



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:55 PM UTC

PDB ID : 8GT0 / pdb_00008gt0
Title : Structure of falcipain and human Stefin A 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

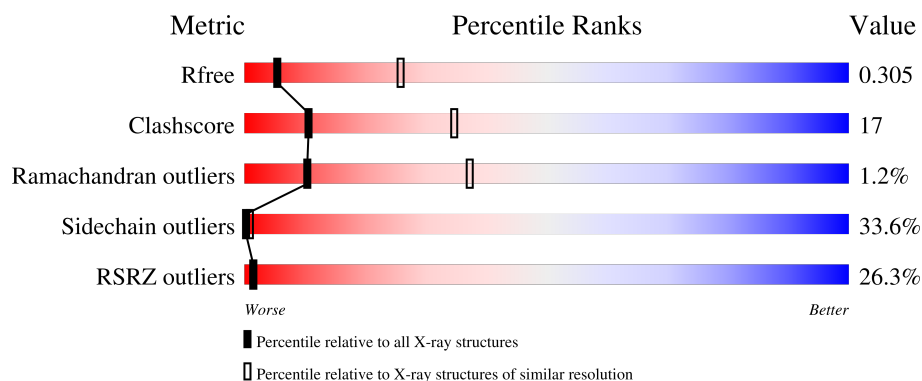
1 Overall quality at a glance

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	
1	C	241	
1	E	241	
2	B	98	
2	D	98	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7032 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.

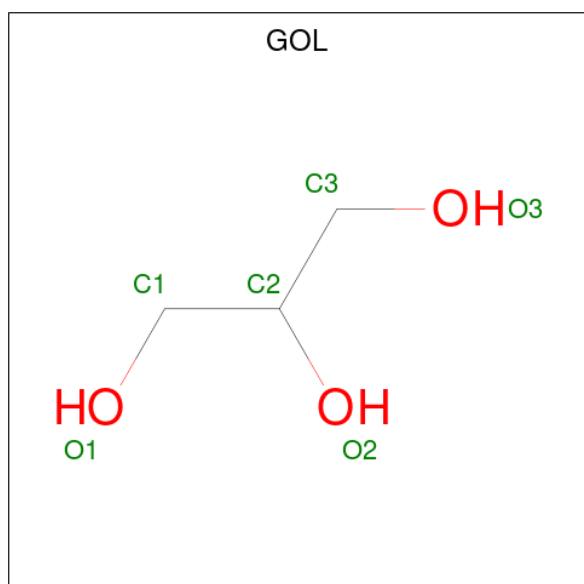
- Molecule 1 is a protein called Cysteine protease falcipain-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1909	1210	314	371	14			
1	C	241	Total	C	N	O	S	0	0	0
			1909	1210	314	371	14			
1	E	18	Total	C	N	O	S	0	0	0
			135	89	22	22	2			

- 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
			775	492	126	155	2			
2	D	98	Total	C	N	O	S	0	0	0
			775	492	126	155	2			

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



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

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

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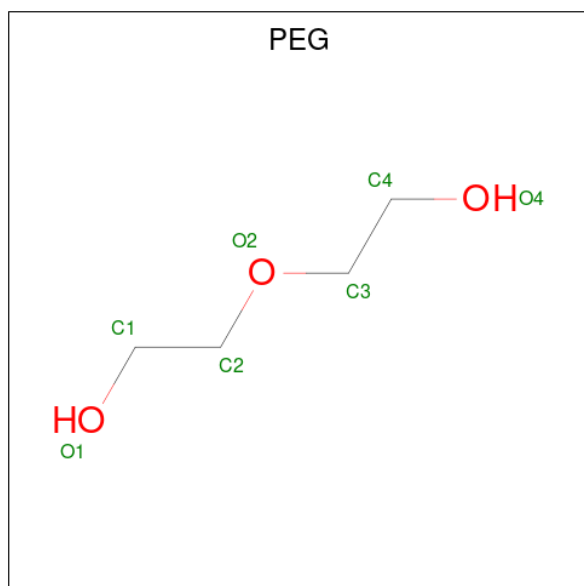
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Na	0	0
			4	4		
4	B	6	Total	Na	0	0
			6	6		
4	C	5	Total	Na	0	0
			5	5		
4	D	8	Total	Na	0	0
			8	8		
4	E	2	Total	Na	0	0
			2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃) (labeled as "Ligand of Interest" by depositor).



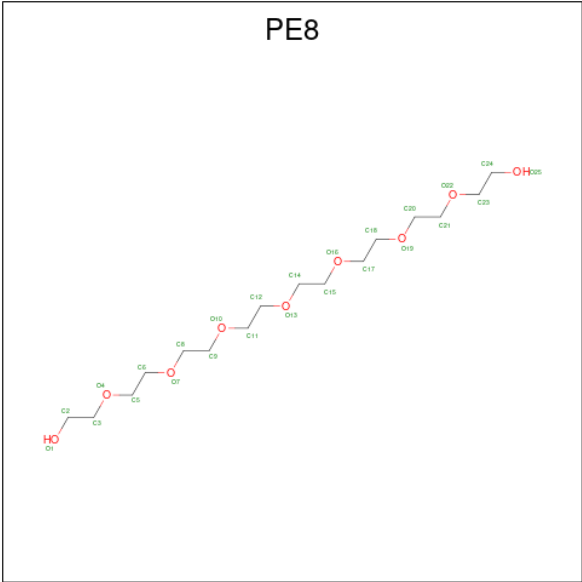
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

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

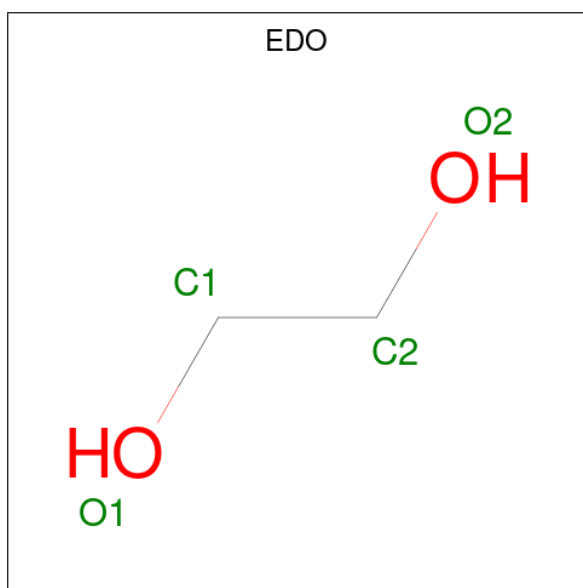
- Molecule 6 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: C₁₆H₃₄O₉) (labeled as "Ligand of Interest" by depositor).



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

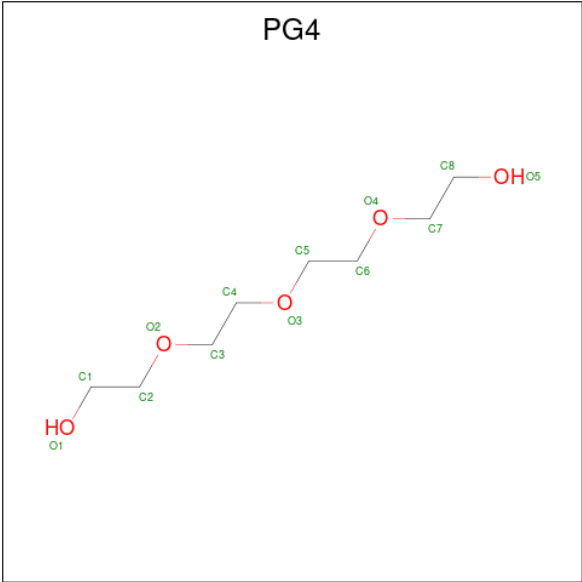
- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂) (labeled as "Ligand

of Interest" by depositor).



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

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅) (labeled as "Ligand of Interest" by depositor).



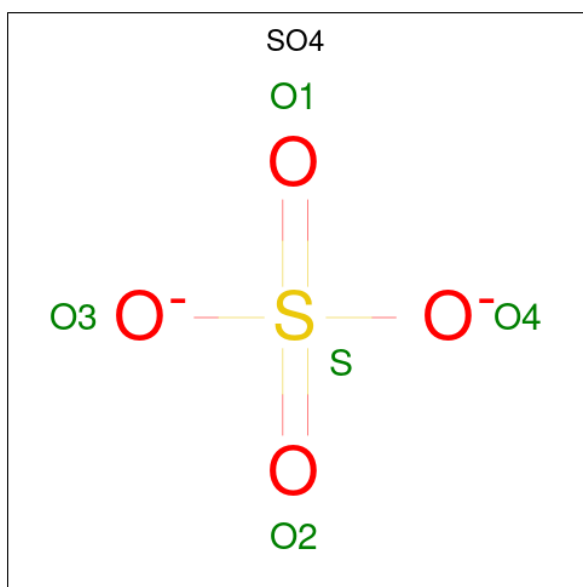
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			13	8	5		
8	A	1	Total	C	O	0	0
			13	8	5		
8	A	1	Total	C	O	0	0
			13	8	5		
8	A	1	Total	C	O	0	0
			13	8	5		
8	A	1	Total	C	O	0	0
			13	8	5		
8	A	1	Total	C	O	0	0
			13	8	5		
8	B	1	Total	C	O	0	0
			13	8	5		
8	B	1	Total	C	O	0	0
			13	8	5		
8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

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

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total	Cl	0	0
			1	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	36	Total	O	0	0
			36	36		

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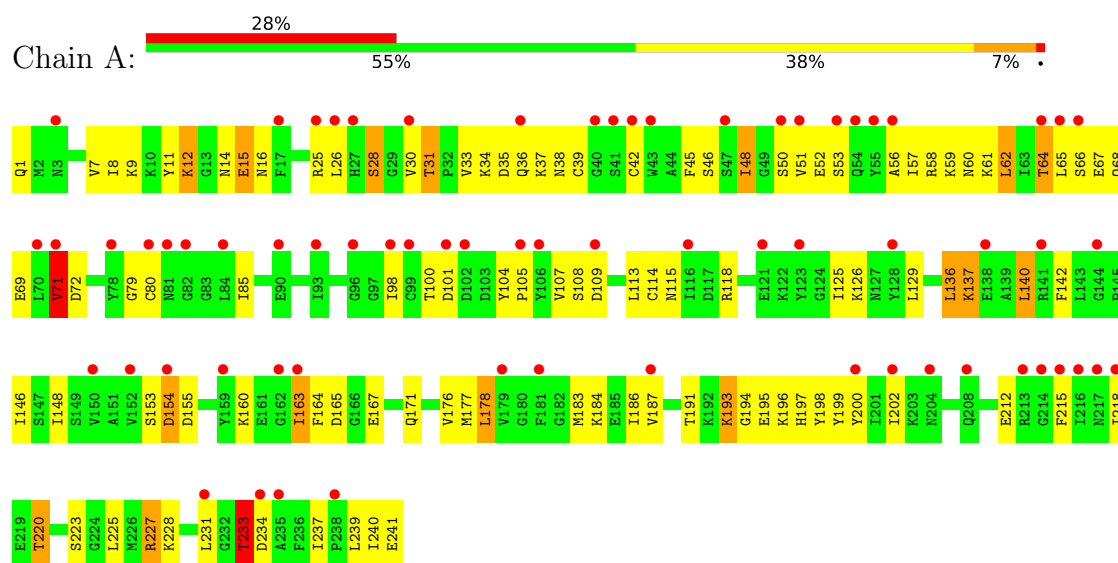
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	36	Total 36	O 36	0	0
11	C	35	Total 35	O 35	0	0
11	D	28	Total 28	O 28	0	0
11	E	9	Total 9	O 9	0	0

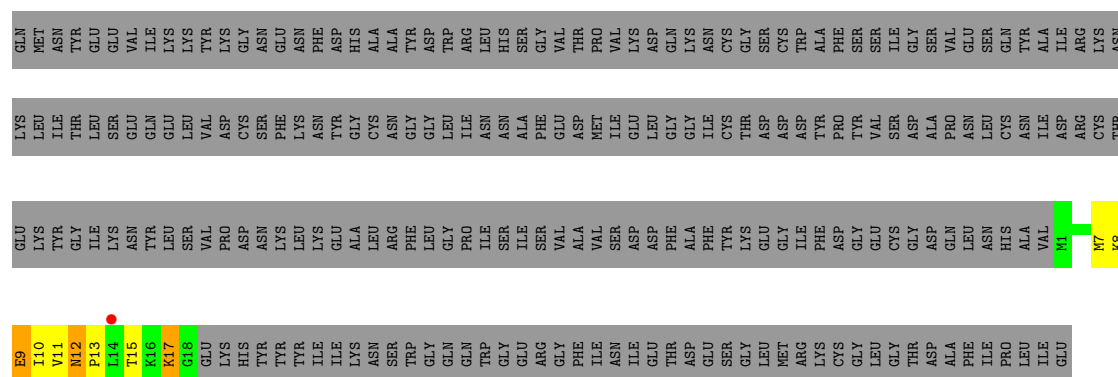
3 Residue-property plots [i](#)

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

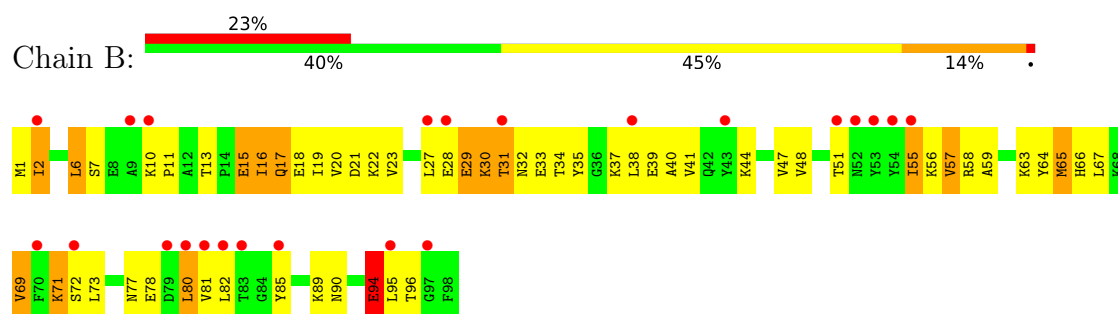
• Molecule 1: Cysteine protease falcipain-2



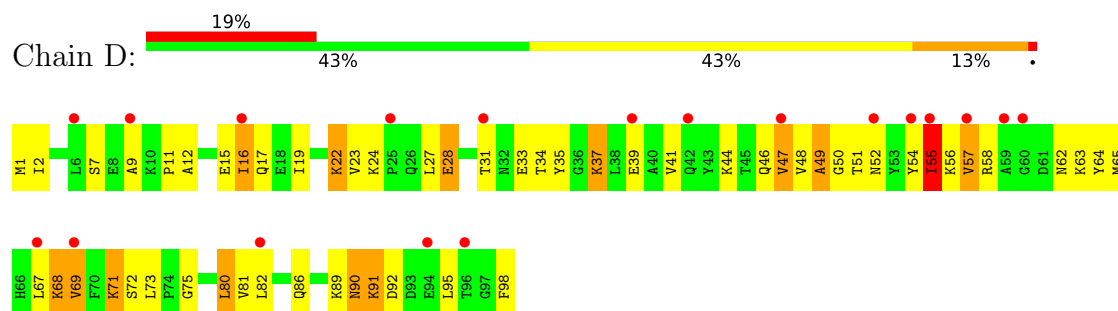
Chain E:  93%



• Molecule 2: Cystatin-A



• Molecule 2: Cystatin-A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.10Å 118.06Å 119.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.99 – 3.28 43.99 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.99-3.28) 99.8 (43.99-3.28)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.278 , 0.299 0.286 , 0.305	Depositor DCC
R_{free} test set	746 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 853.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.045 for -h,l,k	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	7032	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.23	0/1951	0.62	2/2630 (0.1%)
1	C	0.26	0/1951	0.67	0/2630
1	E	0.35	0/136	0.96	0/179
2	B	0.24	0/788	0.69	0/1062
2	D	0.26	0/788	0.64	0/1062
All	All	0.25	0/5614	0.66	2/7563 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	VAL	N-CA-C	-6.60	107.44	113.71
1	A	79	GLY	N-CA-C	5.36	117.82	110.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1909	0	1830	50	0
1	C	1909	0	1830	77	0
1	E	135	0	154	8	0
2	B	775	0	780	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	775	0	780	41	0
3	A	102	0	136	2	0
3	B	126	0	168	2	0
3	C	90	0	120	3	0
3	D	48	0	64	3	0
3	E	18	0	24	1	0
4	A	4	0	0	0	0
4	B	6	0	0	0	0
4	C	5	0	0	0	0
4	D	8	0	0	0	0
4	E	2	0	0	0	0
5	A	49	0	70	3	0
5	B	14	0	20	0	0
5	C	63	0	90	0	0
5	D	14	0	20	2	0
5	E	28	0	40	1	0
6	A	75	0	102	5	0
6	B	125	0	170	7	0
6	C	50	0	68	4	0
6	E	75	0	102	5	0
7	A	20	0	30	0	0
7	B	8	0	12	0	0
7	C	16	0	24	0	0
8	A	130	0	180	8	0
8	B	78	0	108	4	0
8	C	78	0	108	8	0
8	D	104	0	144	3	0
8	E	13	0	18	0	0
9	B	5	0	0	0	0
9	C	5	0	0	0	0
9	D	20	0	0	0	0
9	E	5	0	0	0	0
10	D	1	0	0	0	0
11	A	36	0	0	0	0
11	B	36	0	0	0	0
11	C	35	0	0	1	0
11	D	28	0	0	0	0
11	E	9	0	0	0	0
All	All	7032	0	7192	236	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (236) 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)
2:B:35:TYR:HB3	2:B:38:LEU:HD21	1.59	0.85
8:A:330:PG4:H31	1:C:111:PRO:HG3	1.65	0.78
2:D:19:ILE:HG23	2:D:80:LEU:HD21	1.67	0.77
1:C:45:PHE:HA	1:C:67:GLU:HG2	1.67	0.75
1:C:128:TYR:OH	11:C:401:HOH:O	2.03	0.75
2:D:54:TYR:HB2	2:D:67:LEU:O	1.89	0.72
2:B:71:LYS:HG2	2:B:80:LEU:HB2	1.73	0.70
8:C:337:PG4:H62	3:C:342:GOL:H2	1.72	0.70
1:A:65:LEU:HD23	1:A:98:ILE:HB	1.73	0.70
1:A:39:CYS:H	2:B:48:VAL:HG11	1.55	0.70
3:B:116:GOL:H32	8:B:125:PG4:H41	1.75	0.69
6:A:322:PE8:H122	6:A:322:PE8:H242	1.74	0.69
2:D:19:ILE:HG12	2:D:80:LEU:HD11	1.76	0.68
1:C:31:THR:HG22	1:C:203:LYS:HE3	1.76	0.68
1:C:148:ILE:HG13	1:C:176:VAL:HG23	1.78	0.66
1:C:52:GLU:HG2	1:C:65:LEU:H	1.60	0.65
1:A:11:TYR:HB3	1:A:142:PHE:HB3	1.80	0.64
1:E:11:VAL:HG21	3:E:104:GOL:H2	1.78	0.63
1:A:12:LYS:HG2	1:A:15:GLU:HB3	1.79	0.63
1:A:72:ASP:HB2	1:A:114:CYS:HB2	1.80	0.62
2:B:28:GLU:HA	2:B:32:ASN:HB2	1.81	0.62
2:D:75:GLY:HA3	3:D:124:GOL:H2	1.81	0.62
1:A:186:ILE:HG13	1:A:187:VAL:H	1.67	0.60
1:C:9:LYS:HD2	1:C:10:LYS:HG3	1.83	0.60
1:C:25:ARG:HB3	1:C:30:VAL:HB	1.83	0.59
1:C:159:TYR:HE1	2:D:73:LEU:HB3	1.67	0.59
1:C:186:ILE:HG23	1:C:187:VAL:H	1.67	0.59
1:C:92:MET:HB2	1:C:98:ILE:HD11	1.86	0.57
2:B:58:ARG:HA	2:B:64:TYR:HA	1.86	0.57
2:D:7:SER:O	2:D:44:LYS:HD3	2.05	0.57
1:A:218:ILE:HB	1:A:231:LEU:HD11	1.85	0.57
2:B:40:ALA:HA	2:B:57:VAL:HA	1.88	0.56
2:D:57:VAL:O	2:D:65:MET:N	2.39	0.56
6:E:113:PE8:H121	6:E:113:PE8:H51	1.88	0.56
1:C:199:TYR:HB2	1:C:217:ASN:HB3	1.88	0.56
2:B:56:LYS:HE2	2:B:94:GLU:HG2	1.88	0.55
1:A:64:THR:HG22	1:A:101:ASP:HB2	1.87	0.55
2:D:58:ARG:HA	2:D:64:TYR:HA	1.87	0.55
1:A:36:GLN:HB3	1:A:45:PHE:CE1	2.42	0.55
2:D:27:LEU:HD11	2:D:67:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:MET:HA	2:B:89:LYS:HB2	1.88	0.54
1:C:216:ILE:HD13	1:C:218:ILE:HG12	1.90	0.54
2:B:16:ILE:HG21	6:B:123:PE8:H172	1.88	0.54
1:C:52:GLU:CG	1:C:65:LEU:H	2.20	0.54
6:A:322:PE8:H61	5:A:335:PEG:H12	1.90	0.54
2:D:86:GLN:HB2	2:D:98:PHE:CZ	2.43	0.53
1:A:45:PHE:O	1:A:48:ILE:HG13	2.08	0.53
1:C:84:LEU:O	1:C:88:ALA:HB2	2.09	0.53
1:A:163:ILE:HG23	1:A:199:TYR:HB3	1.89	0.53
1:C:136:LEU:HA	1:C:139:ALA:HB2	1.91	0.53
1:C:48:ILE:O	1:C:52:GLU:HG3	2.09	0.53
1:A:37:LYS:HB2	1:A:108:SER:OG	2.08	0.53
1:C:43:TRP:H	1:C:43:TRP:CD1	2.25	0.53
1:A:187:VAL:HA	1:A:193:LYS:O	2.10	0.52
1:C:69:GLU:HB3	1:C:98:ILE:HG22	1.90	0.52
2:D:12:ALA:HA	2:D:16:ILE:HD11	1.91	0.52
2:D:52:ASN:HB3	2:D:68:LYS:HE2	1.92	0.52
2:B:69:VAL:HB	2:B:80:LEU:HD11	1.91	0.52
2:B:27:LEU:HD22	2:B:31:THR:HB	1.91	0.52
2:D:22:LYS:HB3	2:D:80:LEU:HD22	1.92	0.52
1:A:148:ILE:HG13	1:A:176:VAL:HG23	1.92	0.52
1:E:12:ASN:HB3	5:E:109:PEG:H22	1.90	0.52
1:A:26:LEU:HG	1:C:73:CYS:SG	2.50	0.52
6:B:105:PE8:H92	8:B:126:PG4:H11	1.93	0.51
1:C:164:PHE:HB2	1:C:216:ILE:HD11	1.92	0.51
1:A:136:LEU:O	1:A:140:LEU:HB2	2.10	0.51
1:C:188:ASN:HB3	1:C:195:GLU:HB2	1.93	0.51
2:B:57:VAL:HG23	2:B:65:MET:HG3	1.92	0.51
2:B:66:HIS:HB2	2:B:95:LEU:HD23	1.92	0.51
1:A:38:ASN:O	1:A:109:ASP:HB3	2.10	0.51
8:A:328:PG4:H41	8:A:330:PG4:H52	1.93	0.51
1:C:53:SER:HB3	1:C:145:PRO:HG3	1.93	0.50
2:D:27:LEU:HB3	2:D:35:TYR:HD2	1.76	0.50
6:C:321:PE8:H91	8:C:337:PG4:H22	1.94	0.50
8:A:329:PG4:O5	8:A:337:PG4:H81	2.11	0.50
1:C:149:SER:HA	1:C:175:ALA:HA	1.93	0.50
1:C:157:ALA:HB1	2:D:73:LEU:HD23	1.94	0.50
1:C:159:TYR:CE1	2:D:73:LEU:HB3	2.46	0.50
2:D:31:THR:HG22	2:D:33:GLU:H	1.77	0.49
1:A:71:VAL:HG13	1:A:80:CYS:HB2	1.93	0.49
2:D:54:TYR:O	2:D:55:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:LYS:HE3	2:B:78:GLU:HG2	1.93	0.49
1:C:44:ALA:O	1:C:48:ILE:HG12	2.13	0.49
2:B:64:TYR:HB2	2:B:90:ASN:HA	1.95	0.49
1:C:34:LYS:HB3	1:C:45:PHE:HE2	1.77	0.49
2:D:69:VAL:HG21	2:D:80:LEU:HD23	1.93	0.49
1:C:64:THR:O	1:C:101:ASP:HB3	2.13	0.49
1:C:68:GLN:HB2	1:C:106:TYR:CD1	2.48	0.49
1:A:39:CYS:N	2:B:48:VAL:HG11	2.24	0.49
1:C:24:TRP:HD1	1:C:180:GLY:HA2	1.77	0.48
3:C:303:GOL:H2	8:C:332:PG4:H61	1.95	0.48
1:C:94:GLU:O	8:C:324:PG4:H62	2.13	0.48
2:D:68:LYS:HB2	2:D:98:PHE:CE1	2.48	0.48
1:E:17:LYS:HZ2	1:E:17:LYS:HA	1.78	0.48
6:A:322:PE8:H22	6:A:322:PE8:H52	1.66	0.48
1:E:8:LYS:HD2	1:E:8:LYS:HA	1.62	0.48
1:C:10:LYS:HE3	1:C:10:LYS:HB2	1.53	0.47
1:A:48:ILE:HG21	1:A:66:SER:O	2.14	0.47
1:C:163:ILE:HD11	1:C:199:TYR:HB3	1.95	0.47
1:A:183:MET:HA	1:A:198:TYR:HA	1.97	0.47
2:B:58:ARG:HG2	2:B:64:TYR:CE2	2.49	0.47
1:C:50:SER:HB3	1:C:238:PRO:HG2	1.96	0.47
1:C:63:ILE:HG12	1:C:123:TYR:HD2	1.79	0.47
1:A:56:ALA:O	1:A:60:ASN:HA	2.15	0.47
3:A:345:GOL:H2	8:B:129:PG4:H61	1.96	0.47
1:A:186:ILE:HG13	1:A:187:VAL:N	2.30	0.47
1:C:156:PHE:HE1	1:C:216:ILE:HD12	1.79	0.47
5:D:115:PEG:H11	5:D:115:PEG:H32	1.64	0.47
8:A:344:PG4:H82	3:A:346:GOL:H11	1.97	0.47
1:C:221:ASP:OD1	1:C:221:ASP:N	2.48	0.46
8:A:330:PG4:H82	8:A:330:PG4:H62	1.44	0.46
1:A:183:MET:HE3	1:A:183:MET:HB3	1.86	0.46
1:C:51:VAL:HA	1:C:54:GLN:HG2	1.97	0.46
1:A:115:ASN:HB3	1:A:118:ARG:HG3	1.96	0.46
2:B:21:ASP:HB3	2:B:37:LYS:HG2	1.97	0.46
6:B:131:PE8:H31	6:B:131:PE8:H61	1.58	0.46
1:C:34:LYS:HD2	1:C:34:LYS:HA	1.60	0.46
1:C:135:LYS:HD3	1:C:138:GLU:HB2	1.96	0.46
6:E:114:PE8:H51	6:E:114:PE8:H21	1.46	0.46
1:C:186:ILE:O	1:C:187:VAL:HG13	2.15	0.46
2:D:48:VAL:HG12	2:D:49:ALA:N	2.31	0.46
2:D:67:LEU:HD23	2:D:67:LEU:HA	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:CYS:SG	1:C:109:ASP:HB2	2.56	0.45
1:E:11:VAL:HG23	1:E:13:PRO:HD2	1.97	0.45
2:B:21:ASP:HB3	2:B:37:LYS:HZ2	1.80	0.45
6:A:324:PE8:H182	6:A:324:PE8:H212	1.29	0.45
2:D:48:VAL:O	2:D:50:GLY:N	2.48	0.45
5:D:123:PEG:H41	5:D:123:PEG:H21	1.69	0.45
1:A:164:PHE:HB3	1:A:218:ILE:HG23	1.99	0.45
1:C:48:ILE:HG12	1:C:48:ILE:H	1.57	0.45
1:A:61:LYS:HB3	1:A:61:LYS:HE2	1.42	0.45
1:A:53:SER:O	1:A:57:ILE:HG13	2.16	0.45
1:C:125:ILE:HD12	1:C:125:ILE:HA	1.86	0.45
6:A:322:PE8:H212	6:A:322:PE8:H182	1.62	0.45
1:A:62:LEU:HD22	8:A:330:PG4:H21	1.99	0.45
1:A:148:ILE:HD13	1:A:178:LEU:HG	1.98	0.45
2:B:2:ILE:HD11	2:B:6:LEU:HG	1.98	0.45
1:C:171:GLN:HG2	2:D:1:MET:SD	2.57	0.45
1:A:154:ASP:OD1	1:A:154:ASP:N	2.50	0.45
1:A:178:LEU:HD23	1:A:178:LEU:HA	1.73	0.45
2:D:37:LYS:HA	2:D:37:LYS:HD3	1.27	0.44
2:D:51:THR:O	2:D:71:LYS:HB2	2.16	0.44
1:C:193:LYS:HB3	1:C:193:LYS:HE3	1.62	0.44
1:A:212:GLU:HB2	1:A:215:PHE:O	2.18	0.44
5:A:320:PEG:H22	5:A:320:PEG:H41	1.77	0.44
2:D:64:TYR:CD2	2:D:91:LYS:HB2	2.52	0.44
1:E:9:GLU:O	1:E:10:ILE:HG13	2.17	0.44
1:C:48:ILE:HA	1:C:51:VAL:HG12	2.00	0.44
1:C:190:LEU:O	1:C:191:THR:HB	2.17	0.44
2:D:90:ASN:OD1	2:D:90:ASN:N	2.50	0.44
6:E:114:PE8:H212	6:E:114:PE8:H62	1.99	0.44
1:A:212:GLU:O	1:A:215:PHE:HD1	2.01	0.44
6:B:105:PE8:H82	6:B:105:PE8:H51	1.38	0.44
1:A:227:ARG:H	1:A:227:ARG:HG3	1.29	0.44
8:D:116:PG4:H31	8:D:118:PG4:H42	1.98	0.44
1:A:11:TYR:OH	1:A:58:ARG:NH2	2.51	0.43
8:C:326:PG4:H31	8:C:326:PG4:H51	1.36	0.43
1:A:8:ILE:HD12	1:A:8:ILE:HA	1.89	0.43
2:B:15:GLU:H	2:B:15:GLU:HG2	1.55	0.43
2:B:55:ILE:HD13	2:B:55:ILE:HA	1.68	0.43
1:C:69:GLU:HG2	1:C:104:TYR:CG	2.53	0.43
1:A:227:ARG:HB3	1:A:231:LEU:HB2	2.01	0.43
6:C:321:PE8:H32	3:C:342:GOL:H32	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:324:PG4:H41	8:C:324:PG4:H61	1.22	0.43
8:A:331:PG4:H31	8:A:331:PG4:H11	1.67	0.43
1:C:84:LEU:HD23	1:C:85:ILE:H	1.83	0.43
2:D:46:GLN:HG2	2:D:47:VAL:H	1.83	0.43
8:C:337:PG4:H62	8:C:337:PG4:H82	1.83	0.43
2:D:11:PRO:HB2	3:D:110:GOL:H32	2.00	0.43
2:D:56:LYS:HG2	2:D:65:MET:O	2.18	0.43
8:A:334:PG4:H32	8:A:334:PG4:H12	1.32	0.43
1:C:151:ALA:O	1:C:168:CYS:HB3	2.19	0.43
2:D:28:GLU:CD	2:D:34:THR:HG23	2.44	0.43
8:D:105:PG4:H12	8:D:105:PG4:H32	1.56	0.43
1:A:28:SER:HB2	1:C:115:ASN:HB2	2.00	0.43
1:C:9:LYS:HB3	1:C:9:LYS:HE3	1.68	0.43
1:C:42:CYS:SG	1:C:43:TRP:N	2.92	0.43
2:D:9:ALA:N	2:D:44:LYS:HE2	2.34	0.43
1:C:7:VAL:C	1:C:8:ILE:HD13	2.44	0.42
1:C:48:ILE:HG21	1:C:66:SER:O	2.19	0.42
1:C:186:ILE:HG12	1:C:187:VAL:HG22	2.01	0.42
1:E:13:PRO:O	1:E:15:THR:HG22	2.19	0.42
1:C:72:ASP:HB3	1:C:113:LEU:HA	2.02	0.42
1:C:172:LEU:HB2	2:D:1:MET:N	2.33	0.42
1:E:7:MET:HE2	1:E:7:MET:HB2	1.88	0.42
1:A:200:TYR:CE2	1:A:220:THR:HG21	2.54	0.42
1:C:116:ILE:H	1:C:116:ILE:HG13	1.62	0.42
2:B:30:LYS:HE2	2:B:30:LYS:HB3	1.55	0.42
1:C:188:ASN:HB3	1:C:195:GLU:CB	2.49	0.42
1:C:7:VAL:O	1:C:8:ILE:HD13	2.19	0.42
1:C:184:LYS:HB2	1:C:197:HIS:O	2.19	0.42
1:A:164:PHE:HB3	1:A:218:ILE:HA	2.02	0.42
6:C:321:PE8:H211	6:C:321:PE8:H182	1.65	0.42
1:A:68:GLN:HA	1:A:71:VAL:HB	2.01	0.42
5:A:335:PEG:H42	5:A:335:PEG:H22	1.37	0.42
2:D:39:GLU:HG2	2:D:58:ARG:HD3	2.02	0.42
2:B:38:LEU:HD13	2:B:59:ALA:HB2	2.02	0.42
1:C:146:ILE:HG21	1:C:235:ALA:HB1	2.02	0.42
1:C:192:LYS:HA	1:C:192:LYS:HD3	1.81	0.42
3:B:109:GOL:H32	8:B:125:PG4:H32	2.01	0.42
6:C:321:PE8:H111	8:D:105:PG4:H42	2.02	0.42
2:D:7:SER:C	2:D:44:LYS:HD3	2.44	0.42
6:E:113:PE8:H62	6:E:113:PE8:H31	1.78	0.42
2:B:38:LEU:HD23	2:B:38:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:GLN:HA	3:D:103:GOL:H2	2.02	0.41
8:C:324:PG4:H41	8:C:324:PG4:H81	2.03	0.41
1:A:233:THR:HB	1:A:234:ASP:H	1.80	0.41
1:C:63:ILE:HD12	1:C:63:ILE:HA	1.69	0.41
1:A:186:ILE:O	1:A:194:GLY:HA2	2.20	0.41
2:B:56:LYS:HB3	2:B:56:LYS:HE3	1.85	0.41
1:C:200:TYR:HB2	1:C:218:ILE:O	2.19	0.41
2:D:22:LYS:HB2	2:D:22:LYS:HE3	1.80	0.41
1:A:25:ARG:HA	1:A:30:VAL:HB	2.02	0.41
2:B:29:GLU:H	2:B:29:GLU:HG3	1.44	0.41
2:B:67:LEU:HD23	2:B:67:LEU:HA	1.82	0.41
6:B:105:PE8:H32	6:B:105:PE8:H62	1.71	0.41
1:C:188:ASN:O	1:C:195:GLU:N	2.54	0.41
2:D:19:ILE:O	2:D:23:VAL:HG13	2.21	0.41
2:D:44:LYS:HE3	2:D:95:LEU:HB3	2.02	0.41
1:A:31:THR:HG21	1:A:52:GLU:HB3	2.03	0.41
1:A:104:TYR:HA	1:A:105:PRO:HD3	1.96	0.41
1:C:136:LEU:HA	1:C:136:LEU:HD22	1.84	0.41
2:D:82:LEU:HD12	2:D:82:LEU:HA	1.96	0.41
1:C:154:ASP:OD1	1:C:154:ASP:N	2.54	0.41
1:A:140:LEU:HD12	1:A:178:LEU:HD13	2.03	0.40
6:E:113:PE8:H202	6:E:113:PE8:H172	1.83	0.40
2:B:15:GLU:HG3	6:B:123:PE8:H121	2.03	0.40
1:C:8:ILE:O	1:C:8:ILE:CG2	2.69	0.40
1:C:18:ASP:OD1	1:C:20:ALA:HB3	2.21	0.40
1:C:43:TRP:CE2	1:C:83:GLY:HA3	2.56	0.40
1:C:136:LEU:HD21	1:C:232:GLY:HA3	2.03	0.40
1:A:35:ASP:HB2	1:A:37:LYS:HE3	2.03	0.40
1:C:203:LYS:HG2	1:C:204:ASN:N	2.36	0.40
1:C:227:ARG:HG3	1:C:228:LYS:H	1.87	0.40
1:A:137:LYS:HG2	1:A:200:TYR:CE1	2.57	0.40
2:B:34:THR:N	6:B:131:PE8:O1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	239/241 (99%)	201 (84%)	37 (16%)	1 (0%)	30	60
1	C	239/241 (99%)	191 (80%)	47 (20%)	1 (0%)	30	60
1	E	16/241 (7%)	6 (38%)	10 (62%)	0	100	100
2	B	96/98 (98%)	73 (76%)	19 (20%)	4 (4%)	2	14
2	D	96/98 (98%)	77 (80%)	17 (18%)	2 (2%)	5	26
All	All	686/919 (75%)	548 (80%)	130 (19%)	8 (1%)	10	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	GLN
2	B	77	ASN
2	D	55	ILE
1	A	233	THR
2	B	94	GLU
1	C	28	SER
2	D	49	ALA
2	B	11	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	207/207 (100%)	147 (71%)	60 (29%)	0	1
1	C	207/207 (100%)	130 (63%)	77 (37%)	0	0
1	E	15/207 (7%)	12 (80%)	3 (20%)	1	6
2	B	85/85 (100%)	48 (56%)	37 (44%)	0	0
2	D	85/85 (100%)	61 (72%)	24 (28%)	0	1
All	All	599/791 (76%)	398 (66%)	201 (34%)	0	1

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	7	VAL
1	A	9	LYS
1	A	12	LYS
1	A	14	ASN
1	A	15	GLU
1	A	16	ASN
1	A	28	SER
1	A	31	THR
1	A	33	VAL
1	A	34	LYS
1	A	42	CYS
1	A	46	SER
1	A	48	ILE
1	A	50	SER
1	A	51	VAL
1	A	59	LYS
1	A	62	LEU
1	A	64	THR
1	A	67	GLU
1	A	69	GLU
1	A	71	VAL
1	A	85	ILE
1	A	100	THR
1	A	107	VAL
1	A	113	LEU
1	A	125	ILE
1	A	126	LYS
1	A	129	LEU
1	A	136	LEU
1	A	137	LYS
1	A	140	LEU
1	A	146	ILE
1	A	153	SER
1	A	154	ASP
1	A	155	ASP
1	A	160	LYS
1	A	163	ILE
1	A	165	ASP
1	A	167	GLU
1	A	171	GLN
1	A	177	MET

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Mol	Chain	Res	Type
1	A	178	LEU
1	A	184	LYS
1	A	191	THR
1	A	193	LYS
1	A	195	GLU
1	A	196	LYS
1	A	197	HIS
1	A	202	ILE
1	A	220	THR
1	A	223	SER
1	A	225	LEU
1	A	227	ARG
1	A	228	LYS
1	A	233	THR
1	A	237	ILE
1	A	239	LEU
1	A	240	ILE
1	A	241	GLU
2	B	1	MET
2	B	2	ILE
2	B	6	LEU
2	B	7	SER
2	B	10	LYS
2	B	13	THR
2	B	15	GLU
2	B	16	ILE
2	B	17	GLN
2	B	18	GLU
2	B	19	ILE
2	B	20	VAL
2	B	22	LYS
2	B	23	VAL
2	B	29	GLU
2	B	30	LYS
2	B	31	THR
2	B	33	GLU
2	B	39	GLU
2	B	41	VAL
2	B	44	LYS
2	B	47	VAL
2	B	51	THR
2	B	55	ILE

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Mol	Chain	Res	Type
2	B	57	VAL
2	B	63	LYS
2	B	65	MET
2	B	69	VAL
2	B	71	LYS
2	B	72	SER
2	B	73	LEU
2	B	80	LEU
2	B	81	VAL
2	B	82	LEU
2	B	85	TYR
2	B	94	GLU
2	B	96	THR
1	C	4	TYR
1	C	5	GLU
1	C	8	ILE
1	C	9	LYS
1	C	10	LYS
1	C	12	LYS
1	C	15	GLU
1	C	25	ARG
1	C	26	LEU
1	C	30	VAL
1	C	31	THR
1	C	33	VAL
1	C	34	LYS
1	C	37	LYS
1	C	38	ASN
1	C	39	CYS
1	C	48	ILE
1	C	50	SER
1	C	51	VAL
1	C	61	LYS
1	C	63	ILE
1	C	65	LEU
1	C	68	GLN
1	C	69	GLU
1	C	76	LYS
1	C	84	LEU
1	C	85	ILE
1	C	86	ASN
1	C	91	ASP

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Mol	Chain	Res	Type
1	C	95	LEU
1	C	98	ILE
1	C	100	THR
1	C	101	ASP
1	C	102	ASP
1	C	103	ASP
1	C	107	VAL
1	C	116	ILE
1	C	120	THR
1	C	123	TYR
1	C	125	ILE
1	C	126	LYS
1	C	128	TYR
1	C	129	LEU
1	C	131	VAL
1	C	136	LEU
1	C	137	LYS
1	C	138	GLU
1	C	140	LEU
1	C	141	ARG
1	C	143	LEU
1	C	146	ILE
1	C	147	SER
1	C	154	ASP
1	C	155	ASP
1	C	156	PHE
1	C	165	ASP
1	C	176	VAL
1	C	181	PHE
1	C	186	ILE
1	C	187	VAL
1	C	191	THR
1	C	193	LYS
1	C	195	GLU
1	C	200	TYR
1	C	201	ILE
1	C	202	ILE
1	C	205	SER
1	C	212	GLU
1	C	216	ILE
1	C	218	ILE
1	C	222	GLU

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Mol	Chain	Res	Type
1	C	225	LEU
1	C	226	MET
1	C	228	LYS
1	C	237	ILE
1	C	239	LEU
1	C	240	ILE
2	D	2	ILE
2	D	15	GLU
2	D	16	ILE
2	D	17	GLN
2	D	22	LYS
2	D	24	LYS
2	D	28	GLU
2	D	37	LYS
2	D	41	VAL
2	D	47	VAL
2	D	55	ILE
2	D	57	VAL
2	D	62	ASN
2	D	63	LYS
2	D	68	LYS
2	D	69	VAL
2	D	71	LYS
2	D	72	SER
2	D	80	LEU
2	D	81	VAL
2	D	89	LYS
2	D	90	ASN
2	D	91	LYS
2	D	92	ASP
1	E	9	GLU
1	E	12	ASN
1	E	17	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	77	ASN
1	A	81	ASN
1	A	86	ASN
1	A	134	ASN

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Mol	Chain	Res	Type
1	A	171	GLN
1	C	16	ASN
1	C	27	HIS
1	C	38	ASN
1	C	68	GLN
1	C	127	ASN
2	D	86	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 176 ligands modelled in this entry, 26 are monoatomic - leaving 150 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	D	109	-	5,5,5	0.99	0	5,5,5	1.08	0
8	PG4	B	128	-	12,12,12	0.11	0	11,11,11	0.61	0
3	GOL	A	345	-	5,5,5	0.98	0	5,5,5	1.07	0
8	PG4	D	119	-	12,12,12	0.12	0	11,11,11	0.57	0
7	EDO	B	124	-	3,3,3	0.42	0	2,2,2	0.39	0
3	GOL	B	134	-	5,5,5	1.03	0	5,5,5	1.00	0
3	GOL	B	114	-	5,5,5	0.93	0	5,5,5	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	336	-	3,3,3	0.42	0	2,2,2	0.39	0
8	PG4	E	101	-	12,12,12	0.11	0	11,11,11	0.61	0
5	PEG	D	123	-	6,6,6	0.10	0	5,5,5	0.16	0
3	GOL	D	124	-	5,5,5	0.98	0	5,5,5	0.93	0
8	PG4	C	332	-	12,12,12	0.10	0	11,11,11	0.66	0
5	PEG	C	318	-	6,6,6	0.16	0	5,5,5	0.17	0
5	PEG	C	320	-	6,6,6	0.07	0	5,5,5	0.27	0
9	SO4	E	107	-	4,4,4	0.23	0	6,6,6	0.06	0
8	PG4	A	332	-	12,12,12	0.13	0	11,11,11	0.58	0
9	SO4	D	112	-	4,4,4	0.23	0	6,6,6	0.11	0
8	PG4	C	327	-	12,12,12	0.13	0	11,11,11	0.61	0
3	GOL	C	308	-	5,5,5	0.91	0	5,5,5	1.02	0
7	EDO	C	323	-	3,3,3	0.43	0	2,2,2	0.36	0
7	EDO	A	343	-	3,3,3	0.43	0	2,2,2	0.36	0
3	GOL	B	140	-	5,5,5	1.01	0	5,5,5	1.03	0
5	PEG	E	109	-	6,6,6	0.10	0	5,5,5	0.11	0
8	PG4	D	118	-	12,12,12	0.11	0	11,11,11	0.55	0
6	PE8	A	324	-	24,24,24	0.55	0	23,23,23	0.37	0
3	GOL	C	311	-	5,5,5	0.96	0	5,5,5	0.99	0
3	GOL	D	122	-	5,5,5	0.90	0	5,5,5	1.13	1 (20%)
3	GOL	A	305	-	5,5,5	0.97	0	5,5,5	1.03	0
5	PEG	A	319	-	6,6,6	0.10	0	5,5,5	0.13	0
9	SO4	D	126	-	4,4,4	0.26	0	6,6,6	0.08	0
9	SO4	D	113	-	4,4,4	0.23	0	6,6,6	0.11	0
3	GOL	B	111	-	5,5,5	0.95	0	5,5,5	1.02	0
3	GOL	B	107	-	5,5,5	0.98	0	5,5,5	1.11	0
8	PG4	C	326	-	12,12,12	0.18	0	11,11,11	0.53	0
3	GOL	B	110	-	5,5,5	0.92	0	5,5,5	1.12	0
8	PG4	B	126	-	12,12,12	0.11	0	11,11,11	0.62	0
3	GOL	E	104	-	5,5,5	0.96	0	5,5,5	1.05	0
3	GOL	B	116	-	5,5,5	0.94	0	5,5,5	1.07	0
3	GOL	B	101	-	5,5,5	0.94	0	5,5,5	1.02	0
3	GOL	B	102	-	5,5,5	0.99	0	5,5,5	0.94	0
5	PEG	C	317	-	6,6,6	0.09	0	5,5,5	0.16	0
7	EDO	B	103	-	3,3,3	0.43	0	2,2,2	0.39	0
7	EDO	A	326	-	3,3,3	0.41	0	2,2,2	0.43	0
5	PEG	C	316	-	6,6,6	0.11	0	5,5,5	0.10	0
8	PG4	D	116	-	12,12,12	0.12	0	11,11,11	0.63	0
8	PG4	A	331	-	12,12,12	0.11	0	11,11,11	0.66	0
7	EDO	C	334	-	3,3,3	0.41	0	2,2,2	0.44	0
3	GOL	C	310	-	5,5,5	0.91	0	5,5,5	1.06	0
6	PE8	A	322	-	24,24,24	0.54	0	23,23,23	0.31	0
3	GOL	A	306	-	5,5,5	0.99	0	5,5,5	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PG4	C	325	-	12,12,12	0.12	0	11,11,11	0.62	0
3	GOL	B	132	-	5,5,5	0.93	0	5,5,5	1.10	0
6	PE8	B	131	-	24,24,24	0.54	0	23,23,23	0.25	0
3	GOL	A	303	-	5,5,5	0.96	0	5,5,5	1.07	0
3	GOL	C	338	-	5,5,5	0.92	0	5,5,5	1.12	0
5	PEG	A	335	-	6,6,6	0.17	0	5,5,5	0.23	0
3	GOL	B	115	-	5,5,5	1.02	0	5,5,5	0.94	0
3	GOL	A	346	-	5,5,5	0.98	0	5,5,5	1.01	0
3	GOL	C	341	-	5,5,5	0.94	0	5,5,5	1.22	1 (20%)
8	PG4	B	127	-	12,12,12	0.12	0	11,11,11	0.62	0
3	GOL	A	302	-	5,5,5	0.97	0	5,5,5	1.00	0
3	GOL	A	309	-	5,5,5	0.94	0	5,5,5	1.08	0
8	PG4	A	337	-	12,12,12	0.12	0	11,11,11	0.75	1 (9%)
5	PEG	A	341	-	6,6,6	0.11	0	5,5,5	0.17	0
9	SO4	B	119	-	4,4,4	0.23	0	6,6,6	0.07	0
3	GOL	C	307	-	5,5,5	1.03	0	5,5,5	0.89	0
3	GOL	C	301	-	5,5,5	0.92	0	5,5,5	1.08	0
5	PEG	C	330	-	6,6,6	0.10	0	5,5,5	0.09	0
9	SO4	C	336	-	4,4,4	0.26	0	6,6,6	0.07	0
3	GOL	B	136	-	5,5,5	0.95	0	5,5,5	1.06	0
3	GOL	C	302	-	5,5,5	0.94	0	5,5,5	1.06	0
6	PE8	A	323	-	24,24,24	0.55	0	23,23,23	0.28	0
8	PG4	A	333	-	12,12,12	0.14	0	11,11,11	0.66	0
3	GOL	B	106	-	5,5,5	0.97	0	5,5,5	0.99	0
3	GOL	B	138	-	5,5,5	1.04	0	5,5,5	1.12	0
3	GOL	B	112	-	5,5,5	0.97	0	5,5,5	1.08	0
9	SO4	D	114	-	4,4,4	0.23	0	6,6,6	0.10	0
3	GOL	D	110	-	5,5,5	1.03	0	5,5,5	0.89	0
3	GOL	A	304	-	5,5,5	0.99	0	5,5,5	0.98	0
3	GOL	E	102	-	5,5,5	0.93	0	5,5,5	1.06	0
5	PEG	C	339	-	6,6,6	0.10	0	5,5,5	0.12	0
3	GOL	D	108	-	5,5,5	0.92	0	5,5,5	1.11	0
3	GOL	D	106	-	5,5,5	0.92	0	5,5,5	1.12	0
6	PE8	C	322	-	24,24,24	0.55	0	23,23,23	0.26	0
3	GOL	B	137	-	5,5,5	0.98	0	5,5,5	0.97	0
3	GOL	C	304	-	5,5,5	0.94	0	5,5,5	1.10	0
3	GOL	C	342	-	5,5,5	0.94	0	5,5,5	1.03	0
3	GOL	C	331	-	5,5,5	0.93	0	5,5,5	1.05	0
5	PEG	A	321	-	6,6,6	0.08	0	5,5,5	0.14	0
3	GOL	B	113	-	5,5,5	1.06	0	5,5,5	0.92	0
8	PG4	D	121	-	12,12,12	0.10	0	11,11,11	0.60	0
3	GOL	A	340	-	5,5,5	0.92	0	5,5,5	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	A	320	-	6,6,6	0.12	0	5,5,5	0.06	0
6	PE8	C	321	-	24,24,24	0.55	0	23,23,23	0.37	0
3	GOL	B	130	-	5,5,5	1.01	0	5,5,5	0.87	0
8	PG4	A	329	-	12,12,12	0.14	0	11,11,11	0.52	0
8	PG4	D	117	-	12,12,12	0.11	0	11,11,11	0.60	0
6	PE8	B	121	-	24,24,24	0.55	0	23,23,23	0.27	0
5	PEG	B	120	-	6,6,6	0.11	0	5,5,5	0.08	0
5	PEG	E	110	-	6,6,6	0.11	0	5,5,5	0.13	0
5	PEG	C	315	-	6,6,6	0.09	0	5,5,5	0.14	0
8	PG4	A	334	-	12,12,12	0.12	0	11,11,11	0.68	0
8	PG4	A	344	-	12,12,12	0.11	0	11,11,11	0.62	0
3	GOL	A	312	-	5,5,5	0.96	0	5,5,5	1.08	0
8	PG4	B	129	4	12,12,12	0.12	0	11,11,11	0.55	0
3	GOL	A	311	-	5,5,5	0.92	0	5,5,5	1.05	0
8	PG4	D	101	-	12,12,12	0.12	0	11,11,11	0.61	0
3	GOL	B	109	-	5,5,5	0.99	0	5,5,5	1.00	0
3	GOL	D	107	-	5,5,5	0.93	0	5,5,5	1.08	0
3	GOL	A	308	-	5,5,5	0.99	0	5,5,5	0.96	0
3	GOL	A	314	-	5,5,5	1.00	0	5,5,5	0.91	0
5	PEG	D	115	-	6,6,6	0.12	0	5,5,5	0.12	0
7	EDO	C	328	-	3,3,3	0.42	0	2,2,2	0.39	0
3	GOL	E	103	-	5,5,5	0.95	0	5,5,5	1.05	0
6	PE8	B	123	-	24,24,24	0.55	0	23,23,23	0.30	0
5	PEG	B	139	-	6,6,6	0.11	0	5,5,5	0.10	0
3	GOL	B	135	-	5,5,5	0.97	0	5,5,5	1.05	0
5	PEG	A	342	-	6,6,6	0.11	0	5,5,5	0.11	0
8	PG4	B	104	-	12,12,12	0.11	0	11,11,11	0.74	0
5	PEG	C	340	-	6,6,6	0.09	0	5,5,5	0.12	0
8	PG4	A	338	-	12,12,12	0.13	0	11,11,11	0.59	0
3	GOL	C	306	-	5,5,5	0.92	0	5,5,5	1.08	0
8	PG4	A	330	-	12,12,12	0.11	0	11,11,11	0.60	0
5	PEG	A	318	-	6,6,6	0.12	0	5,5,5	0.07	0
6	PE8	E	112	-	24,24,24	0.54	0	23,23,23	0.30	0
8	PG4	D	127	-	12,12,12	0.10	0	11,11,11	0.65	0
3	GOL	C	303	-	5,5,5	0.95	0	5,5,5	1.06	0
3	GOL	A	310	-	5,5,5	1.00	0	5,5,5	0.98	0
3	GOL	C	305	-	5,5,5	0.92	0	5,5,5	1.12	0
8	PG4	B	125	-	12,12,12	0.09	0	11,11,11	0.69	0
3	GOL	A	313	-	5,5,5	0.89	0	5,5,5	1.13	0
5	PEG	C	319	-	6,6,6	0.14	0	5,5,5	0.05	0
6	PE8	E	114	-	24,24,24	0.54	0	23,23,23	0.31	0
8	PG4	D	105	-	12,12,12	0.13	0	11,11,11	0.77	0
6	PE8	B	105	-	24,24,24	0.54	0	23,23,23	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PE8	E	113	-	24,24,24	0.54	0	23,23,23	0.26	0
5	PEG	E	111	-	6,6,6	0.11	0	5,5,5	0.07	0
8	PG4	C	324	-	12,12,12	0.15	0	11,11,11	0.41	0
3	GOL	B	108	-	5,5,5	0.93	0	5,5,5	1.04	0
6	PE8	B	122	-	24,24,24	0.54	0	23,23,23	0.27	0
7	EDO	A	325	-	3,3,3	0.43	0	2,2,2	0.37	0
8	PG4	A	328	-	12,12,12	0.14	0	11,11,11	0.50	0
3	GOL	C	309	-	5,5,5	0.94	0	5,5,5	1.08	0
3	GOL	A	301	-	5,5,5	0.93	0	5,5,5	1.09	0
5	PEG	E	108	-	6,6,6	0.10	0	5,5,5	0.11	0
7	EDO	A	327	-	3,3,3	0.42	0	2,2,2	0.40	0
3	GOL	D	103	-	5,5,5	0.97	0	5,5,5	1.00	0
8	PG4	C	337	-	12,12,12	0.12	0	11,11,11	0.57	0
3	GOL	A	307	-	5,5,5	1.01	0	5,5,5	0.95	0
7	EDO	C	329	-	3,3,3	0.42	0	2,2,2	0.40	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
3	GOL	D	109	-	-	4/4/4/4	-
8	PG4	B	128	-	-	6/10/10/10	-
3	GOL	A	345	-	-	4/4/4/4	-
8	PG4	D	119	-	-	6/10/10/10	-
7	EDO	B	124	-	-	0/1/1/1	-
3	GOL	B	134	-	-	4/4/4/4	-
3	GOL	B	114	-	-	2/4/4/4	-
7	EDO	A	336	-	-	1/1/1/1	-
8	PG4	E	101	-	-	8/10/10/10	-
5	PEG	D	123	-	-	2/4/4/4	-
3	GOL	D	124	-	-	2/4/4/4	-
8	PG4	C	332	-	-	3/10/10/10	-
5	PEG	C	318	-	-	3/4/4/4	-
5	PEG	C	320	-	-	2/4/4/4	-
8	PG4	A	332	-	-	6/10/10/10	-
8	PG4	C	327	-	-	6/10/10/10	-
3	GOL	C	308	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	C	323	-	-	1/1/1/1	-
7	EDO	A	343	-	-	1/1/1/1	-
3	GOL	B	140	-	-	2/4/4/4	-
5	PEG	E	109	-	-	2/4/4/4	-
8	PG4	D	118	-	-	4/10/10/10	-
6	PE8	A	324	-	-	16/22/22/22	-
3	GOL	C	311	-	-	2/4/4/4	-
3	GOL	D	122	-	-	2/4/4/4	-
3	GOL	A	305	-	-	4/4/4/4	-
5	PEG	A	319	-	-	3/4/4/4	-
3	GOL	B	111	-	-	3/4/4/4	-
3	GOL	B	107	-	-	3/4/4/4	-
8	PG4	C	326	-	-	7/10/10/10	-
3	GOL	B	110	-	-	2/4/4/4	-
8	PG4	B	126	-	-	7/10/10/10	-
3	GOL	E	104	-	-	2/4/4/4	-
3	GOL	B	116	-	-	1/4/4/4	-
3	GOL	B	101	-	-	2/4/4/4	-
3	GOL	B	102	-	-	2/4/4/4	-
5	PEG	C	317	-	-	4/4/4/4	-
7	EDO	B	103	-	-	1/1/1/1	-
7	EDO	A	326	-	-	1/1/1/1	-
5	PEG	C	316	-	-	2/4/4/4	-
8	PG4	D	116	-	-	5/10/10/10	-
8	PG4	A	331	-	-	8/10/10/10	-
7	EDO	C	334	-	-	1/1/1/1	-
3	GOL	C	310	-	-	2/4/4/4	-
6	PE8	A	322	-	-	13/22/22/22	-
3	GOL	A	306	-	-	4/4/4/4	-
8	PG4	C	325	-	-	8/10/10/10	-
3	GOL	B	132	-	-	4/4/4/4	-
6	PE8	B	131	-	-	13/22/22/22	-
3	GOL	A	303	-	-	2/4/4/4	-
3	GOL	C	338	-	-	2/4/4/4	-
5	PEG	A	335	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	115	-	-	4/4/4/4	-
3	GOL	A	346	-	-	0/4/4/4	-
3	GOL	C	341	-	-	4/4/4/4	-
8	PG4	B	127	-	-	5/10/10/10	-
3	GOL	A	302	-	-	0/4/4/4	-
3	GOL	A	309	-	-	0/4/4/4	-
8	PG4	A	337	-	-	7/10/10/10	-
5	PEG	A	341	-	-	3/4/4/4	-
3	GOL	C	307	-	-	4/4/4/4	-
3	GOL	C	301	-	-	2/4/4/4	-
5	PEG	C	330	-	-	1/4/4/4	-
3	GOL	B	136	-	-	2/4/4/4	-
3	GOL	C	302	-	-	4/4/4/4	-
6	PE8	A	323	-	-	11/22/22/22	-
8	PG4	A	333	-	-	5/10/10/10	-
3	GOL	B	106	-	-	2/4/4/4	-
3	GOL	B	138	-	-	4/4/4/4	-
3	GOL	B	112	-	-	4/4/4/4	-
3	GOL	D	110	-	-	2/4/4/4	-
3	GOL	A	304	-	-	1/4/4/4	-
3	GOL	E	102	-	-	2/4/4/4	-
5	PEG	C	339	-	-	2/4/4/4	-
3	GOL	D	108	-	-	2/4/4/4	-
3	GOL	D	106	-	-	2/4/4/4	-
6	PE8	C	322	-	-	13/22/22/22	-
3	GOL	B	137	-	-	2/4/4/4	-
3	GOL	C	304	-	-	1/4/4/4	-
3	GOL	C	342	-	-	2/4/4/4	-
3	GOL	C	331	-	-	1/4/4/4	-
5	PEG	A	321	-	-	1/4/4/4	-
3	GOL	B	113	-	-	0/4/4/4	-
8	PG4	D	121	-	-	6/10/10/10	-
3	GOL	A	340	-	-	2/4/4/4	-
5	PEG	A	320	-	-	2/4/4/4	-
6	PE8	C	321	-	-	10/22/22/22	-
3	GOL	B	130	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PG4	A	329	-	-	4/10/10/10	-
8	PG4	D	117	-	-	5/10/10/10	-
6	PE8	B	121	-	-	13/22/22/22	-
5	PEG	B	120	-	-	1/4/4/4	-
5	PEG	E	110	-	-	3/4/4/4	-
5	PEG	C	315	-	-	2/4/4/4	-
8	PG4	A	334	-	-	6/10/10/10	-
8	PG4	A	344	-	-	5/10/10/10	-
3	GOL	A	312	-	-	4/4/4/4	-
8	PG4	B	129	4	-	7/10/10/10	-
3	GOL	A	311	-	-	0/4/4/4	-
8	PG4	D	101	-	-	4/10/10/10	-
3	GOL	B	109	-	-	2/4/4/4	-
3	GOL	D	107	-	-	2/4/4/4	-
3	GOL	A	308	-	-	3/4/4/4	-
3	GOL	A	314	-	-	4/4/4/4	-
5	PEG	D	115	-	-	2/4/4/4	-
7	EDO	C	328	-	-	1/1/1/1	-
3	GOL	E	103	-	-	0/4/4/4	-
6	PE8	B	123	-	-	16/22/22/22	-
5	PEG	B	139	-	-	0/4/4/4	-
3	GOL	B	135	-	-	4/4/4/4	-
5	PEG	A	342	-	-	3/4/4/4	-
8	PG4	B	104	-	-	3/10/10/10	-
5	PEG	C	340	-	-	4/4/4/4	-
8	PG4	A	338	-	-	6/10/10/10	-
3	GOL	C	306	-	-	4/4/4/4	-
8	PG4	A	330	-	-	6/10/10/10	-
5	PEG	A	318	-	-	3/4/4/4	-
6	PE8	E	112	-	-	14/22/22/22	-
8	PG4	D	127	-	-	8/10/10/10	-
3	GOL	C	303	-	-	3/4/4/4	-
3	GOL	A	310	-	-	2/4/4/4	-
3	GOL	C	305	-	-	4/4/4/4	-
8	PG4	B	125	-	-	5/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	313	-	-	0/4/4/4	-
5	PEG	C	319	-	-	4/4/4/4	-
6	PE8	E	114	-	-	15/22/22/22	-
8	PG4	D	105	-	-	3/10/10/10	-
6	PE8	B	105	-	-	15/22/22/22	-
6	PE8	E	113	-	-	16/22/22/22	-
5	PEG	E	111	-	-	3/4/4/4	-
8	PG4	C	324	-	-	7/10/10/10	-
3	GOL	B	108	-	-	2/4/4/4	-
6	PE8	B	122	-	-	13/22/22/22	-
7	EDO	A	325	-	-	1/1/1/1	-
8	PG4	A	328	-	-	6/10/10/10	-
3	GOL	C	309	-	-	2/4/4/4	-
3	GOL	A	301	-	-	2/4/4/4	-
5	PEG	E	108	-	-	2/4/4/4	-
7	EDO	A	327	-	-	1/1/1/1	-
3	GOL	D	103	-	-	2/4/4/4	-
8	PG4	C	337	-	-	3/10/10/10	-
3	GOL	A	307	-	-	2/4/4/4	-
7	EDO	C	329	-	-	1/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	341	GOL	C3-C2-C1	-2.07	104.19	111.80
8	A	337	PG4	C5-O3-C4	-2.04	104.35	113.26
3	D	122	GOL	C3-C2-C1	-2.00	104.45	111.80

There are no chirality outliers.

All (571) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	GOL	C1-C2-C3-O3
3	A	303	GOL	O1-C1-C2-O2
3	A	303	GOL	O1-C1-C2-C3
3	A	305	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	306	GOL	O1-C1-C2-C3
3	A	306	GOL	C1-C2-C3-O3
3	A	306	GOL	O2-C2-C3-O3
3	A	307	GOL	C1-C2-C3-O3
3	A	308	GOL	O1-C1-C2-C3
3	A	312	GOL	O1-C1-C2-C3
3	A	312	GOL	C1-C2-C3-O3
3	A	340	GOL	O1-C1-C2-C3
3	A	345	GOL	O1-C1-C2-C3
3	A	345	GOL	C1-C2-C3-O3
3	B	107	GOL	O1-C1-C2-C3
3	B	108	GOL	O1-C1-C2-C3
3	B	110	GOL	O2-C2-C3-O3
3	B	112	GOL	C1-C2-C3-O3
3	B	114	GOL	O1-C1-C2-C3
3	B	115	GOL	O1-C1-C2-C3
3	B	115	GOL	C1-C2-C3-O3
3	B	115	GOL	O2-C2-C3-O3
3	B	130	GOL	O1-C1-C2-C3
3	B	130	GOL	C1-C2-C3-O3
3	B	132	GOL	O1-C1-C2-C3
3	B	132	GOL	C1-C2-C3-O3
3	B	134	GOL	O1-C1-C2-O2
3	B	134	GOL	O1-C1-C2-C3
3	B	134	GOL	C1-C2-C3-O3
3	B	135	GOL	C1-C2-C3-O3
3	B	136	GOL	C1-C2-C3-O3
3	B	137	GOL	O1-C1-C2-C3
3	C	301	GOL	C1-C2-C3-O3
3	C	302	GOL	O1-C1-C2-O2
3	C	302	GOL	O1-C1-C2-C3
3	C	302	GOL	C1-C2-C3-O3
3	C	303	GOL	C1-C2-C3-O3
3	C	305	GOL	O1-C1-C2-C3
3	C	305	GOL	C1-C2-C3-O3
3	C	306	GOL	C1-C2-C3-O3
3	C	307	GOL	C1-C2-C3-O3
3	C	308	GOL	O1-C1-C2-O2
3	C	308	GOL	O1-C1-C2-C3
3	C	311	GOL	O1-C1-C2-C3
3	C	338	GOL	C1-C2-C3-O3
3	C	341	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	C	341	GOL	C1-C2-C3-O3
3	D	103	GOL	O1-C1-C2-C3
3	D	107	GOL	O1-C1-C2-O2
3	D	107	GOL	O1-C1-C2-C3
3	D	109	GOL	O1-C1-C2-C3
3	D	109	GOL	C1-C2-C3-O3
3	D	110	GOL	C1-C2-C3-O3
3	D	122	GOL	O1-C1-C2-C3
3	E	102	GOL	O1-C1-C2-C3
6	E	112	PE8	C20-C21-O22-C23
8	C	326	PG4	C1-C2-O2-C3
8	D	105	PG4	C1-C2-O2-C3
5	A	335	PEG	C4-C3-O2-C2
6	A	324	PE8	C21-C20-O19-C18
6	B	105	PE8	C5-C6-O7-C8
6	C	321	PE8	C8-C9-O10-C11
8	C	324	PG4	C6-C5-O3-C4
8	C	324	PG4	C8-C7-O4-C6
8	D	116	PG4	C4-C3-O2-C2
6	A	322	PE8	C21-C20-O19-C18
8	C	326	PG4	C3-C4-O3-C5
5	C	318	PEG	C1-C2-O2-C3
6	B	131	PE8	C14-C15-O16-C17
6	B	122	PE8	C8-C9-O10-C11
8	A	329	PG4	C5-C6-O4-C7
8	A	334	PG4	C1-C2-O2-C3
5	C	319	PEG	C1-C2-O2-C3
8	A	331	PG4	C1-C2-O2-C3
6	B	105	PE8	C14-C15-O16-C17
6	B	131	PE8	C17-C18-O19-C20
8	C	326	PG4	O4-C7-C8-O5
8	D	127	PG4	O4-C7-C8-O5
6	E	113	PE8	C14-C15-O16-C17
6	E	114	PE8	C2-C3-O4-C5
8	A	337	PG4	C4-C3-O2-C2
6	E	113	PE8	C17-C18-O19-C20
6	A	322	PE8	O7-C8-C9-O10
6	B	123	PE8	O13-C14-C15-O16
6	C	321	PE8	O19-C20-C21-O22
6	E	112	PE8	O16-C17-C18-O19
8	C	324	PG4	O3-C5-C6-O4
8	D	127	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
6	B	105	PE8	O19-C20-C21-O22
6	B	123	PE8	O16-C17-C18-O19
6	A	324	PE8	O19-C20-C21-O22
6	B	105	PE8	O4-C5-C6-O7
8	B	128	PG4	C1-C2-O2-C3
8	B	127	PG4	O3-C5-C6-O4
6	B	123	PE8	O7-C8-C9-O10
6	E	112	PE8	O13-C14-C15-O16
8	C	326	PG4	O2-C3-C4-O3
8	A	332	PG4	O2-C3-C4-O3
8	B	104	PG4	O3-C5-C6-O4
8	B	129	PG4	O2-C3-C4-O3
6	B	105	PE8	O10-C11-C12-O13
8	B	129	PG4	O3-C5-C6-O4
8	C	325	PG4	C1-C2-O2-C3
6	C	322	PE8	O19-C20-C21-O22
6	E	114	PE8	O4-C5-C6-O7
5	E	111	PEG	C4-C3-O2-C2
6	B	121	PE8	O10-C11-C12-O13
8	D	127	PG4	C1-C2-O2-C3
8	D	121	PG4	O2-C3-C4-O3
6	A	323	PE8	O13-C14-C15-O16
6	B	122	PE8	O16-C17-C18-O19
6	B	131	PE8	O10-C11-C12-O13
3	A	306	GOL	O1-C1-C2-O2
3	A	312	GOL	O1-C1-C2-O2
3	B	108	GOL	O1-C1-C2-O2
3	B	112	GOL	O2-C2-C3-O3
3	B	130	GOL	O1-C1-C2-O2
3	B	132	GOL	O1-C1-C2-O2
3	B	135	GOL	O2-C2-C3-O3
3	C	338	GOL	O2-C2-C3-O3
3	C	341	GOL	O2-C2-C3-O3
3	D	103	GOL	O1-C1-C2-O2
3	D	110	GOL	O2-C2-C3-O3
3	D	124	GOL	O1-C1-C2-O2
6	B	121	PE8	O4-C5-C6-O7
6	B	123	PE8	O4-C5-C6-O7
6	E	112	PE8	O4-C5-C6-O7
6	C	322	PE8	O4-C5-C6-O7
8	D	117	PG4	O2-C3-C4-O3
5	A	318	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
5	A	321	PEG	O1-C1-C2-O2
5	B	120	PEG	O2-C3-C4-O4
5	C	316	PEG	O1-C1-C2-O2
5	C	318	PEG	O2-C3-C4-O4
5	C	340	PEG	O1-C1-C2-O2
5	E	110	PEG	O1-C1-C2-O2
6	B	105	PE8	O22-C23-C24-O25
6	C	321	PE8	O22-C23-C24-O25
8	A	328	PG4	O4-C7-C8-O5
8	A	330	PG4	O1-C1-C2-O2
8	A	334	PG4	O4-C7-C8-O5
8	A	338	PG4	O1-C1-C2-O2
8	B	128	PG4	O4-C7-C8-O5
8	B	129	PG4	O4-C7-C8-O5
8	C	324	PG4	O1-C1-C2-O2
8	C	327	PG4	O1-C1-C2-O2
8	D	101	PG4	O1-C1-C2-O2
8	E	101	PG4	O1-C1-C2-O2
6	C	322	PE8	C5-C6-O7-C8
6	C	322	PE8	O13-C14-C15-O16
6	B	131	PE8	O7-C8-C9-O10
8	A	332	PG4	O3-C5-C6-O4
6	A	323	PE8	O7-C8-C9-O10
6	E	114	PE8	O19-C20-C21-O22
8	C	327	PG4	O2-C3-C4-O3
5	A	318	PEG	O1-C1-C2-O2
5	A	342	PEG	O1-C1-C2-O2
5	C	317	PEG	O1-C1-C2-O2
5	D	115	PEG	O1-C1-C2-O2
5	E	111	PEG	O2-C3-C4-O4
8	A	328	PG4	O1-C1-C2-O2
8	A	329	PG4	O1-C1-C2-O2
8	A	331	PG4	O1-C1-C2-O2
8	A	332	PG4	O1-C1-C2-O2
8	B	104	PG4	O1-C1-C2-O2
8	B	125	PG4	O4-C7-C8-O5
8	B	129	PG4	O1-C1-C2-O2
8	C	325	PG4	O4-C7-C8-O5
8	D	101	PG4	O4-C7-C8-O5
8	D	121	PG4	O1-C1-C2-O2
6	A	322	PE8	C2-C3-O4-C5
6	C	321	PE8	O7-C8-C9-O10

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Mol	Chain	Res	Type	Atoms
5	D	123	PEG	C4-C3-O2-C2
6	C	321	PE8	C21-C20-O19-C18
8	D	118	PG4	C6-C5-O3-C4
8	E	101	PG4	O3-C5-C6-O4
8	A	337	PG4	C5-C6-O4-C7
8	B	128	PG4	O3-C5-C6-O4
8	E	101	PG4	O2-C3-C4-O3
8	A	330	PG4	C8-C7-O4-C6
8	A	328	PG4	O2-C3-C4-O3
3	A	305	GOL	O1-C1-C2-C3
3	A	310	GOL	C1-C2-C3-O3
3	A	314	GOL	O1-C1-C2-C3
3	A	314	GOL	C1-C2-C3-O3
3	B	102	GOL	C1-C2-C3-O3
3	B	106	GOL	O1-C1-C2-C3
3	B	109	GOL	C1-C2-C3-O3
3	B	110	GOL	C1-C2-C3-O3
3	B	111	GOL	O1-C1-C2-C3
3	B	112	GOL	O1-C1-C2-C3
3	B	135	GOL	O1-C1-C2-C3
3	B	138	GOL	O1-C1-C2-C3
3	B	140	GOL	C1-C2-C3-O3
3	C	307	GOL	O1-C1-C2-C3
3	C	309	GOL	O1-C1-C2-C3
3	C	341	GOL	O1-C1-C2-C3
3	C	342	GOL	O1-C1-C2-C3
3	D	124	GOL	O1-C1-C2-C3
3	E	104	GOL	C1-C2-C3-O3
6	B	121	PE8	O22-C23-C24-O25
6	B	131	PE8	O1-C2-C3-O4
6	E	112	PE8	O22-C23-C24-O25
8	E	101	PG4	O4-C7-C8-O5
6	B	105	PE8	C6-C5-O4-C3
8	A	333	PG4	O3-C5-C6-O4
6	E	114	PE8	O10-C11-C12-O13
3	A	301	GOL	O2-C2-C3-O3
3	A	307	GOL	O2-C2-C3-O3
3	A	308	GOL	O1-C1-C2-O2
3	A	314	GOL	O2-C2-C3-O3
3	A	345	GOL	O1-C1-C2-O2
3	B	107	GOL	O1-C1-C2-O2
3	B	112	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	114	GOL	O1-C1-C2-O2
3	B	115	GOL	O1-C1-C2-O2
3	B	132	GOL	O2-C2-C3-O3
3	B	134	GOL	O2-C2-C3-O3
3	B	136	GOL	O2-C2-C3-O3
3	B	137	GOL	O1-C1-C2-O2
3	C	301	GOL	O2-C2-C3-O3
3	C	302	GOL	O2-C2-C3-O3
3	C	303	GOL	O2-C2-C3-O3
3	C	305	GOL	O1-C1-C2-O2
3	C	306	GOL	O2-C2-C3-O3
3	C	307	GOL	O2-C2-C3-O3
3	C	309	GOL	O1-C1-C2-O2
3	D	109	GOL	O2-C2-C3-O3
3	D	122	GOL	O1-C1-C2-O2
3	E	102	GOL	O1-C1-C2-O2
8	A	337	PG4	O3-C5-C6-O4
8	D	127	PG4	O3-C5-C6-O4
6	B	105	PE8	O16-C17-C18-O19
6	E	113	PE8	O13-C14-C15-O16
8	A	338	PG4	O3-C5-C6-O4
5	A	341	PEG	O1-C1-C2-O2
5	E	108	PEG	O1-C1-C2-O2
6	E	113	PE8	O22-C23-C24-O25
6	E	114	PE8	O1-C2-C3-O4
8	B	126	PG4	O4-C7-C8-O5
8	C	327	PG4	O4-C7-C8-O5
8	C	332	PG4	O4-C7-C8-O5
8	D	105	PG4	O1-C1-C2-O2
6	B	121	PE8	O13-C14-C15-O16
6	B	123	PE8	C14-C15-O16-C17
6	E	113	PE8	C6-C5-O4-C3
8	A	333	PG4	O2-C3-C4-O3
6	E	114	PE8	O16-C17-C18-O19
5	C	316	PEG	O2-C3-C4-O4
8	A	331	PG4	O4-C7-C8-O5
8	D	119	PG4	O4-C7-C8-O5
6	A	322	PE8	O19-C20-C21-O22
6	A	323	PE8	O16-C17-C18-O19
6	B	122	PE8	O13-C14-C15-O16
6	E	114	PE8	O13-C14-C15-O16
8	B	128	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
6	B	105	PE8	O13-C14-C15-O16
6	B	123	PE8	O10-C11-C12-O13
6	B	131	PE8	C6-C5-O4-C3
6	B	121	PE8	O19-C20-C21-O22
8	C	324	PG4	O2-C3-C4-O3
8	A	334	PG4	O2-C3-C4-O3
8	C	326	PG4	O3-C5-C6-O4
8	A	344	PG4	O2-C3-C4-O3
8	B	126	PG4	O2-C3-C4-O3
5	A	335	PEG	O2-C3-C4-O4
5	C	339	PEG	O2-C3-C4-O4
5	C	340	PEG	O2-C3-C4-O4
5	E	110	PEG	O2-C3-C4-O4
6	B	122	PE8	O22-C23-C24-O25
8	A	334	PG4	O1-C1-C2-O2
8	C	325	PG4	O1-C1-C2-O2
8	D	118	PG4	O4-C7-C8-O5
8	D	121	PG4	O4-C7-C8-O5
6	C	321	PE8	O16-C17-C18-O19
5	D	115	PEG	C1-C2-O2-C3
3	A	305	GOL	O2-C2-C3-O3
3	A	340	GOL	O1-C1-C2-O2
3	A	345	GOL	O2-C2-C3-O3
3	B	106	GOL	O1-C1-C2-O2
3	B	109	GOL	O2-C2-C3-O3
3	B	130	GOL	O2-C2-C3-O3
3	B	135	GOL	O1-C1-C2-O2
3	C	305	GOL	O2-C2-C3-O3
3	C	307	GOL	O1-C1-C2-O2
3	C	311	GOL	O1-C1-C2-O2
3	E	104	GOL	O2-C2-C3-O3
8	A	328	PG4	O3-C5-C6-O4
8	A	328	PG4	C1-C2-O2-C3
6	A	323	PE8	O10-C11-C12-O13
6	A	323	PE8	O4-C5-C6-O7
8	C	327	PG4	O3-C5-C6-O4
6	E	113	PE8	O10-C11-C12-O13
5	C	315	PEG	O1-C1-C2-O2
5	C	319	PEG	O1-C1-C2-O2
8	D	117	PG4	O3-C5-C6-O4
7	C	334	EDO	O1-C1-C2-O2
6	C	321	PE8	O4-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
6	A	324	PE8	O4-C5-C6-O7
5	C	339	PEG	O1-C1-C2-O2
8	B	125	PG4	O1-C1-C2-O2
8	D	117	PG4	O4-C7-C8-O5
8	B	129	PG4	C6-C5-O3-C4
8	A	334	PG4	O3-C5-C6-O4
6	A	322	PE8	O4-C5-C6-O7
6	C	322	PE8	O10-C11-C12-O13
8	A	338	PG4	O2-C3-C4-O3
6	A	322	PE8	O10-C11-C12-O13
5	A	342	PEG	O2-C3-C4-O4
3	A	308	GOL	O2-C2-C3-O3
3	A	310	GOL	O2-C2-C3-O3
3	A	312	GOL	O2-C2-C3-O3
3	A	314	GOL	O1-C1-C2-O2
3	B	101	GOL	O2-C2-C3-O3
3	C	308	GOL	O2-C2-C3-O3
3	D	109	GOL	O1-C1-C2-O2
8	A	329	PG4	O3-C5-C6-O4
8	B	127	PG4	O2-C3-C4-O3
8	C	325	PG4	O3-C5-C6-O4
6	A	324	PE8	O13-C14-C15-O16
6	A	322	PE8	O13-C14-C15-O16
8	D	116	PG4	O3-C5-C6-O4
7	A	325	EDO	O1-C1-C2-O2
7	A	343	EDO	O1-C1-C2-O2
6	A	324	PE8	O7-C8-C9-O10
8	B	126	PG4	O3-C5-C6-O4
8	D	116	PG4	O2-C3-C4-O3
8	A	330	PG4	O3-C5-C6-O4
5	E	111	PEG	O1-C1-C2-O2
3	A	304	GOL	O2-C2-C3-O3
3	B	140	GOL	O2-C2-C3-O3
3	C	303	GOL	O1-C1-C2-O2
3	C	310	GOL	O2-C2-C3-O3
3	C	331	GOL	O2-C2-C3-O3
3	C	342	GOL	O1-C1-C2-O2
3	D	108	GOL	O2-C2-C3-O3
6	B	105	PE8	C9-C8-O7-C6
8	B	127	PG4	C5-C6-O4-C7
8	A	338	PG4	C3-C4-O3-C5
8	C	332	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
8	D	118	PG4	C5-C6-O4-C7
8	E	101	PG4	C5-C6-O4-C7
5	A	341	PEG	O2-C3-C4-O4
5	C	320	PEG	O2-C3-C4-O4
5	E	109	PEG	O1-C1-C2-O2
8	D	117	PG4	O1-C1-C2-O2
5	E	109	PEG	C1-C2-O2-C3
6	A	323	PE8	C18-C17-O16-C15
6	A	324	PE8	C9-C8-O7-C6
6	B	123	PE8	C21-C20-O19-C18
8	A	334	PG4	C5-C6-O4-C7
8	B	126	PG4	C8-C7-O4-C6
8	D	119	PG4	C3-C4-O3-C5
6	A	324	PE8	C24-C23-O22-C21
6	B	131	PE8	C21-C20-O19-C18
6	B	131	PE8	C24-C23-O22-C21
8	A	337	PG4	C8-C7-O4-C6
8	A	331	PG4	C5-C6-O4-C7
8	D	119	PG4	C4-C3-O2-C2
8	A	331	PG4	C3-C4-O3-C5
6	A	322	PE8	C17-C18-O19-C20
6	A	324	PE8	C18-C17-O16-C15
6	B	123	PE8	C8-C9-O10-C11
6	B	123	PE8	C24-C23-O22-C21
6	E	112	PE8	C2-C3-O4-C5
6	E	112	PE8	C11-C12-O13-C14
8	C	332	PG4	C8-C7-O4-C6
6	A	323	PE8	C14-C15-O16-C17
6	A	323	PE8	C20-C21-O22-C23
6	E	113	PE8	C12-C11-O10-C9
8	B	126	PG4	C4-C3-O2-C2
8	D	105	PG4	C8-C7-O4-C6
3	B	101	GOL	C1-C2-C3-O3
3	B	138	GOL	C1-C2-C3-O3
3	C	306	GOL	O1-C1-C2-C3
3	D	108	GOL	C1-C2-C3-O3
6	E	112	PE8	C5-C6-O7-C8
6	E	114	PE8	C14-C15-O16-C17
8	A	332	PG4	C6-C5-O3-C4
6	E	114	PE8	C21-C20-O19-C18
8	B	126	PG4	C3-C4-O3-C5
8	E	101	PG4	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
6	A	324	PE8	C20-C21-O22-C23
6	B	121	PE8	C21-C20-O19-C18
6	B	122	PE8	C20-C21-O22-C23
6	C	322	PE8	C12-C11-O10-C9
5	A	341	PEG	C1-C2-O2-C3
5	C	330	PEG	C4-C3-O2-C2
8	C	325	PG4	C8-C7-O4-C6
8	A	333	PG4	C1-C2-O2-C3
5	C	317	PEG	C1-C2-O2-C3
5	C	340	PEG	C1-C2-O2-C3
6	E	114	PE8	C12-C11-O10-C9
6	C	322	PE8	C20-C21-O22-C23
8	A	344	PG4	C4-C3-O2-C2
8	A	344	PG4	C5-C6-O4-C7
5	A	319	PEG	O1-C1-C2-O2
8	D	127	PG4	O1-C1-C2-O2
6	B	121	PE8	O16-C17-C18-O19
6	E	114	PE8	C18-C17-O16-C15
6	C	322	PE8	O16-C17-C18-O19
6	C	321	PE8	C18-C17-O16-C15
6	A	322	PE8	C15-C14-O13-C12
6	E	113	PE8	C9-C8-O7-C6
8	D	116	PG4	C3-C4-O3-C5
6	A	324	PE8	C2-C3-O4-C5
8	B	126	PG4	C1-C2-O2-C3
6	A	324	PE8	C17-C18-O19-C20
6	B	123	PE8	C15-C14-O13-C12
8	A	328	PG4	C5-C6-O4-C7
6	C	322	PE8	C17-C18-O19-C20
6	A	324	PE8	C14-C15-O16-C17
6	B	122	PE8	C17-C18-O19-C20
8	D	127	PG4	C8-C7-O4-C6
6	B	105	PE8	C17-C18-O19-C20
6	B	122	PE8	C18-C17-O16-C15
6	E	114	PE8	C6-C5-O4-C3
5	C	317	PEG	C4-C3-O2-C2
6	B	123	PE8	C18-C17-O16-C15
6	B	131	PE8	C11-C12-O13-C14
8	B	128	PG4	O1-C1-C2-O2
8	A	333	PG4	C5-C6-O4-C7
8	D	118	PG4	C8-C7-O4-C6
8	C	337	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
5	A	319	PEG	C4-C3-O2-C2
6	C	322	PE8	C21-C20-O19-C18
8	B	127	PG4	C1-C2-O2-C3
6	B	122	PE8	C5-C6-O7-C8
3	B	111	GOL	O1-C1-C2-O2
8	C	326	PG4	C5-C6-O4-C7
8	A	330	PG4	C6-C5-O3-C4
8	B	128	PG4	C5-C6-O4-C7
8	C	337	PG4	C1-C2-O2-C3
5	C	319	PEG	O2-C3-C4-O4
6	A	324	PE8	O22-C23-C24-O25
6	C	321	PE8	O1-C2-C3-O4
6	B	121	PE8	C18-C17-O16-C15
6	C	322	PE8	C2-C3-O4-C5
8	A	338	PG4	C5-C6-O4-C7
8	D	119	PG4	C1-C2-O2-C3
6	E	114	PE8	C20-C21-O22-C23
8	C	324	PG4	C3-C4-O3-C5
8	E	101	PG4	C1-C2-O2-C3
5	A	319	PEG	C1-C2-O2-C3
6	E	113	PE8	C5-C6-O7-C8
5	A	342	PEG	C1-C2-O2-C3
5	C	318	PEG	O1-C1-C2-O2
6	A	323	PE8	C17-C18-O19-C20
8	A	344	PG4	C8-C7-O4-C6
6	E	114	PE8	C17-C18-O19-C20
6	A	323	PE8	C24-C23-O22-C21
6	B	121	PE8	C11-C12-O13-C14
6	B	131	PE8	C9-C8-O7-C6
5	E	110	PEG	C1-C2-O2-C3
3	B	102	GOL	O2-C2-C3-O3
3	D	106	GOL	O2-C2-C3-O3
6	C	321	PE8	O13-C14-C15-O16
6	B	123	PE8	C17-C18-O19-C20
8	B	104	PG4	C3-C4-O3-C5
6	E	113	PE8	O7-C8-C9-O10
6	E	112	PE8	C18-C17-O16-C15
6	A	324	PE8	C12-C11-O10-C9
6	E	112	PE8	C8-C9-O10-C11
6	A	322	PE8	C5-C6-O7-C8
5	C	320	PEG	C1-C2-O2-C3
8	B	125	PG4	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
6	E	113	PE8	C20-C21-O22-C23
8	C	327	PG4	C8-C7-O4-C6
8	A	337	PG4	O1-C1-C2-O2
6	B	121	PE8	C9-C8-O7-C6
6	C	322	PE8	C8-C9-O10-C11
8	A	332	PG4	C4-C3-O2-C2
6	B	105	PE8	C21-C20-O19-C18
6	A	324	PE8	C11-C12-O13-C14
6	A	322	PE8	C6-C5-O4-C3
8	C	325	PG4	C5-C6-O4-C7
8	D	121	PG4	C5-C6-O4-C7
6	B	105	PE8	C8-C9-O10-C11
8	C	325	PG4	C6-C5-O3-C4
8	D	127	PG4	C3-C4-O3-C5
8	A	329	PG4	C1-C2-O2-C3
5	E	108	PEG	O2-C3-C4-O4
6	B	123	PE8	C9-C8-O7-C6
8	C	327	PG4	C5-C6-O4-C7
6	B	121	PE8	C14-C15-O16-C17
8	D	101	PG4	C8-C7-O4-C6
3	C	304	GOL	C1-C2-C3-O3
3	C	310	GOL	C1-C2-C3-O3
3	D	106	GOL	C1-C2-C3-O3
5	A	335	PEG	C1-C2-O2-C3
6	B	122	PE8	C21-C20-O19-C18
8	B	127	PG4	C4-C3-O2-C2
3	B	138	GOL	O2-C2-C3-O3
5	C	340	PEG	C4-C3-O2-C2
5	A	318	PEG	C1-C2-O2-C3
8	D	121	PG4	C3-C4-O3-C5
8	B	129	PG4	C3-C4-O3-C5
6	B	121	PE8	O1-C2-C3-O4
5	A	320	PEG	C4-C3-O2-C2
6	E	113	PE8	C8-C9-O10-C11
8	D	121	PG4	C4-C3-O2-C2
6	C	322	PE8	C15-C14-O13-C12
6	A	324	PE8	O10-C11-C12-O13
6	E	112	PE8	O7-C8-C9-O10
8	C	325	PG4	C4-C3-O2-C2
3	A	305	GOL	O1-C1-C2-O2
3	B	111	GOL	O2-C2-C3-O3
8	C	324	PG4	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
7	A	326	EDO	O1-C1-C2-O2
7	A	327	EDO	O1-C1-C2-O2
7	A	336	EDO	O1-C1-C2-O2
7	B	103	EDO	O1-C1-C2-O2
7	C	328	EDO	O1-C1-C2-O2
7	C	329	EDO	O1-C1-C2-O2
6	B	123	PE8	C6-C5-O4-C3
5	C	317	PEG	O2-C3-C4-O4
8	E	101	PG4	C8-C7-O4-C6
8	A	332	PG4	C3-C4-O3-C5
6	B	122	PE8	O7-C8-C9-O10
6	B	131	PE8	O13-C14-C15-O16
5	C	319	PEG	C4-C3-O2-C2
6	B	123	PE8	C11-C12-O13-C14
3	B	107	GOL	C1-C2-C3-O3
8	D	101	PG4	C3-C4-O3-C5
6	B	122	PE8	C24-C23-O22-C21
6	B	105	PE8	C15-C14-O13-C12
8	A	330	PG4	C3-C4-O3-C5
3	B	116	GOL	O1-C1-C2-O2
3	B	138	GOL	O1-C1-C2-O2
8	A	331	PG4	C8-C7-O4-C6
6	E	112	PE8	O10-C11-C12-O13
8	D	127	PG4	C4-C3-O2-C2
6	E	114	PE8	C11-C12-O13-C14
8	D	117	PG4	C8-C7-O4-C6
6	A	322	PE8	C11-C12-O13-C14
6	A	323	PE8	O19-C20-C21-O22
5	D	123	PEG	C1-C2-O2-C3
8	A	330	PG4	O4-C7-C8-O5
6	E	112	PE8	O19-C20-C21-O22
6	E	113	PE8	C18-C17-O16-C15
6	B	105	PE8	C11-C12-O13-C14
6	A	322	PE8	C24-C23-O22-C21
6	B	121	PE8	O7-C8-C9-O10
8	D	119	PG4	O3-C5-C6-O4
8	A	331	PG4	C6-C5-O3-C4
6	B	122	PE8	O10-C11-C12-O13
6	E	113	PE8	C21-C20-O19-C18
8	C	326	PG4	C6-C5-O3-C4
6	B	131	PE8	O22-C23-C24-O25
3	C	306	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	B	131	PE8	O19-C20-C21-O22
6	E	112	PE8	C9-C8-O7-C6
7	C	323	EDO	O1-C1-C2-O2
5	A	320	PEG	O1-C1-C2-O2
6	B	123	PE8	O22-C23-C24-O25
8	A	337	PG4	C6-C5-O3-C4
5	C	315	PEG	C4-C3-O2-C2
6	B	122	PE8	C11-C12-O13-C14
8	B	129	PG4	C4-C3-O2-C2
8	B	125	PG4	O3-C5-C6-O4
8	C	337	PG4	C8-C7-O4-C6
8	A	333	PG4	C3-C4-O3-C5
8	A	338	PG4	C6-C5-O3-C4
8	A	337	PG4	O2-C3-C4-O3
8	A	331	PG4	O3-C5-C6-O4
8	D	119	PG4	O2-C3-C4-O3
8	D	116	PG4	O4-C7-C8-O5
6	E	113	PE8	O16-C17-C18-O19
8	B	125	PG4	O2-C3-C4-O3
6	E	113	PE8	O4-C5-C6-O7
8	A	344	PG4	O3-C5-C6-O4

There are no ring outliers.

40 monomers are involved in 50 short contacts:

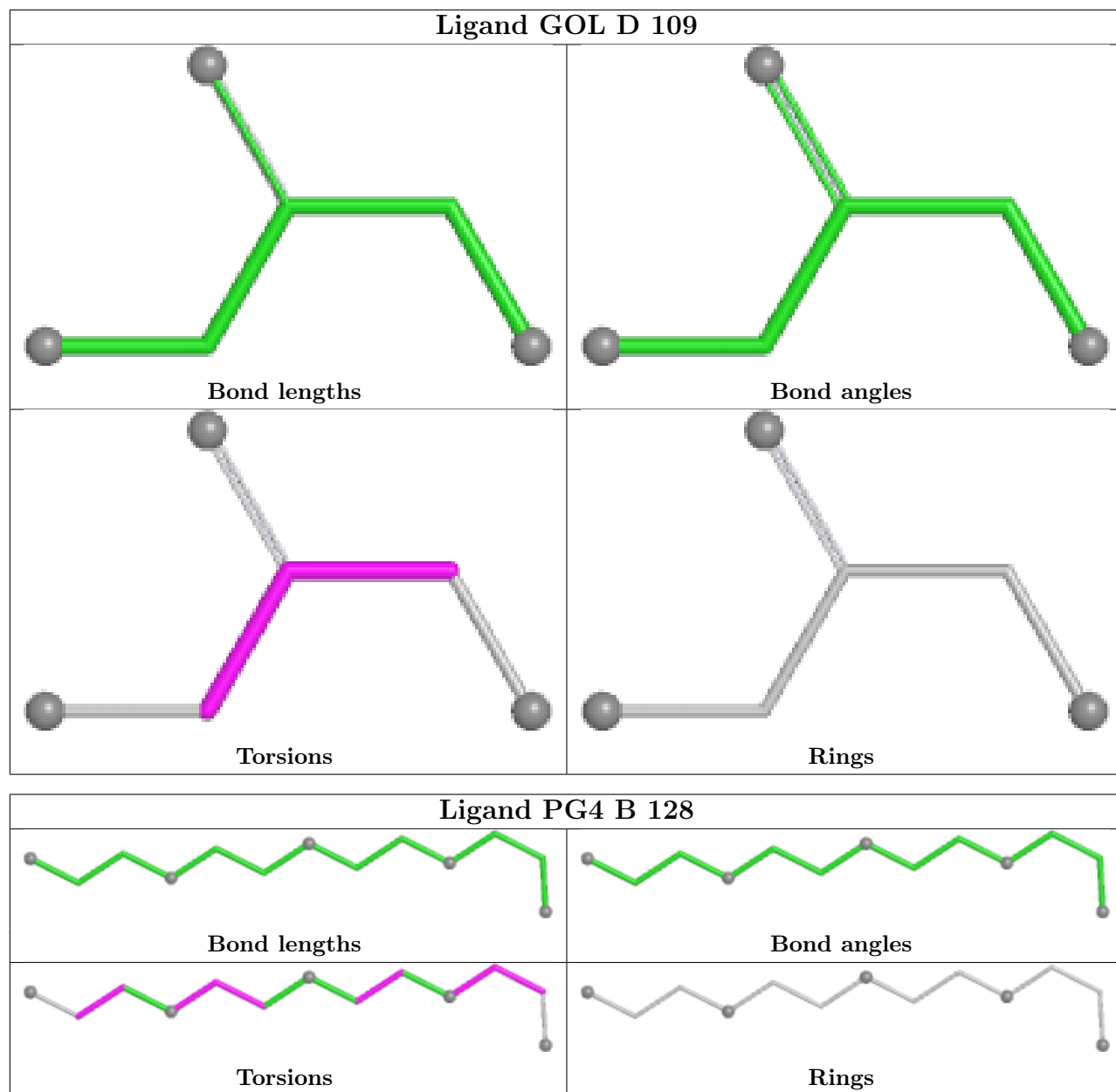
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	345	GOL	1	0
5	D	123	PEG	1	0
3	D	124	GOL	1	0
8	C	332	PG4	1	0
5	E	109	PEG	1	0
8	D	118	PG4	1	0
6	A	324	PE8	1	0
8	C	326	PG4	1	0
8	B	126	PG4	1	0
3	E	104	GOL	1	0
3	B	116	GOL	1	0
8	D	116	PG4	1	0
8	A	331	PG4	1	0
6	A	322	PE8	4	0
6	B	131	PE8	2	0
5	A	335	PEG	2	0

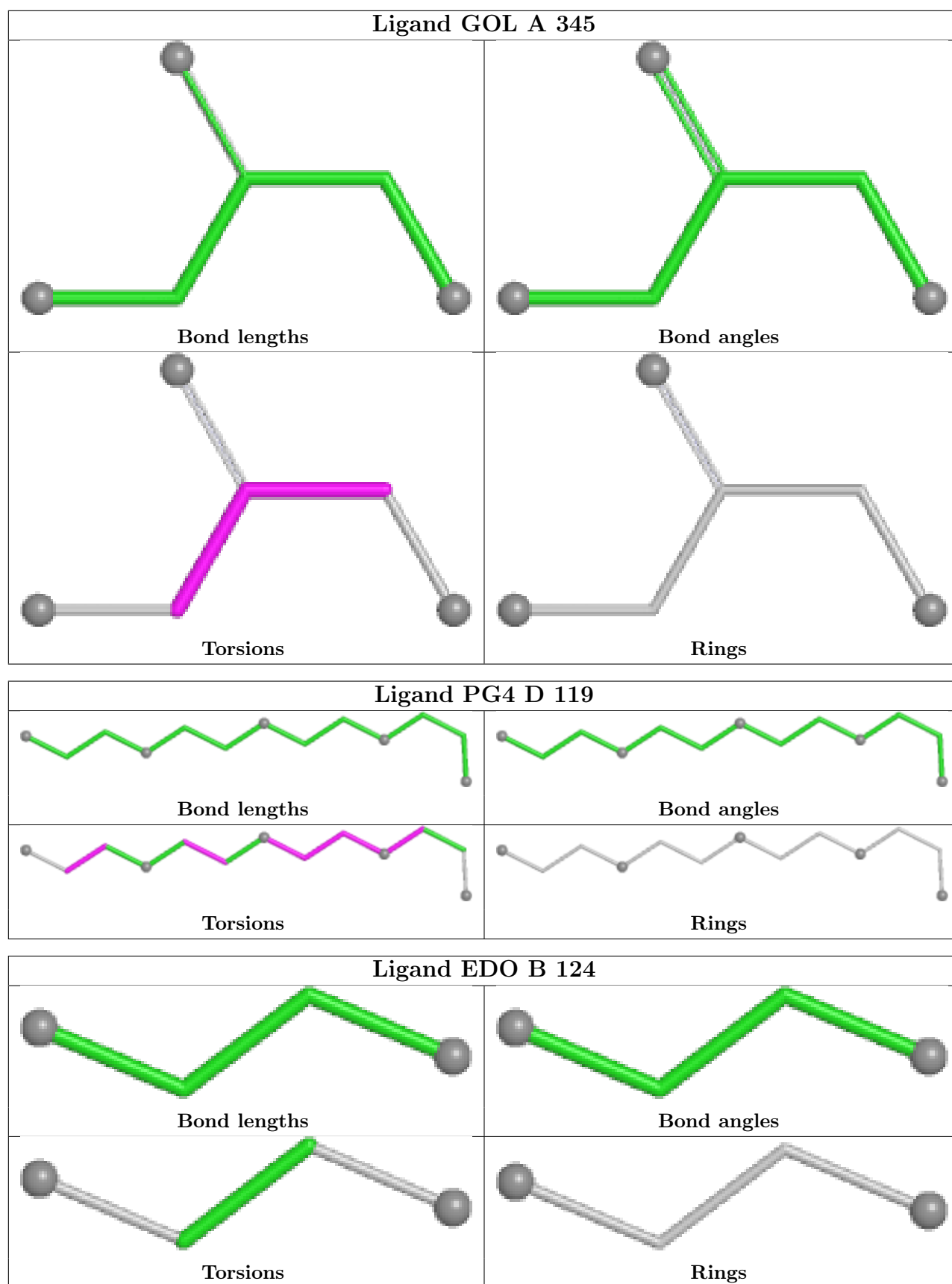
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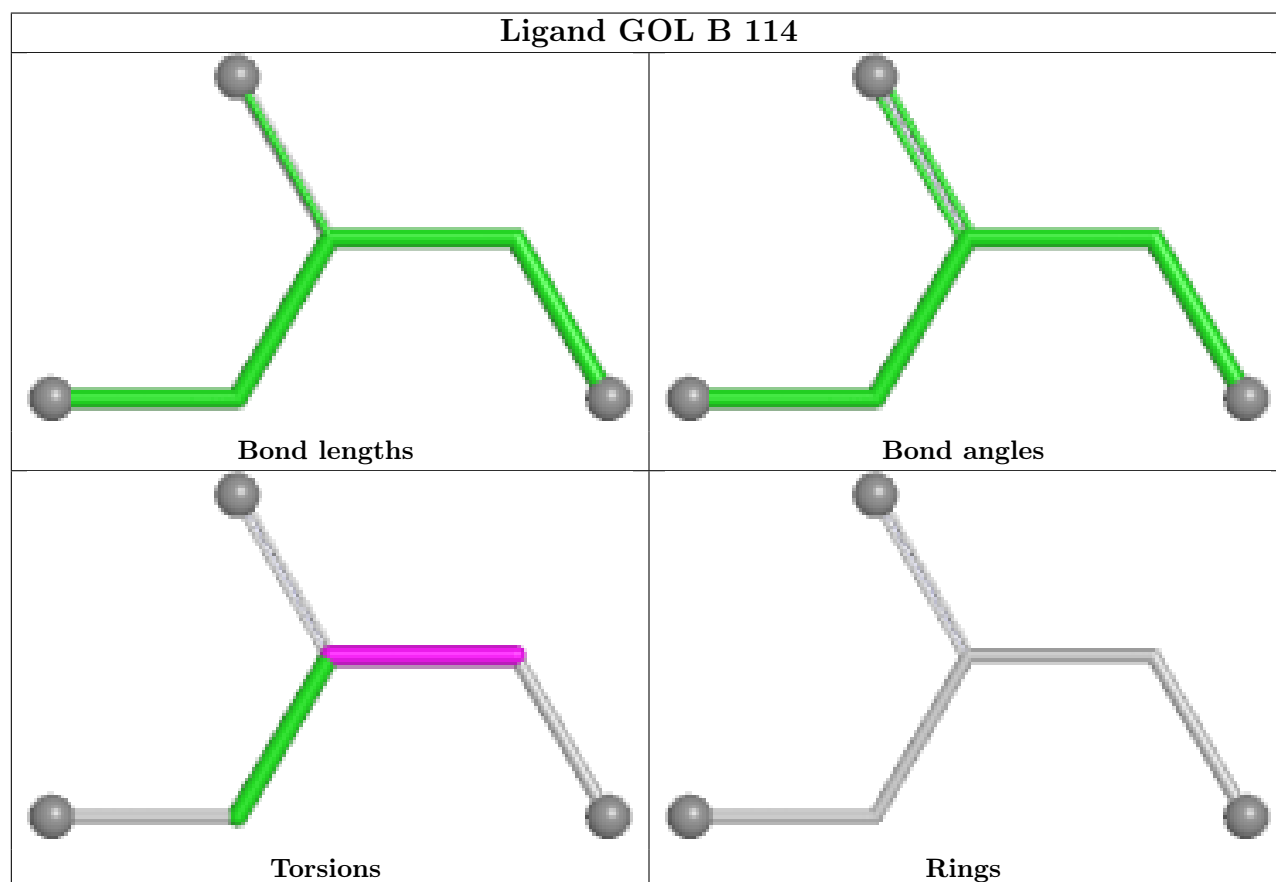
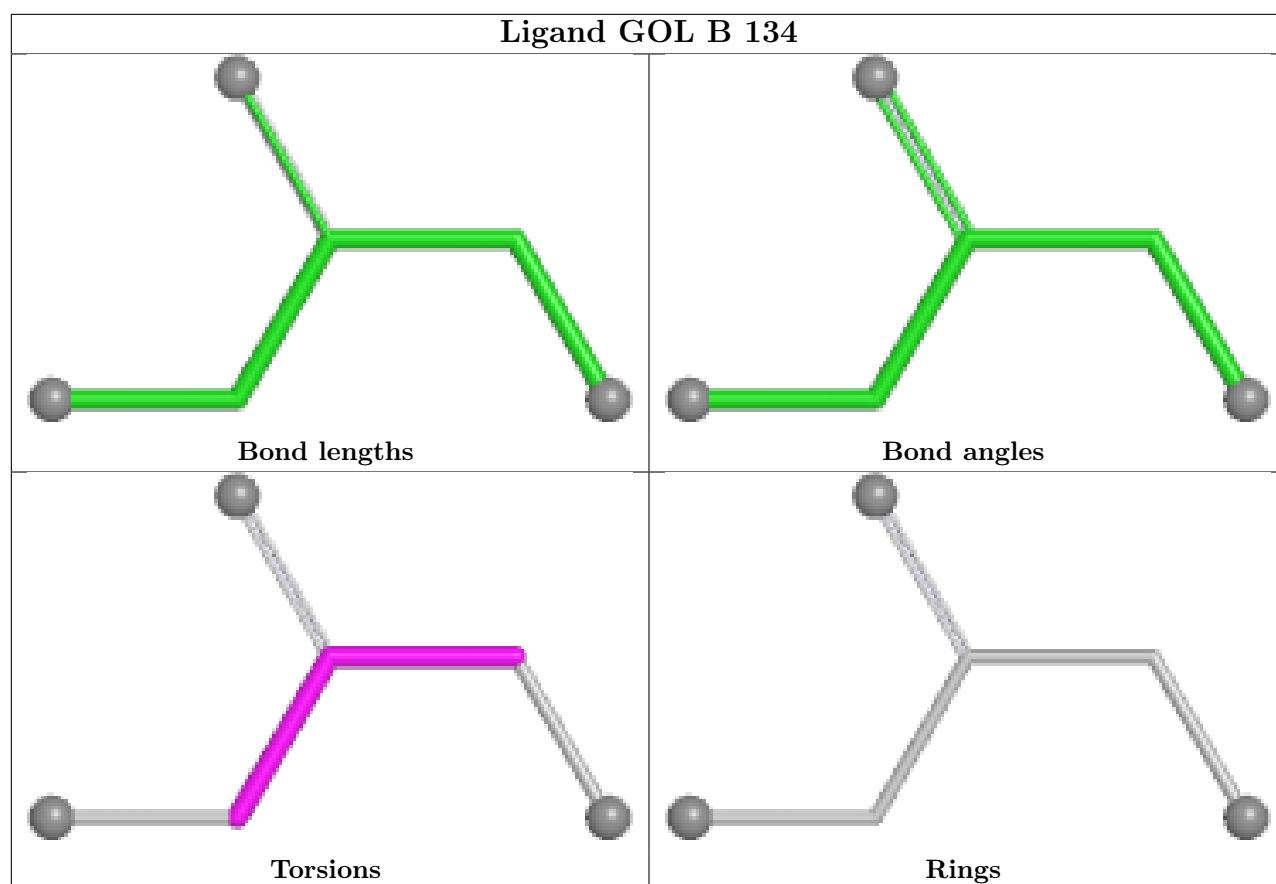
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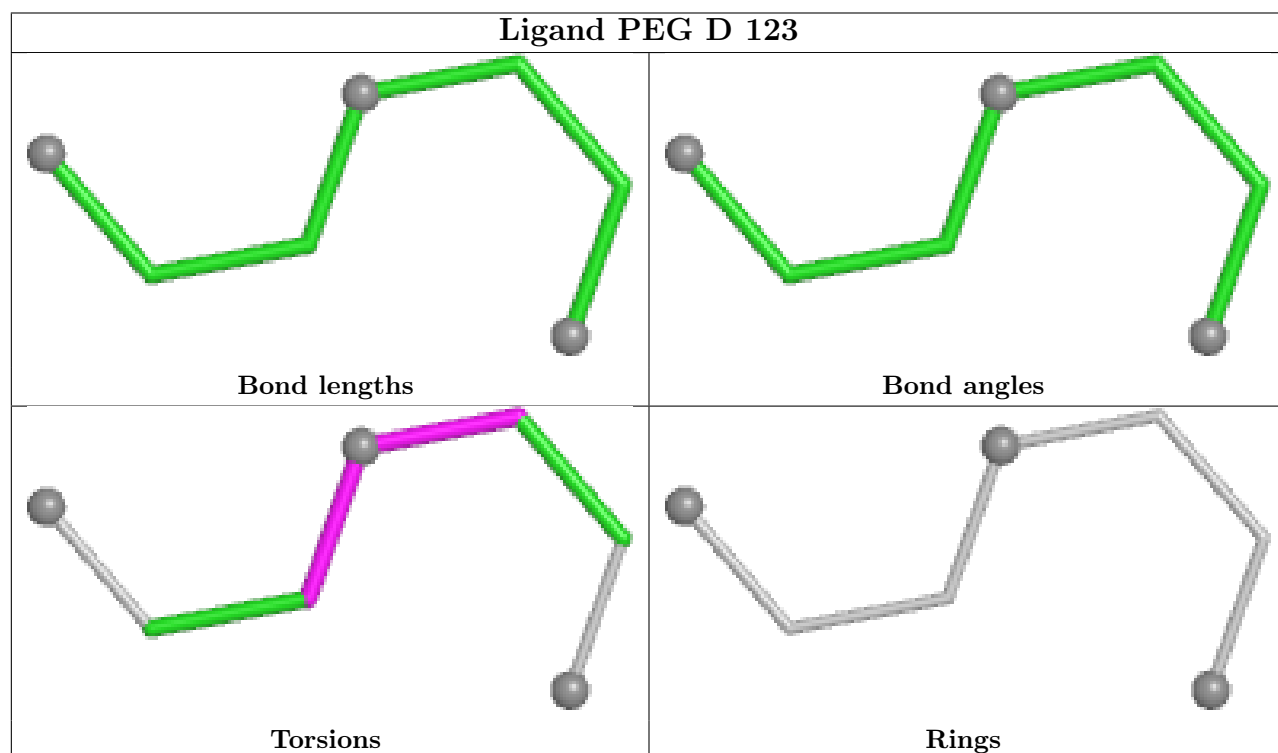
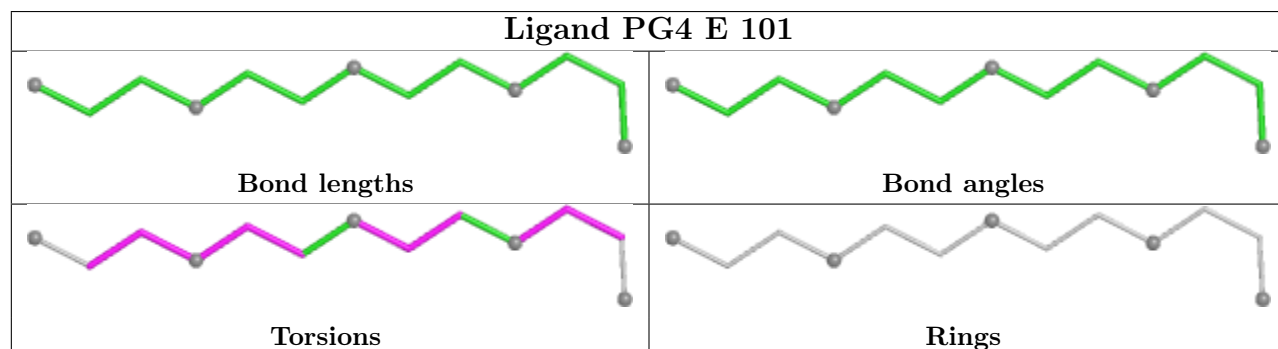
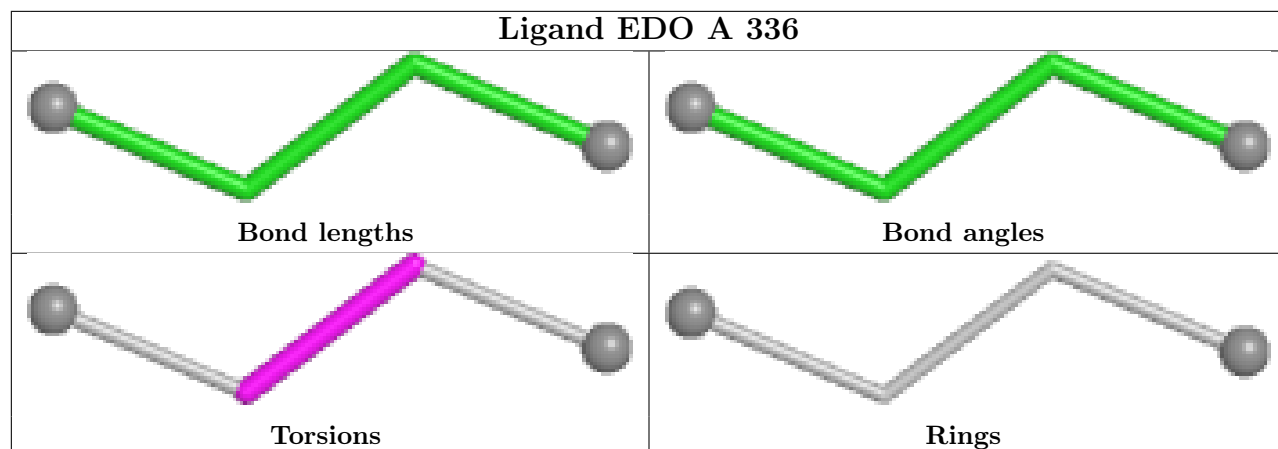
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	346	GOL	1	0
8	A	337	PG4	1	0
3	D	110	GOL	1	0
3	C	342	GOL	2	0
5	A	320	PEG	1	0
6	C	321	PE8	4	0
8	A	329	PG4	1	0
8	A	334	PG4	1	0
8	A	344	PG4	1	0
8	B	129	PG4	1	0
3	B	109	GOL	1	0
5	D	115	PEG	1	0
6	B	123	PE8	2	0
8	A	330	PG4	4	0
3	C	303	GOL	1	0
8	B	125	PG4	2	0
6	E	114	PE8	2	0
8	D	105	PG4	2	0
6	B	105	PE8	3	0
6	E	113	PE8	3	0
8	C	324	PG4	3	0
8	A	328	PG4	1	0
3	D	103	GOL	1	0
8	C	337	PG4	3	0

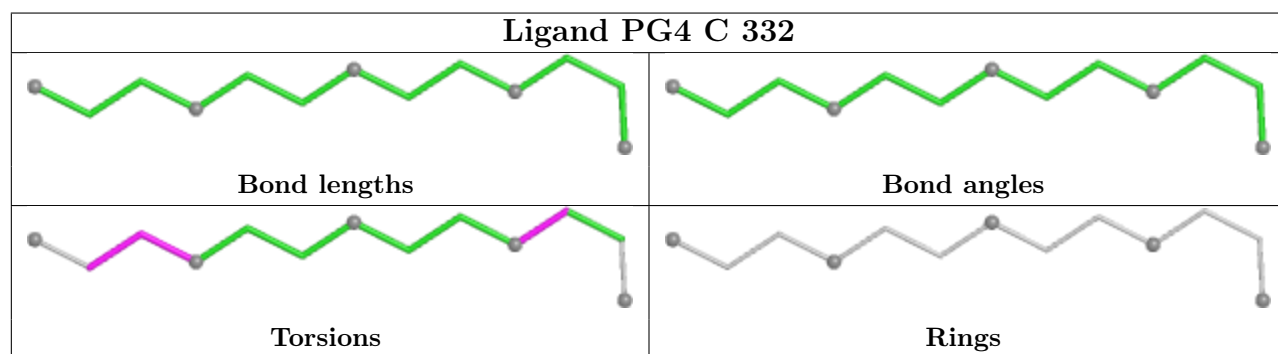
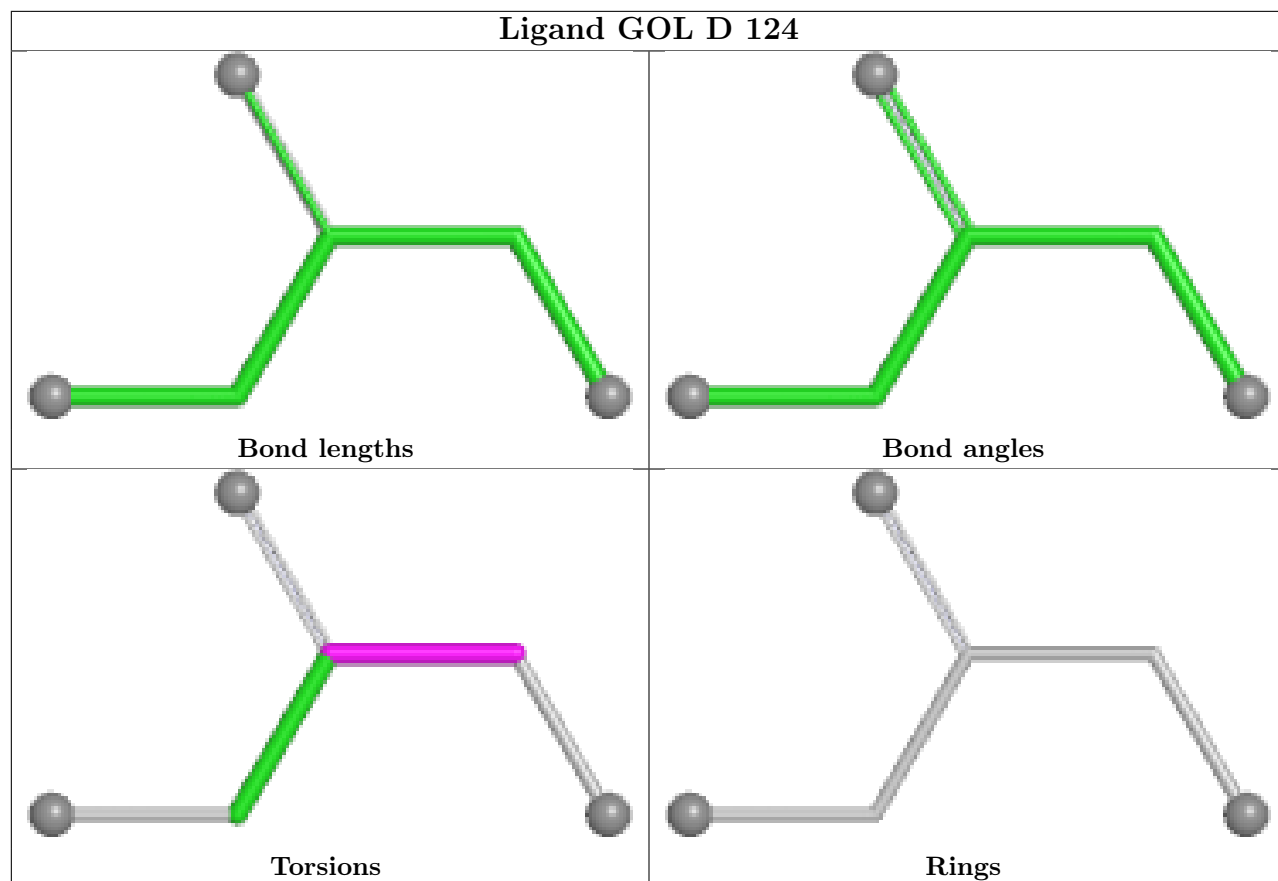
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

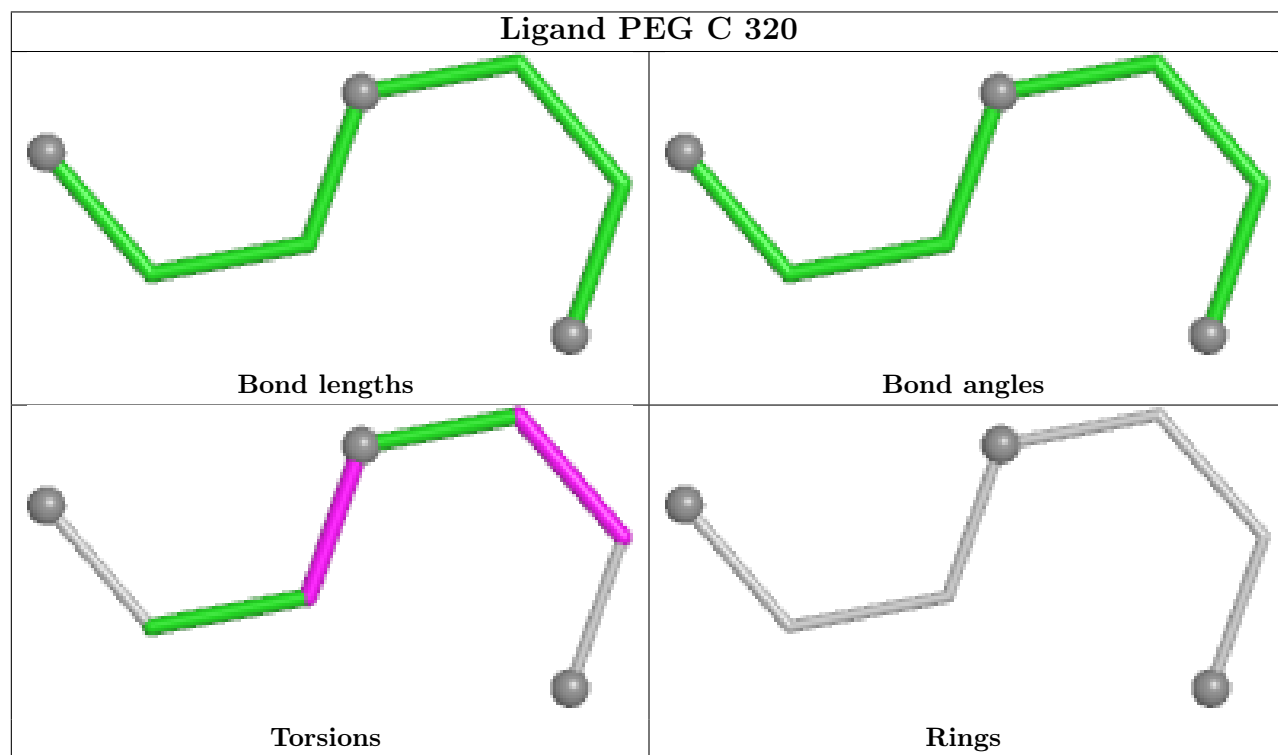
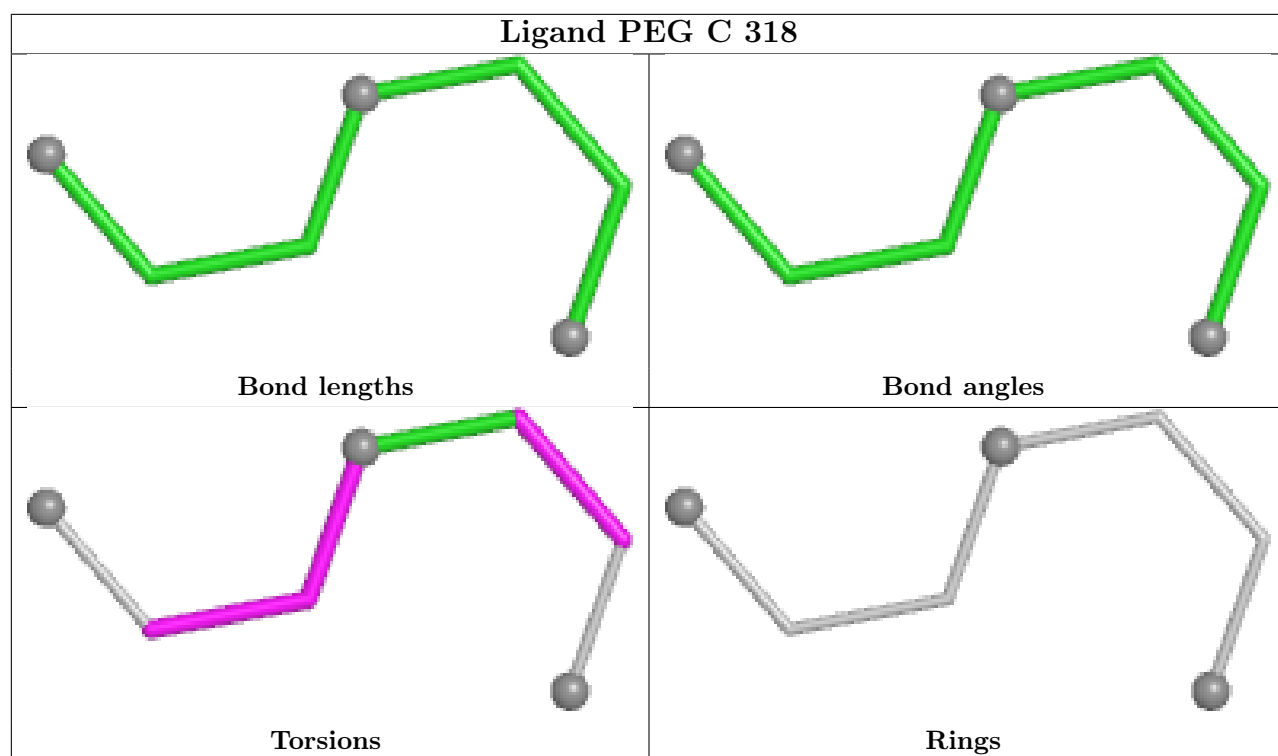


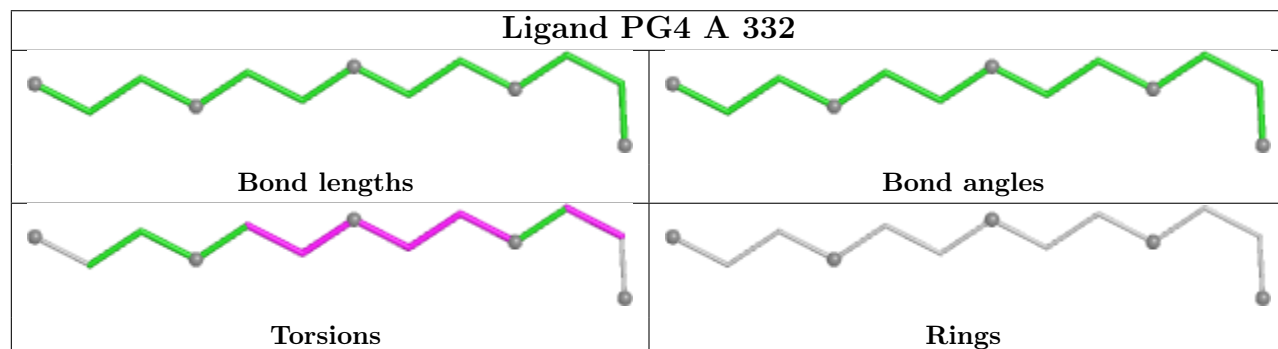
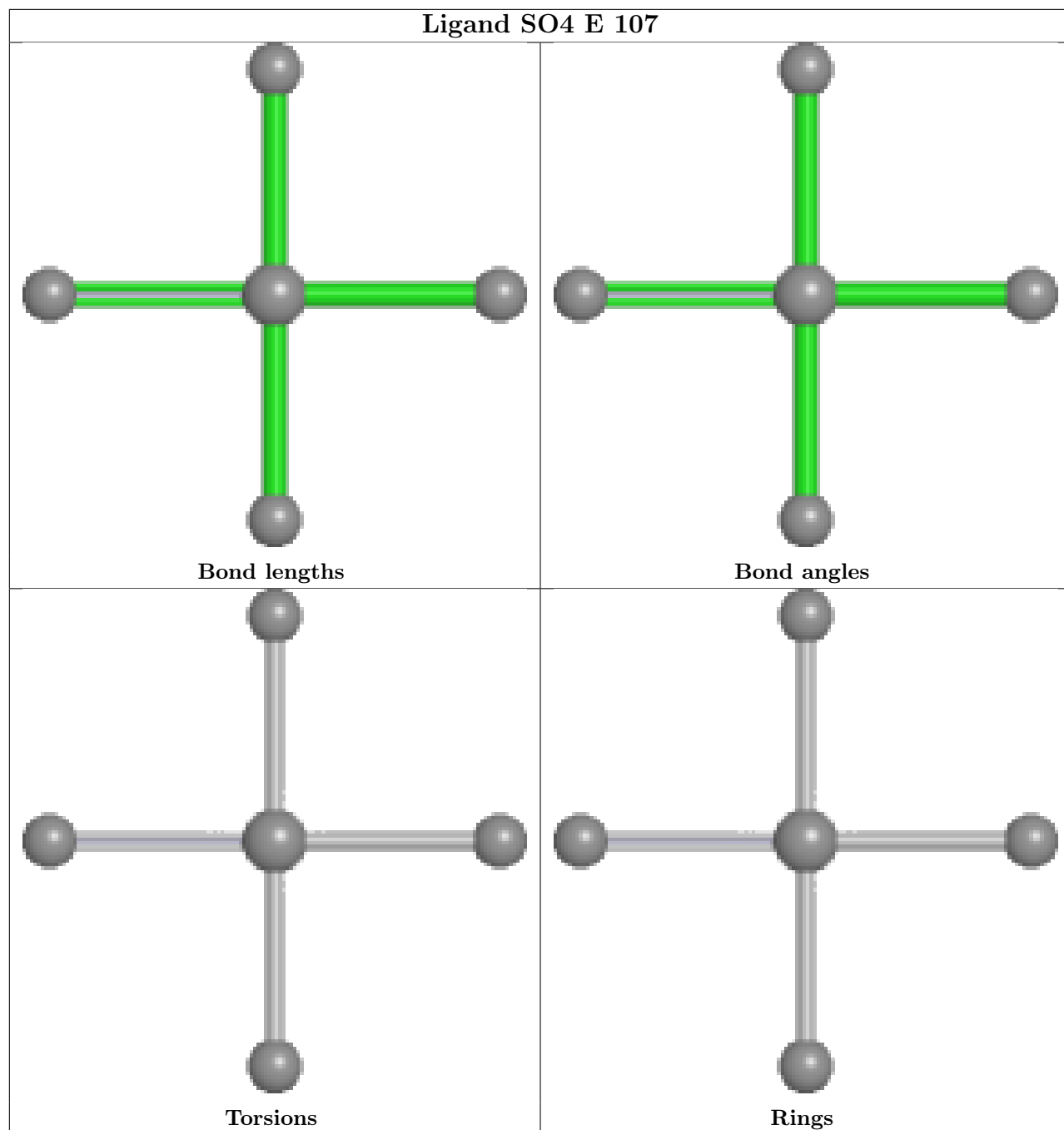


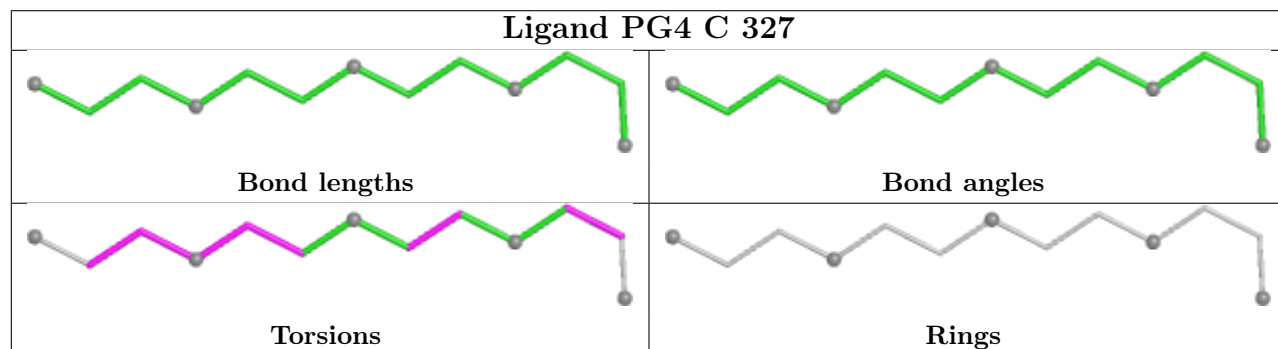
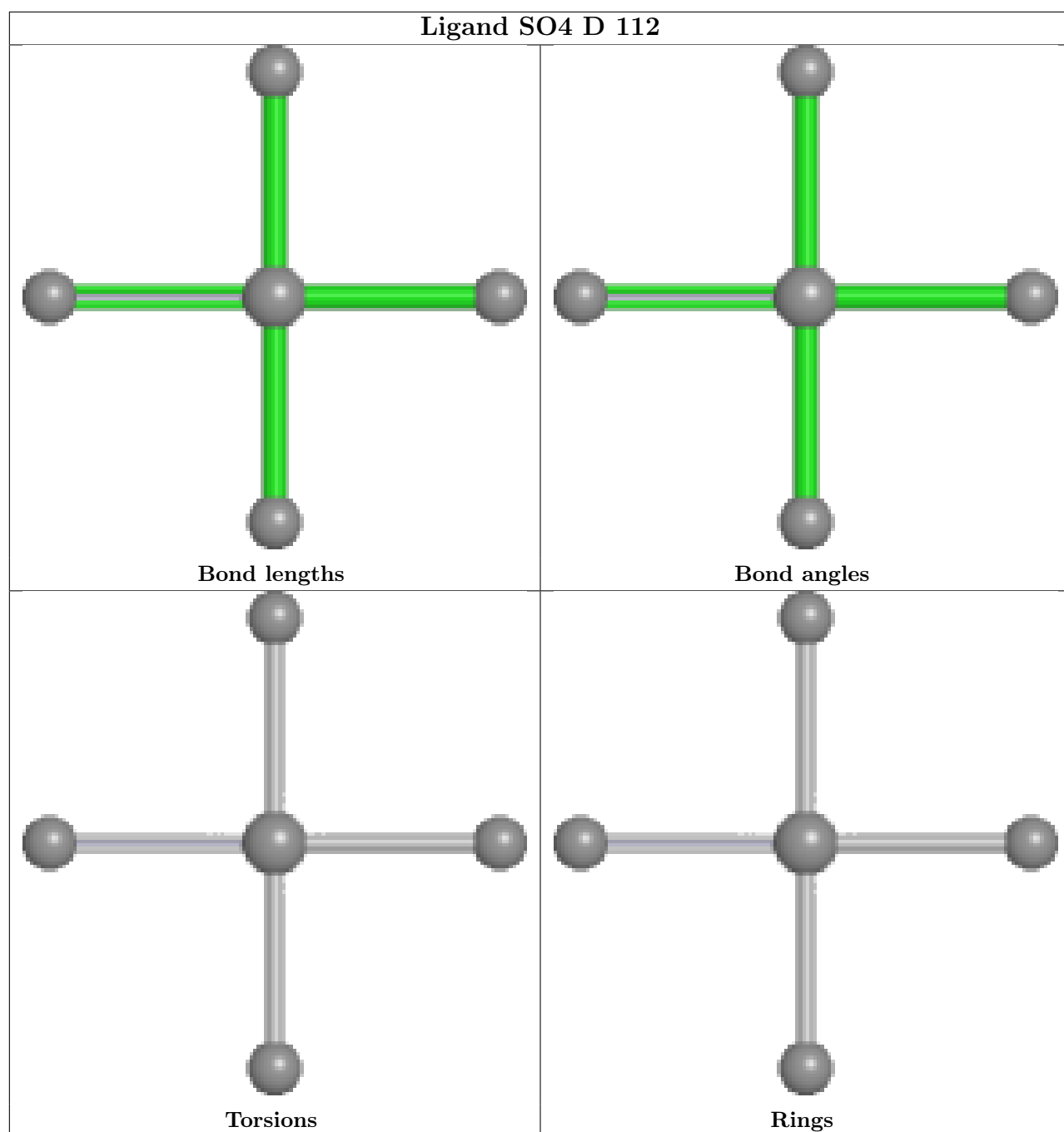


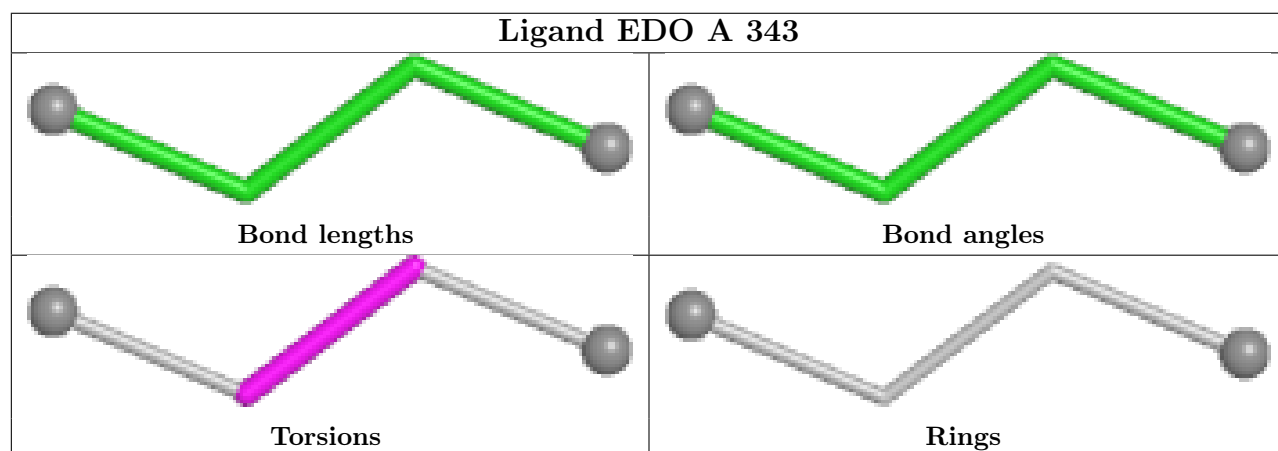
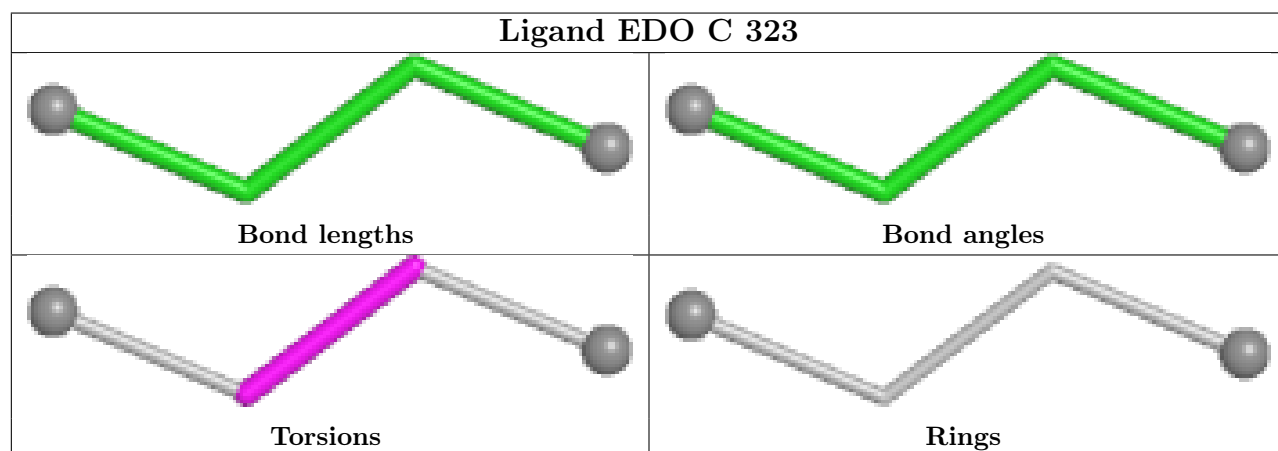
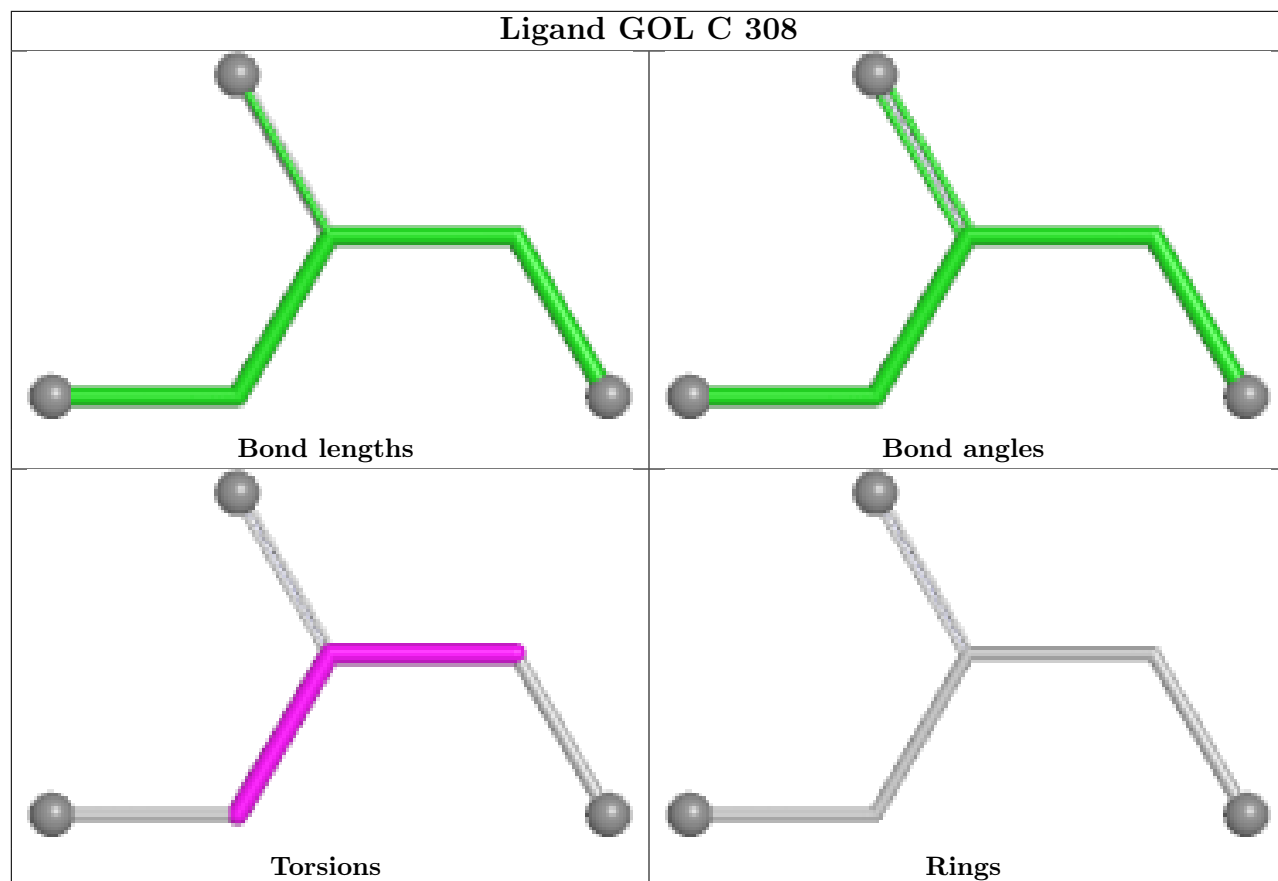


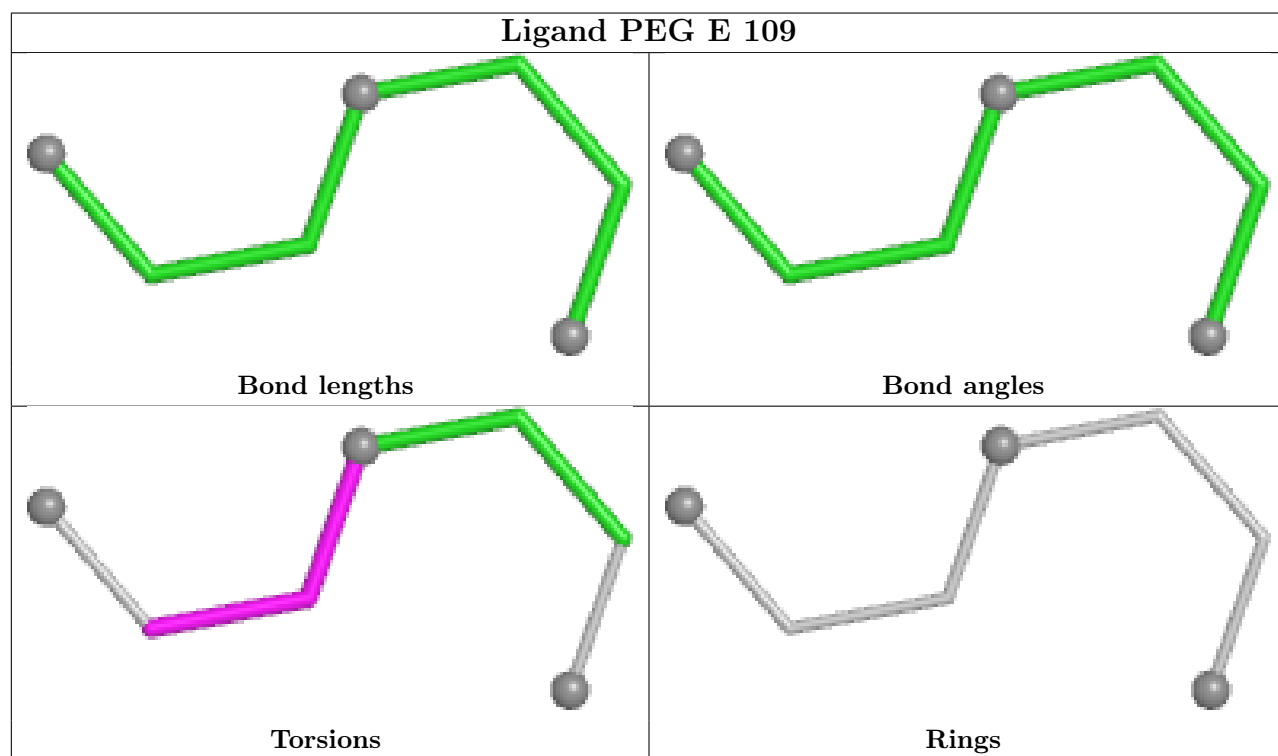
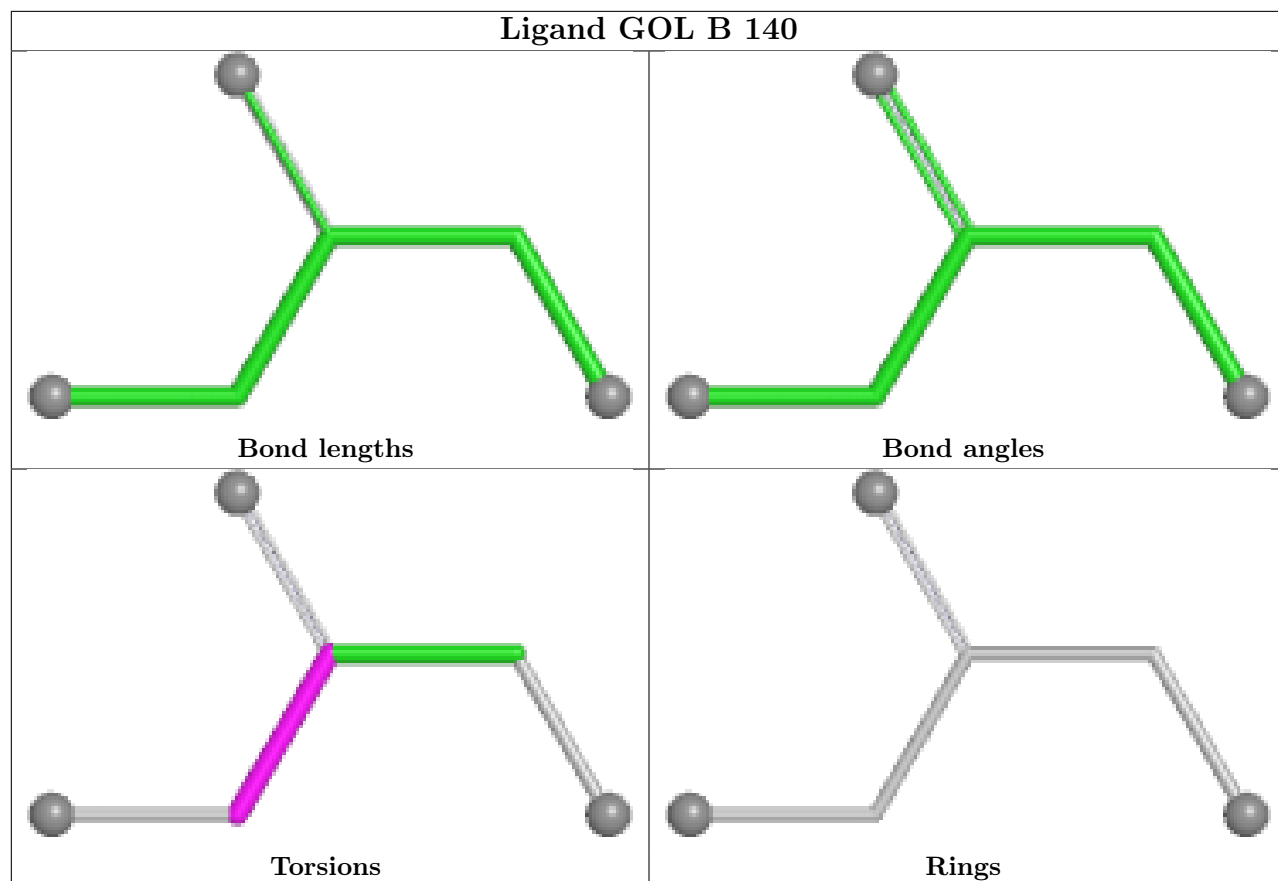


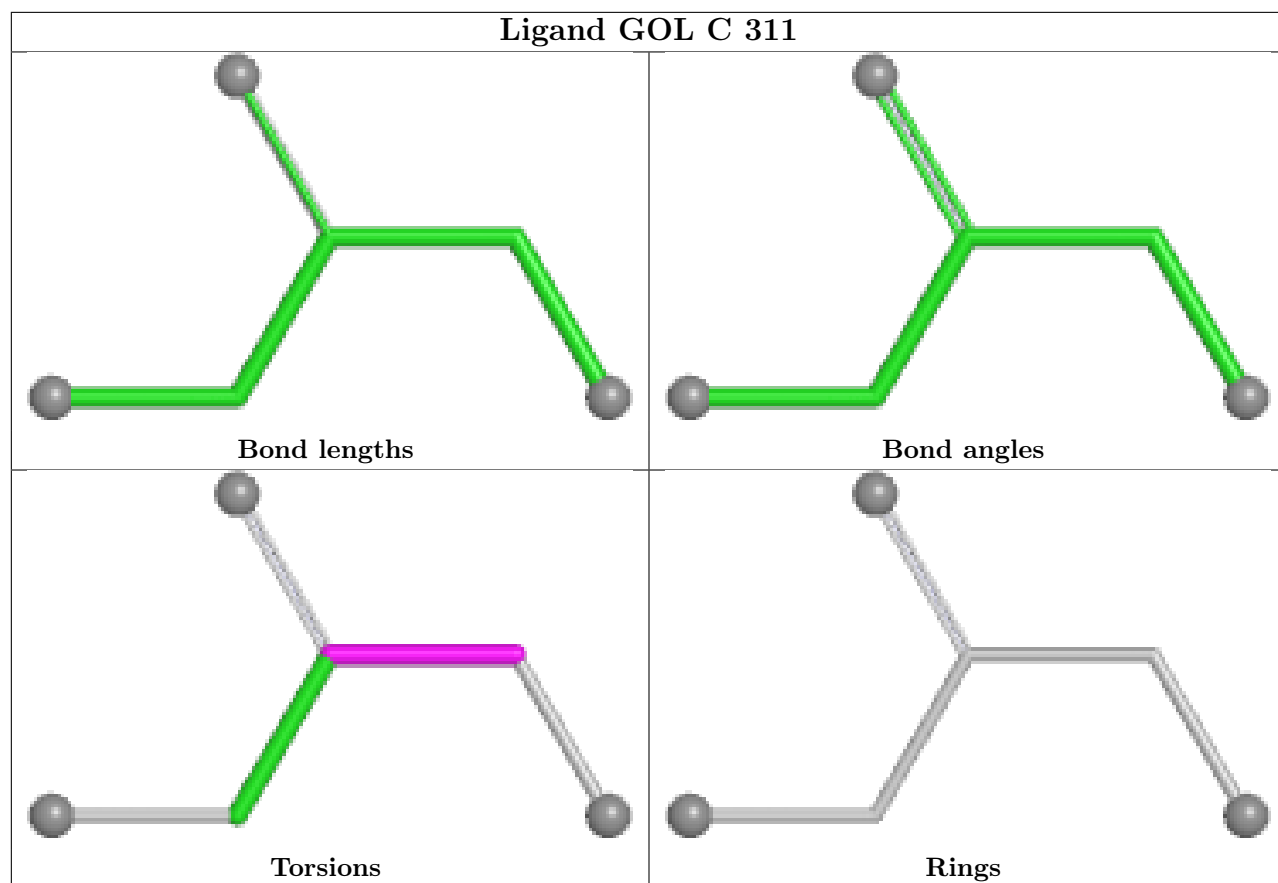
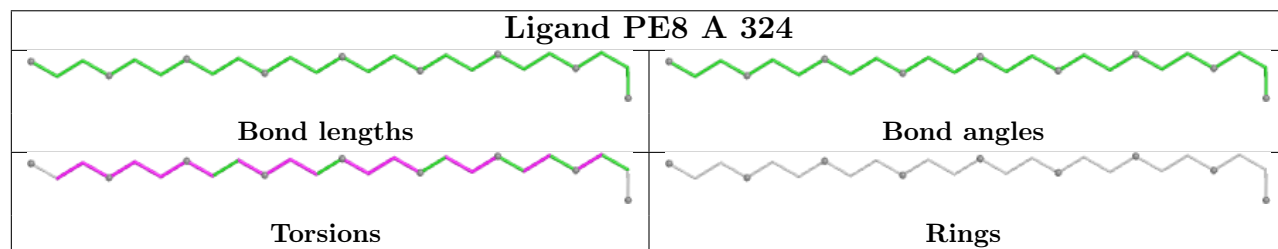
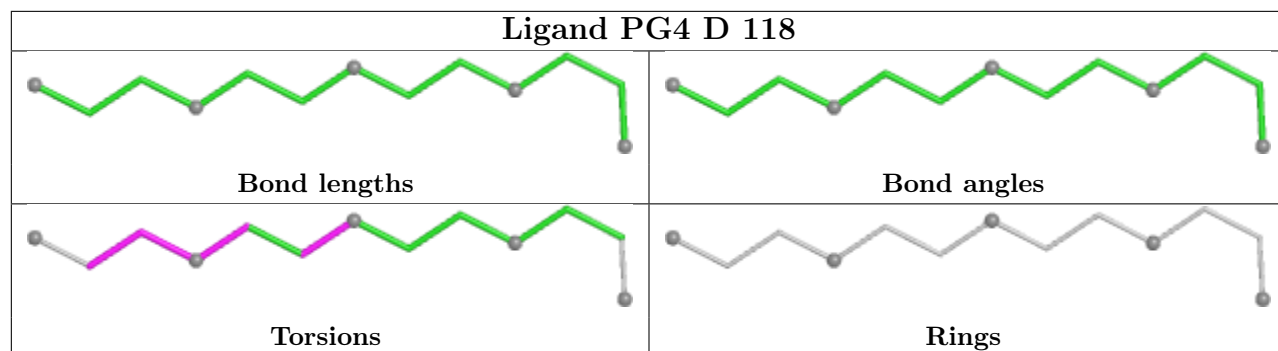


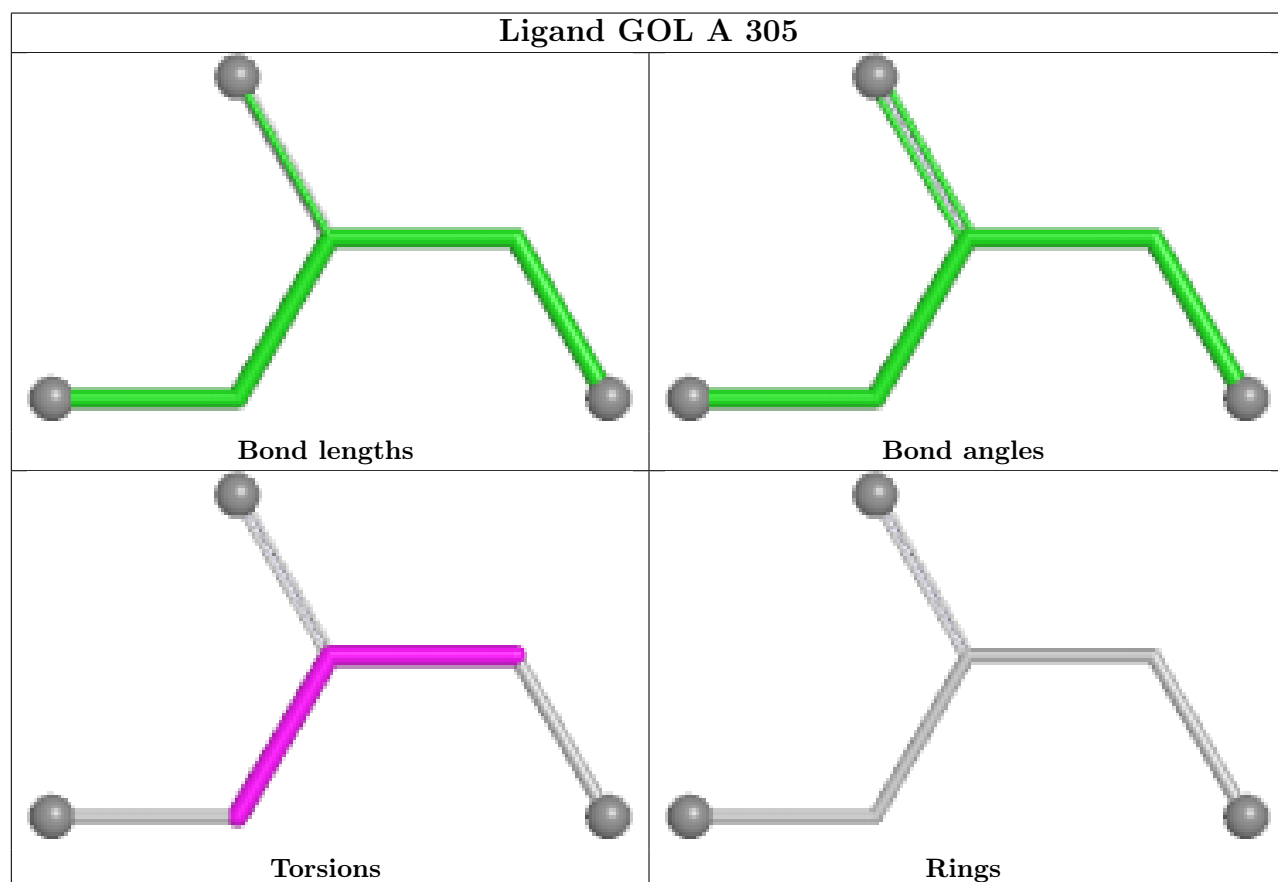
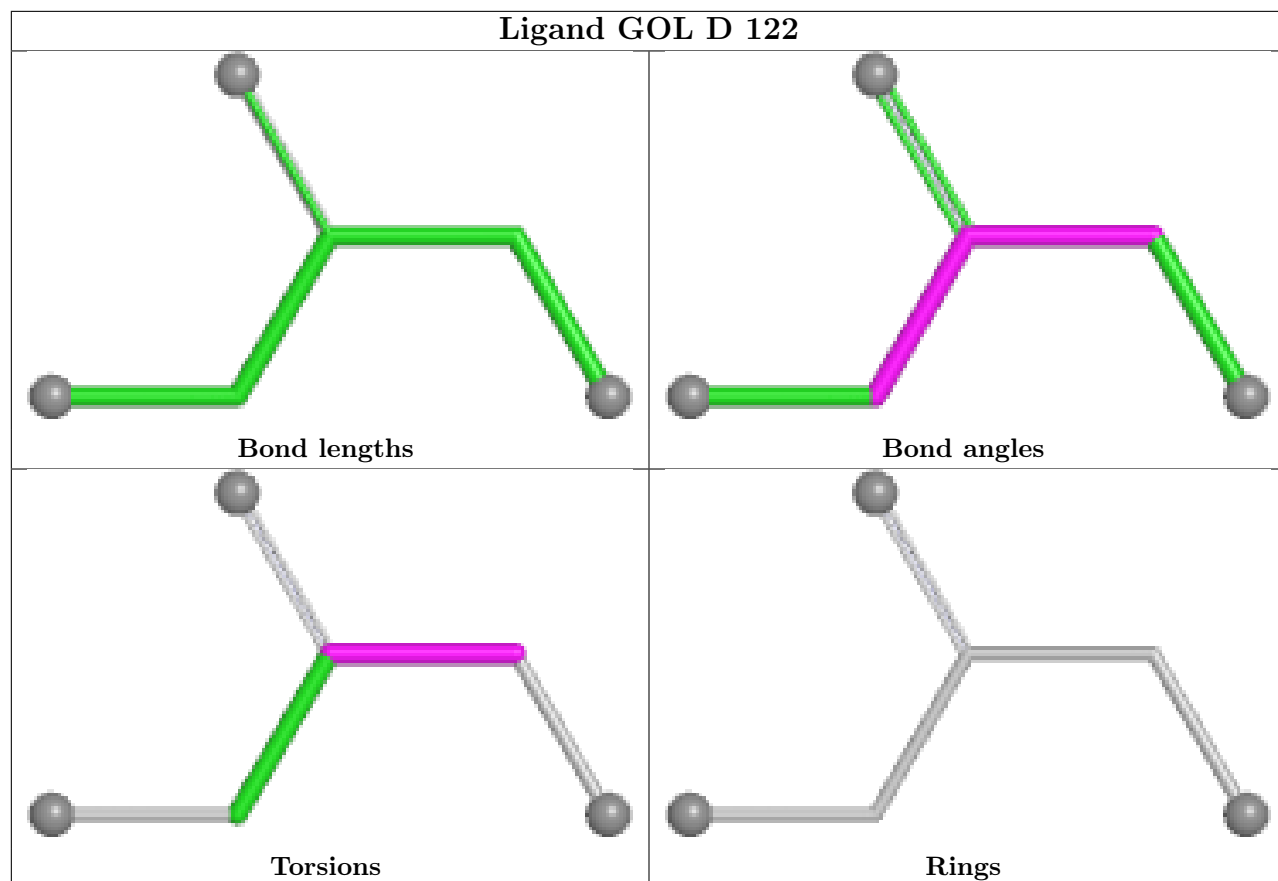


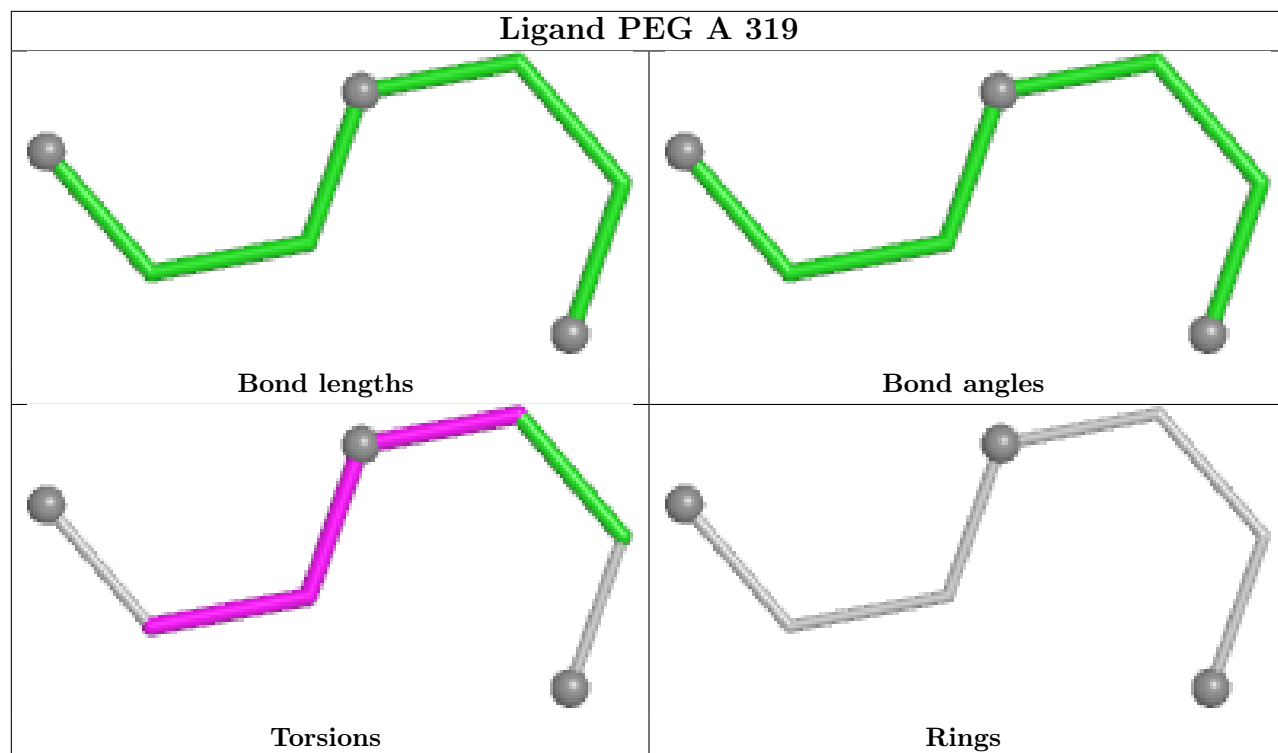


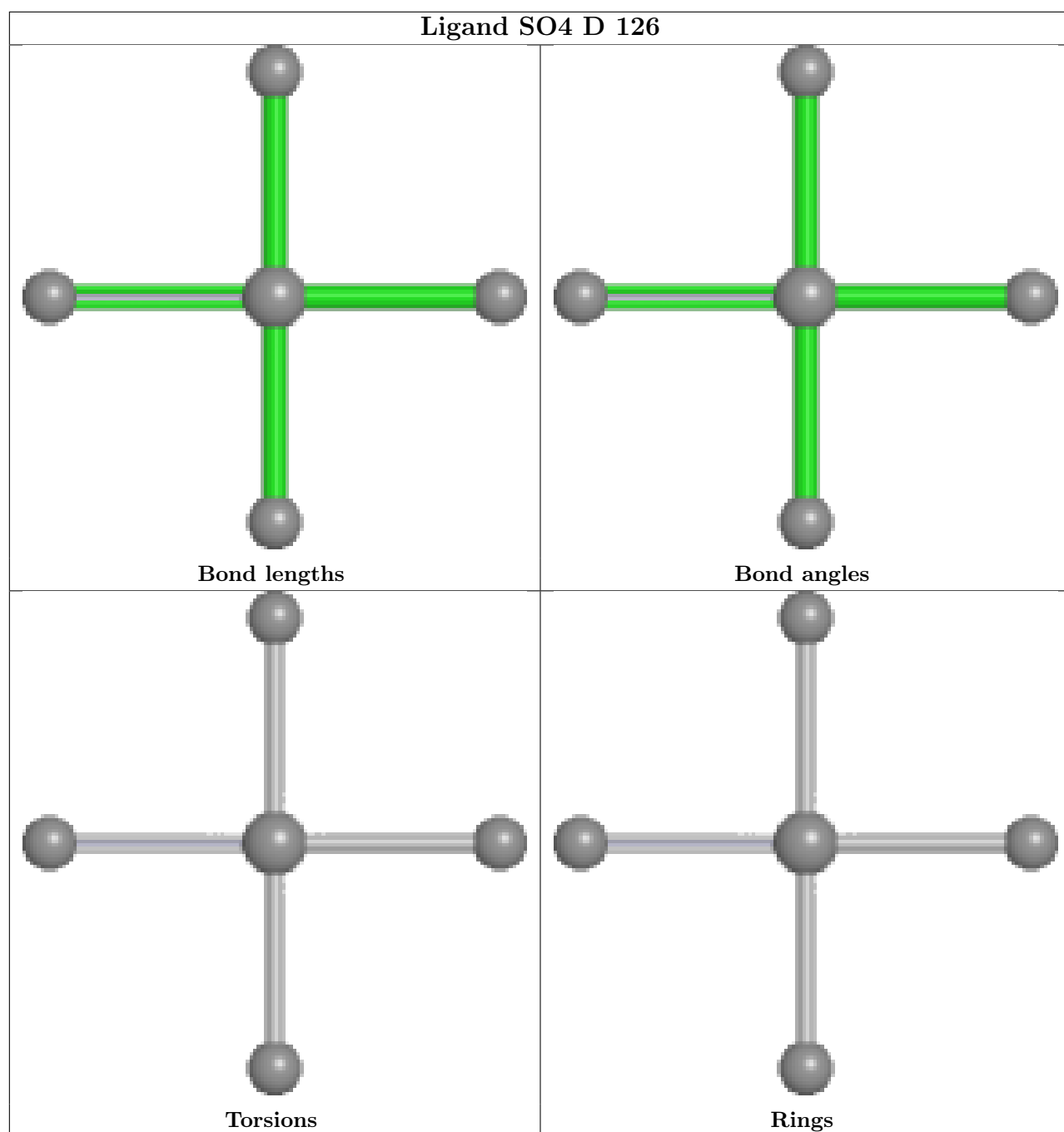


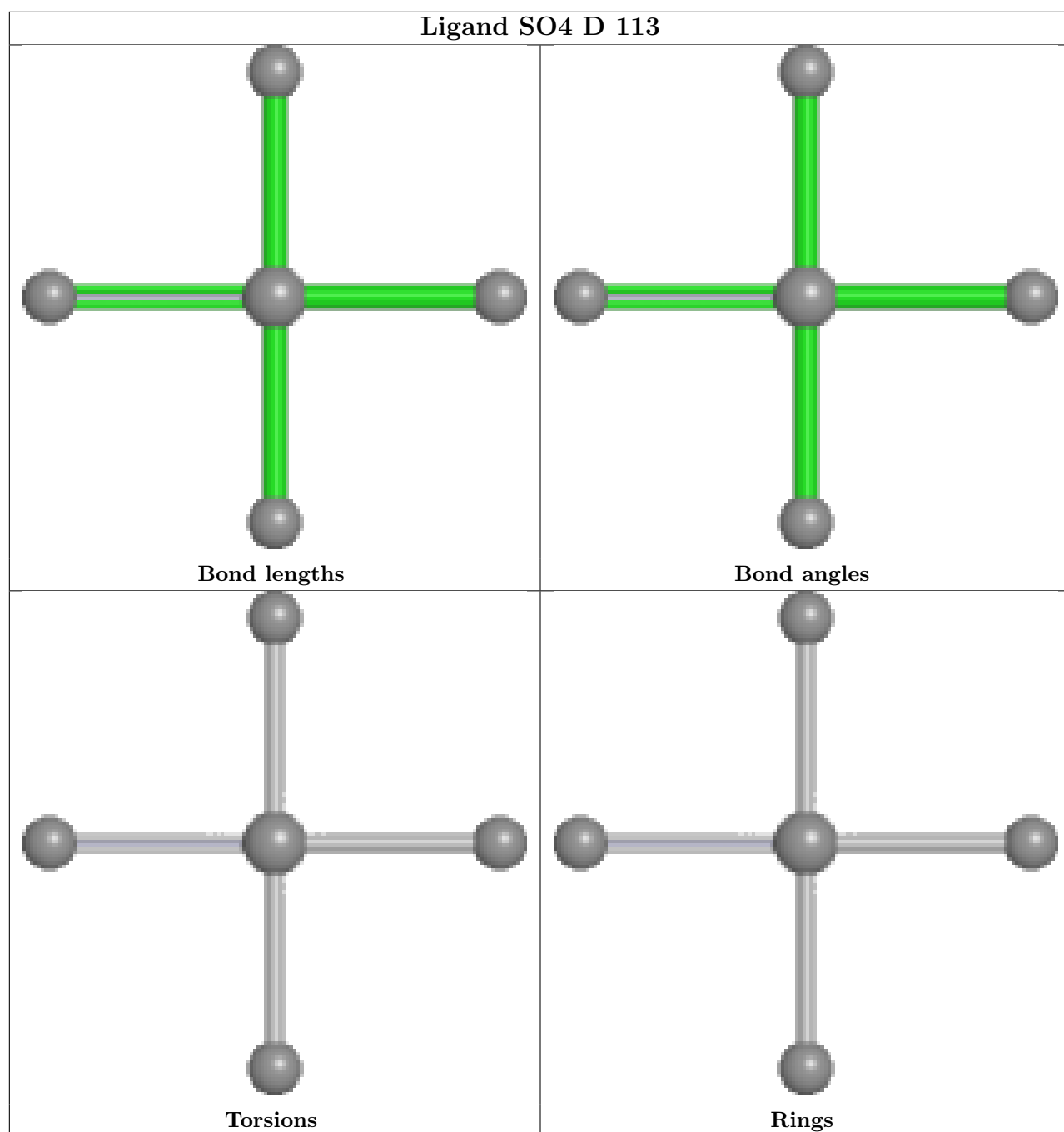


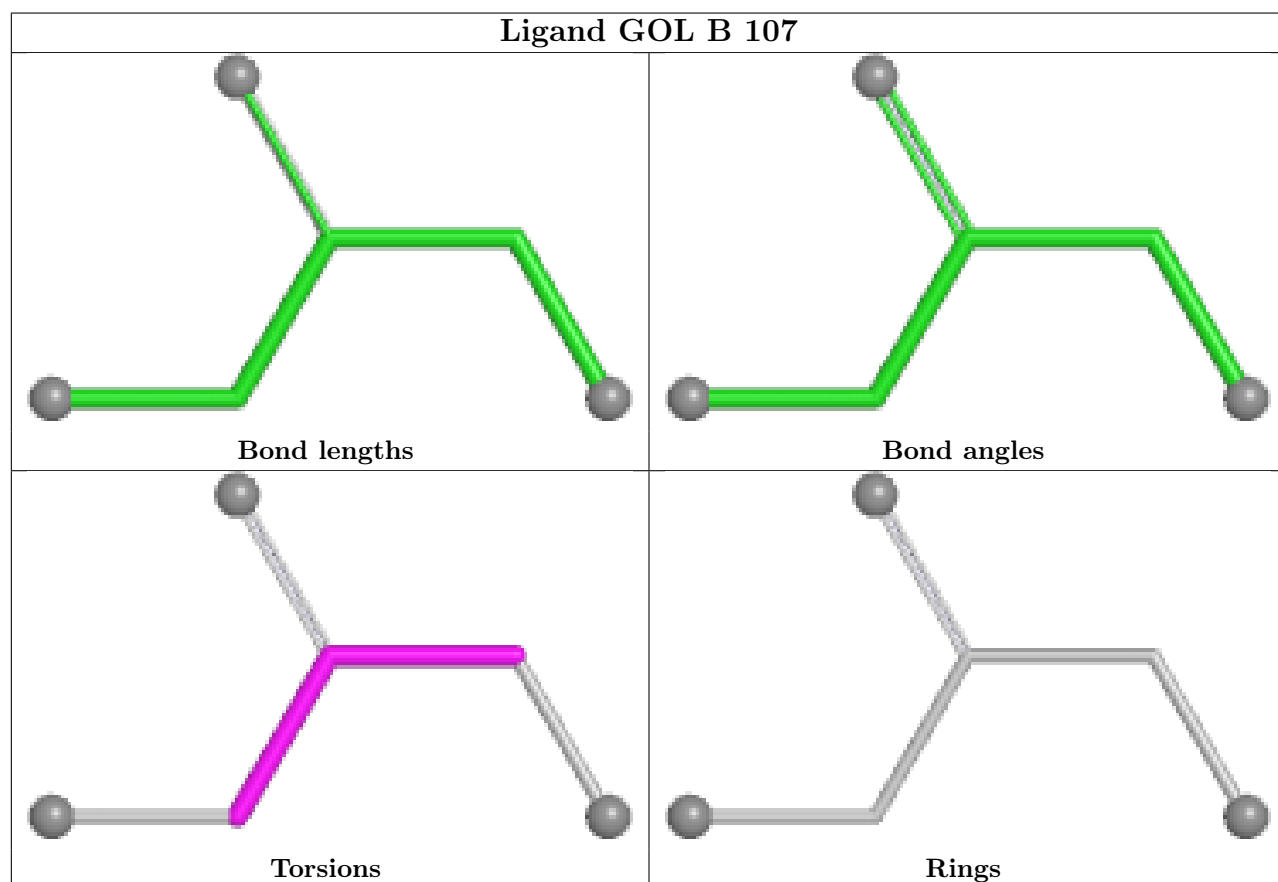
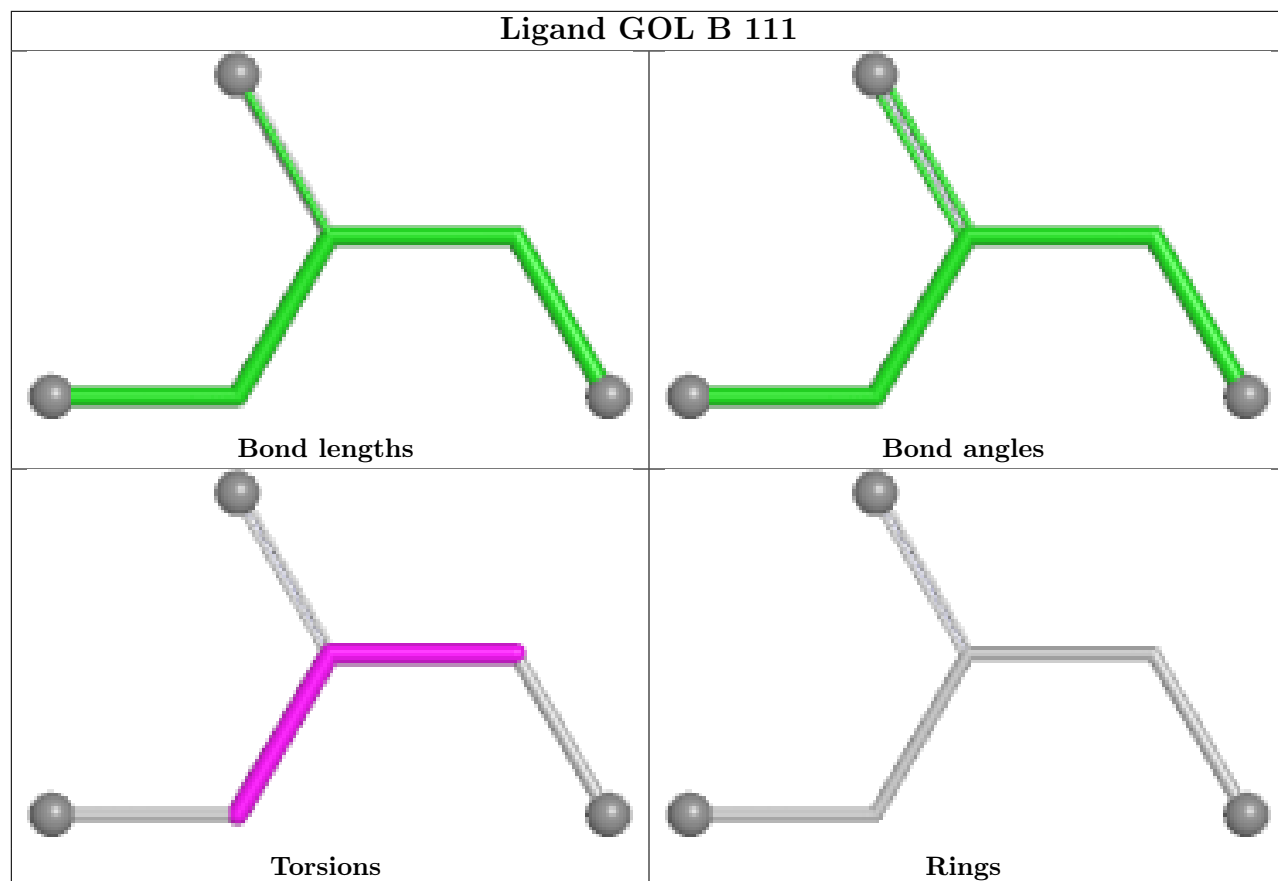


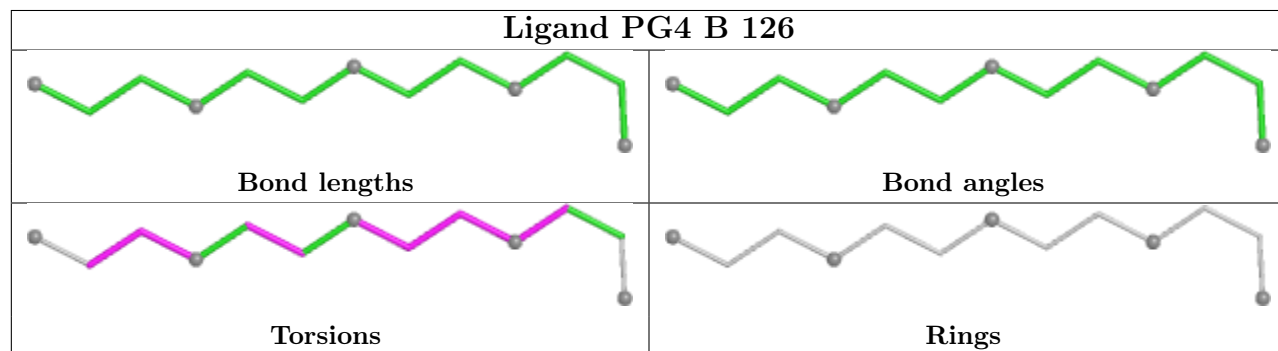
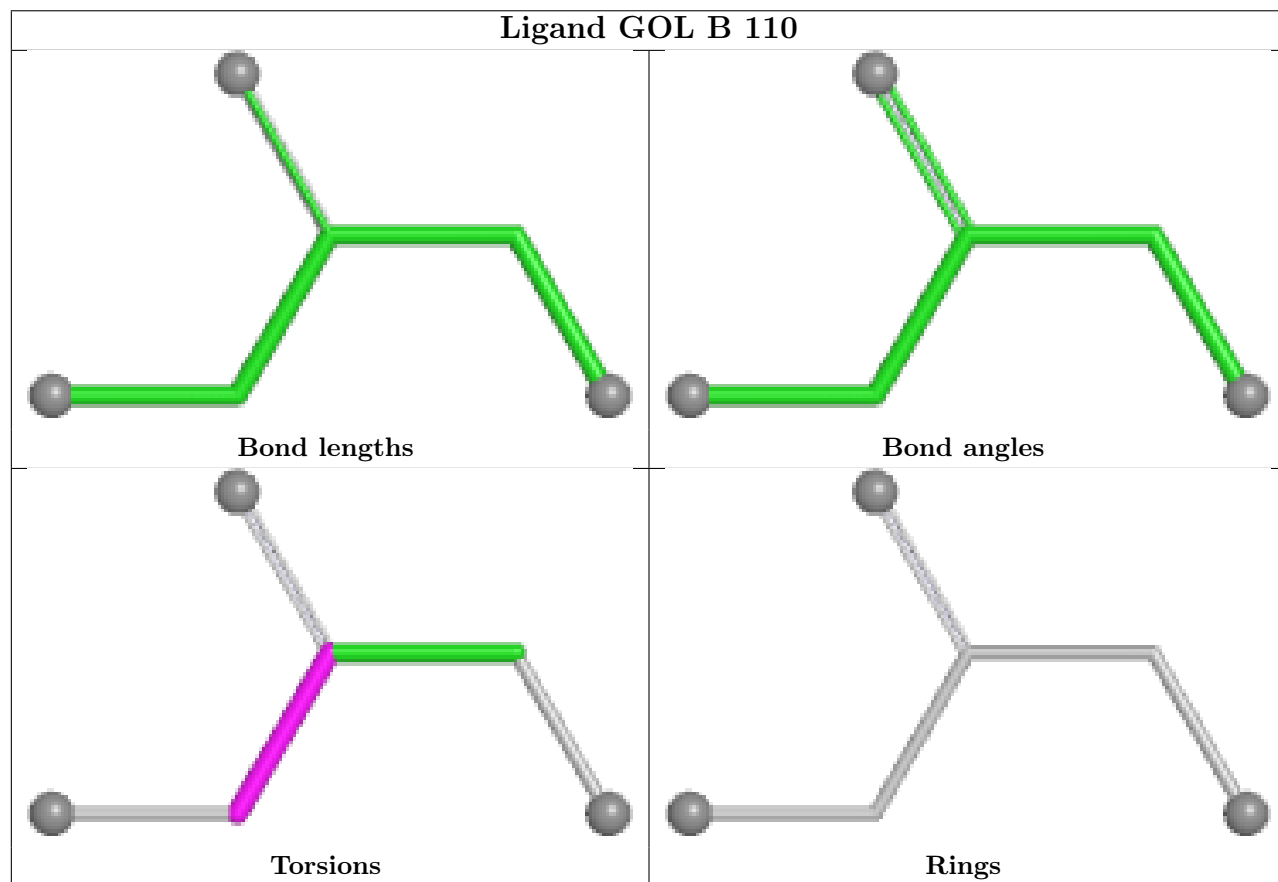
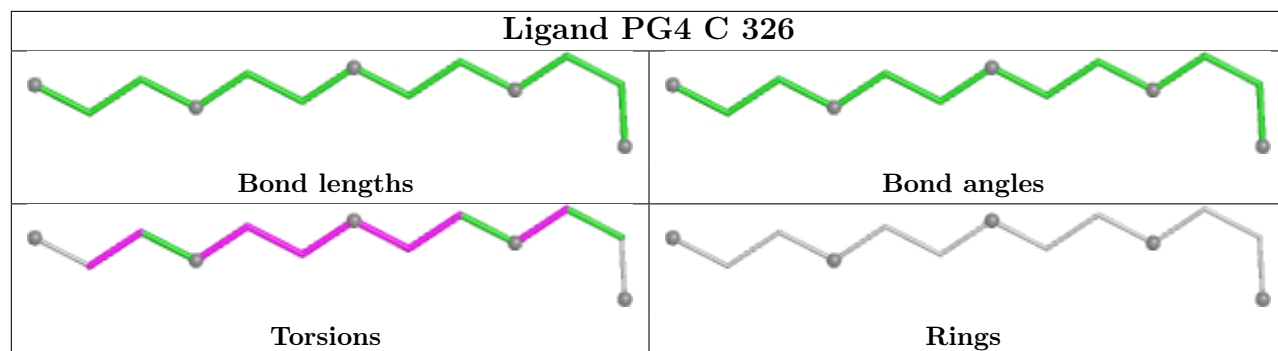


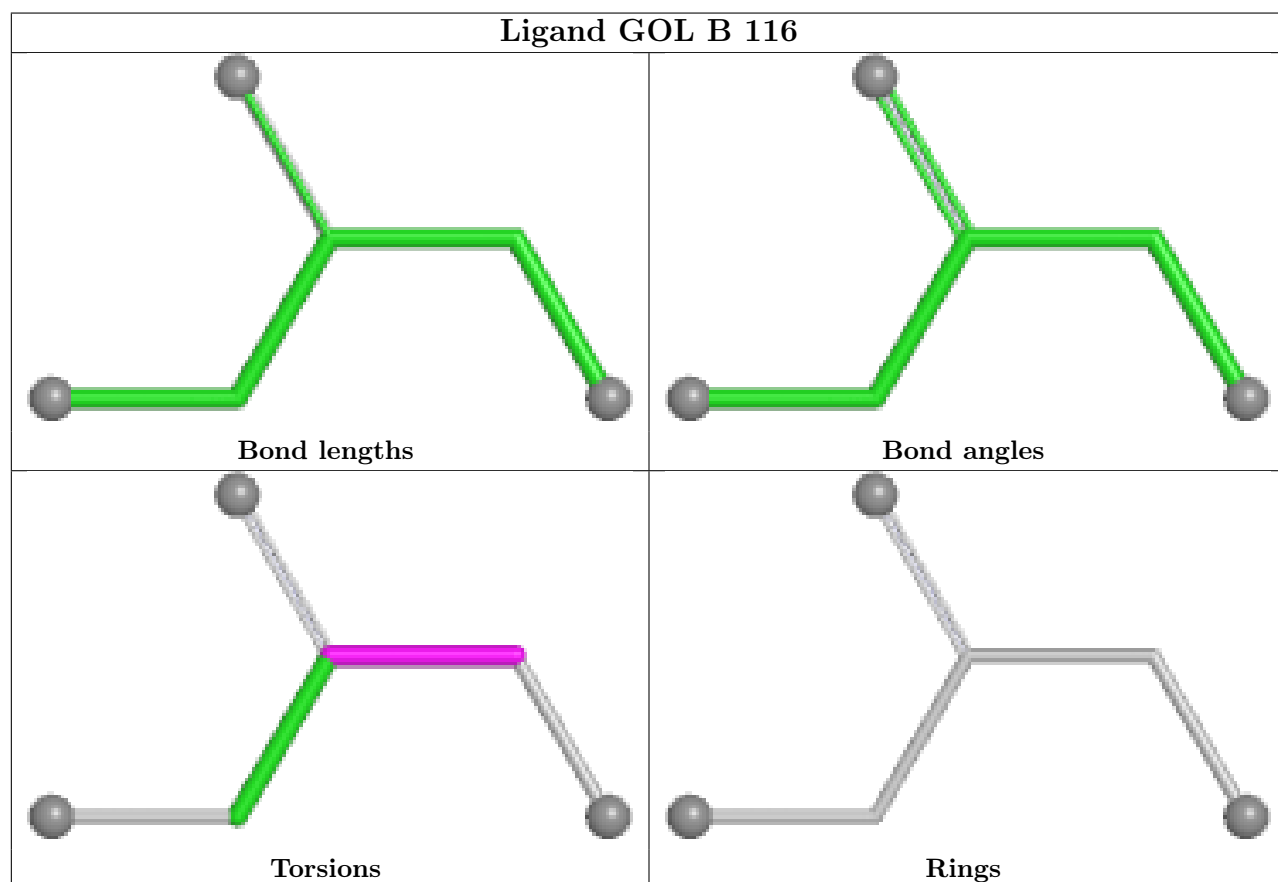
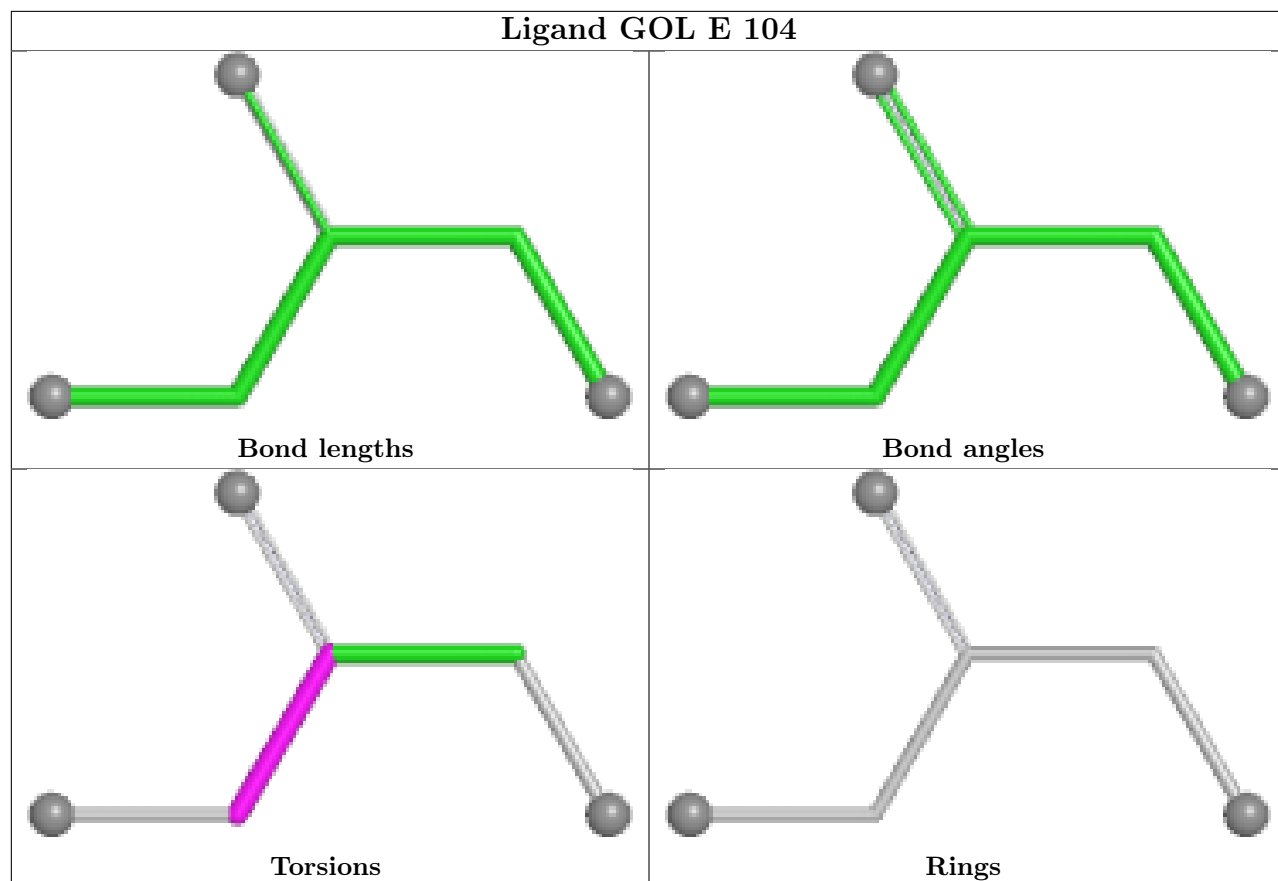


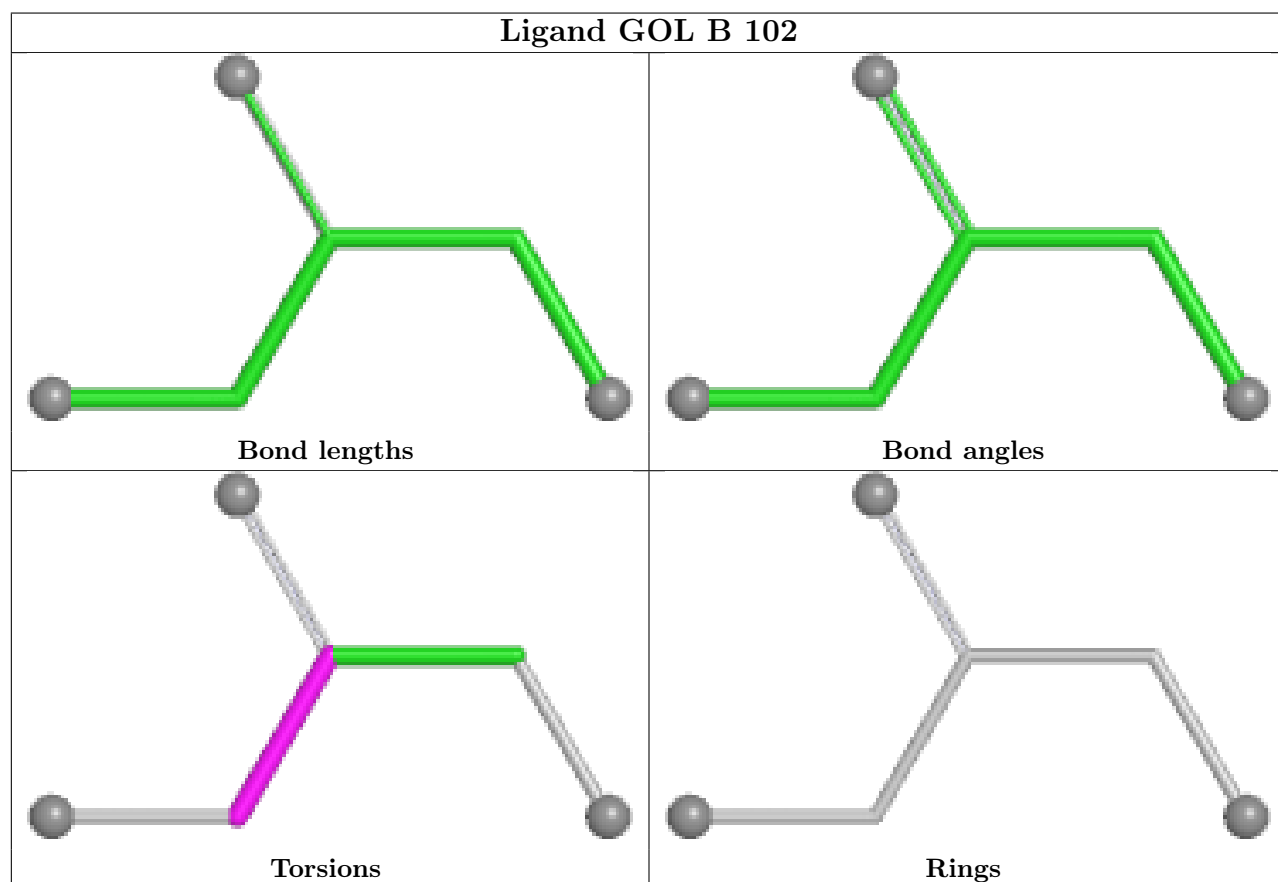
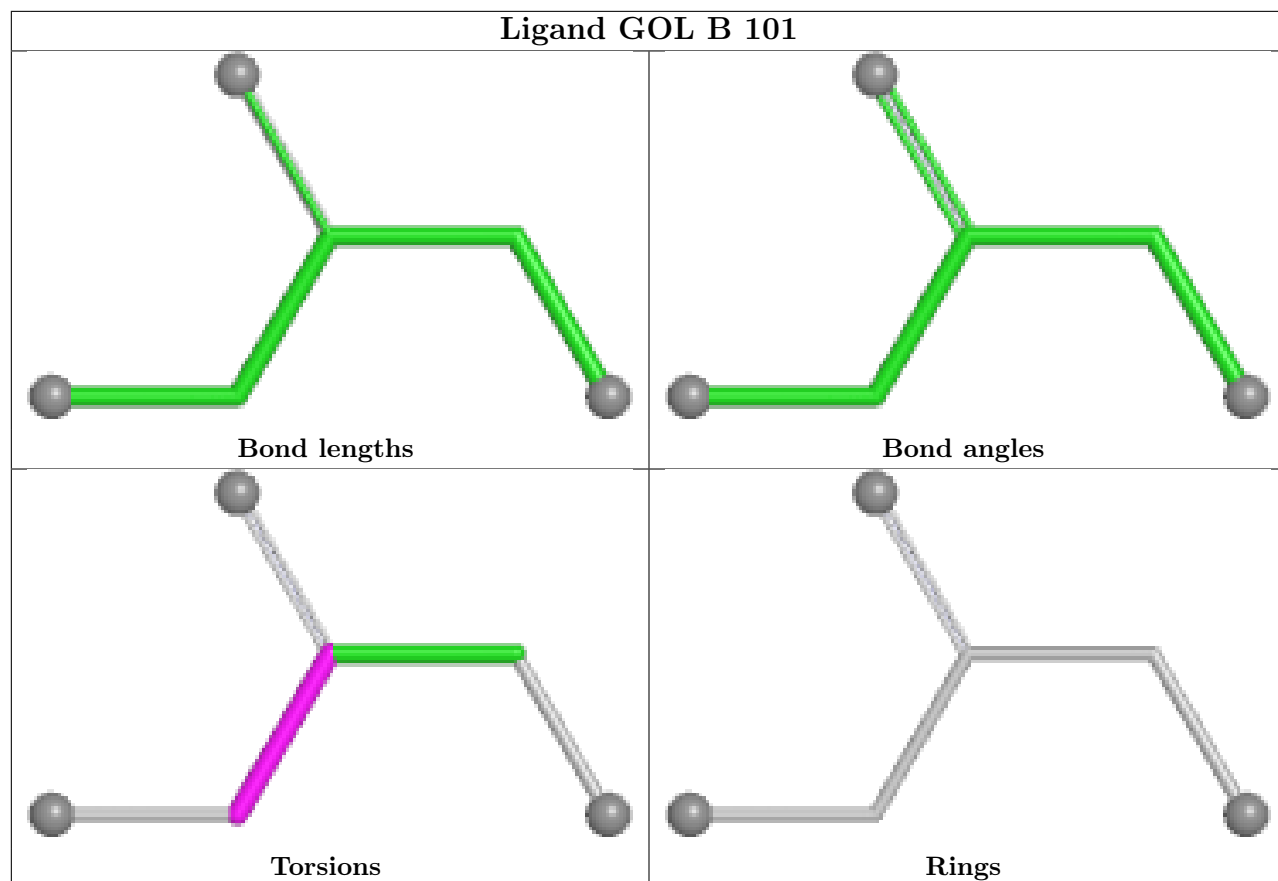


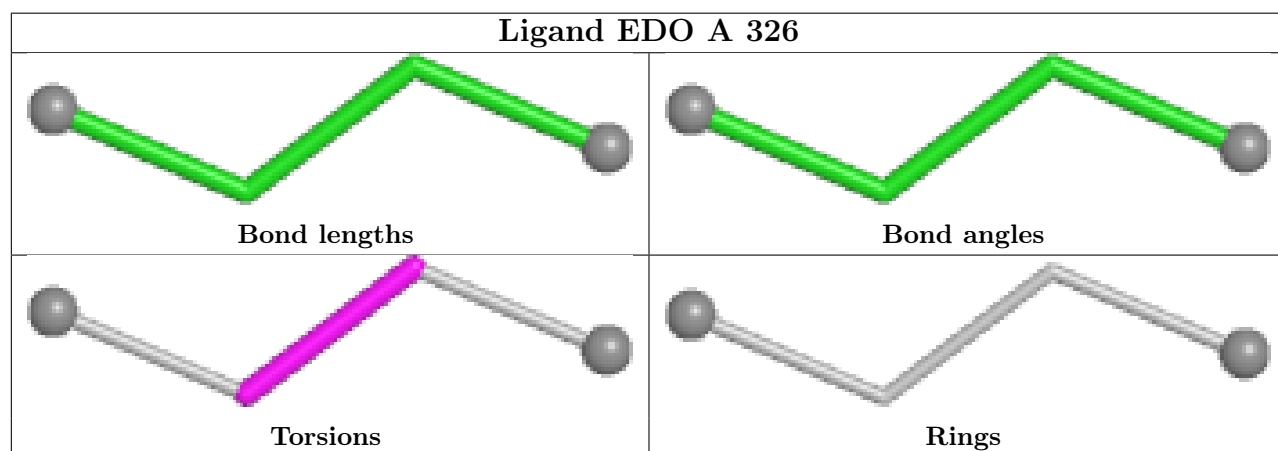
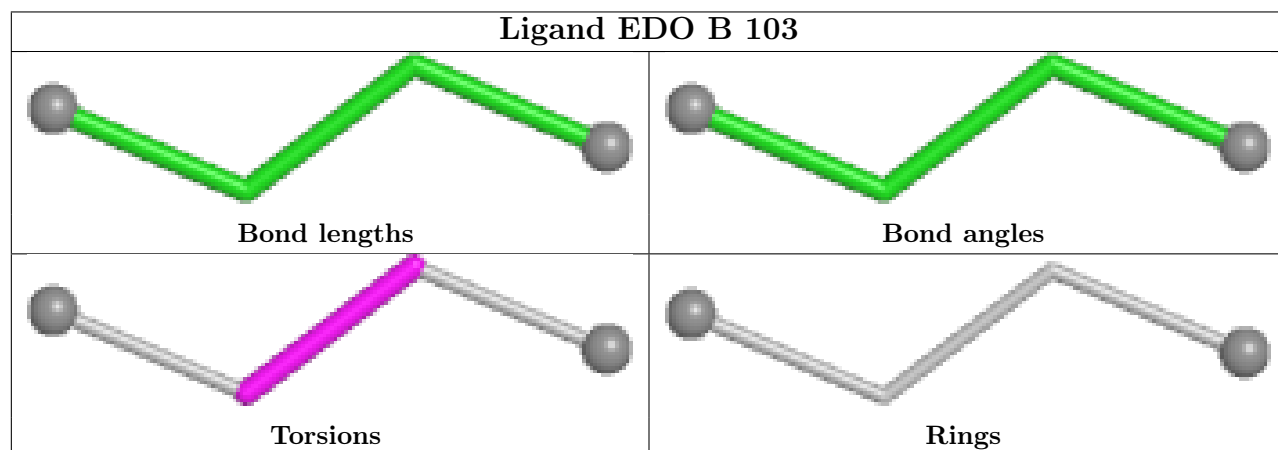
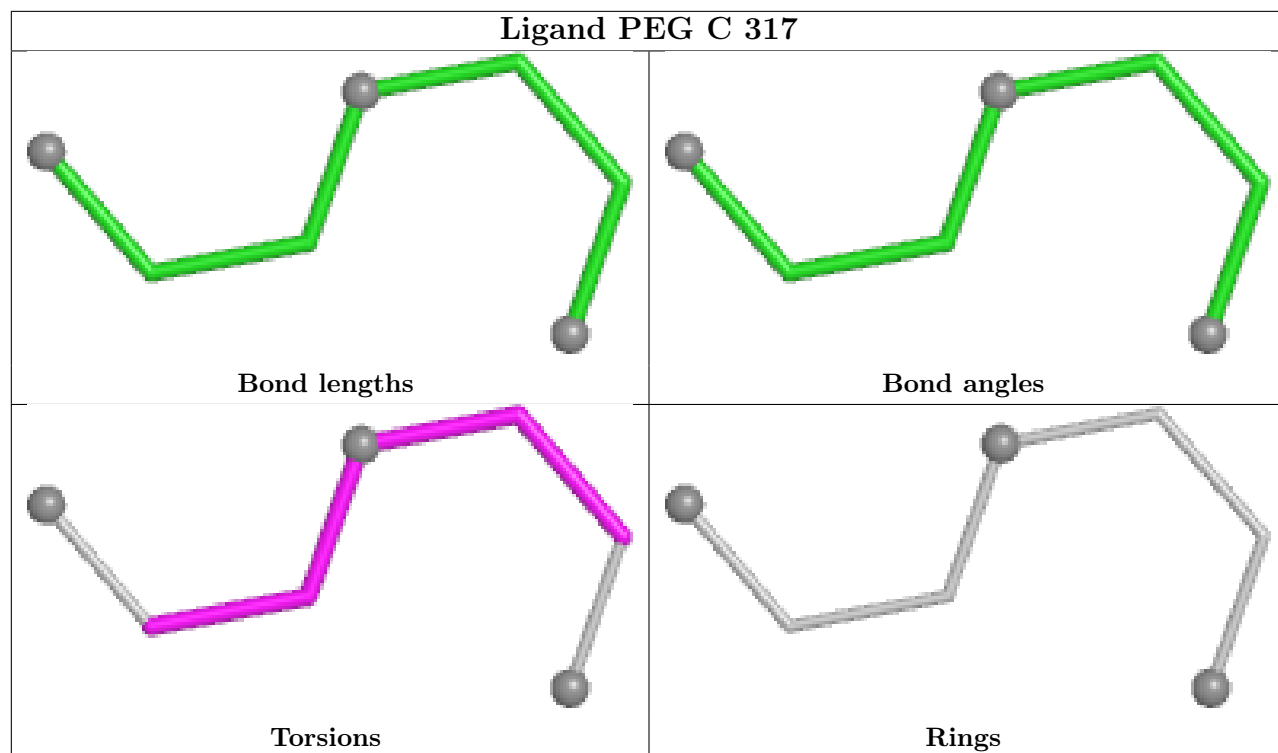


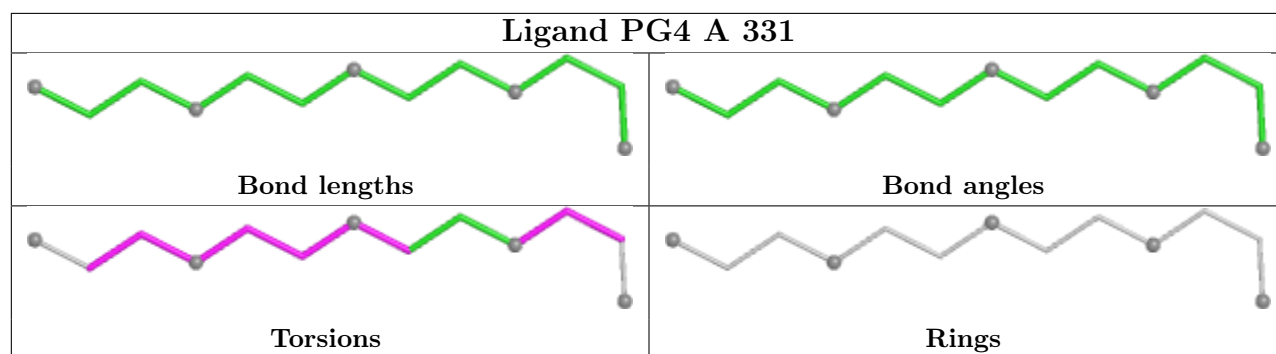
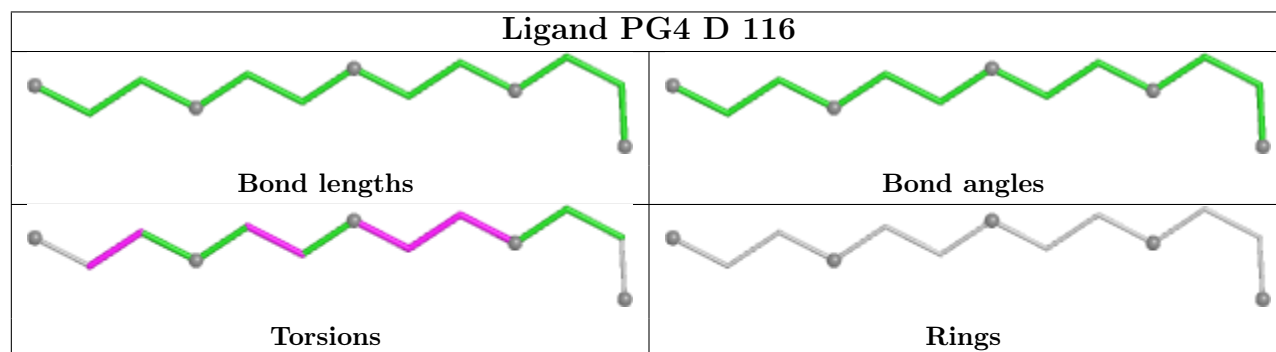
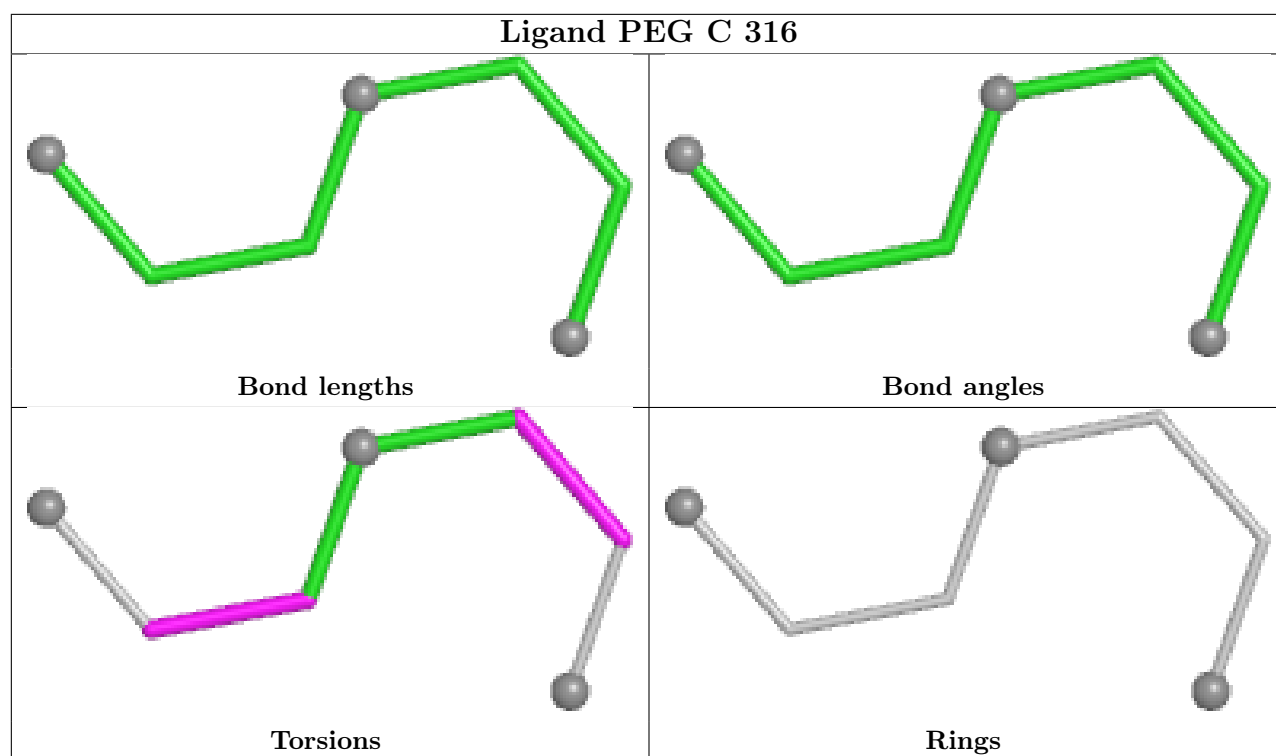


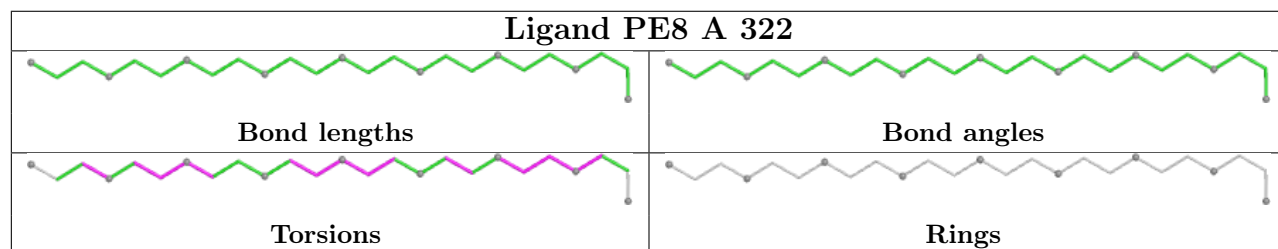
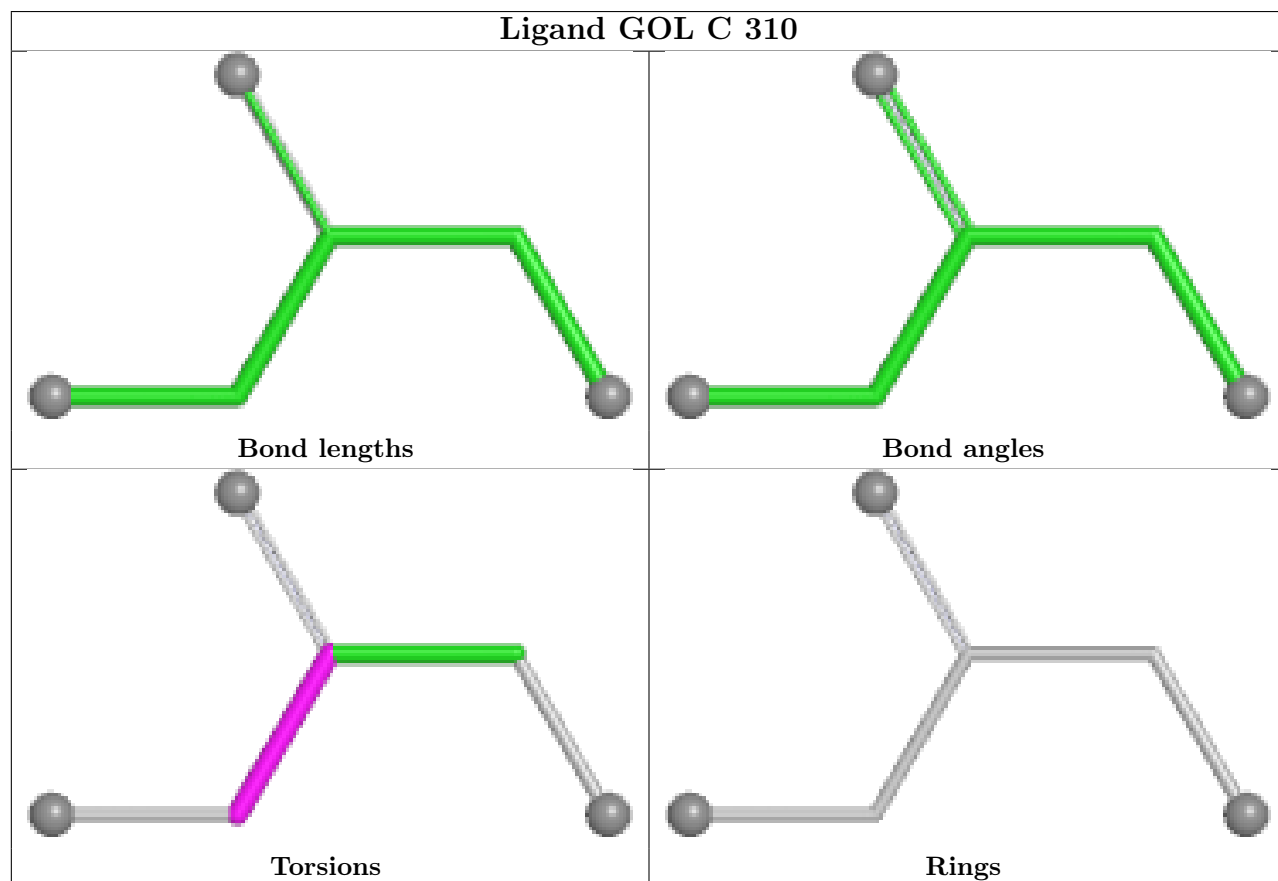
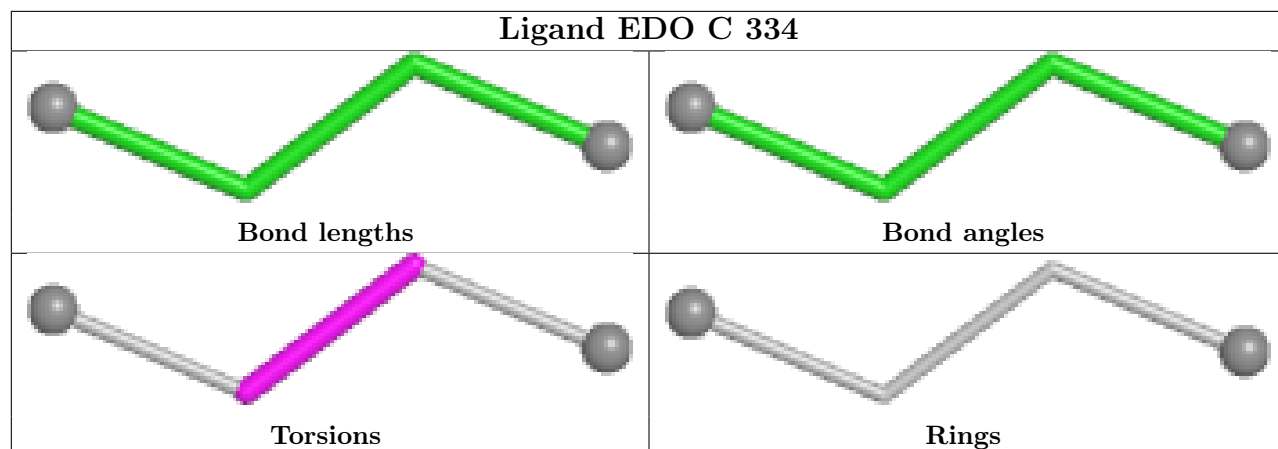


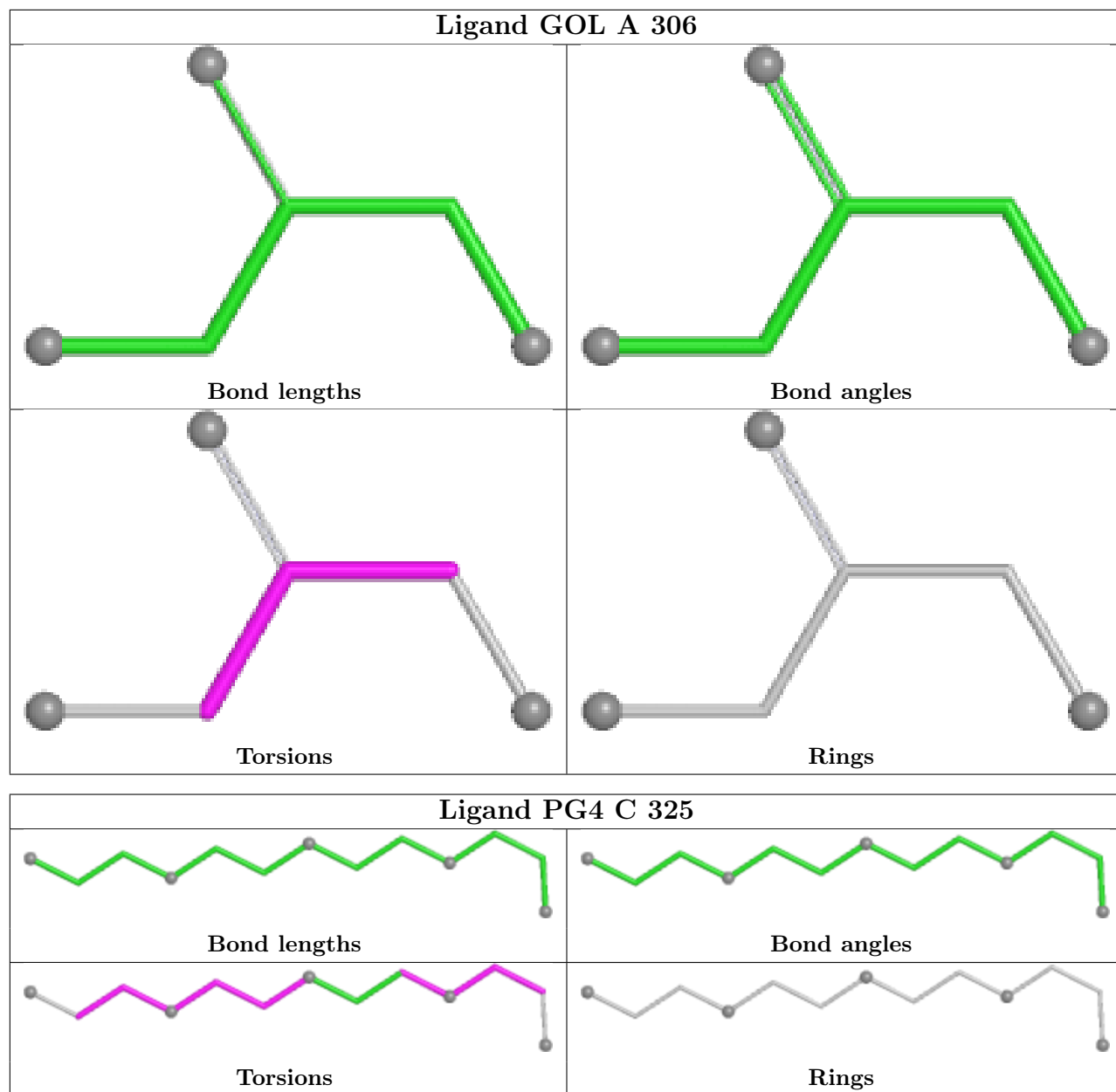


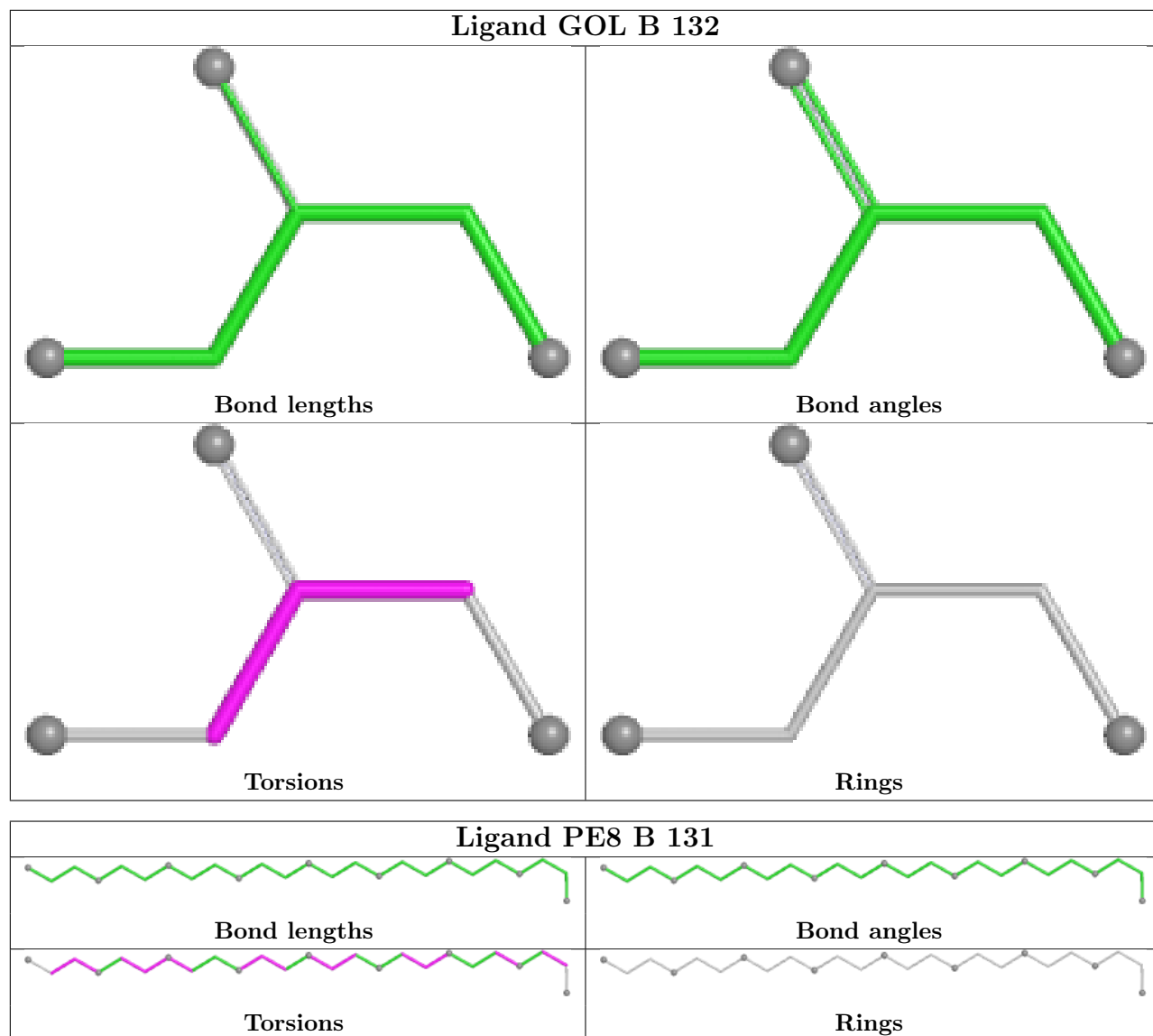


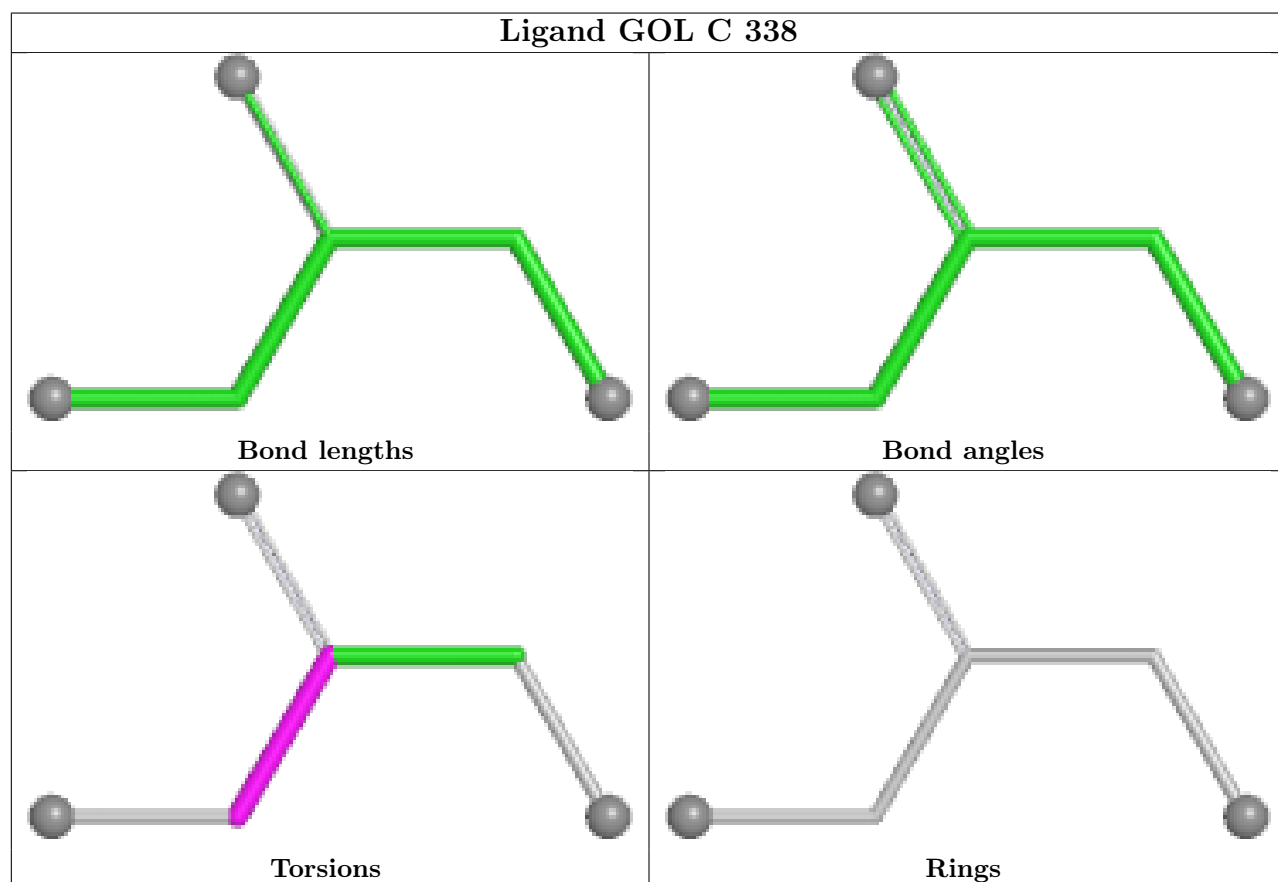
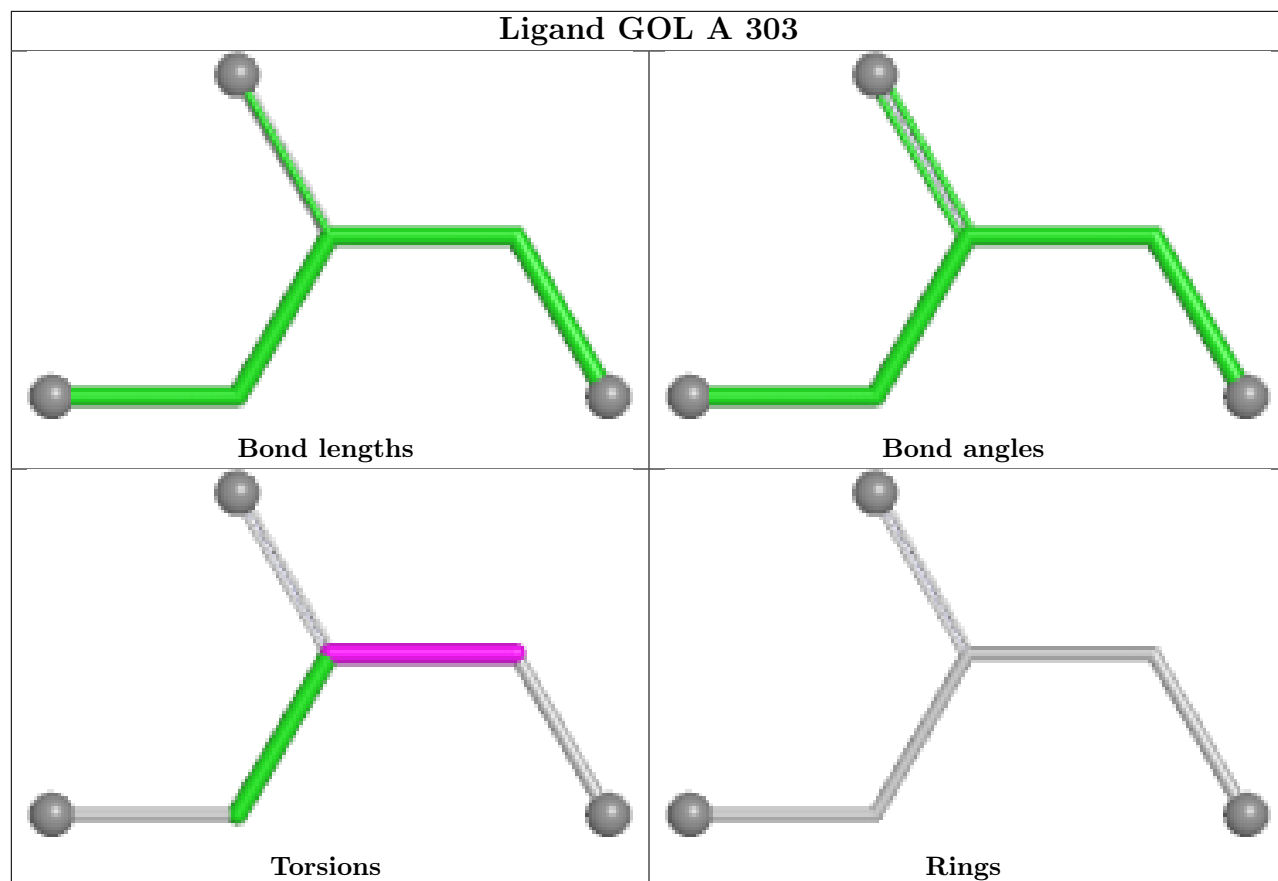


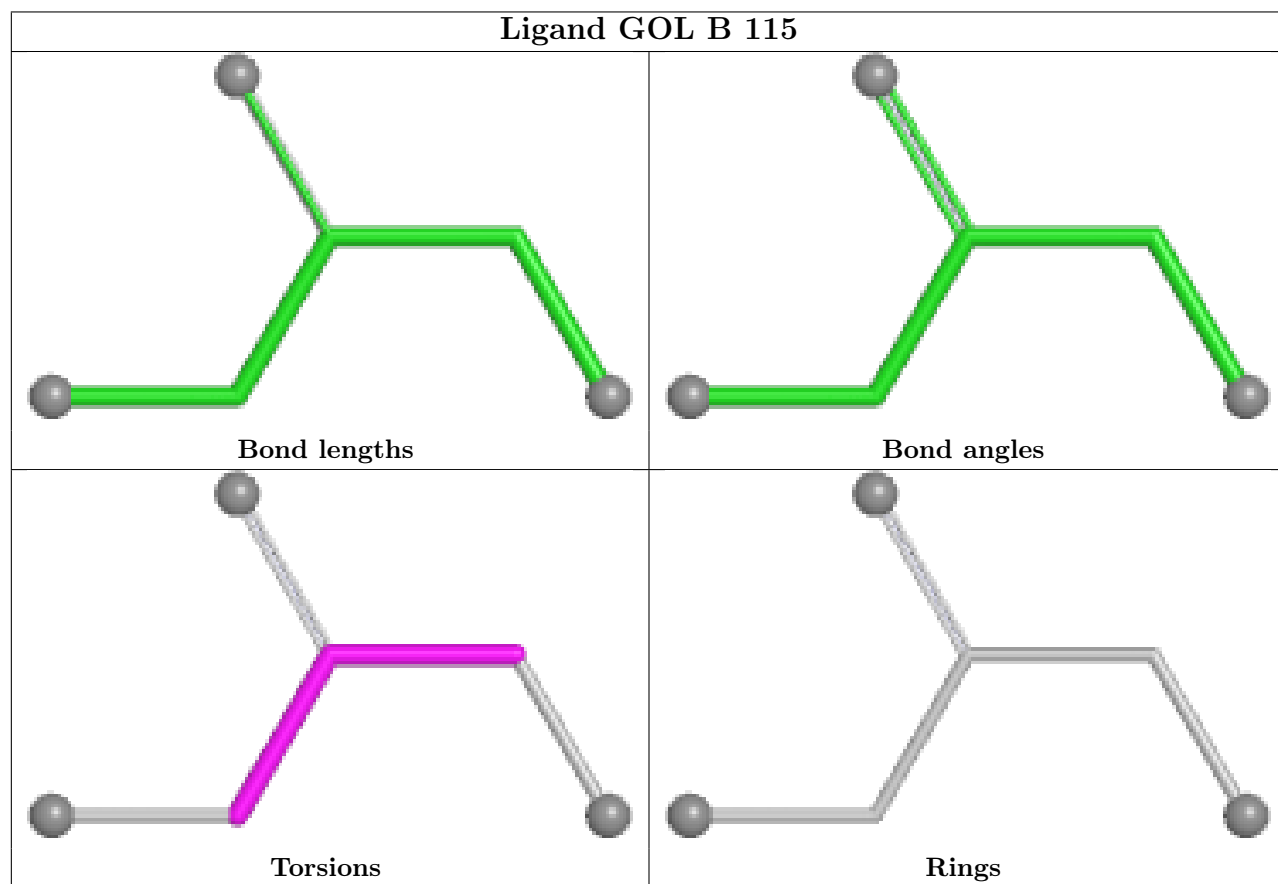
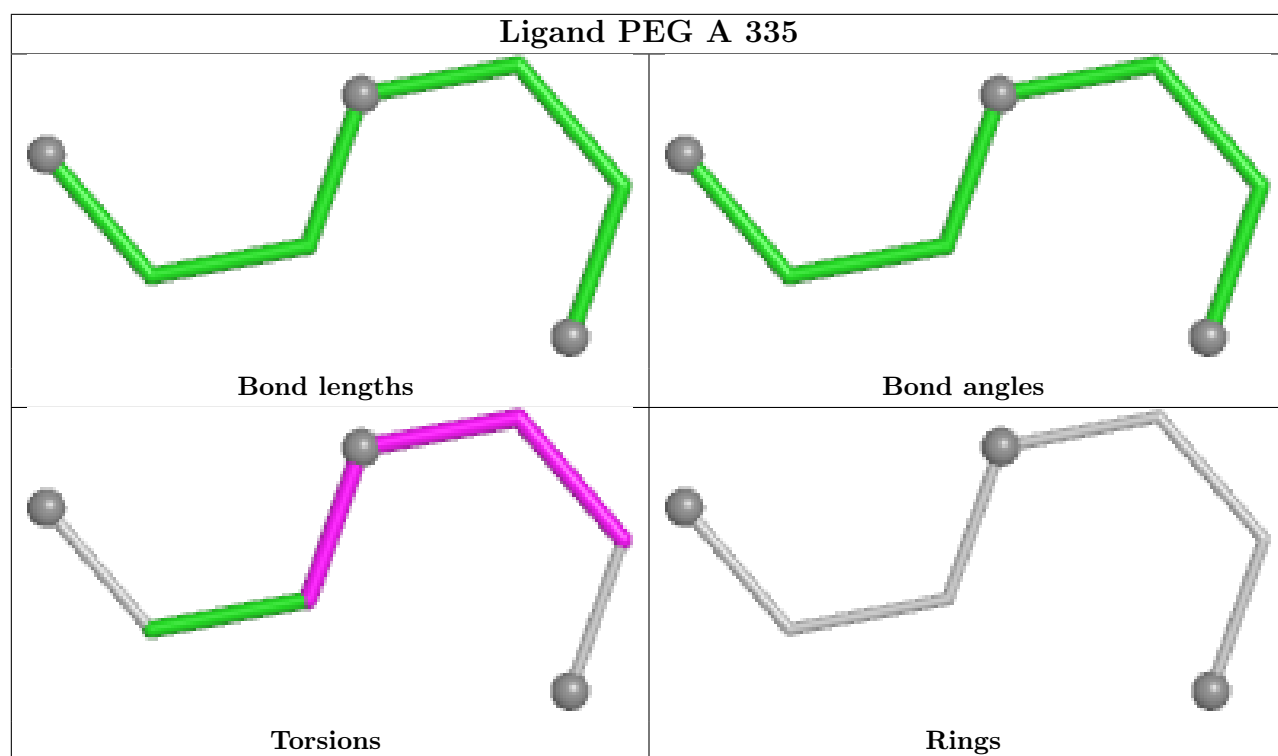


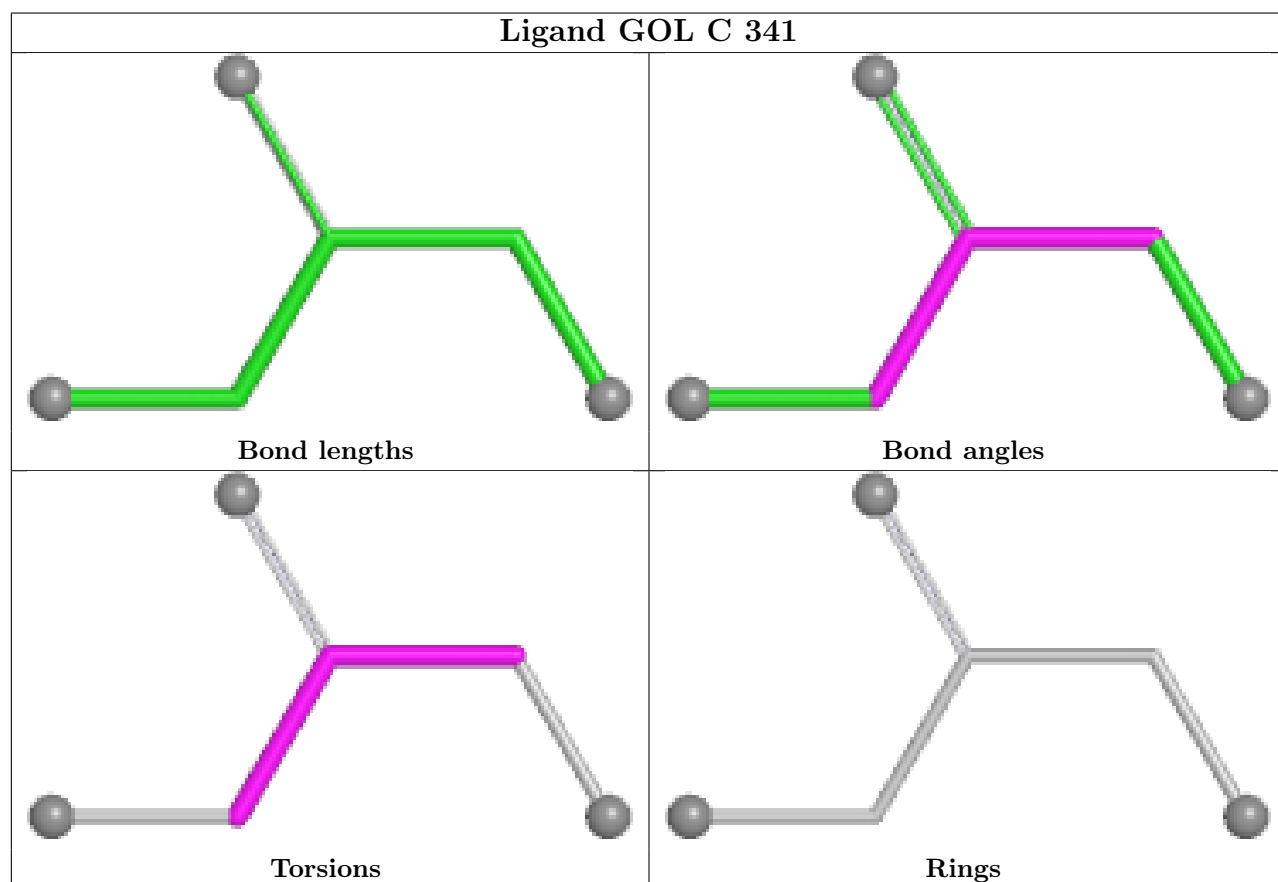
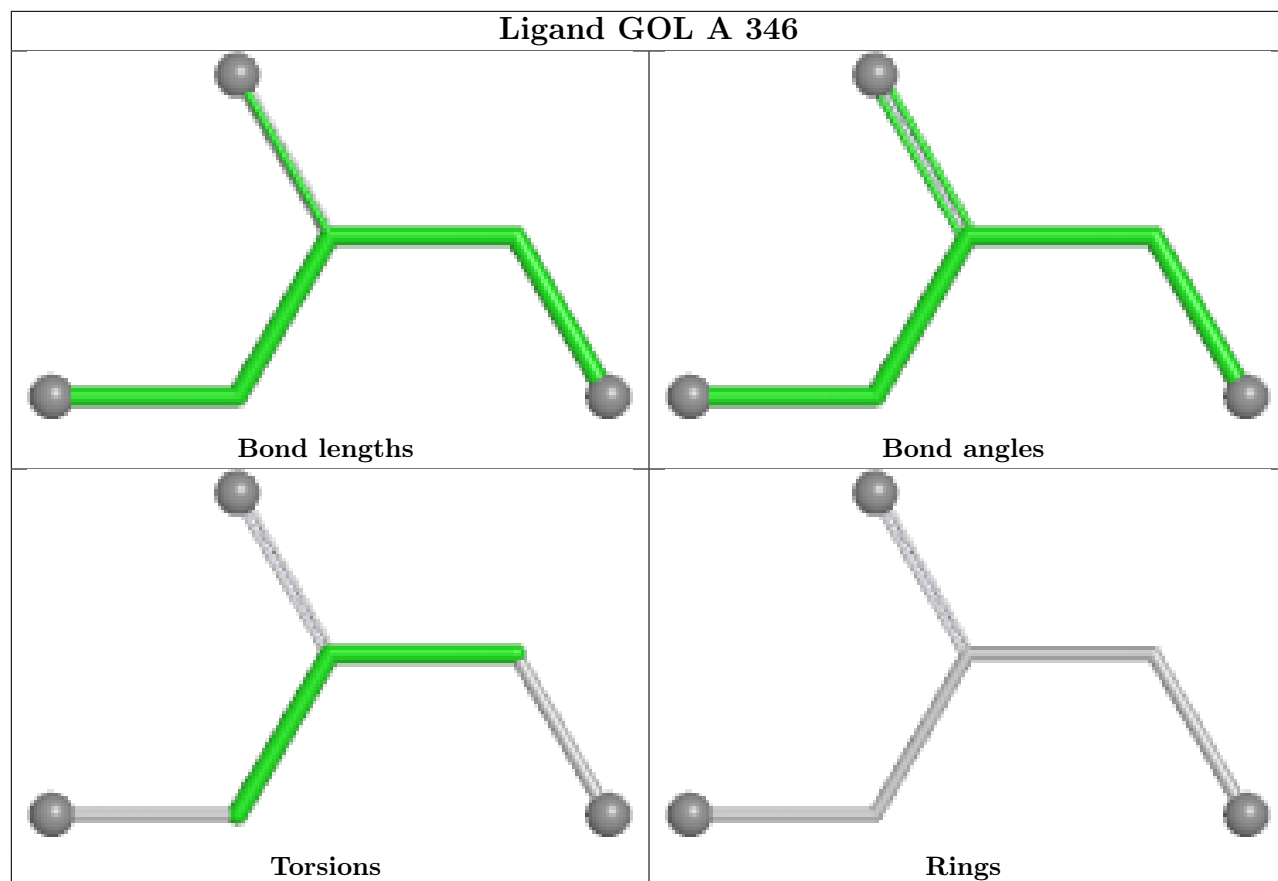


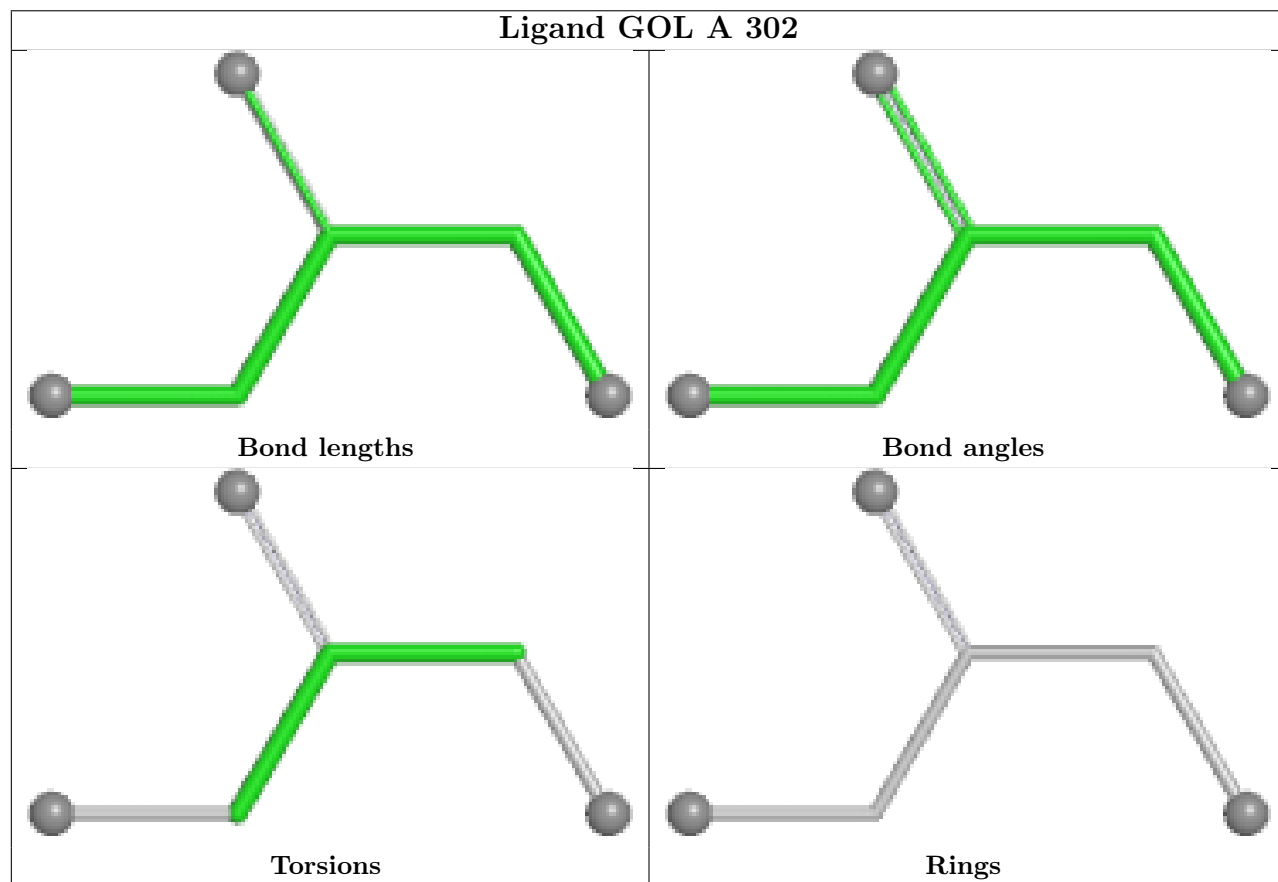
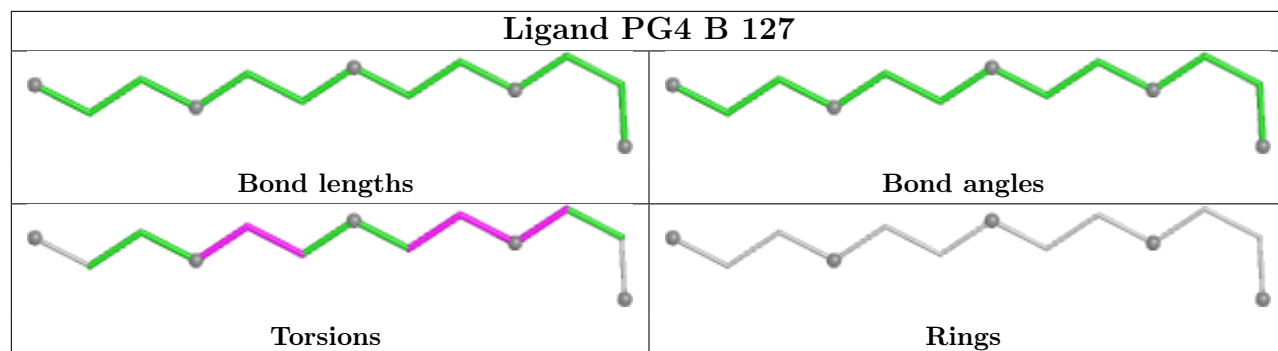


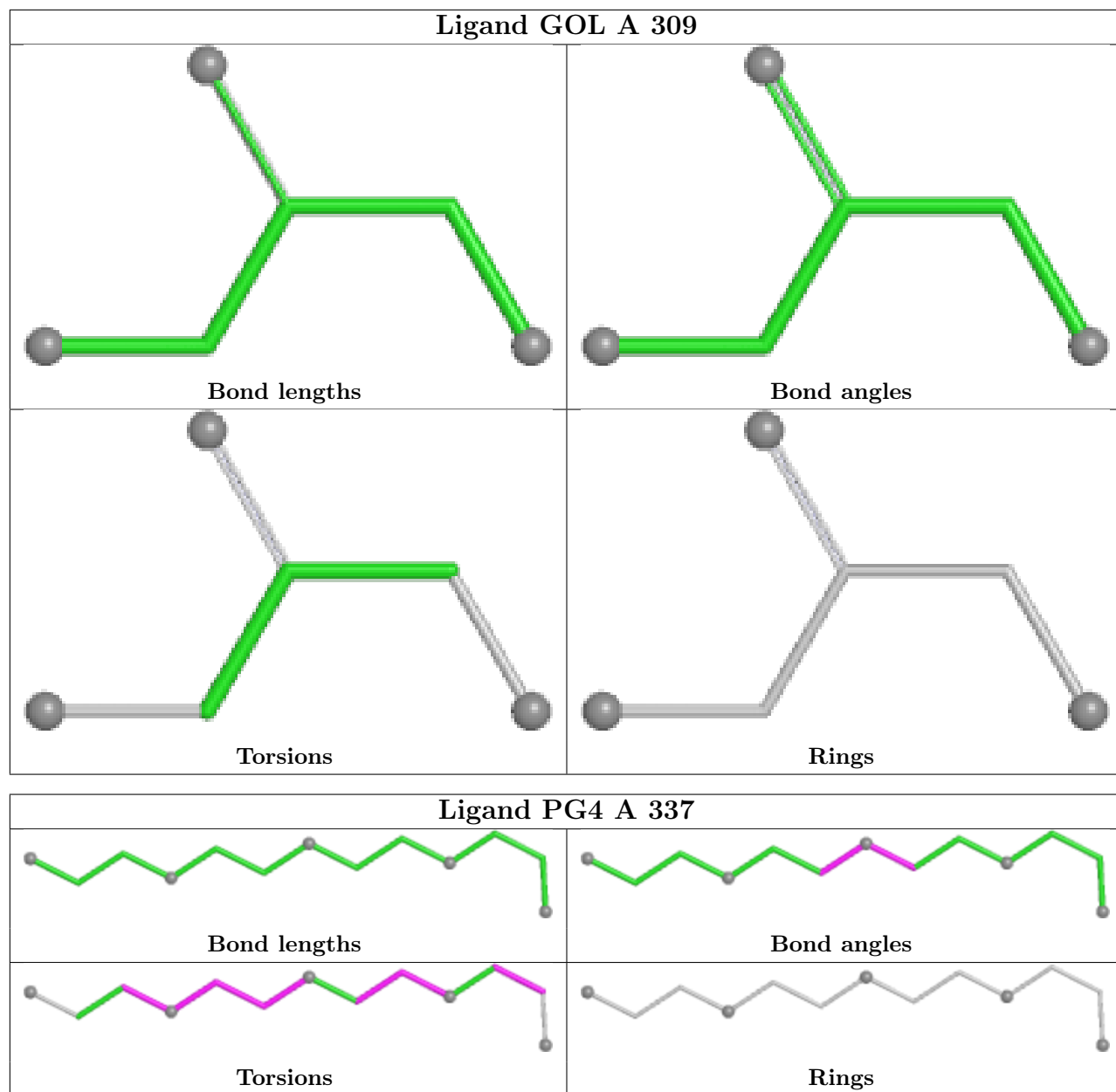


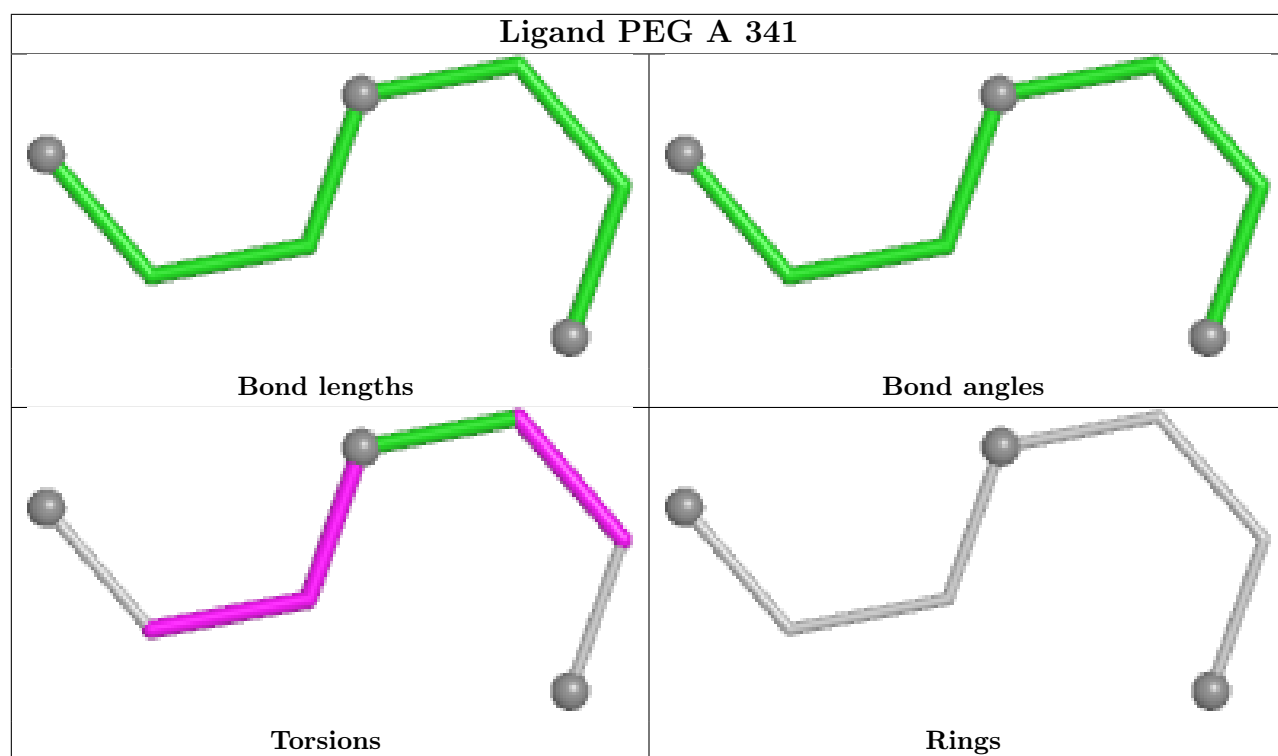


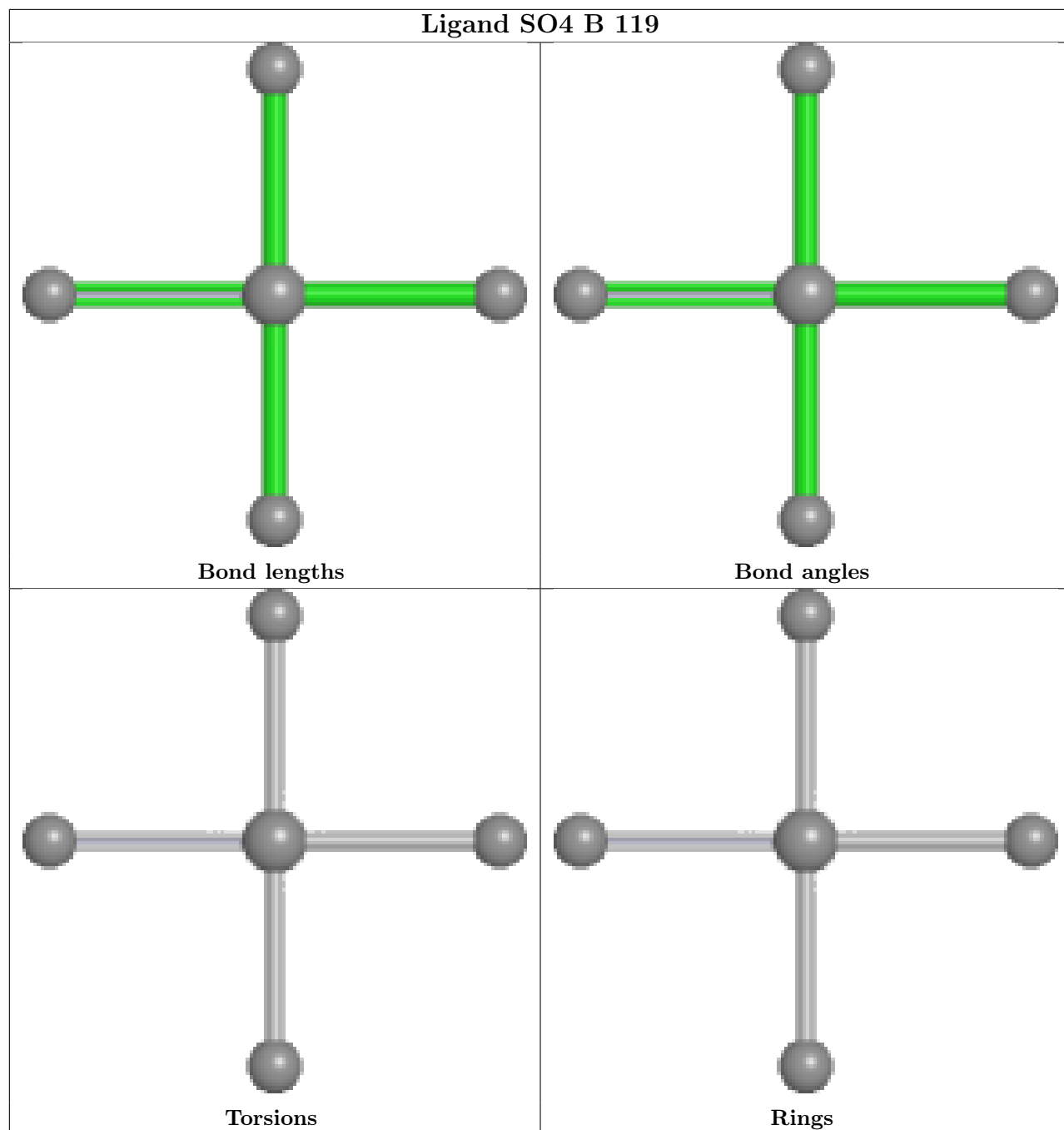


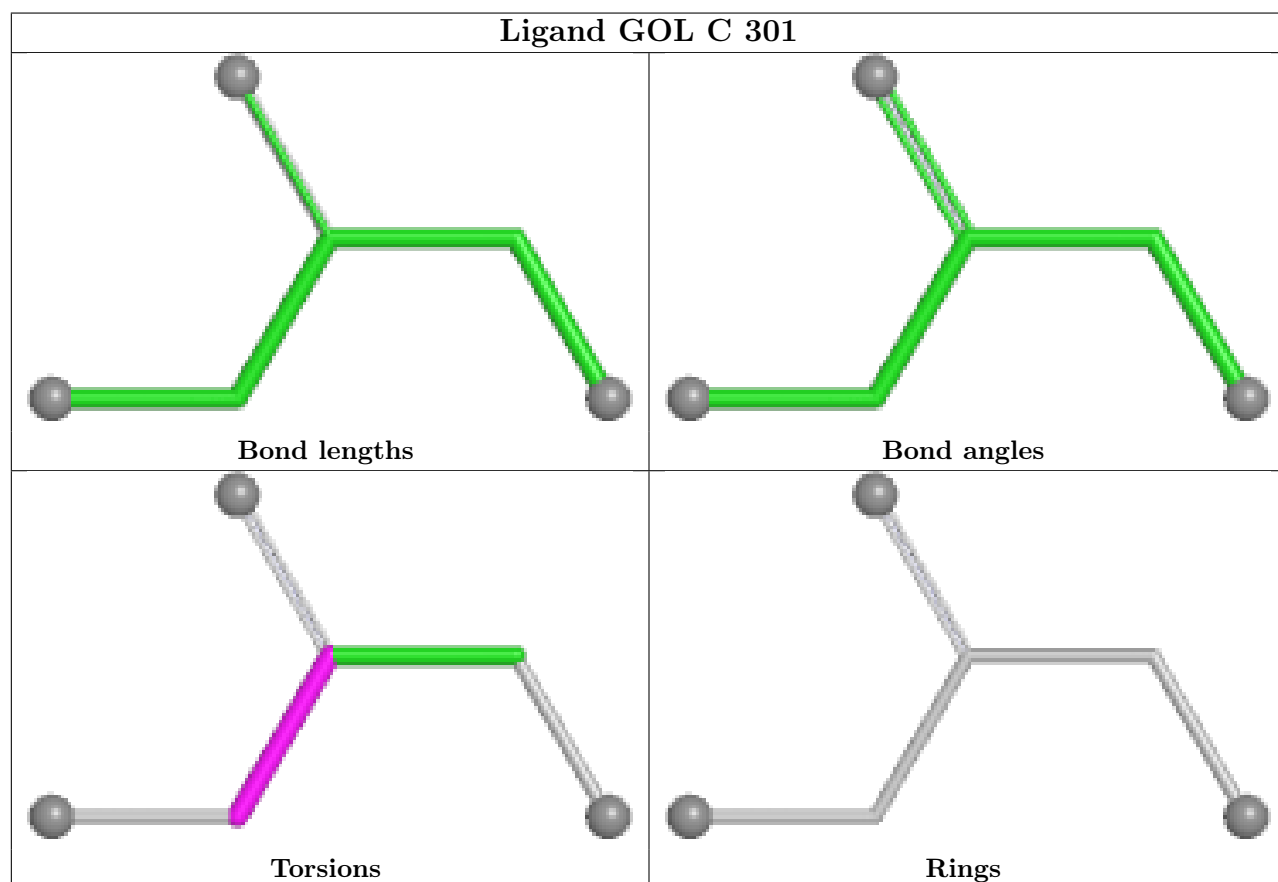
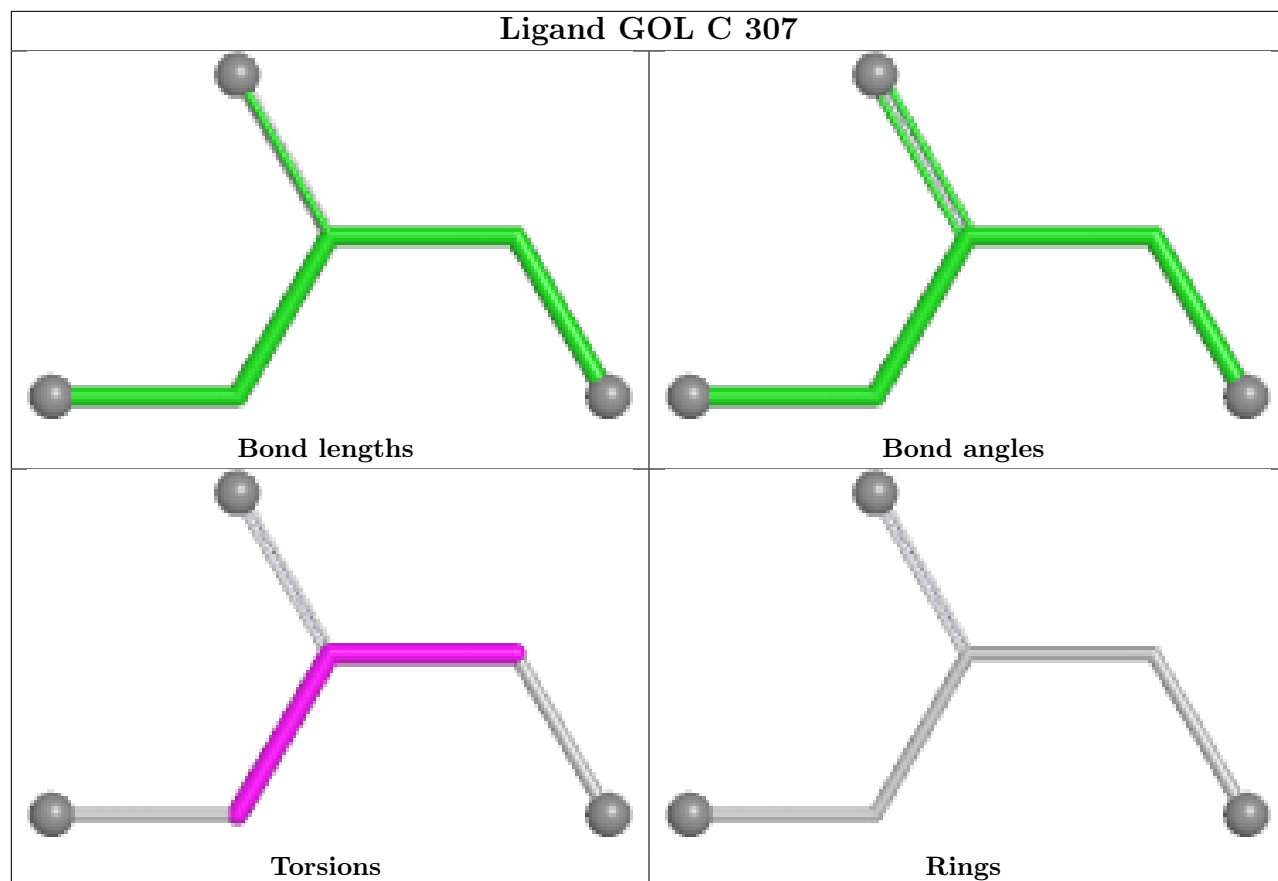


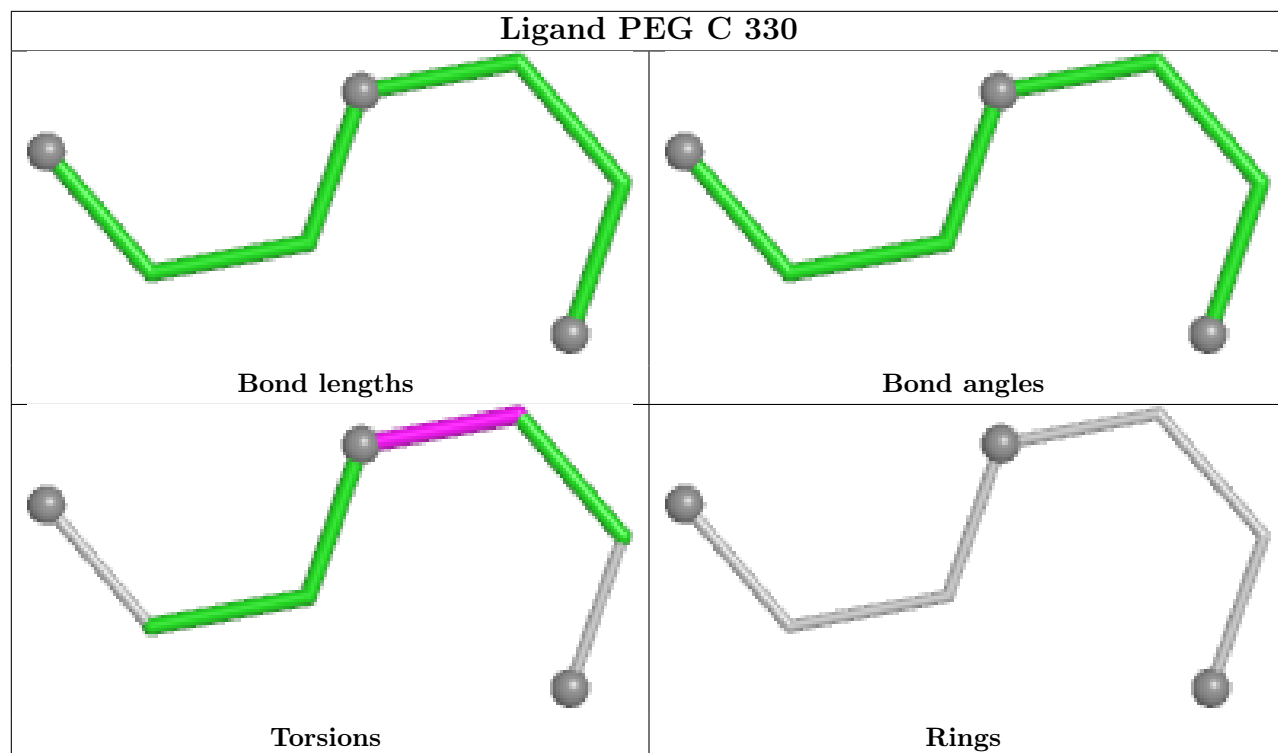


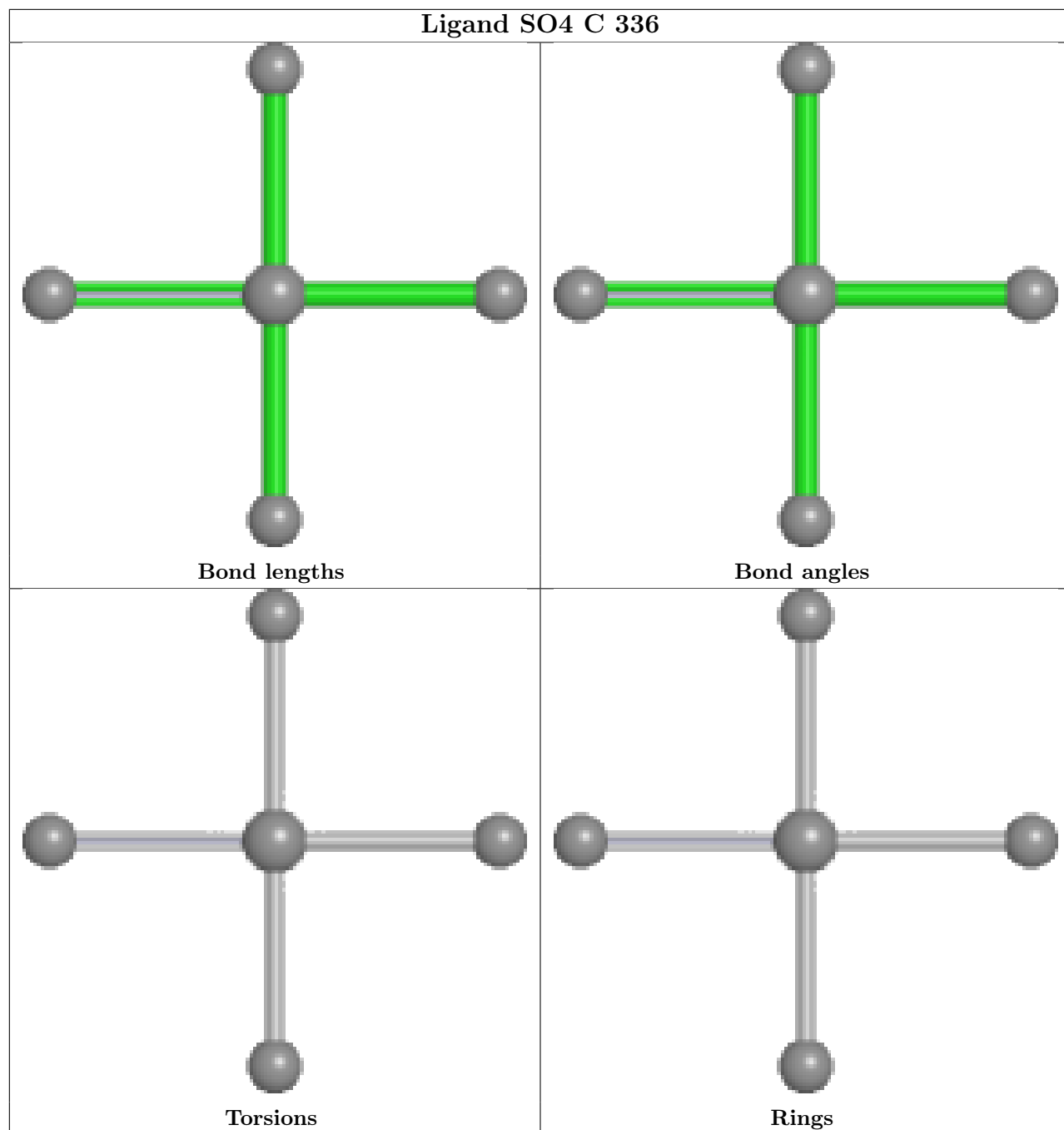


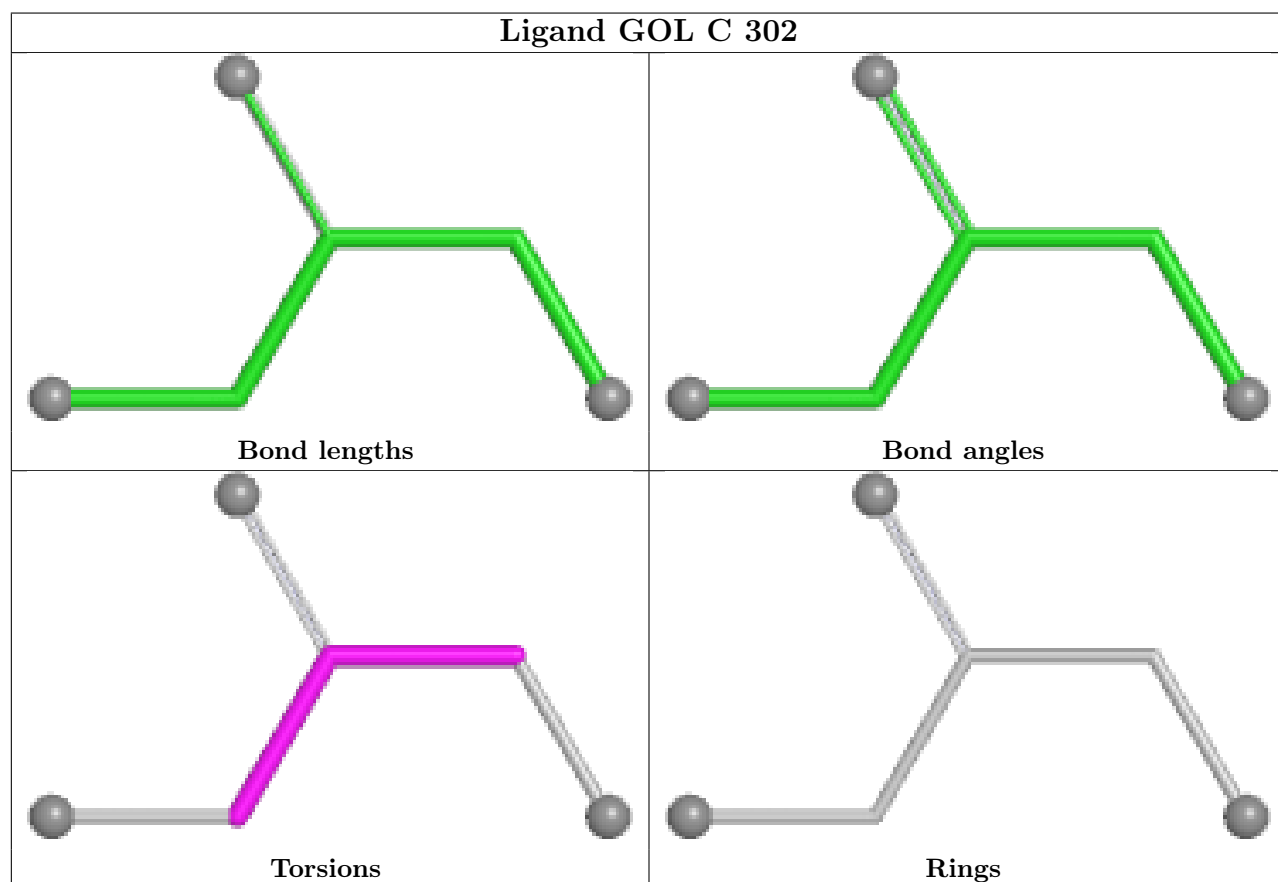
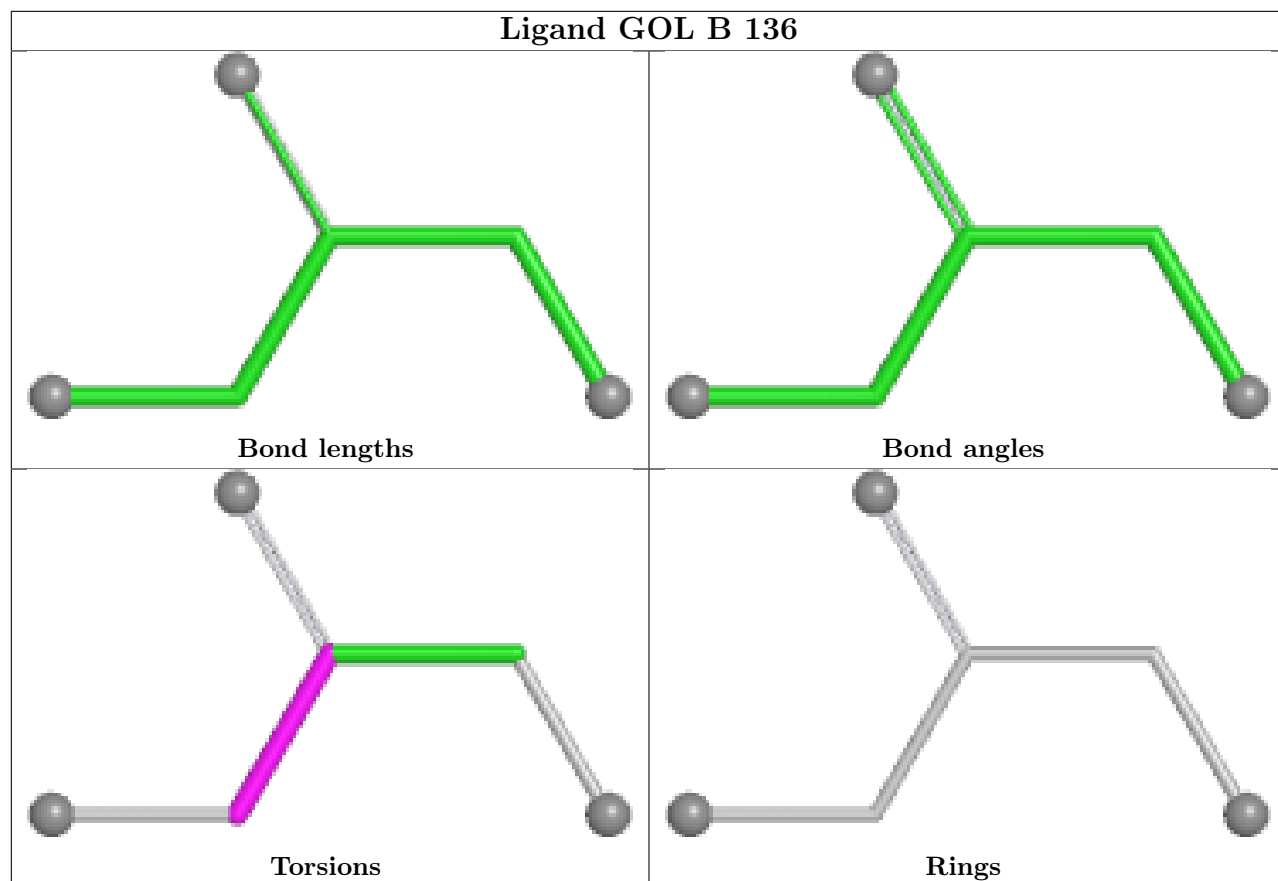


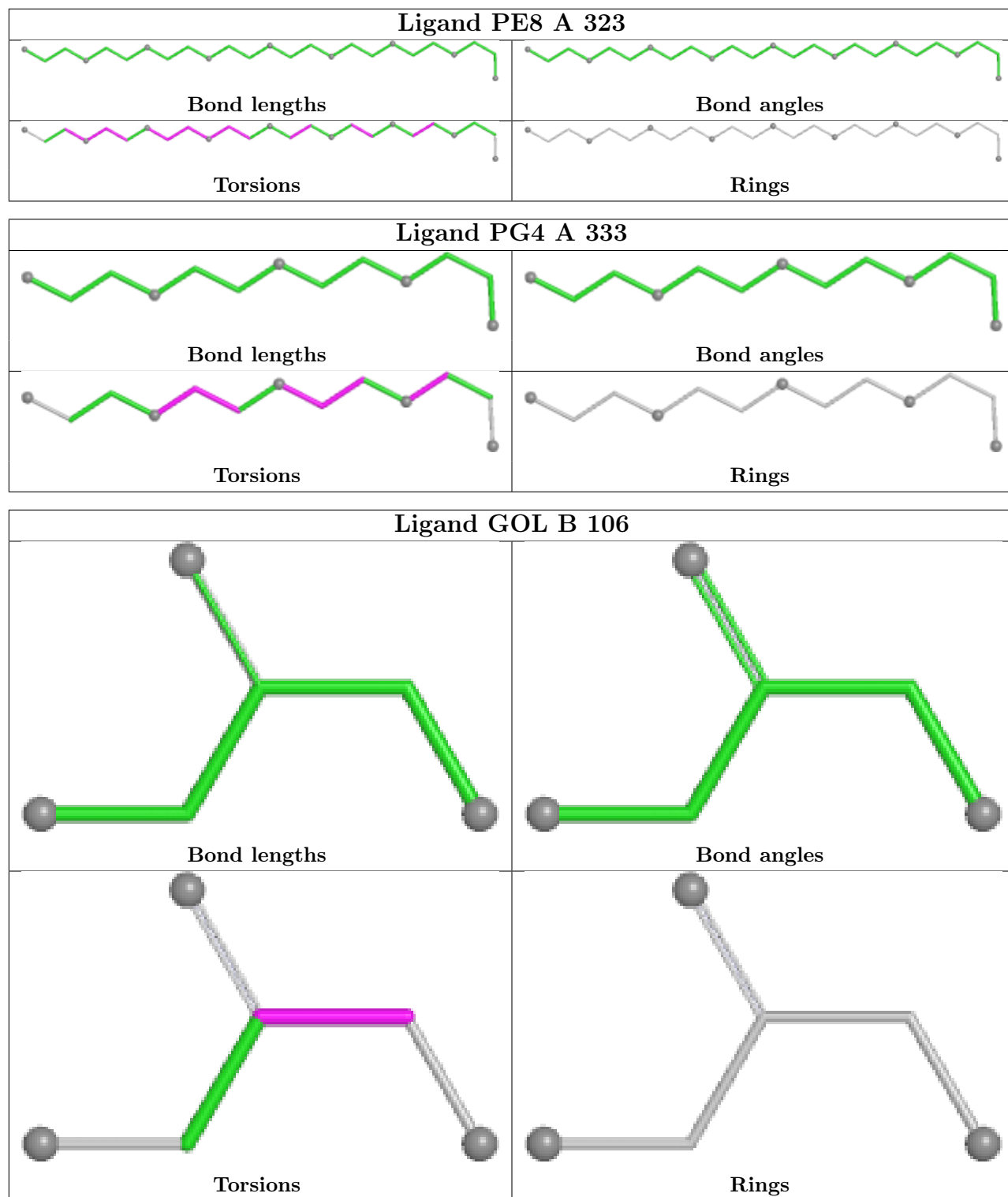


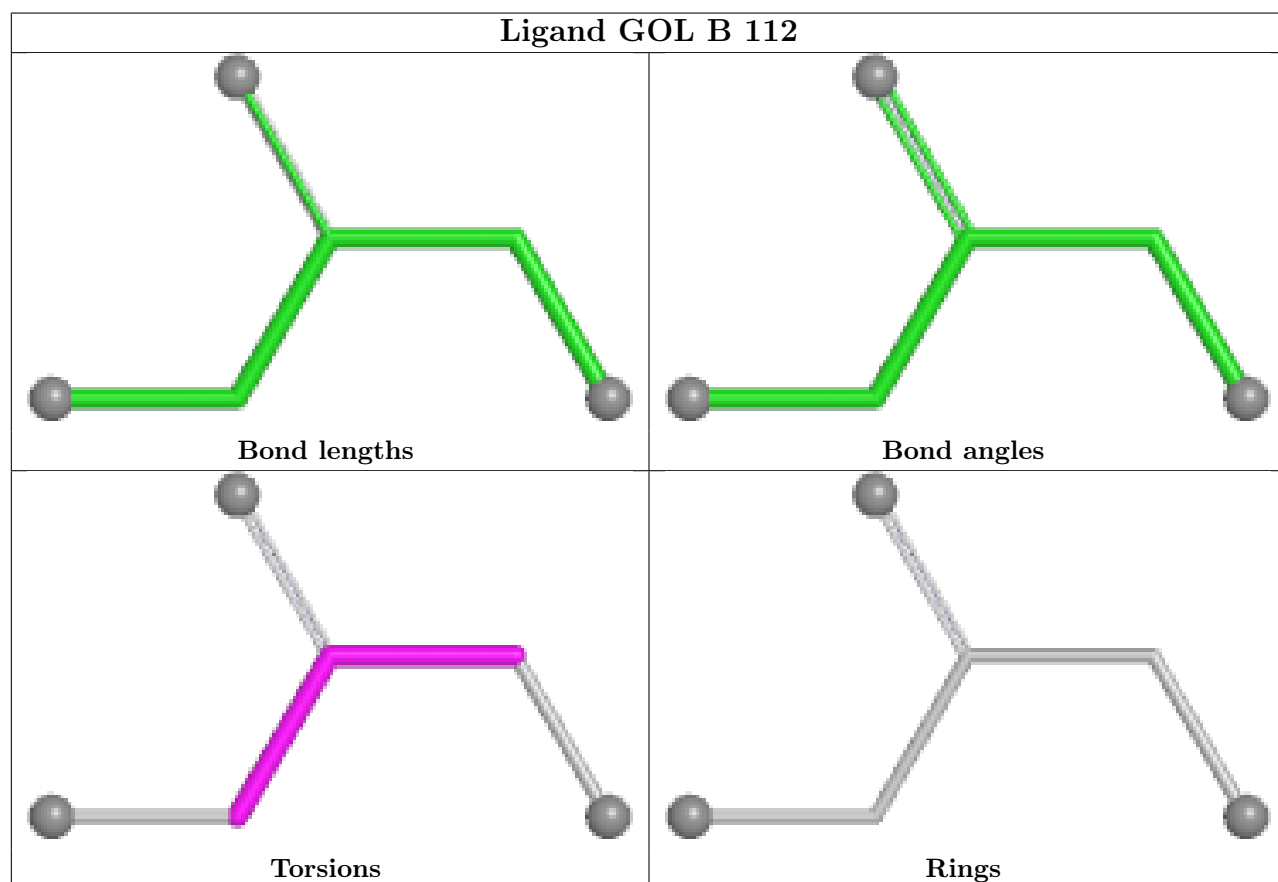
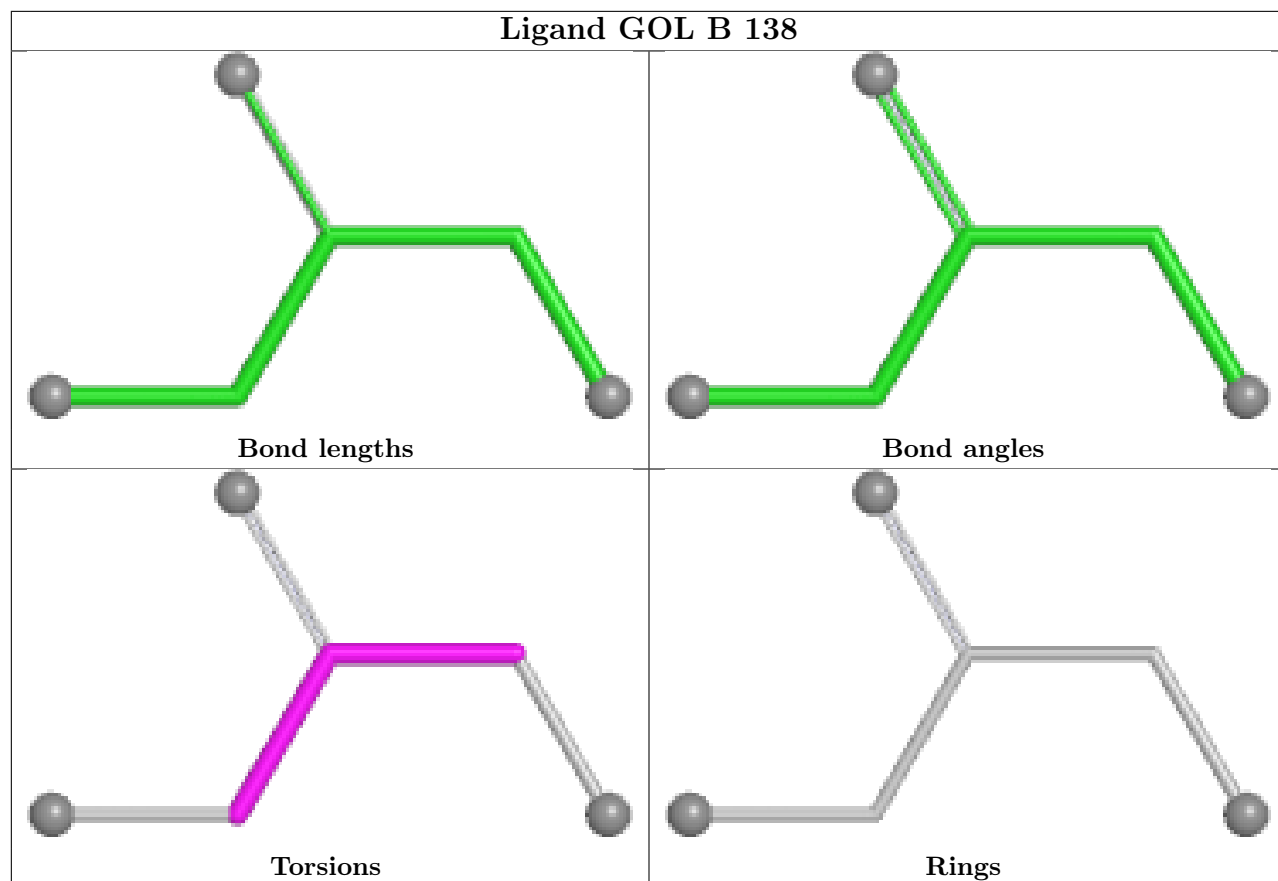


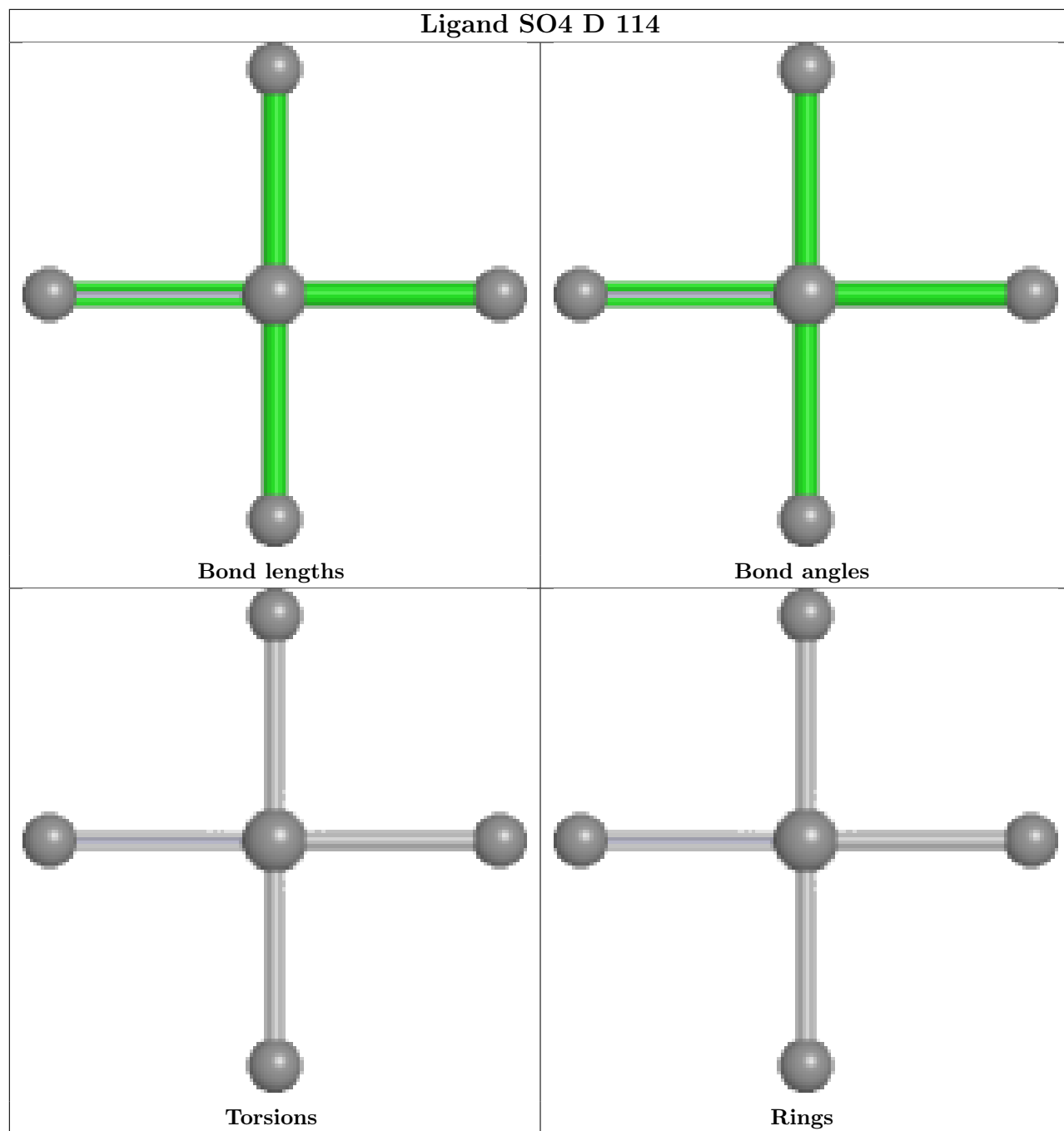


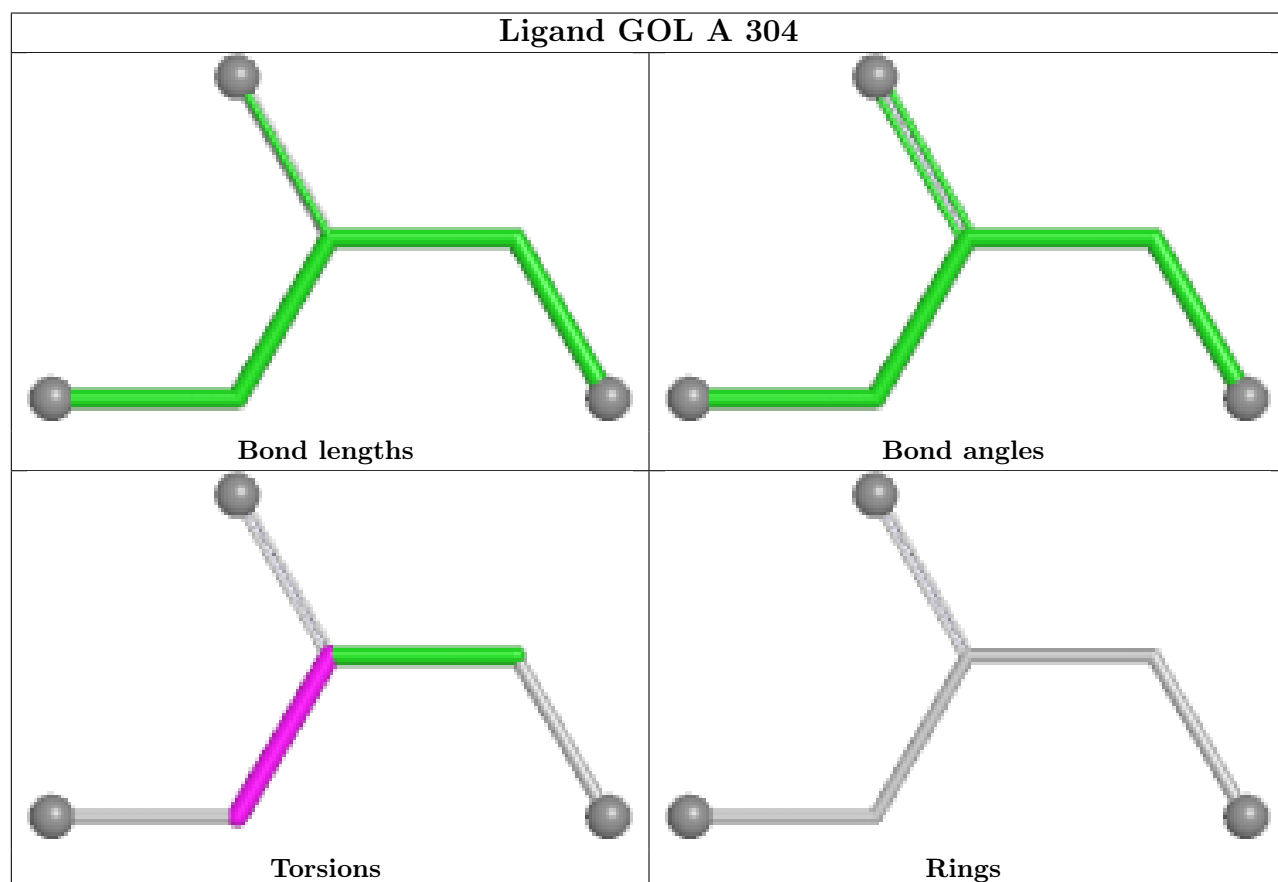
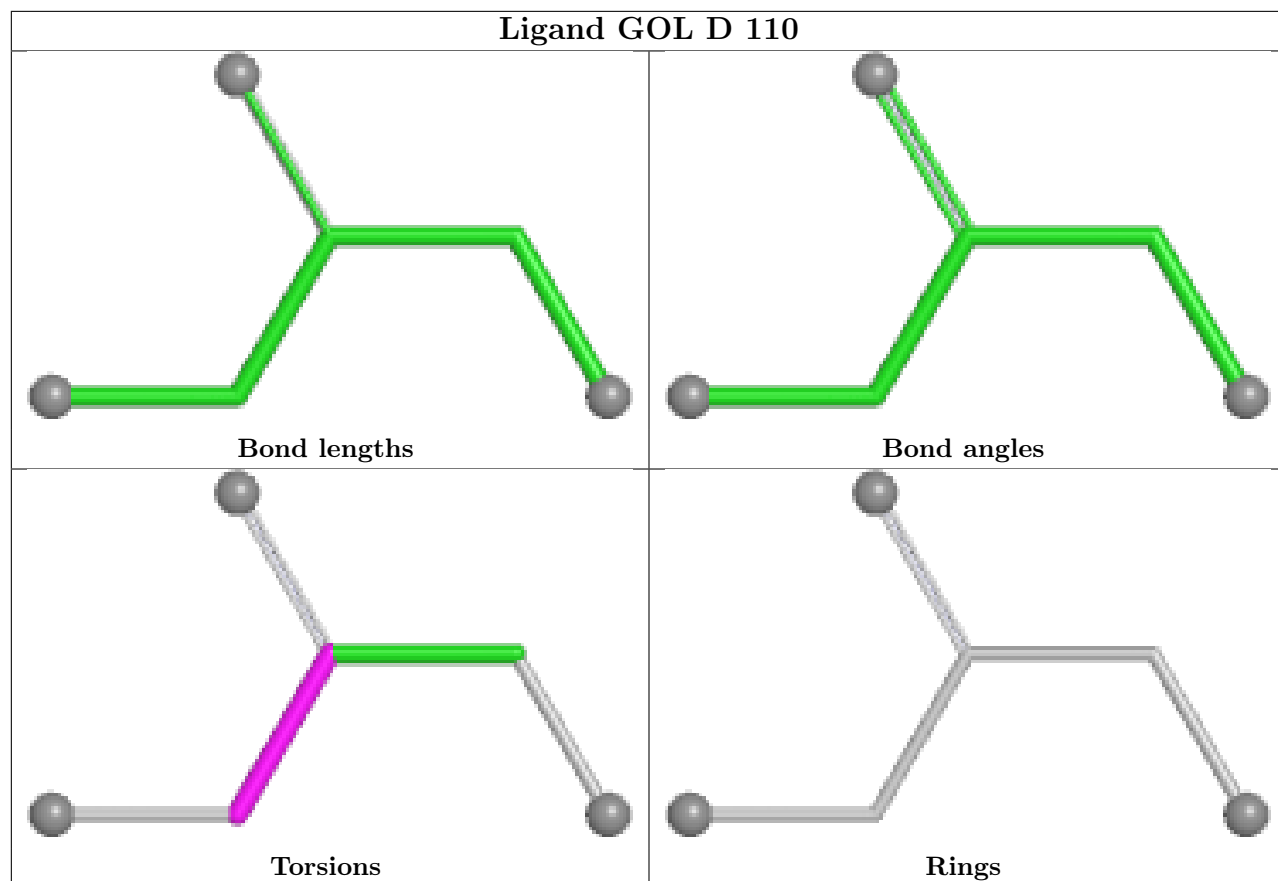




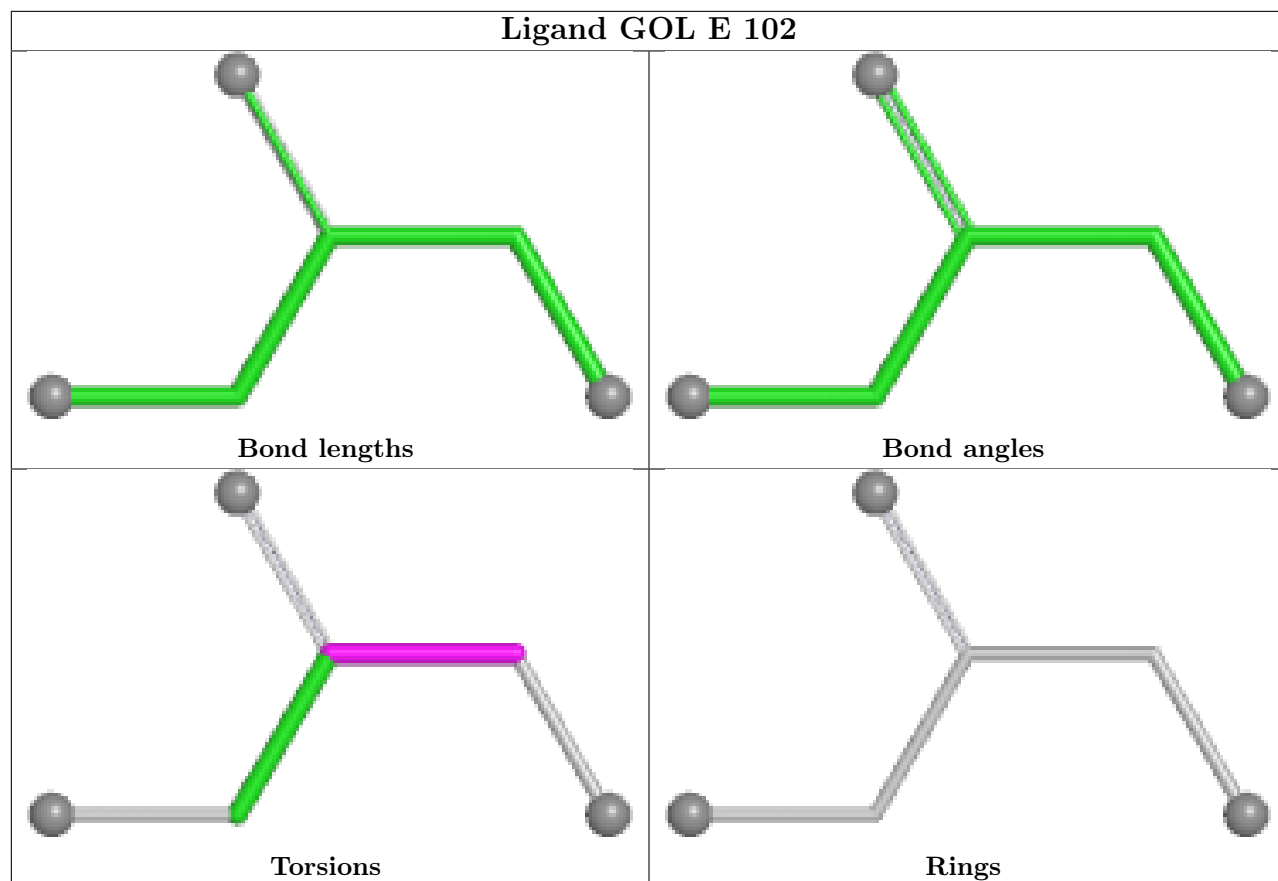




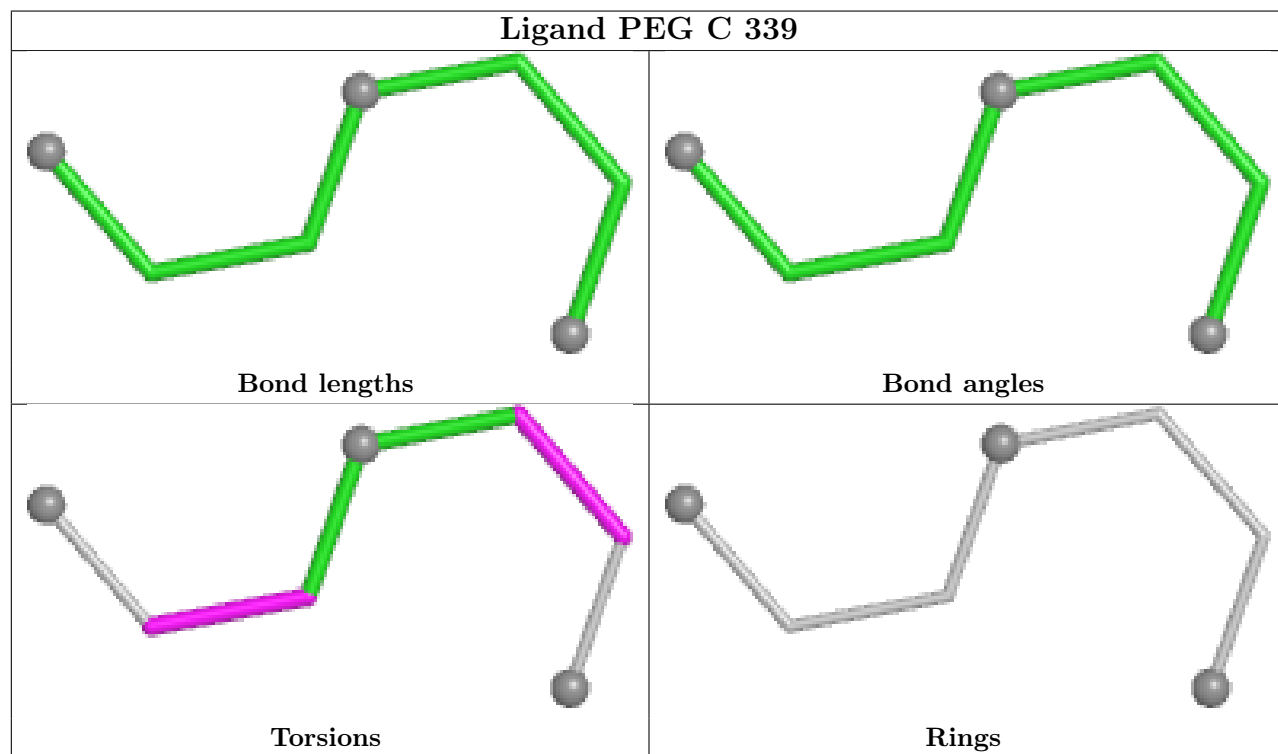


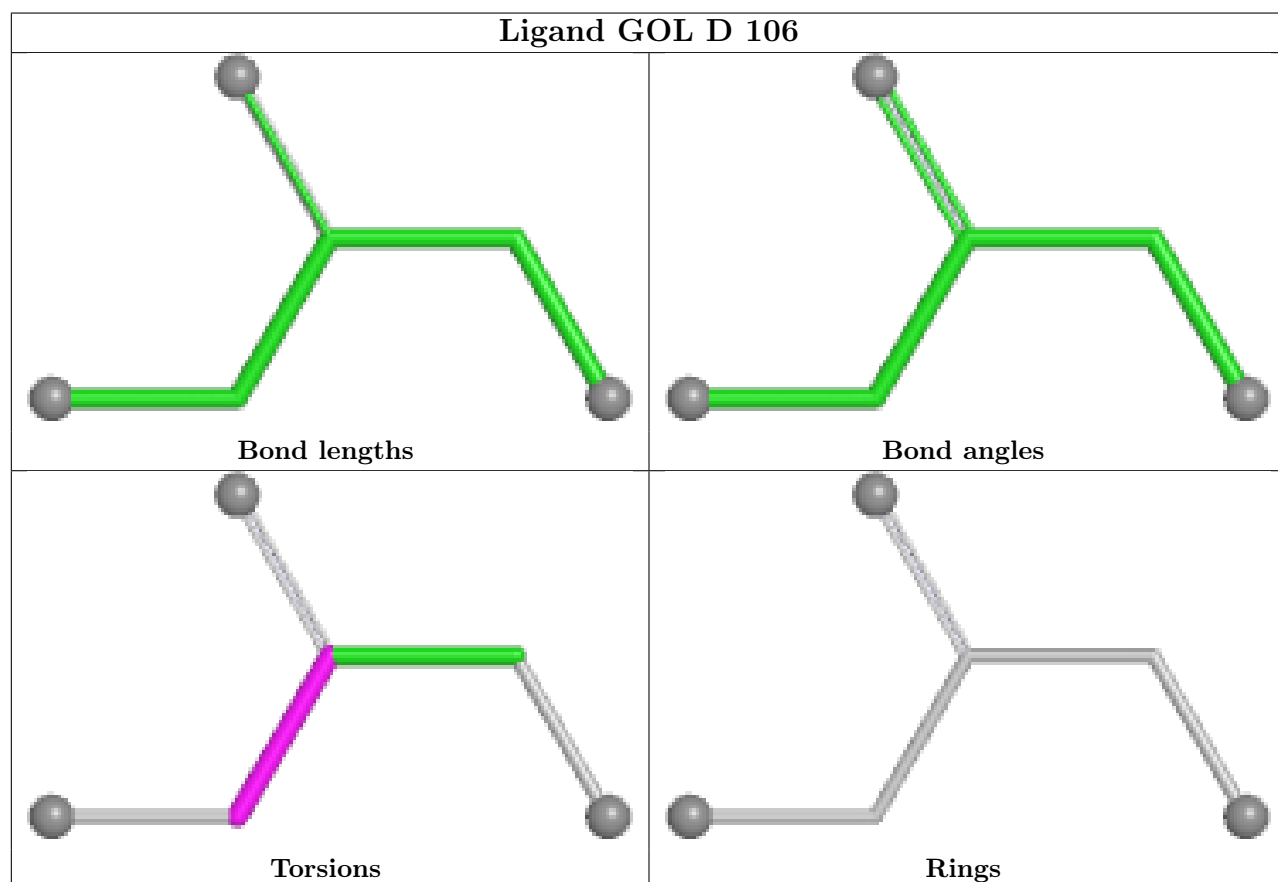
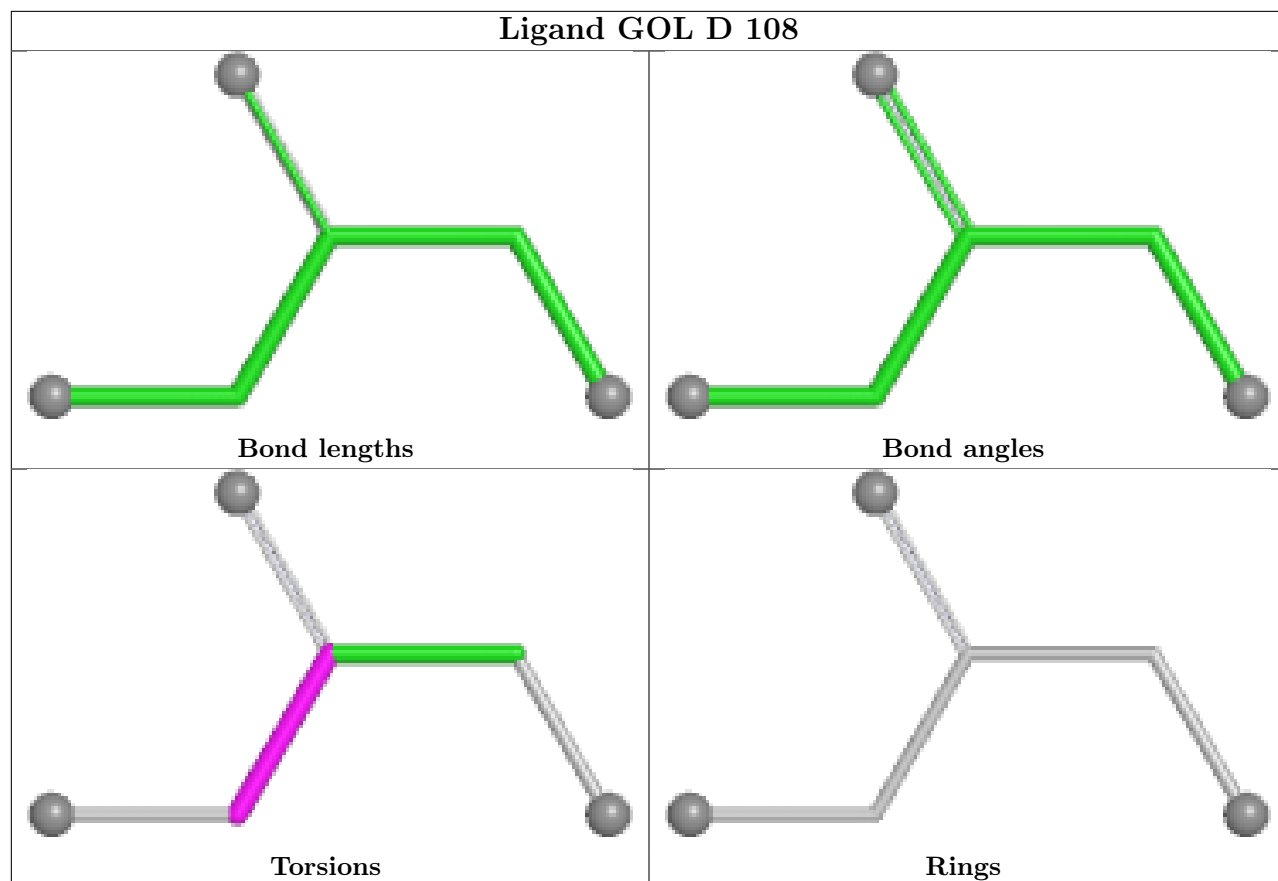


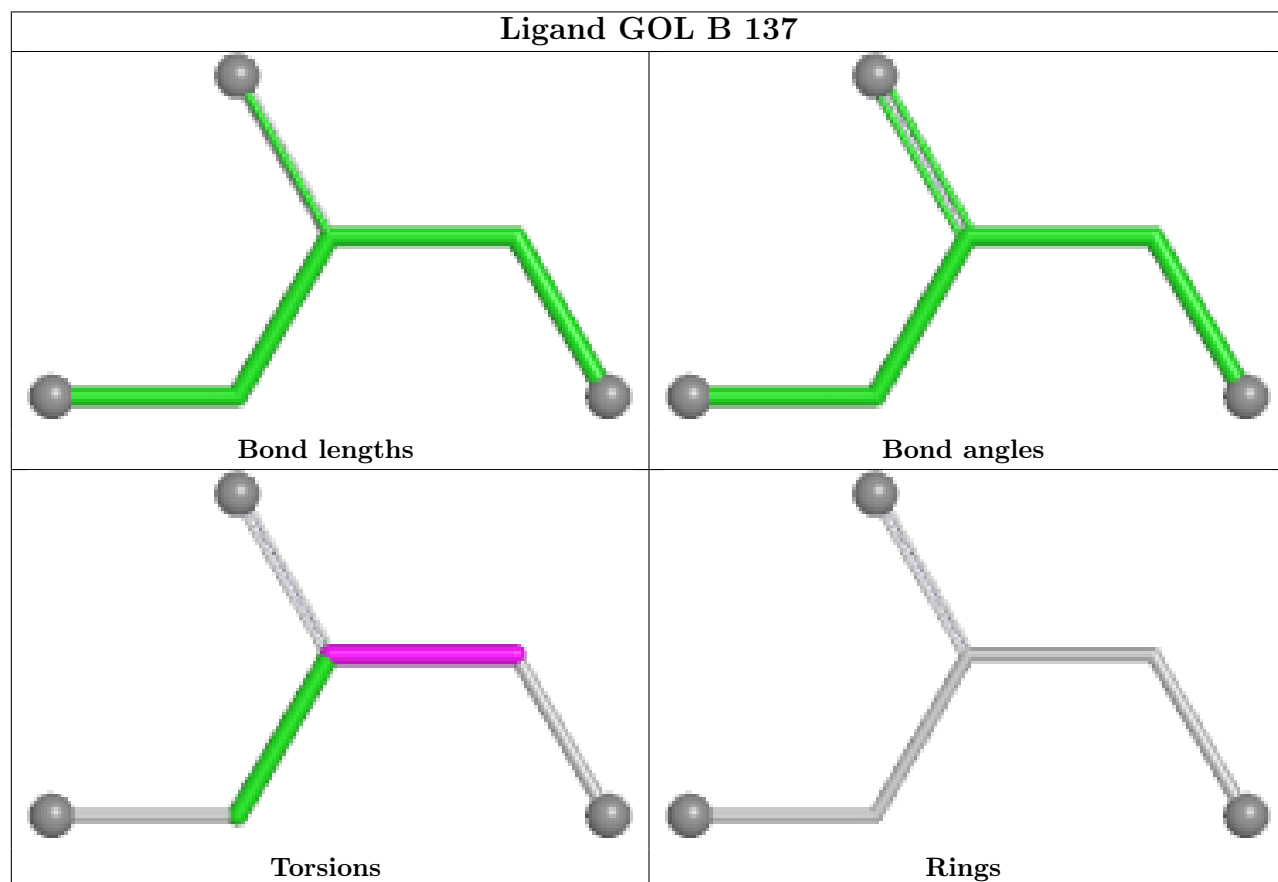
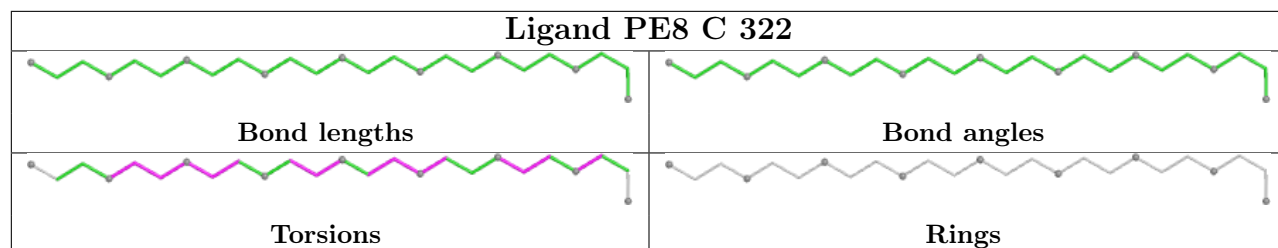
Ligand GOL E 102

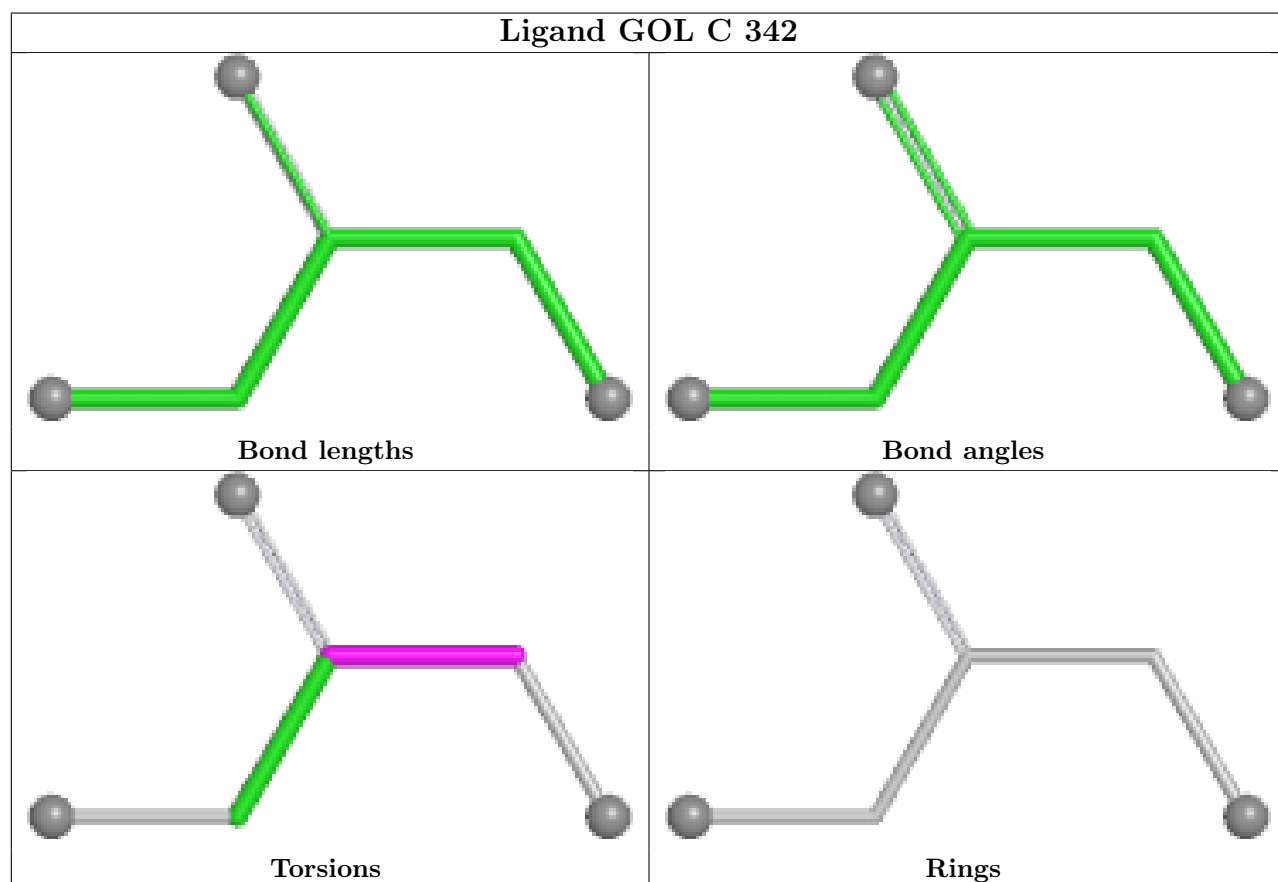
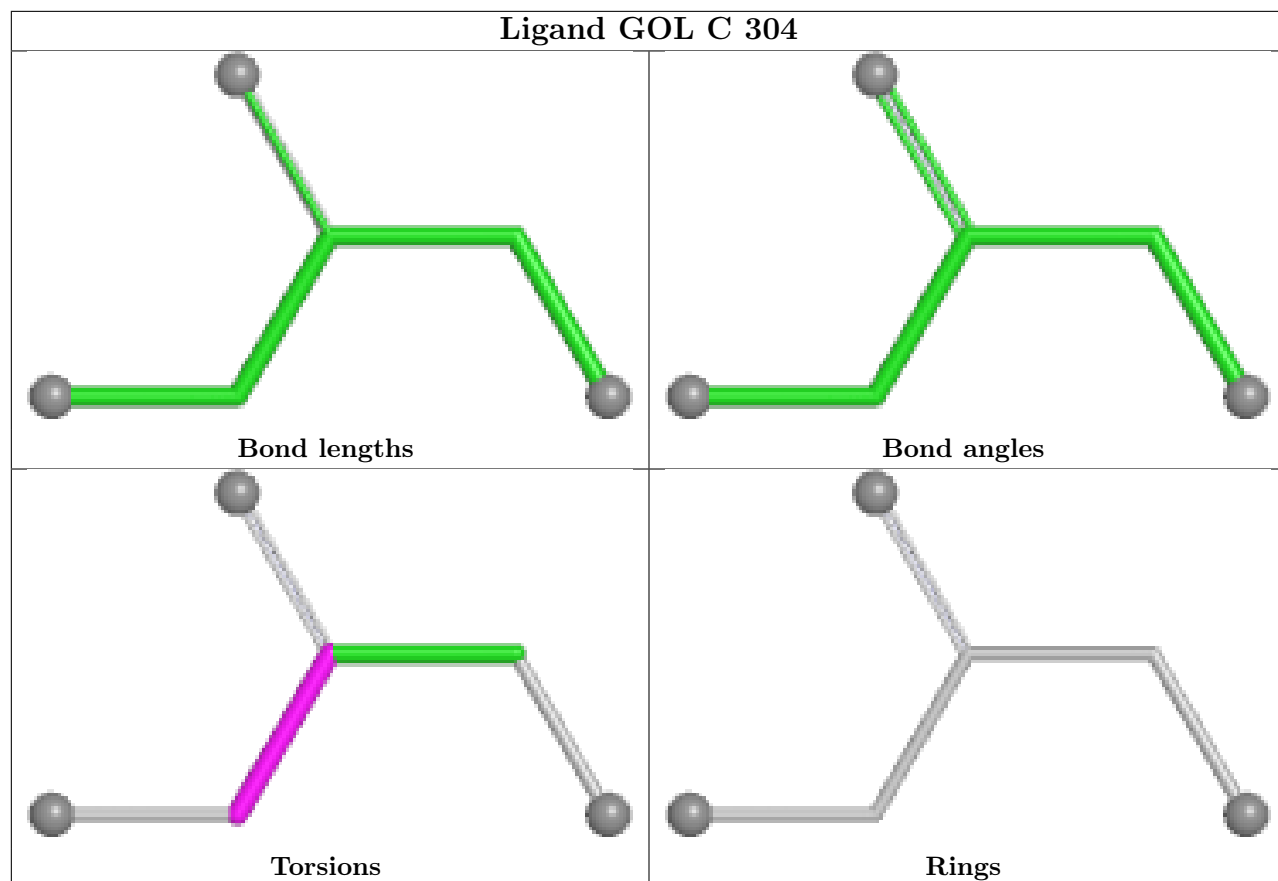


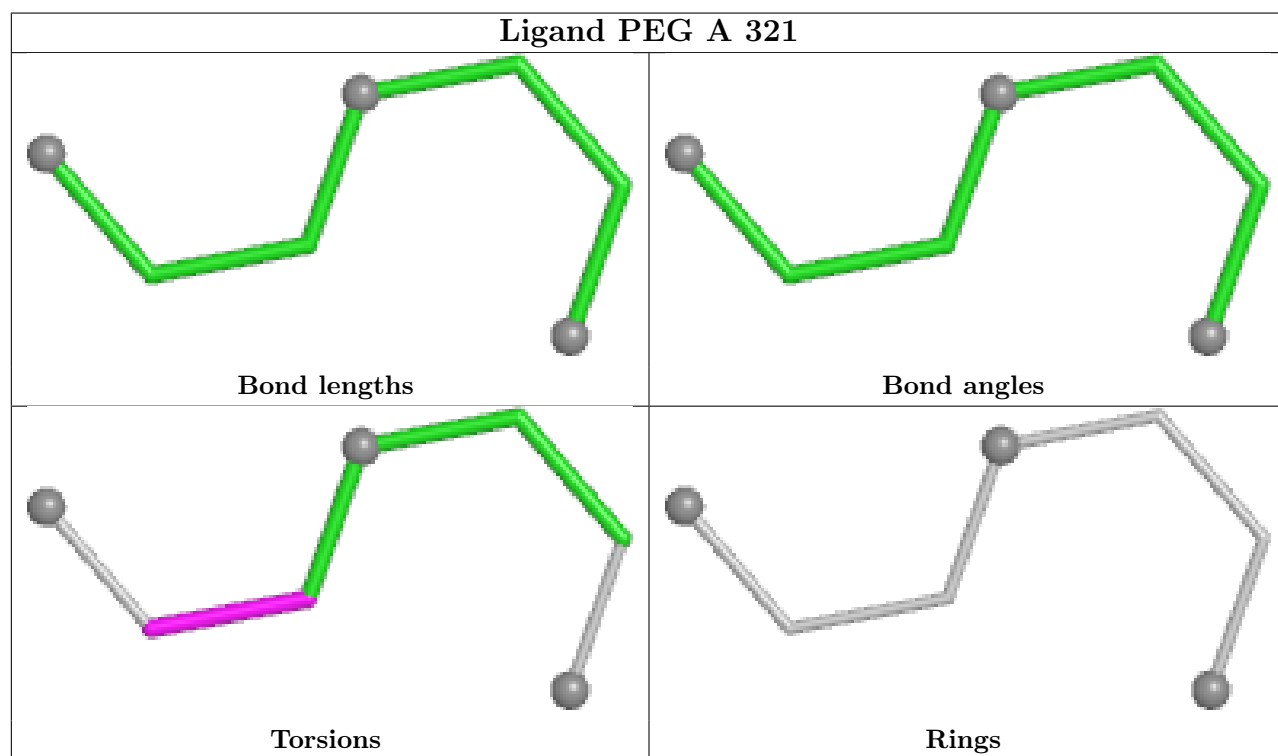
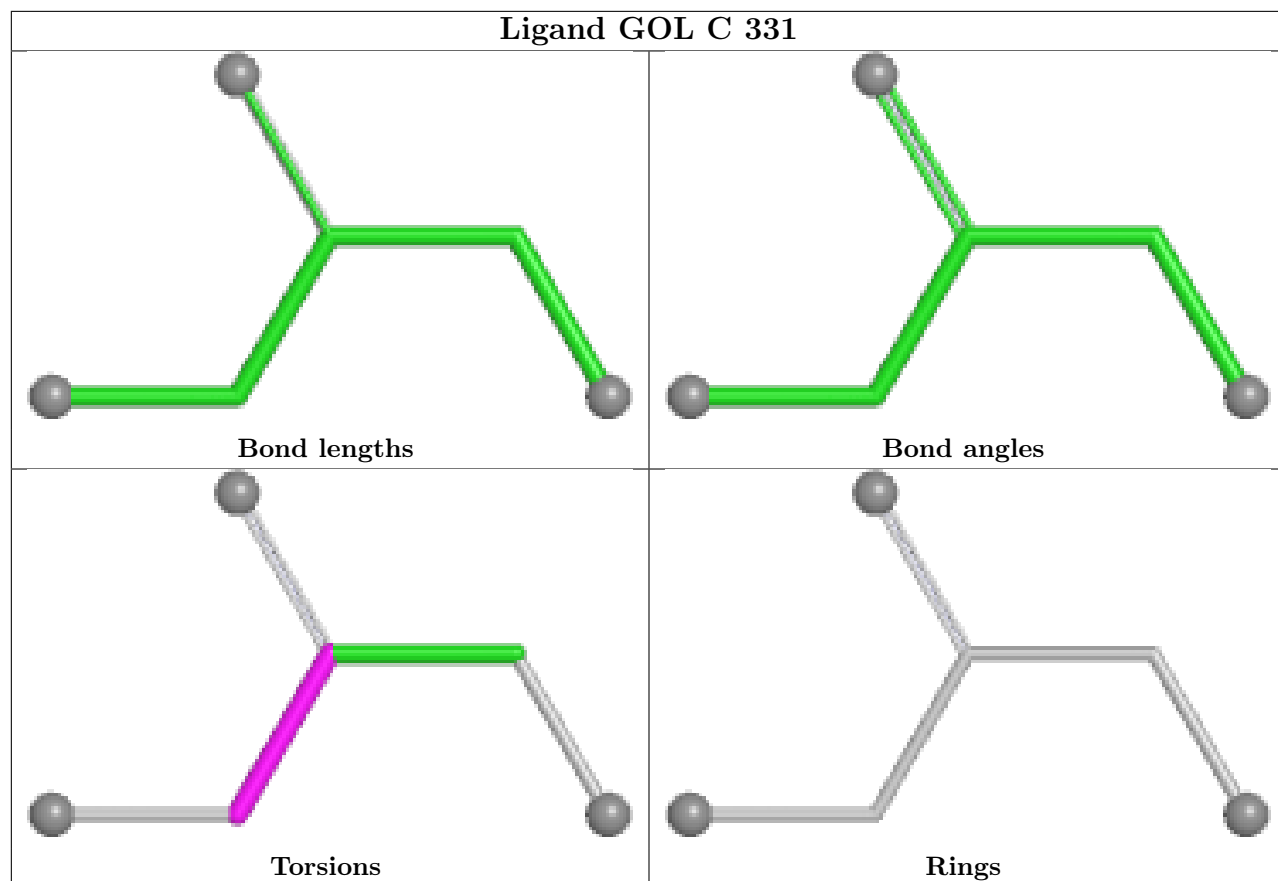
Ligand PEG C 339

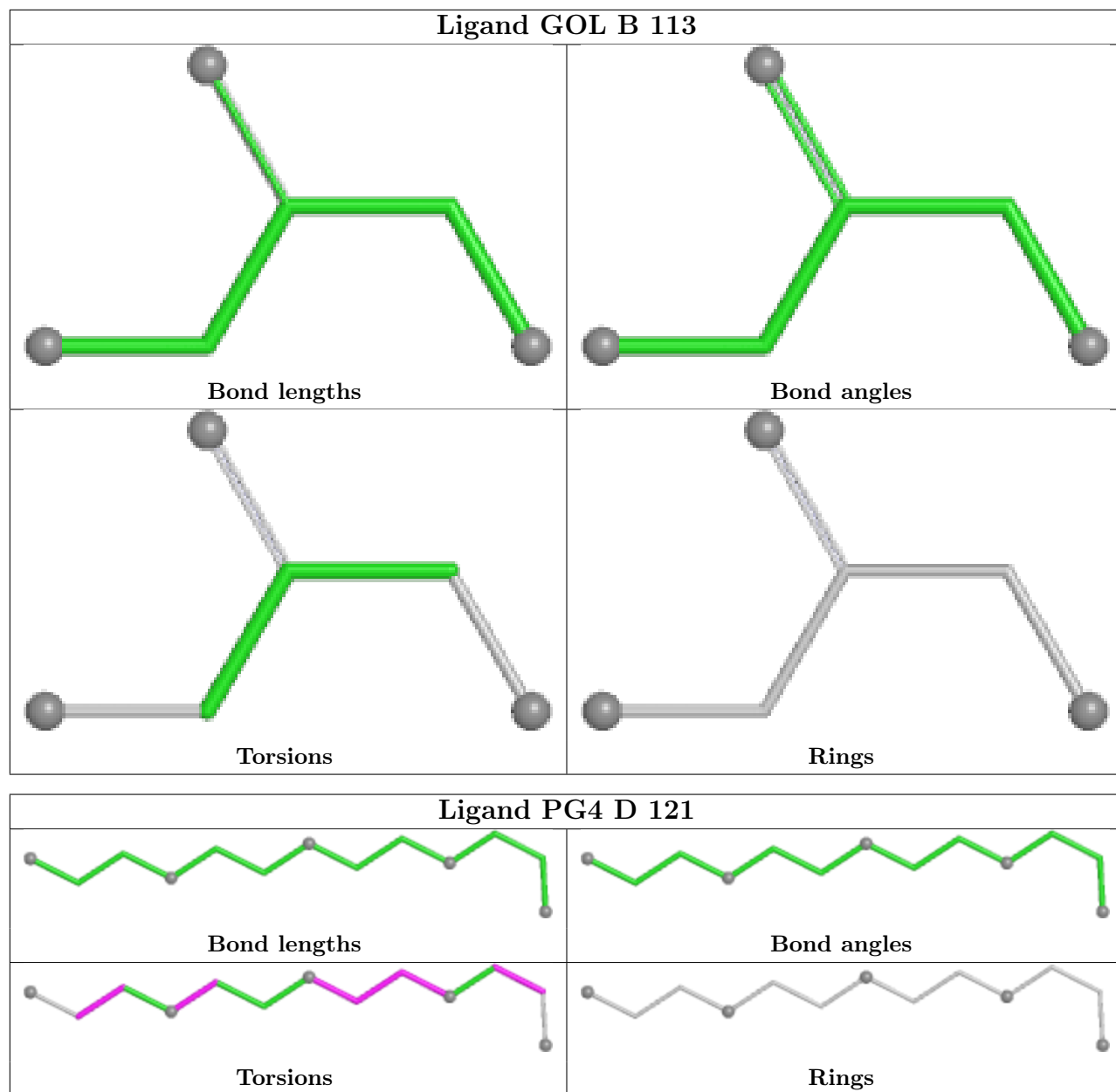


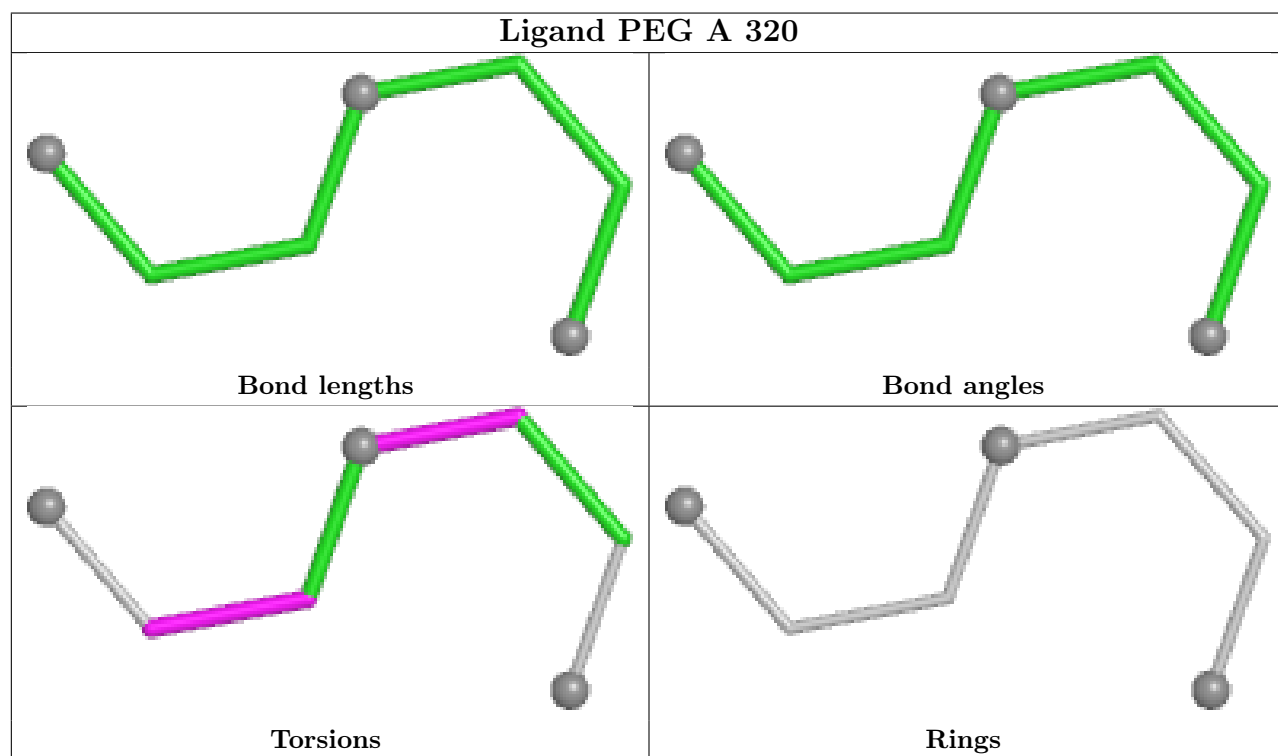
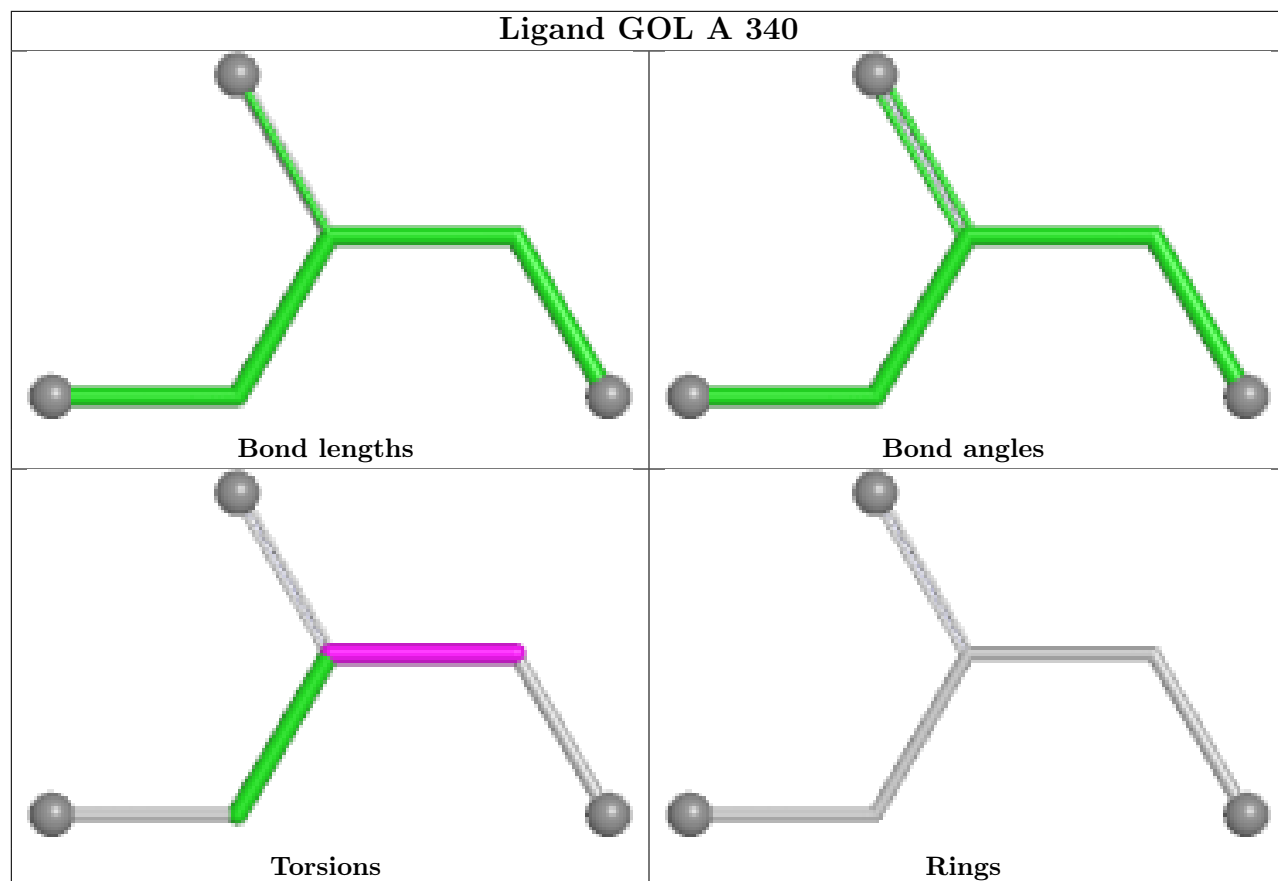


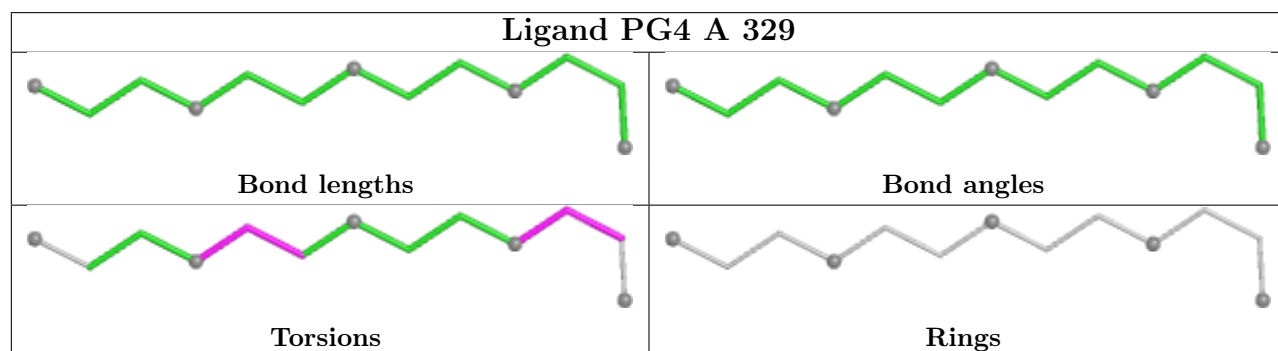
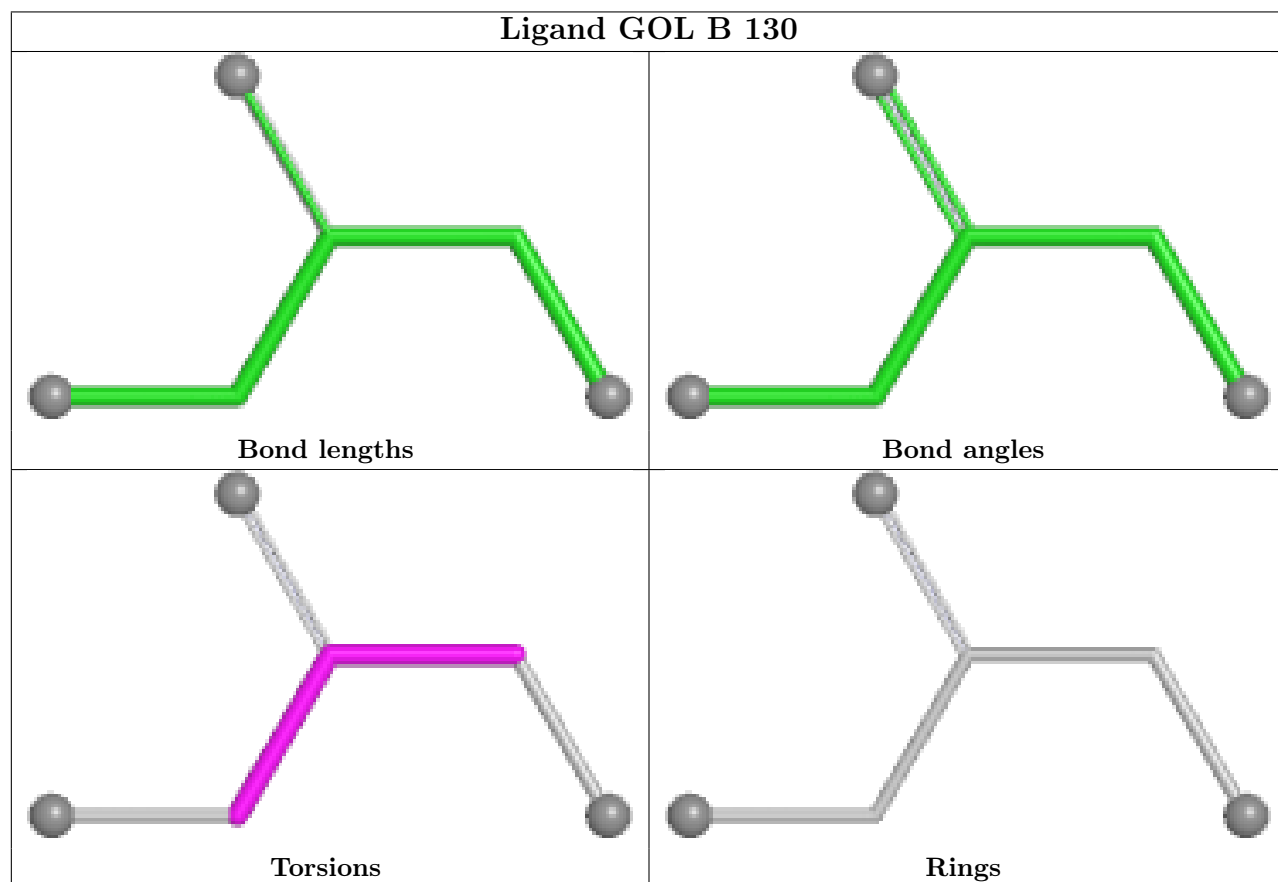
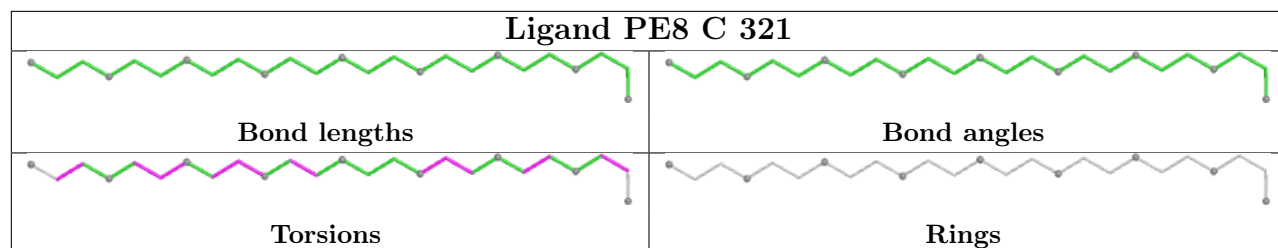


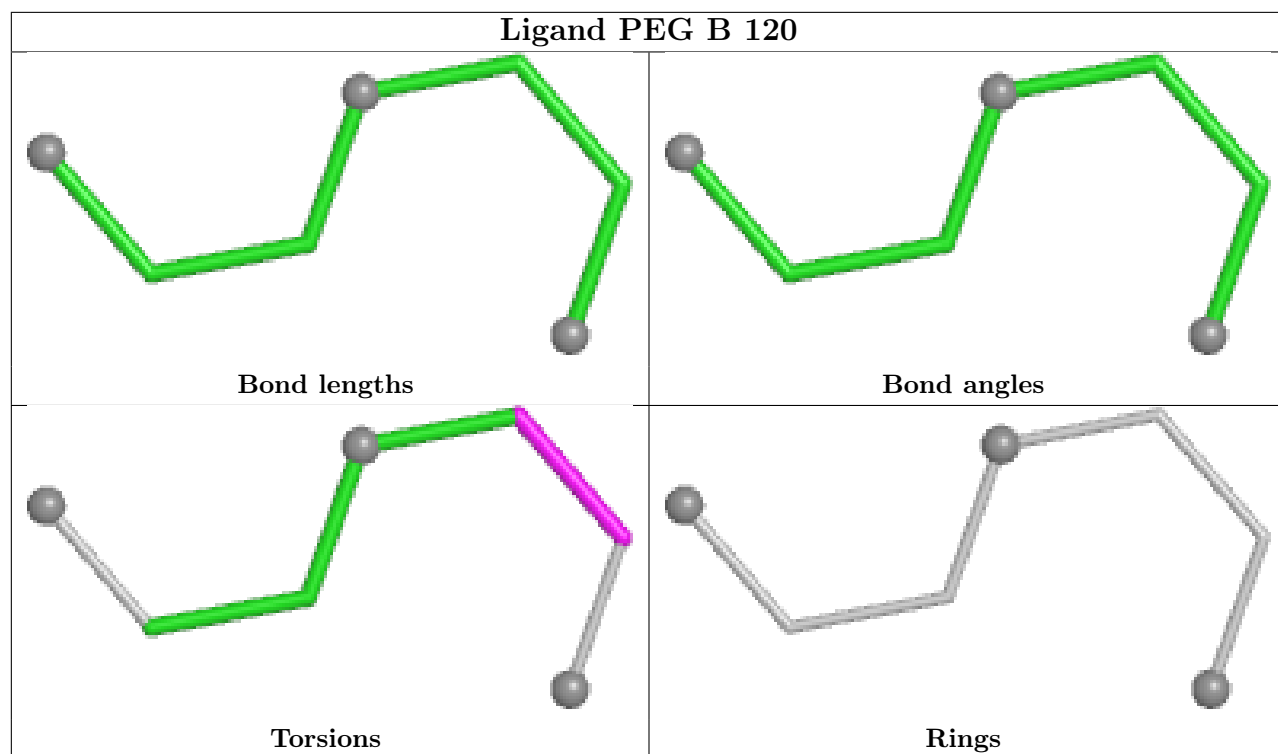
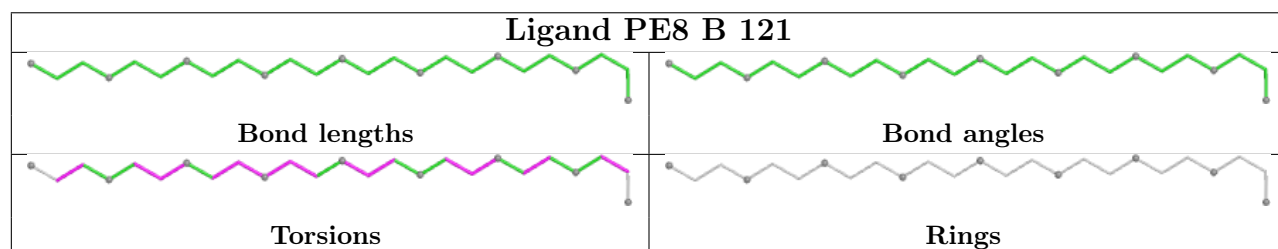
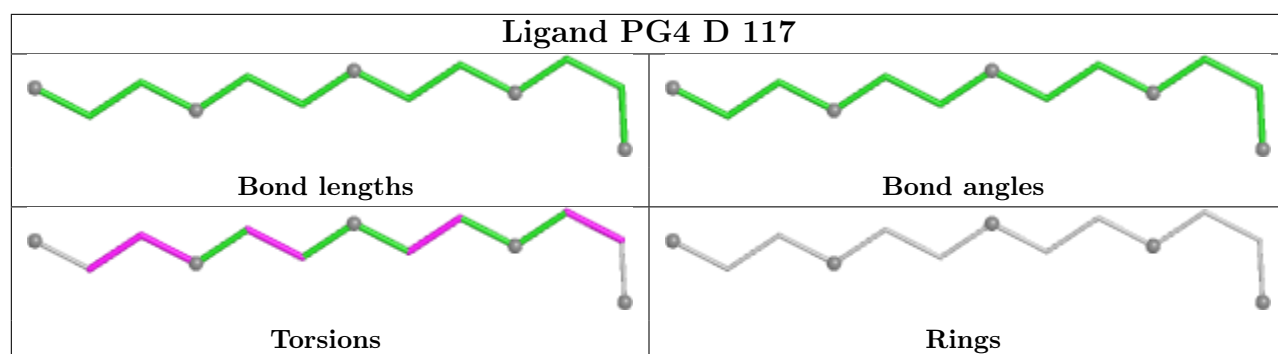


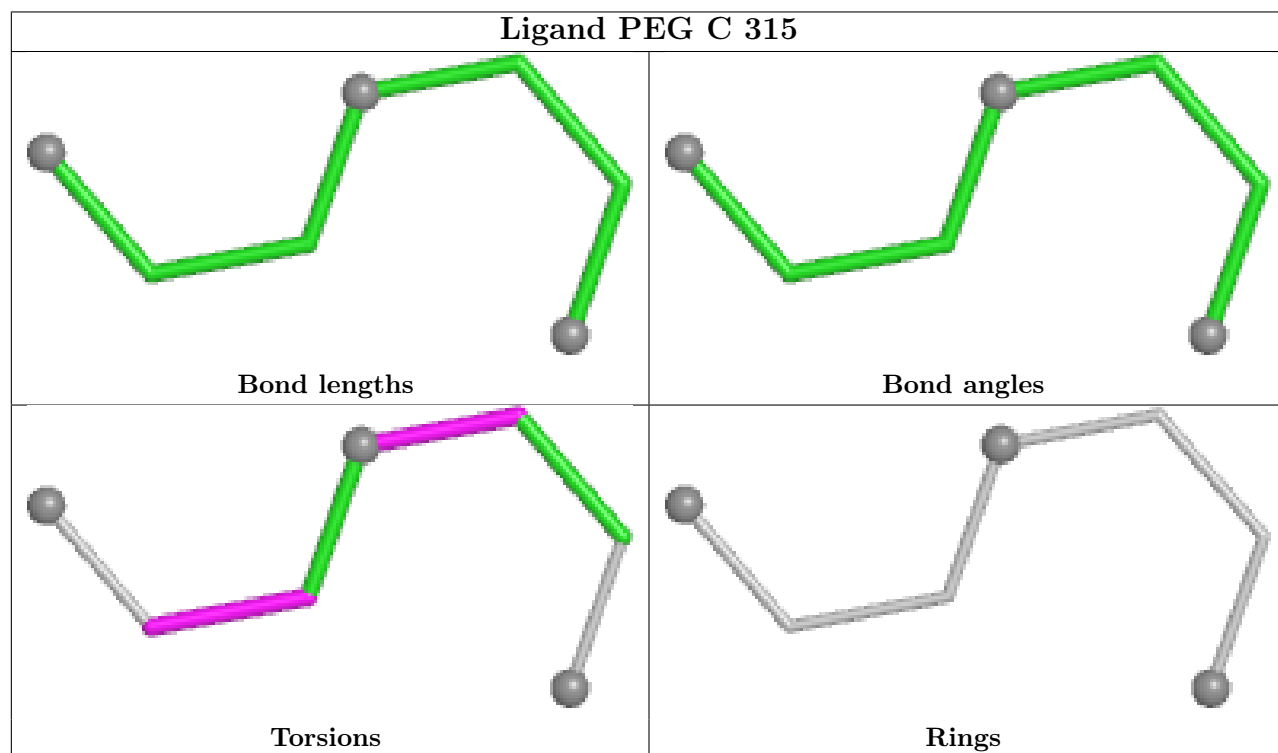
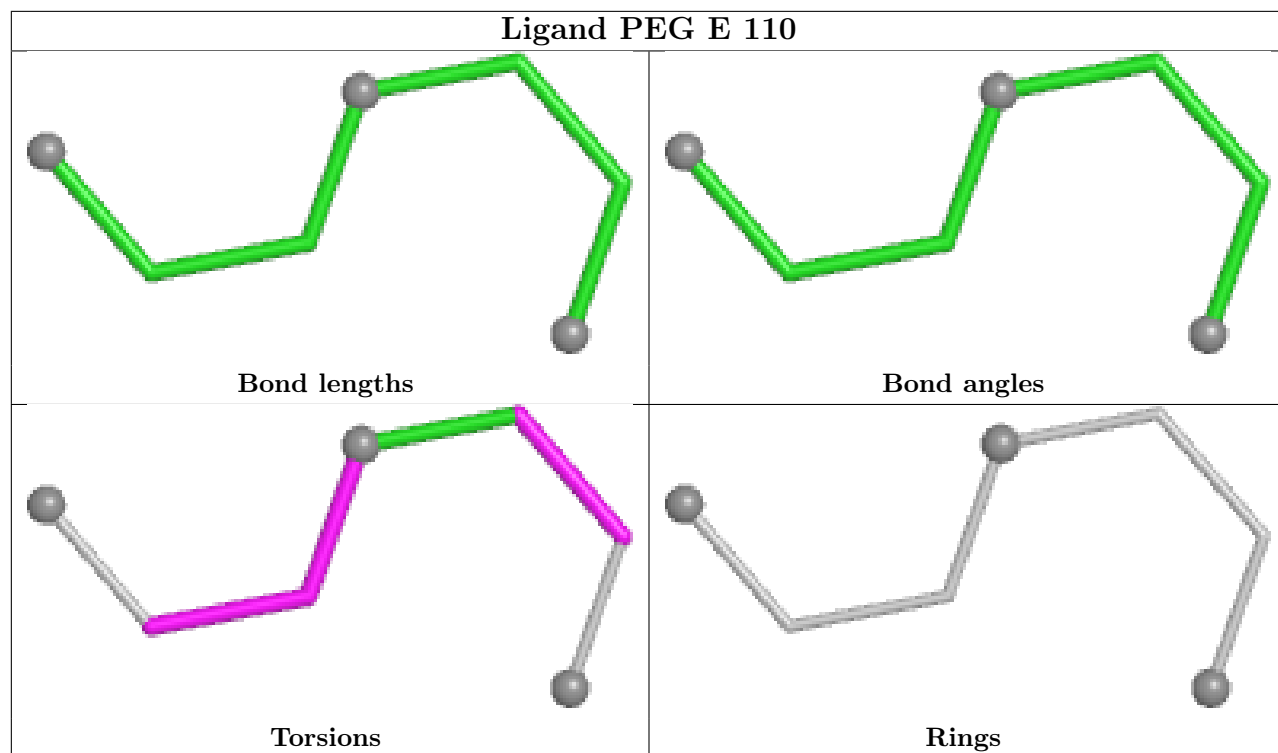


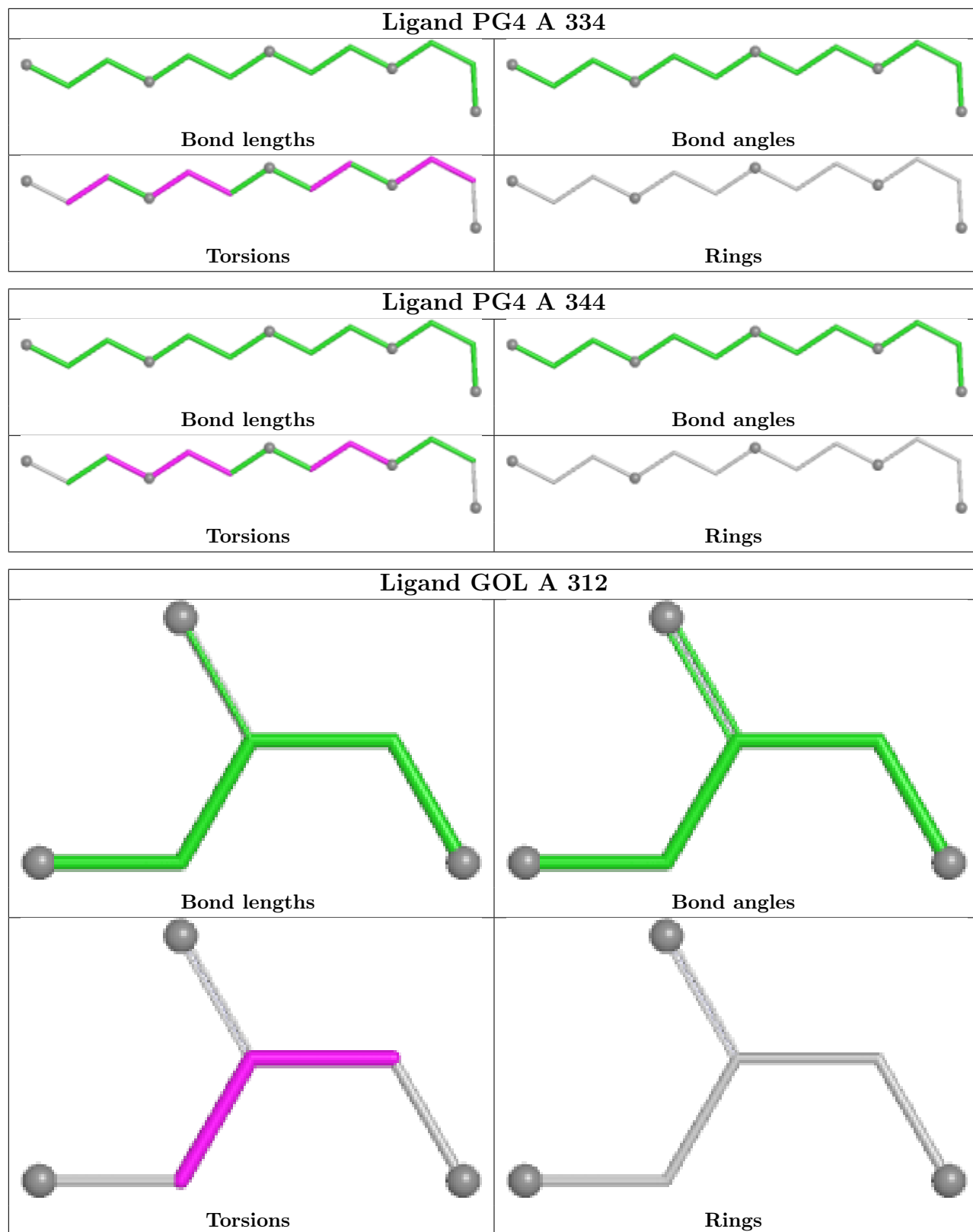


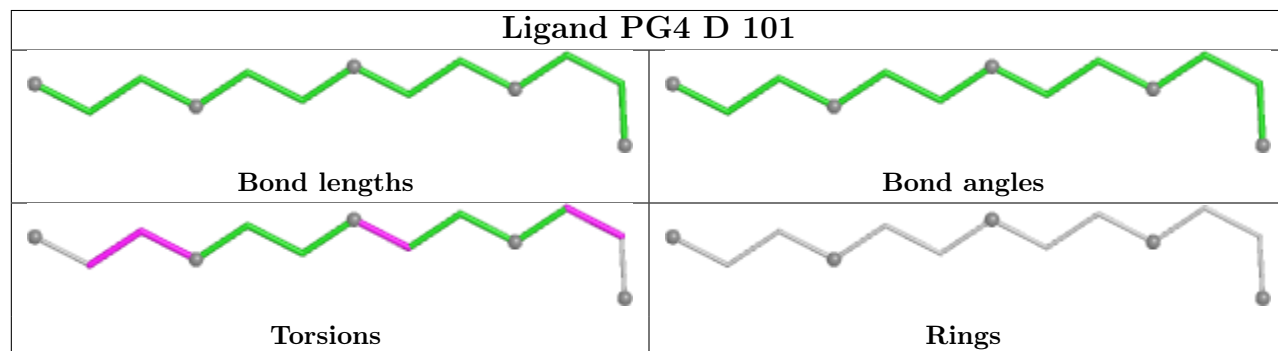
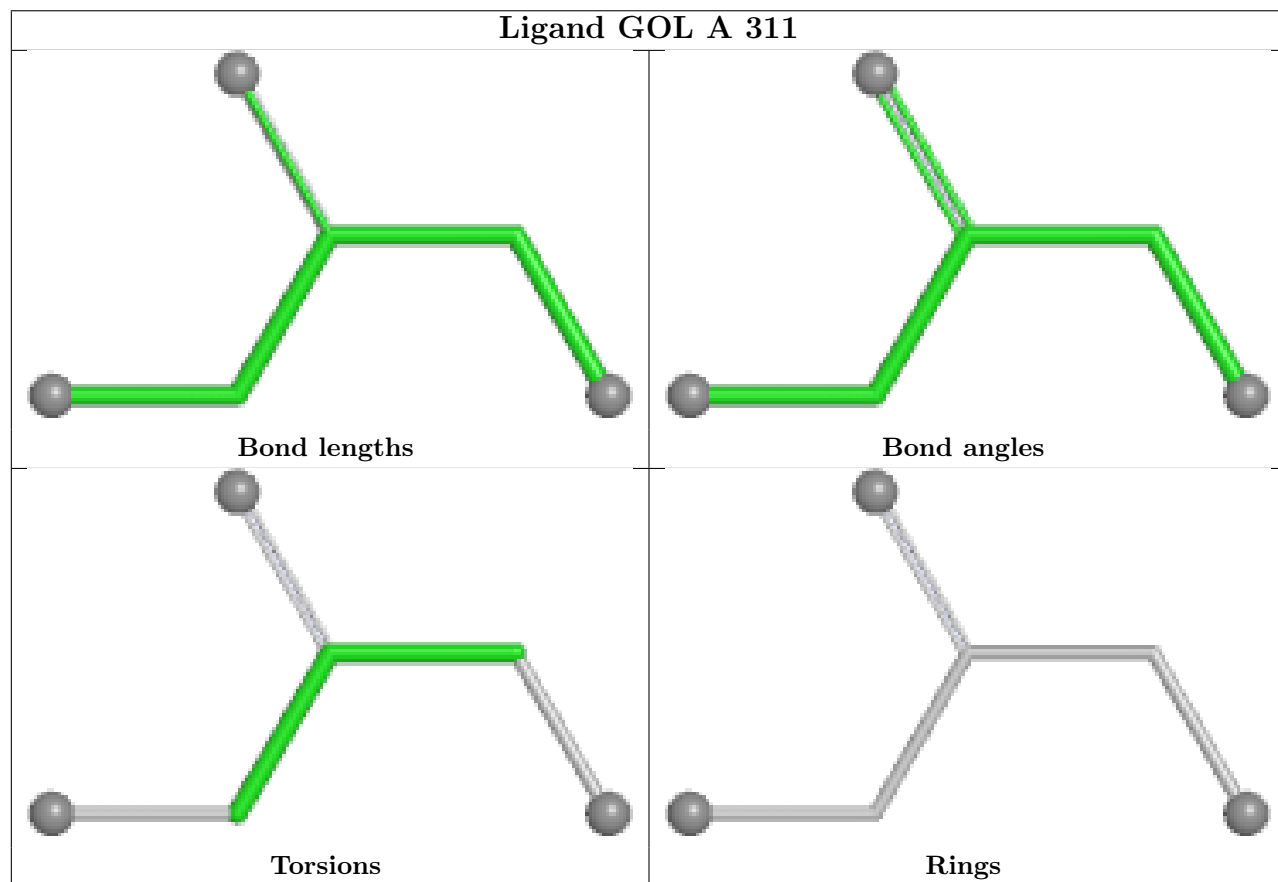
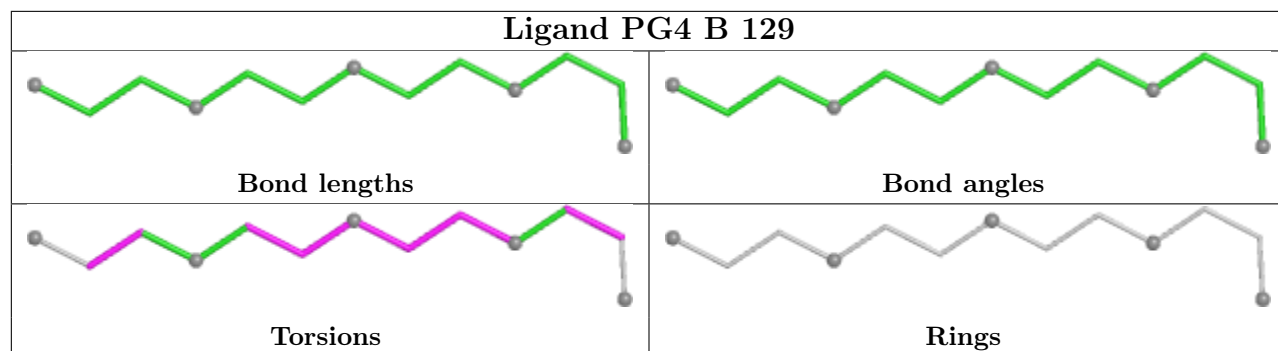


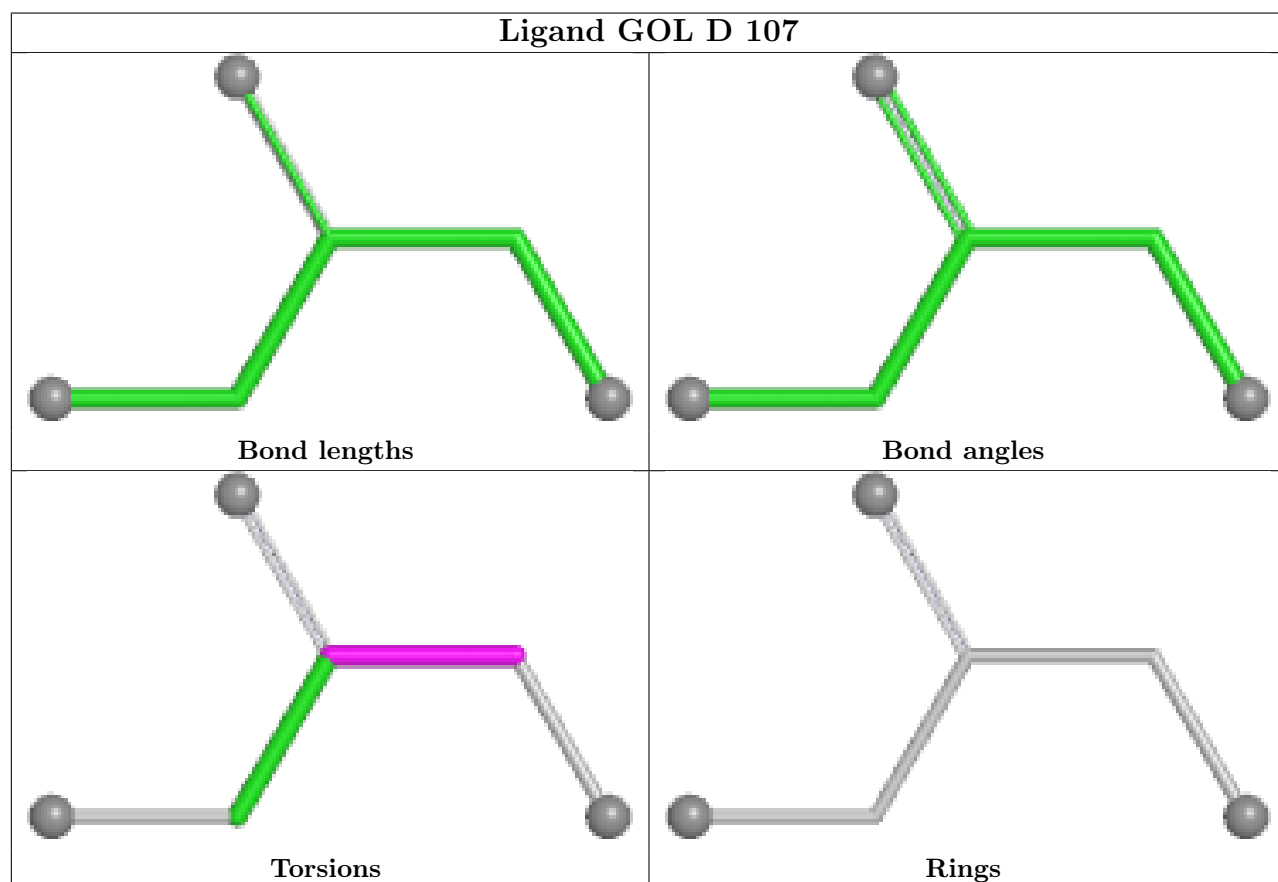
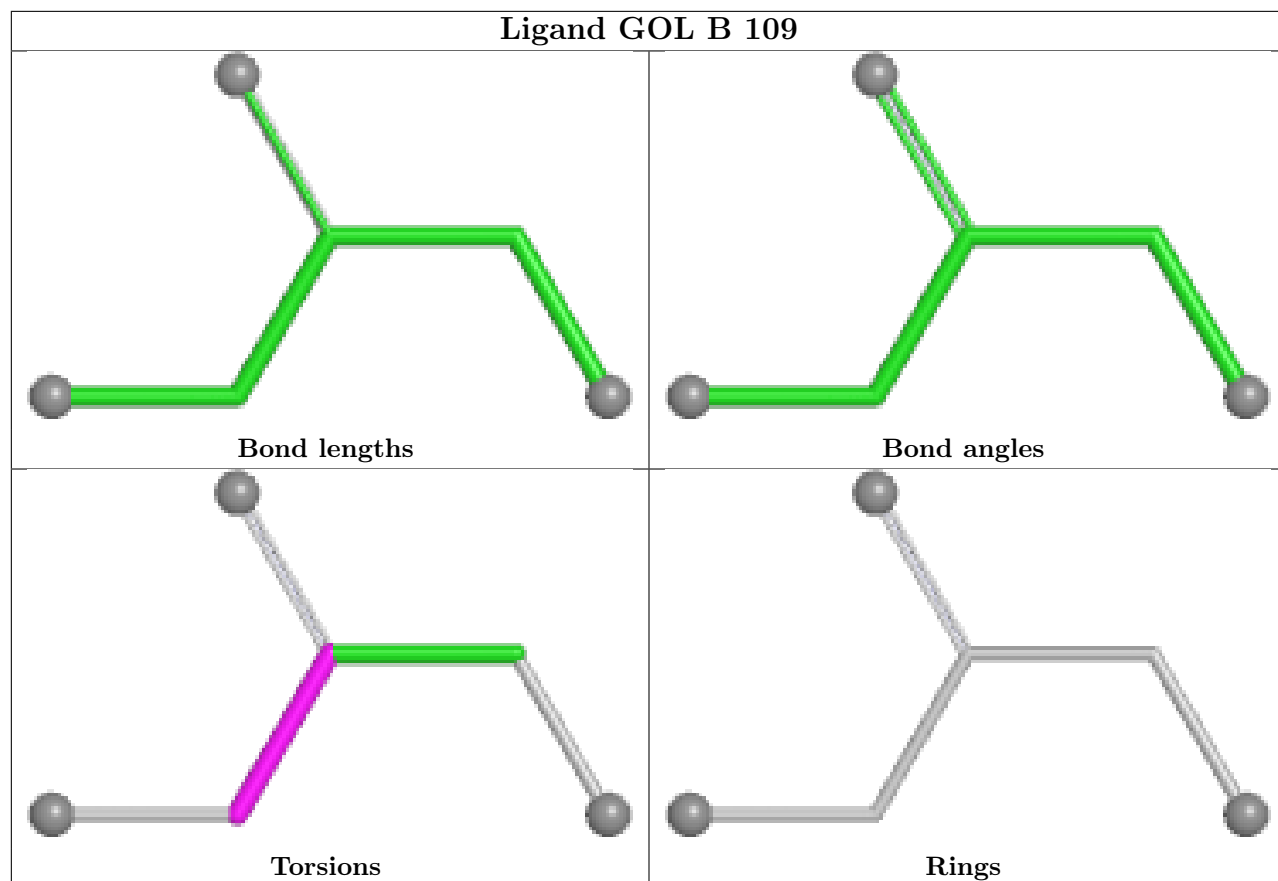


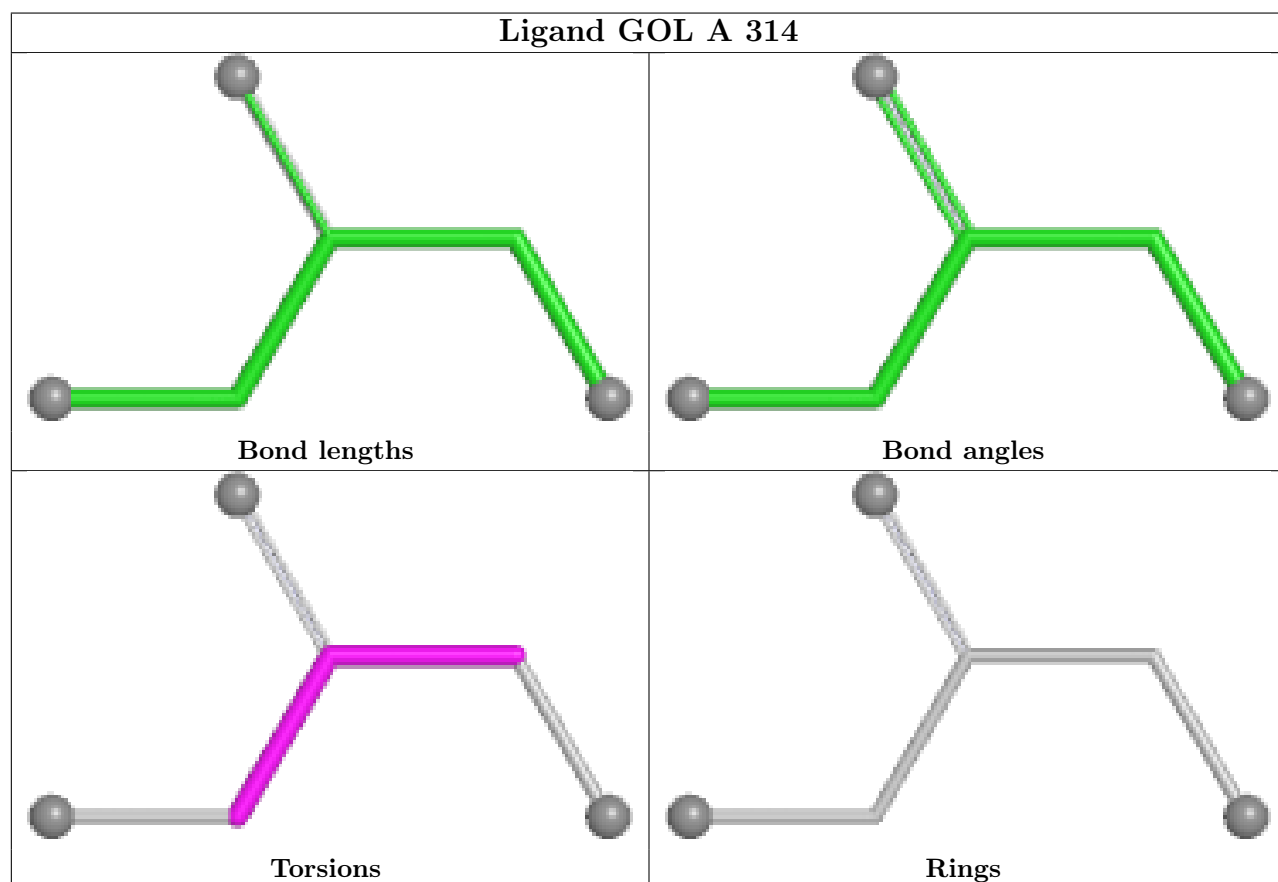
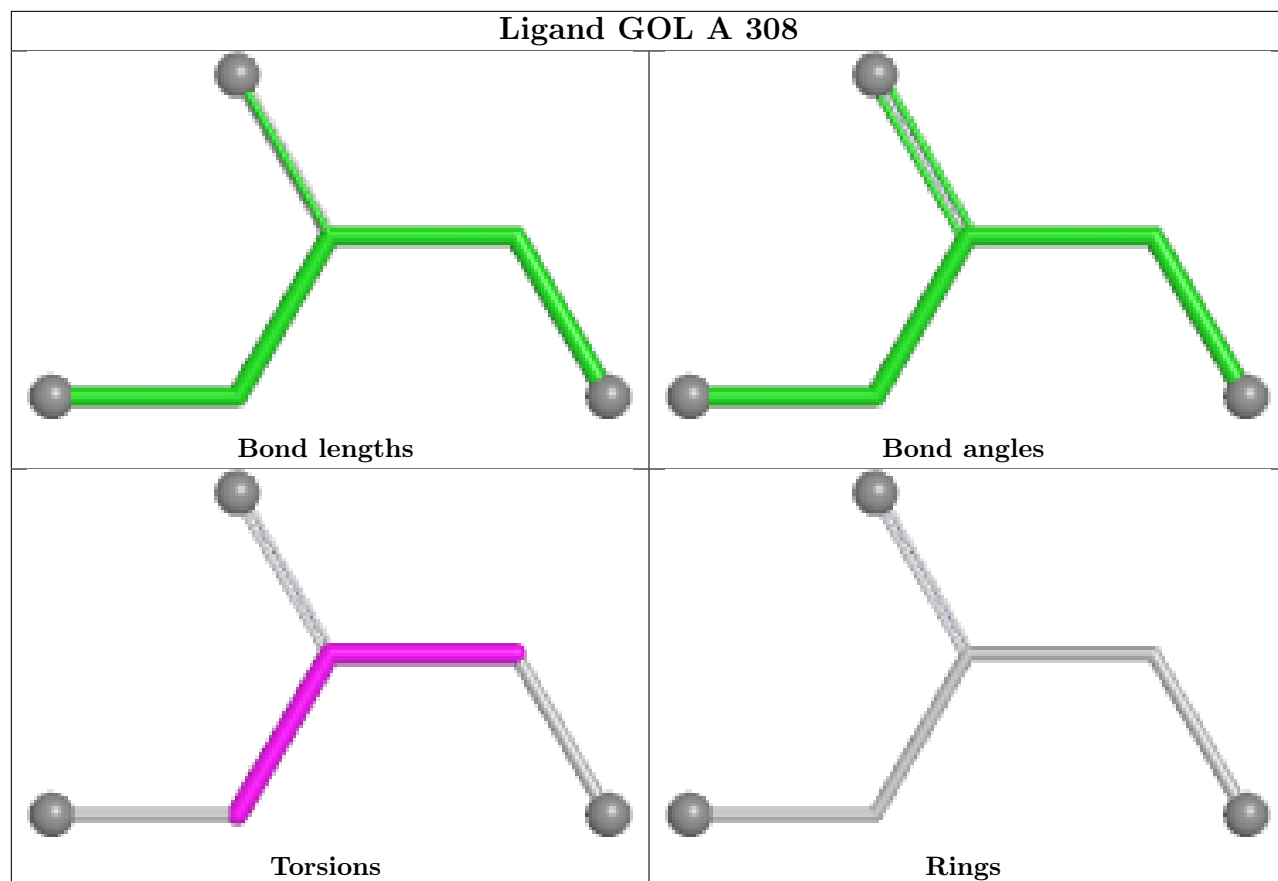


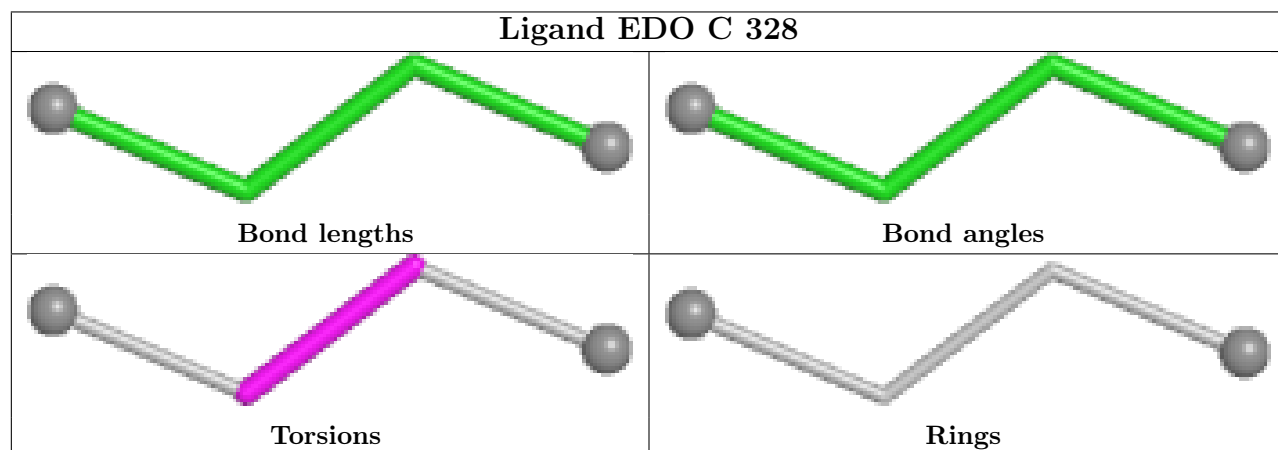
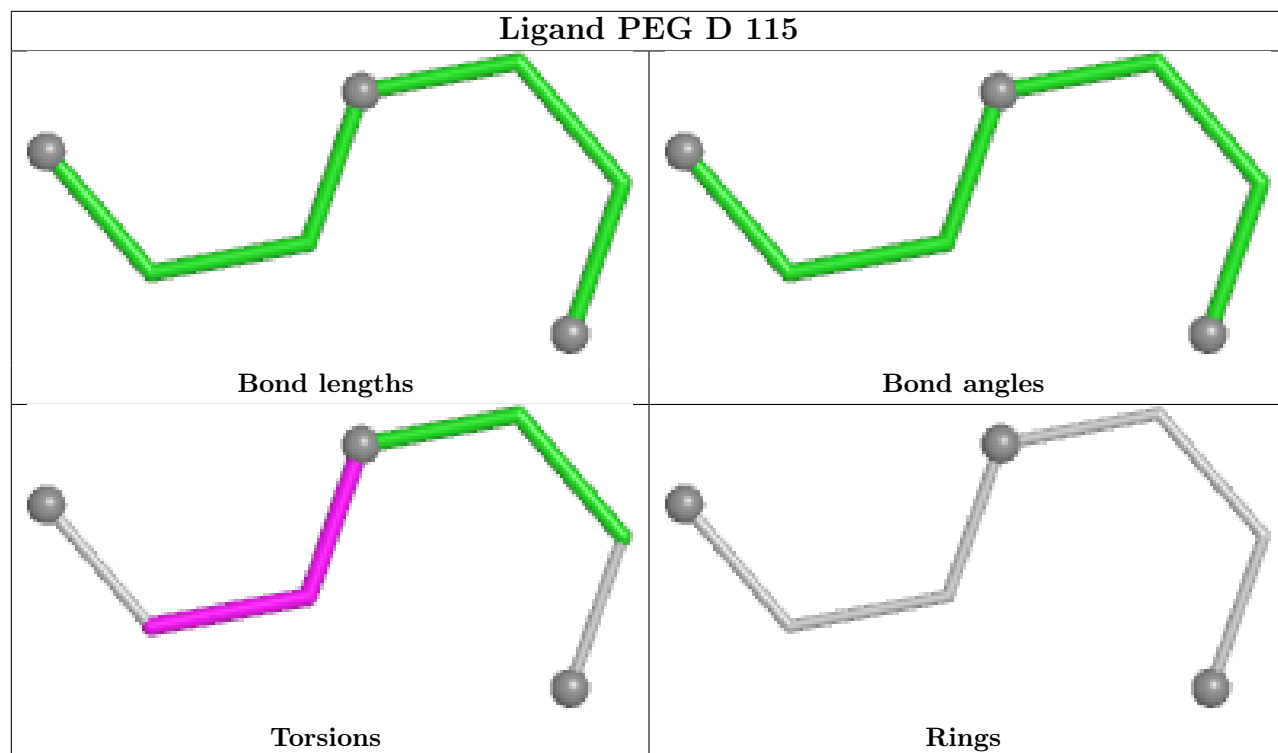


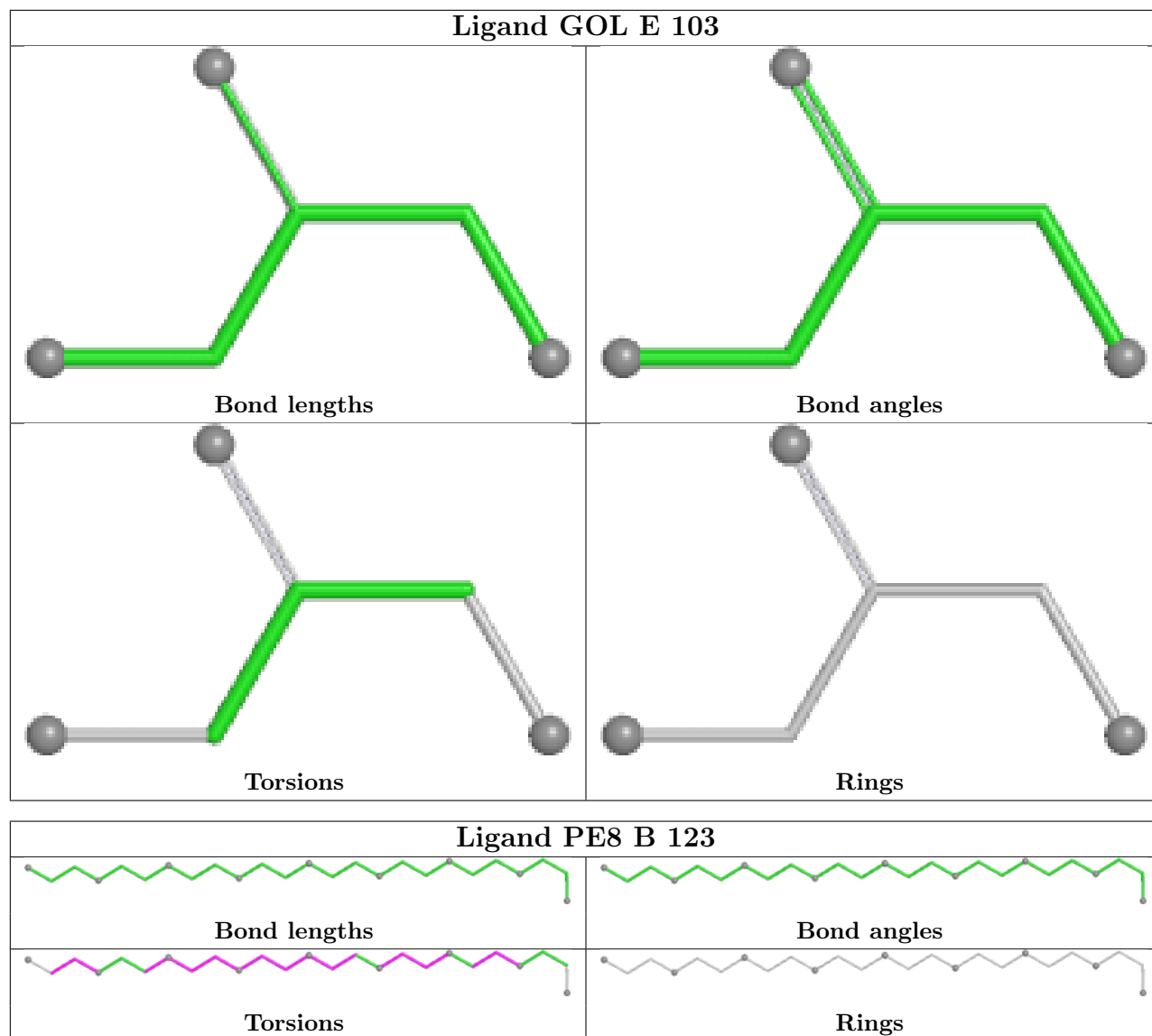


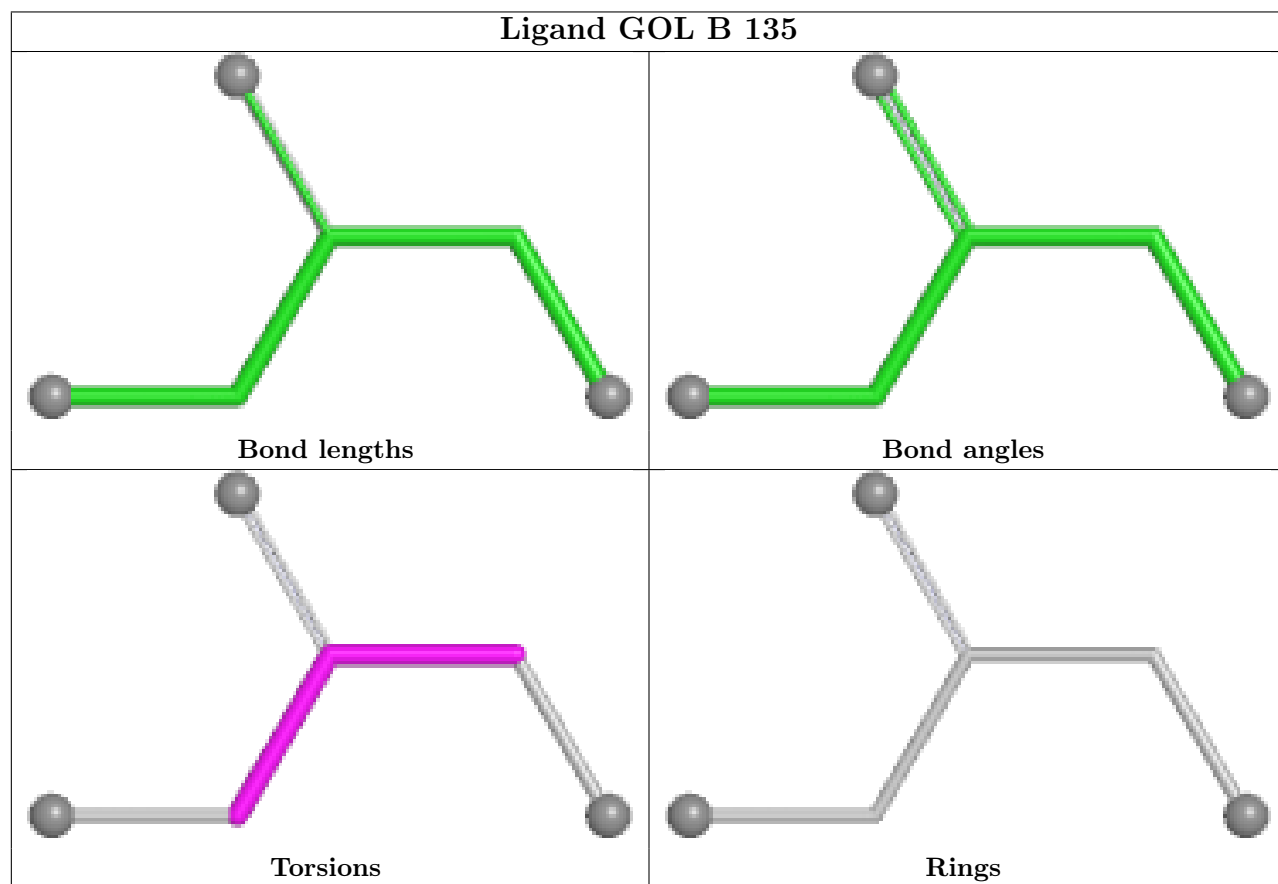
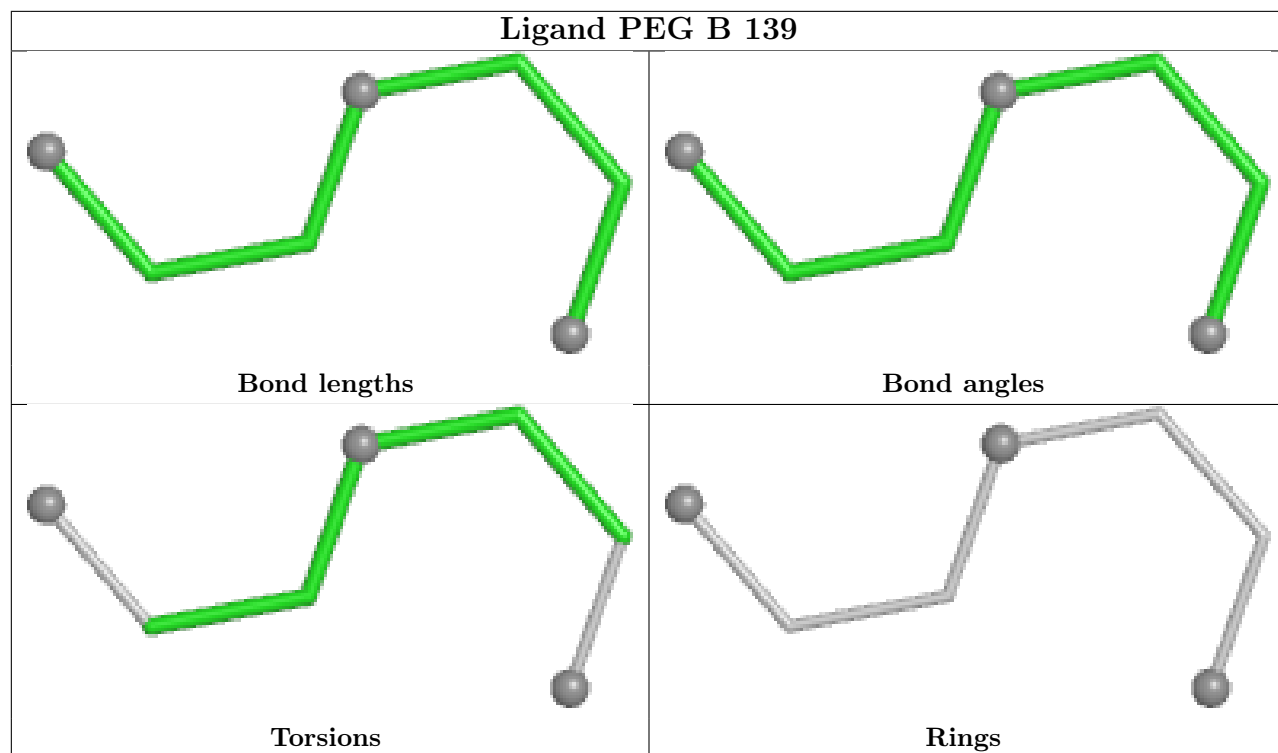


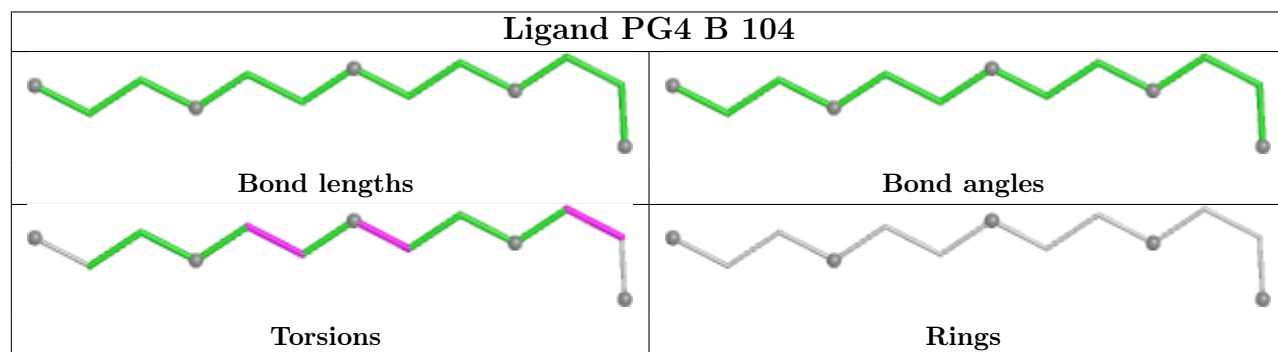
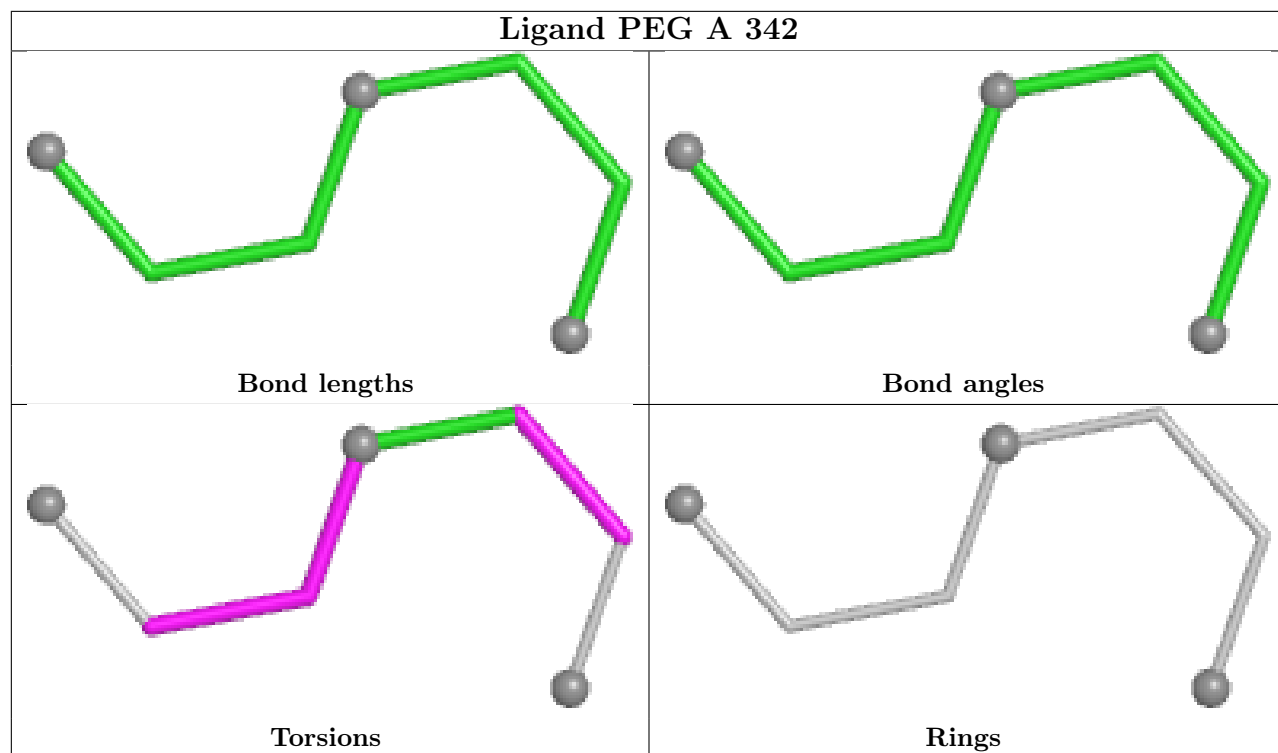


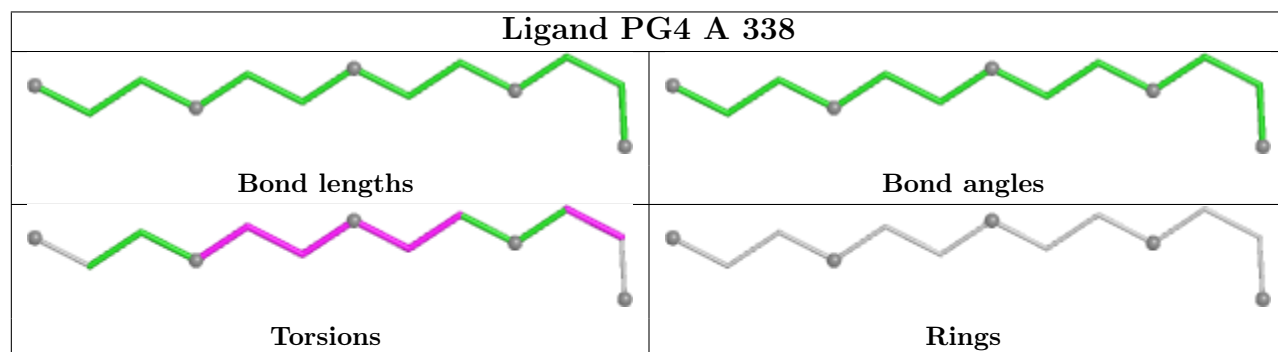
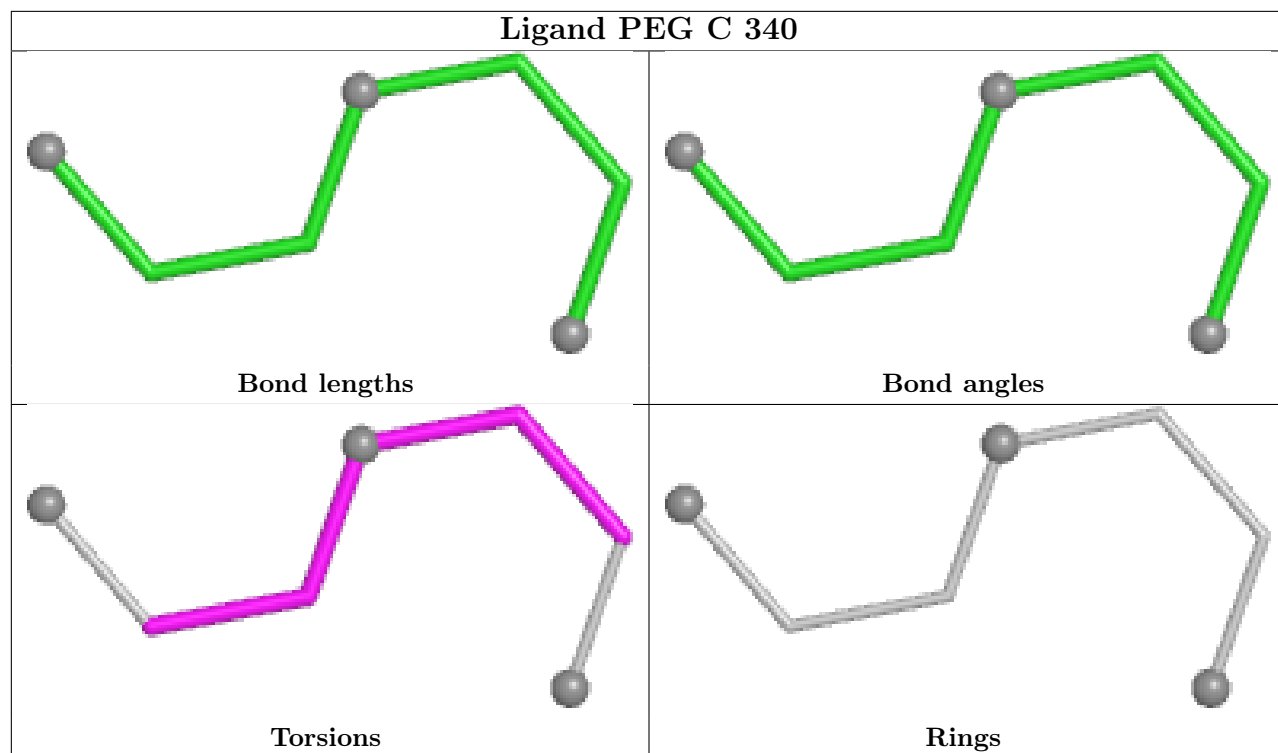


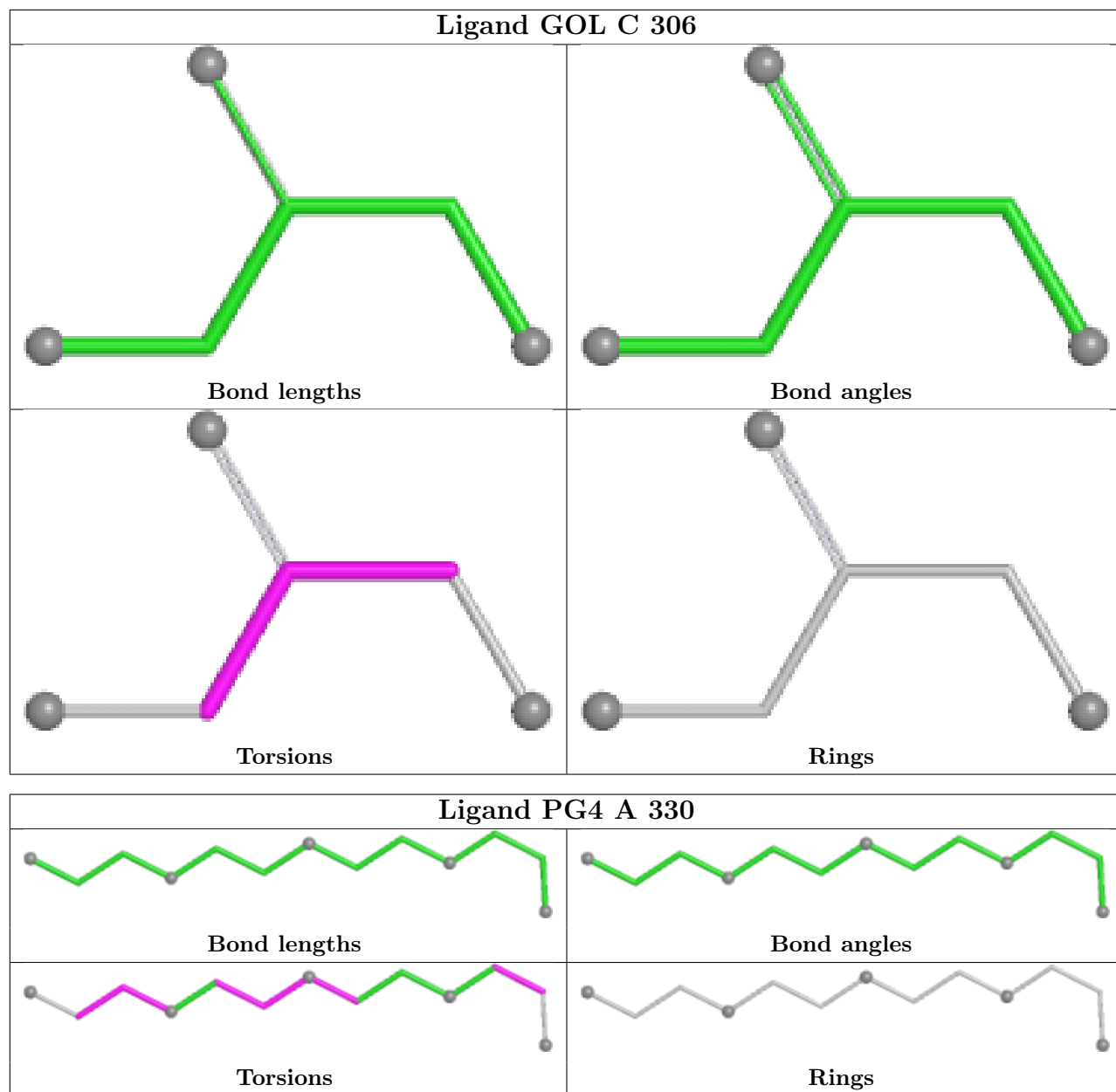


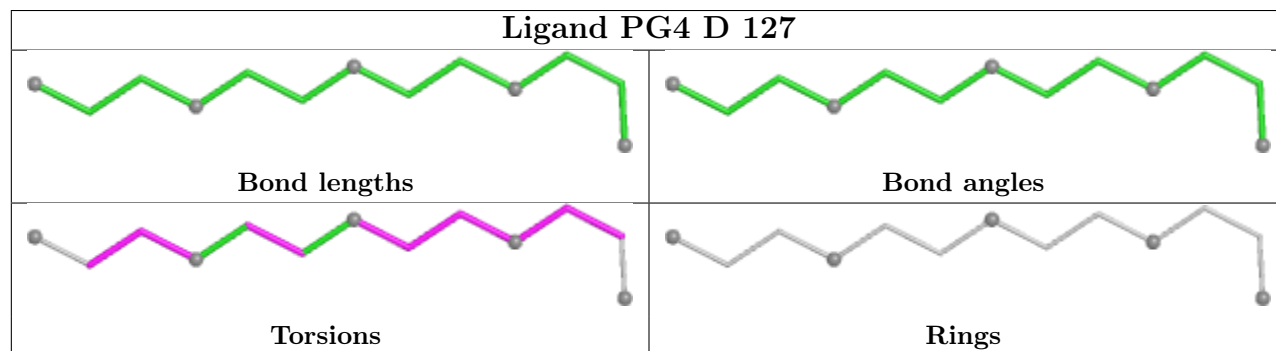
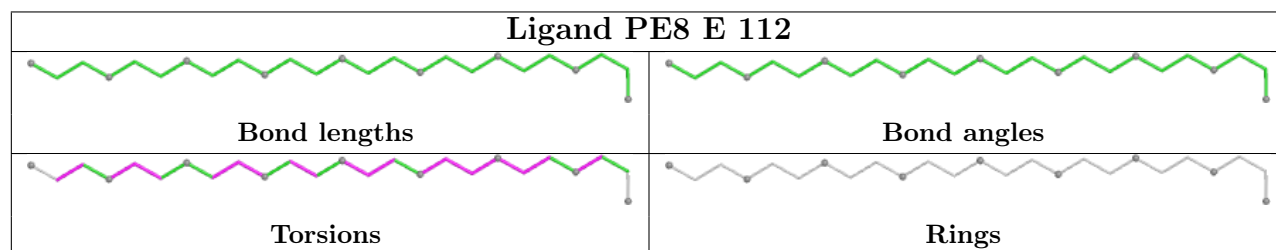
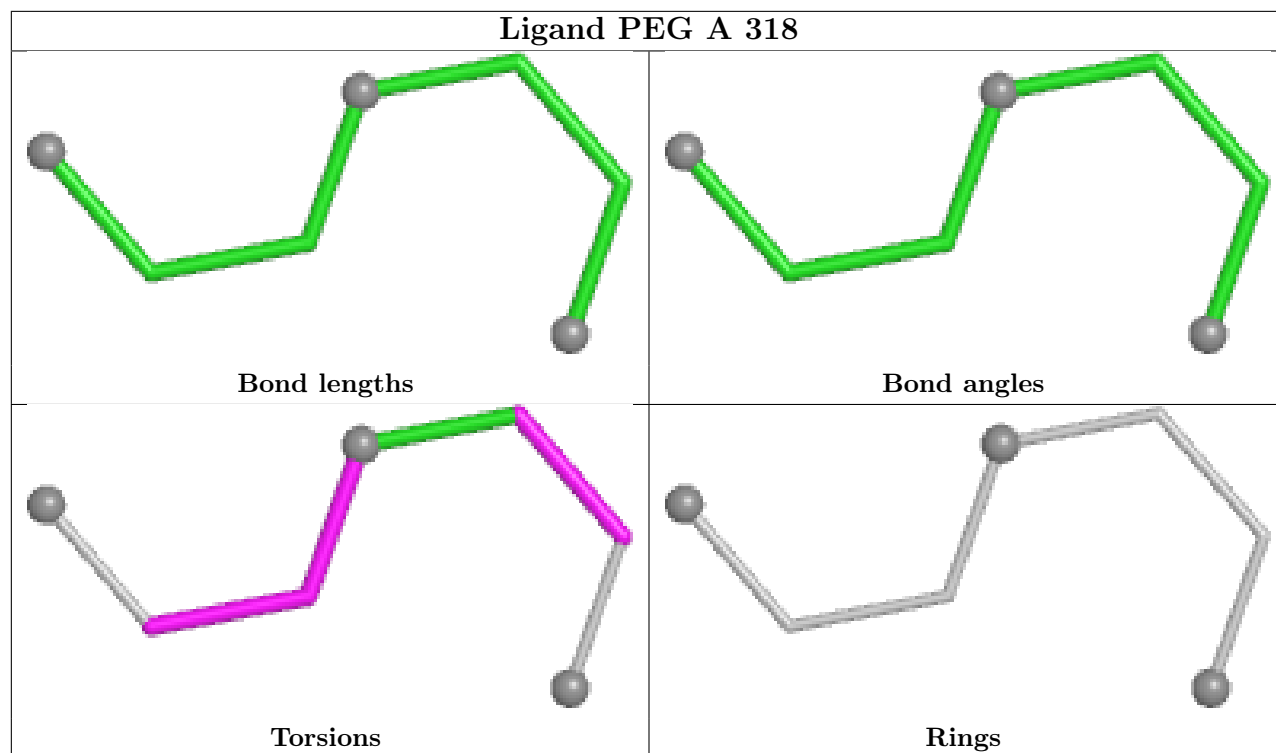


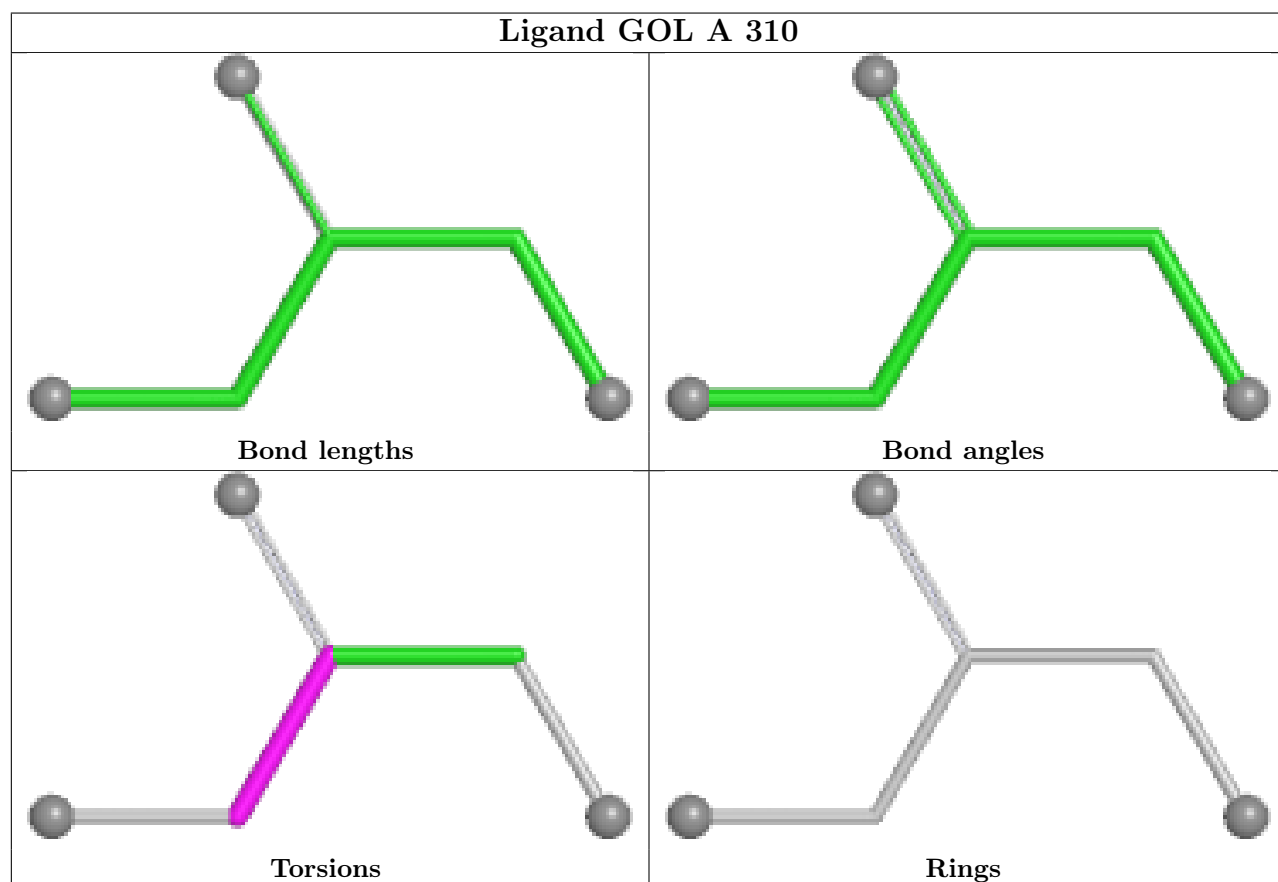
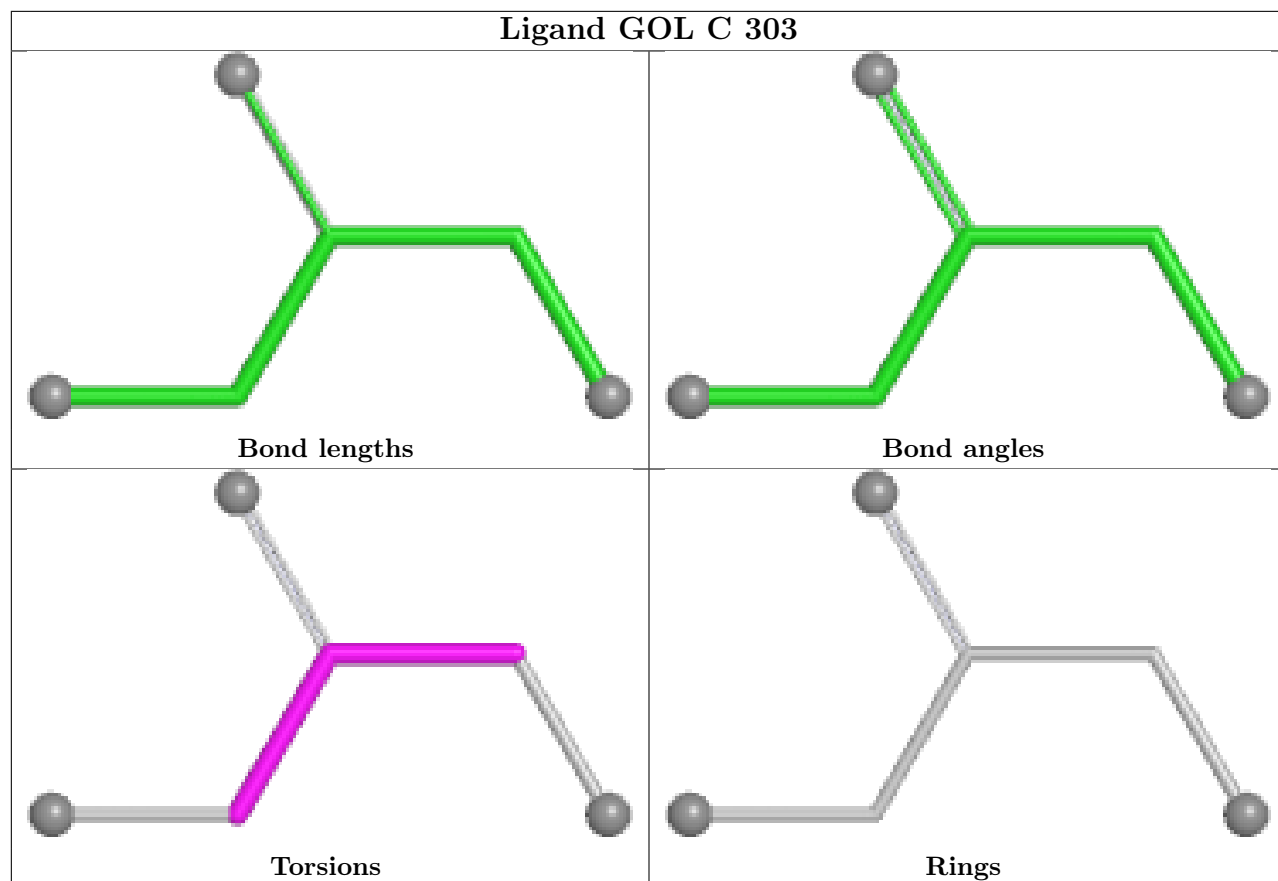


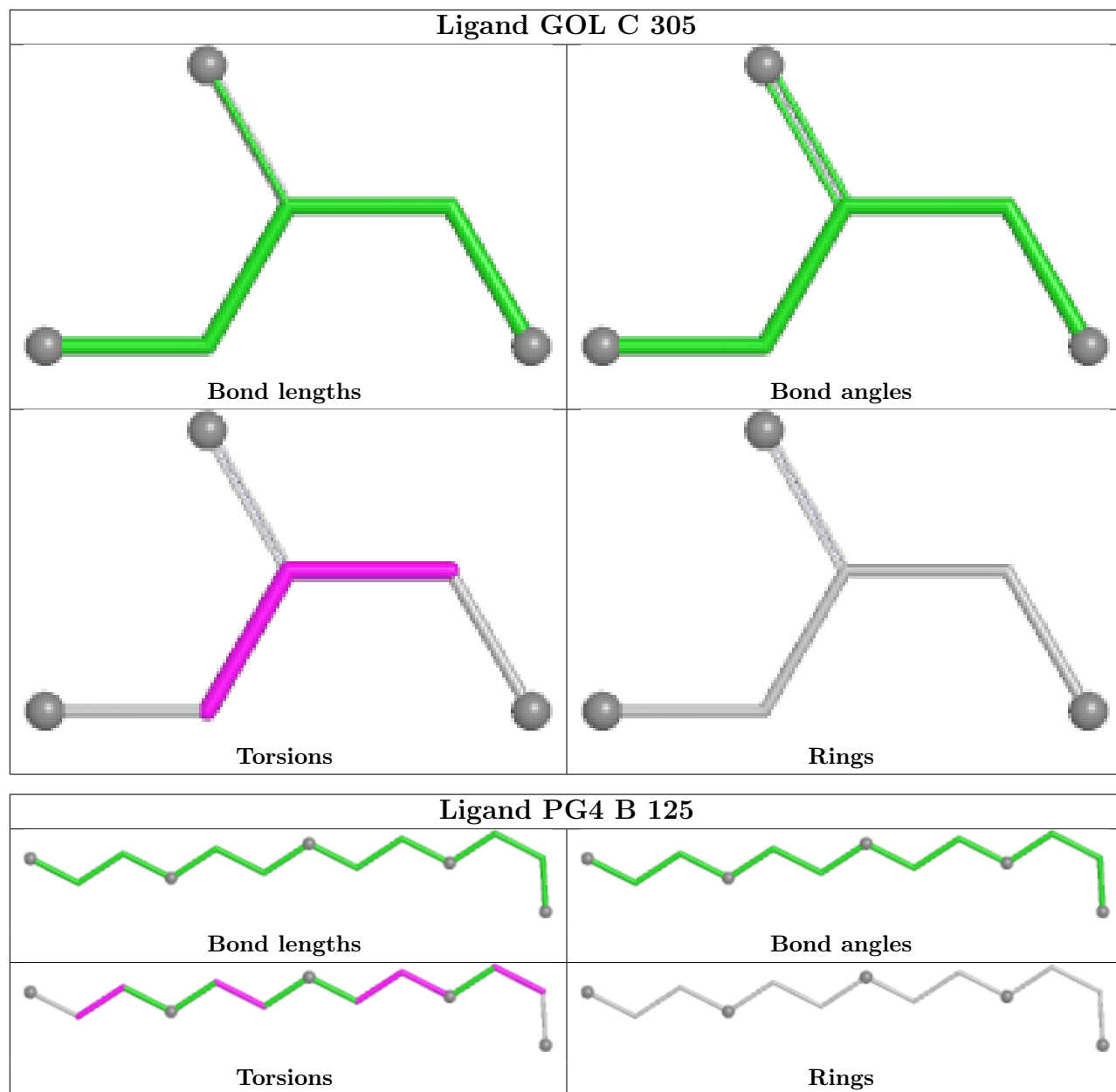


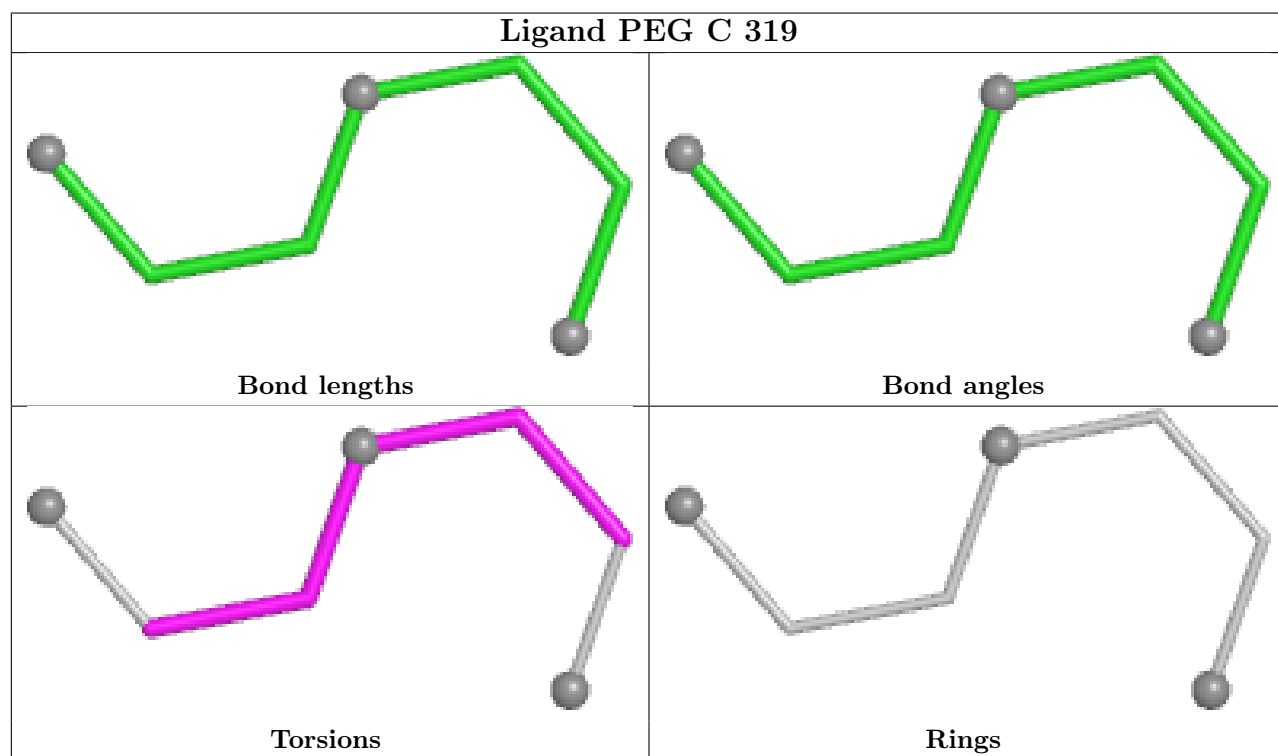
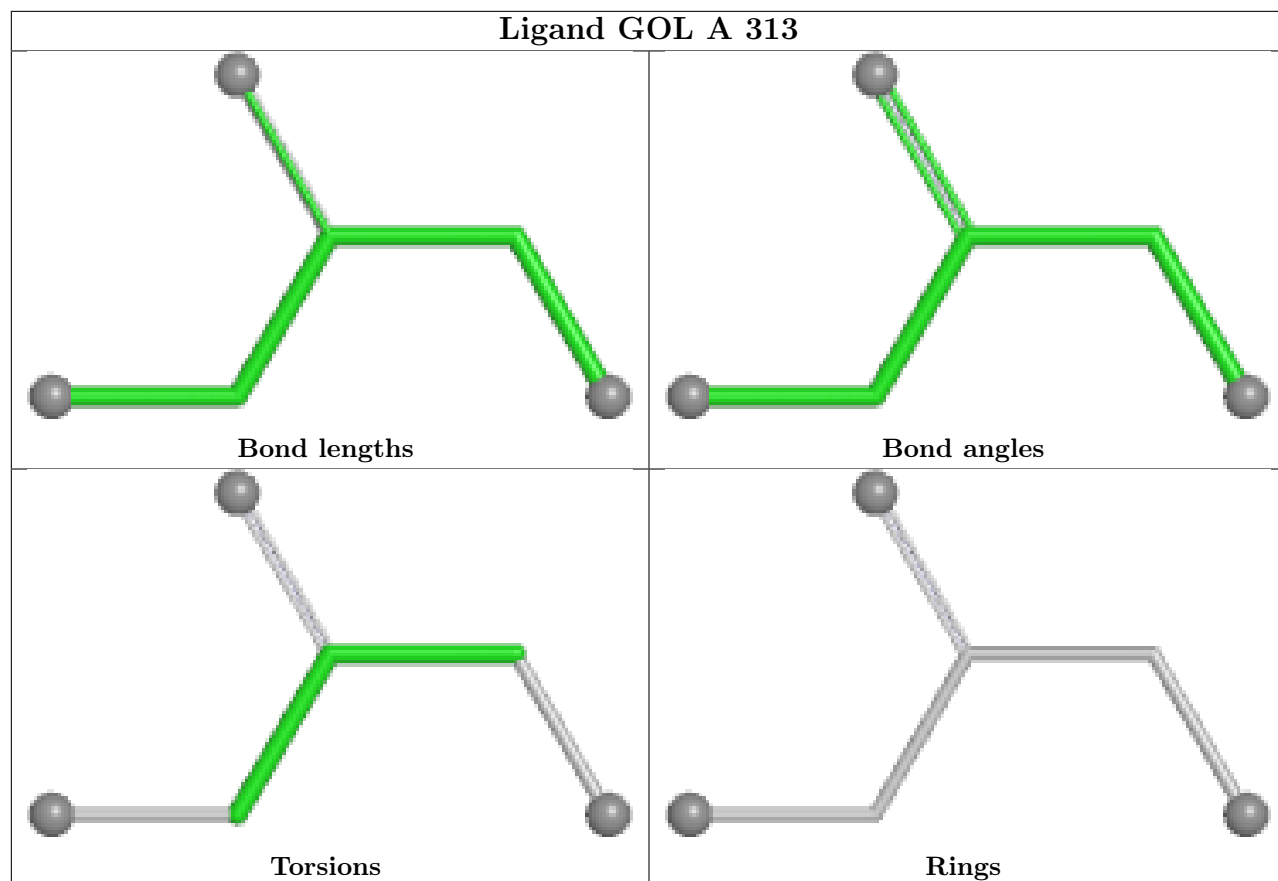


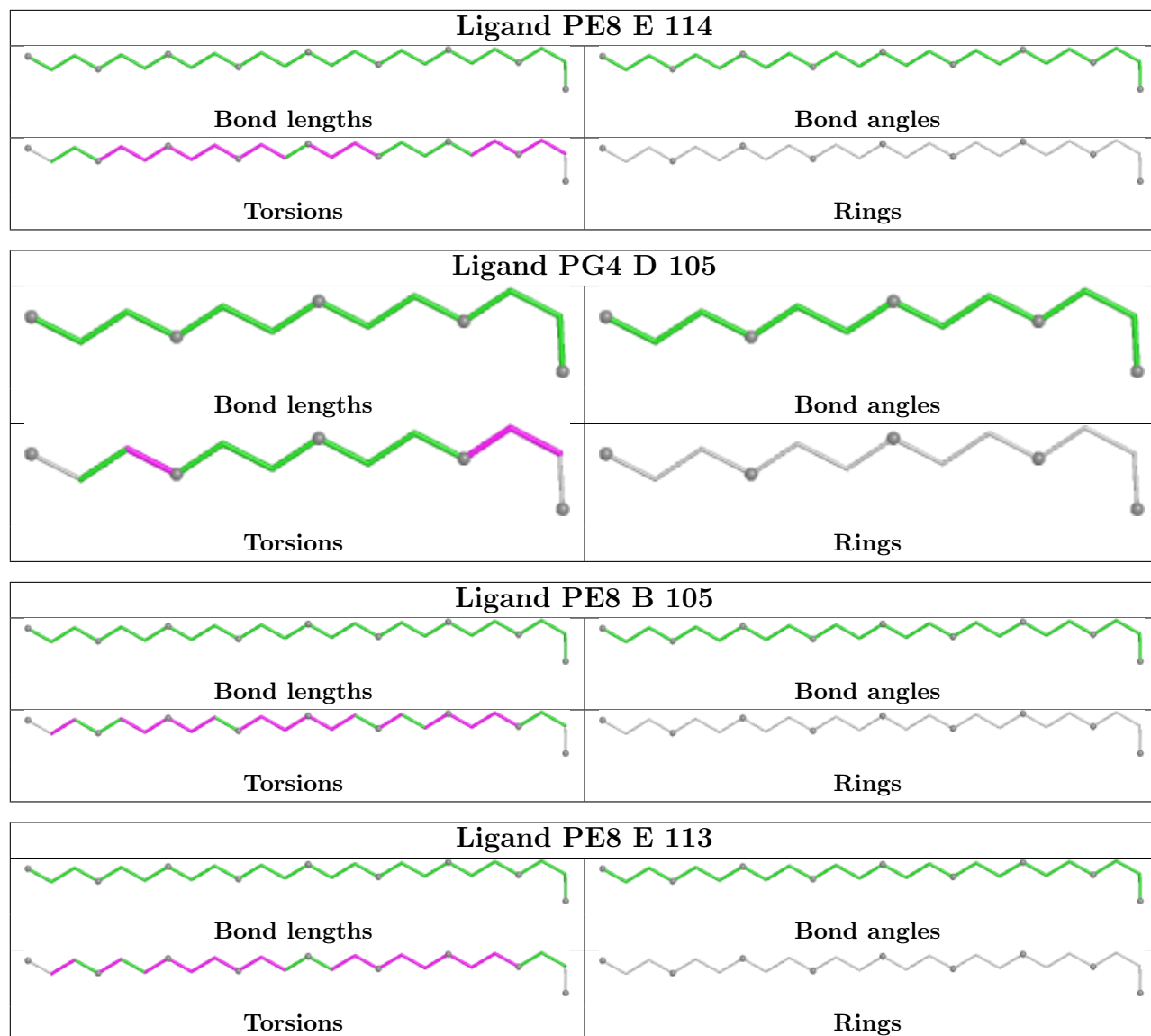


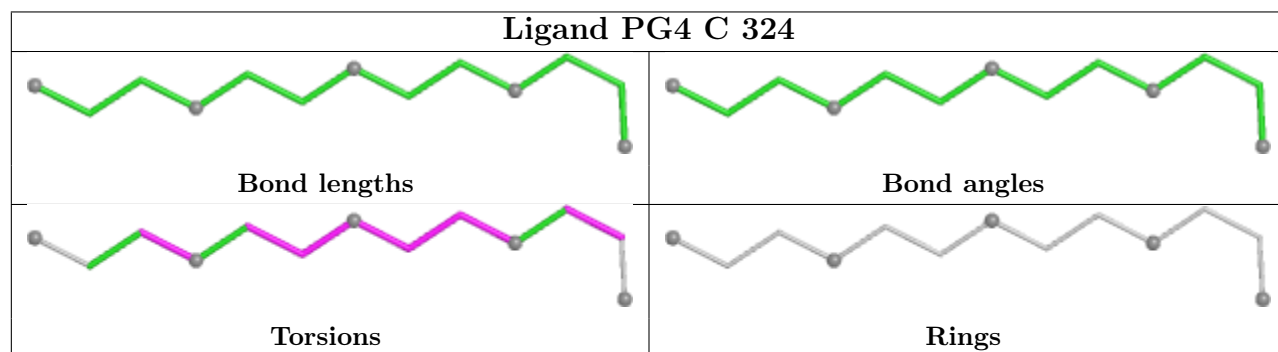
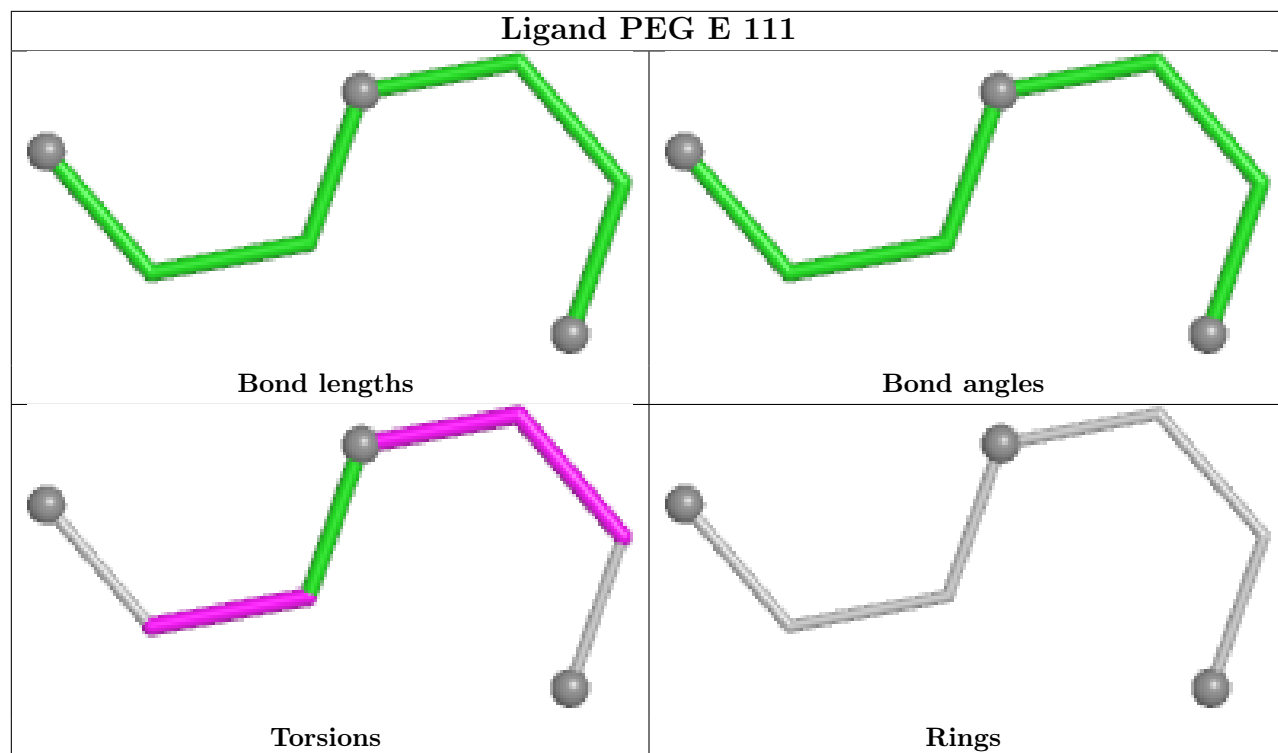


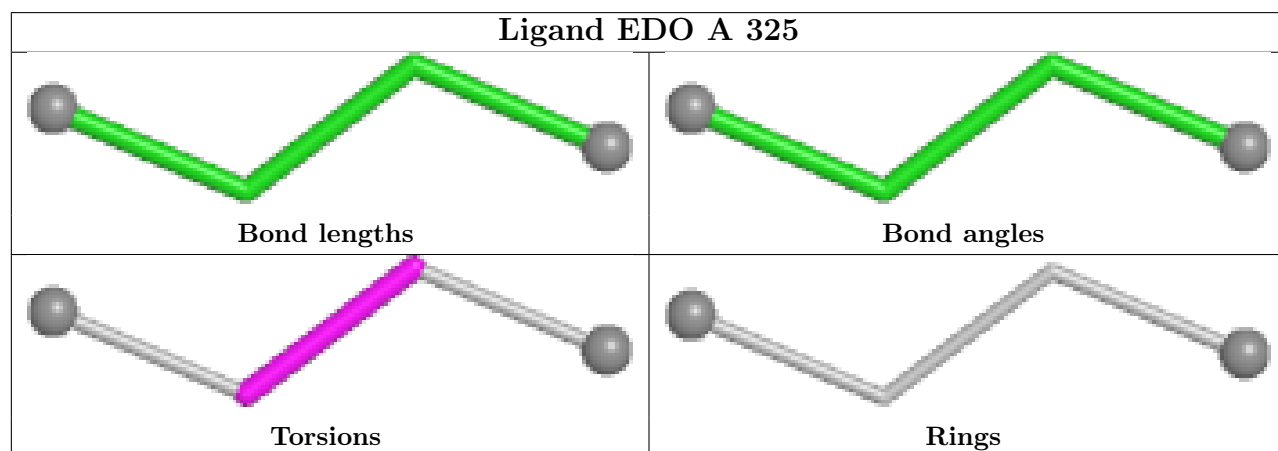
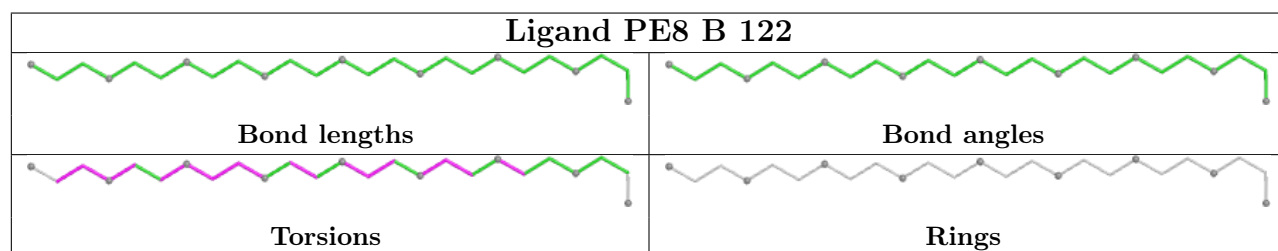
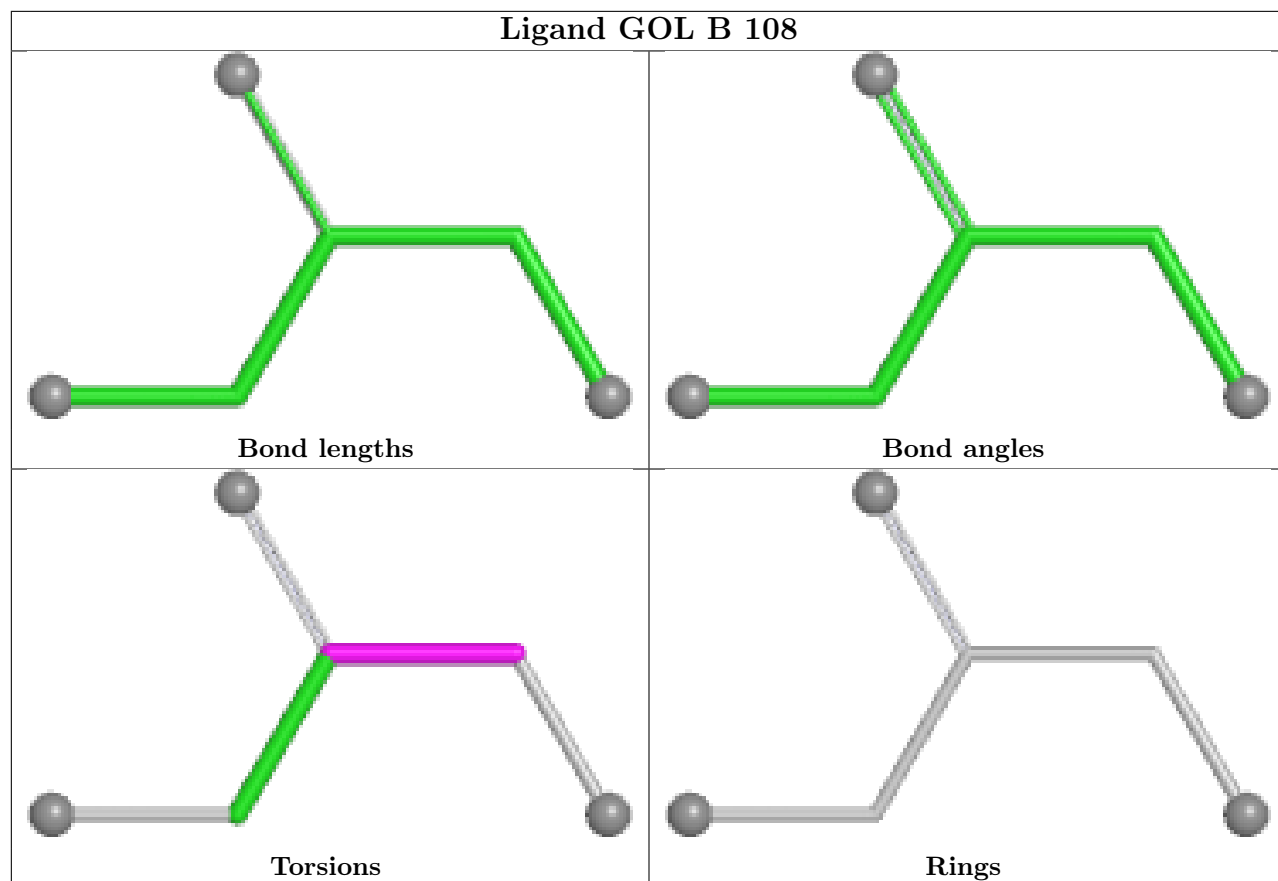


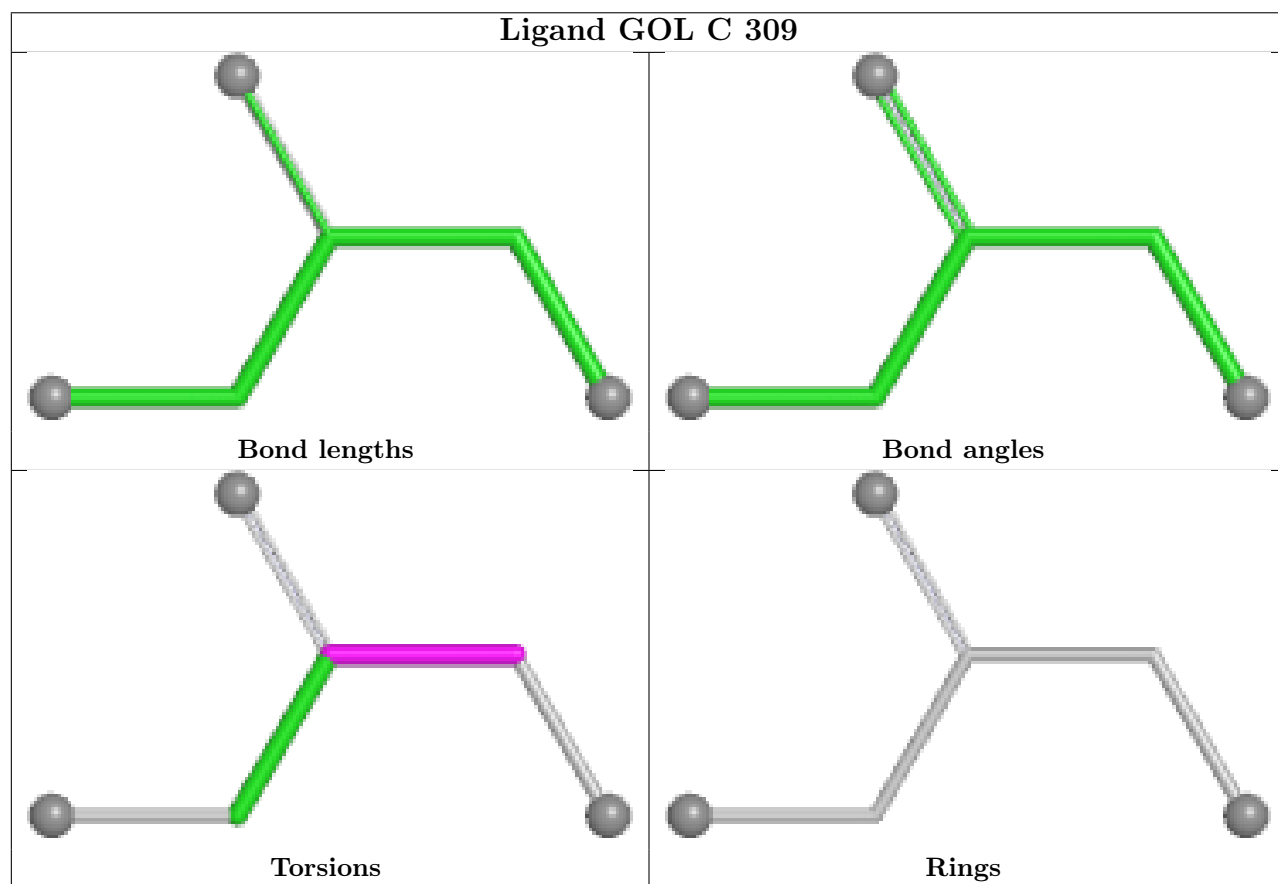
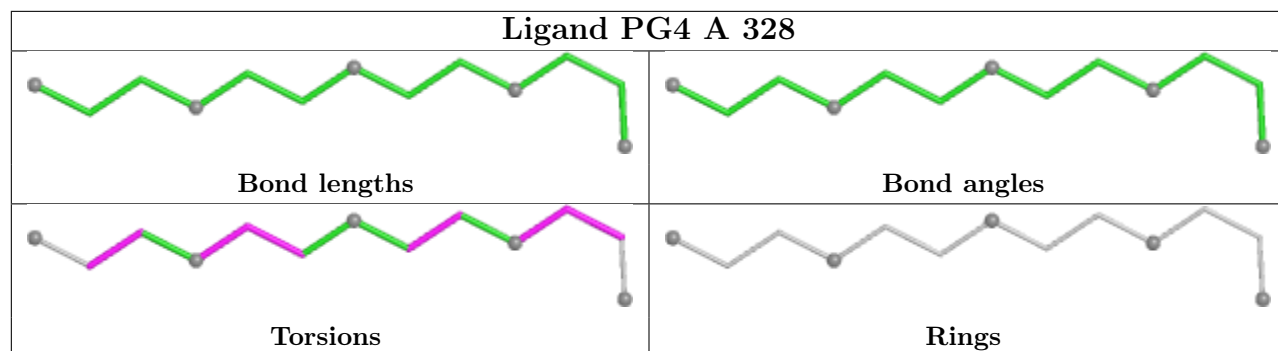


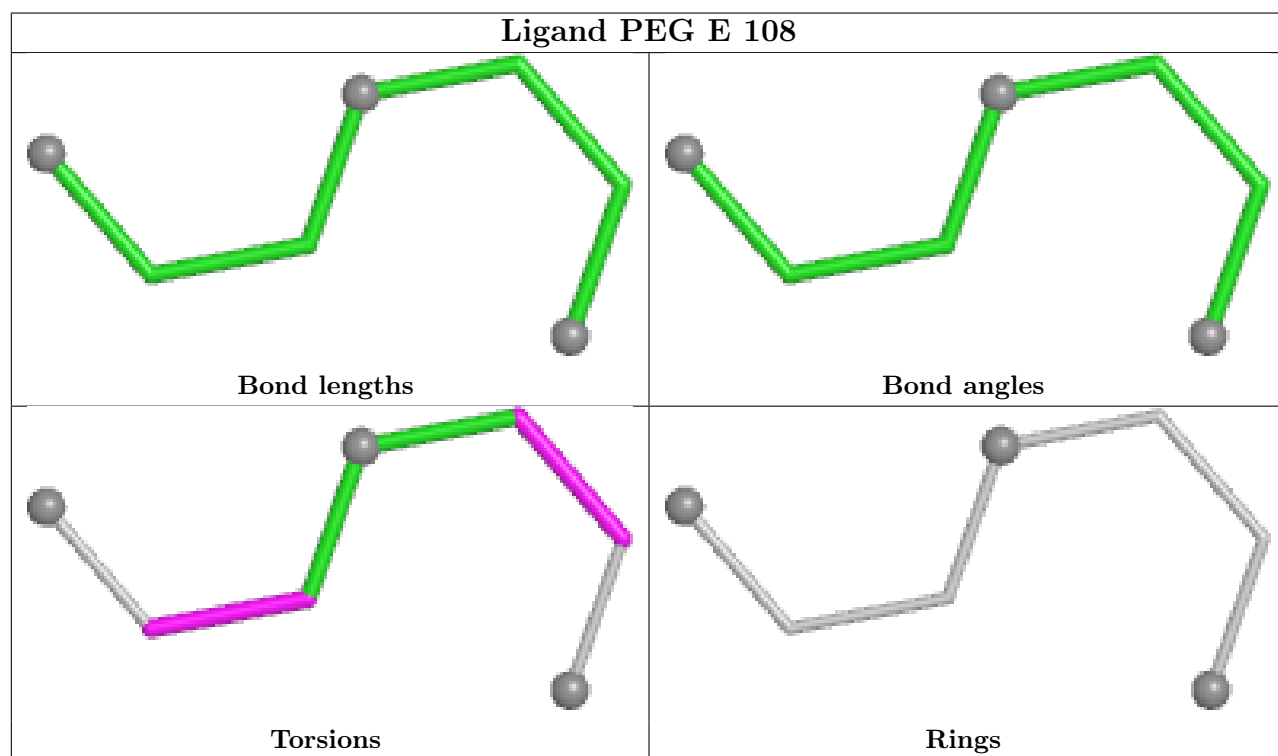
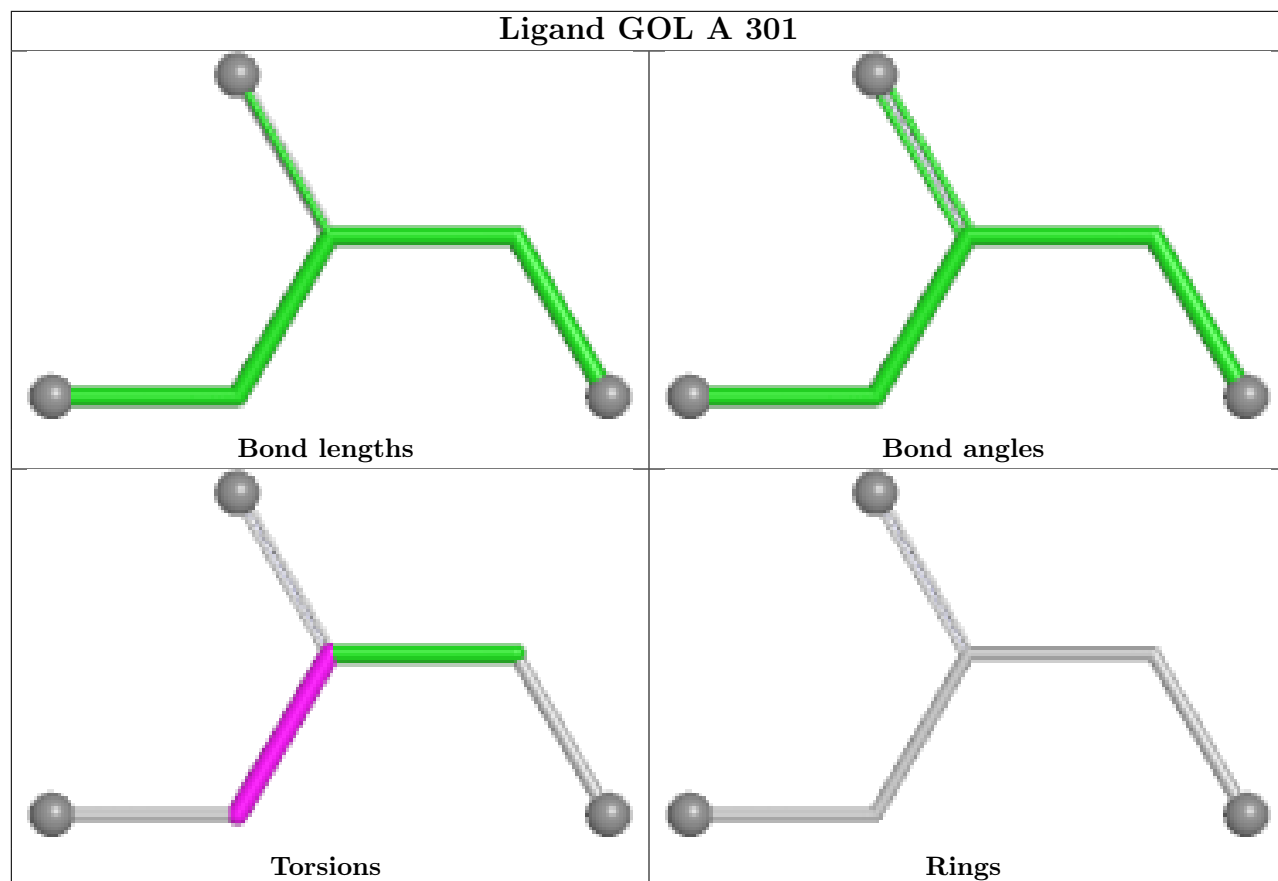


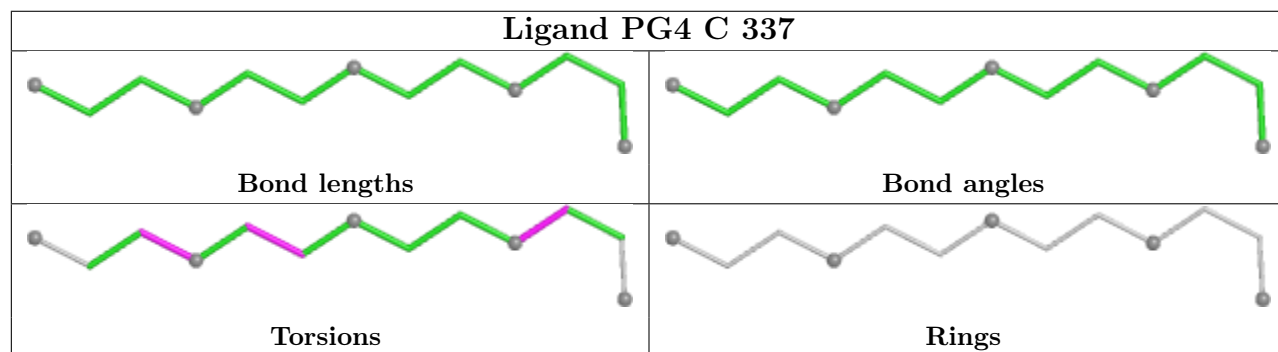
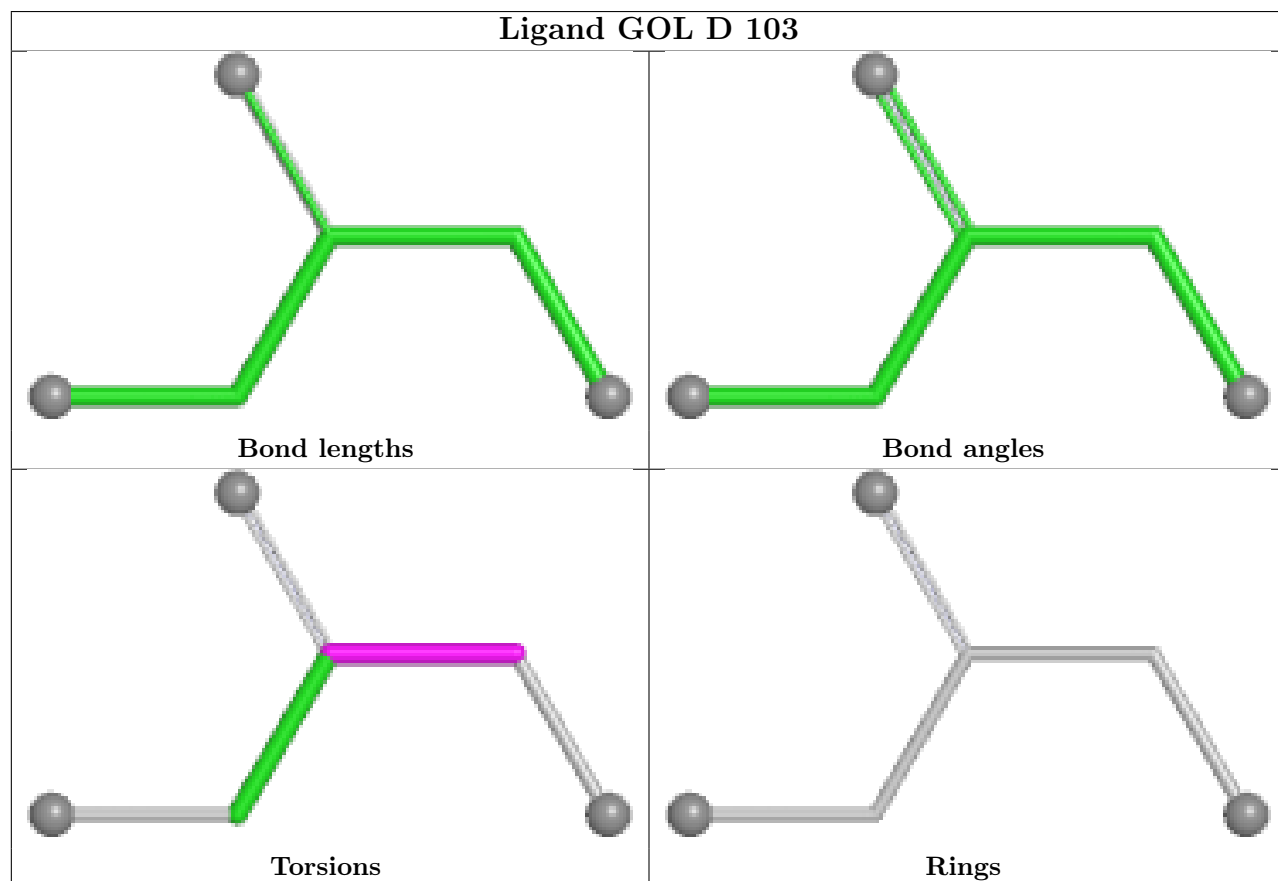
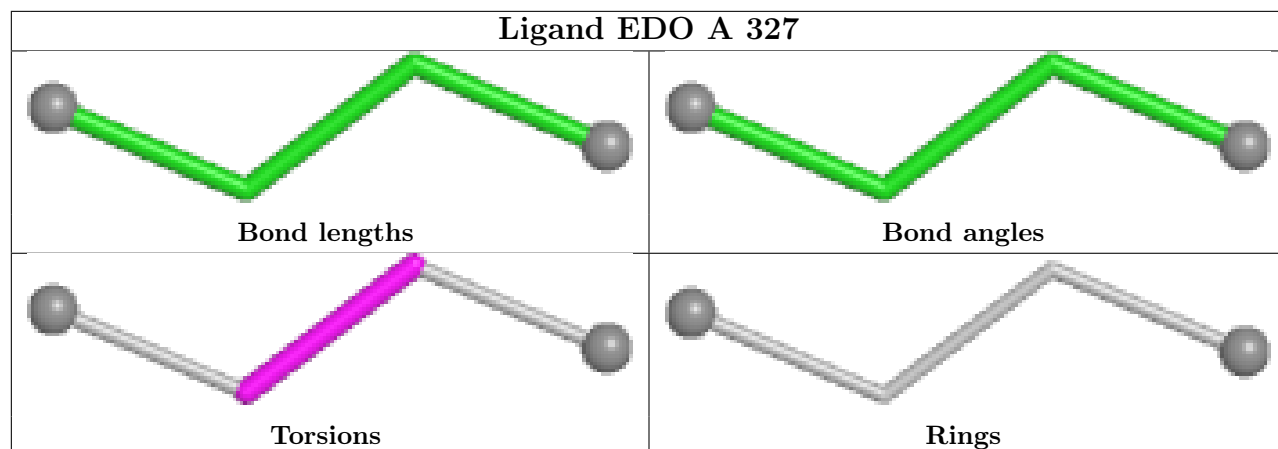


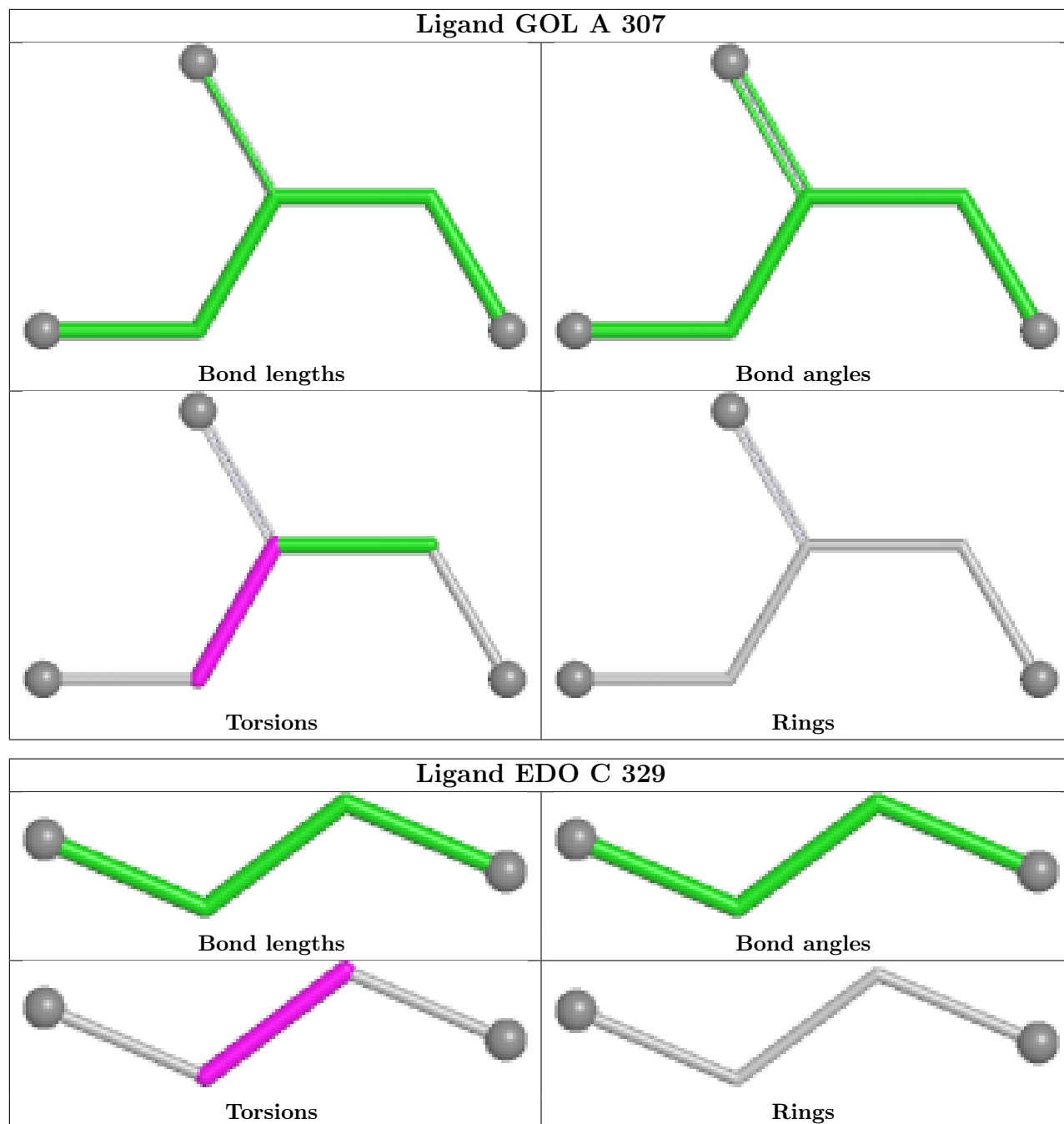












5.7 Other polymers [i](#)

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(Å ²)	Q<0.9
1	A	241/241 (100%)	1.49	68 (28%)  	31, 50, 63, 71	0
1	C	241/241 (100%)	1.60	72 (29%)  	36, 54, 64, 76	0
1	E	18/241 (7%)	0.71	1 (5%)  	37, 56, 69, 72	0
2	B	98/98 (100%)	1.44	23 (23%)  	42, 64, 78, 85	0
2	D	98/98 (100%)	1.37	19 (19%)  	36, 54, 66, 69	0
All	All	696/919 (75%)	1.48	183 (26%)  	31, 53, 70, 85	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	149	SER	7.0
1	C	116	ILE	6.6
1	C	28	SER	6.4
1	A	51	VAL	6.2
2	D	54	TYR	6.2
1	C	178	LEU	5.9
1	C	70	LEU	5.5
2	D	96	THR	5.4
2	D	42	GLN	4.5
1	C	114	CYS	4.5
1	C	210	TRP	4.3
1	C	104	TYR	4.3
1	C	113	LEU	4.3
1	A	26	LEU	4.3
1	C	127	ASN	4.2
1	C	147	SER	4.2
1	A	47	SER	4.2
1	C	47	SER	4.1
2	B	51	THR	4.1
2	B	53	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	237	ILE	3.9
1	A	217	ASN	3.8
1	C	231	LEU	3.8
2	B	97	GLY	3.8
1	C	103	ASP	3.7
2	D	57	VAL	3.7
1	C	66	SER	3.7
1	A	141	ARG	3.7
1	A	43	TRP	3.6
1	A	204	ASN	3.6
2	B	81	VAL	3.6
1	C	155	ASP	3.6
1	A	234	ASP	3.5
2	B	52	ASN	3.5
1	A	162	GLY	3.5
1	C	115	ASN	3.5
1	A	106	TYR	3.4
1	C	86	ASN	3.4
1	A	25	ARG	3.3
1	C	214	GLY	3.3
1	C	24	TRP	3.3
1	A	163	ILE	3.3
1	A	40	GLY	3.3
1	A	53	SER	3.2
2	D	31	THR	3.2
1	C	145	PRO	3.2
2	B	83	THR	3.2
1	A	70	LEU	3.2
2	D	60	GLY	3.1
1	A	101	ASP	3.0
1	A	213	ARG	3.0
1	C	71	VAL	3.0
1	C	138	GLU	3.0
1	C	65	LEU	2.9
1	A	159	TYR	2.9
1	C	146	ILE	2.9
1	C	185	GLU	2.9
1	C	88	ALA	2.9
1	A	27	HIS	2.9
2	B	80	LEU	2.9
1	A	152	VAL	2.9
1	A	36	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	97	GLY	2.9
1	A	98	ILE	2.9
1	A	90	GLU	2.8
2	B	72	SER	2.8
1	C	173	ASN	2.8
1	C	112	ASN	2.8
1	A	54	GLN	2.8
1	A	41	SER	2.8
1	A	64	THR	2.8
1	A	17	PHE	2.8
1	A	202	ILE	2.8
1	A	216	ILE	2.8
1	A	99	CYS	2.7
1	C	46	SER	2.7
1	C	232	GLY	2.7
2	D	59	ALA	2.7
1	C	158	PHE	2.7
1	A	179	VAL	2.7
1	C	143	LEU	2.7
1	A	56	ALA	2.7
1	A	154	ASP	2.7
1	C	36	GLN	2.7
1	A	187	VAL	2.7
1	C	200	TYR	2.7
2	B	38	LEU	2.7
2	B	82	LEU	2.7
2	D	6	LEU	2.7
1	A	102	ASP	2.7
1	C	23	ASP	2.7
1	C	139	ALA	2.6
1	C	174	HIS	2.6
2	B	54	TYR	2.6
1	C	98	ILE	2.6
1	C	148	ILE	2.6
2	D	55	ILE	2.6
1	C	72	ASP	2.6
1	C	150	VAL	2.5
1	C	176	VAL	2.5
2	D	52	ASN	2.5
1	C	63	ILE	2.5
1	A	200	TYR	2.5
1	A	42	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	79	ASP	2.5
1	C	55	TYR	2.5
1	A	65	LEU	2.5
1	C	168	CYS	2.5
1	C	181	PHE	2.5
2	B	31	THR	2.5
1	C	53	SER	2.5
1	A	116	ILE	2.5
1	A	3	ASN	2.5
1	A	82	GLY	2.5
2	B	9	ALA	2.4
1	C	216	ILE	2.4
2	B	70	PHE	2.4
2	D	82	LEU	2.4
1	A	181	PHE	2.4
1	C	117	ASP	2.4
1	A	30	VAL	2.4
1	C	163	ILE	2.3
2	D	39	GLU	2.3
1	A	50	SER	2.3
2	B	2	ILE	2.3
2	D	94	GLU	2.3
1	C	51	VAL	2.3
2	D	69	VAL	2.3
1	C	184	LYS	2.3
1	C	8	ILE	2.3
1	A	109	ASP	2.3
1	C	124	GLY	2.3
1	C	177	MET	2.3
1	A	66	SER	2.3
2	B	10	LYS	2.3
1	A	214	GLY	2.2
1	A	81	ASN	2.2
2	D	47	VAL	2.2
2	D	9	ALA	2.2
2	B	43	TYR	2.2
1	A	231	LEU	2.2
1	A	150	VAL	2.2
1	A	55	TYR	2.2
1	A	208	GLN	2.2
1	C	48	ILE	2.2
1	C	2	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	157	ALA	2.2
1	C	83	GLY	2.2
1	C	7	VAL	2.1
1	C	22	TYR	2.1
2	B	85	TYR	2.1
1	A	93	ILE	2.1
1	A	235	ALA	2.1
1	C	151	ALA	2.1
1	C	89	PHE	2.1
1	A	123	TYR	2.1
2	D	16	ILE	2.1
1	A	84	LEU	2.1
1	C	159	TYR	2.1
1	A	238	PRO	2.1
1	C	238	PRO	2.1
1	A	80	CYS	2.1
1	E	14	LEU	2.1
2	B	55	ILE	2.1
2	D	67	LEU	2.1
1	A	78	TYR	2.1
1	A	96	GLY	2.1
1	A	105	PRO	2.1
1	A	218	ILE	2.1
1	C	198	TYR	2.1
1	A	121	GLU	2.1
1	C	205	SER	2.0
1	A	215	PHE	2.0
2	D	25	PRO	2.0
1	A	138	GLU	2.0
2	B	28	GLU	2.0
1	A	71	VAL	2.0
1	A	128	TYR	2.0
1	A	144	GLY	2.0
1	C	156	PHE	2.0
1	C	52	GLU	2.0
2	B	27	LEU	2.0
2	B	95	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	B	143	1/1	0.45	0.15	29,29,29,29	0
4	NA	D	104	1/1	0.58	0.18	41,41,41,41	0
3	GOL	B	114	6/6	0.64	0.13	33,37,42,48	0
7	EDO	C	328	4/4	0.64	0.24	44,45,47,48	0
3	GOL	A	303	6/6	0.67	0.17	46,53,58,60	0
3	GOL	C	303	6/6	0.68	0.16	50,67,68,72	0
3	GOL	A	310	6/6	0.68	0.21	39,46,54,61	0
5	PEG	C	316	7/7	0.69	0.15	37,47,51,57	0
3	GOL	C	307	6/6	0.69	0.12	45,51,53,56	0
5	PEG	A	320	7/7	0.71	0.16	38,49,57,61	0
8	PG4	C	327	13/13	0.71	0.14	45,53,57,59	0
9	SO4	B	119	5/5	0.72	0.12	78,80,90,96	0
3	GOL	B	137	6/6	0.73	0.12	28,41,44,55	0
5	PEG	E	108	7/7	0.73	0.15	45,53,58,62	0
6	PE8	C	321	25/25	0.73	0.12	36,44,50,51	0
4	NA	D	129	1/1	0.74	0.08	34,34,34,34	0
8	PG4	C	332	13/13	0.74	0.15	38,46,57,57	0
5	PEG	A	342	7/7	0.74	0.16	34,36,45,46	0
3	GOL	C	302	6/6	0.75	0.14	43,53,58,59	0
3	GOL	A	314	6/6	0.75	0.16	32,33,40,42	0
7	EDO	A	336	4/4	0.75	0.26	48,51,52,53	0
5	PEG	A	319	7/7	0.75	0.15	29,36,40,43	0
3	GOL	B	116	6/6	0.75	0.13	46,48,51,52	0
3	GOL	C	331	6/6	0.75	0.16	22,26,34,35	0
3	GOL	B	101	6/6	0.75	0.13	30,38,42,54	0
8	PG4	C	324	13/13	0.76	0.12	46,53,62,62	0
7	EDO	A	327	4/4	0.76	0.09	54,57,63,63	0
3	GOL	B	115	6/6	0.76	0.15	31,40,57,67	0
3	GOL	C	308	6/6	0.76	0.16	30,42,48,54	0
3	GOL	B	110	6/6	0.77	0.11	38,41,45,46	0
5	PEG	C	320	7/7	0.77	0.17	18,25,32,36	0
5	PEG	D	123	7/7	0.77	0.11	39,41,51,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	B	117	1/1	0.78	0.10	30,30,30,30	0
3	GOL	C	306	6/6	0.78	0.13	42,47,52,52	0
6	PE8	E	112	25/25	0.78	0.13	16,39,48,52	0
3	GOL	A	308	6/6	0.78	0.17	41,44,45,47	0
5	PEG	A	335	7/7	0.78	0.19	30,31,38,40	0
4	NA	D	111	1/1	0.79	0.15	35,35,35,35	0
3	GOL	B	102	6/6	0.79	0.13	44,53,61,63	0
5	PEG	E	109	7/7	0.79	0.15	32,43,52,56	0
8	PG4	A	330	13/13	0.79	0.15	28,36,50,53	0
6	PE8	B	105	25/25	0.79	0.12	36,45,54,55	0
3	GOL	D	108	6/6	0.79	0.15	12,16,21,24	0
3	GOL	D	124	6/6	0.79	0.12	35,45,50,53	0
6	PE8	E	114	25/25	0.79	0.11	34,42,47,49	0
3	GOL	D	122	6/6	0.80	0.14	2,11,18,21	0
3	GOL	D	107	6/6	0.80	0.13	16,23,30,34	0
3	GOL	C	304	6/6	0.80	0.14	35,41,48,52	0
8	PG4	D	101	13/13	0.80	0.18	33,55,67,69	0
8	PG4	D	117	13/13	0.80	0.13	43,51,59,60	0
8	PG4	A	337	13/13	0.80	0.13	27,30,52,52	0
5	PEG	D	115	7/7	0.81	0.13	27,38,42,47	0
3	GOL	E	103	6/6	0.81	0.12	29,38,39,45	0
3	GOL	C	310	6/6	0.81	0.12	33,44,46,48	0
6	PE8	E	113	25/25	0.81	0.13	18,31,39,44	0
3	GOL	C	309	6/6	0.81	0.16	41,46,49,55	0
8	PG4	B	127	13/13	0.81	0.12	32,40,54,57	0
8	PG4	A	331	13/13	0.82	0.11	34,49,60,63	0
3	GOL	D	110	6/6	0.82	0.12	40,45,51,51	0
3	GOL	D	106	6/6	0.82	0.13	22,26,30,32	0
3	GOL	B	138	6/6	0.82	0.15	20,29,36,39	0
5	PEG	C	330	7/7	0.82	0.12	38,41,47,50	0
6	PE8	B	122	25/25	0.82	0.11	20,32,41,44	0
6	PE8	B	123	25/25	0.82	0.13	22,43,56,64	0
8	PG4	A	328	13/13	0.82	0.14	30,39,47,48	0
8	PG4	D	118	13/13	0.82	0.13	24,43,50,51	0
3	GOL	B	109	6/6	0.82	0.18	37,40,47,48	0
8	PG4	C	325	13/13	0.83	0.13	36,45,53,54	0
3	GOL	A	307	6/6	0.83	0.14	38,42,44,45	0
5	PEG	C	318	7/7	0.83	0.16	32,33,50,50	0
8	PG4	B	104	13/13	0.83	0.10	20,30,35,35	0
8	PG4	D	116	13/13	0.83	0.14	24,36,40,41	0
8	PG4	B	125	13/13	0.83	0.12	37,44,50,50	0
5	PEG	C	319	7/7	0.83	0.13	50,54,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PE8	A	324	25/25	0.83	0.10	22,33,51,54	0
3	GOL	A	309	6/6	0.84	0.09	33,40,50,50	0
3	GOL	C	311	6/6	0.84	0.08	37,48,49,53	0
5	PEG	A	341	7/7	0.84	0.10	14,24,29,34	0
8	PG4	A	338	13/13	0.84	0.11	24,40,57,59	0
8	PG4	D	105	13/13	0.84	0.14	29,36,47,61	0
3	GOL	B	111	6/6	0.84	0.11	43,46,53,55	0
7	EDO	C	329	4/4	0.84	0.11	38,43,43,45	0
7	EDO	C	334	4/4	0.84	0.12	31,33,38,41	0
3	GOL	B	113	6/6	0.84	0.14	29,38,44,48	0
9	SO4	D	113	5/5	0.84	0.10	52,62,65,67	0
3	GOL	C	342	6/6	0.85	0.12	28,34,36,37	0
8	PG4	A	332	13/13	0.85	0.17	24,34,46,53	0
3	GOL	A	311	6/6	0.85	0.09	23,27,30,31	0
5	PEG	C	317	7/7	0.85	0.14	37,41,44,50	0
6	PE8	B	131	25/25	0.85	0.12	20,33,46,53	0
4	NA	C	333	1/1	0.85	0.12	31,31,31,31	0
6	PE8	C	322	25/25	0.85	0.10	15,31,41,44	0
8	PG4	D	119	13/13	0.85	0.11	15,24,28,30	0
8	PG4	D	127	13/13	0.85	0.10	19,26,32,34	0
3	GOL	B	130	6/6	0.85	0.13	37,44,50,52	0
9	SO4	C	336	5/5	0.85	0.11	44,51,56,62	0
3	GOL	B	136	6/6	0.85	0.13	23,31,35,35	0
5	PEG	C	339	7/7	0.86	0.10	24,26,31,33	0
3	GOL	A	346	6/6	0.86	0.13	32,34,37,43	0
8	PG4	B	128	13/13	0.86	0.12	27,33,41,46	0
8	PG4	B	129	13/13	0.86	0.12	25,27,32,33	0
4	NA	A	316	1/1	0.86	0.16	15,15,15,15	0
3	GOL	B	140	6/6	0.86	0.21	25,28,31,32	0
3	GOL	D	109	6/6	0.86	0.10	22,24,25,26	0
6	PE8	A	322	25/25	0.86	0.10	20,31,42,48	0
4	NA	B	144	1/1	0.86	0.07	26,26,26,26	0
5	PEG	B	120	7/7	0.87	0.08	24,27,28,28	0
8	PG4	D	121	13/13	0.87	0.09	9,23,29,30	0
5	PEG	C	315	7/7	0.87	0.08	17,34,38,39	0
8	PG4	B	126	13/13	0.87	0.12	26,33,45,48	0
7	EDO	A	343	4/4	0.87	0.14	34,37,39,43	0
9	SO4	D	112	5/5	0.87	0.10	47,57,65,75	0
3	GOL	B	135	6/6	0.87	0.09	20,30,35,35	0
6	PE8	A	323	25/25	0.88	0.10	9,18,28,29	0
3	GOL	B	112	6/6	0.88	0.10	34,36,40,41	0
4	NA	A	339	1/1	0.88	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	107	6/6	0.88	0.10	8,22,36,42	0
7	EDO	A	326	4/4	0.88	0.10	22,24,26,28	0
3	GOL	A	345	6/6	0.88	0.11	28,29,35,47	0
5	PEG	E	111	7/7	0.88	0.11	28,38,47,49	0
8	PG4	E	101	13/13	0.88	0.10	16,25,34,34	0
8	PG4	A	334	13/13	0.88	0.10	29,40,45,51	0
4	NA	D	128	1/1	0.88	0.11	44,44,44,44	0
7	EDO	C	323	4/4	0.88	0.16	32,37,48,50	0
8	PG4	A	344	13/13	0.88	0.07	33,37,47,51	0
4	NA	D	102	1/1	0.89	0.12	37,37,37,37	0
7	EDO	B	124	4/4	0.89	0.09	32,38,45,46	0
3	GOL	C	301	6/6	0.89	0.08	34,35,40,40	0
3	GOL	A	304	6/6	0.89	0.14	21,26,27,27	0
3	GOL	A	312	6/6	0.89	0.08	26,38,45,50	0
3	GOL	B	108	6/6	0.89	0.11	27,36,41,50	0
5	PEG	E	110	7/7	0.89	0.11	18,22,25,29	0
5	PEG	A	318	7/7	0.89	0.11	15,19,33,33	0
3	GOL	A	305	6/6	0.89	0.10	35,40,44,47	0
3	GOL	B	132	6/6	0.89	0.07	28,34,44,46	0
5	PEG	A	321	7/7	0.89	0.10	19,35,41,43	0
3	GOL	D	103	6/6	0.89	0.10	37,45,54,56	0
8	PG4	C	337	13/13	0.89	0.10	11,27,35,35	0
4	NA	B	142	1/1	0.90	0.09	8,8,8,8	0
3	GOL	A	313	6/6	0.90	0.08	7,19,27,28	0
5	PEG	B	139	7/7	0.90	0.07	23,28,38,41	0
3	GOL	E	102	6/6	0.90	0.08	32,37,40,41	0
4	NA	C	314	1/1	0.90	0.12	13,13,13,13	0
7	EDO	B	103	4/4	0.90	0.08	20,20,20,21	0
3	GOL	A	340	6/6	0.90	0.07	22,29,33,33	0
8	PG4	A	333	13/13	0.90	0.09	14,20,24,24	0
4	NA	E	105	1/1	0.90	0.15	35,35,35,35	0
9	SO4	D	114	5/5	0.90	0.16	40,46,47,48	0
8	PG4	C	326	13/13	0.91	0.07	23,36,39,39	0
3	GOL	E	104	6/6	0.91	0.07	29,32,34,35	0
4	NA	B	118	1/1	0.91	0.11	59,59,59,59	0
3	GOL	C	338	6/6	0.91	0.09	14,23,33,34	0
3	GOL	A	306	6/6	0.91	0.17	22,34,39,39	0
6	PE8	B	121	25/25	0.91	0.09	20,27,33,37	0
5	PEG	C	340	7/7	0.92	0.07	19,26,36,39	0
3	GOL	A	301	6/6	0.92	0.11	25,28,30,36	0
3	GOL	B	134	6/6	0.92	0.08	18,21,35,42	0
3	GOL	A	302	6/6	0.92	0.08	12,16,22,24	0

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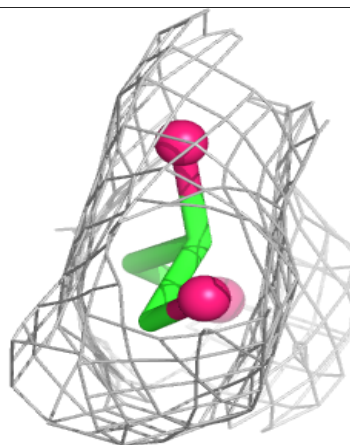
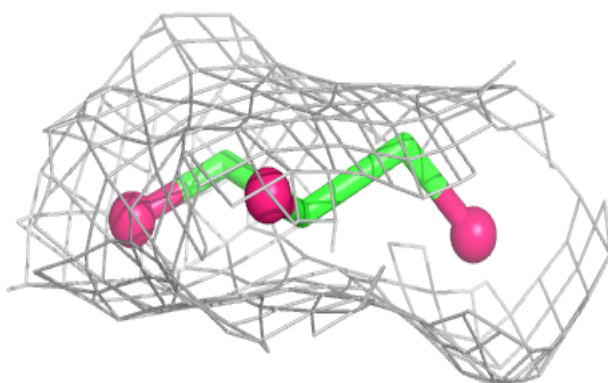
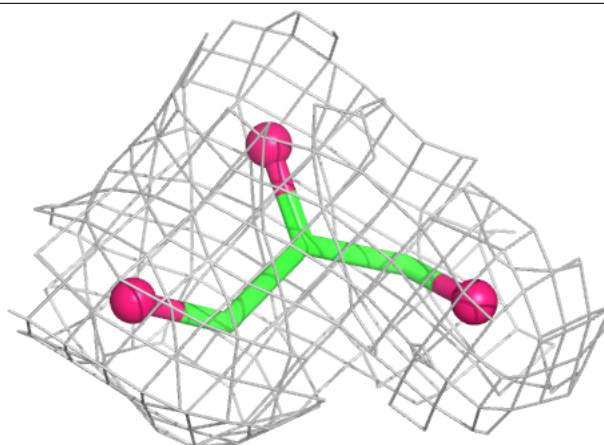
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	A	325	4/4	0.92	0.10	24,27,30,31	0
9	SO4	D	126	5/5	0.92	0.12	39,48,58,66	0
8	PG4	A	329	13/13	0.93	0.06	18,33,51,54	0
4	NA	B	133	1/1	0.93	0.17	26,26,26,26	0
3	GOL	C	341	6/6	0.93	0.08	11,27,37,45	0
4	NA	C	312	1/1	0.93	0.15	30,30,30,30	0
9	SO4	E	107	5/5	0.93	0.09	49,50,57,61	0
3	GOL	B	106	6/6	0.94	0.12	26,31,32,36	0
4	NA	C	335	1/1	0.94	0.08	19,19,19,19	0
10	CL	D	120	1/1	0.94	0.04	41,41,41,41	0
4	NA	C	313	1/1	0.95	0.03	34,34,34,34	0
4	NA	D	125	1/1	0.95	0.10	35,35,35,35	0
4	NA	A	315	1/1	0.95	0.12	14,14,14,14	0
4	NA	A	317	1/1	0.95	0.07	21,21,21,21	0
3	GOL	C	305	6/6	0.96	0.06	5,14,21,24	0
4	NA	D	130	1/1	0.96	0.06	10,10,10,10	0
4	NA	E	106	1/1	0.97	0.10	16,16,16,16	0
4	NA	D	131	1/1	0.98	0.06	10,10,10,10	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.

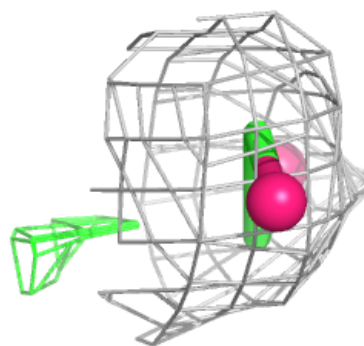
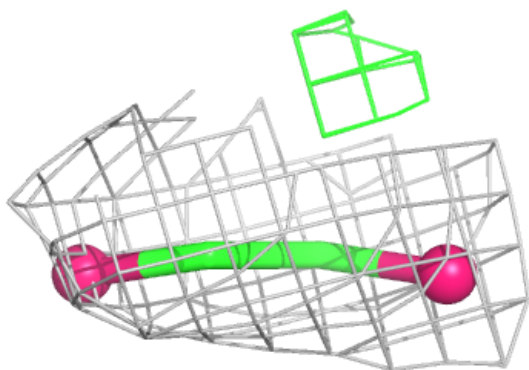
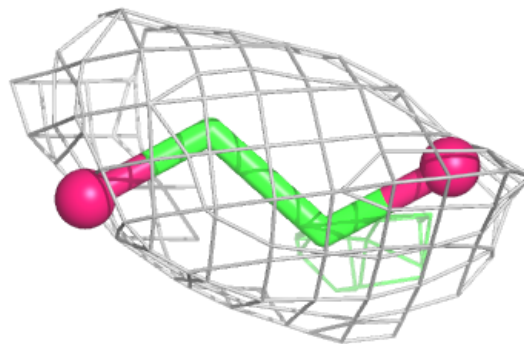
Electron density around GOL B 114:

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



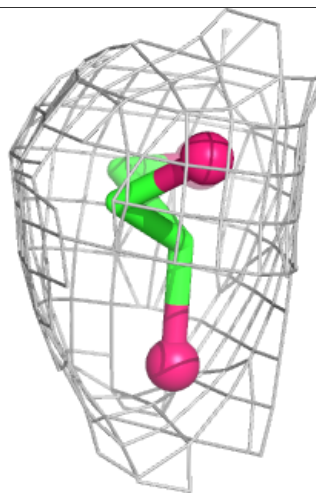
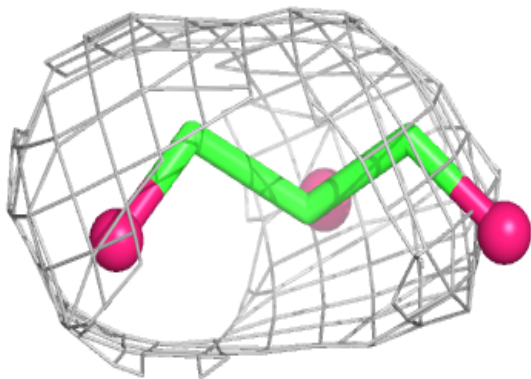
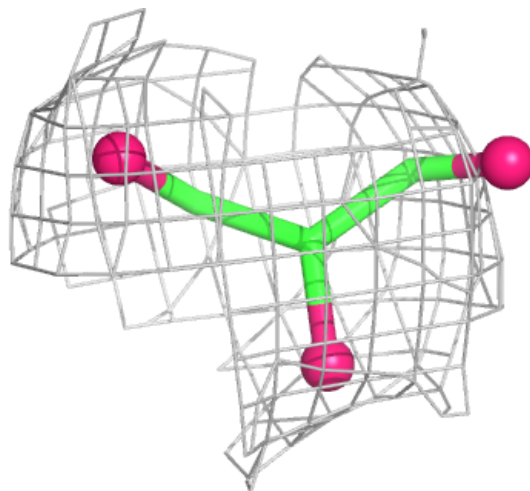
Electron density around EDO C 328:

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



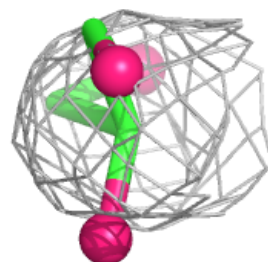
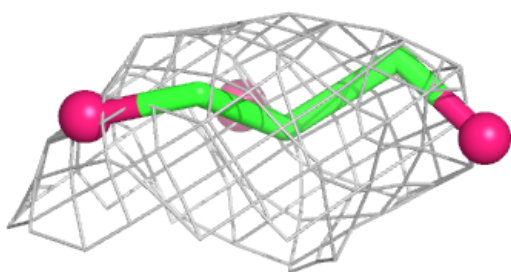
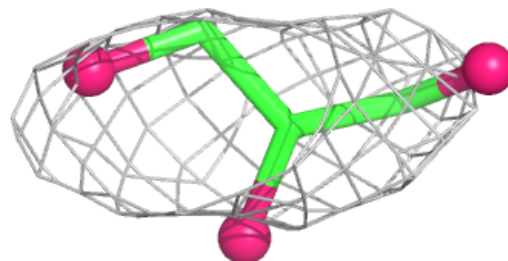
Electron density around GOL A 303:

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

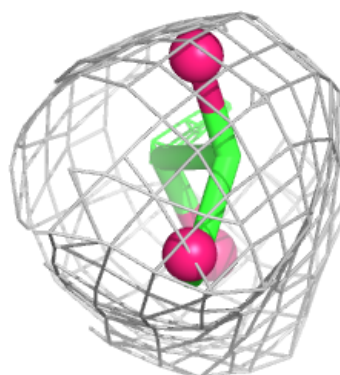
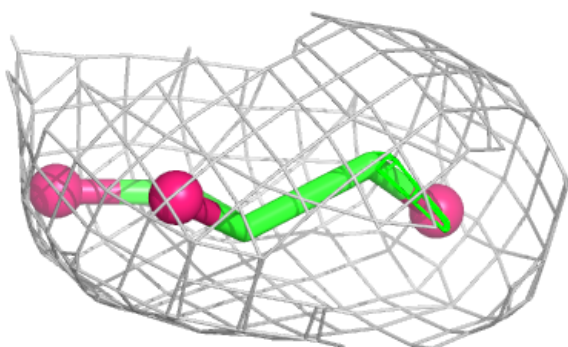
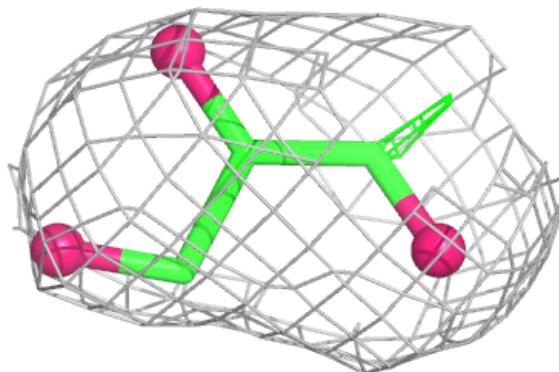


Electron density around GOL C 303:

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

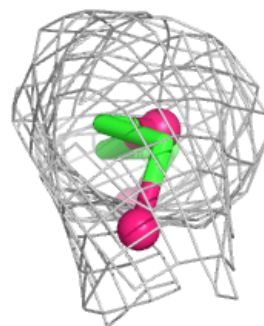
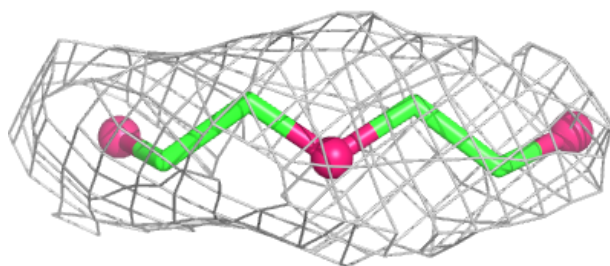
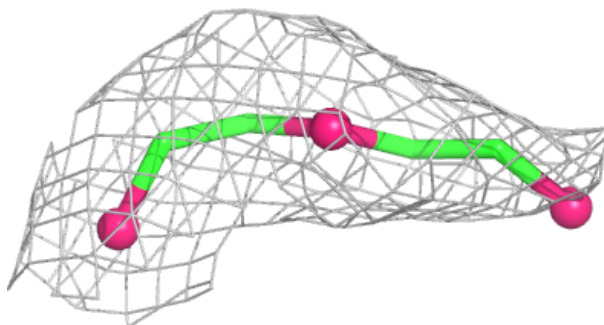
**Electron density around GOL A 310:**

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



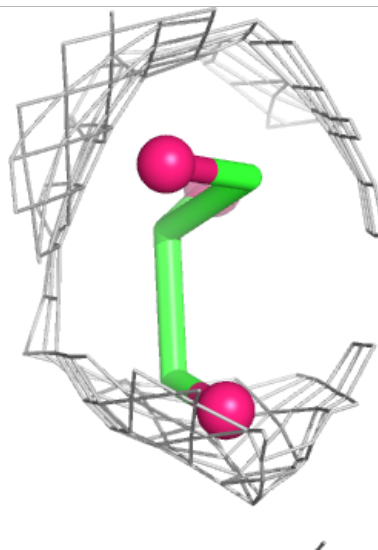
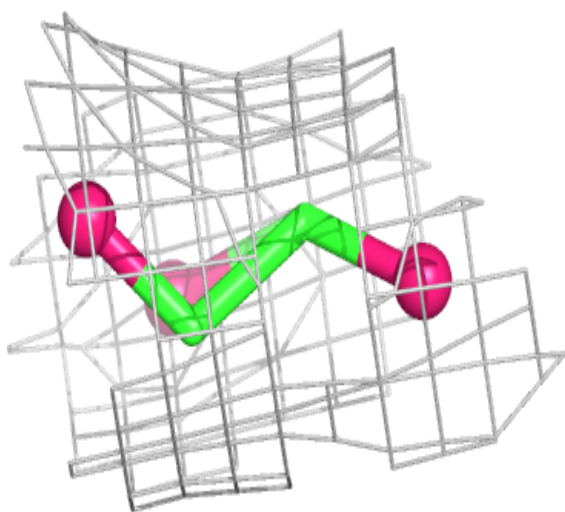
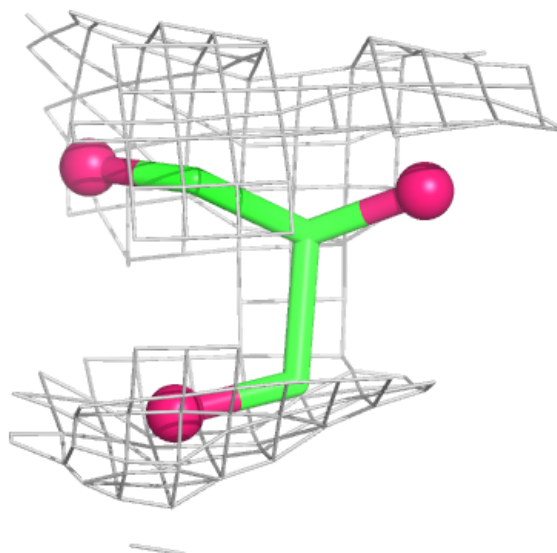
Electron density around PEG C 316:

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



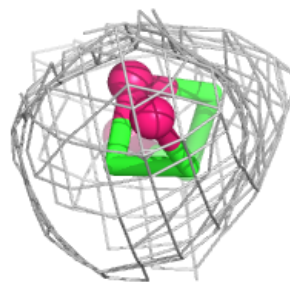
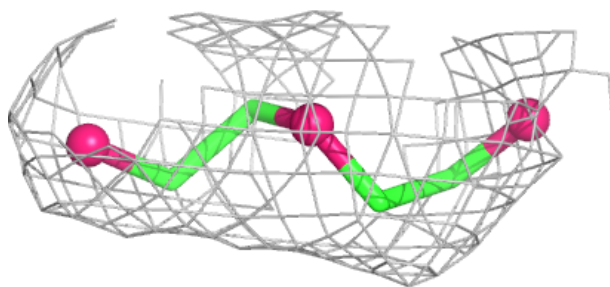
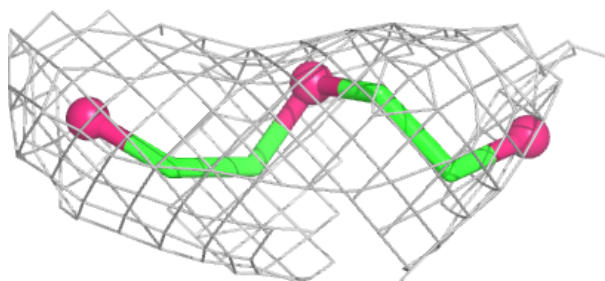
Electron density around GOL C 307:

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

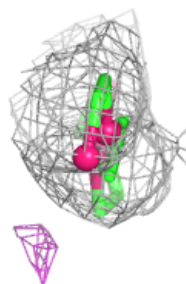
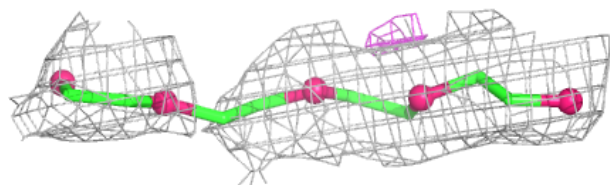
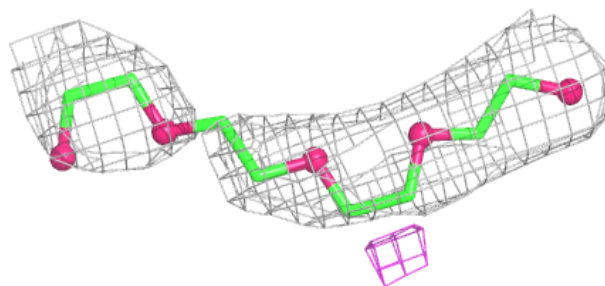


Electron density around PEG A 320:

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

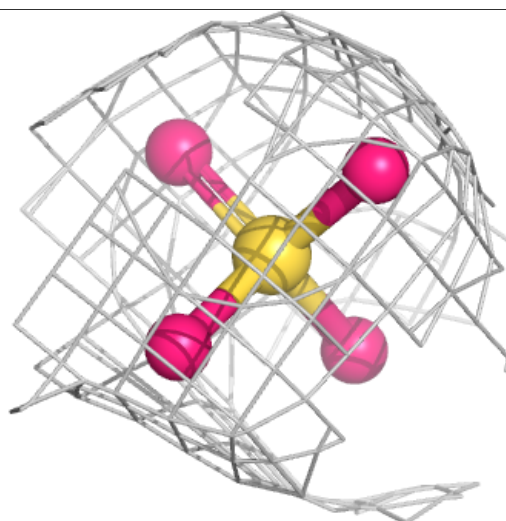
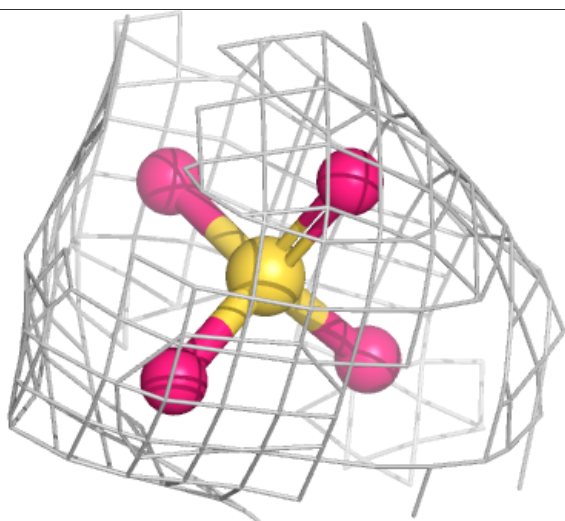
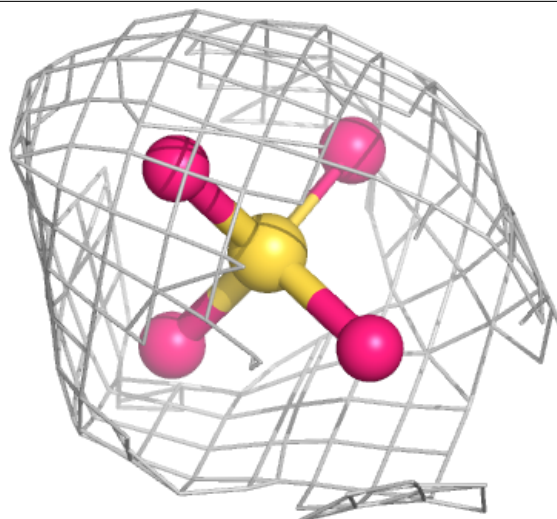
**Electron density around PG4 C 327:**

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



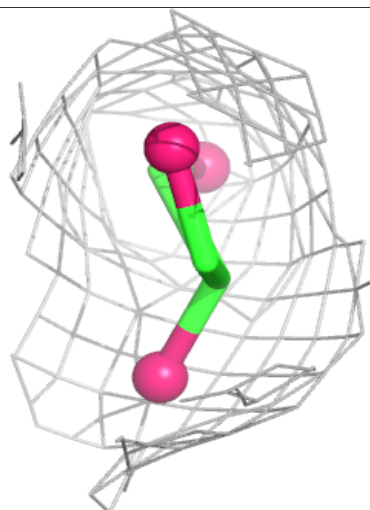
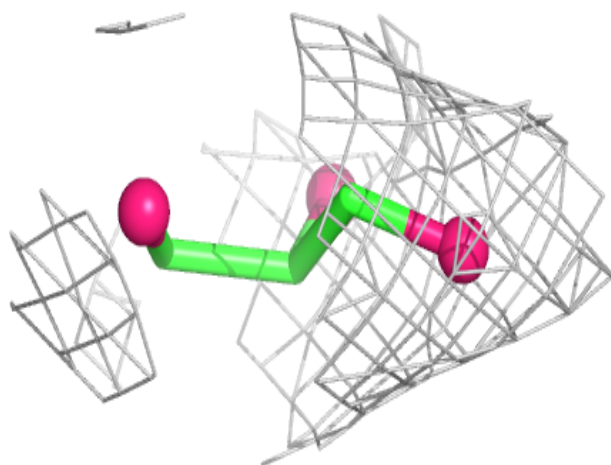
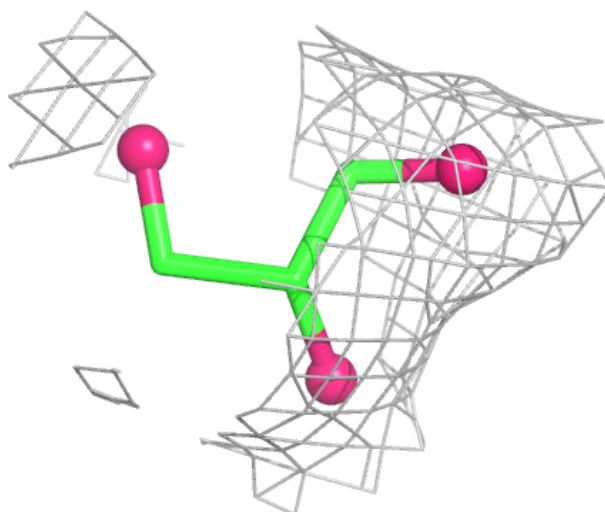
Electron density around SO4 B 119:

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



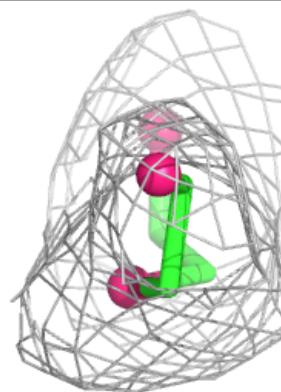
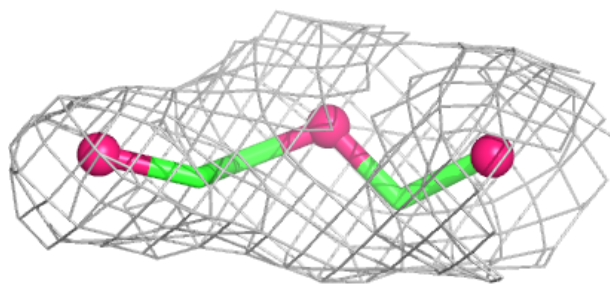
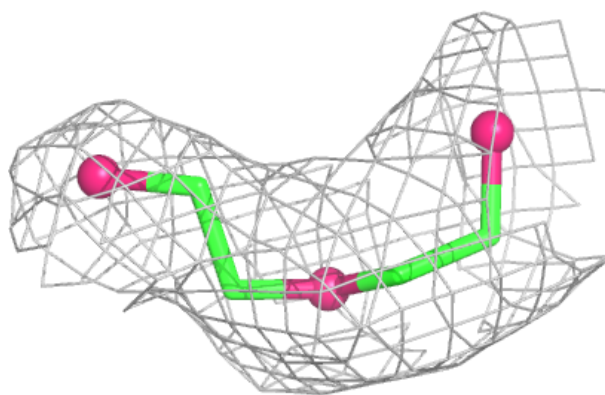
Electron density around GOL B 137:

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

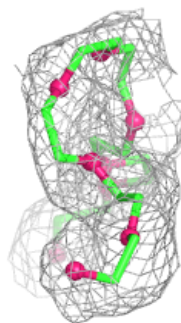
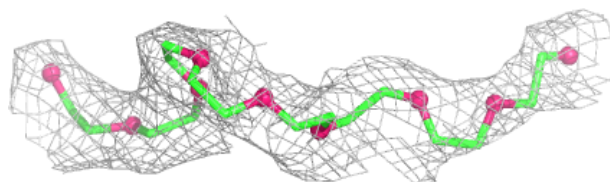
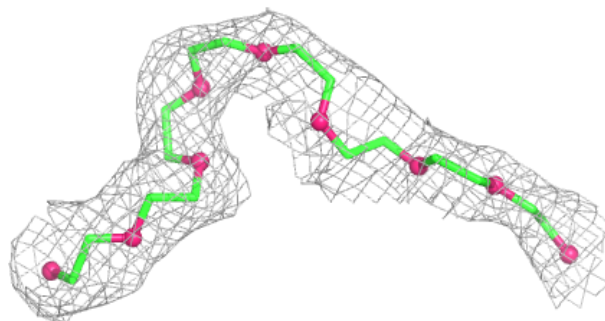


Electron density around PEG E 108:

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

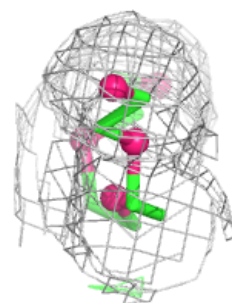
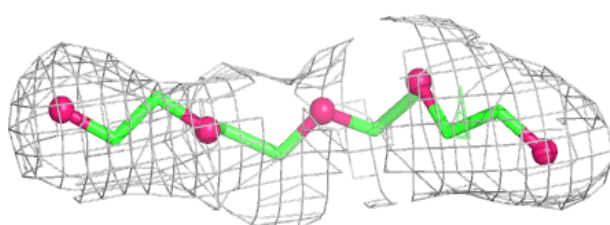
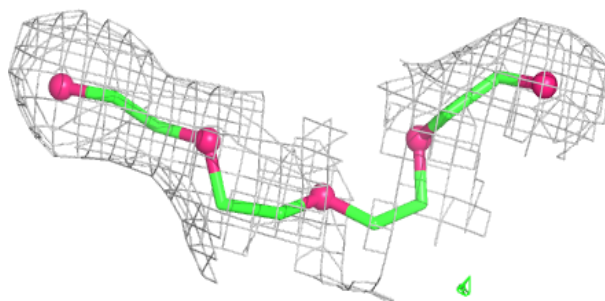
**Electron density around PE8 C 321:**

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

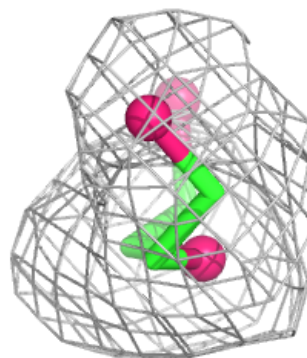
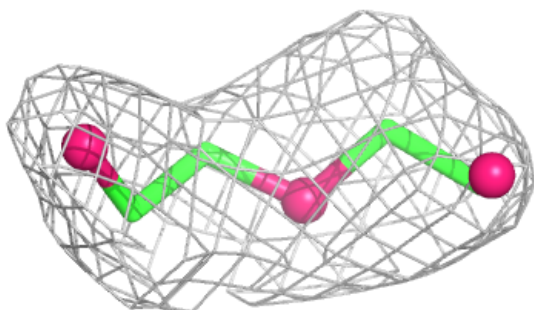
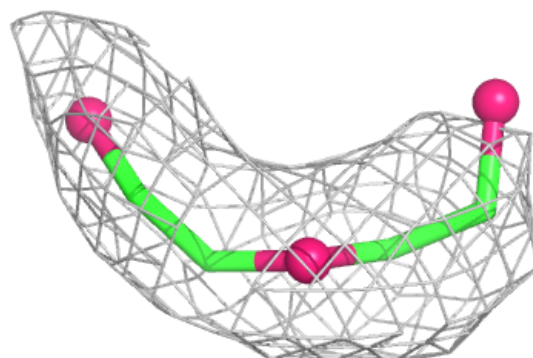


Electron density around PG4 C 332:

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

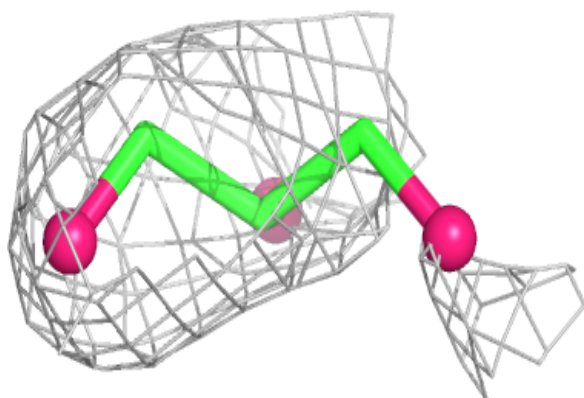
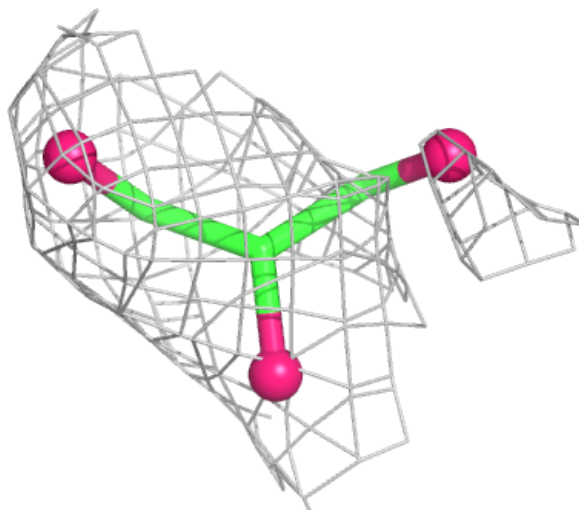
**Electron density around PEG A 342:**

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



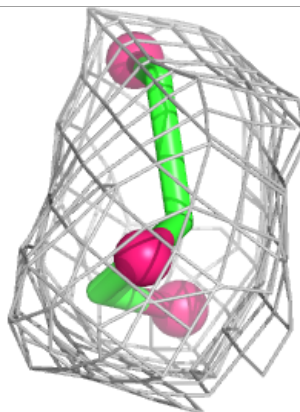
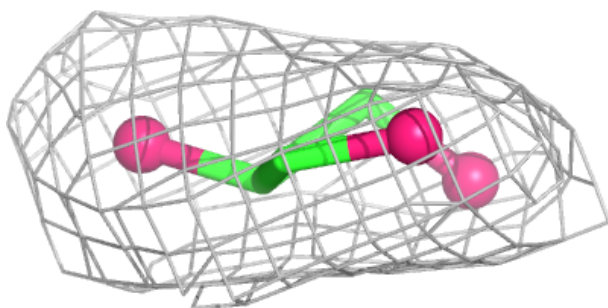
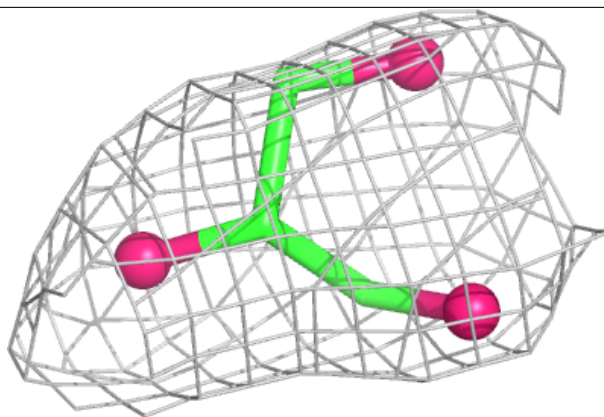
Electron density around GOL C 302:

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

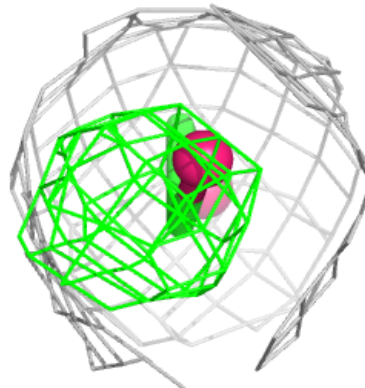
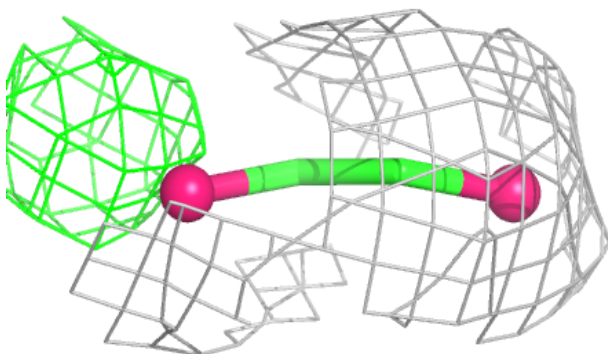
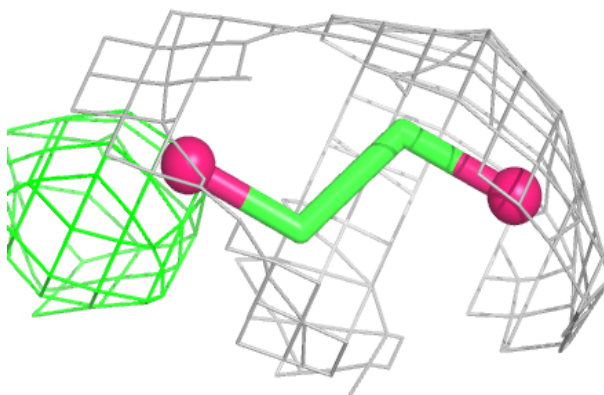


Electron density around GOL A 314:

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

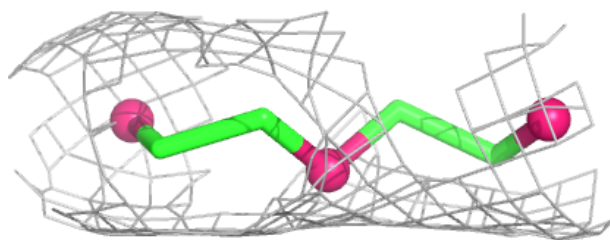
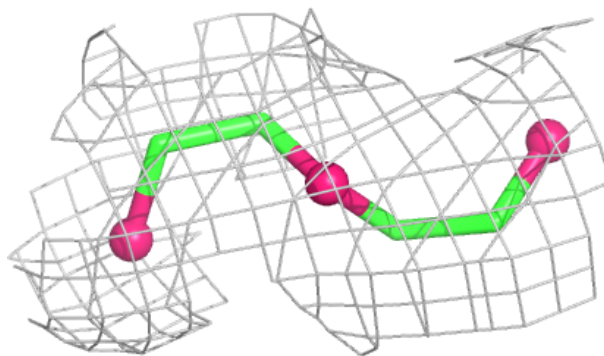
**Electron density around EDO A 336:**

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

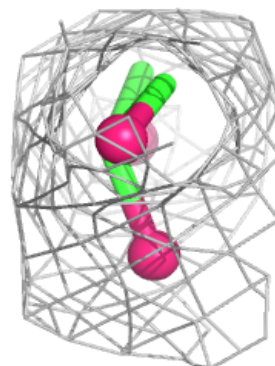
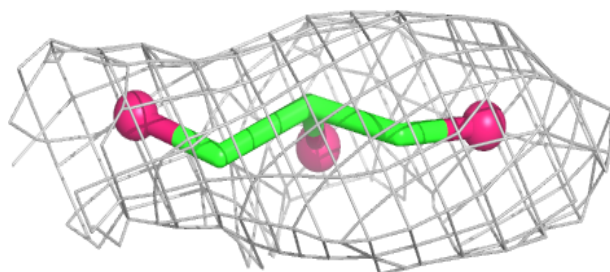
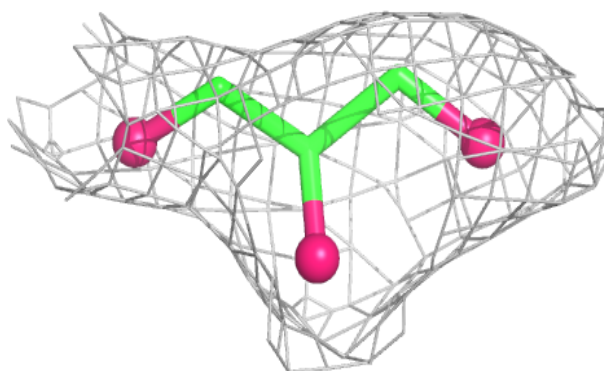


Electron density around PEG A 319:

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

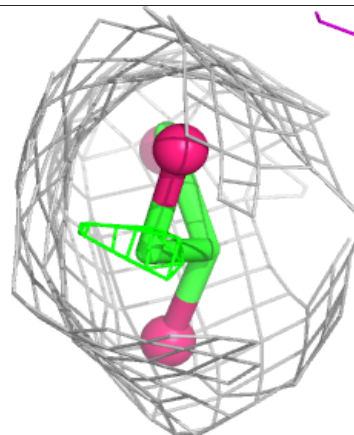
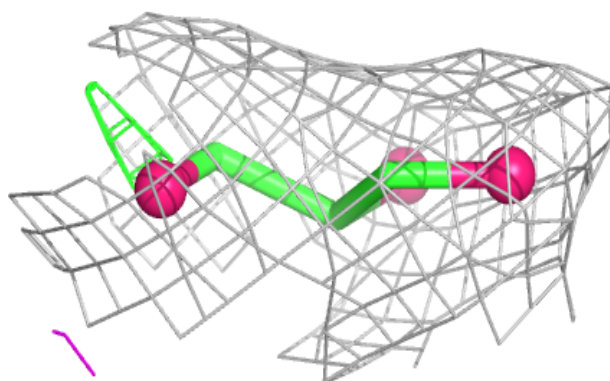
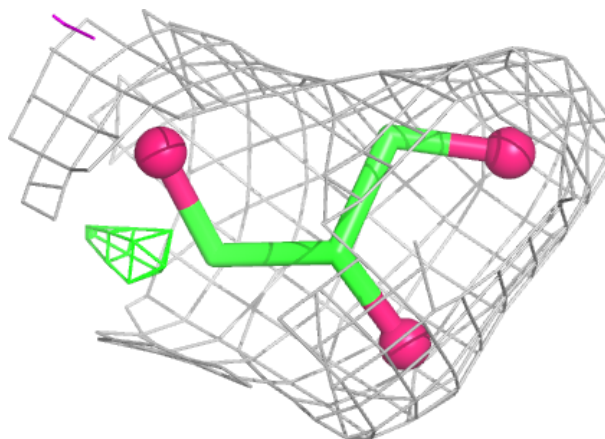
**Electron density around GOL B 116:**

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

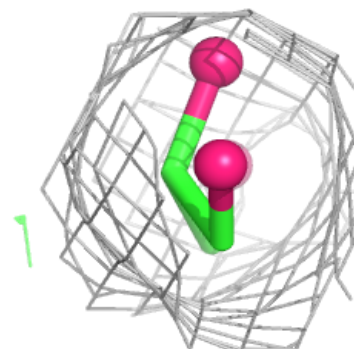
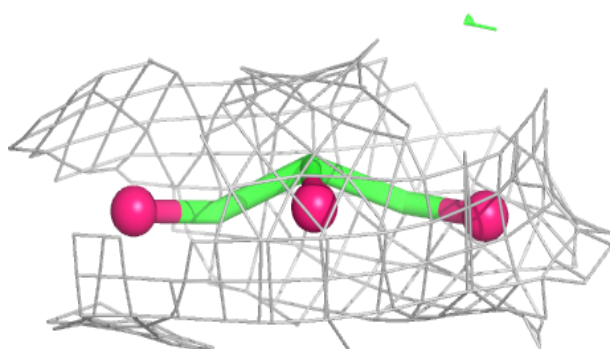
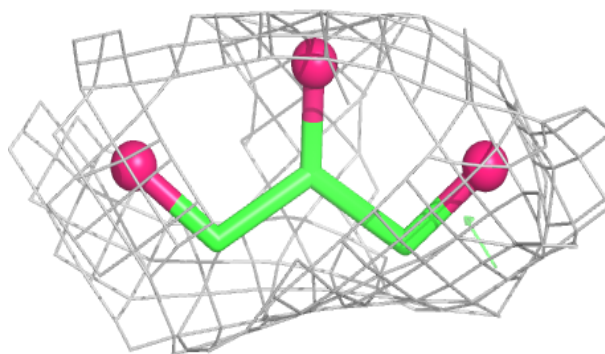


Electron density around GOL C 331:

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

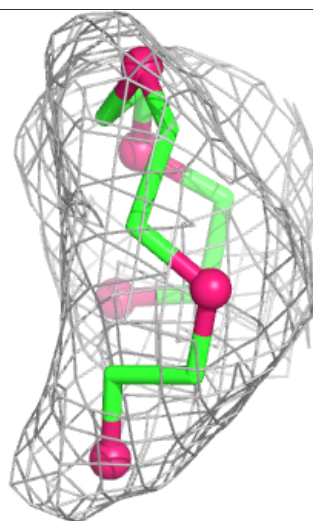
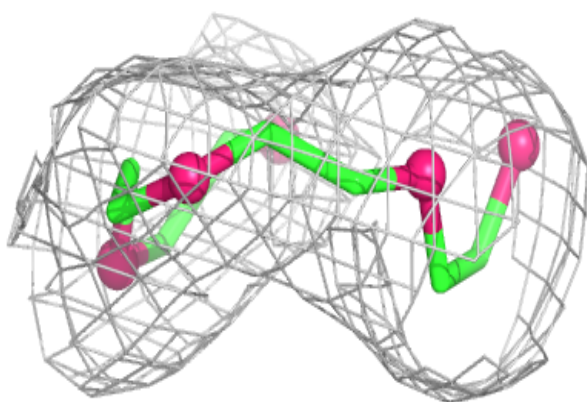
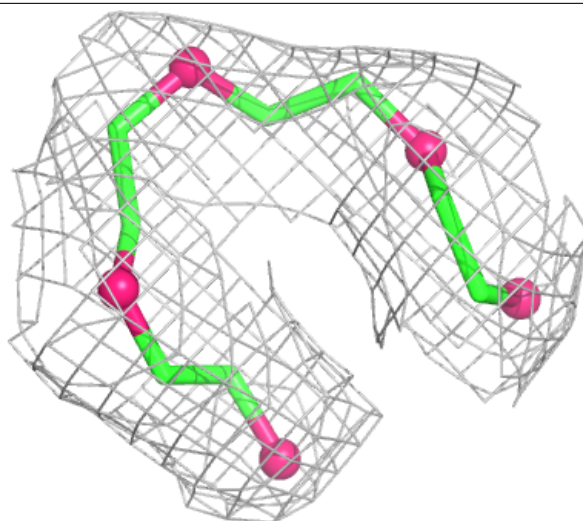
**Electron density around GOL B 101:**

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



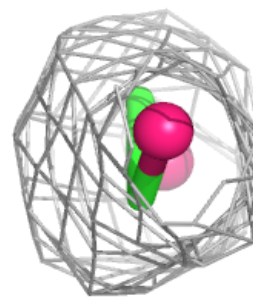
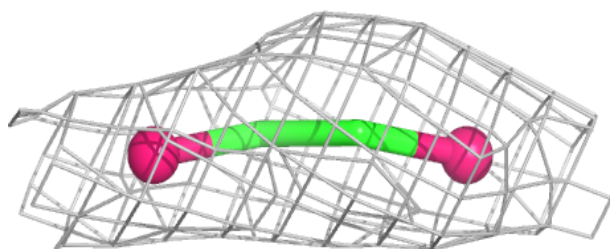
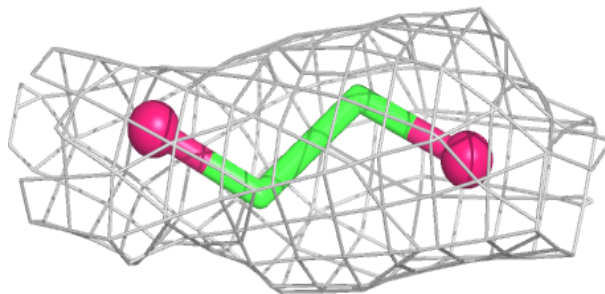
Electron density around PG4 C 324:

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



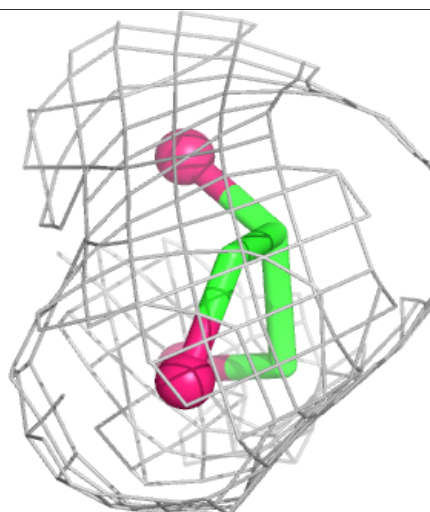
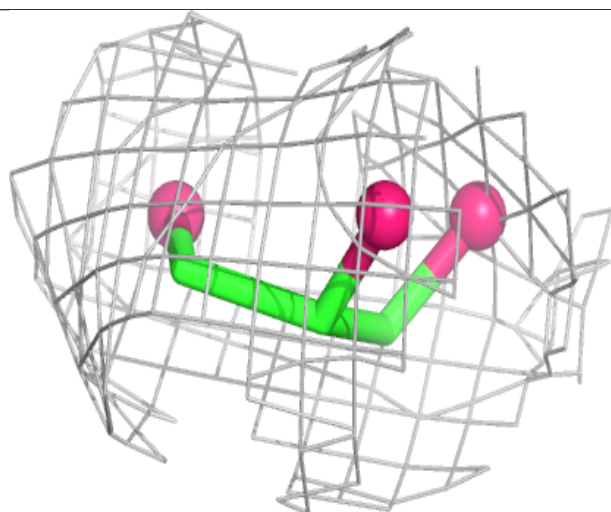
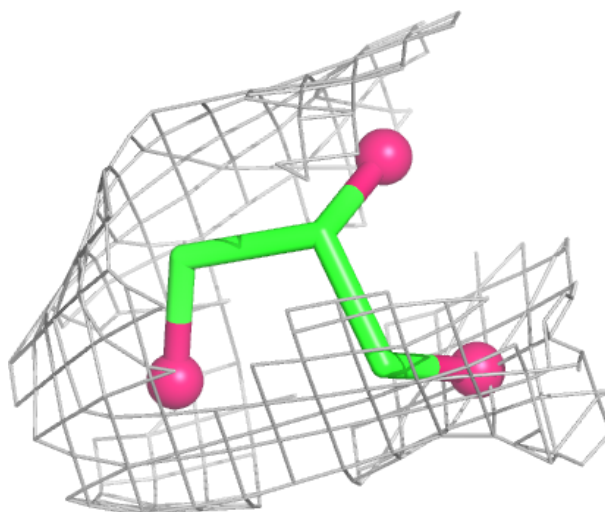
Electron density around EDO A 327:

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



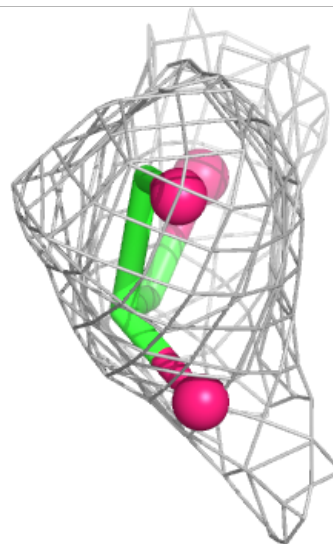
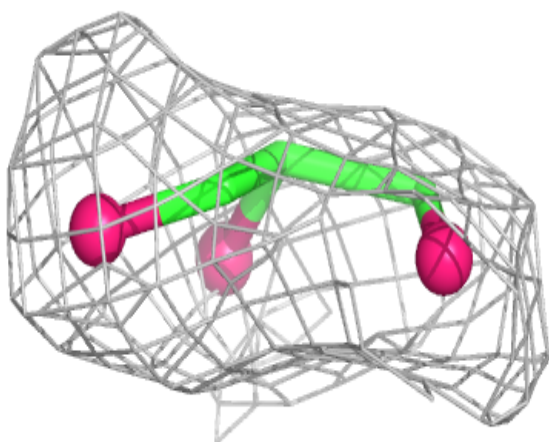
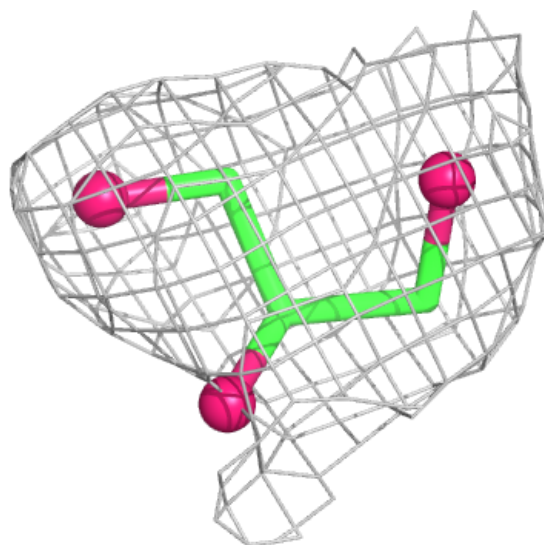
Electron density around GOL B 115:

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



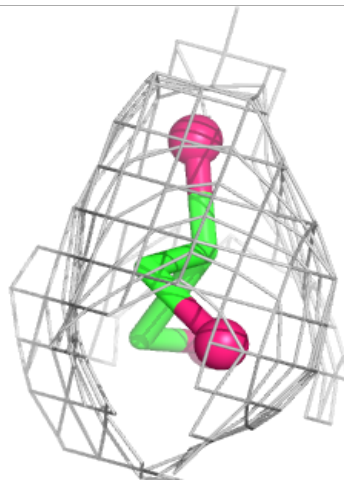
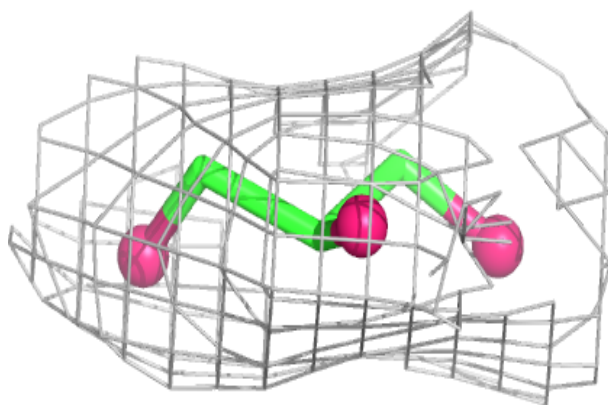
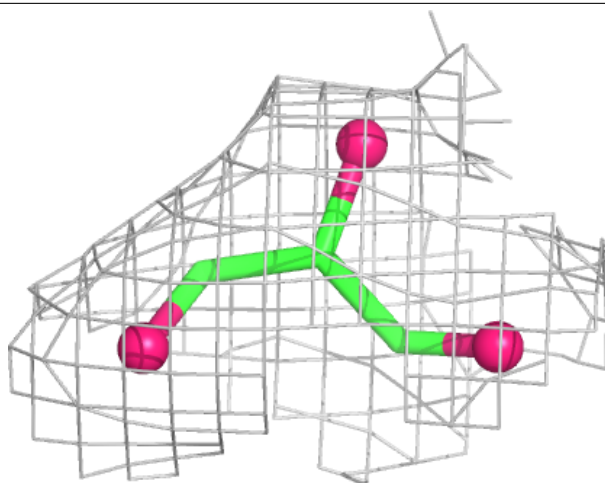
Electron density around GOL C 308:

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



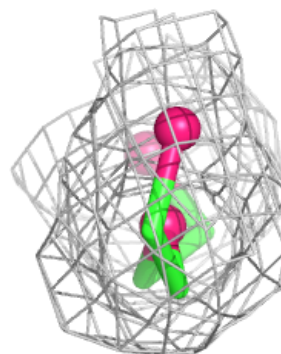
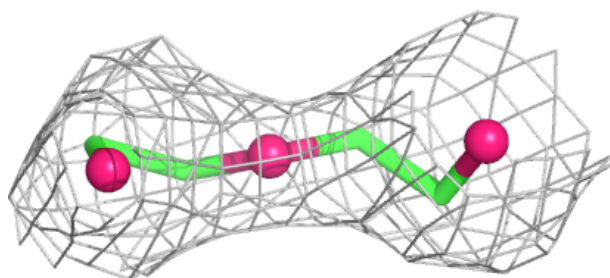
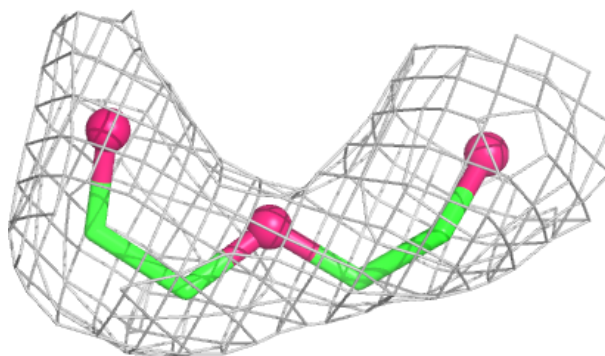
Electron density around GOL B 110:

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

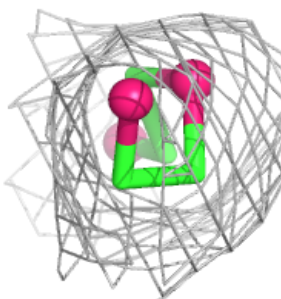
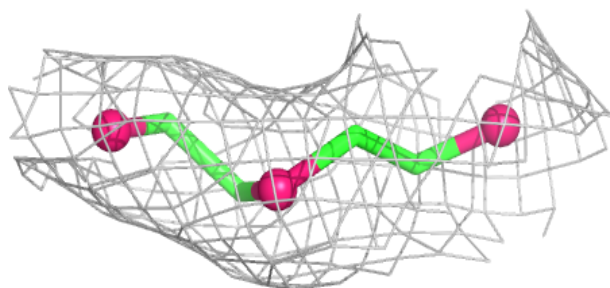
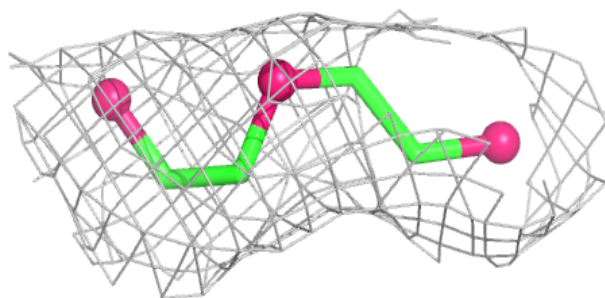


Electron density around PEG C 320:

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

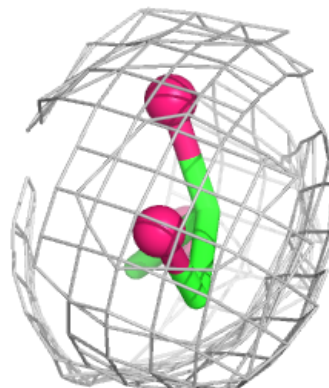
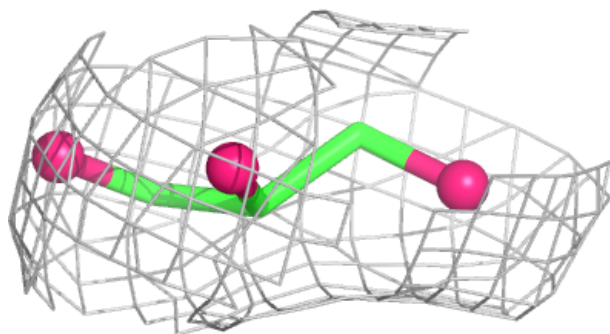
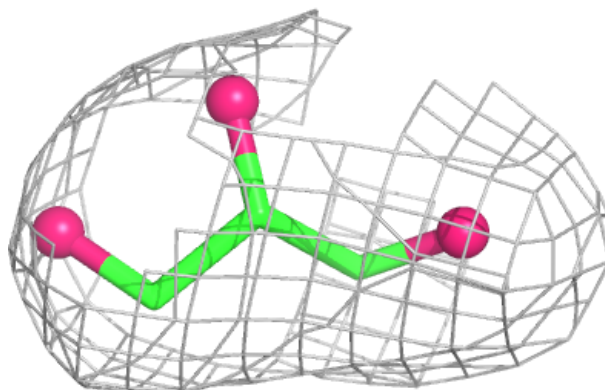
**Electron density around PEG D 123:**

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

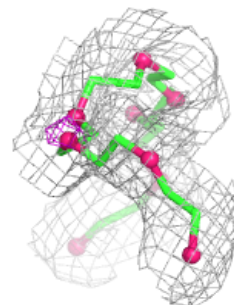
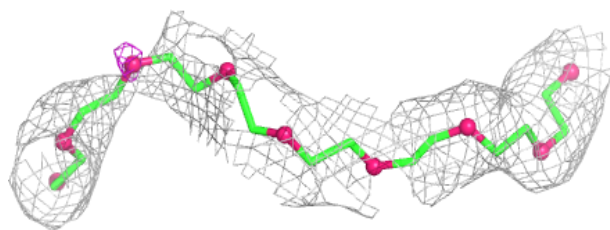
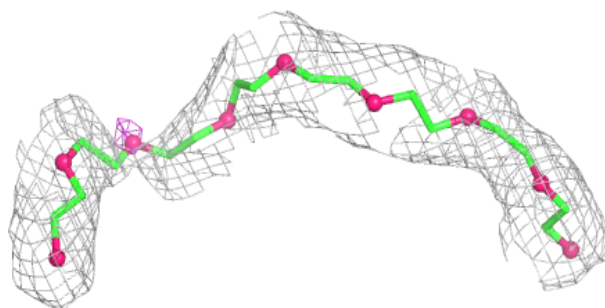


Electron density around GOL C 306:

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

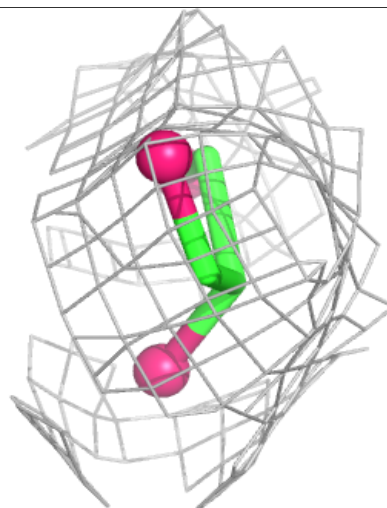
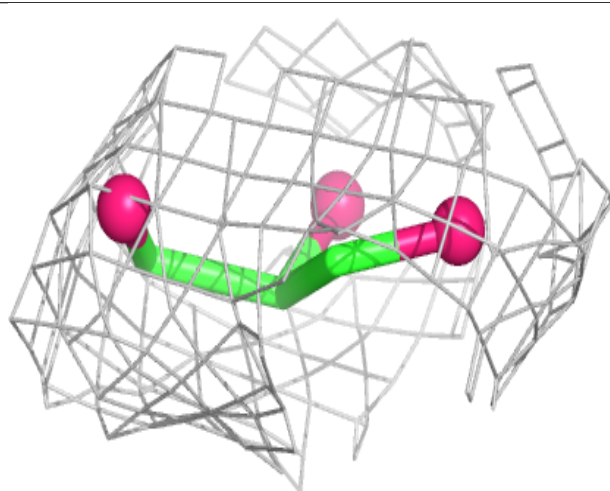
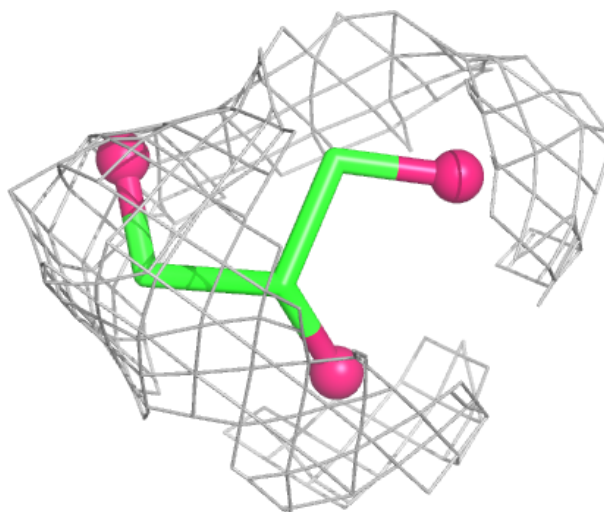
**Electron density around PE8 E 112:**

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



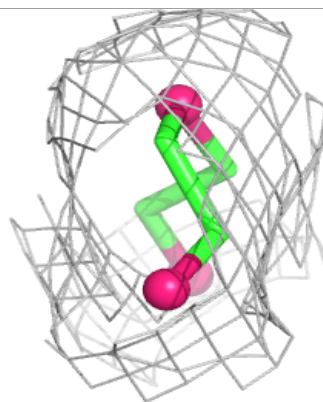
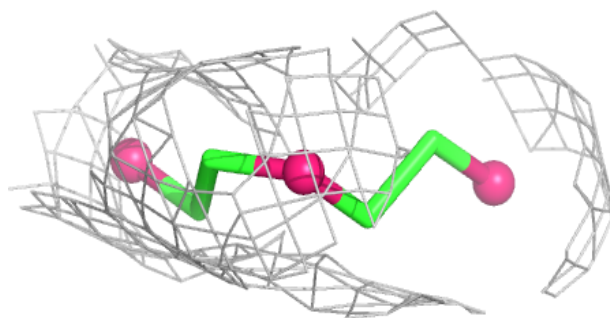
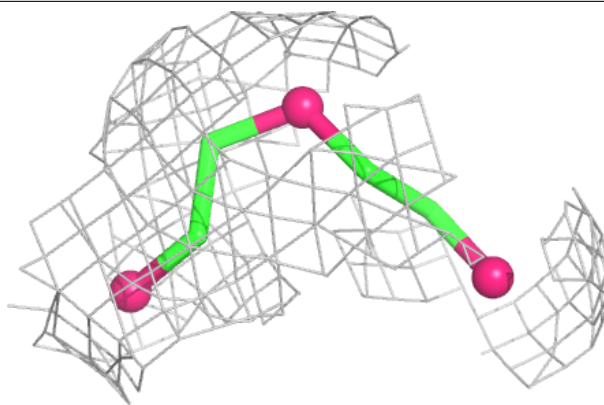
Electron density around GOL A 308:

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



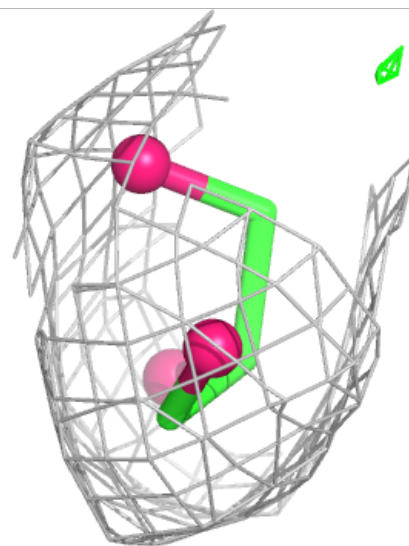
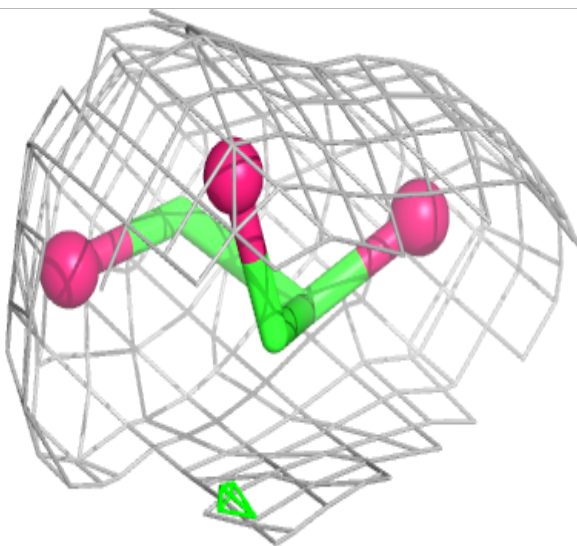
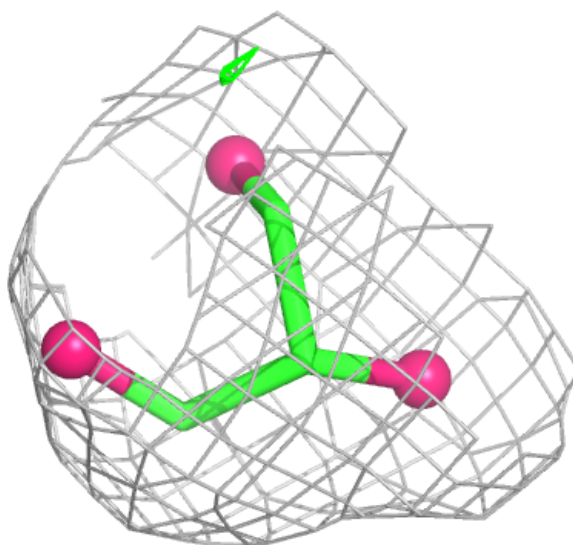
Electron density around PEG A 335:

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



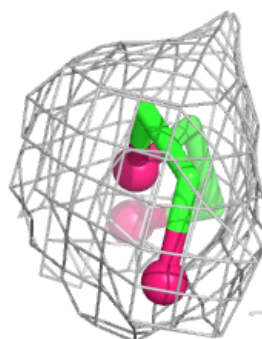
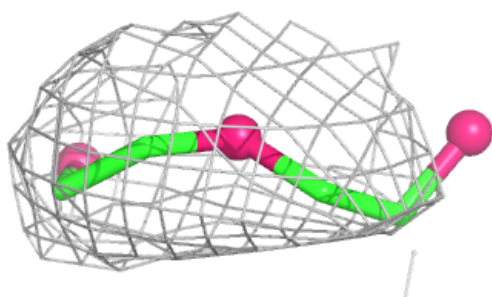
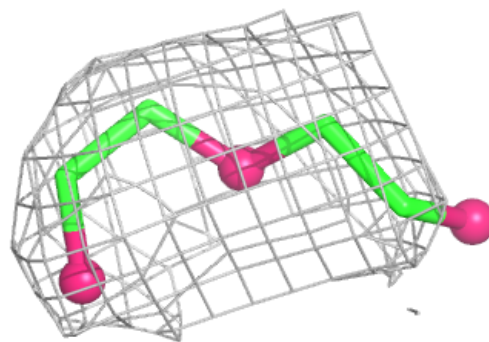
Electron density around GOL B 102:

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

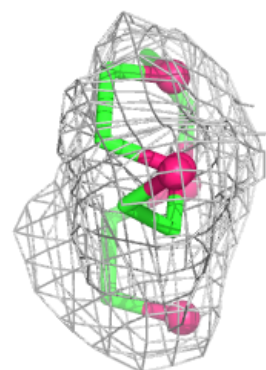
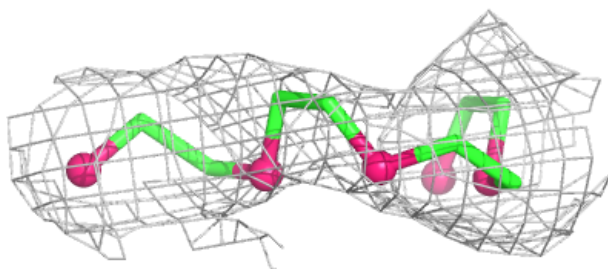


Electron density around PEG E 109:

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

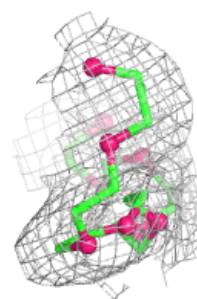
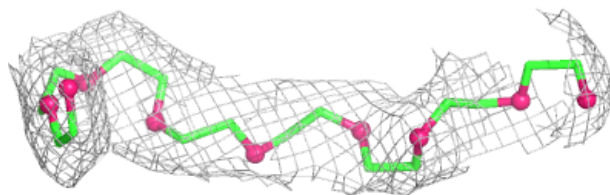
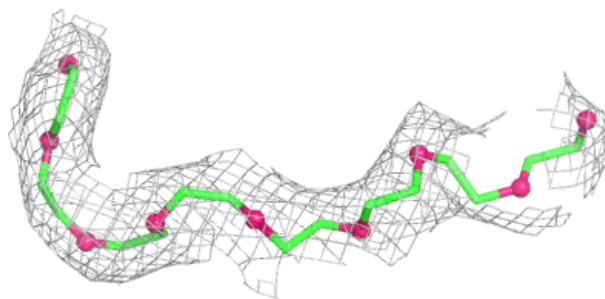
**Electron density around PG4 A 330:**

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

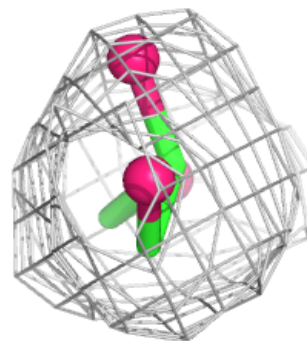
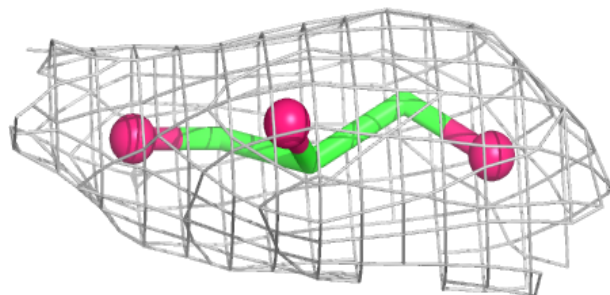
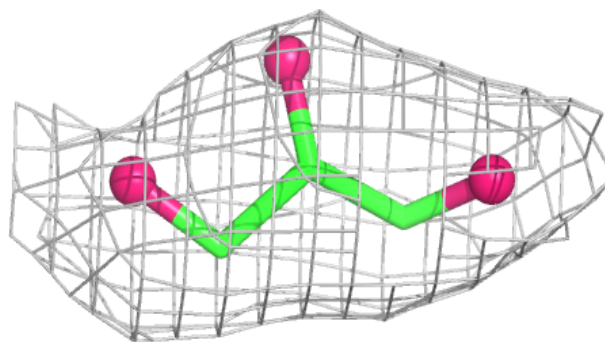


Electron density around PE8 B 105:

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

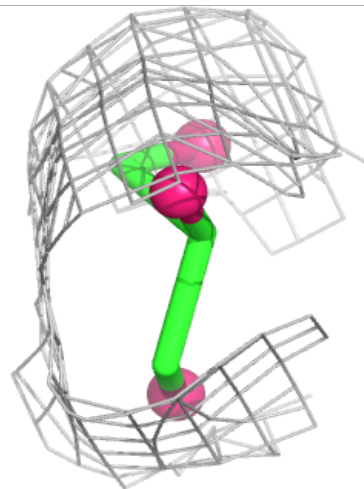
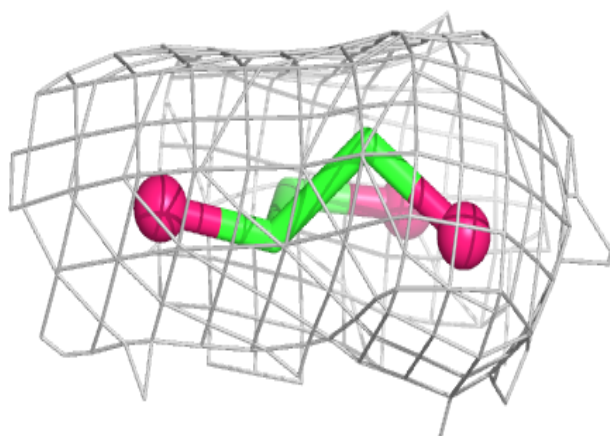
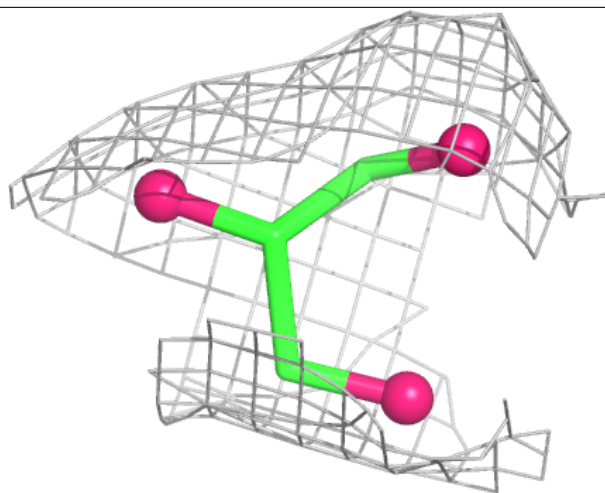
**Electron density around GOL D 108:**

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



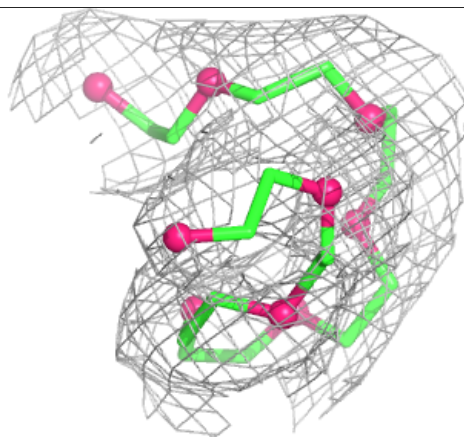
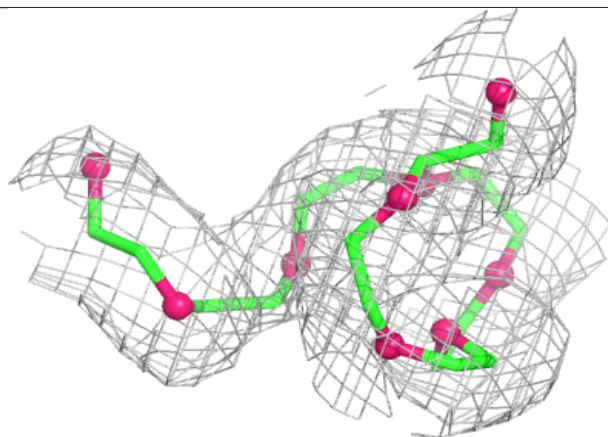
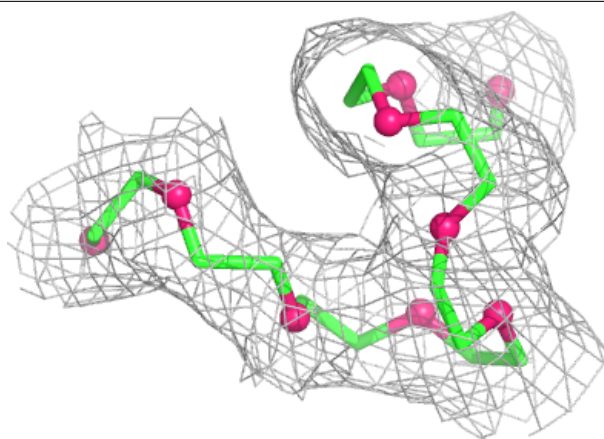
Electron density around GOL D 124:

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

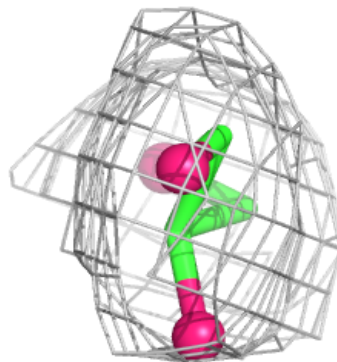
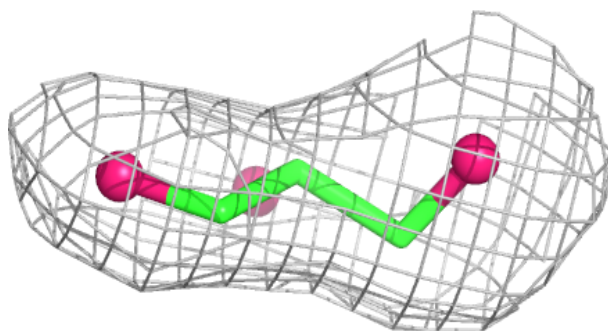
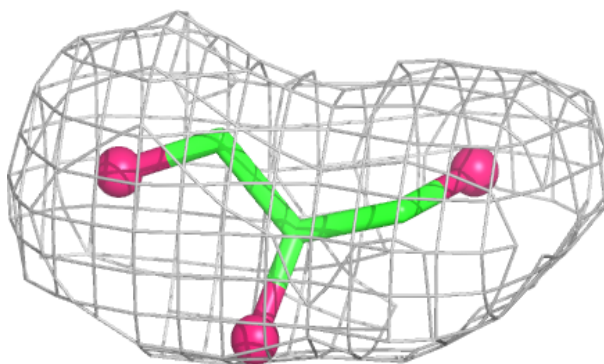


Electron density around PE8 E 114:

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

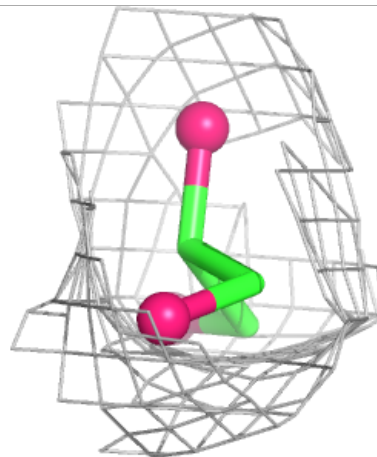
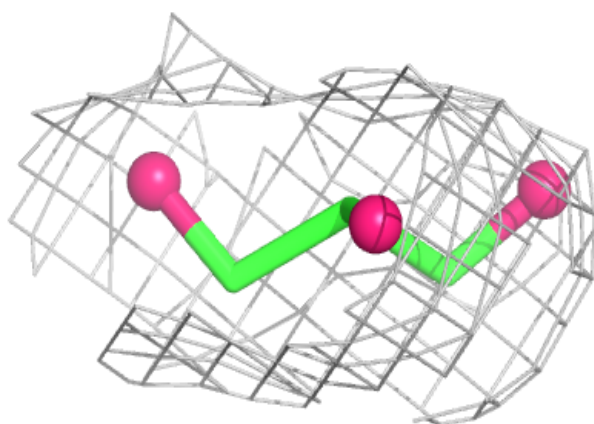
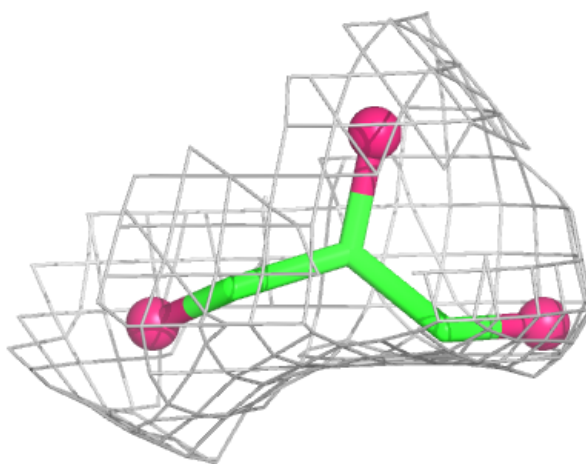
**Electron density around GOL D 122:**

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



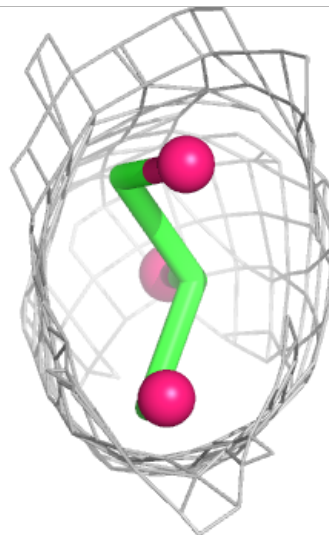
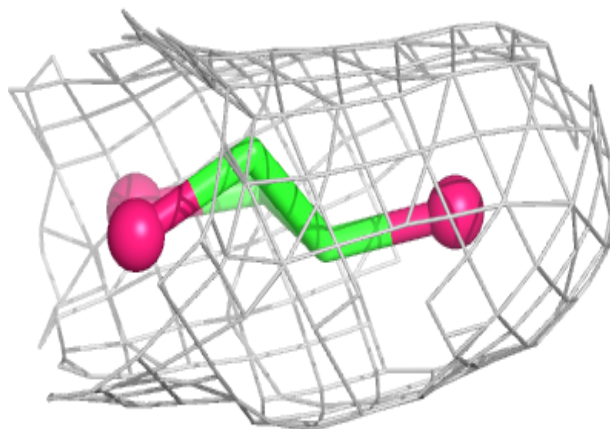
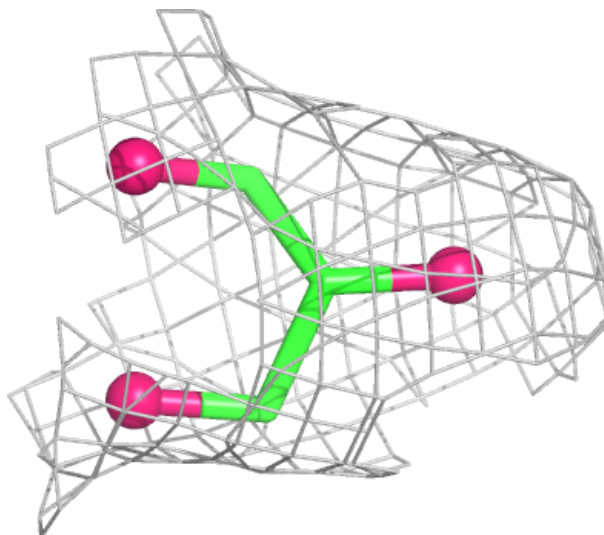
Electron density around GOL D 107:

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



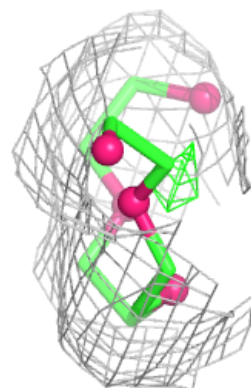
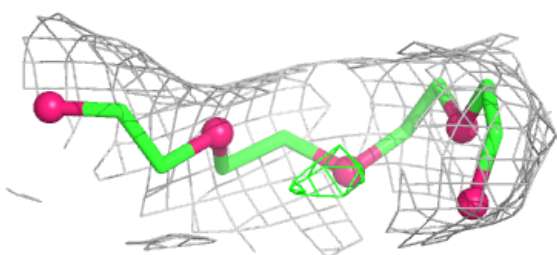
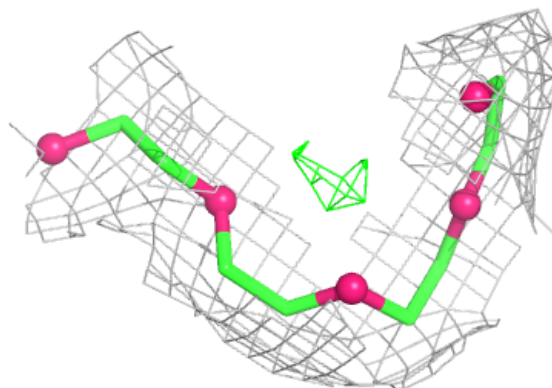
Electron density around GOL C 304:

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

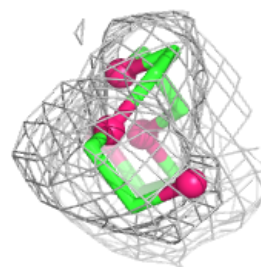
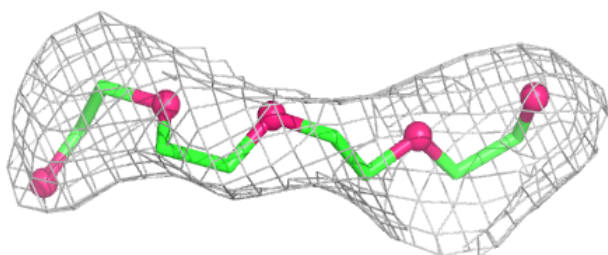
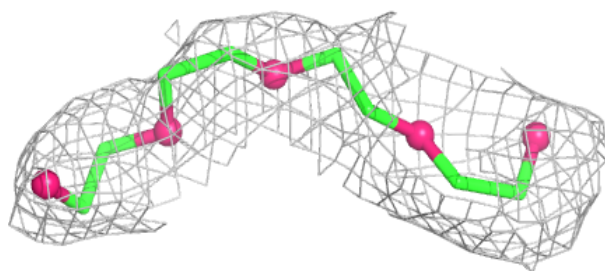


Electron density around PG4 D 101:

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

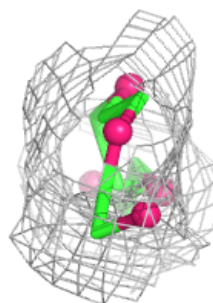
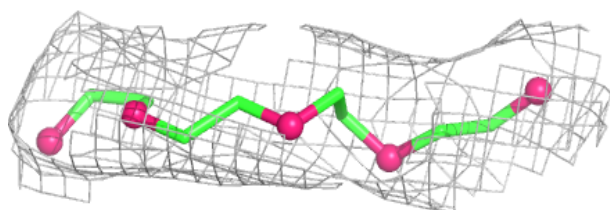
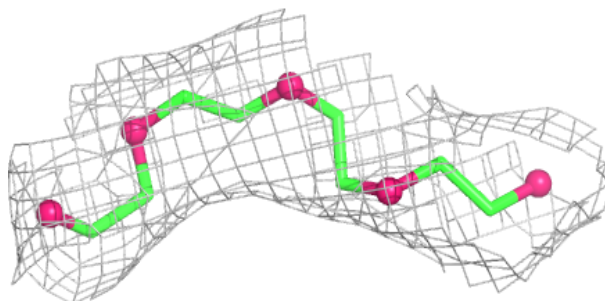
**Electron density around PG4 D 117:**

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

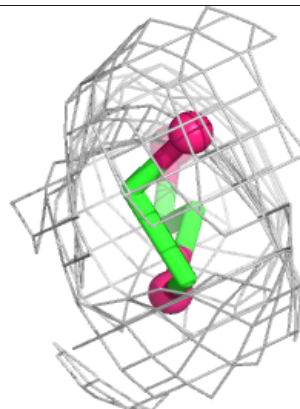
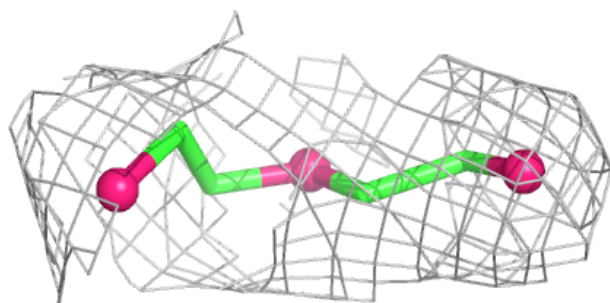
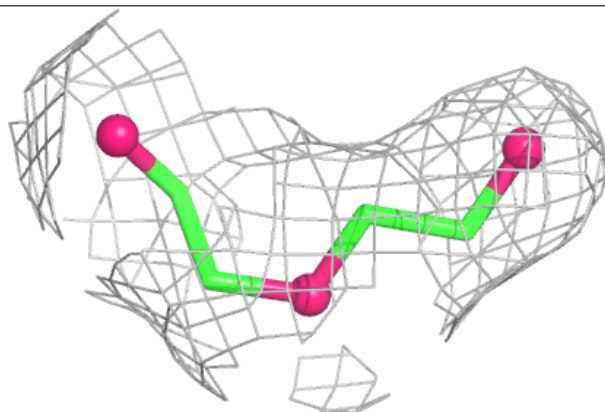


Electron density around PG4 A 337:

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

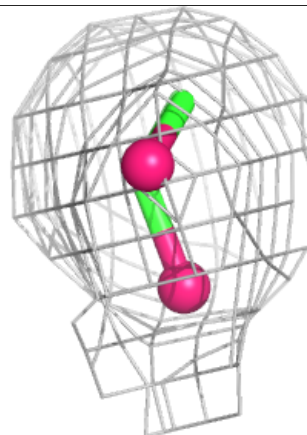
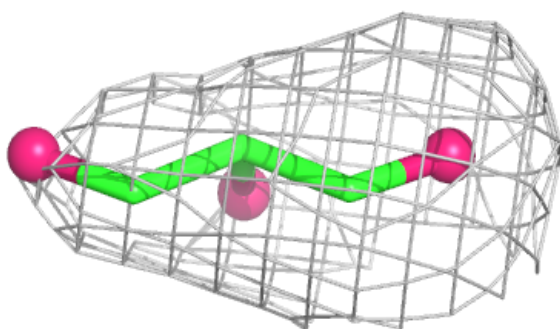
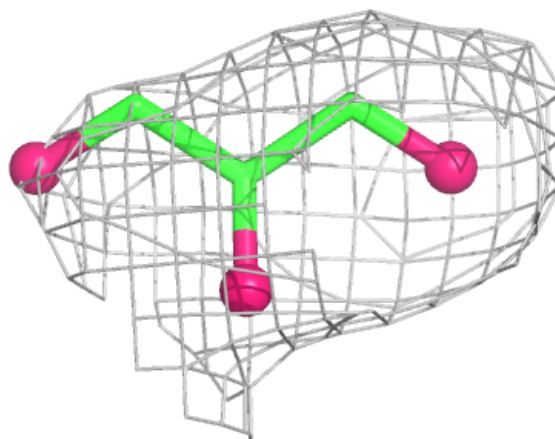
**Electron density around PEG D 115:**

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



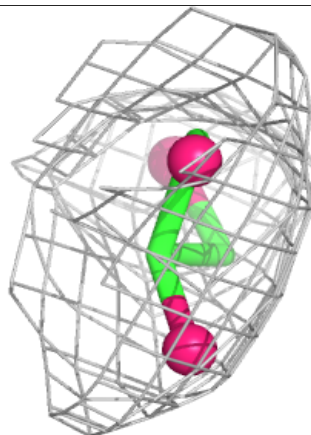
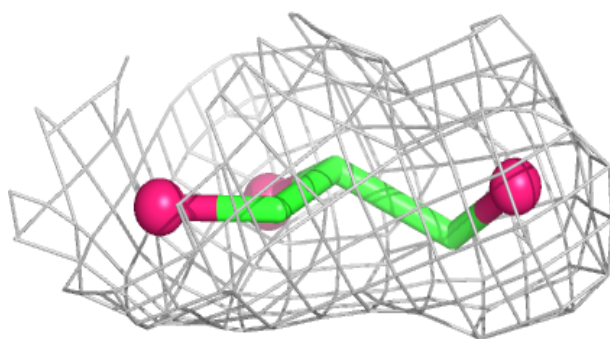
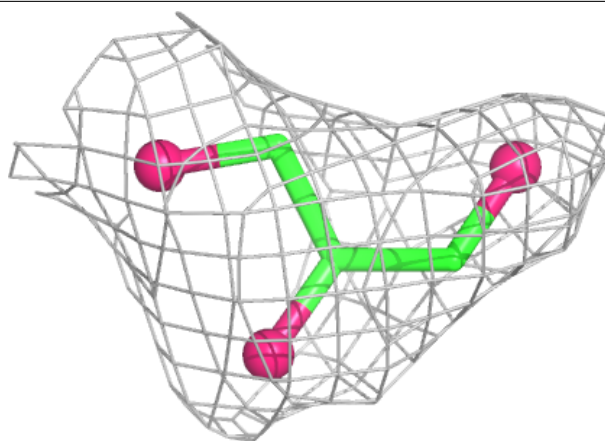
Electron density around GOL E 103:

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

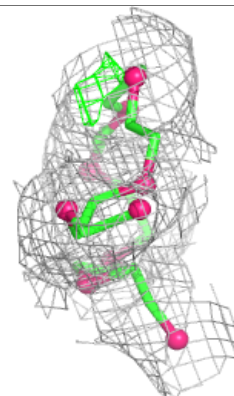
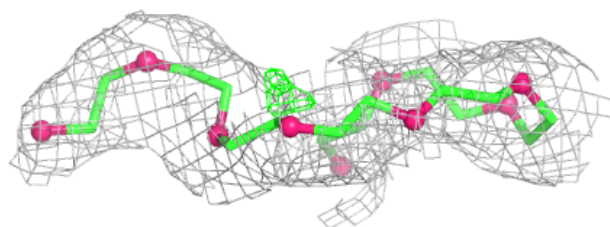
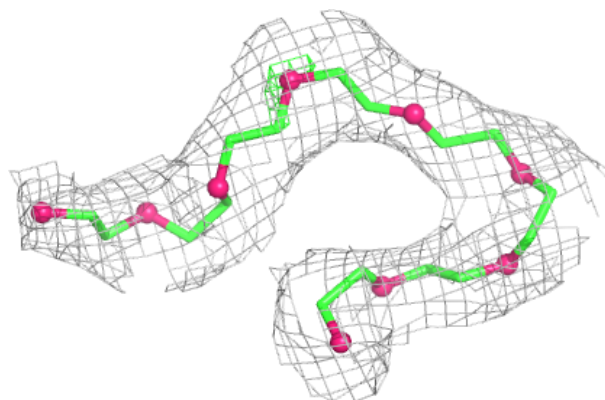


Electron density around GOL C 310:

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

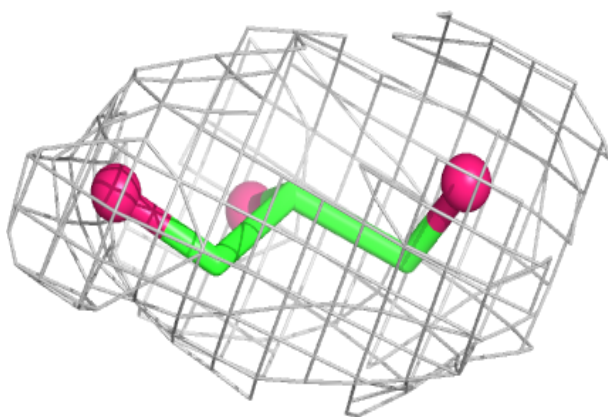
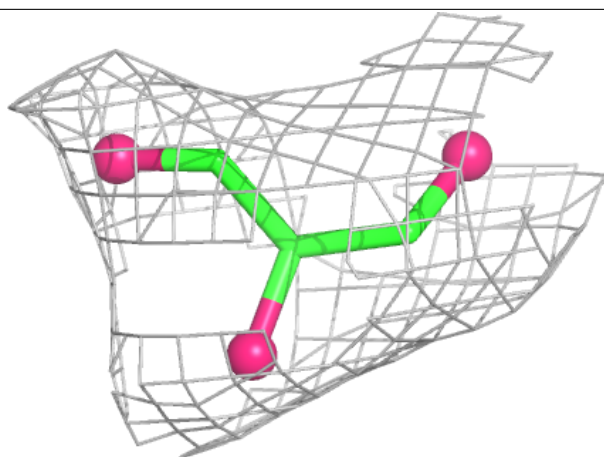
**Electron density around PE8 E 113:**

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



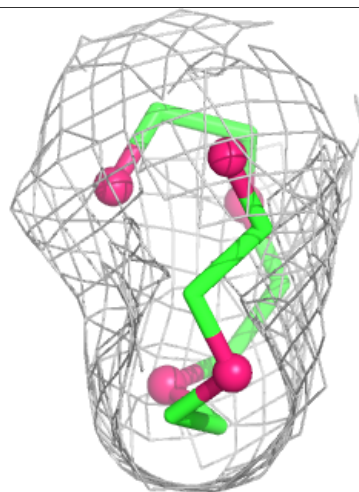
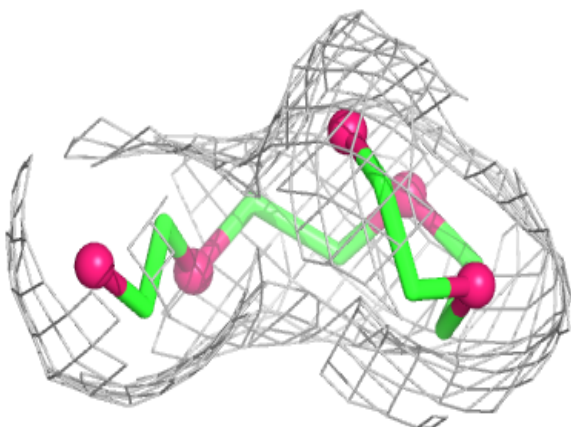
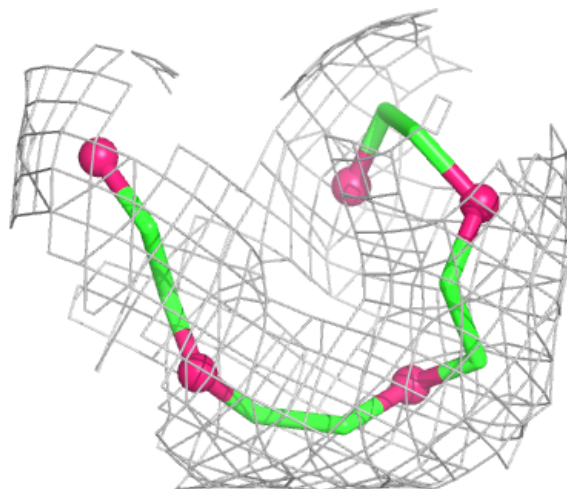
Electron density around GOL C 309:

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



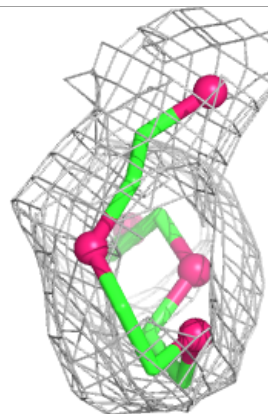
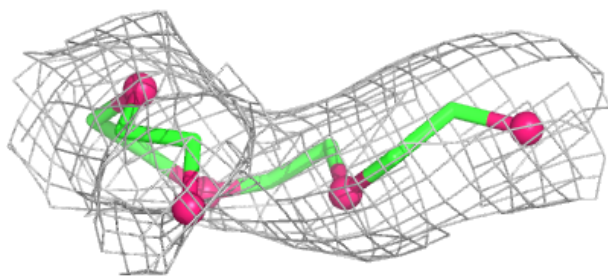
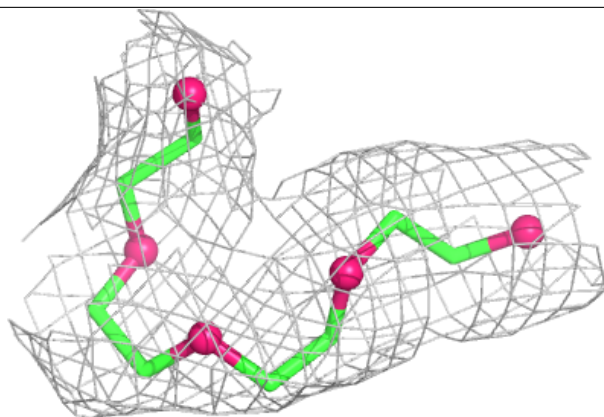
Electron density around PG4 B 127:

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

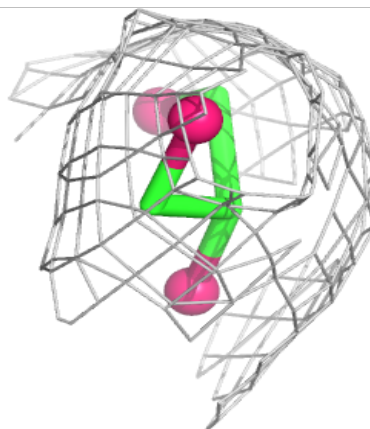
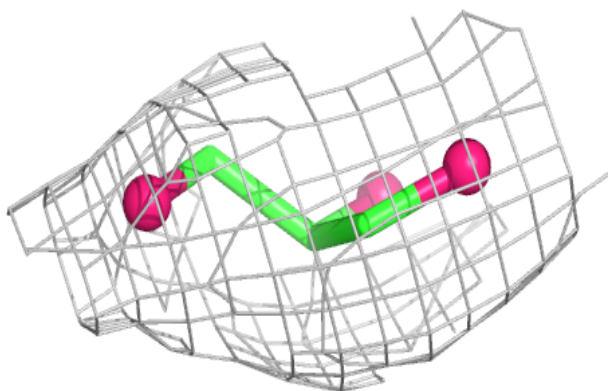
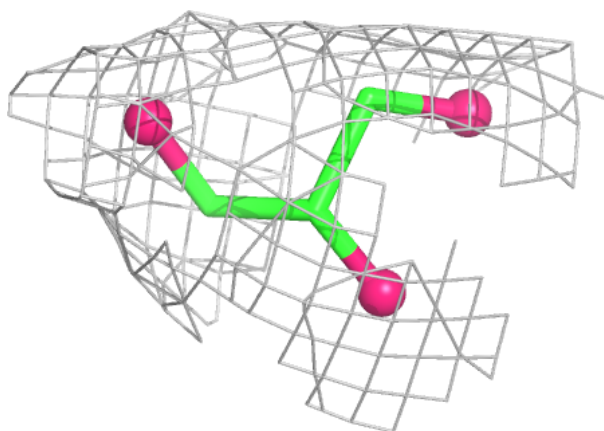


Electron density around PG4 A 331:

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

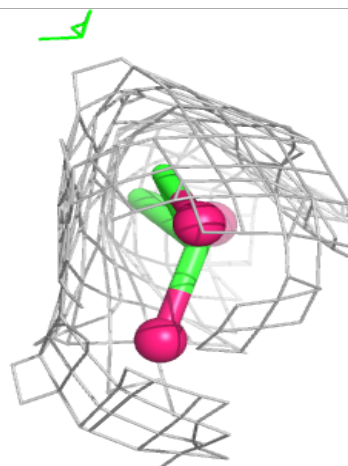
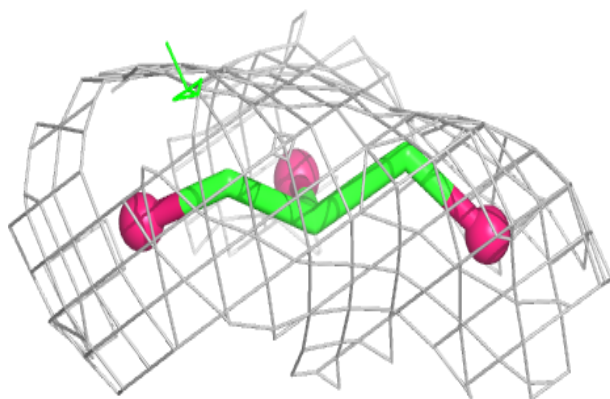
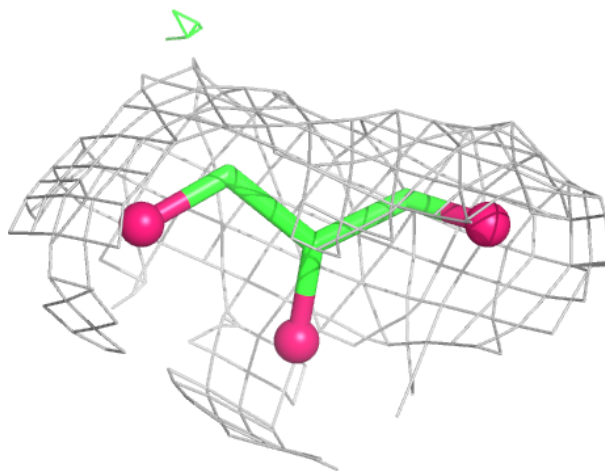
**Electron density around GOL D 110:**

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



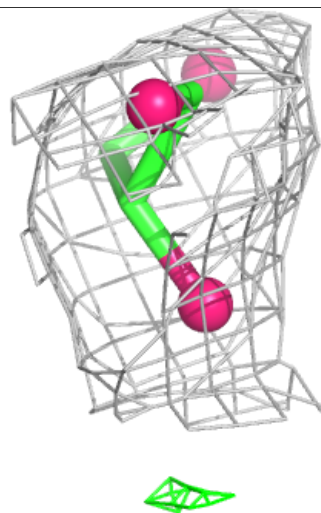
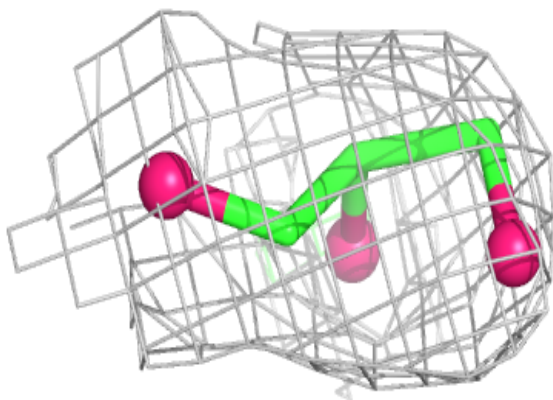
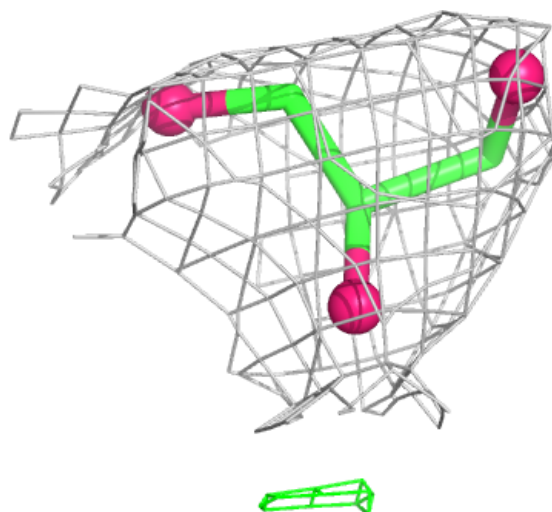
Electron density around GOL D 106:

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



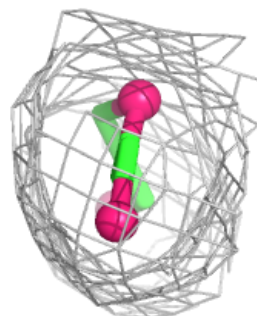
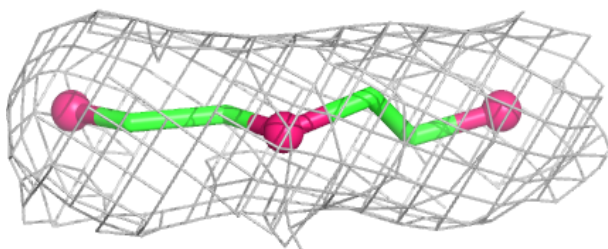
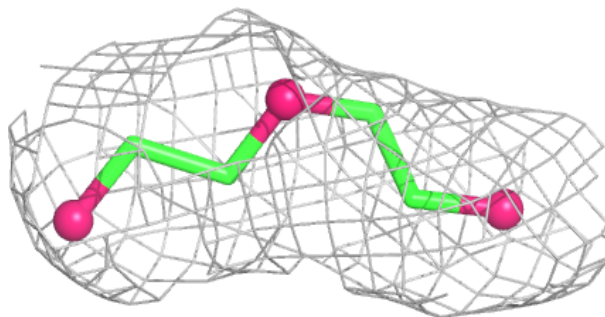
Electron density around GOL B 138:

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

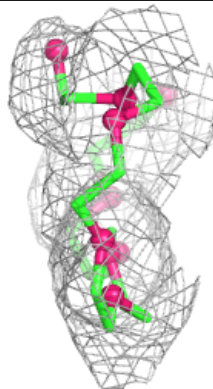
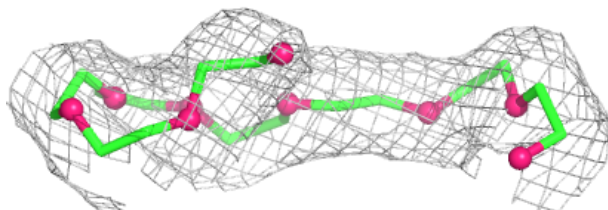
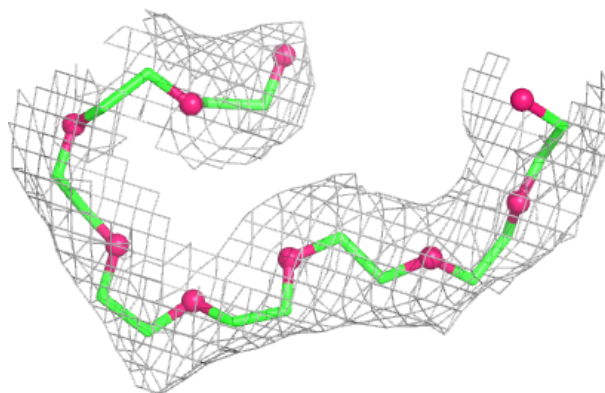


Electron density around PEG C 330:

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

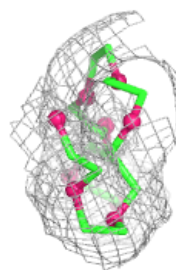
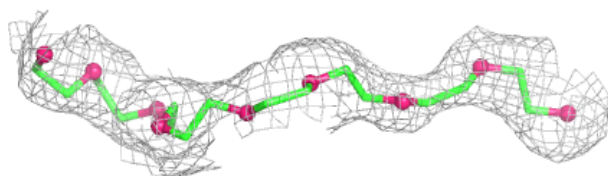
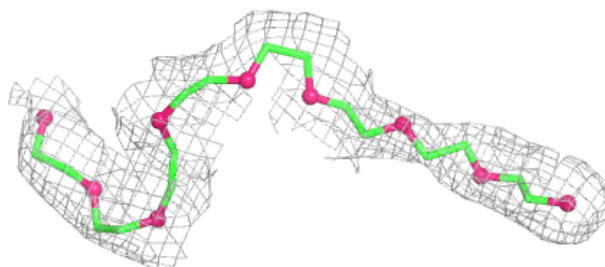
**Electron density around PE8 B 122:**

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

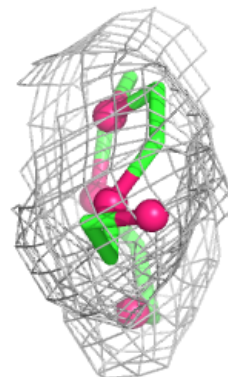
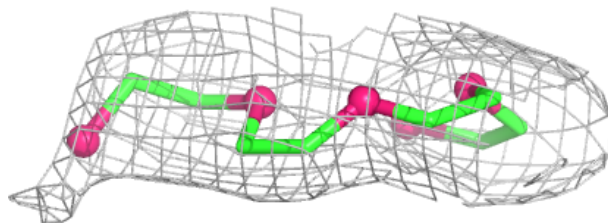
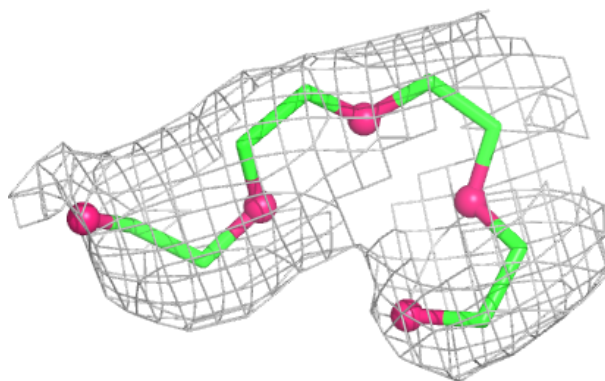


Electron density around PE8 B 123:

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

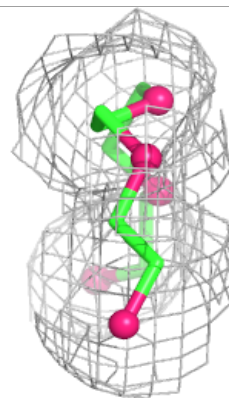
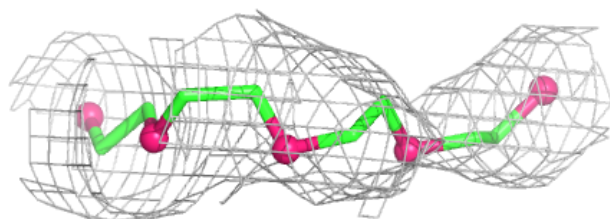
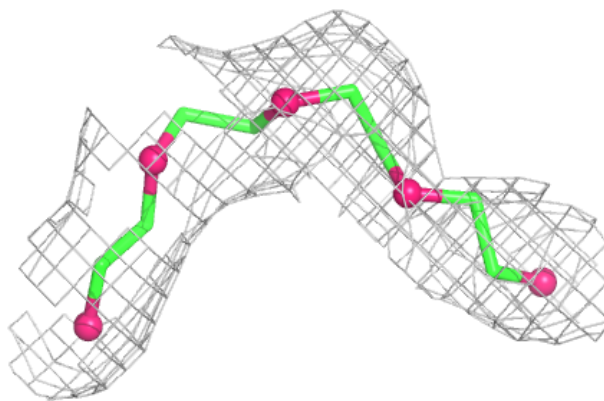
**Electron density around PG4 A 328:**

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

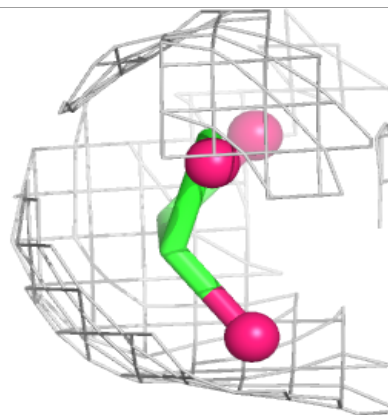
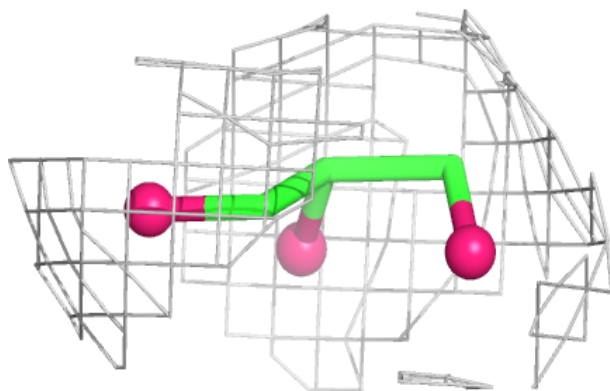
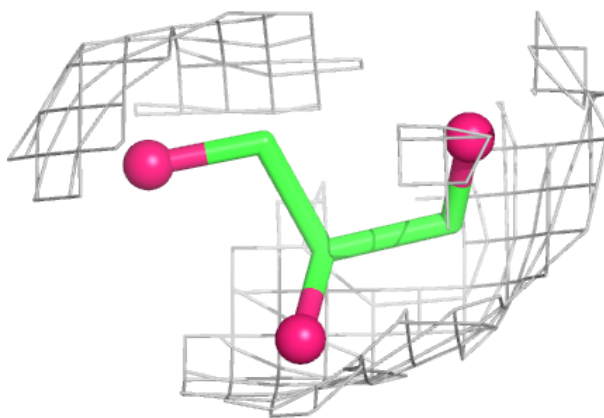


Electron density around PG4 D 118:

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

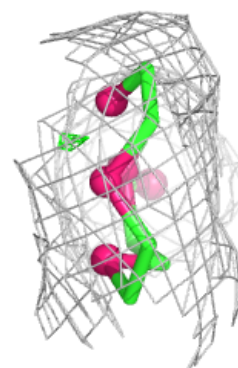
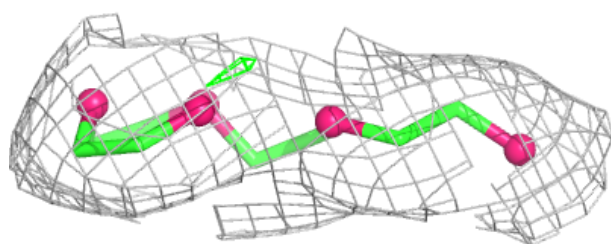
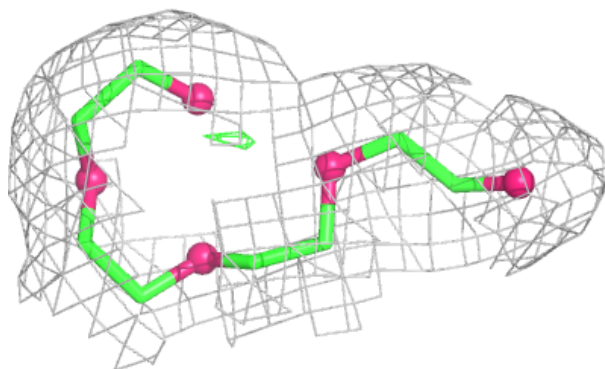
**Electron density around GOL B 109:**

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

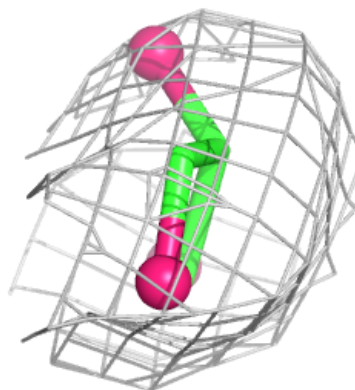
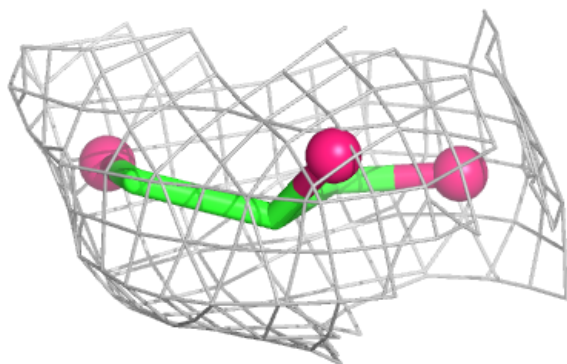
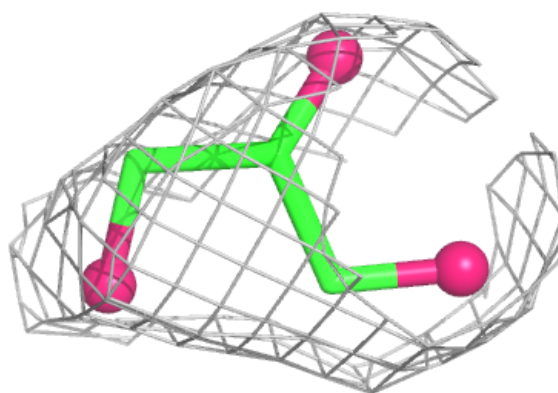


Electron density around PG4 C 325:

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

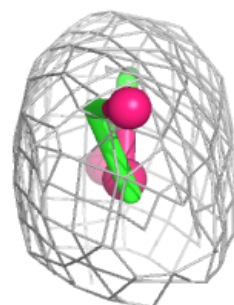
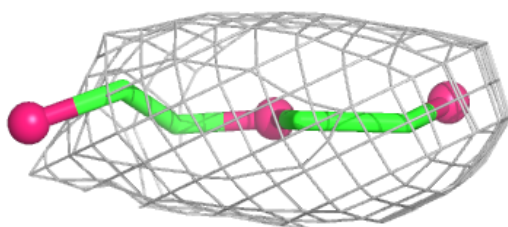
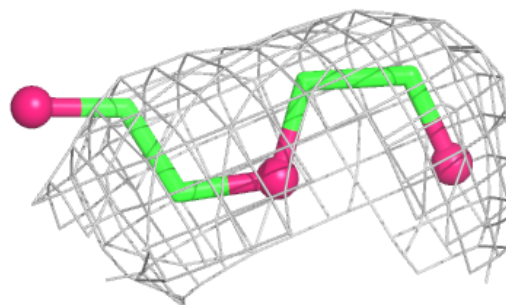
**Electron density around GOL A 307:**

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

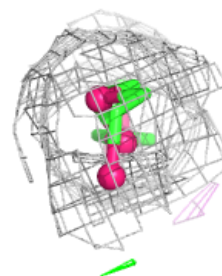
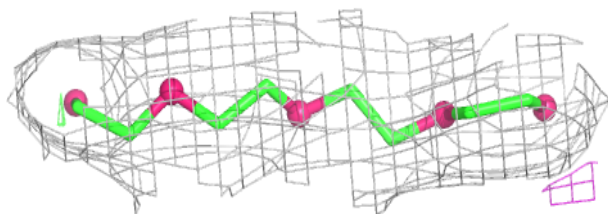
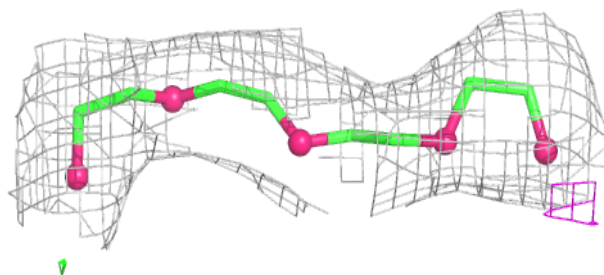


Electron density around PEG C 318:

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

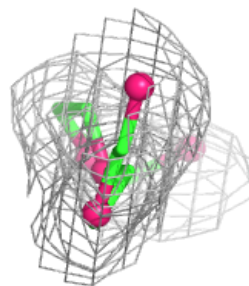
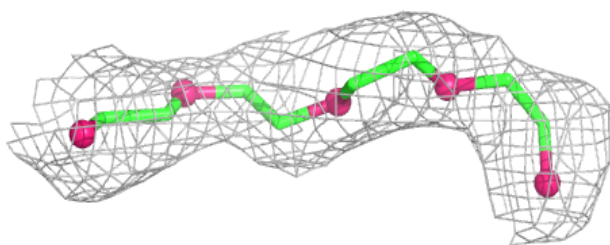
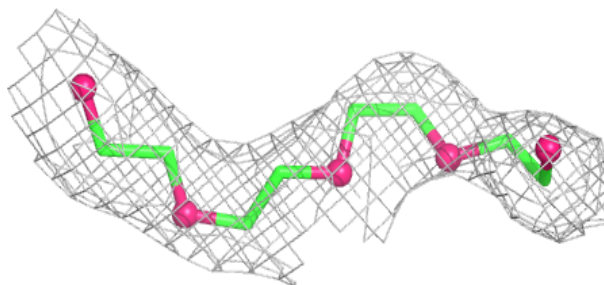
**Electron density around PG4 B 104:**

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

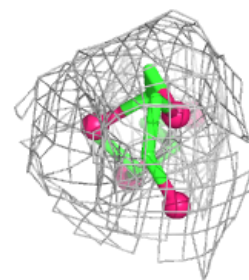
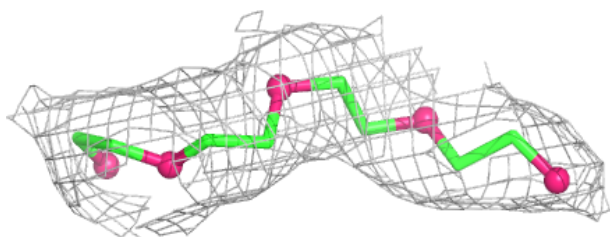
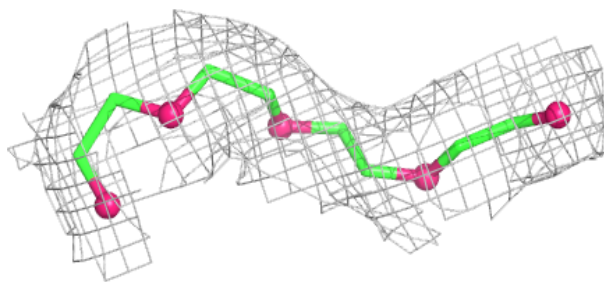


Electron density around PG4 D 116:

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

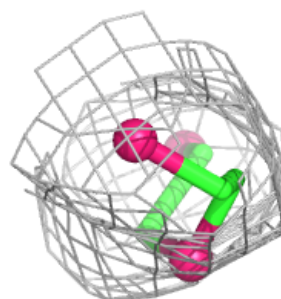
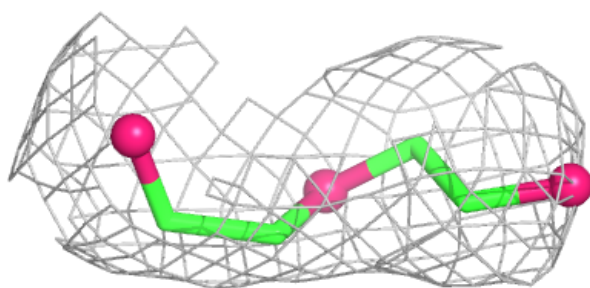
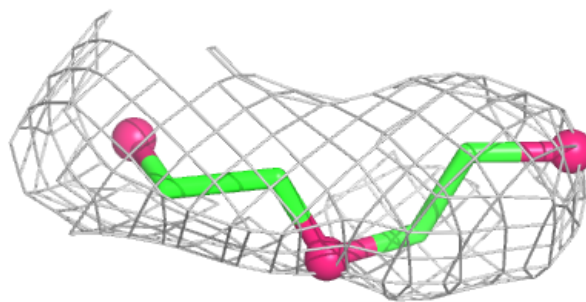
**Electron density around PG4 B 125:**

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

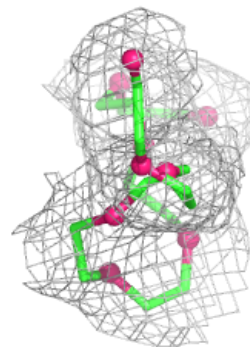
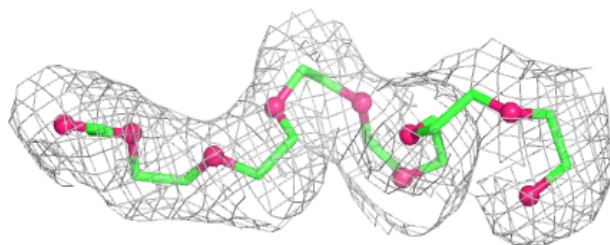
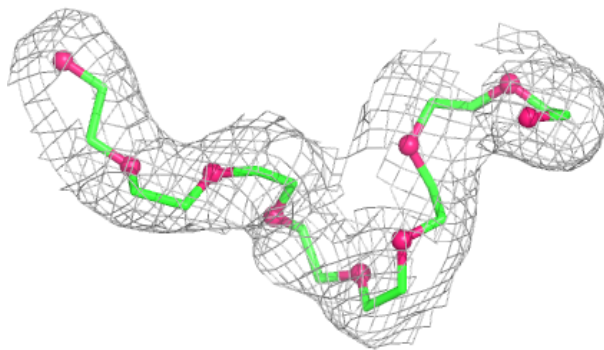


Electron density around PEG C 319:

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

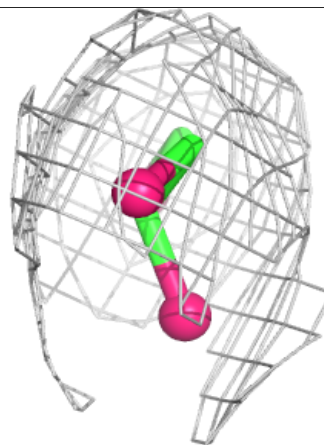
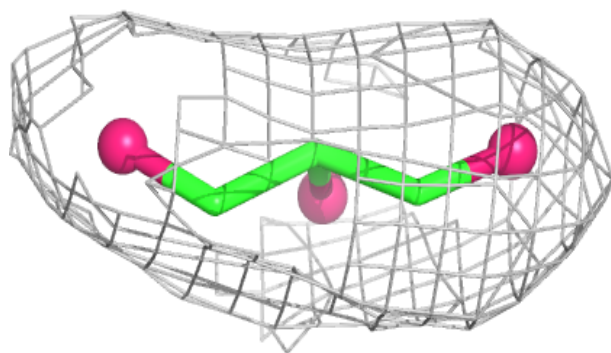
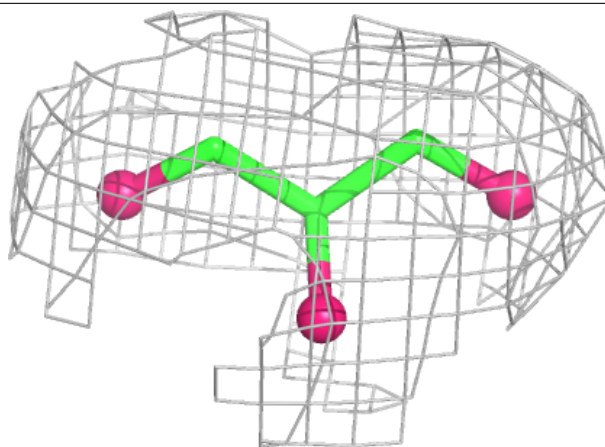
**Electron density around PE8 A 324:**

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



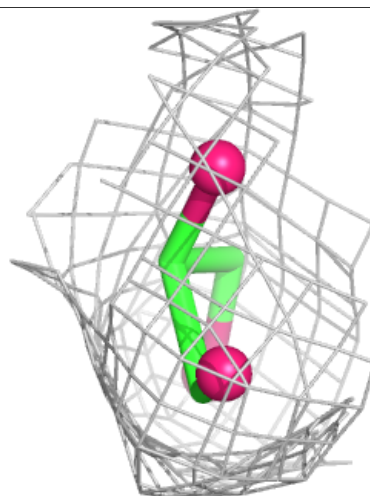
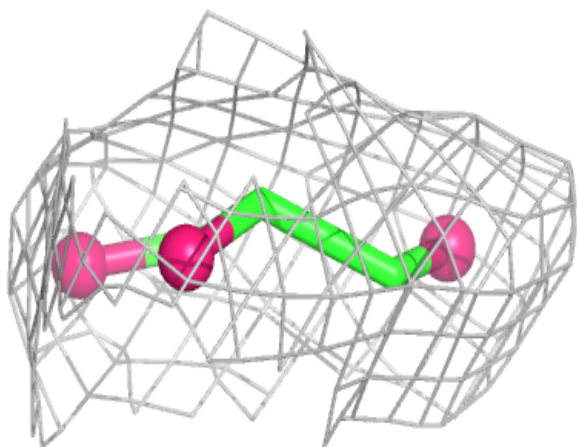
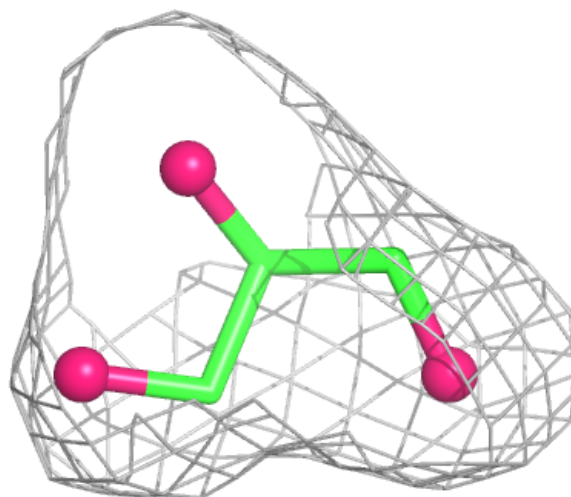
Electron density around GOL A 309:

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



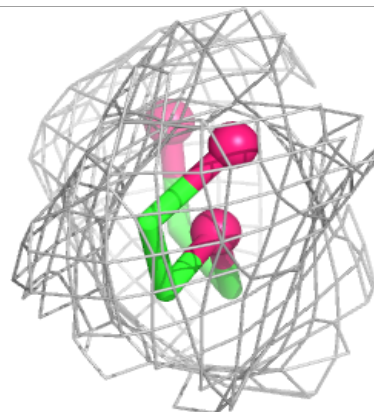
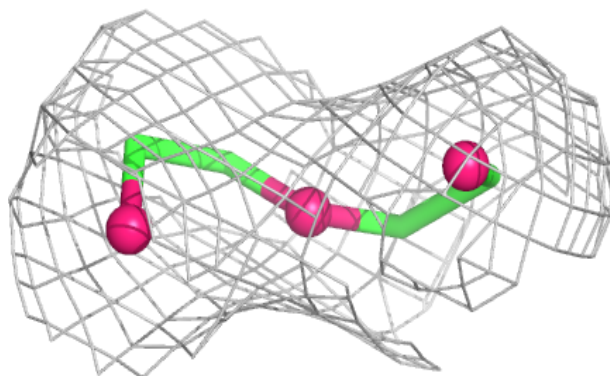
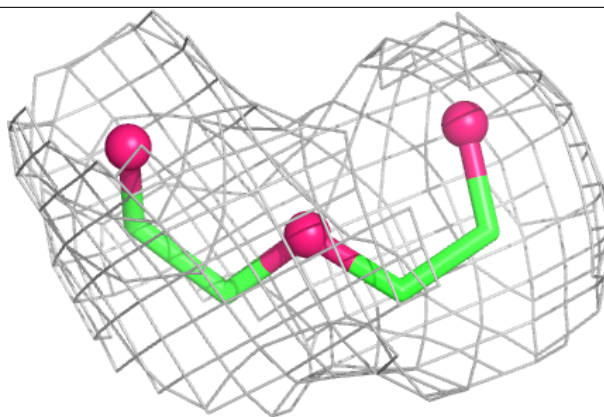
Electron density around GOL C 311:

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

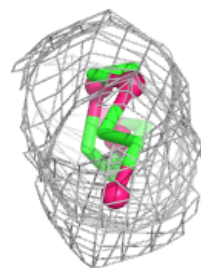
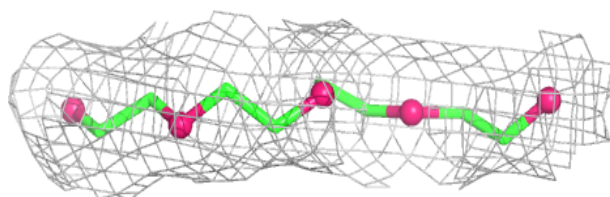
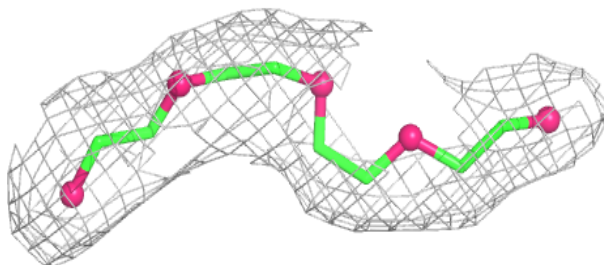


Electron density around PEG A 341:

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

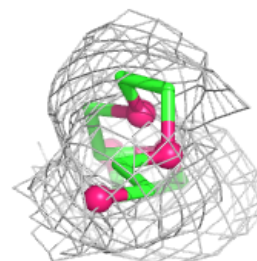
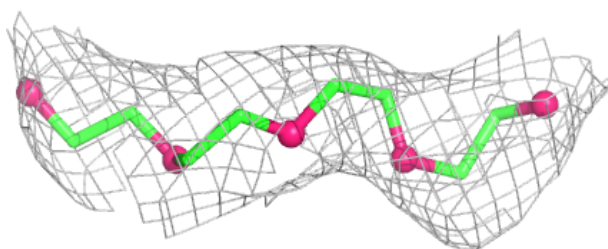
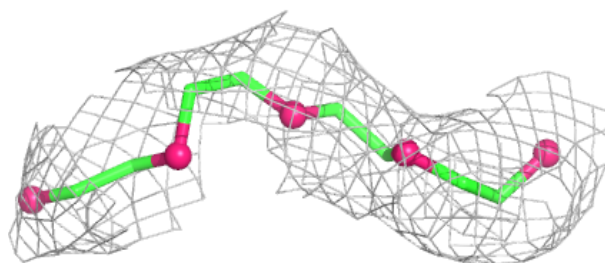
**Electron density around PG4 A 338:**

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



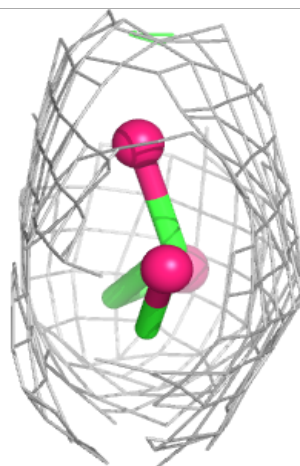
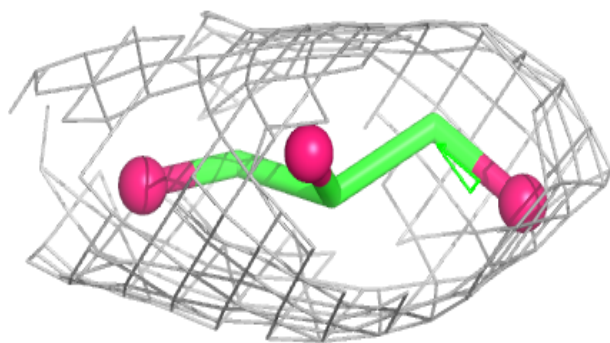
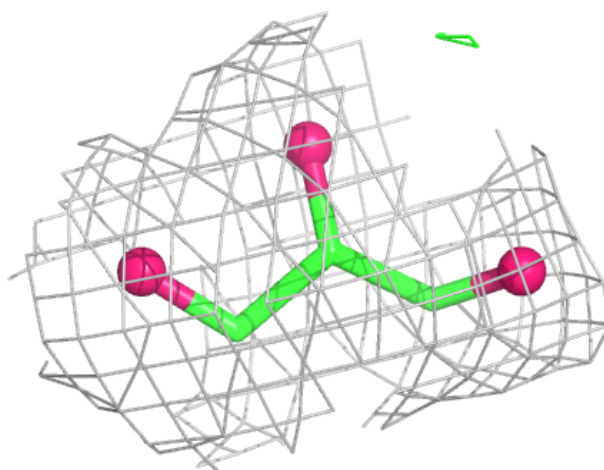
Electron density around PG4 D 105:

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



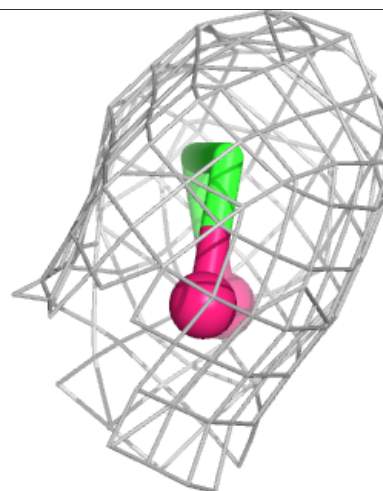
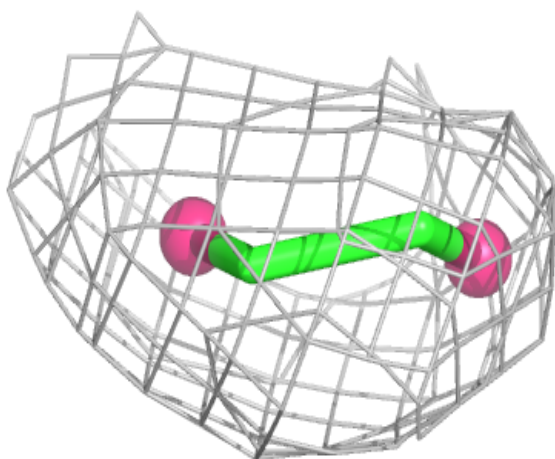
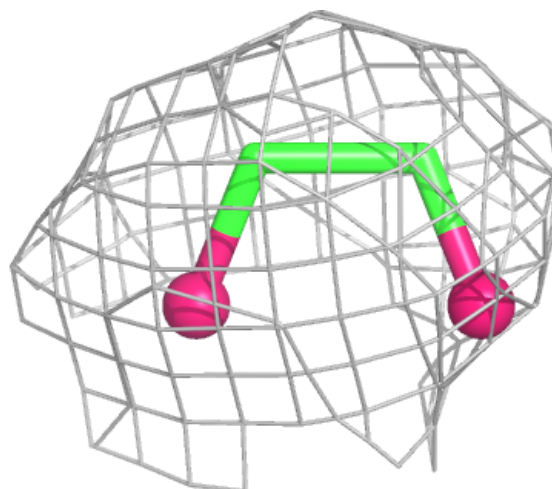
Electron density around GOL B 111:

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



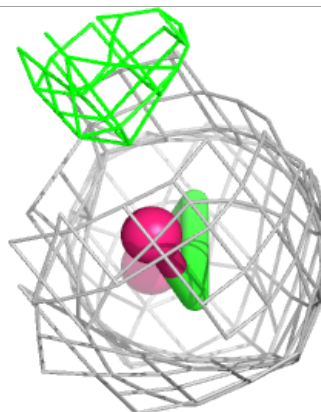
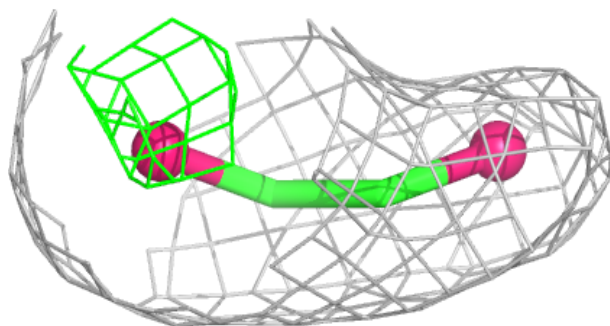
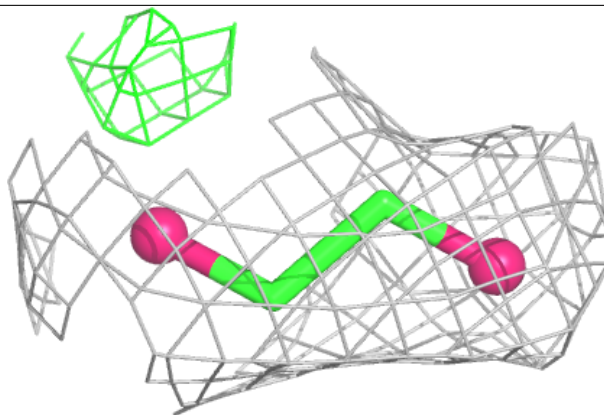
Electron density around EDO C 329:

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

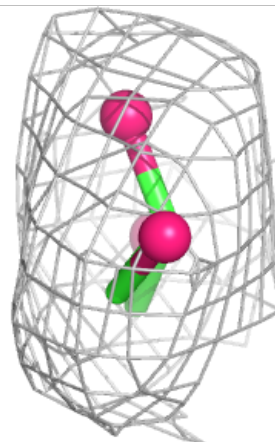
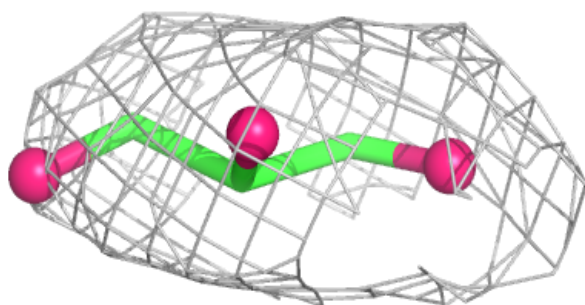
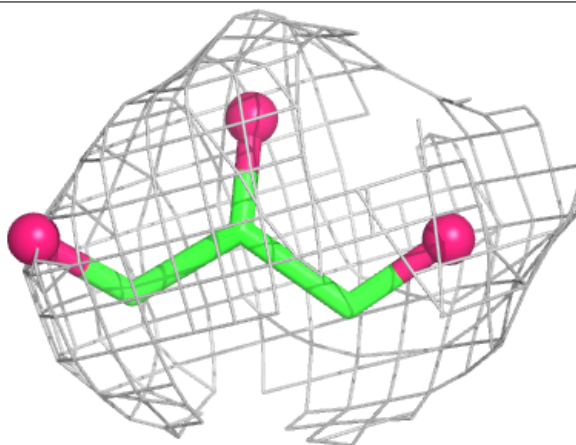


Electron density around EDO C 334:

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

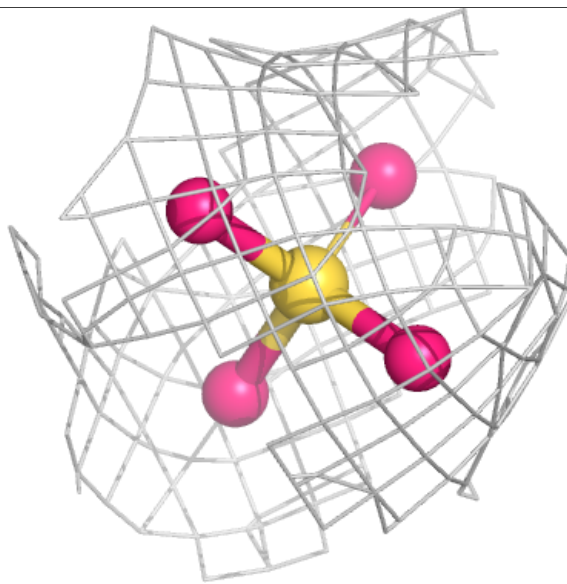
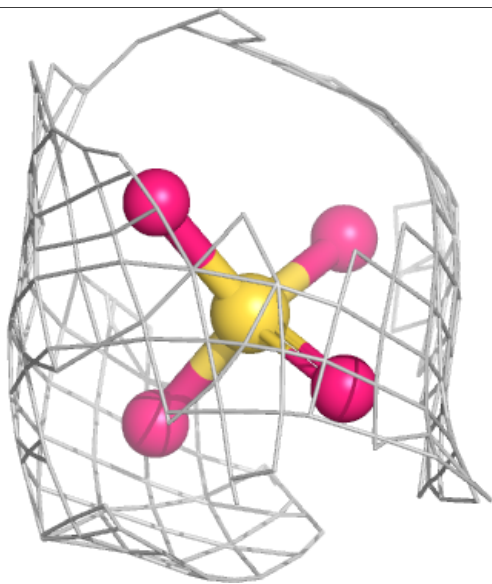
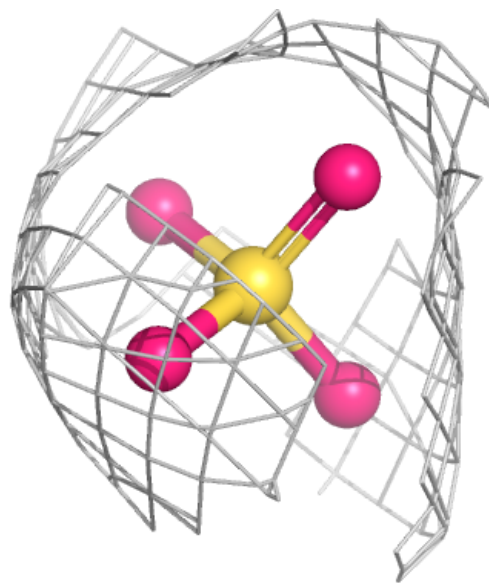
**Electron density around GOL B 113:**

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



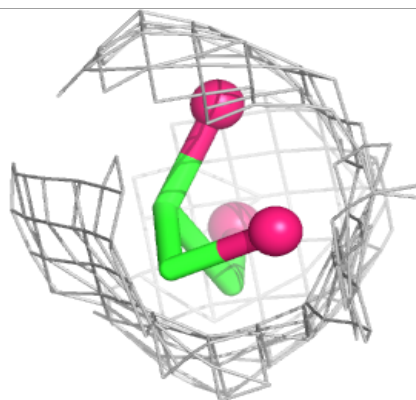
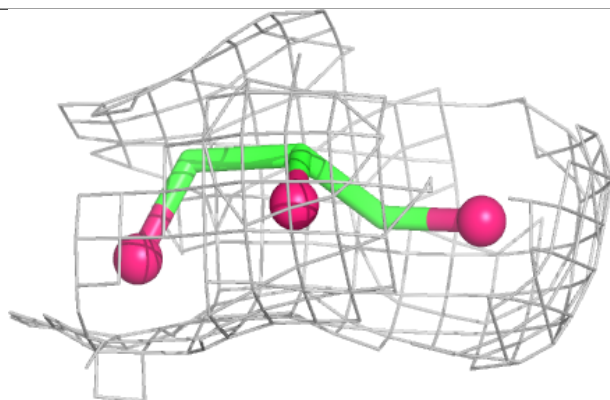
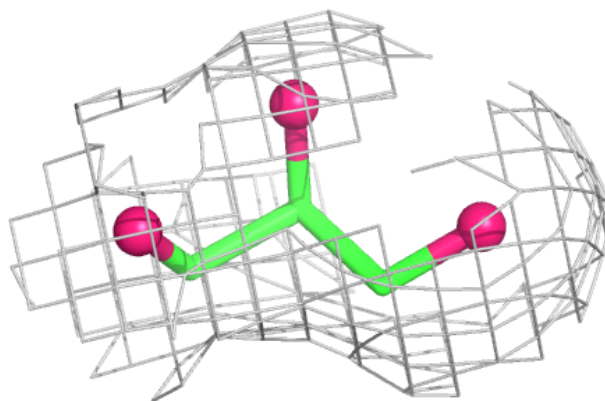
Electron density around SO4 D 113:

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

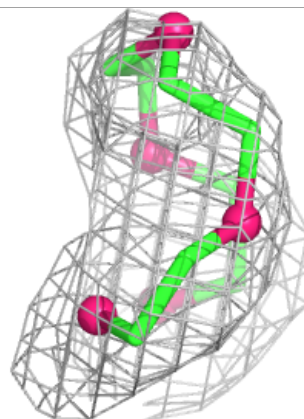
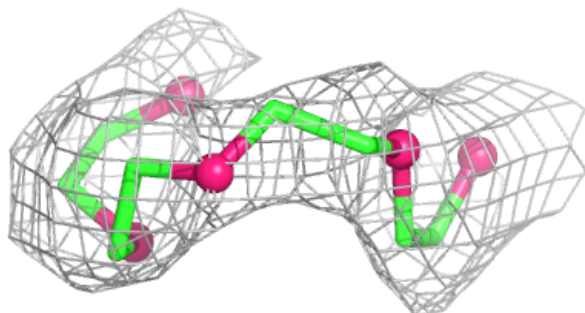
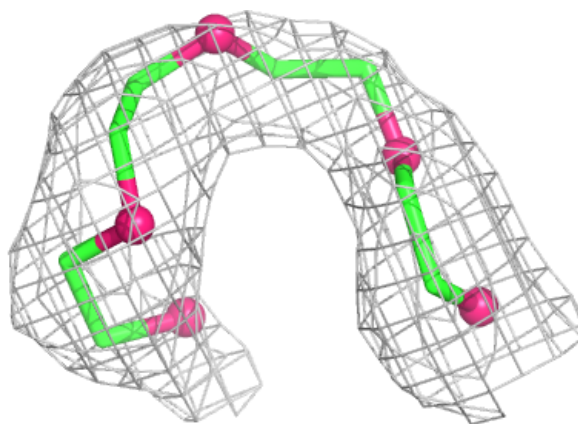


Electron density around GOL C 342:

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

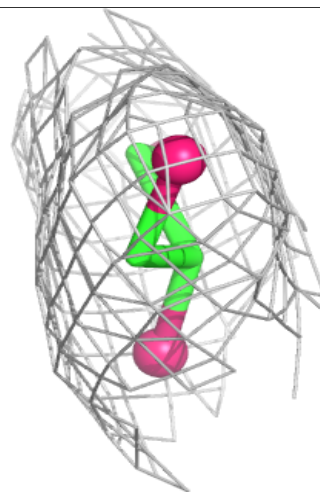
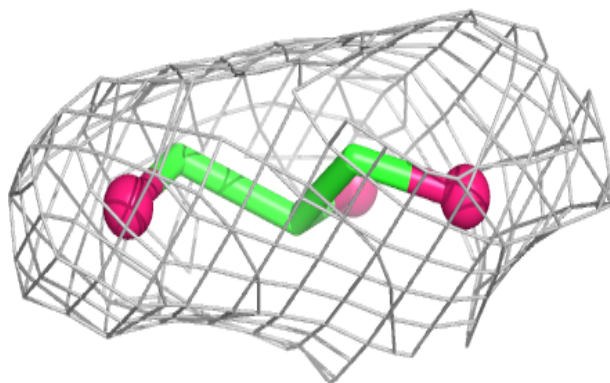
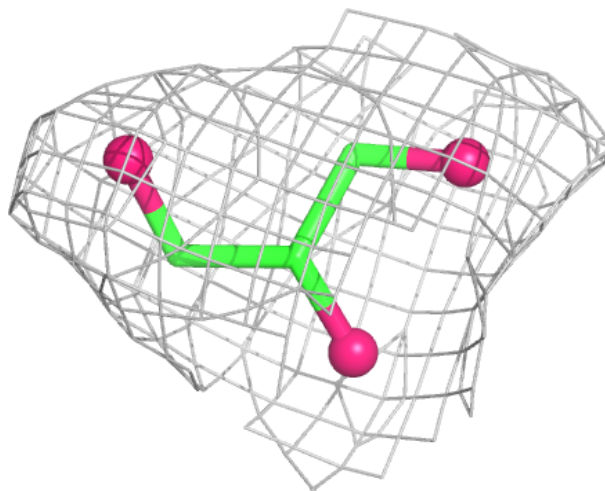
**Electron density around PG4 A 332:**

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



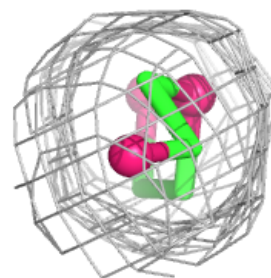
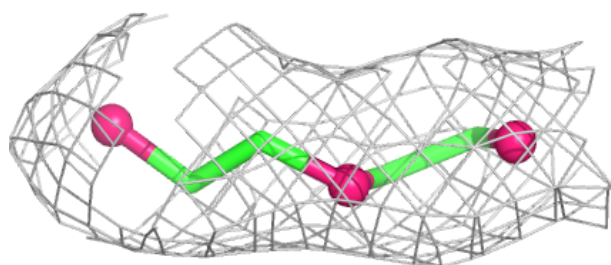
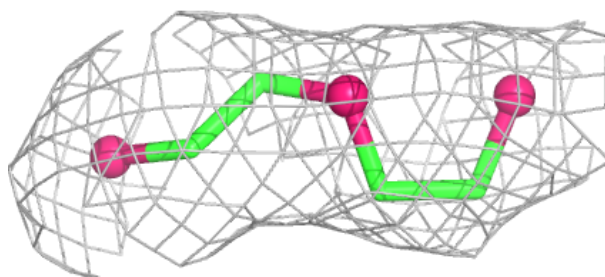
Electron density around GOL A 311:

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



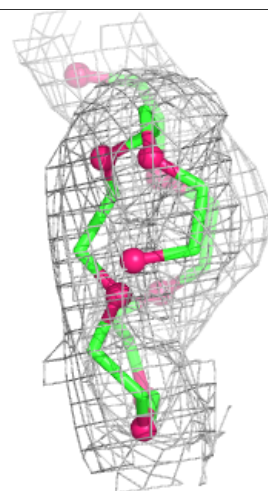
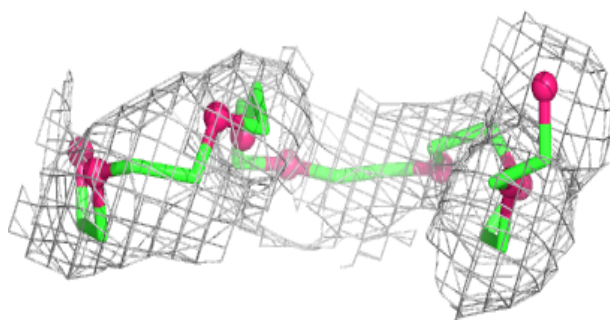
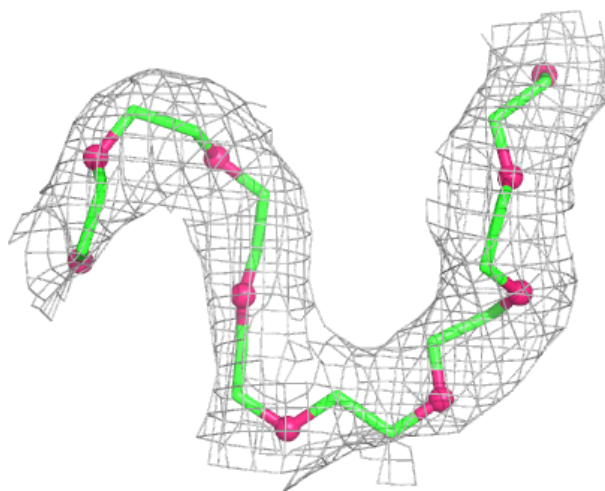
Electron density around PEG C 317:

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



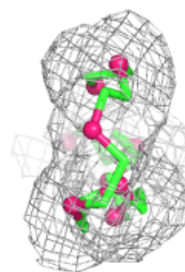
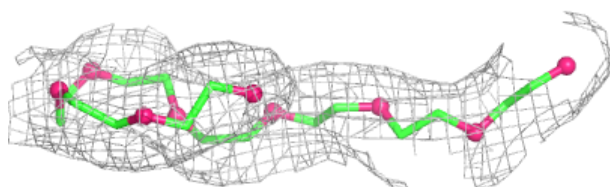
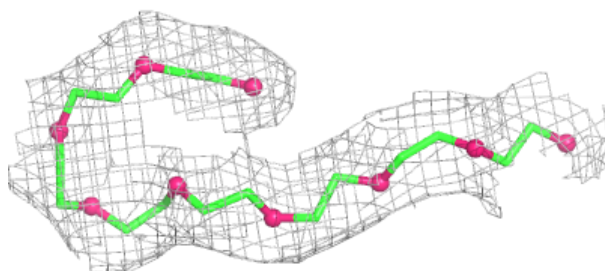
Electron density around PE8 B 131:

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

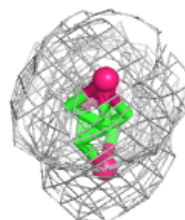
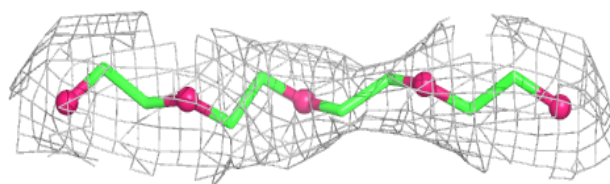
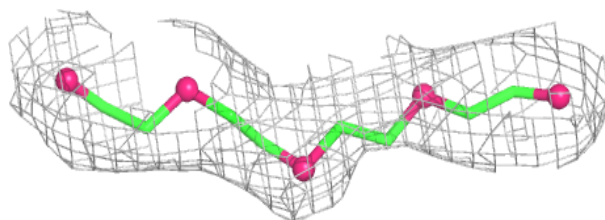


Electron density around PE8 C 322:

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

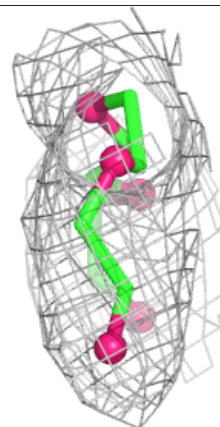
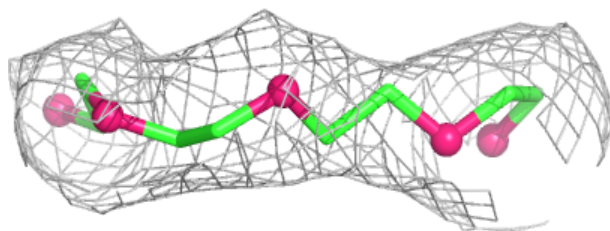
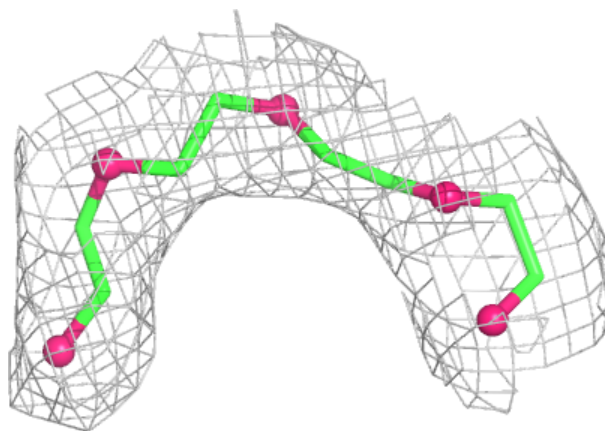
**Electron density around PG4 D 119:**

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



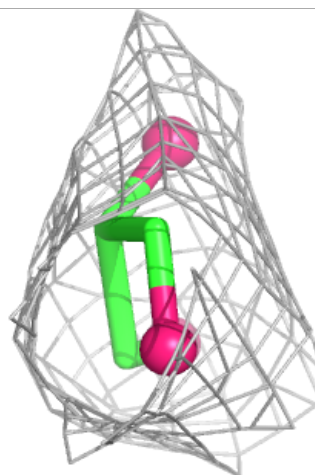
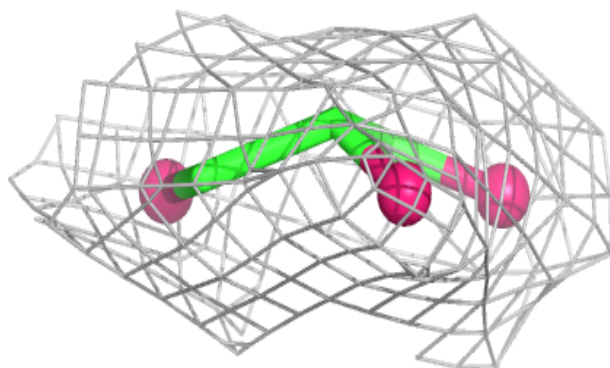
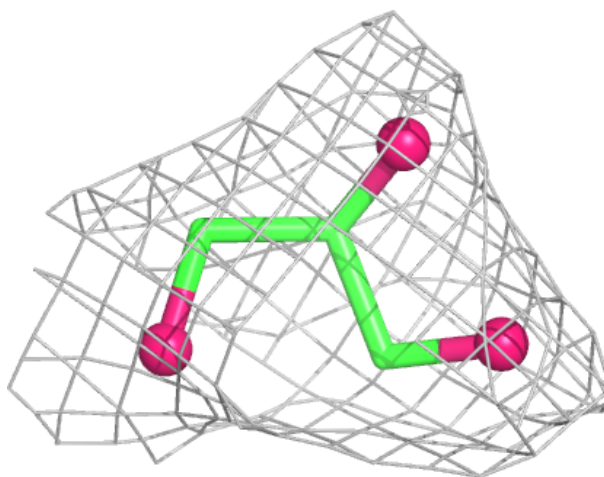
Electron density around PG4 D 127:

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



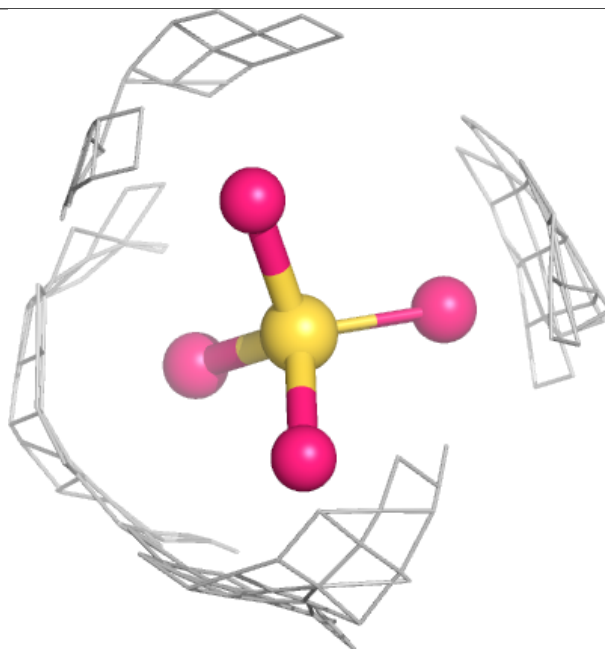
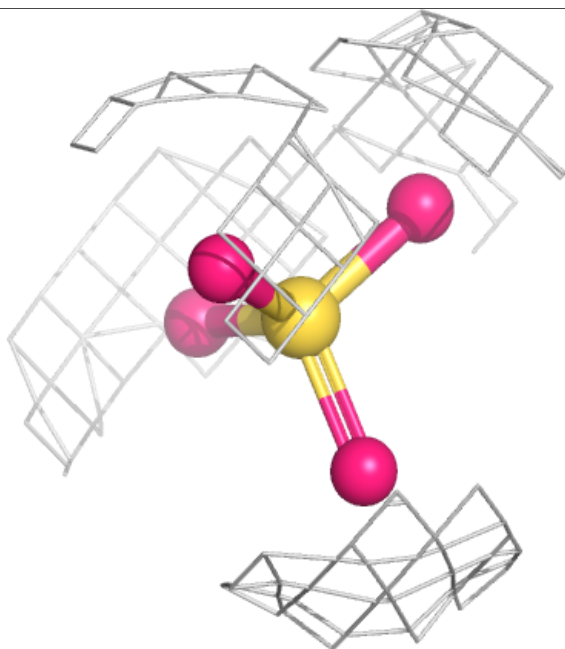
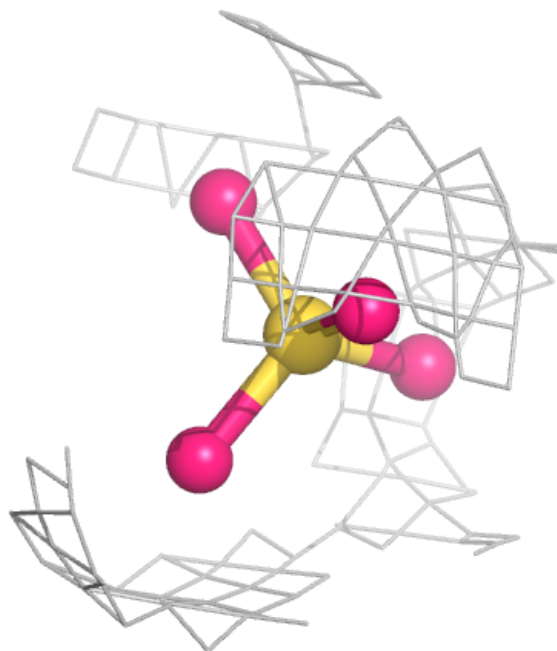
Electron density around GOL B 130:

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



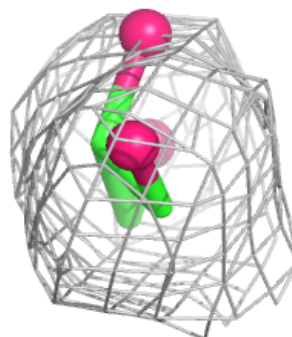
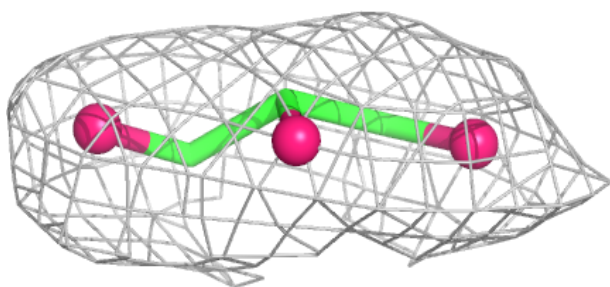
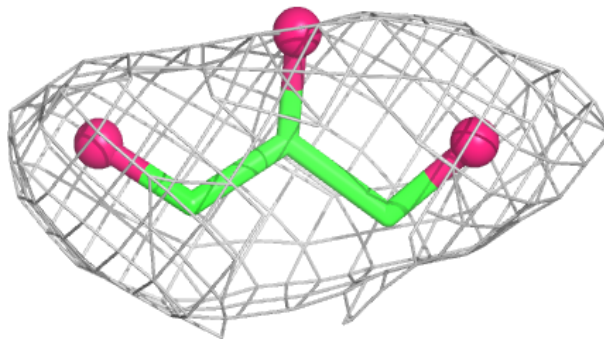
Electron density around SO4 C 336:

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

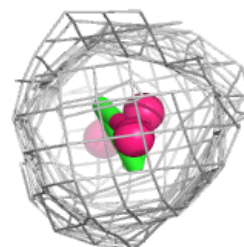
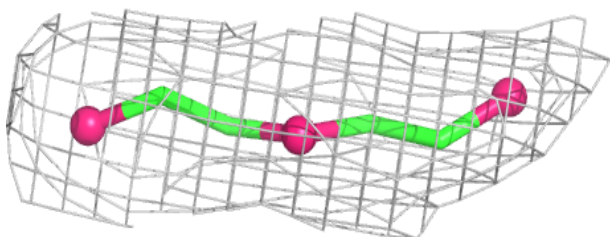
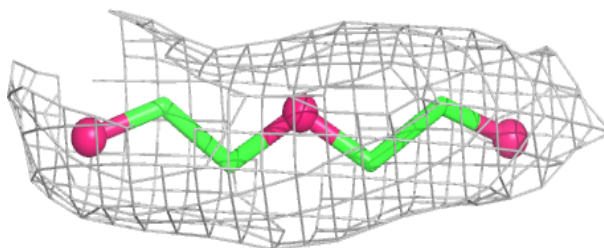


Electron density around GOL B 136:

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

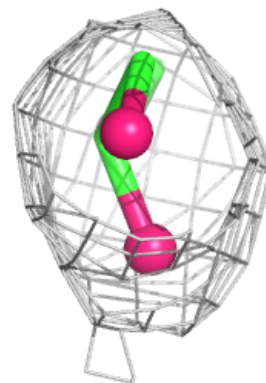
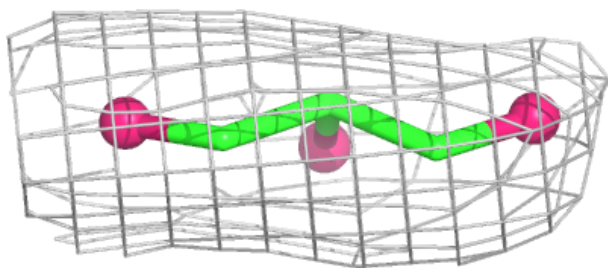
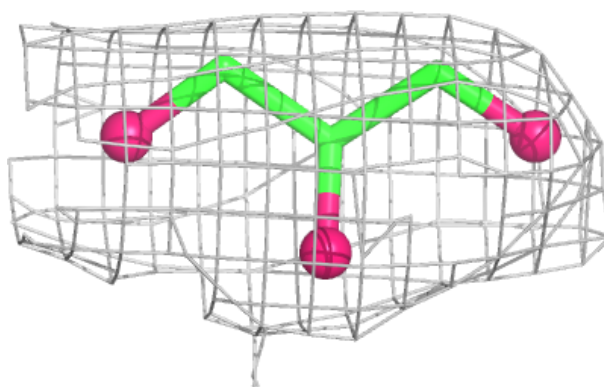
**Electron density around PEG C 339:**

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

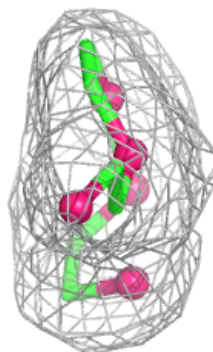
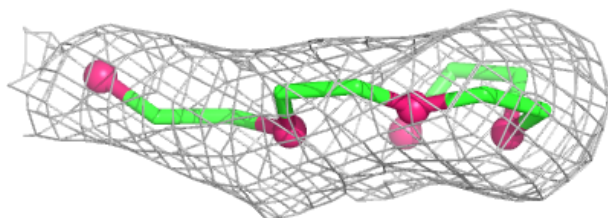
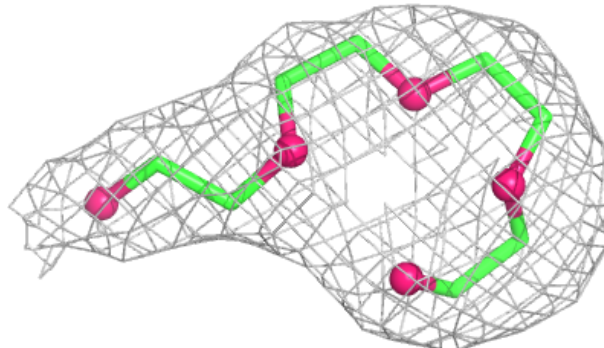


Electron density around GOL A 346:

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

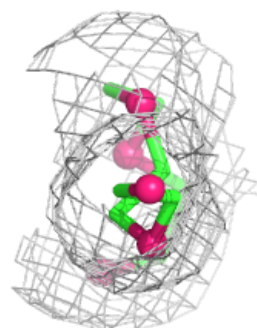
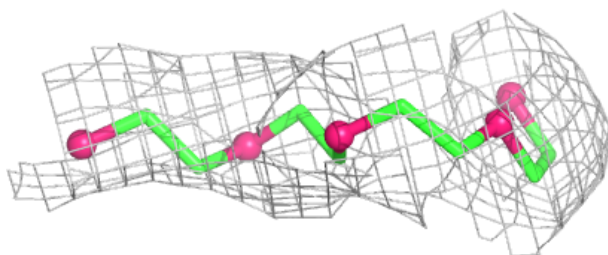
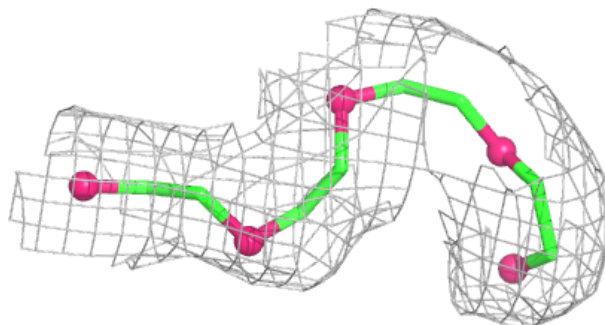
**Electron density around PG4 B 128:**

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

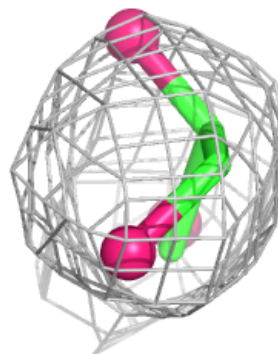
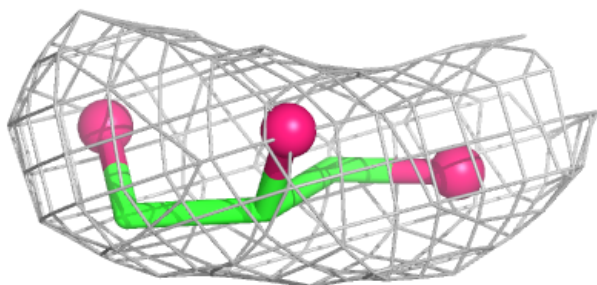
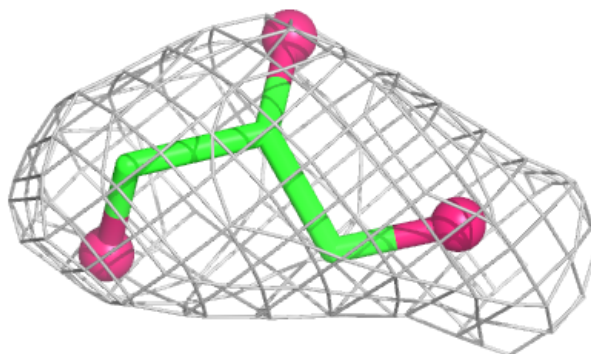


Electron density around PG4 B 129:

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

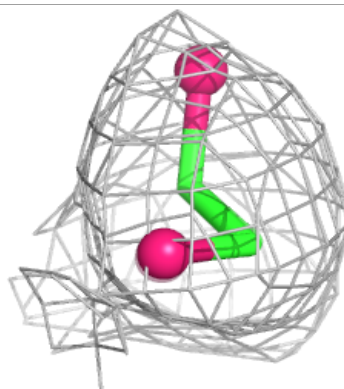
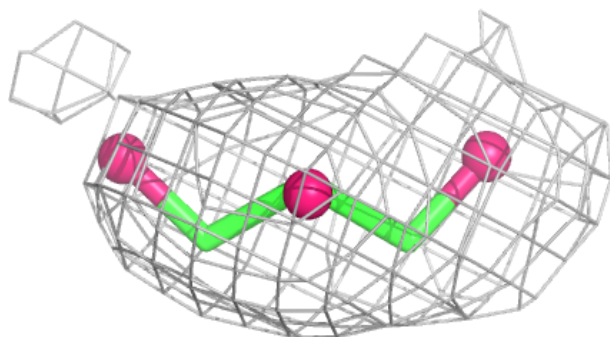
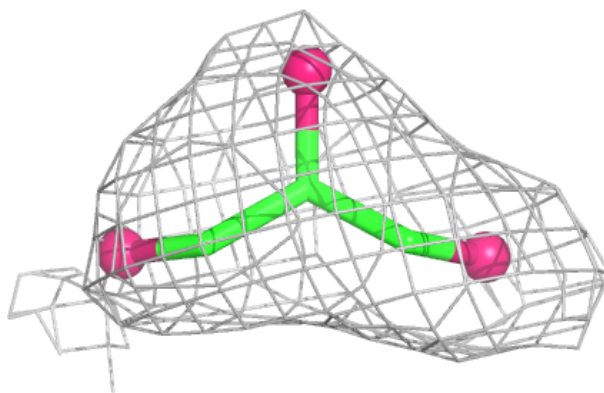
**Electron density around GOL B 140:**

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

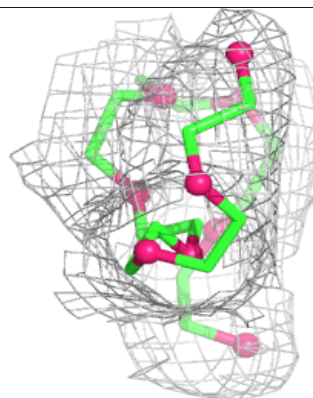
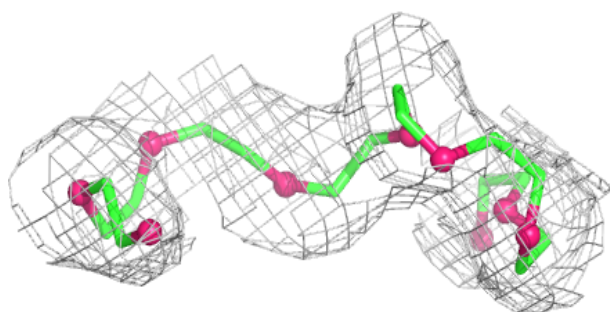
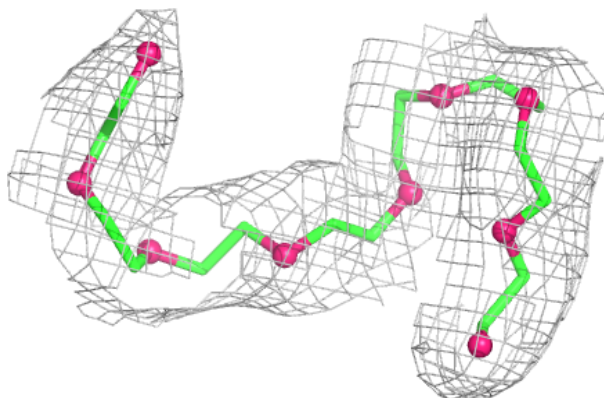


Electron density around GOL D 109:

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

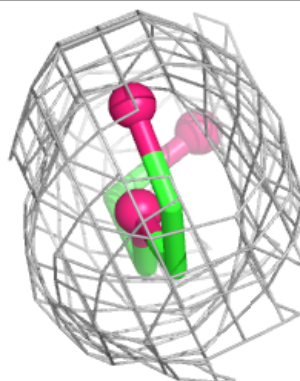
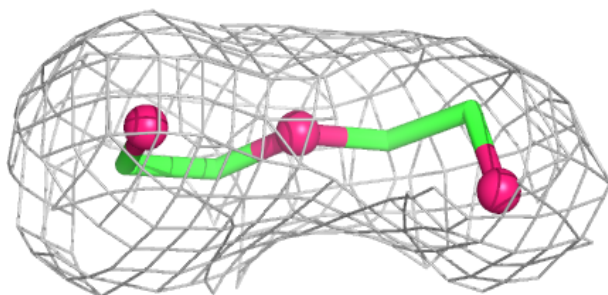
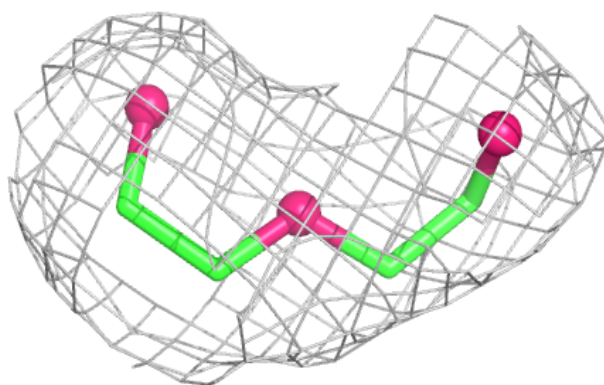
**Electron density around PE8 A 322:**

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

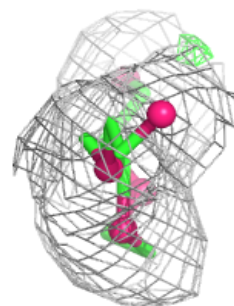
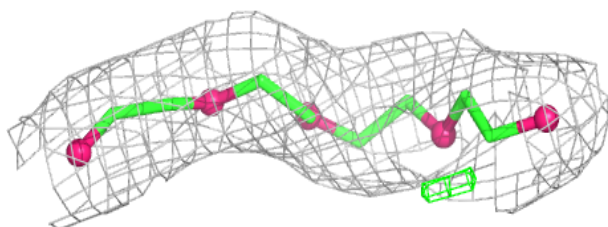
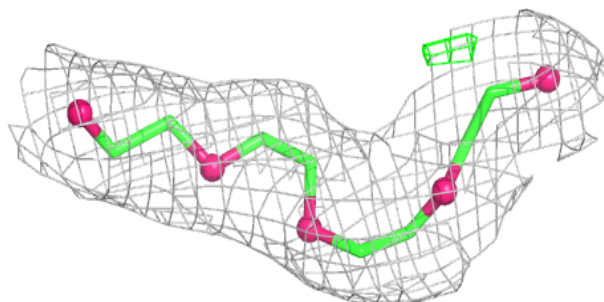


Electron density around PEG B 120:

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

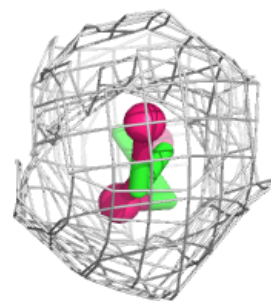
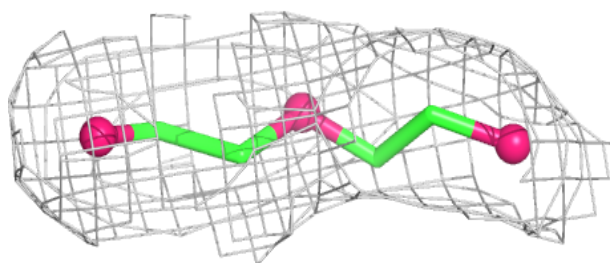
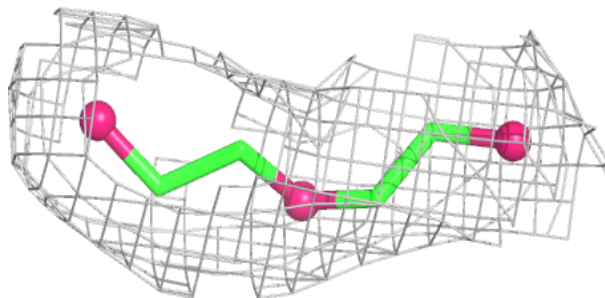
**Electron density around PG4 D 121:**

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

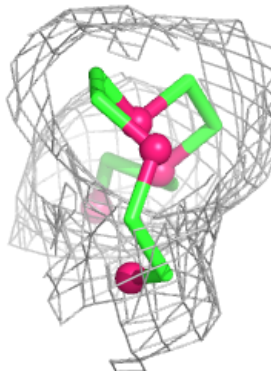
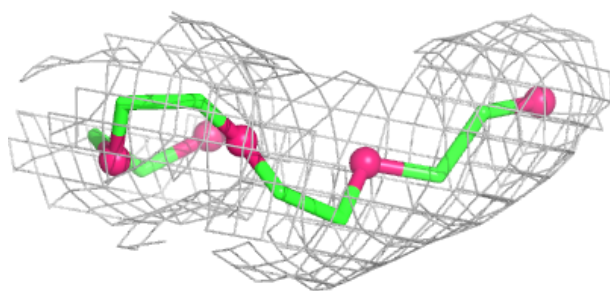
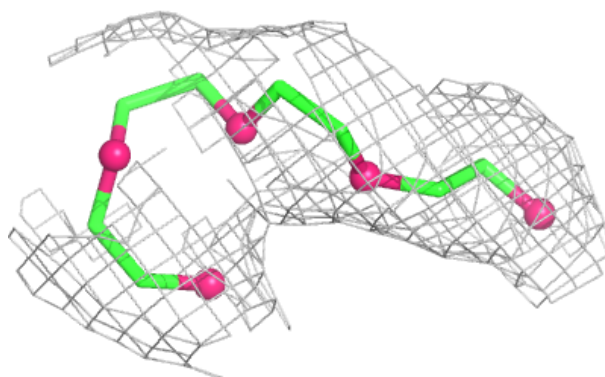


Electron density around PEG C 315:

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

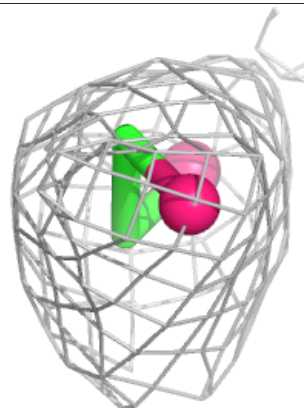
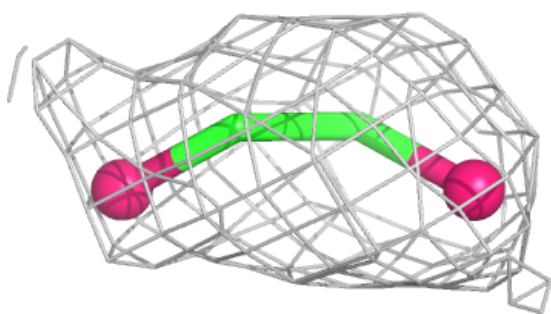
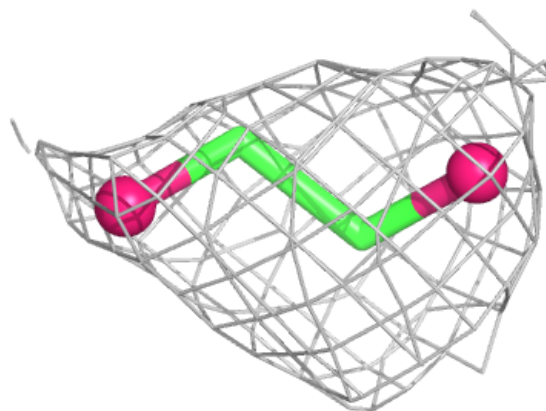
**Electron density around PG4 B 126:**

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



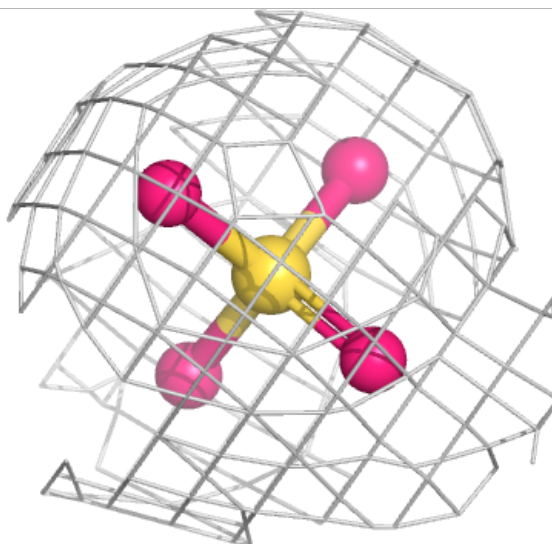
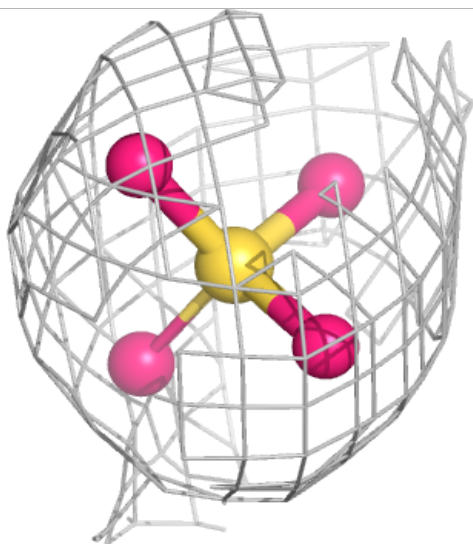
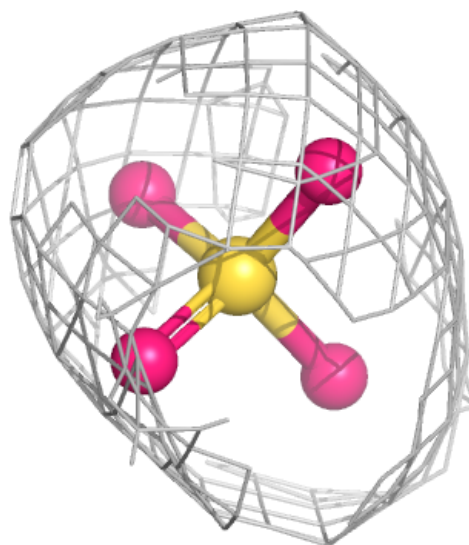
Electron density around EDO A 343:

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



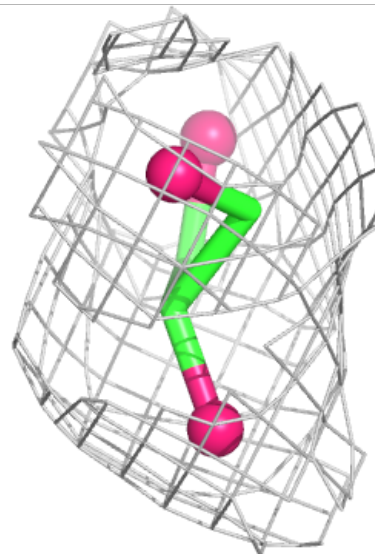
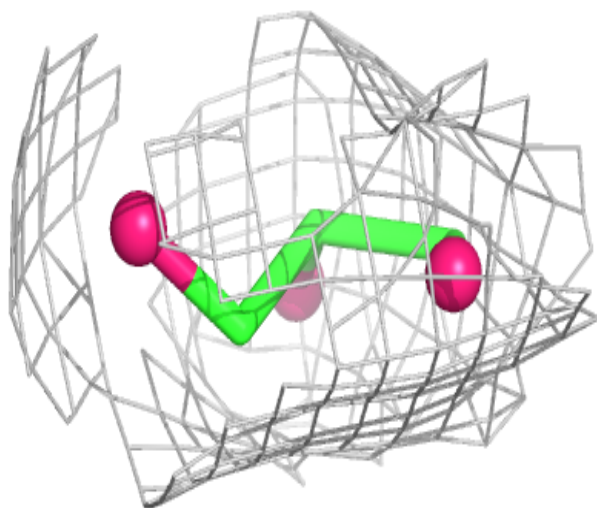
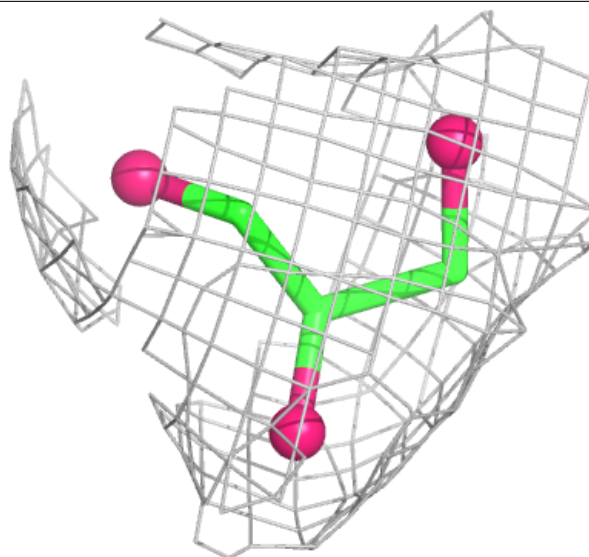
Electron density around SO4 D 112:

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



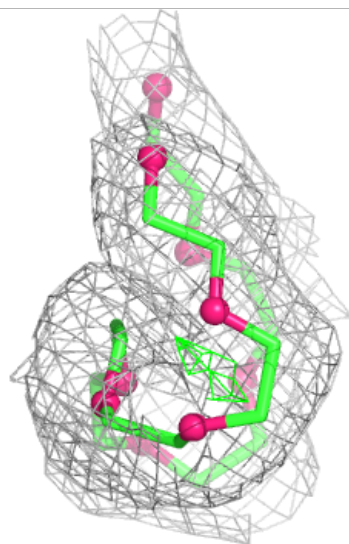
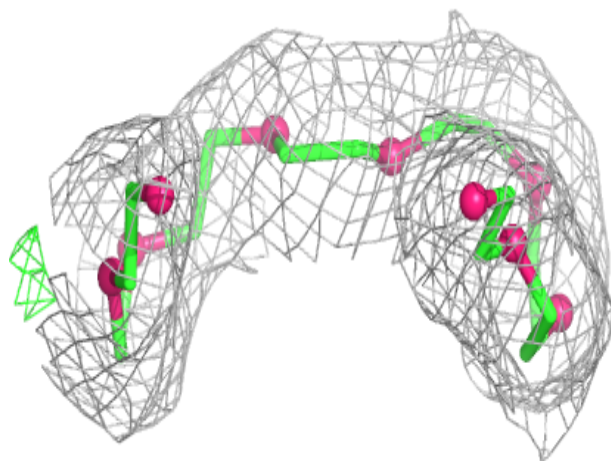
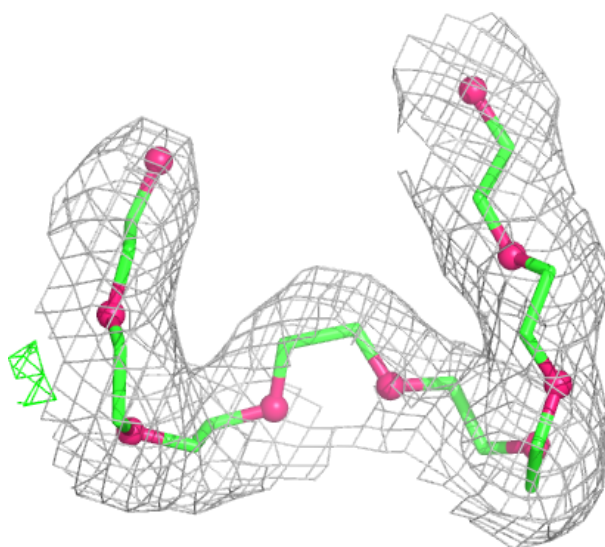
Electron density around GOL B 135:

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



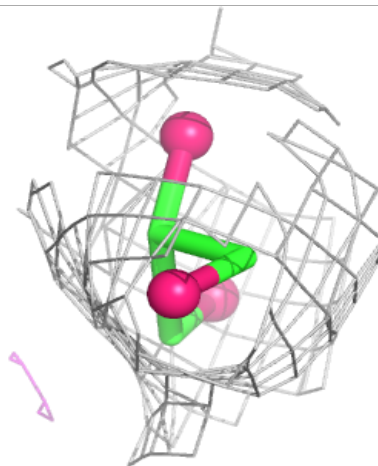
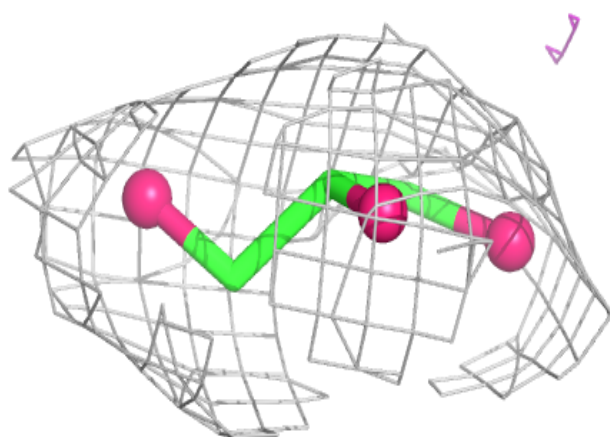
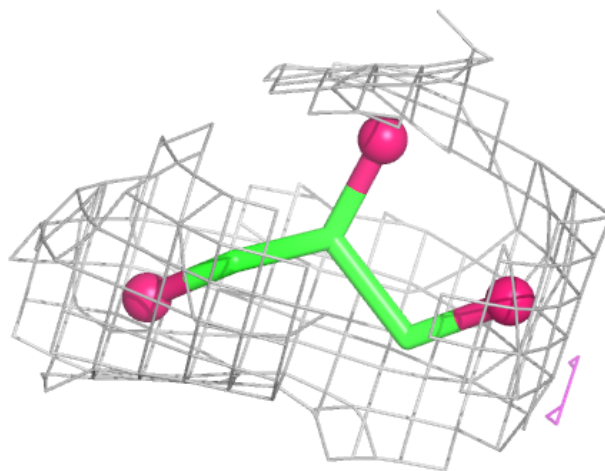
Electron density around PE8 A 323:

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



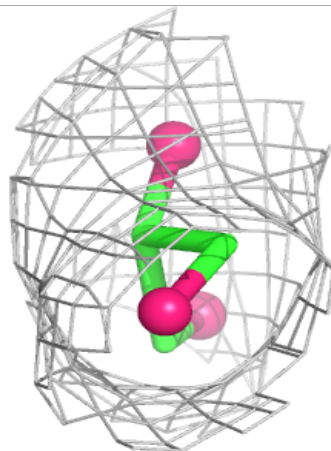
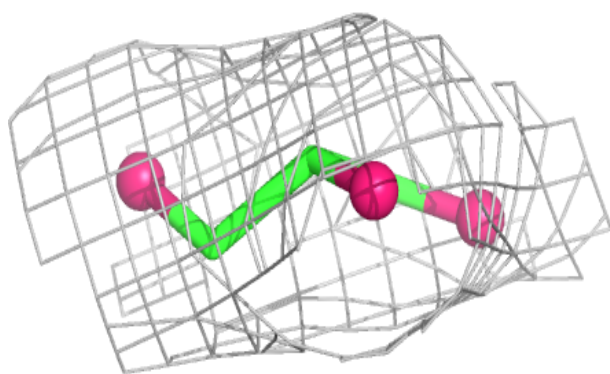
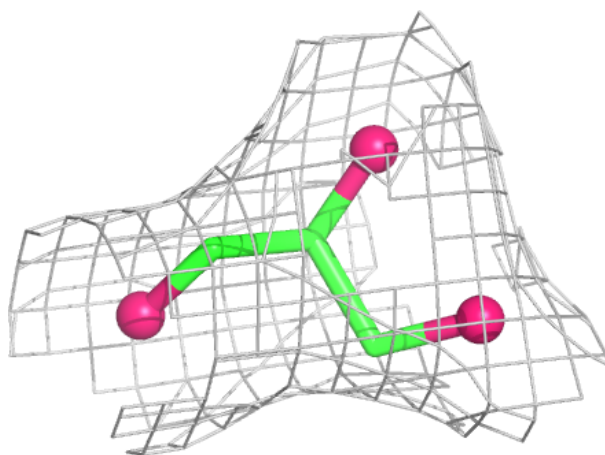
Electron density around GOL B 112:

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



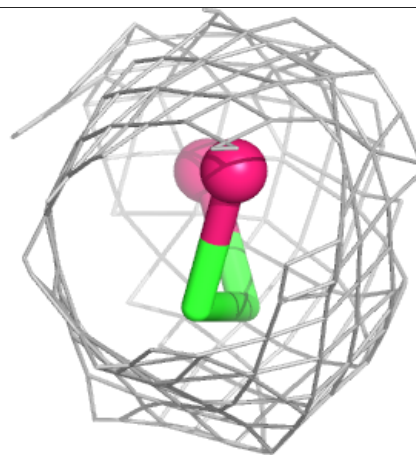
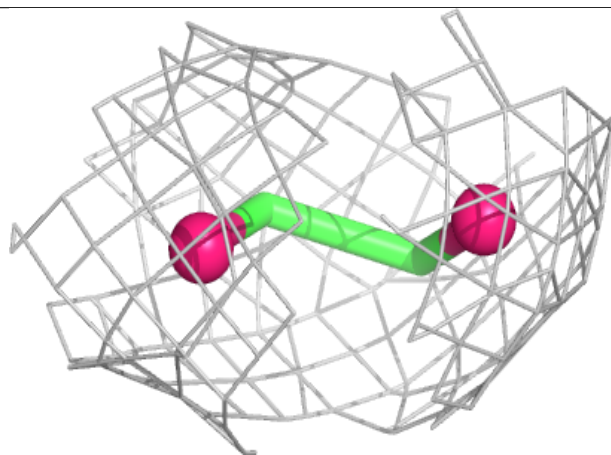
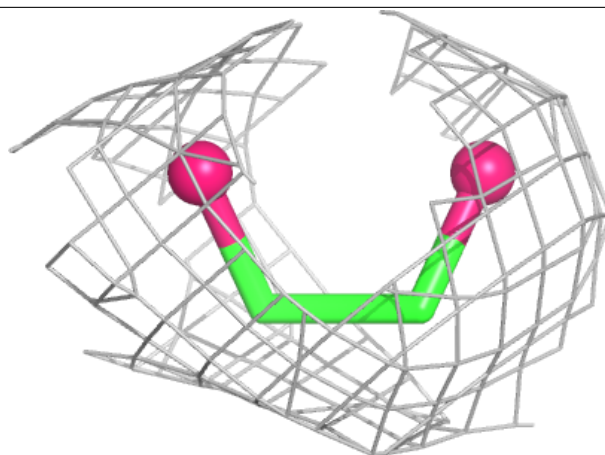
Electron density around GOL B 107:

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

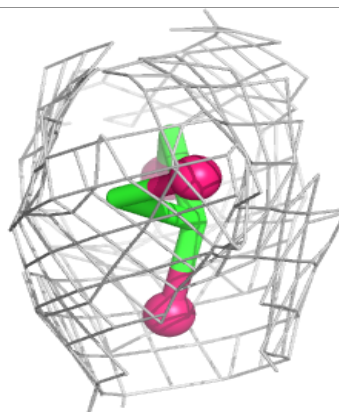
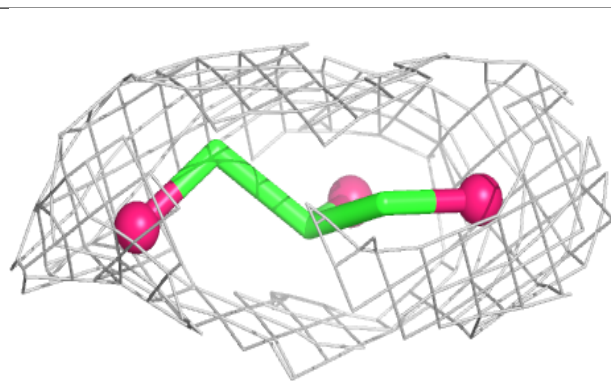
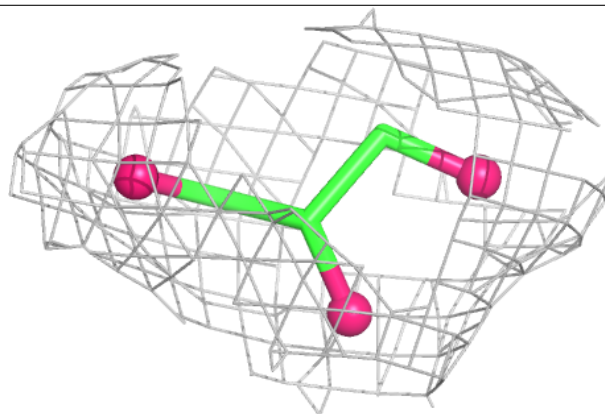


Electron density around EDO A 326:

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

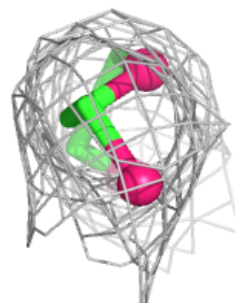
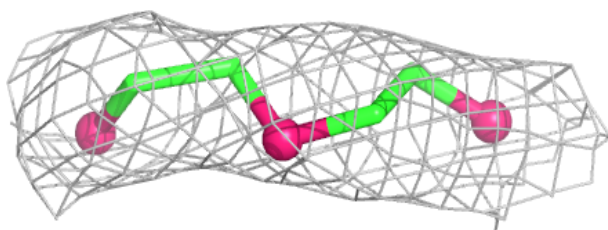
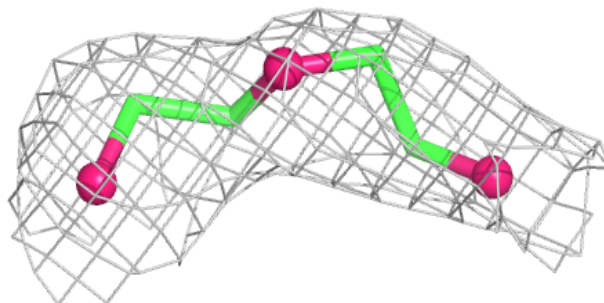
**Electron density around GOL A 345:**

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

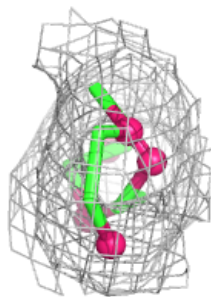
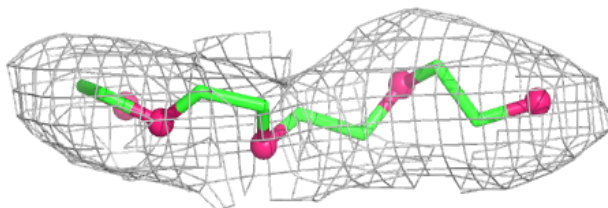


Electron density around PEG E 111:

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

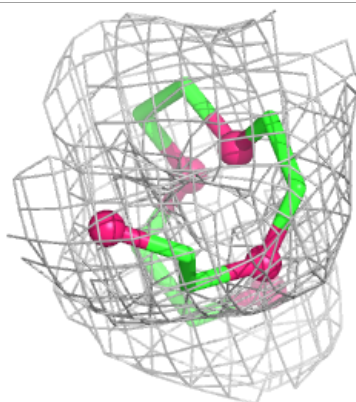
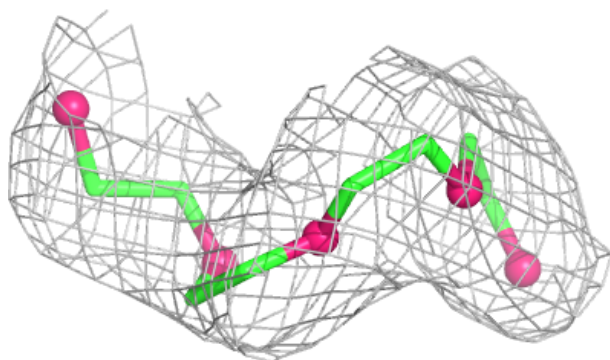
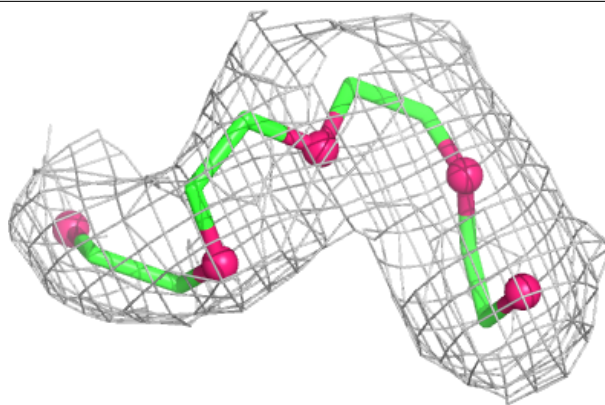
**Electron density around PG4 E 101:**

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

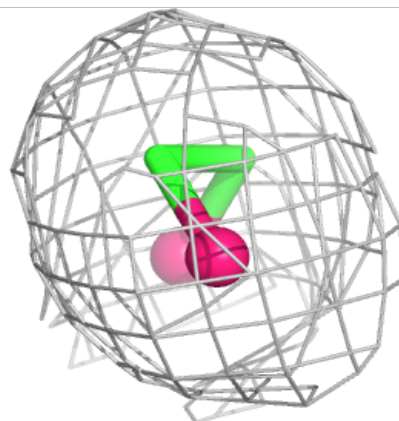
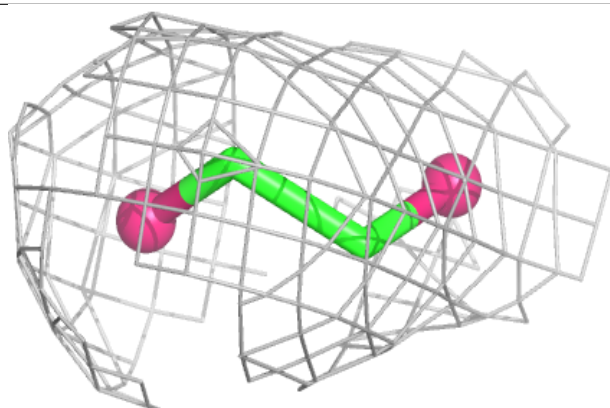
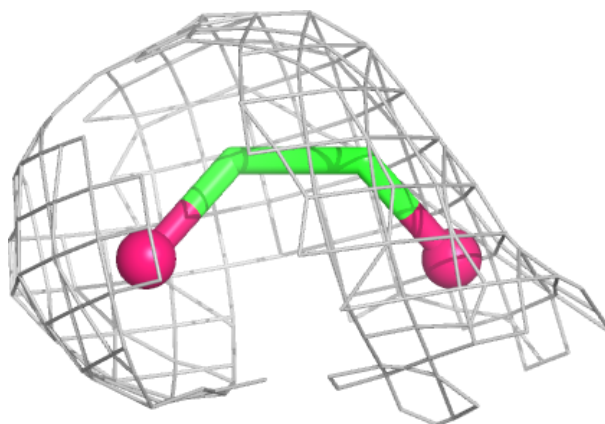


Electron density around PG4 A 334:

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

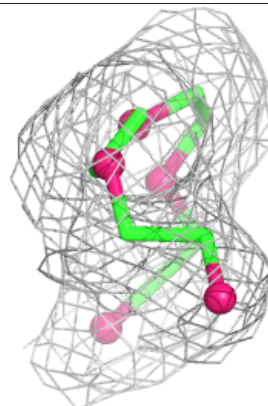
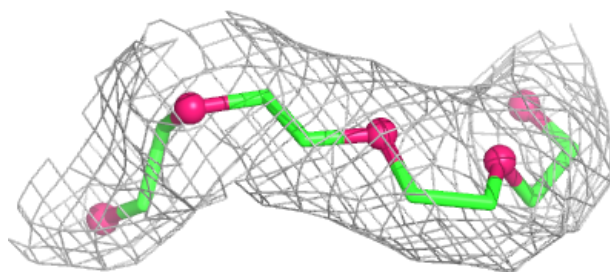
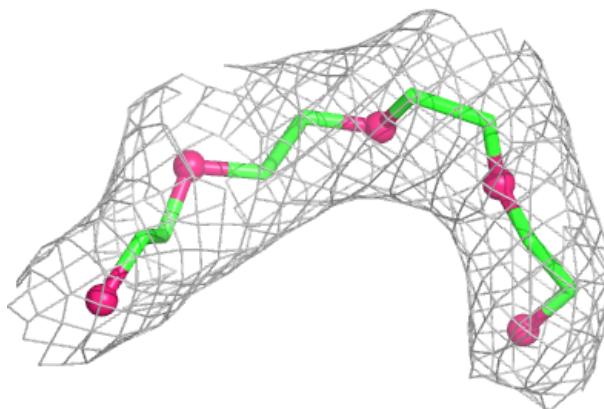
**Electron density around EDO C 323:**

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

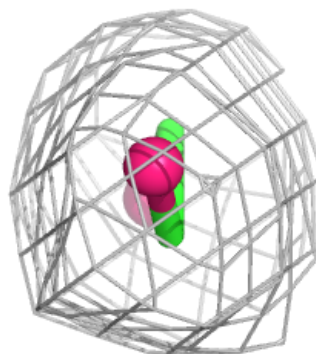
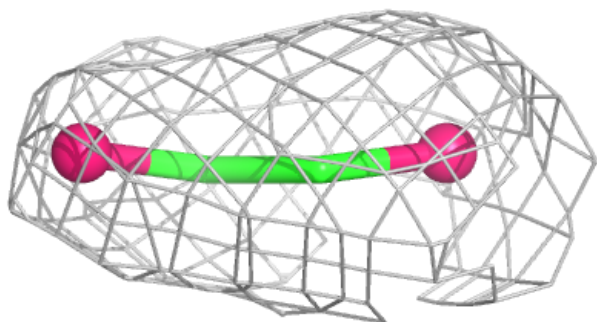
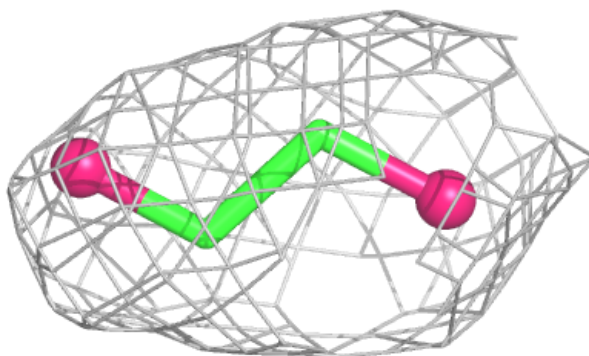


Electron density around PG4 A 344:

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

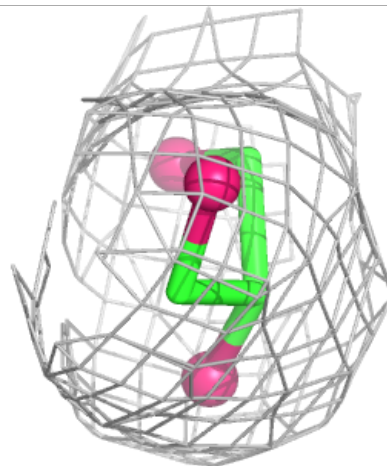
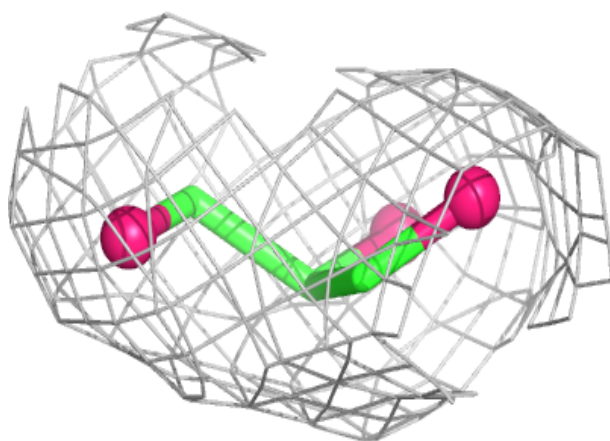
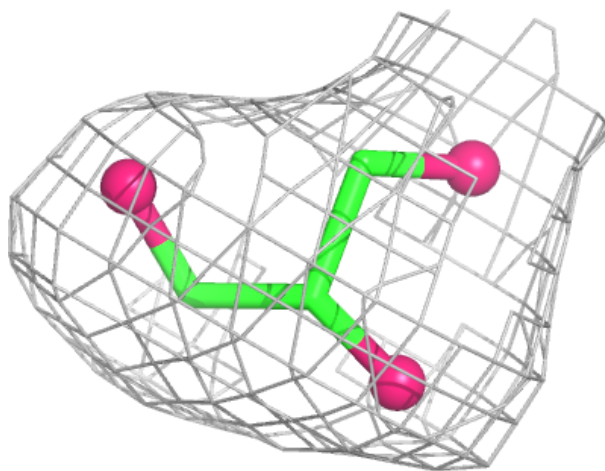
**Electron density around EDO B 124:**

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



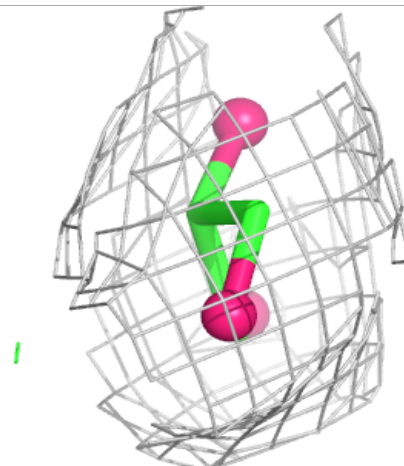
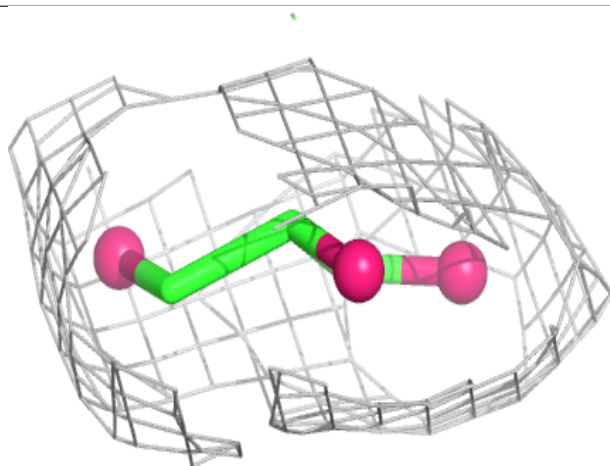
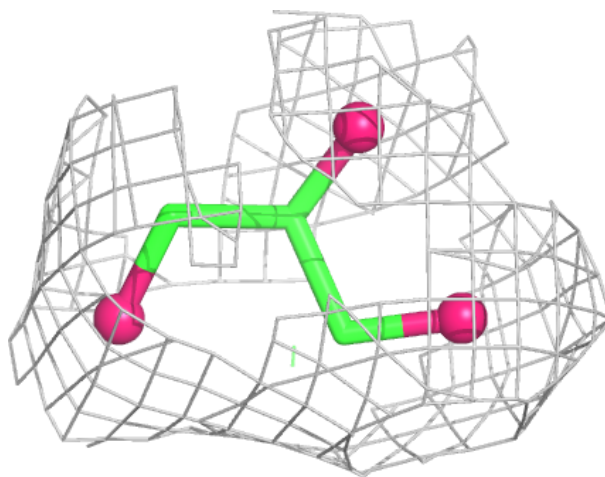
Electron density around GOL C 301:

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



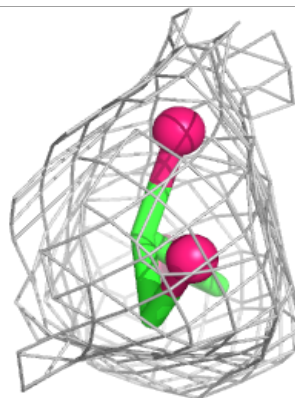
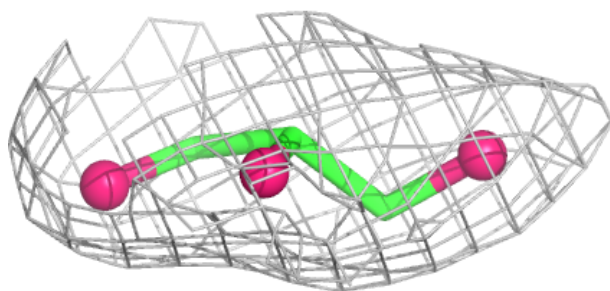
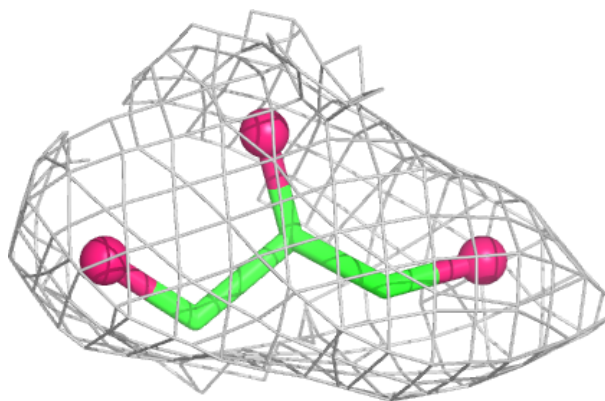
Electron density around GOL A 304:

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



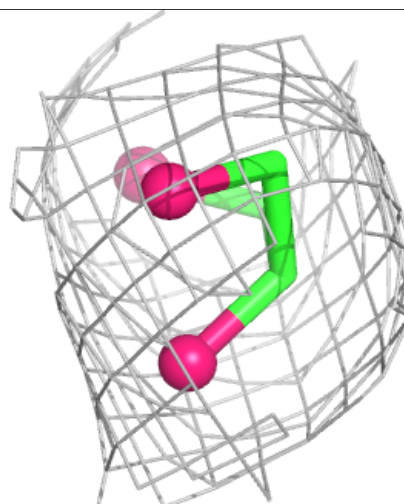
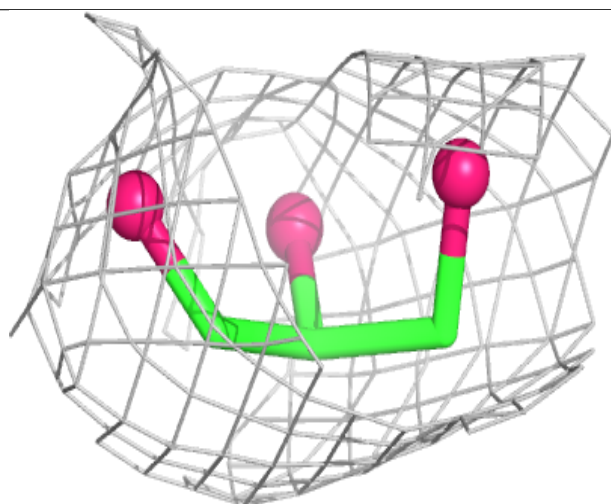
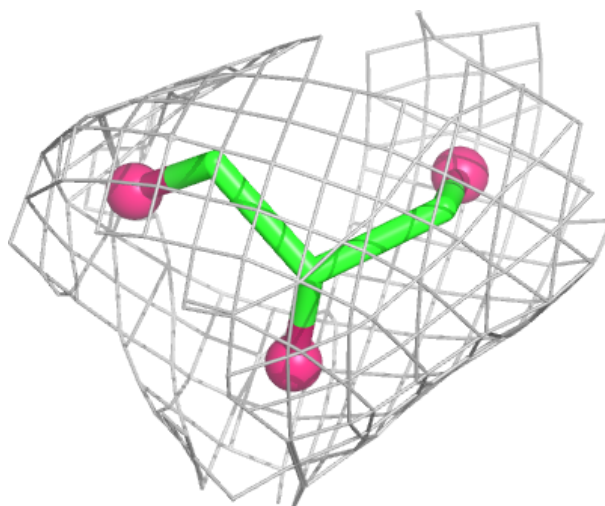
Electron density around GOL A 312:

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



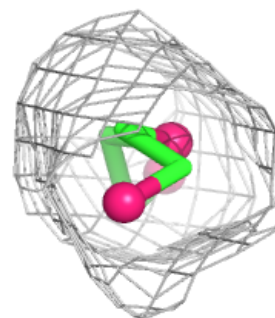
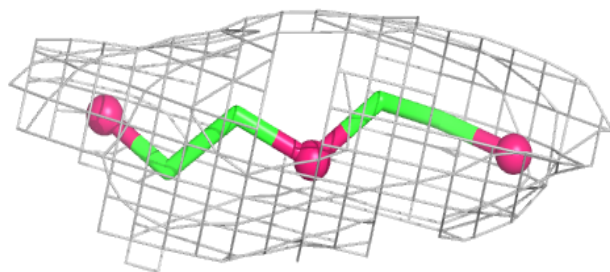
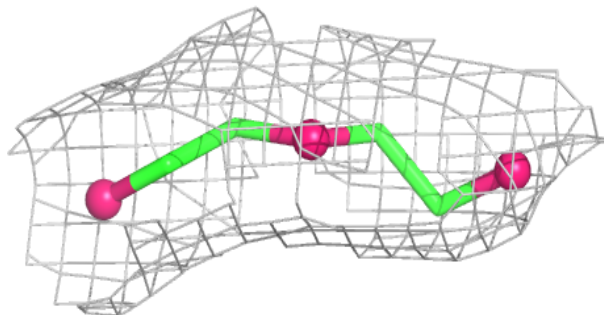
Electron density around GOL B 108:

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

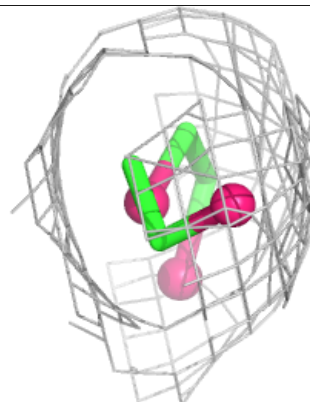
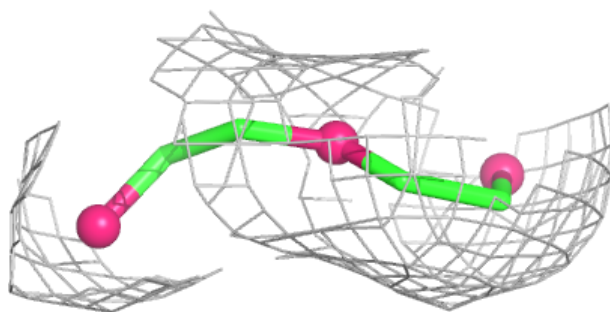
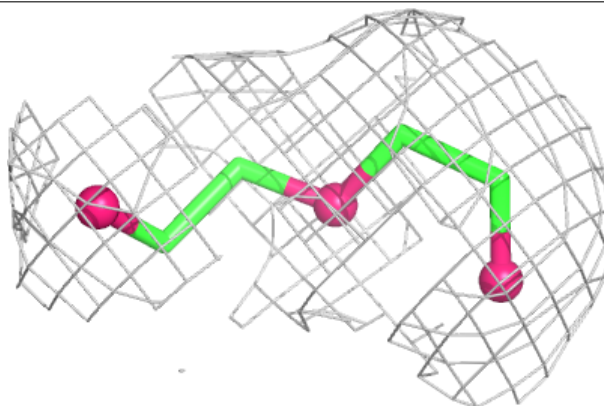


Electron density around PEG E 110:

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

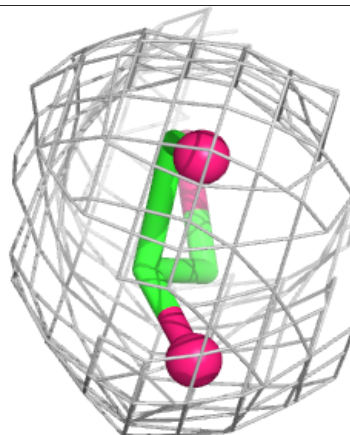
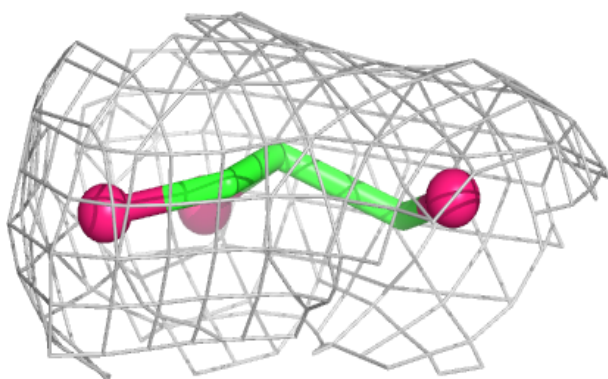
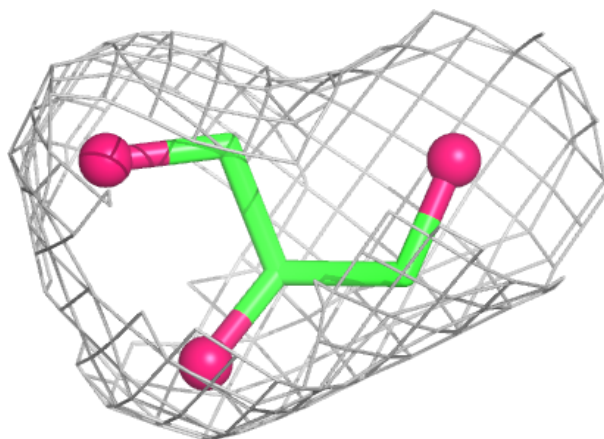
**Electron density around PEG A 318:**

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

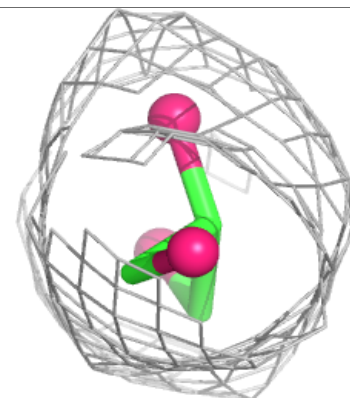
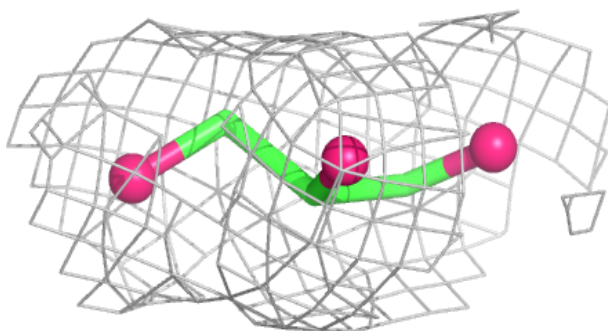
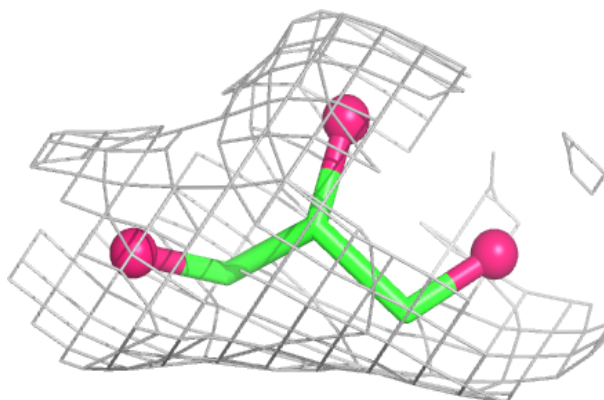


Electron density around GOL A 305:

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

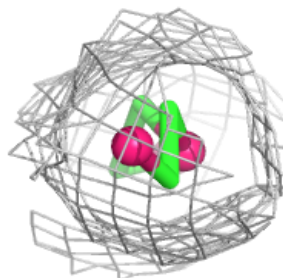
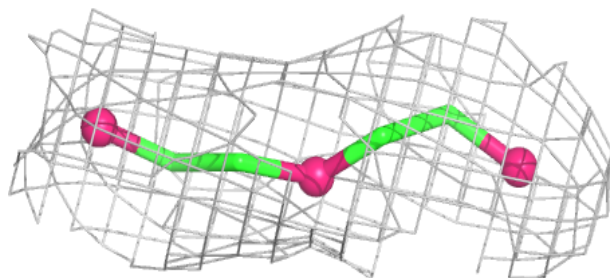
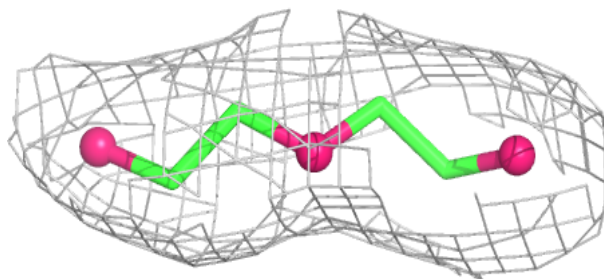
**Electron density around GOL B 132:**

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

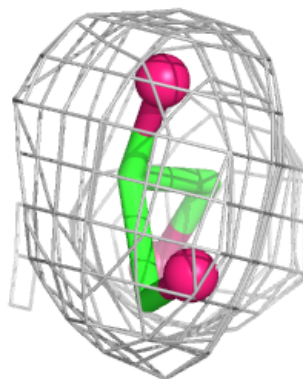
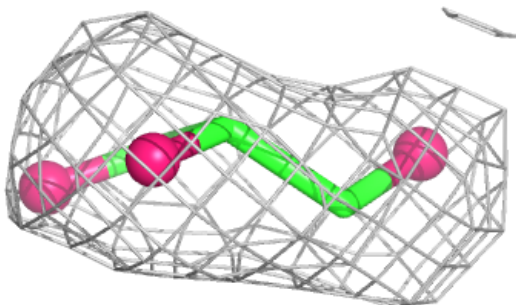
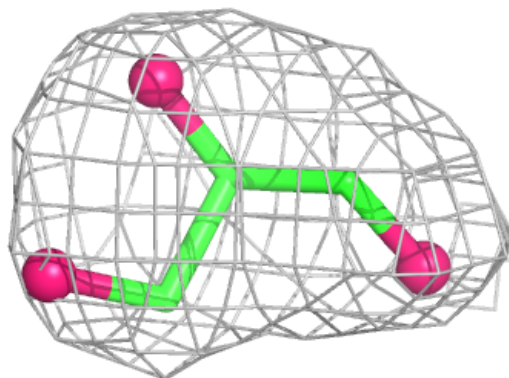


Electron density around PEG A 321:

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

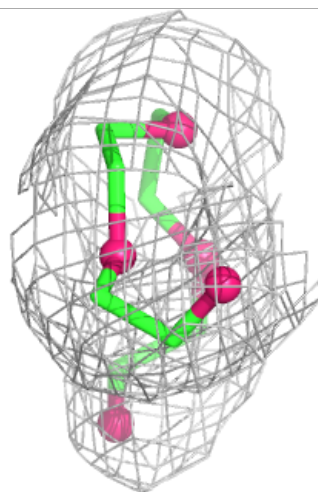
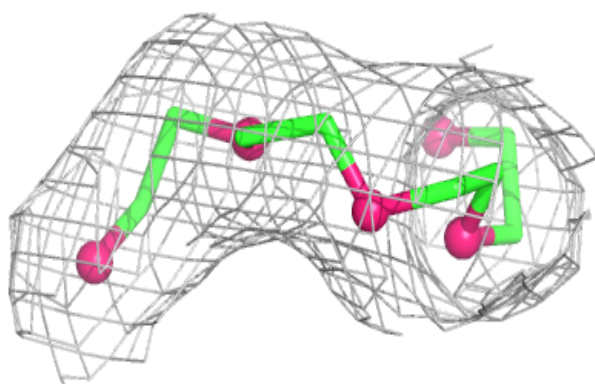
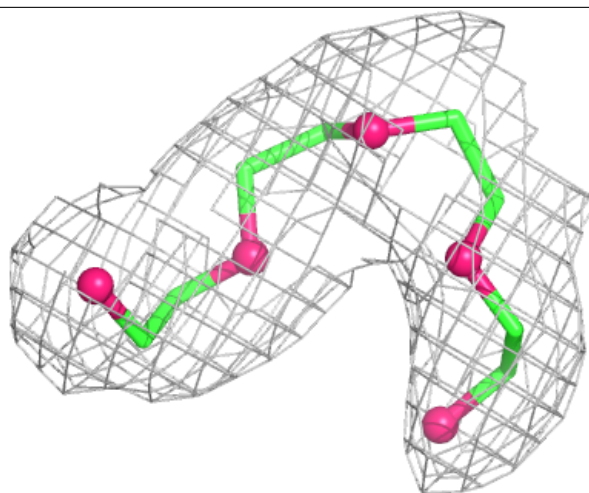
**Electron density around GOL D 103:**

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



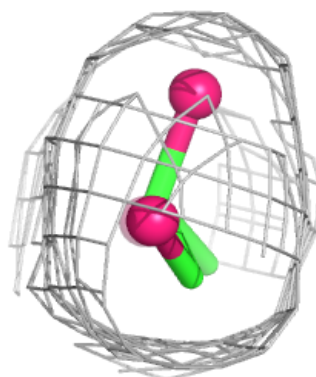
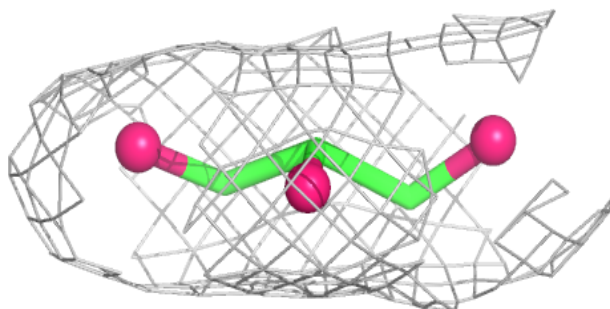
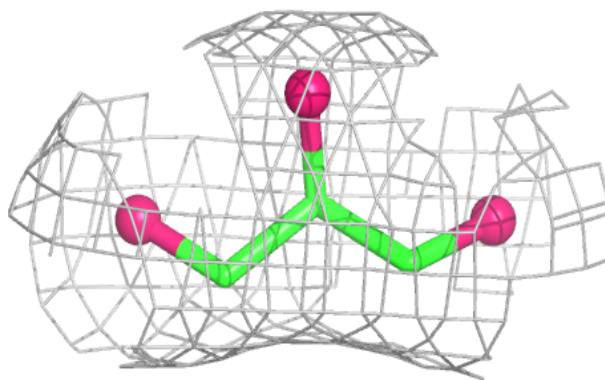
Electron density around PG4 C 337:

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

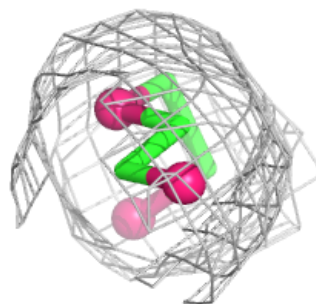
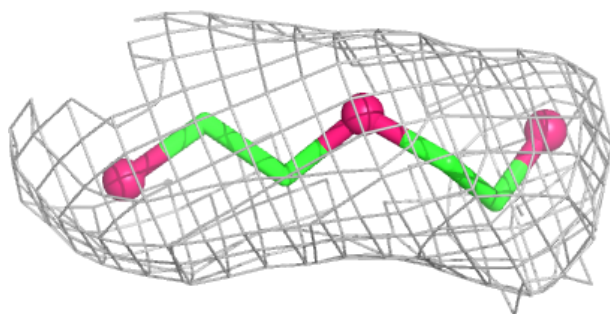
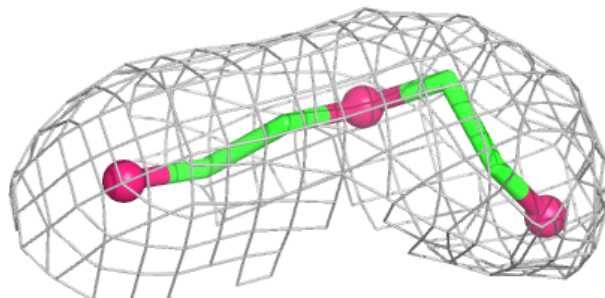


Electron density around GOL A 313:

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

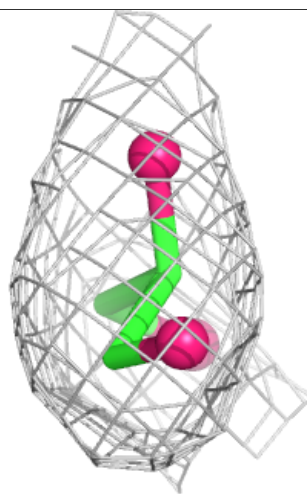
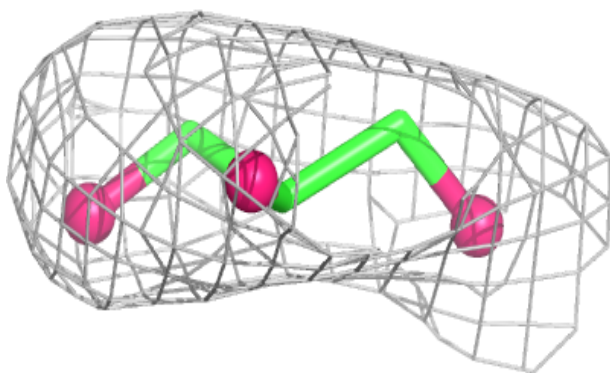
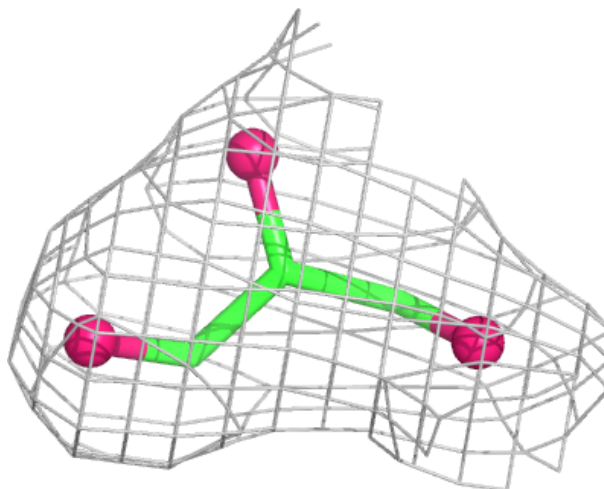
**Electron density around PEG B 139:**

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



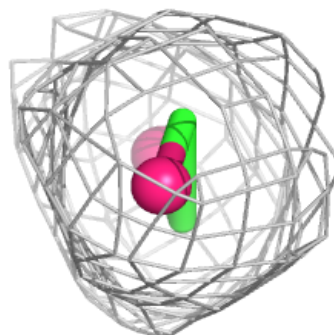
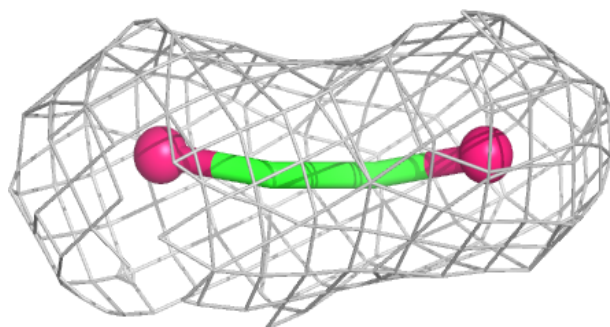
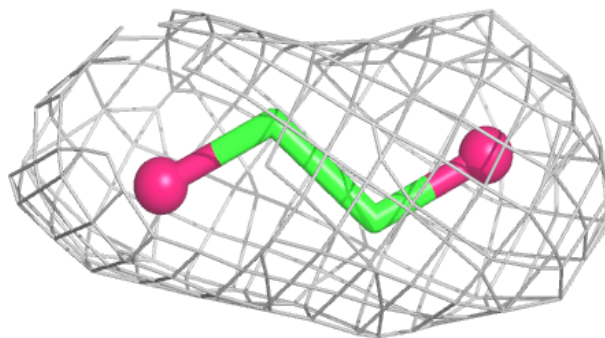
Electron density around GOL E 102:

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

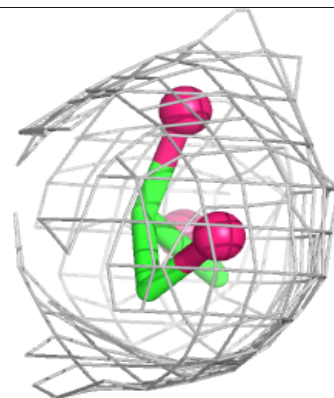
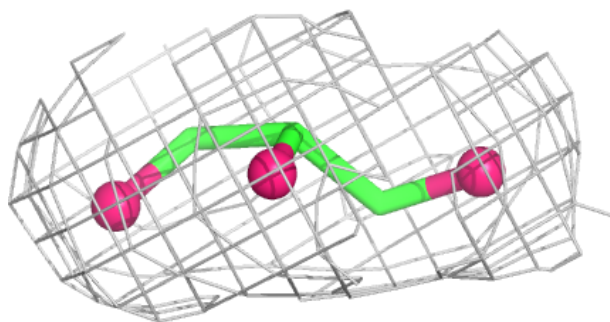
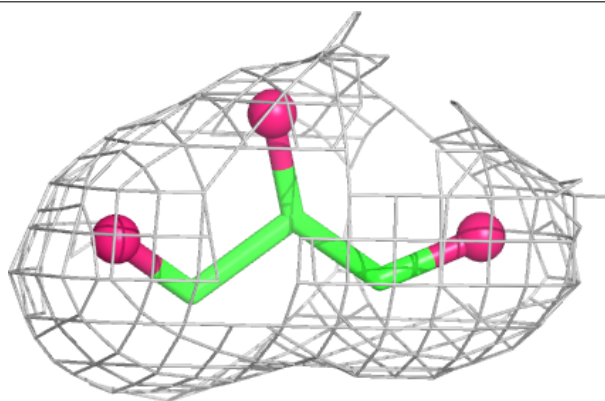


Electron density around EDO B 103:

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

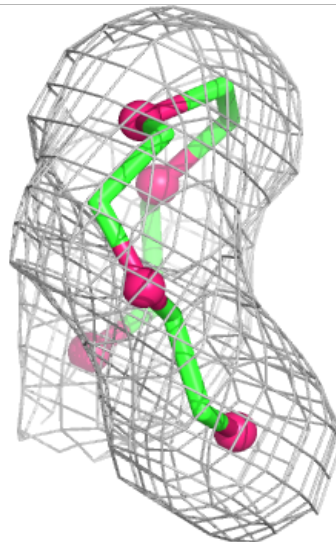
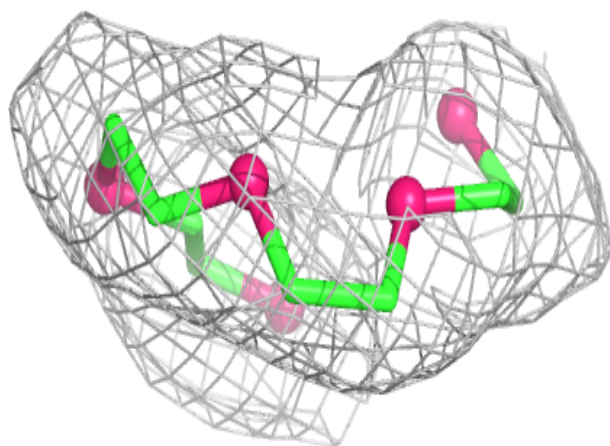
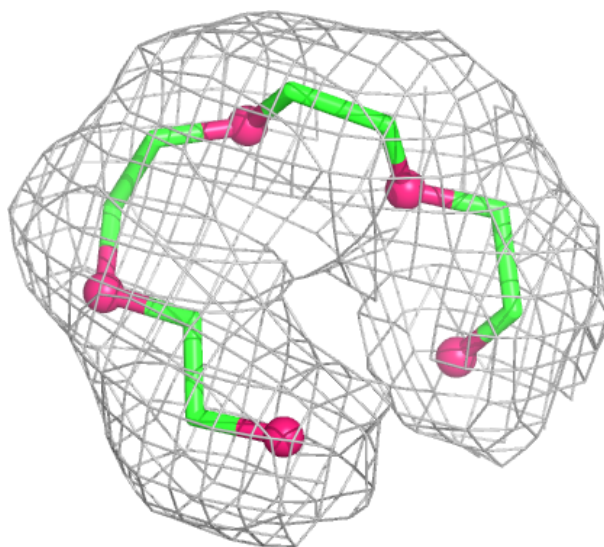
**Electron density around GOL A 340:**

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



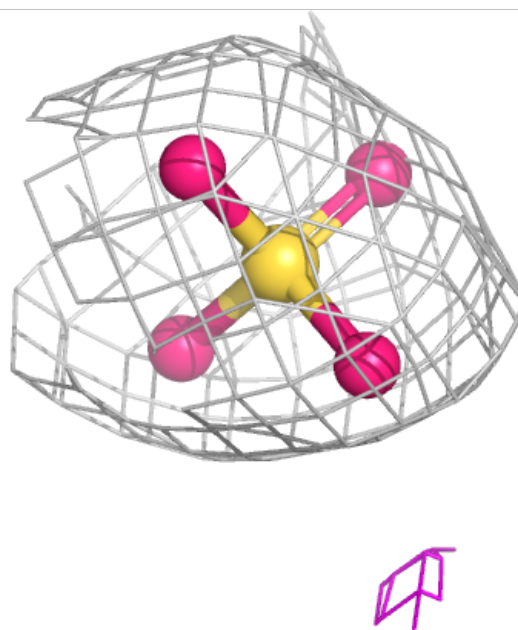
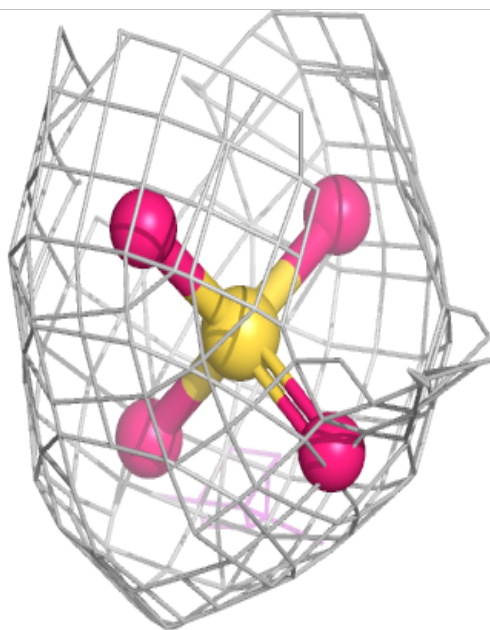
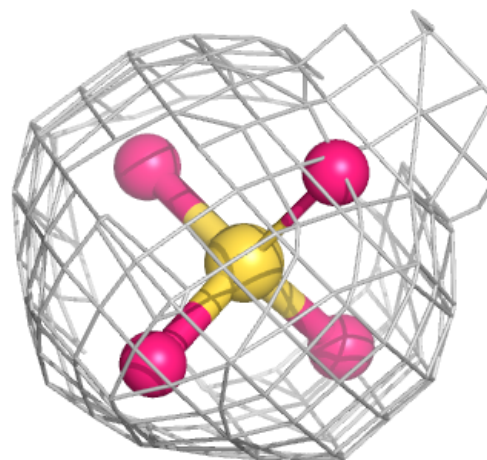
Electron density around PG4 A 333:

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



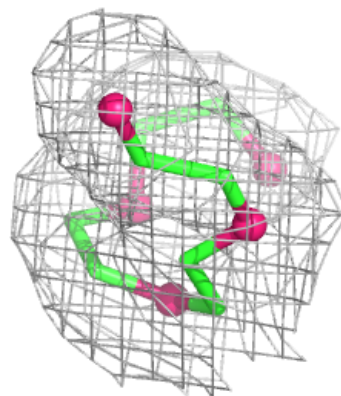
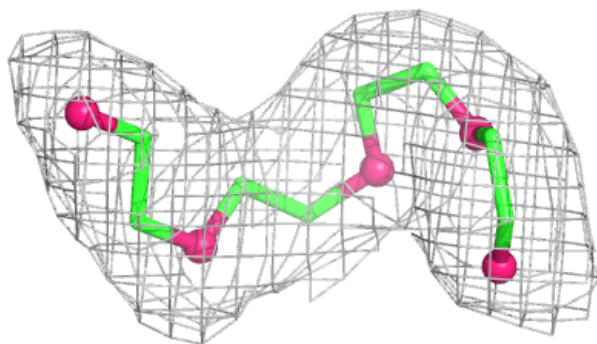
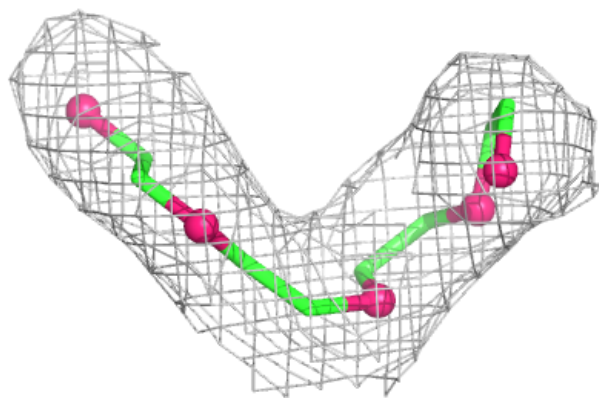
Electron density around SO4 D 114:

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



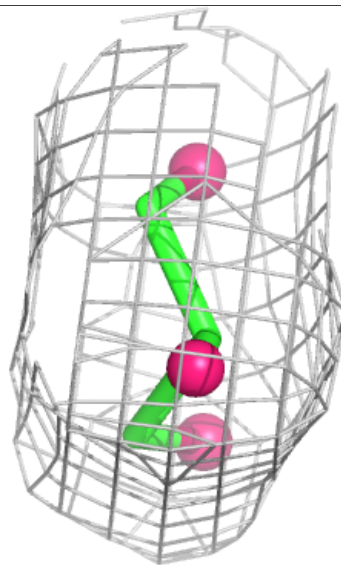
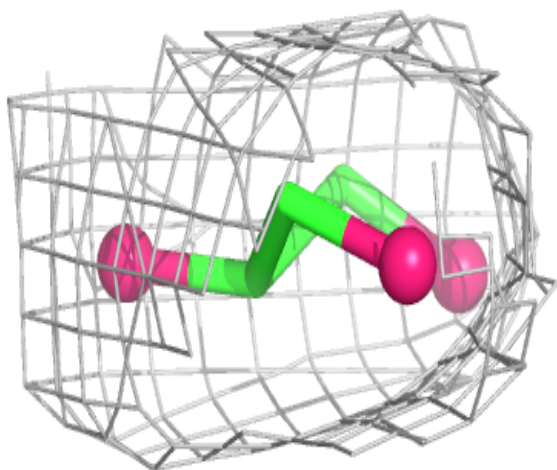
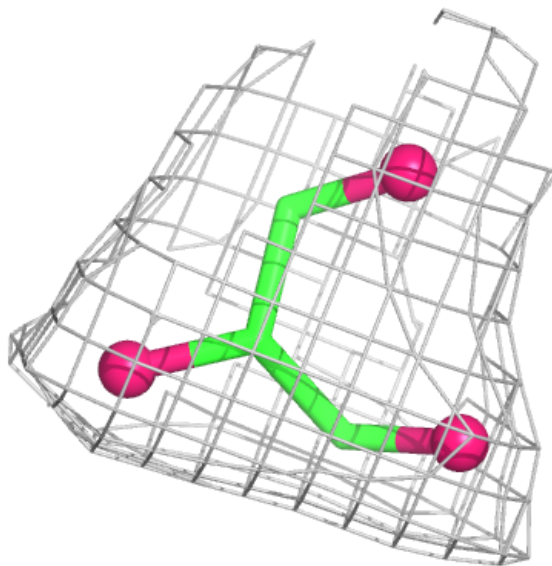
Electron density around PG4 C 326:

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



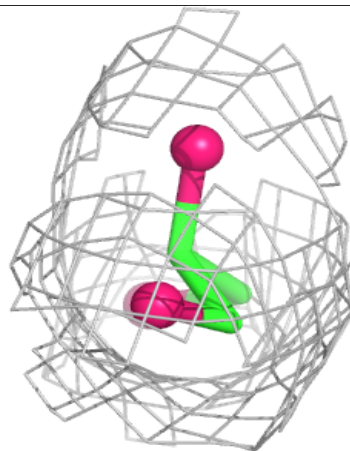
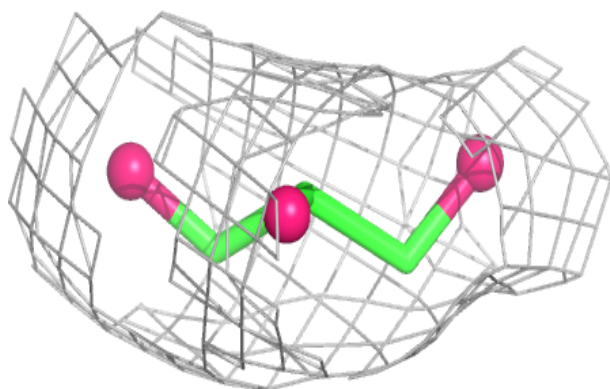
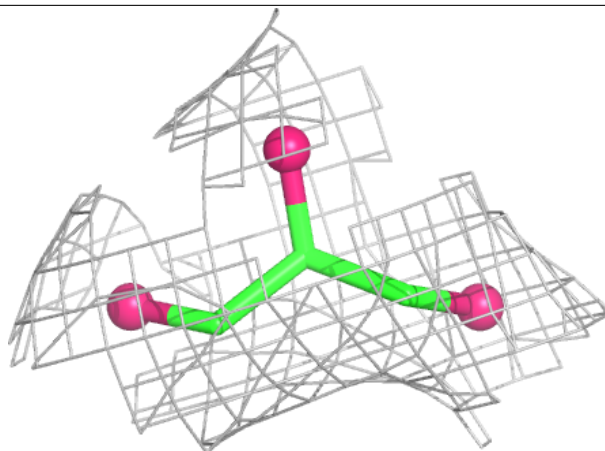
Electron density around GOL E 104:

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



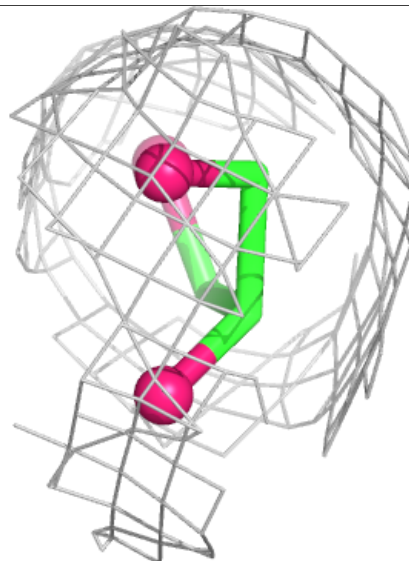
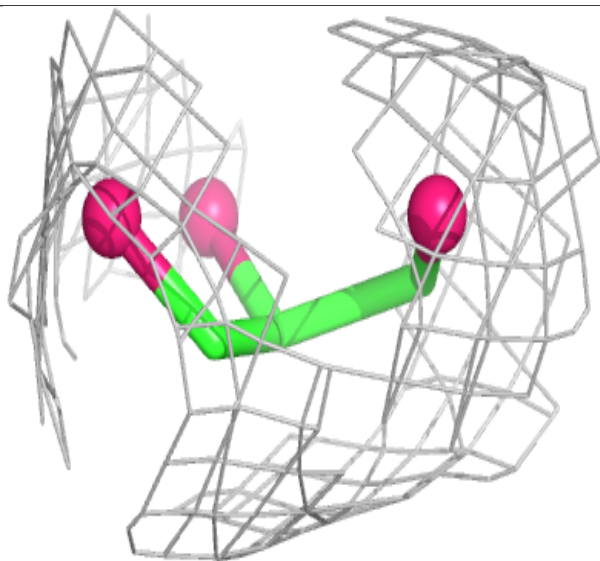
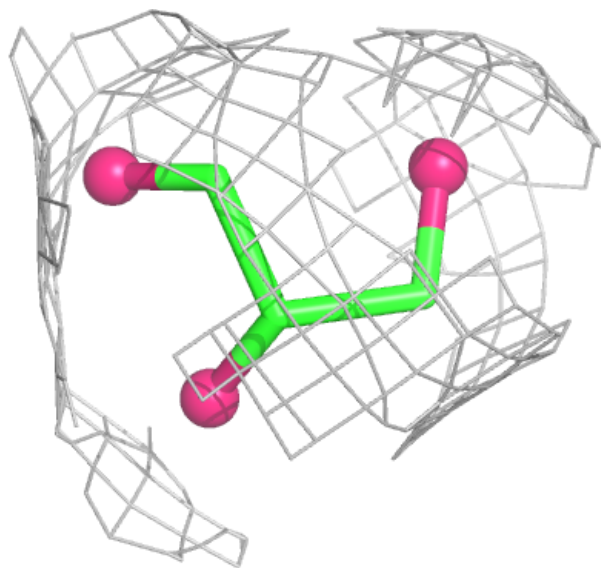
Electron density around GOL C 338:

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



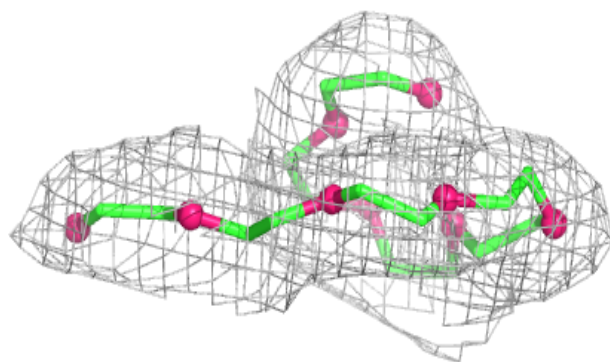
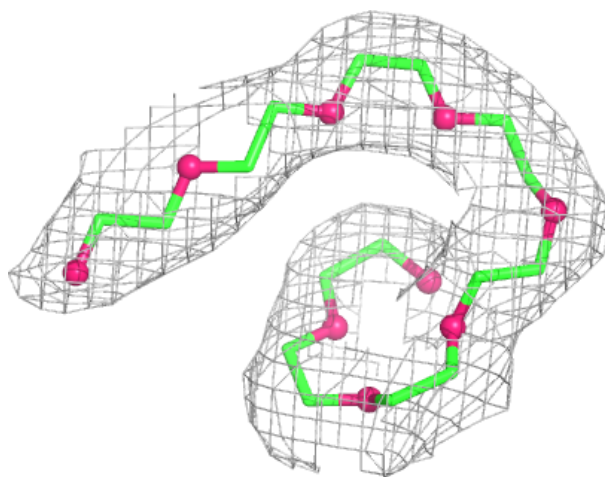
Electron density around GOL A 306:

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



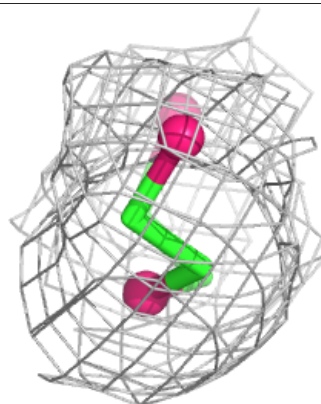
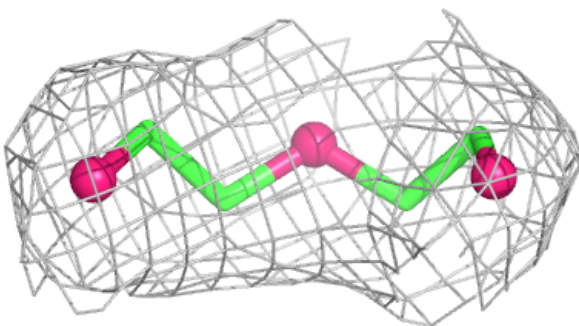
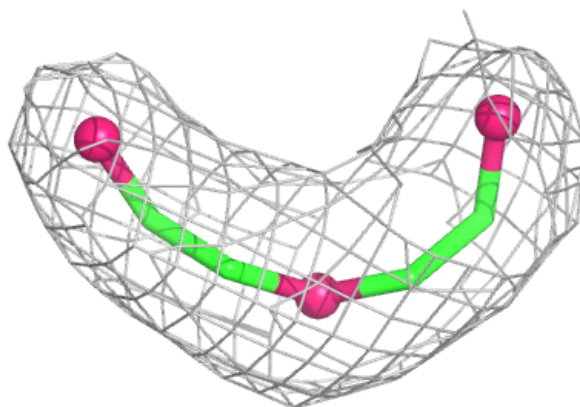
Electron density around PE8 B 121:

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



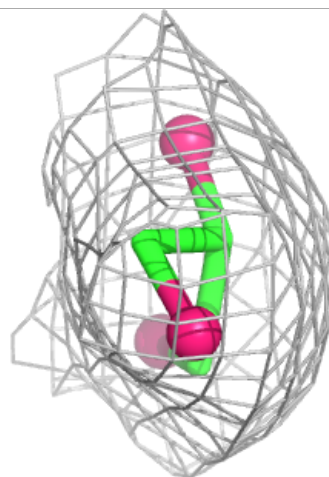
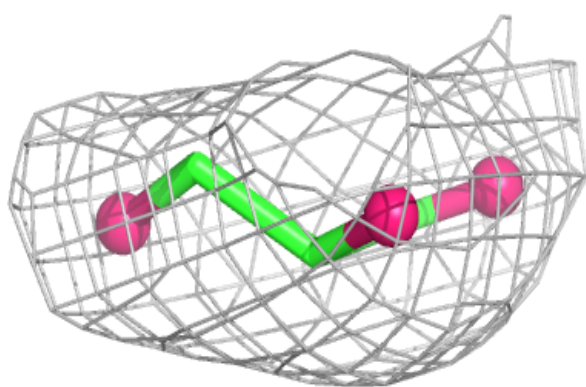
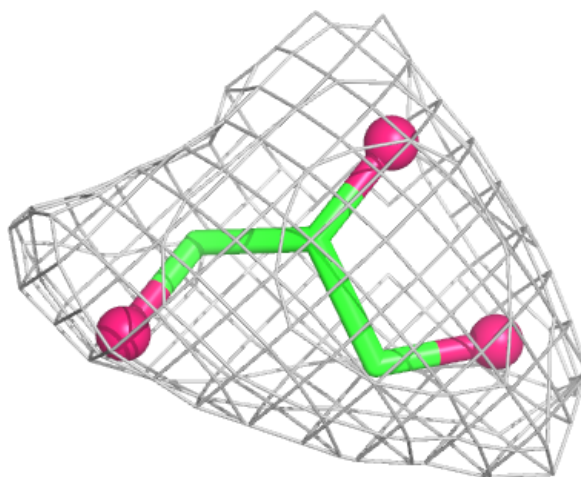
Electron density around PEG C 340:

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



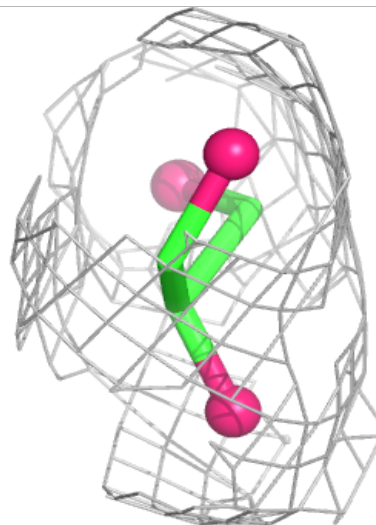
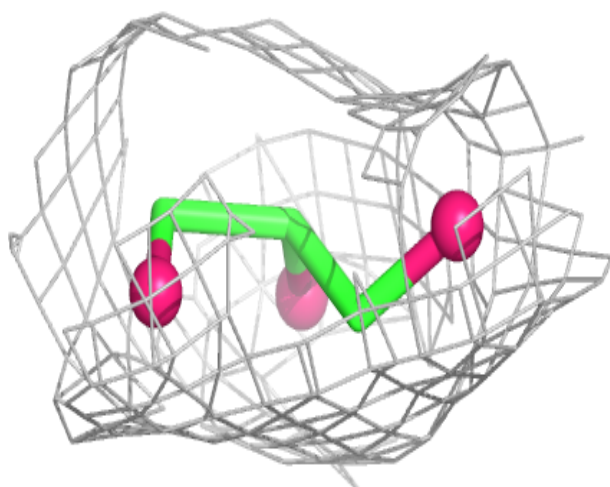
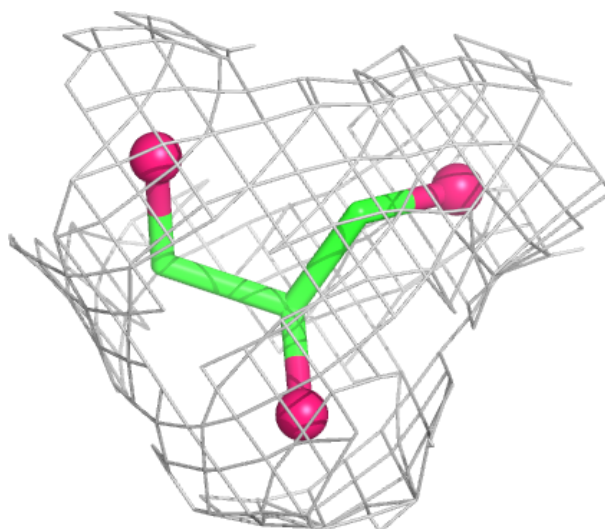
Electron density around GOL A 301:

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



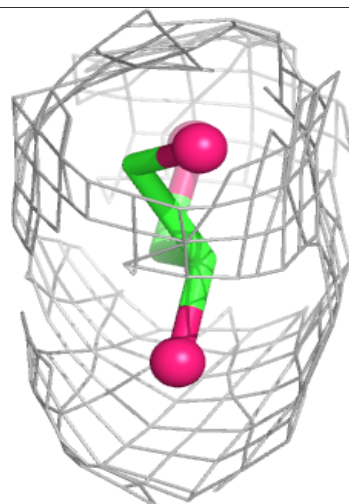
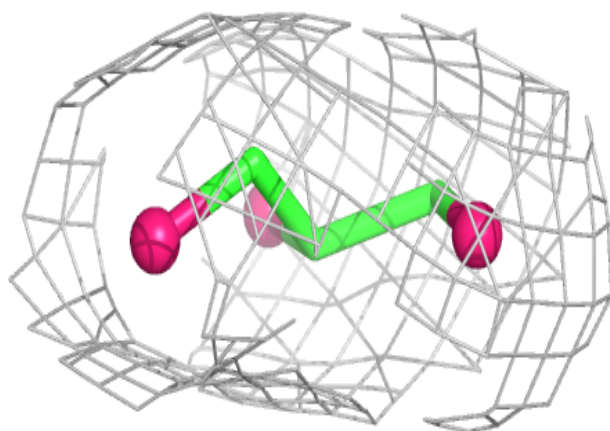
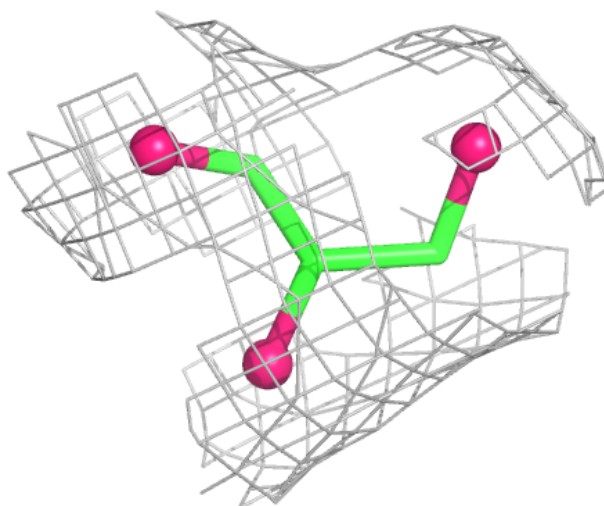
Electron density around GOL B 134:

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



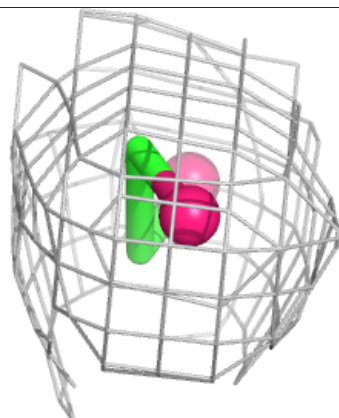
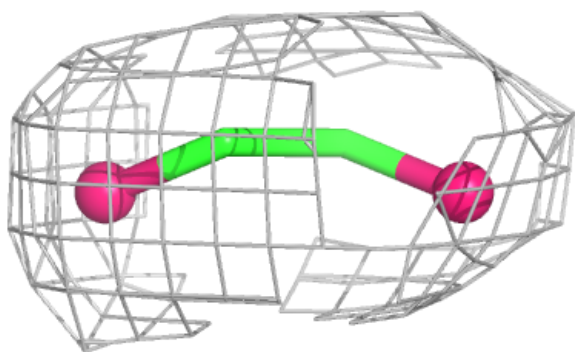
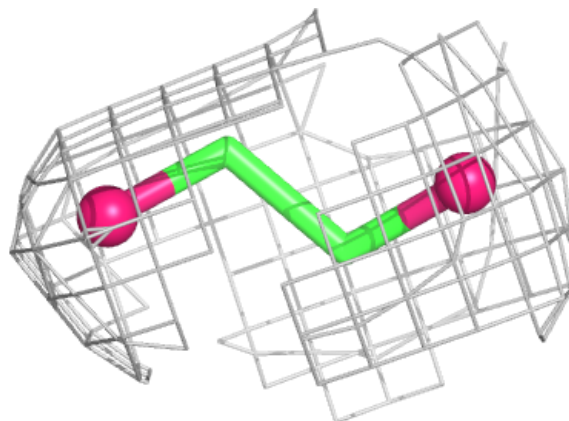
Electron density around GOL A 302:

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



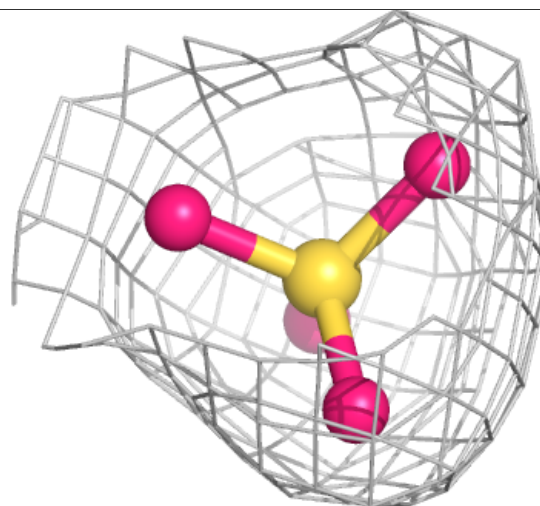
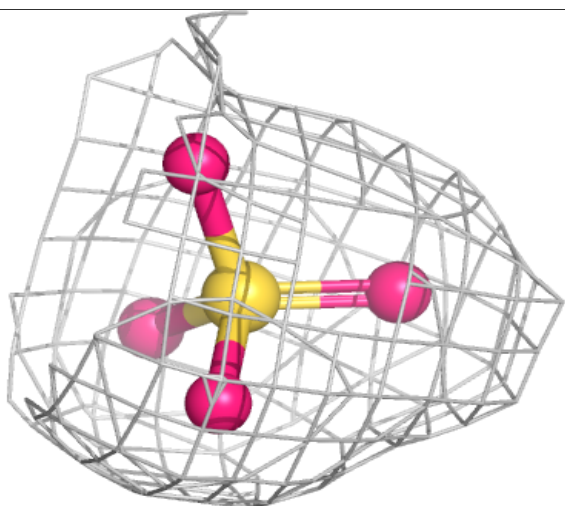
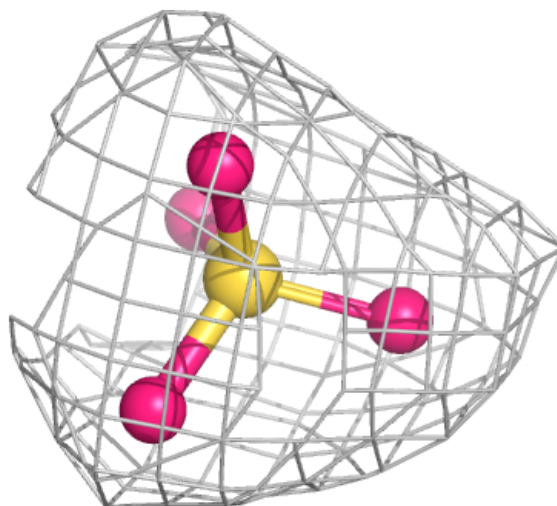
Electron density around EDO A 325:

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



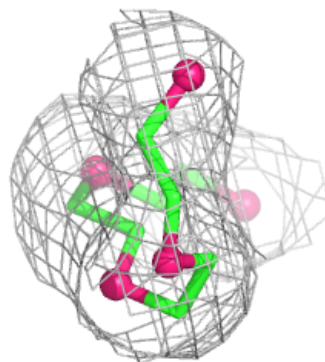
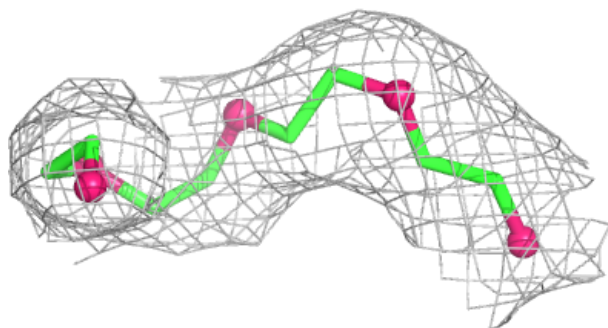
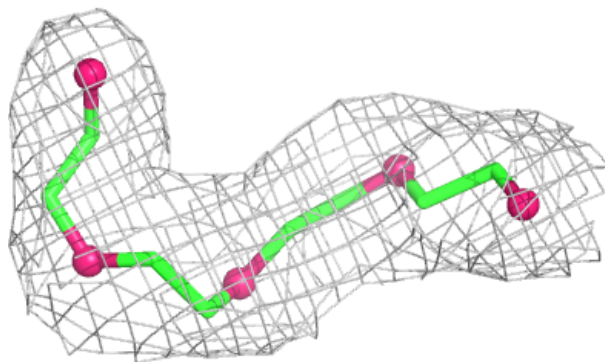
Electron density around SO4 D 126:

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

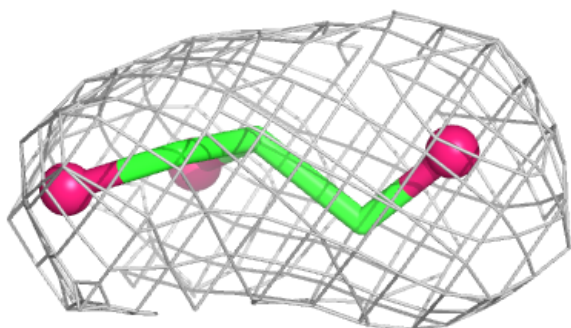
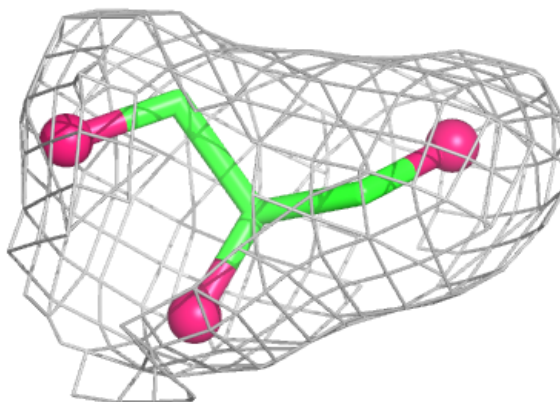


Electron density around PG4 A 329:

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

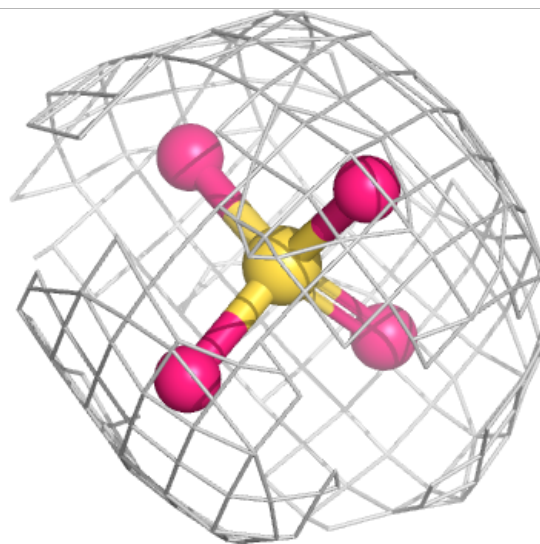
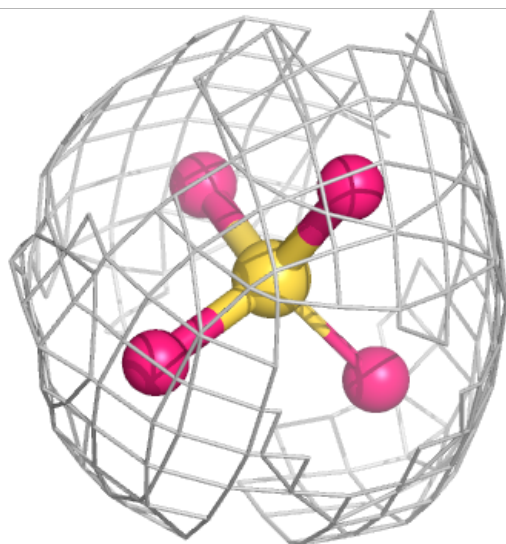
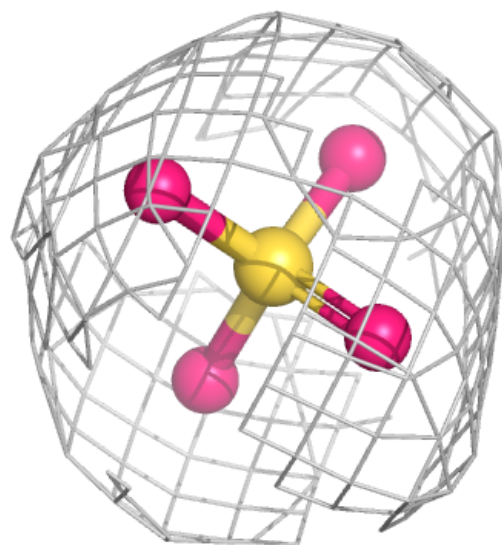
**Electron density around GOL C 341:**

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



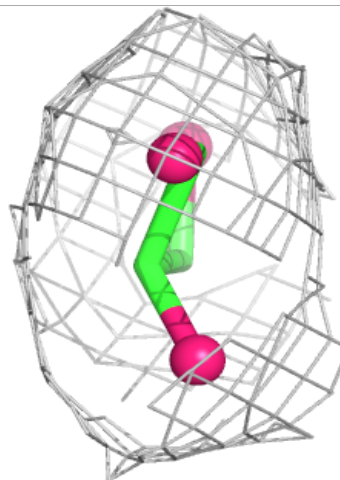
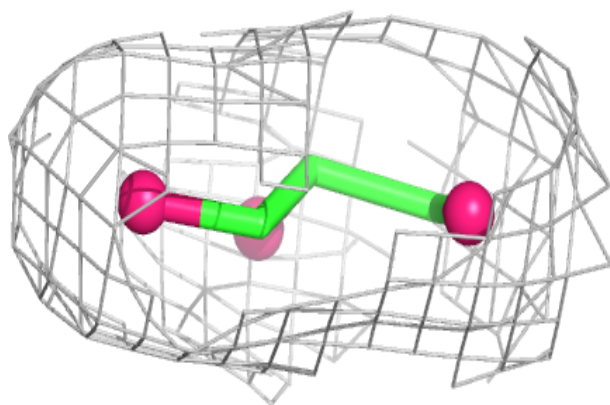
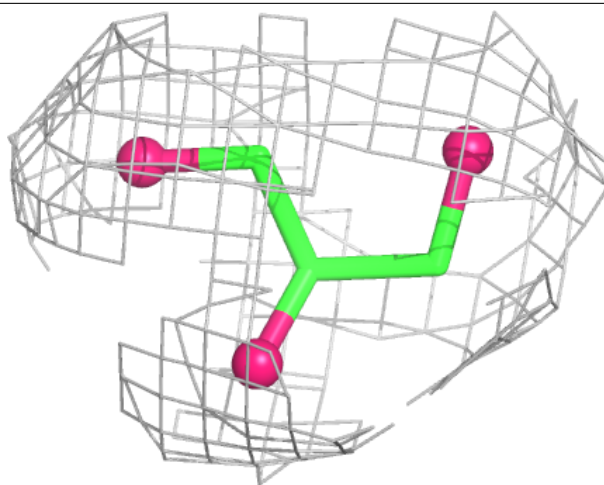
Electron density around SO4 E 107:

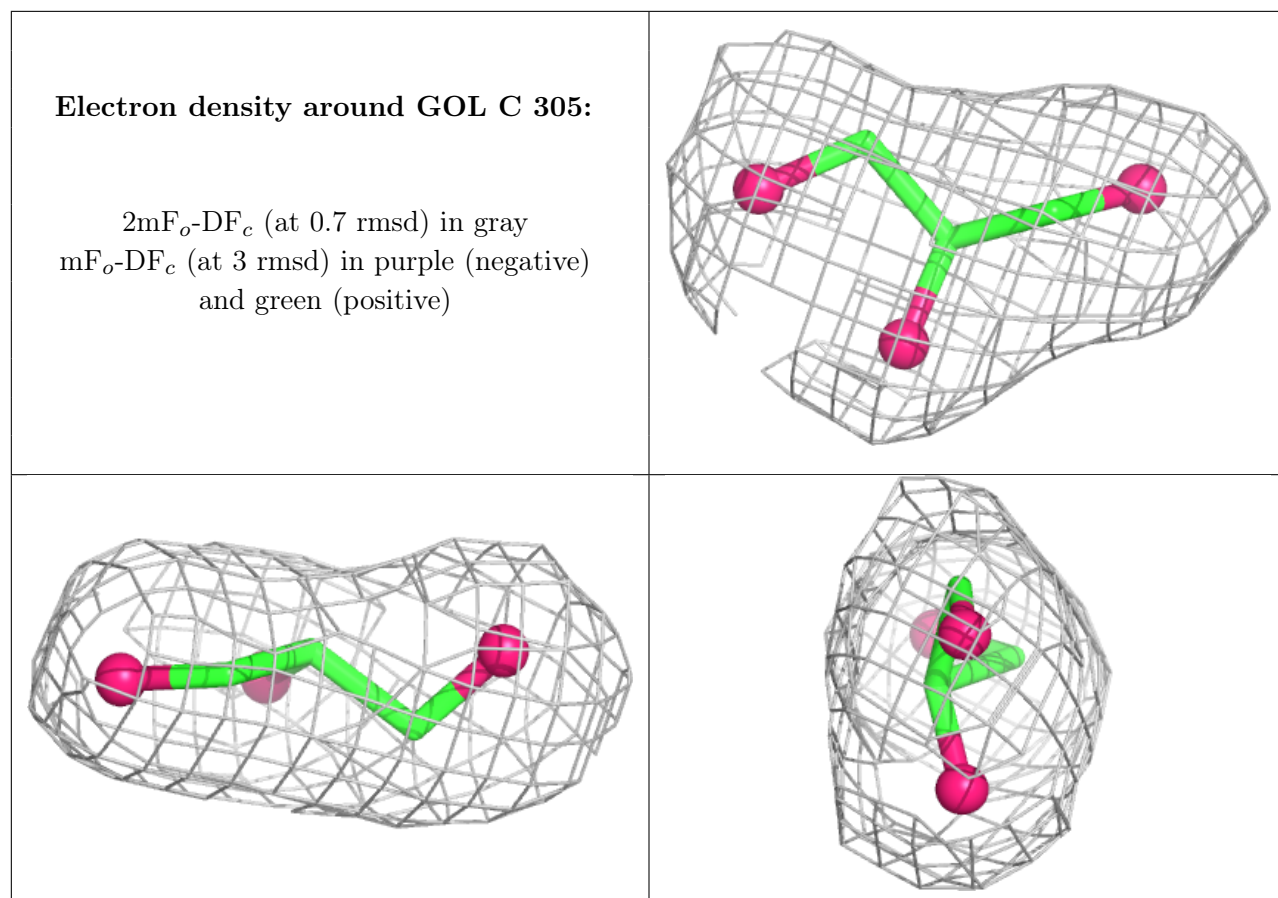
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.