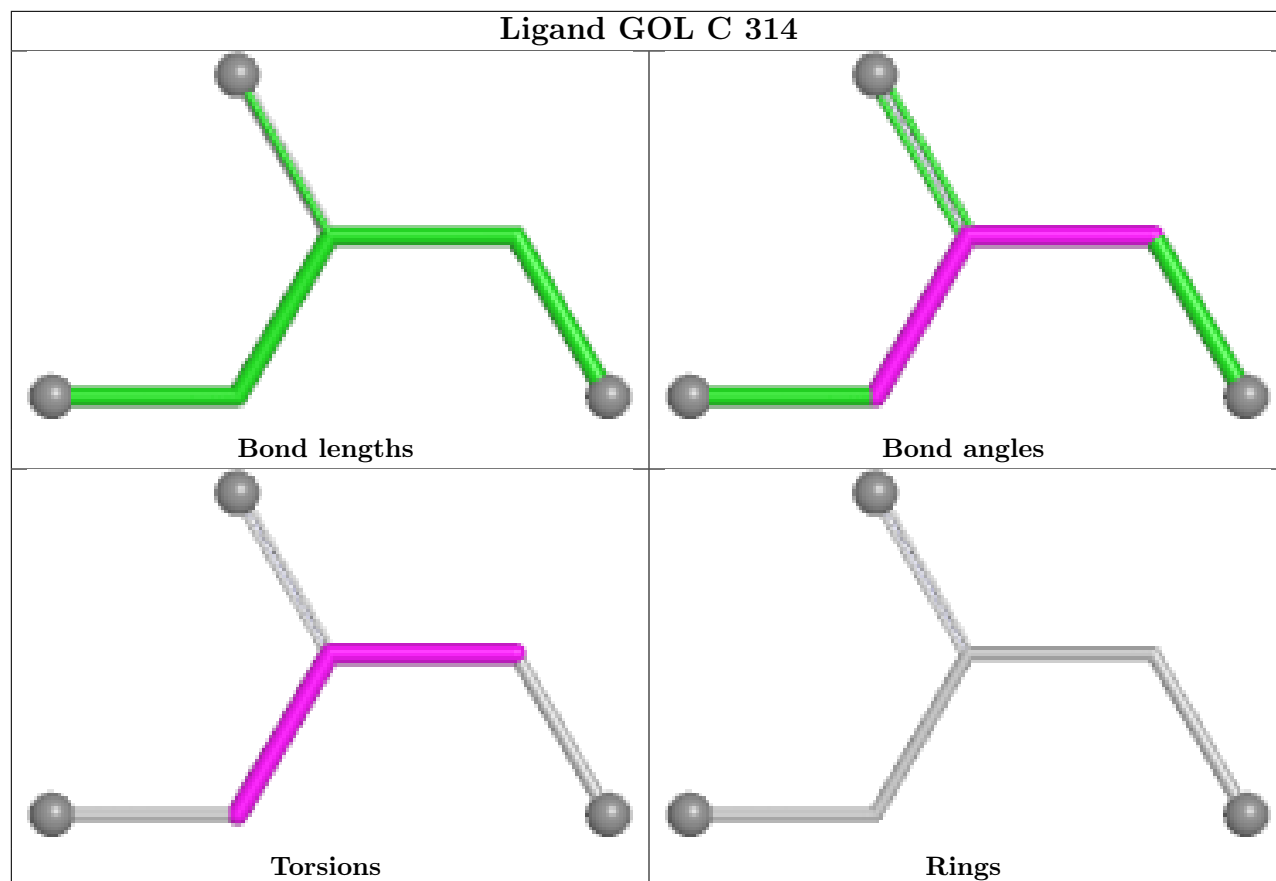
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

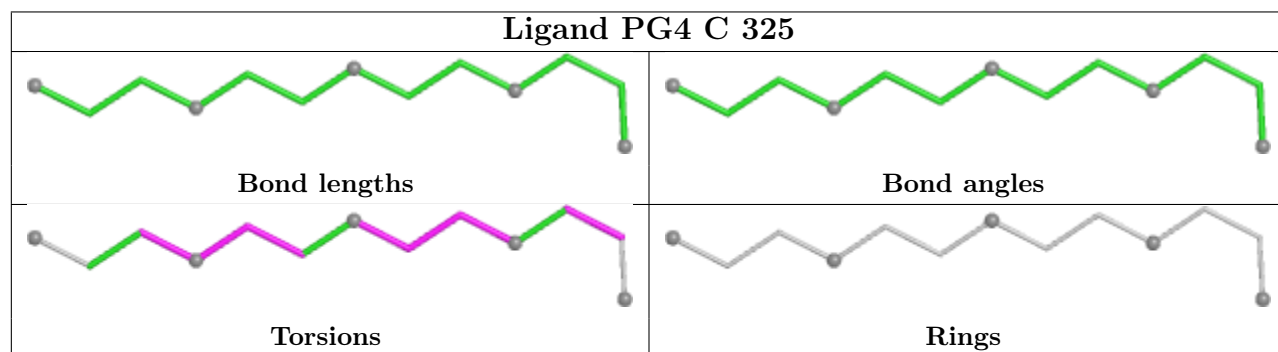
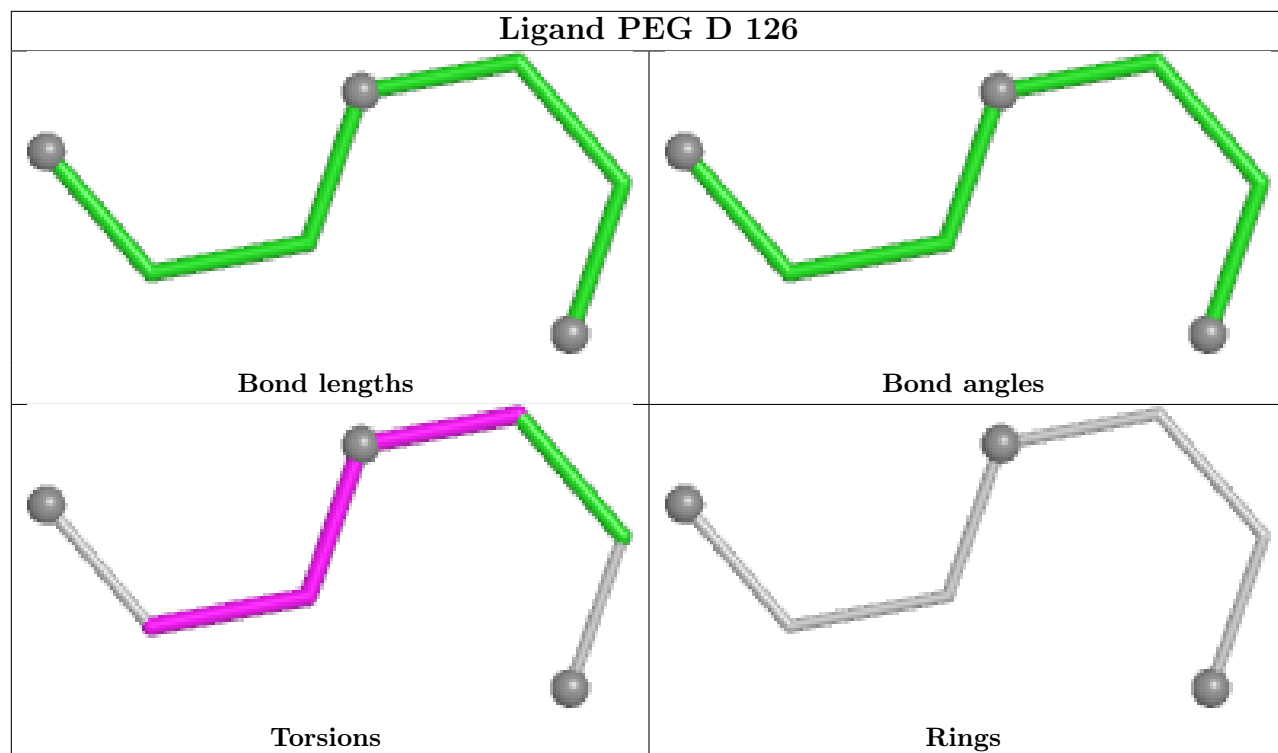


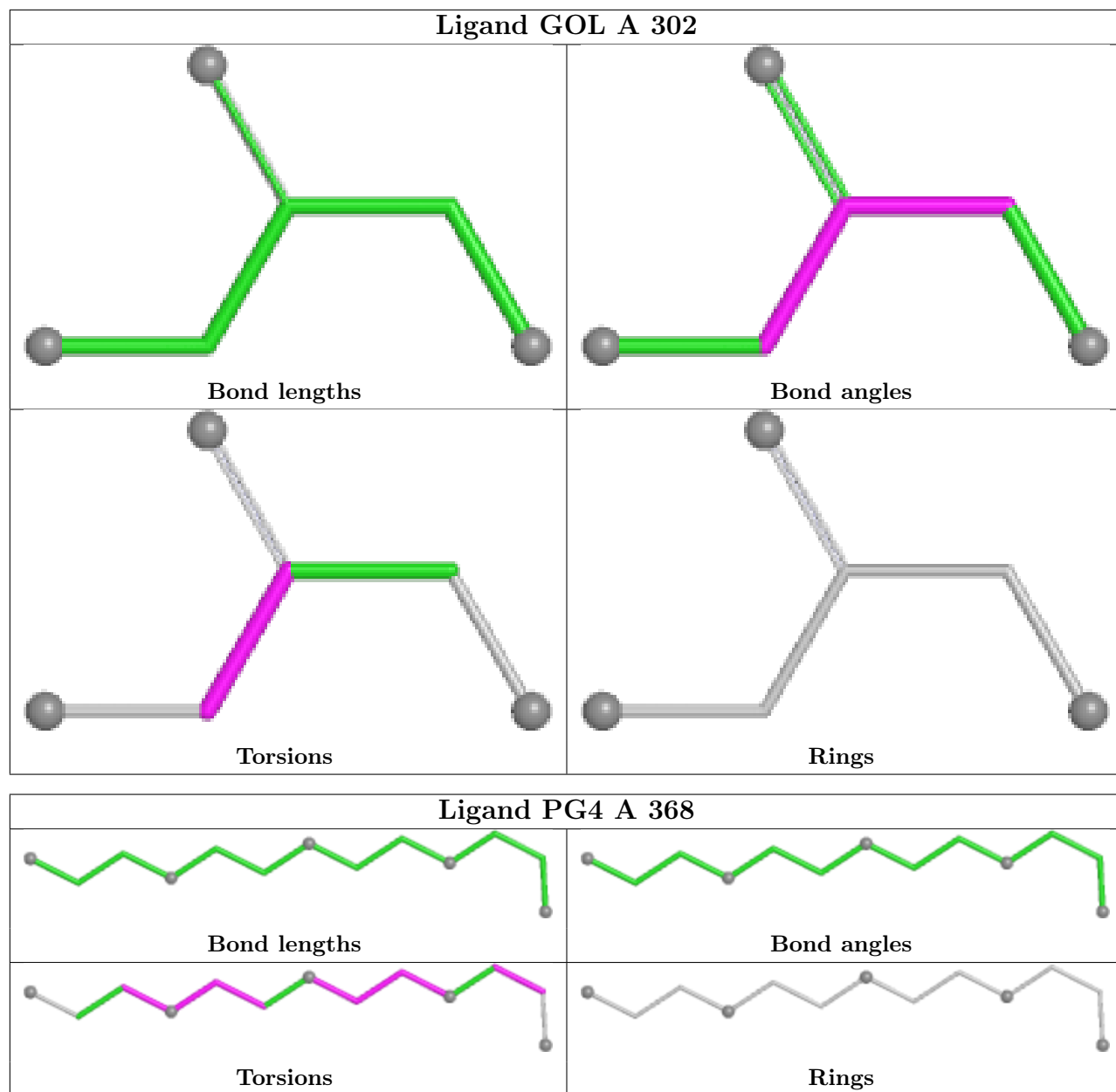


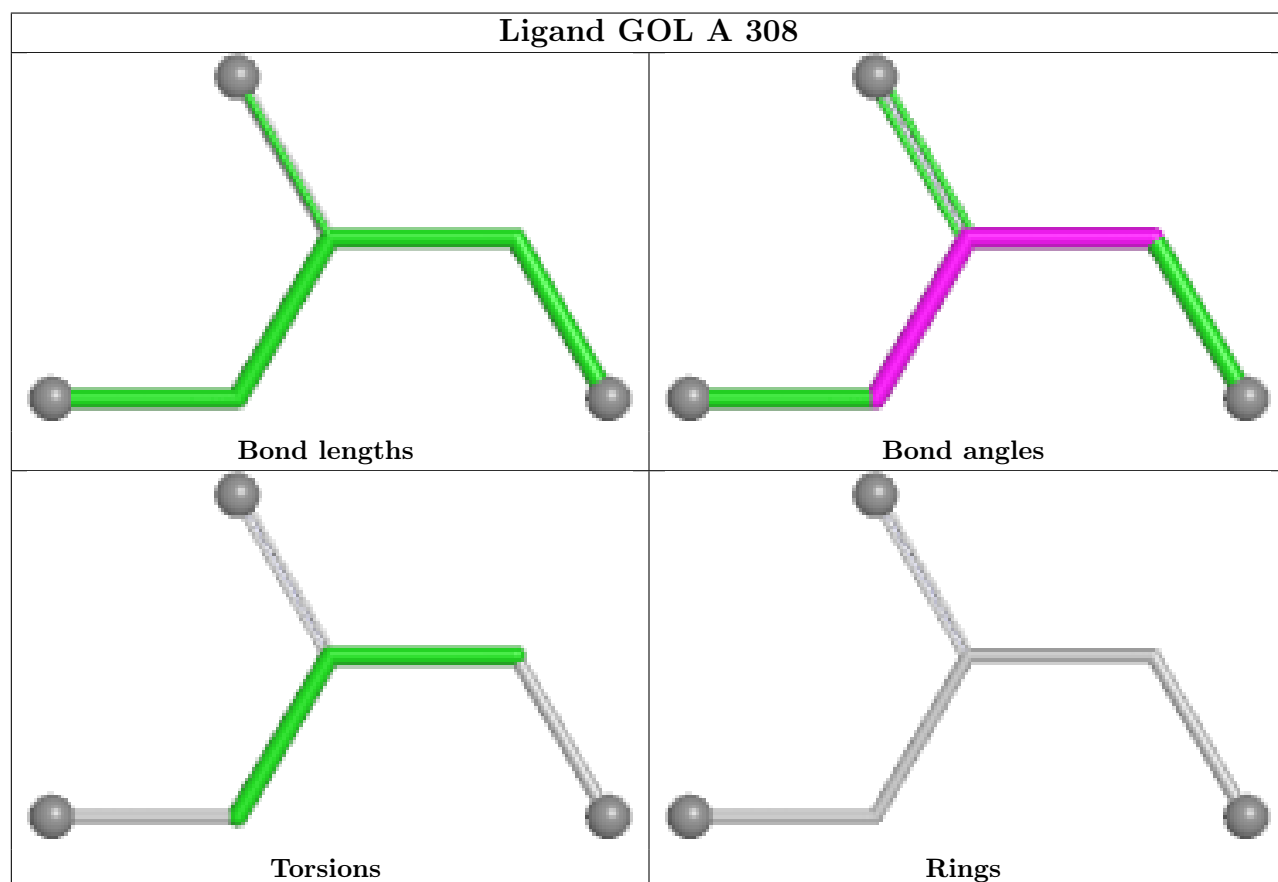
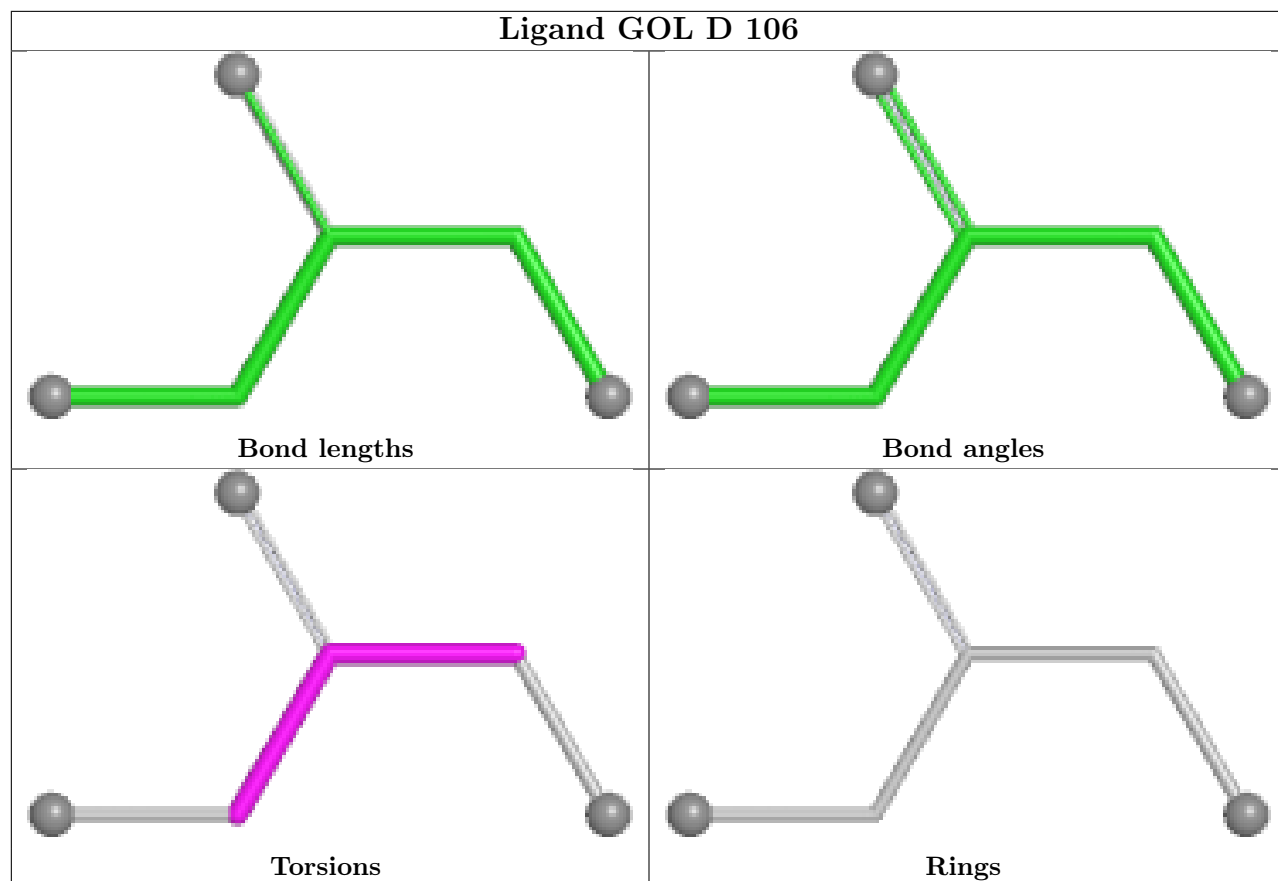


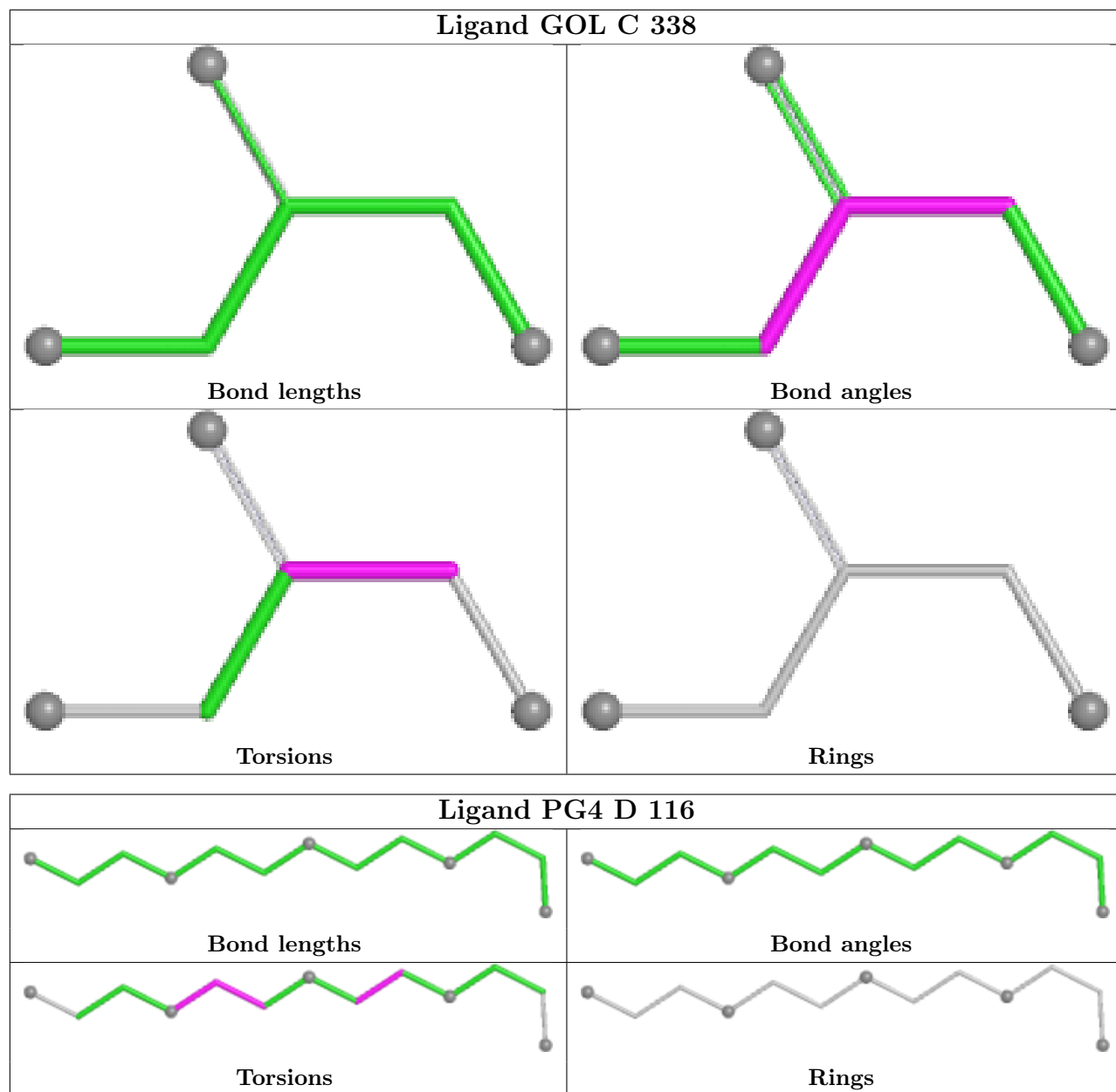


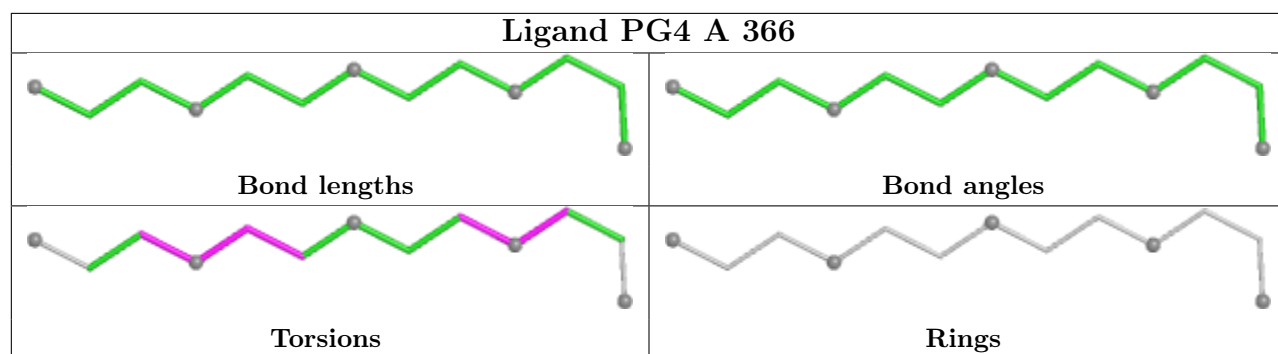
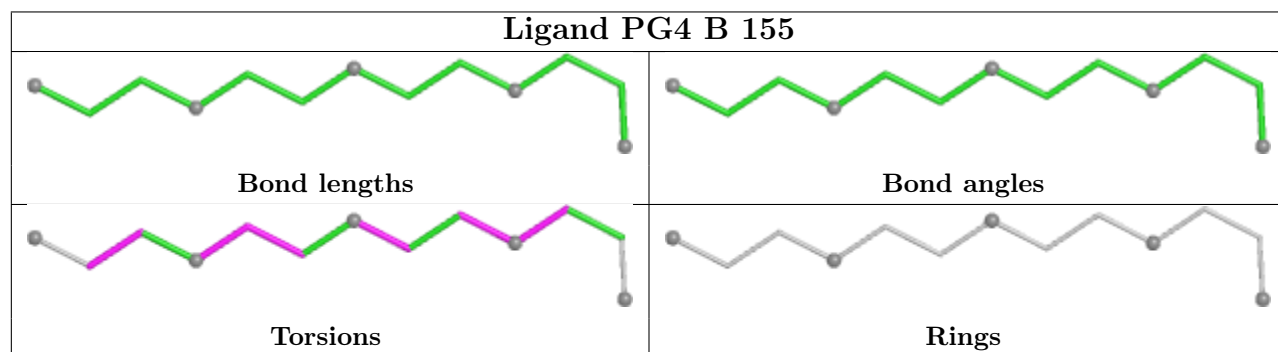
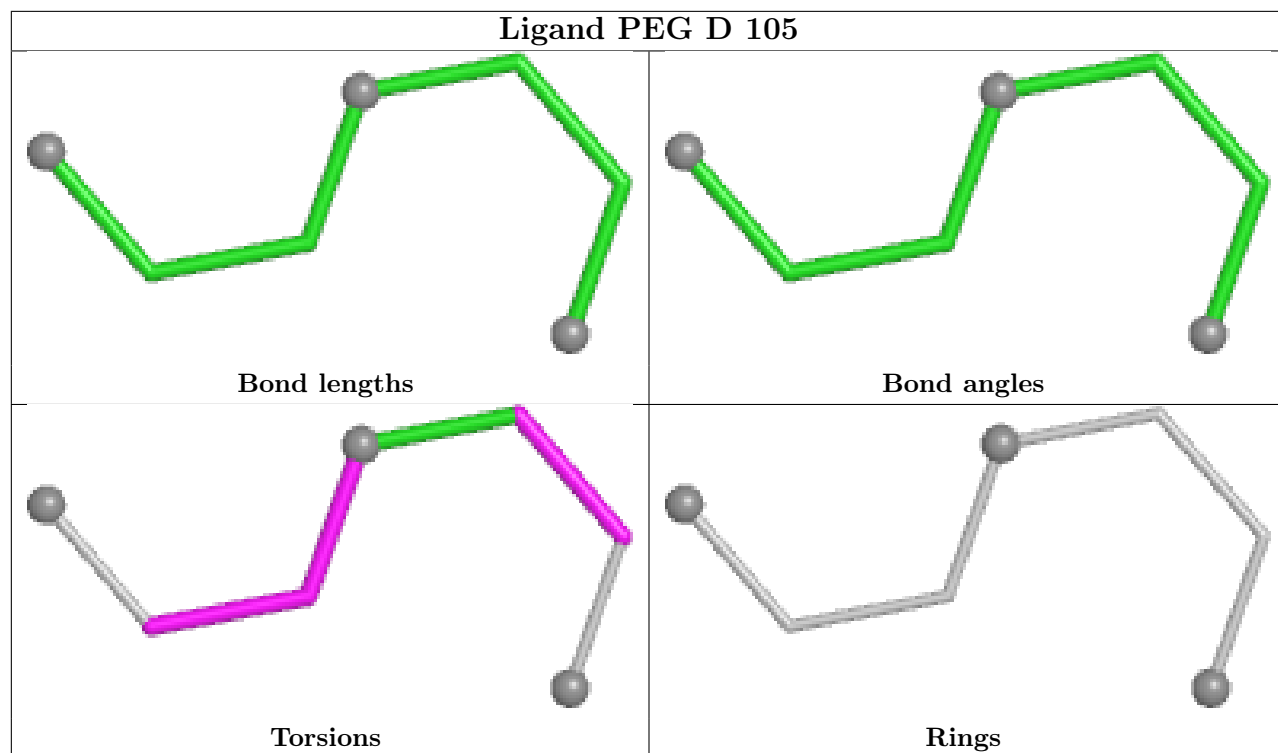


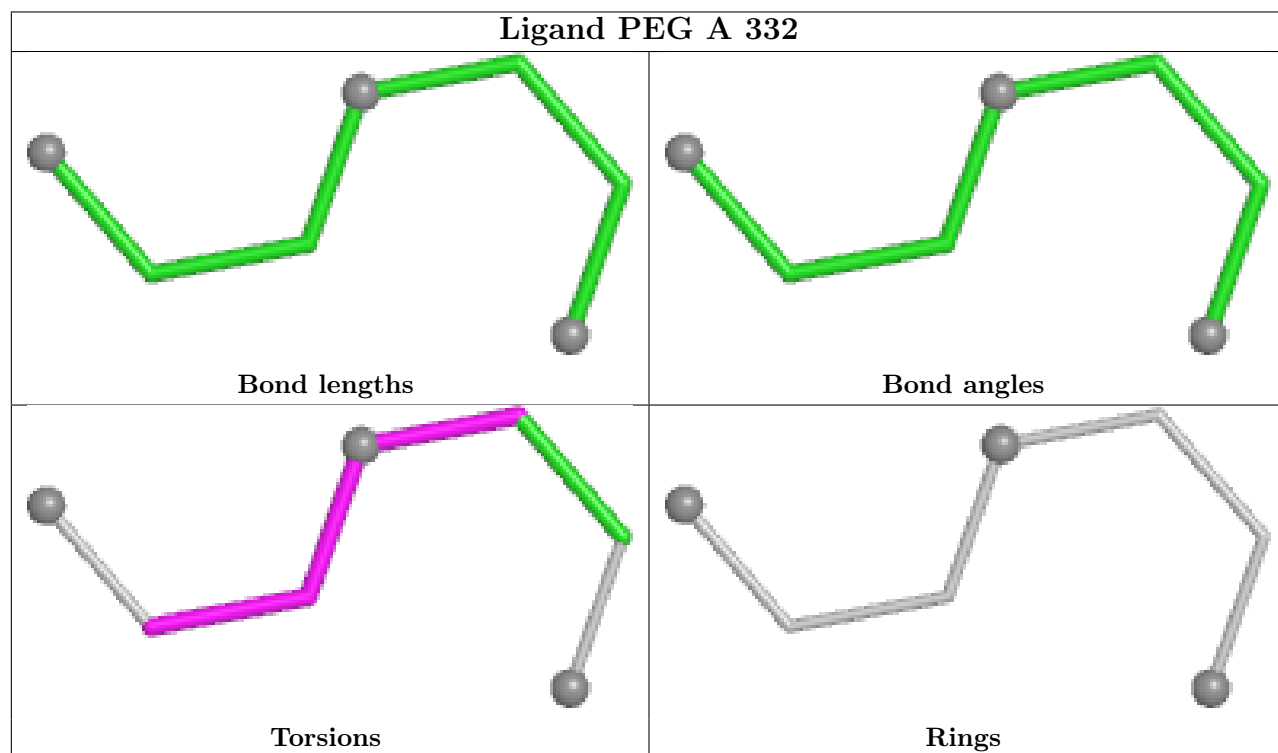
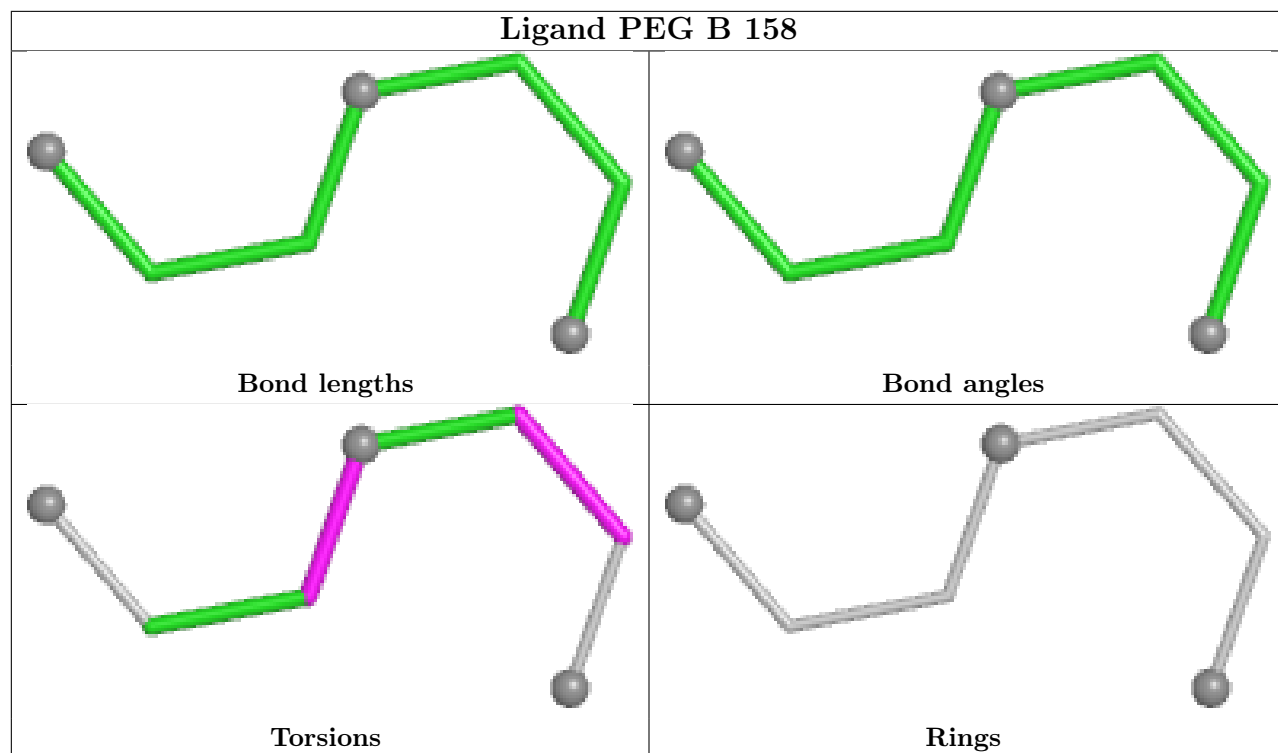


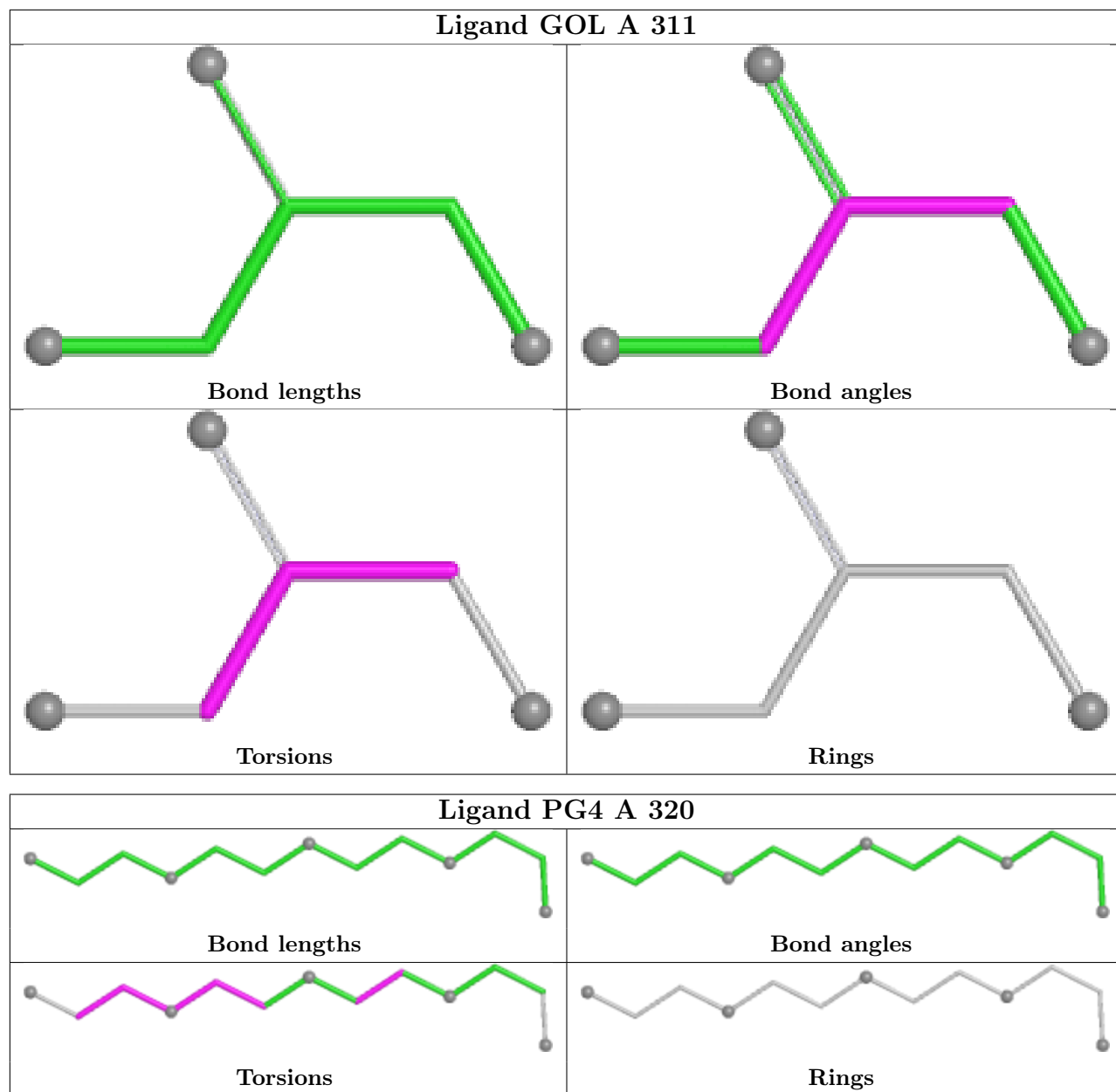


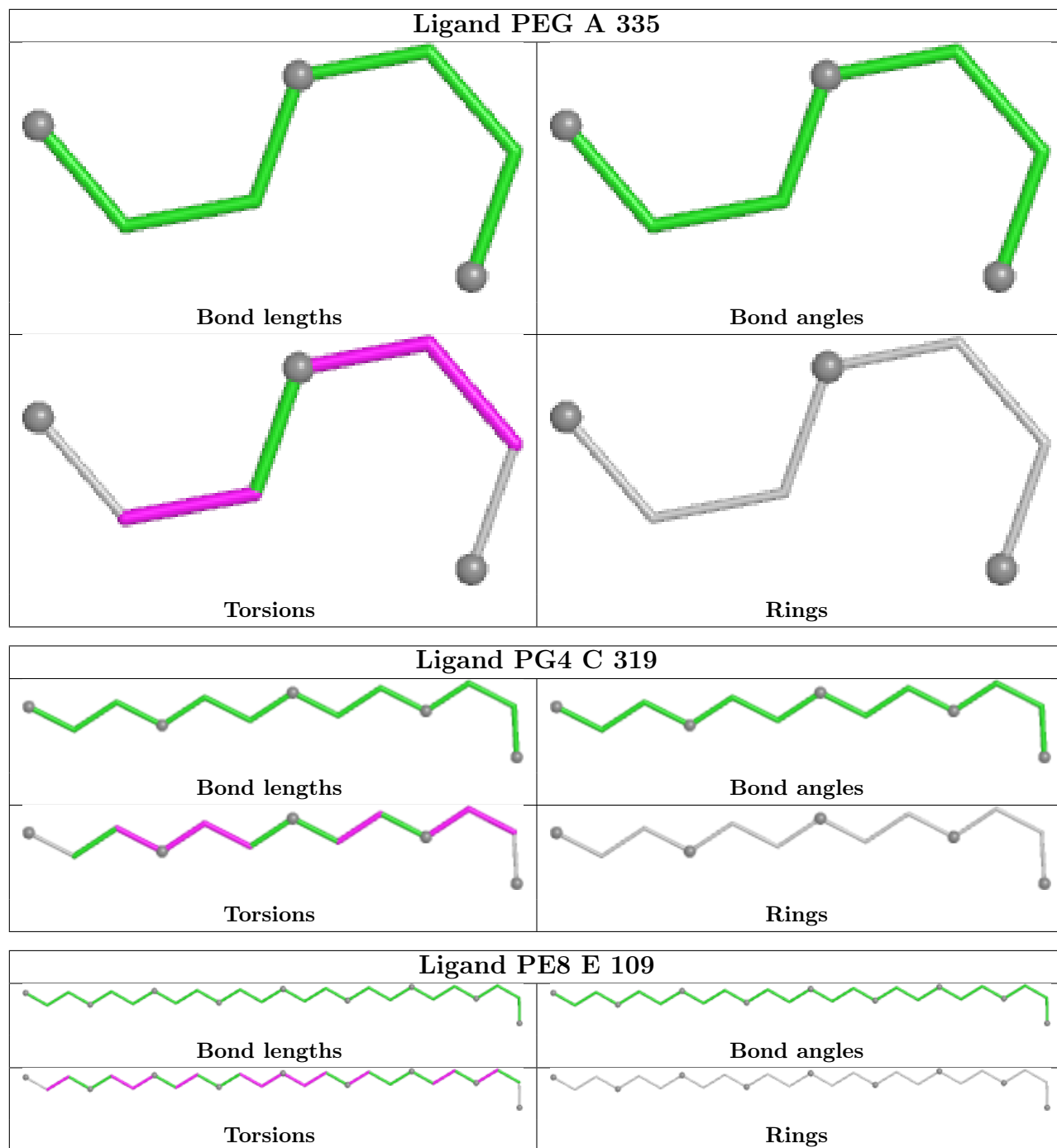


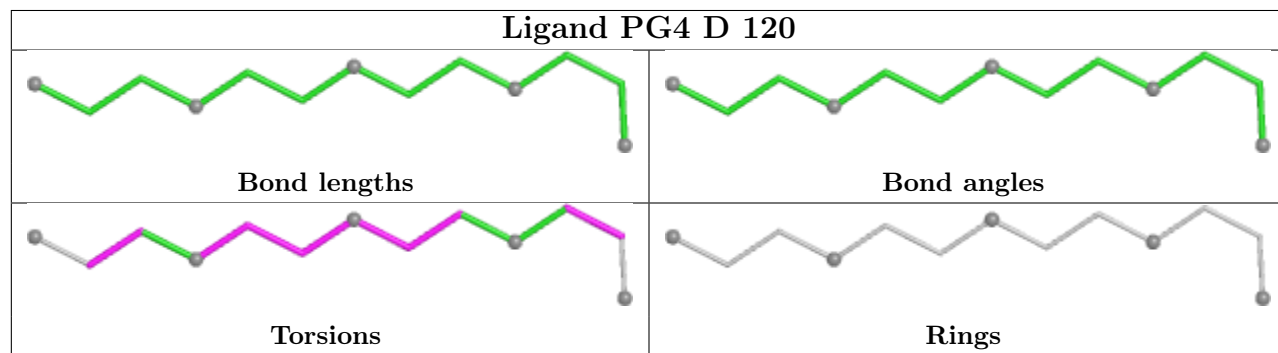
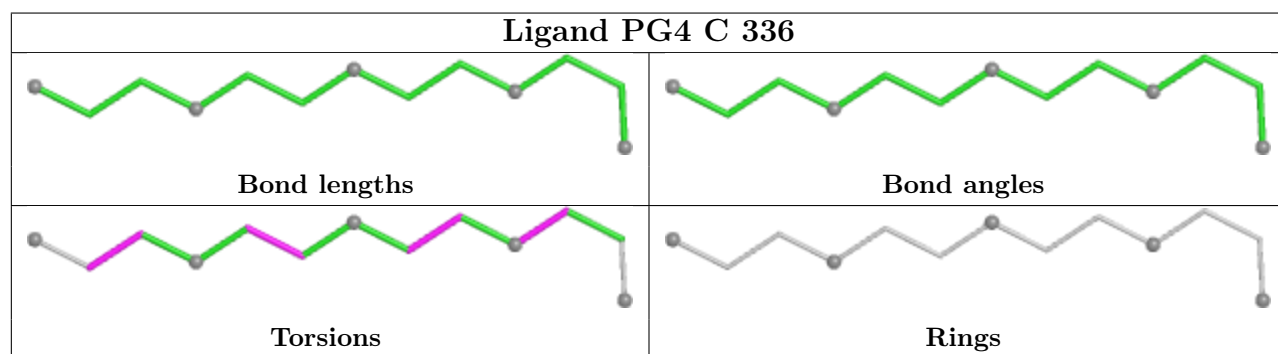
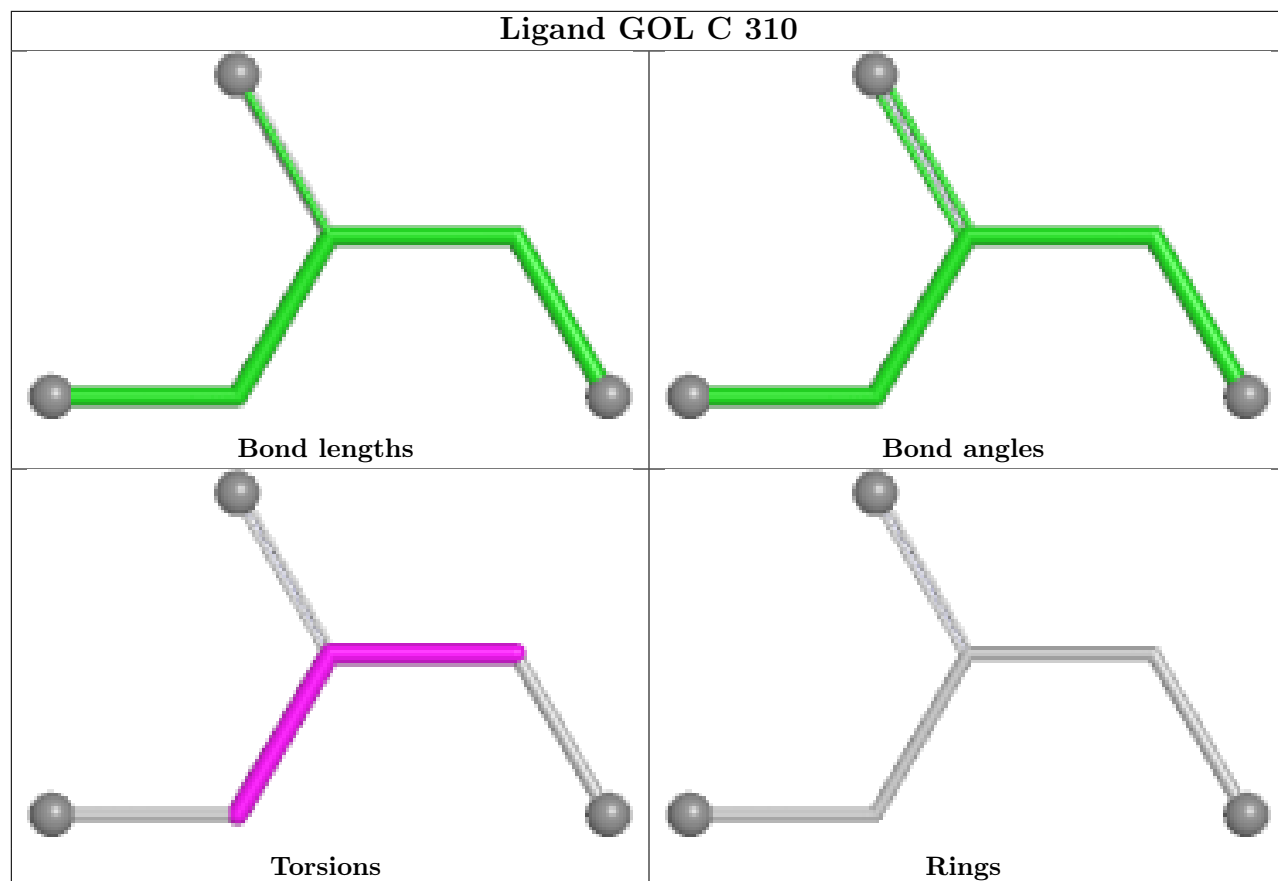


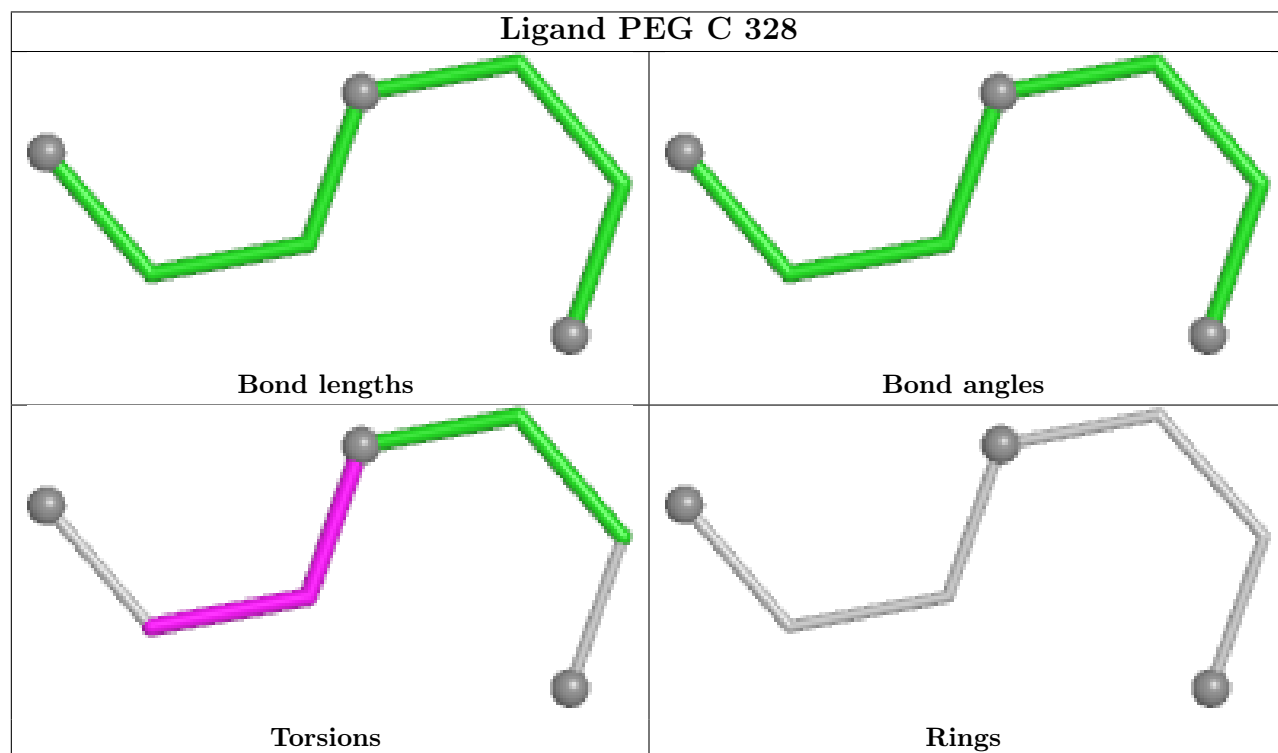
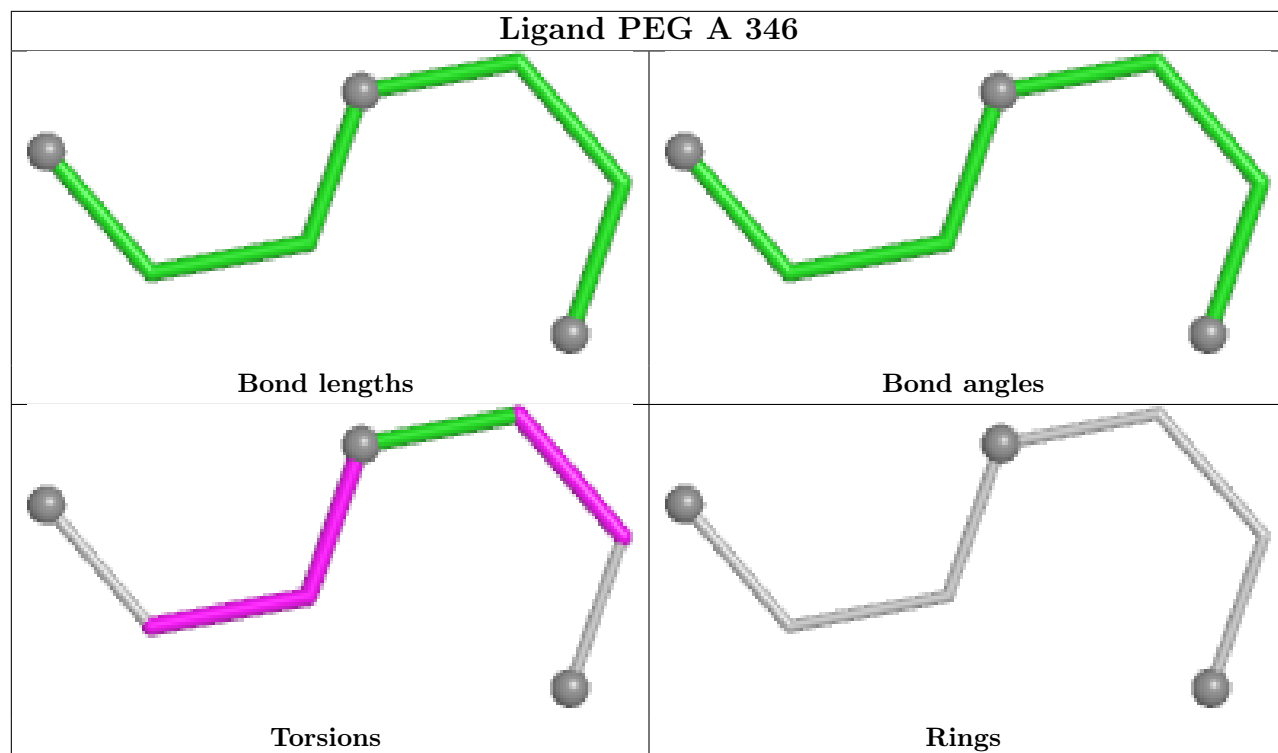


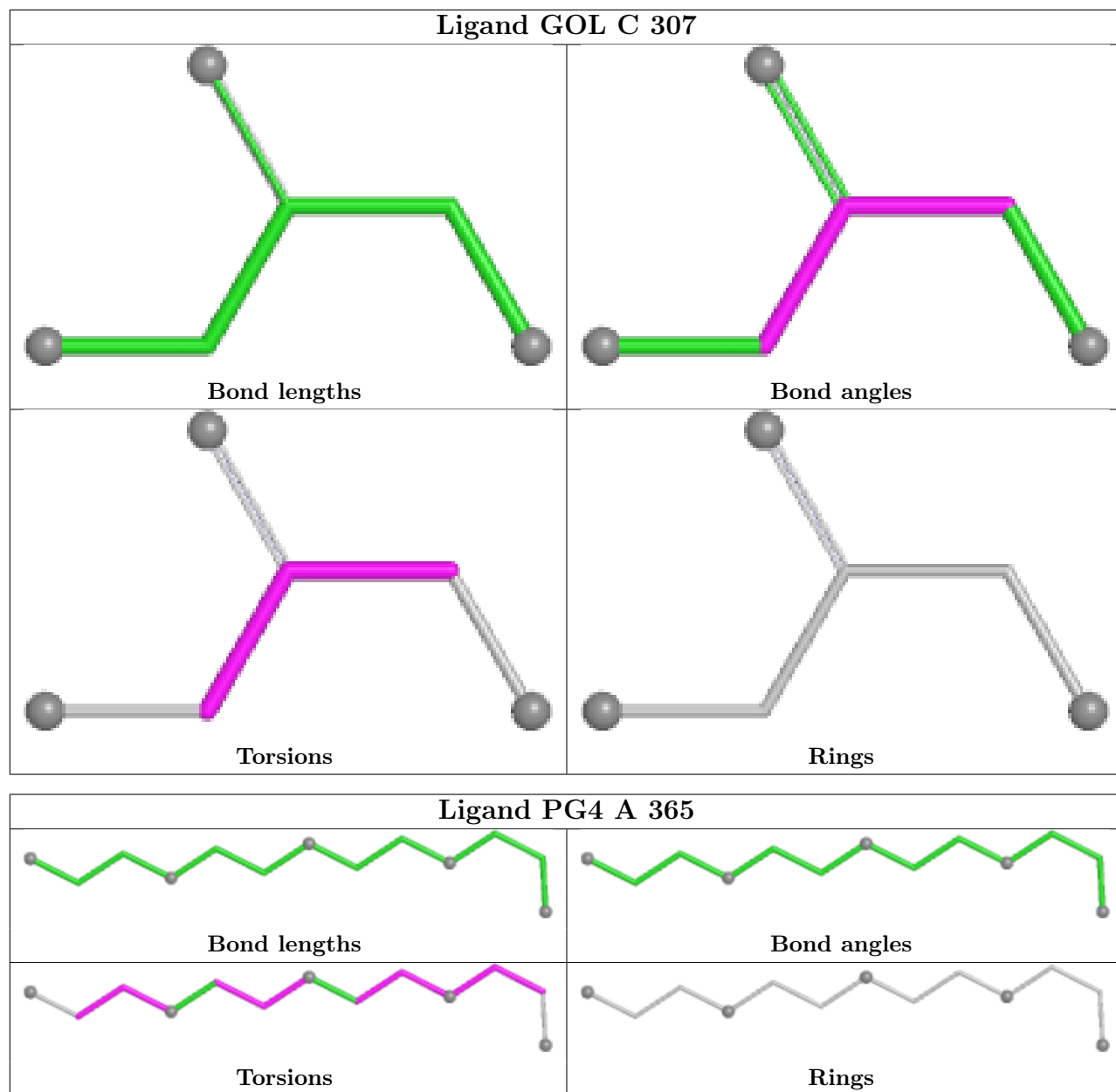


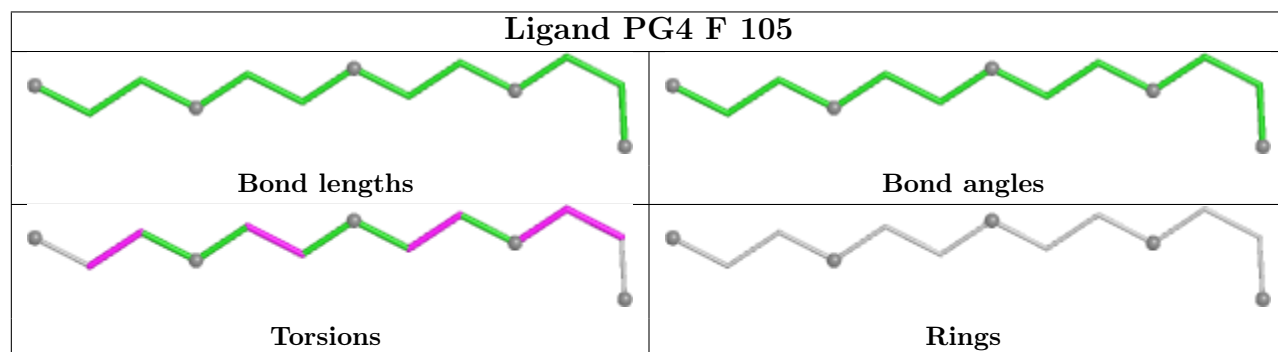
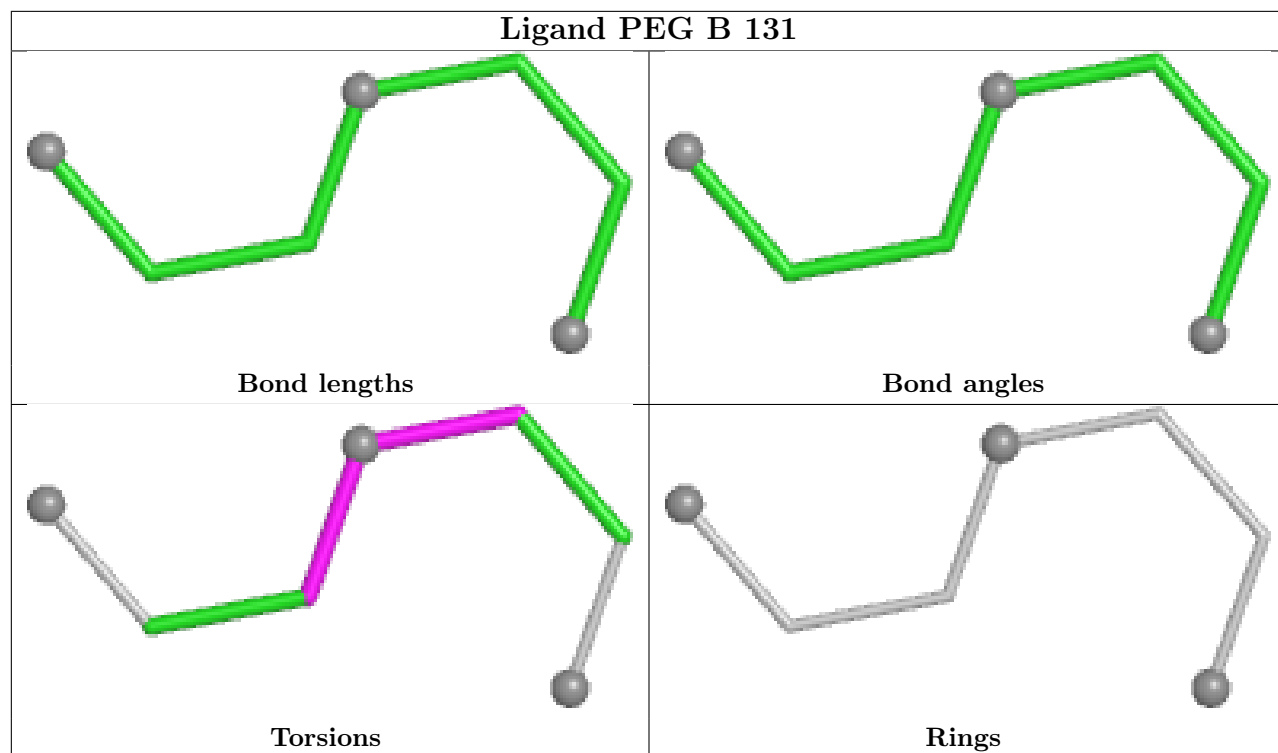


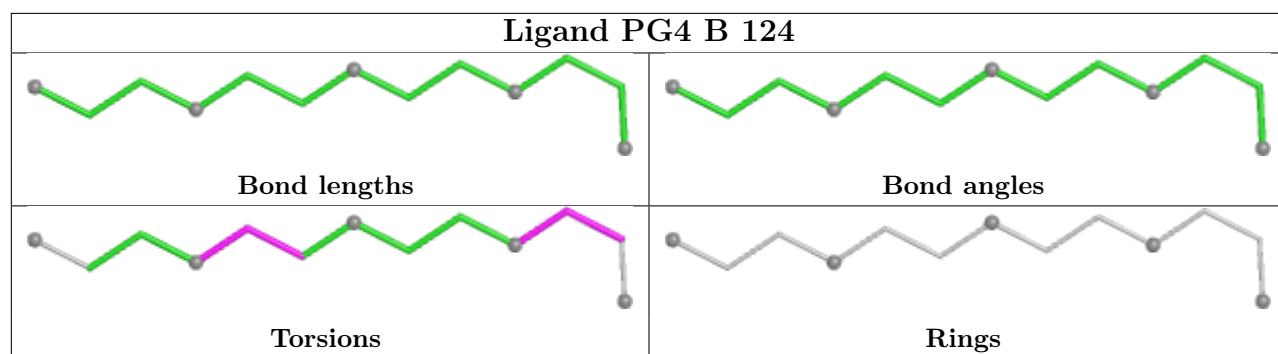
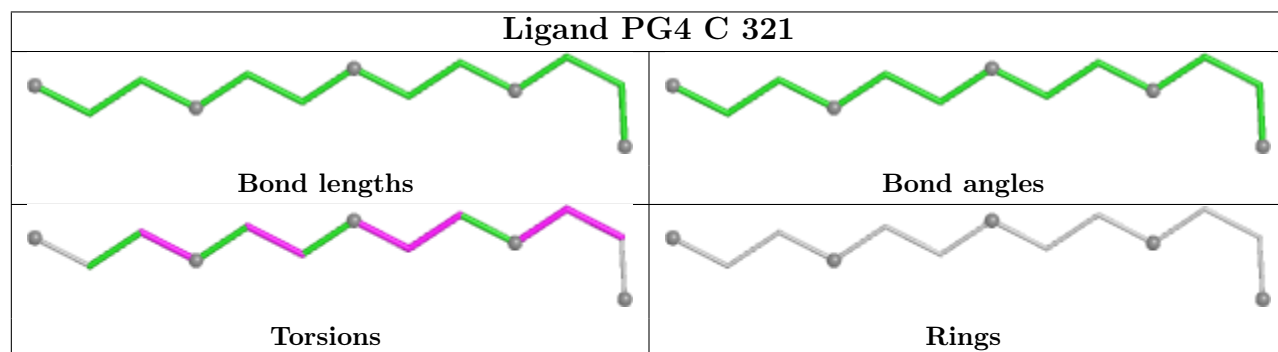
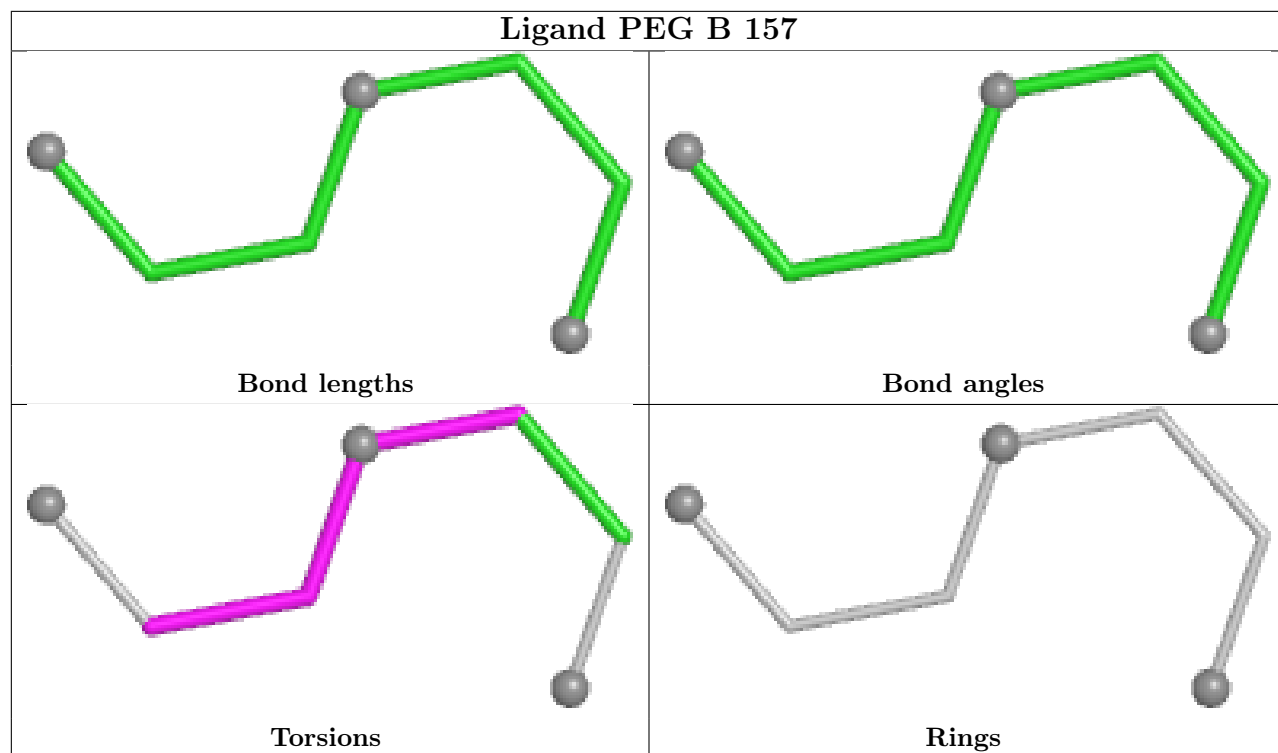


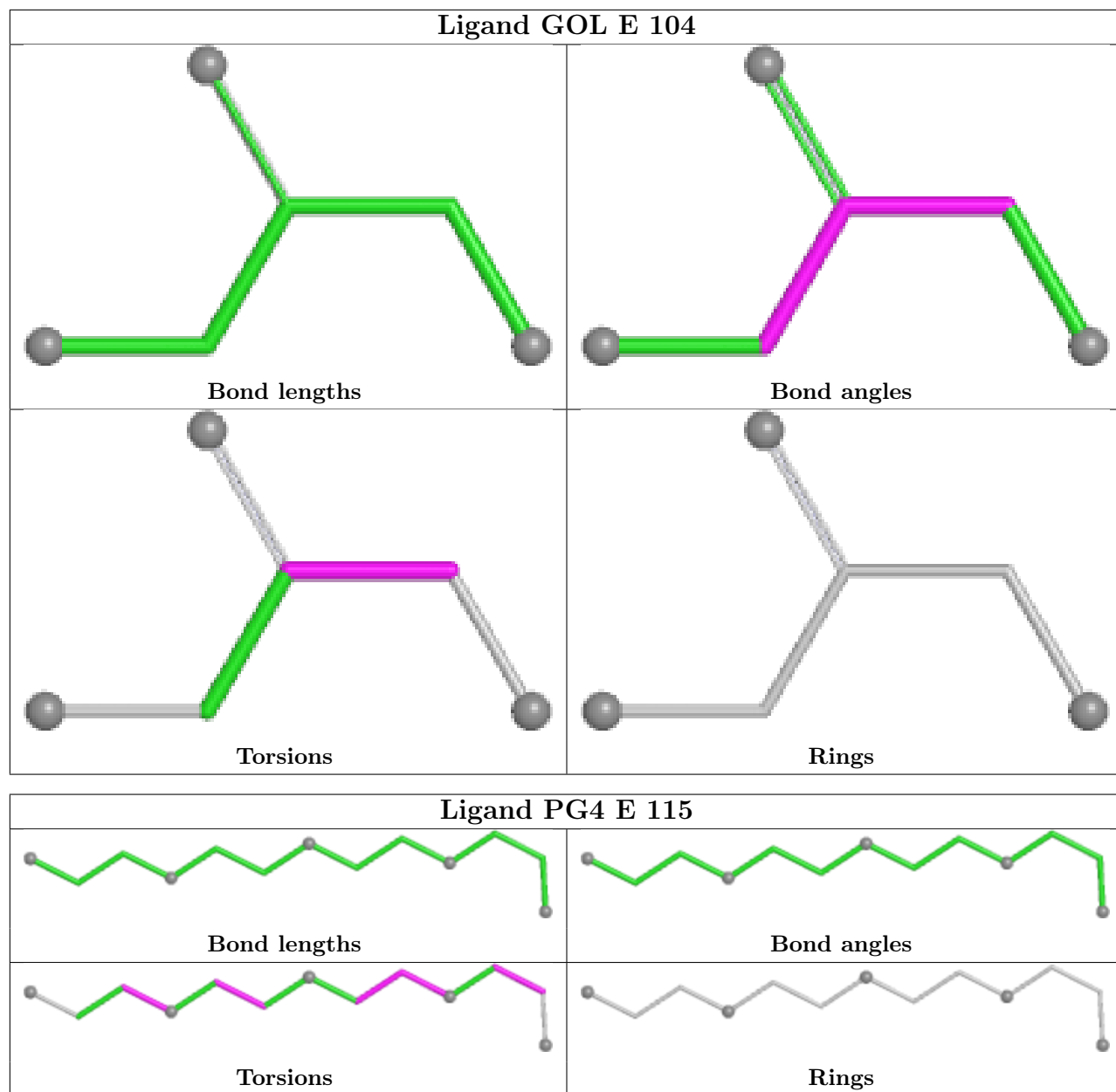


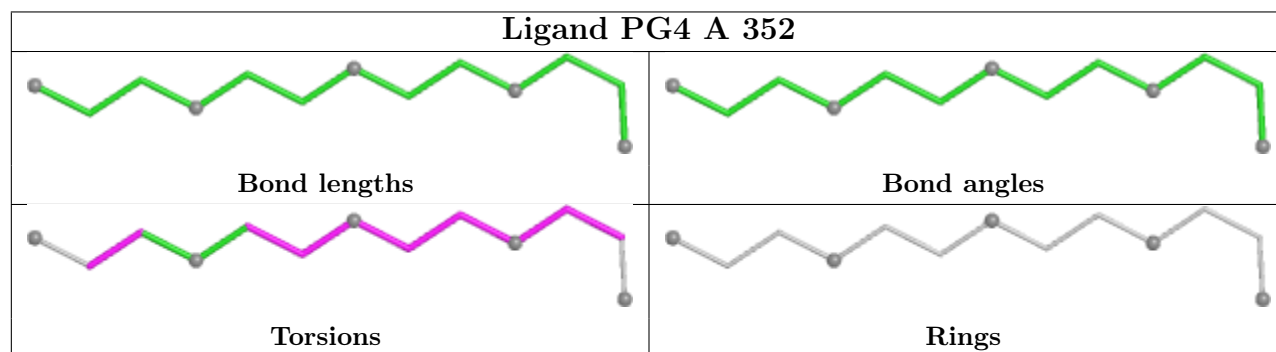
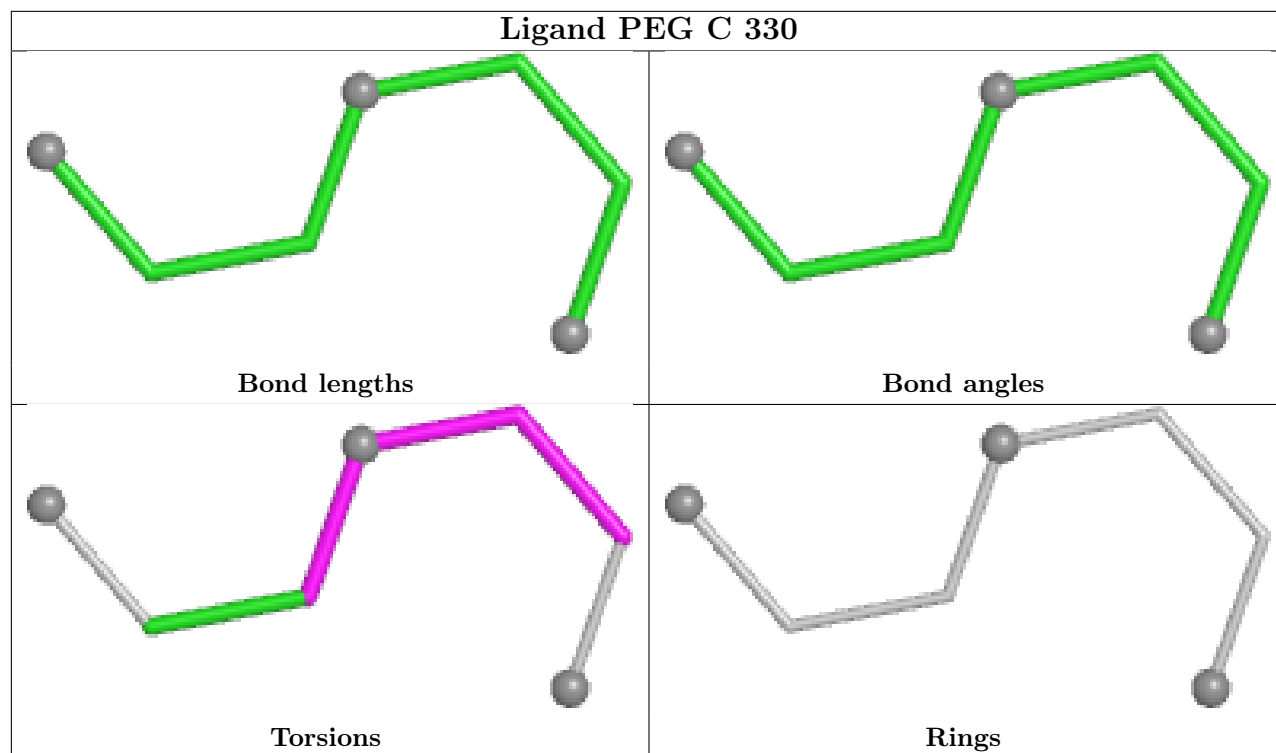


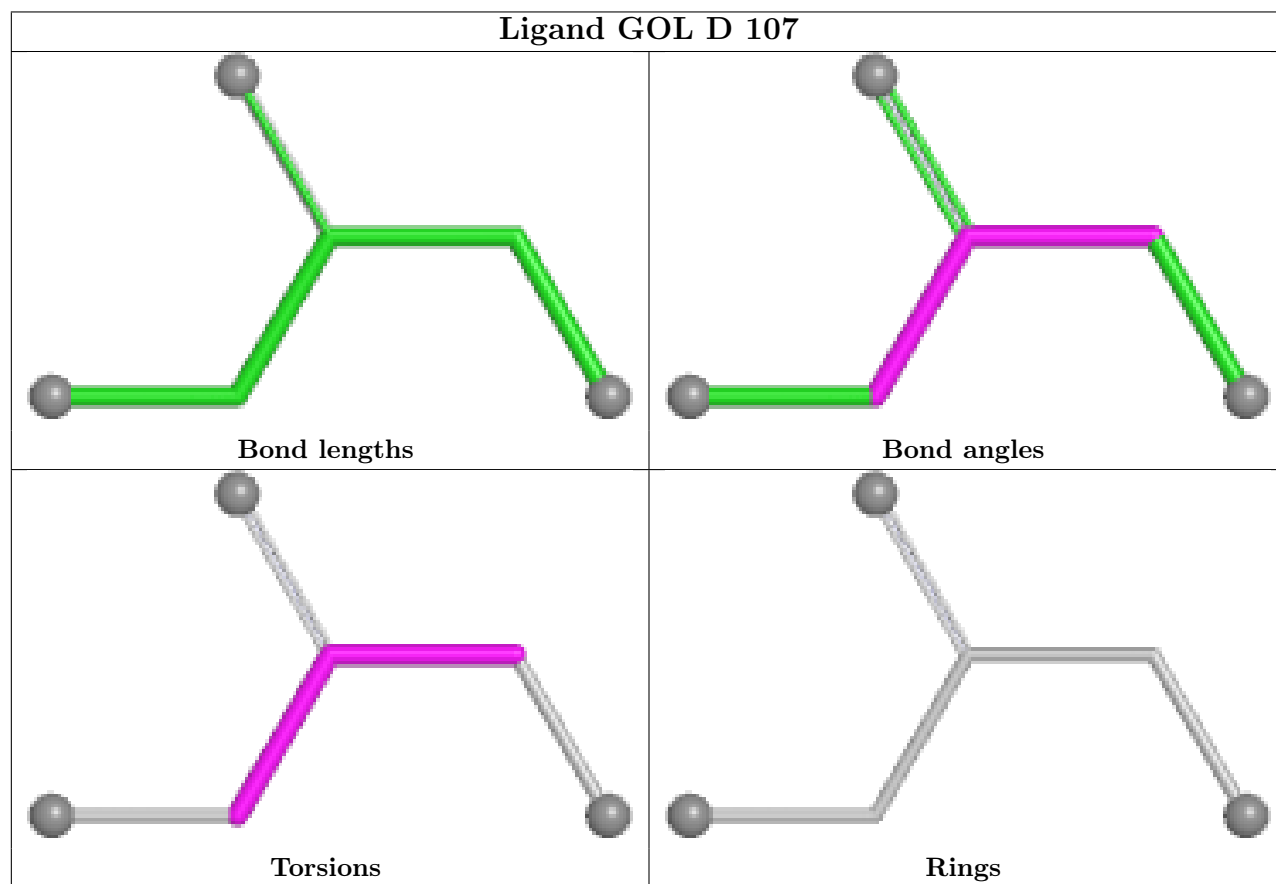
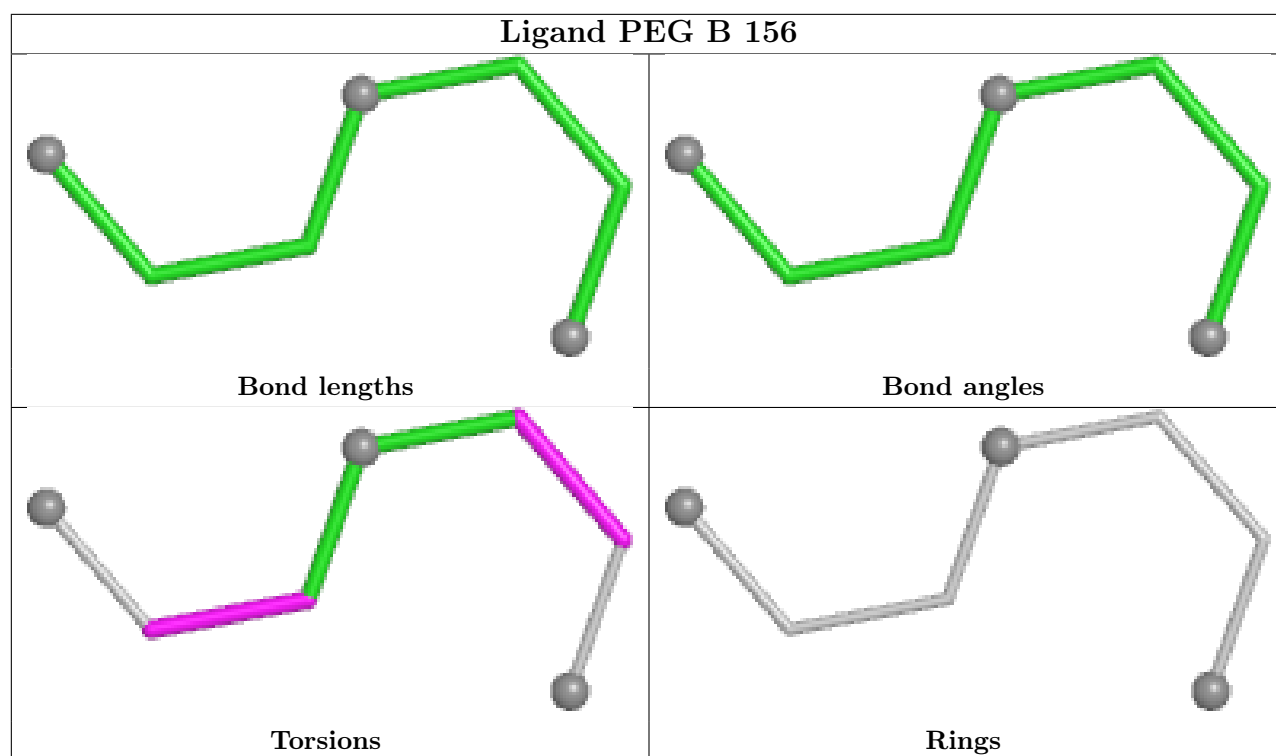


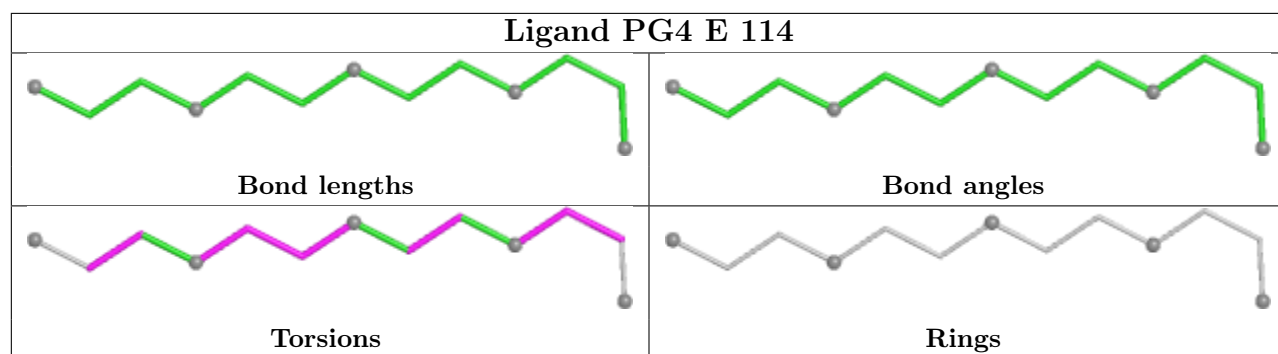
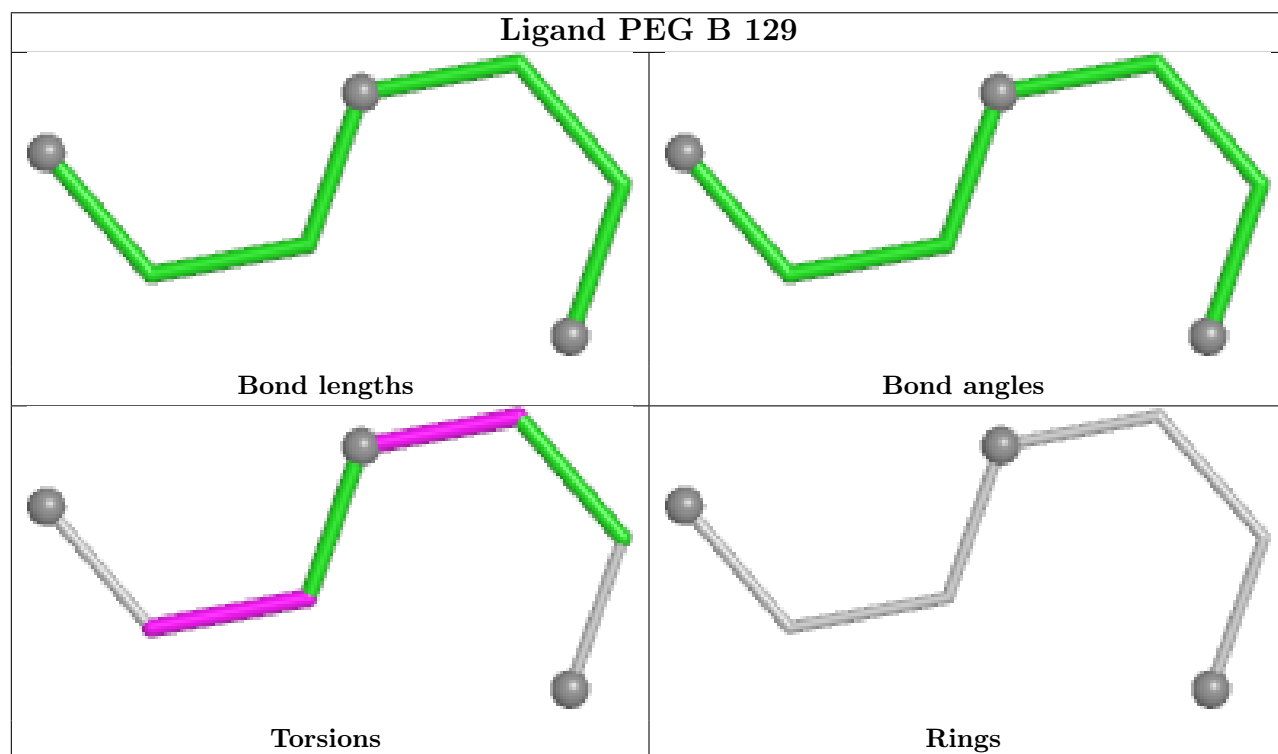
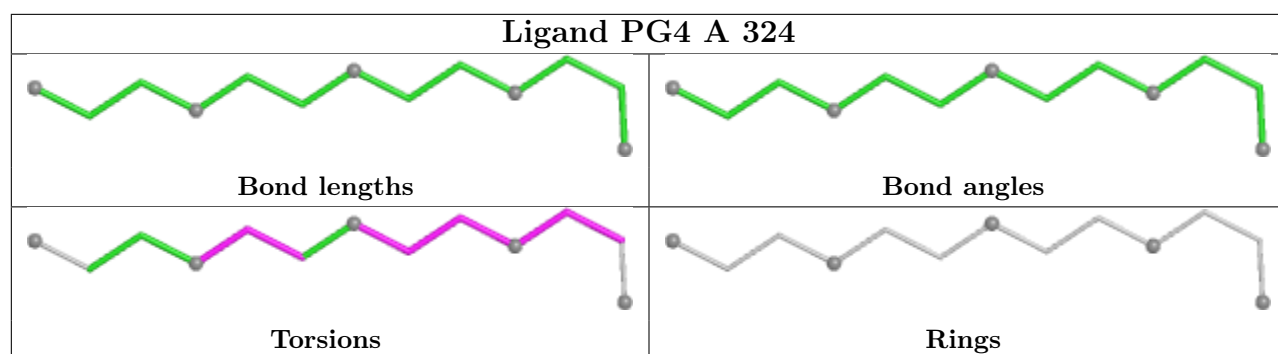


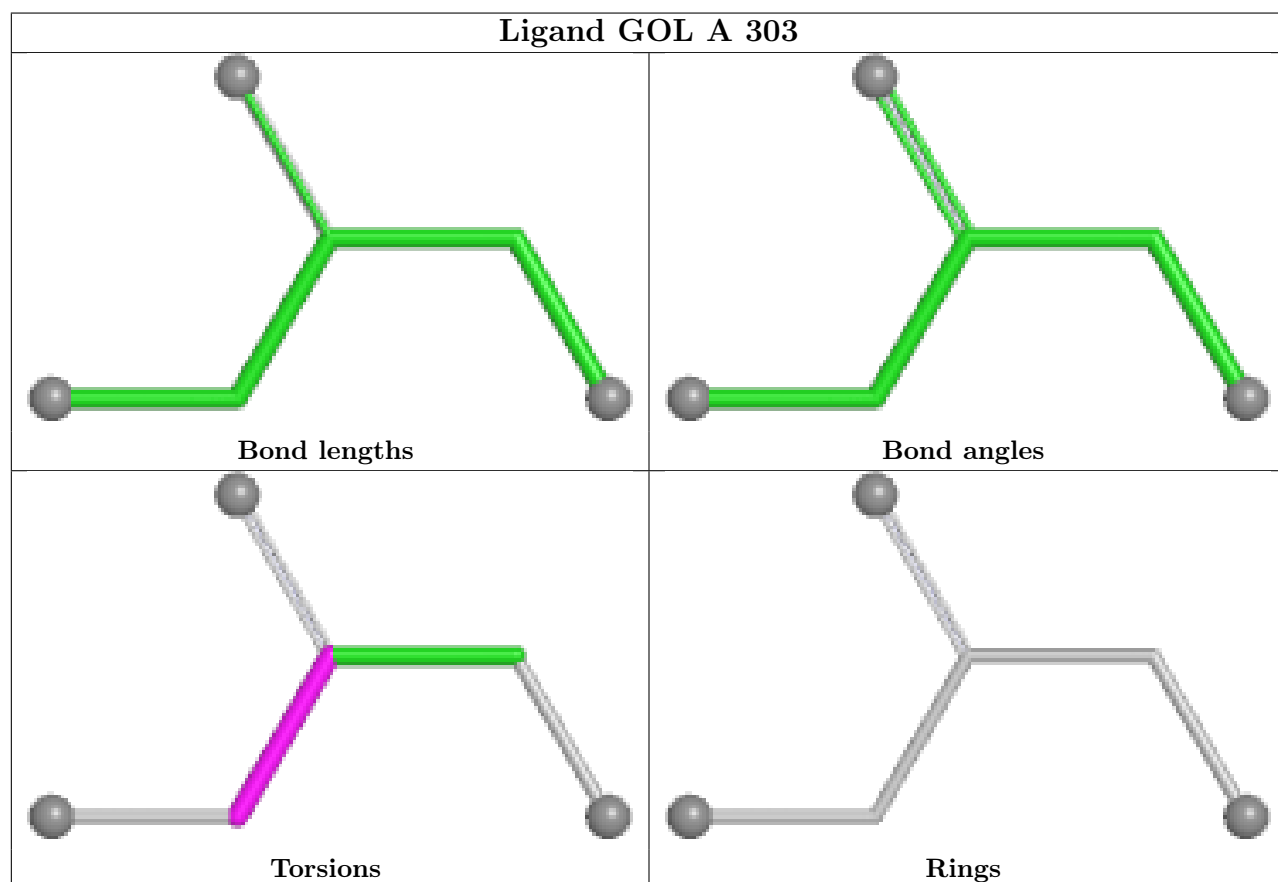
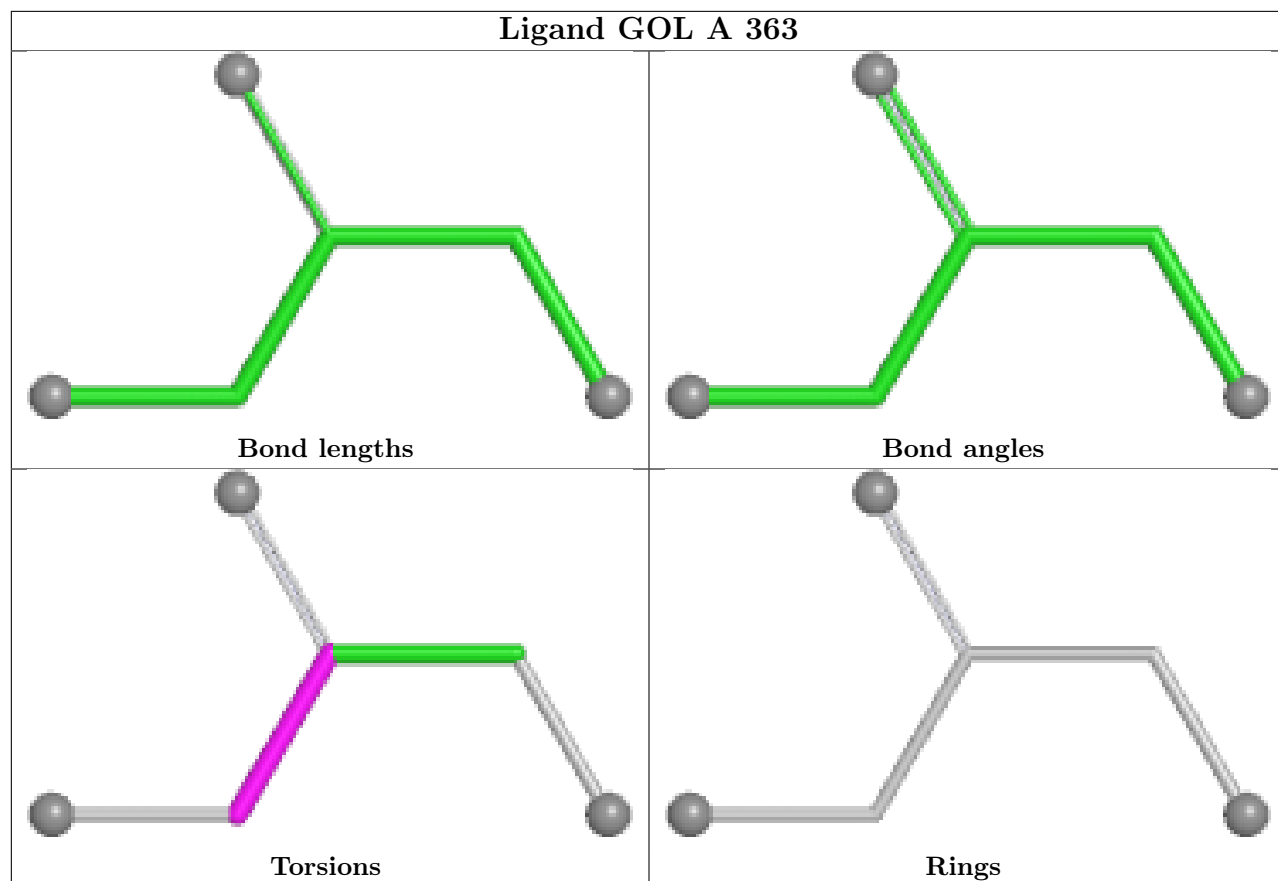


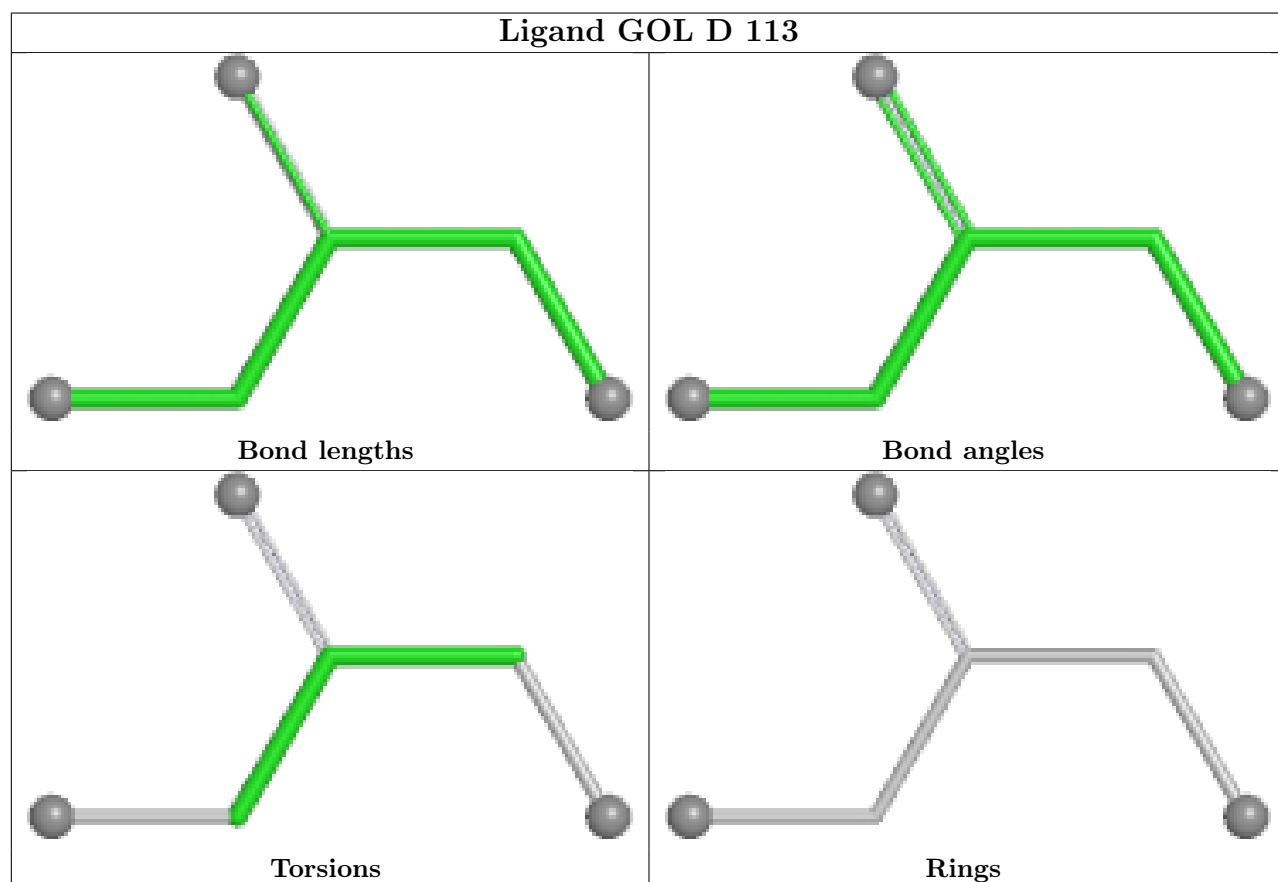
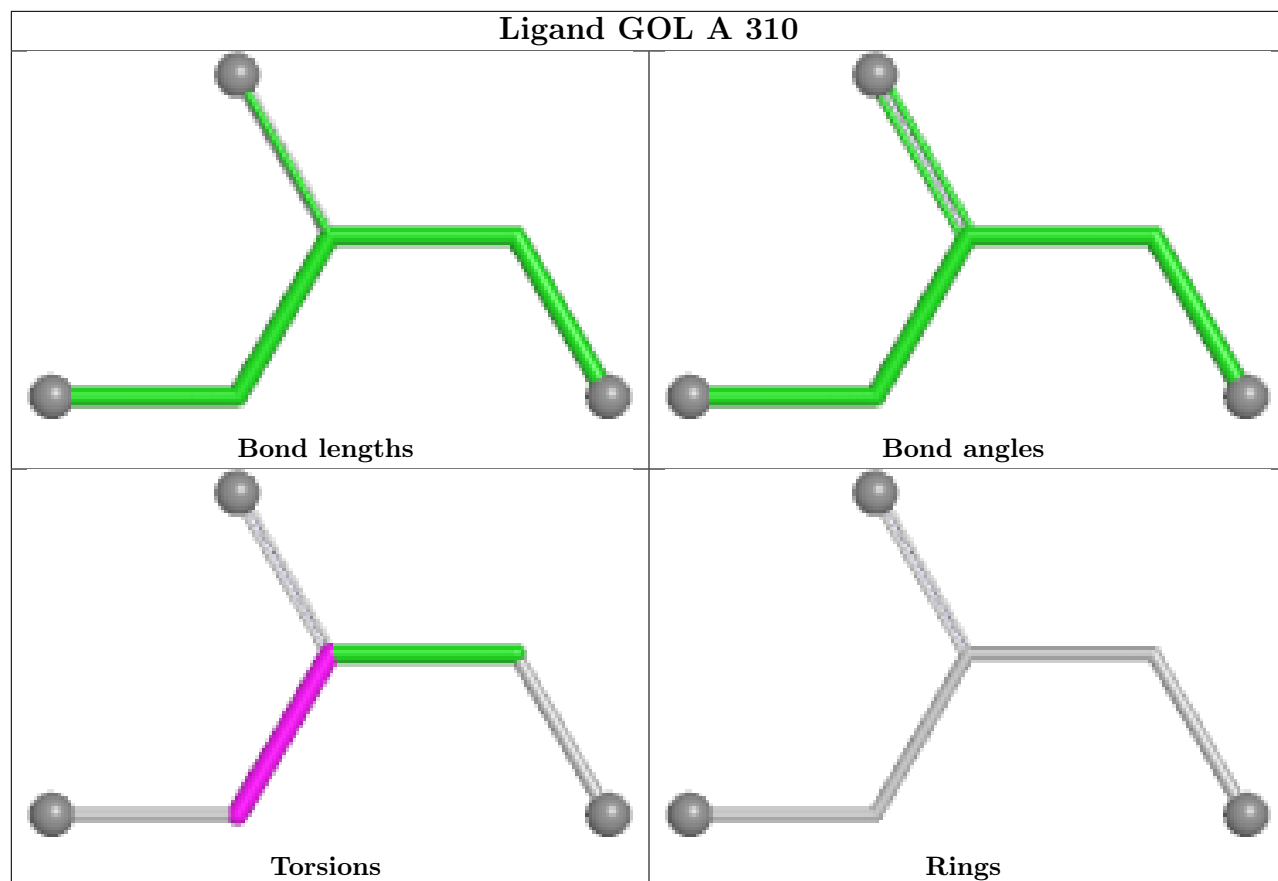


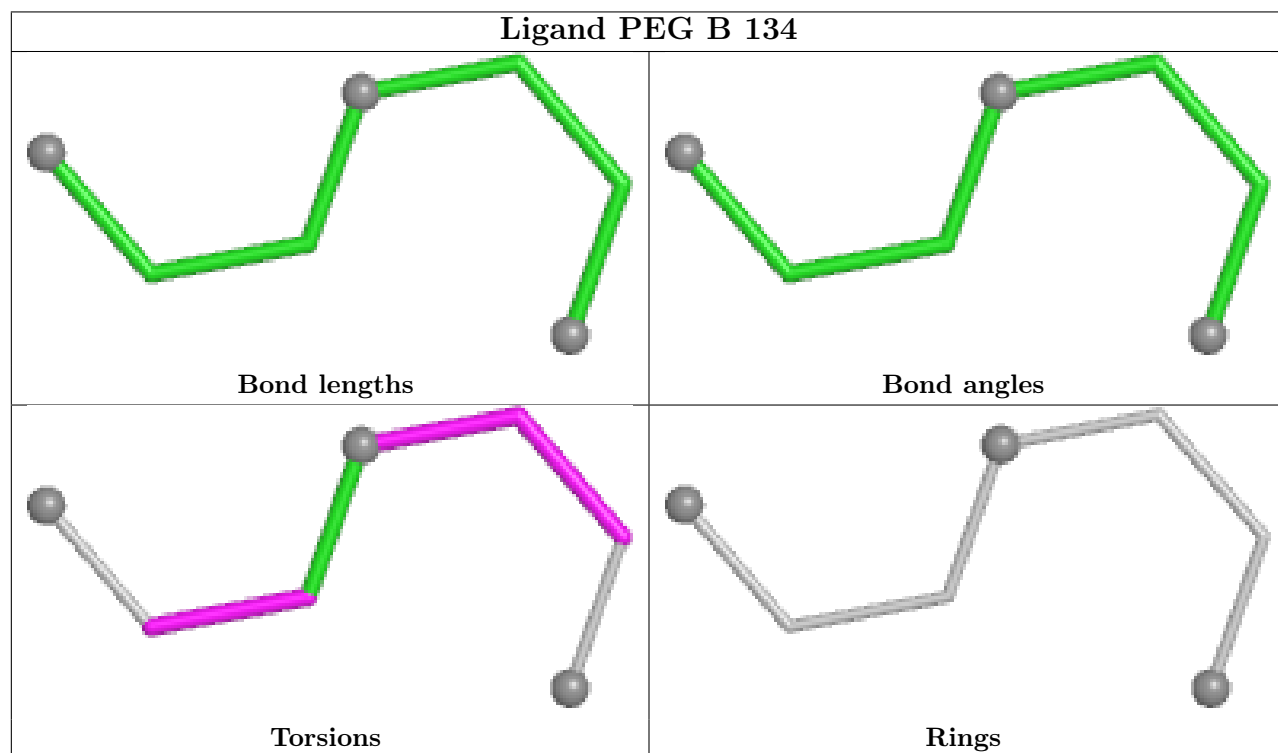
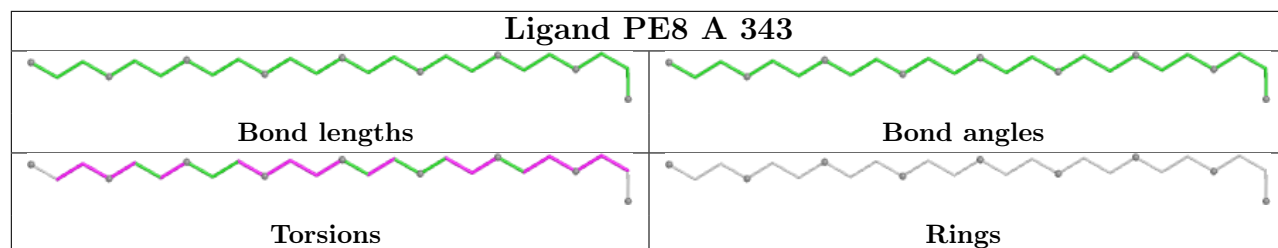


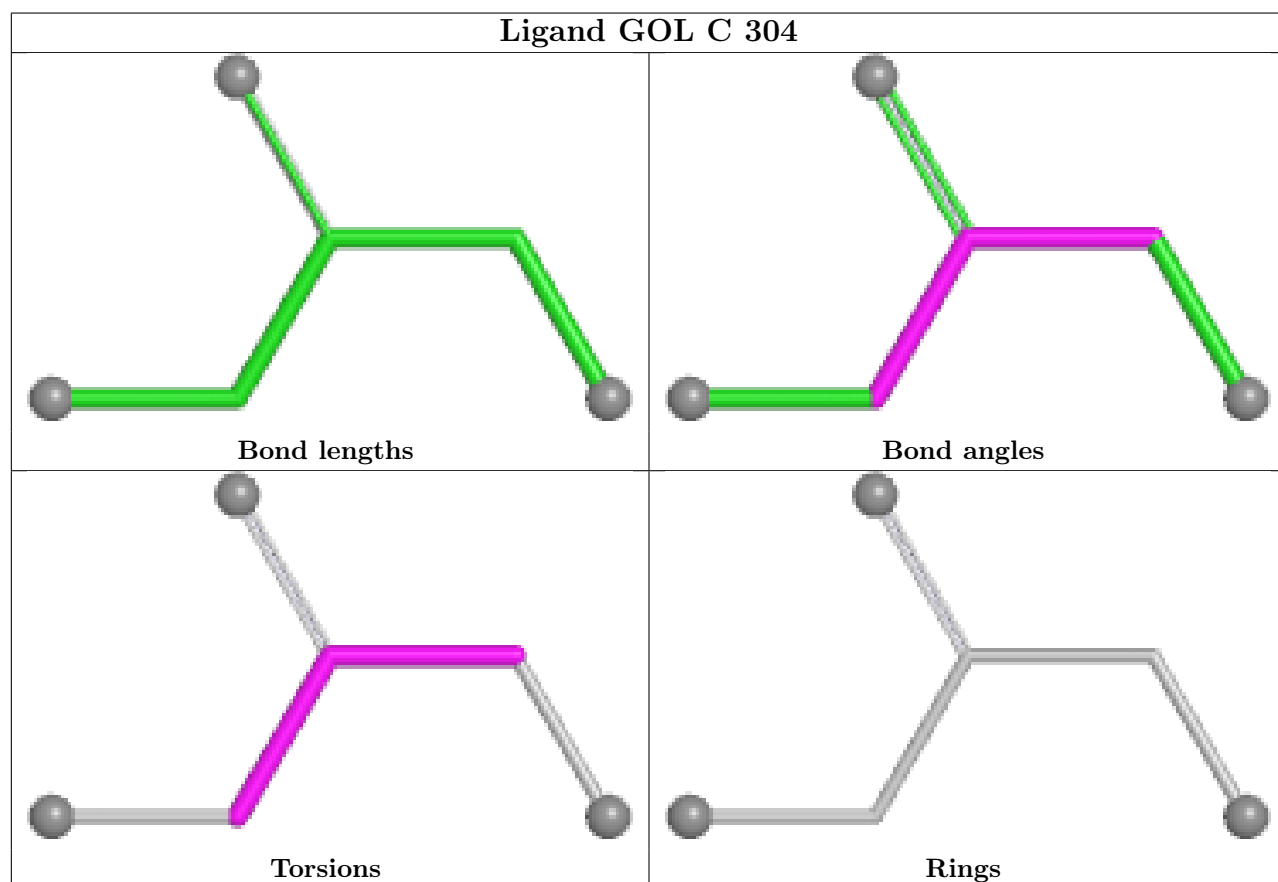
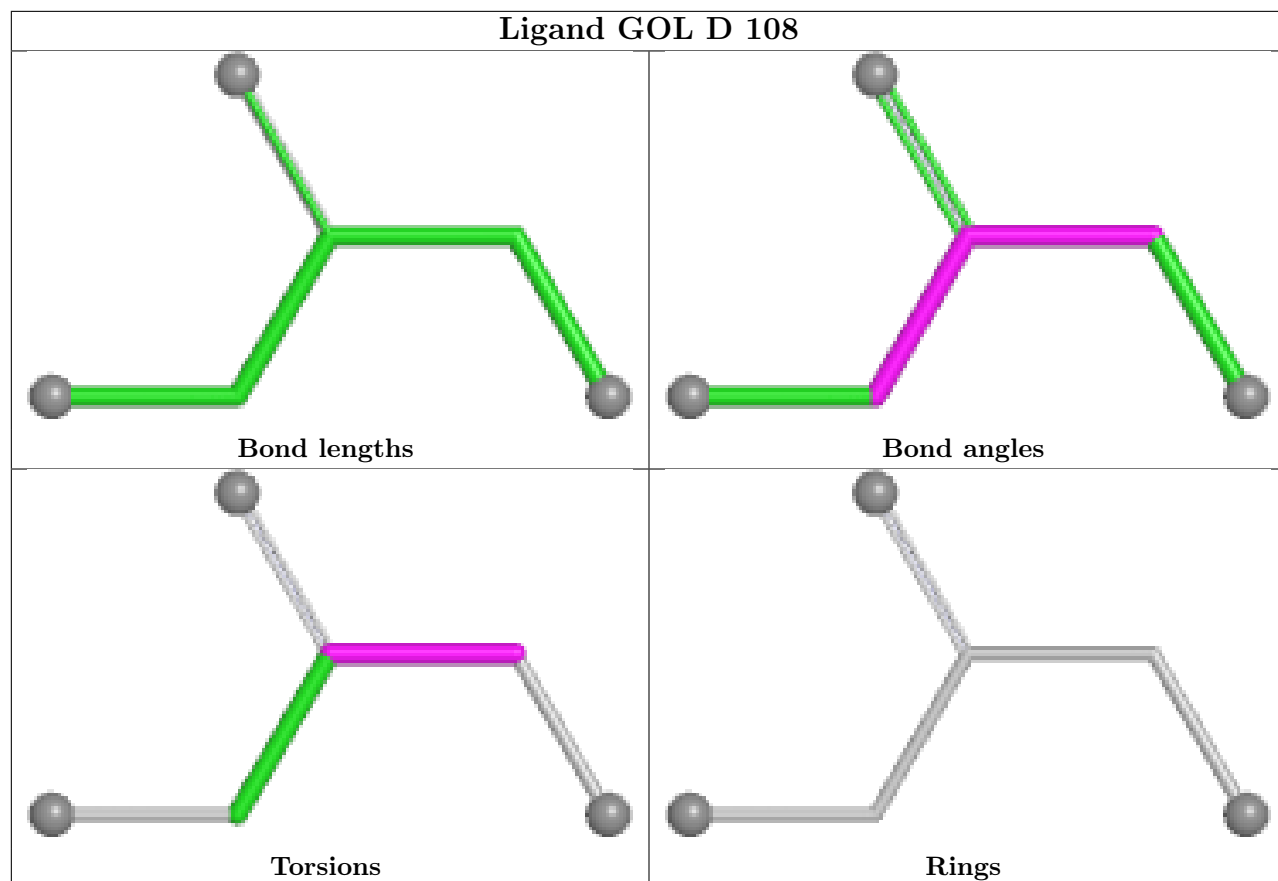


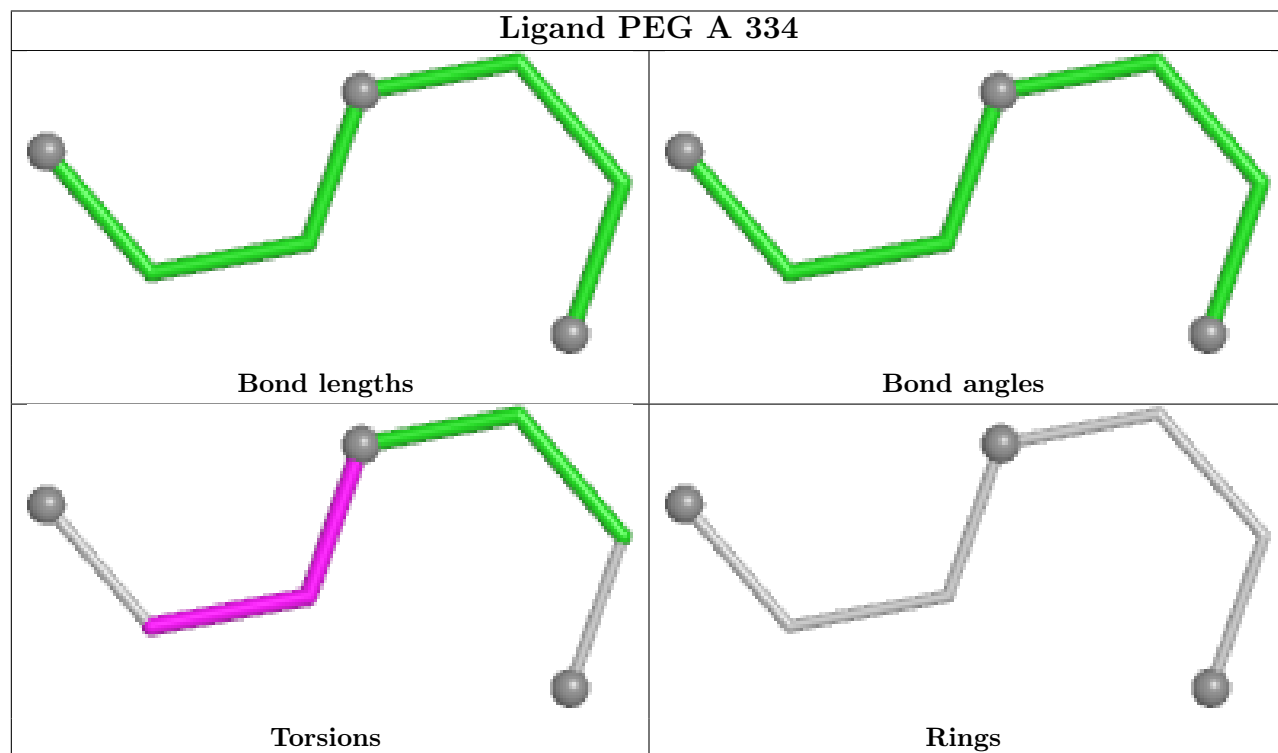
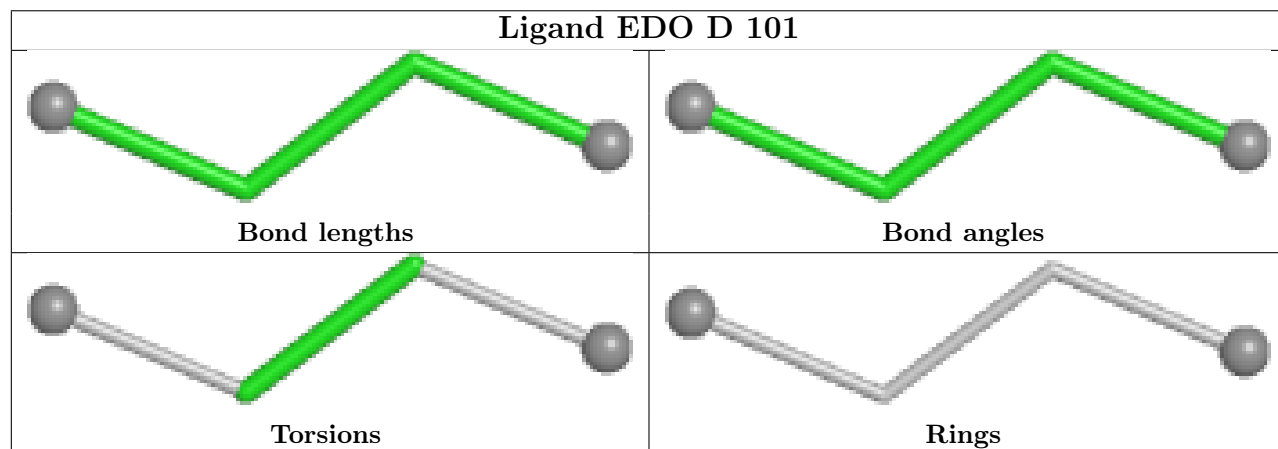
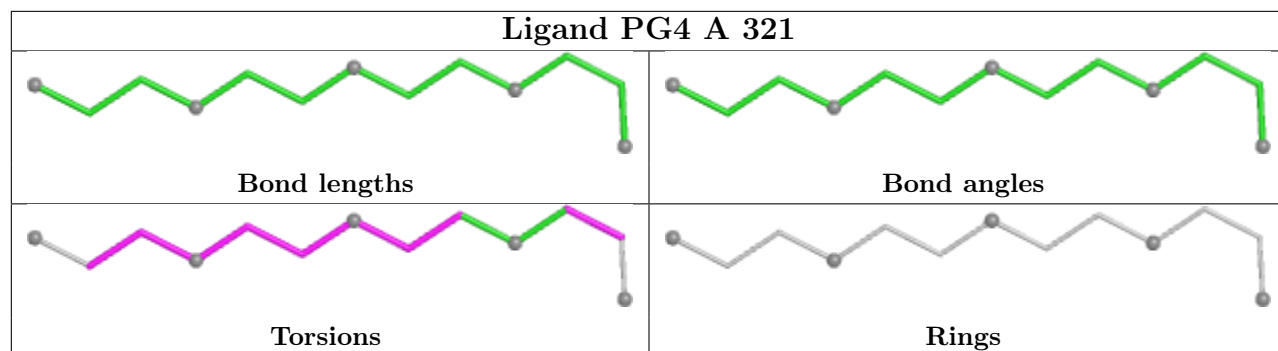


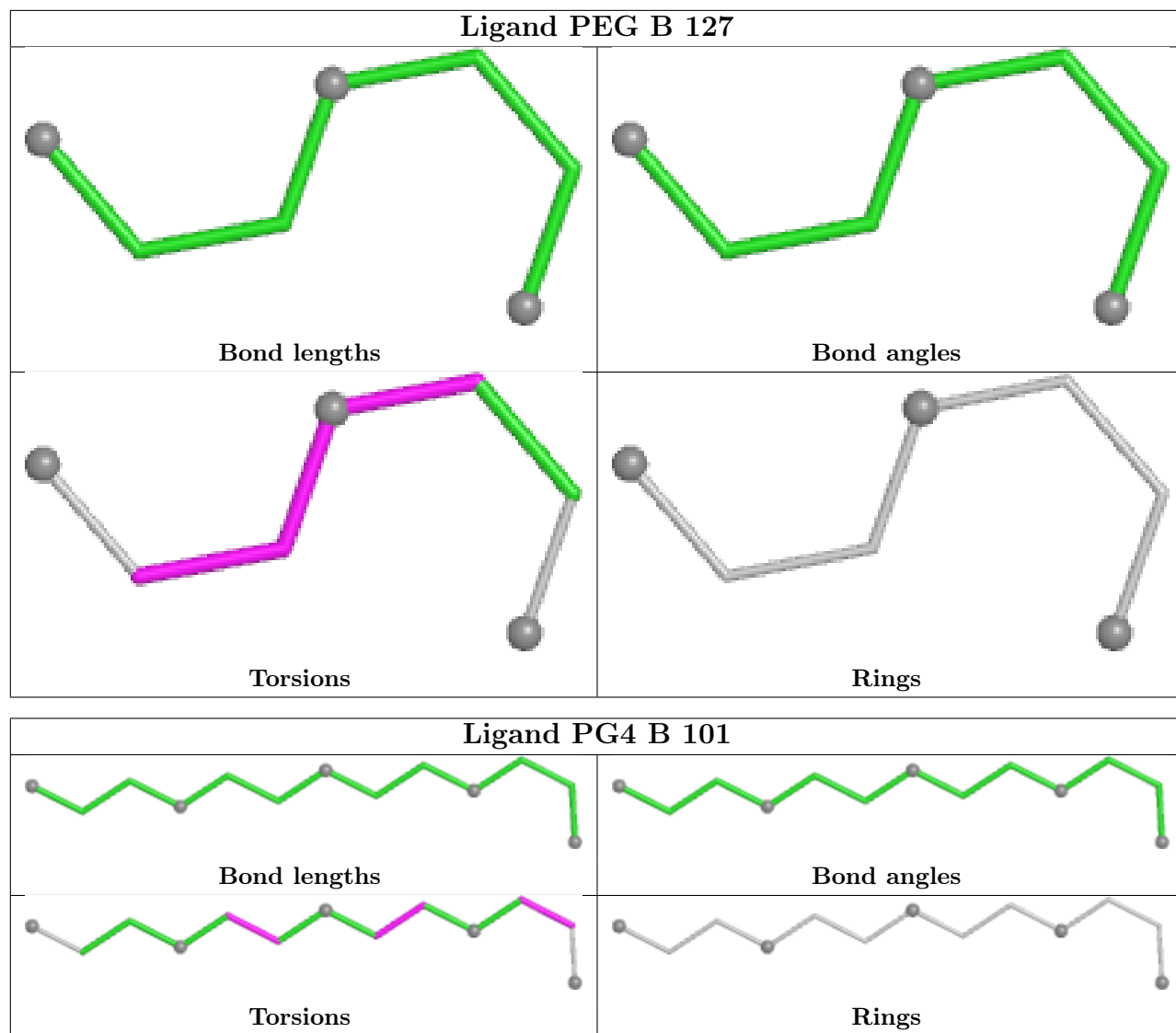


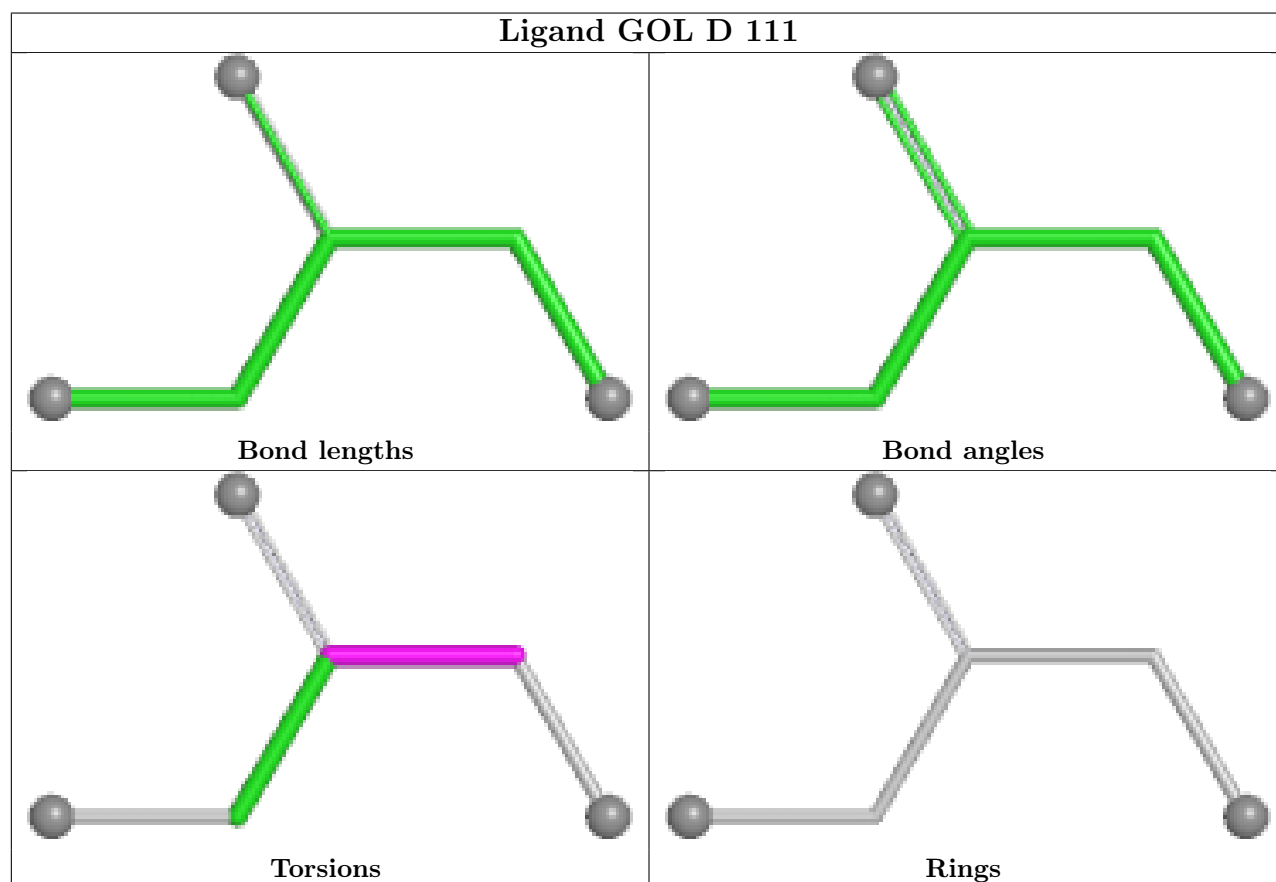
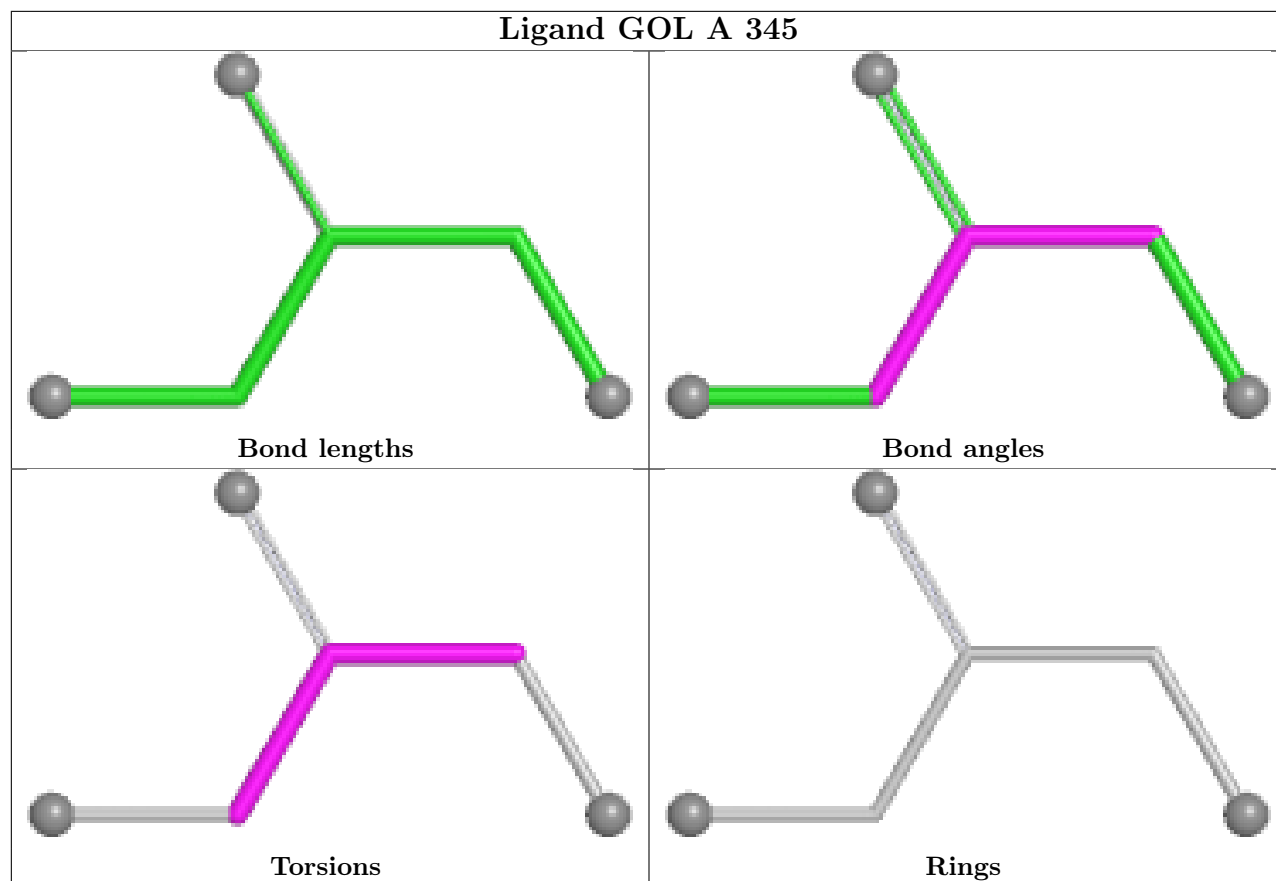


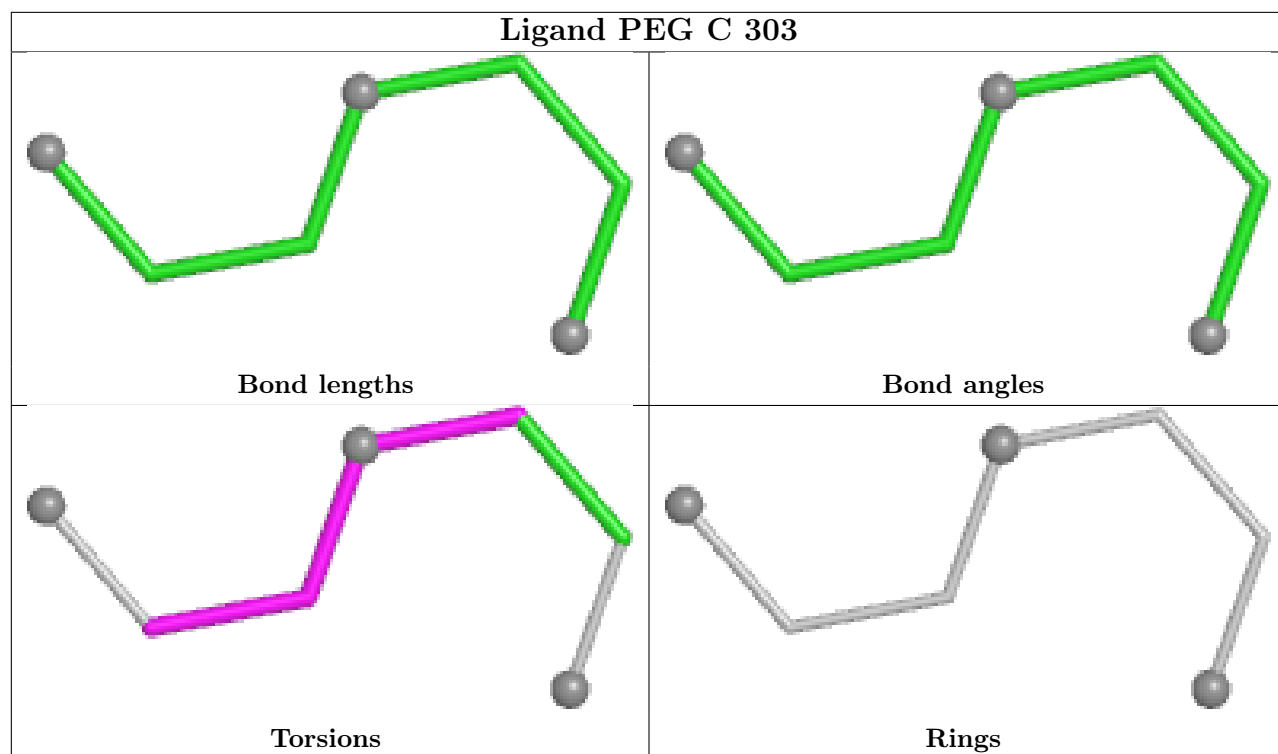
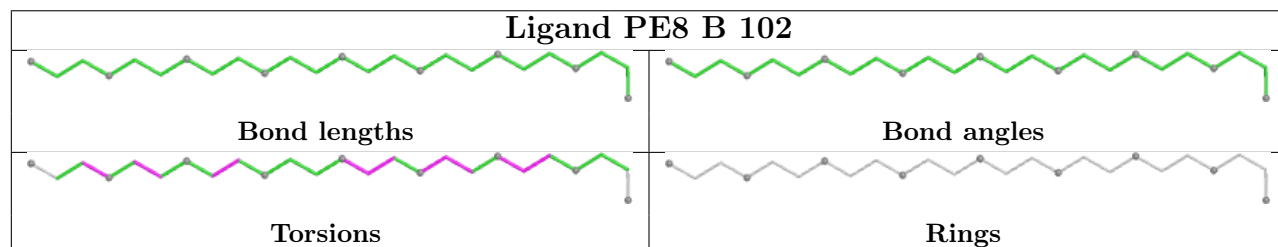
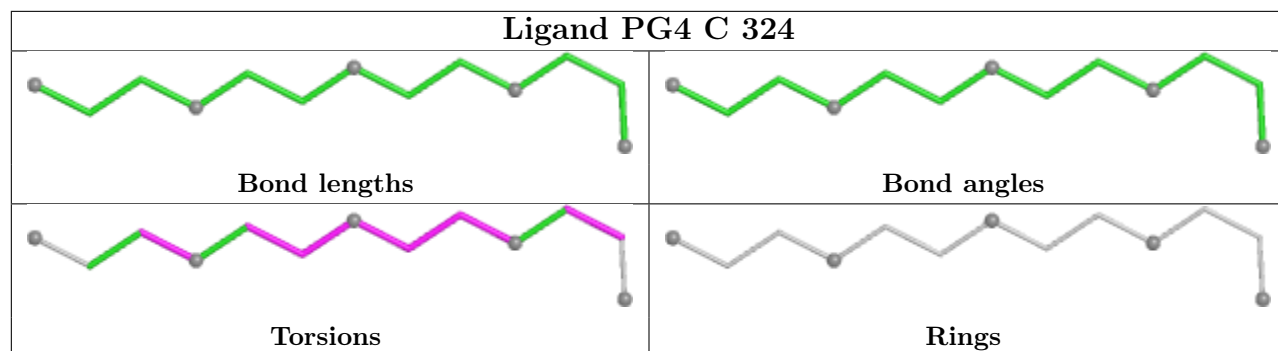


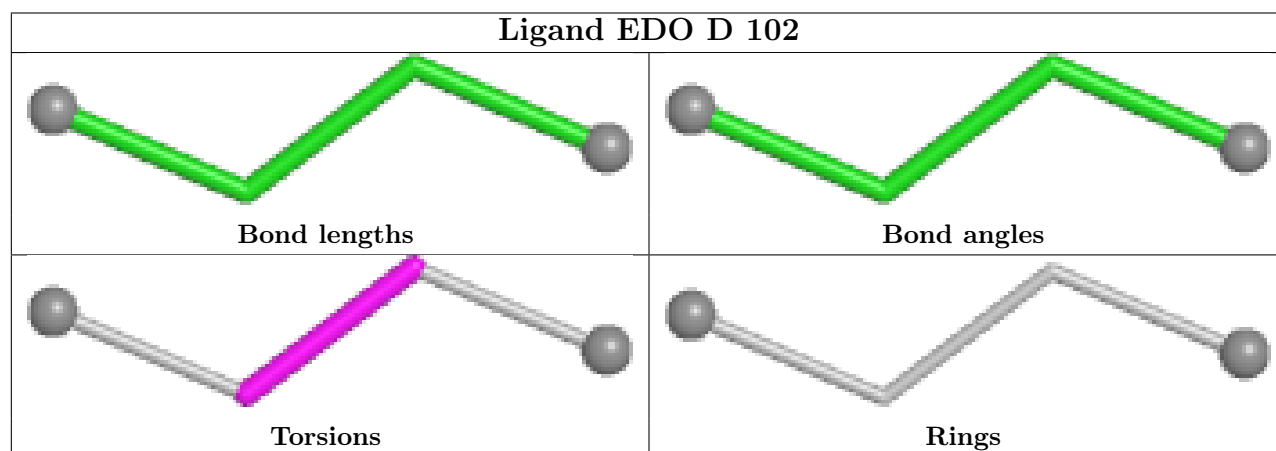
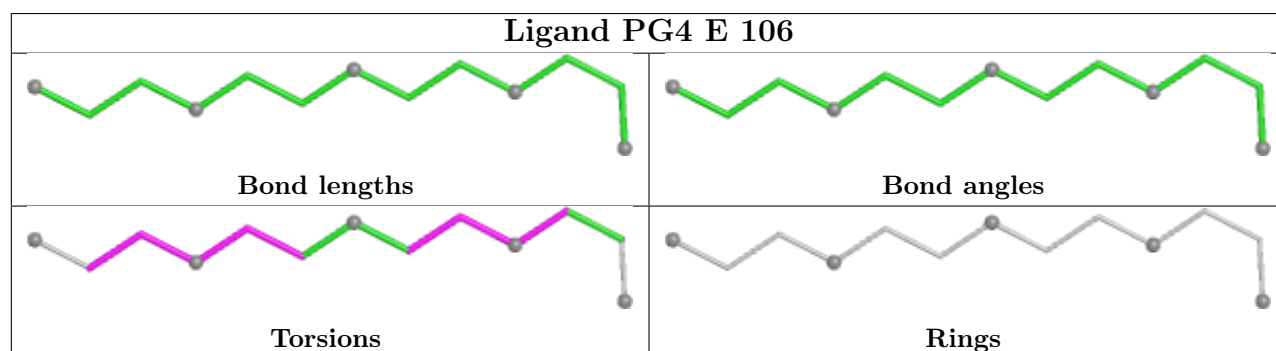
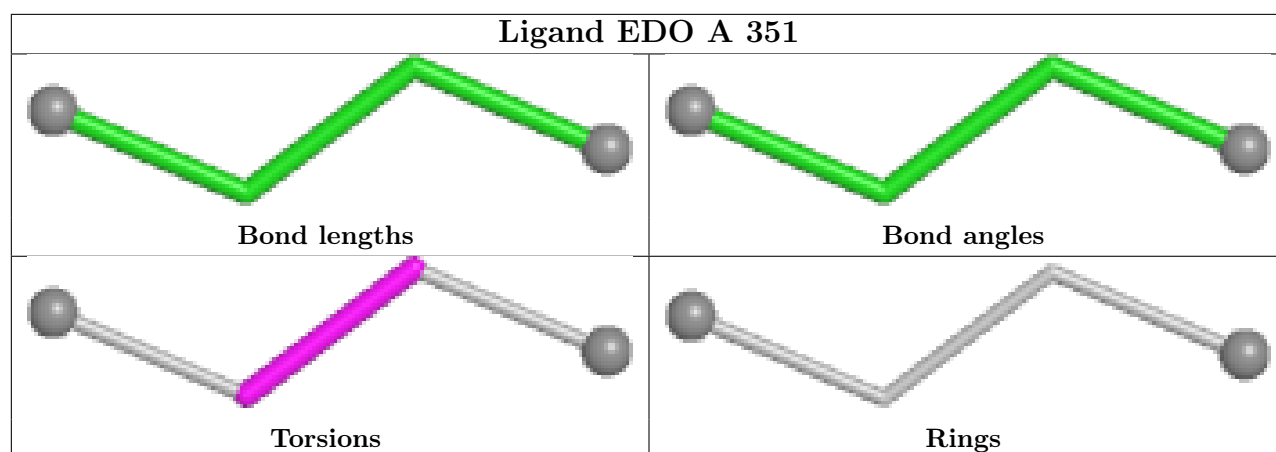


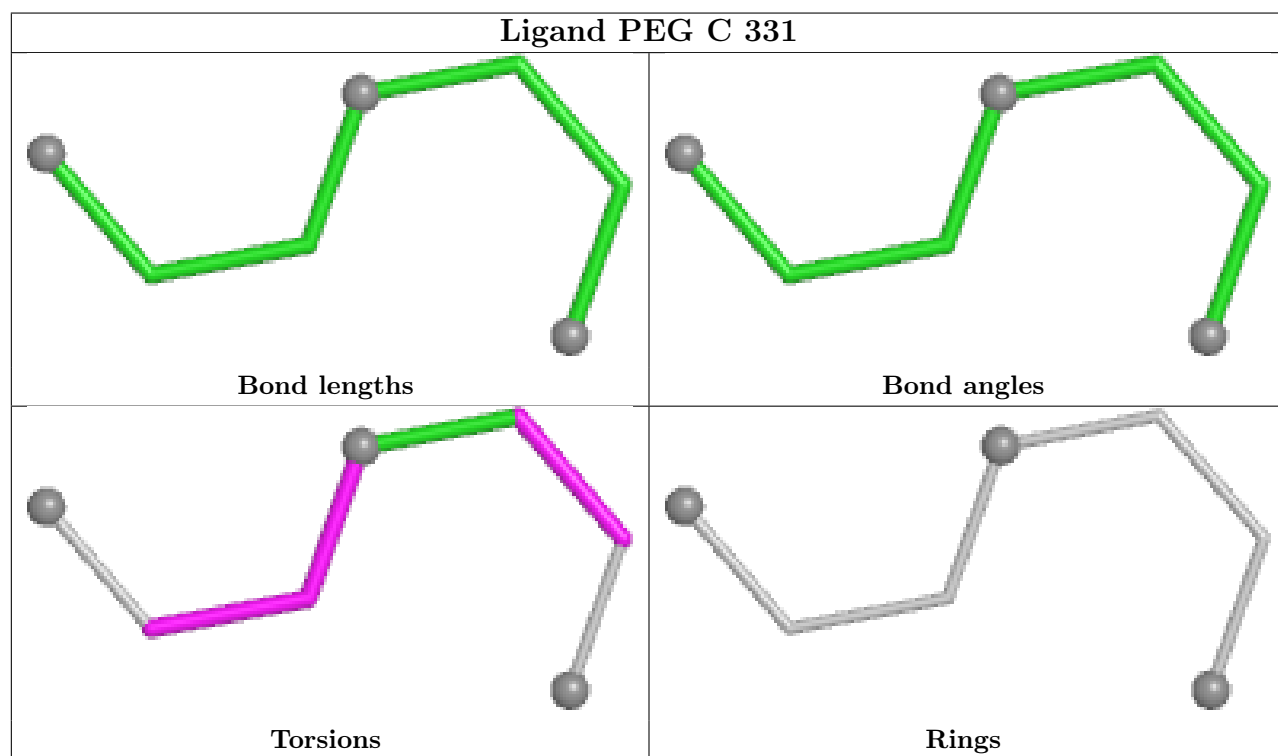
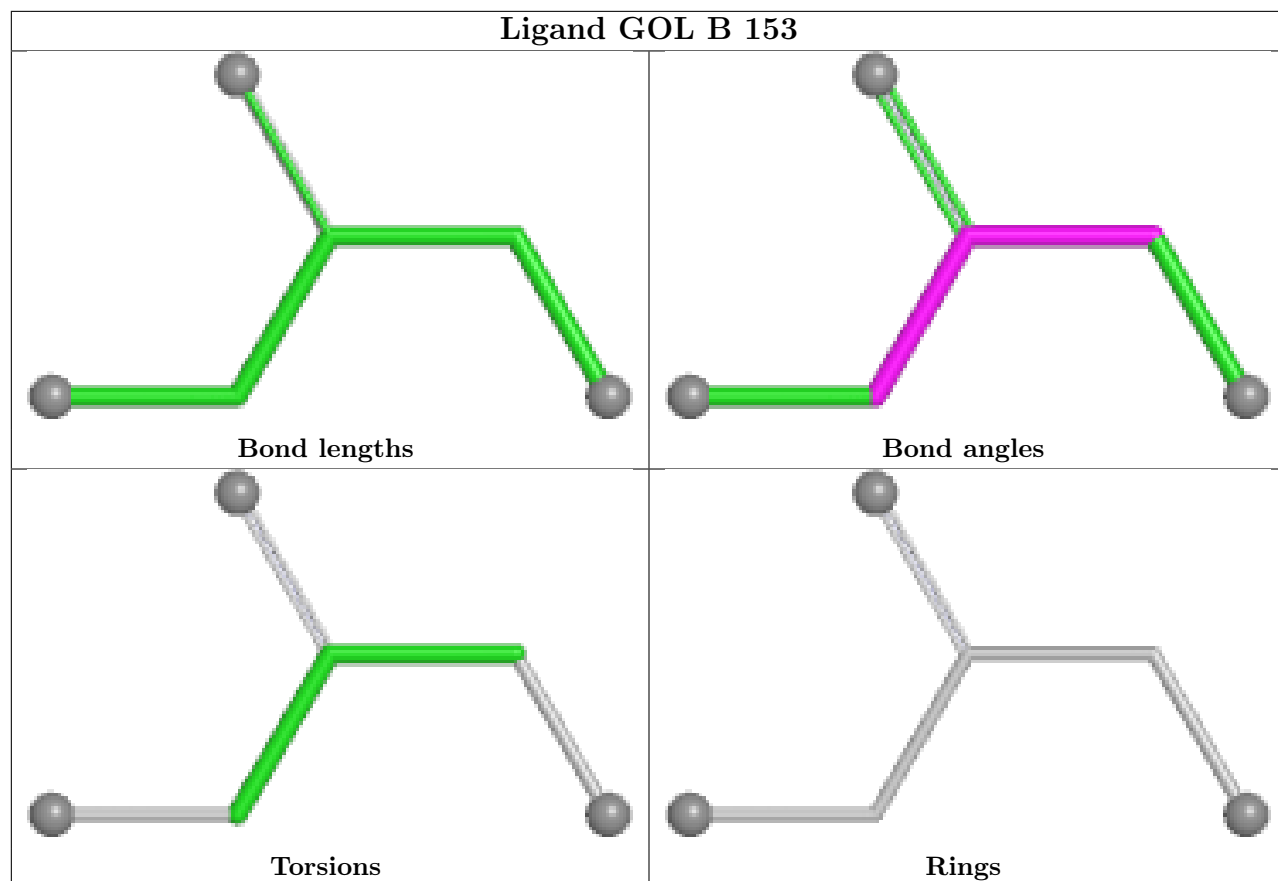


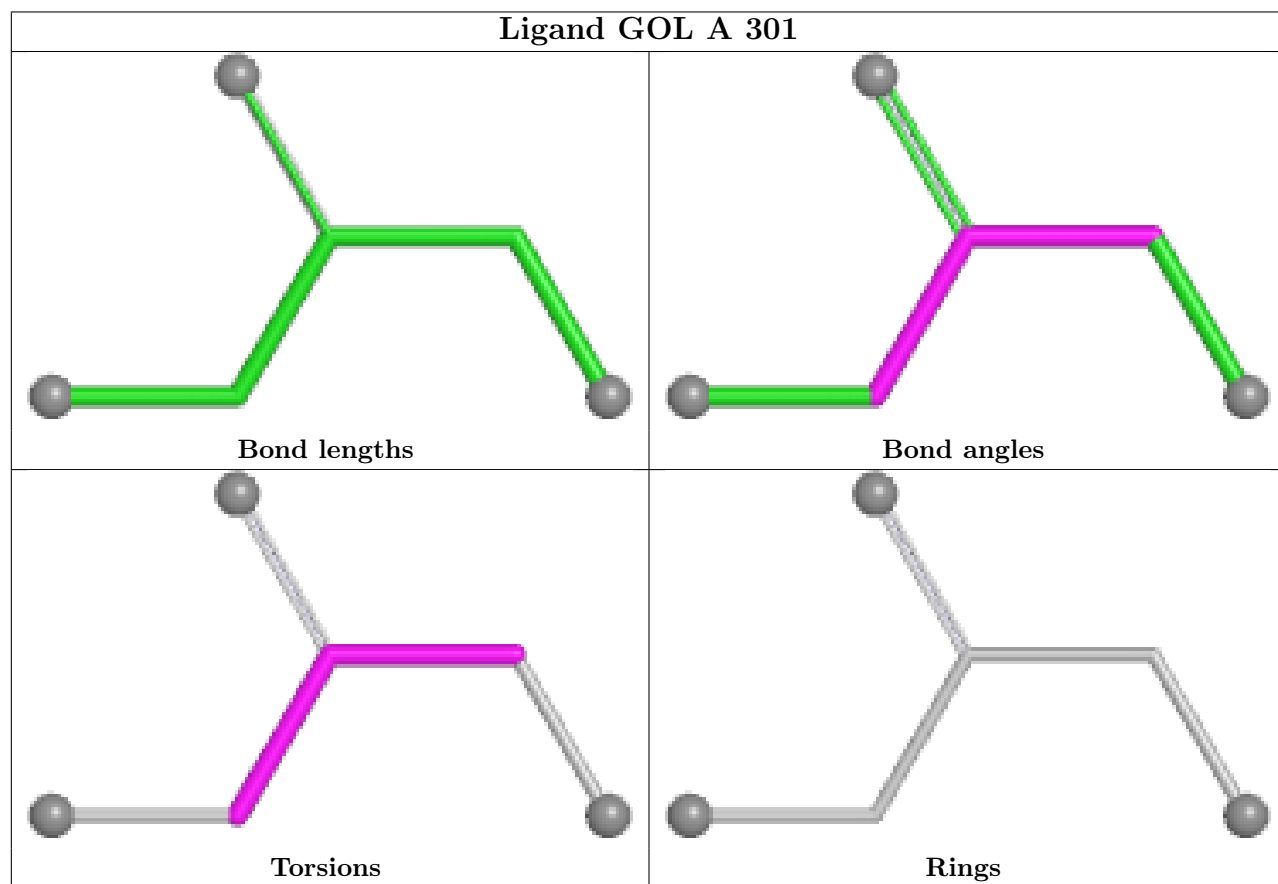
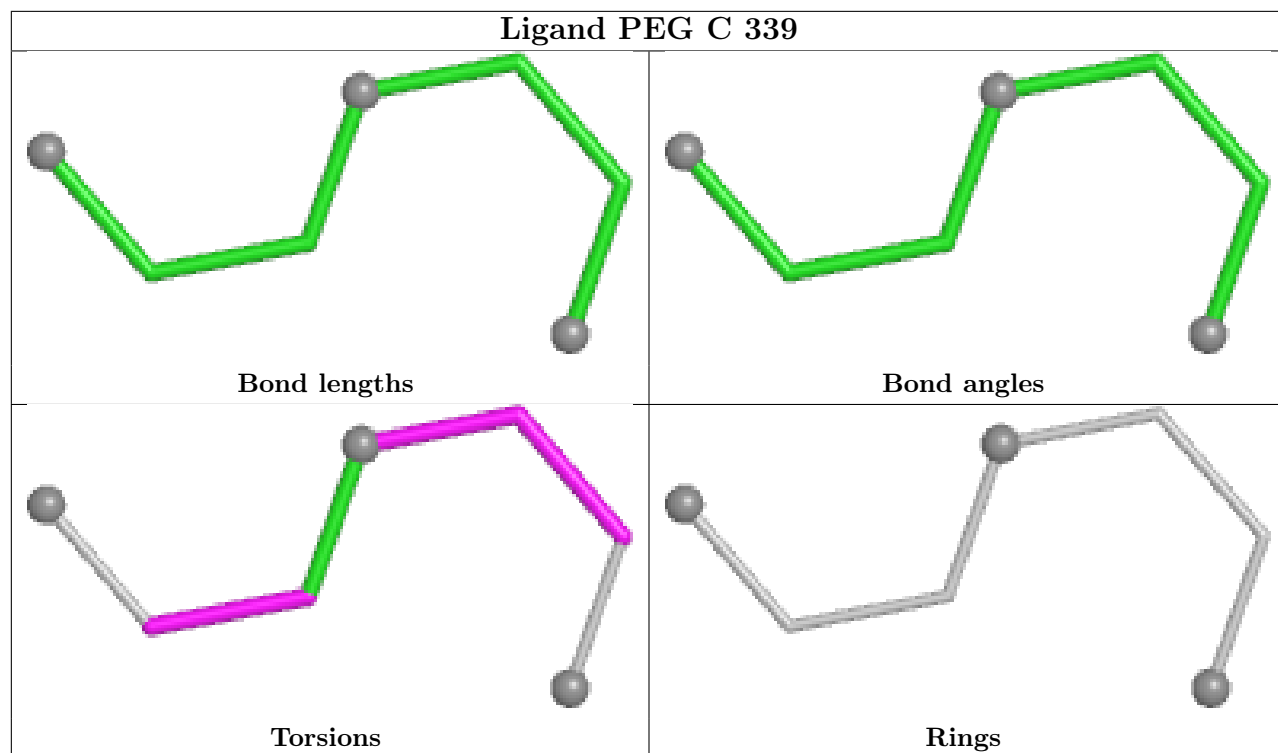


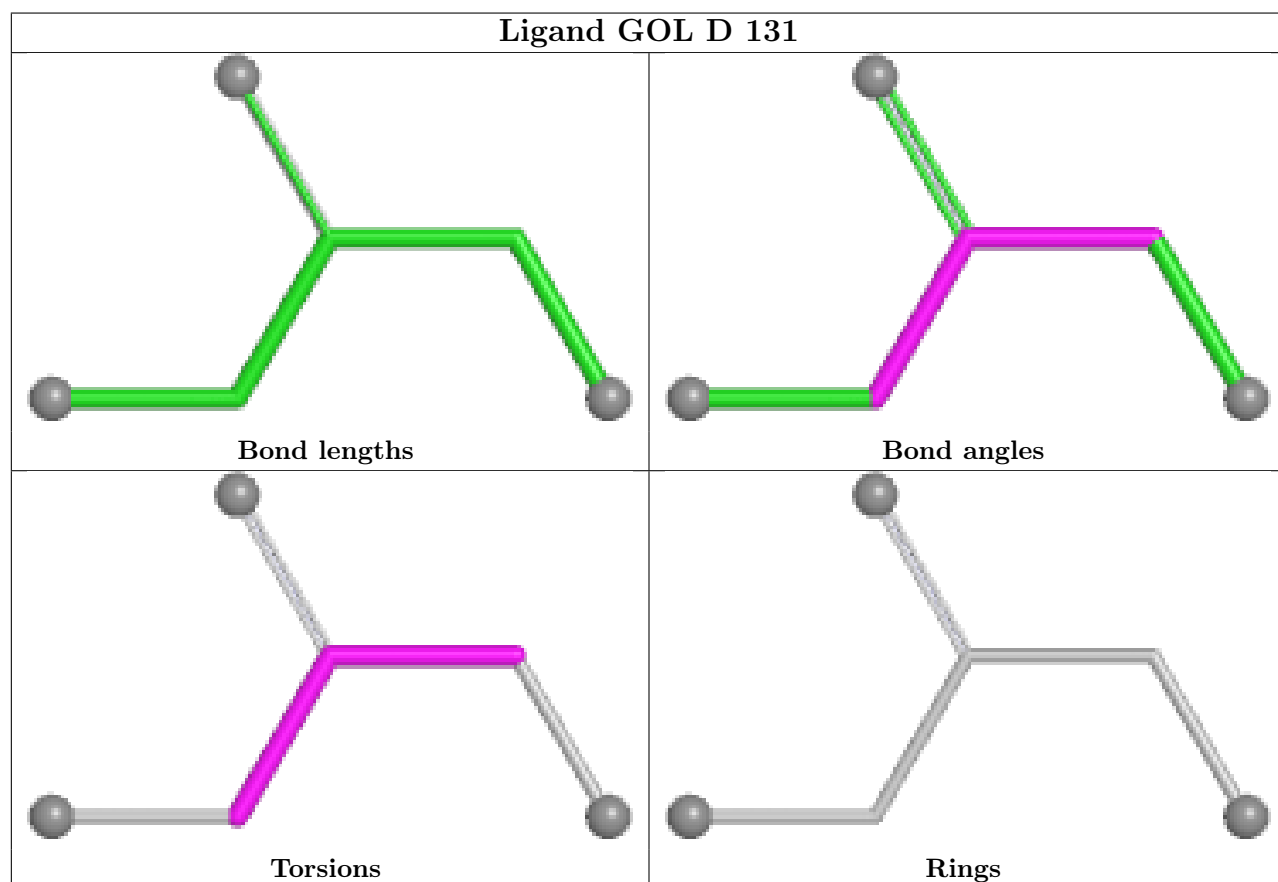
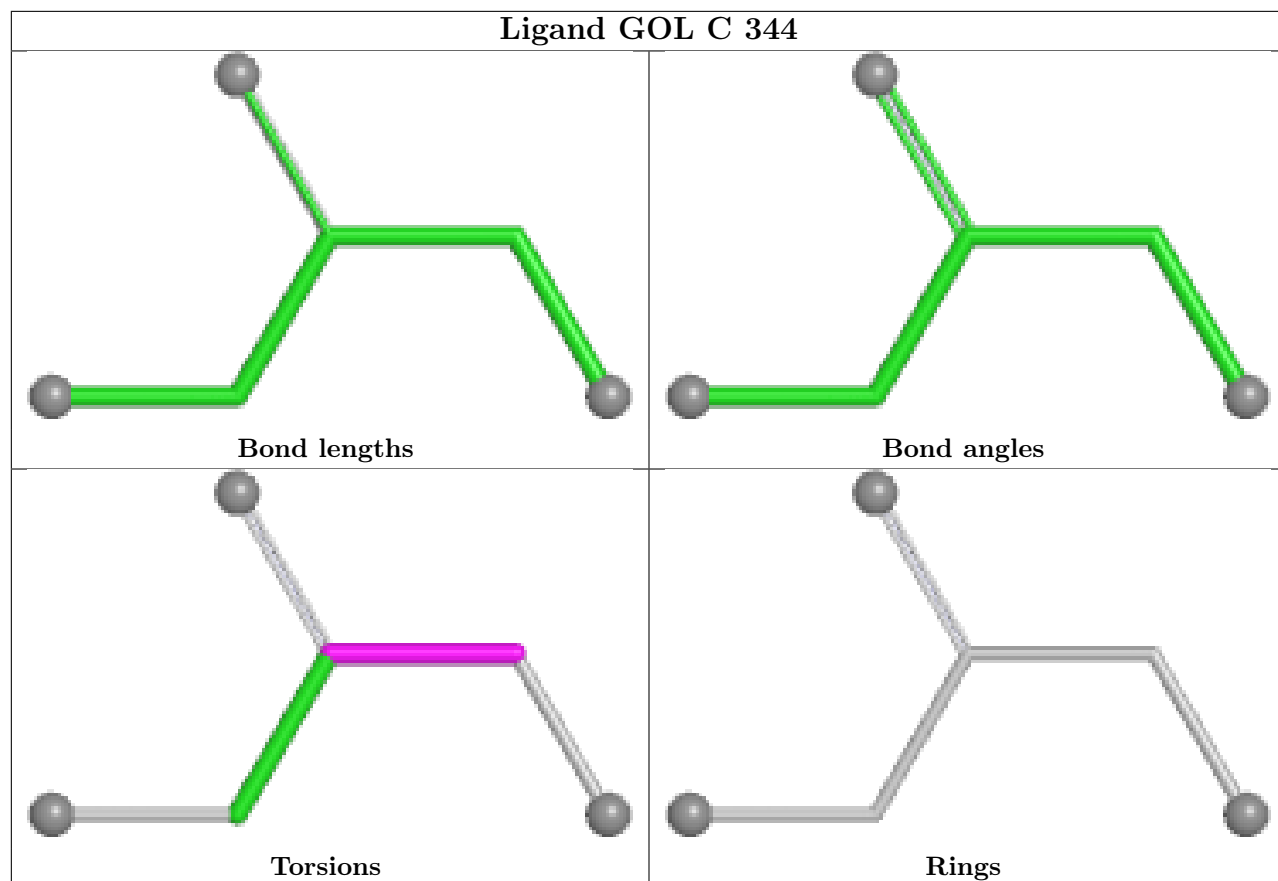


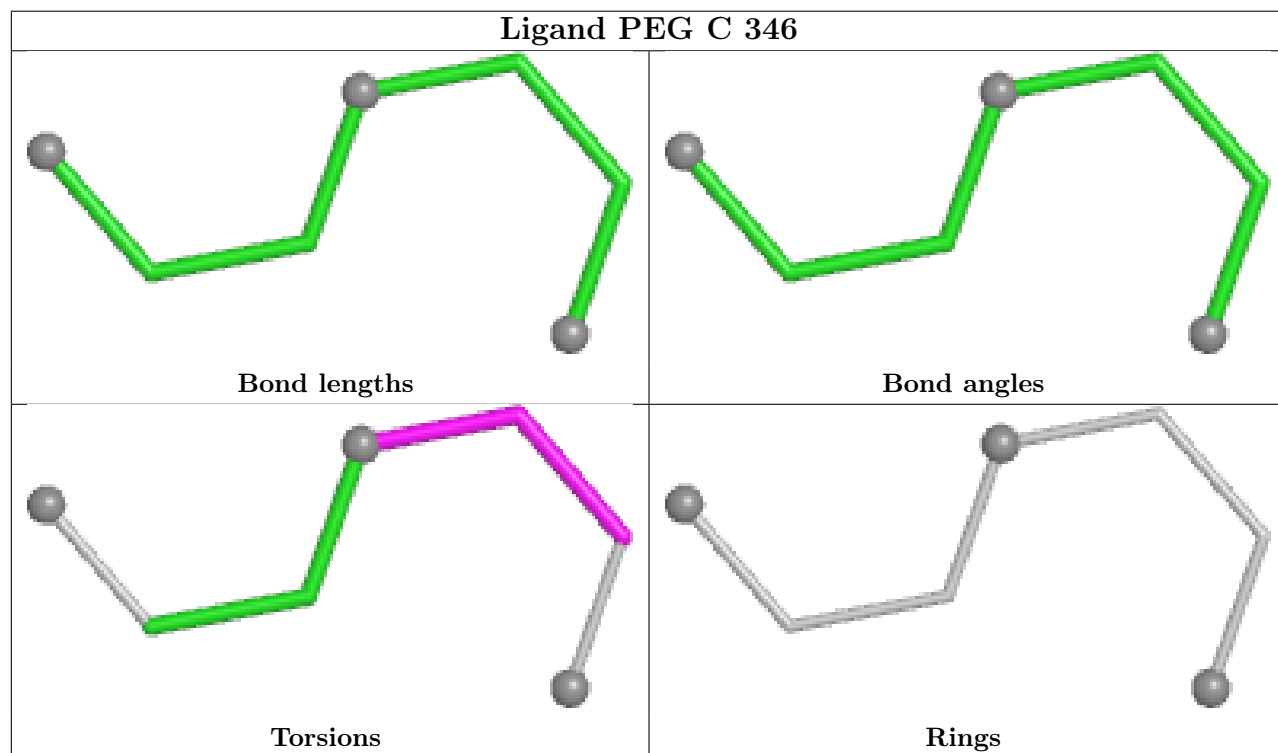
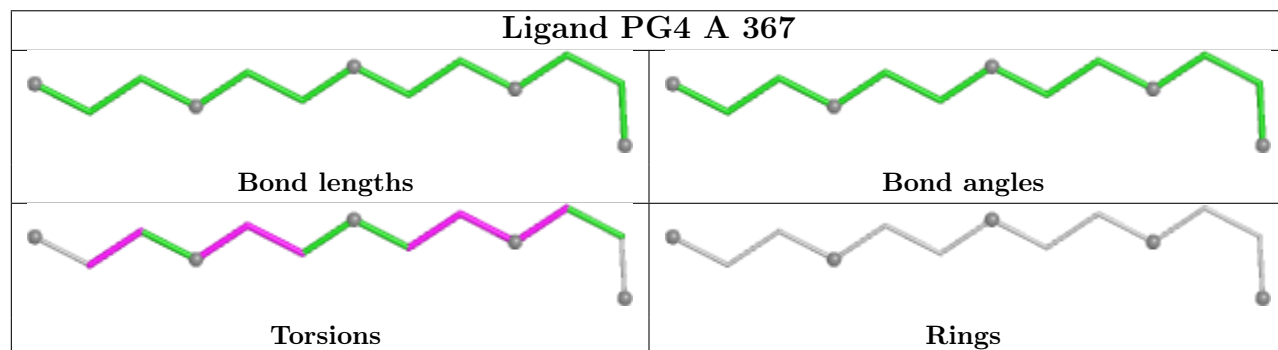
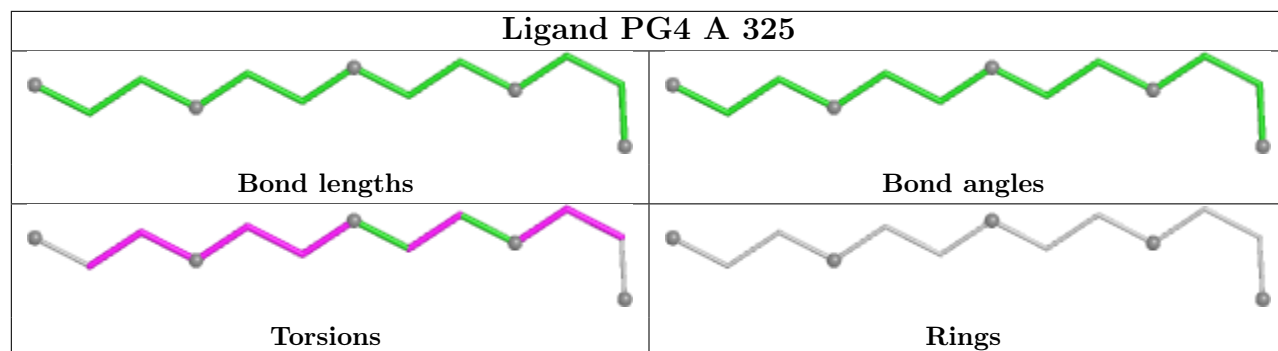


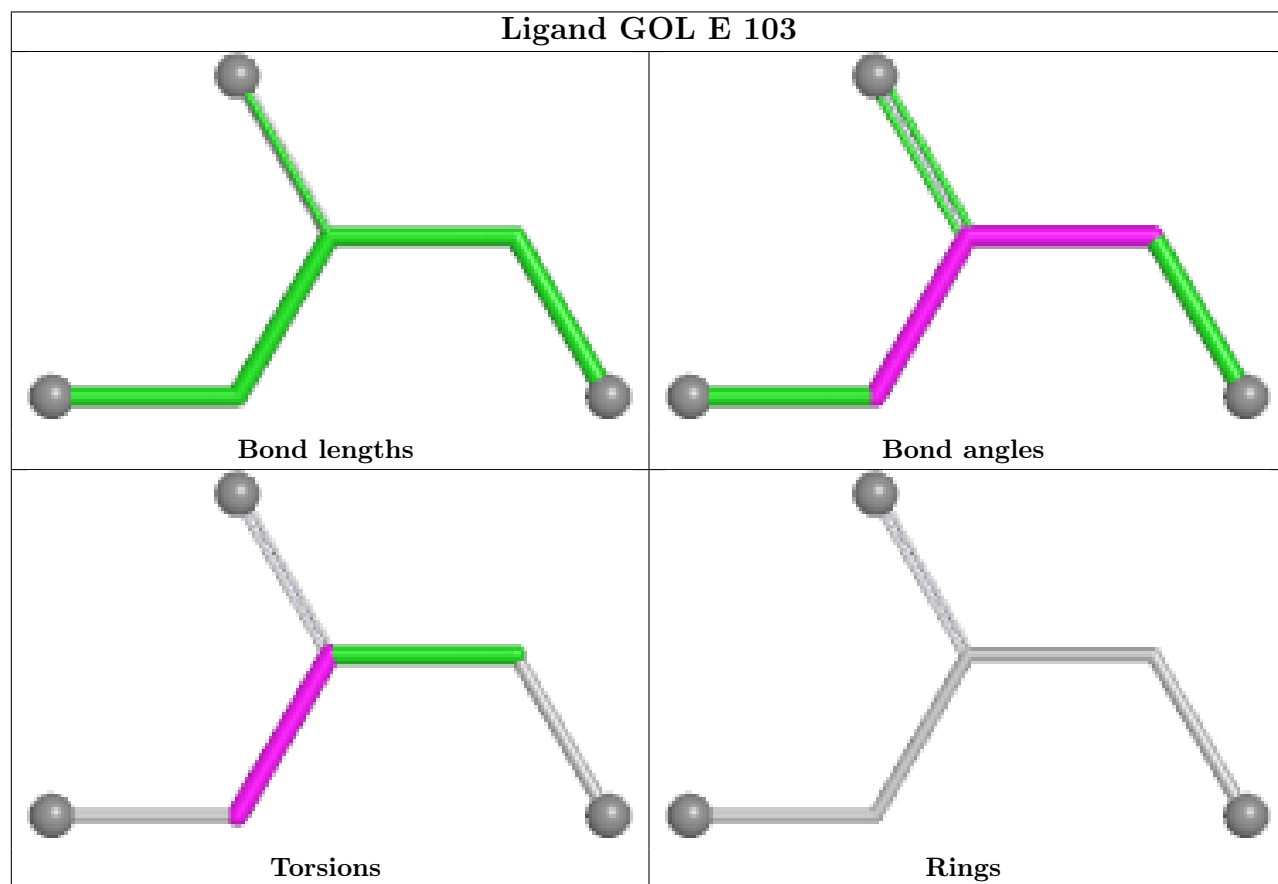
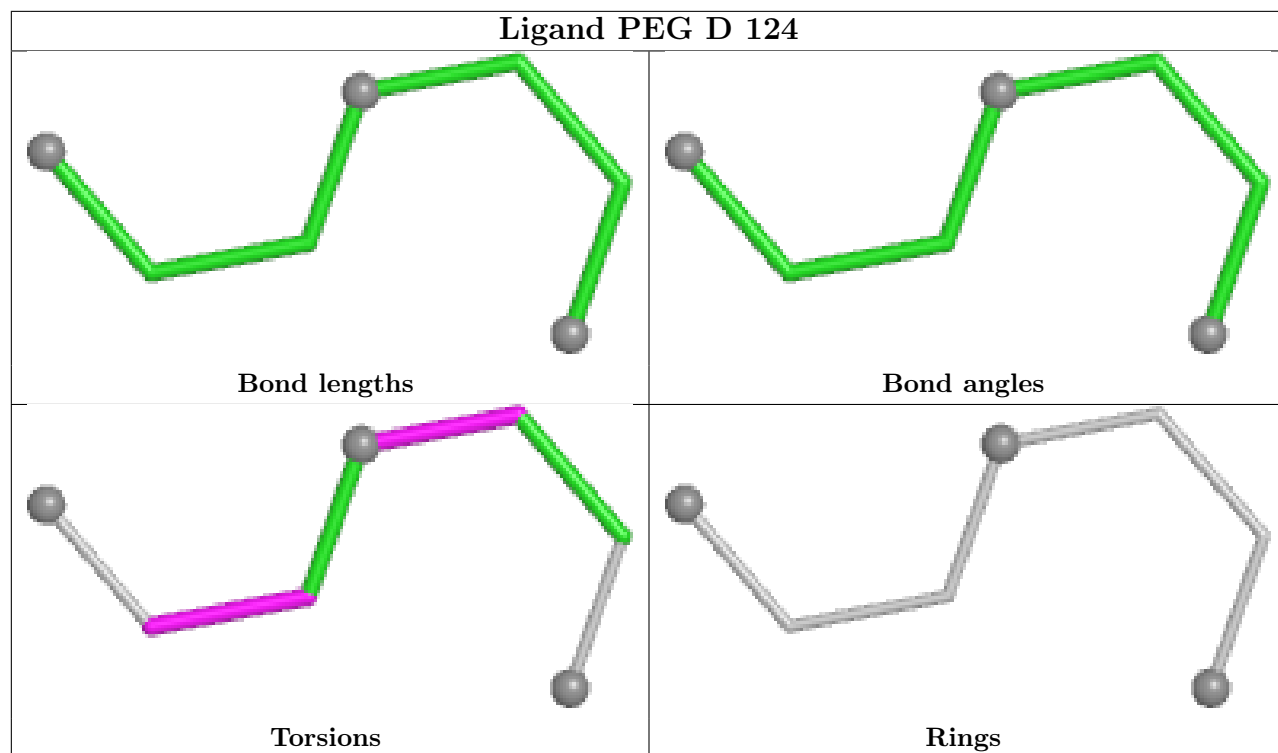


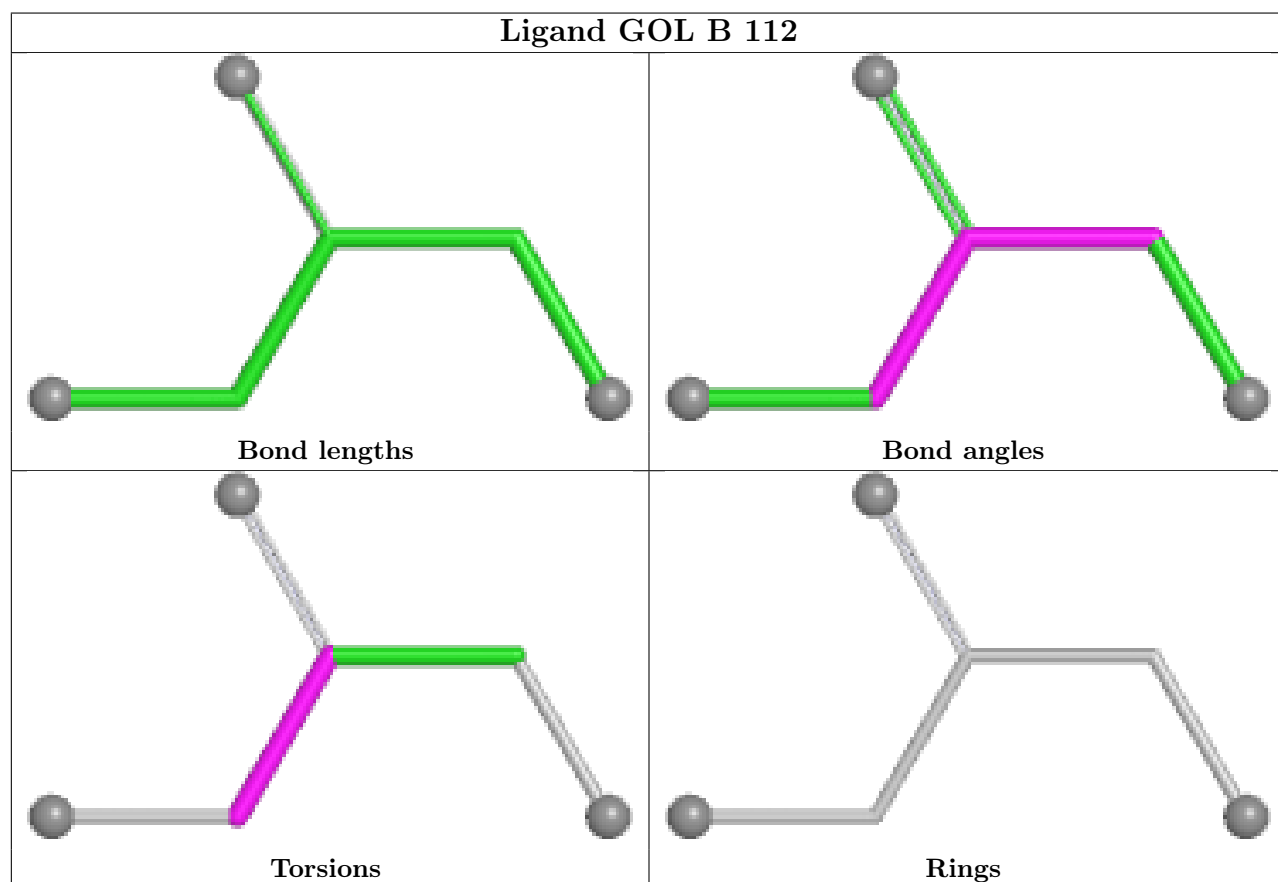
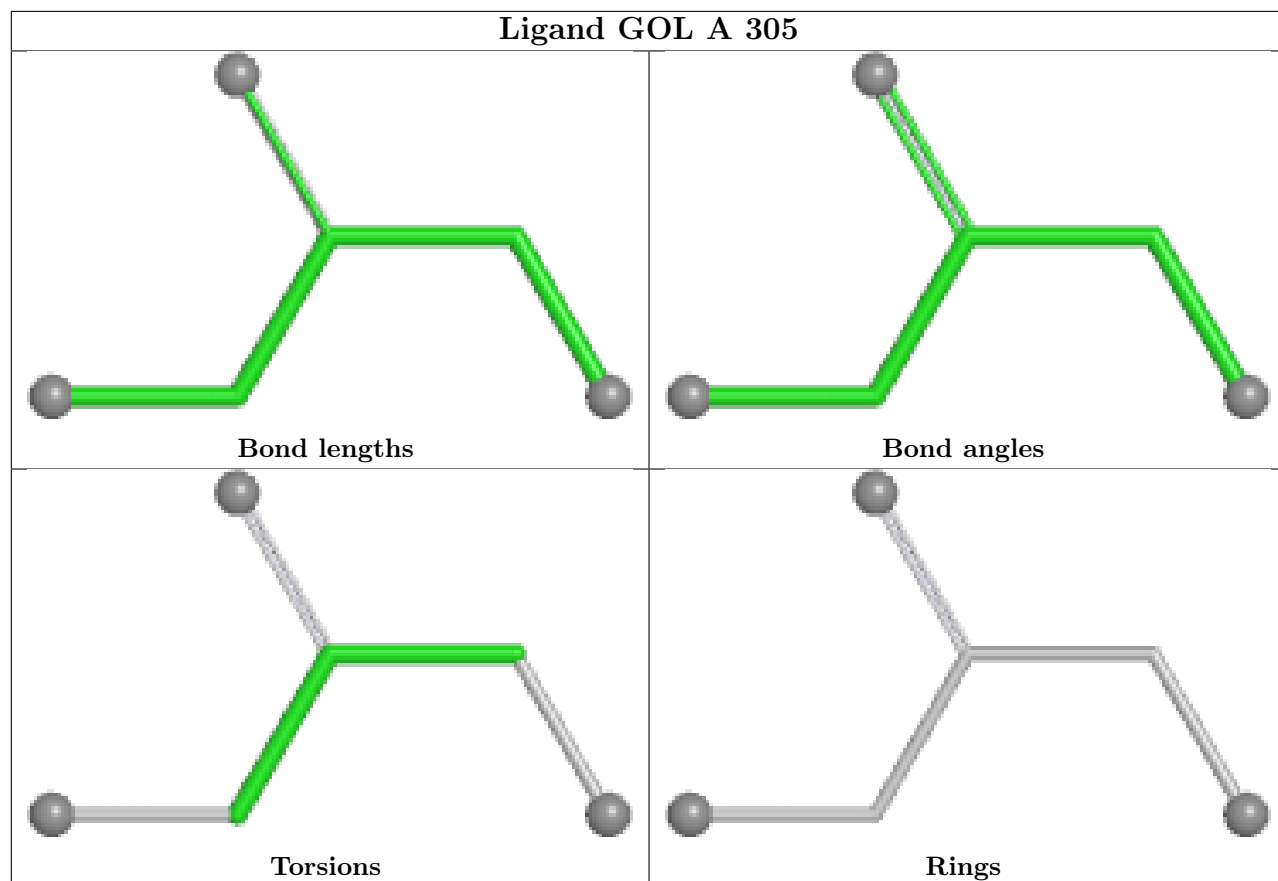


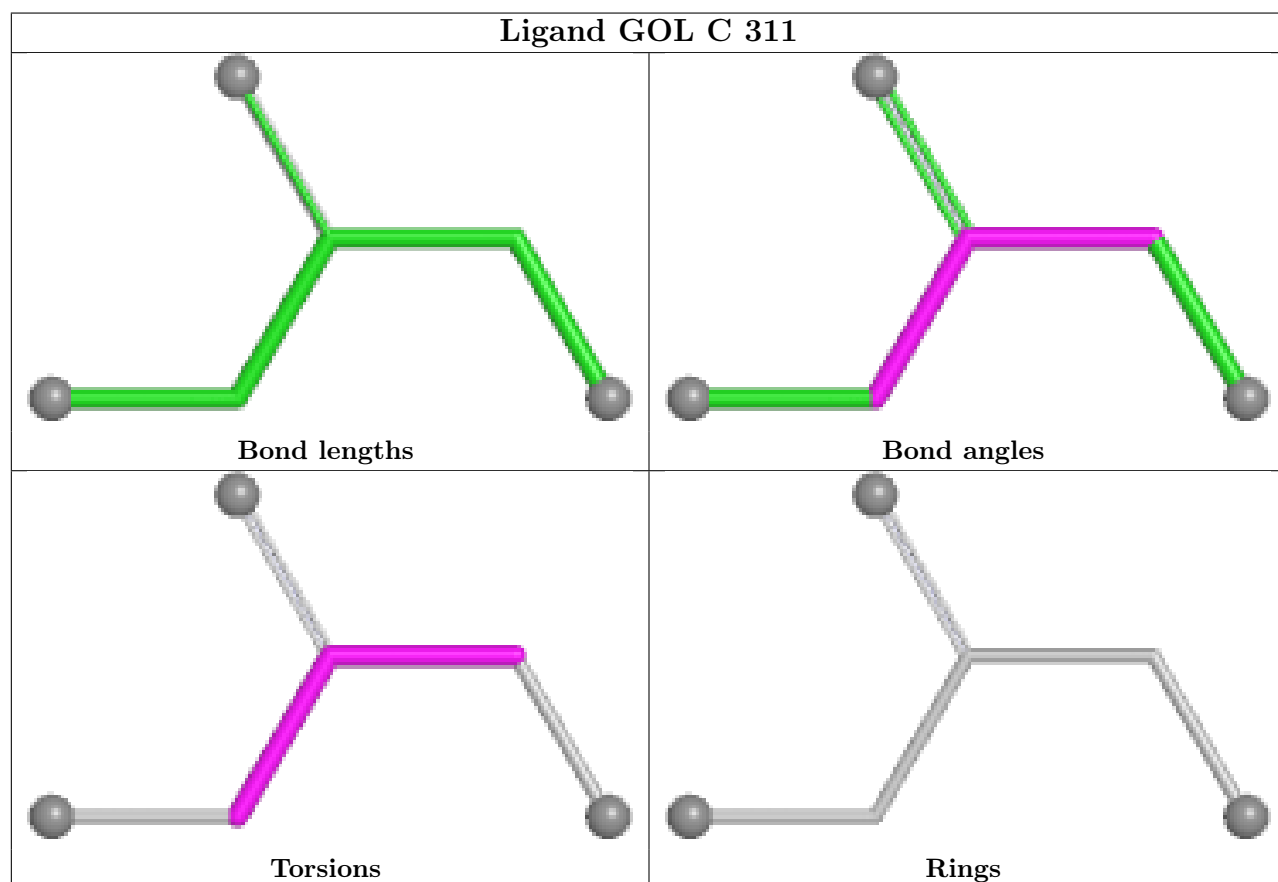
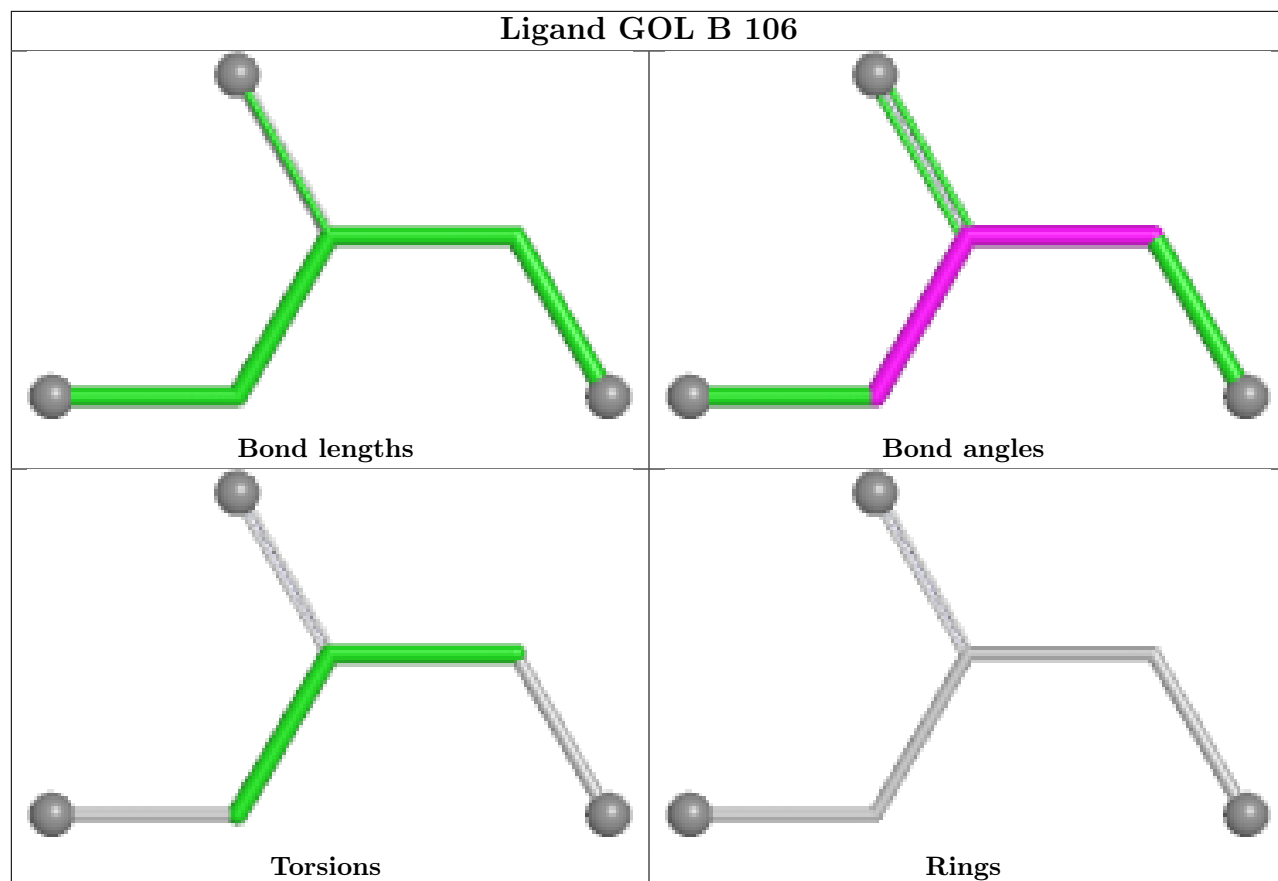


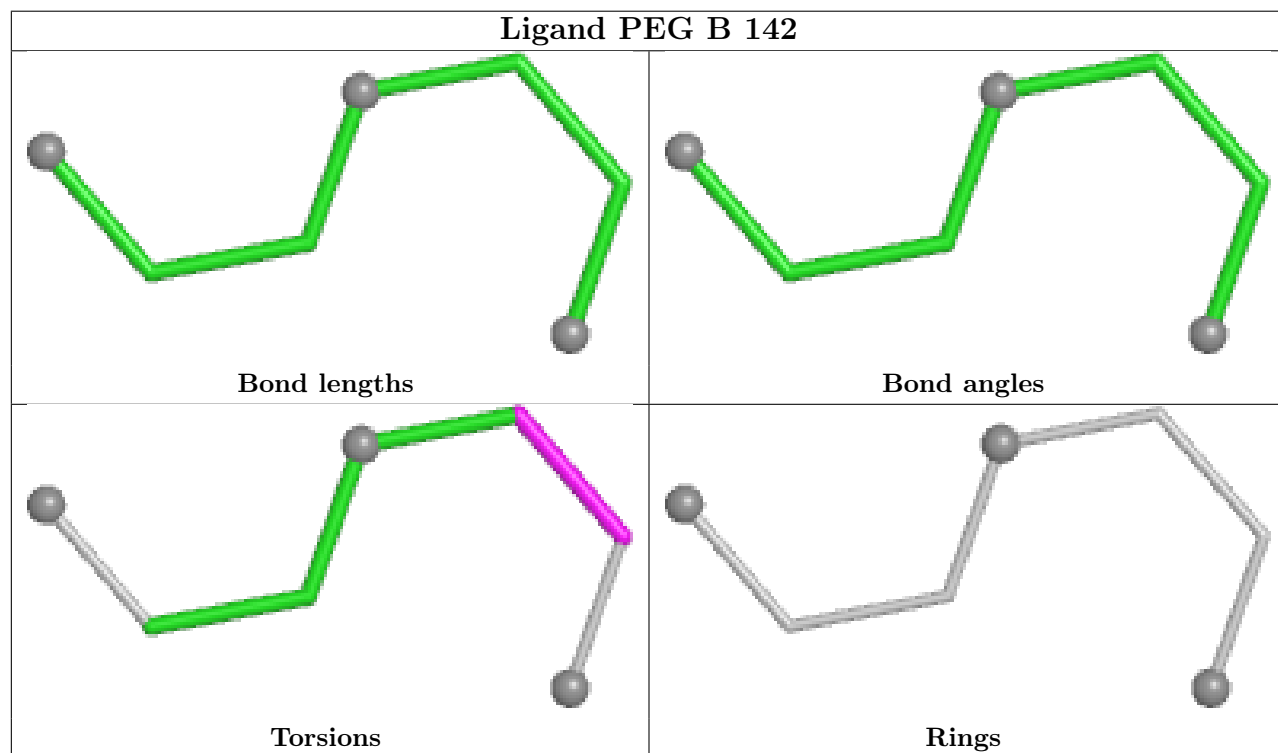
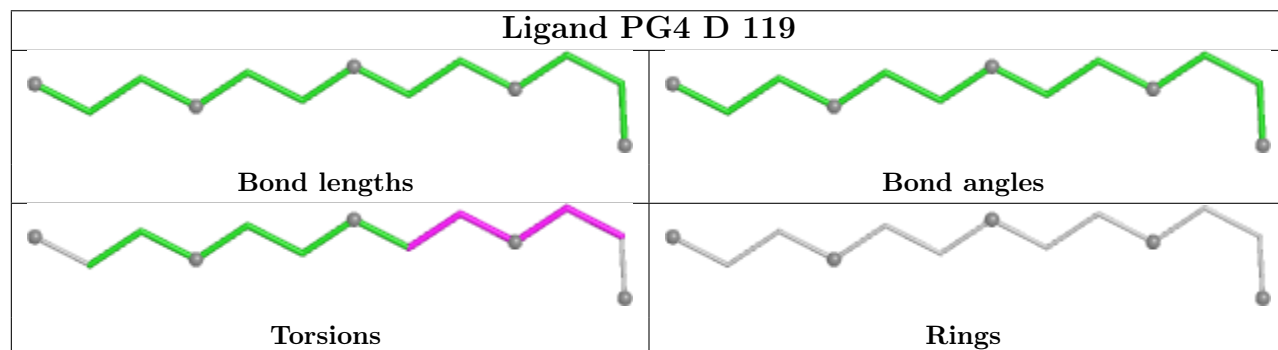
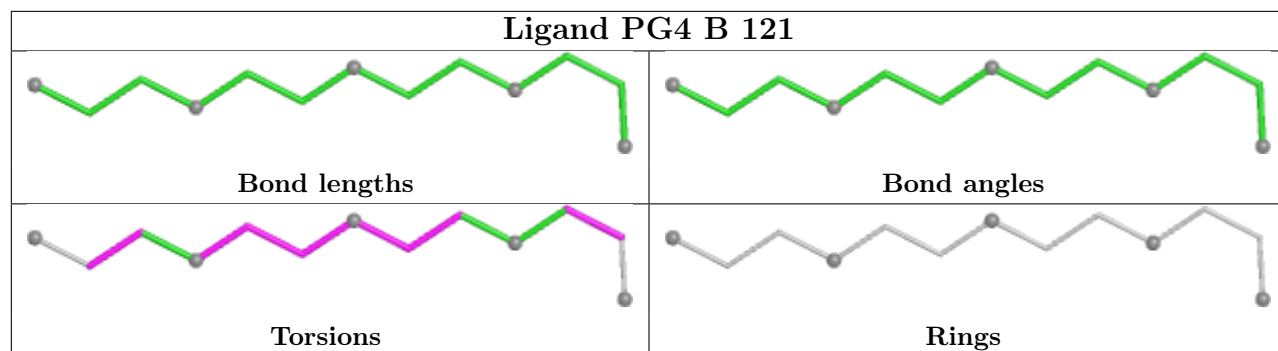


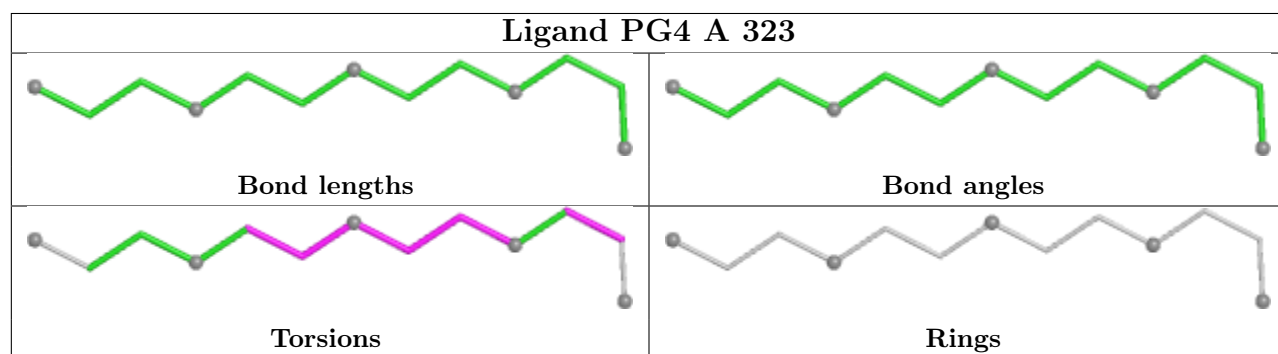
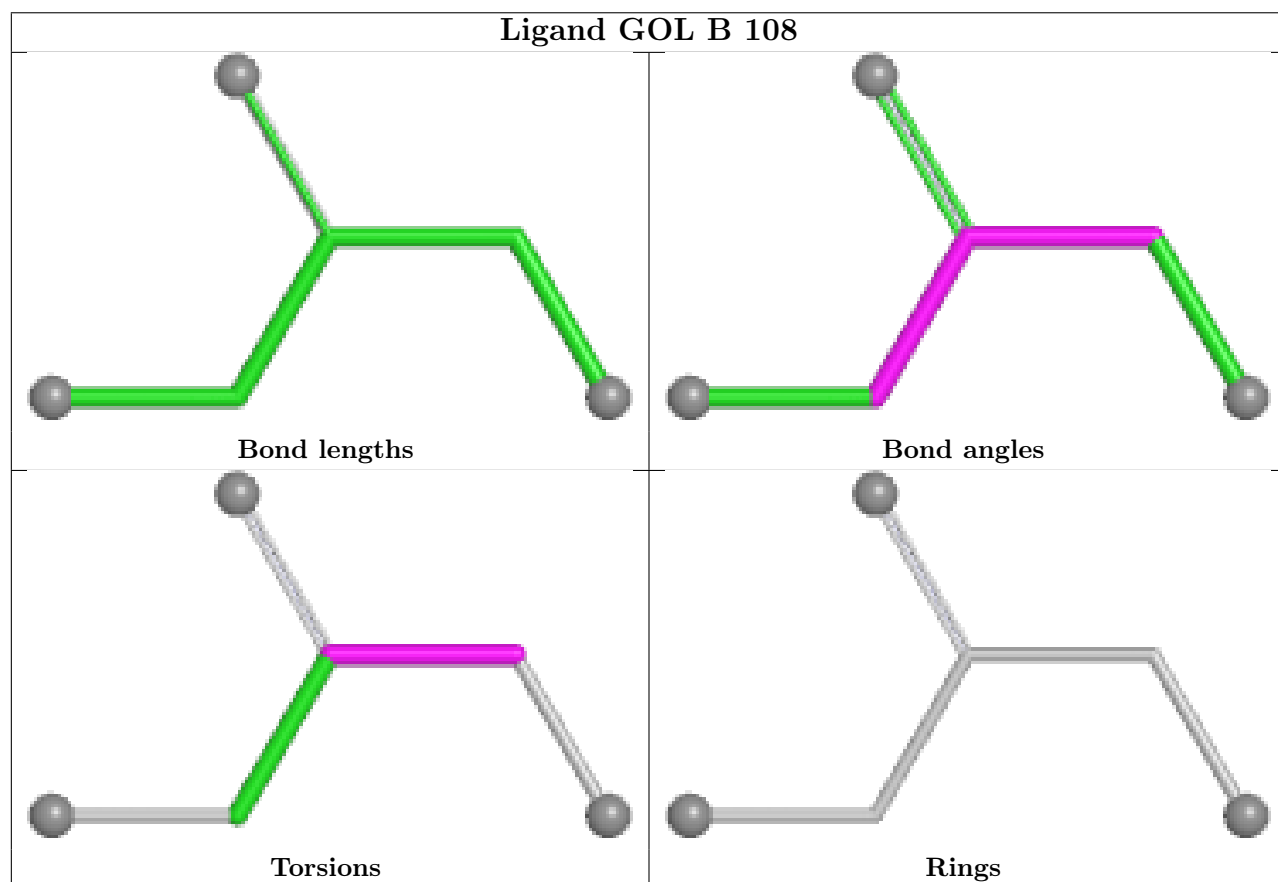
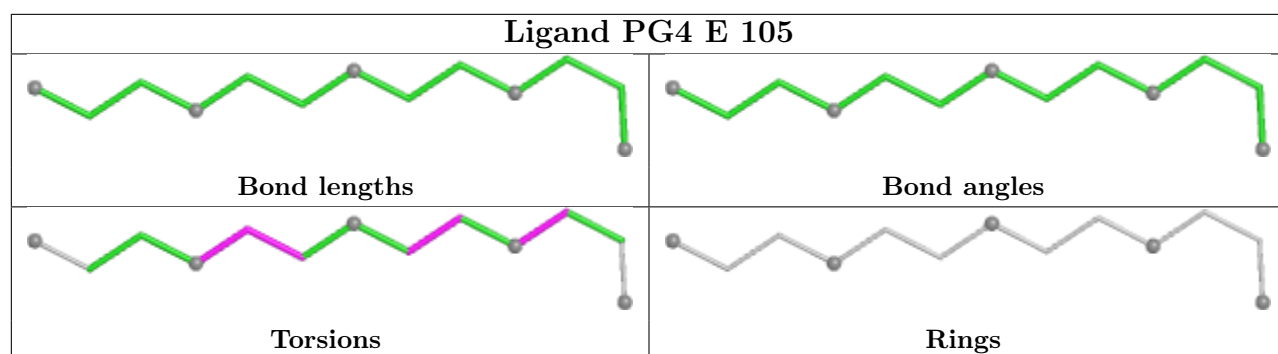


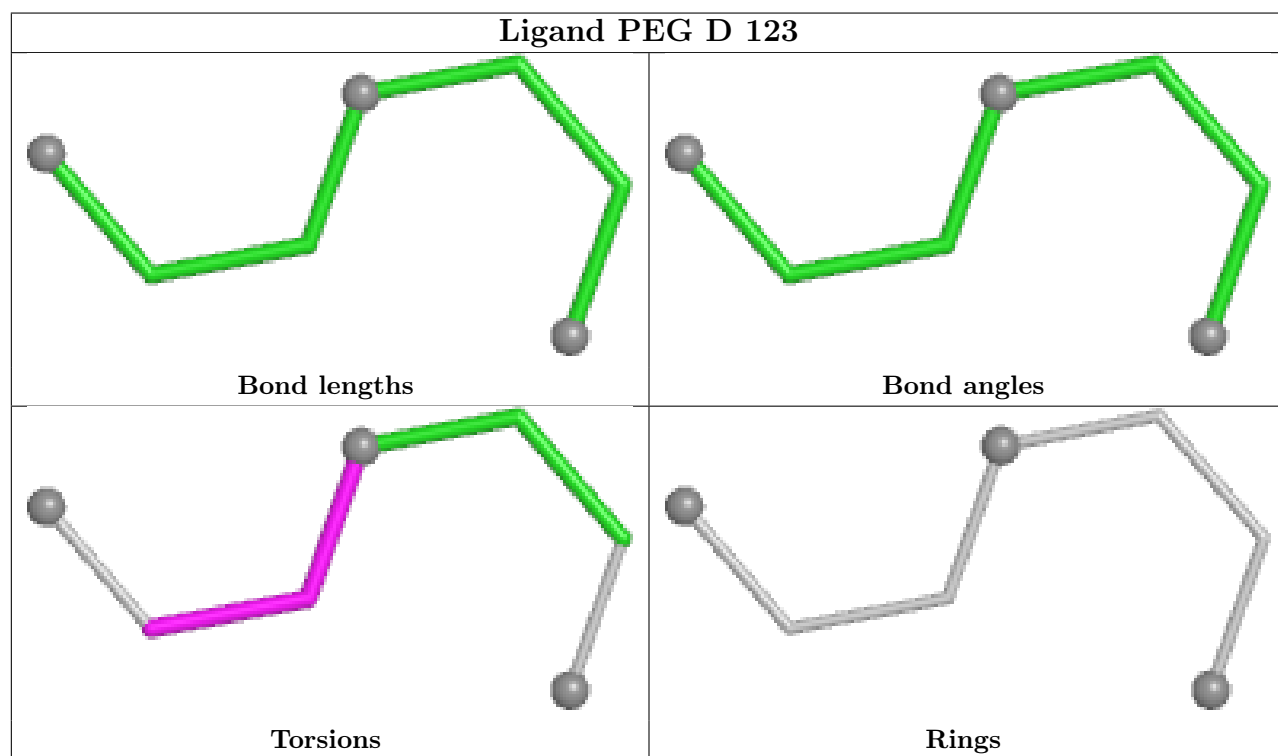
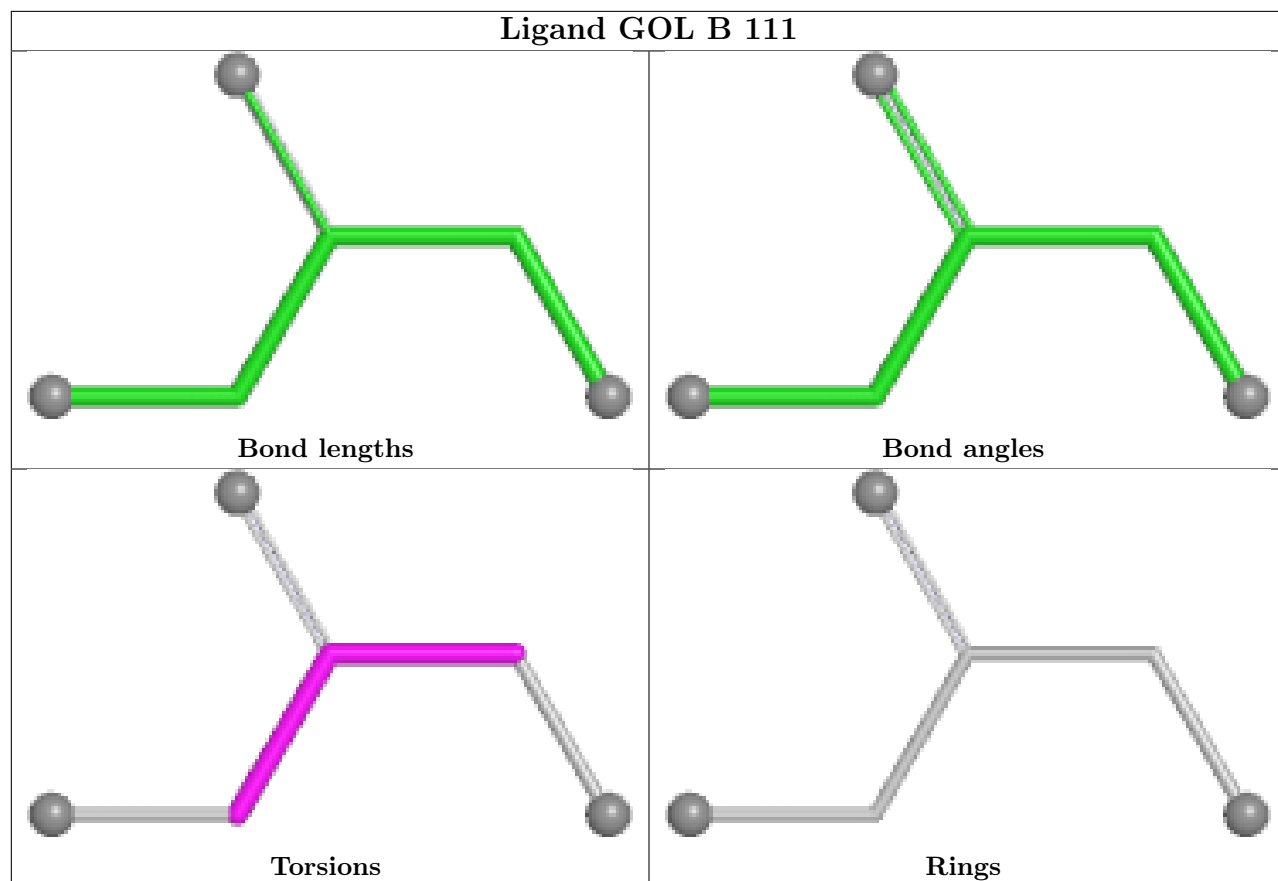


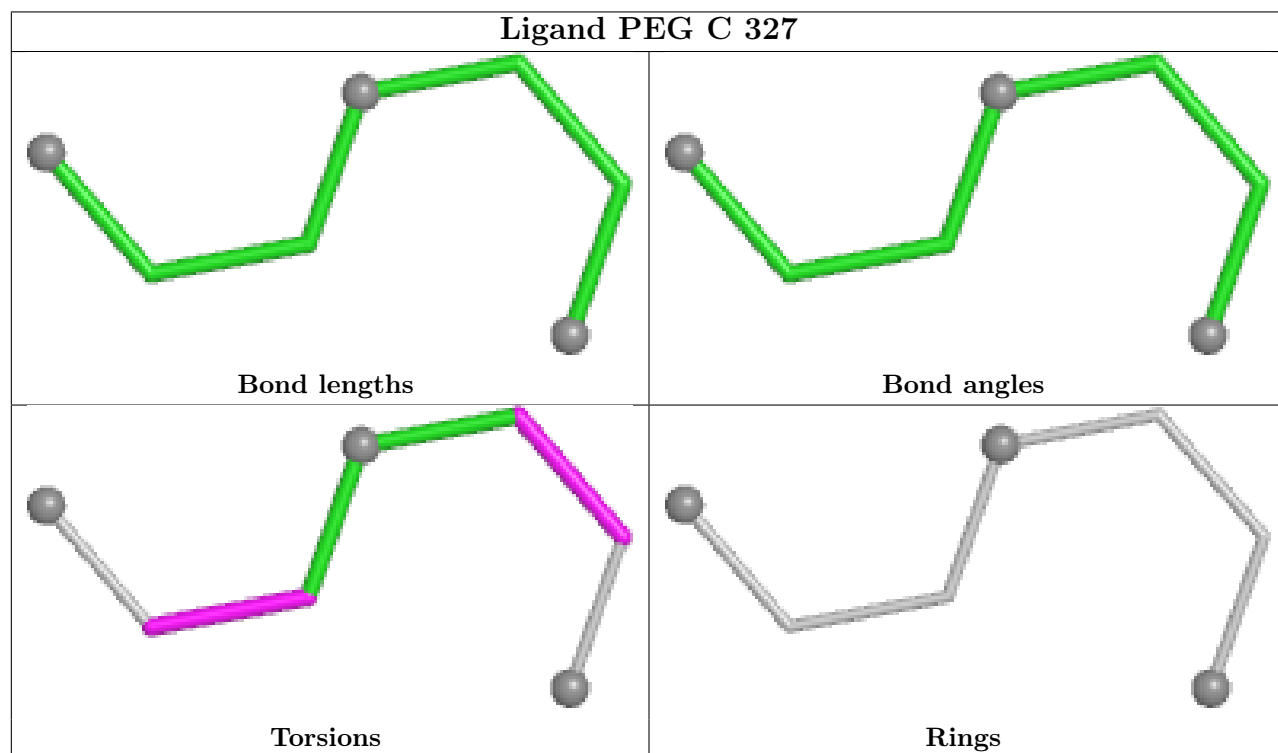
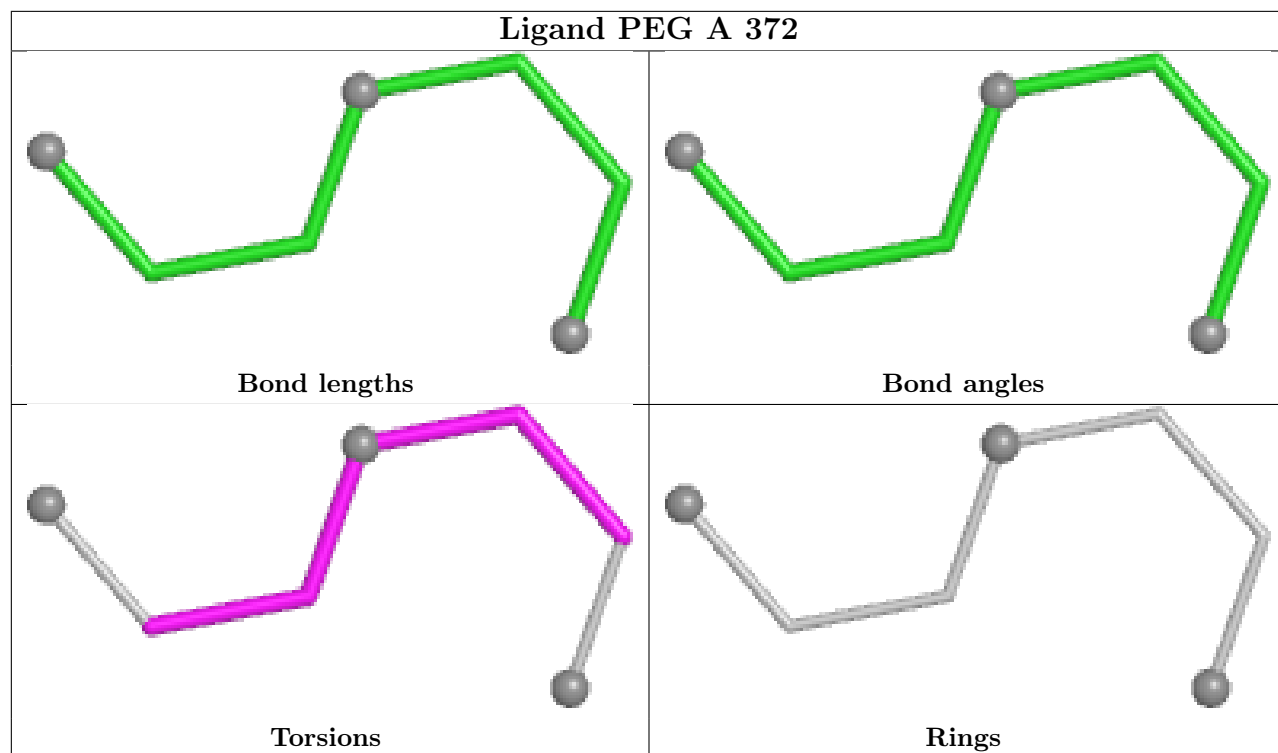


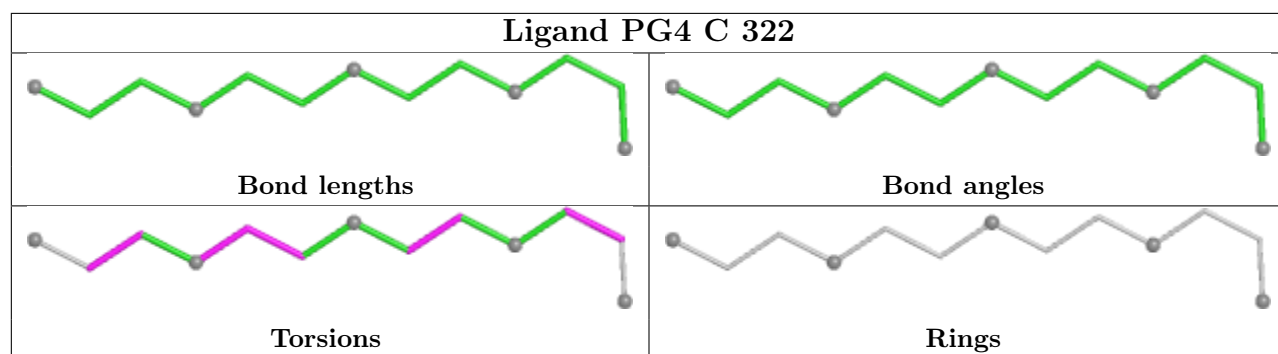
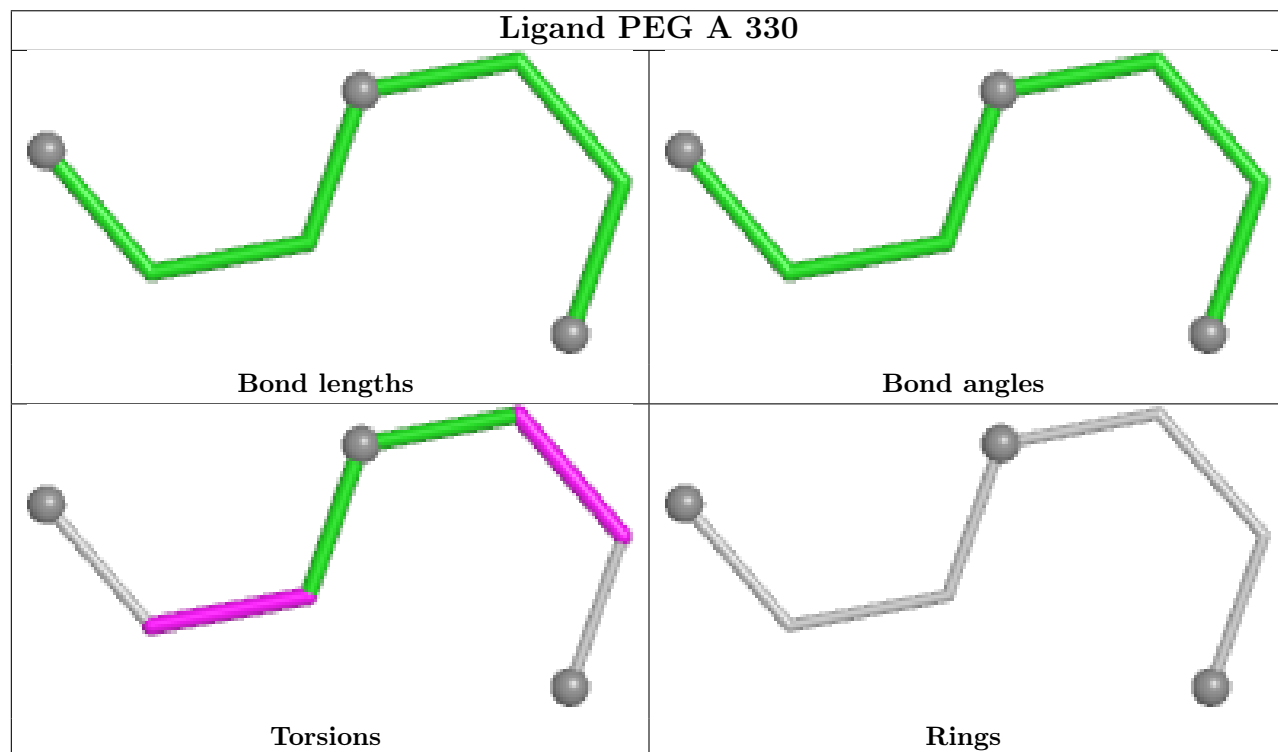
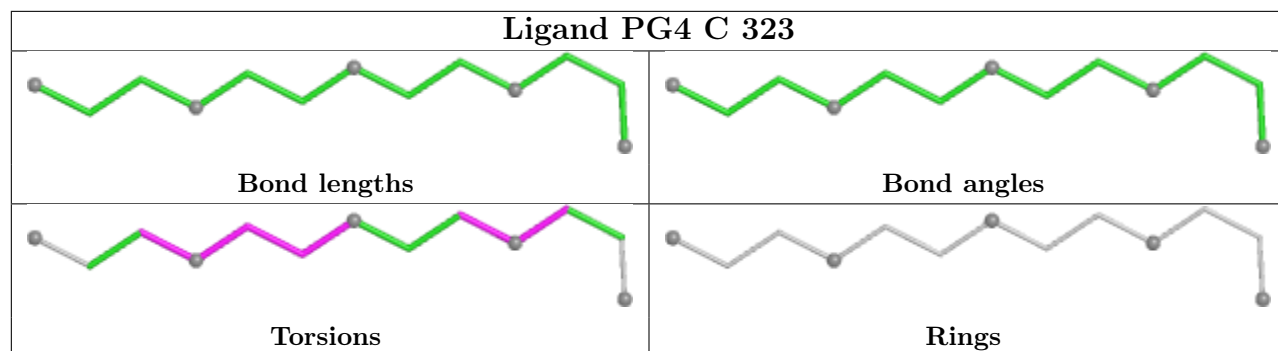


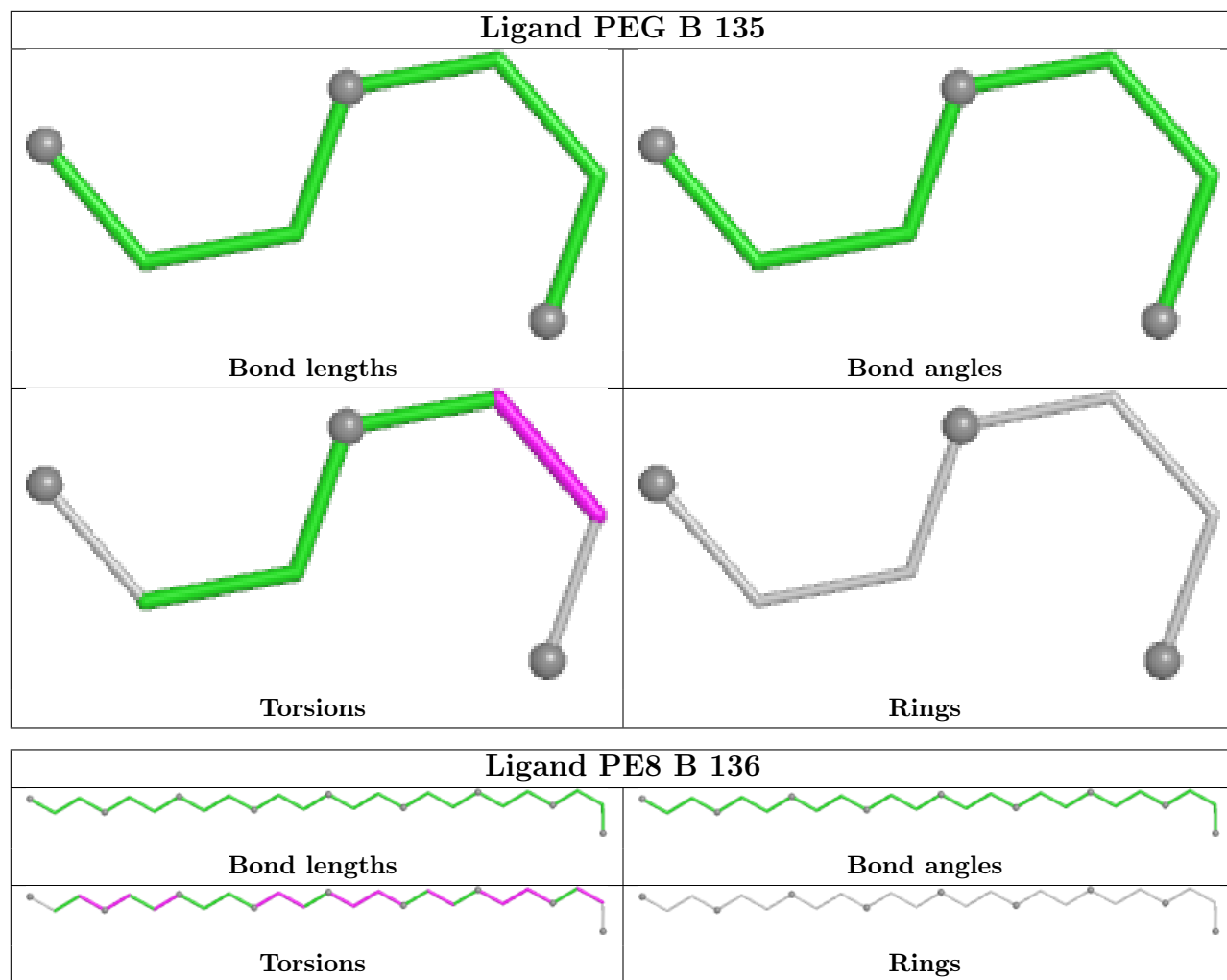


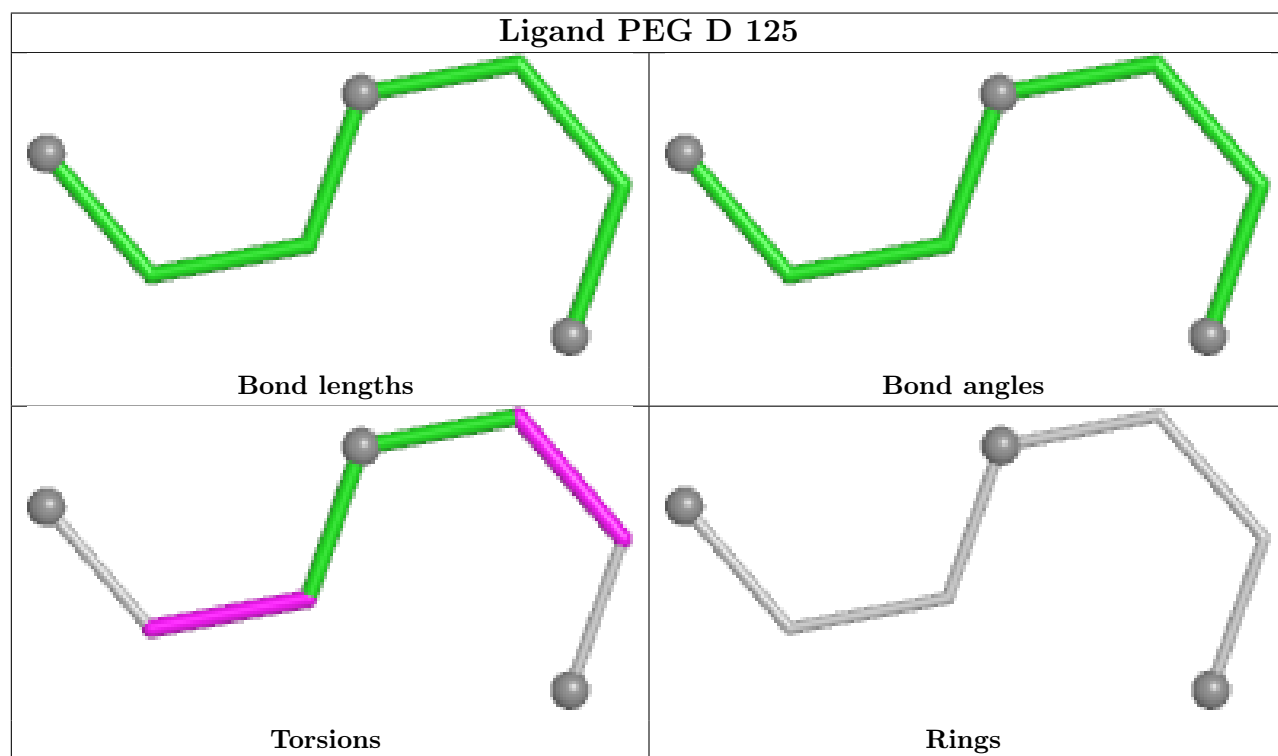
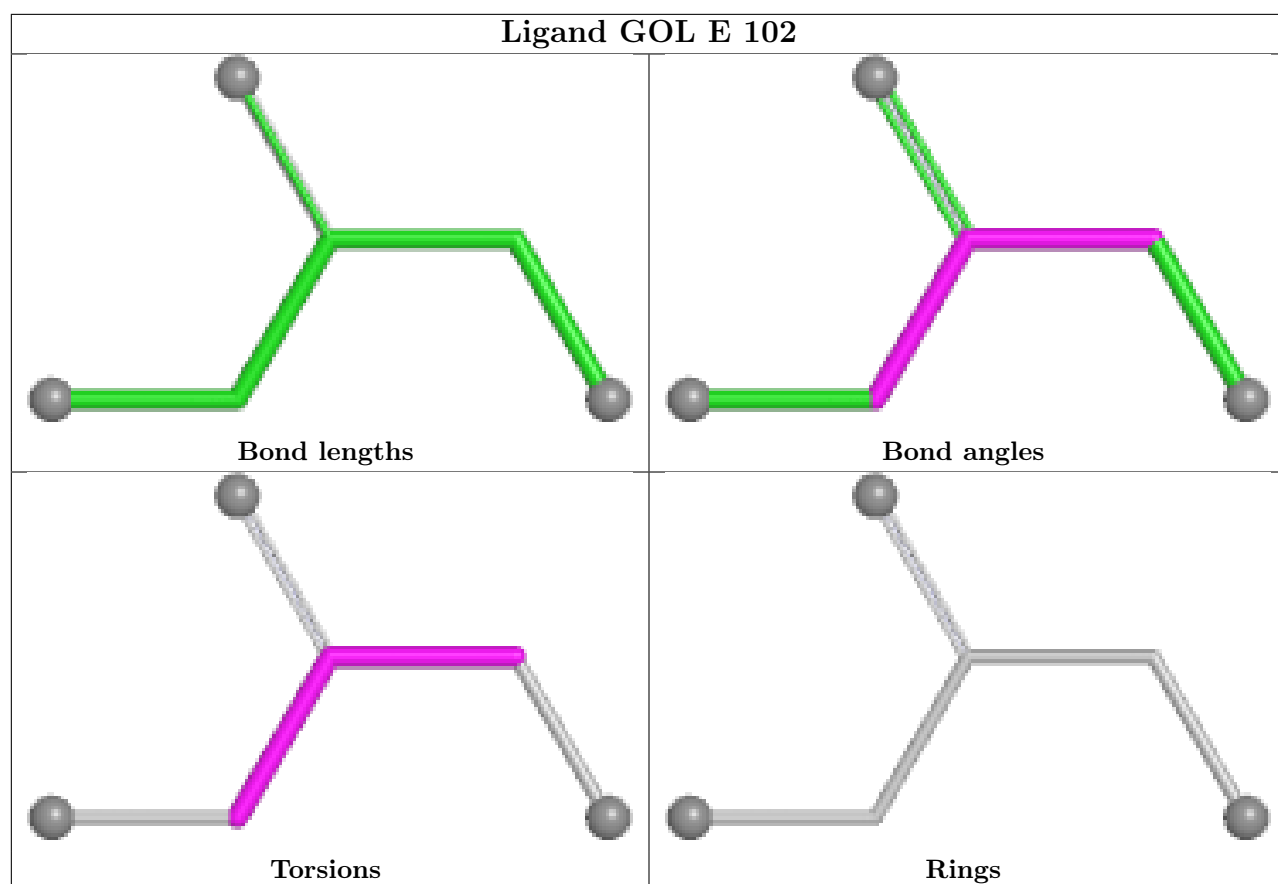


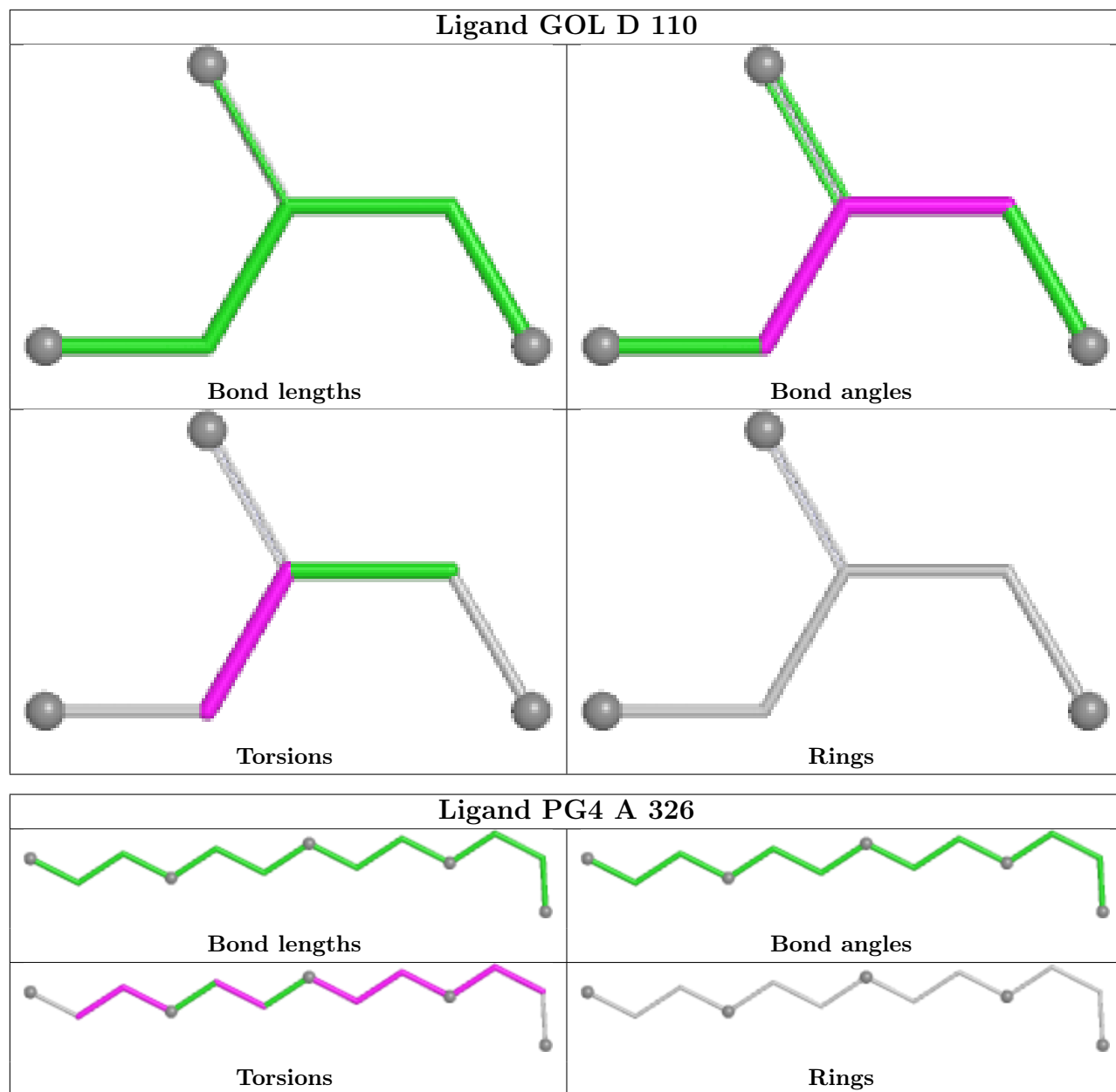


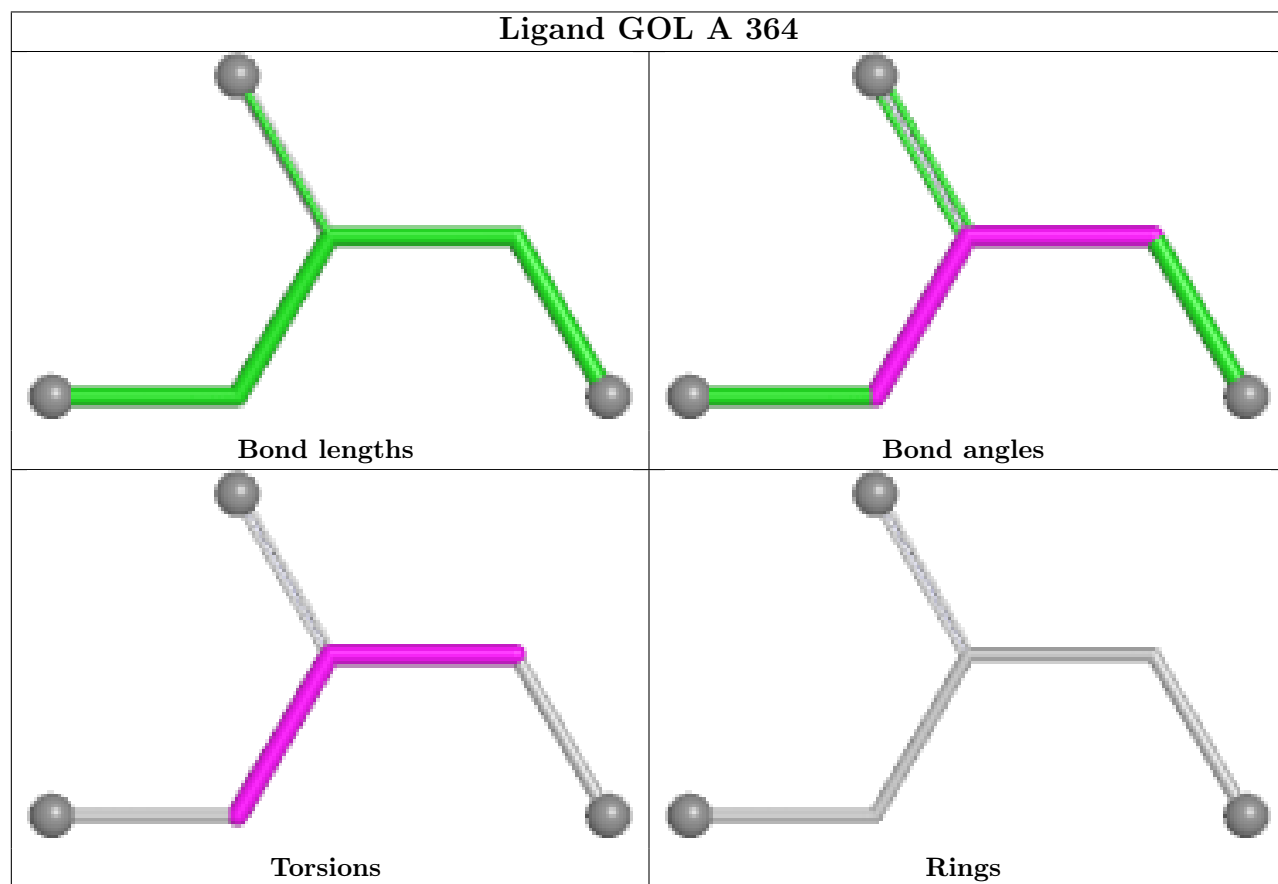
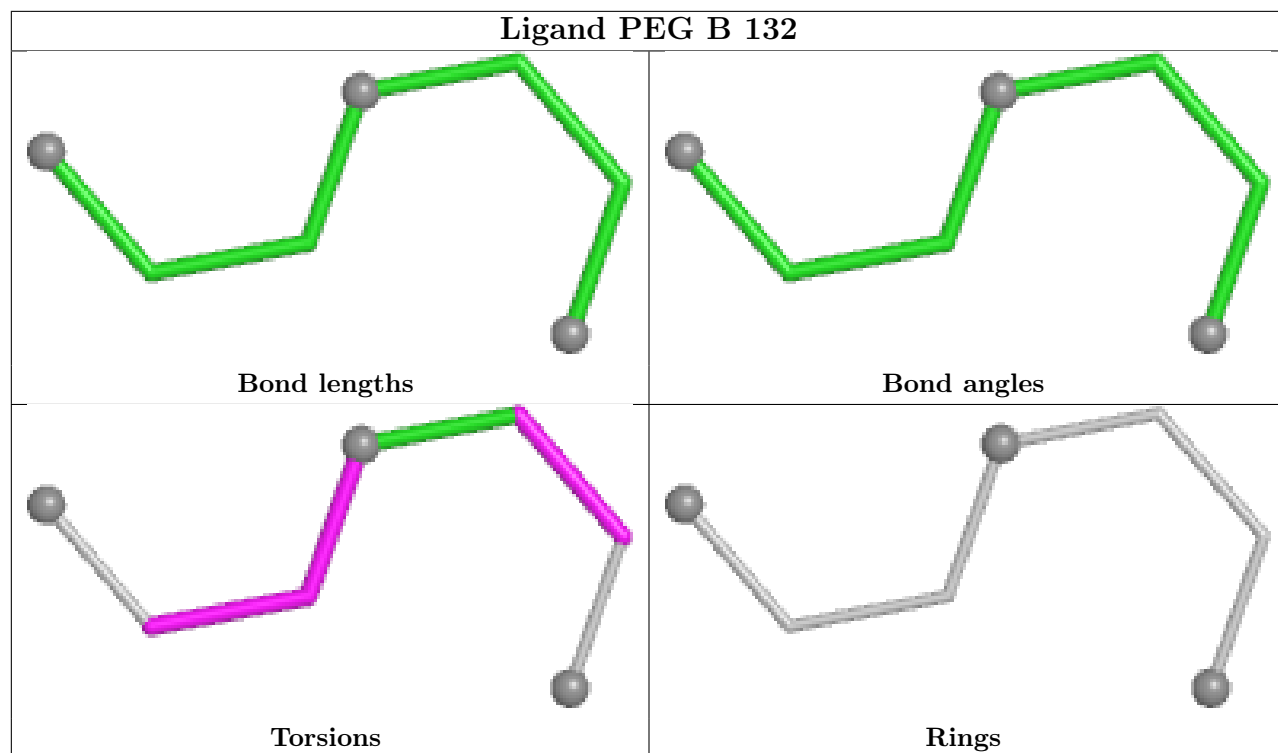


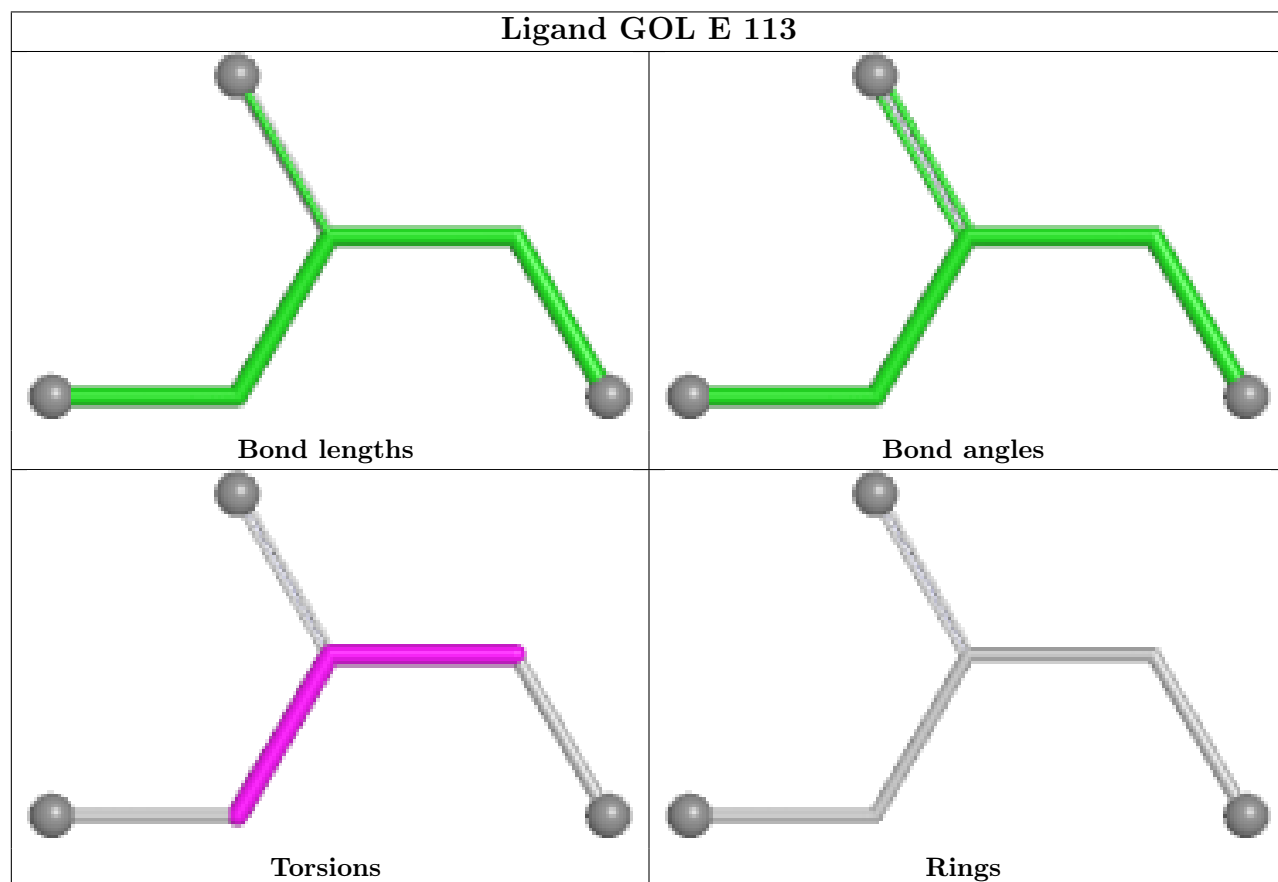
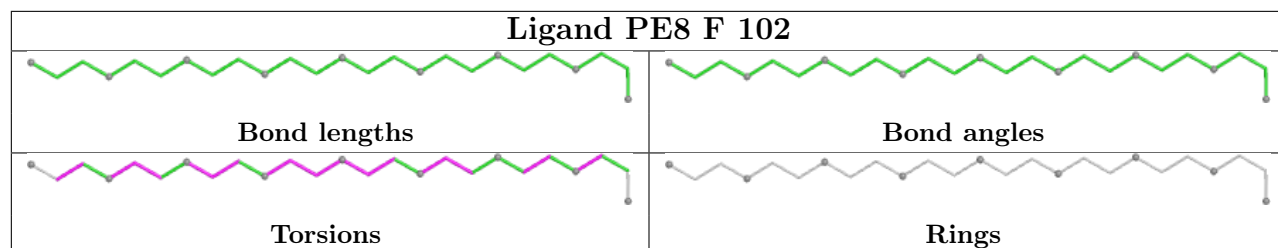


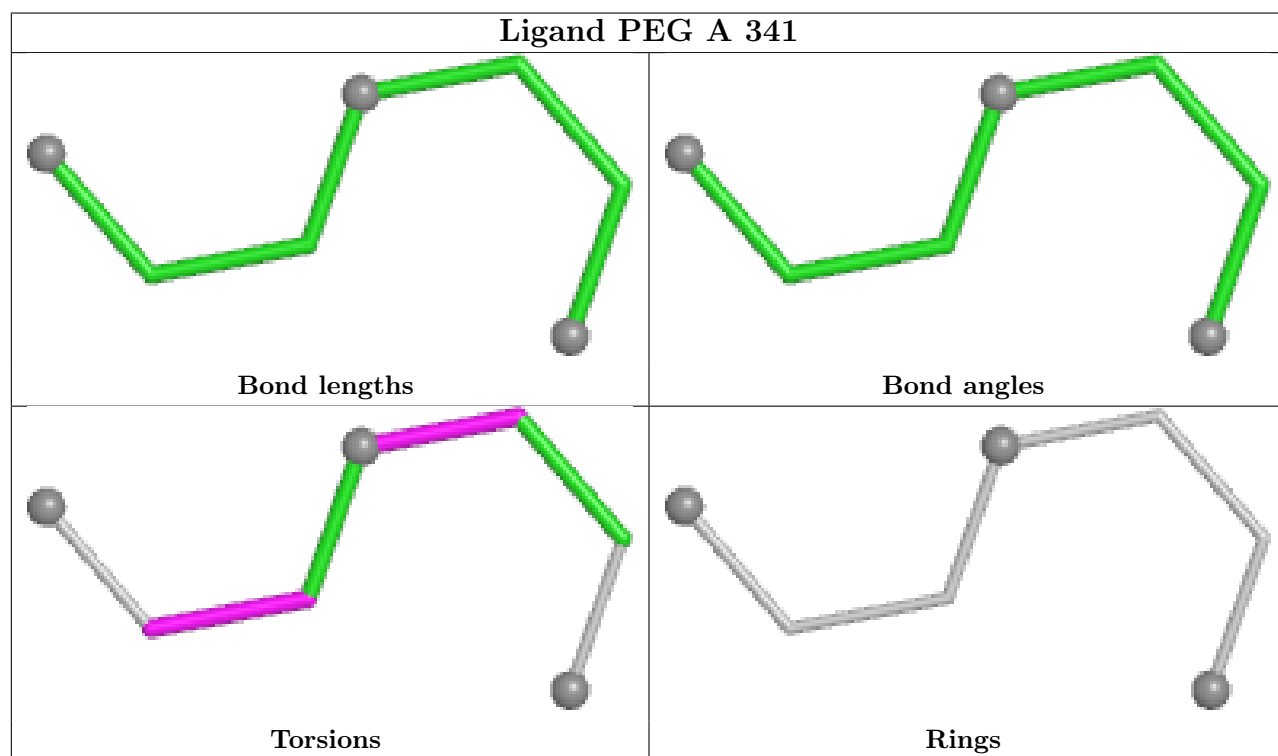
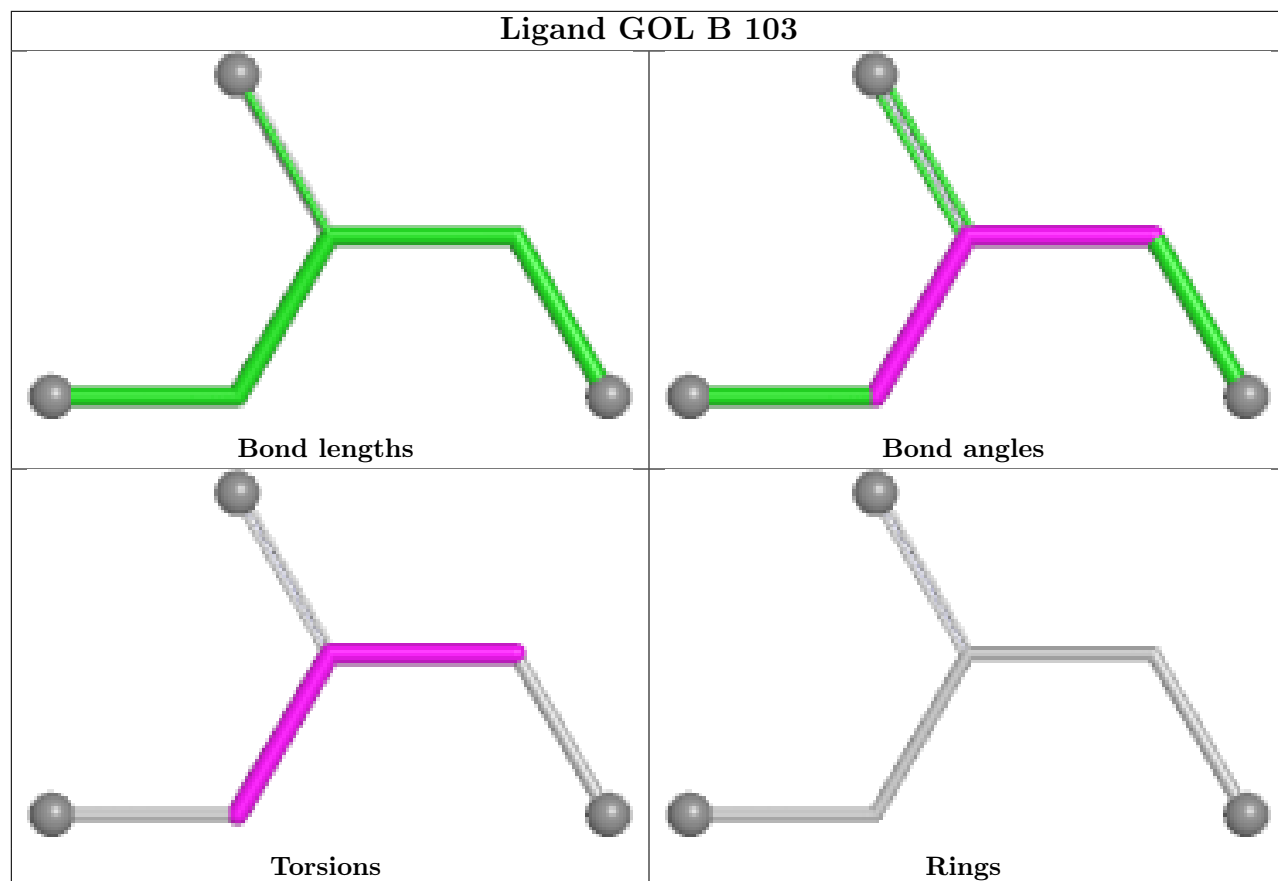


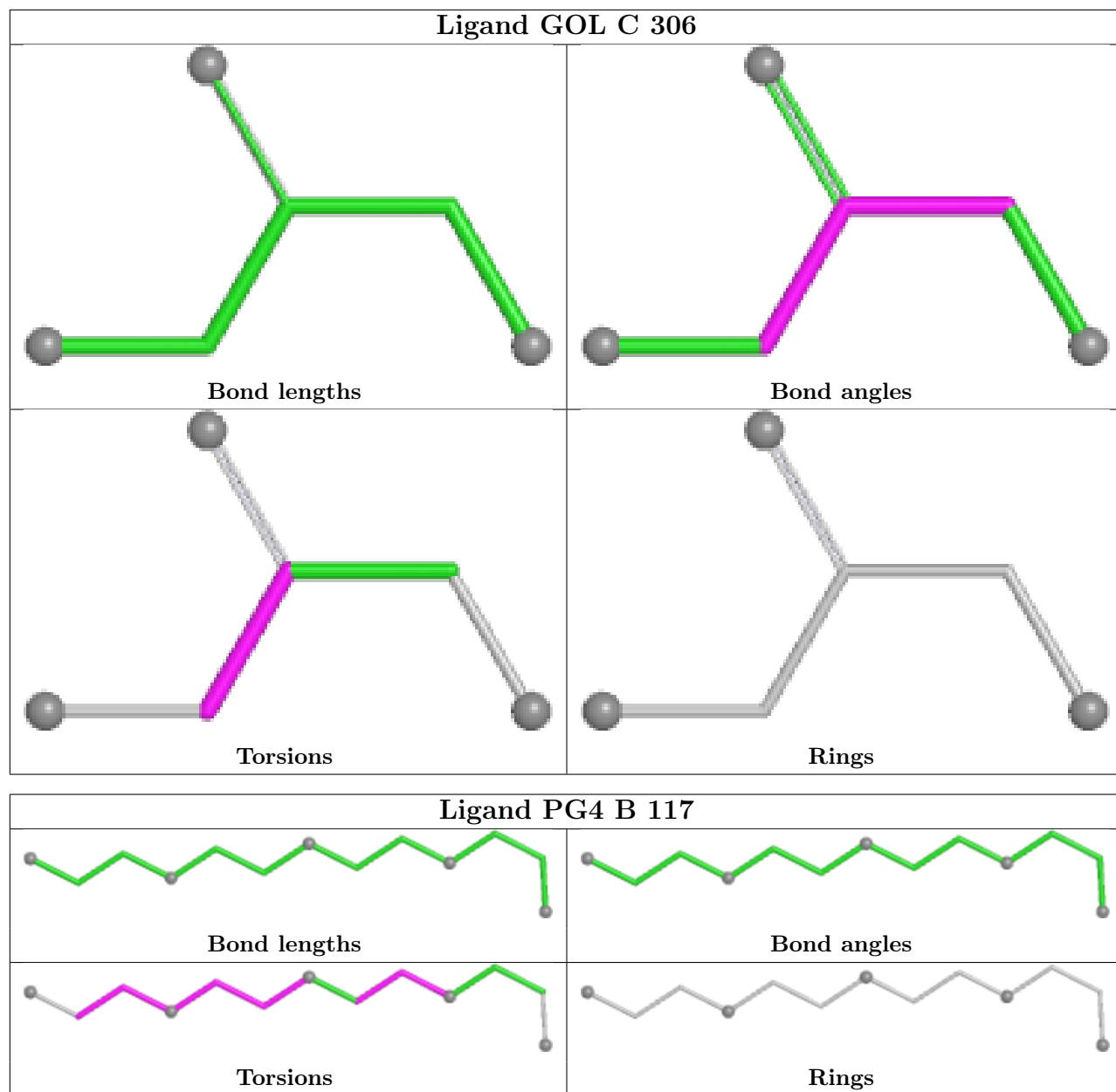


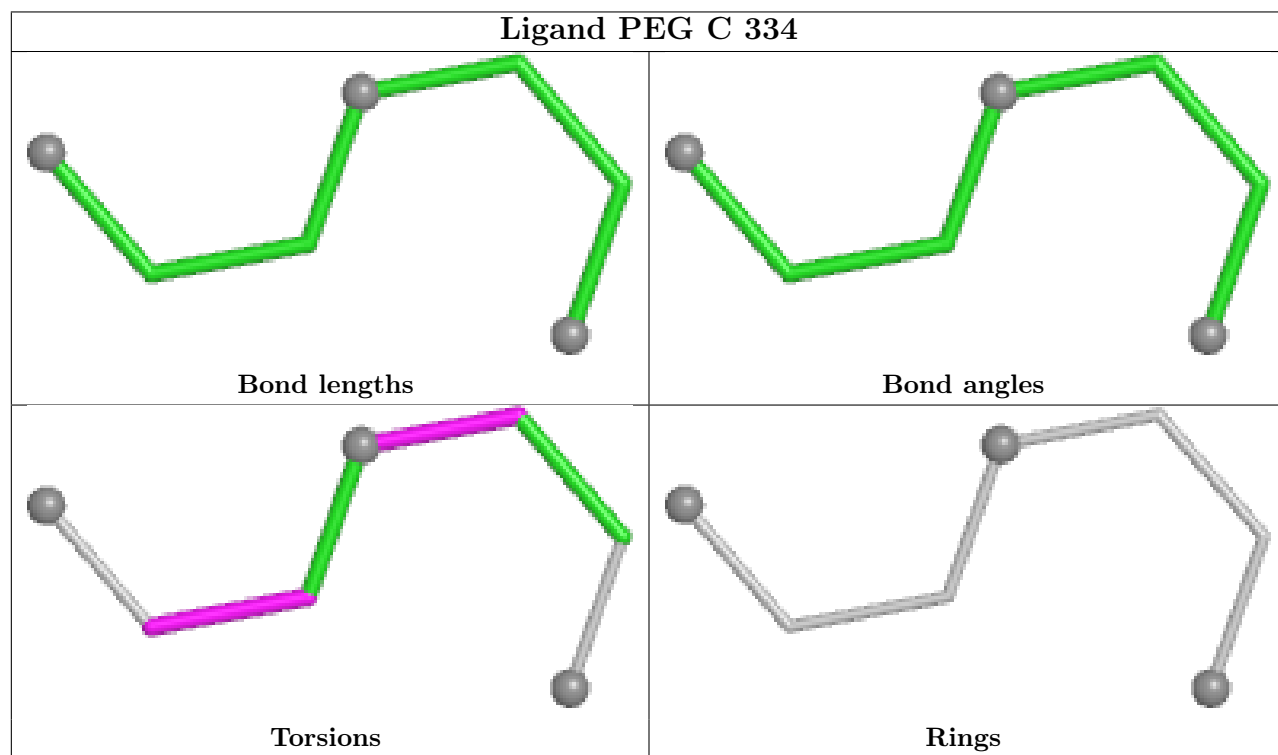
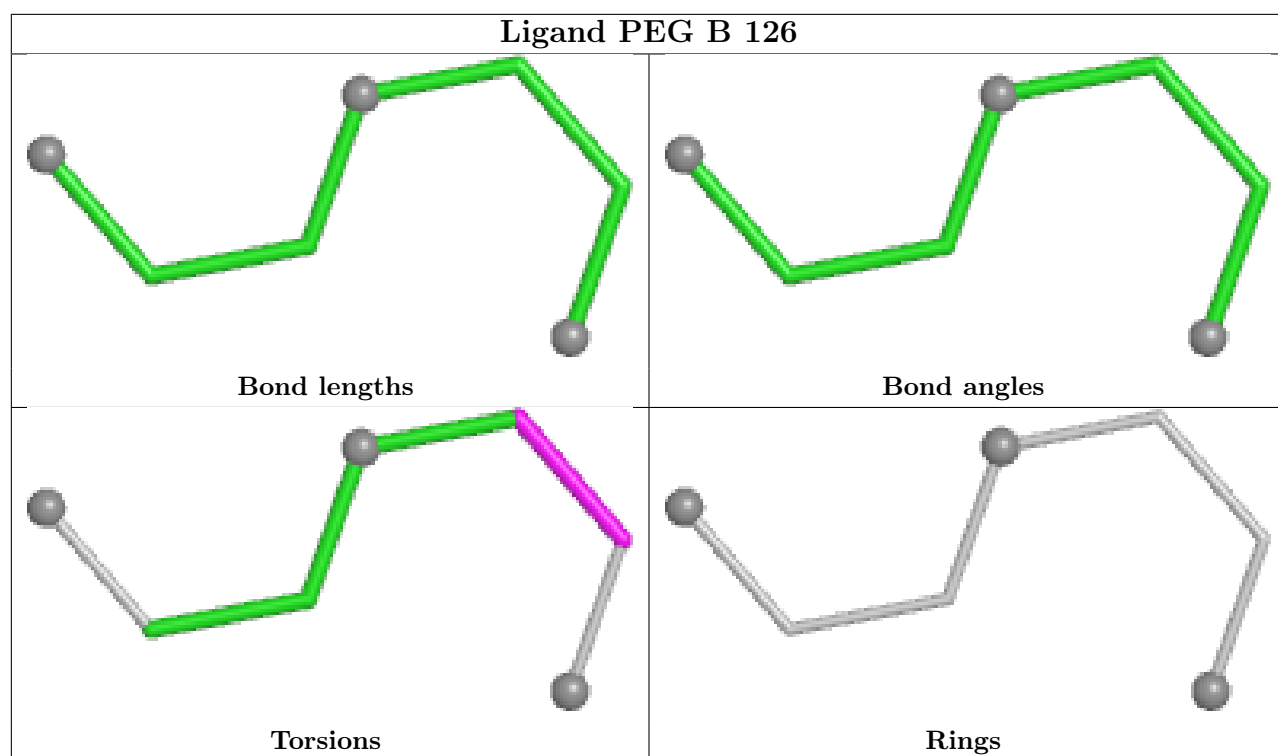


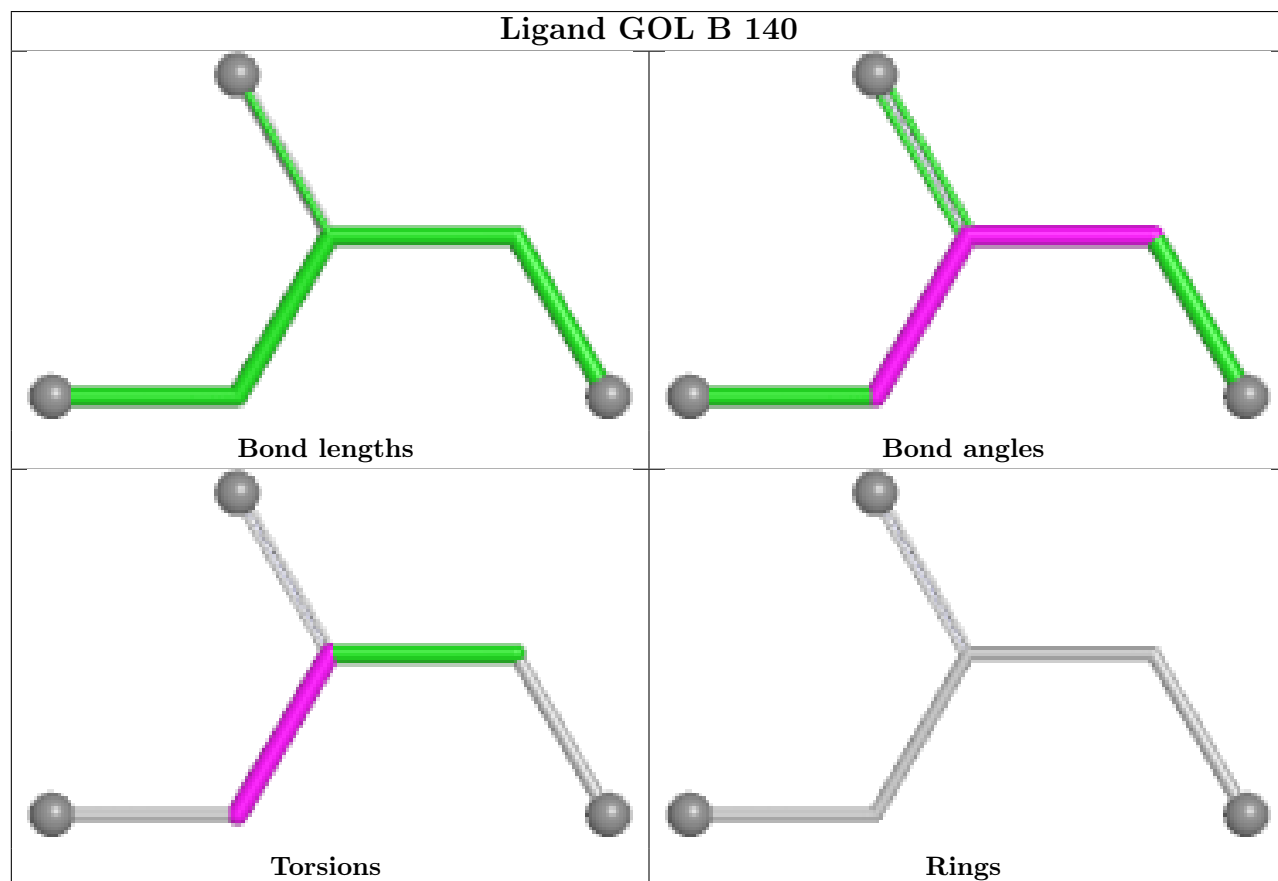
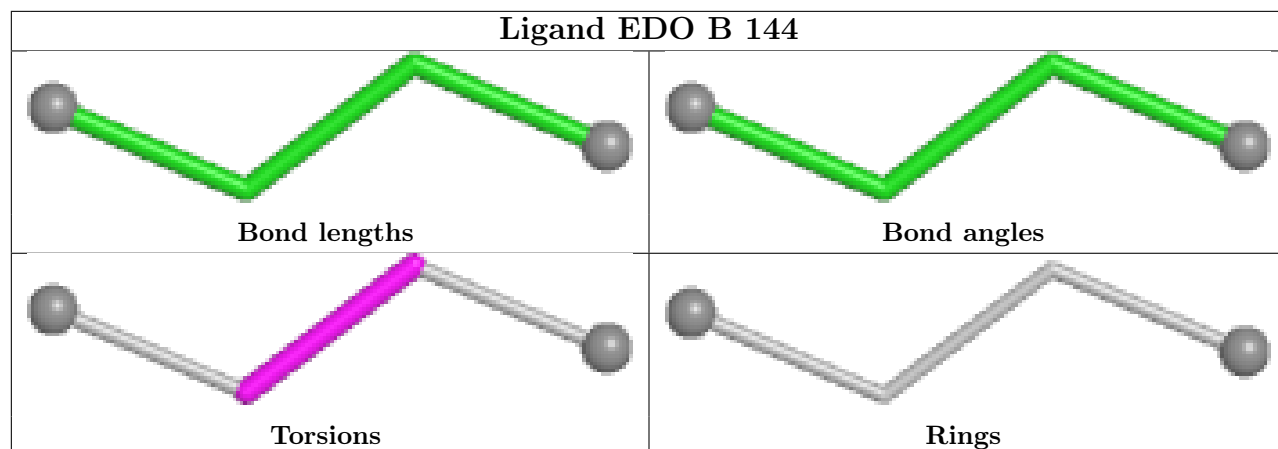


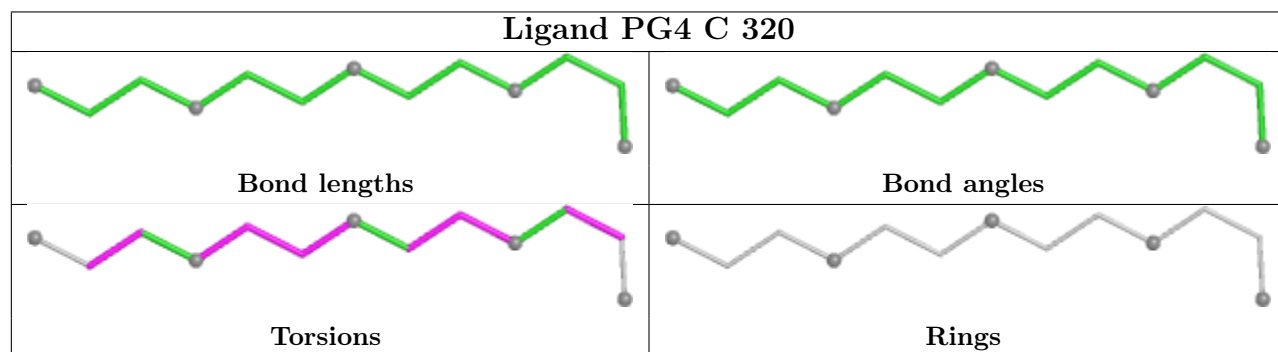
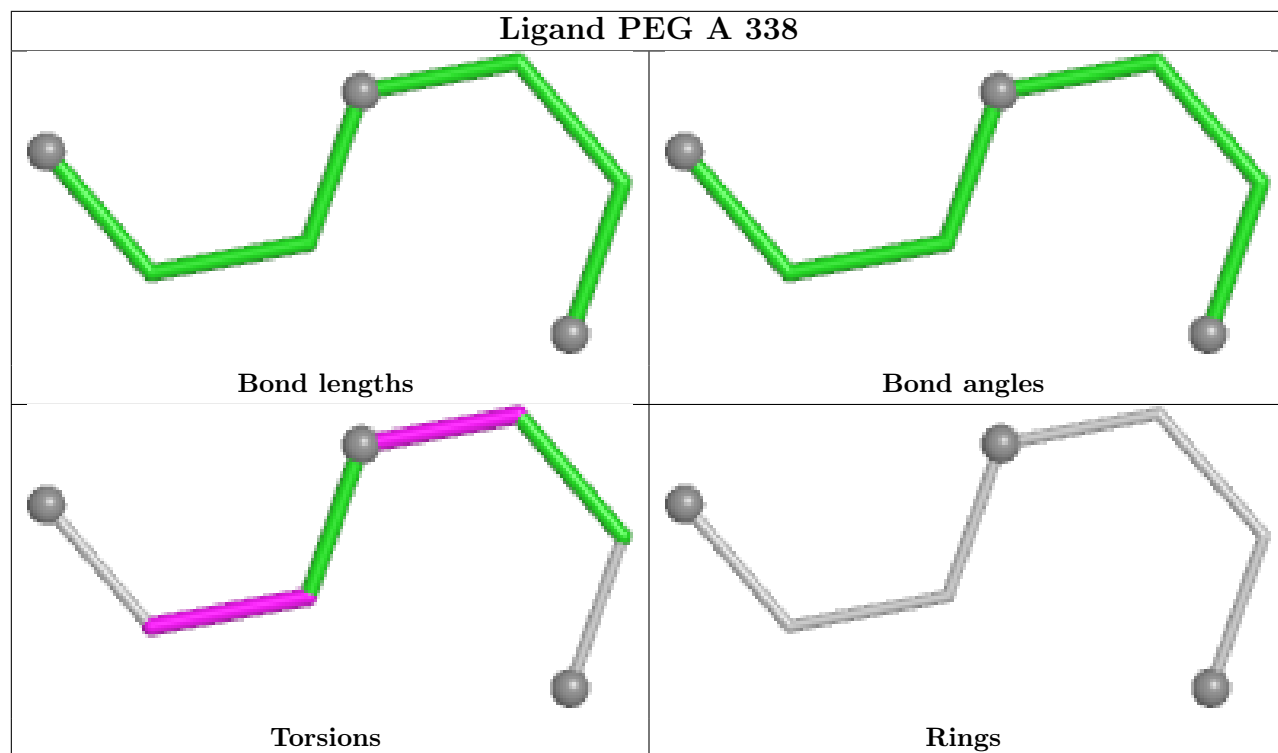


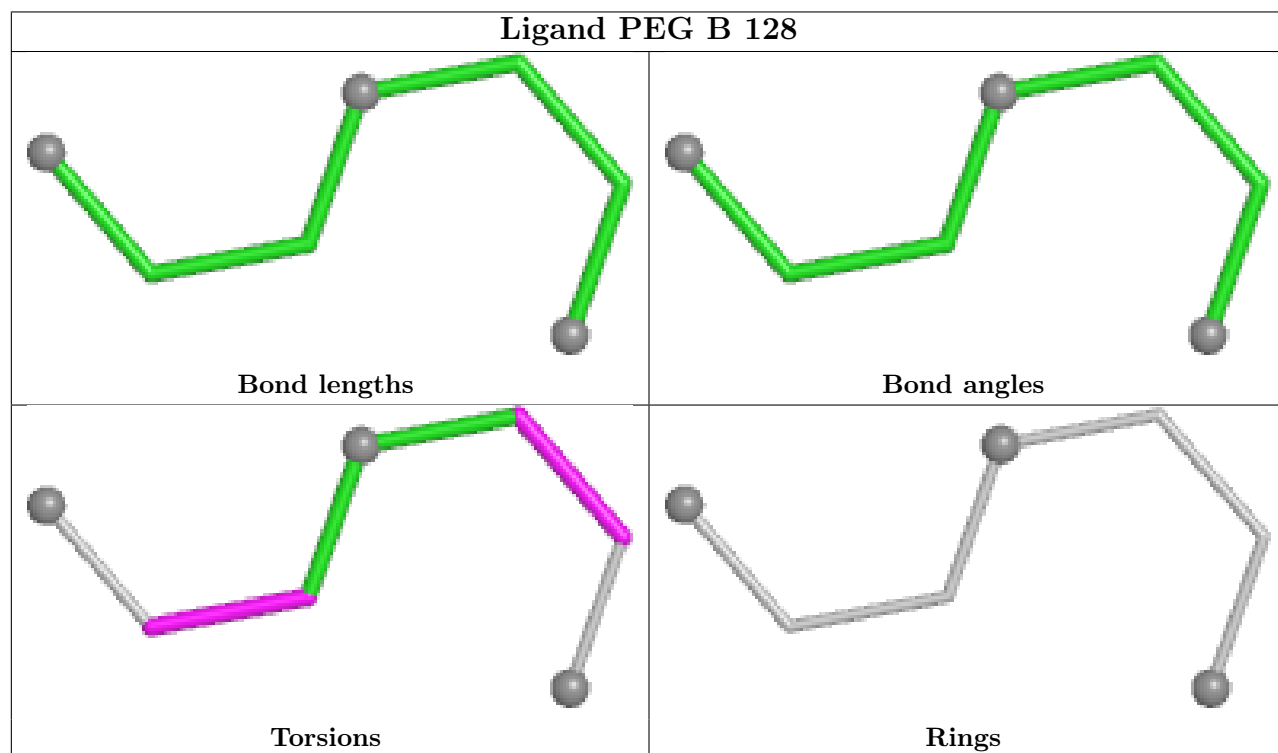
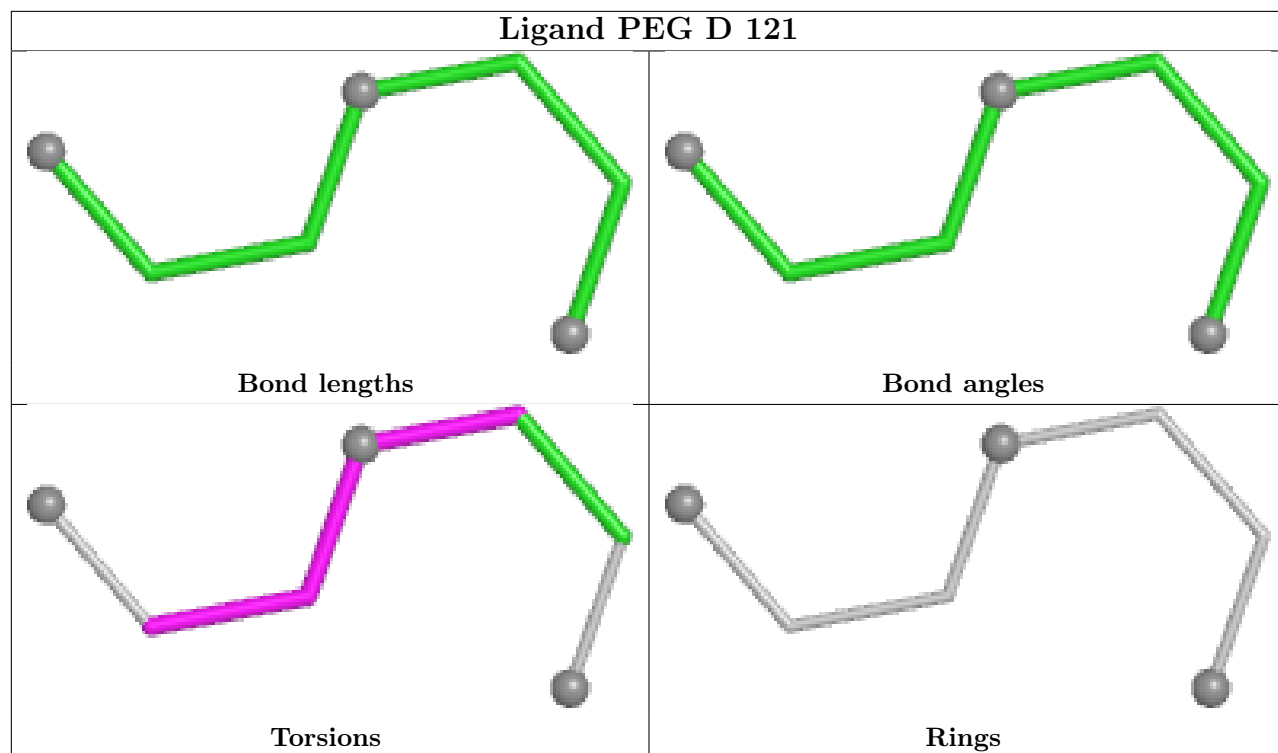


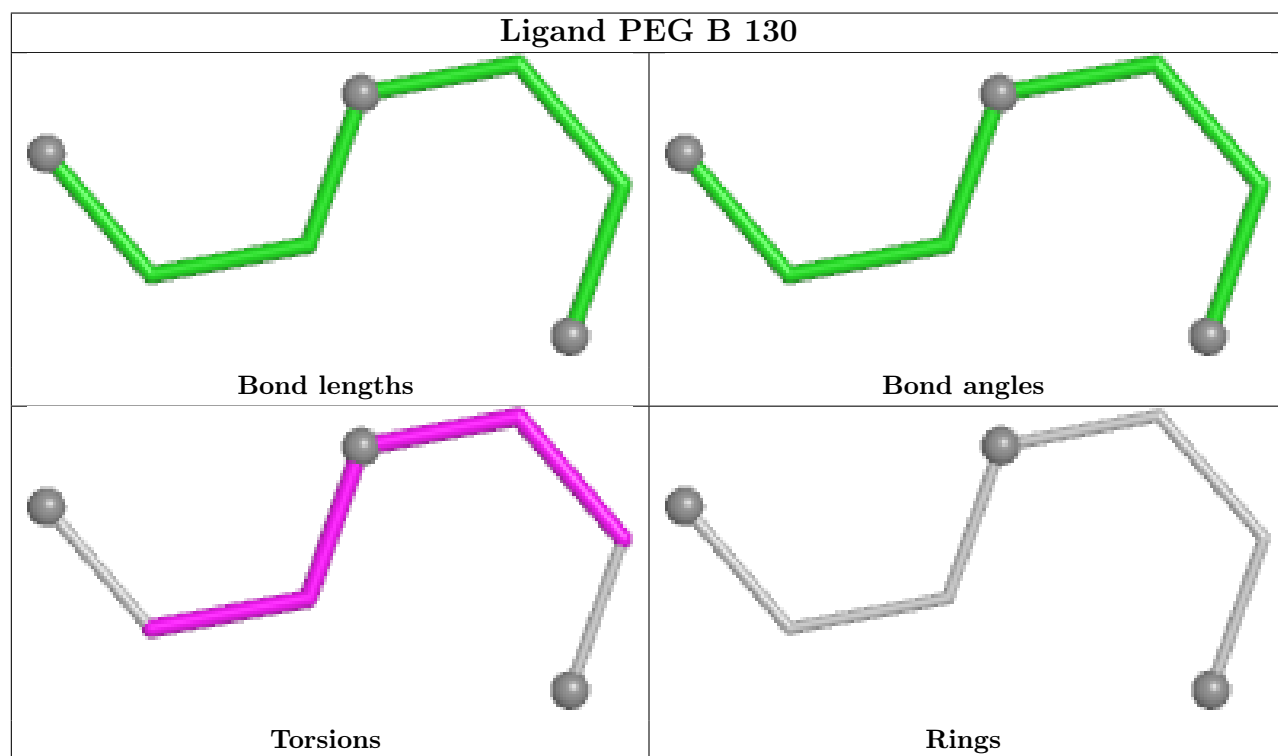
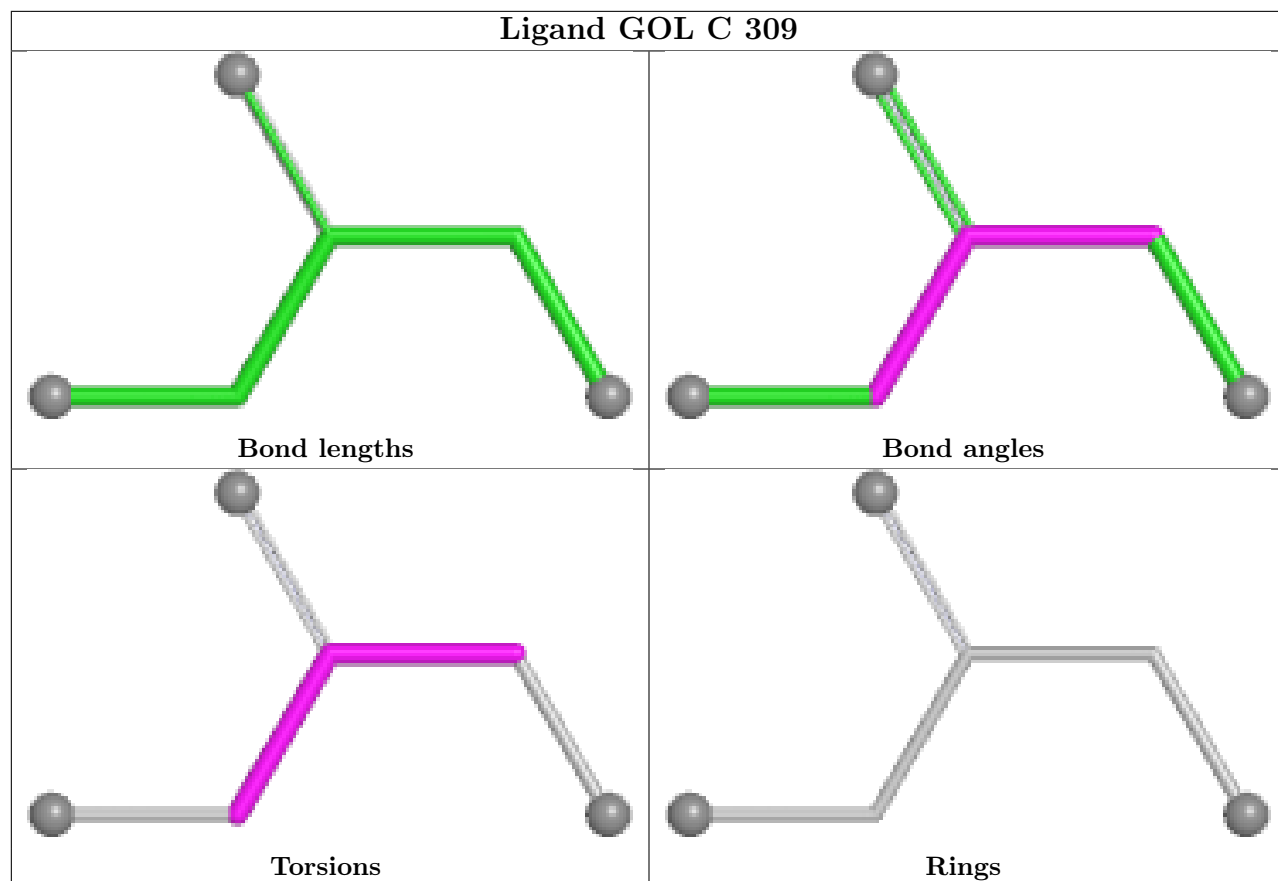


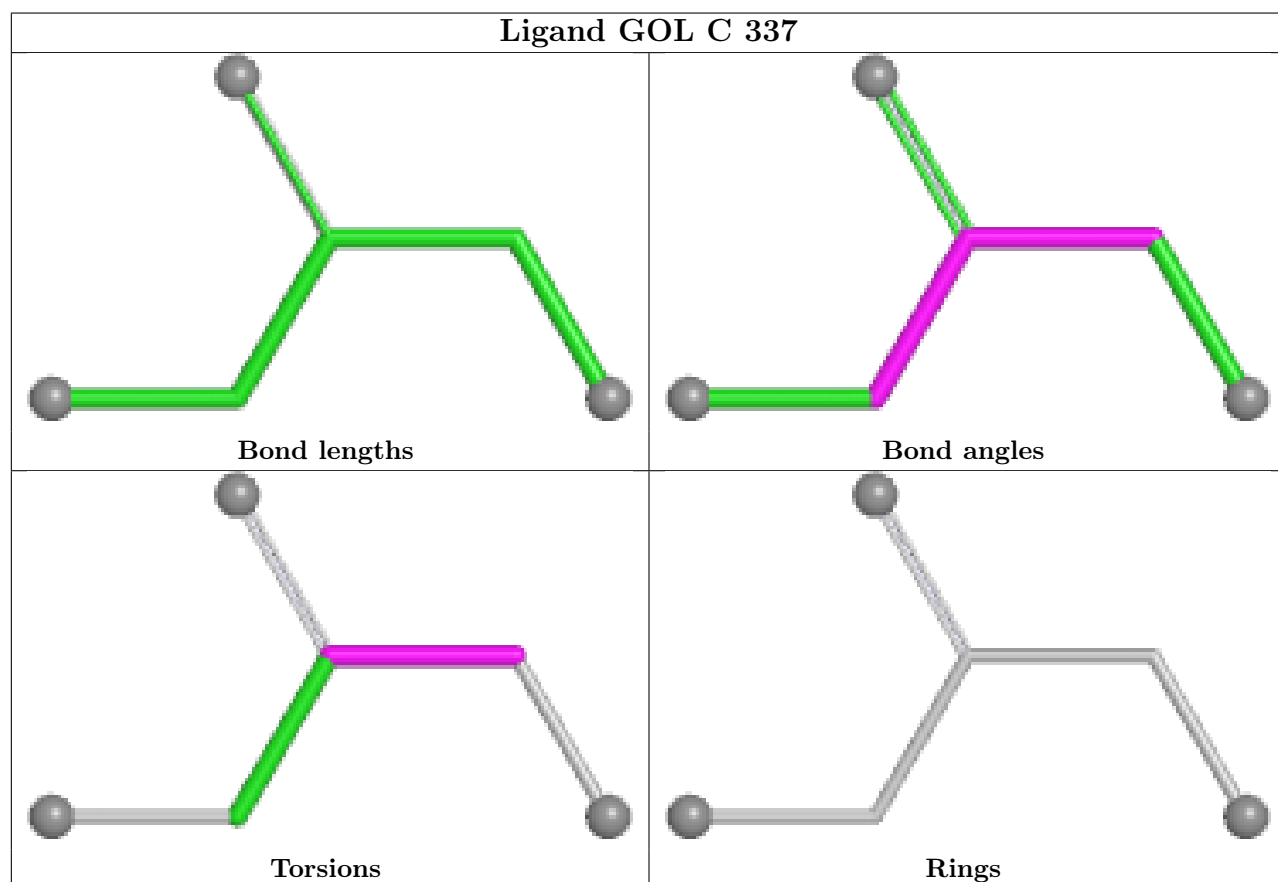
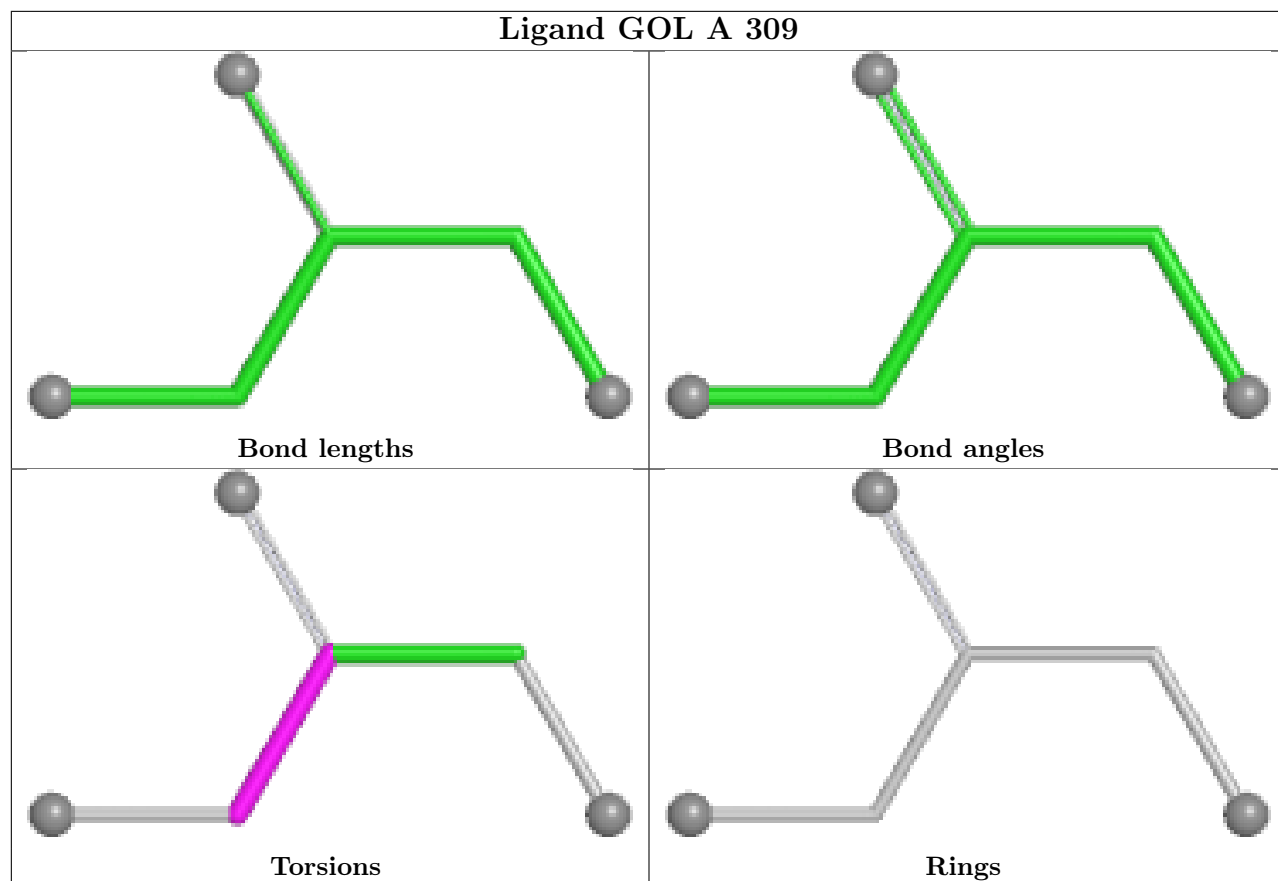


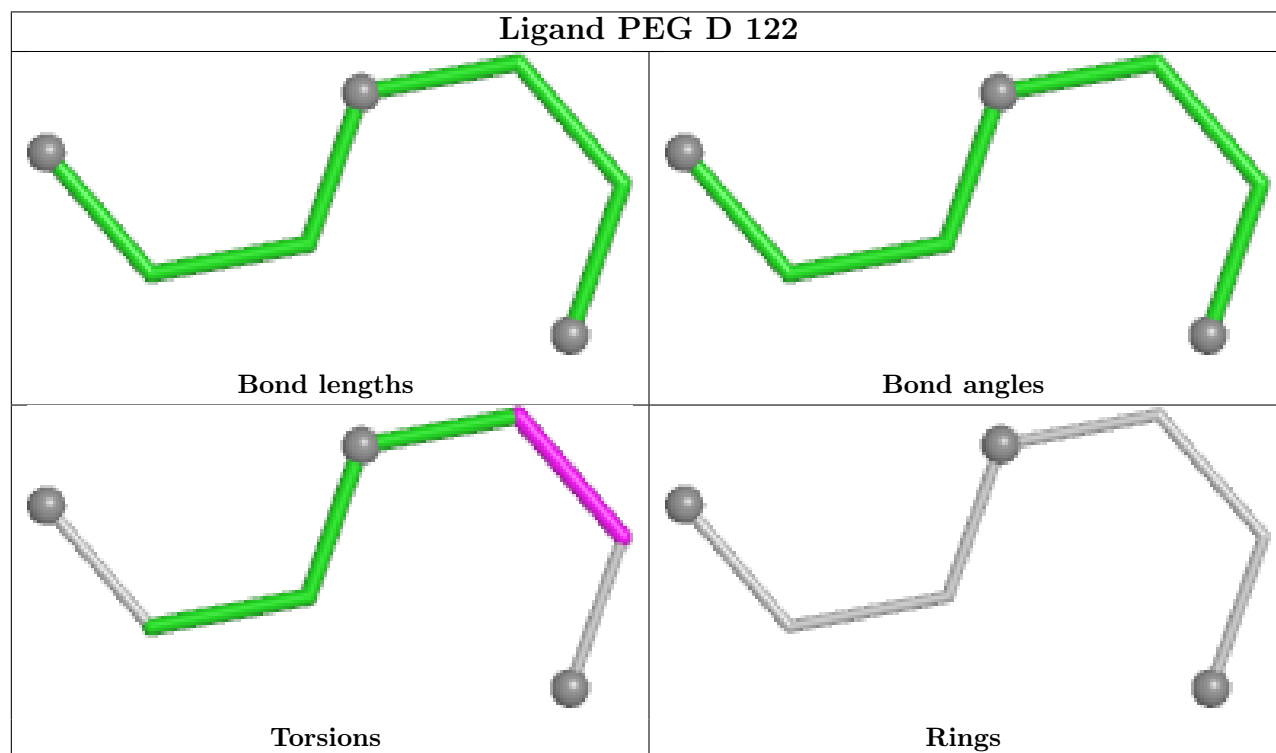
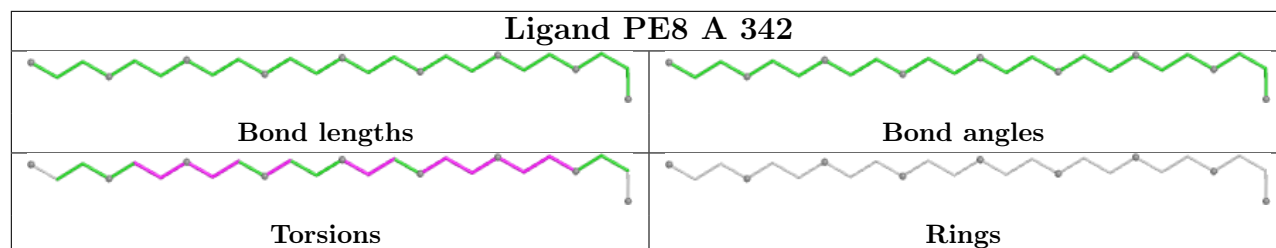


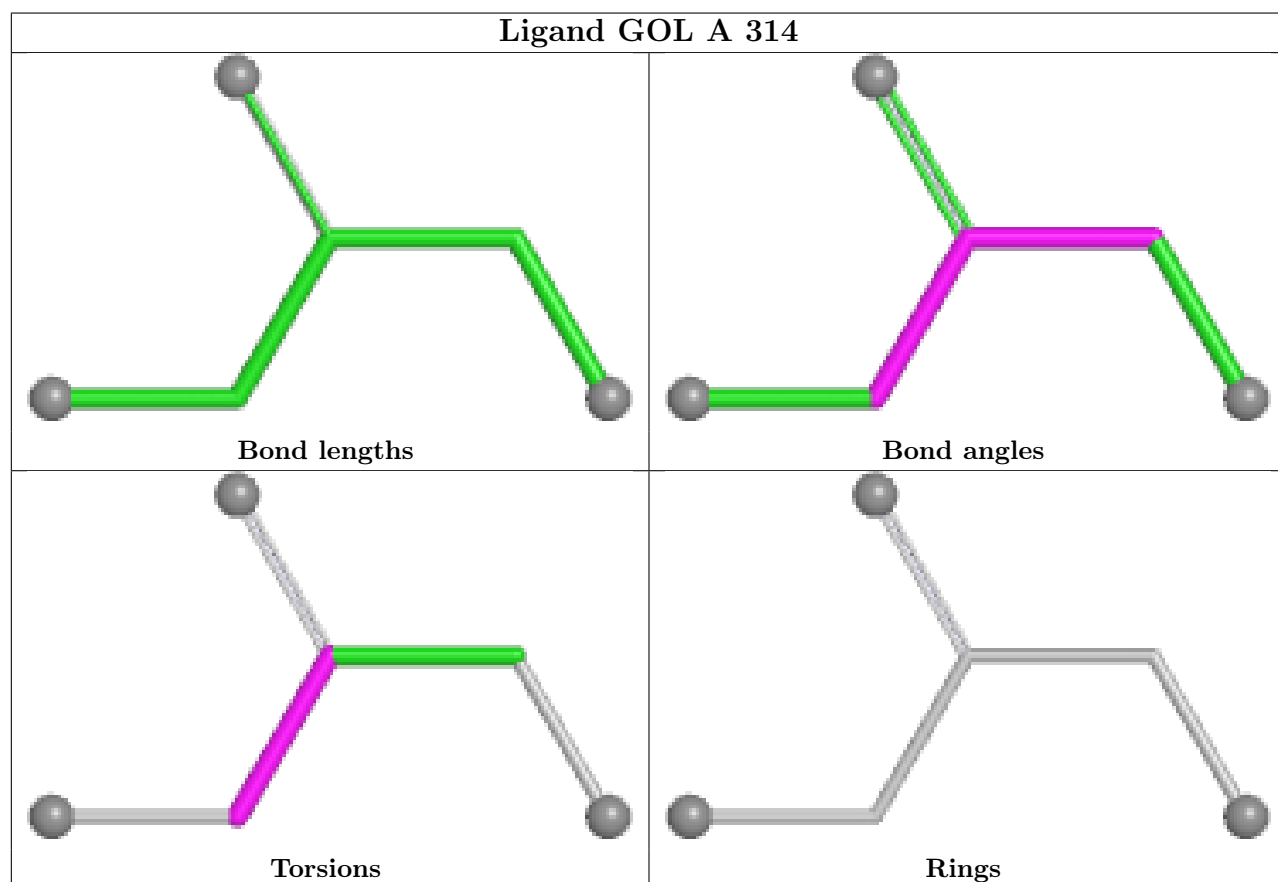
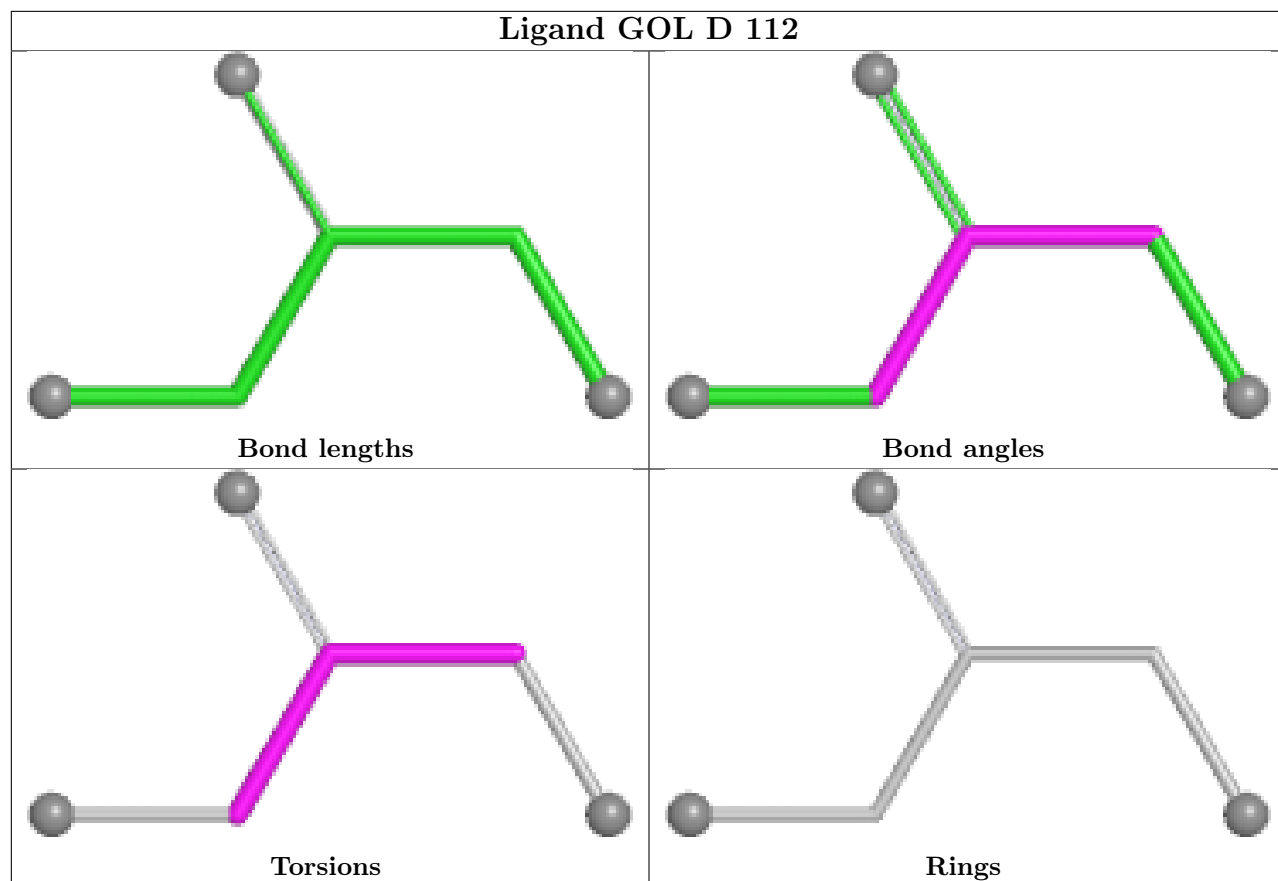


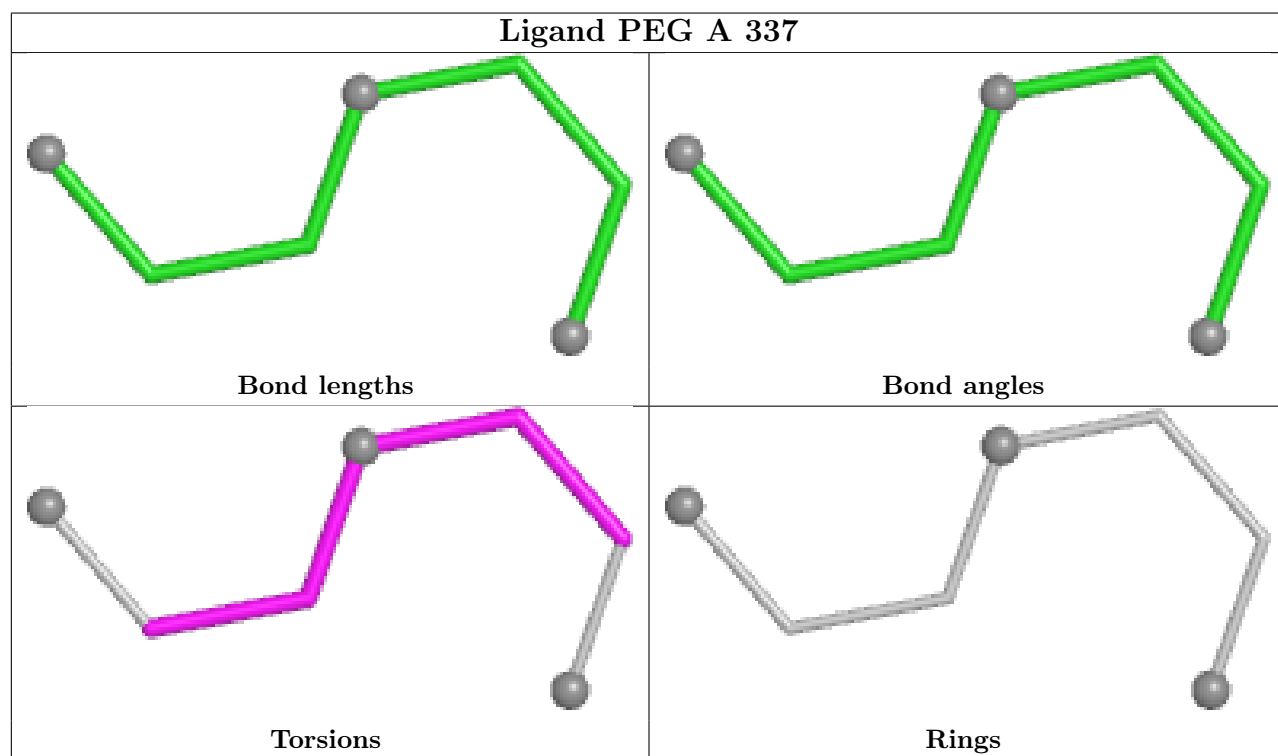
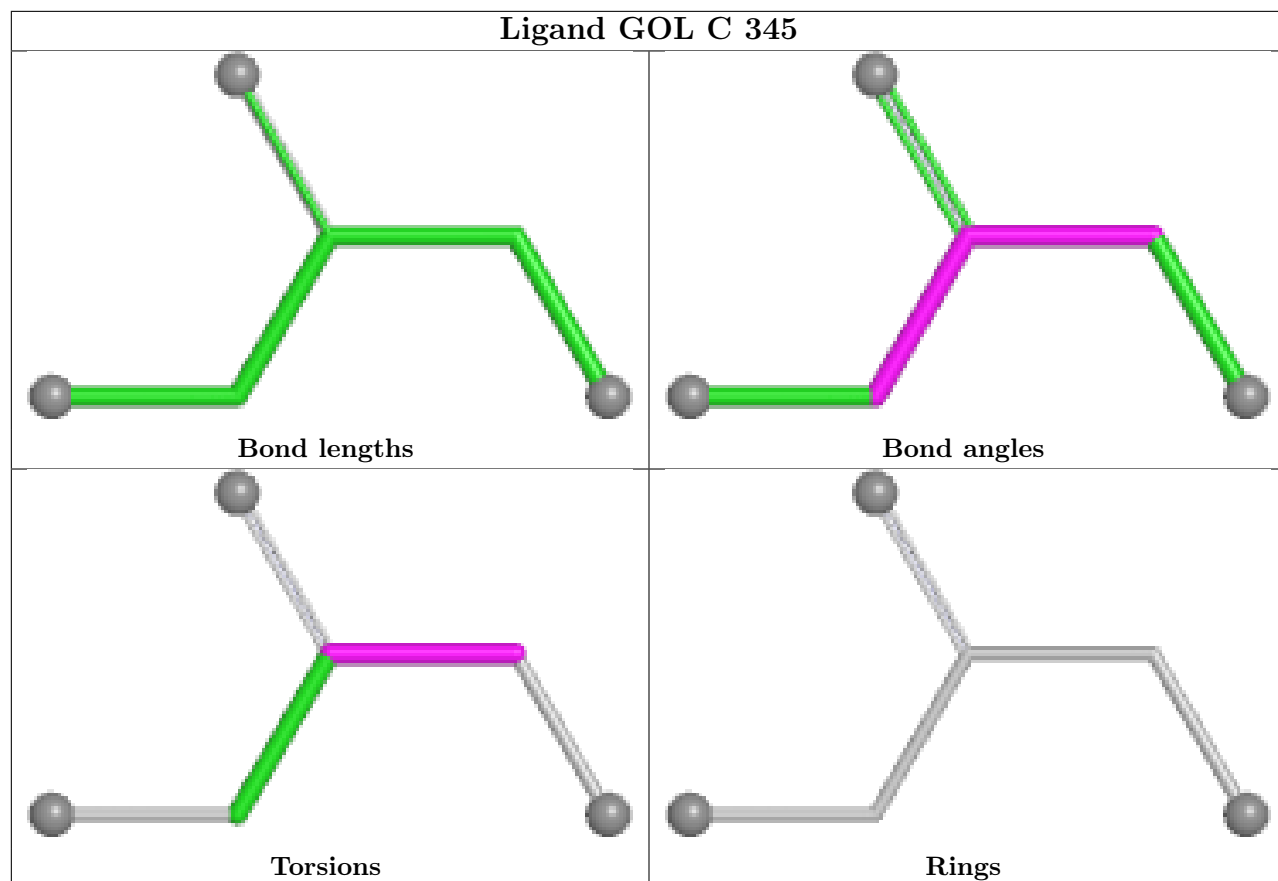


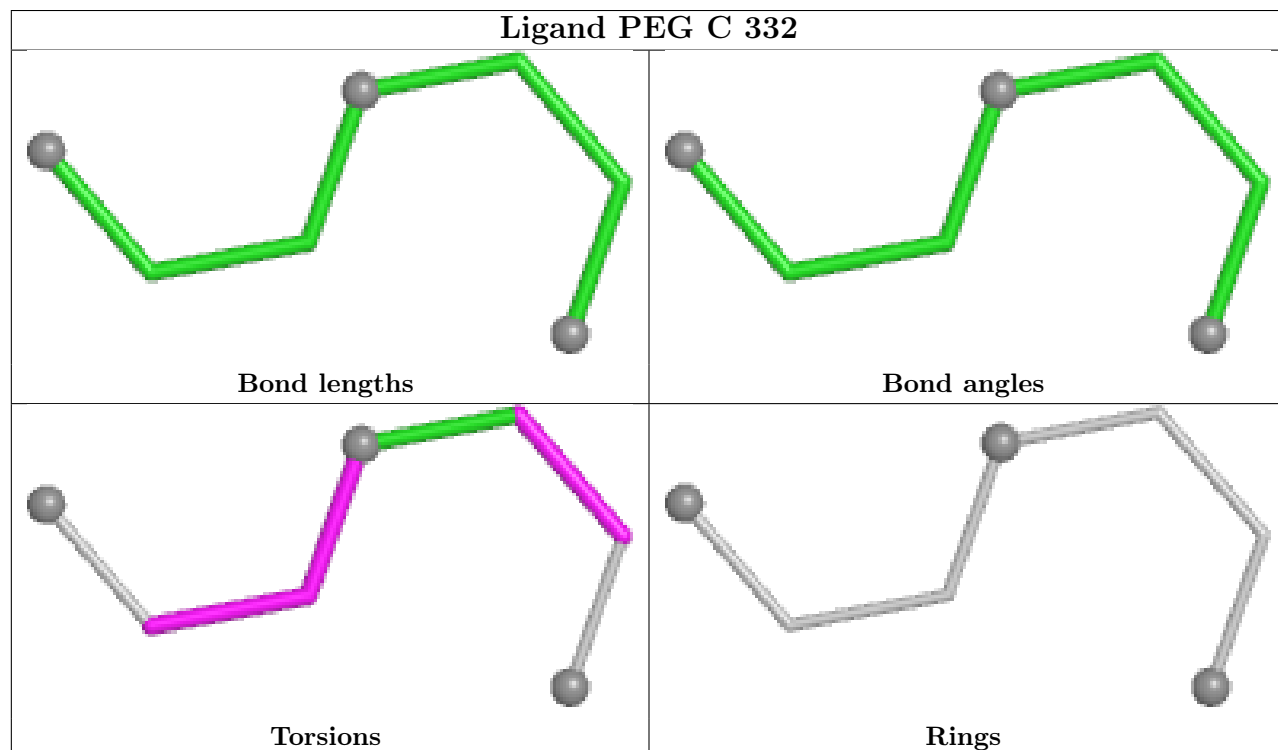
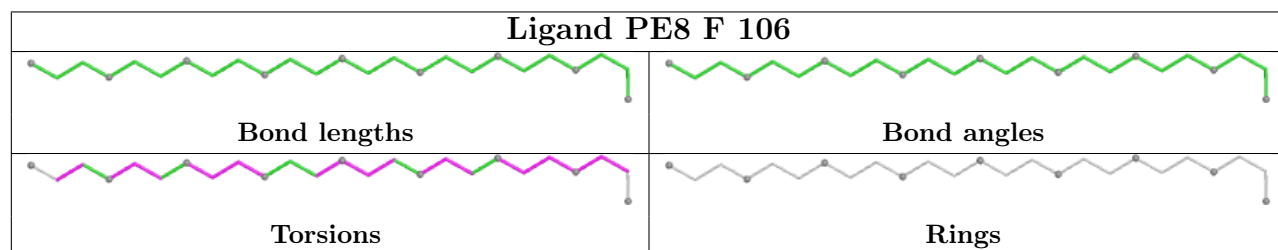
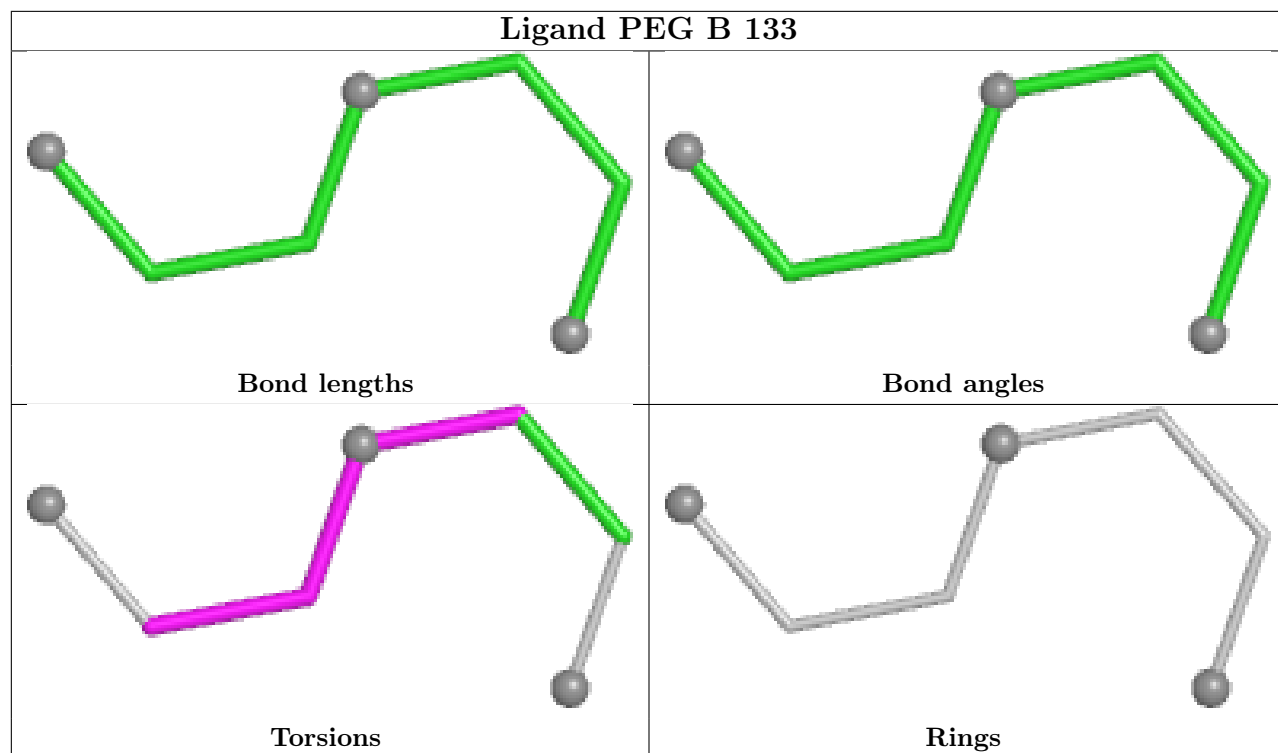


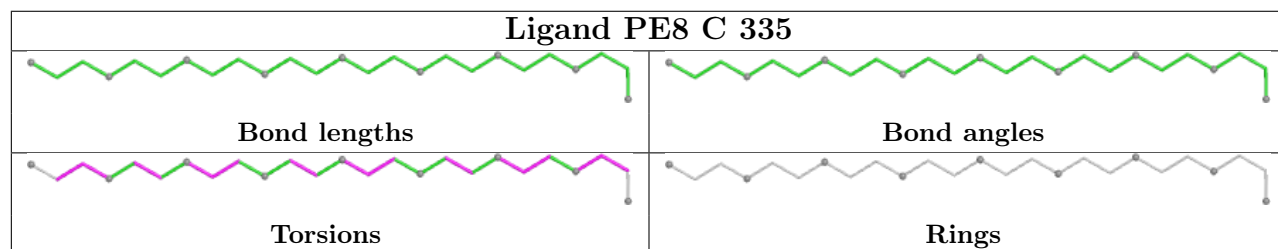
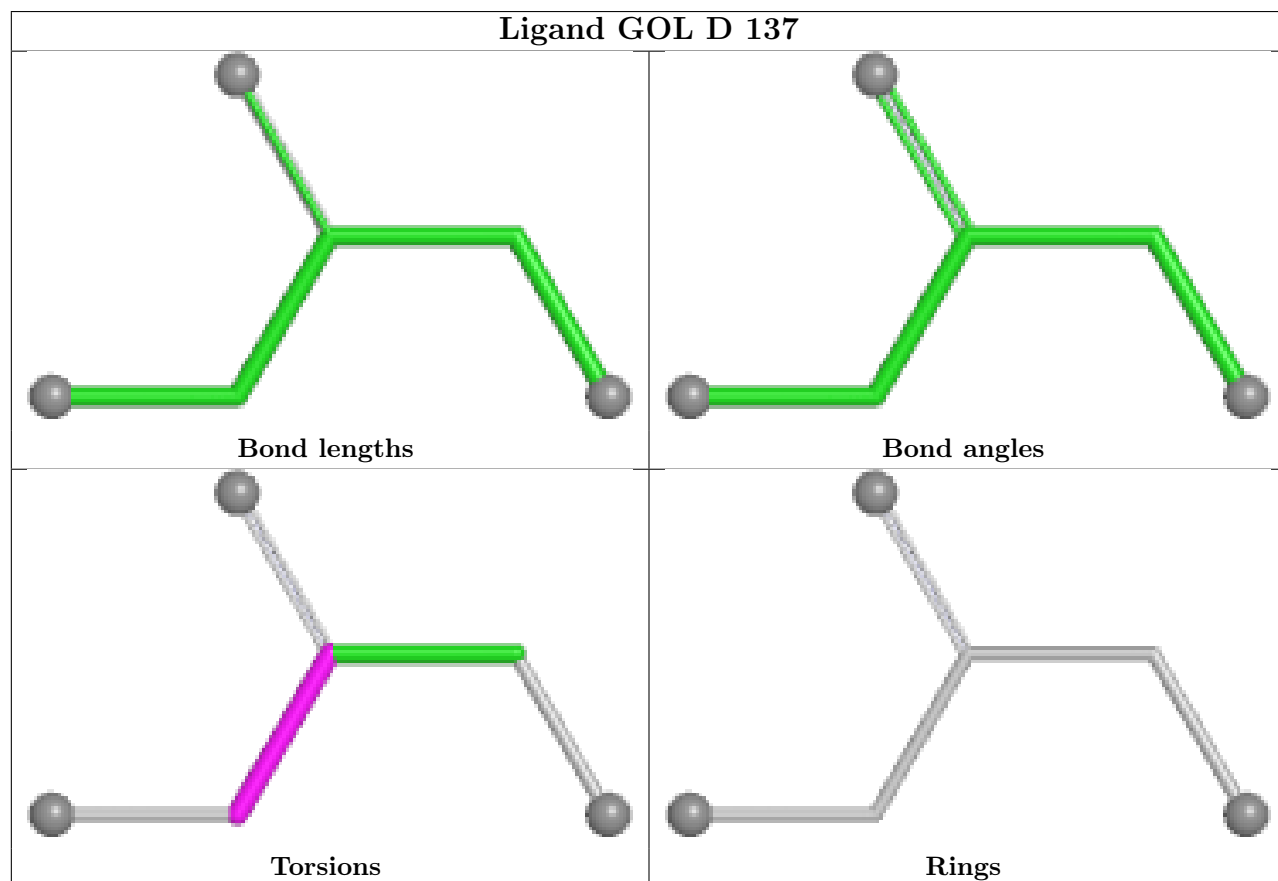
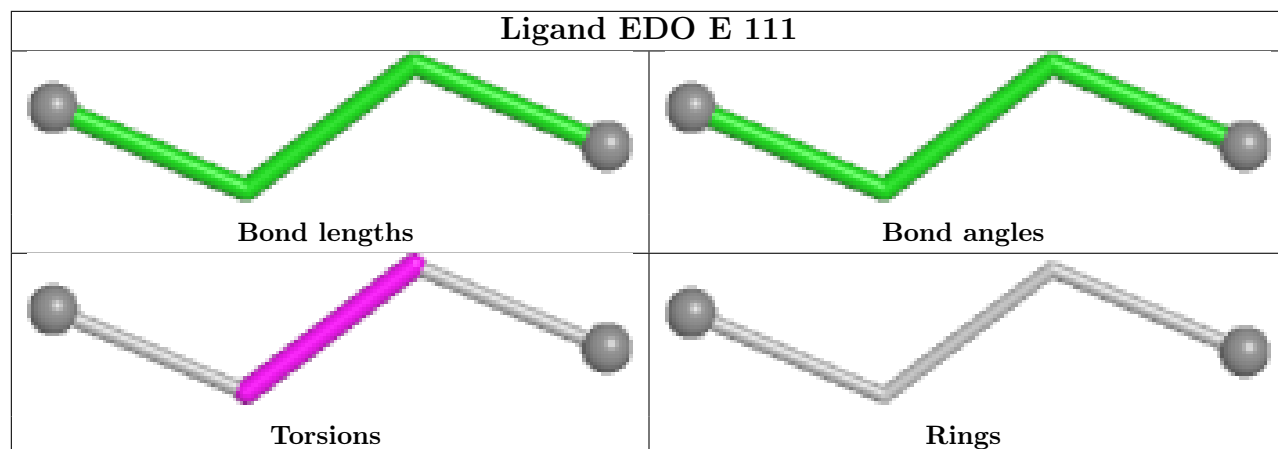


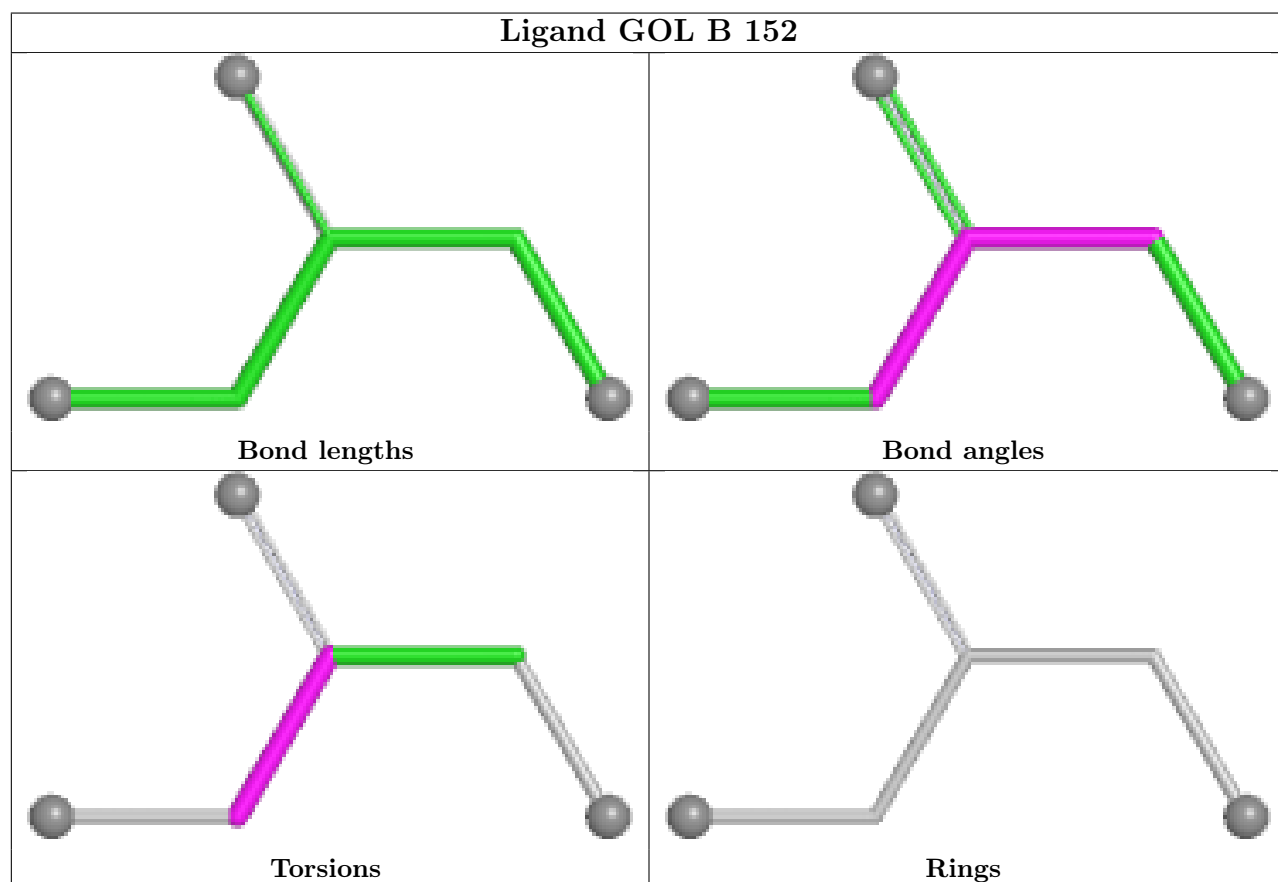
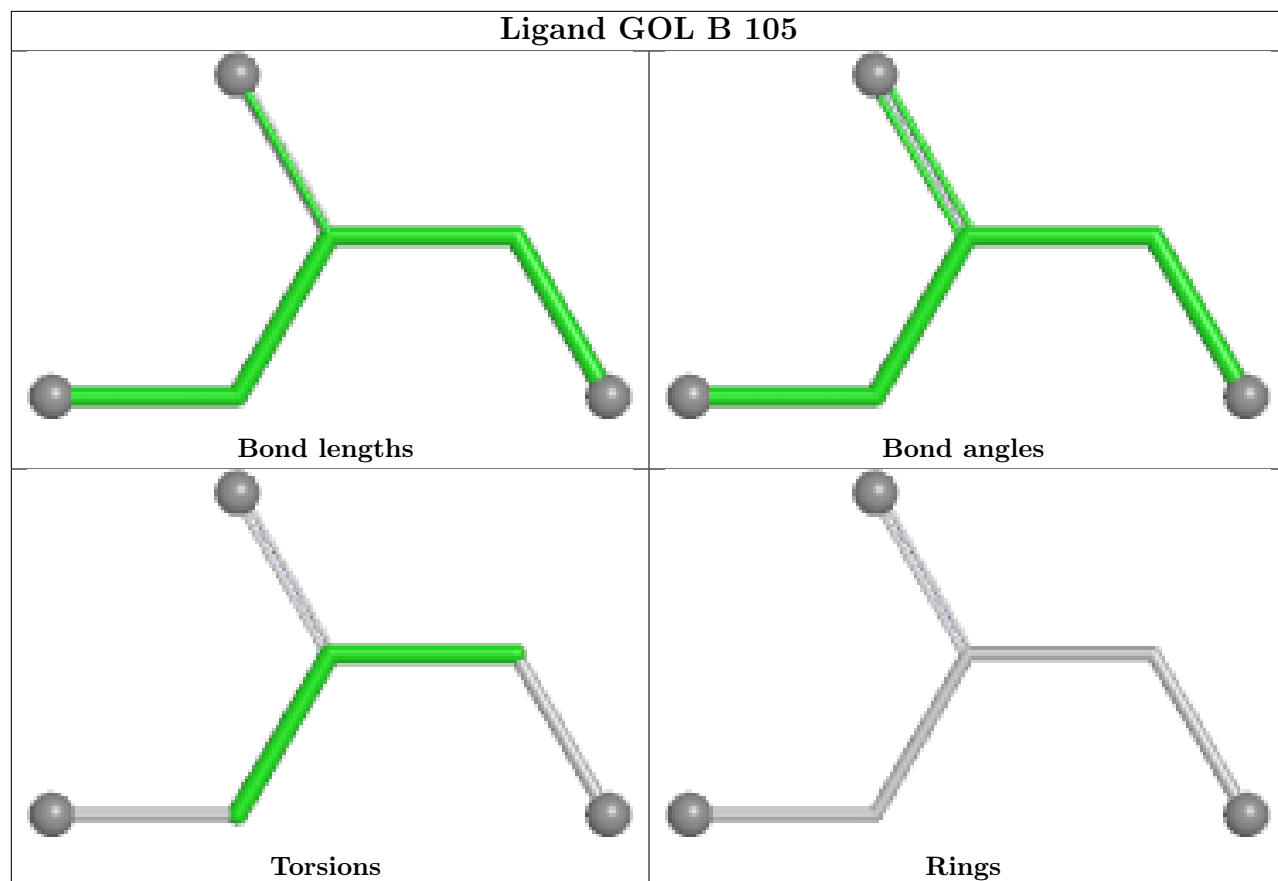


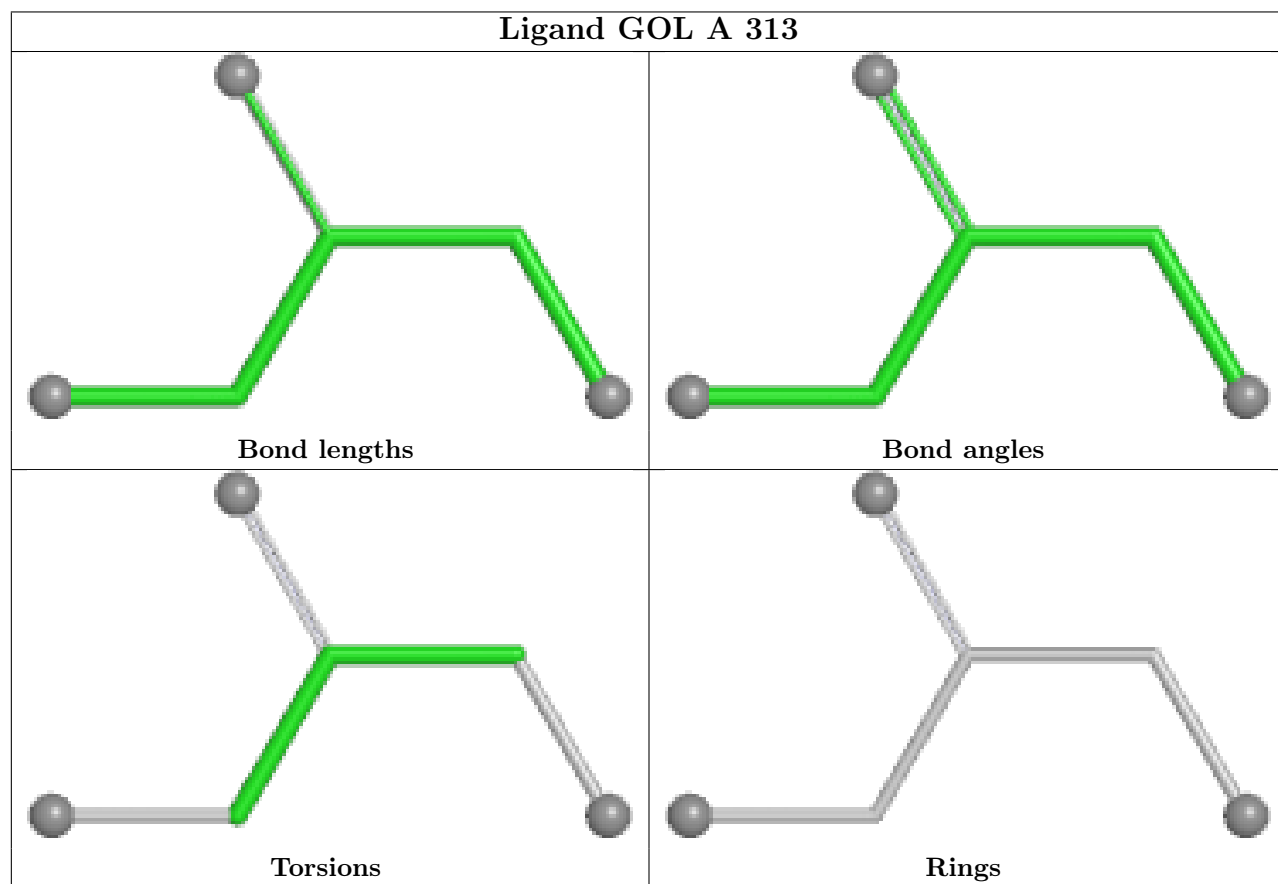
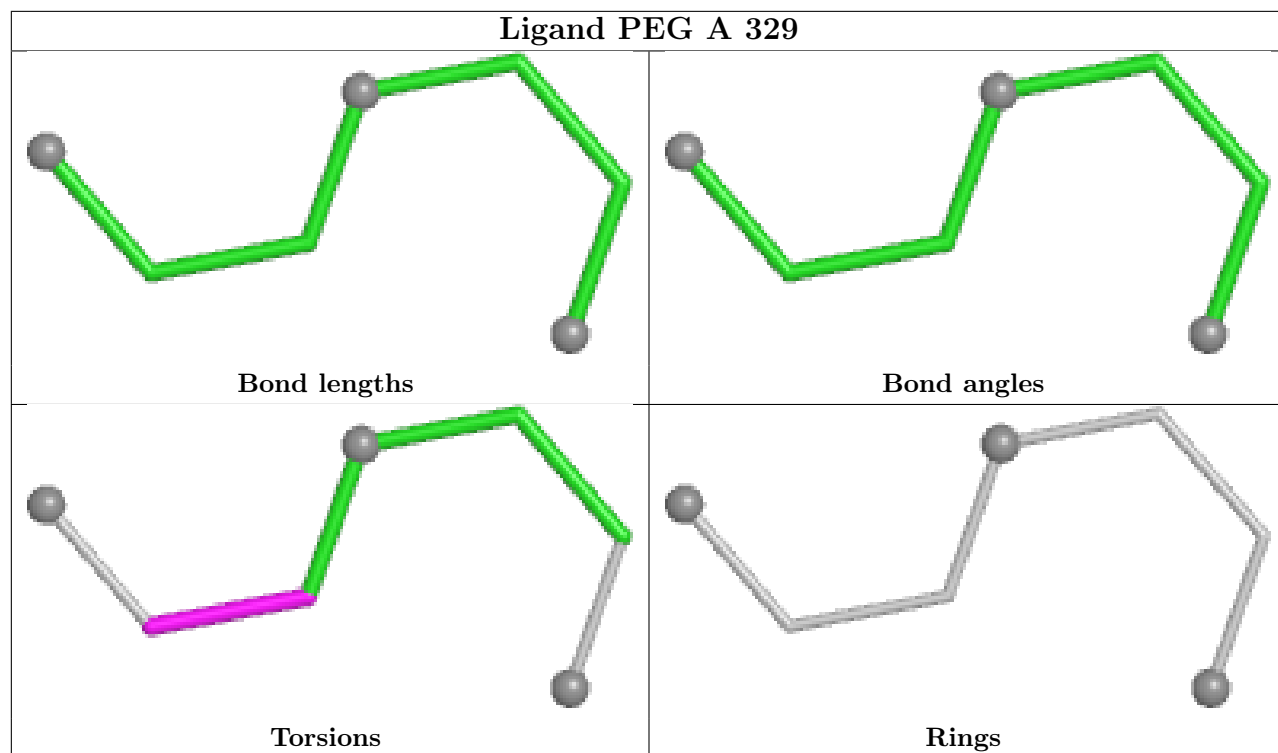


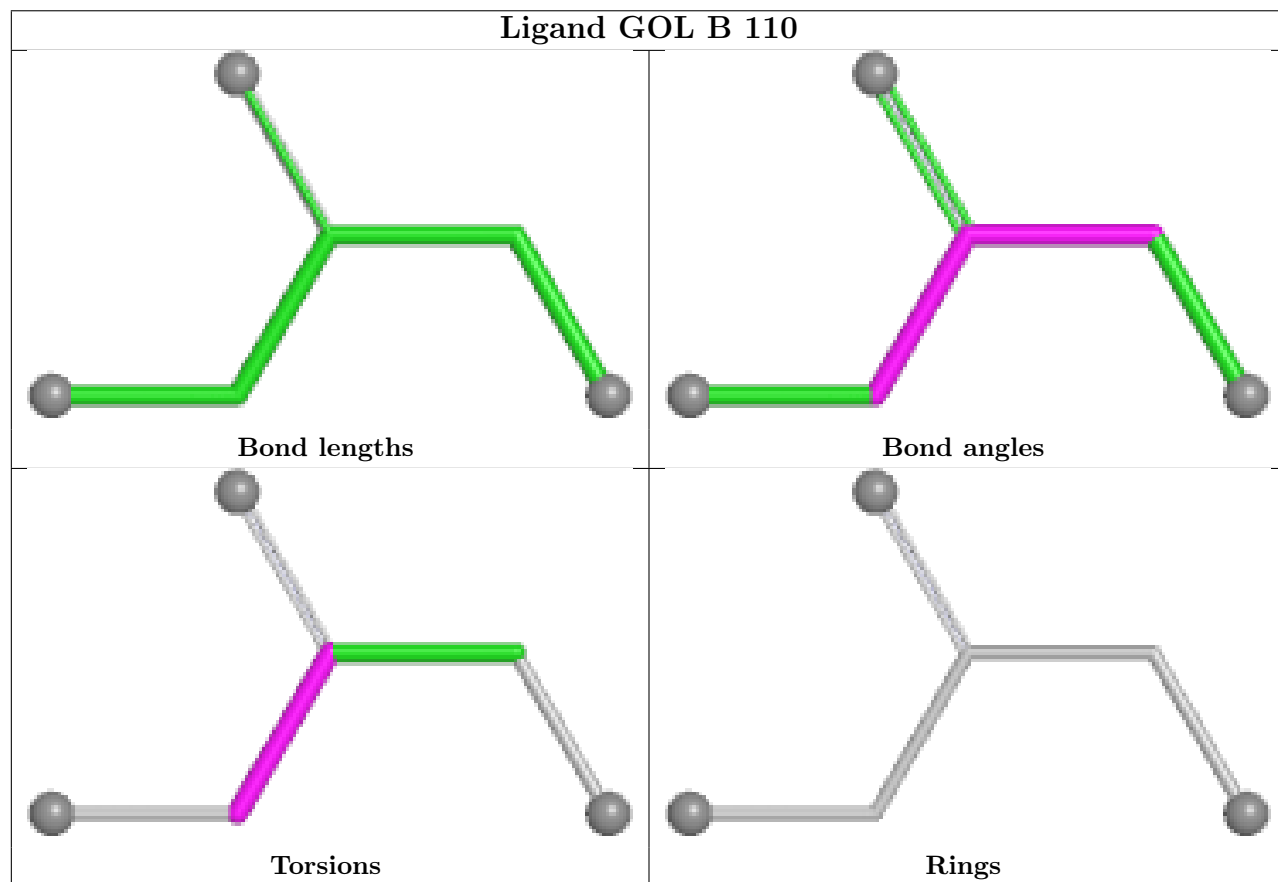
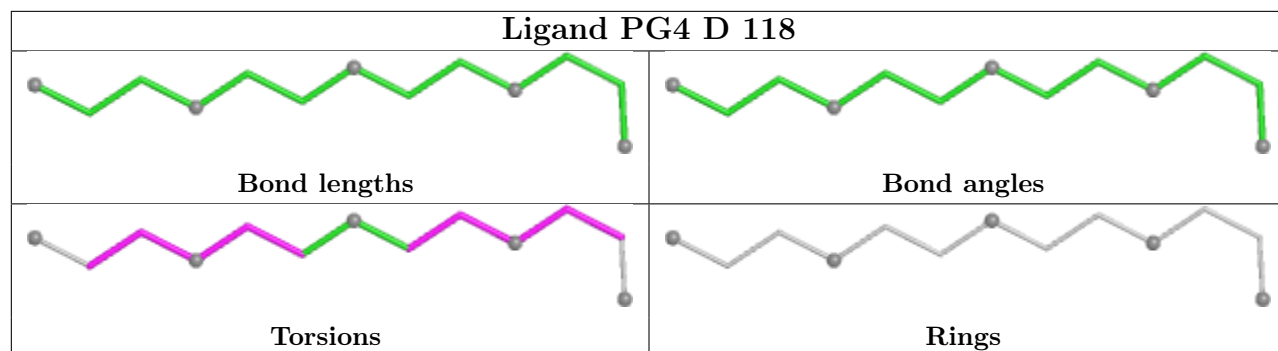


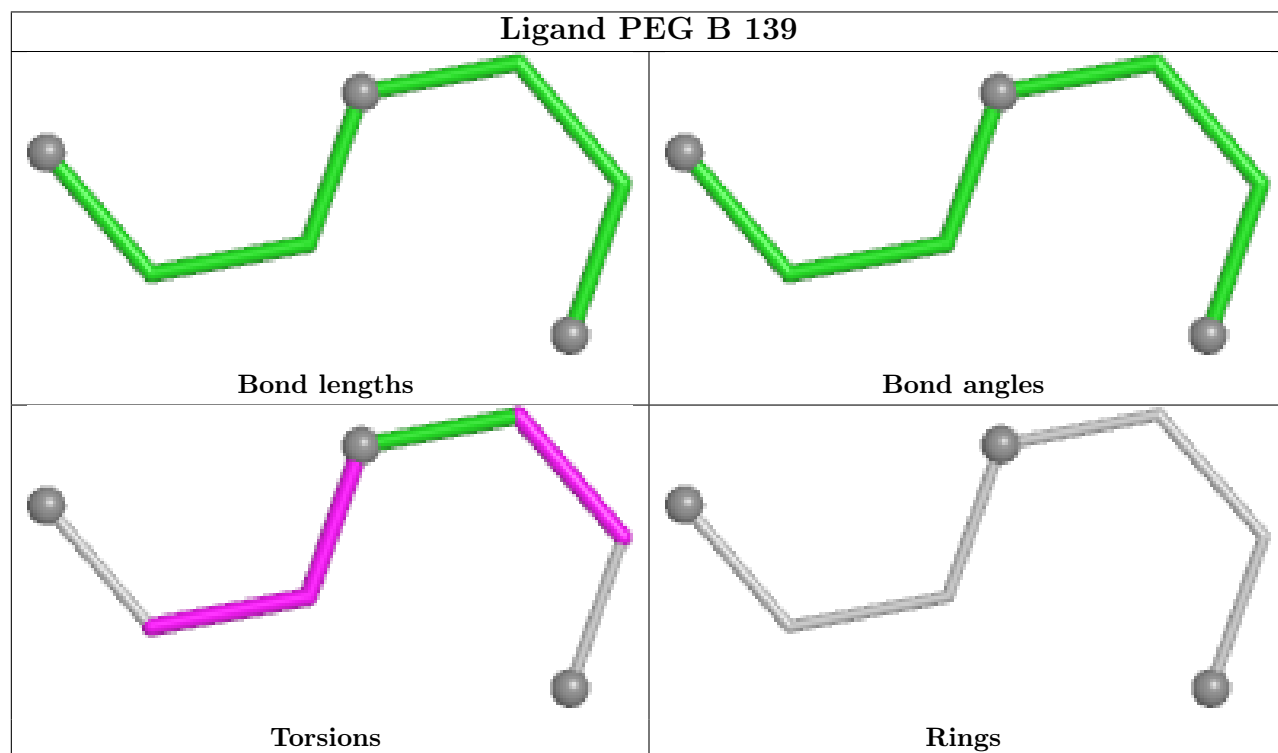
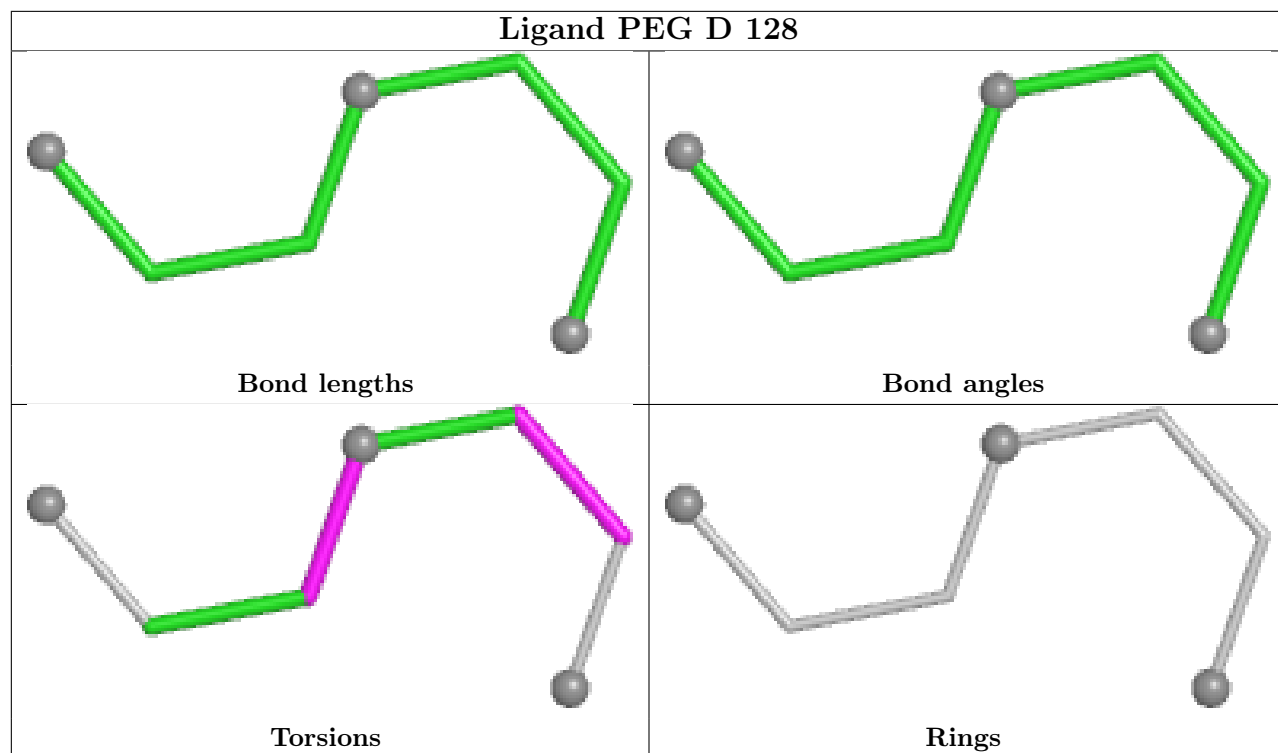


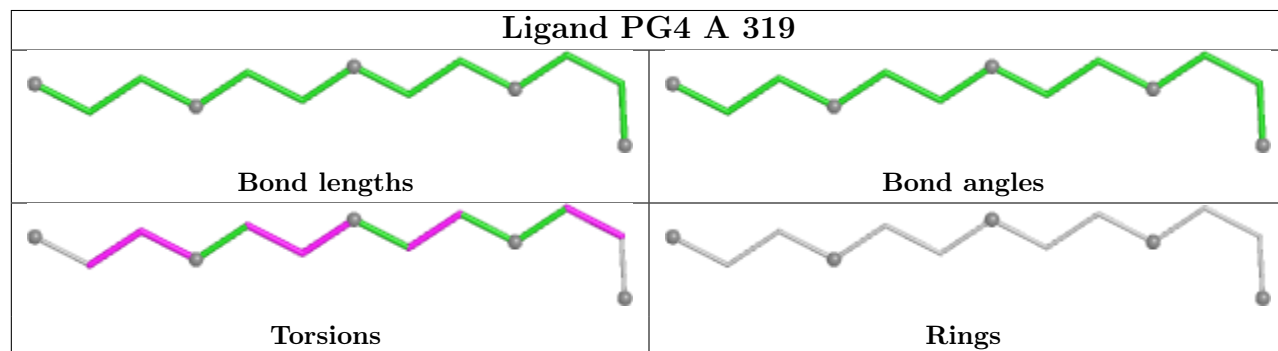
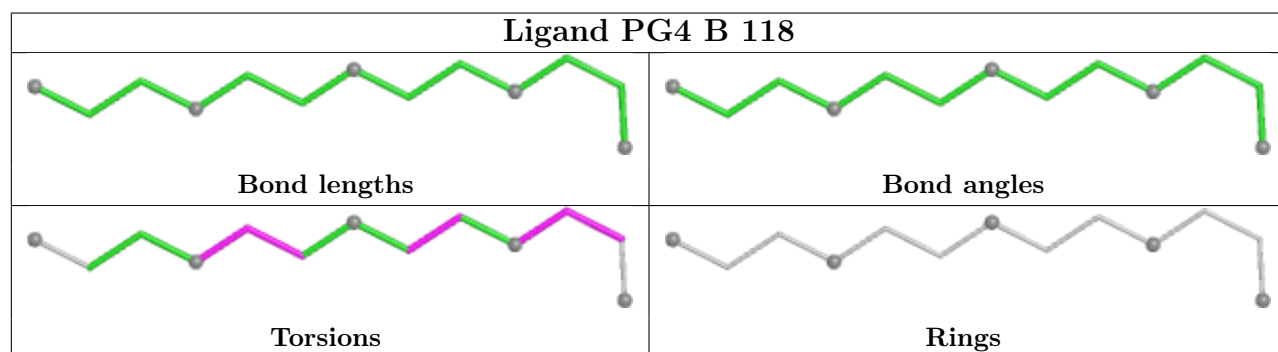
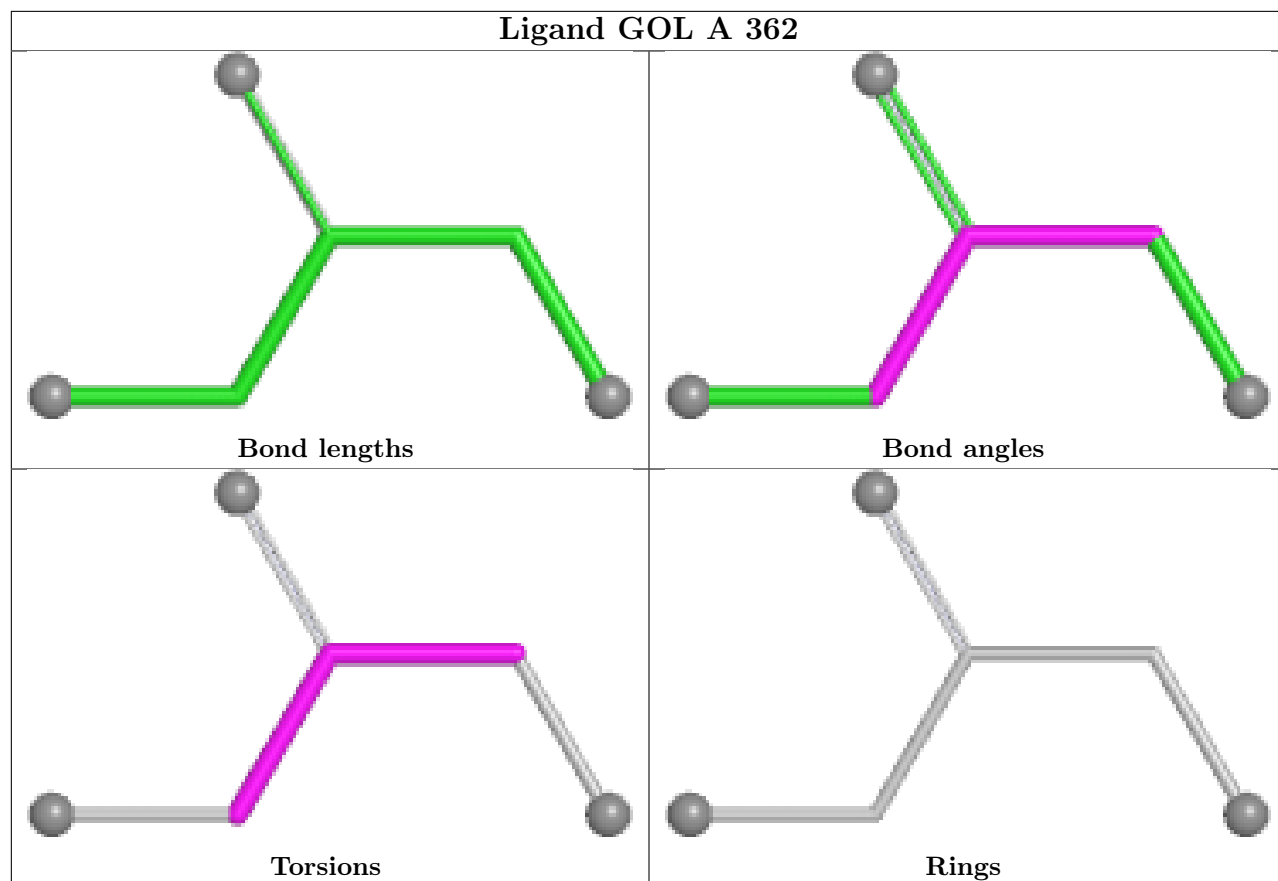


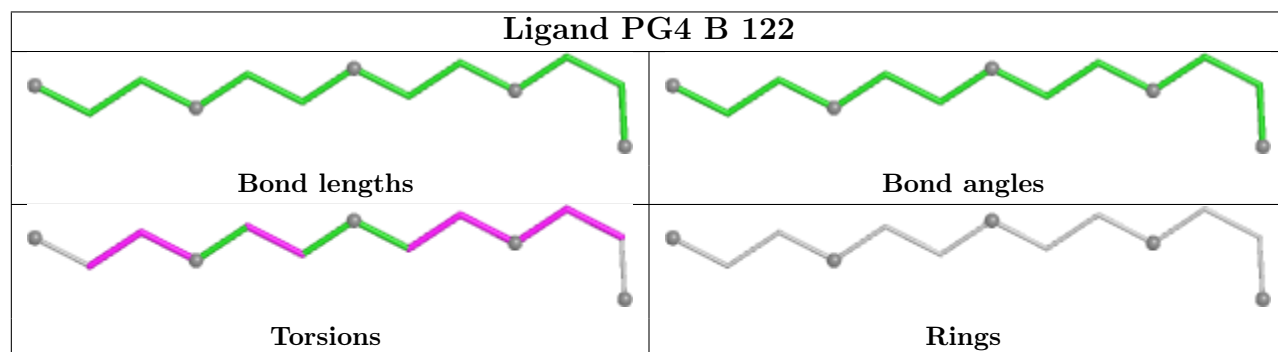
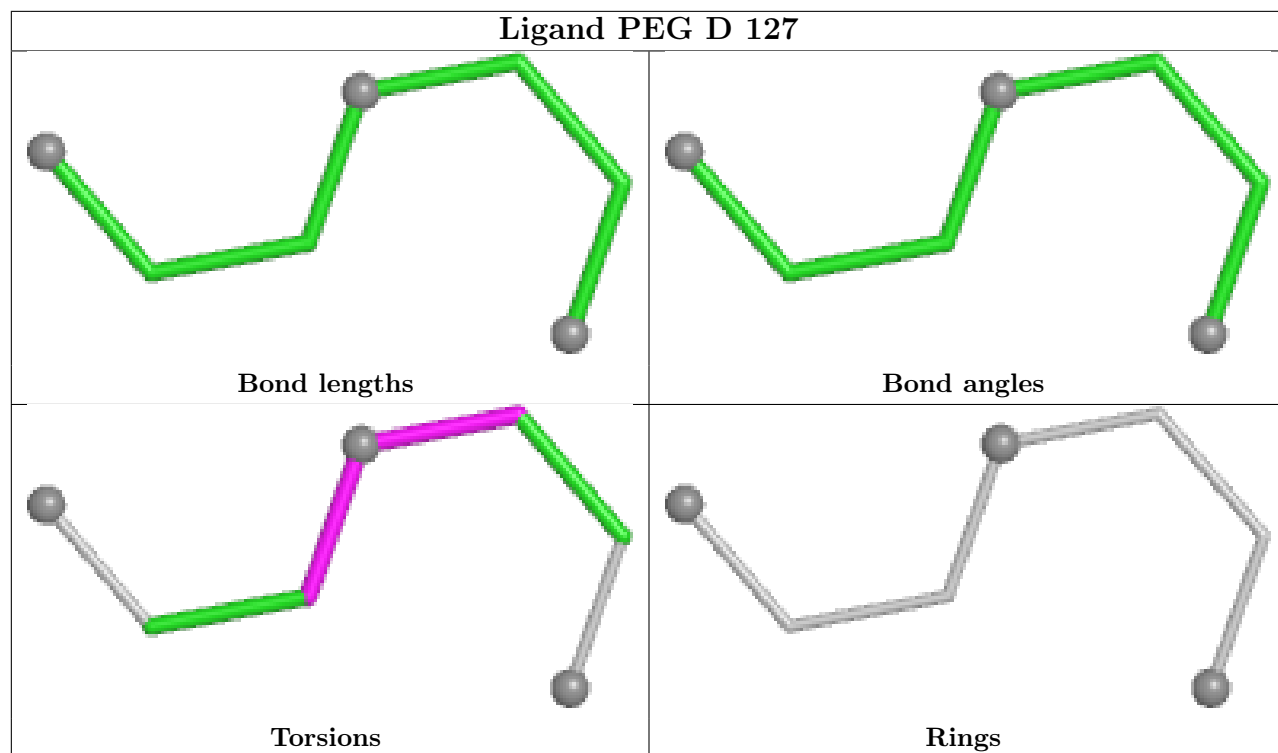


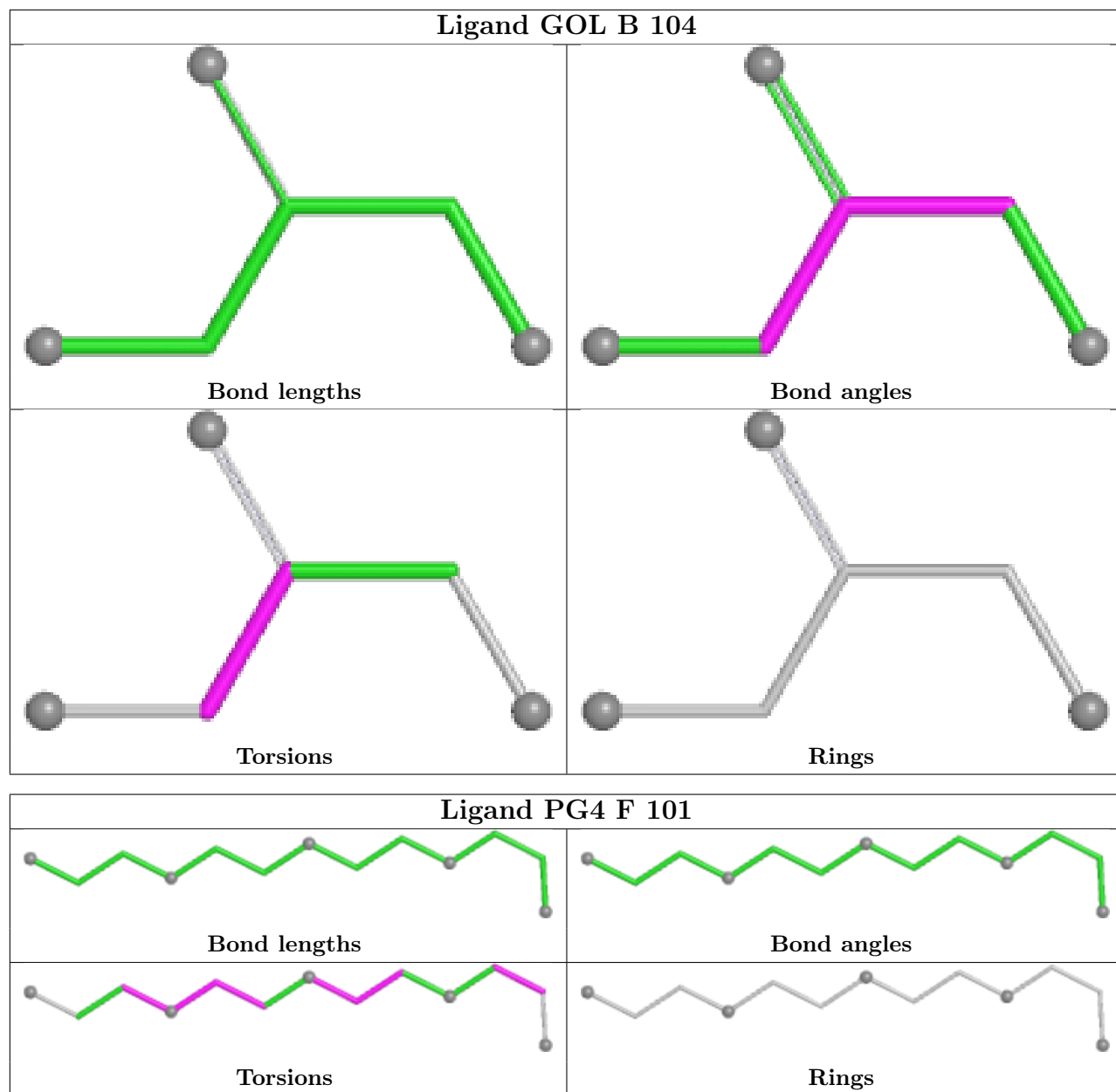


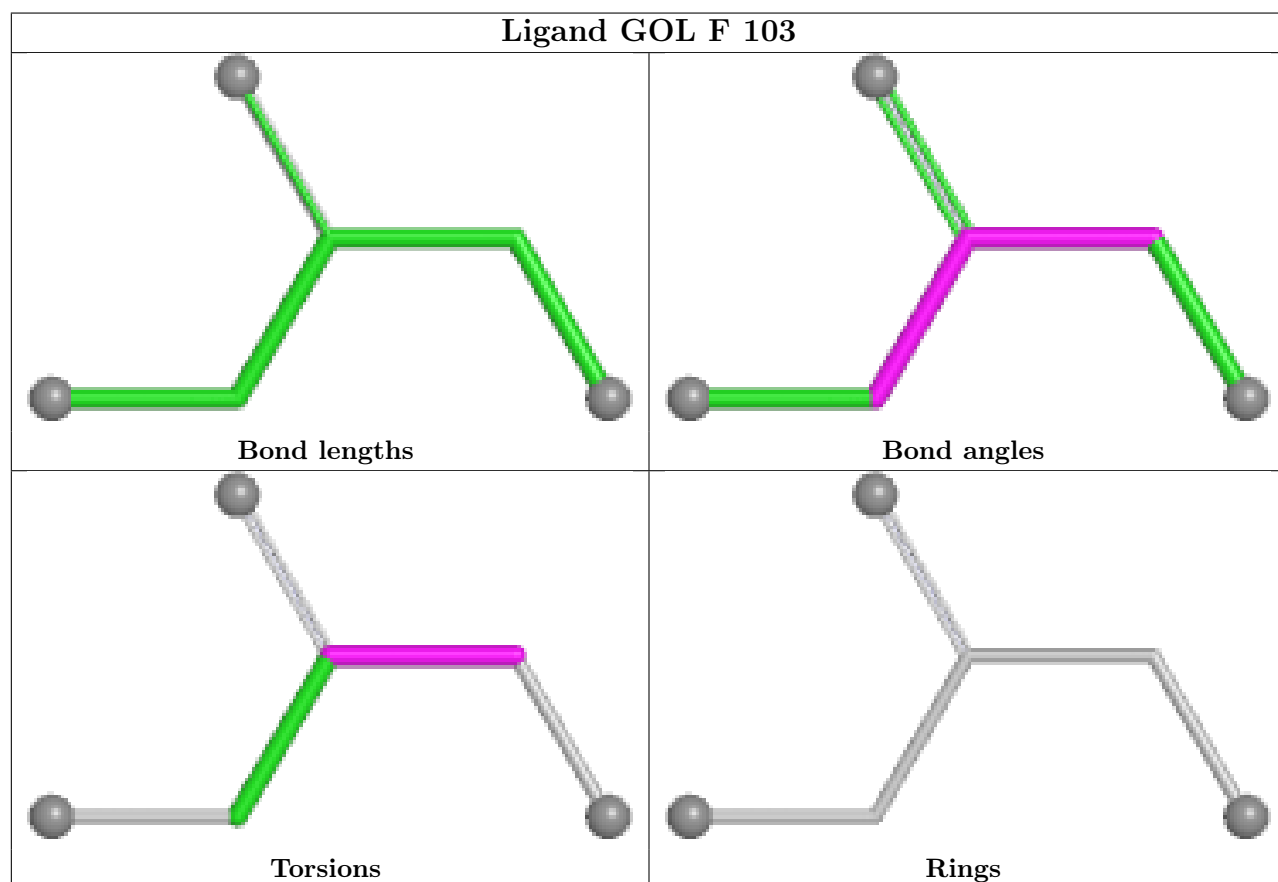
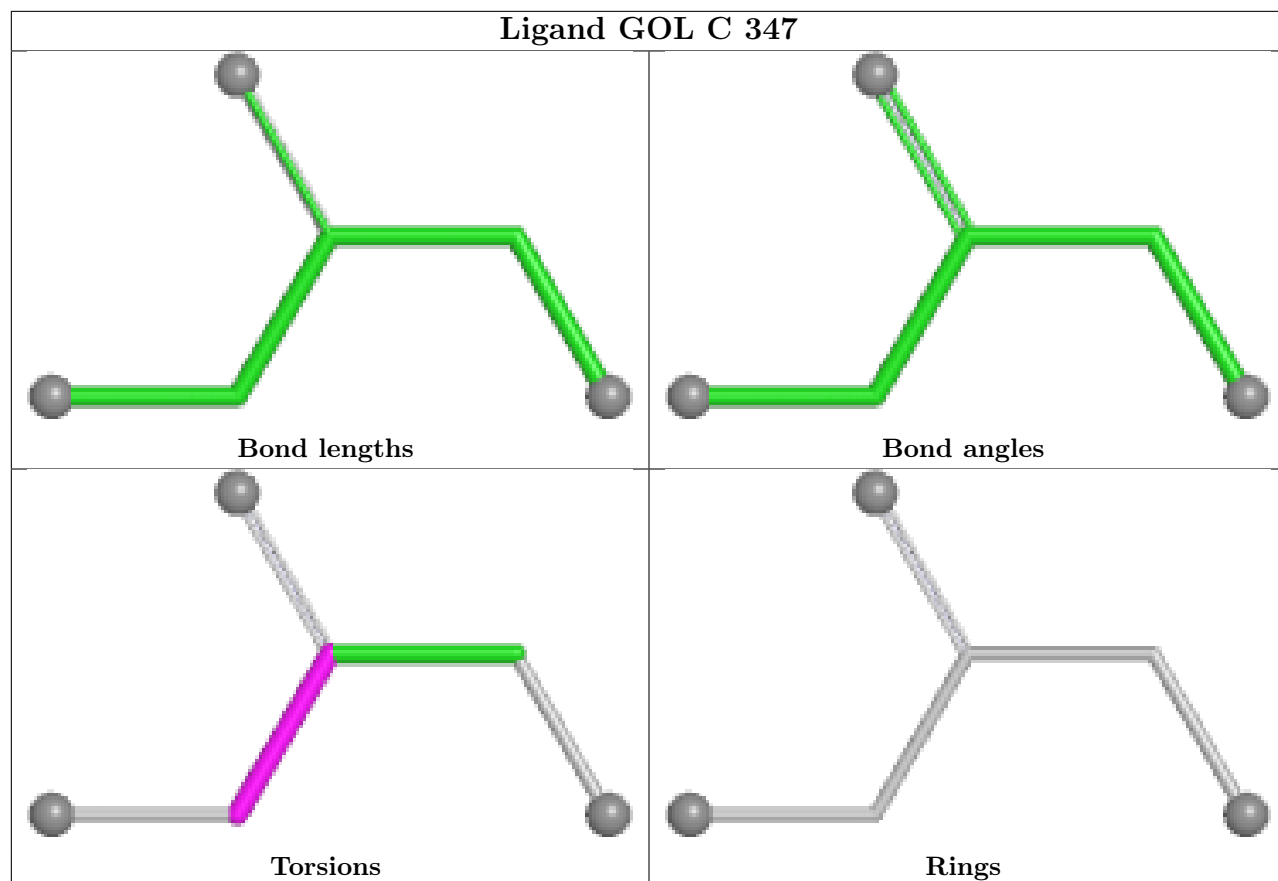


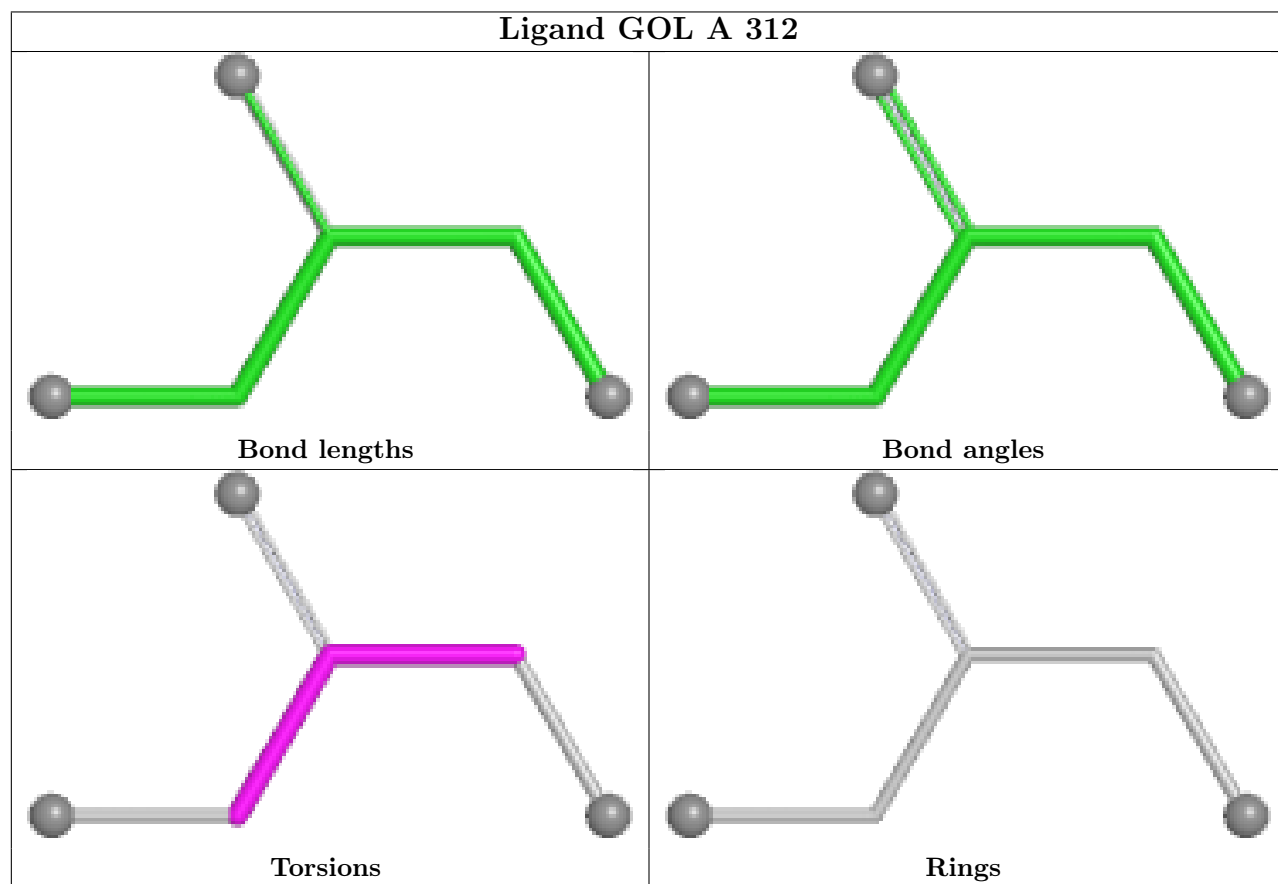
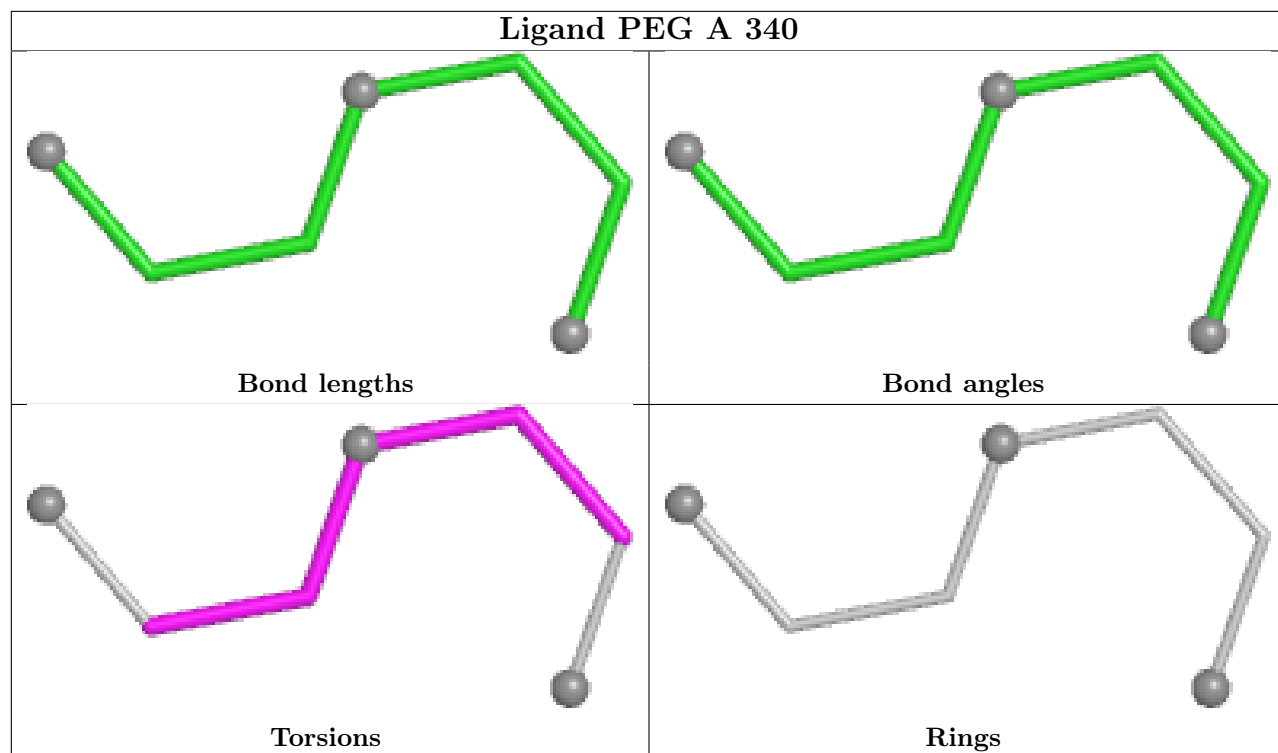


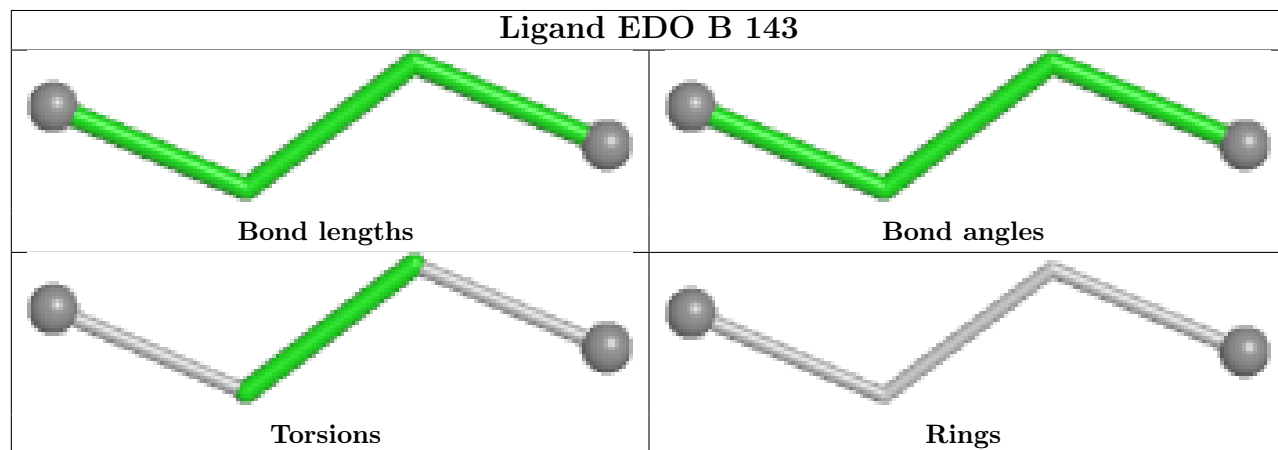
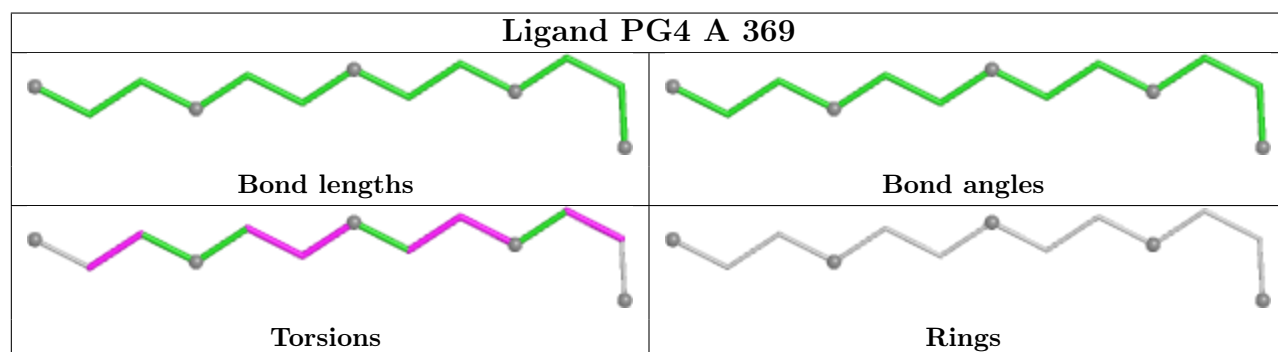
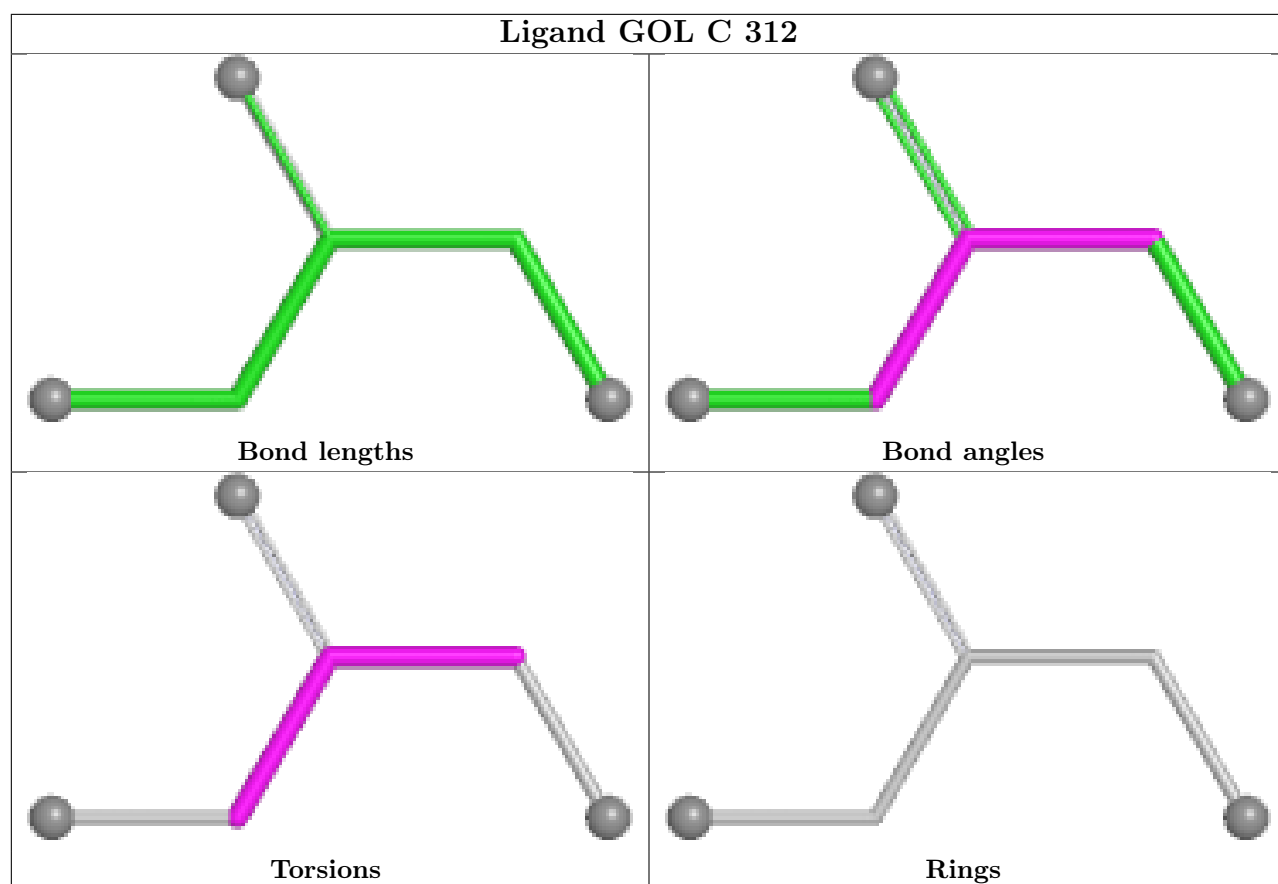


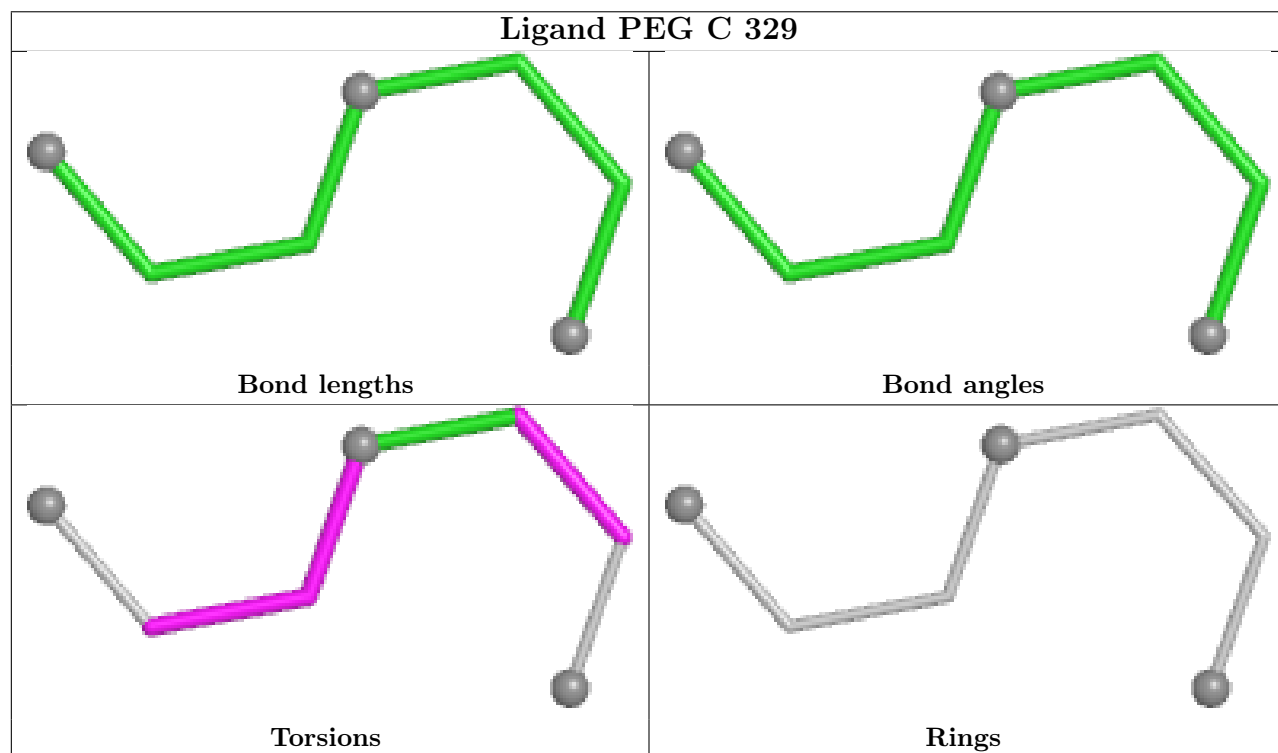
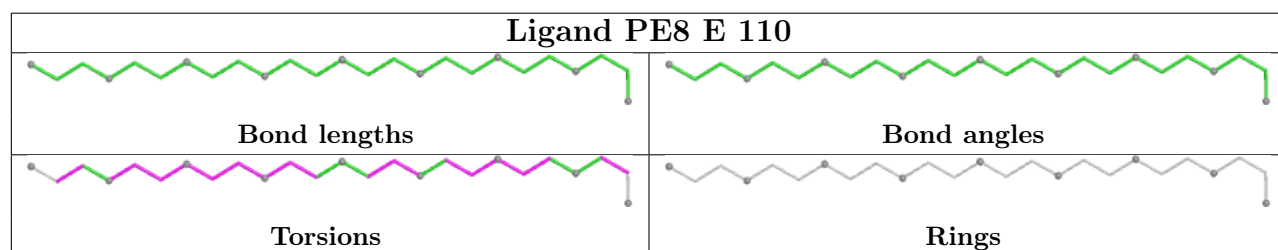
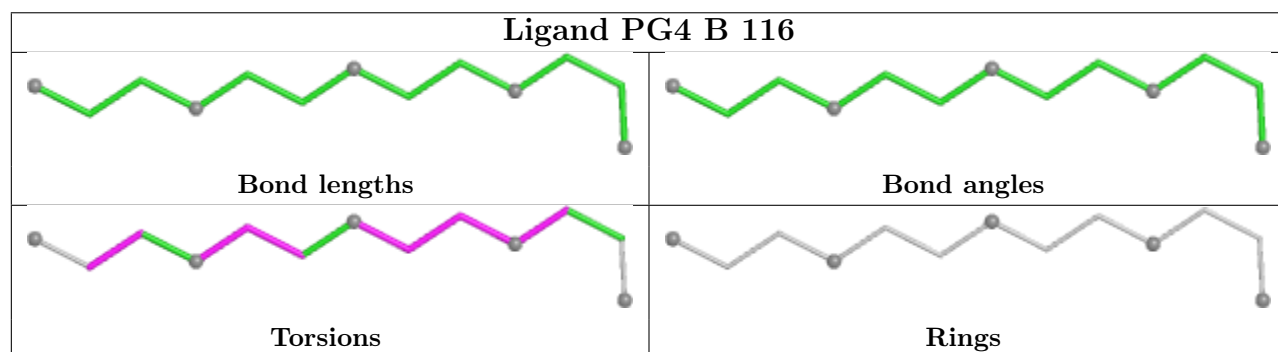
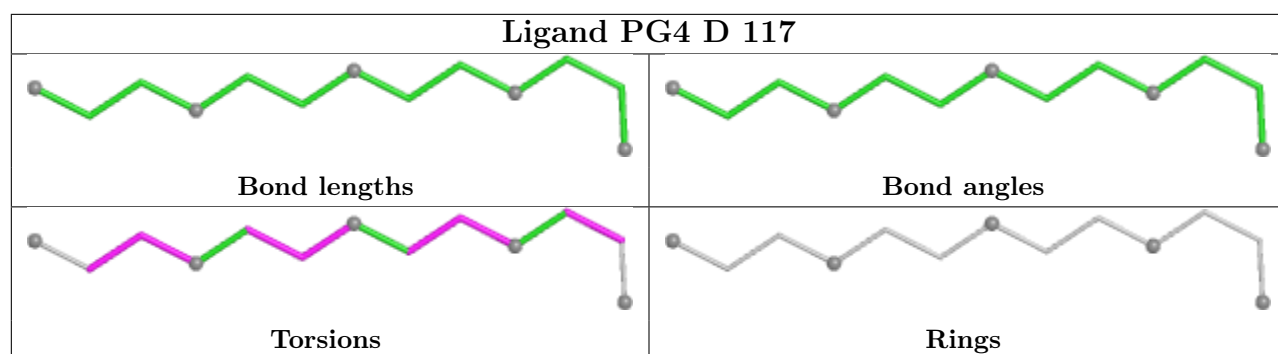


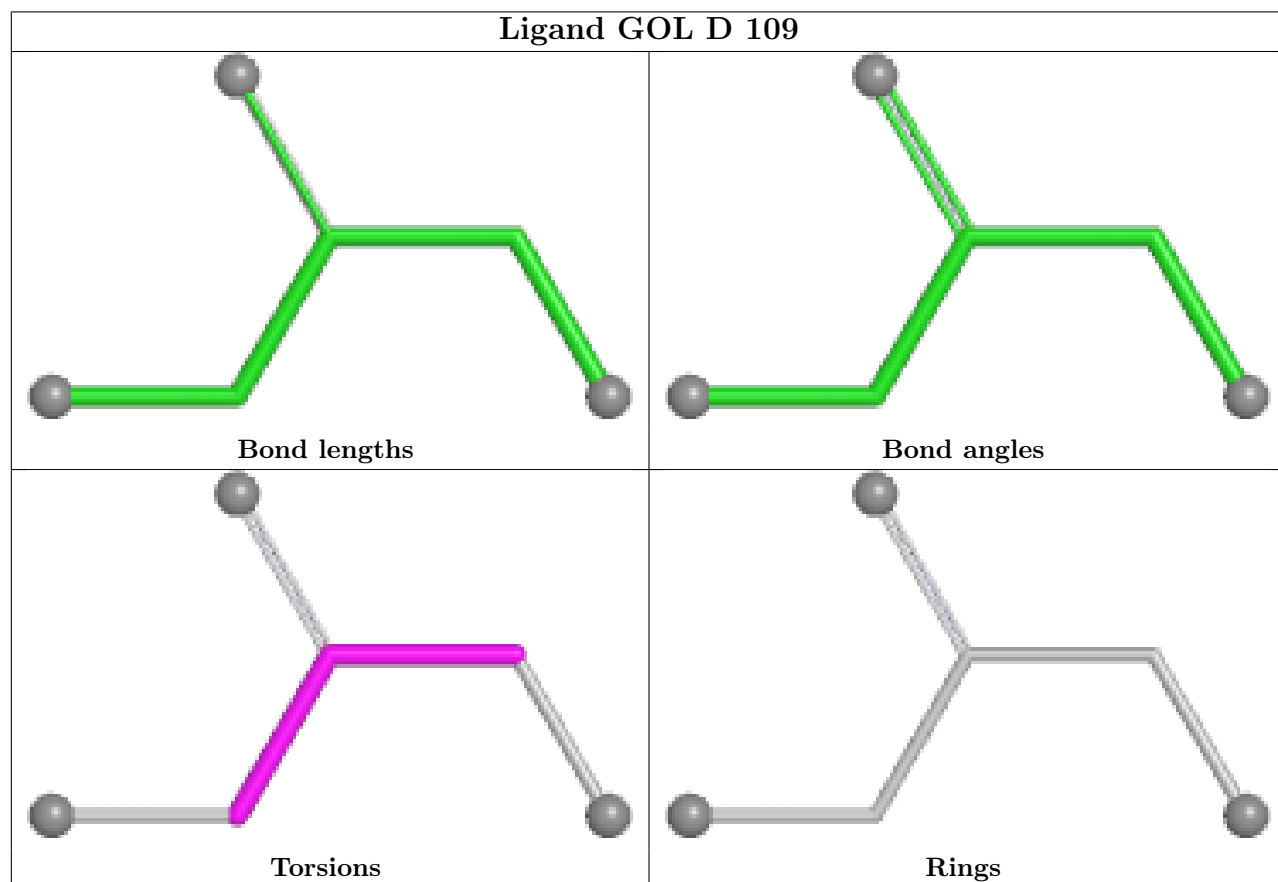
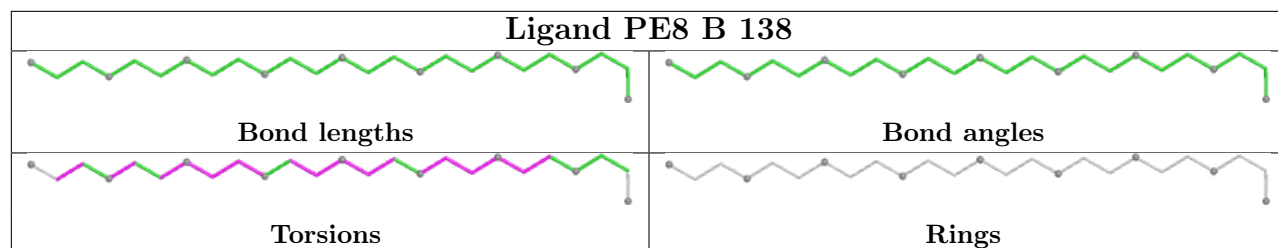


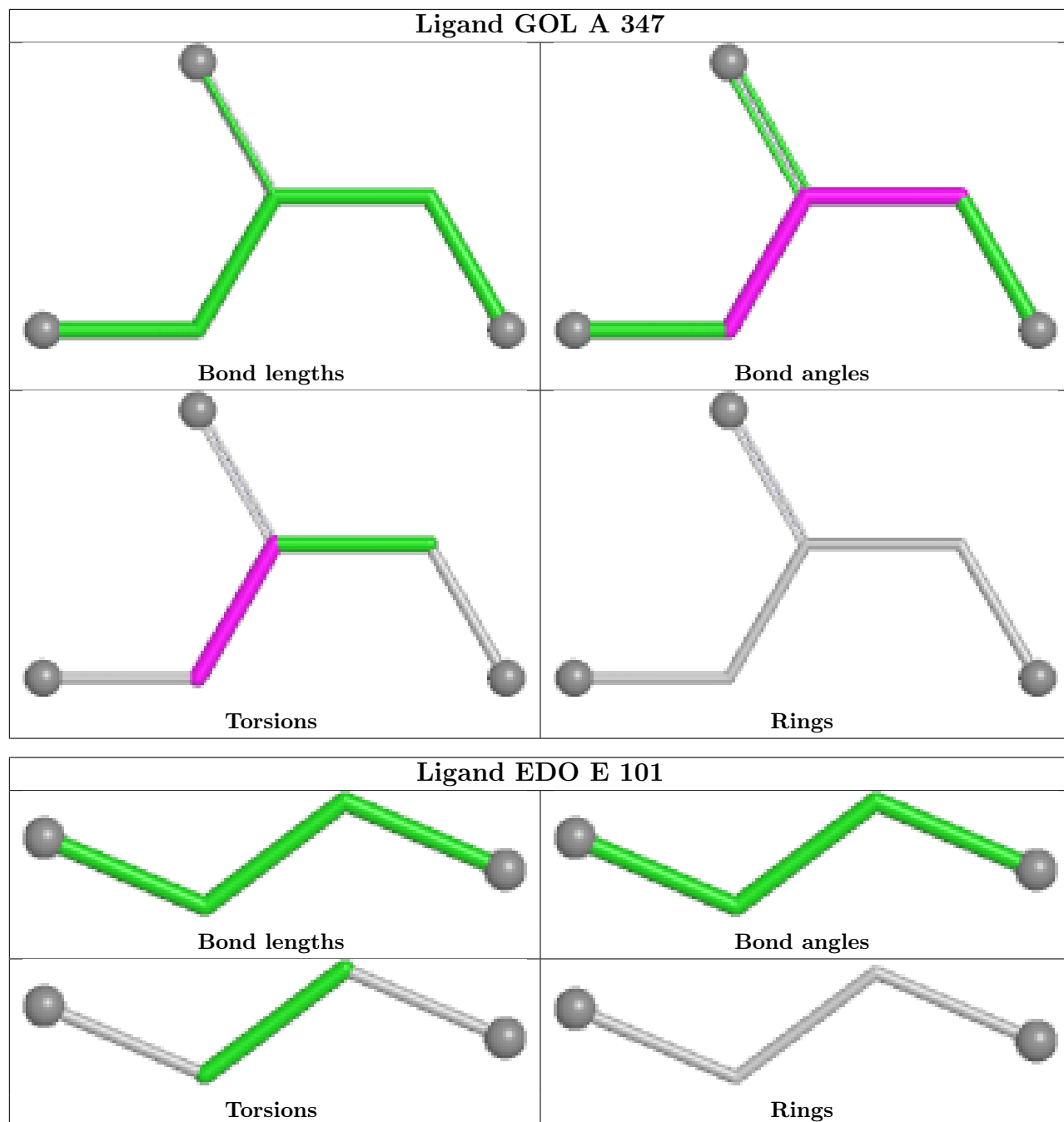


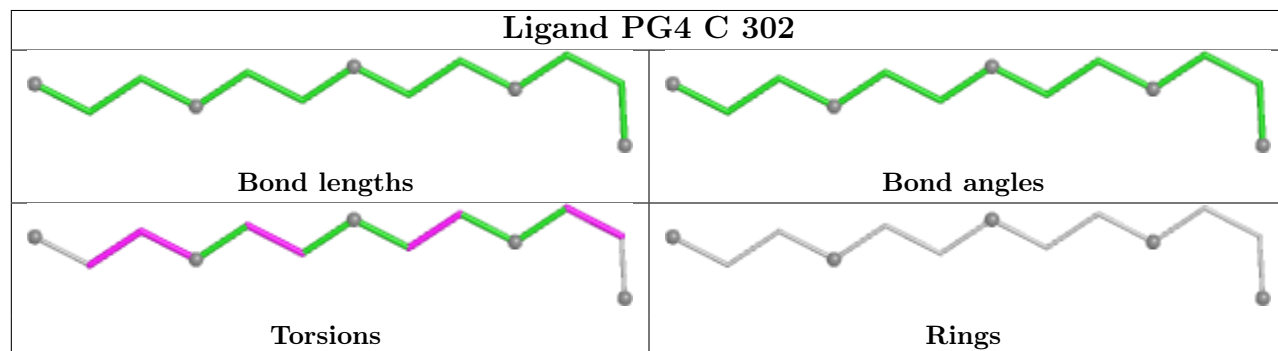
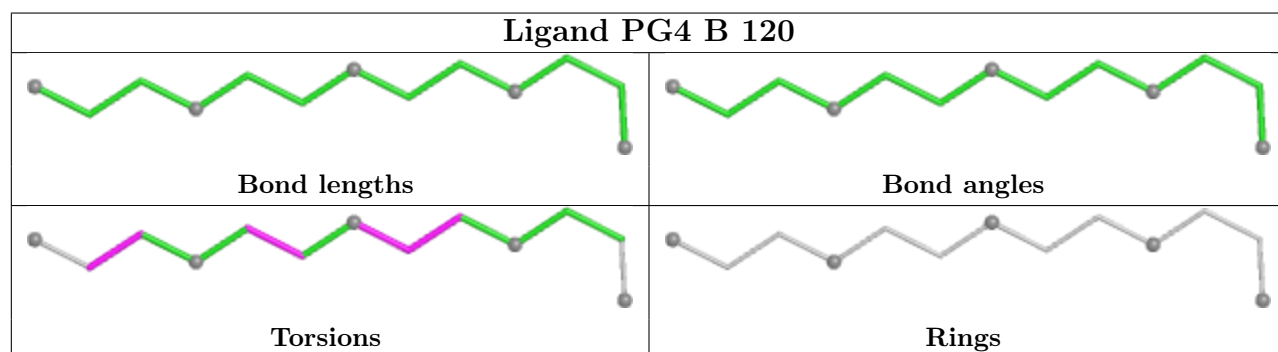
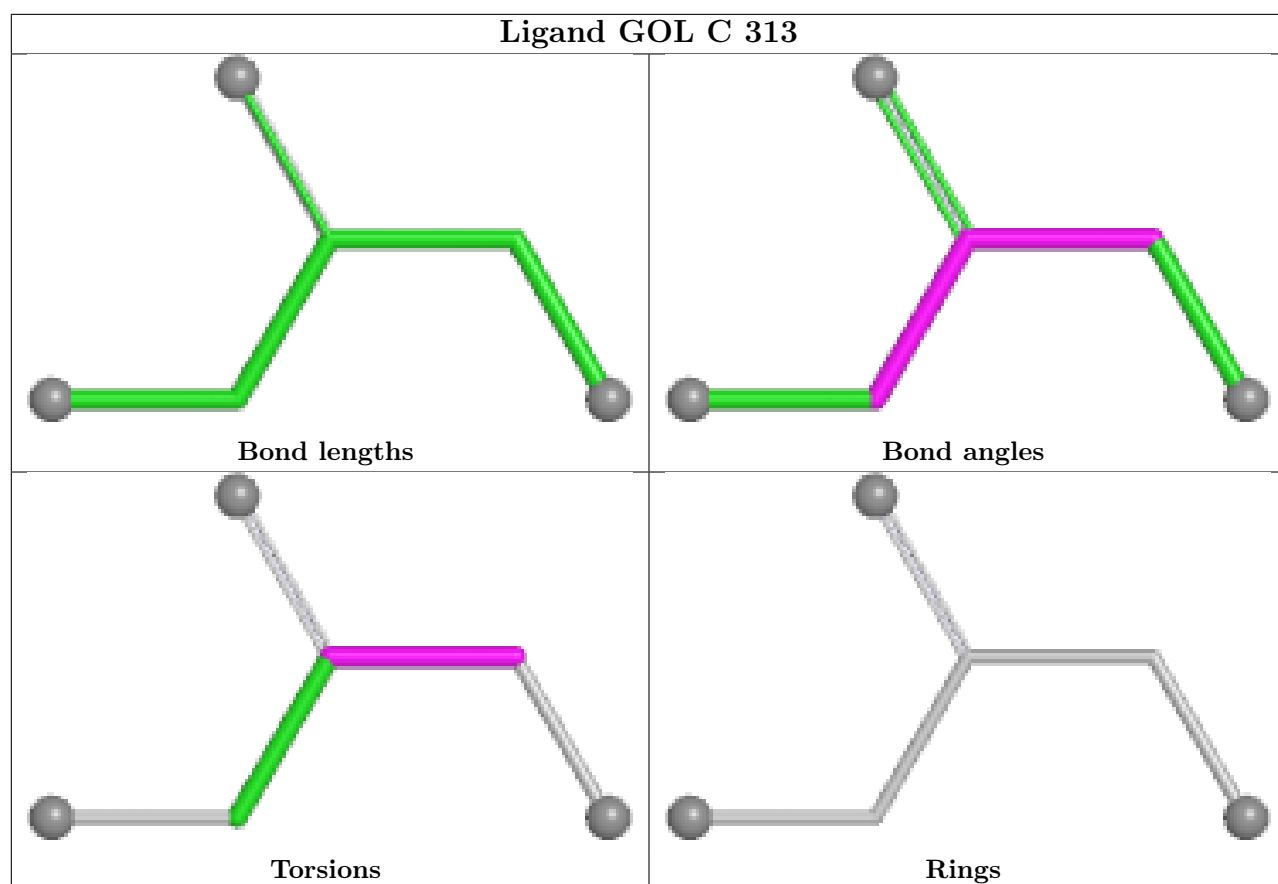


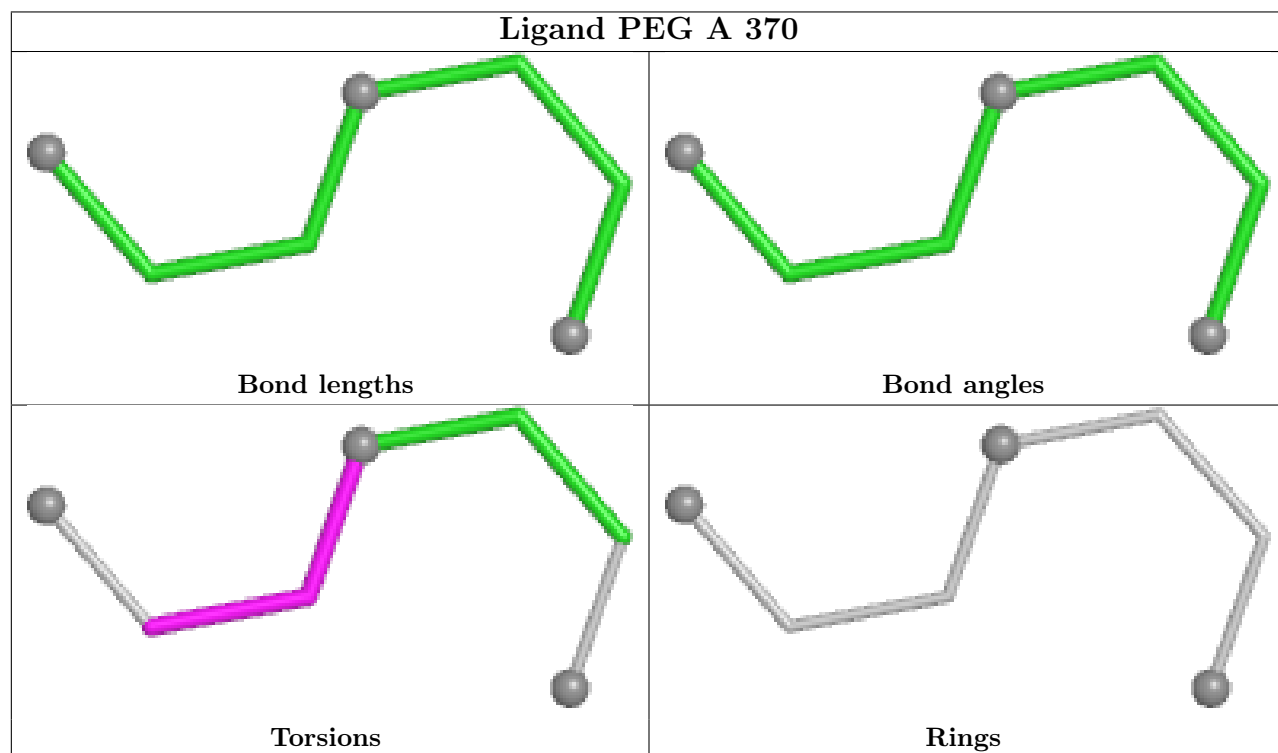
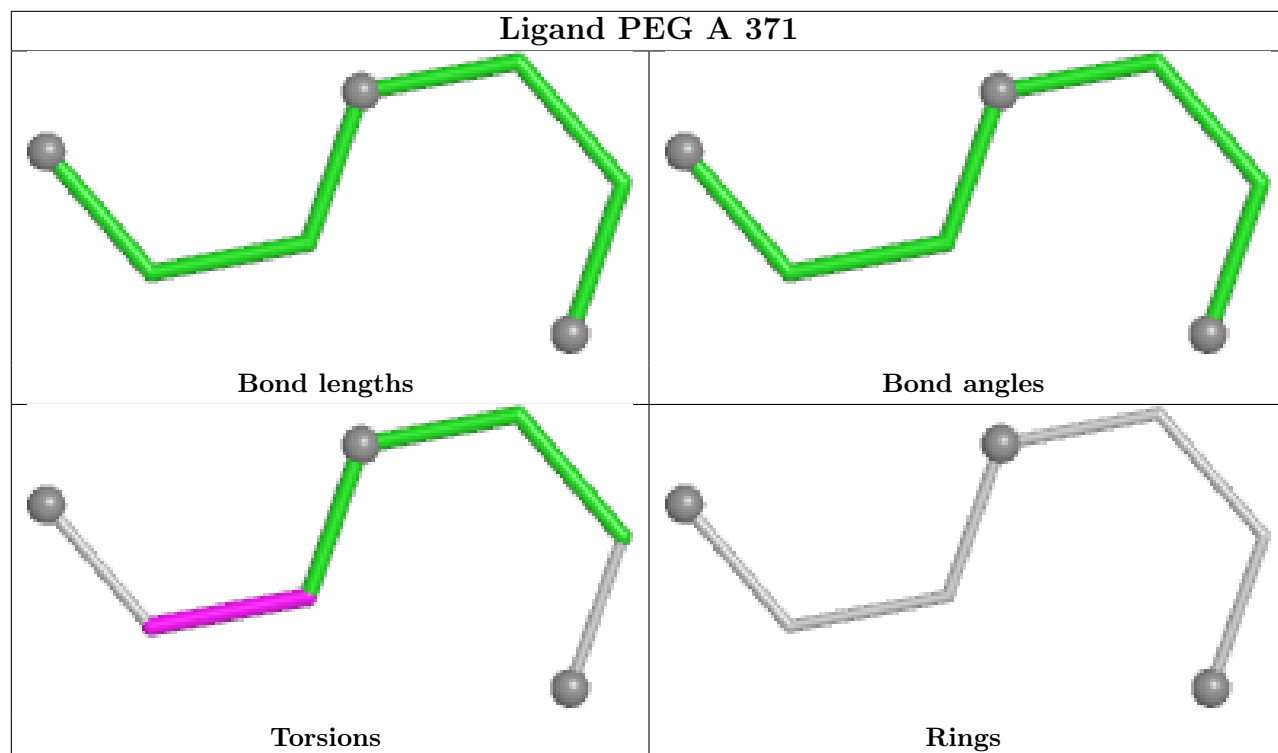


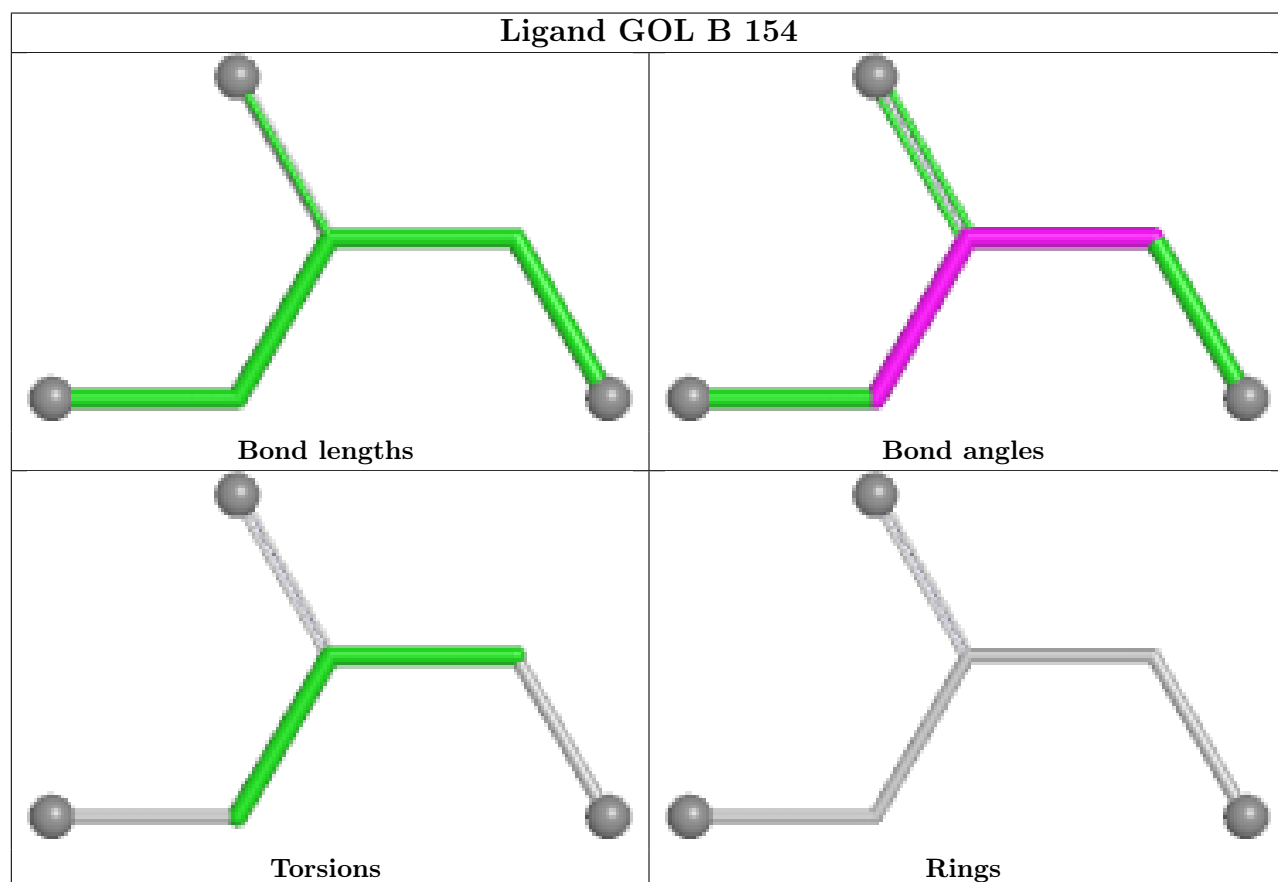
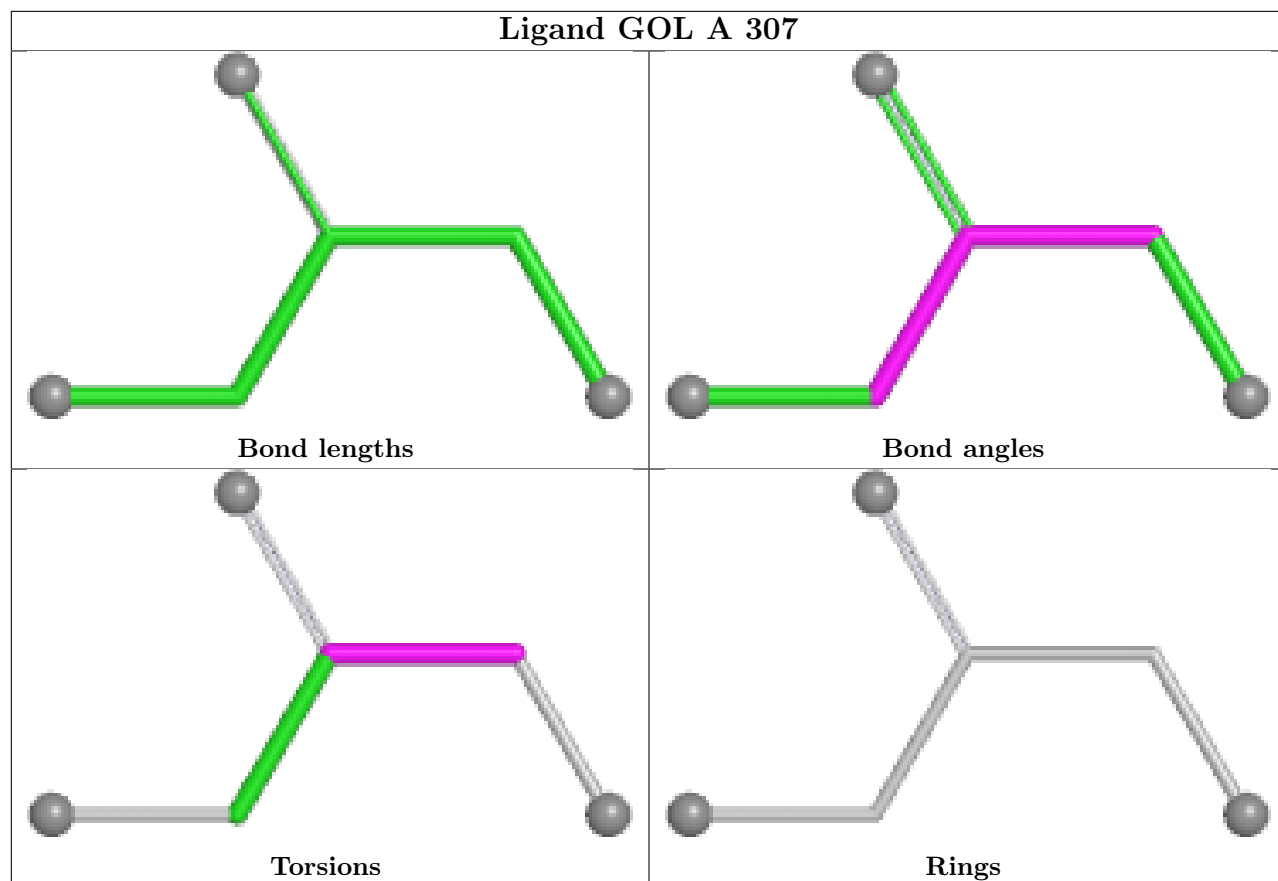


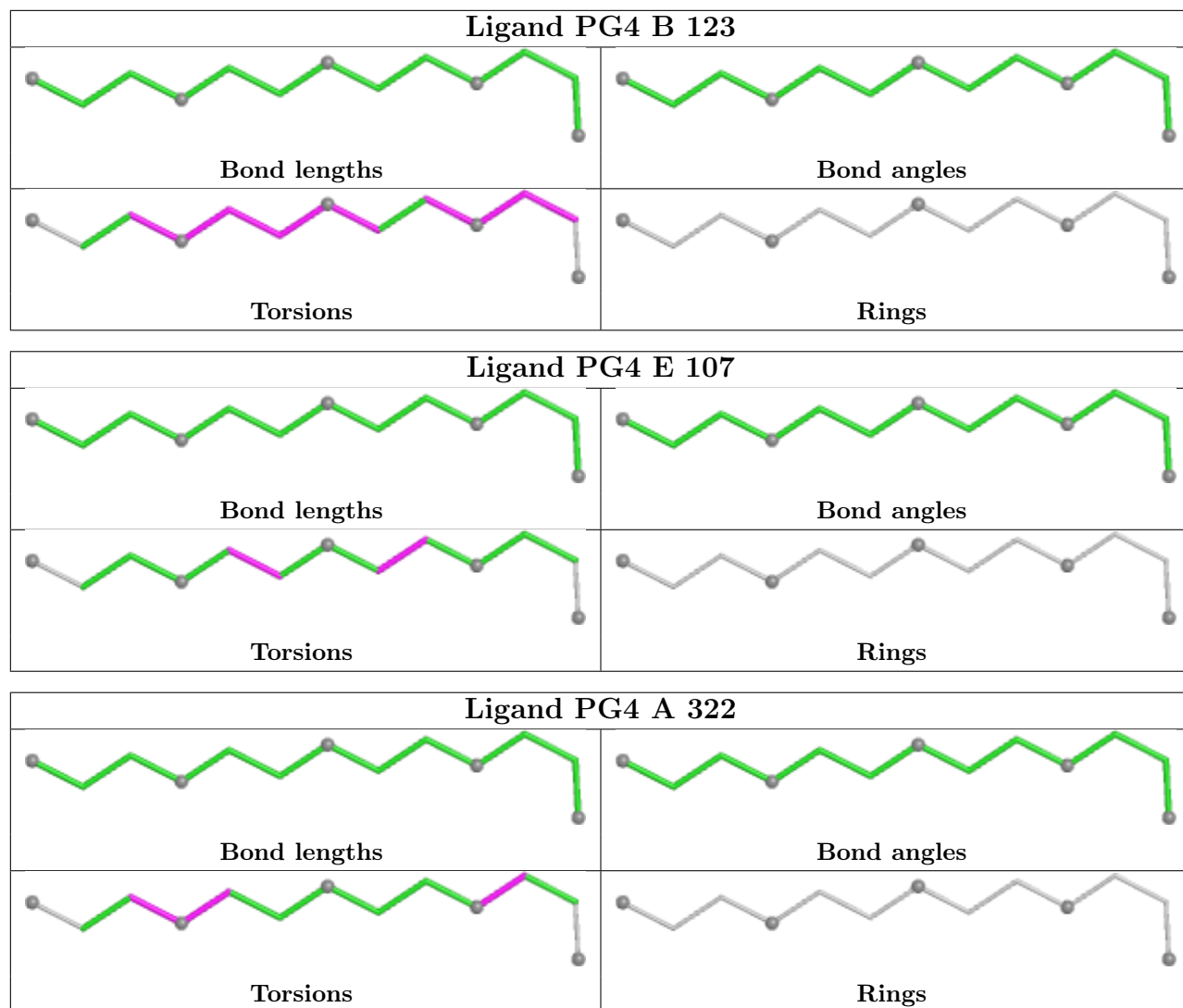


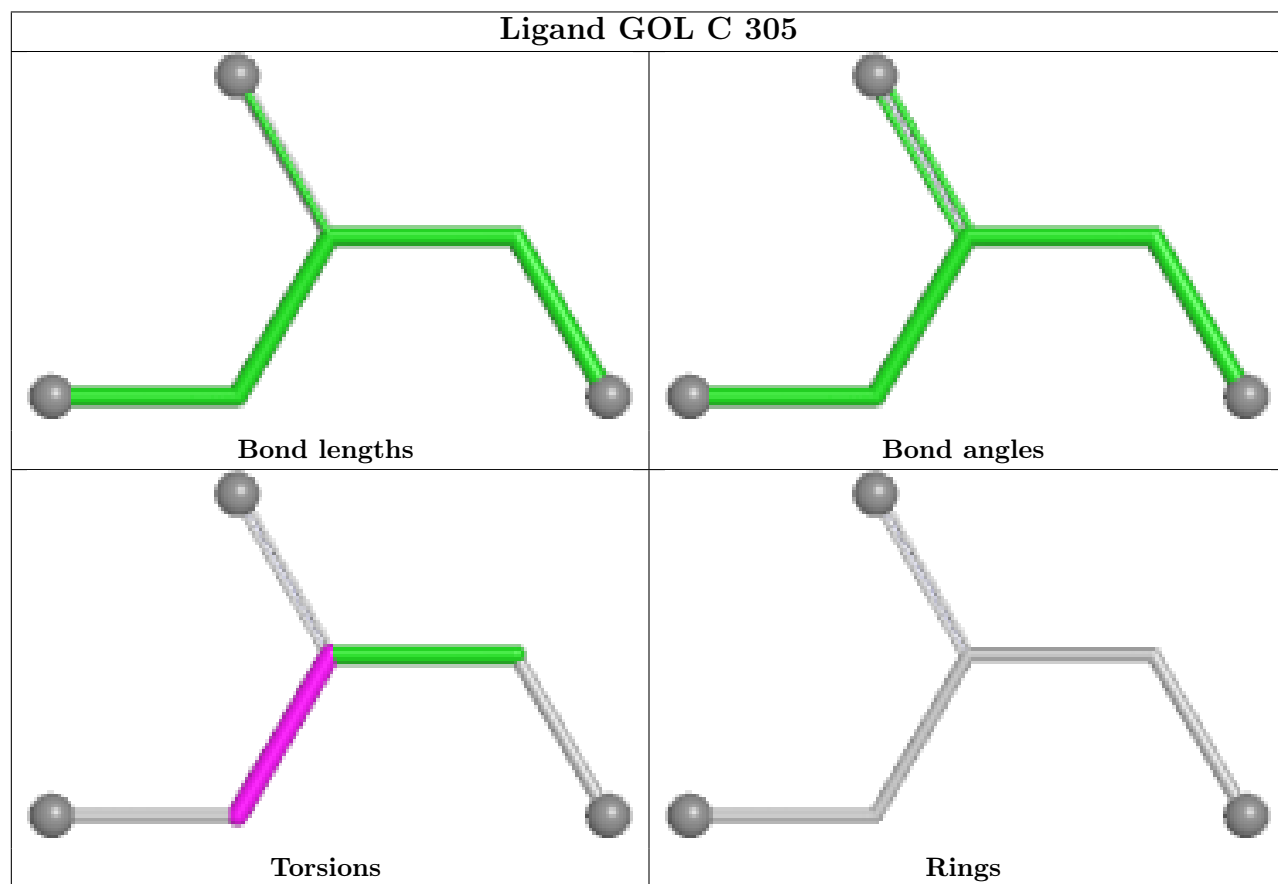
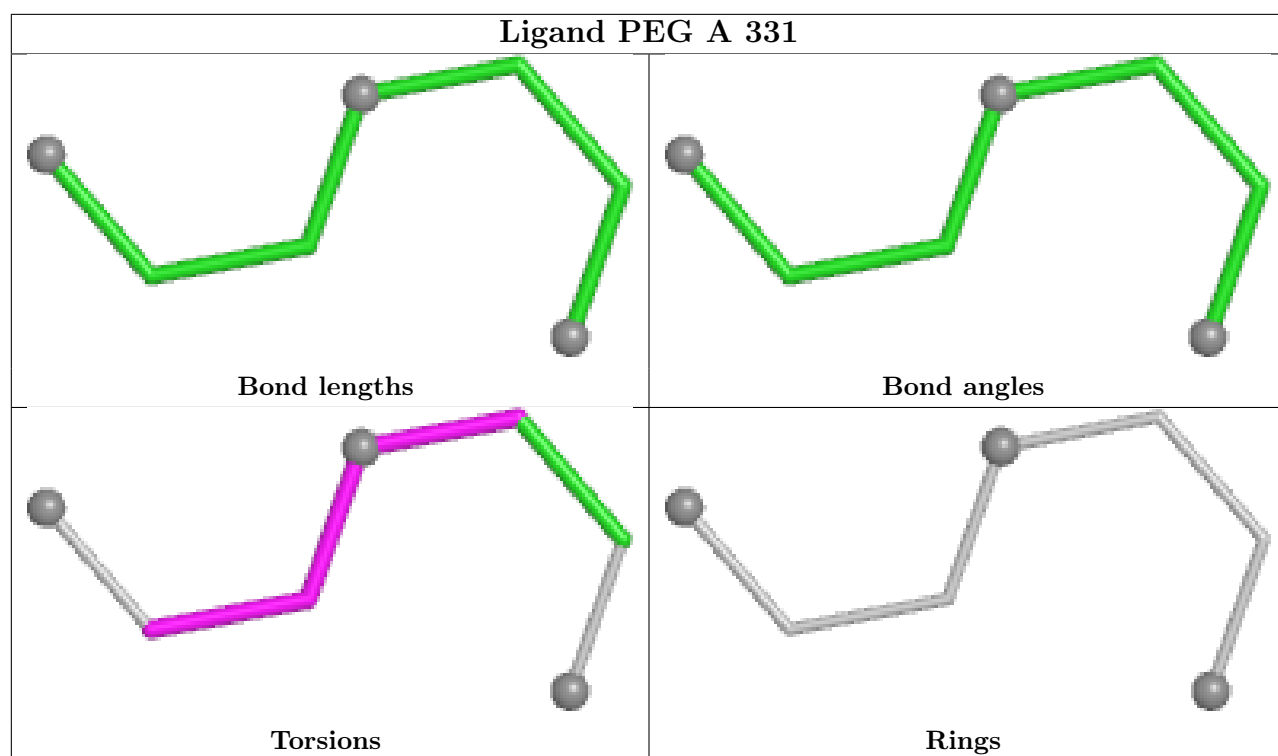


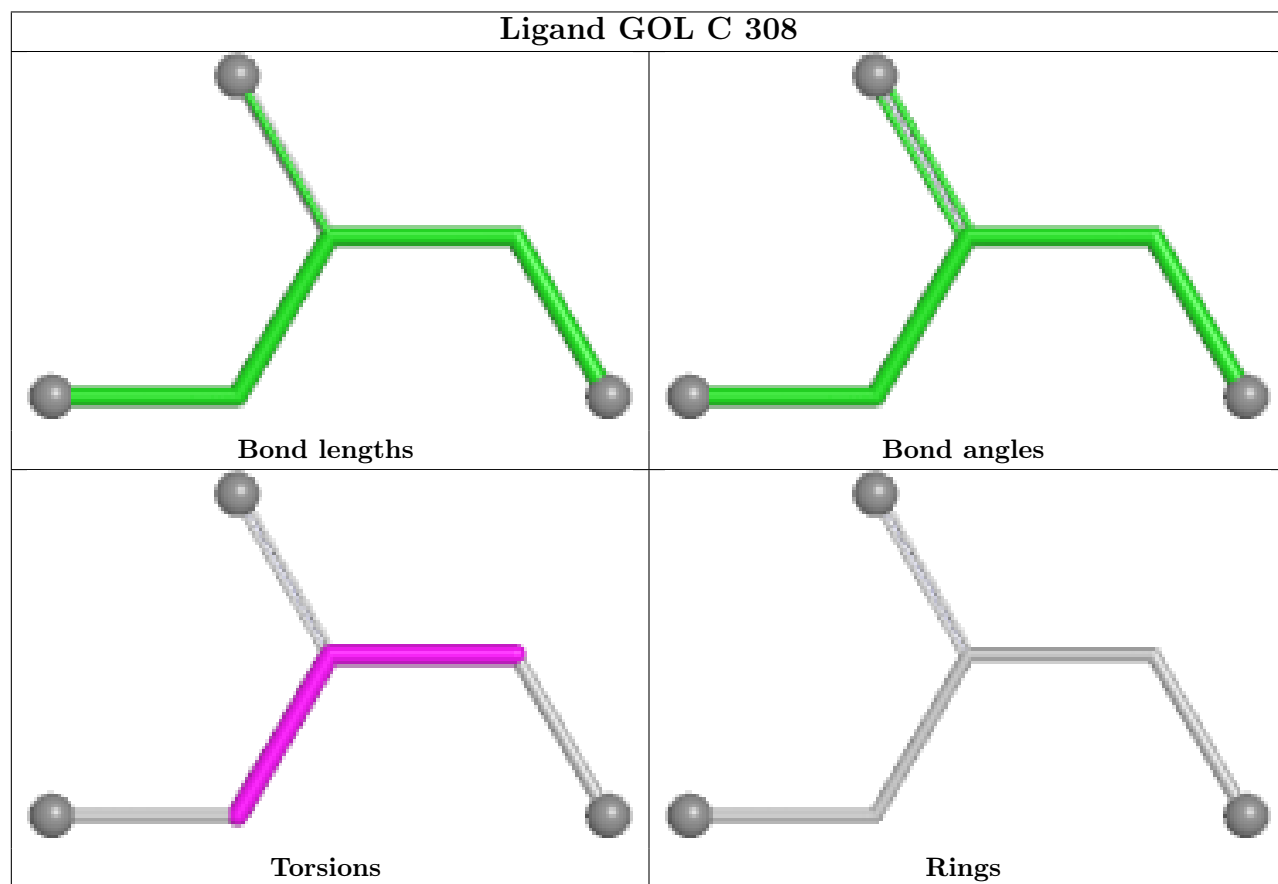
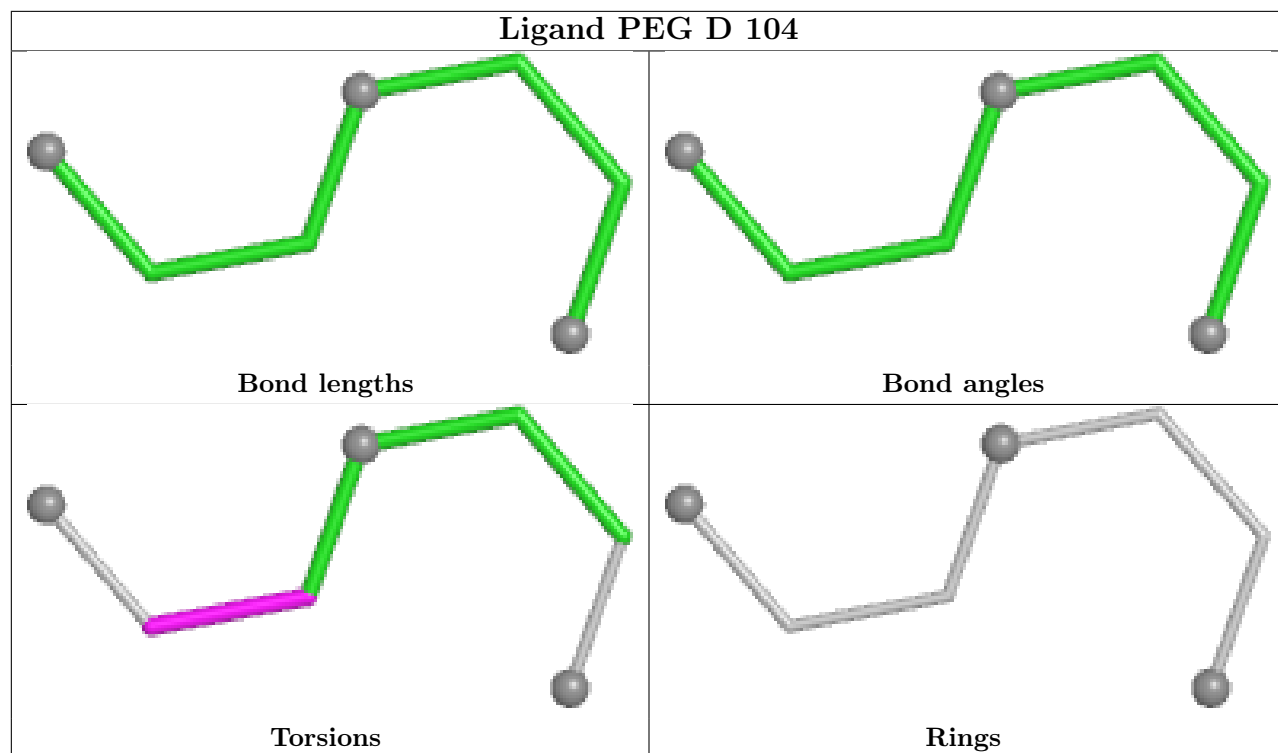


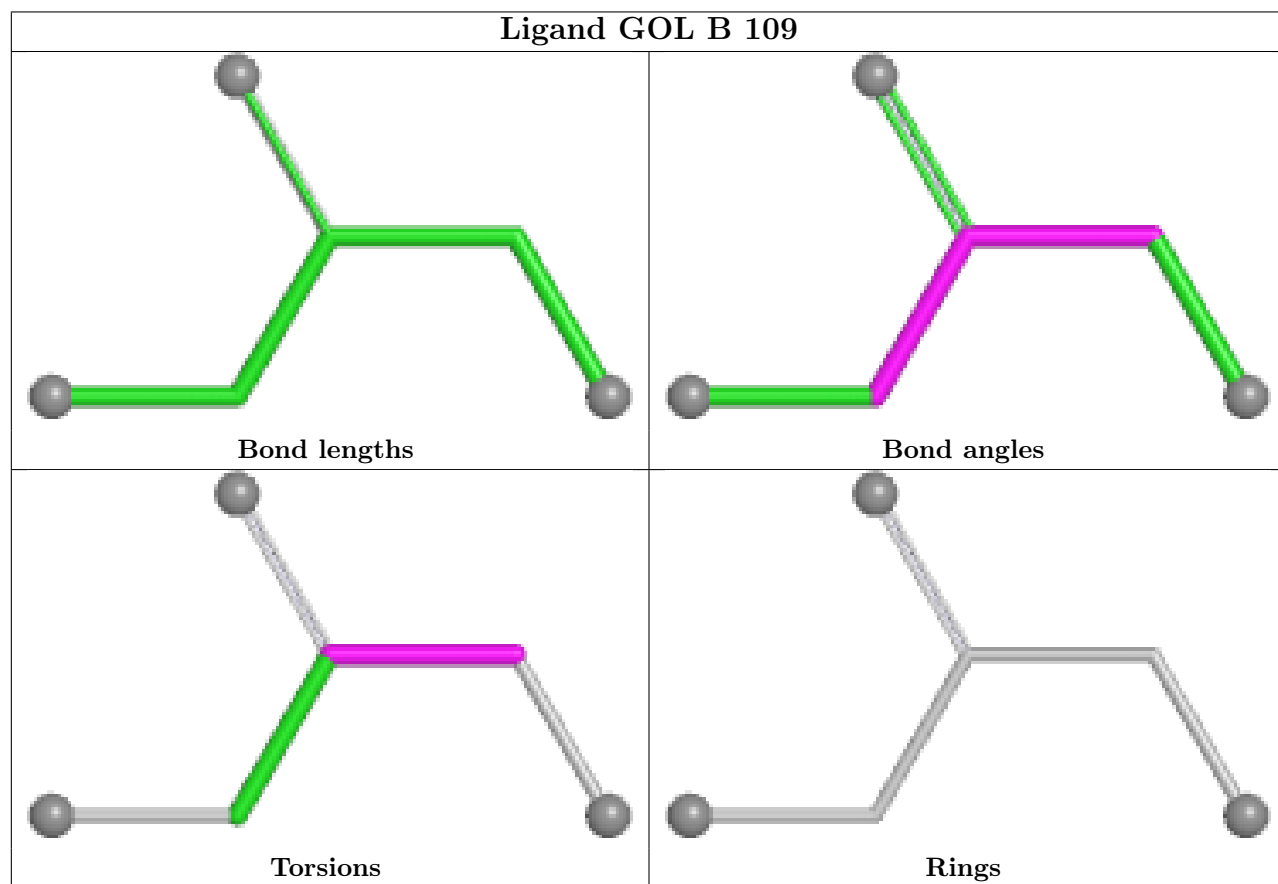
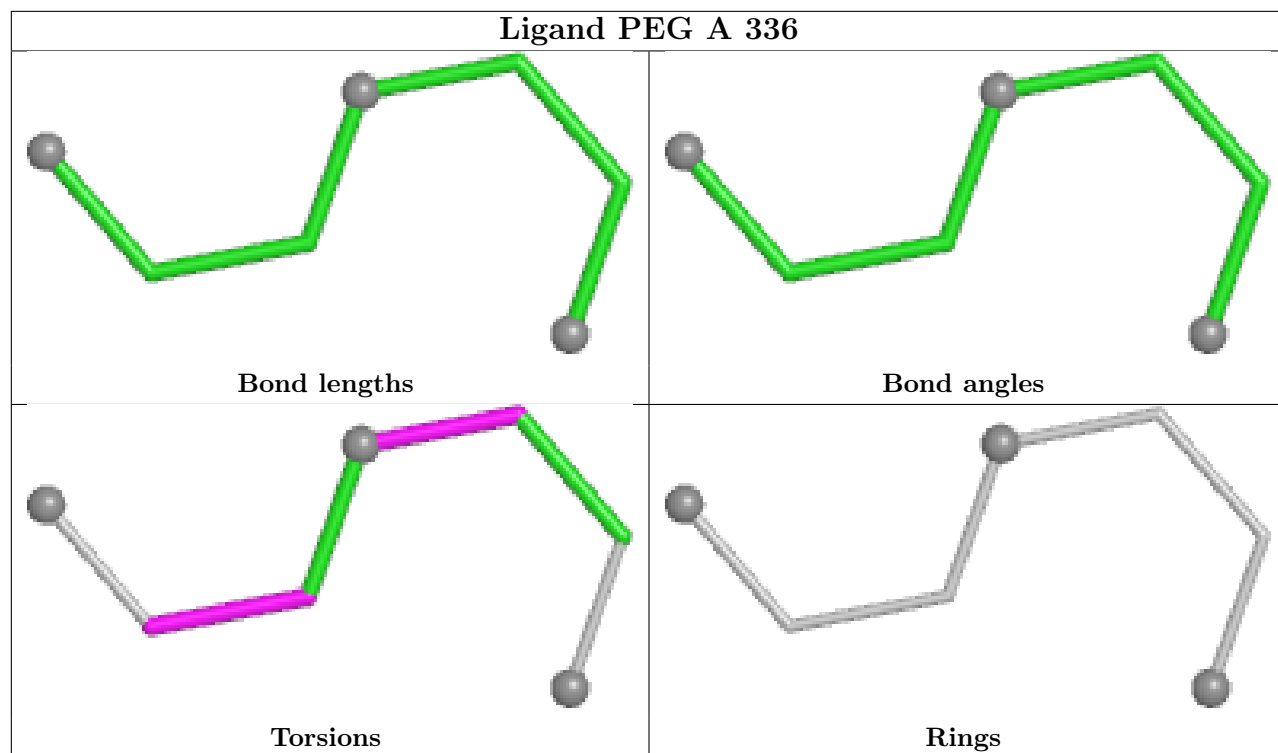


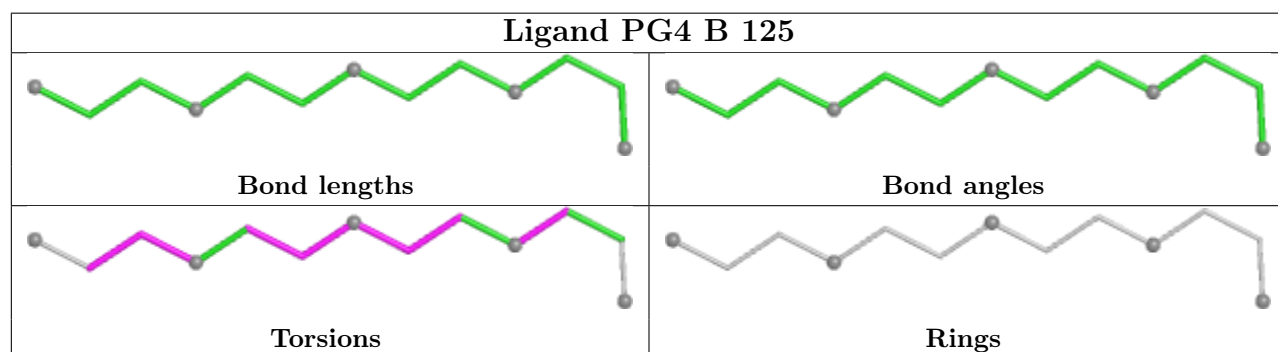
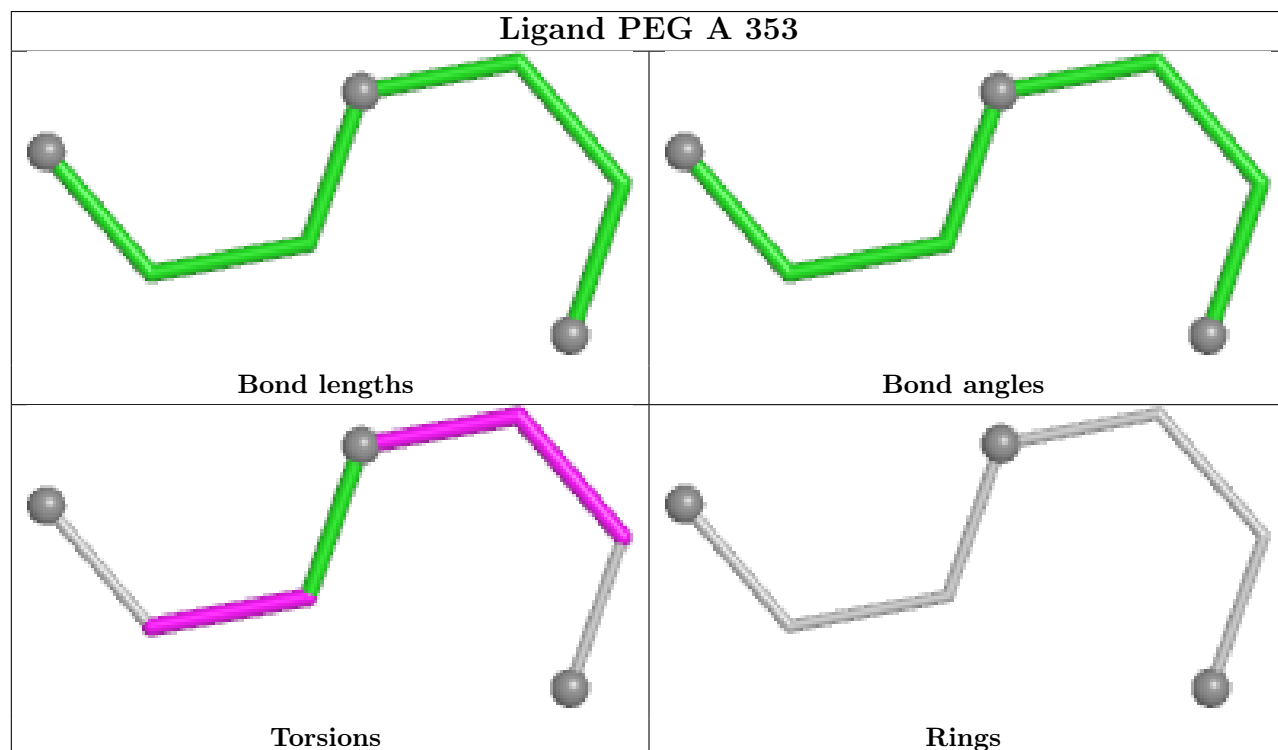
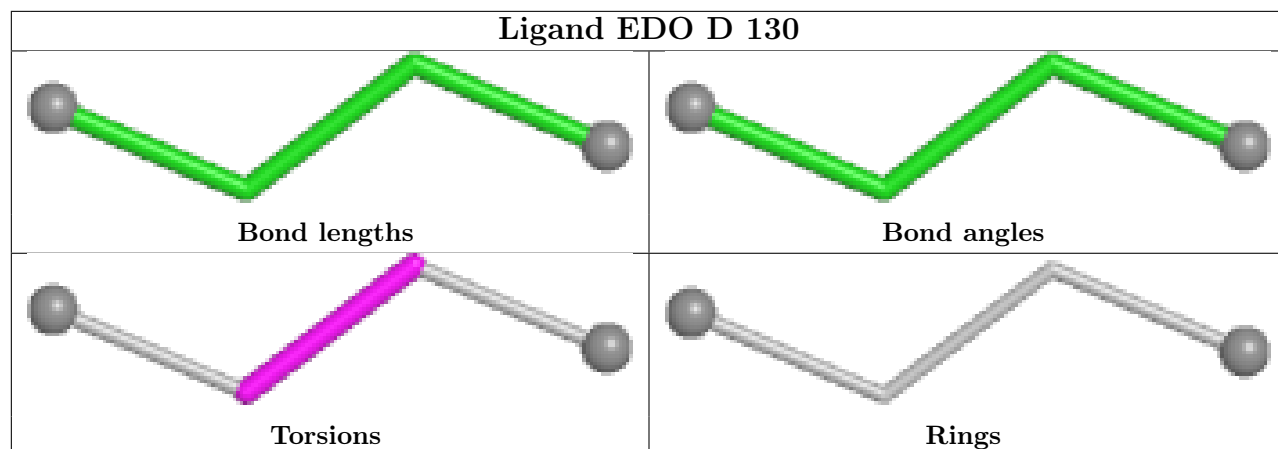


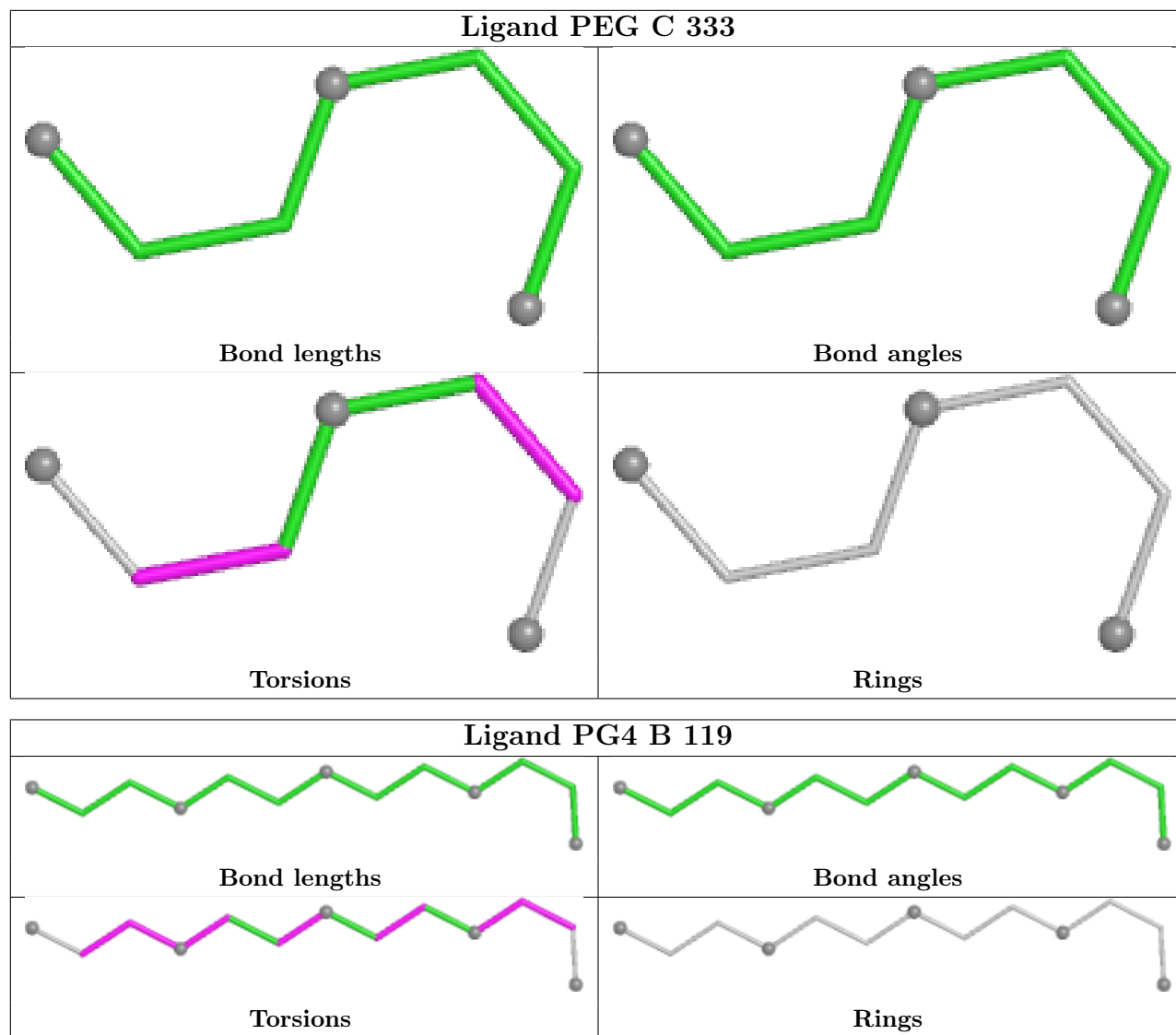












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	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%)

All (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
1	A	211	GLY	4.9
1	C	119	CYS	4.6
2	B	40	ALA	4.4
1	C	115	ASN	4.3
1	C	88	ALA	4.2
1	C	81	ASN	4.1
1	C	70	LEU	4.0
1	A	221	ASP	4.0
1	C	186	ILE	4.0
2	B	53	TYR	3.9
1	C	66	SER	3.8
1	C	155	ASP	3.6
1	A	45	PHE	3.5
1	C	77	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	90	ASN	3.3
2	B	83	THR	3.3
1	C	48	ILE	3.3
2	D	8	GLU	3.3
1	A	36	GLN	3.2
1	A	65	LEU	3.2
2	B	84	GLY	3.1
1	A	33	VAL	3.1
2	B	4	GLY	3.1
1	A	140	LEU	3.0
2	D	69	VAL	3.0
1	A	24	TRP	3.0
1	C	72	ASP	3.0
1	C	51	VAL	3.0
1	C	69	GLU	3.0
2	D	44	LYS	3.0
1	C	89	PHE	3.0
1	A	150	VAL	3.0
1	A	43	TRP	2.9
1	A	47	SER	2.9
2	D	60	GLY	2.9
1	C	177	MET	2.9
2	B	26	GLN	2.9
2	D	16	ILE	2.9
1	A	83	GLY	2.9
2	B	46	GLN	2.8
1	A	3	ASN	2.8
2	B	27	LEU	2.8
1	C	113	LEU	2.7
1	A	41	SER	2.7
1	C	229	CYS	2.7
2	B	57	VAL	2.7
1	A	77	ASN	2.7
1	C	99	CYS	2.6
2	B	9	ALA	2.6
2	B	48	VAL	2.6
1	A	142	PHE	2.6
1	A	72	ASP	2.6
1	A	214	GLY	2.6
1	C	230	GLY	2.6
1	A	84	LEU	2.6
2	B	55	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	65	MET	2.5
2	D	72	SER	2.5
2	D	92	ASP	2.5
1	A	70	LEU	2.5
1	C	157	ALA	2.5
2	B	32	ASN	2.5
1	A	93	ILE	2.5
2	D	68	ARG	2.5
1	A	204	ASN	2.5
2	B	39	GLU	2.5
1	A	48	ILE	2.4
2	B	19	ILE	2.4
1	C	8	ILE	2.4
1	C	226	MET	2.4
1	A	81	ASN	2.4
1	C	124	GLY	2.4
1	C	127	ASN	2.4
1	C	91	ASP	2.4
1	C	223	SER	2.4
1	A	38	ASN	2.3
1	A	175	ALA	2.3
1	A	156	PHE	2.3
1	A	146	ILE	2.3
1	A	163	ILE	2.3
2	B	68	ARG	2.3
2	D	2	ILE	2.3
4	F	1	VAL	2.3
2	D	93	ASP	2.3
1	A	63	ILE	2.3
1	A	85	ILE	2.3
1	C	100	THR	2.3
1	A	19	HIS	2.2
1	A	87	ASN	2.2
1	C	165	ASP	2.2
1	C	237	ILE	2.2
1	A	116	ILE	2.2
1	A	232	GLY	2.2
2	D	84	GLY	2.2
1	A	196	LYS	2.2
1	C	137	LYS	2.2
1	C	147	SER	2.2
1	C	194	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	3	PRO	2.2
1	C	176	VAL	2.2
1	A	201	ILE	2.2
2	D	27	LEU	2.2
1	A	152	VAL	2.1
1	C	85	ILE	2.1
1	C	98	ILE	2.1
1	C	36	GLN	2.1
1	C	173	ASN	2.1
2	B	56	LYS	2.1
1	A	15	GLU	2.1
1	A	205	SER	2.1
1	C	201	ILE	2.1
1	A	158	PHE	2.1
1	C	227	ARG	2.1
1	C	18	ASP	2.1
1	A	46	SER	2.0
1	C	133	ASP	2.0
1	C	144	GLY	2.0
1	C	61	LYS	2.0
1	C	218	ILE	2.0
1	C	114	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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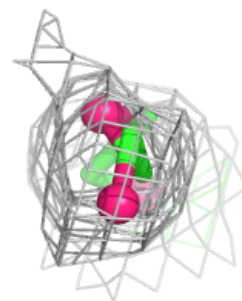
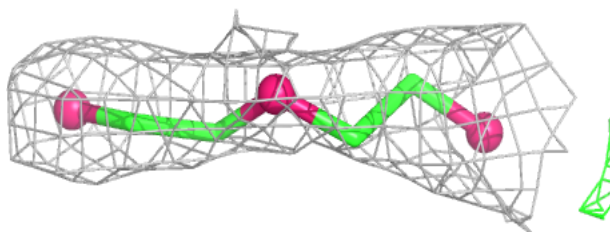
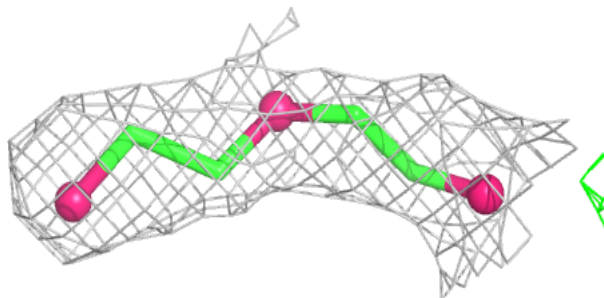
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	364	6/6	0.89	0.09	36,43,49,55	0
5	GOL	A	304	6/6	0.89	0.08	38,44,50,55	0
6	NA	D	129	1/1	0.89	0.20	82,82,82,82	0
10	PE8	B	137	25/25	0.89	0.08	20,49,64,72	0
10	PE8	B	138	25/25	0.89	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)

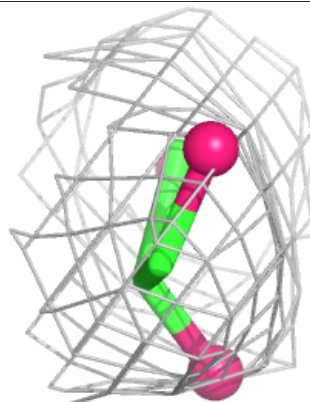
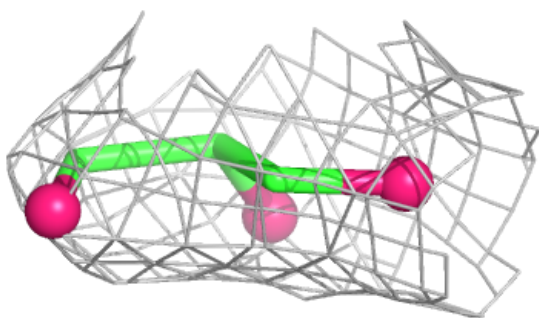
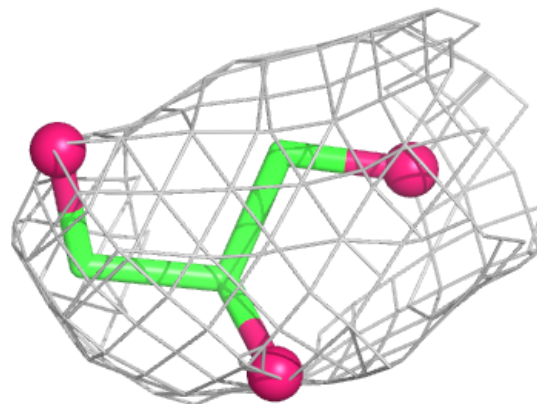
**Electron density around EDO B 143:**

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



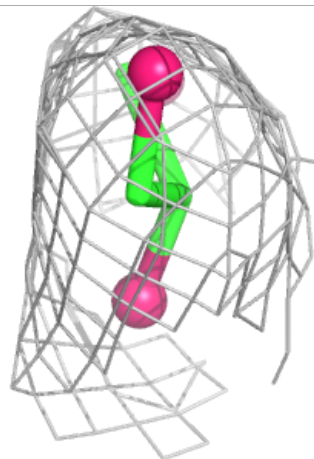
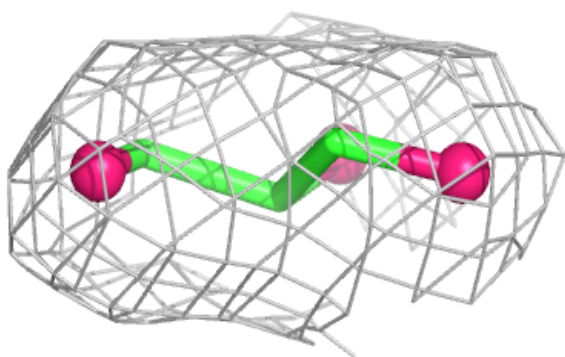
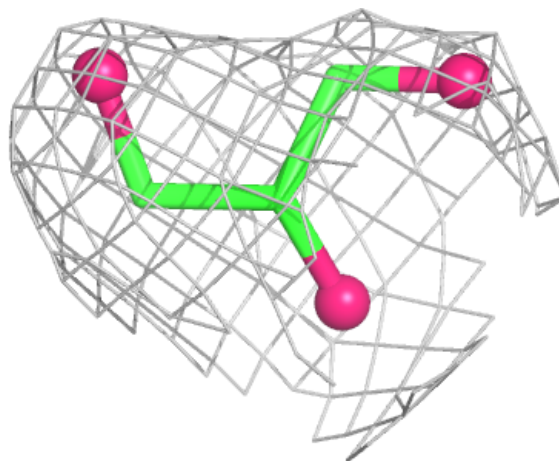
Electron density around GOL C 305:

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



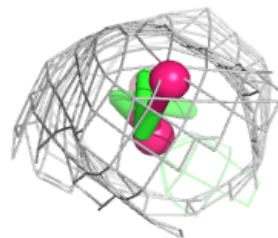
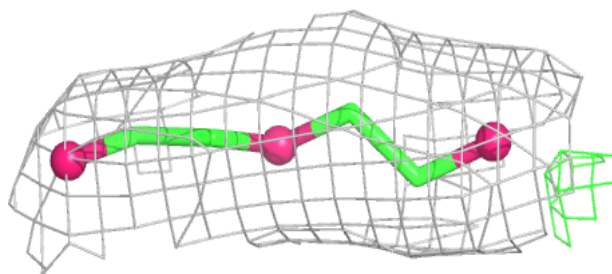
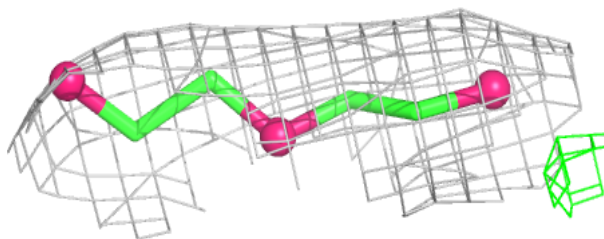
Electron density around GOL D 113:

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

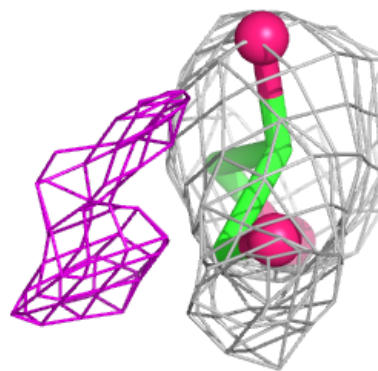
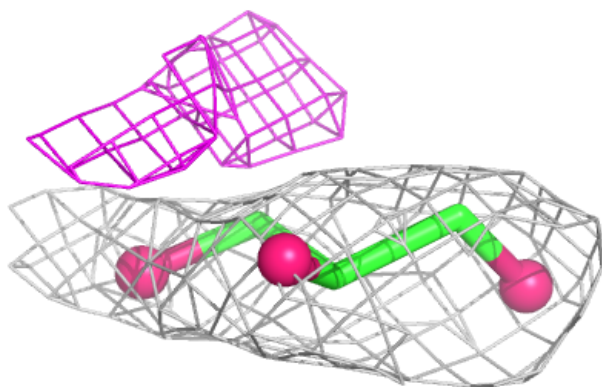
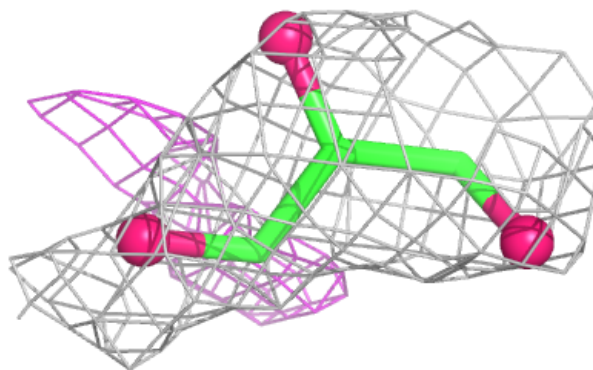


Electron density around PEG A 338:

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

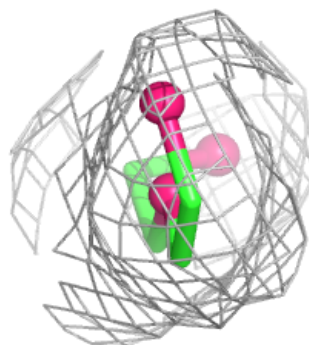
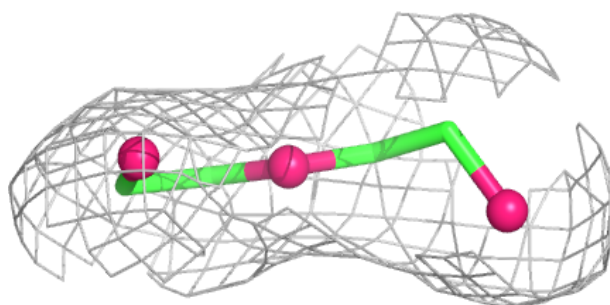
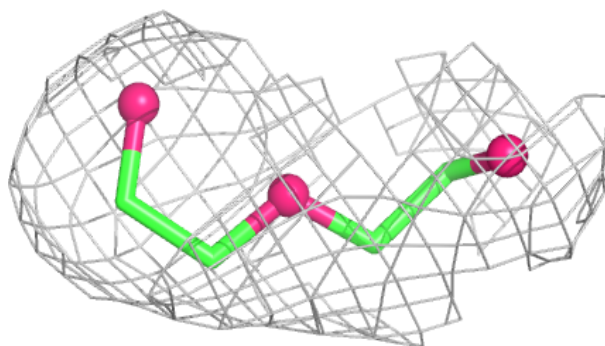
**Electron density around GOL F 103:**

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

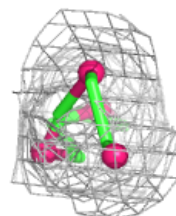
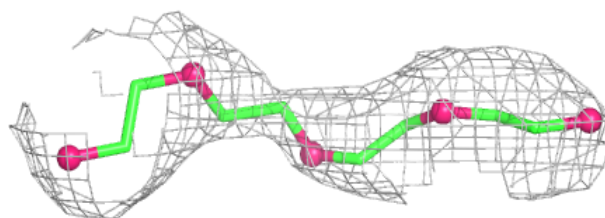


Electron density around PEG B 128:

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

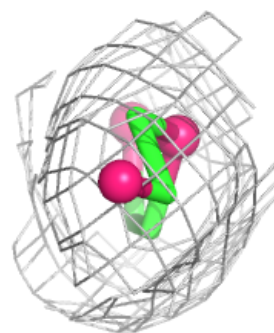
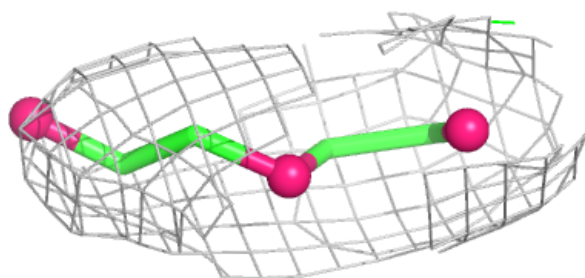
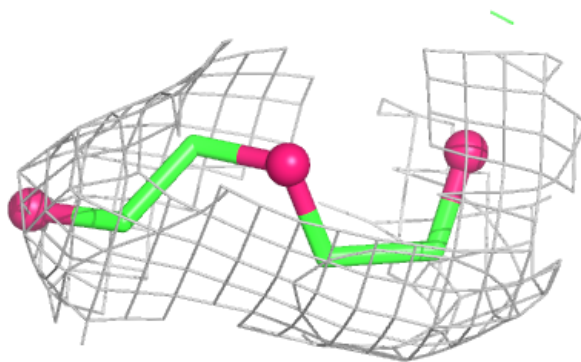
**Electron density around PG4 E 105:**

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



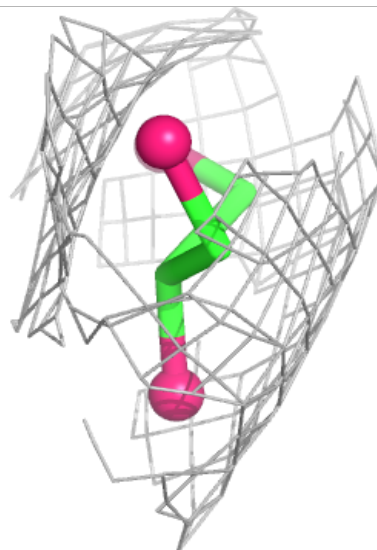
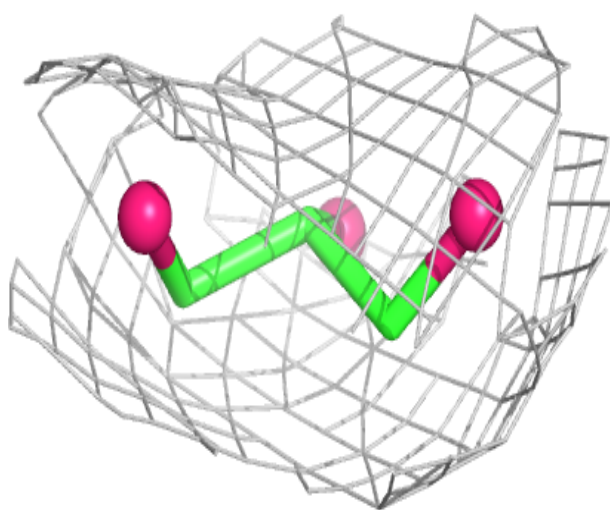
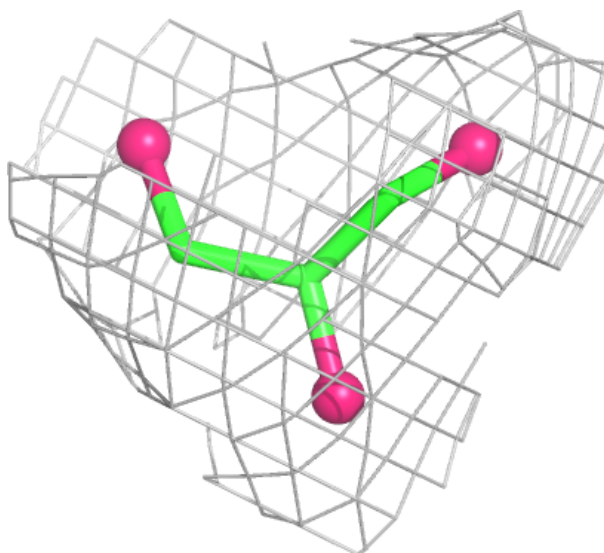
Electron density around PEG B 133:

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



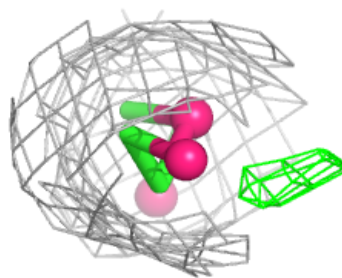
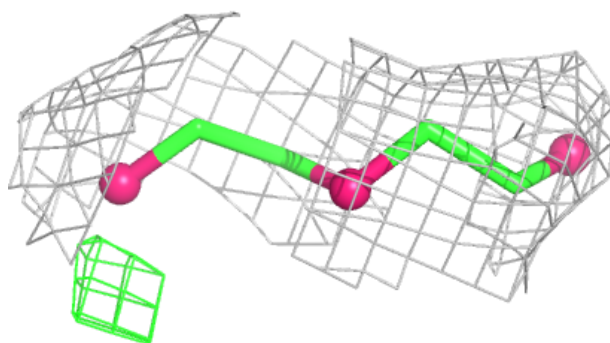
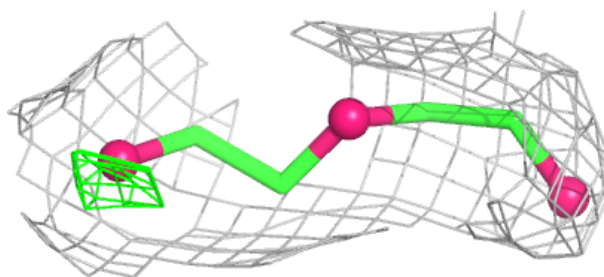
Electron density around GOL D 107:

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



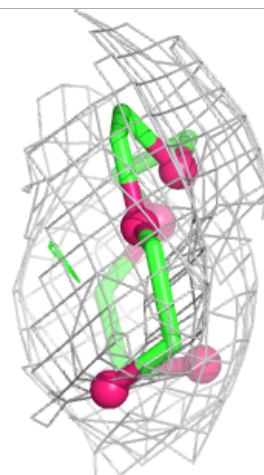
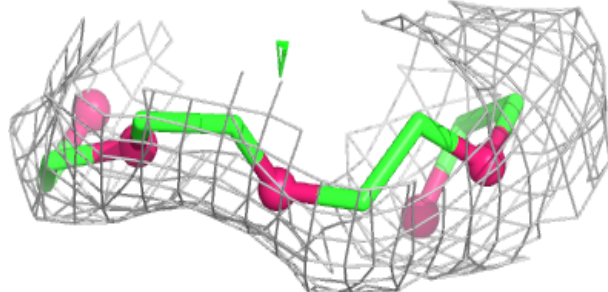
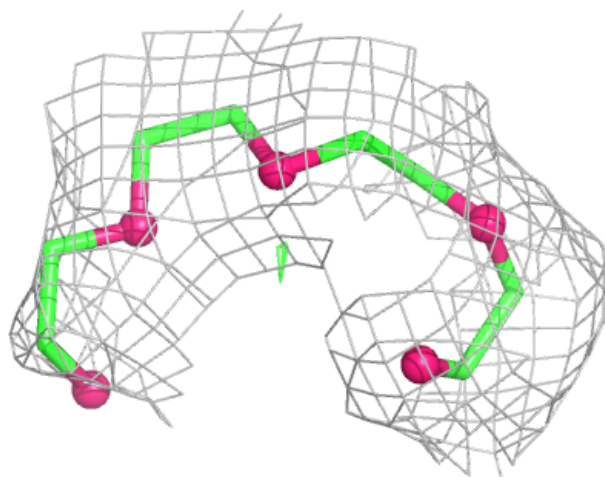
Electron density around PEG A 337:

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



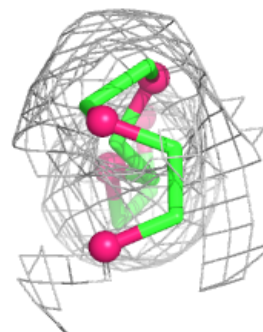
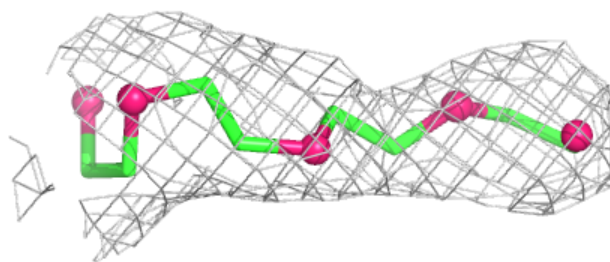
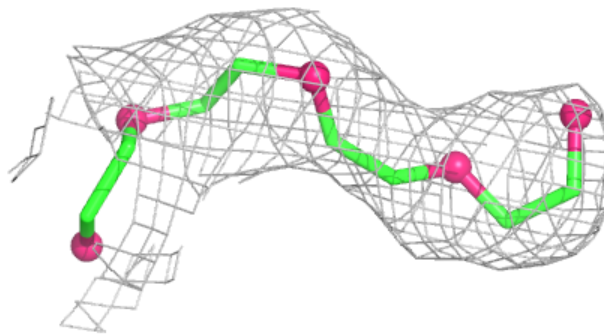
Electron density around PG4 B 101:

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



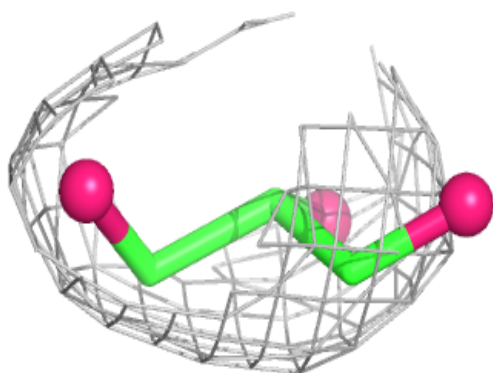
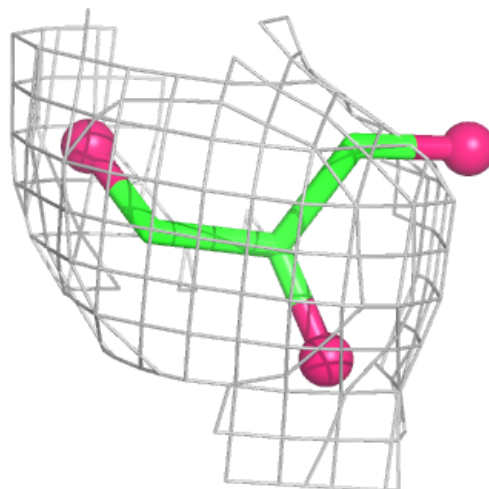
Electron density around PG4 A 325:

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



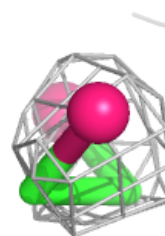
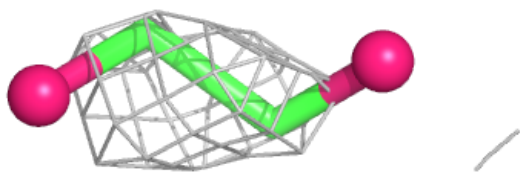
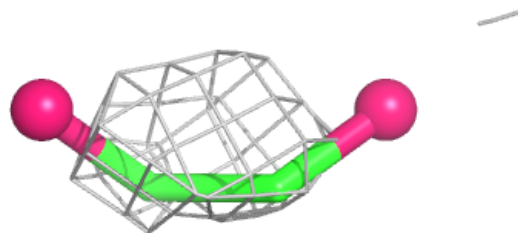
Electron density around GOL E 103:

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



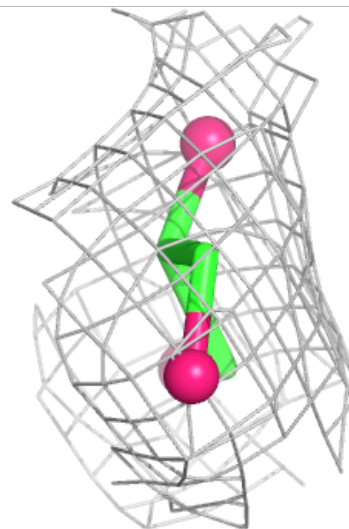
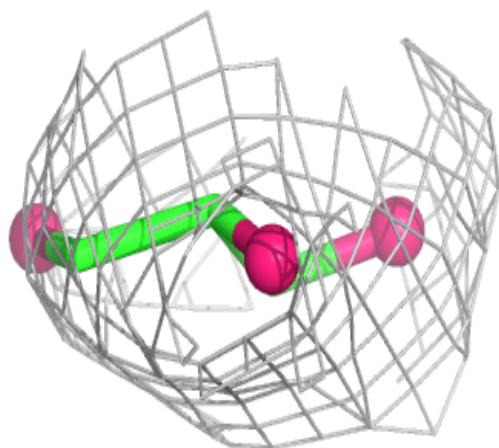
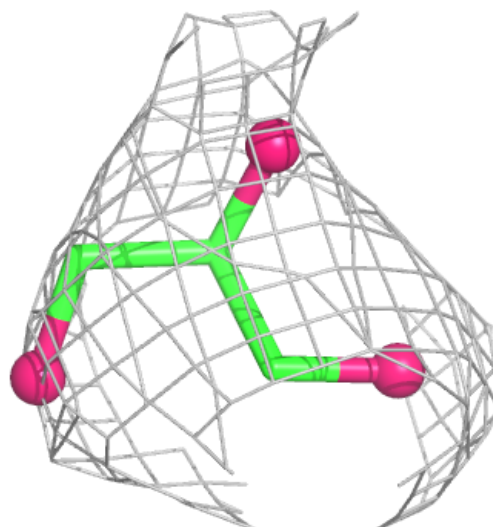
Electron density around EDO A 351:

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



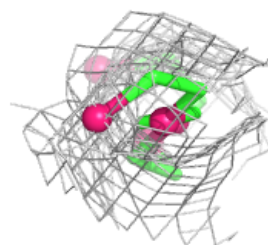
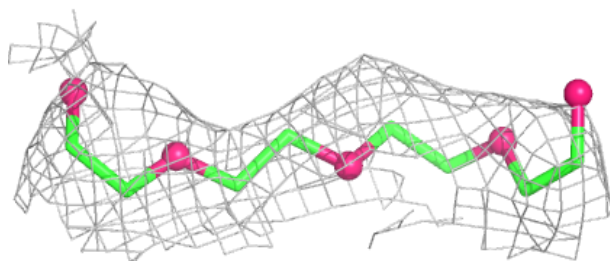
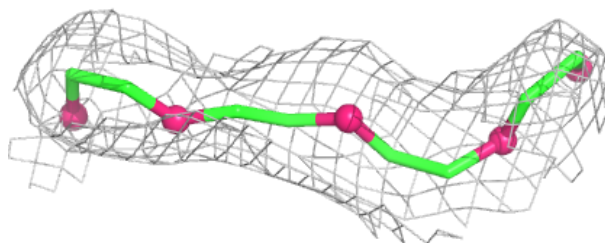
Electron density around GOL B 105:

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

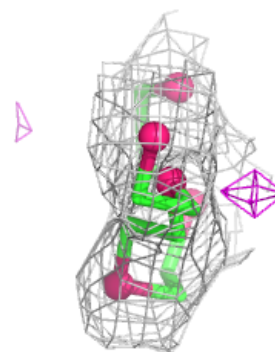
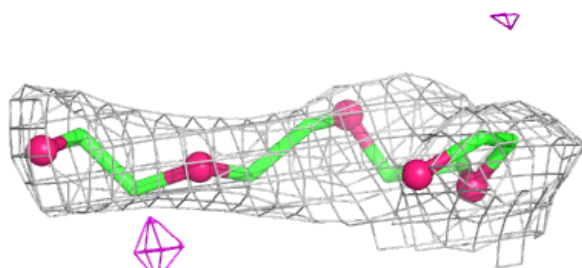
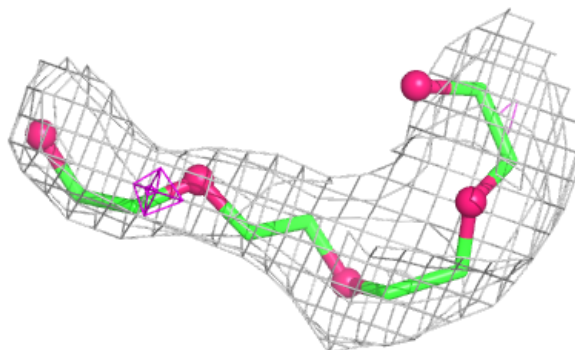


Electron density around PG4 C 322:

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

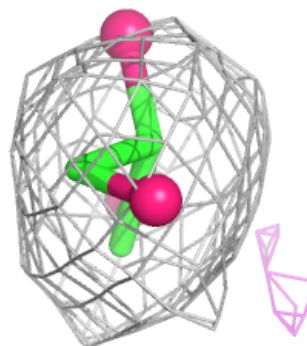
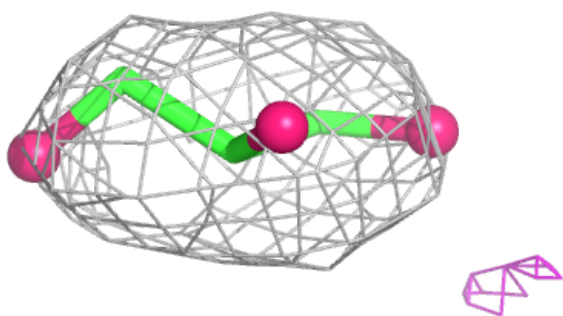
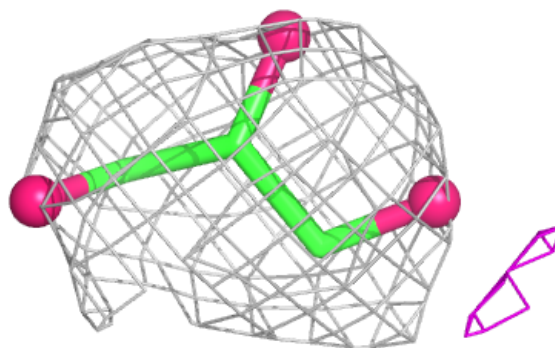
**Electron density around PG4 A 326:**

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

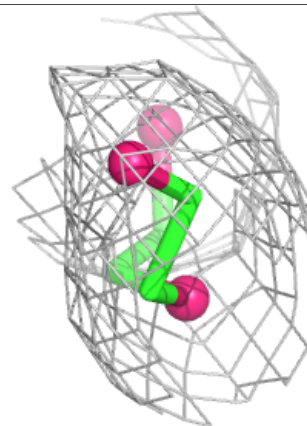
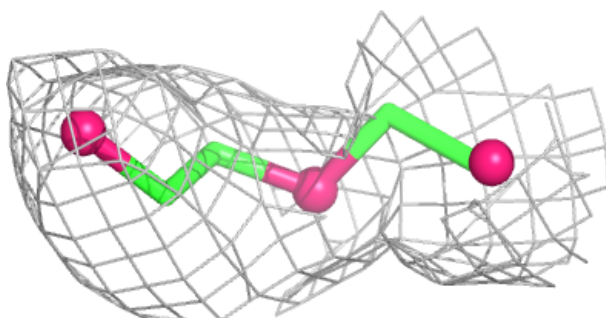
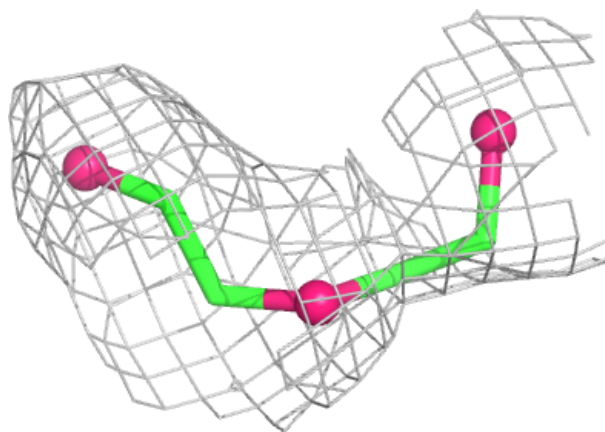


Electron density around GOL C 311:

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

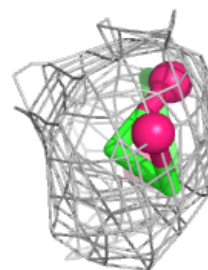
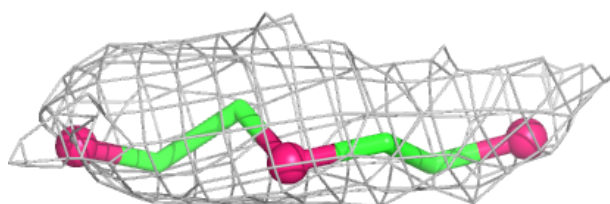
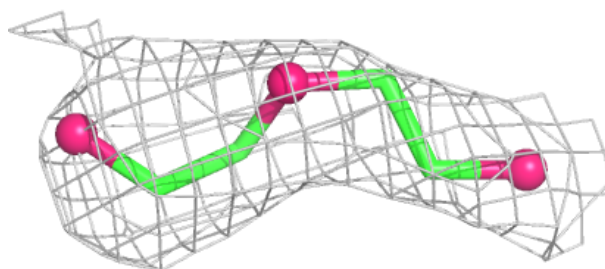
**Electron density around PEG B 134:**

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

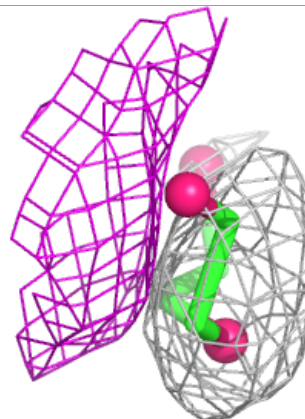
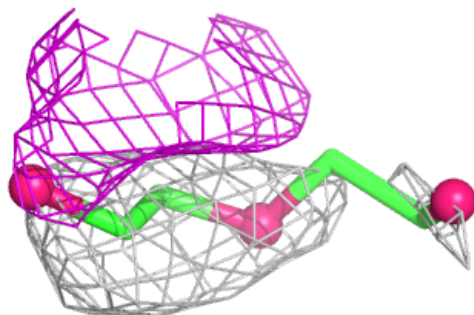
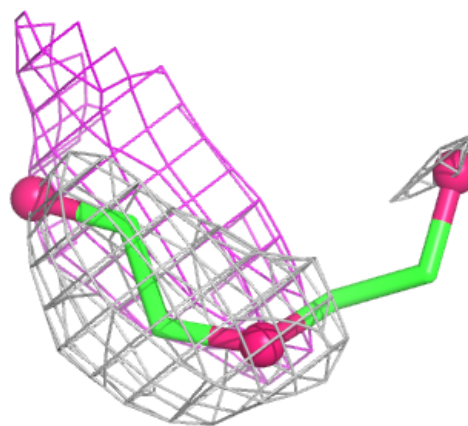


Electron density around PEG A 341:

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

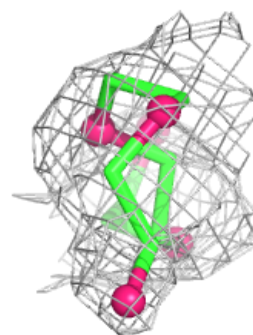
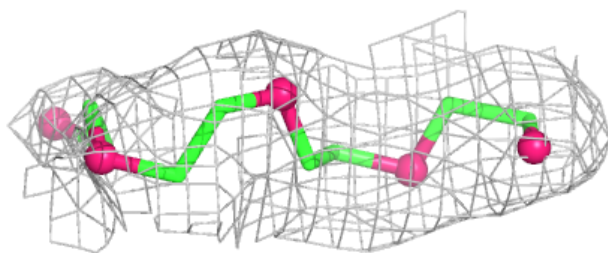
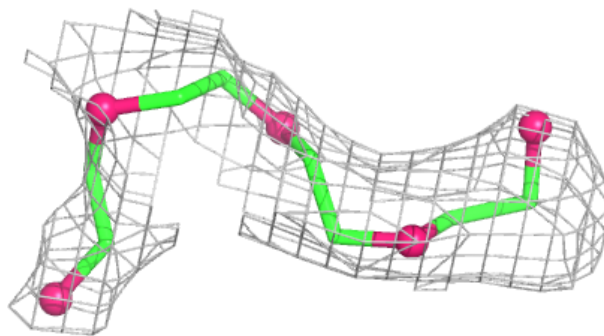
**Electron density around PEG D 104:**

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

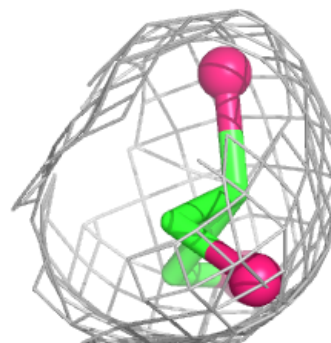
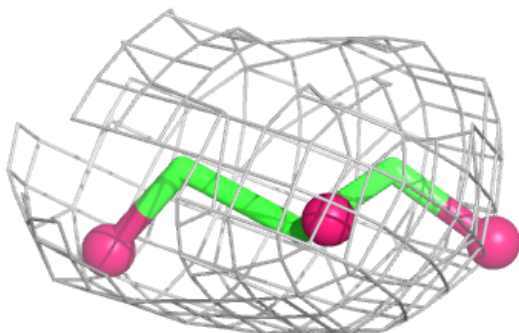
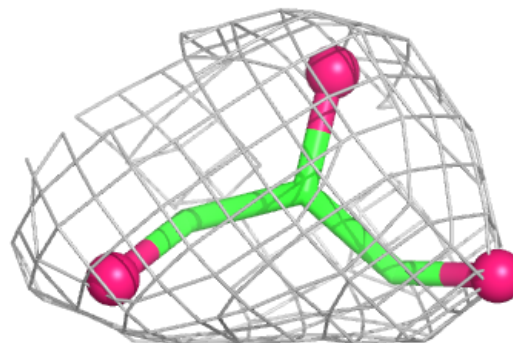


Electron density around PG4 A 323:

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

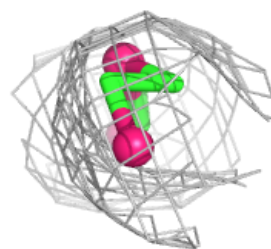
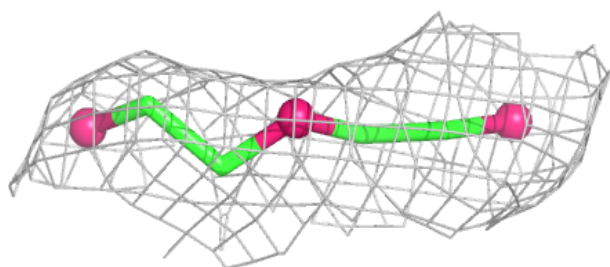
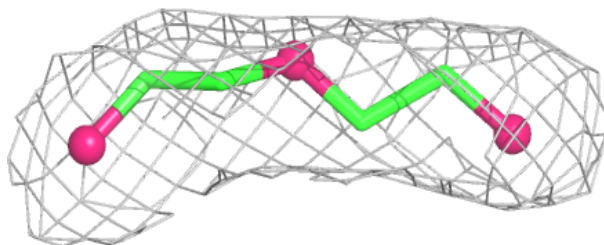
**Electron density around GOL B 104:**

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

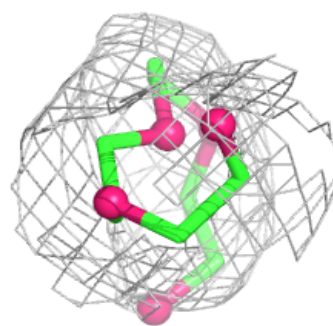
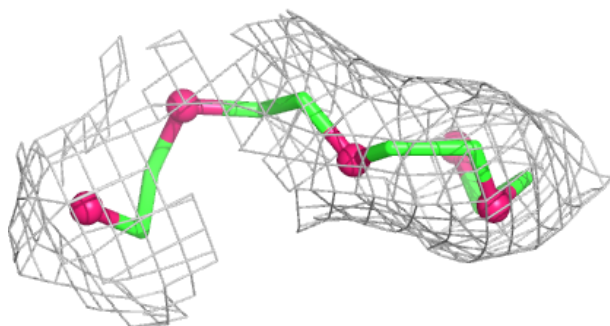
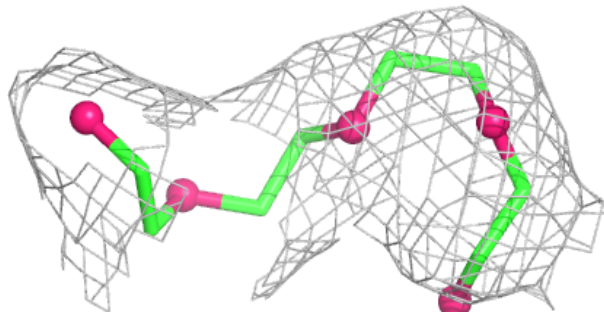


Electron density around PEG A 335:

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

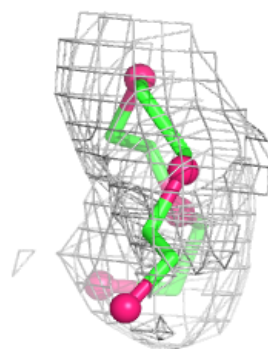
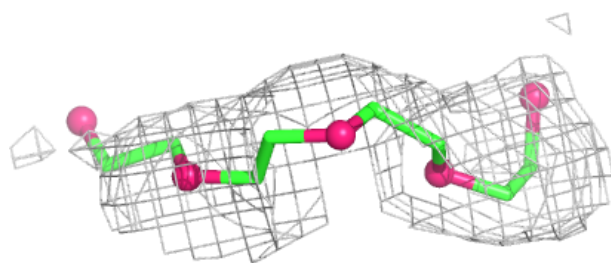
**Electron density around PG4 A 324:**

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

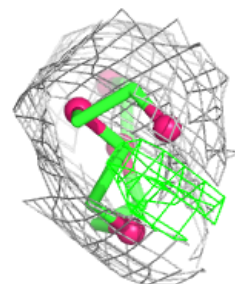
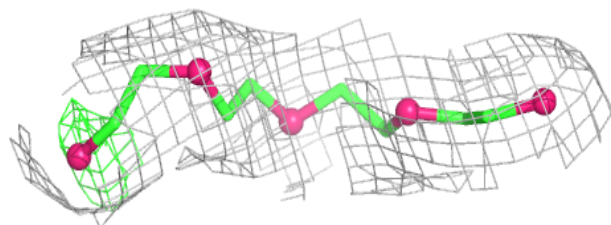
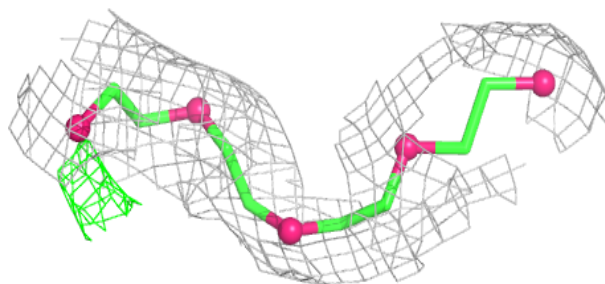


Electron density around PG4 C 324:

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

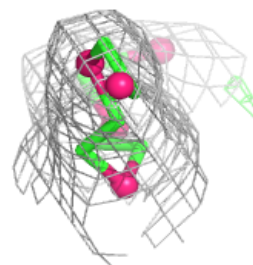
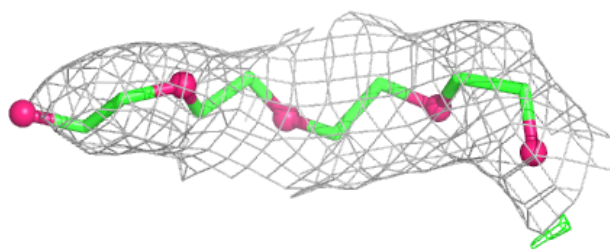
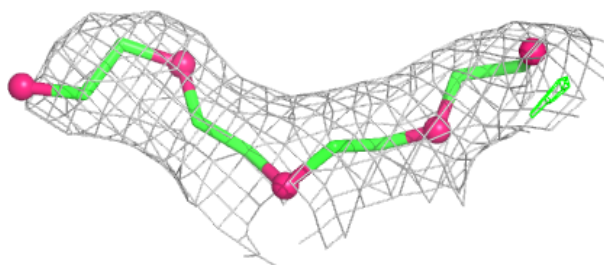
**Electron density around PG4 D 120:**

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

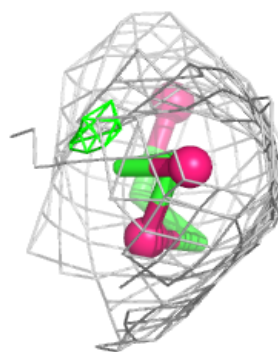
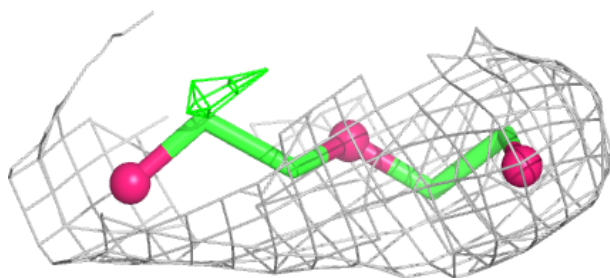
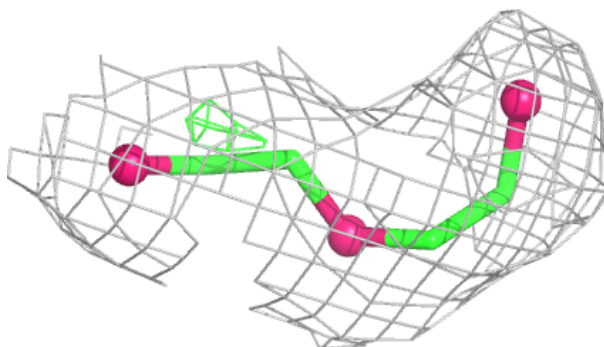


Electron density around PG4 B 118:

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

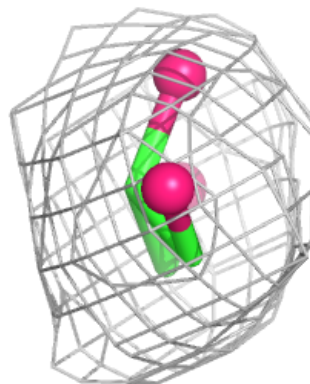
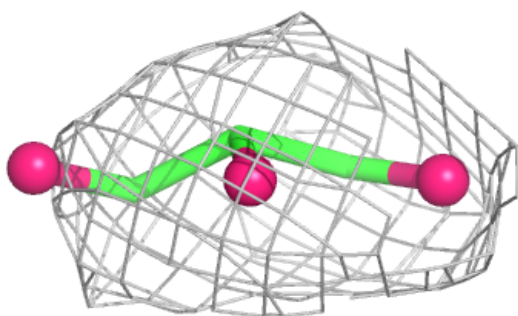
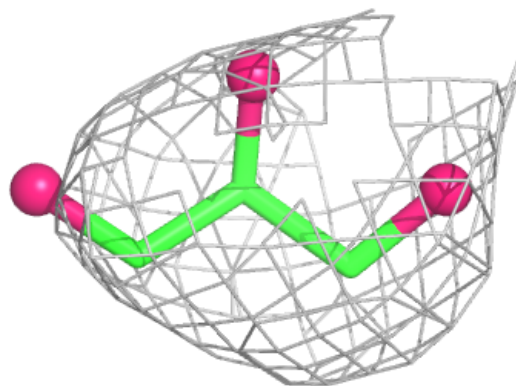
**Electron density around PEG A 330:**

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



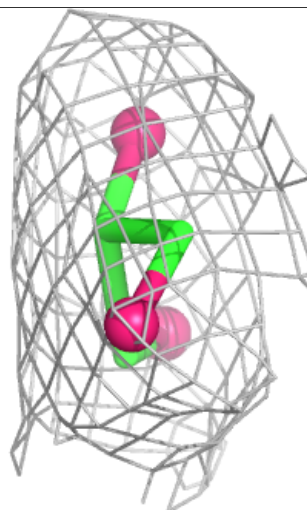
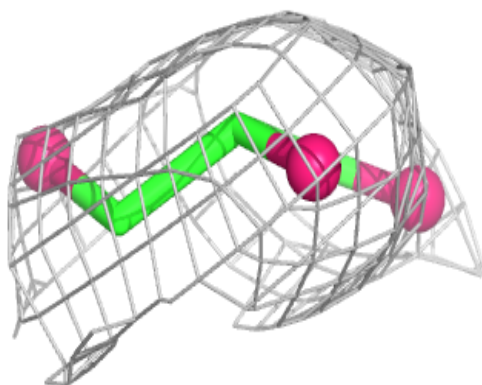
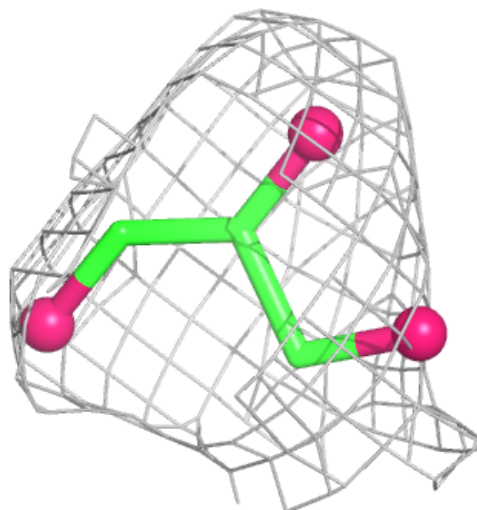
Electron density around GOL B 140:

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



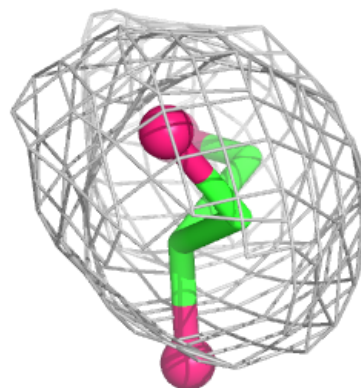
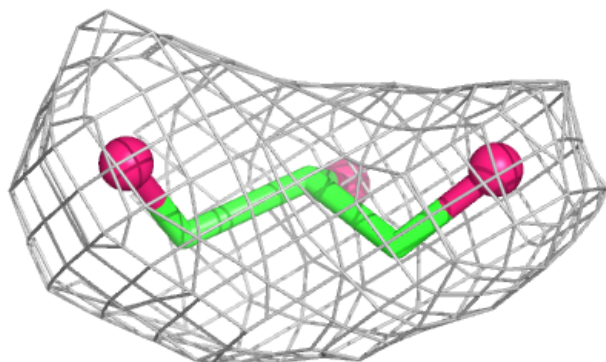
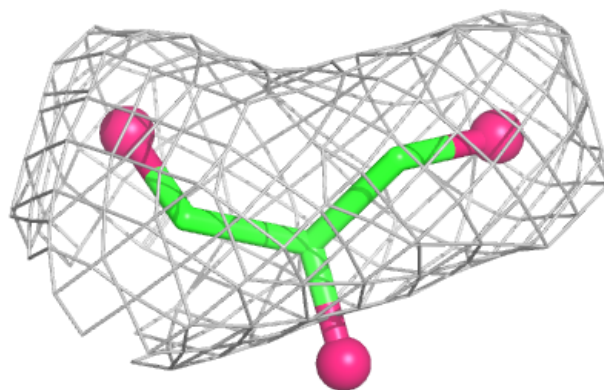
Electron density around GOL A 306:

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

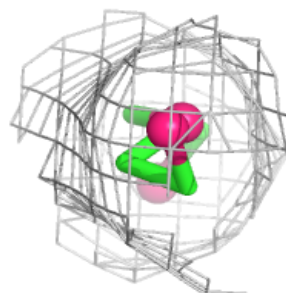
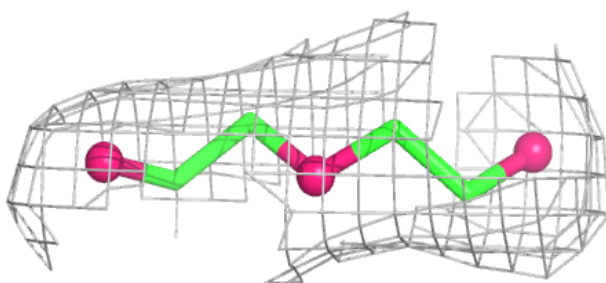
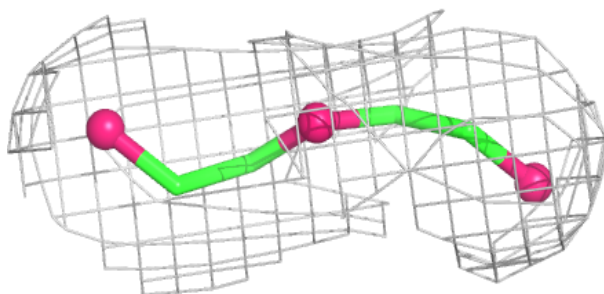


Electron density around GOL B 152:

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

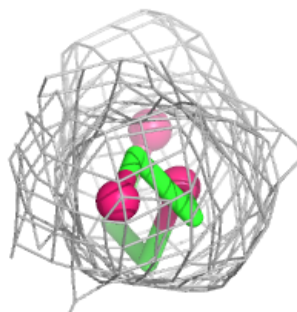
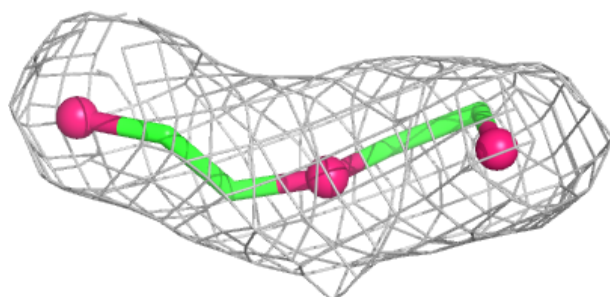
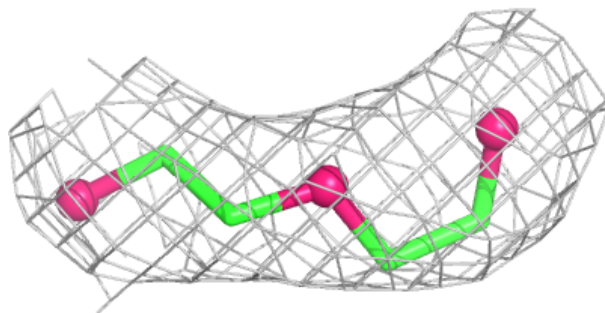
**Electron density around PEG D 105:**

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

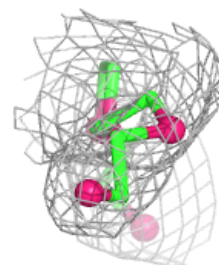
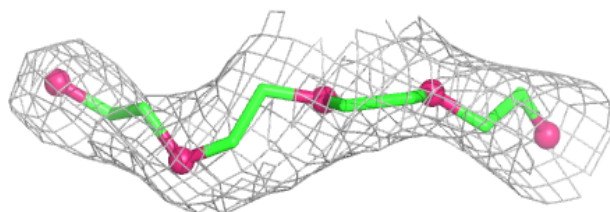
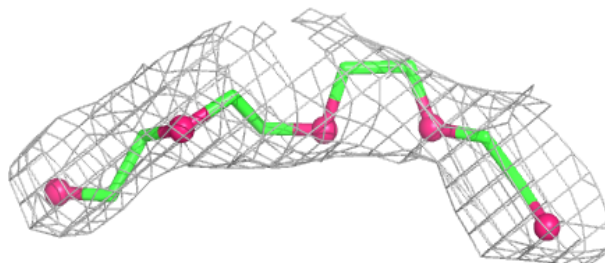


Electron density around PEG B 132:

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

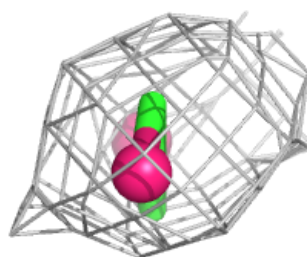
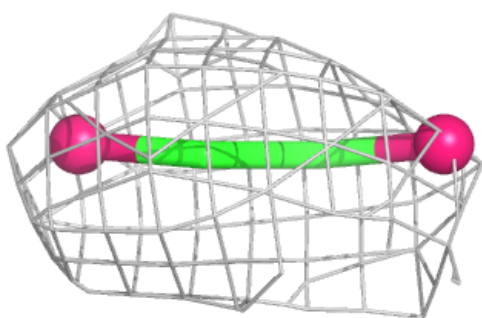
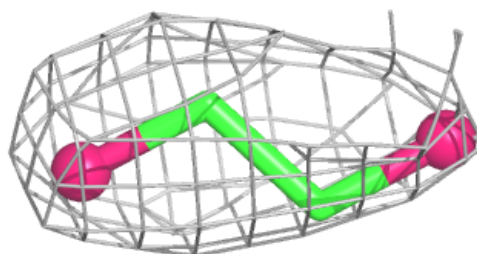
**Electron density around PG4 C 320:**

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

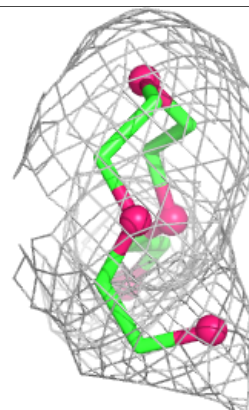
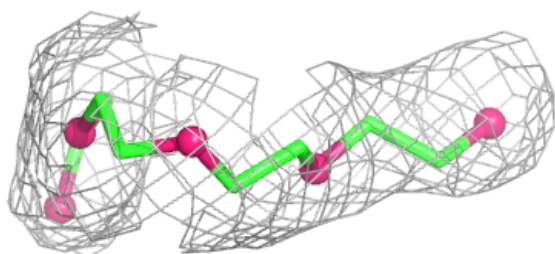
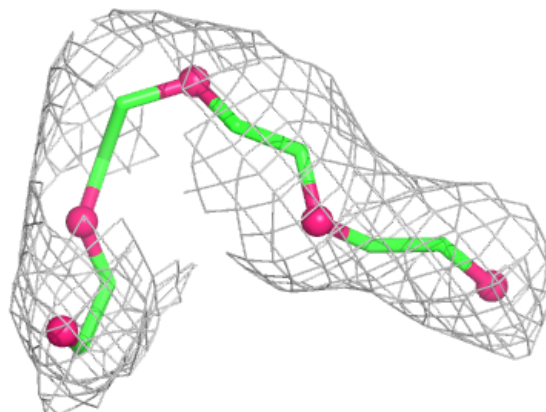


Electron density around EDO D 101:

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

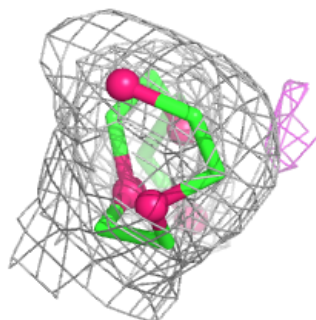
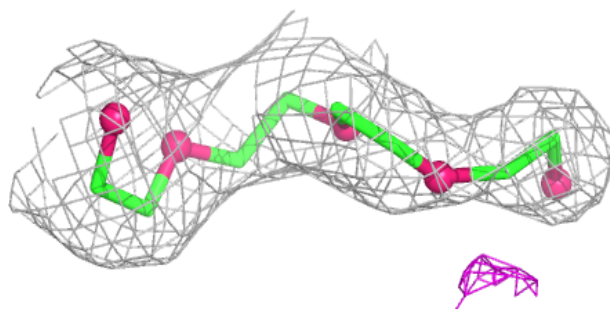
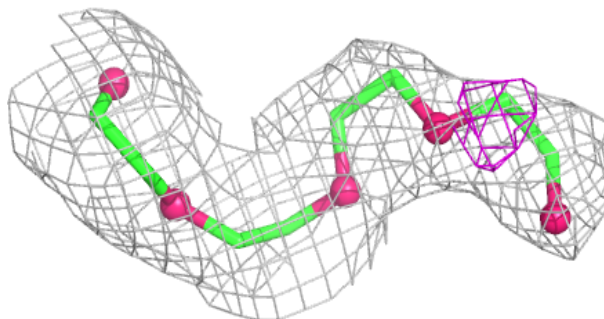
**Electron density around PG4 D 117:**

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

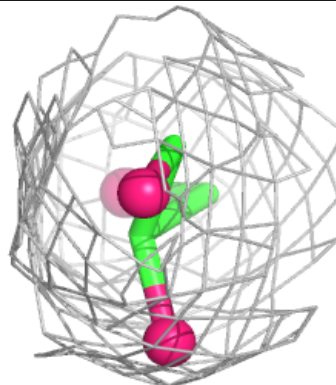
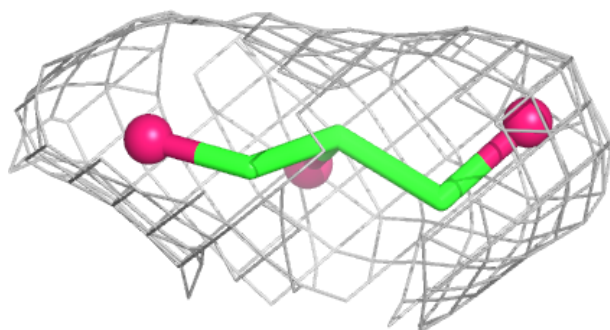
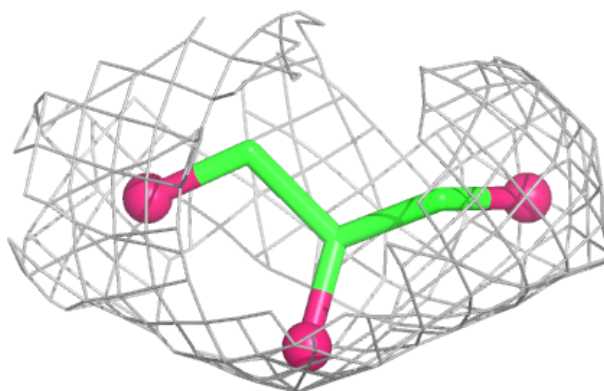


Electron density around PG4 A 368:

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

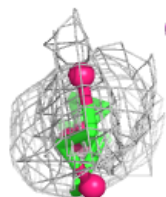
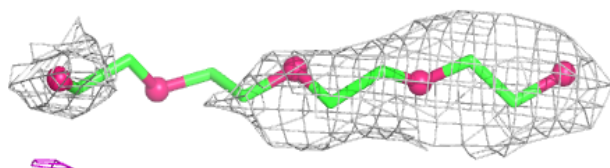
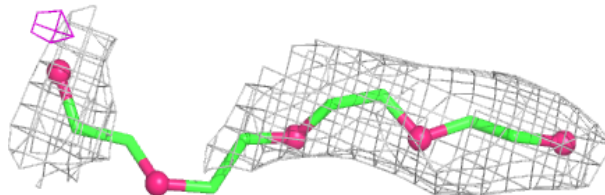
**Electron density around GOL B 108:**

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

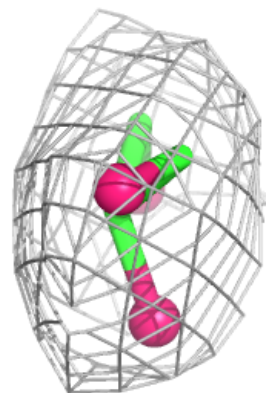
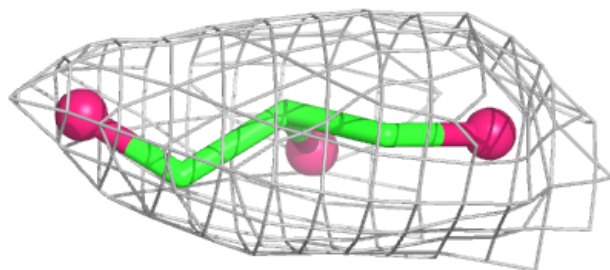
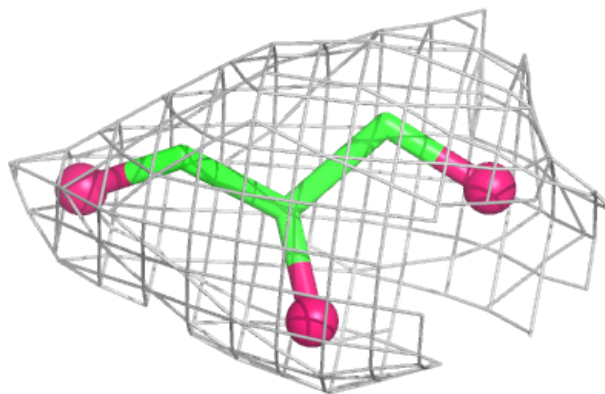


Electron density around PG4 C 302:

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

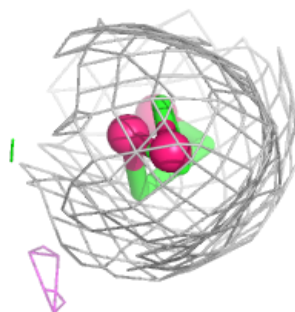
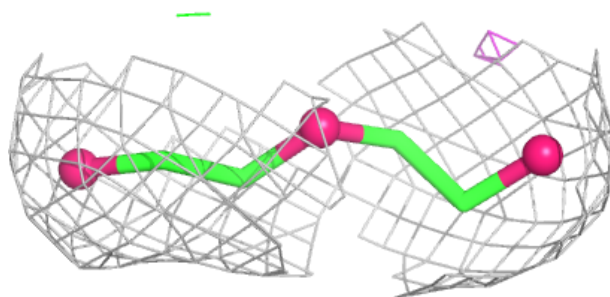
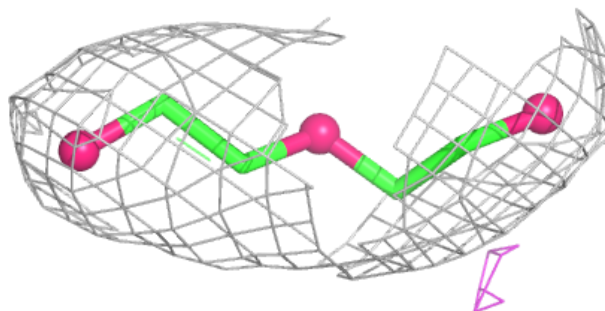
**Electron density around GOL C 309:**

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



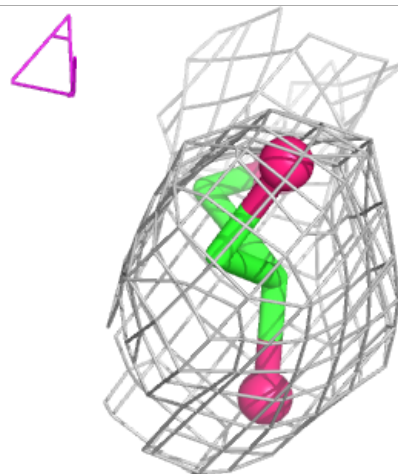
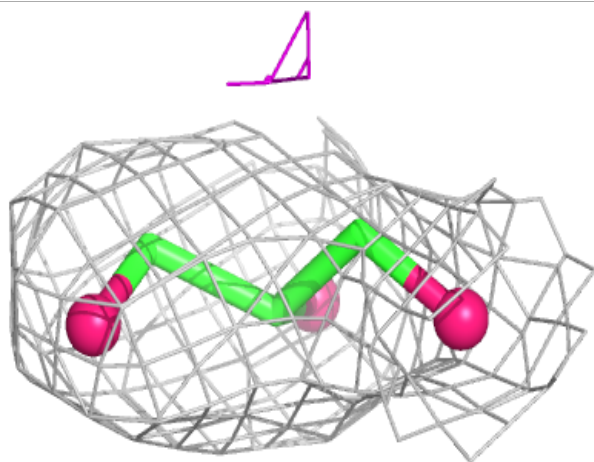
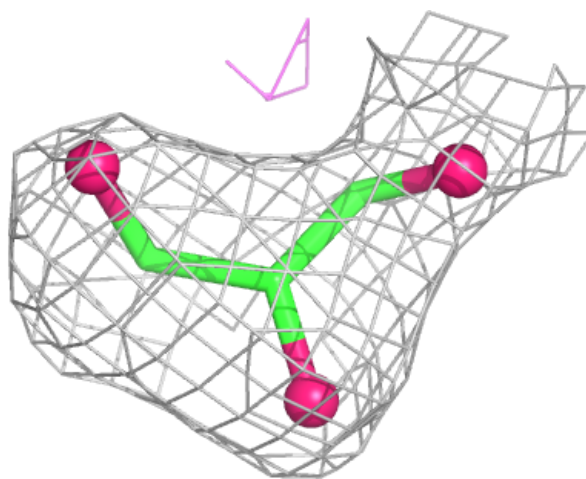
Electron density around PEG A 339:

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



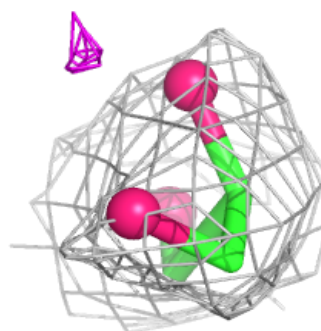
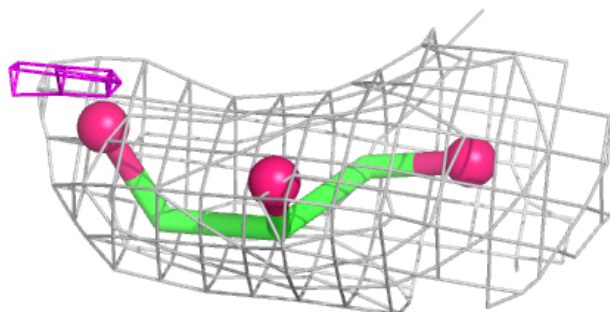
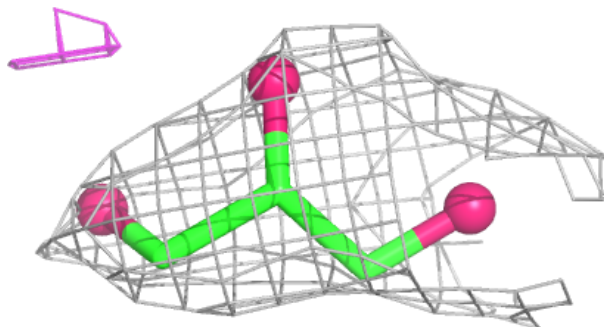
Electron density around GOL E 104:

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

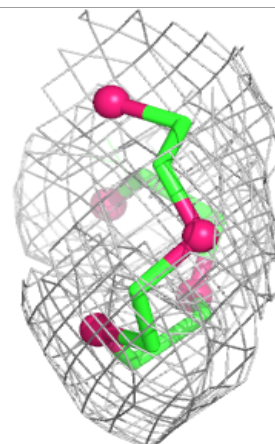
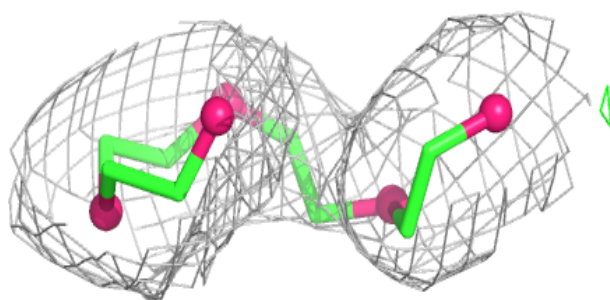
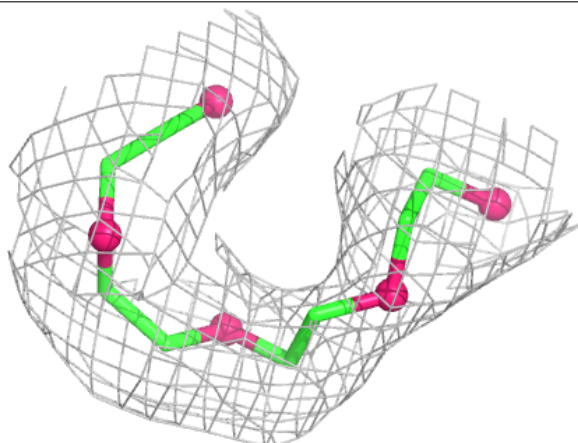


Electron density around GOL D 110:

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

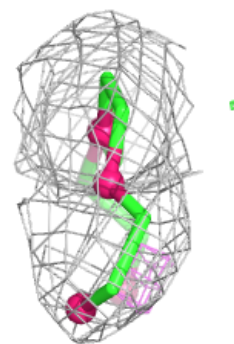
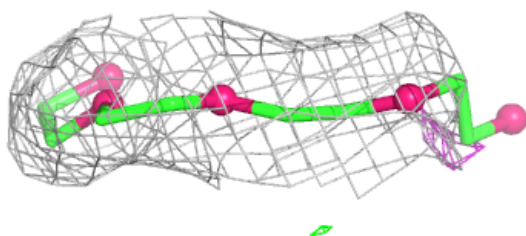
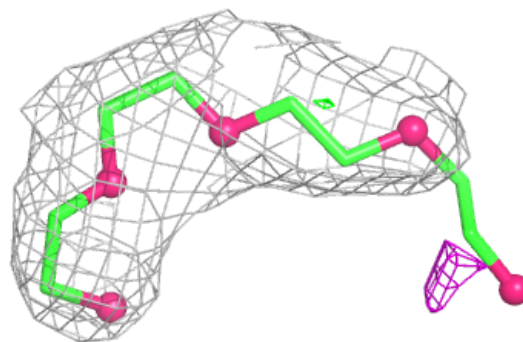
**Electron density around PG4 E 106:**

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



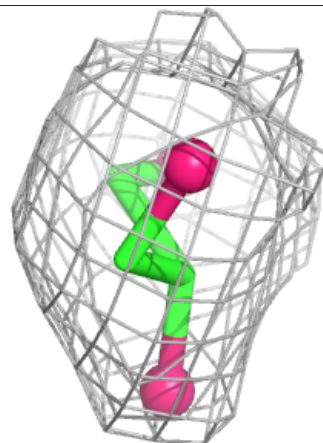
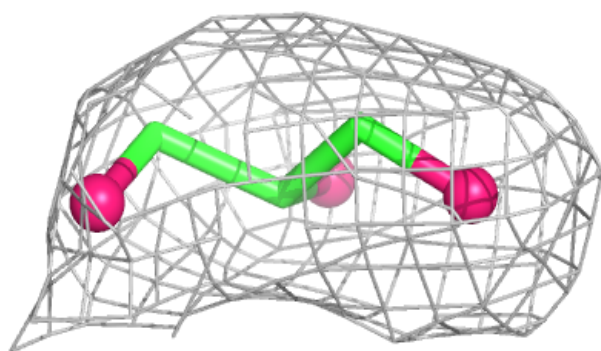
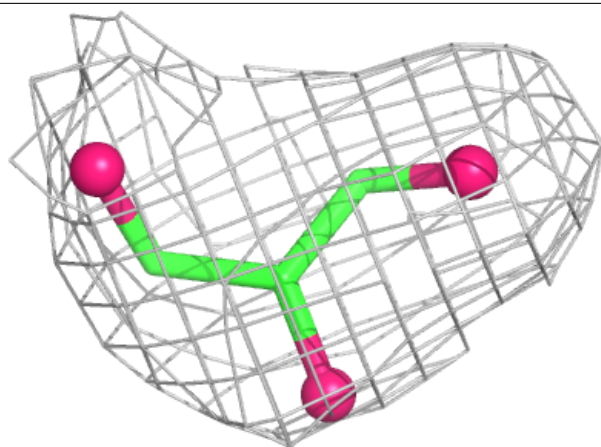
Electron density around PG4 C 336:

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



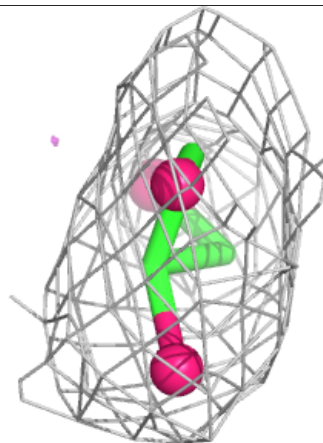
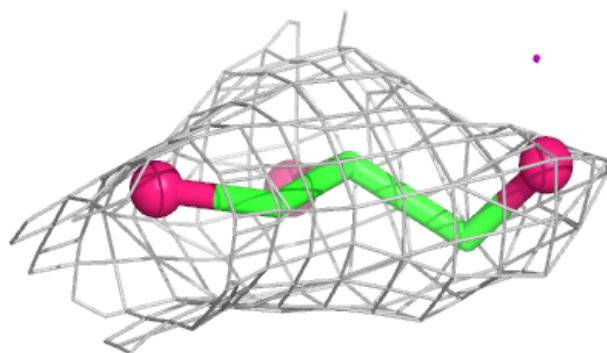
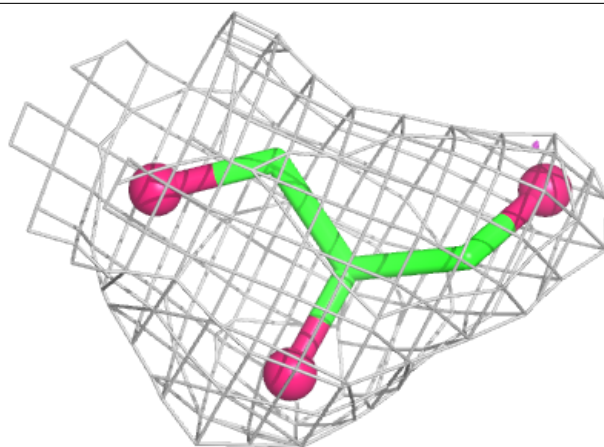
Electron density around GOL B 109:

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

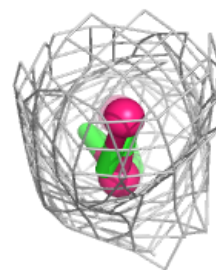
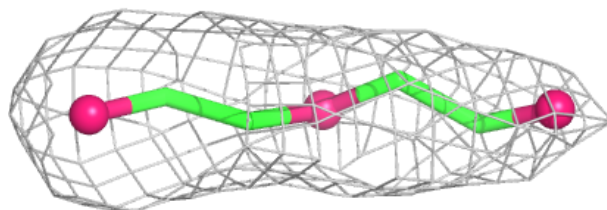
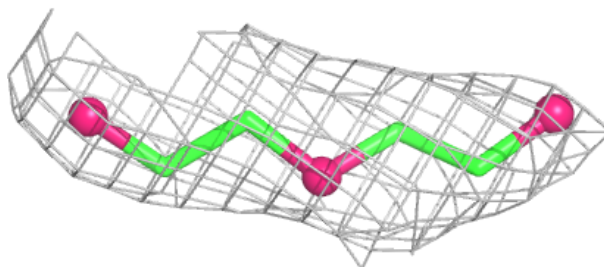


Electron density around GOL A 362:

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

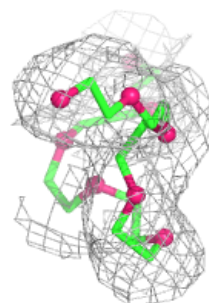
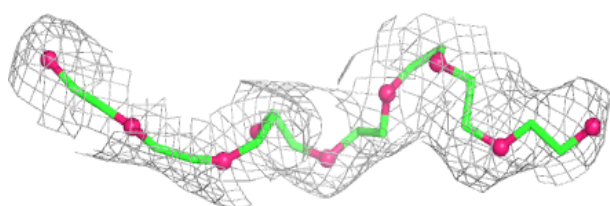
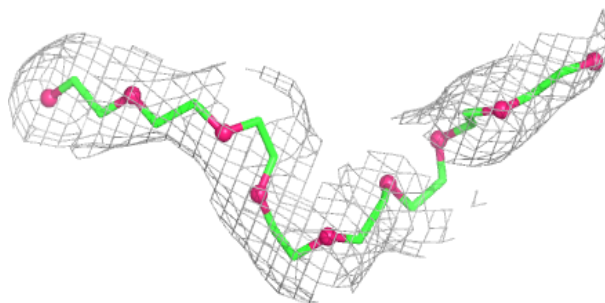
**Electron density around PEG D 127:**

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

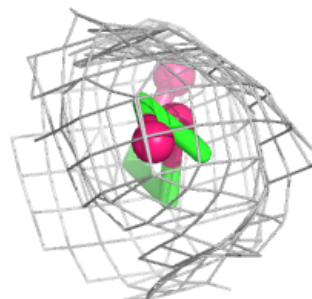
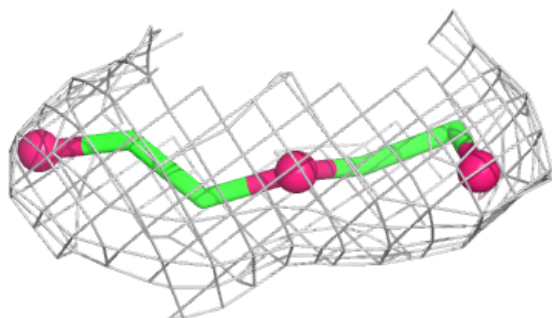
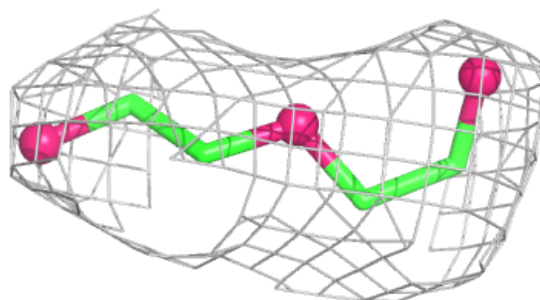


Electron density around PE8 A 342:

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

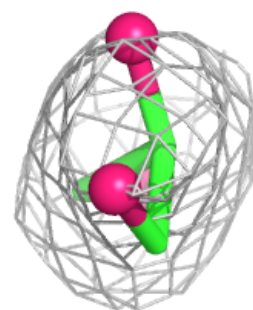
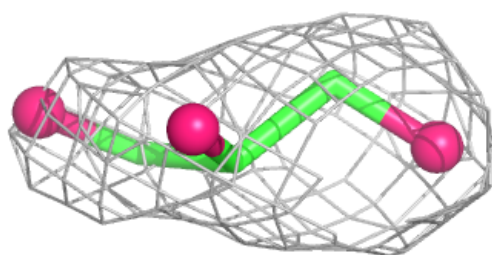
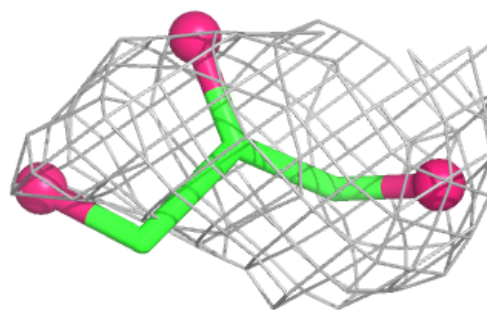
**Electron density around PEG A 336:**

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



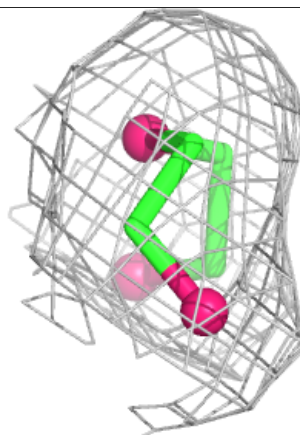
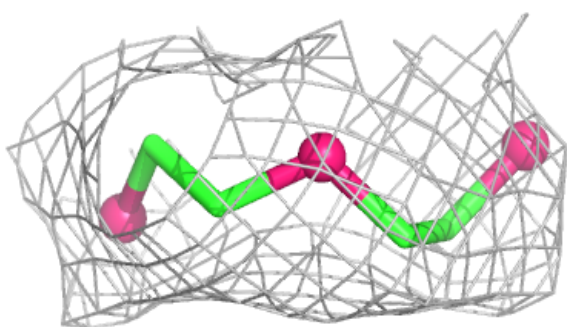
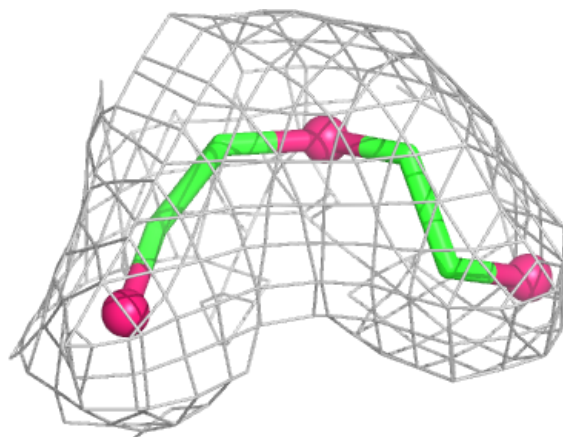
Electron density around GOL A 345:

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



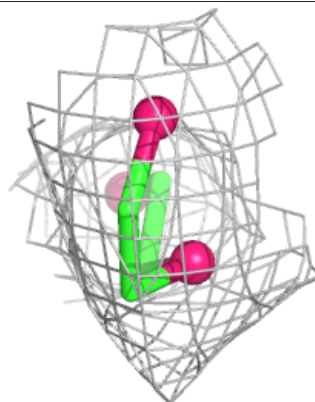
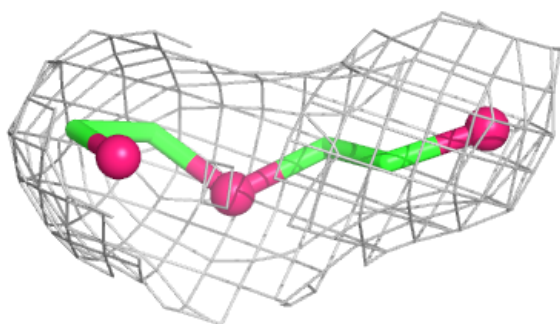
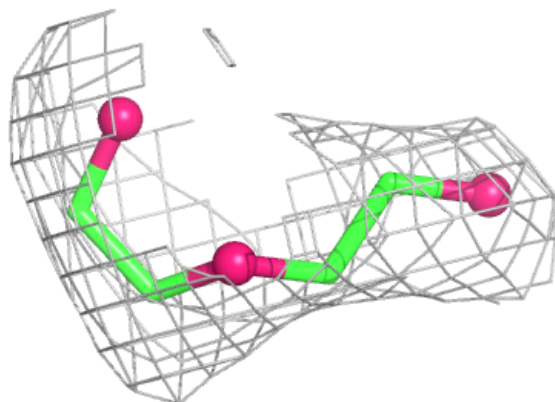
Electron density around PEG A 332:

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

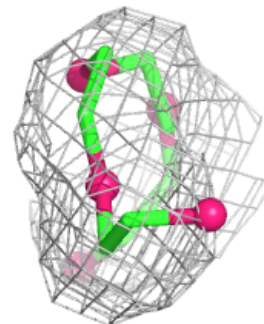
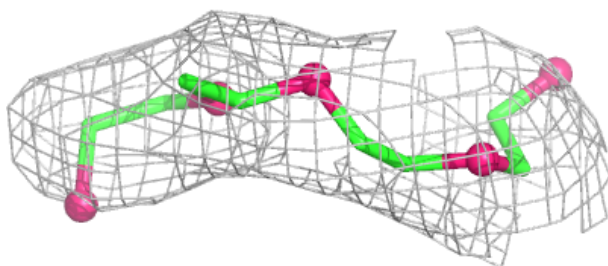
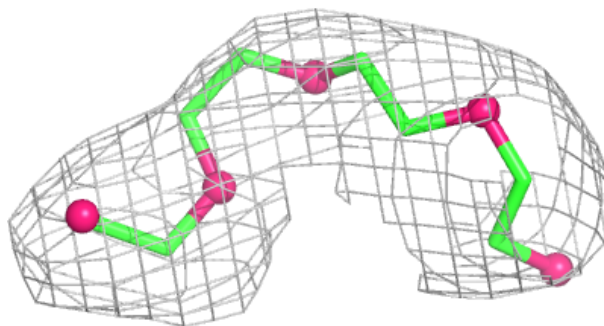


Electron density around PEG A 333:

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

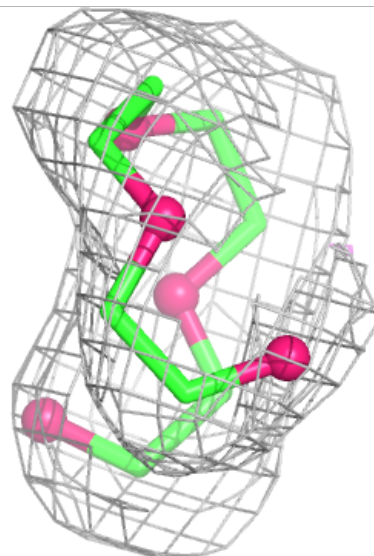
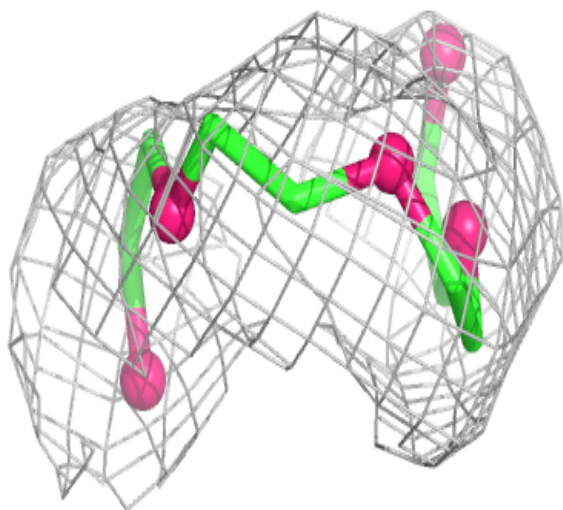
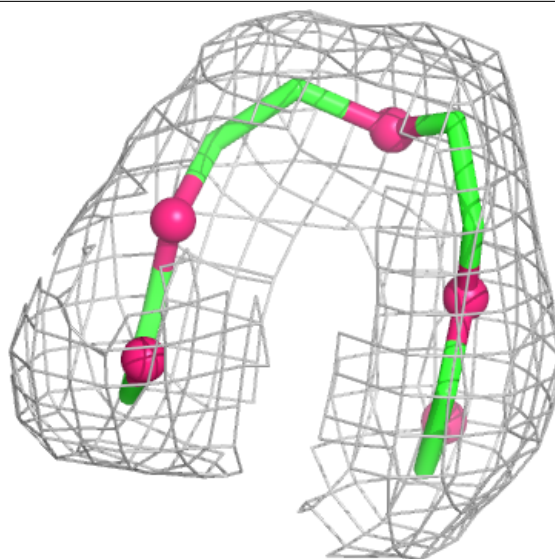
**Electron density around PG4 B 125:**

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



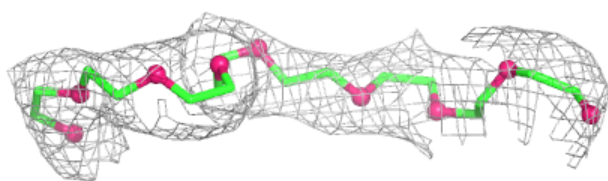
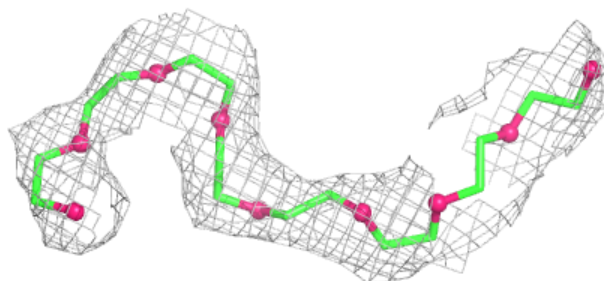
Electron density around PG4 A 369:

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

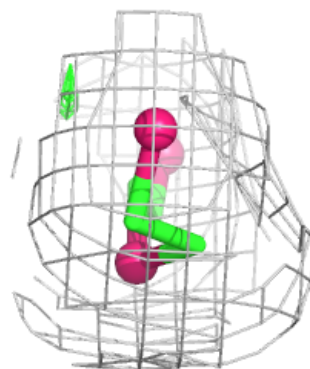
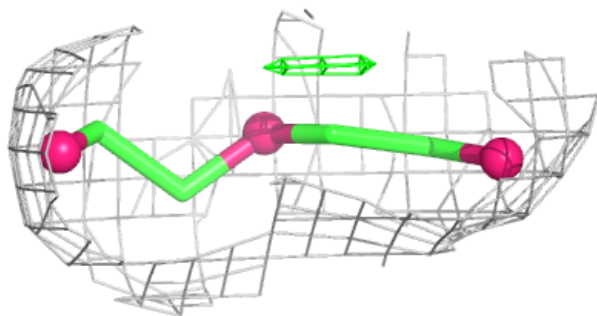
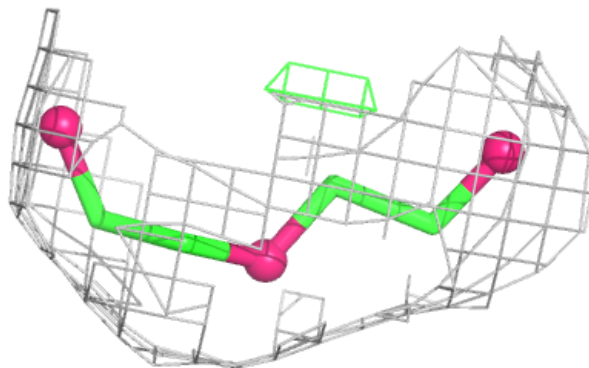


Electron density around PE8 F 106:

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

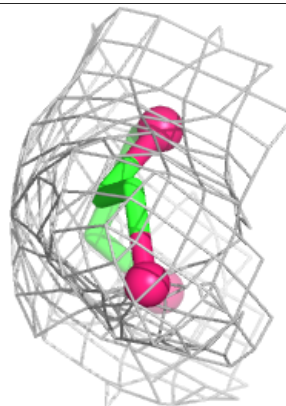
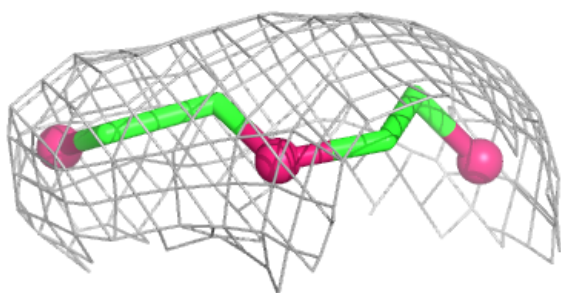
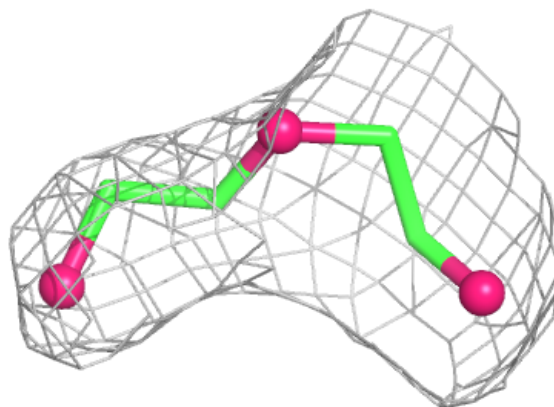
**Electron density around PEG C 330:**

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

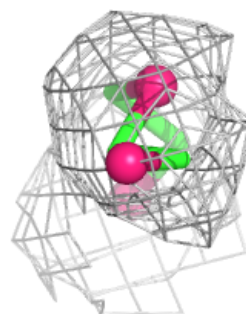
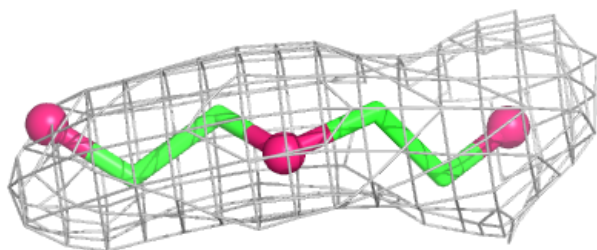
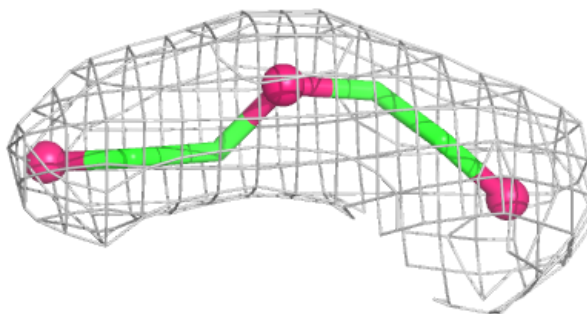


Electron density around PEG C 331:

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

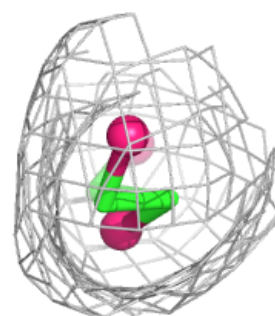
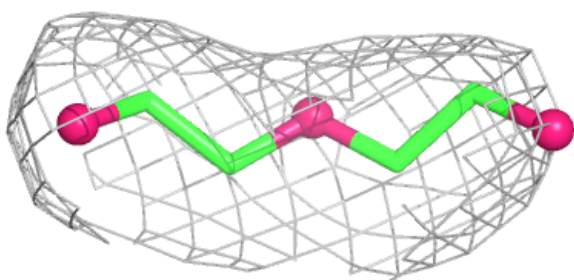
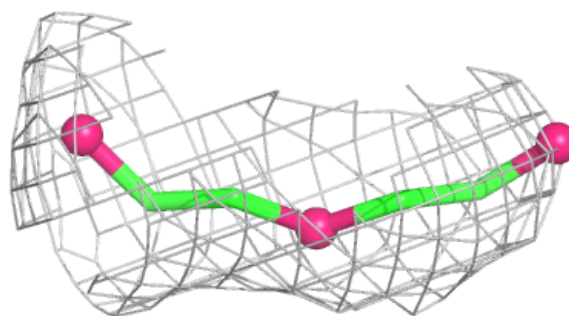
**Electron density around PEG C 332:**

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

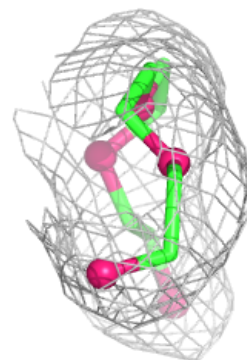
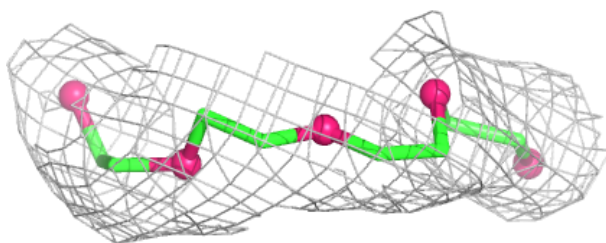
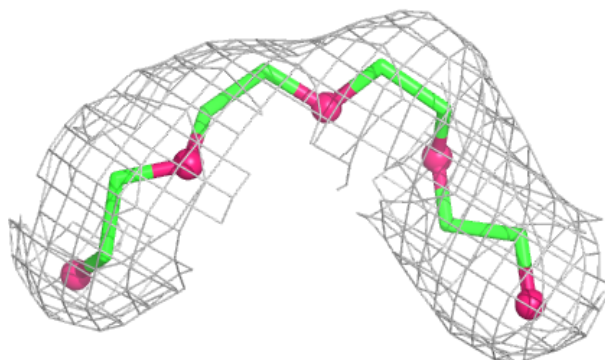


Electron density around PEG B 135:

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

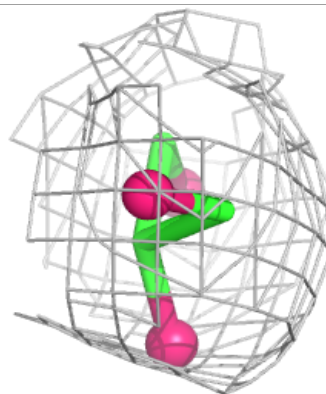
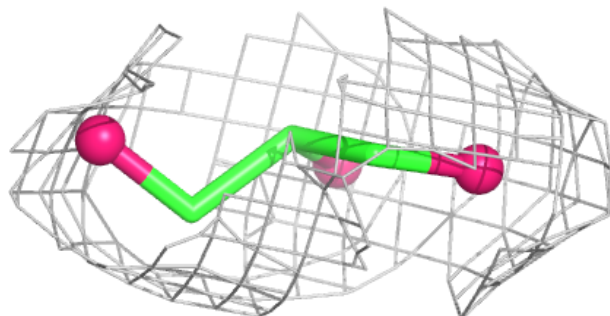
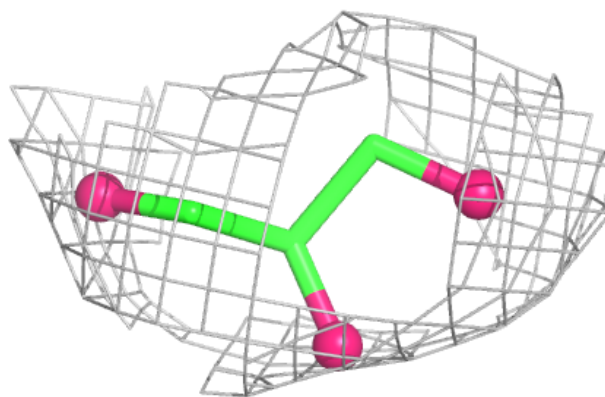
**Electron density around PG4 B 124:**

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

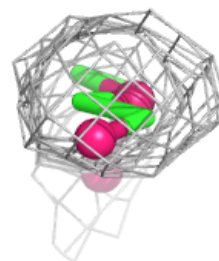
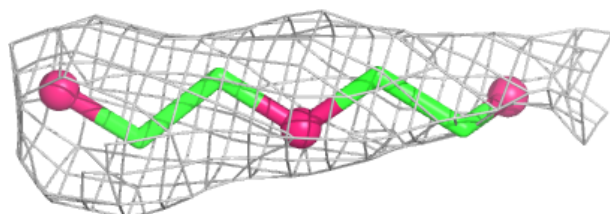
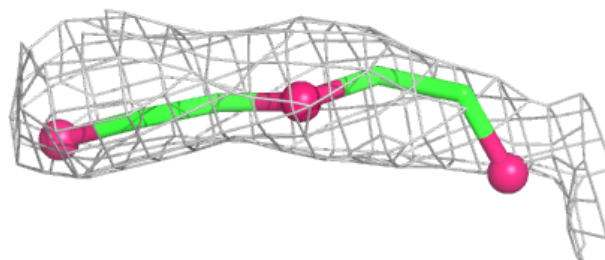


Electron density around GOL B 103:

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

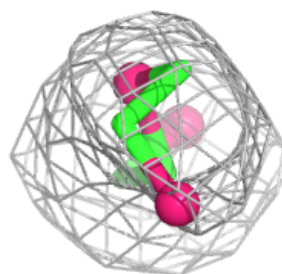
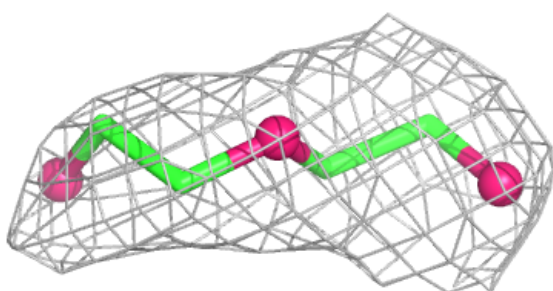
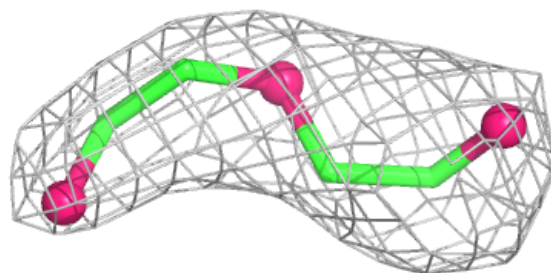
**Electron density around PEG A 329:**

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

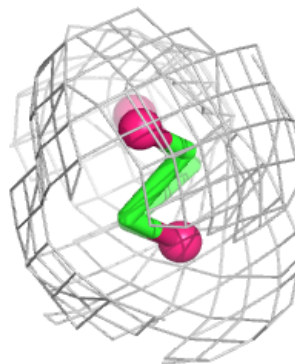
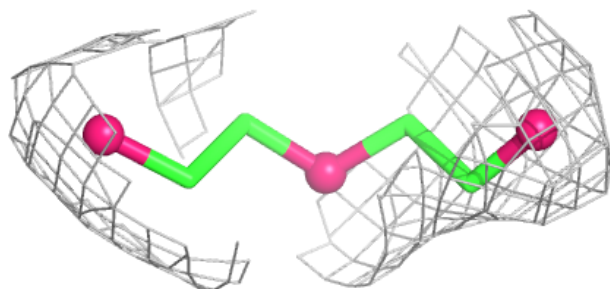
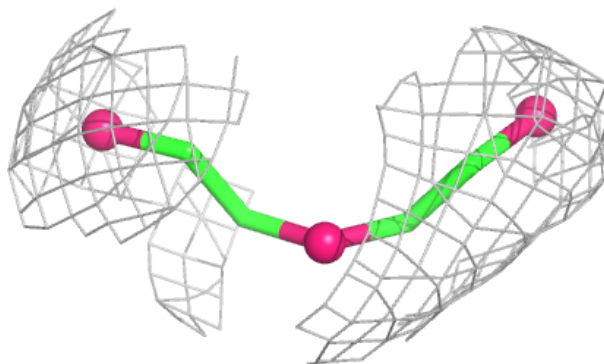


Electron density around PEG A 371:

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

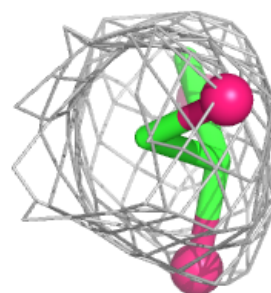
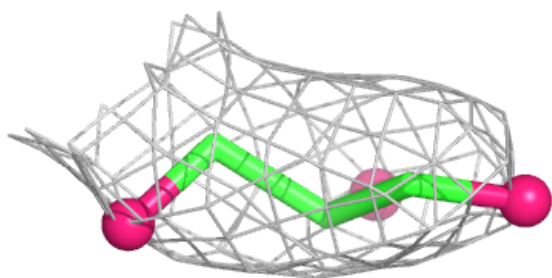
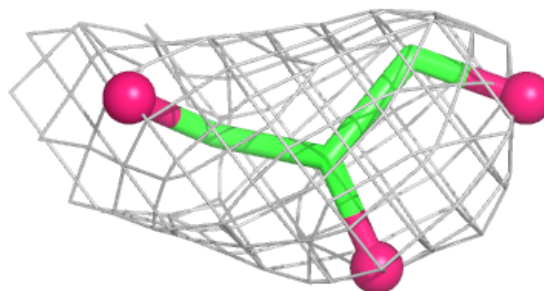
**Electron density around PEG D 121:**

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

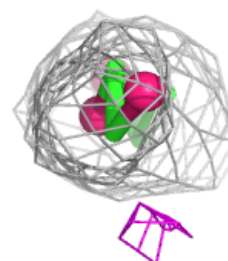
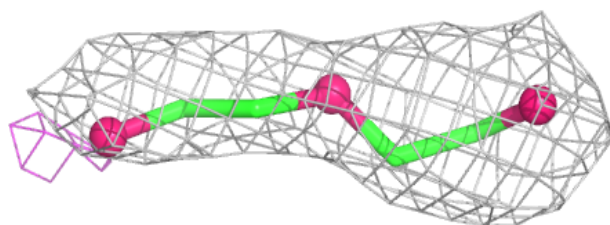
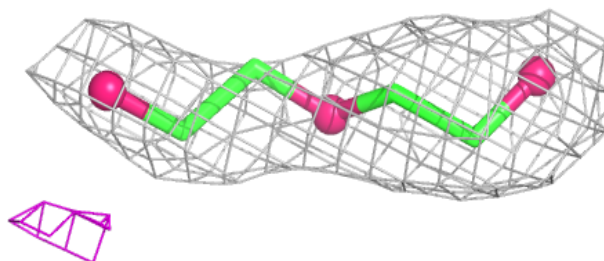


Electron density around GOL C 307:

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

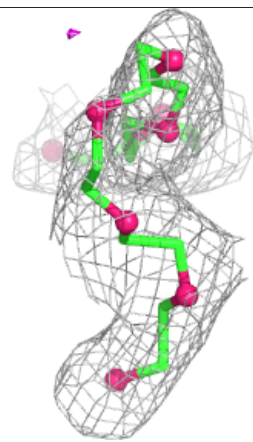
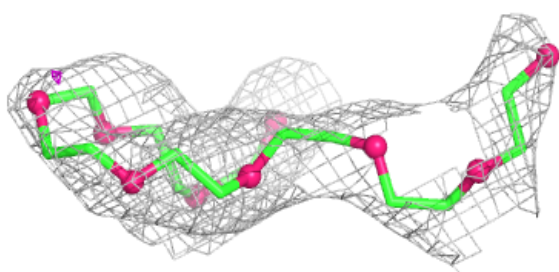
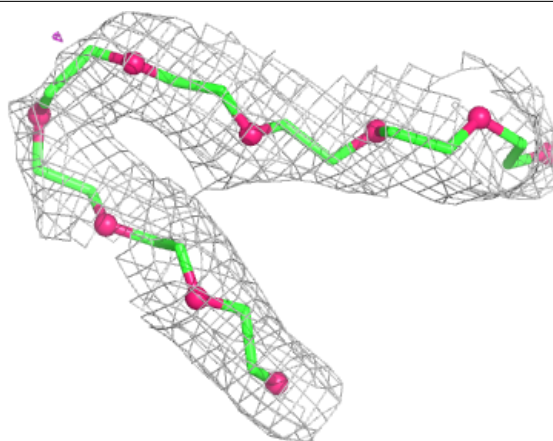
**Electron density around PEG D 128:**

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



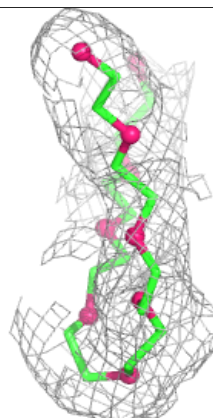
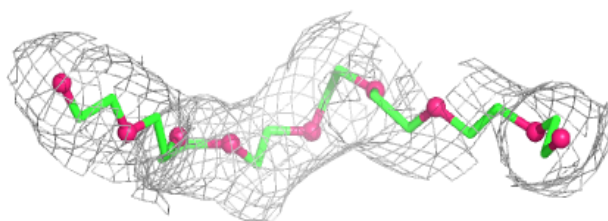
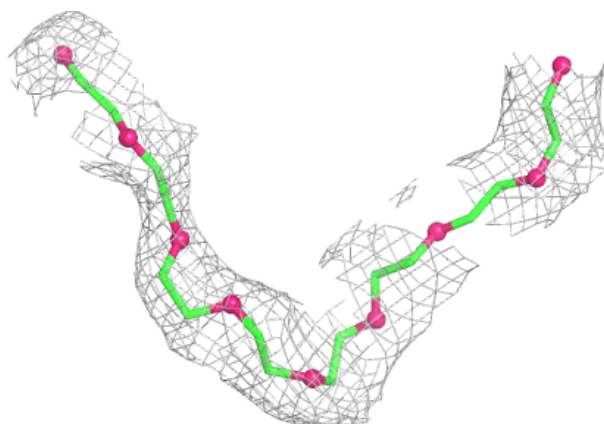
Electron density around PE8 A 344:

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

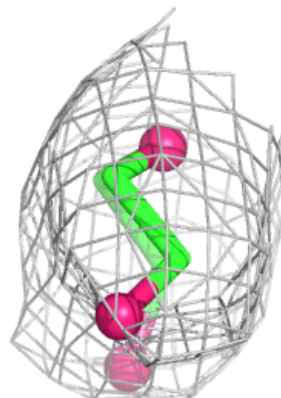
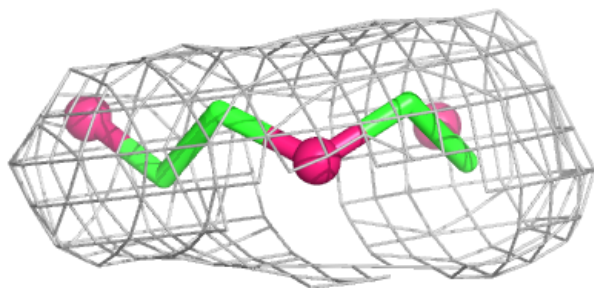
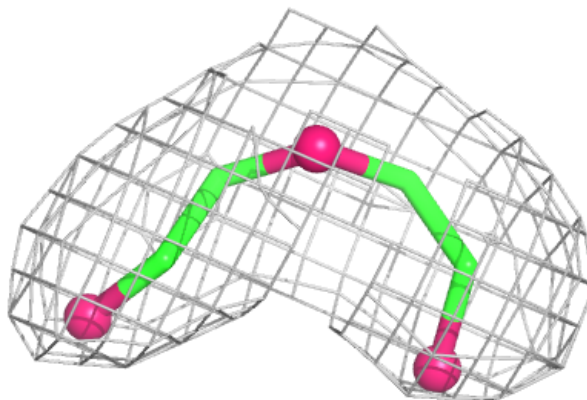


Electron density around PE8 B 102:

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

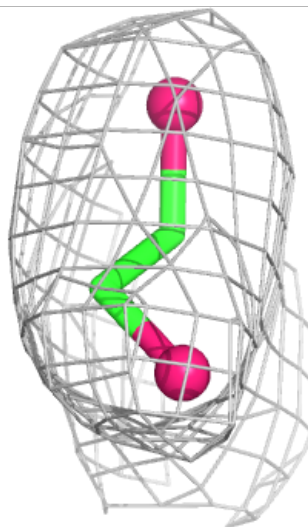
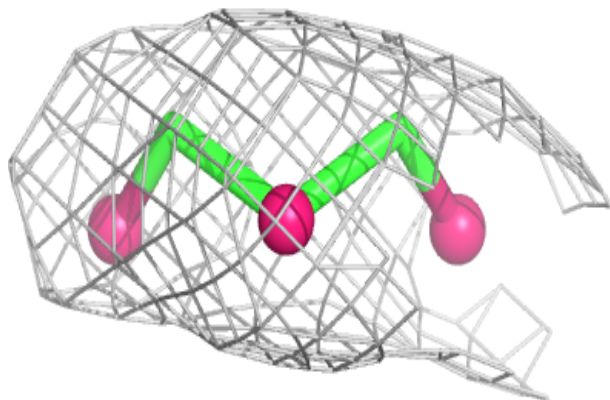
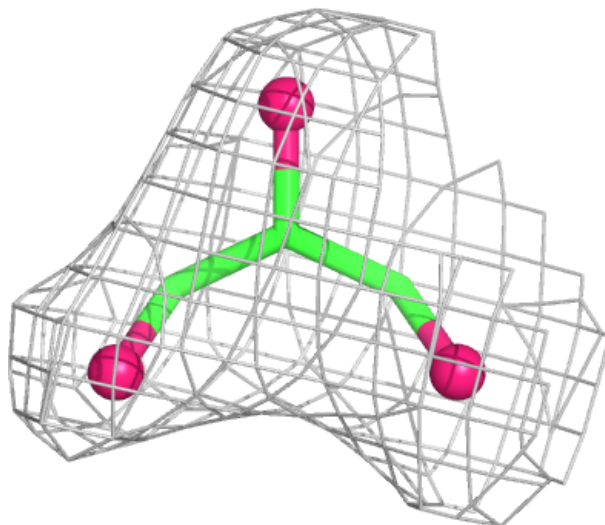
**Electron density around PEG B 130:**

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



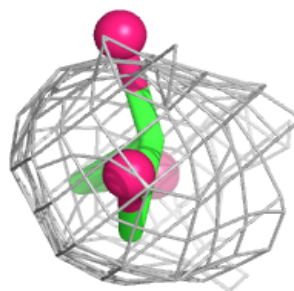
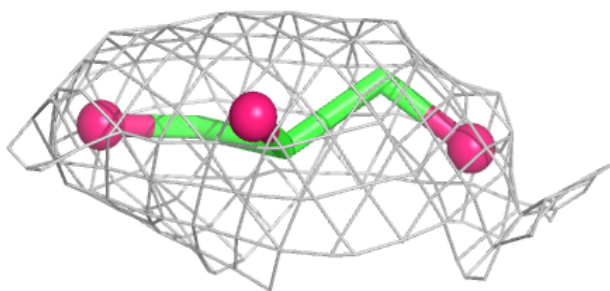
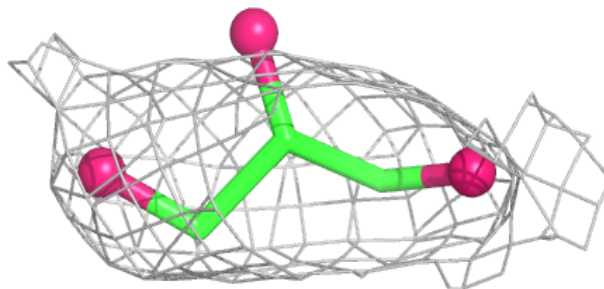
Electron density around GOL C 314:

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

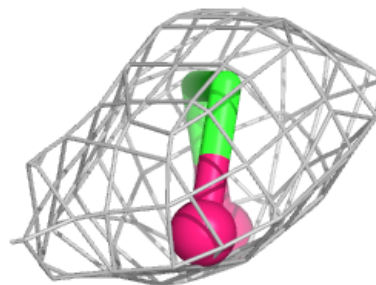
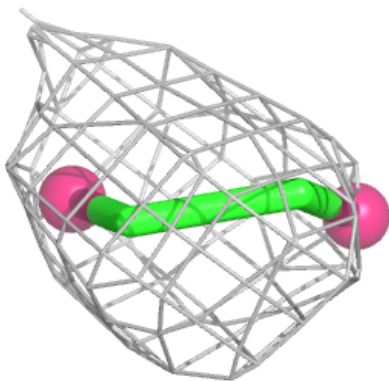
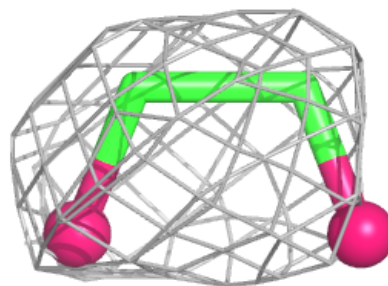


Electron density around GOL D 131:

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

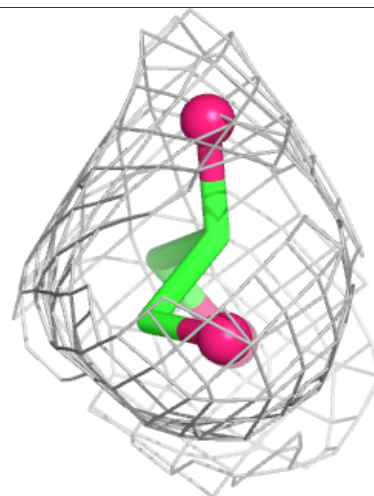
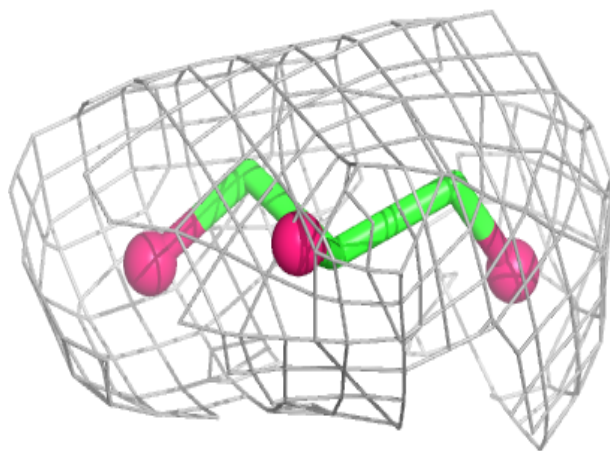
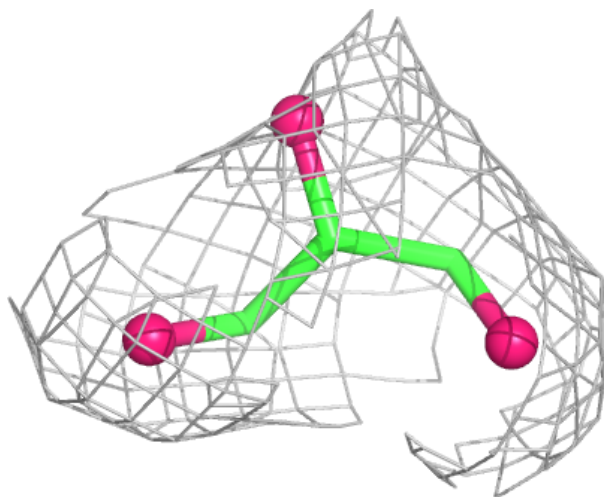
**Electron density around EDO B 144:**

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



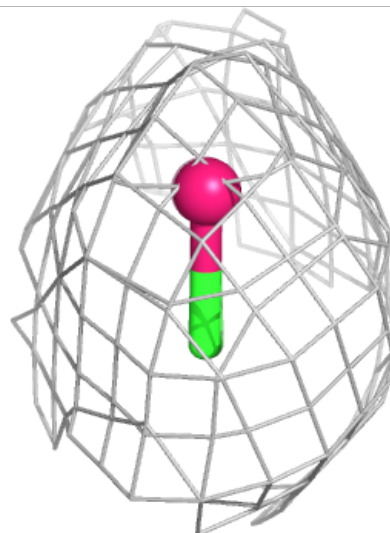
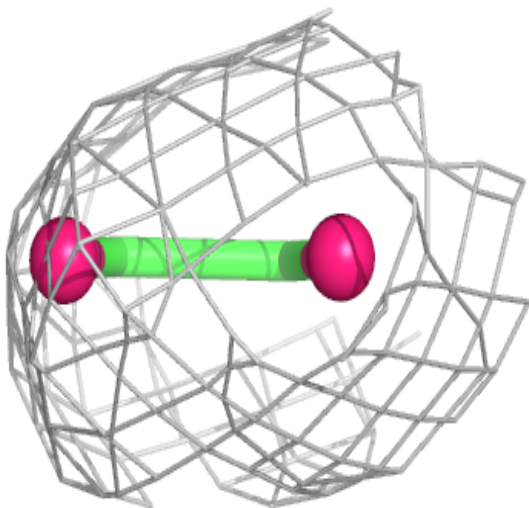
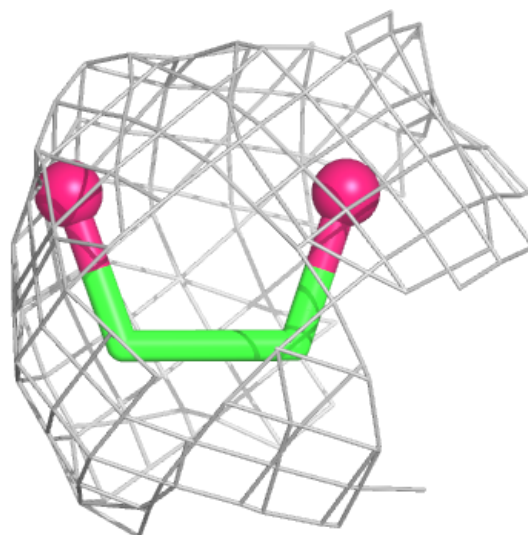
Electron density around GOL C 338:

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



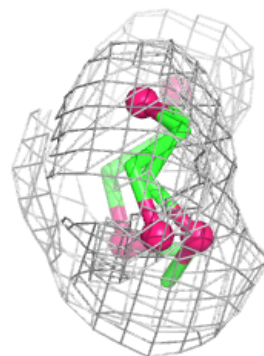
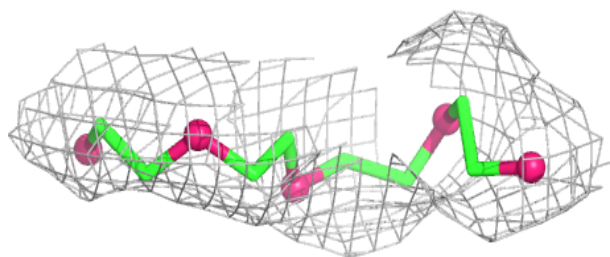
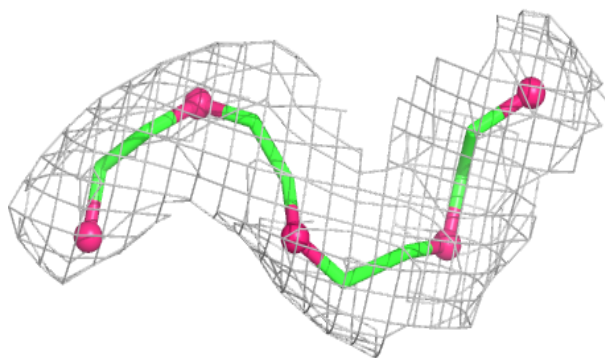
Electron density around EDO E 111:

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

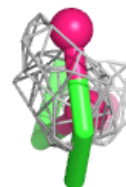
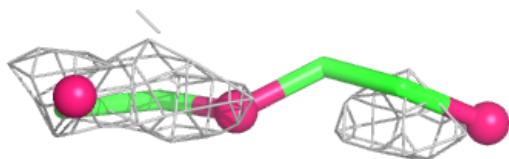
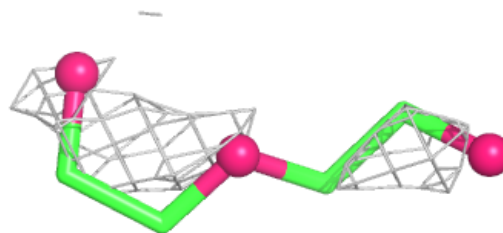


Electron density around PG4 D 118:

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

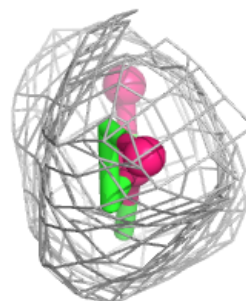
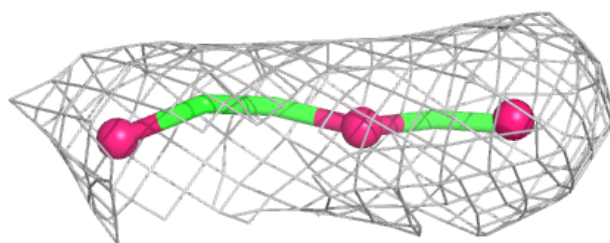
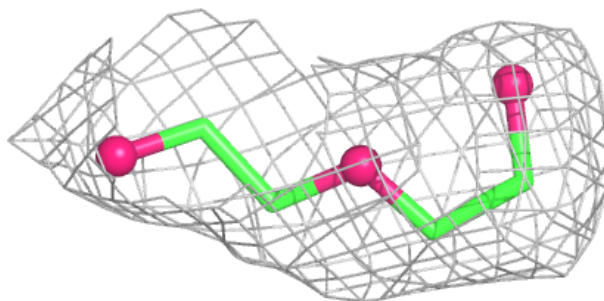
**Electron density around PEG C 333:**

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

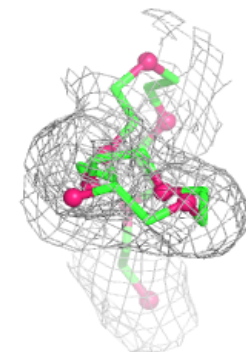
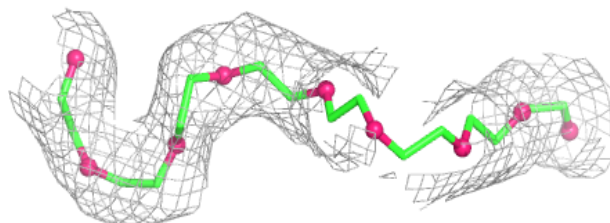
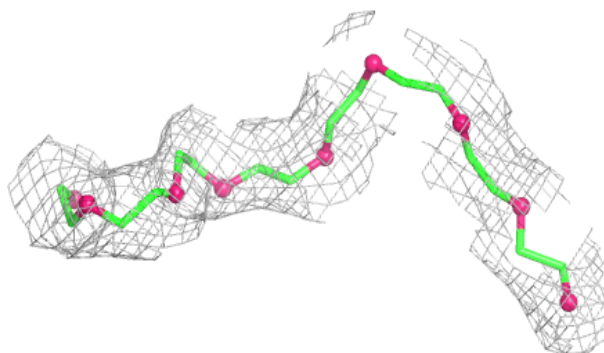


Electron density around PEG C 327:

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

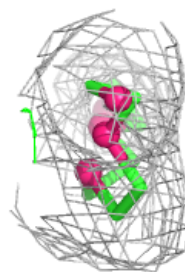
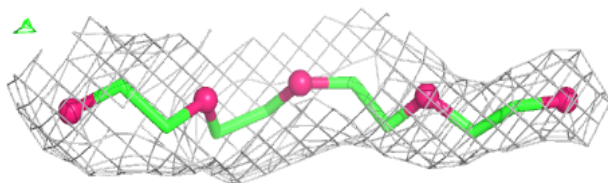
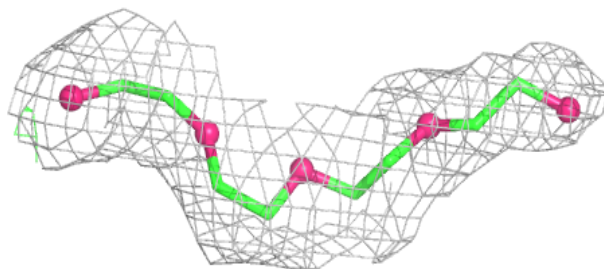
**Electron density around PE8 A 343:**

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

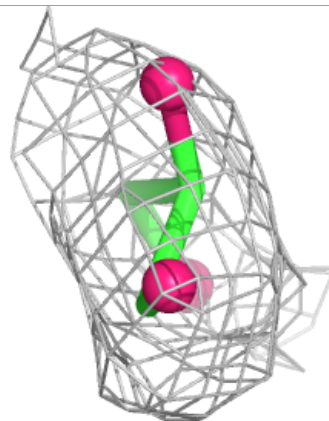
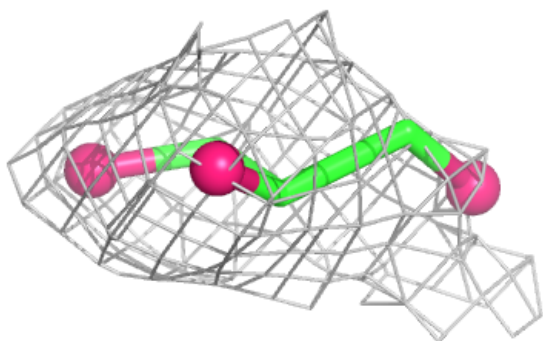
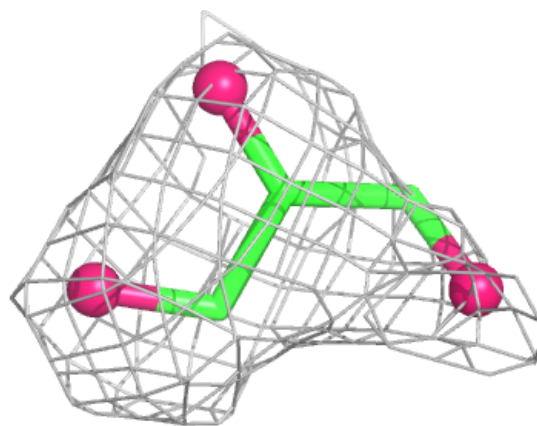


Electron density around PG4 D 103:

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

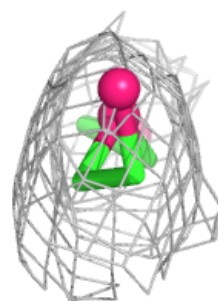
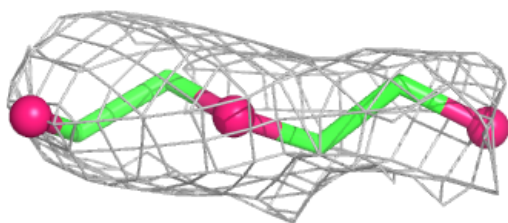
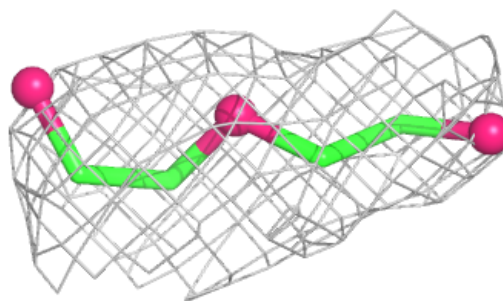
**Electron density around GOL A 303:**

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

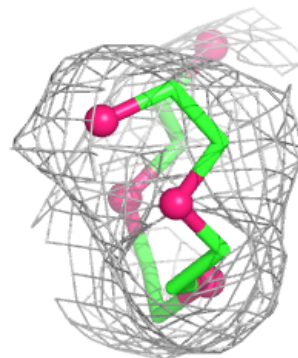
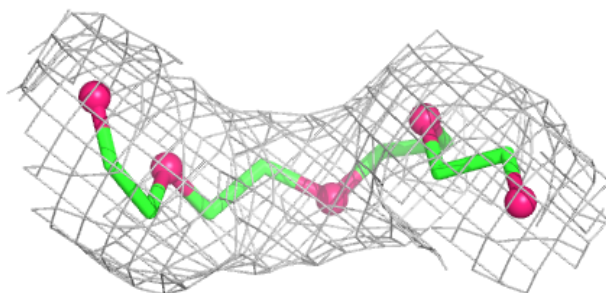
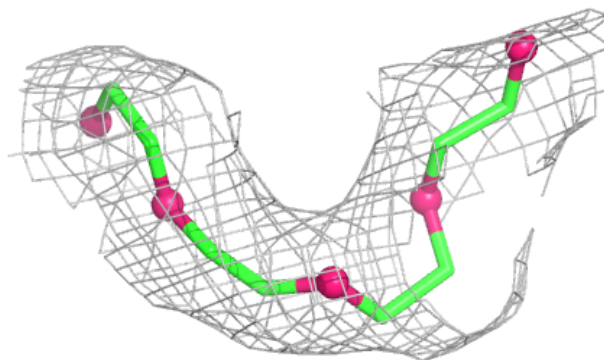


Electron density around PEG D 126:

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

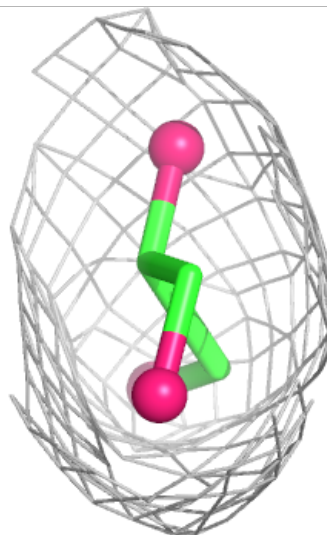
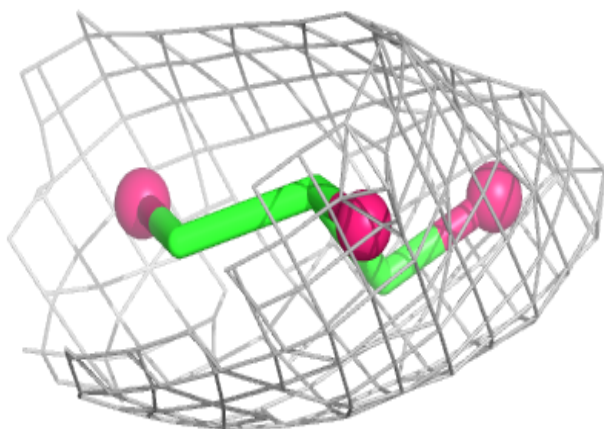
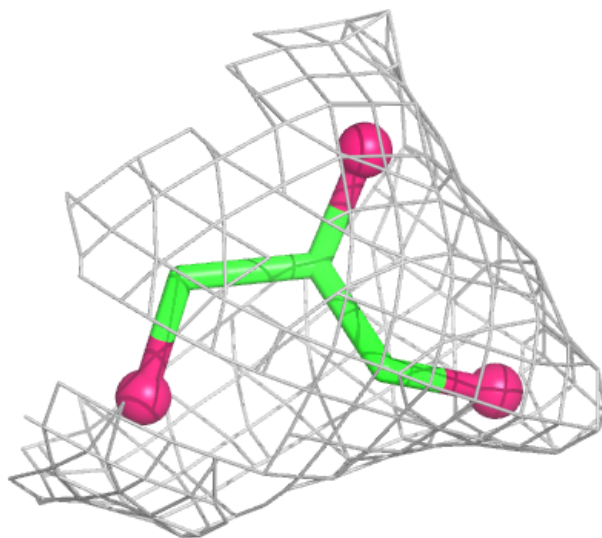
**Electron density around PG4 B 155:**

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



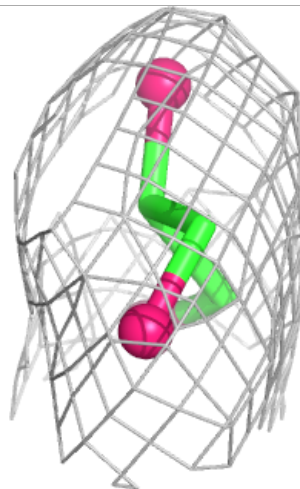
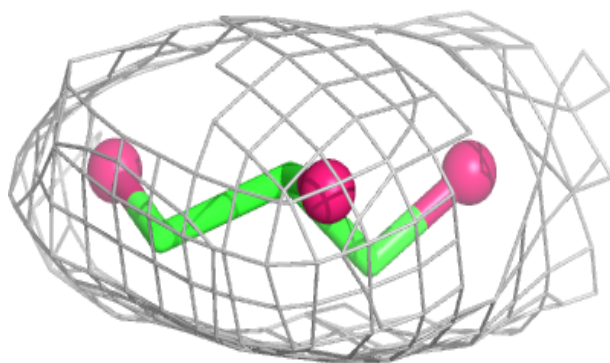
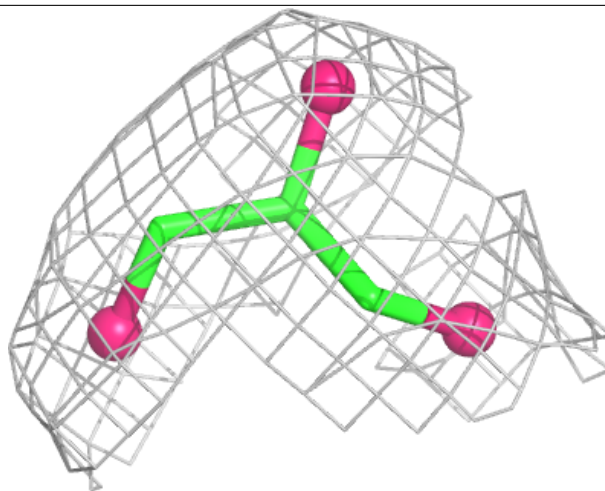
Electron density around GOL B 107:

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



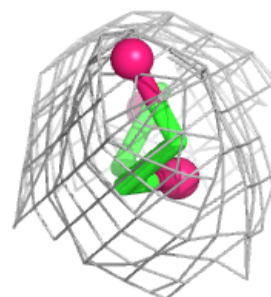
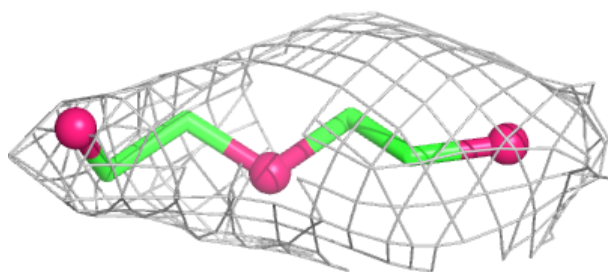
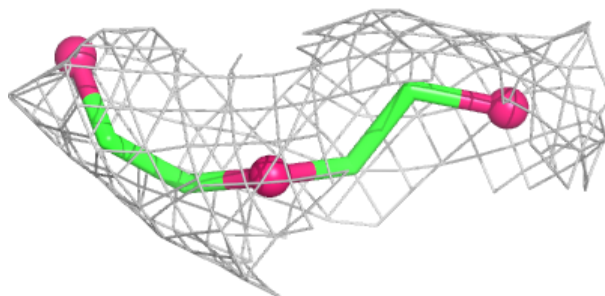
Electron density around GOL A 301:

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

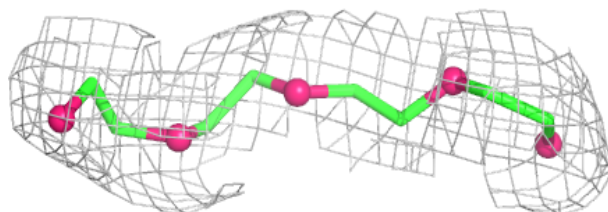
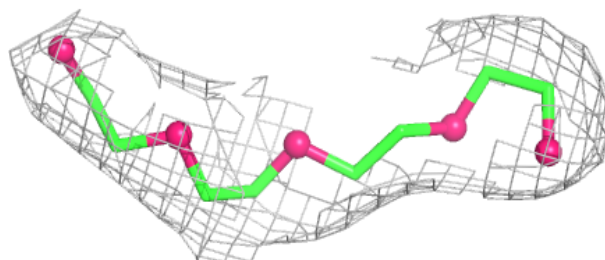


Electron density around PEG C 329:

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

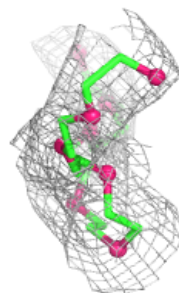
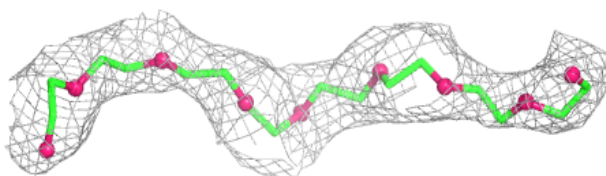
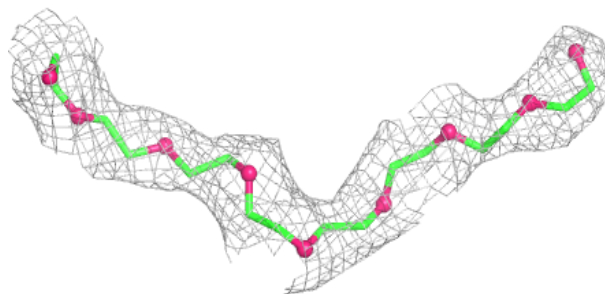
**Electron density around PG4 B 119:**

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

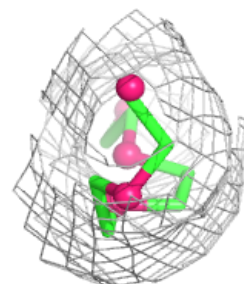
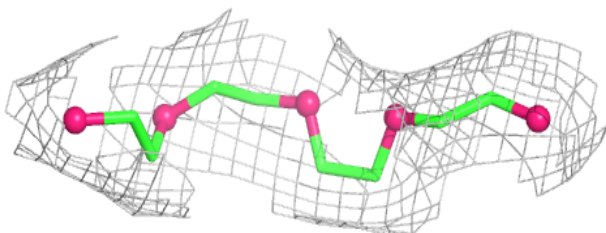
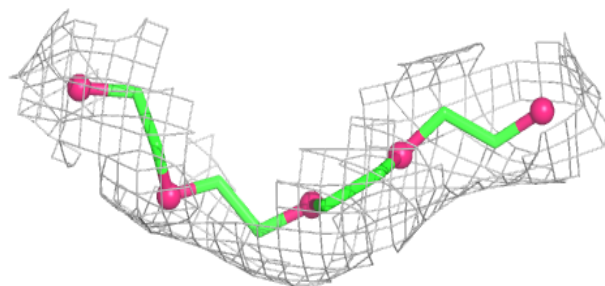


Electron density around PE8 F 102:

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

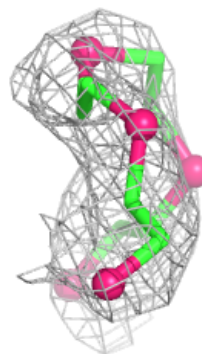
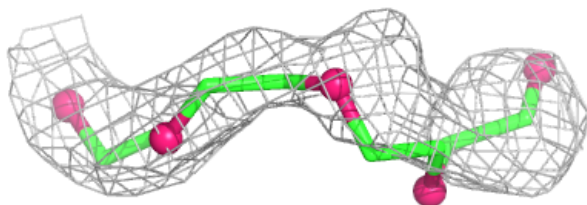
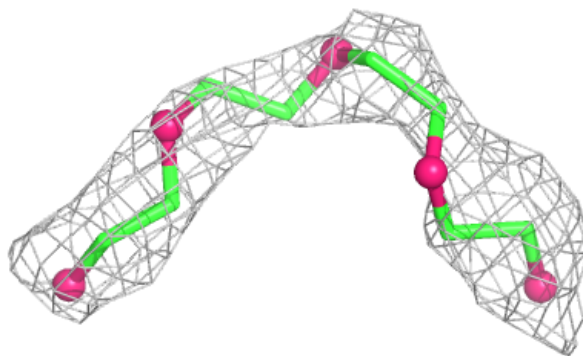
**Electron density around PG4 E 114:**

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

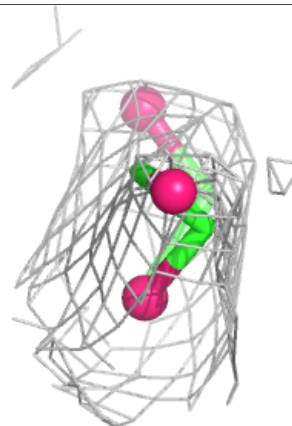
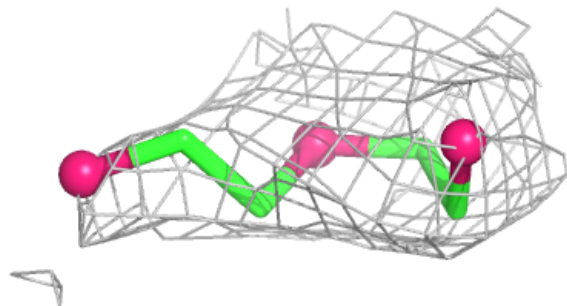
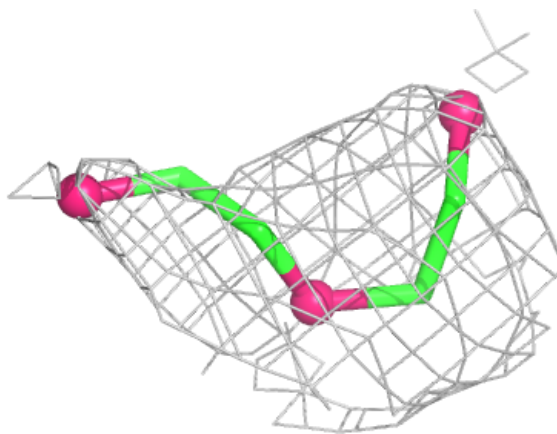


Electron density around PG4 C 325:

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

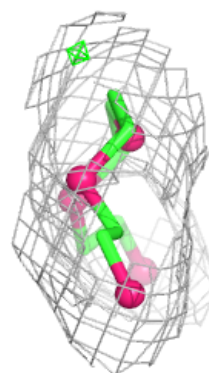
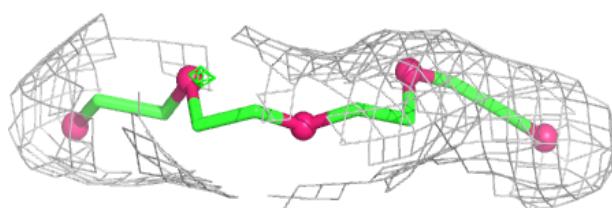
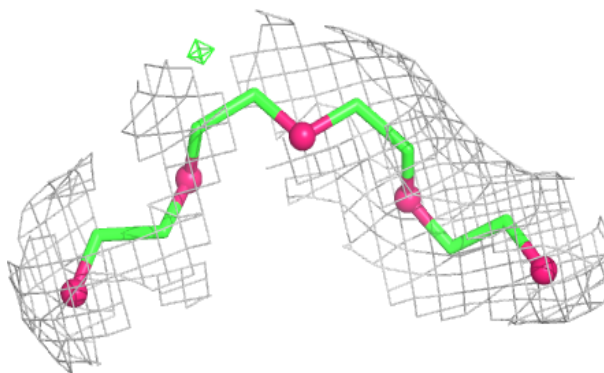
**Electron density around PEG A 331:**

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

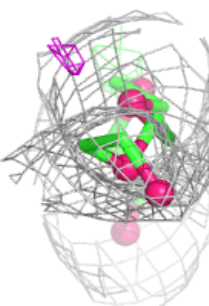
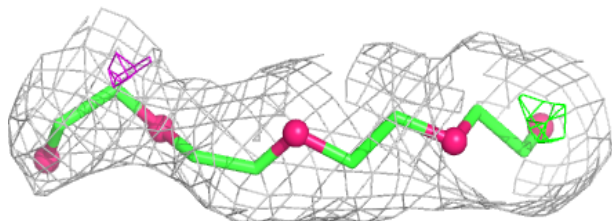
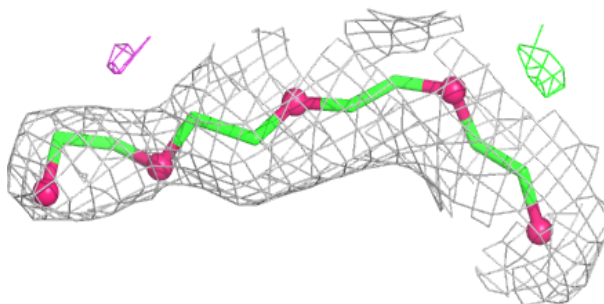


Electron density around PG4 A 322:

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

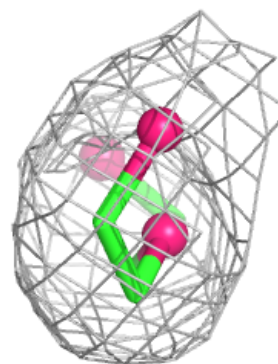
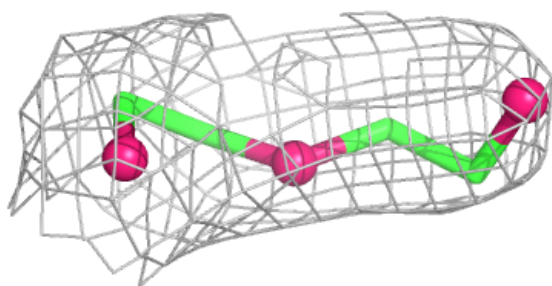
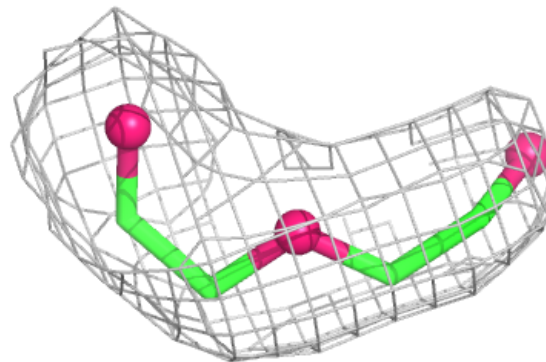
**Electron density around PG4 D 116:**

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



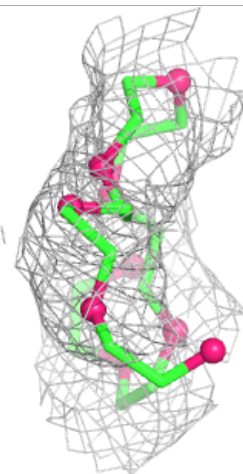
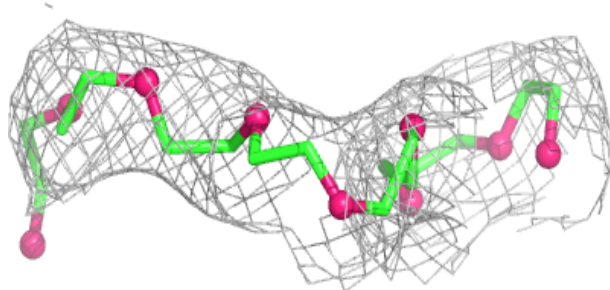
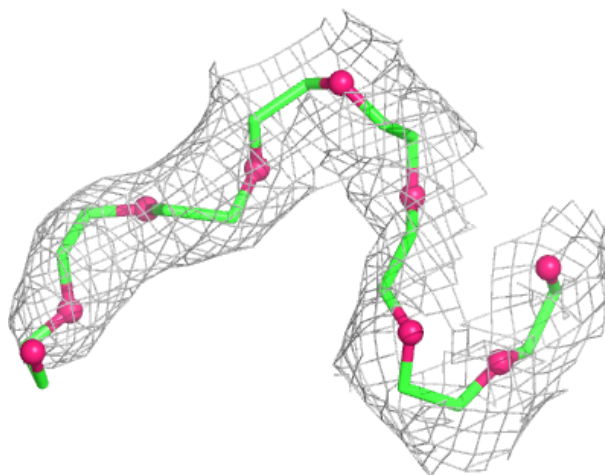
Electron density around PEG C 339:

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



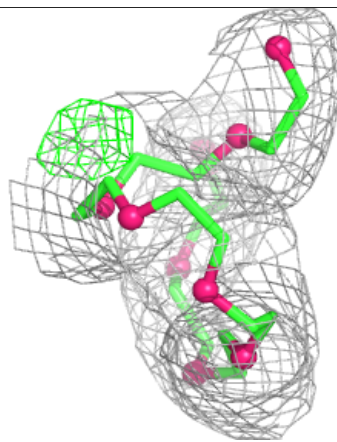
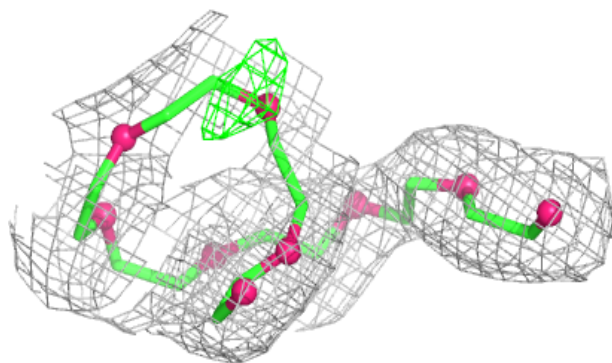
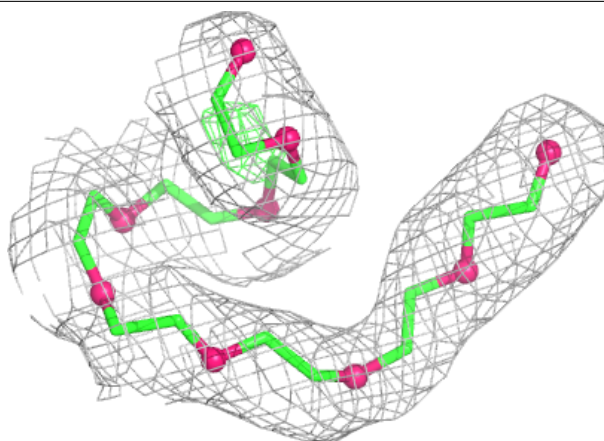
Electron density around PE8 B 136:

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



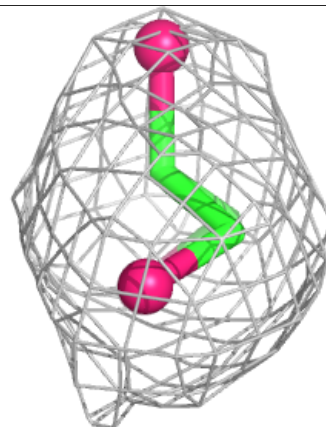
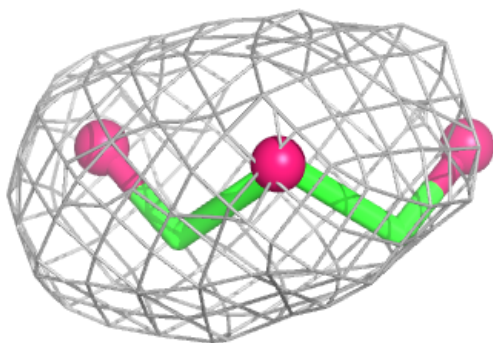
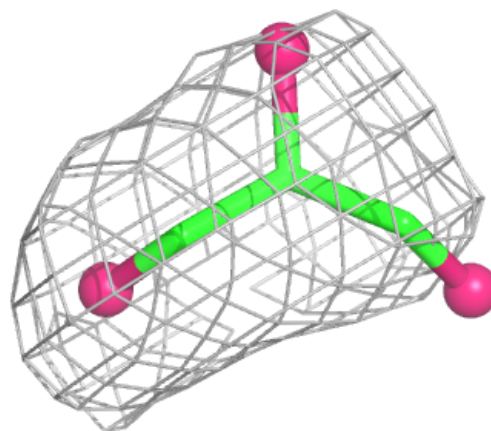
Electron density around PE8 E 110:

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



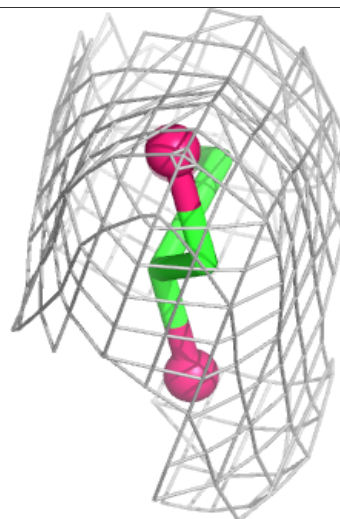
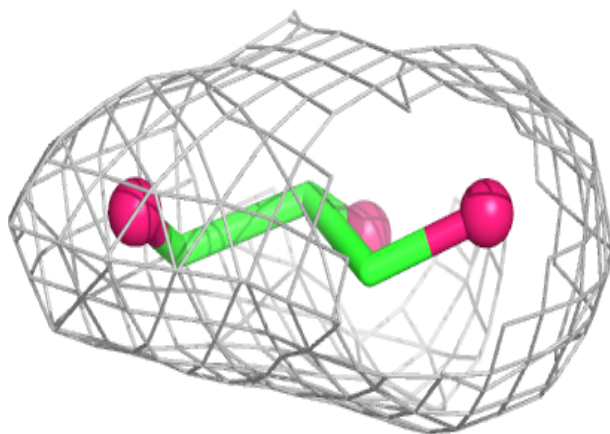
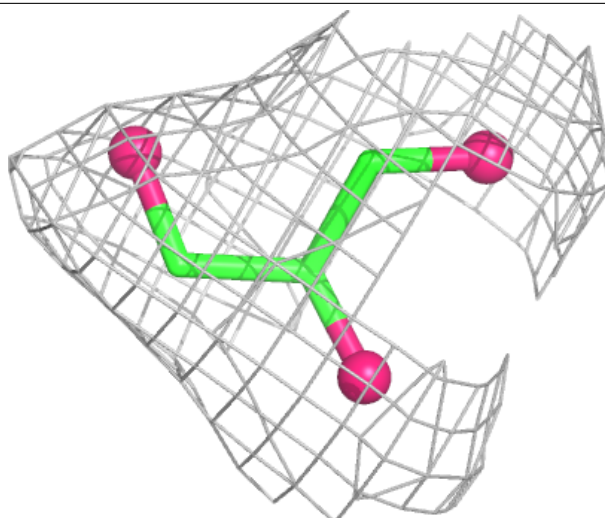
Electron density around GOL C 312:

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



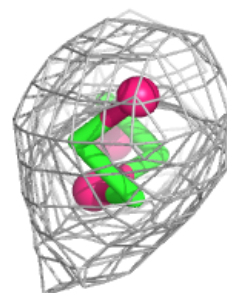
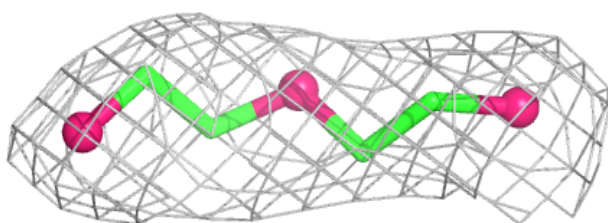
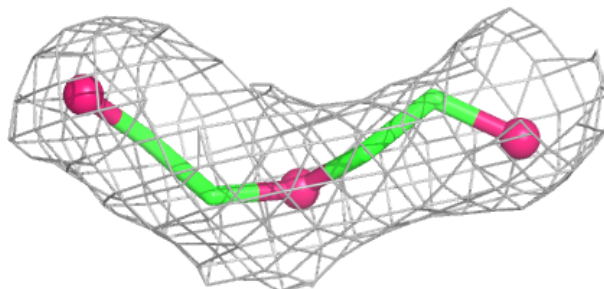
Electron density around GOL A 305:

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

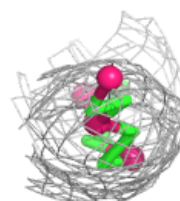
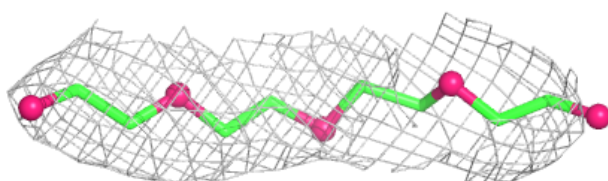
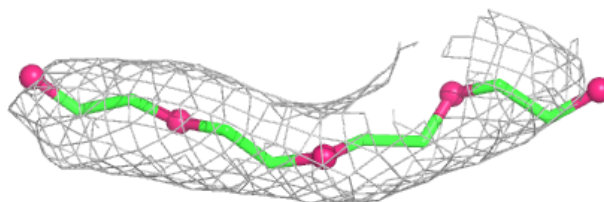


Electron density around PEG A 353:

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

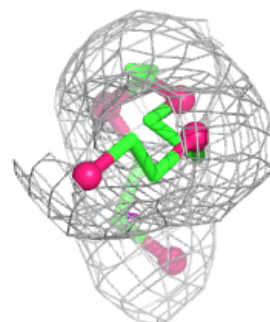
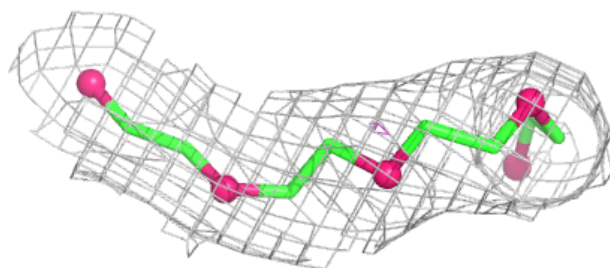
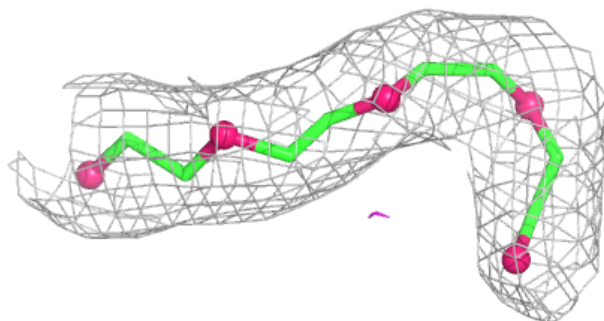
**Electron density around PG4 B 120:**

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

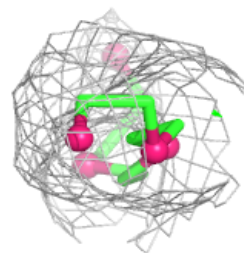
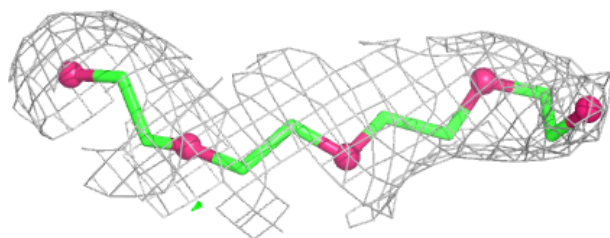
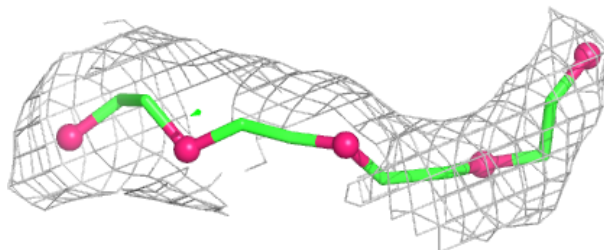


Electron density around PG4 A 320:

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

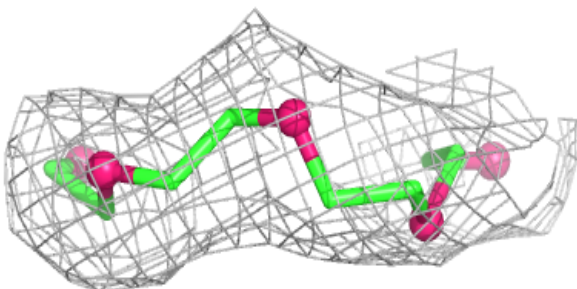
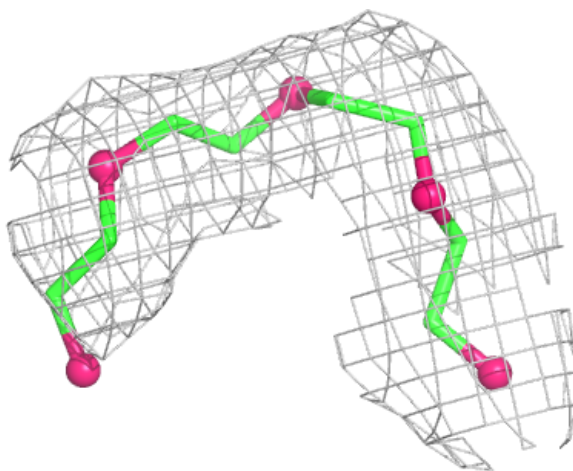
**Electron density around PG4 C 319:**

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



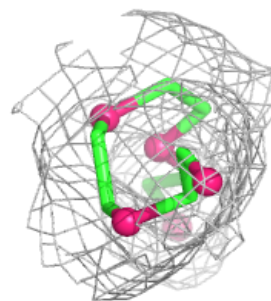
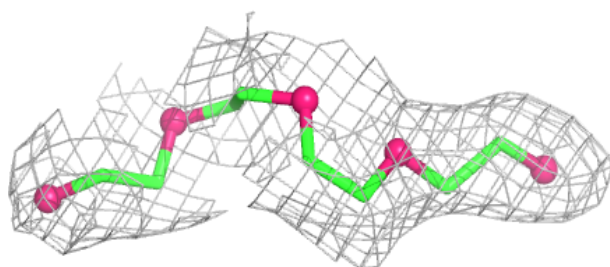
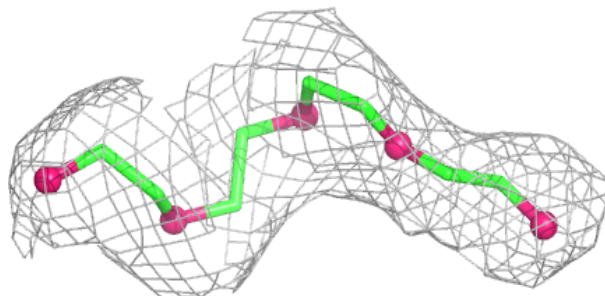
Electron density around PG4 A 321:

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



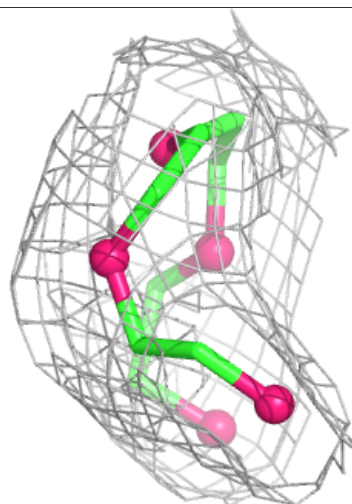
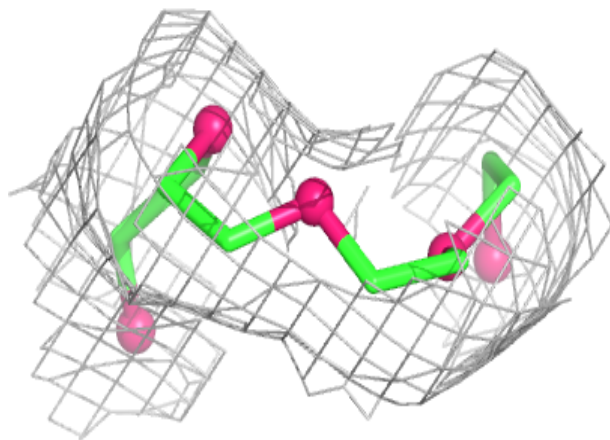
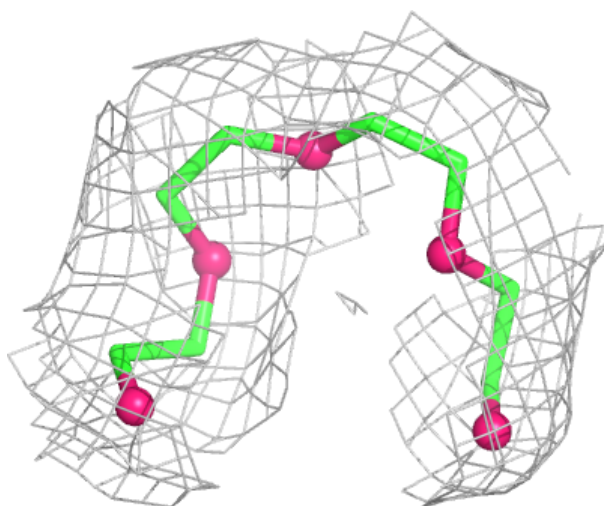
Electron density around PG4 A 352:

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



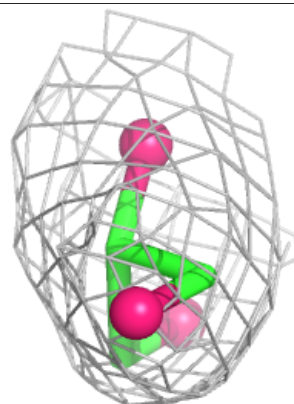
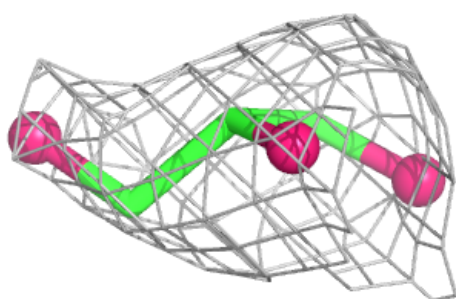
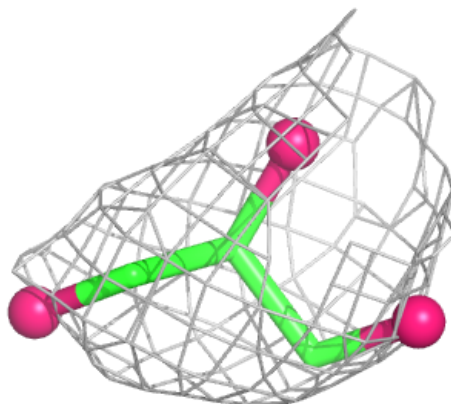
Electron density around PG4 D 119:

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

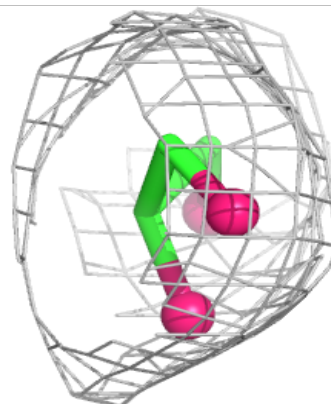
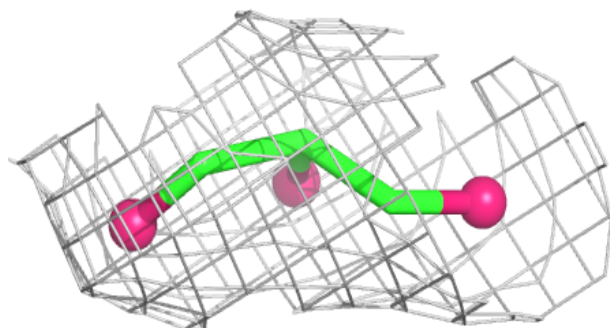
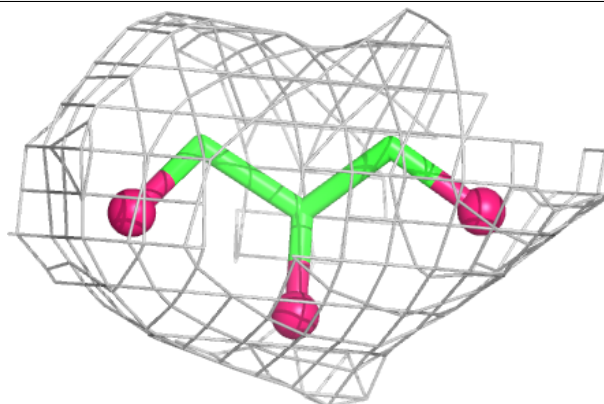


Electron density around GOL C 310:

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

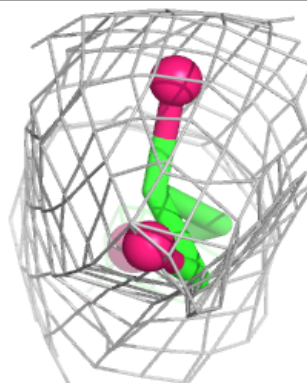
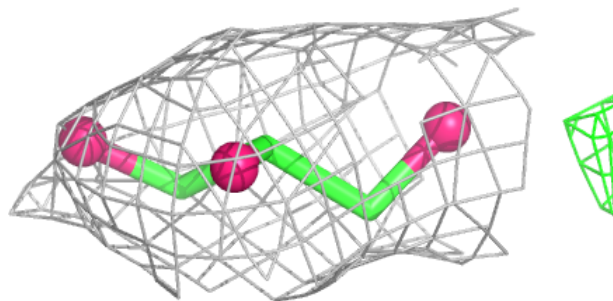
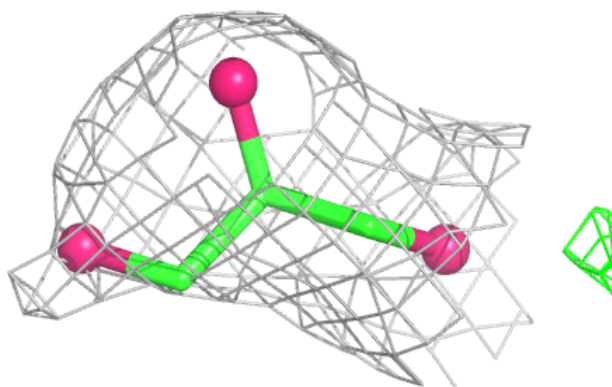
**Electron density around GOL C 306:**

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



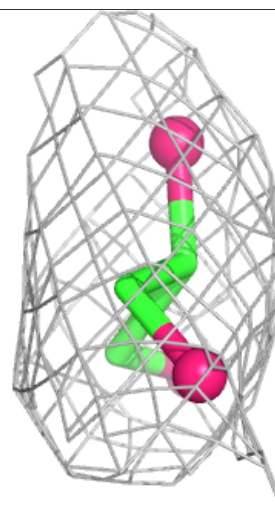
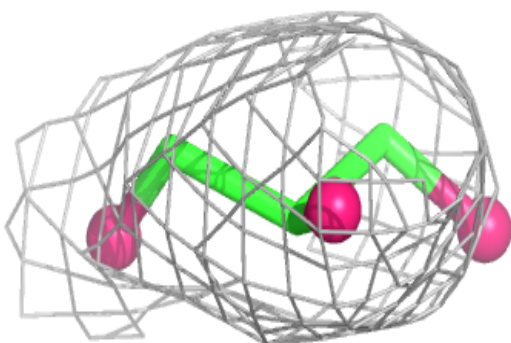
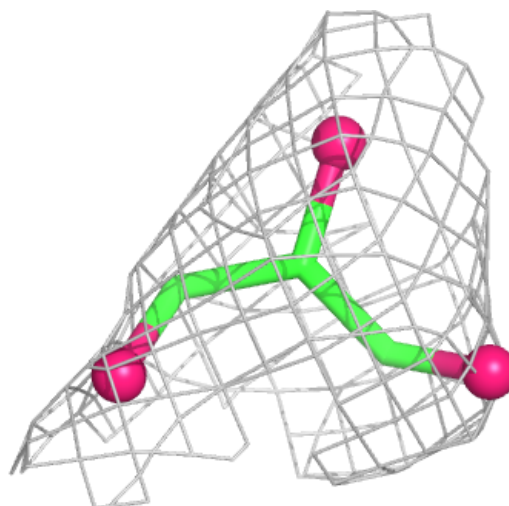
Electron density around GOL A 314:

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



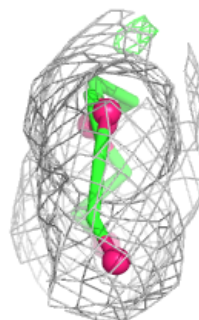
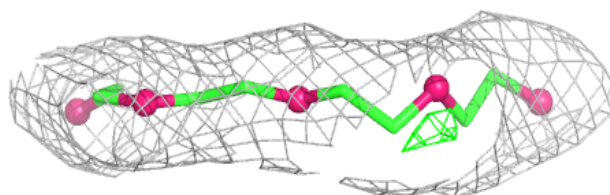
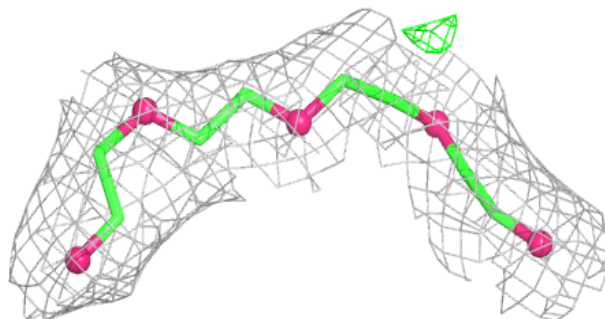
Electron density around GOL A 302:

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

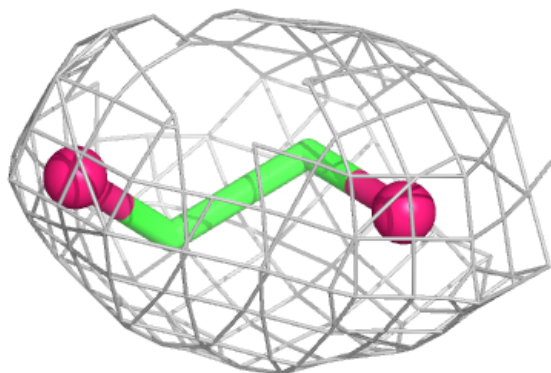
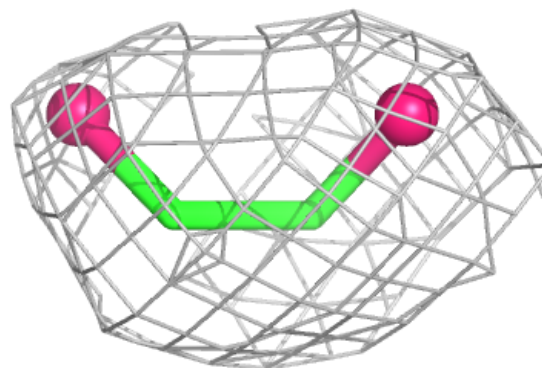


Electron density around PG4 F 105:

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

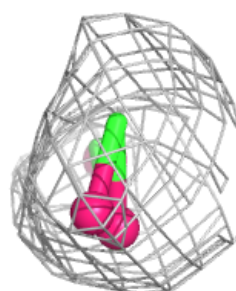
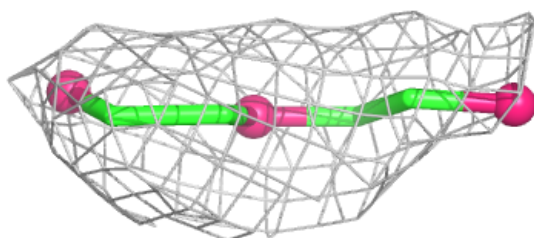
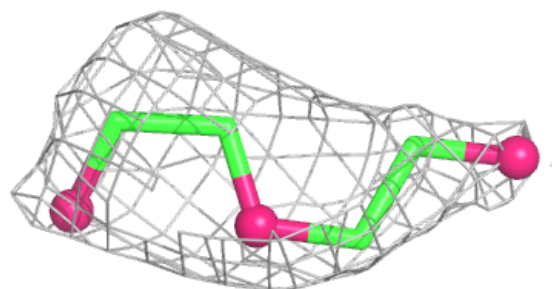
**Electron density around EDO D 130:**

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

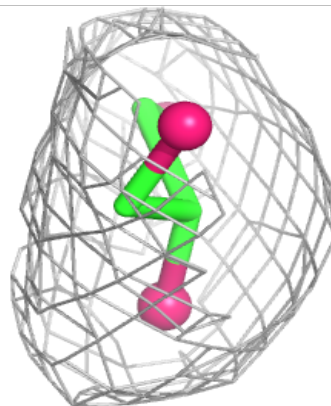
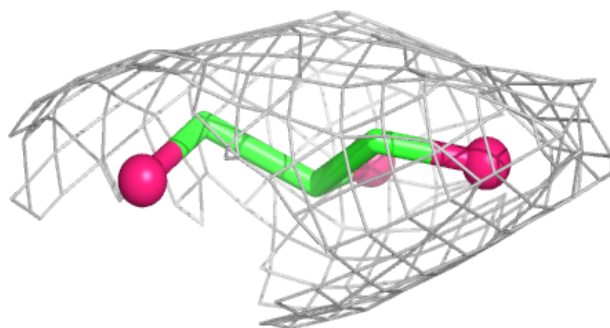
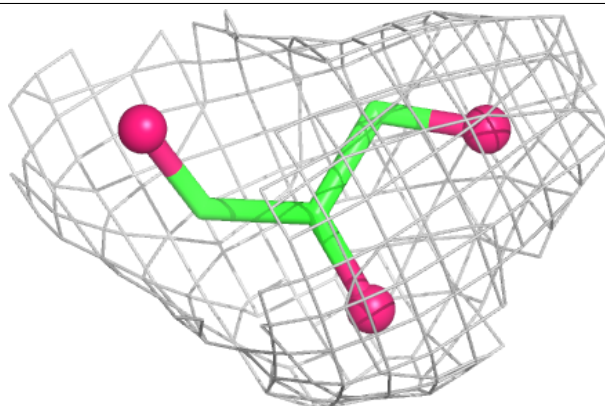


Electron density around PEG C 334:

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

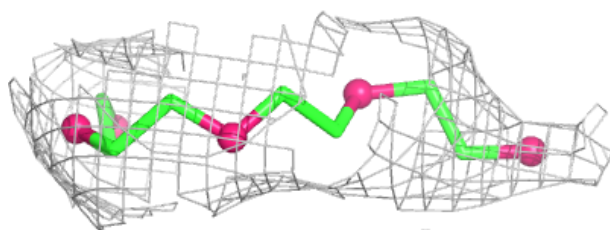
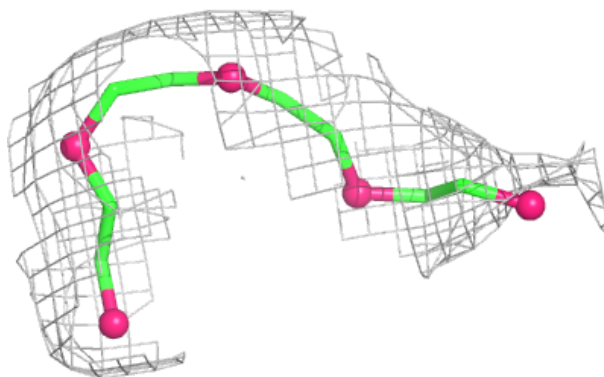
**Electron density around GOL B 153:**

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

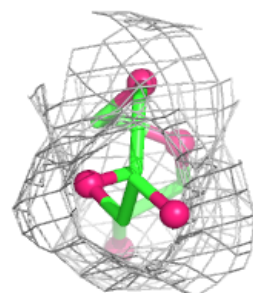
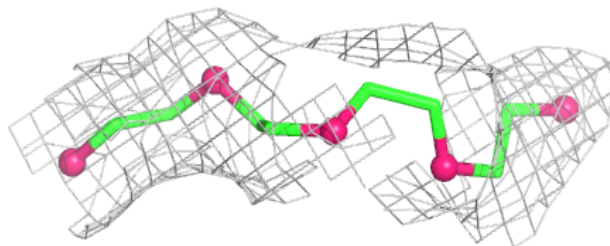
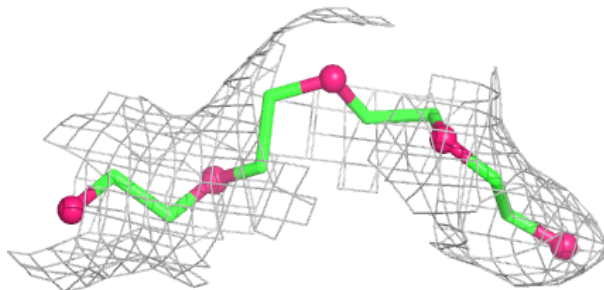


Electron density around PG4 B 122:

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

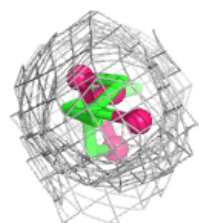
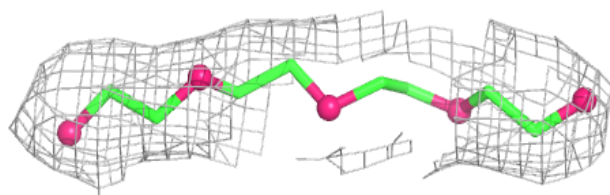
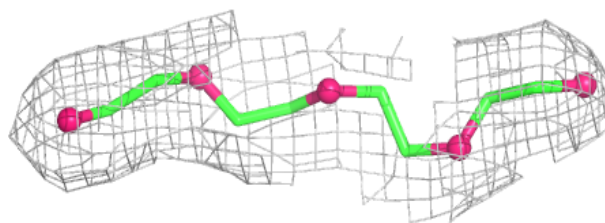
**Electron density around PG4 C 323:**

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

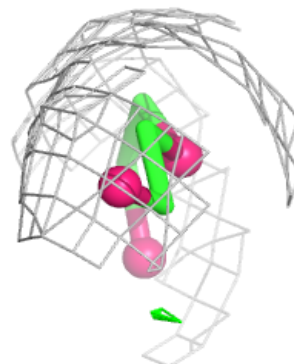
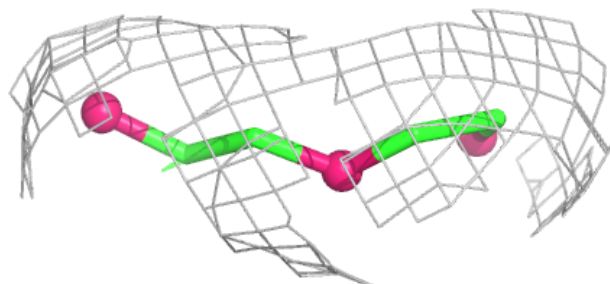
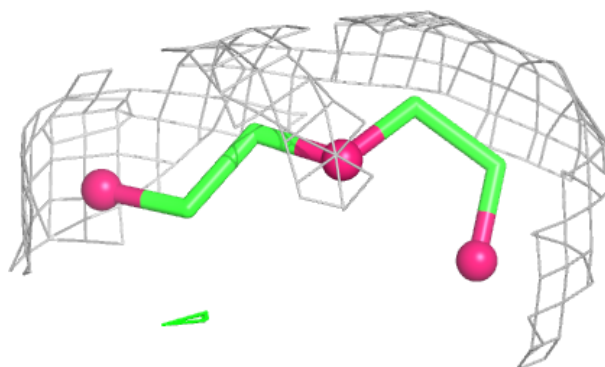


Electron density around PG4 E 115:

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

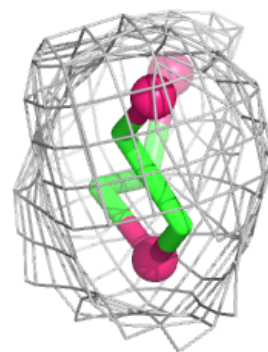
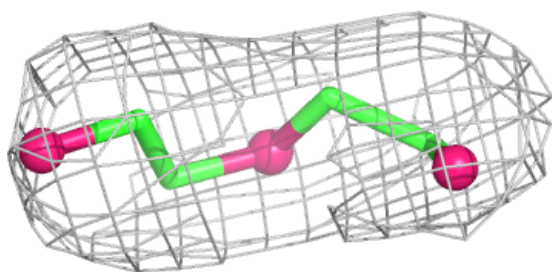
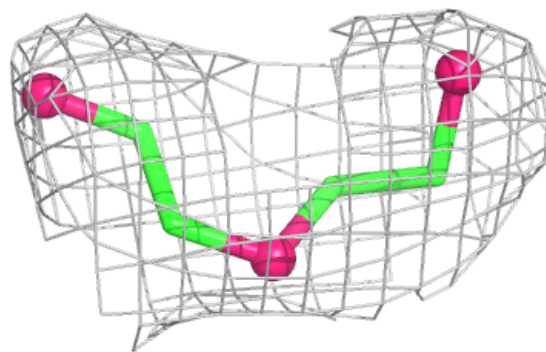
**Electron density around PEG A 370:**

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



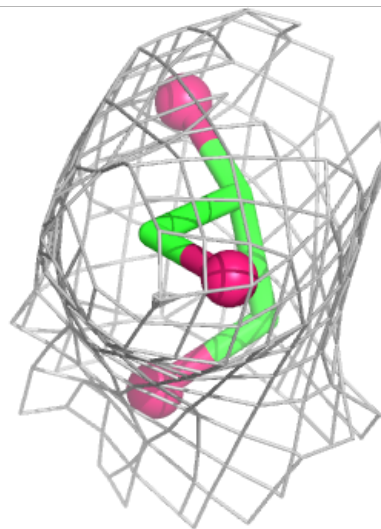
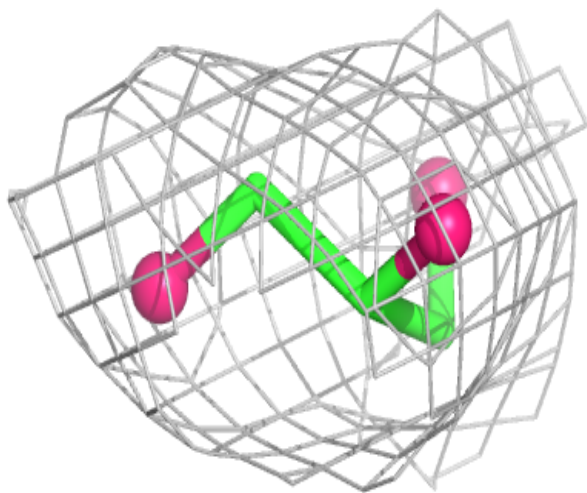
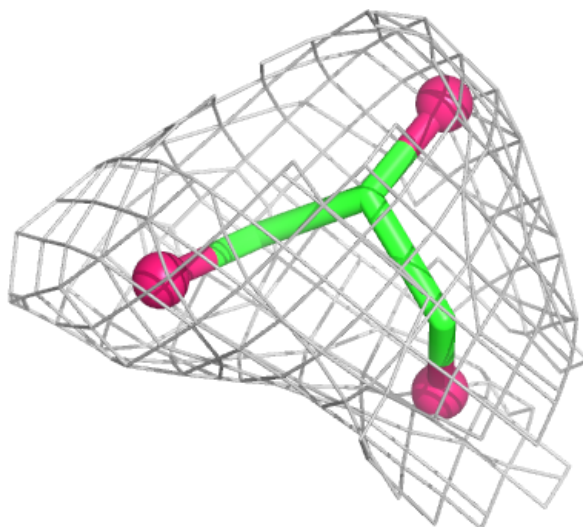
Electron density around PEG B 157:

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



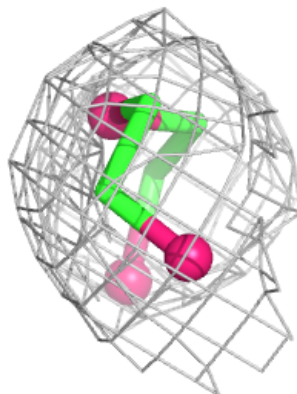
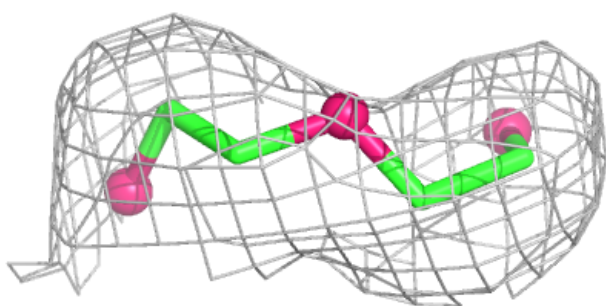
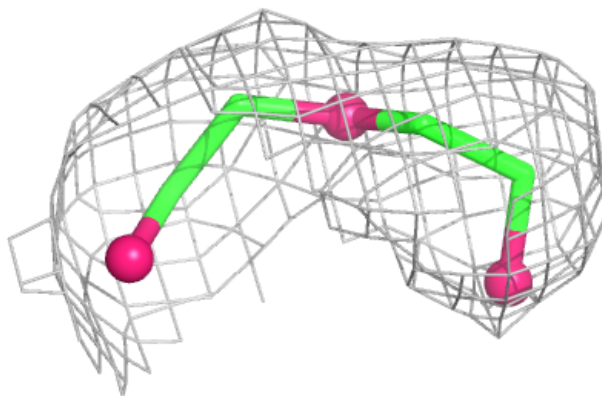
Electron density around GOL E 113:

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



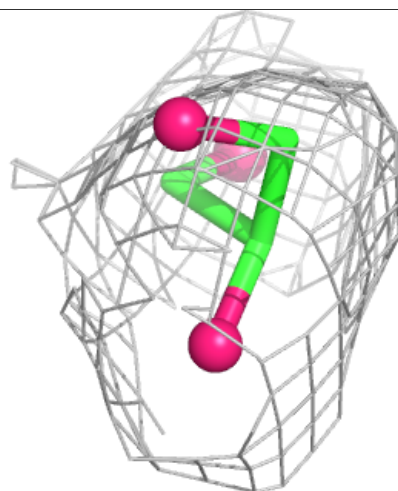
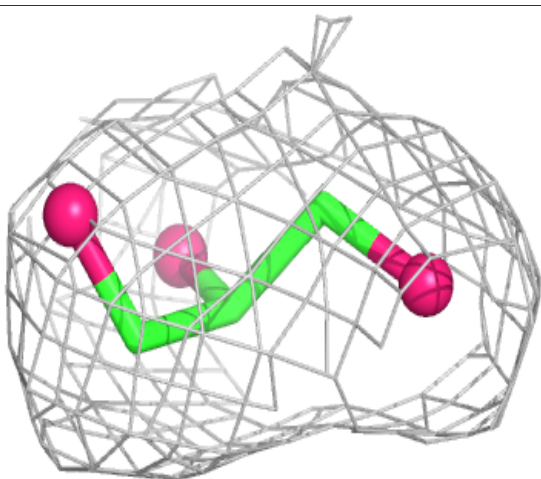
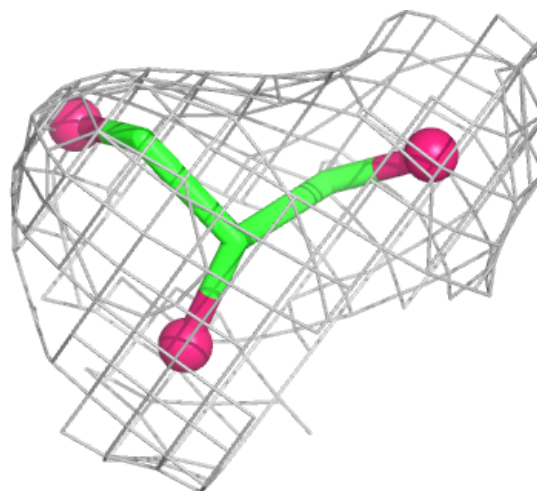
Electron density around PEG A 334:

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



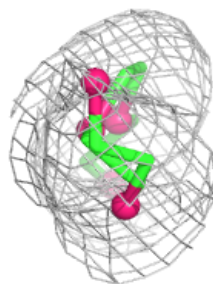
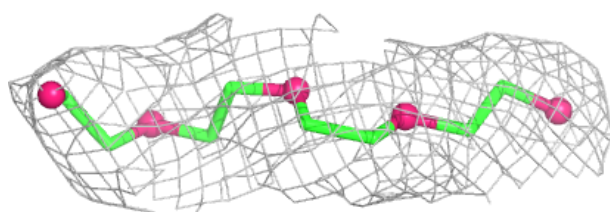
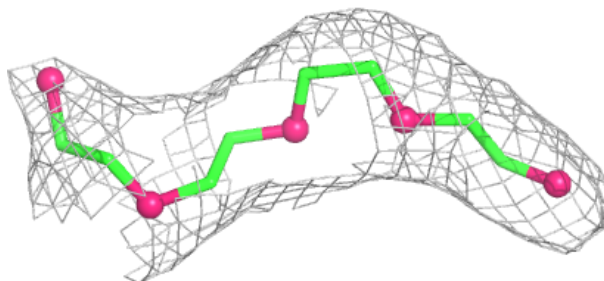
Electron density around GOL C 344:

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

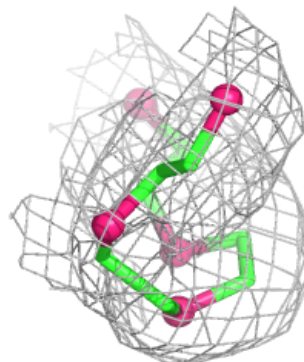
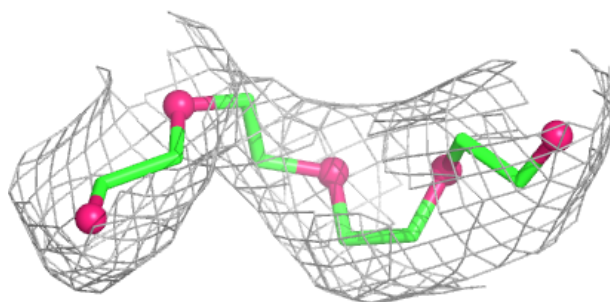
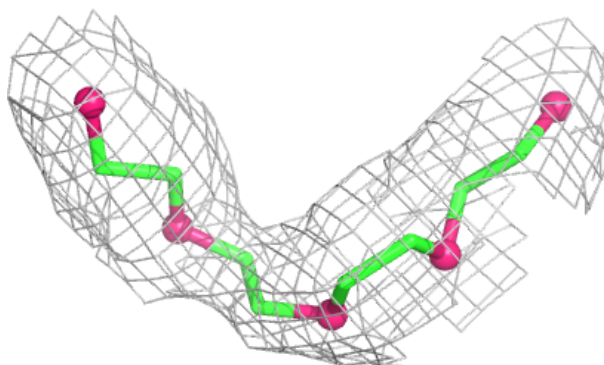


Electron density around PG4 A 319:

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

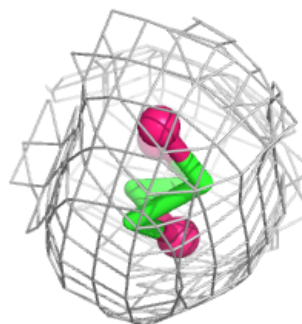
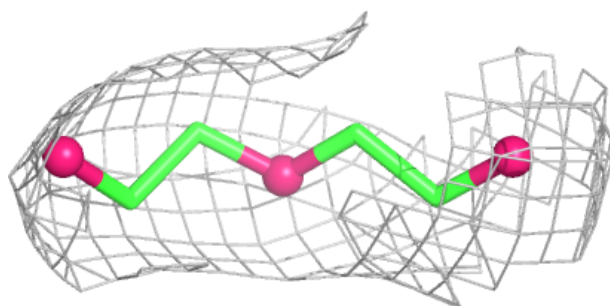
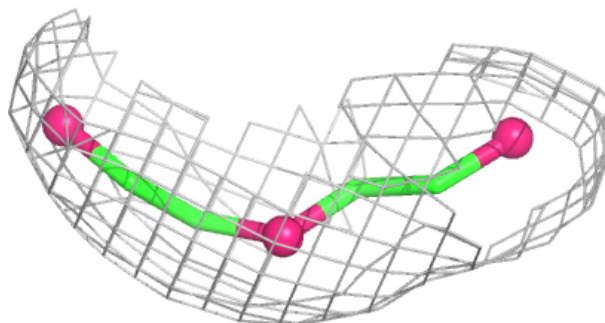
**Electron density around PG4 B 121:**

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



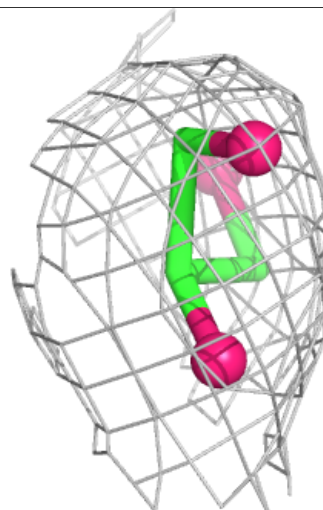
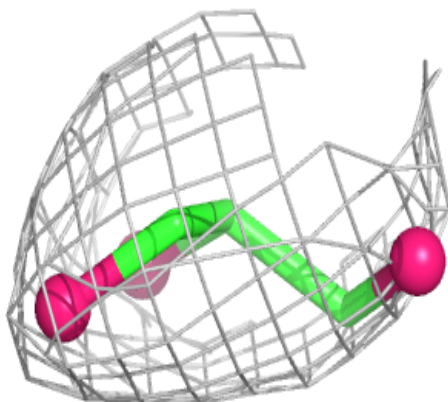
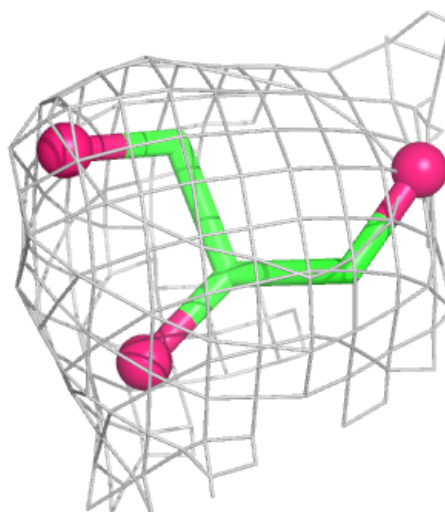
Electron density around PEG C 346:

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



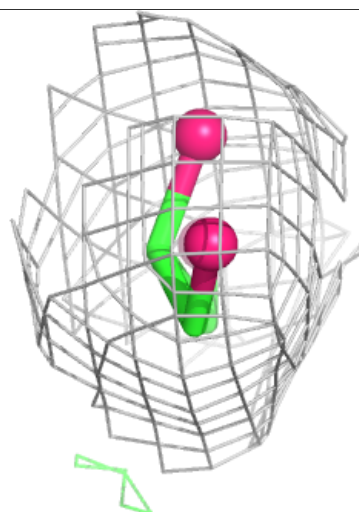
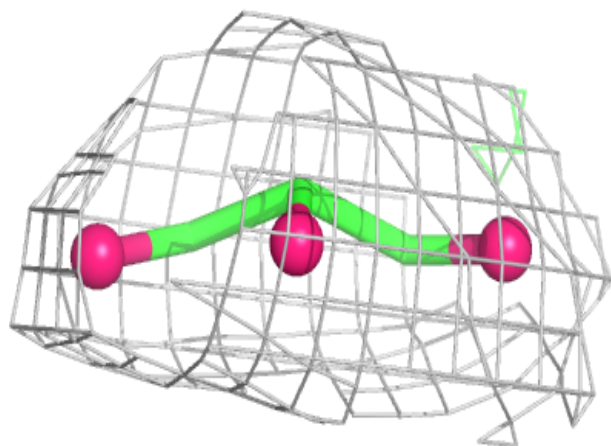
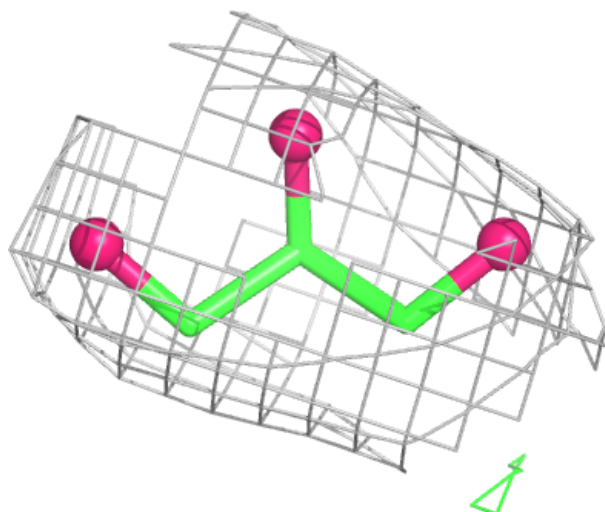
Electron density around GOL C 347:

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



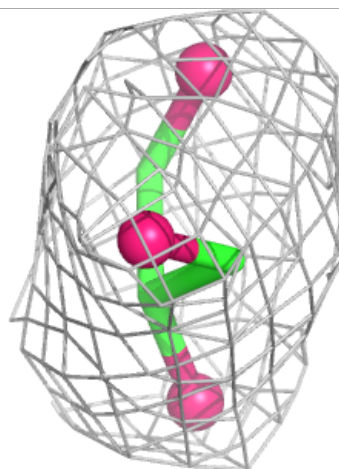
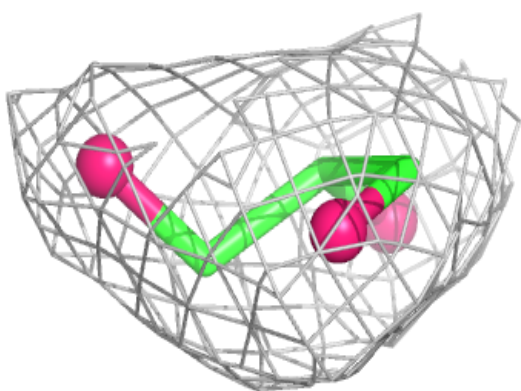
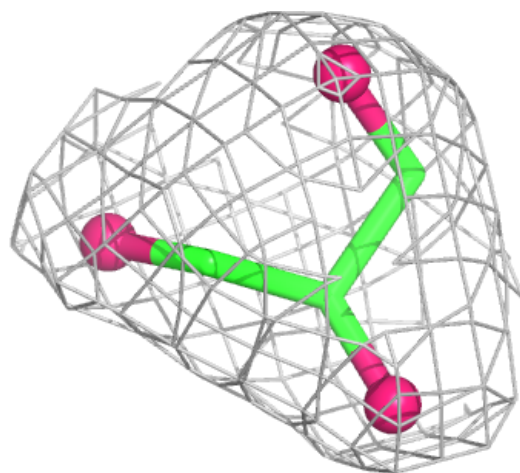
Electron density around GOL A 307:

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



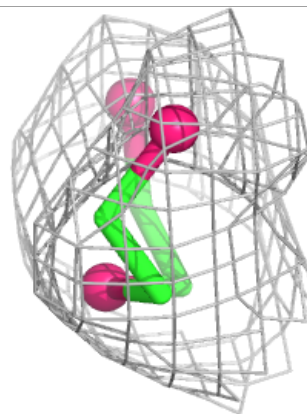
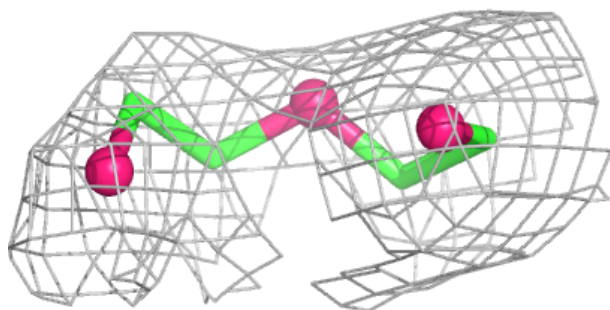
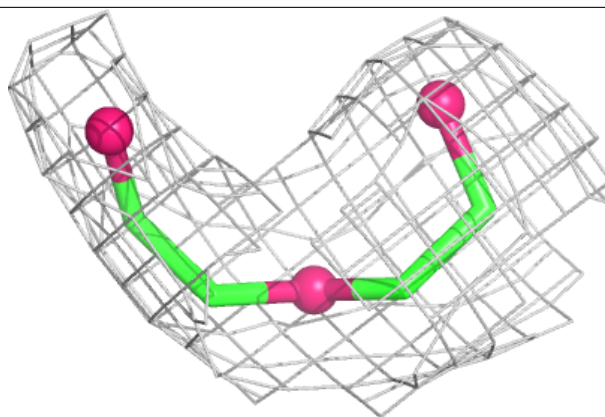
Electron density around GOL B 111:

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

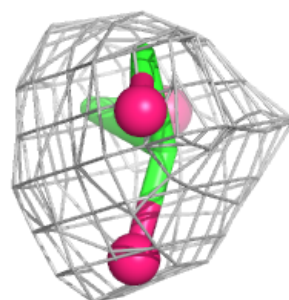
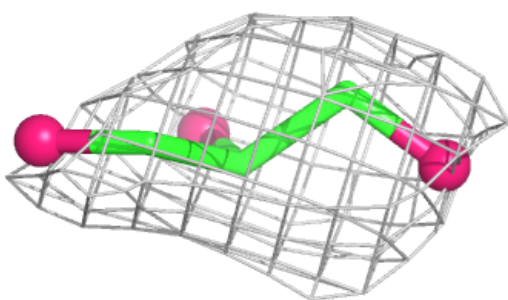
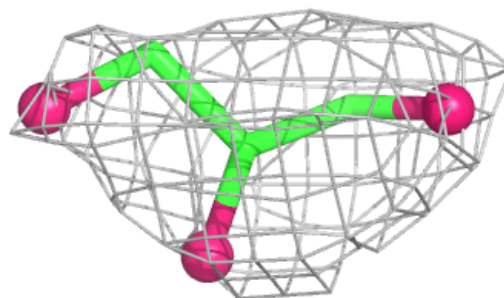


Electron density around PEG C 303:

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

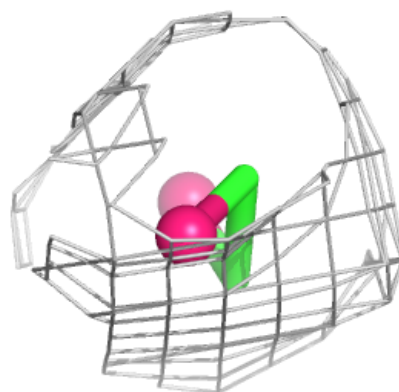
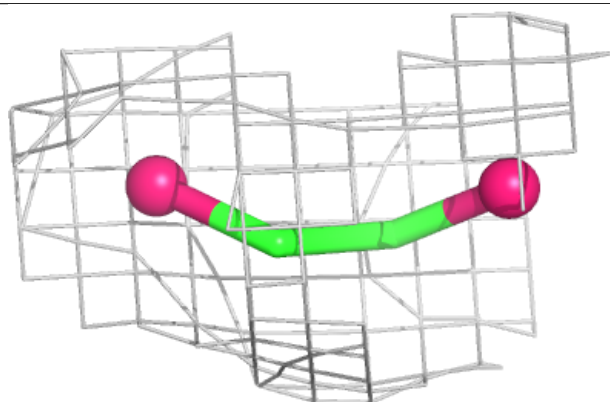
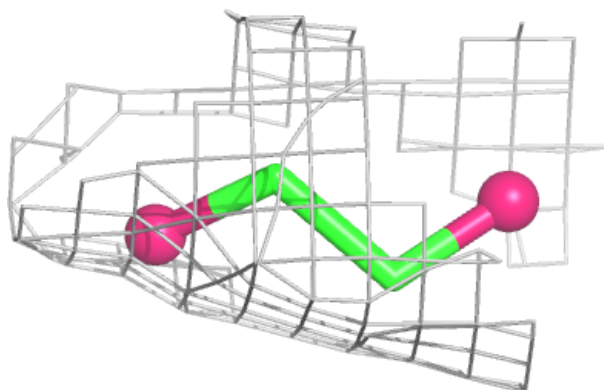
**Electron density around GOL C 304:**

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



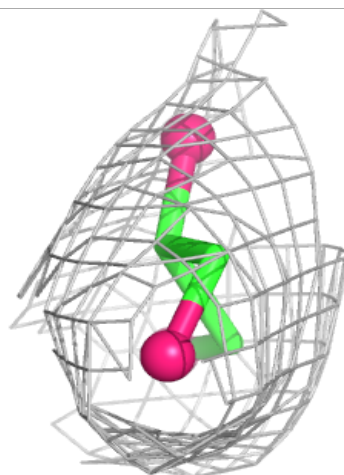
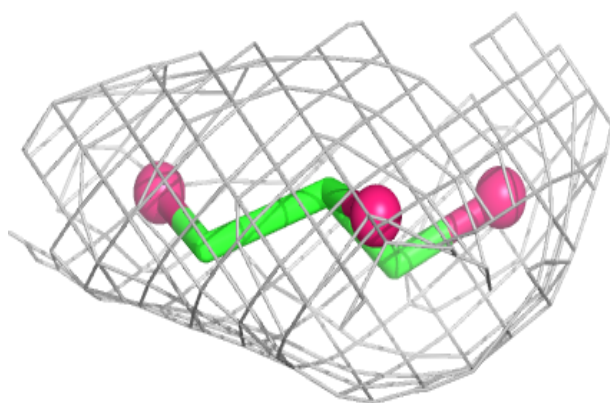
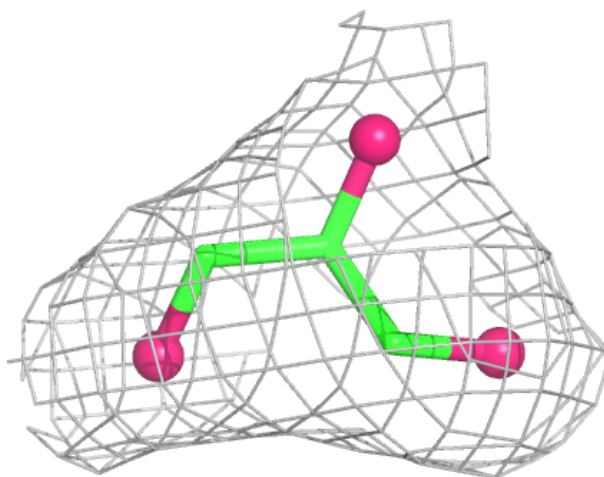
Electron density around EDO D 102:

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



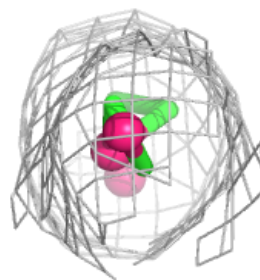
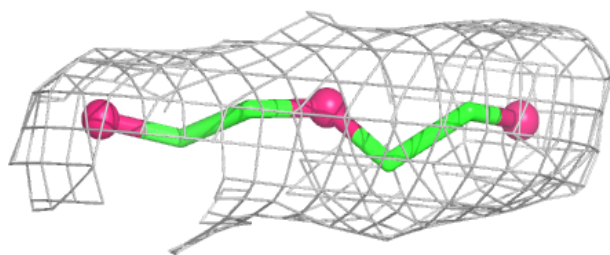
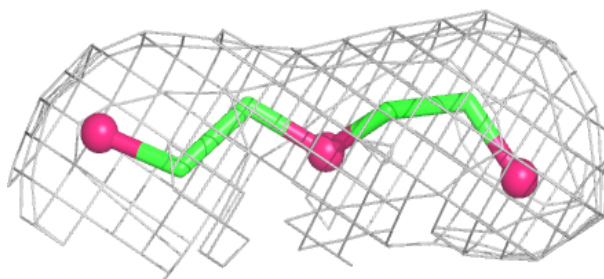
Electron density around GOL A 308:

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

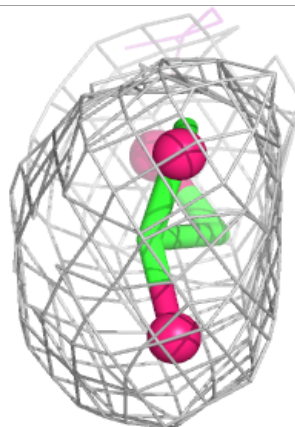
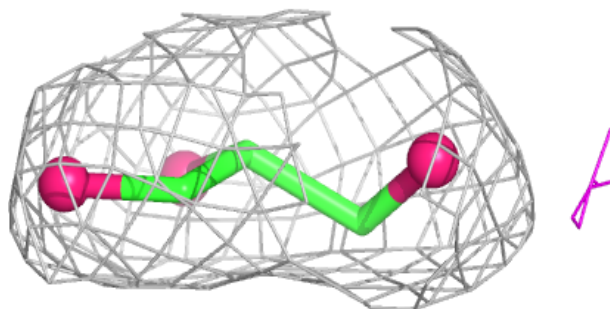
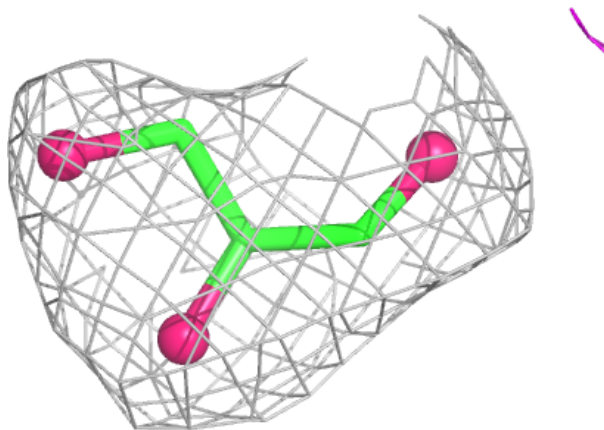


Electron density around PEG A 372:

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

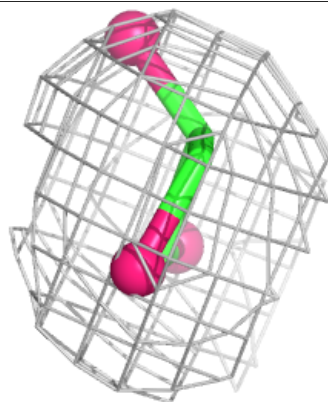
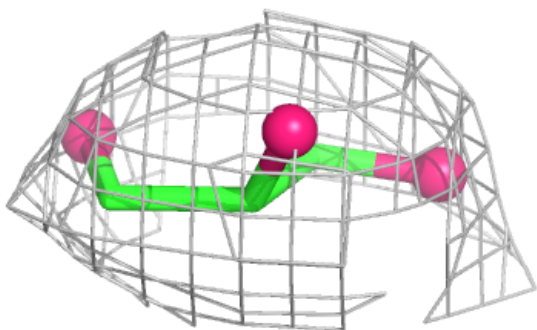
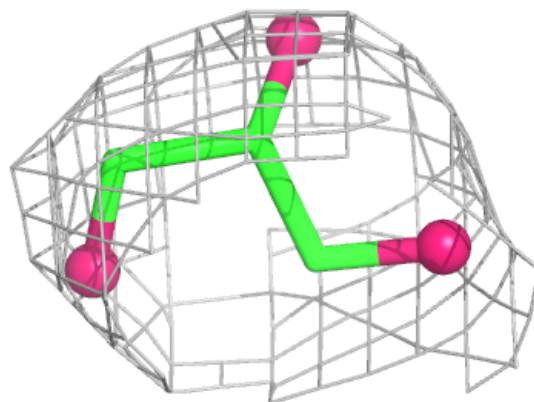
**Electron density around GOL D 109:**

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

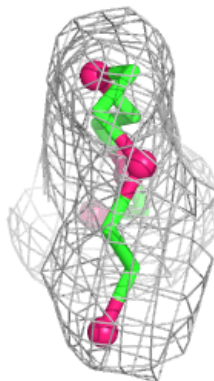
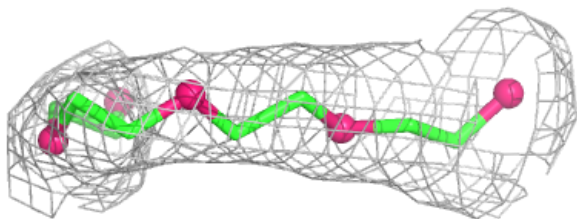
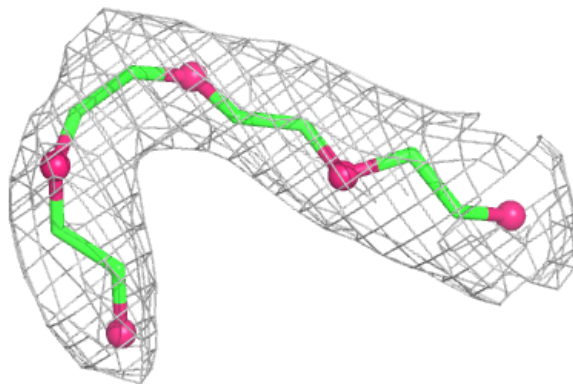


Electron density around GOL A 310:

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

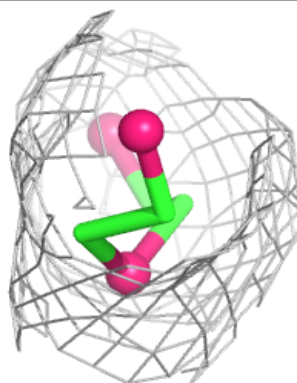
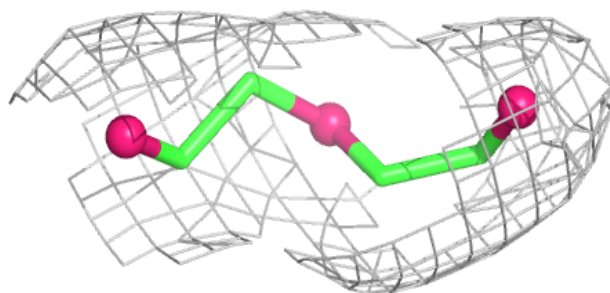
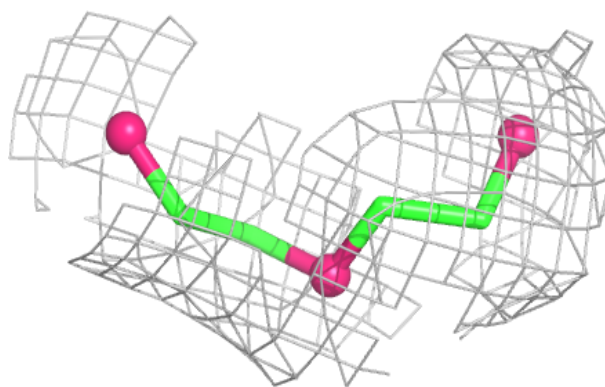
**Electron density around PG4 B 116:**

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

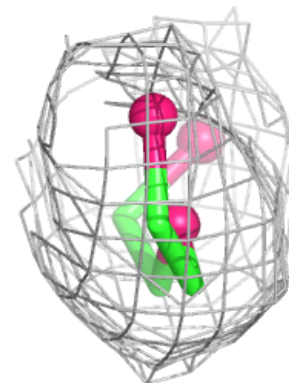
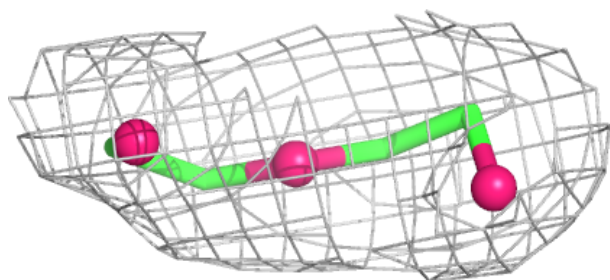
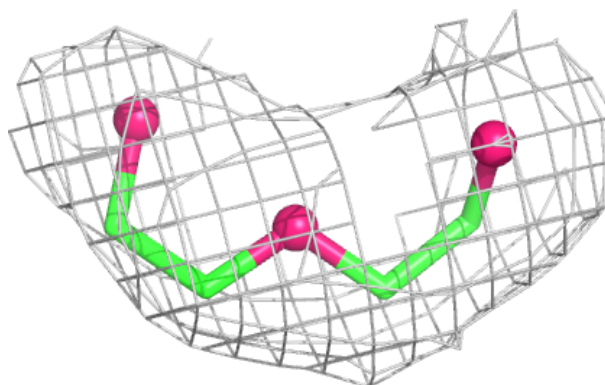


Electron density around PEG B 139:

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

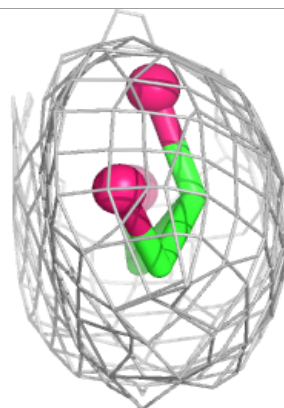
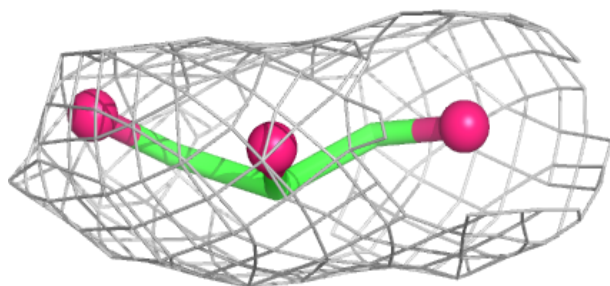
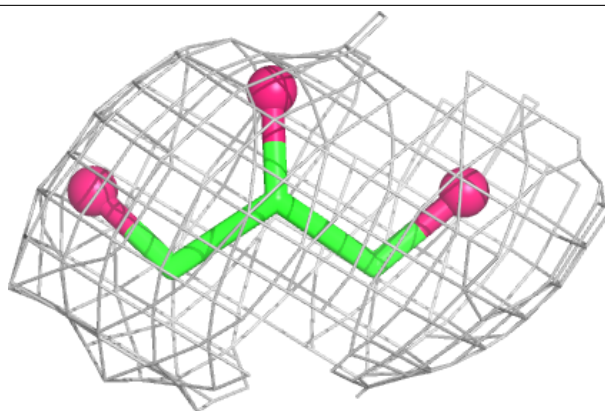
**Electron density around PEG B 142:**

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

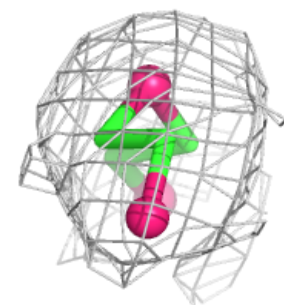
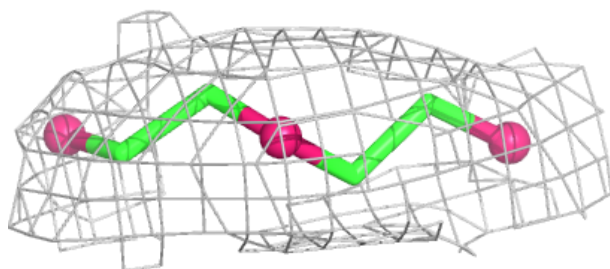
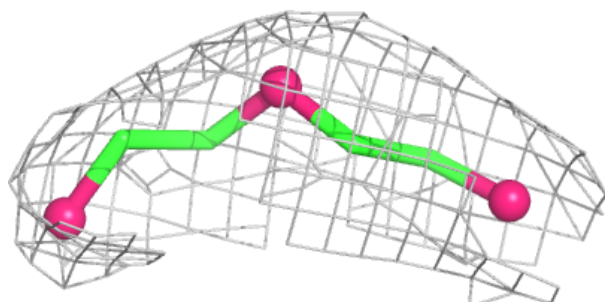


Electron density around GOL D 112:

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

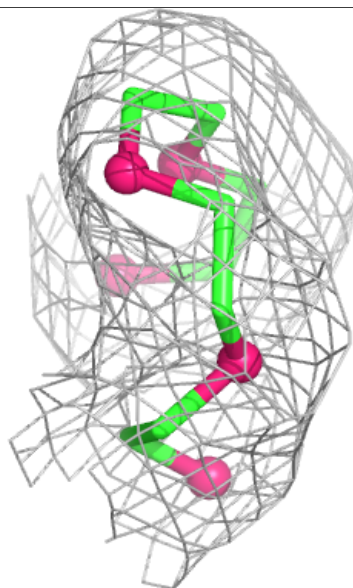
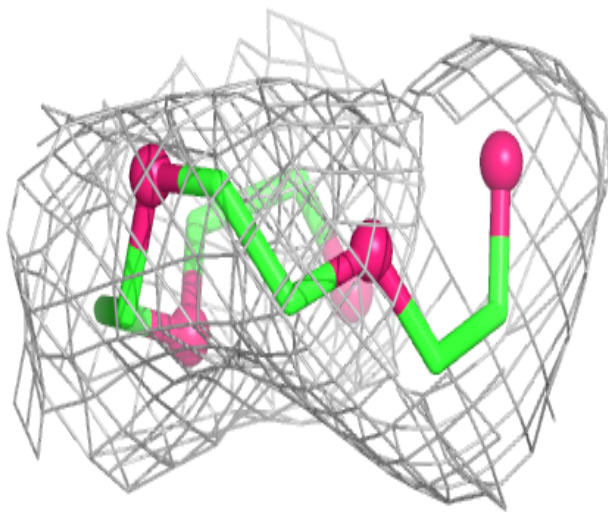
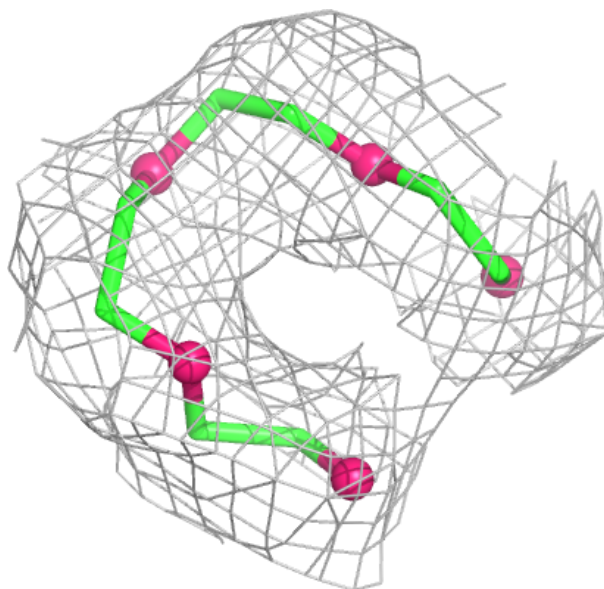
**Electron density around PEG D 123:**

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



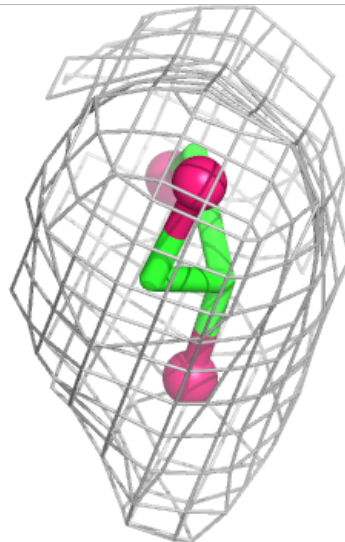
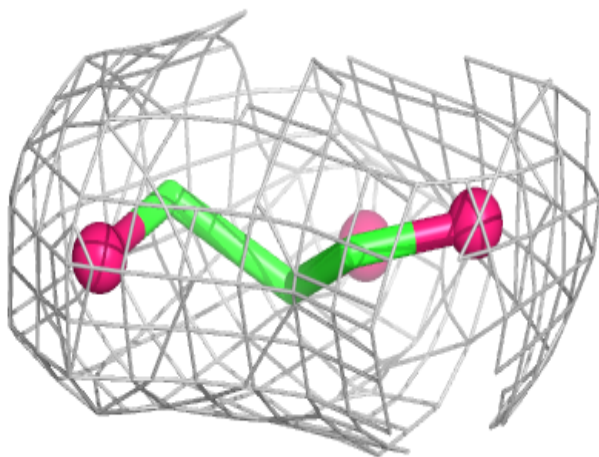
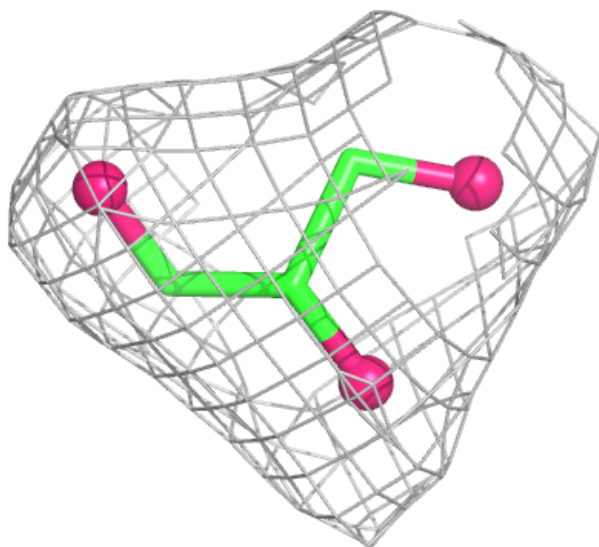
Electron density around PG4 F 101:

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



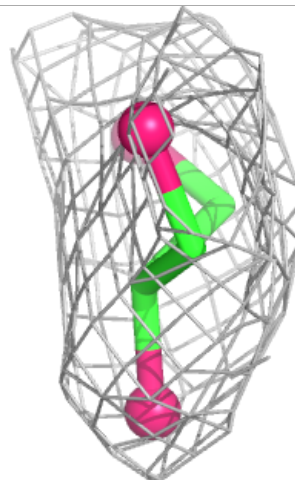
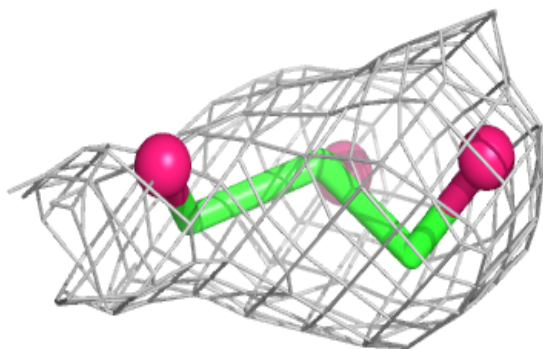
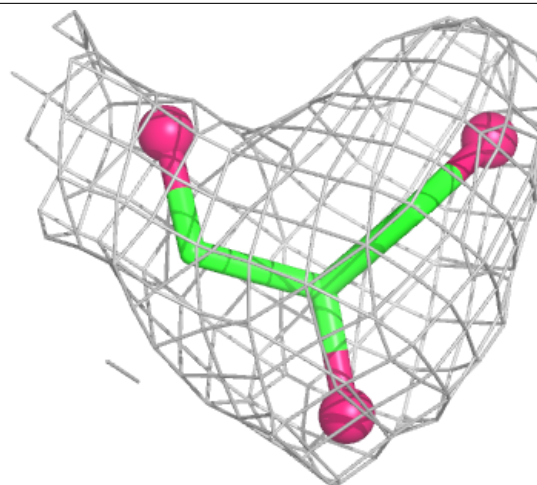
Electron density around GOL A 363:

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



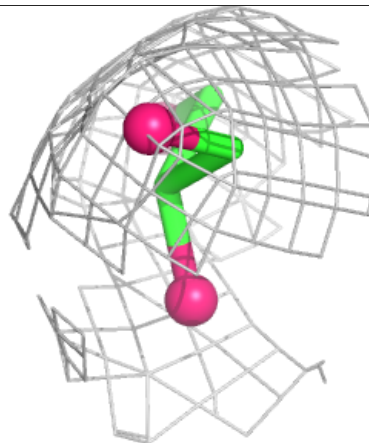
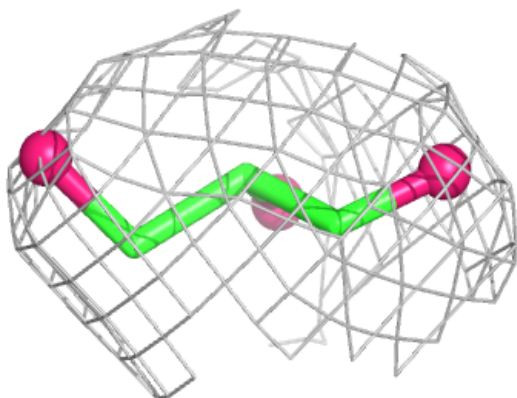
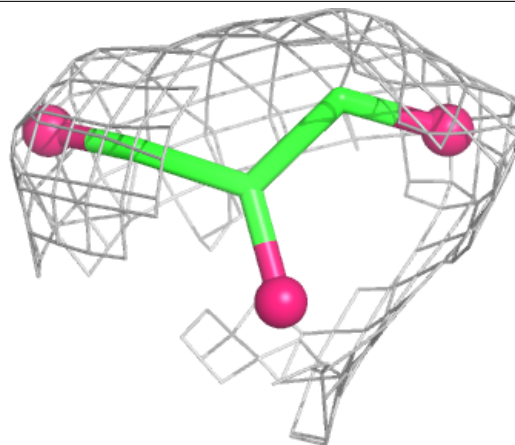
Electron density around GOL C 313:

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



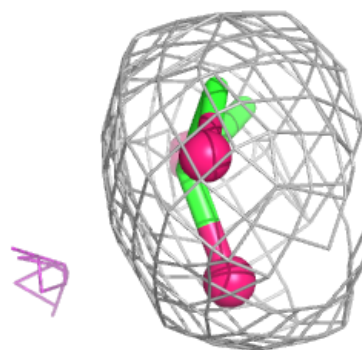
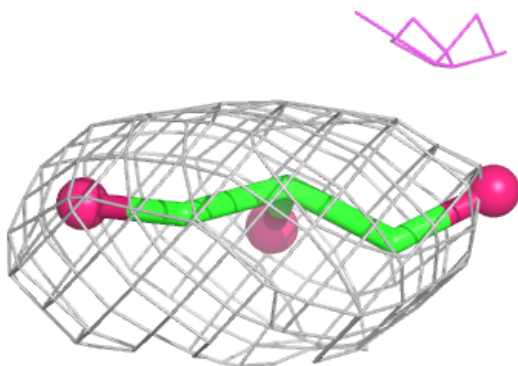
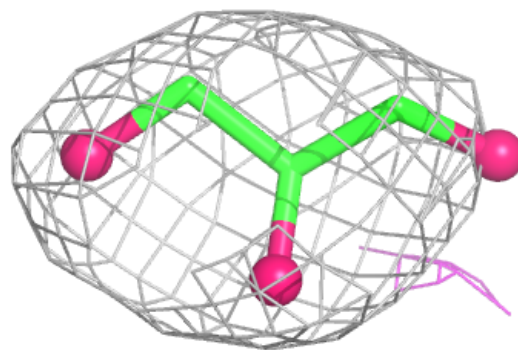
Electron density around GOL A 347:

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



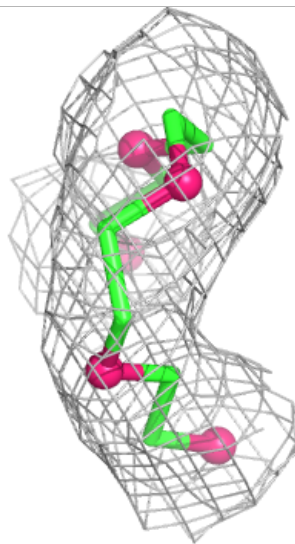
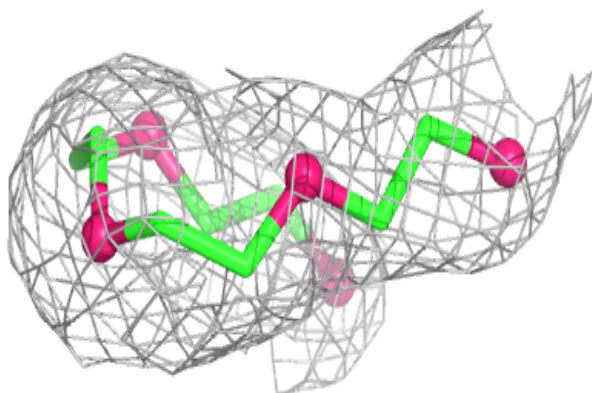
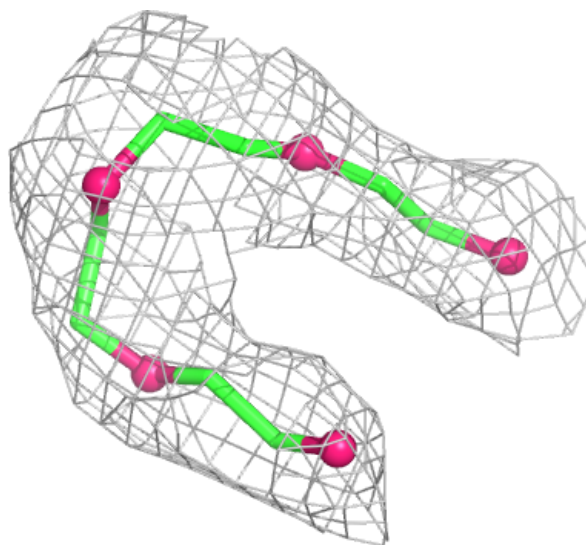
Electron density around GOL B 110:

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



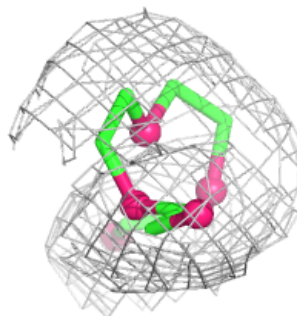
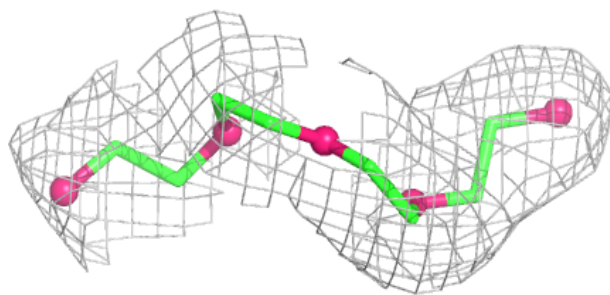
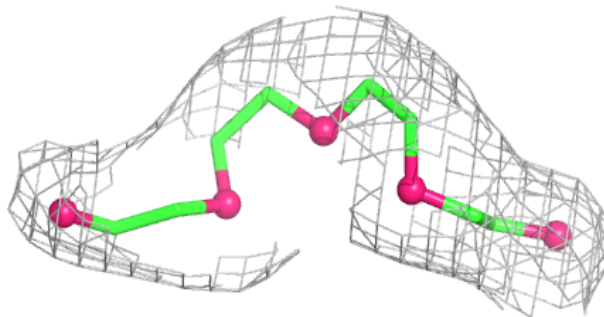
Electron density around PG4 E 107:

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

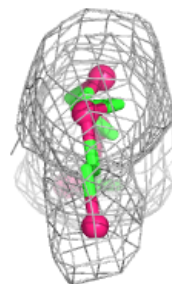
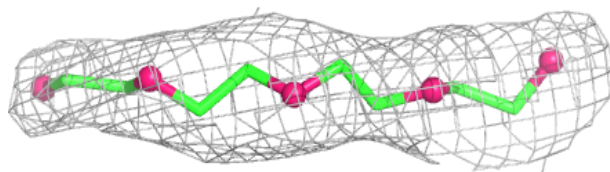
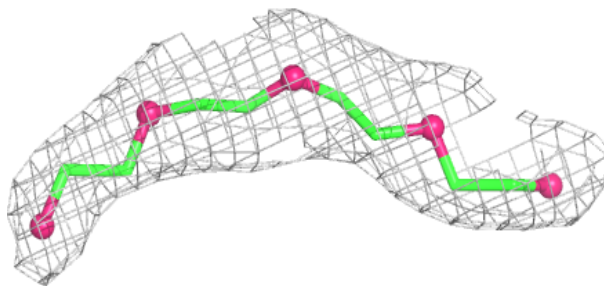


Electron density around PG4 A 367:

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

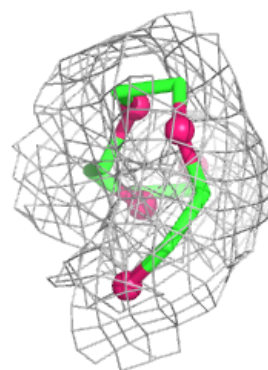
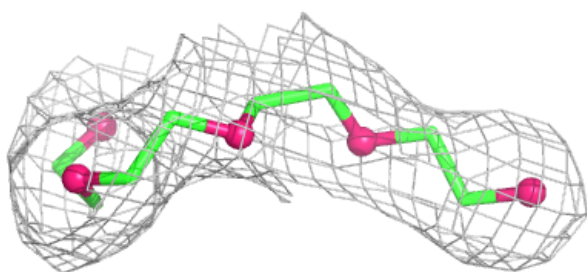
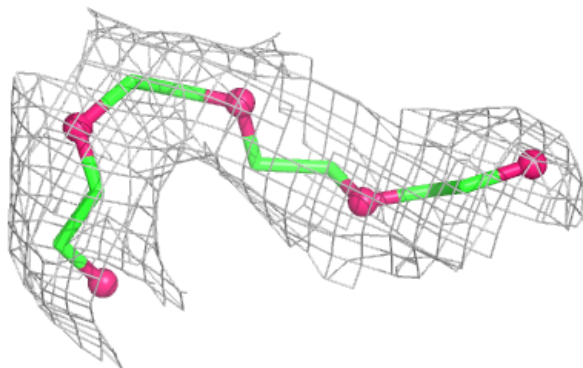
**Electron density around PG4 B 117:**

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

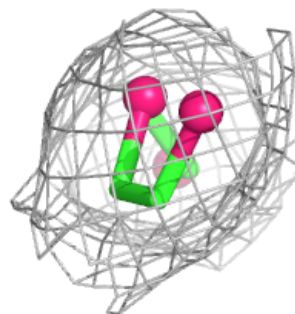
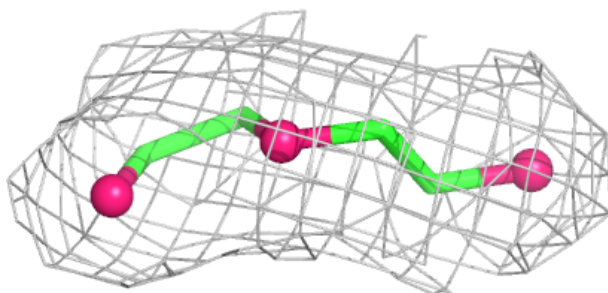
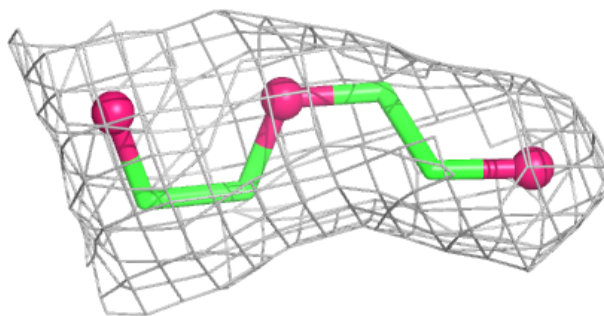


Electron density around PG4 C 321:

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

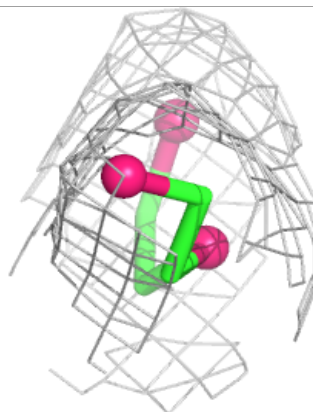
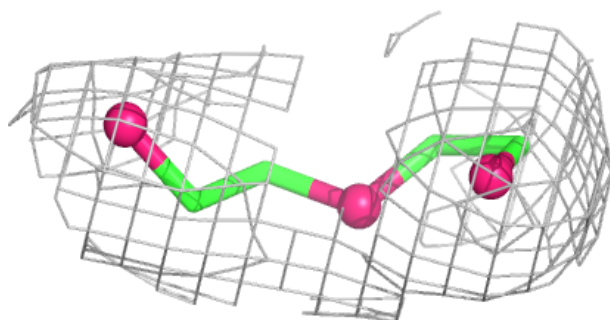
**Electron density around PEG D 124:**

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

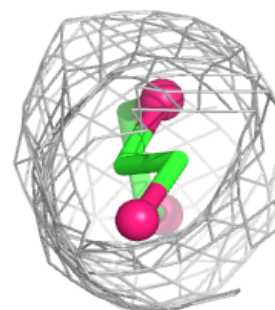
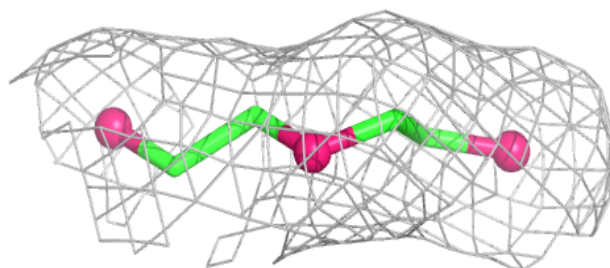
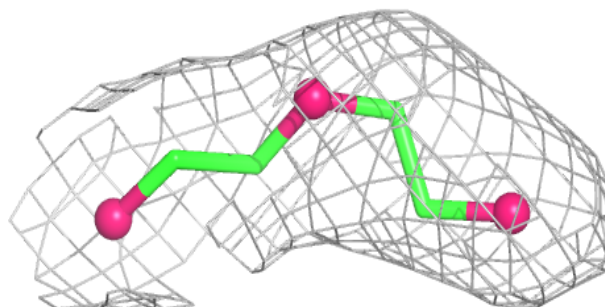


Electron density around PEG D 125:

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

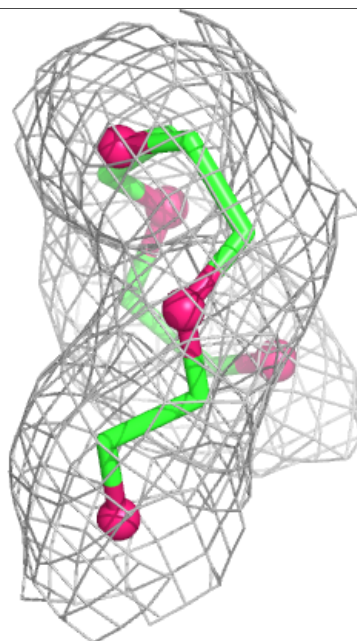
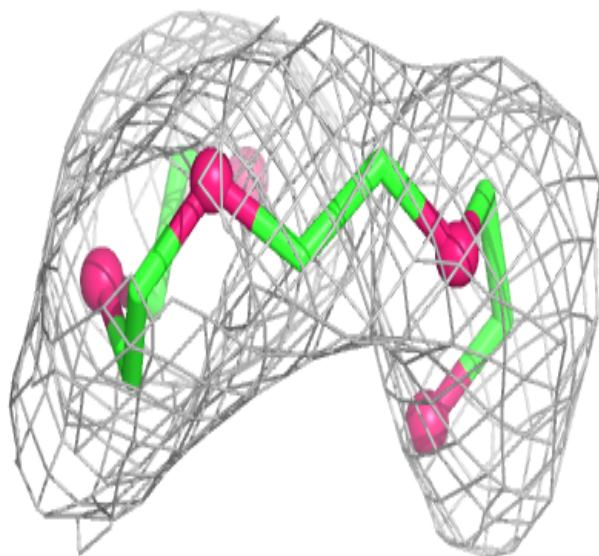
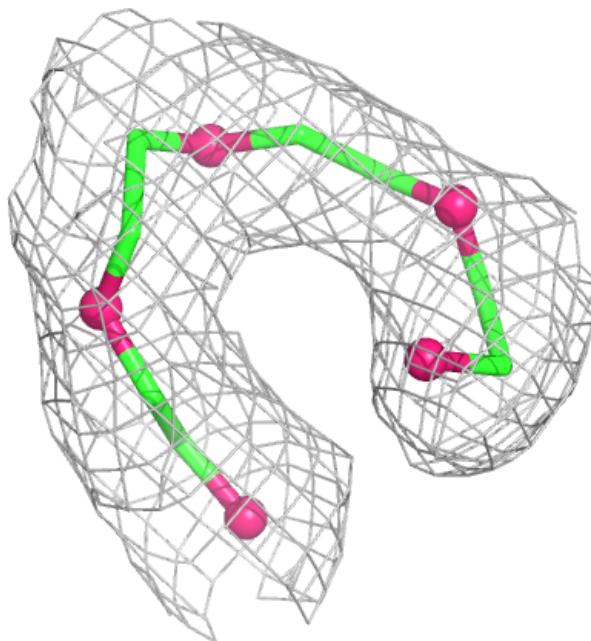
**Electron density around PEG C 328:**

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



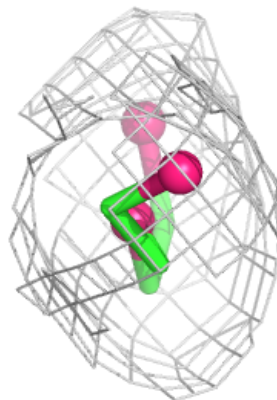
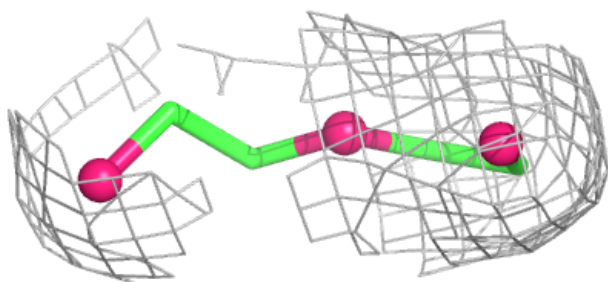
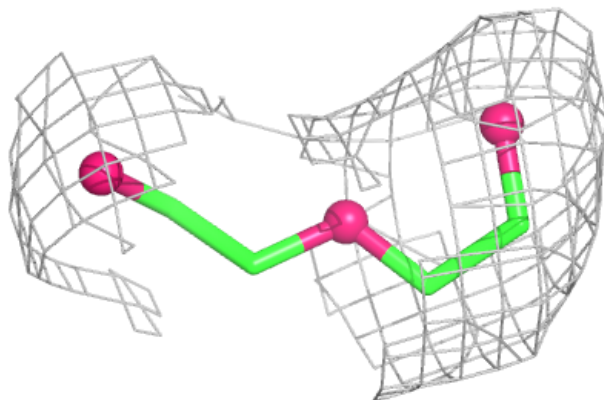
Electron density around PG4 A 366:

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



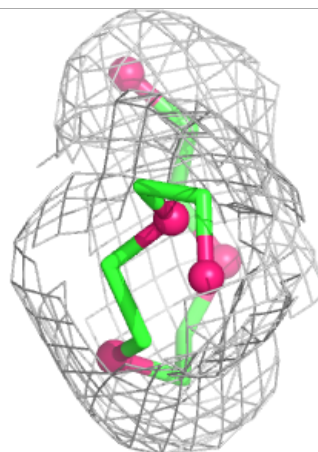
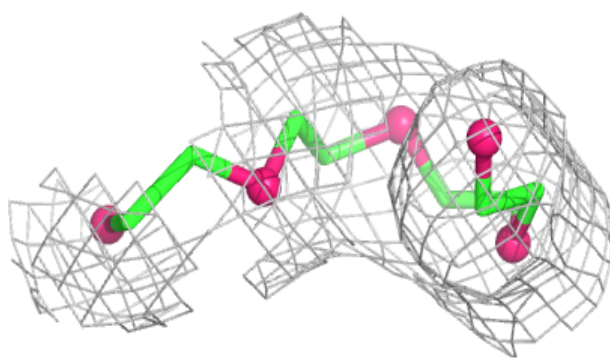
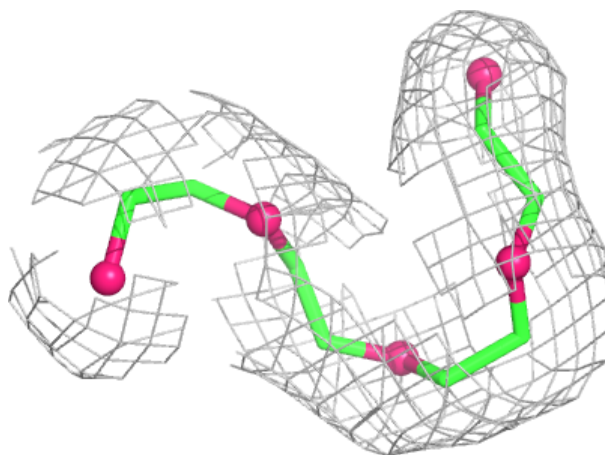
Electron density around PEG B 156:

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



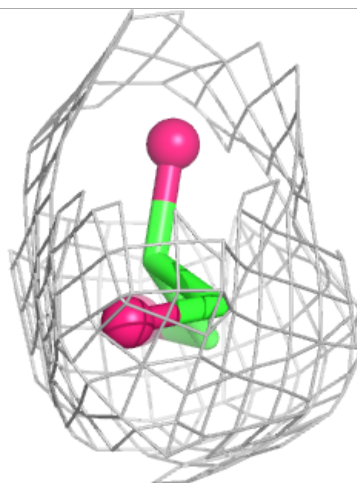
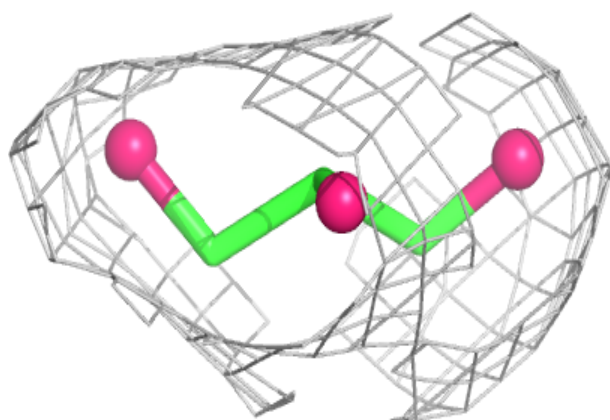
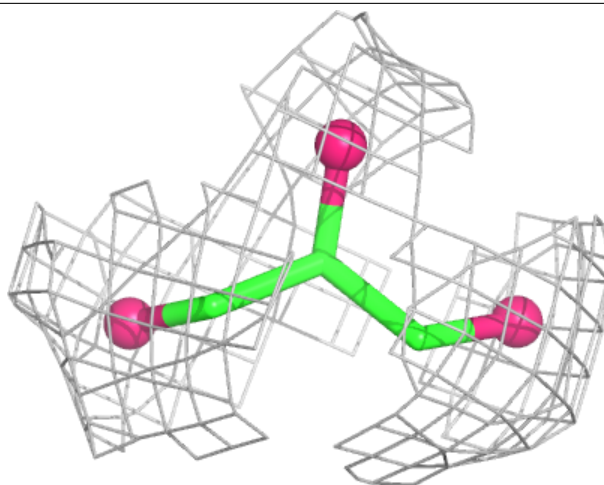
Electron density around PG4 B 123:

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



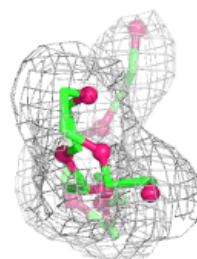
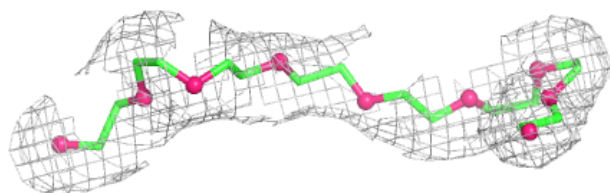
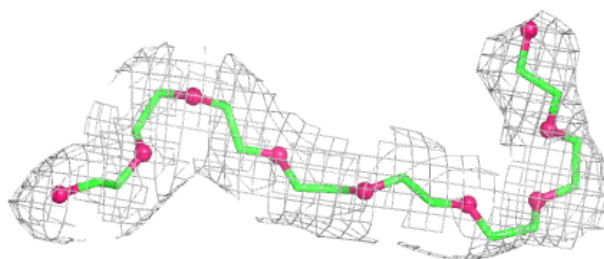
Electron density around GOL C 337:

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

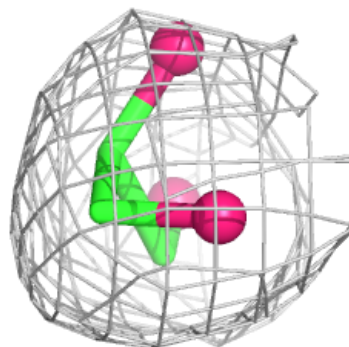
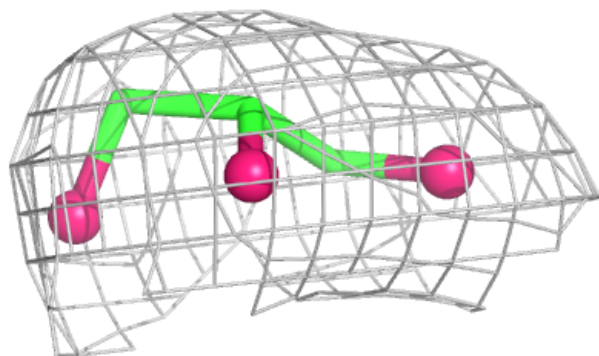
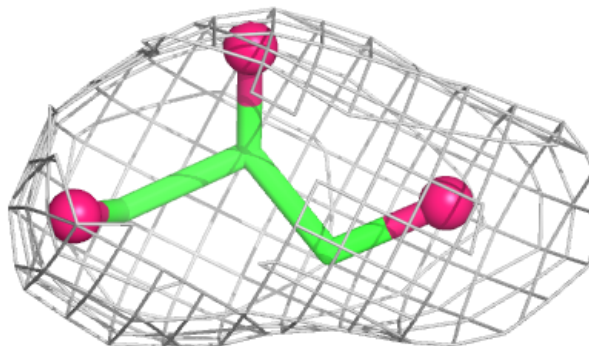


Electron density around PE8 C 335:

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

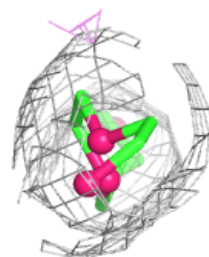
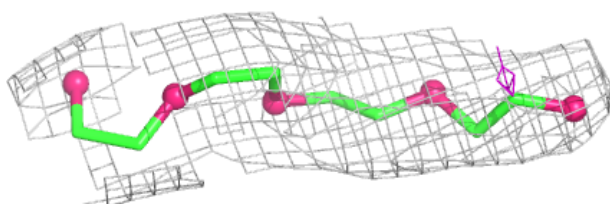
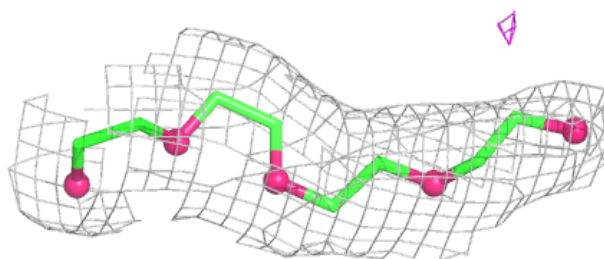
**Electron density around GOL B 106:**

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

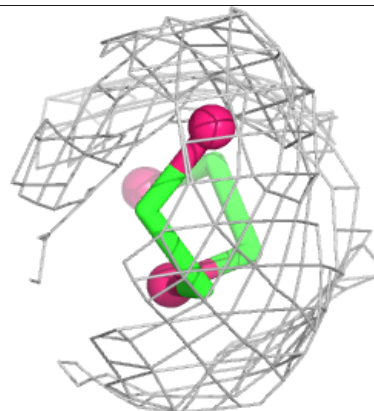
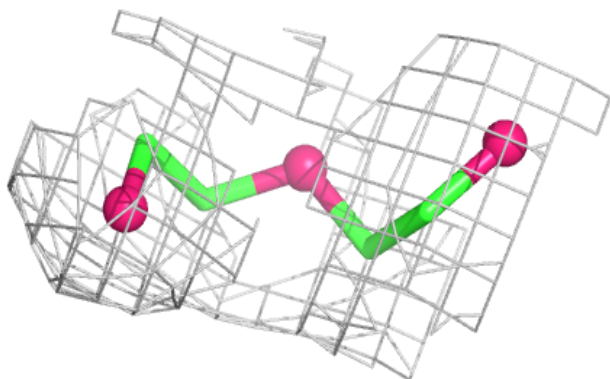
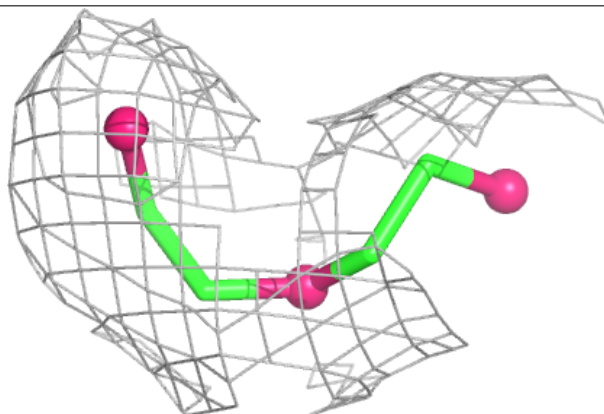


Electron density around PG4 A 365:

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

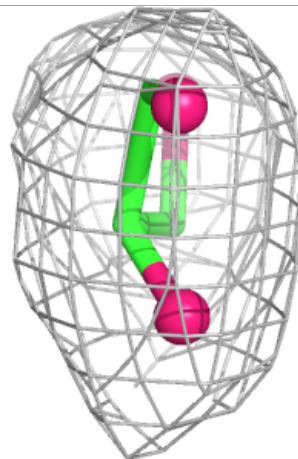
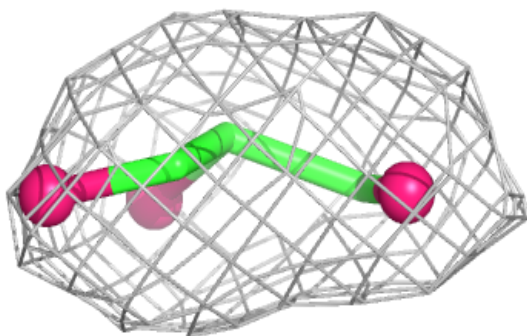
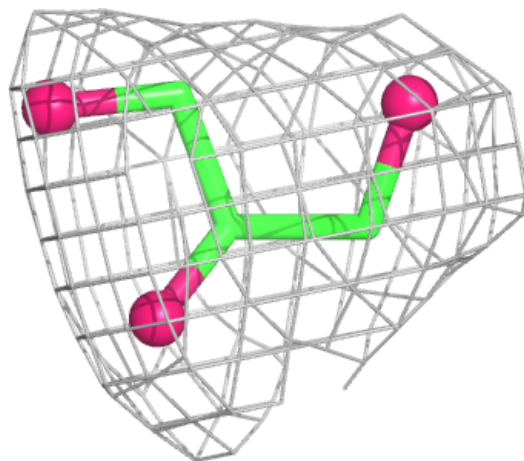
**Electron density around PEG B 127:**

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



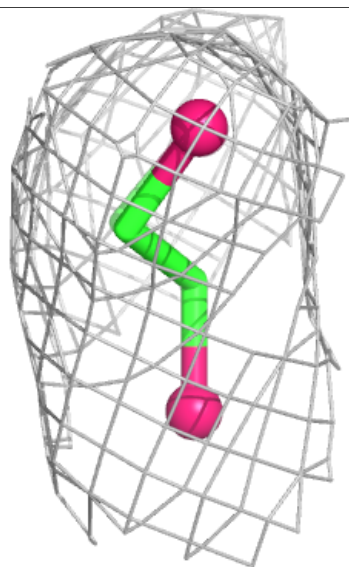
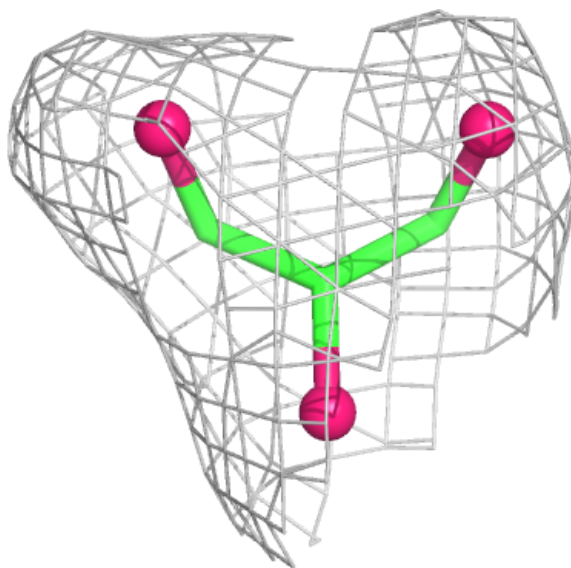
Electron density around GOL A 312:

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



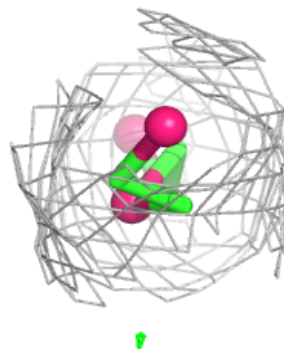
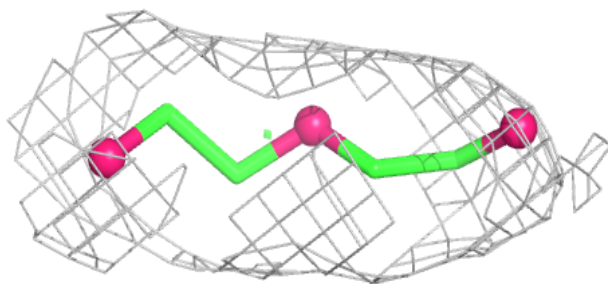
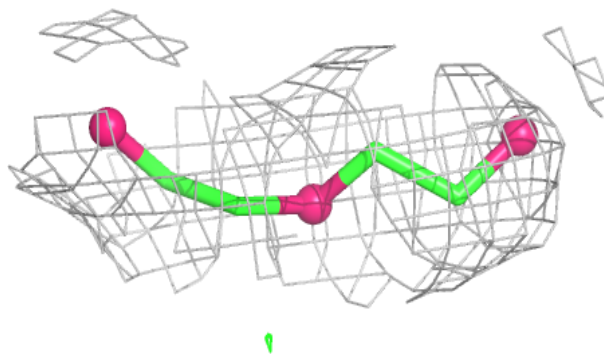
Electron density around GOL A 311:

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

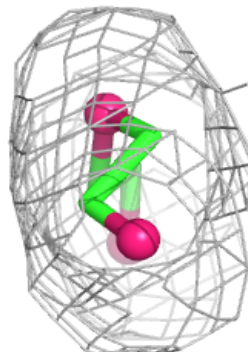
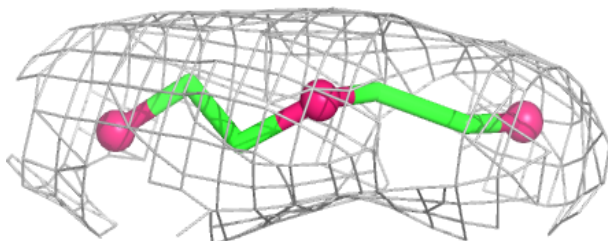
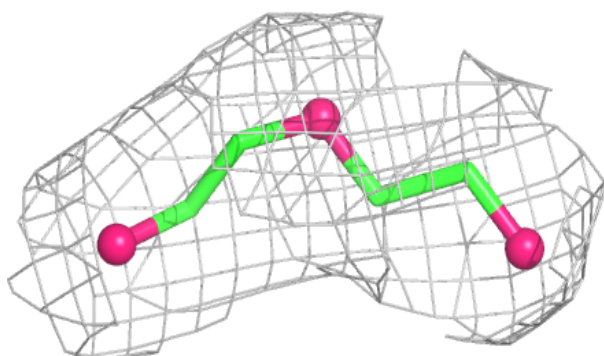


Electron density around PEG A 340:

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

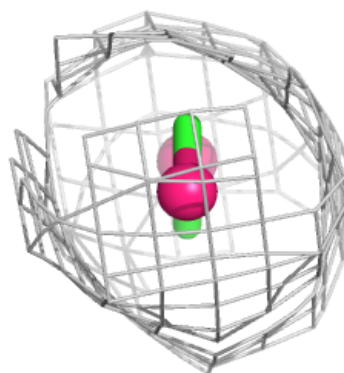
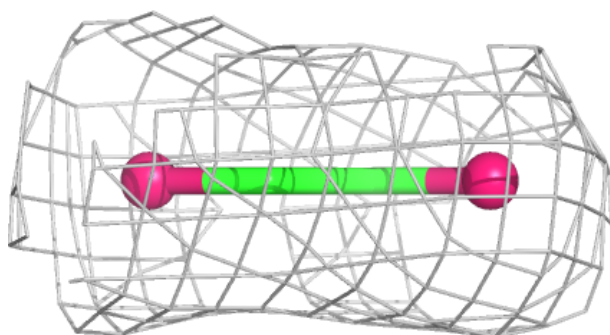
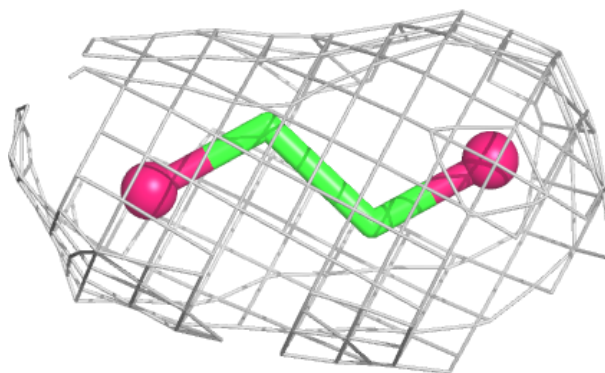
**Electron density around PEG B 131:**

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

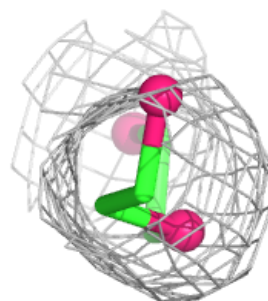
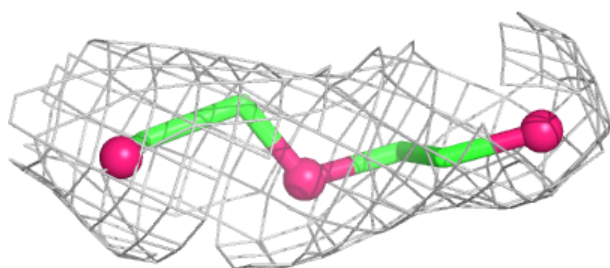
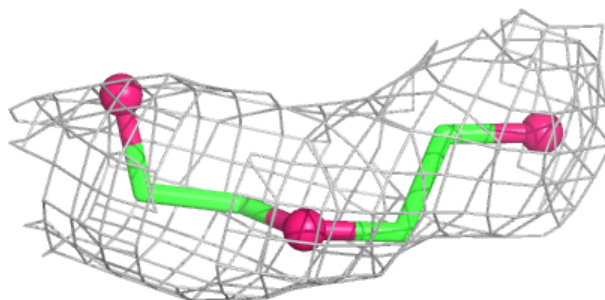


Electron density around EDO E 101:

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

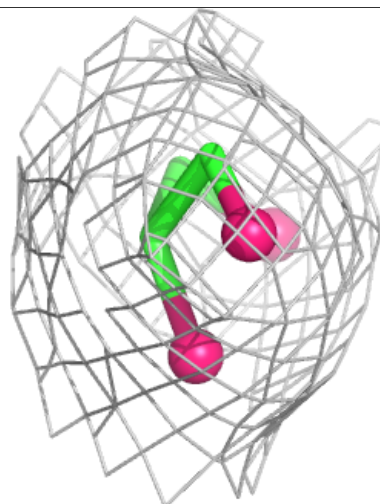
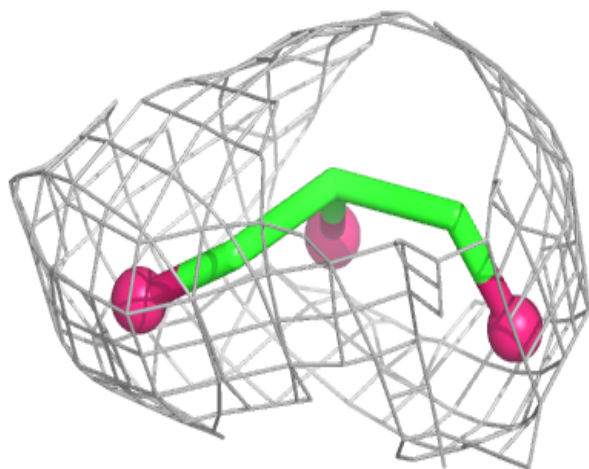
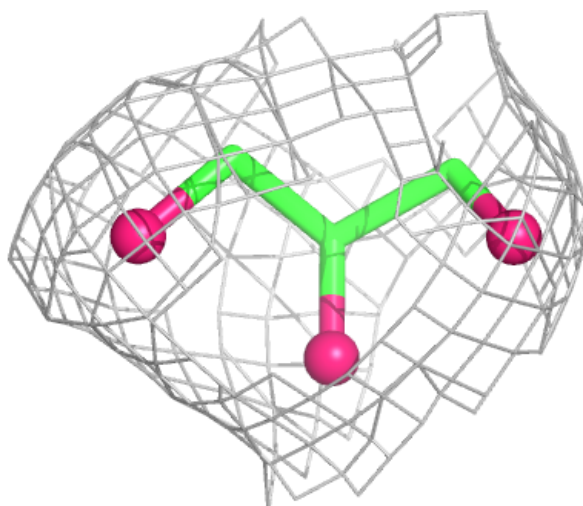
**Electron density around PEG D 122:**

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



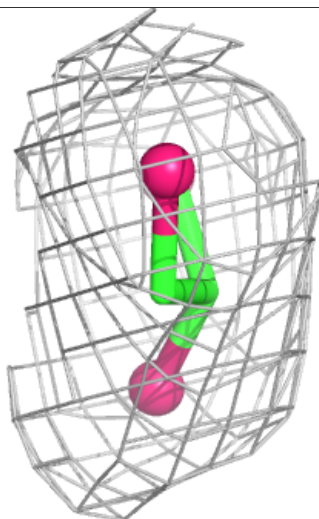
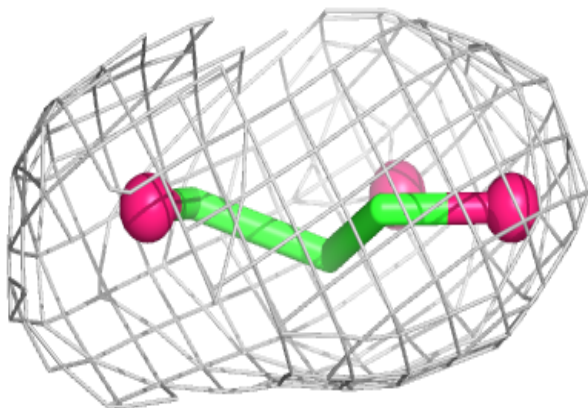
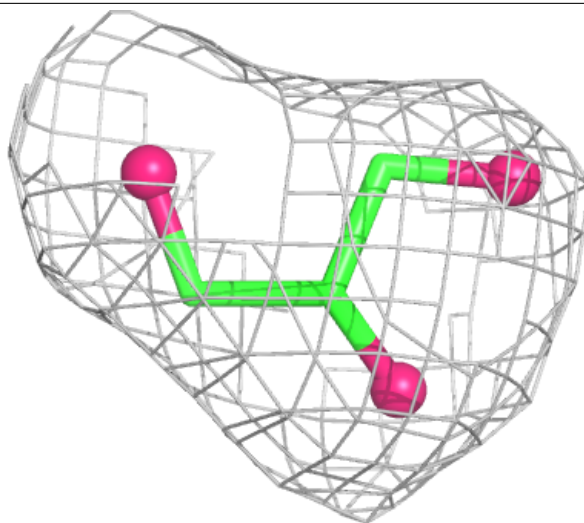
Electron density around GOL E 102:

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



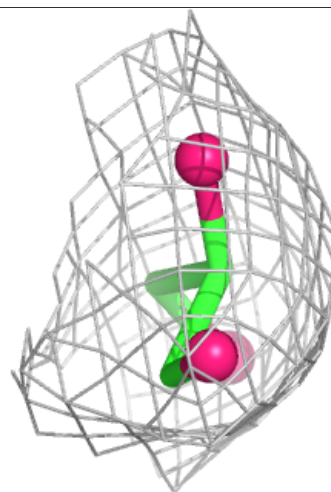
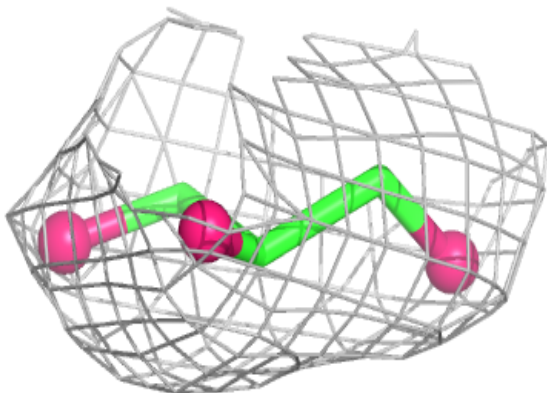
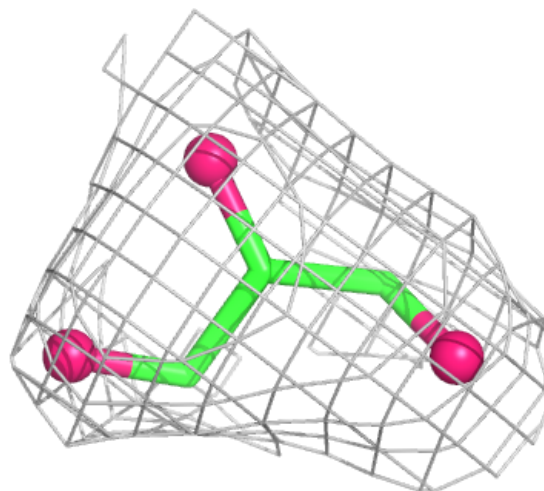
Electron density around GOL D 106:

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



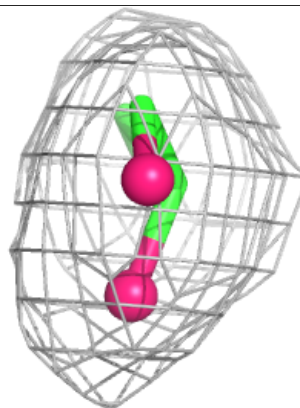
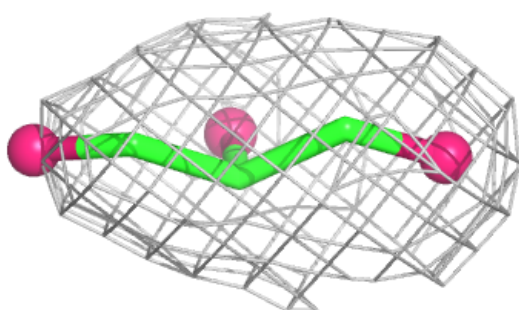
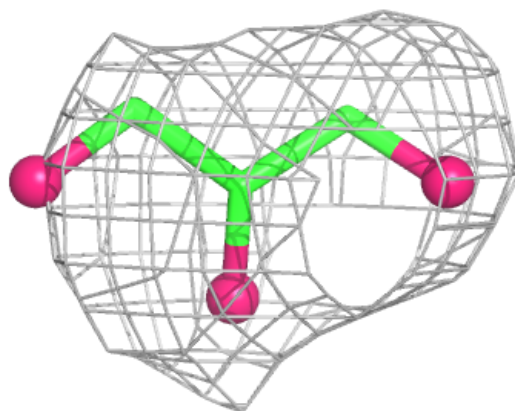
Electron density around GOL C 345:

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

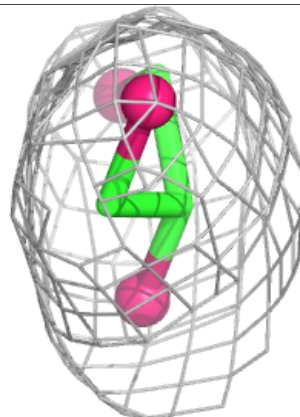
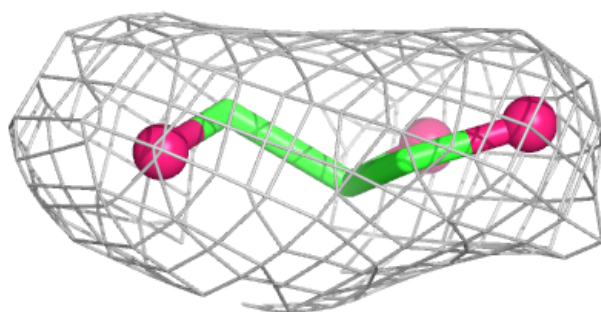
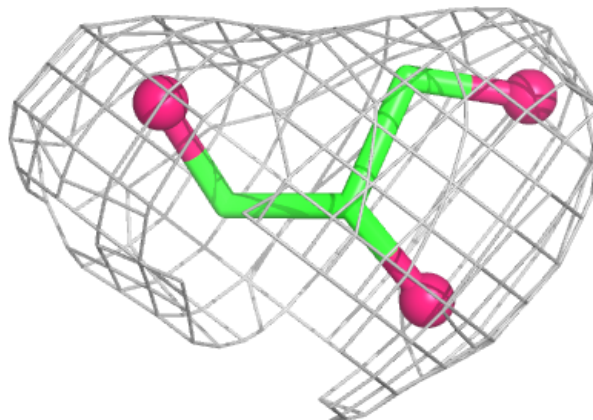


Electron density around GOL D 108:

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

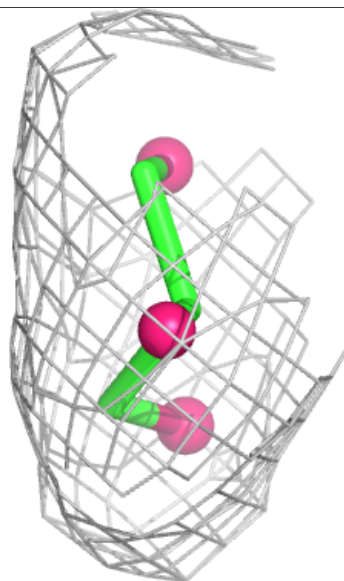
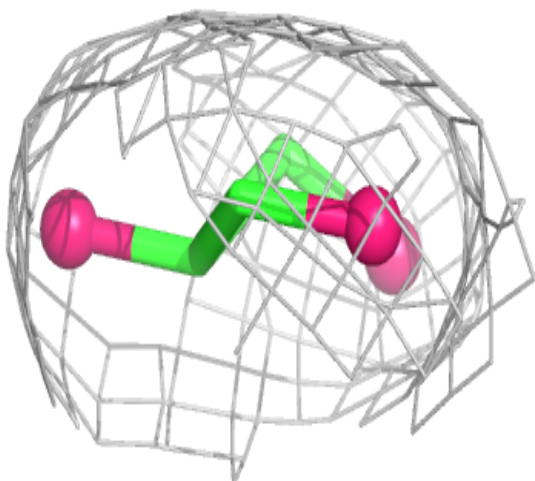
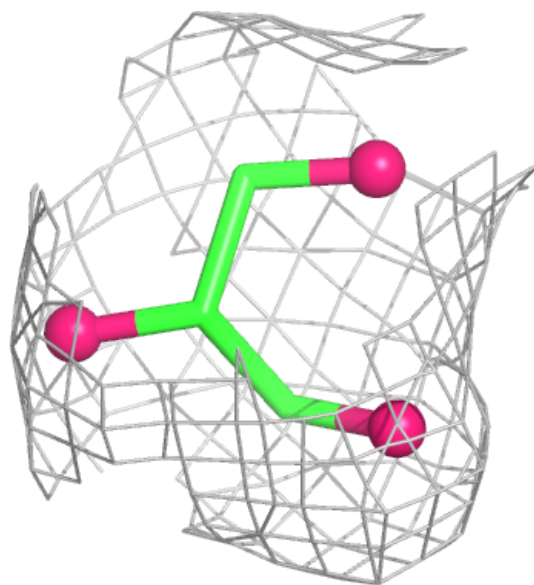
**Electron density around GOL A 373:**

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



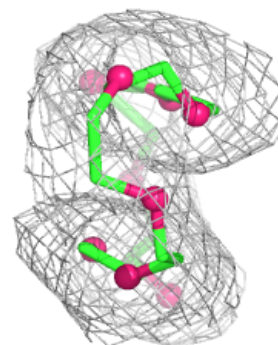
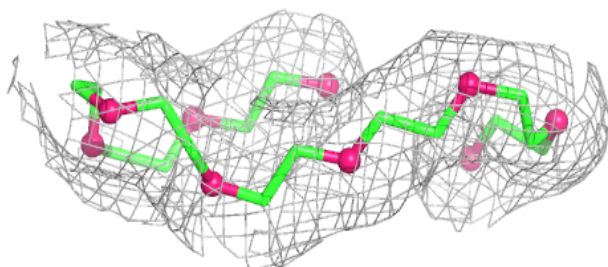
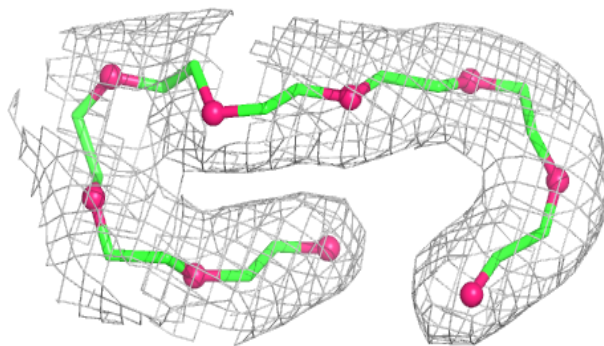
Electron density around GOL D 137:

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

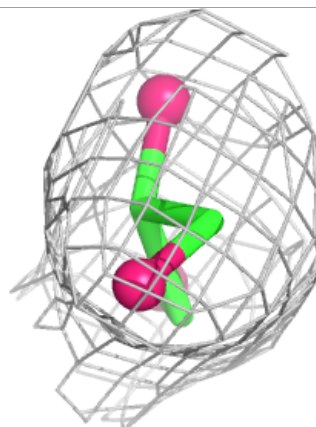
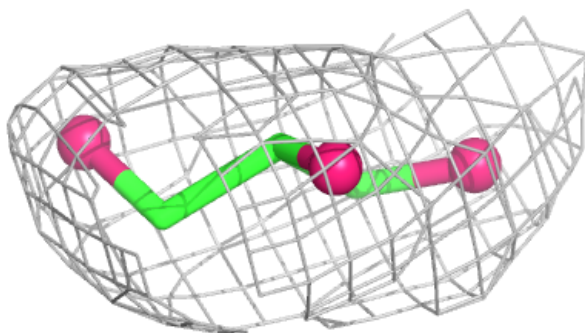
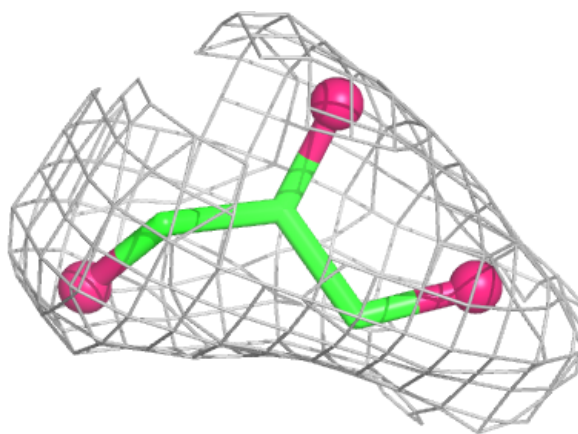


Electron density around PE8 E 109:

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

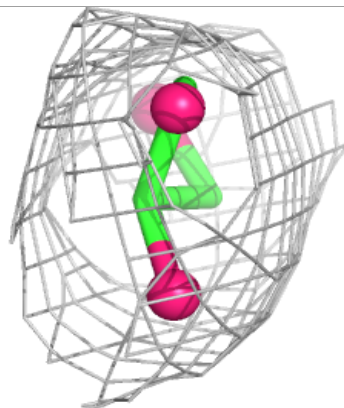
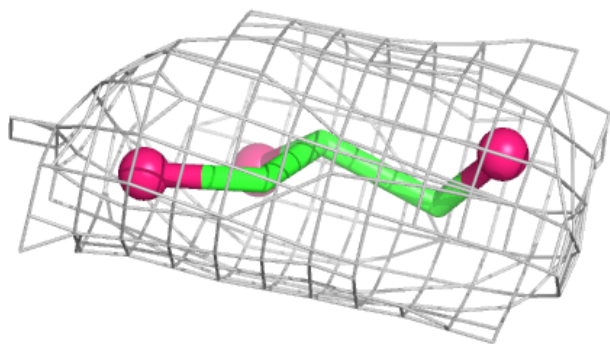
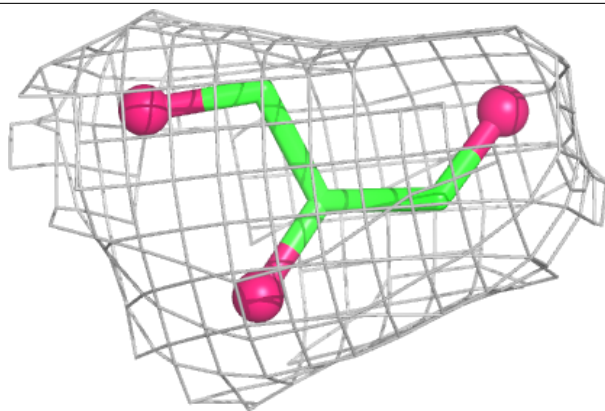
**Electron density around GOL A 364:**

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



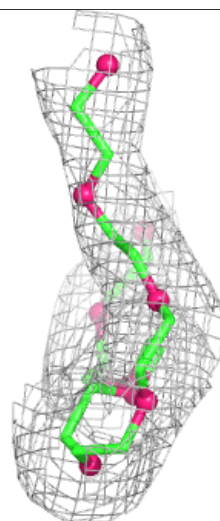
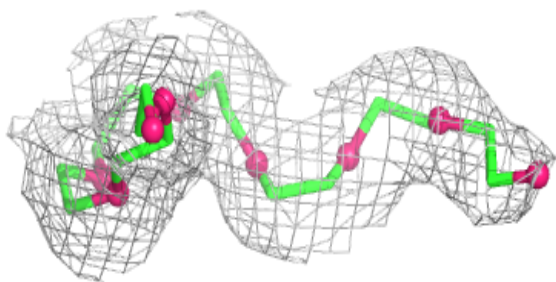
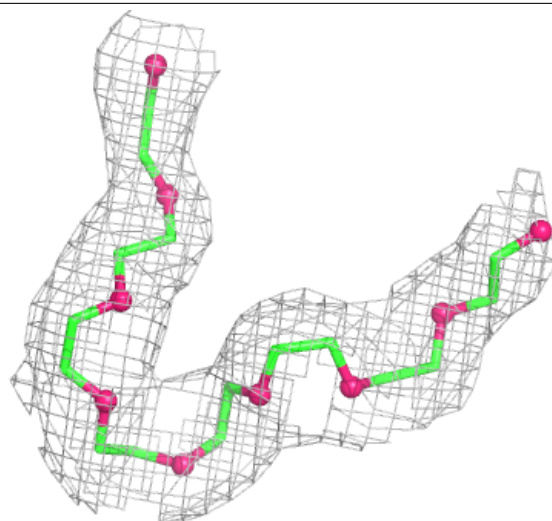
Electron density around GOL A 304:

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



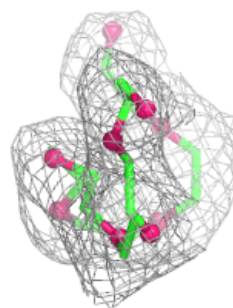
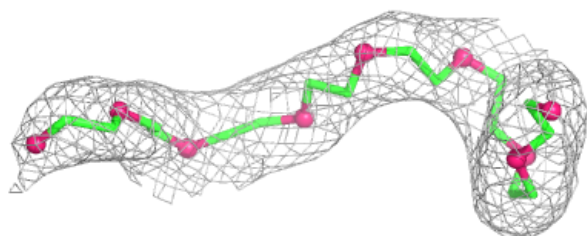
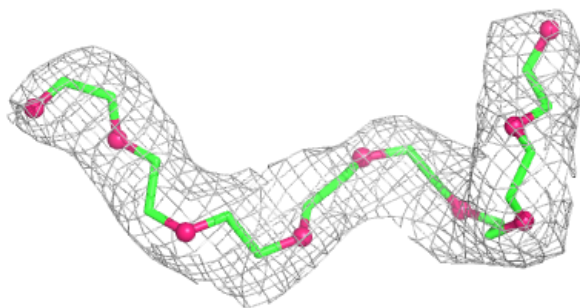
Electron density around PE8 B 137:

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

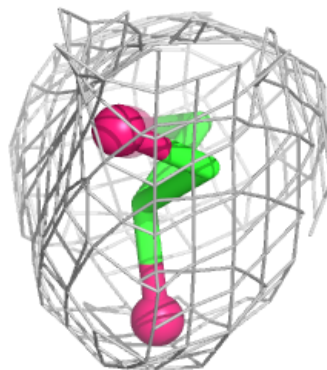
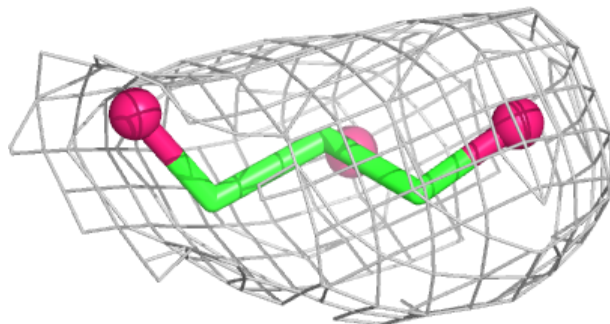
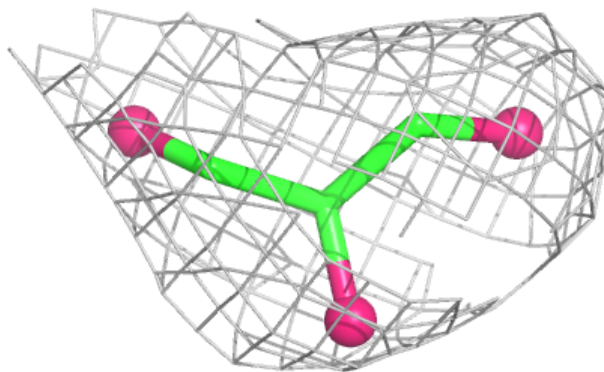


Electron density around PE8 B 138:

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

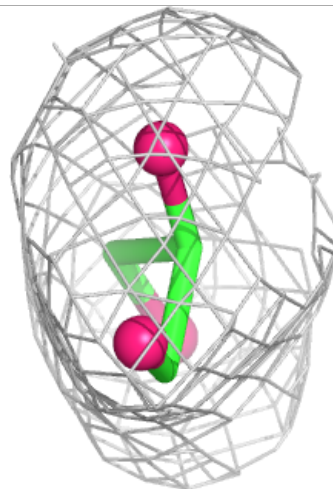
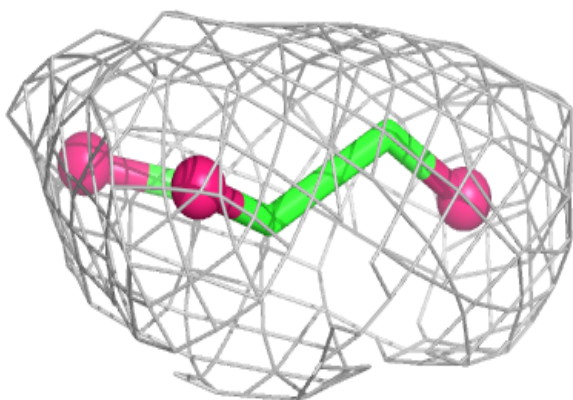
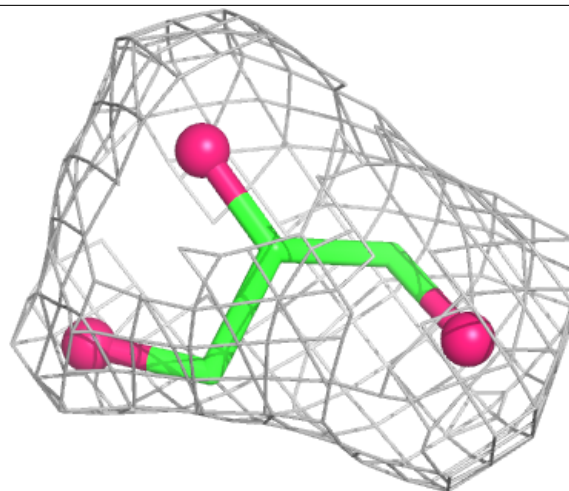
**Electron density around GOL B 112:**

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



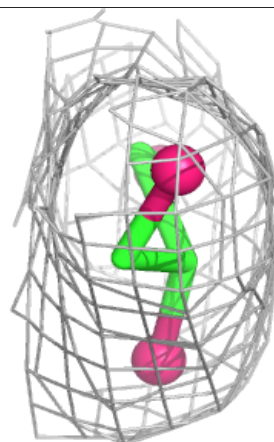
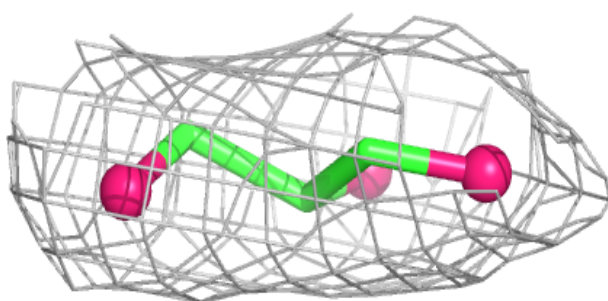
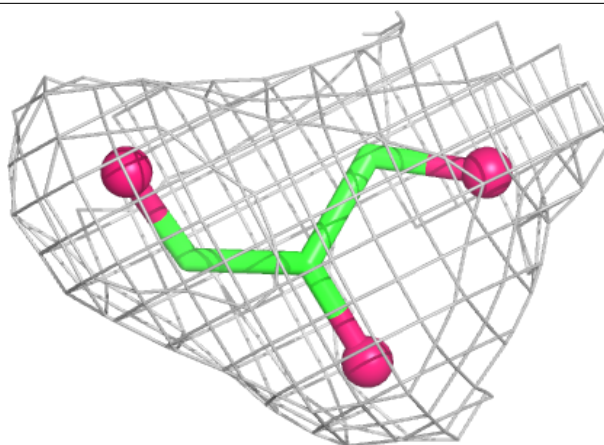
Electron density around GOL A 309:

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

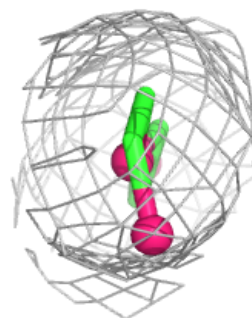
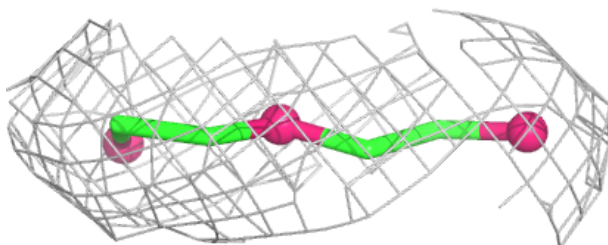
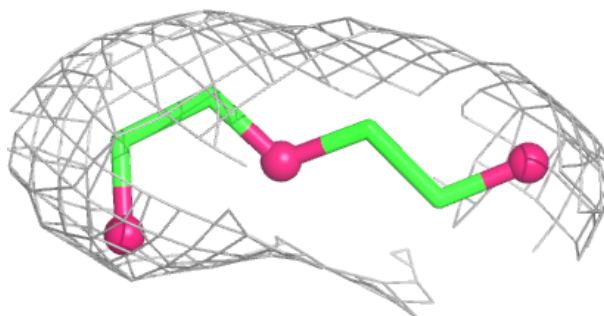


Electron density around GOL A 313:

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

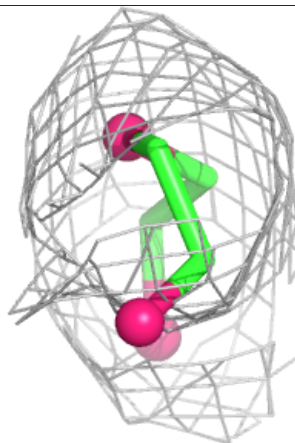
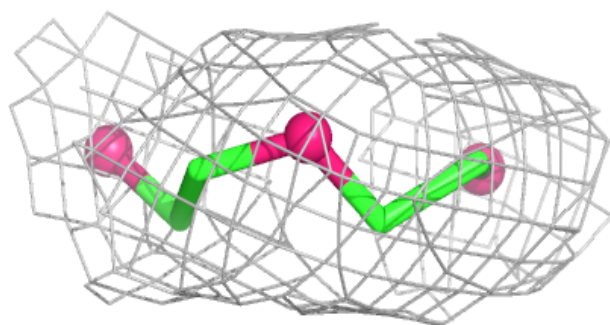
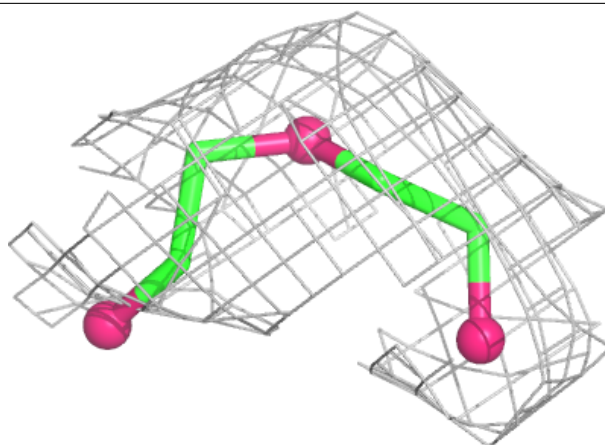
**Electron density around PEG B 126:**

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



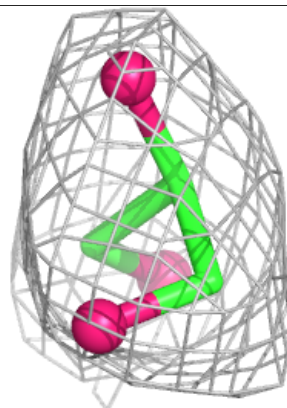
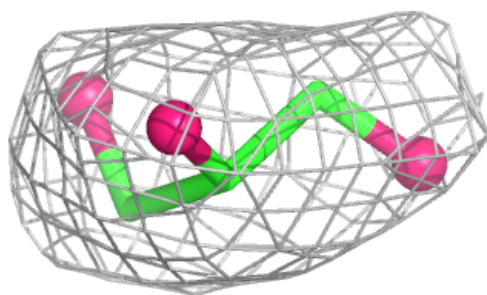
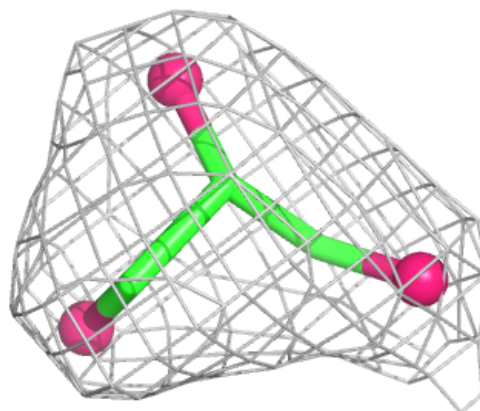
Electron density around PEG A 346:

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



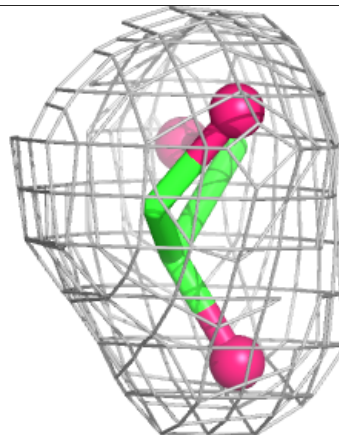
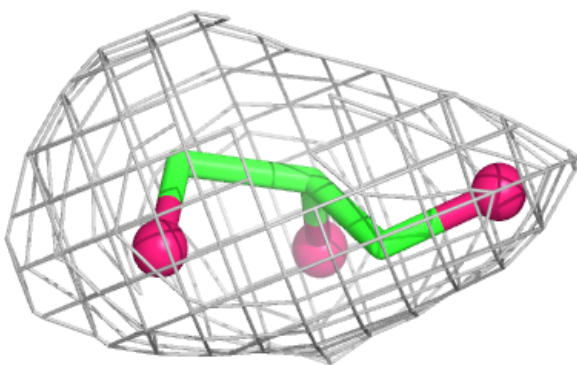
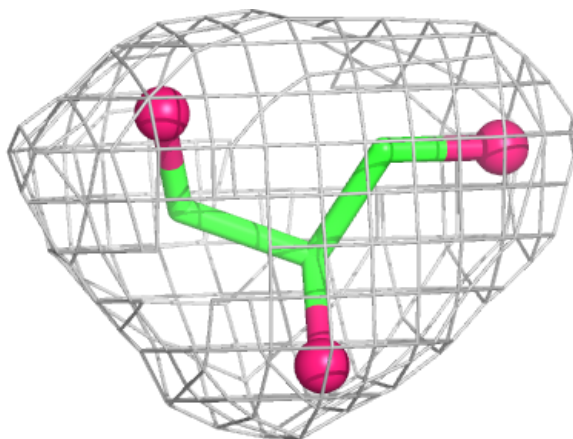
Electron density around GOL D 111:

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



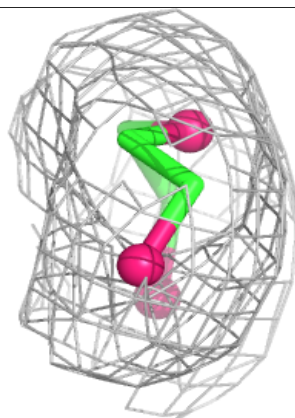
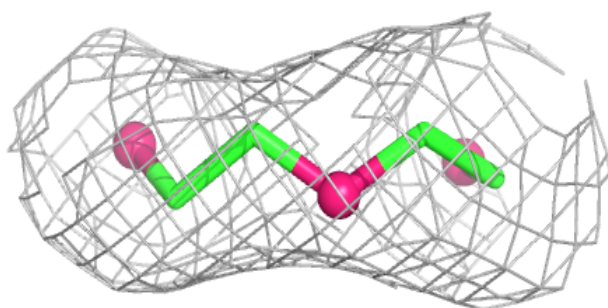
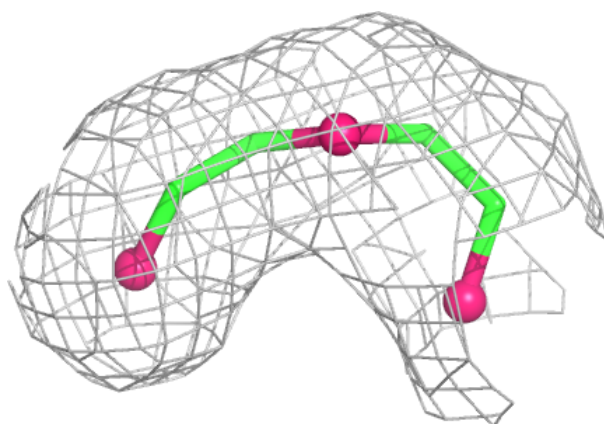
Electron density around GOL C 308:

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

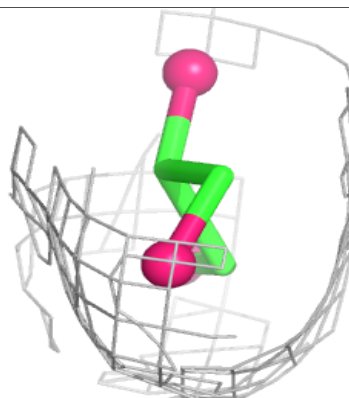
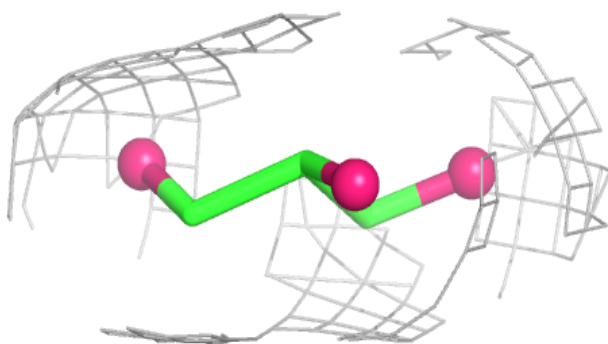


Electron density around PEG B 158:

$2mF_o-DF_c$ (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.