wwPDB Geometry-Only Validation Summary Report

Jun 12, 2024 – 09:57 PM EDT

PDB ID	:	3K2S
Title	:	Solution structure of double super helix model
Authors	:	Wu, Z.; Gogonea, V.; Lee, X.; Wagner, M.A.; Li, X.-M.; Huang, Y.; Undurti, A.; May, R.P.; Haertlein, M.; Moulin, M.; Gutsche, I.; Zaccai, G.; Didonato, J.A.; Hazen, L.S.
Deposited on	:	2009-09-30
Resolution	:	Not provided

This is a wwPDB Geometry-Only Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

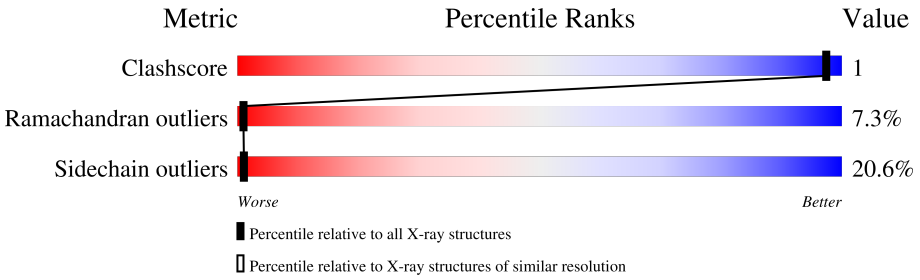
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION SCATTERING

The reported resolution of this entry is unknown.

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))
Clashscore	141614	-
Ramachandran outliers	138981	-
Sidechain outliers	138945	-

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	243	71% 23%
1	B	243	69% 25% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	POV	A	308	X	-	-	-
2	POV	A	316	X	-	-	-
2	POV	A	318	X	-	-	-
2	POV	A	319	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	POV	A	322	X	-	-	-
2	POV	A	326	X	-	-	-
2	POV	A	365	X	-	-	-
2	POV	A	368	X	-	-	-
2	POV	A	378	X	-	-	-
2	POV	A	380	X	-	-	-
2	POV	A	383	X	-	-	-
2	POV	A	385	X	-	-	-
2	POV	A	400	X	-	-	-
2	POV	A	410	X	-	-	-
2	POV	B	303	X	-	-	-
2	POV	B	321	X	-	-	-
2	POV	B	328	X	-	-	-
2	POV	B	329	X	-	-	-
2	POV	B	330	X	-	-	-
2	POV	B	346	X	-	-	-
2	POV	B	347	X	-	-	-
2	POV	B	362	X	-	-	-
2	POV	B	364	X	-	-	-
2	POV	B	367	X	-	-	-

2 Entry composition (i)

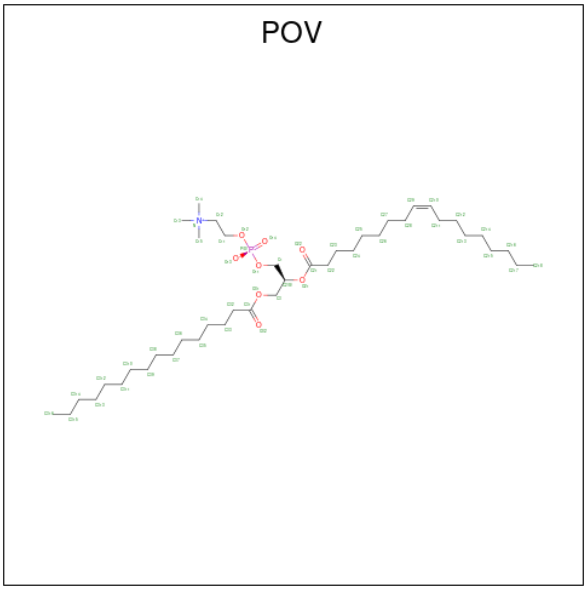
There are 3 unique types of molecules in this entry. The entry contains 14920 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Apolipoprotein A-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1980	1241	347	389	3			
1	B	243	Total	C	N	O	S	0	0	0
			1980	1241	347	389	3			

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	A	1	Total	C	N	O	P	0	0
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2	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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2	A	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0
2	B	1	Total 52	C 42	N 1	O 8	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
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2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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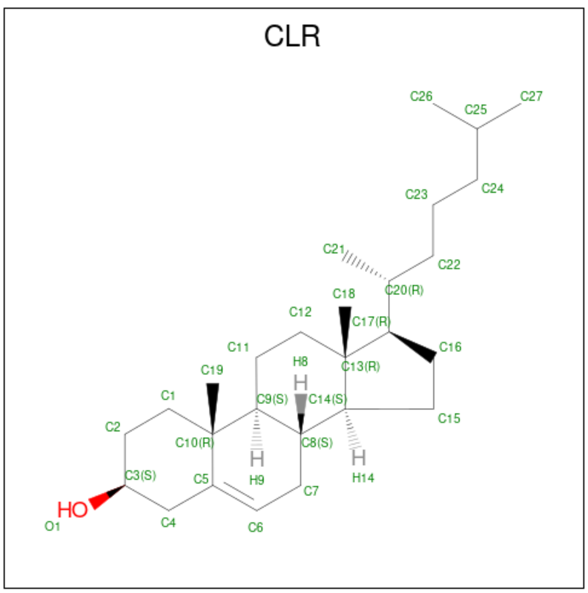
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O P 52 42 1 8 1	0	0
2	B	1	Total C N O P 52 42 1 8 1	0	0
2	B	1	Total C N O P 52 42 1 8 1	0	0
2	B	1	Total C N O P 52 42 1 8 1	0	0
2	B	1	Total C N O P 52 42 1 8 1	0	0
2	B	1	Total C N O P 52 42 1 8 1	0	0
2	B	1	Total C N O P 52 42 1 8 1	0	0

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 28 27 1	0	0
3	A	1	Total C O 28 27 1	0	0
3	A	1	Total C O 28 27 1	0	0
3	A	1	Total C O 28 27 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 28 27 1	0	0
3	A	1	Total C O 28 27 1	0	0
3	A	1	Total C O 28 27 1	0	0
3	A	1	Total C O 28 27 1	0	0
3	A	1	Total C O 28 27 1	0	0
3	A	1	Total C O 28 27 1	0	0
3	B	1	Total C O 28 27 1	0	0
3	B	1	Total C O 28 27 1	0	0
3	B	1	Total C O 28 27 1	0	0
3	B	1	Total C O 28 27 1	0	0
3	B	1	Total C O 28 27 1	0	0
3	B	1	Total C O 28 27 1	0	0
3	B	1	Total C O 28 27 1	0	0
3	B	1	Total C O 28 27 1	0	0
3	B	1	Total C O 28 27 1	0	0
3	B	1	Total C O 28 27 1	0	0

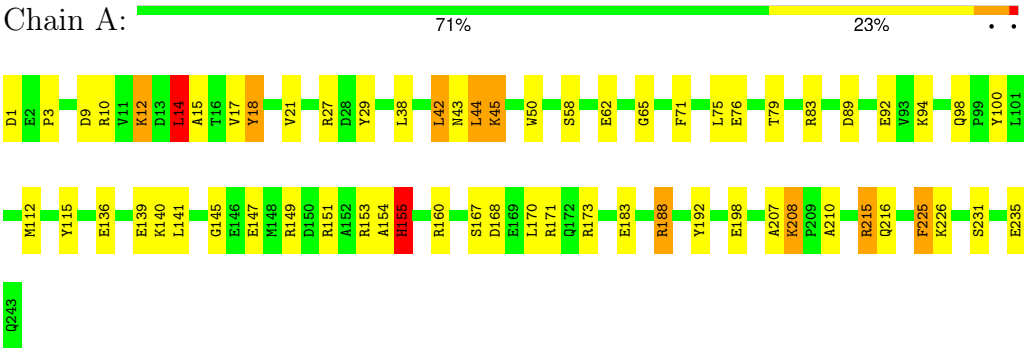
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

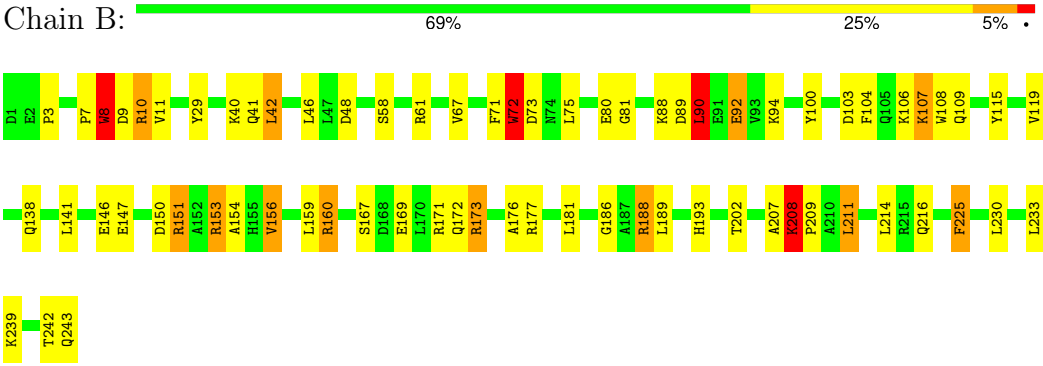
• Molecule 1: Apolipoprotein A-I

Chain A:



• Molecule 1: Apolipoprotein A-I

Chain B:



4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, POV

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	0.82	0/2015	1.35	20/2714 (0.7%)
1	B	0.82	0/2015	1.35	12/2714 (0.4%)
All	All	0.82	0/4030	1.35	32/5428 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	9
All	All	0	14

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	188	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	A	149	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	8	TRP	O-C-N	-7.79	110.24	122.70
1	B	151	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	B	8	TRP	CB-CG-CD2	7.20	135.96	126.60

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	167	SER	Peptide
1	A	168	ASP	Peptide
1	A	236	TYR	Peptide
1	A	237	THR	Peptide

4.2 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	1980	0	1968	8	0
1	B	1980	0	1968	9	0
2	A	5772	0	9102	5	0
2	B	4628	0	7298	12	0
3	A	280	0	460	2	0
3	B	280	0	460	1	0
All	All	14920	0	21256	27	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 1.

The worst 5 of 27 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LYS:HB3	1:A:15:ALA:HB2	1.82	0.62
1:A:44:LEU:HD12	1:A:45:LYS:H	1.67	0.60
1:B:115:TYR:CE1	1:B:119:VAL:HG21	2.37	0.60
1:A:12:LYS:CB	1:A:15:ALA:HB2	2.37	0.54
1:A:210:ALA:HB1	3:A:402:CLR:H181	1.91	0.52

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	241/243 (99%)	192 (80%)	37 (15%)	12 (5%)	2 2
1	B	241/243 (99%)	181 (75%)	37 (15%)	23 (10%)	0 0
All	All	482/486 (99%)	373 (77%)	74 (15%)	35 (7%)	1 1

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	B	8	TRP
1	B	10	ARG
1	B	160	ARG
1	B	172	GLN

4.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	214/214 (100%)	171 (80%)	43 (20%)	1 1
1	B	214/214 (100%)	169 (79%)	45 (21%)	1 1
All	All	428/428 (100%)	340 (79%)	88 (21%)	1 1

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	94	LYS

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Mol	Chain	Res	Type
1	B	171	ARG
1	B	104	PHE
1	B	138	GLN
1	B	189	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	GLN

4.3.3 RNA (i)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

220 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	POV	A	366	-	51,51,51	0.88	2 (3%)	57,59,59	0.78	2 (3%)
2	POV	A	396	-	51,51,51	0.84	2 (3%)	57,59,59	0.56	0
3	CLR	A	405	-	31,31,31	0.81	0	48,48,48	0.88	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	POV	B	341	-	51,51,51	0.97	2 (3%)	57,59,59	0.69	1 (1%)
2	POV	A	345	-	51,51,51	0.92	2 (3%)	57,59,59	0.67	1 (1%)
2	POV	A	353	-	51,51,51	0.89	2 (3%)	57,59,59	0.60	1 (1%)
3	CLR	A	402	-	31,31,31	0.81	0	48,48,48	1.34	6 (12%)
2	POV	B	317	-	51,51,51	0.88	2 (3%)	57,59,59	0.64	1 (1%)
2	POV	B	353	-	51,51,51	0.87	2 (3%)	57,59,59	0.76	2 (3%)
2	POV	A	415	-	51,51,51	0.88	3 (5%)	57,59,59	0.54	0
2	POV	A	392	-	51,51,51	0.91	2 (3%)	57,59,59	0.48	0
2	POV	B	326	-	51,51,51	0.89	2 (3%)	57,59,59	0.64	1 (1%)
3	CLR	B	394	-	31,31,31	0.89	1 (3%)	48,48,48	1.00	2 (4%)
2	POV	B	328	-	51,51,51	0.92	2 (3%)	57,59,59	0.51	0
2	POV	B	342	-	51,51,51	0.92	2 (3%)	57,59,59	0.57	0
2	POV	B	309	-	51,51,51	0.87	2 (3%)	57,59,59	0.67	0
2	POV	A	383	-	51,51,51	0.93	2 (3%)	57,59,59	0.51	0
2	POV	B	330	-	51,51,51	0.91	2 (3%)	57,59,59	0.51	0
2	POV	A	317	-	51,51,51	0.93	2 (3%)	57,59,59	0.51	0
2	POV	B	305	-	51,51,51	0.89	2 (3%)	57,59,59	0.53	0
2	POV	A	338	-	51,51,51	0.92	2 (3%)	57,59,59	0.49	0
2	POV	A	395	-	51,51,51	0.92	2 (3%)	57,59,59	0.69	1 (1%)
2	POV	B	347	-	51,51,51	0.88	2 (3%)	57,59,59	0.69	1 (1%)
2	POV	B	343	-	51,51,51	0.94	2 (3%)	57,59,59	0.56	0
2	POV	A	335	-	51,51,51	0.91	2 (3%)	57,59,59	0.50	0
2	POV	B	350	-	51,51,51	0.93	2 (3%)	57,59,59	0.62	0
2	POV	B	357	-	51,51,51	0.96	2 (3%)	57,59,59	0.74	1 (1%)
2	POV	B	314	-	51,51,51	0.87	2 (3%)	57,59,59	0.56	0
2	POV	B	384	-	51,51,51	0.92	2 (3%)	57,59,59	0.57	0
2	POV	B	379	-	51,51,51	0.92	2 (3%)	57,59,59	0.67	1 (1%)
2	POV	B	362	-	51,51,51	0.92	2 (3%)	57,59,59	0.61	0
2	POV	A	379	-	51,51,51	0.87	2 (3%)	57,59,59	0.51	0
2	POV	A	397	-	51,51,51	0.90	2 (3%)	57,59,59	0.54	0
2	POV	B	339	-	51,51,51	0.95	2 (3%)	57,59,59	0.85	3 (5%)
2	POV	A	337	-	51,51,51	0.89	2 (3%)	57,59,59	0.57	0
2	POV	B	389	-	51,51,51	0.90	2 (3%)	57,59,59	0.69	1 (1%)
2	POV	A	322	-	51,51,51	0.88	2 (3%)	57,59,59	0.64	1 (1%)
2	POV	B	366	-	51,51,51	0.89	2 (3%)	57,59,59	0.67	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	POV	B	358	-	51,51,51	0.87	2 (3%)	57,59,59	0.80	1 (1%)
2	POV	A	334	-	51,51,51	0.98	2 (3%)	57,59,59	0.65	1 (1%)
2	POV	A	390	-	51,51,51	0.91	2 (3%)	57,59,59	0.49	0
2	POV	B	302	-	51,51,51	0.90	2 (3%)	57,59,59	0.73	1 (1%)
2	POV	B	325	-	51,51,51	0.88	2 (3%)	57,59,59	0.61	0
2	POV	A	393	-	51,51,51	0.91	2 (3%)	57,59,59	0.55	0
2	POV	A	347	-	51,51,51	0.88	2 (3%)	57,59,59	0.50	0
2	POV	A	363	-	51,51,51	0.93	2 (3%)	57,59,59	0.55	0
2	POV	A	308	-	51,51,51	0.92	2 (3%)	57,59,59	0.55	0
2	POV	B	356	-	51,51,51	0.92	2 (3%)	57,59,59	0.59	1 (1%)
2	POV	B	371	-	51,51,51	0.93	2 (3%)	57,59,59	0.59	0
2	POV	A	343	-	51,51,51	0.89	2 (3%)	57,59,59	0.69	1 (1%)
3	CLR	B	391	-	31,31,31	0.74	0	48,48,48	1.00	3 (6%)
3	CLR	B	396	-	31,31,31	0.83	1 (3%)	48,48,48	1.20	5 (10%)
2	POV	A	348	-	51,51,51	0.91	2 (3%)	57,59,59	0.55	0
2	POV	A	310	-	51,51,51	0.89	2 (3%)	57,59,59	0.65	1 (1%)
2	POV	A	325	-	51,51,51	0.86	2 (3%)	57,59,59	0.66	1 (1%)
2	POV	A	309	-	51,51,51	0.90	2 (3%)	57,59,59	0.63	1 (1%)
2	POV	B	310	-	51,51,51	0.94	2 (3%)	57,59,59	0.68	2 (3%)
2	POV	B	375	-	51,51,51	0.93	2 (3%)	57,59,59	0.47	0
3	CLR	B	390	-	31,31,31	0.69	0	48,48,48	0.97	3 (6%)
2	POV	B	352	-	51,51,51	0.85	2 (3%)	57,59,59	0.59	1 (1%)
2	POV	A	386	-	51,51,51	0.95	2 (3%)	57,59,59	0.49	0
2	POV	B	376	-	51,51,51	0.89	2 (3%)	57,59,59	0.52	0
2	POV	A	323	-	51,51,51	0.92	2 (3%)	57,59,59	0.50	0
2	POV	B	368	-	51,51,51	0.90	2 (3%)	57,59,59	0.71	1 (1%)
2	POV	B	320	-	51,51,51	0.94	2 (3%)	57,59,59	0.62	1 (1%)
3	CLR	B	393	-	31,31,31	0.73	0	48,48,48	1.02	2 (4%)
2	POV	A	408	-	51,51,51	0.93	2 (3%)	57,59,59	0.52	0
3	CLR	B	399	-	31,31,31	0.79	0	48,48,48	0.97	3 (6%)
2	POV	A	371	-	51,51,51	0.87	2 (3%)	57,59,59	0.56	0
2	POV	A	387	-	51,51,51	0.91	2 (3%)	57,59,59	0.65	0
2	POV	A	305	-	51,51,51	0.93	2 (3%)	57,59,59	0.66	1 (1%)
2	POV	A	394	-	51,51,51	0.91	2 (3%)	57,59,59	0.50	0
2	POV	B	345	-	51,51,51	0.93	2 (3%)	57,59,59	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	POV	B	385	-	51,51,51	0.88	2 (3%)	57,59,59	0.53	0
2	POV	B	387	-	51,51,51	0.86	2 (3%)	57,59,59	0.55	0
2	POV	A	311	-	51,51,51	0.90	2 (3%)	57,59,59	0.61	1 (1%)
2	POV	B	344	-	51,51,51	0.89	2 (3%)	57,59,59	0.64	0
2	POV	A	362	-	51,51,51	0.92	2 (3%)	57,59,59	0.78	1 (1%)
2	POV	B	383	-	51,51,51	0.90	2 (3%)	57,59,59	0.65	1 (1%)
3	CLR	A	421	-	31,31,31	0.74	0	48,48,48	0.99	3 (6%)
2	POV	A	414	-	51,51,51	0.90	2 (3%)	57,59,59	0.65	0
2	POV	A	375	-	51,51,51	0.90	2 (3%)	57,59,59	0.52	0
2	POV	B	315	-	51,51,51	0.96	2 (3%)	57,59,59	0.57	0
2	POV	B	364	-	51,51,51	0.89	2 (3%)	57,59,59	0.57	0
2	POV	A	332	-	51,51,51	0.87	2 (3%)	57,59,59	0.54	0
2	POV	B	307	-	51,51,51	0.94	2 (3%)	57,59,59	0.74	1 (1%)
2	POV	B	318	-	51,51,51	0.92	2 (3%)	57,59,59	0.66	1 (1%)
2	POV	B	332	-	51,51,51	0.91	2 (3%)	57,59,59	0.55	0
2	POV	A	314	-	51,51,51	0.93	2 (3%)	57,59,59	0.61	1 (1%)
2	POV	A	327	-	51,51,51	0.93	2 (3%)	57,59,59	0.68	1 (1%)
2	POV	B	329	-	51,51,51	0.90	2 (3%)	57,59,59	0.50	0
2	POV	A	411	-	51,51,51	0.93	2 (3%)	57,59,59	0.72	2 (3%)
2	POV	B	381	-	51,51,51	0.96	2 (3%)	57,59,59	0.51	0
2	POV	B	388	-	51,51,51	0.91	2 (3%)	57,59,59	0.65	1 (1%)
2	POV	A	381	-	51,51,51	0.89	2 (3%)	57,59,59	0.46	0
2	POV	A	324	-	51,51,51	0.92	2 (3%)	57,59,59	0.51	0
2	POV	A	352	-	51,51,51	0.90	2 (3%)	57,59,59	0.70	1 (1%)
2	POV	A	374	-	51,51,51	0.92	2 (3%)	57,59,59	0.68	0
2	POV	B	331	-	51,51,51	0.91	2 (3%)	57,59,59	0.84	3 (5%)
2	POV	B	382	-	51,51,51	0.89	2 (3%)	57,59,59	0.68	2 (3%)
2	POV	B	321	-	51,51,51	0.94	2 (3%)	57,59,59	0.68	2 (3%)
2	POV	A	329	-	51,51,51	0.87	2 (3%)	57,59,59	0.78	1 (1%)
2	POV	A	361	-	51,51,51	0.89	2 (3%)	57,59,59	0.64	1 (1%)
2	POV	B	323	-	51,51,51	0.91	2 (3%)	57,59,59	0.71	2 (3%)
2	POV	A	359	-	51,51,51	0.87	2 (3%)	57,59,59	0.77	2 (3%)
2	POV	B	359	-	51,51,51	0.91	2 (3%)	57,59,59	0.55	0
2	POV	B	336	-	51,51,51	0.89	2 (3%)	57,59,59	0.60	0
2	POV	B	354	-	51,51,51	0.93	2 (3%)	57,59,59	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	POV	A	331	-	51,51,51	0.88	2 (3%)	57,59,59	0.69	2 (3%)
2	POV	A	412	-	51,51,51	0.92	2 (3%)	57,59,59	0.62	1 (1%)
2	POV	A	328	-	51,51,51	0.91	2 (3%)	57,59,59	0.59	0
2	POV	A	350	-	51,51,51	0.90	2 (3%)	57,59,59	0.47	0
2	POV	A	370	-	51,51,51	0.93	2 (3%)	57,59,59	0.54	0
2	POV	A	398	-	51,51,51	0.92	2 (3%)	57,59,59	0.60	0
2	POV	A	358	-	51,51,51	0.88	2 (3%)	57,59,59	0.62	1 (1%)
2	POV	A	382	-	51,51,51	0.92	2 (3%)	57,59,59	0.50	0
2	POV	B	367	-	51,51,51	0.91	2 (3%)	57,59,59	0.68	1 (1%)
2	POV	A	372	-	51,51,51	0.91	2 (3%)	57,59,59	0.54	0
2	POV	B	355	-	51,51,51	0.87	2 (3%)	57,59,59	0.54	0
2	POV	A	377	-	51,51,51	0.90	2 (3%)	57,59,59	0.55	0
2	POV	A	340	-	51,51,51	0.87	2 (3%)	57,59,59	0.57	0
2	POV	A	302	-	51,51,51	0.87	2 (3%)	57,59,59	0.62	1 (1%)
2	POV	A	319	-	51,51,51	0.89	2 (3%)	57,59,59	0.68	1 (1%)
2	POV	B	340	-	51,51,51	0.90	3 (5%)	57,59,59	0.78	2 (3%)
3	CLR	B	398	-	31,31,31	0.79	0	48,48,48	0.95	3 (6%)
2	POV	A	312	-	51,51,51	0.95	2 (3%)	57,59,59	0.61	1 (1%)
2	POV	B	327	-	51,51,51	0.93	2 (3%)	57,59,59	0.67	1 (1%)
2	POV	B	348	-	51,51,51	0.89	2 (3%)	57,59,59	0.62	1 (1%)
2	POV	B	369	-	51,51,51	0.90	2 (3%)	57,59,59	0.59	0
2	POV	B	319	-	51,51,51	0.93	2 (3%)	57,59,59	0.56	1 (1%)
2	POV	B	372	-	51,51,51	0.86	2 (3%)	57,59,59	0.59	0
3	CLR	A	404	-	31,31,31	0.86	1 (3%)	48,48,48	1.01	2 (4%)
2	POV	A	315	-	51,51,51	0.90	2 (3%)	57,59,59	0.66	1 (1%)
2	POV	A	384	-	51,51,51	0.92	2 (3%)	57,59,59	0.80	2 (3%)
2	POV	A	355	-	51,51,51	1.00	2 (3%)	57,59,59	0.63	1 (1%)
2	POV	A	339	-	51,51,51	0.92	2 (3%)	57,59,59	0.51	0
2	POV	A	344	-	51,51,51	0.96	2 (3%)	57,59,59	0.63	0
2	POV	A	380	-	51,51,51	0.91	2 (3%)	57,59,59	0.47	0
2	POV	B	380	-	51,51,51	0.92	2 (3%)	57,59,59	0.77	2 (3%)
3	CLR	B	392	-	31,31,31	0.76	0	48,48,48	1.28	5 (10%)
3	CLR	A	420	-	31,31,31	0.90	0	48,48,48	1.17	3 (6%)
2	POV	A	369	-	51,51,51	0.91	2 (3%)	57,59,59	0.63	1 (1%)
2	POV	A	304	-	51,51,51	0.89	2 (3%)	57,59,59	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	POV	A	376	-	51,51,51	0.89	2 (3%)	57,59,59	0.71	1 (1%)
2	POV	A	368	-	51,51,51	0.90	2 (3%)	57,59,59	0.49	0
2	POV	A	367	-	51,51,51	0.95	2 (3%)	57,59,59	0.56	0
2	POV	B	338	-	51,51,51	0.90	2 (3%)	57,59,59	0.62	0
2	POV	B	373	-	51,51,51	1.00	2 (3%)	57,59,59	0.77	2 (3%)
2	POV	A	399	-	51,51,51	0.94	2 (3%)	57,59,59	0.55	0
2	POV	A	416	-	51,51,51	0.87	2 (3%)	57,59,59	0.51	0
2	POV	A	306	-	51,51,51	0.89	2 (3%)	57,59,59	0.49	0
2	POV	B	346	-	51,51,51	0.90	2 (3%)	57,59,59	0.65	0
2	POV	B	316	-	51,51,51	0.89	2 (3%)	57,59,59	0.59	0
3	CLR	A	401	-	31,31,31	0.90	0	48,48,48	0.98	1 (2%)
2	POV	B	360	-	51,51,51	0.89	2 (3%)	57,59,59	0.73	2 (3%)
2	POV	A	303	-	51,51,51	0.91	2 (3%)	57,59,59	0.59	1 (1%)
2	POV	B	303	-	51,51,51	0.87	2 (3%)	57,59,59	0.50	0
2	POV	B	312	-	51,51,51	0.91	2 (3%)	57,59,59	0.56	0
2	POV	A	354	-	51,51,51	0.93	2 (3%)	57,59,59	0.63	0
2	POV	A	356	-	51,51,51	0.93	2 (3%)	57,59,59	0.60	0
2	POV	B	374	-	51,51,51	0.93	2 (3%)	57,59,59	0.64	1 (1%)
3	CLR	B	397	-	31,31,31	0.83	0	48,48,48	0.92	2 (4%)
2	POV	A	342	-	51,51,51	0.88	2 (3%)	57,59,59	0.59	0
2	POV	A	407	-	51,51,51	0.91	2 (3%)	57,59,59	0.65	1 (1%)
2	POV	A	346	-	51,51,51	0.90	2 (3%)	57,59,59	0.53	0
2	POV	A	388	-	51,51,51	0.87	2 (3%)	57,59,59	0.49	0
2	POV	B	313	-	51,51,51	0.90	2 (3%)	57,59,59	0.79	2 (3%)
2	POV	A	410	-	51,51,51	0.89	2 (3%)	57,59,59	0.55	0
2	POV	B	361	-	51,51,51	0.92	2 (3%)	57,59,59	0.80	1 (1%)
2	POV	A	330	-	51,51,51	0.87	2 (3%)	57,59,59	0.63	1 (1%)
2	POV	A	320	-	51,51,51	0.90	2 (3%)	57,59,59	0.57	0
2	POV	A	333	-	51,51,51	0.92	2 (3%)	57,59,59	0.72	1 (1%)
2	POV	B	311	-	51,51,51	0.98	2 (3%)	57,59,59	0.54	1 (1%)
2	POV	A	413	-	51,51,51	0.90	2 (3%)	57,59,59	0.63	1 (1%)
2	POV	A	360	-	51,51,51	0.93	2 (3%)	57,59,59	0.55	0
2	POV	B	308	-	51,51,51	0.86	2 (3%)	57,59,59	0.50	0
2	POV	A	417	-	51,51,51	0.90	2 (3%)	57,59,59	0.67	1 (1%)
2	POV	B	349	-	51,51,51	0.90	2 (3%)	57,59,59	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	POV	A	357	-	51,51,51	0.92	2 (3%)	57,59,59	0.67	1 (1%)
2	POV	B	335	-	51,51,51	0.92	2 (3%)	57,59,59	0.51	0
2	POV	B	377	-	51,51,51	0.83	2 (3%)	57,59,59	0.63	0
2	POV	A	313	-	51,51,51	0.90	2 (3%)	57,59,59	0.54	0
2	POV	B	333	-	51,51,51	0.90	2 (3%)	57,59,59	0.66	0
2	POV	B	337	-	51,51,51	0.90	2 (3%)	57,59,59	0.63	1 (1%)
2	POV	A	326	-	51,51,51	0.91	2 (3%)	57,59,59	0.55	0
2	POV	A	364	-	51,51,51	0.87	2 (3%)	57,59,59	0.57	0
3	CLR	A	419	-	31,31,31	0.92	0	48,48,48	1.23	3 (6%)
2	POV	A	318	-	51,51,51	0.93	2 (3%)	57,59,59	0.70	1 (1%)
2	POV	A	389	-	51,51,51	0.91	2 (3%)	57,59,59	0.61	0
2	POV	B	322	-	51,51,51	0.93	2 (3%)	57,59,59	0.49	0
2	POV	B	370	-	51,51,51	0.95	2 (3%)	57,59,59	0.59	0
2	POV	B	386	-	51,51,51	0.95	2 (3%)	57,59,59	0.57	0
2	POV	B	334	-	51,51,51	0.91	2 (3%)	57,59,59	0.77	1 (1%)
2	POV	B	378	-	51,51,51	0.86	2 (3%)	57,59,59	0.69	1 (1%)
2	POV	A	378	-	51,51,51	0.90	2 (3%)	57,59,59	0.64	2 (3%)
2	POV	A	349	-	51,51,51	0.87	2 (3%)	57,59,59	0.61	0
2	POV	B	351	-	51,51,51	0.90	2 (3%)	57,59,59	0.66	1 (1%)
2	POV	A	336	-	51,51,51	0.88	2 (3%)	57,59,59	0.67	1 (1%)
2	POV	A	385	-	51,51,51	0.90	2 (3%)	57,59,59	0.51	0
2	POV	A	391	-	51,51,51	0.92	2 (3%)	57,59,59	0.64	1 (1%)
2	POV	A	400	-	51,51,51	0.88	2 (3%)	57,59,59	0.58	0
3	CLR	A	406	-	31,31,31	0.84	1 (3%)	48,48,48	0.96	3 (6%)
2	POV	B	363	-	51,51,51	0.91	2 (3%)	57,59,59	0.50	0
2	POV	A	307	-	51,51,51	0.89	2 (3%)	57,59,59	0.52	0
2	POV	A	365	-	51,51,51	0.91	2 (3%)	57,59,59	0.63	0
2	POV	B	304	-	51,51,51	0.89	2 (3%)	57,59,59	0.64	1 (1%)
2	POV	A	351	-	51,51,51	0.87	2 (3%)	57,59,59	0.60	0
2	POV	B	306	-	51,51,51	0.92	2 (3%)	57,59,59	0.62	1 (1%)
2	POV	A	409	-	51,51,51	0.93	2 (3%)	57,59,59	0.73	1 (1%)
2	POV	B	365	-	51,51,51	0.88	2 (3%)	57,59,59	0.64	1 (1%)
3	CLR	A	403	-	31,31,31	0.83	0	48,48,48	1.02	2 (4%)
2	POV	A	301	-	51,51,51	0.88	2 (3%)	57,59,59	0.53	0
2	POV	B	301	-	51,51,51	0.93	2 (3%)	57,59,59	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CLR	A	418	-	31,31,31	0.82	0	48,48,48	1.04	2 (4%)
2	POV	B	324	-	51,51,51	0.96	2 (3%)	57,59,59	0.70	1 (1%)
2	POV	A	373	-	51,51,51	0.91	2 (3%)	57,59,59	0.51	0
2	POV	A	321	-	51,51,51	0.93	2 (3%)	57,59,59	0.64	0
3	CLR	B	395	-	31,31,31	0.76	0	48,48,48	1.06	4 (8%)
2	POV	A	341	-	51,51,51	0.95	2 (3%)	57,59,59	0.70	1 (1%)
2	POV	A	316	-	51,51,51	0.88	2 (3%)	57,59,59	0.69	2 (3%)

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
2	POV	A	366	-	-	9/55/55/55	-
2	POV	A	396	-	-	11/55/55/55	-
3	CLR	A	405	-	-	2/10/68/68	0/4/4/4
2	POV	B	341	-	-	14/55/55/55	-
2	POV	A	345	-	-	8/55/55/55	-
2	POV	A	353	-	-	13/55/55/55	-
3	CLR	A	402	-	-	4/10/68/68	0/4/4/4
2	POV	B	317	-	-	10/55/55/55	-
2	POV	B	353	-	-	5/55/55/55	-
2	POV	A	415	-	-	13/55/55/55	-
2	POV	A	392	-	-	8/55/55/55	-
2	POV	B	326	-	-	10/55/55/55	-
3	CLR	B	394	-	-	0/10/68/68	0/4/4/4
2	POV	B	328	-	1/1/5/7	7/55/55/55	-
2	POV	B	342	-	-	6/55/55/55	-
2	POV	B	309	-	-	6/55/55/55	-
2	POV	A	383	-	1/1/5/7	8/55/55/55	-
2	POV	B	330	-	1/1/5/7	12/55/55/55	-
2	POV	A	317	-	-	12/55/55/55	-
2	POV	B	305	-	-	8/55/55/55	-
2	POV	A	338	-	-	11/55/55/55	-
2	POV	A	395	-	-	14/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	B	347	-	1/1/5/7	13/55/55/55	-
2	POV	B	343	-	-	13/55/55/55	-
2	POV	A	335	-	-	8/55/55/55	-
2	POV	B	350	-	-	8/55/55/55	-
2	POV	B	357	-	-	12/55/55/55	-
2	POV	B	314	-	-	8/55/55/55	-
2	POV	B	384	-	-	11/55/55/55	-
2	POV	B	379	-	-	14/55/55/55	-
2	POV	B	362	-	1/1/5/7	11/55/55/55	-
2	POV	A	379	-	-	5/55/55/55	-
2	POV	A	397	-	-	9/55/55/55	-
2	POV	B	339	-	-	11/55/55/55	-
2	POV	A	337	-	-	4/55/55/55	-
2	POV	B	389	-	-	8/55/55/55	-
2	POV	A	322	-	1/1/5/7	12/55/55/55	-
2	POV	B	366	-	-	9/55/55/55	-
2	POV	B	358	-	-	16/55/55/55	-
2	POV	A	334	-	-	13/55/55/55	-
2	POV	A	390	-	-	11/55/55/55	-
2	POV	B	302	-	-	15/55/55/55	-
2	POV	B	325	-	-	5/55/55/55	-
2	POV	A	393	-	-	17/55/55/55	-
2	POV	A	347	-	-	14/55/55/55	-
2	POV	A	363	-	-	14/55/55/55	-
2	POV	A	308	-	1/1/5/7	7/55/55/55	-
2	POV	B	356	-	-	5/55/55/55	-
2	POV	B	371	-	-	11/55/55/55	-
2	POV	A	343	-	-	8/55/55/55	-
3	CLR	B	391	-	-	0/10/68/68	0/4/4/4
3	CLR	B	396	-	-	5/10/68/68	0/4/4/4
2	POV	A	348	-	-	12/55/55/55	-
2	POV	A	310	-	-	12/55/55/55	-
2	POV	A	325	-	-	14/55/55/55	-
2	POV	A	309	-	-	4/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	B	310	-	-	7/55/55/55	-
2	POV	B	375	-	-	6/55/55/55	-
3	CLR	B	390	-	-	2/10/68/68	0/4/4/4
2	POV	B	352	-	-	8/55/55/55	-
2	POV	A	386	-	-	8/55/55/55	-
2	POV	B	376	-	-	7/55/55/55	-
2	POV	A	323	-	-	9/55/55/55	-
2	POV	B	368	-	-	8/55/55/55	-
2	POV	B	320	-	-	11/55/55/55	-
3	CLR	B	393	-	-	0/10/68/68	0/4/4/4
2	POV	A	408	-	-	13/55/55/55	-
3	CLR	B	399	-	-	4/10/68/68	0/4/4/4
2	POV	A	371	-	-	10/55/55/55	-
2	POV	A	387	-	-	9/55/55/55	-
2	POV	A	305	-	-	8/55/55/55	-
2	POV	A	394	-	-	12/55/55/55	-
2	POV	B	345	-	-	12/55/55/55	-
2	POV	B	385	-	-	8/55/55/55	-
2	POV	B	387	-	-	9/55/55/55	-
2	POV	A	311	-	-	16/55/55/55	-
2	POV	B	344	-	-	9/55/55/55	-
2	POV	A	362	-	-	11/55/55/55	-
2	POV	B	383	-	-	12/55/55/55	-
3	CLR	A	421	-	-	2/10/68/68	0/4/4/4
2	POV	A	414	-	-	5/55/55/55	-
2	POV	A	375	-	-	7/55/55/55	-
2	POV	B	315	-	-	4/55/55/55	-
2	POV	B	364	-	1/1/5/7	9/55/55/55	-
2	POV	A	332	-	-	9/55/55/55	-
2	POV	B	307	-	-	14/55/55/55	-
2	POV	B	318	-	-	11/55/55/55	-
2	POV	B	332	-	-	11/55/55/55	-
2	POV	A	314	-	-	8/55/55/55	-
2	POV	B	329	-	1/1/5/7	5/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	A	327	-	-	15/55/55/55	-
2	POV	A	411	-	-	15/55/55/55	-
2	POV	B	381	-	-	15/55/55/55	-
2	POV	B	388	-	-	10/55/55/55	-
2	POV	A	381	-	-	8/55/55/55	-
2	POV	A	324	-	-	11/55/55/55	-
2	POV	A	352	-	-	13/55/55/55	-
2	POV	A	374	-	-	6/55/55/55	-
2	POV	B	331	-	-	13/55/55/55	-
2	POV	B	382	-	-	14/55/55/55	-
2	POV	B	321	-	1/1/5/7	9/55/55/55	-
2	POV	A	329	-	-	9/55/55/55	-
2	POV	A	361	-	-	5/55/55/55	-
2	POV	B	323	-	-	11/55/55/55	-
2	POV	A	359	-	-	15/55/55/55	-
2	POV	B	359	-	-	8/55/55/55	-
2	POV	B	336	-	-	12/55/55/55	-
2	POV	B	354	-	-	10/55/55/55	-
2	POV	A	331	-	-	15/55/55/55	-
2	POV	A	412	-	-	6/55/55/55	-
2	POV	A	328	-	-	8/55/55/55	-
2	POV	A	350	-	-	9/55/55/55	-
2	POV	A	370	-	-	11/55/55/55	-
2	POV	A	398	-	-	8/55/55/55	-
2	POV	A	358	-	-	6/55/55/55	-
2	POV	B	367	-	1/1/5/7	10/55/55/55	-
2	POV	A	382	-	-	10/55/55/55	-
2	POV	A	372	-	-	8/55/55/55	-
2	POV	B	355	-	-	10/55/55/55	-
2	POV	A	377	-	-	6/55/55/55	-
2	POV	A	340	-	-	9/55/55/55	-
2	POV	A	302	-	-	8/55/55/55	-
2	POV	A	319	-	1/1/5/7	11/55/55/55	-
2	POV	B	340	-	-	11/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	B	398	-	-	1/10/68/68	0/4/4/4
2	POV	A	312	-	-	9/55/55/55	-
2	POV	B	327	-	-	10/55/55/55	-
2	POV	B	348	-	-	8/55/55/55	-
2	POV	B	369	-	-	11/55/55/55	-
2	POV	B	319	-	-	11/55/55/55	-
2	POV	B	372	-	-	7/55/55/55	-
3	CLR	A	404	-	-	3/10/68/68	0/4/4/4
2	POV	A	315	-	-	13/55/55/55	-
2	POV	A	384	-	-	16/55/55/55	-
2	POV	A	355	-	-	6/55/55/55	-
2	POV	A	339	-	-	12/55/55/55	-
2	POV	A	344	-	-	8/55/55/55	-
2	POV	A	380	-	1/1/5/7	11/55/55/55	-
2	POV	B	380	-	-	9/55/55/55	-
3	CLR	B	392	-	-	4/10/68/68	0/4/4/4
3	CLR	A	420	-	-	1/10/68/68	0/4/4/4
2	POV	A	369	-	-	9/55/55/55	-
2	POV	A	304	-	-	9/55/55/55	-
2	POV	A	376	-	-	13/55/55/55	-
2	POV	A	368	-	1/1/5/7	8/55/55/55	-
2	POV	A	367	-	-	4/55/55/55	-
2	POV	B	338	-	-	10/55/55/55	-
2	POV	B	373	-	-	12/55/55/55	-
2	POV	A	399	-	-	12/55/55/55	-
2	POV	A	416	-	-	8/55/55/55	-
2	POV	B	346	-	1/1/5/7	13/55/55/55	-
2	POV	A	306	-	-	5/55/55/55	-
2	POV	B	316	-	-	6/55/55/55	-
3	CLR	A	401	-	-	0/10/68/68	0/4/4/4
2	POV	B	360	-	-	13/55/55/55	-
2	POV	A	303	-	-	10/55/55/55	-
2	POV	B	303	-	1/1/5/7	8/55/55/55	-
2	POV	B	312	-	-	10/55/55/55	-
2	POV	A	354	-	-	16/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	A	356	-	-	10/55/55/55	-
2	POV	B	374	-	-	18/55/55/55	-
3	CLR	B	397	-	-	0/10/68/68	0/4/4/4
2	POV	A	342	-	-	7/55/55/55	-
2	POV	A	407	-	-	7/55/55/55	-
2	POV	A	346	-	-	9/55/55/55	-
2	POV	A	388	-	-	6/55/55/55	-
2	POV	B	313	-	-	9/55/55/55	-
2	POV	A	410	-	1/1/5/7	8/55/55/55	-
2	POV	B	361	-	-	14/55/55/55	-
2	POV	A	330	-	-	6/55/55/55	-
2	POV	A	320	-	-	8/55/55/55	-
2	POV	A	333	-	-	6/55/55/55	-
2	POV	B	311	-	-	13/55/55/55	-
2	POV	A	413	-	-	8/55/55/55	-
2	POV	A	360	-	-	9/55/55/55	-
2	POV	B	308	-	-	5/55/55/55	-
2	POV	A	417	-	-	6/55/55/55	-
2	POV	B	349	-	-	10/55/55/55	-
2	POV	A	357	-	-	8/55/55/55	-
2	POV	B	335	-	-	6/55/55/55	-
2	POV	B	377	-	-	6/55/55/55	-
2	POV	A	313	-	-	16/55/55/55	-
2	POV	B	333	-	-	9/55/55/55	-
2	POV	B	337	-	-	2/55/55/55	-
2	POV	A	326	-	1/1/5/7	8/55/55/55	-
2	POV	A	364	-	-	10/55/55/55	-
3	CLR	A	419	-	-	1/10/68/68	0/4/4/4
2	POV	A	318	-	1/1/5/7	11/55/55/55	-
2	POV	A	389	-	-	14/55/55/55	-
2	POV	B	322	-	-	10/55/55/55	-
2	POV	B	370	-	-	11/55/55/55	-
2	POV	B	386	-	-	7/55/55/55	-
2	POV	B	334	-	-	11/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	B	378	-	-	16/55/55/55	-
2	POV	A	378	-	1/1/5/7	16/55/55/55	-
2	POV	A	349	-	-	9/55/55/55	-
2	POV	B	351	-	-	6/55/55/55	-
2	POV	A	385	-	1/1/5/7	8/55/55/55	-
2	POV	A	336	-	-	12/55/55/55	-
2	POV	A	400	-	1/1/5/7	8/55/55/55	-
2	POV	A	391	-	-	5/55/55/55	-
3	CLR	A	406	-	-	0/10/68/68	0/4/4/4
2	POV	B	363	-	-	2/55/55/55	-
2	POV	A	307	-	-	6/55/55/55	-
2	POV	A	365	-	1/1/5/7	11/55/55/55	-
2	POV	B	304	-	-	11/55/55/55	-
2	POV	A	351	-	-	9/55/55/55	-
2	POV	B	306	-	-	10/55/55/55	-
2	POV	A	409	-	-	11/55/55/55	-
2	POV	B	365	-	-	8/55/55/55	-
3	CLR	A	403	-	-	0/10/68/68	0/4/4/4
2	POV	A	301	-	-	11/55/55/55	-
2	POV	B	301	-	-	7/55/55/55	-
3	CLR	A	418	-	-	2/10/68/68	0/4/4/4
2	POV	B	324	-	-	10/55/55/55	-
2	POV	A	373	-	-	6/55/55/55	-
2	POV	A	321	-	-	11/55/55/55	-
3	CLR	B	395	-	-	0/10/68/68	0/4/4/4
2	POV	A	341	-	-	11/55/55/55	-
2	POV	A	316	-	1/1/5/7	4/55/55/55	-

The worst 5 of 406 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	POV	O21-C2	-3.76	1.37	1.46
2	A	317	POV	O21-C2	-3.76	1.37	1.46
2	B	341	POV	O21-C2	-3.74	1.37	1.46
2	B	362	POV	O21-C2	-3.72	1.37	1.46
2	B	324	POV	O21-C2	-3.71	1.37	1.46

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	392	CLR	C16-C17-C20	4.81	119.46	112.18
2	A	362	POV	O31-C3-C2	4.15	120.36	108.40
3	B	399	CLR	C4-C5-C10	4.07	121.63	116.42
2	B	361	POV	O21-C2-C1	4.02	122.78	108.34
2	B	334	POV	C26-C27-C28	3.97	132.94	113.86

5 of 24 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	308	POV	C2
2	A	316	POV	C2
2	A	318	POV	C2
2	A	319	POV	C2
2	A	322	POV	C2

5 of 1964 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	POV	C11-O12-P-O11
2	A	301	POV	C11-O12-P-O13
2	A	301	POV	C11-O12-P-O14
2	A	301	POV	O12-C11-C12-N
2	A	305	POV	C11-O12-P-O14

There are no ring outliers.

18 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	396	POV	1	0
3	A	402	CLR	2	0
2	B	314	POV	1	0
2	B	339	POV	1	0
2	B	302	POV	1	0
3	B	393	CLR	1	0
2	A	311	POV	1	0
2	B	329	POV	1	0
2	B	388	POV	1	0
2	B	331	POV	2	0
2	A	412	POV	1	0
2	B	373	POV	1	0
2	B	303	POV	1	0

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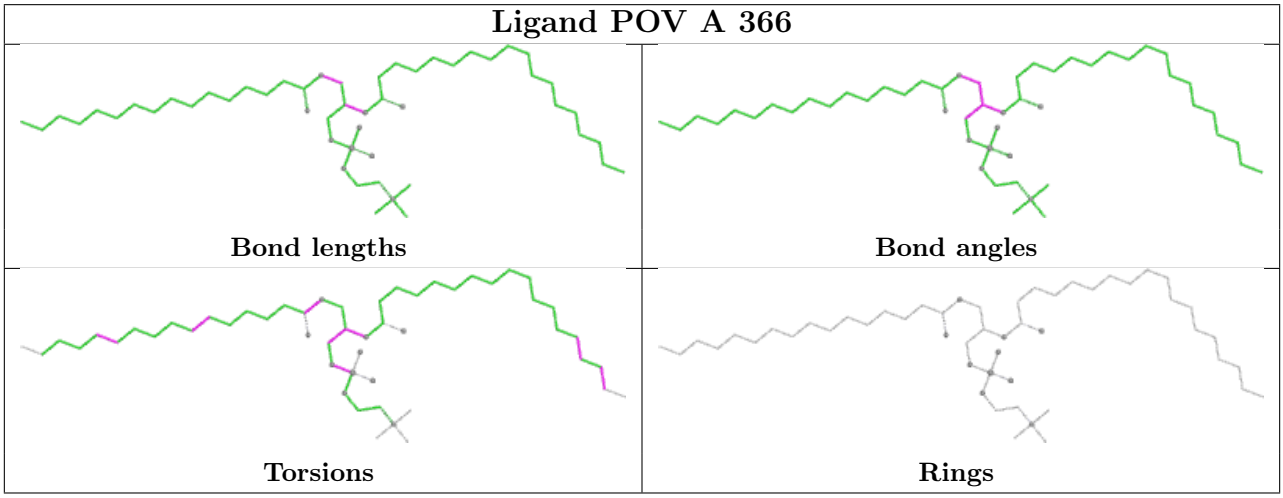
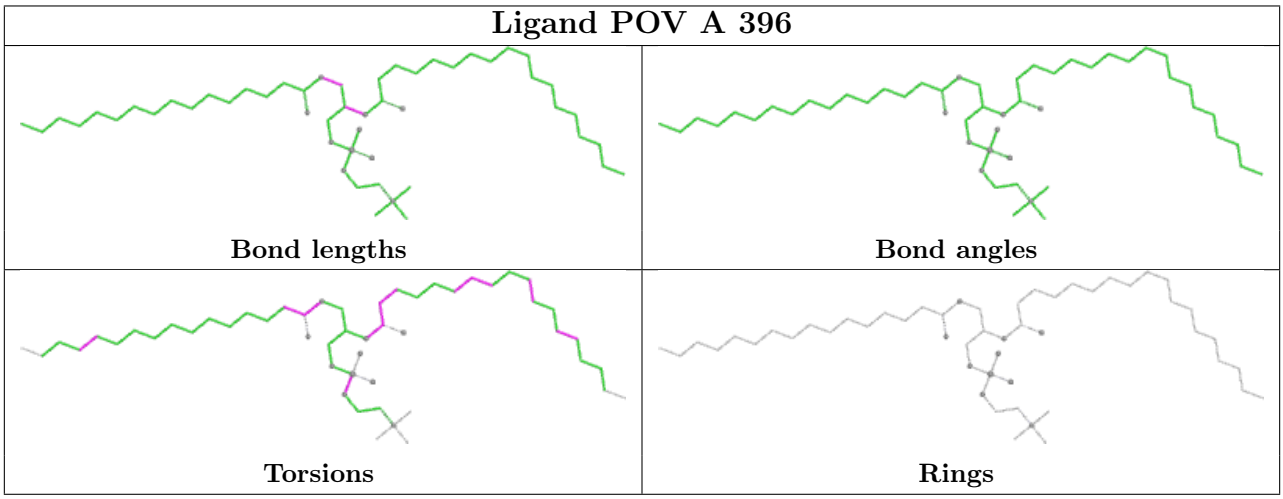
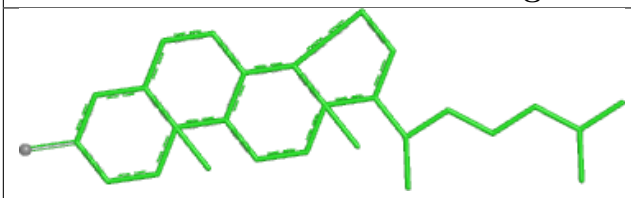
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	313	POV	1	0
2	B	349	POV	1	0
2	A	357	POV	1	0
2	A	318	POV	1	0
2	B	334	POV	1	0

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

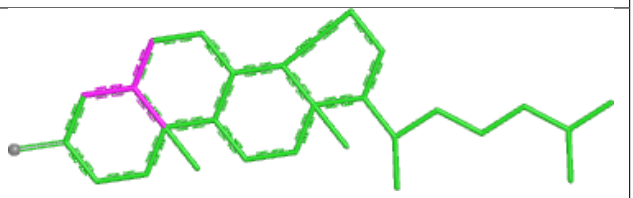




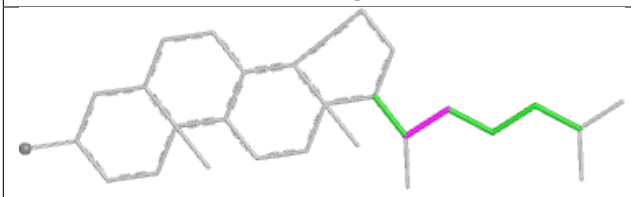
Ligand CLR A 405



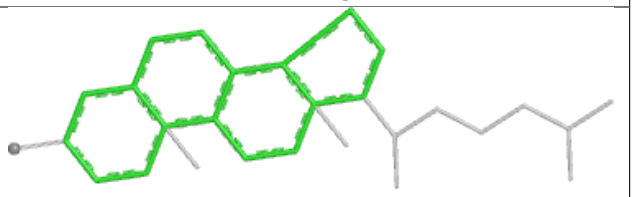
Bond lengths



Bond angles

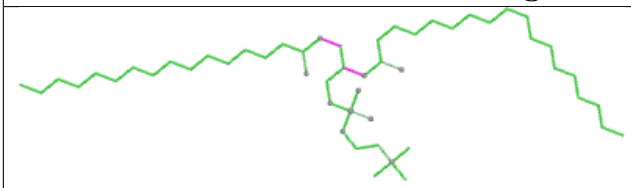


Torsions

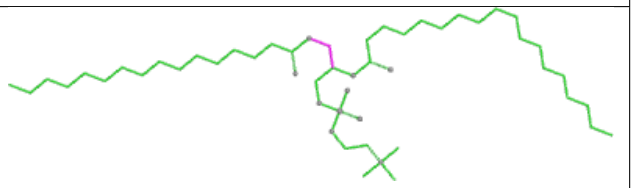


Rings

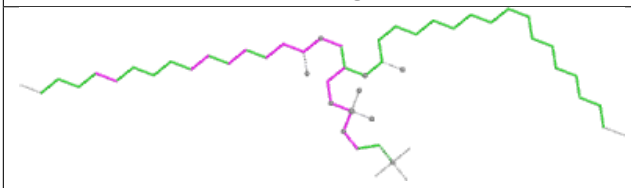
Ligand POV B 341



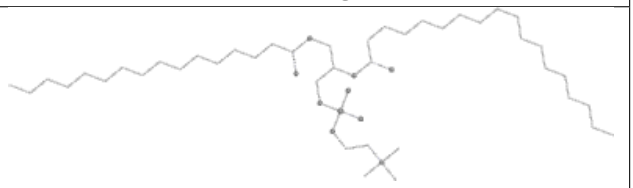
Bond lengths



Bond angles

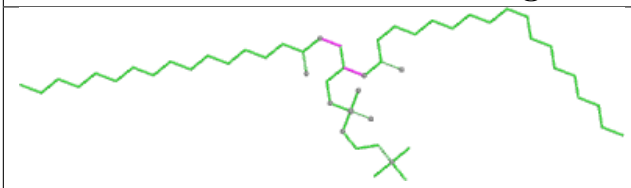


Torsions

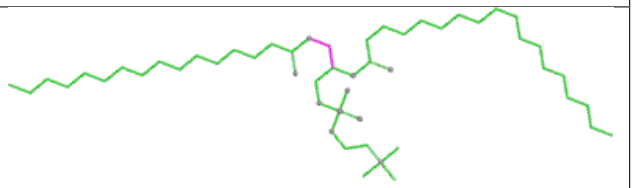


Rings

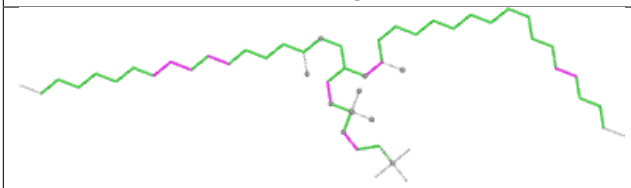
Ligand POV A 345



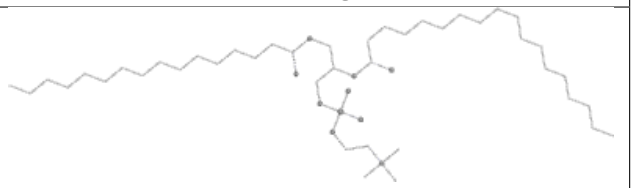
Bond lengths



Bond angles

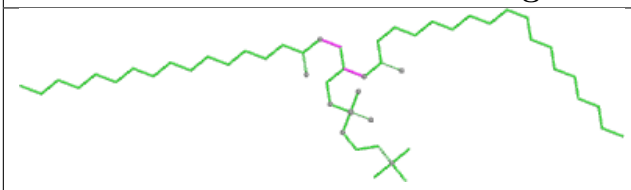


Torsions

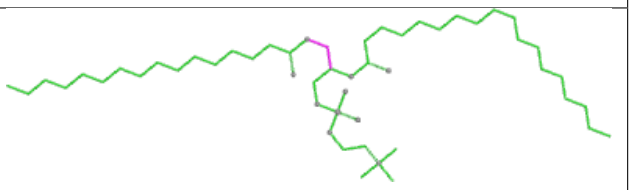


Rings

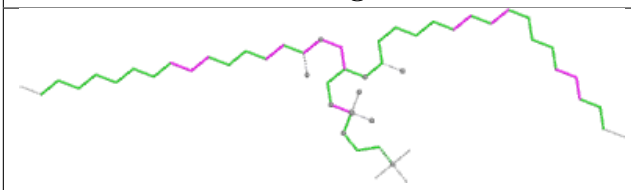
Ligand POV A 353



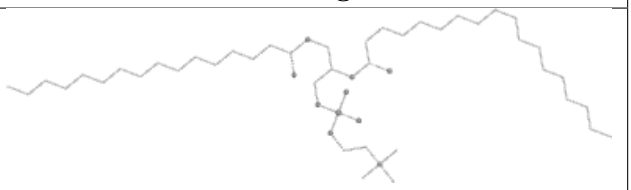
Bond lengths



Bond angles

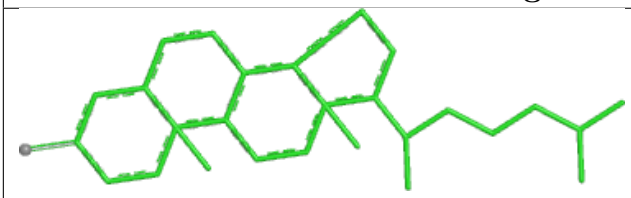


Torsions

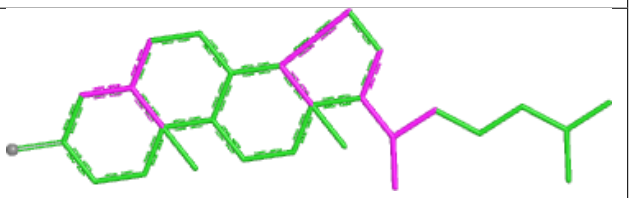


Rings

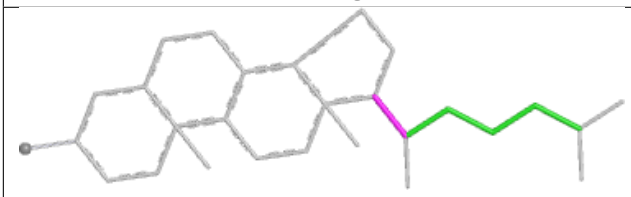
Ligand CLR A 402



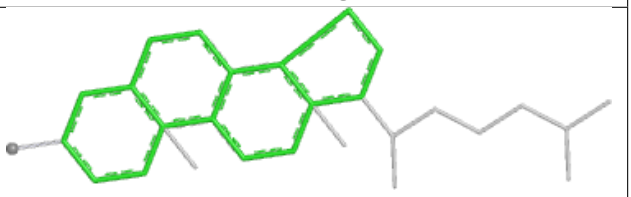
Bond lengths



Bond angles

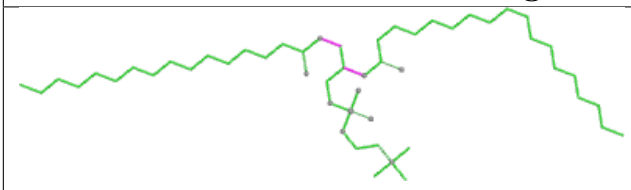


Torsions

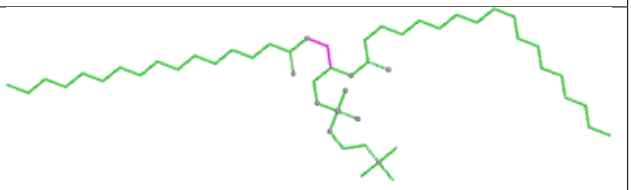


Rings

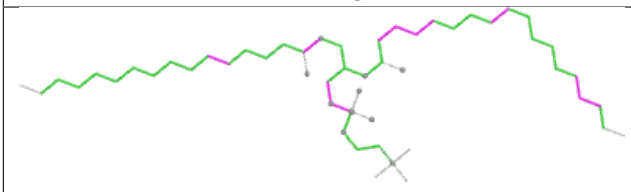
Ligand POV B 317



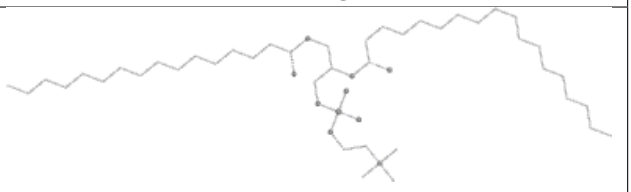
Bond lengths



Bond angles

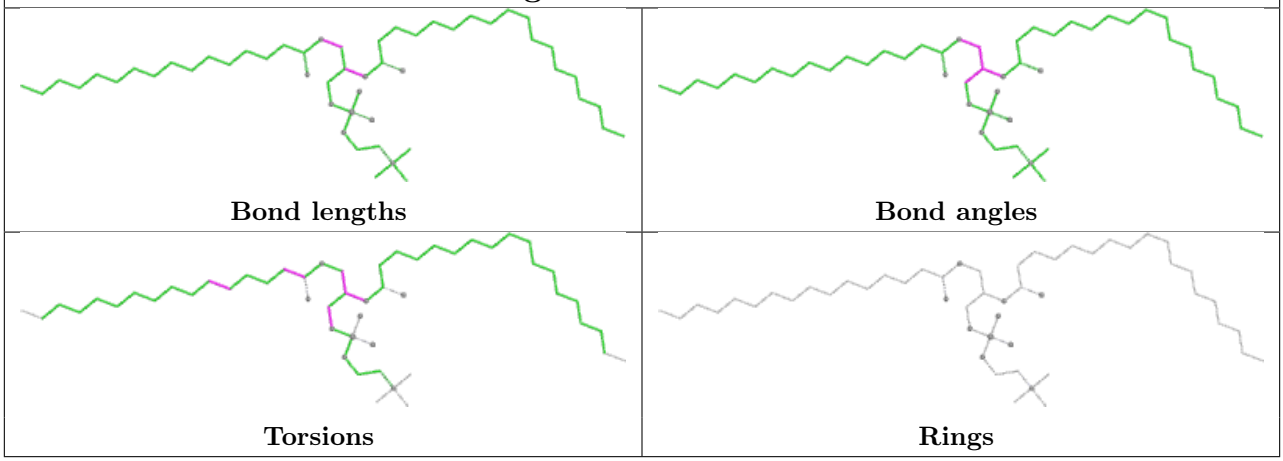


Torsions



Rings

Ligand POV B 353



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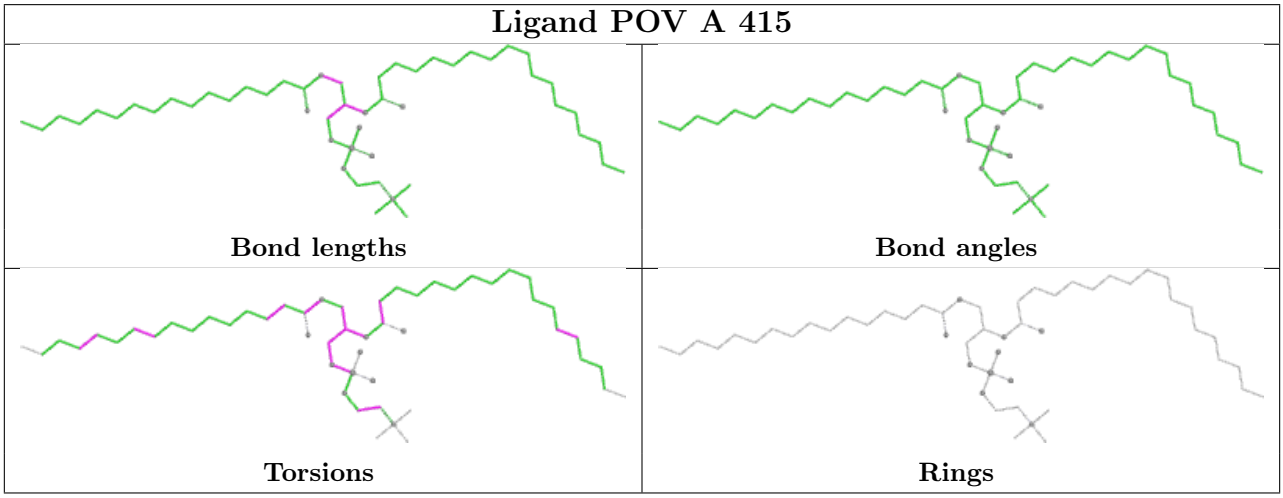

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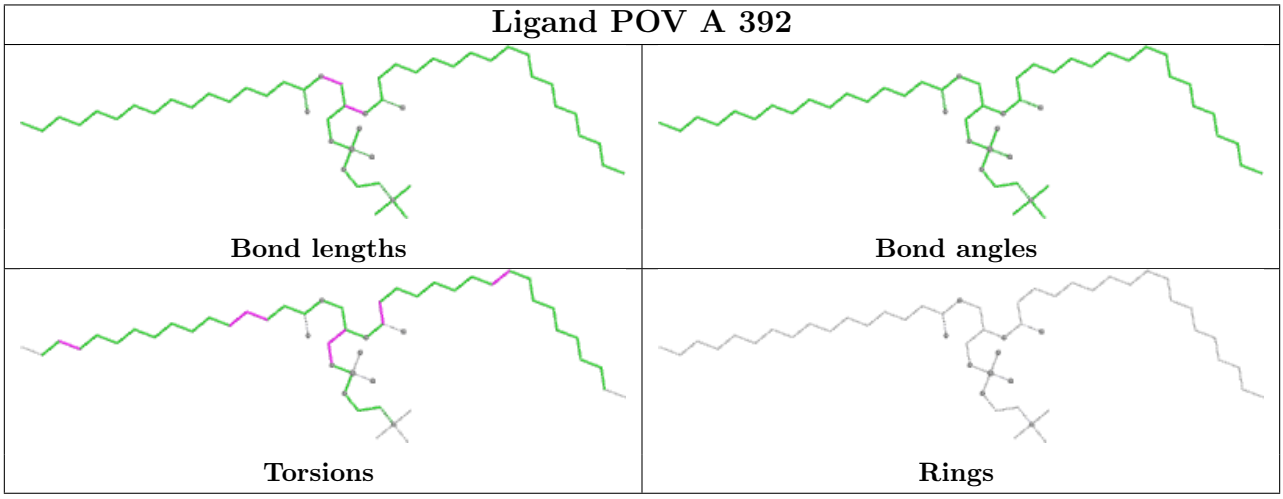

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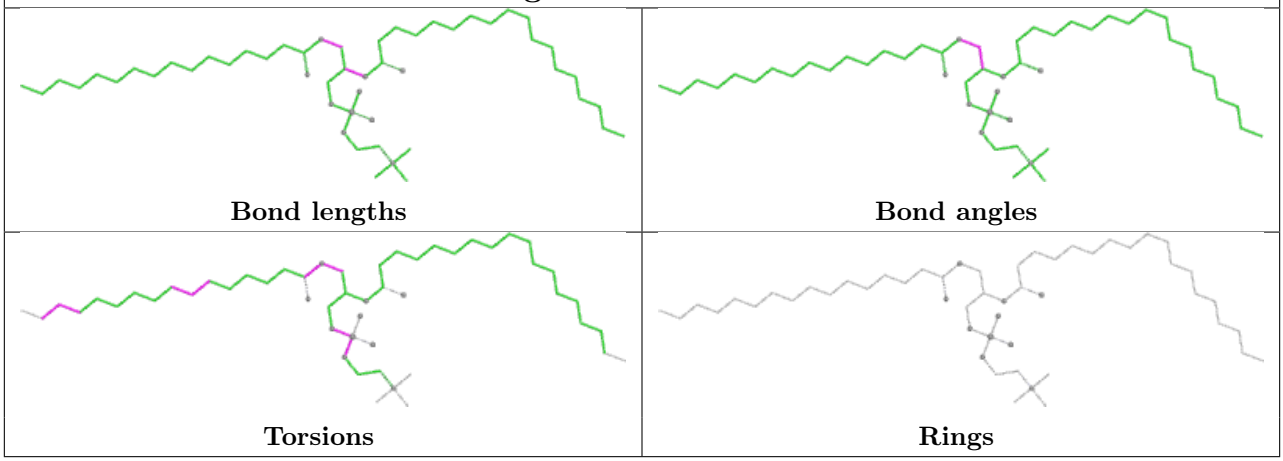

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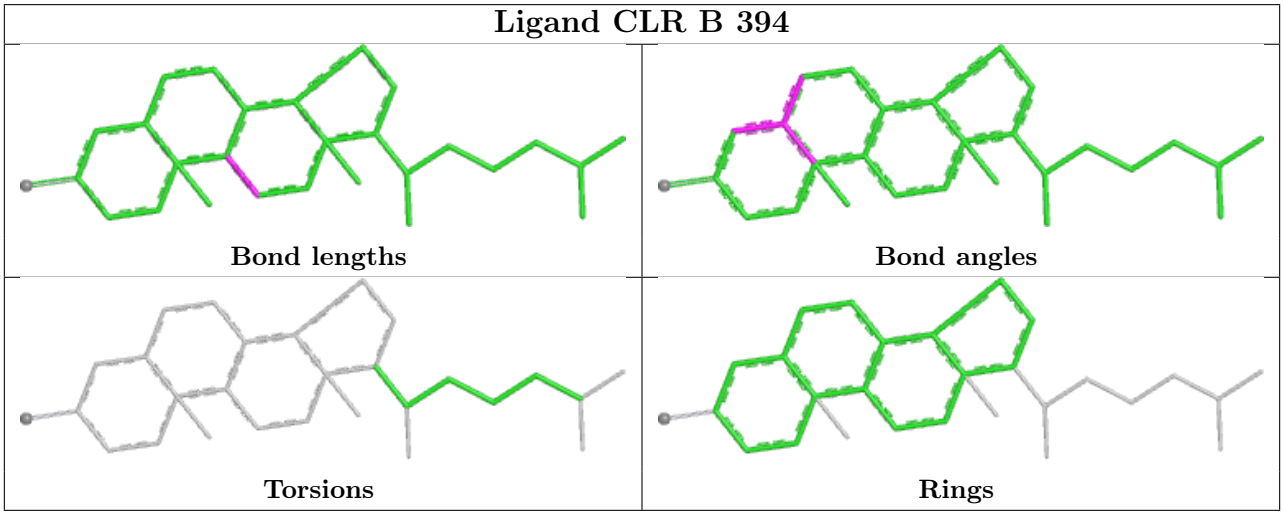
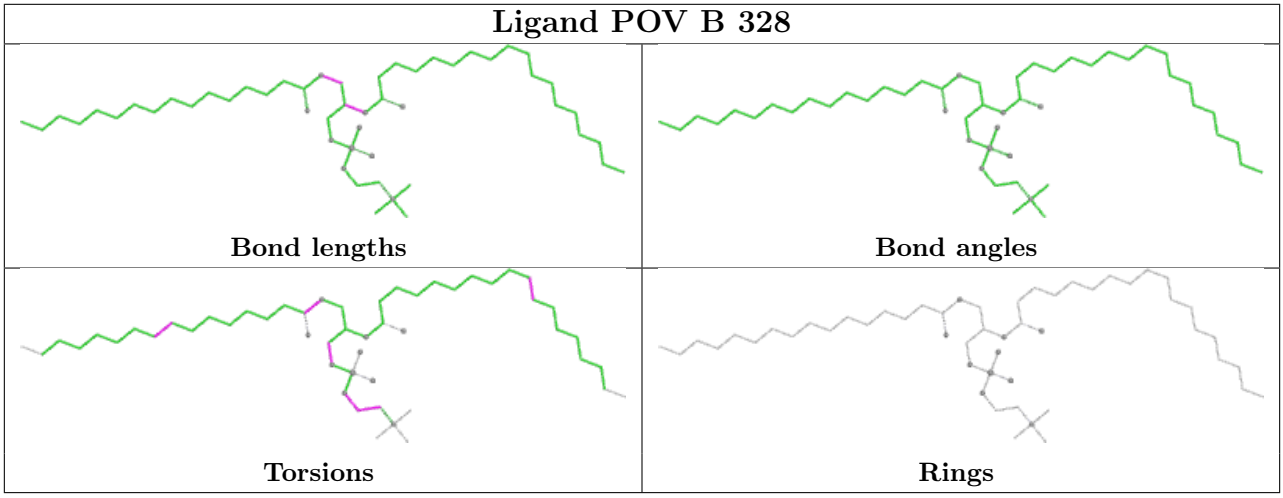


Ligand POV B 328



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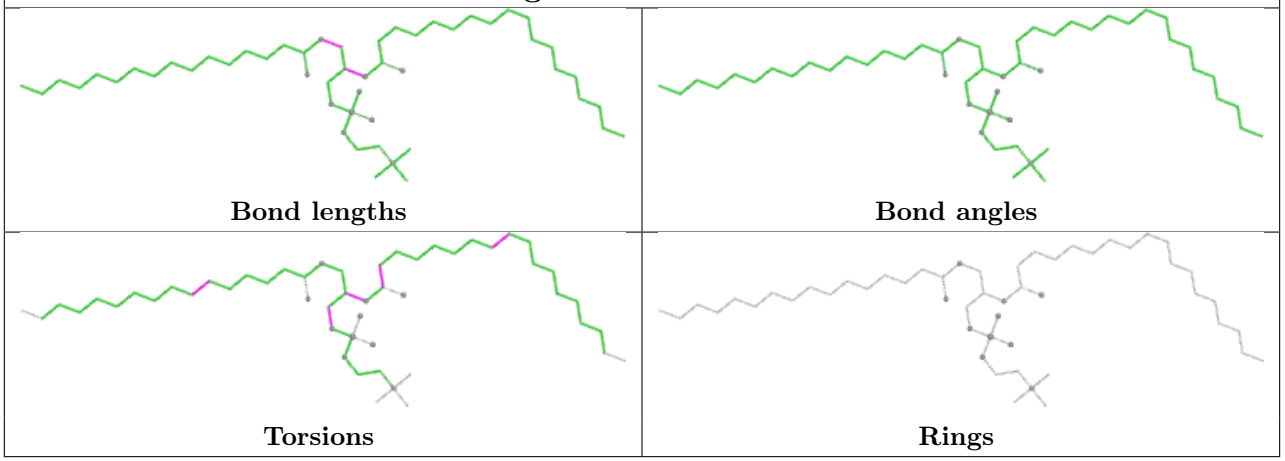

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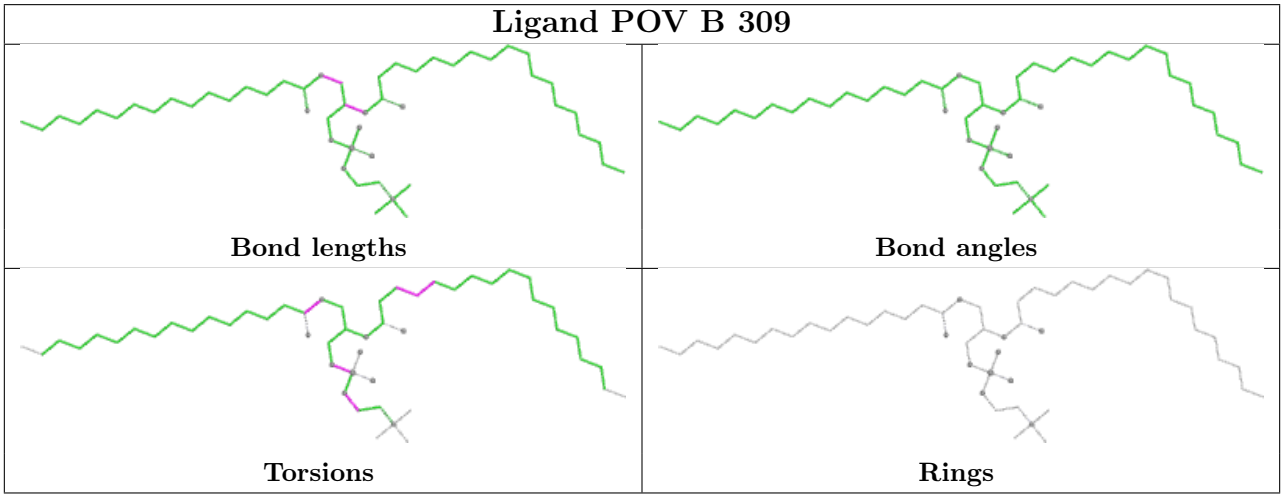

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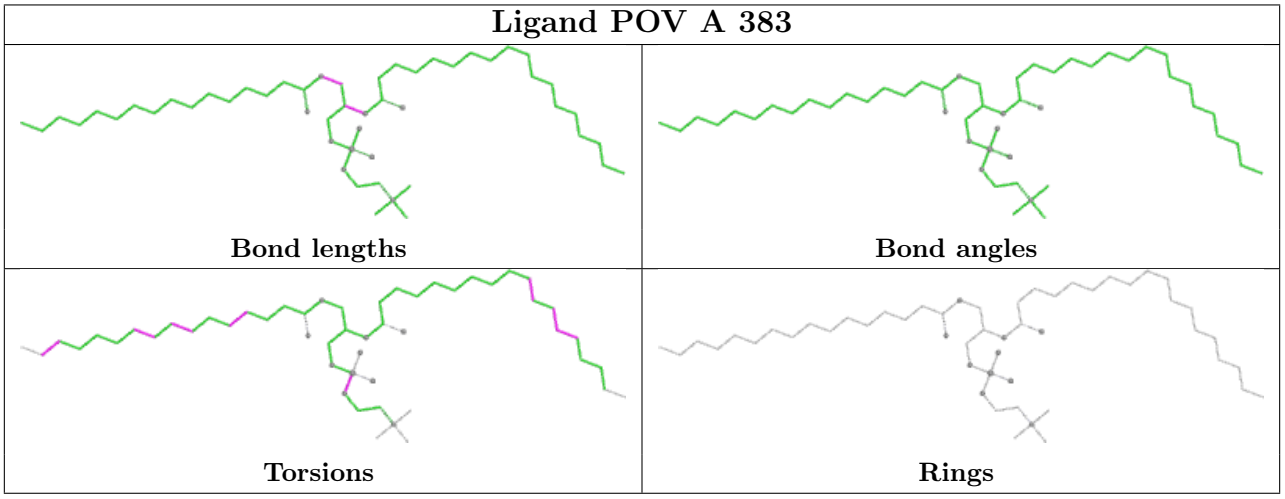

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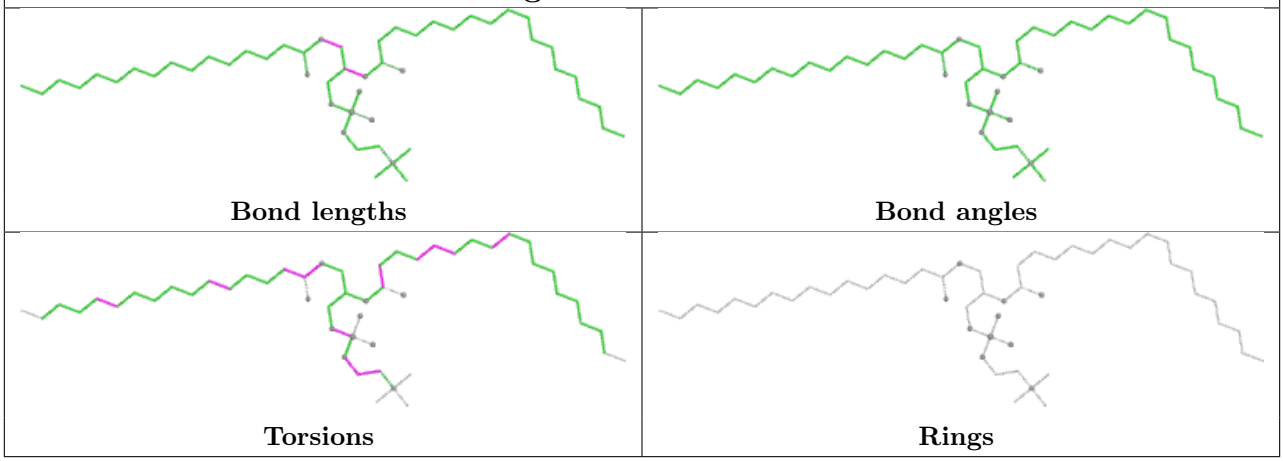

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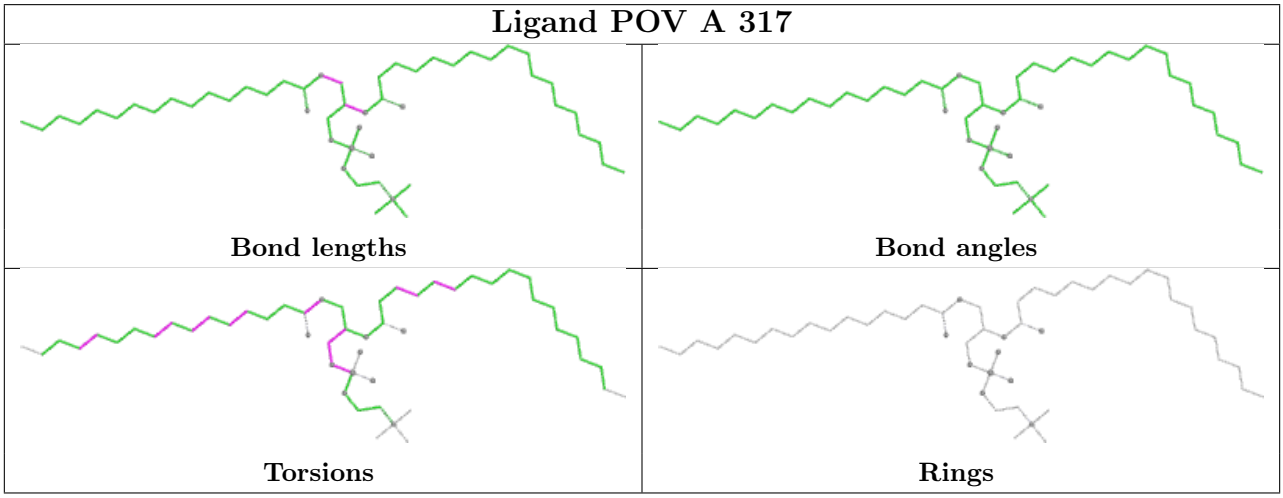

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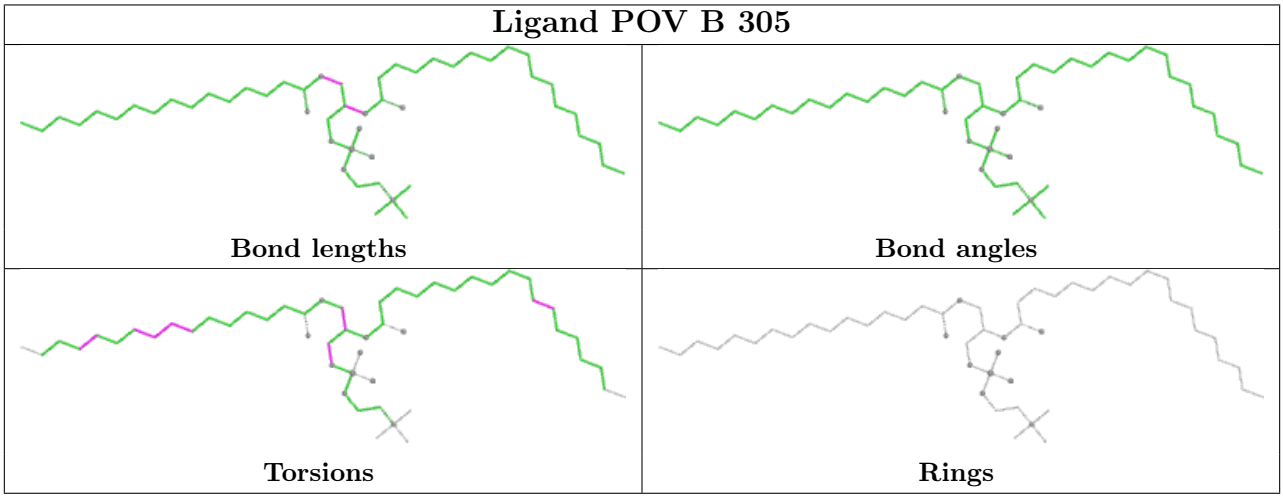

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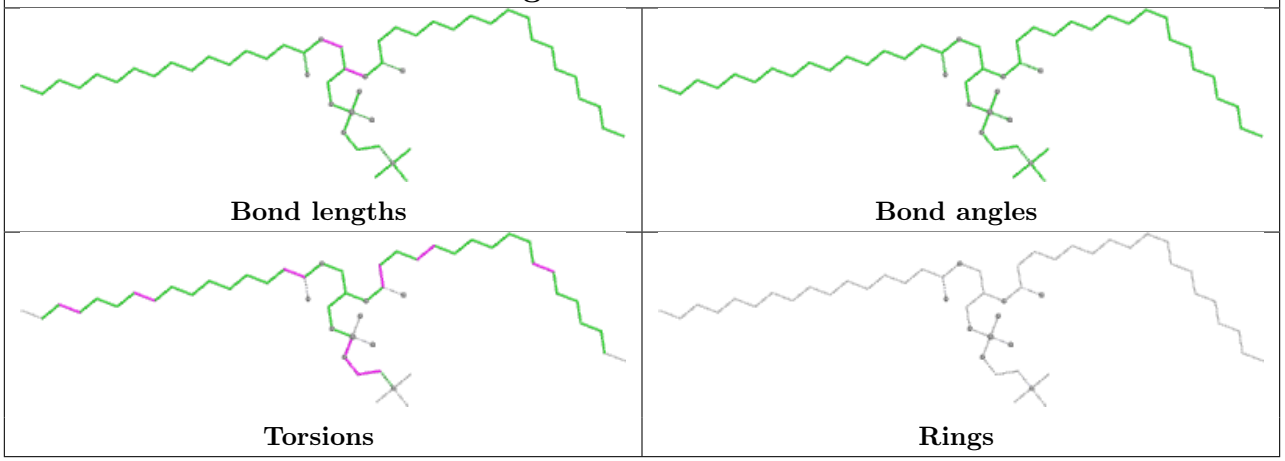

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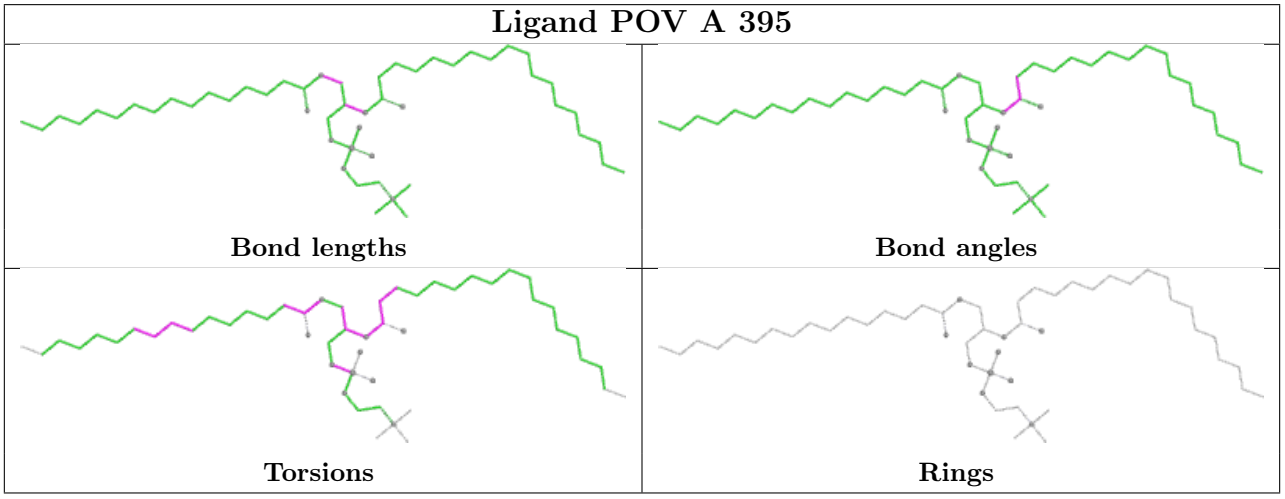

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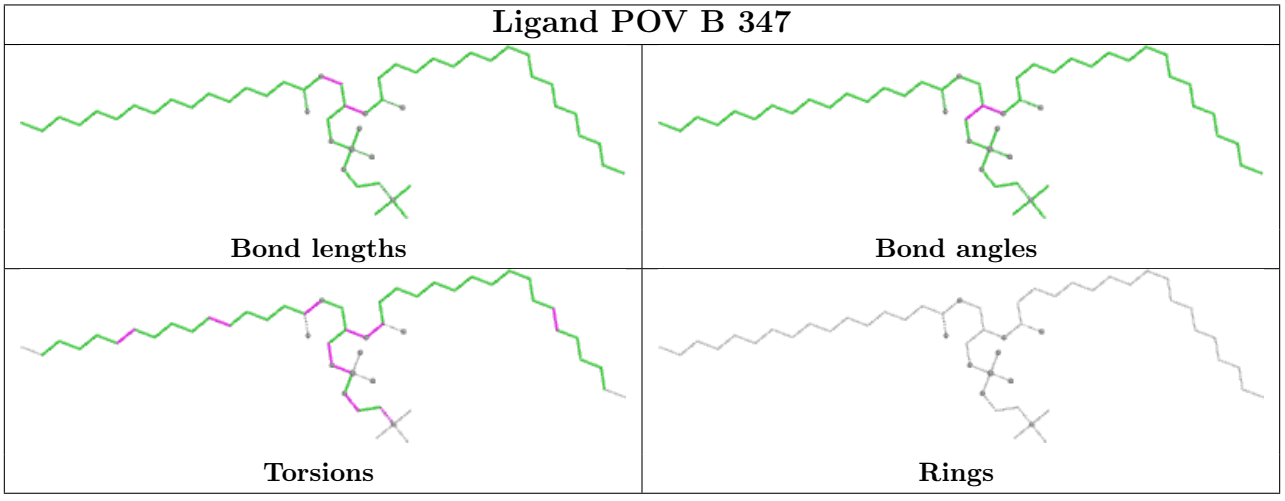

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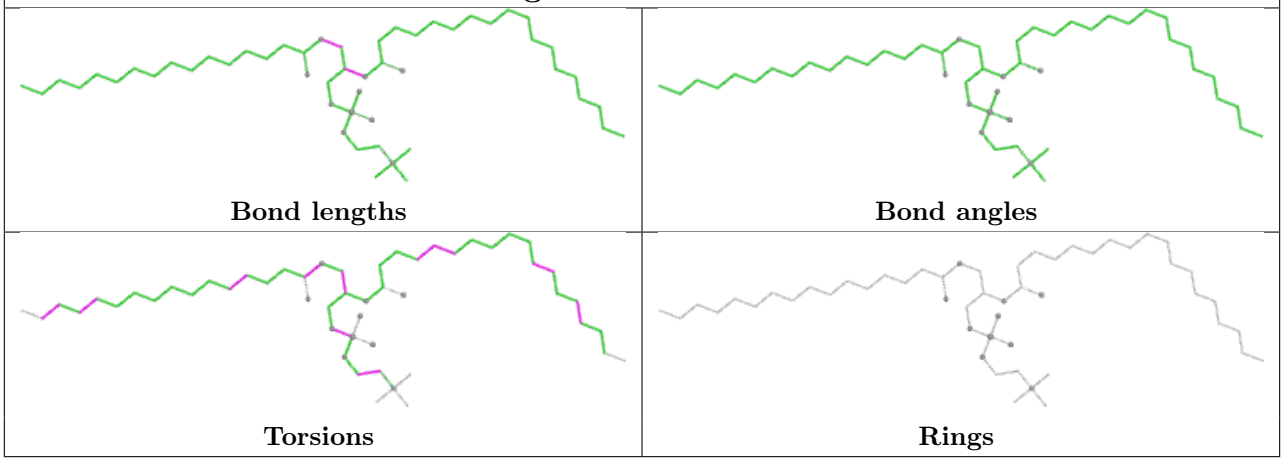

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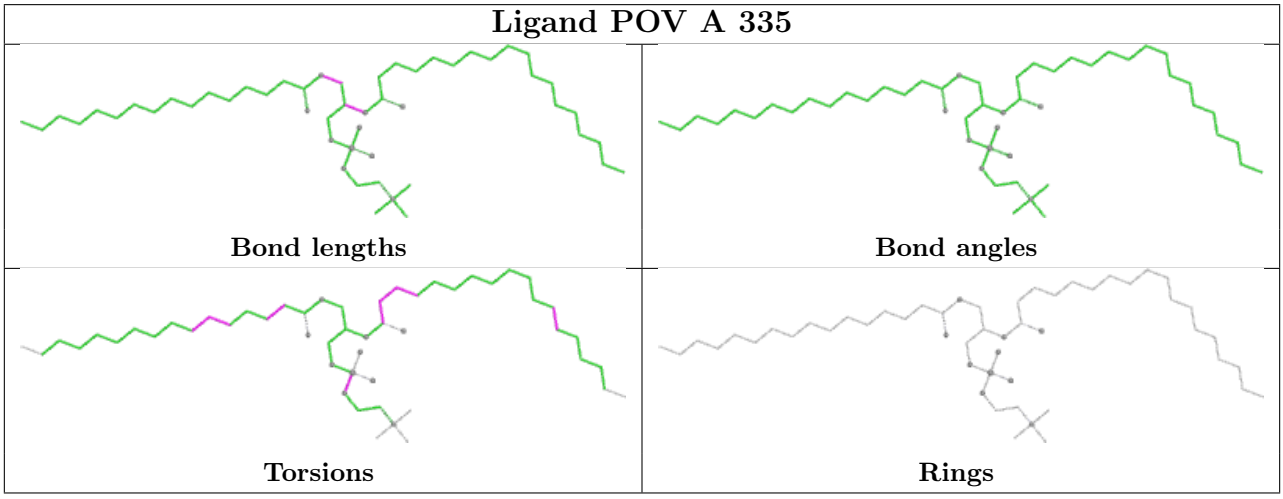

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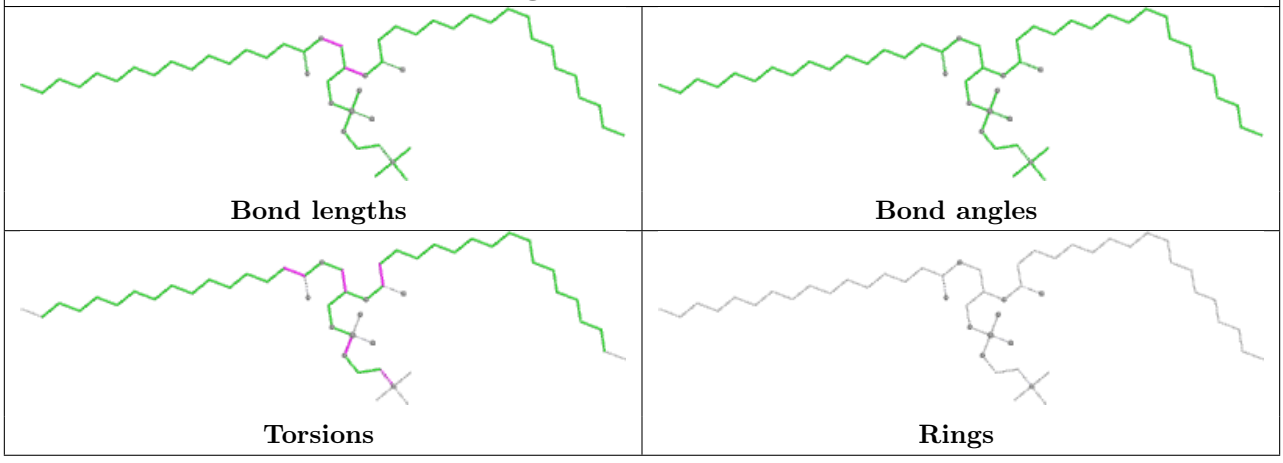

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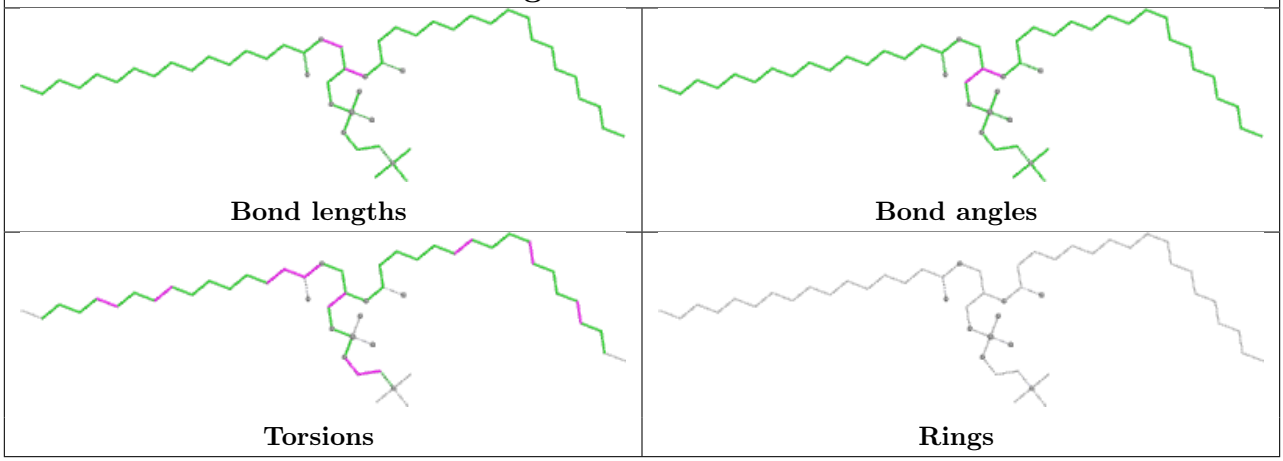

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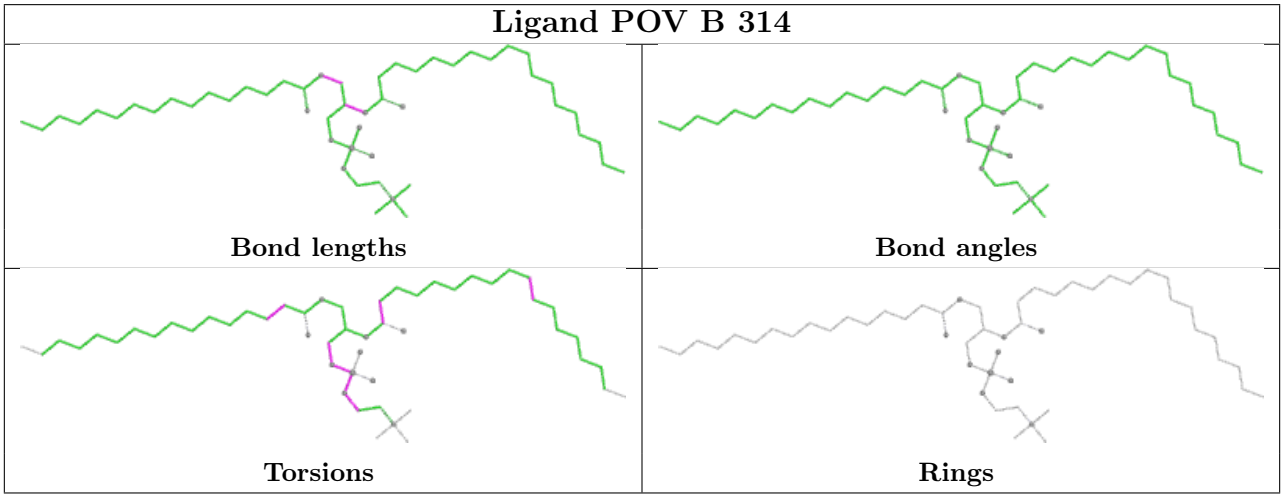

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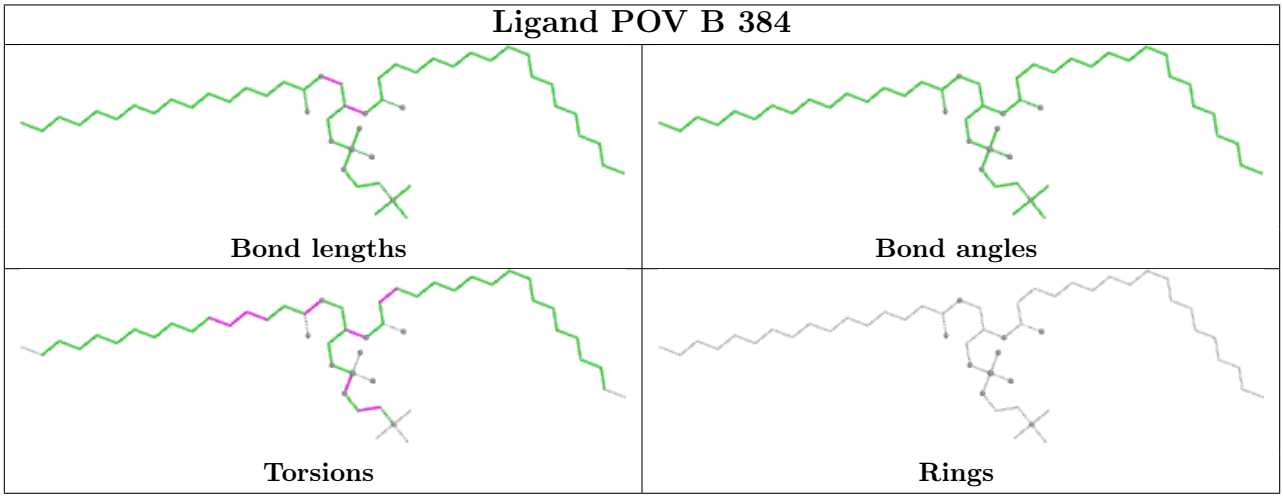

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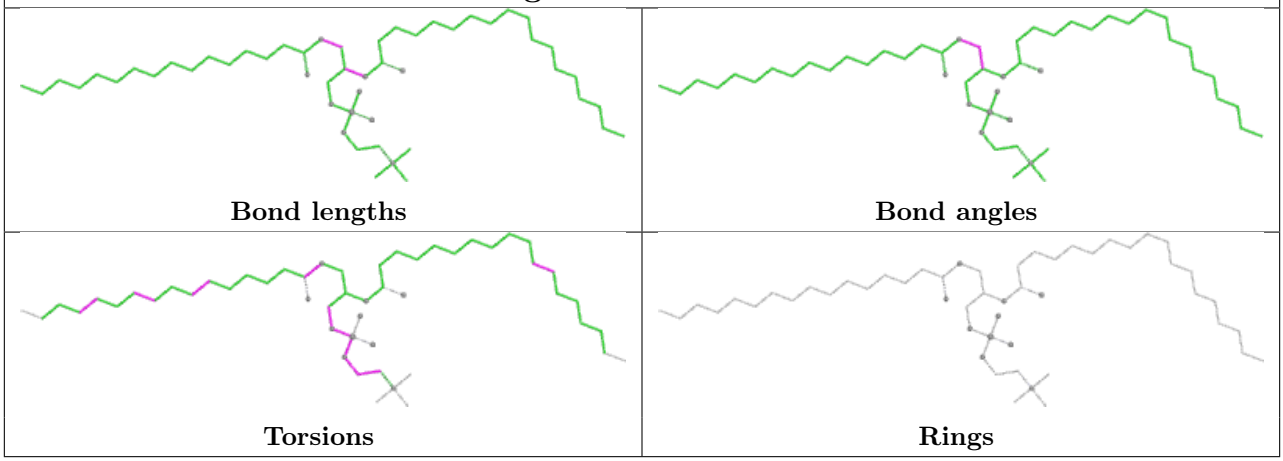

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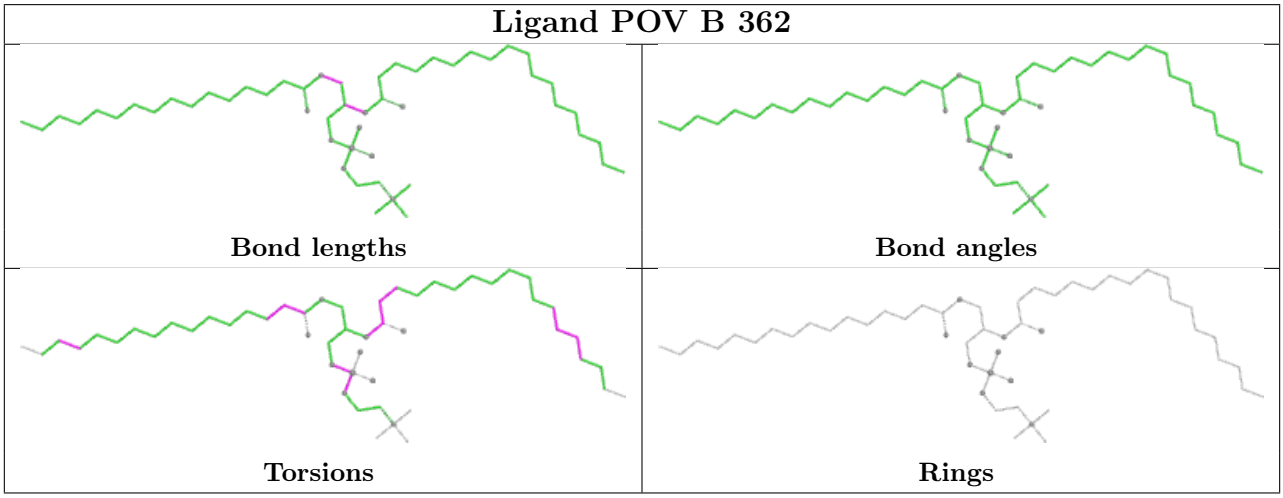

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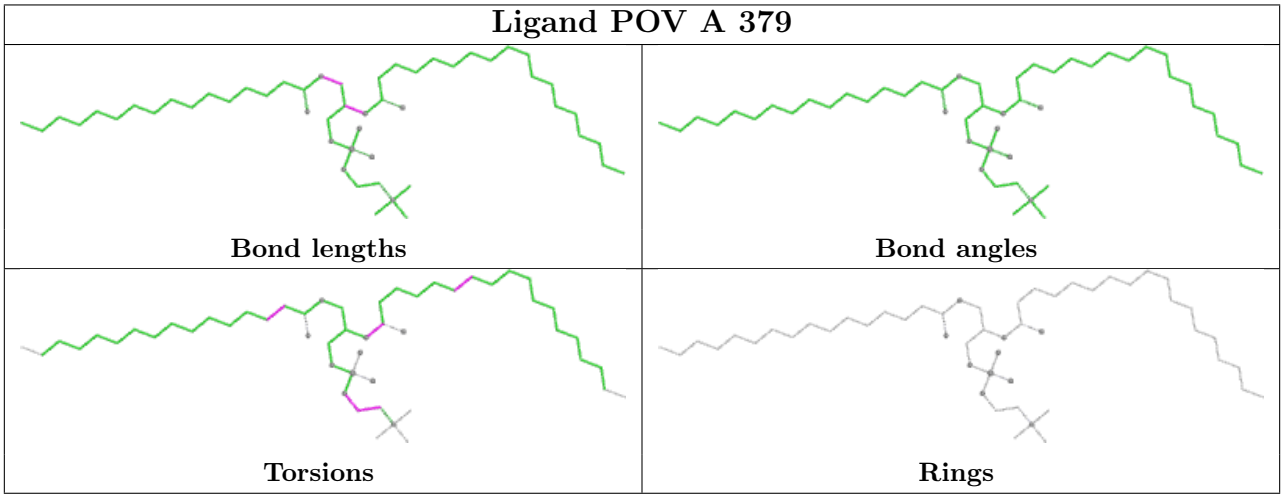

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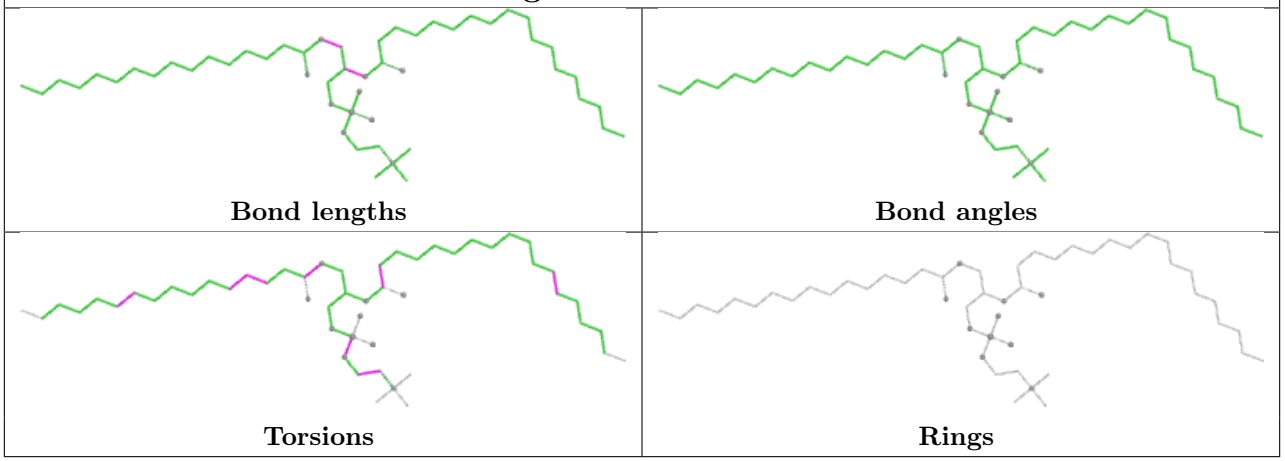

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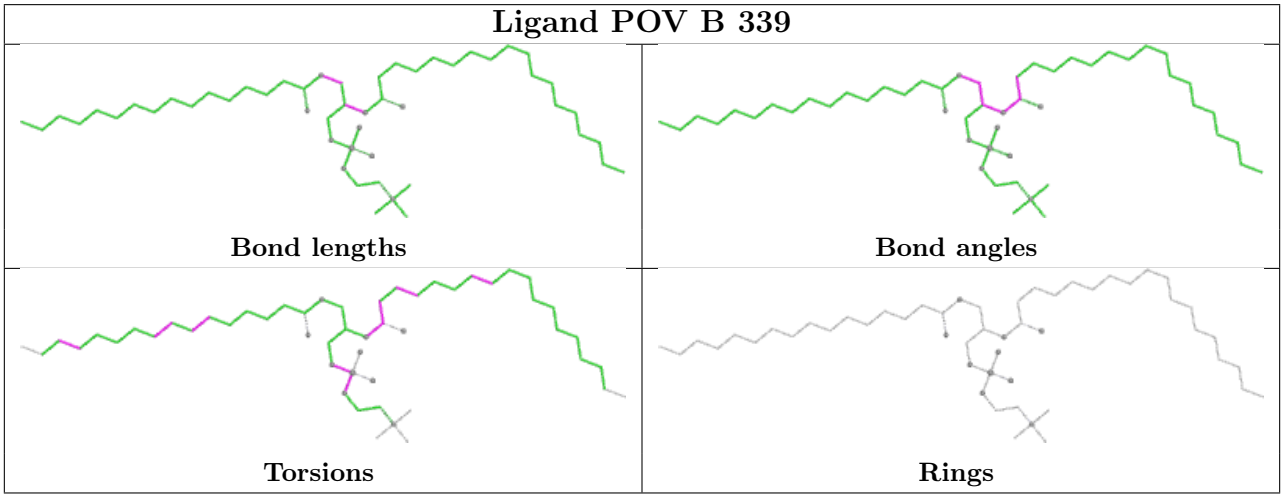

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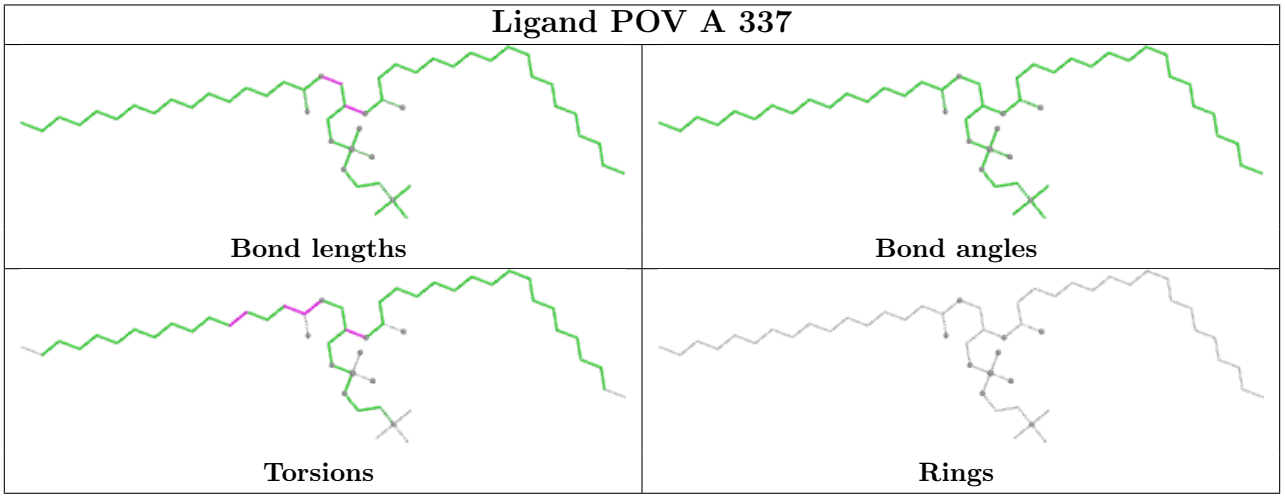

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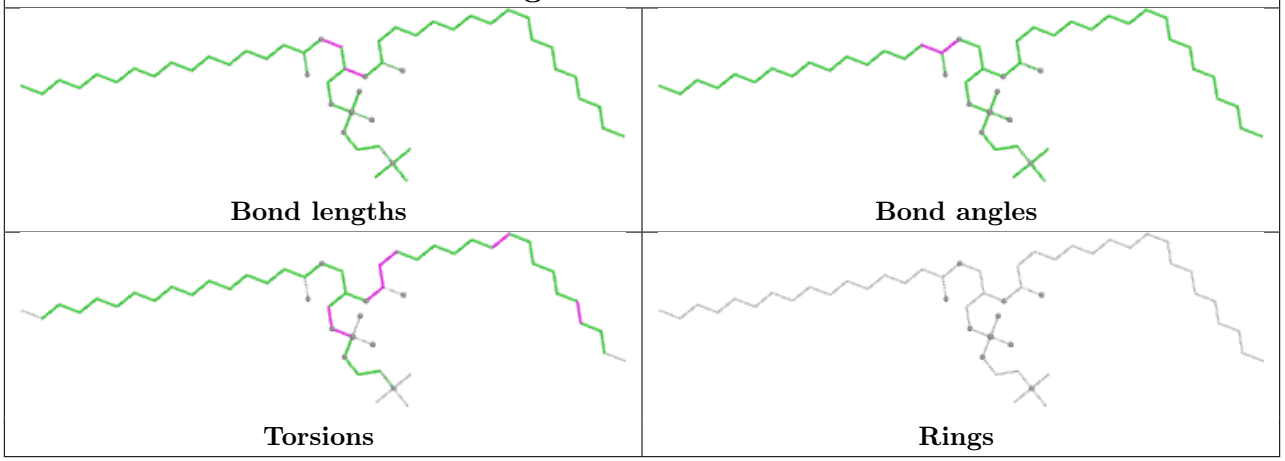

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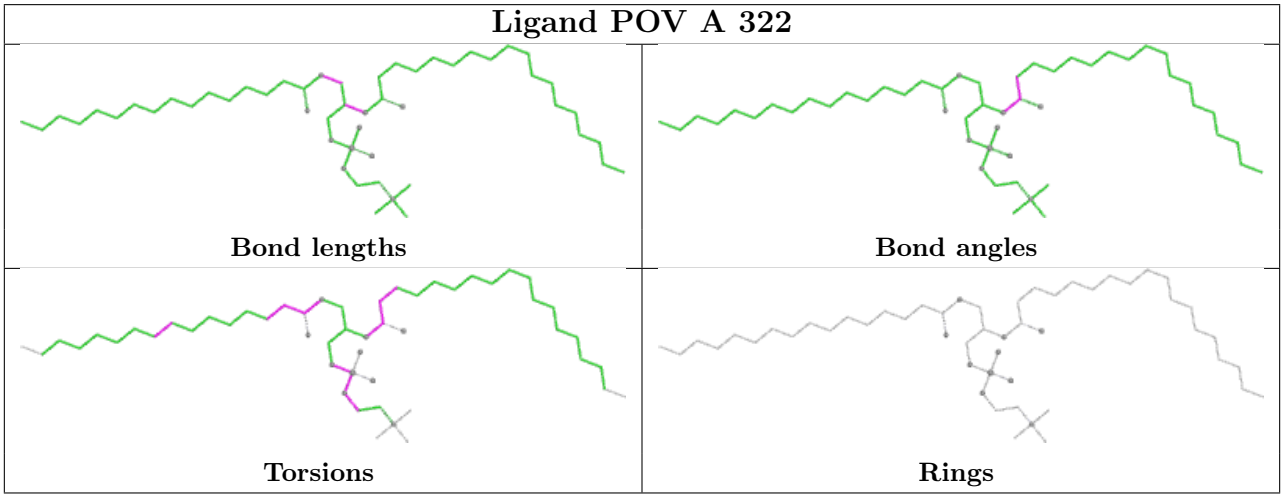

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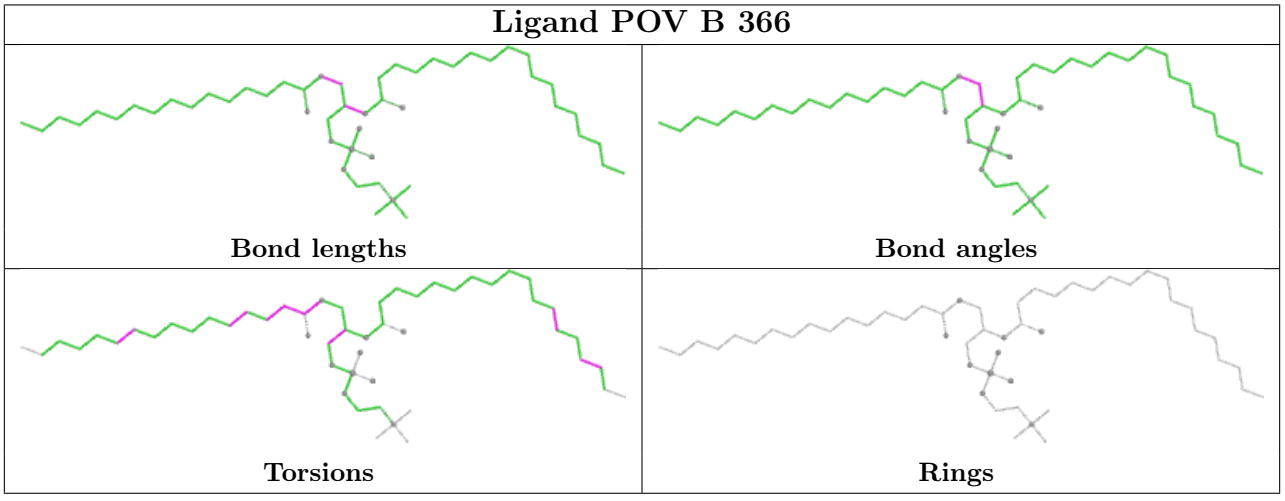

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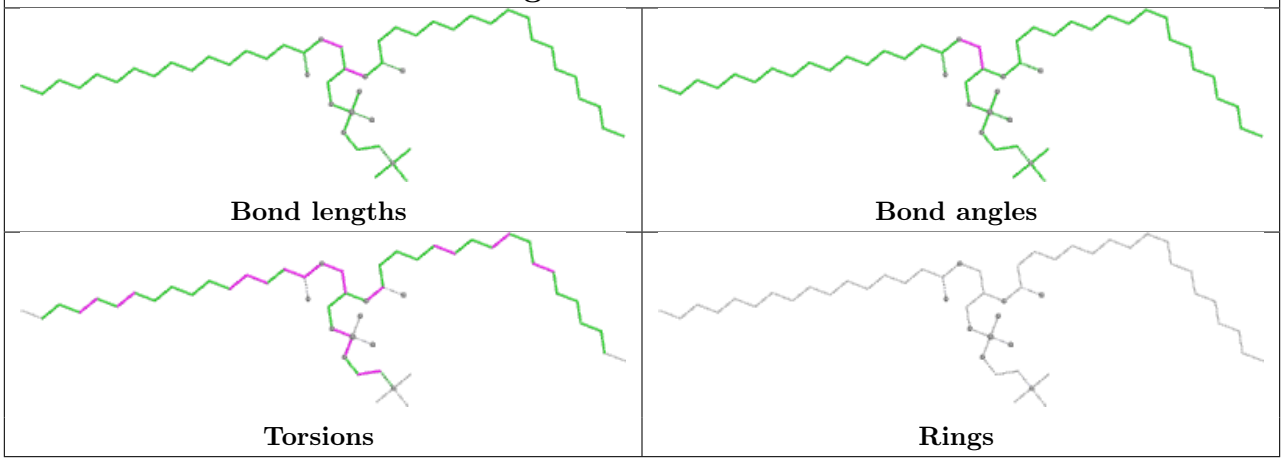

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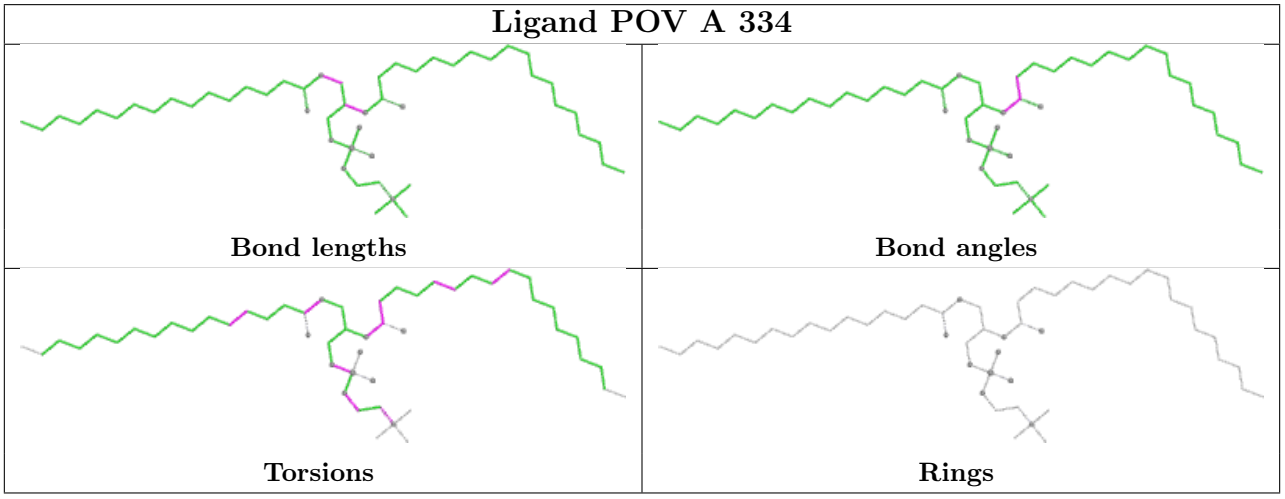

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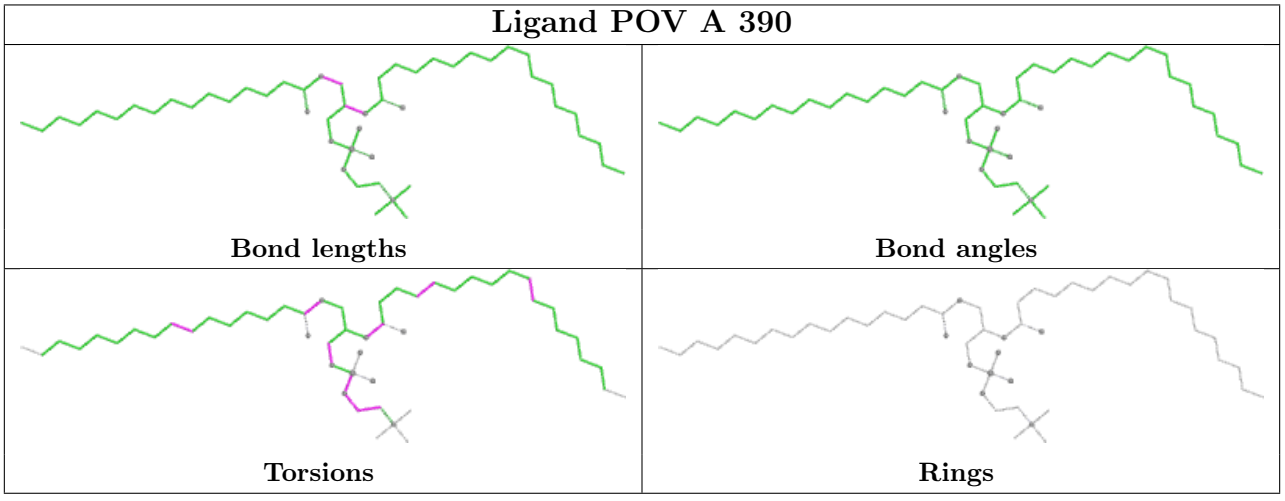

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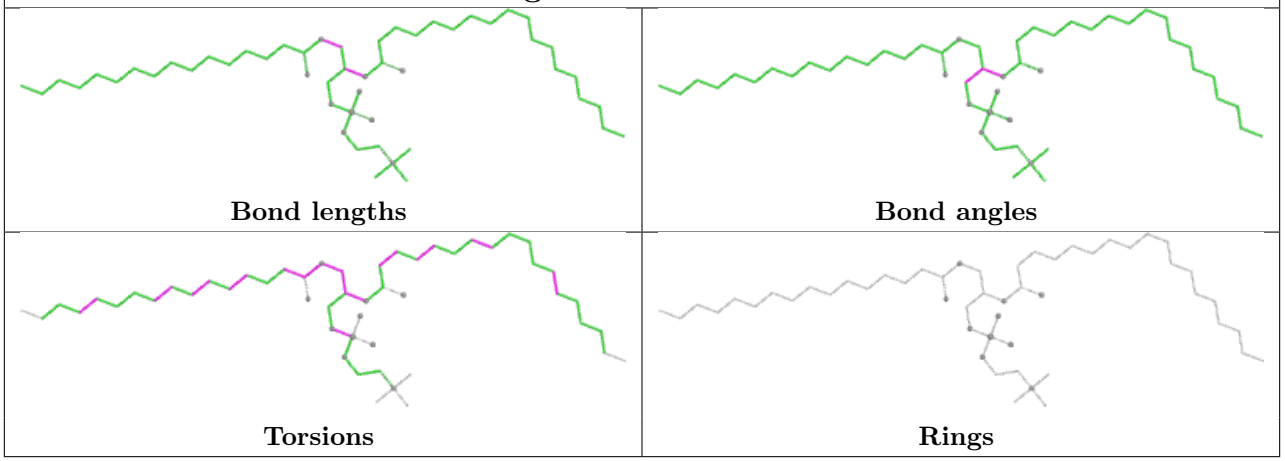

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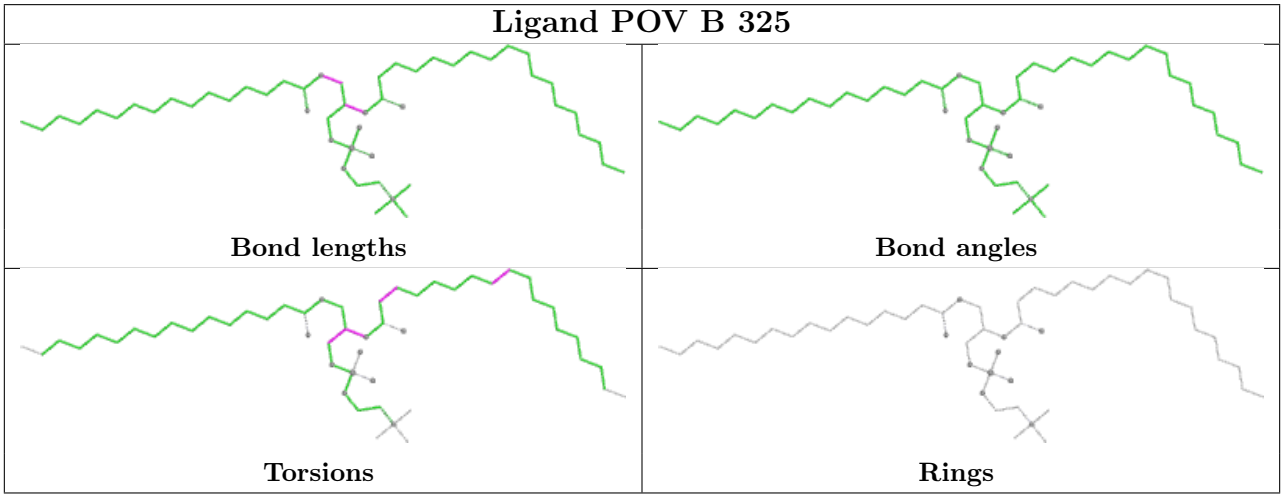

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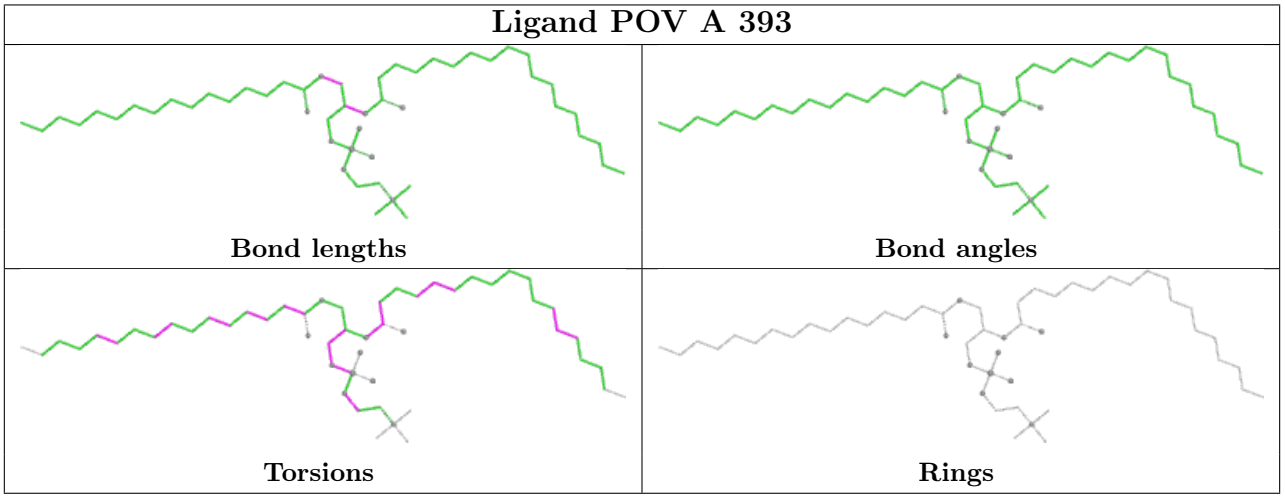

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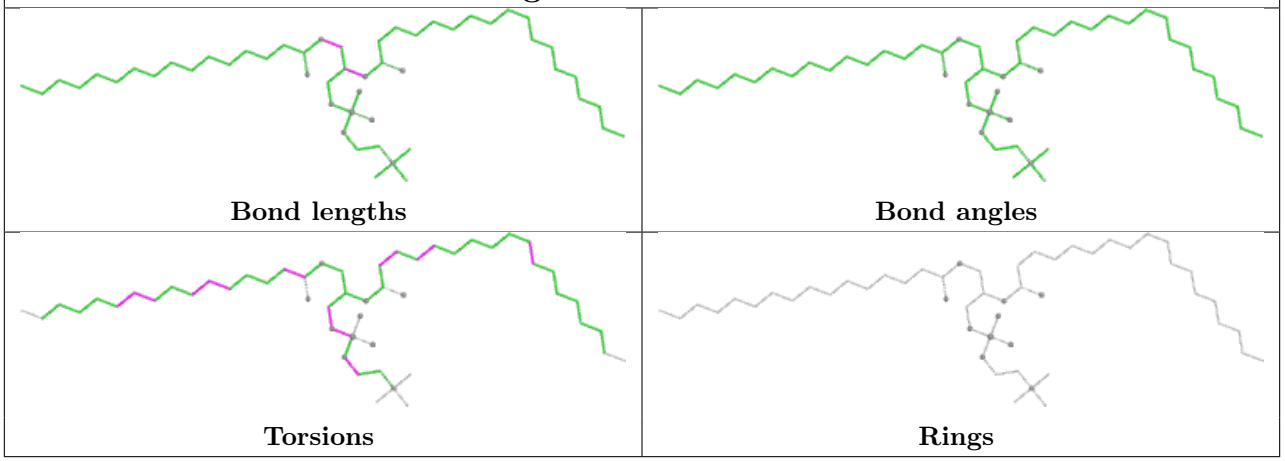

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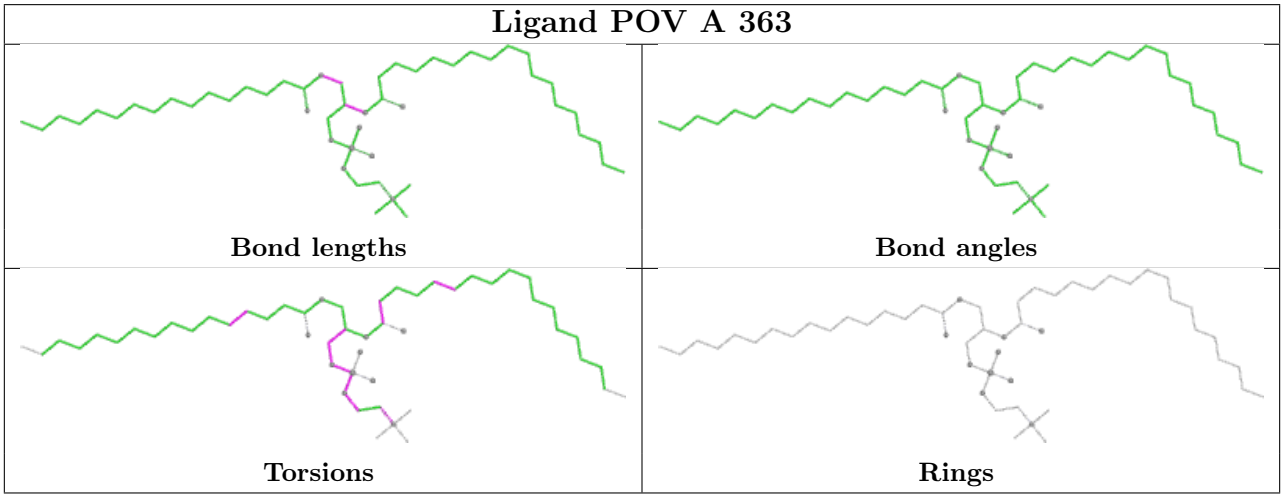

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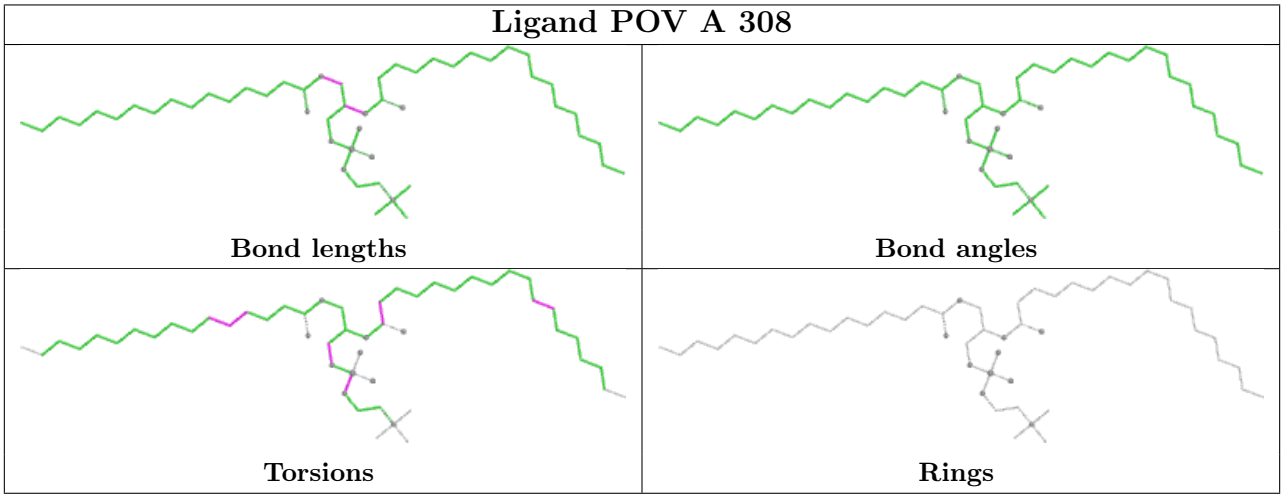

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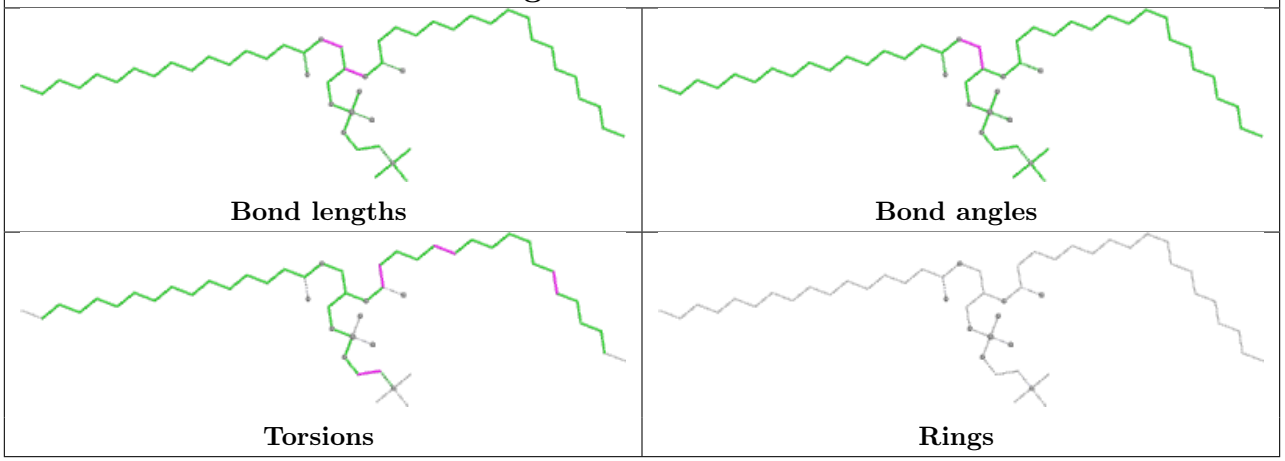

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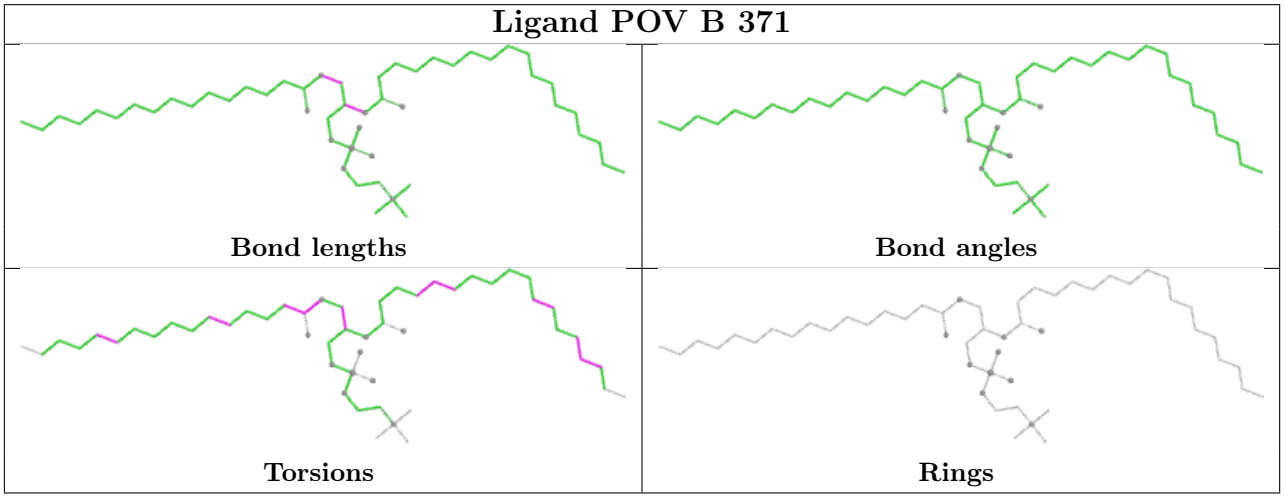

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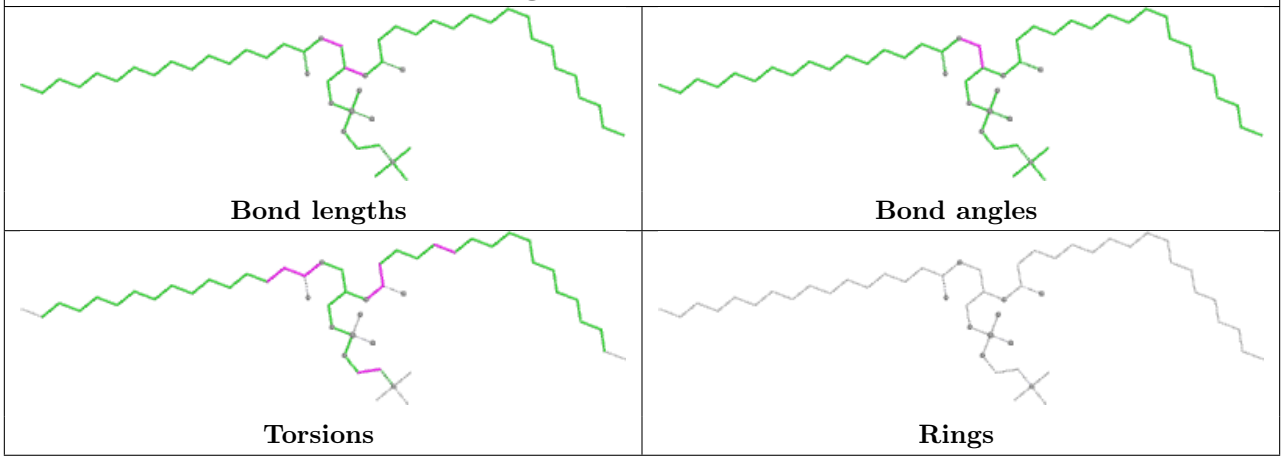

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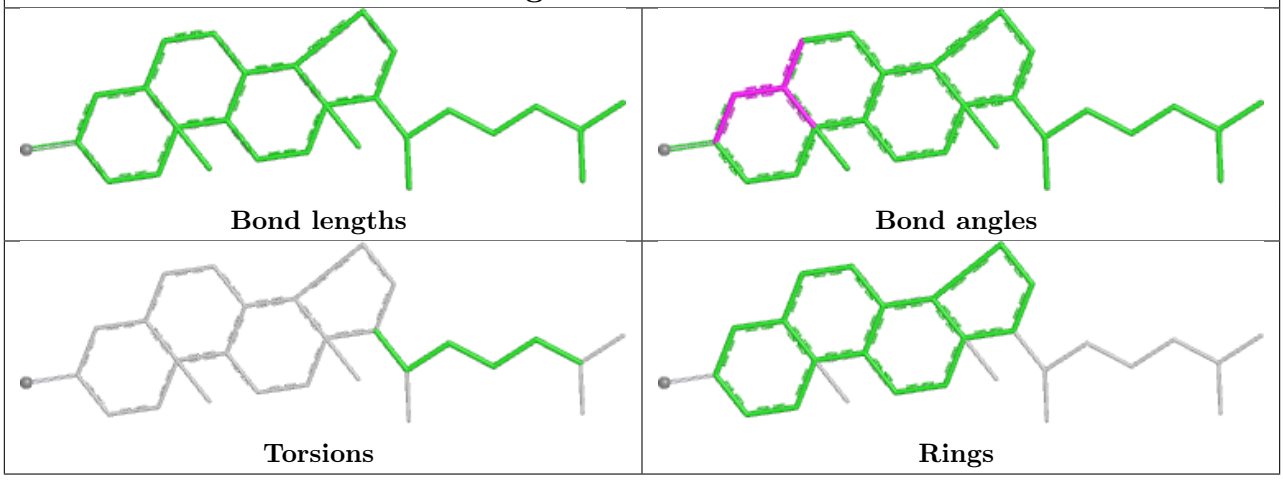

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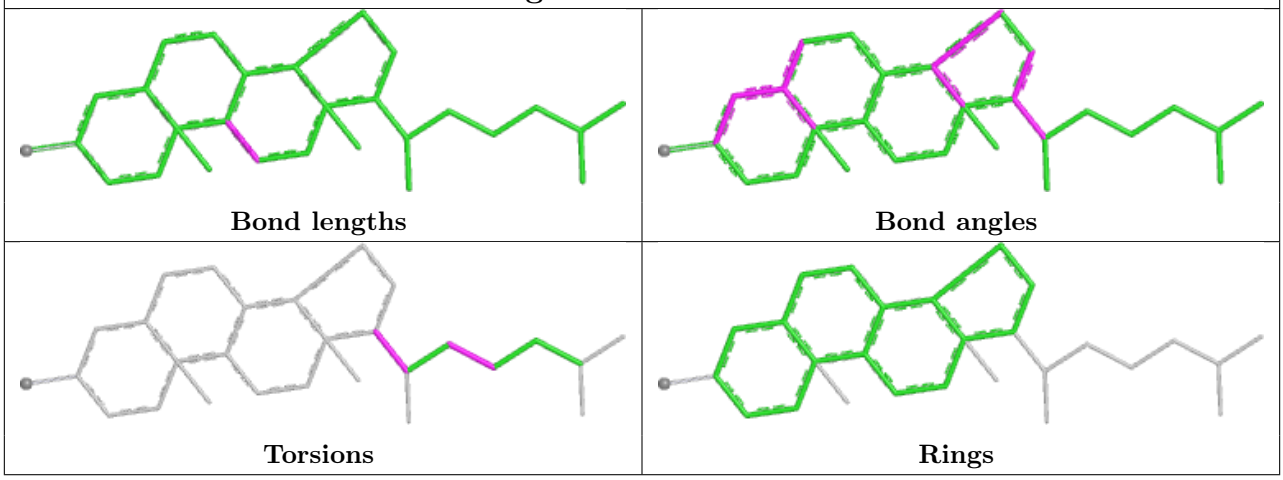

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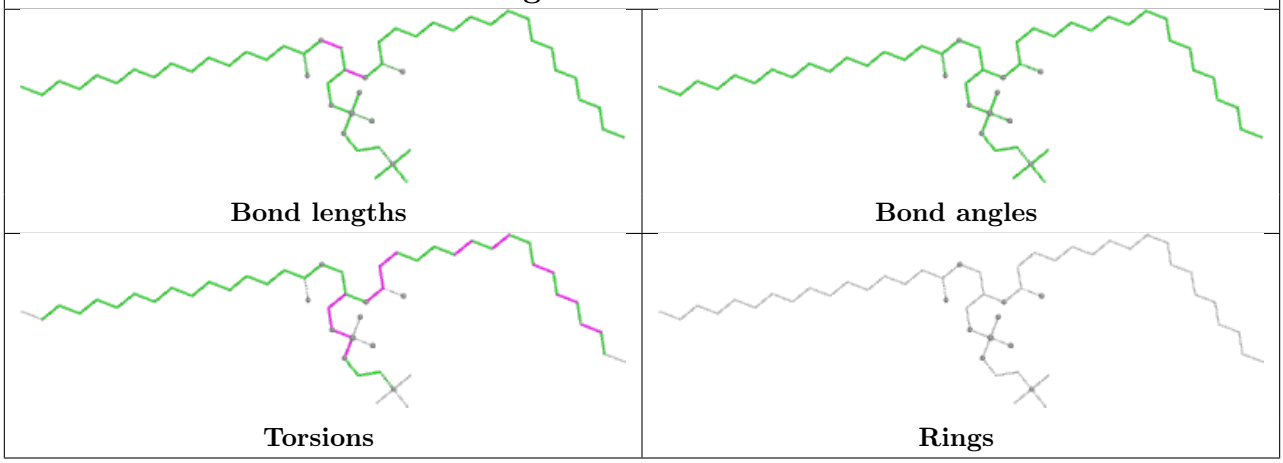

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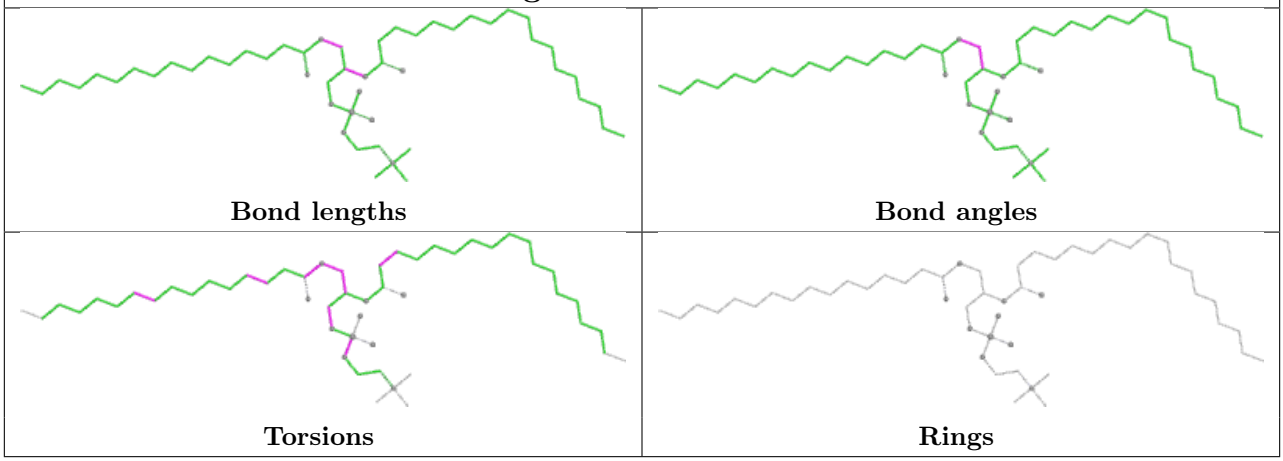

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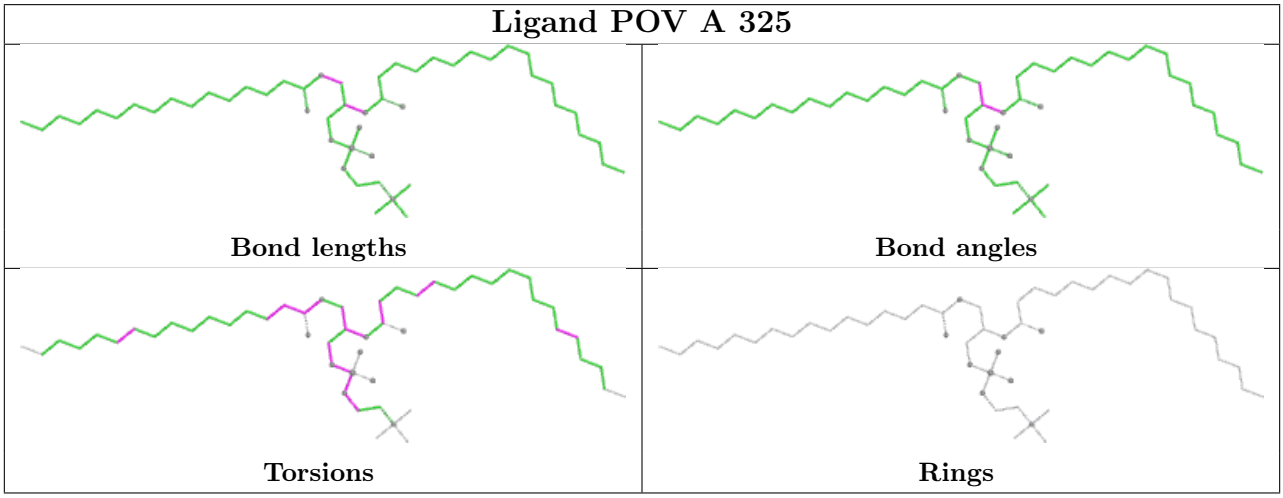

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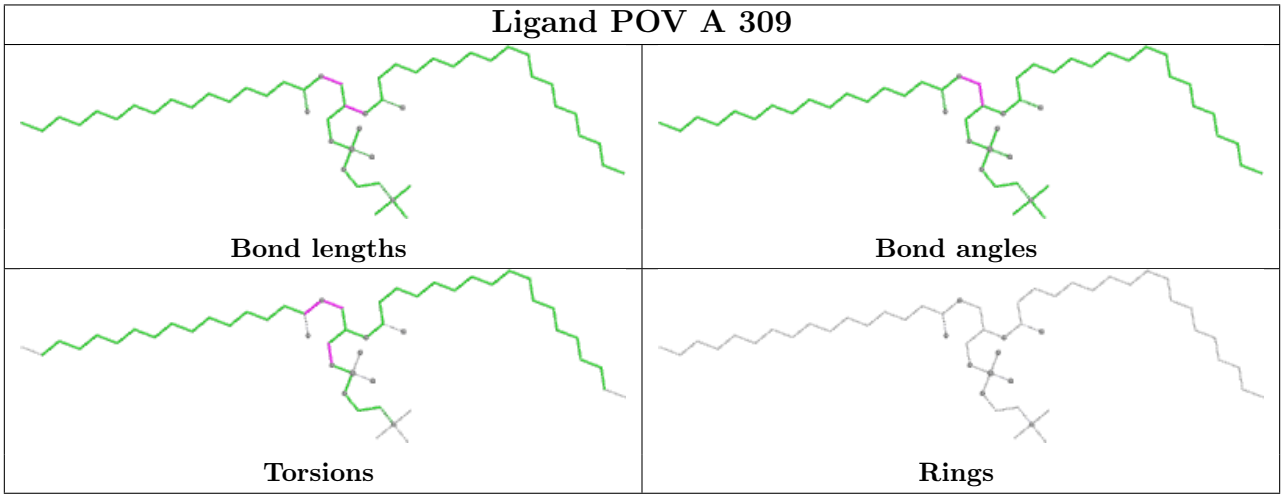

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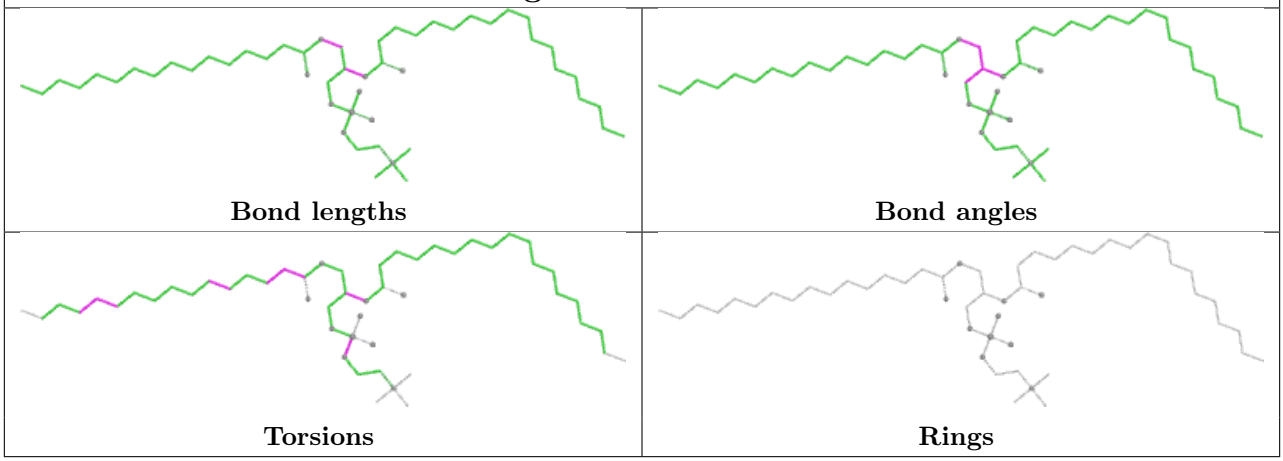

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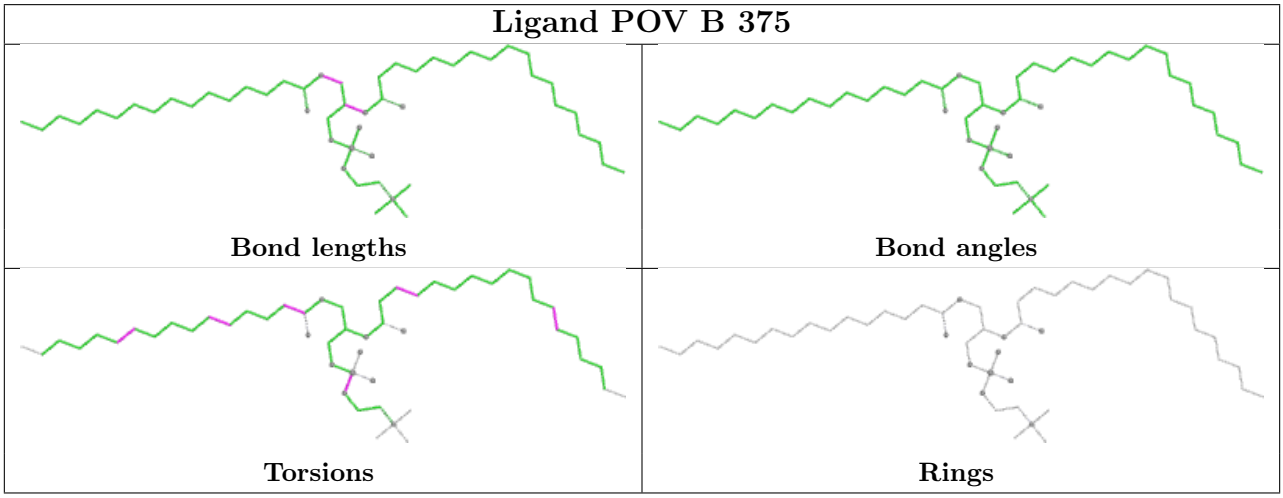

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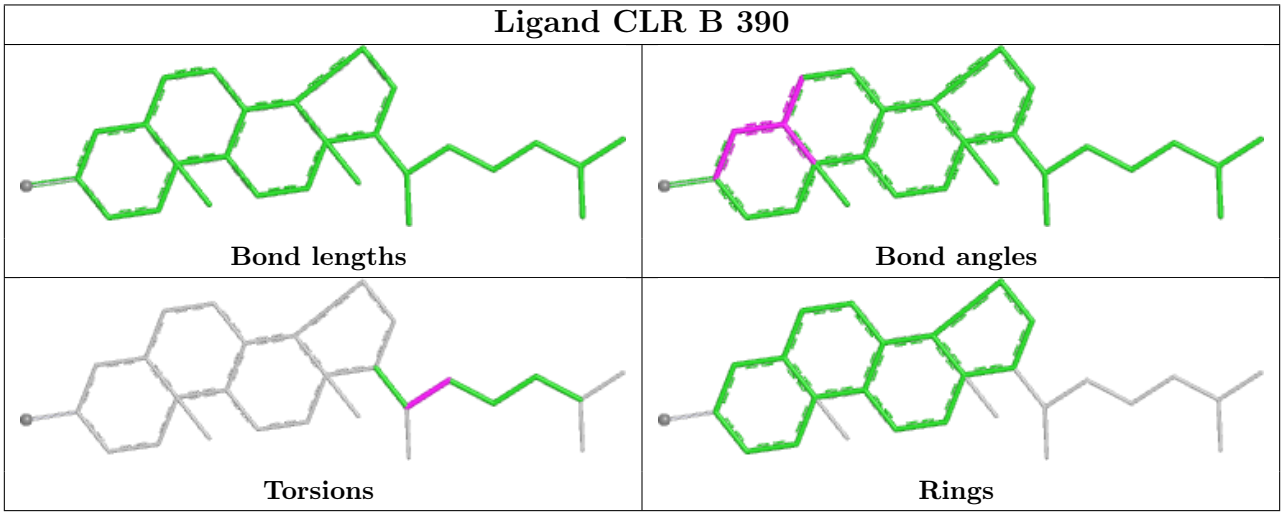

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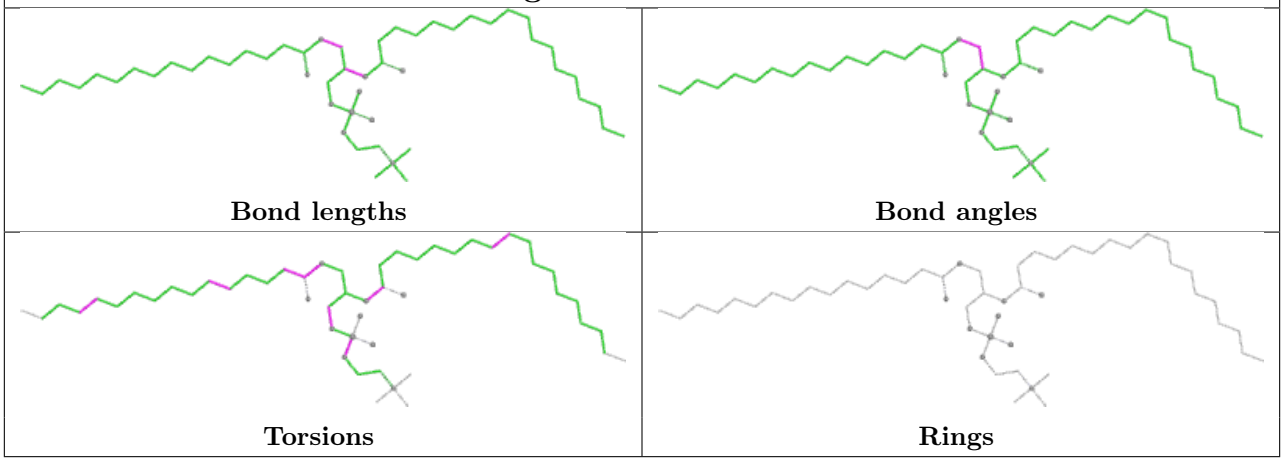

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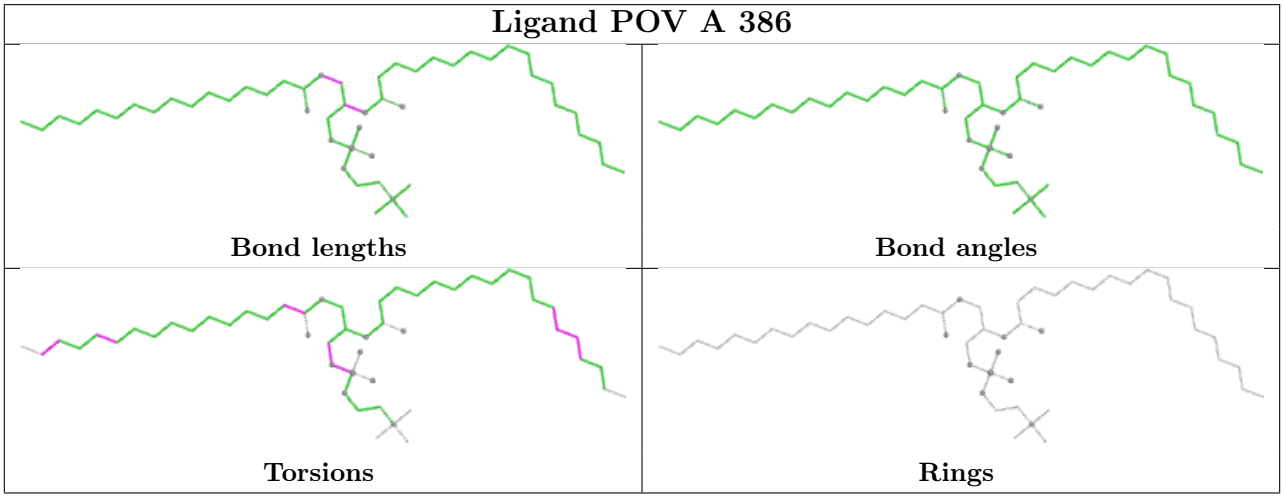

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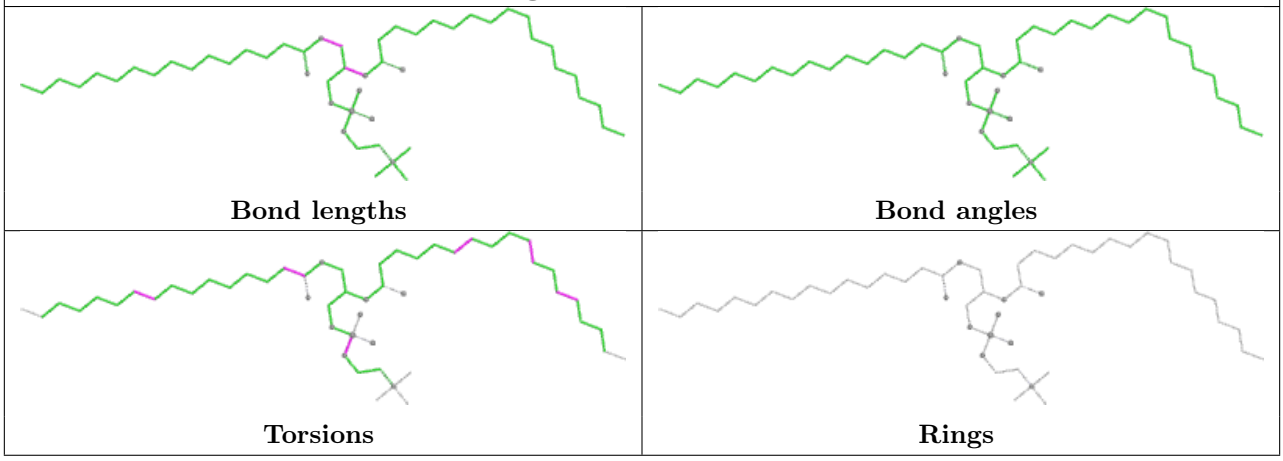

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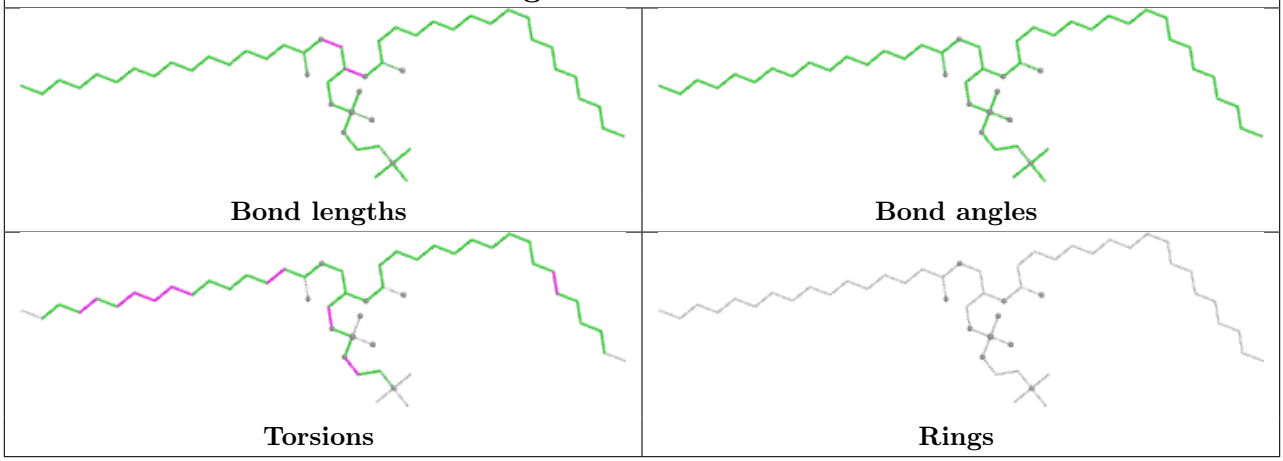

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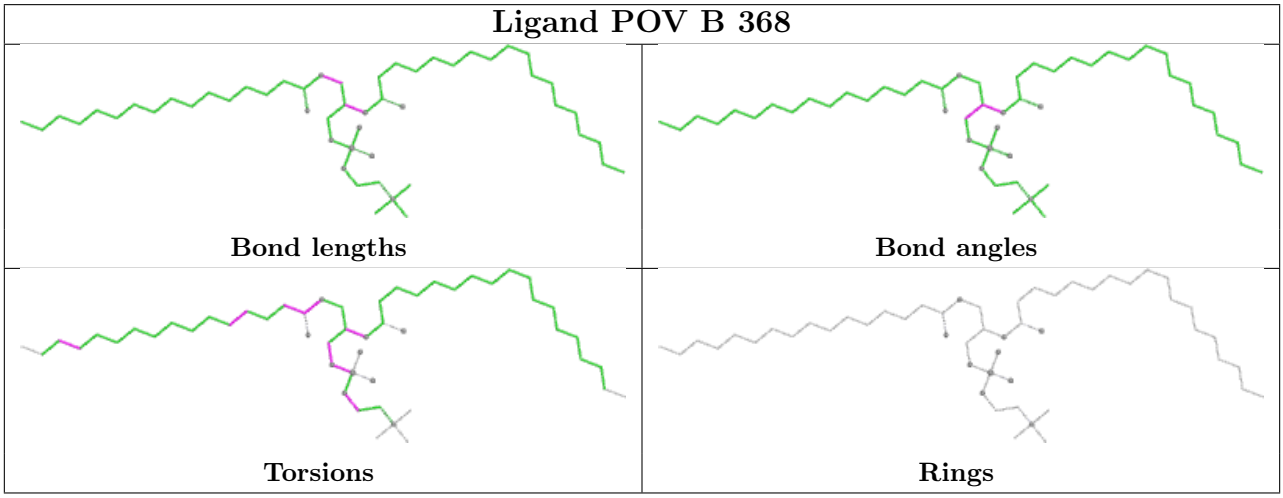

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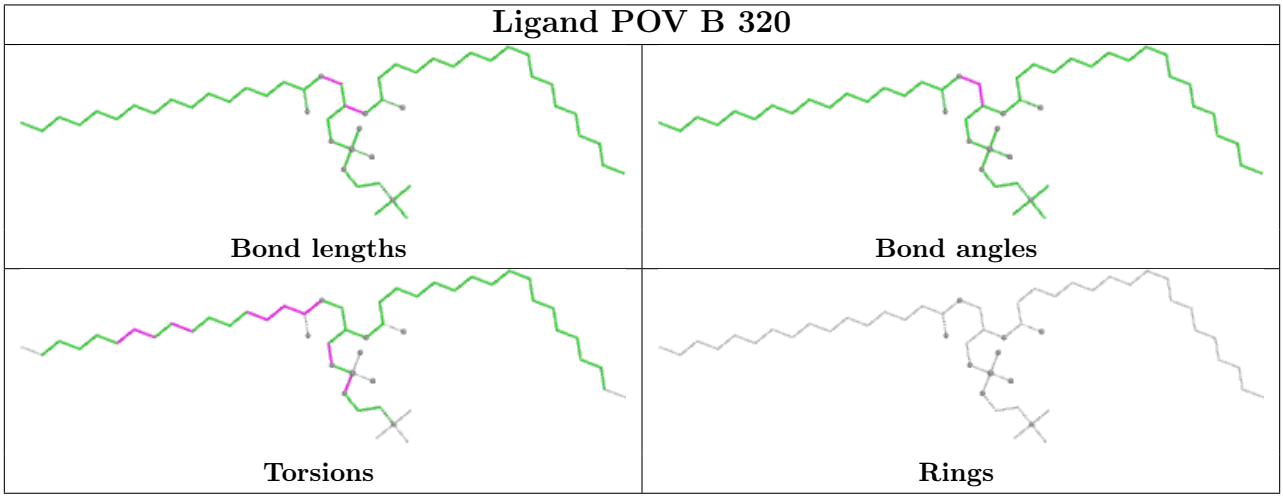
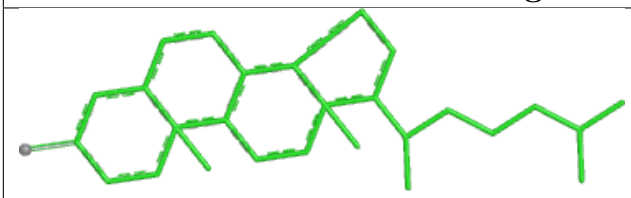
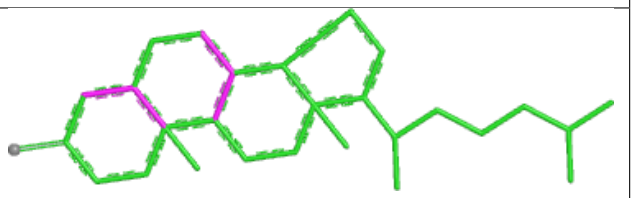


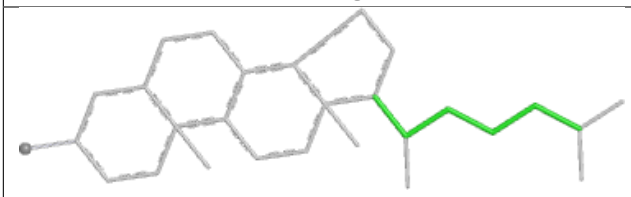
Ligand CLR B 393



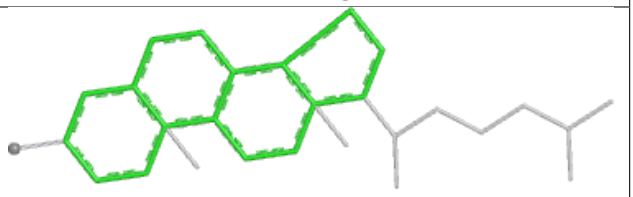
Bond lengths



Bond angles

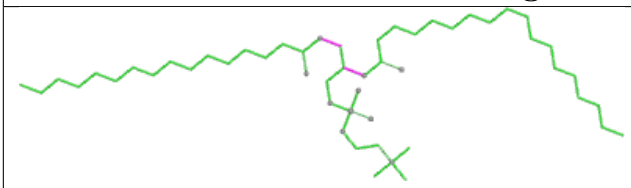


Torsions

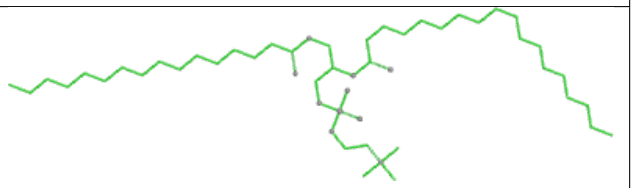


Rings

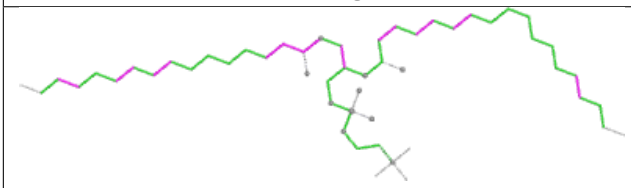
Ligand POV A 408



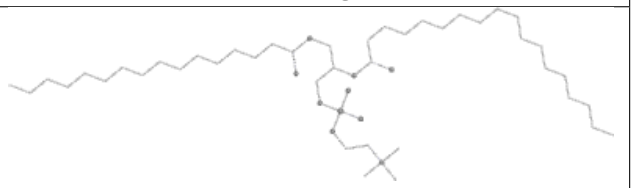
Bond lengths



Bond angles

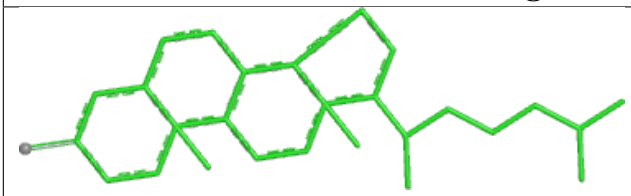


Torsions

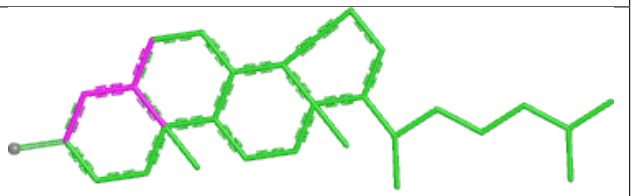


Rings

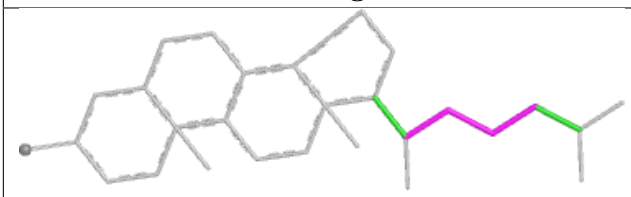
Ligand CLR B 399



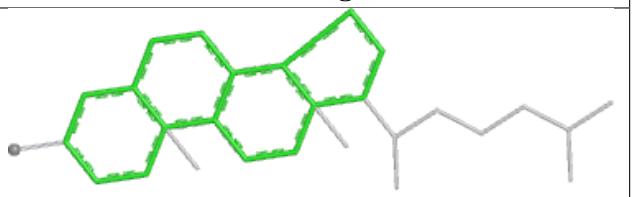
Bond lengths



Bond angles

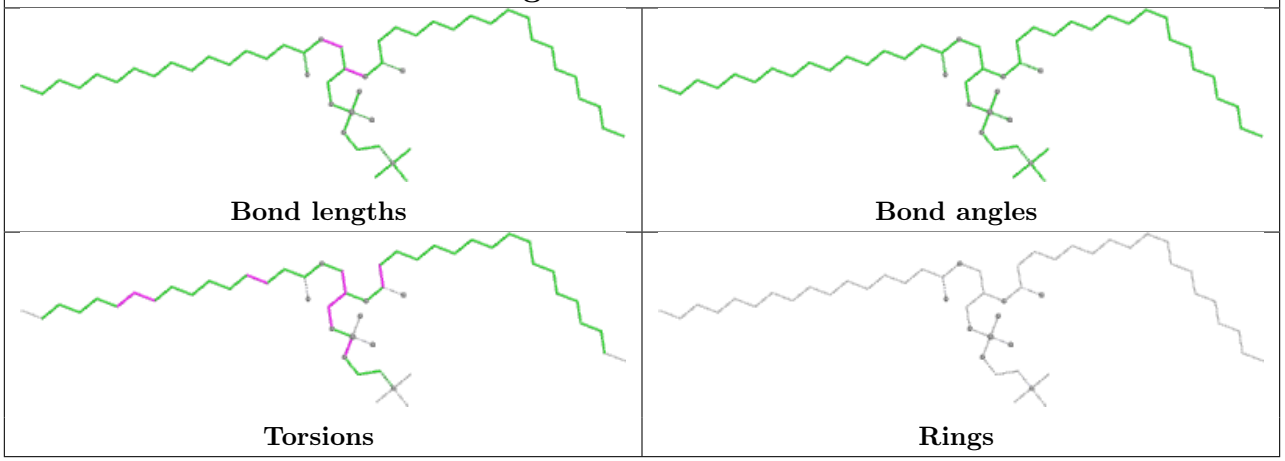


Torsions

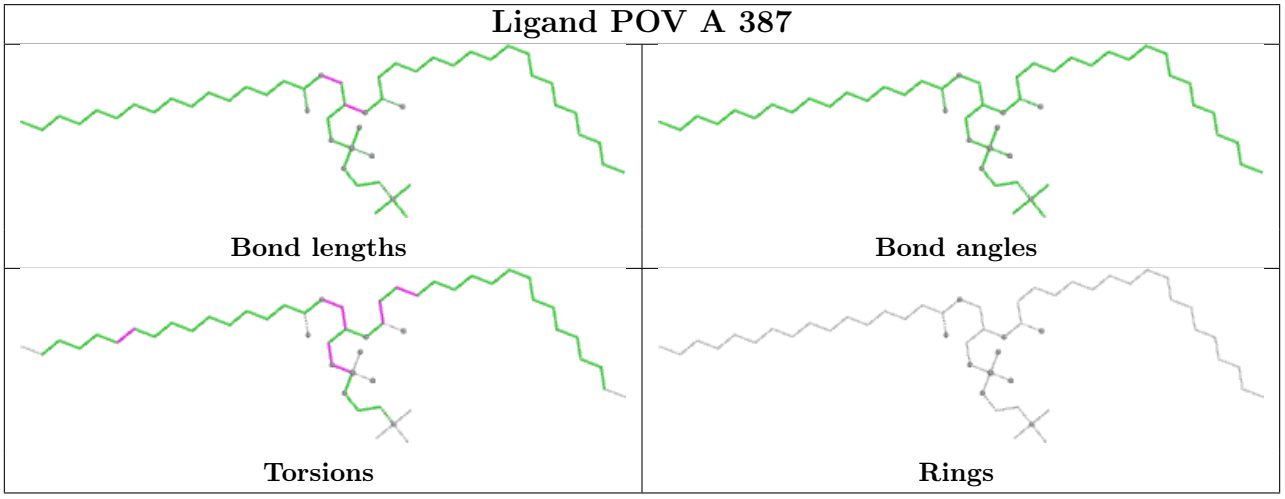


Rings

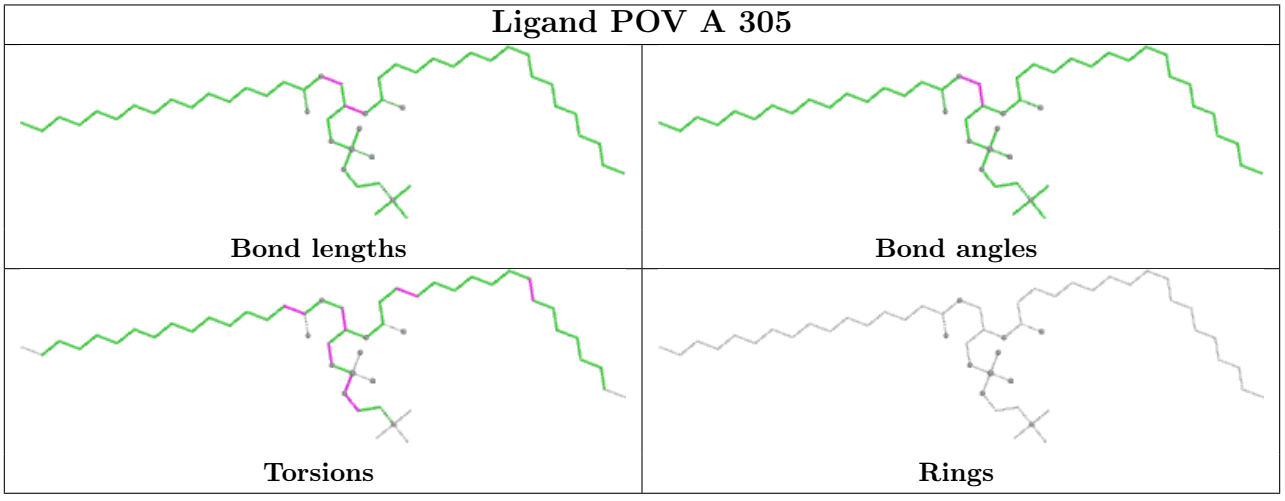
Ligand POV A 371



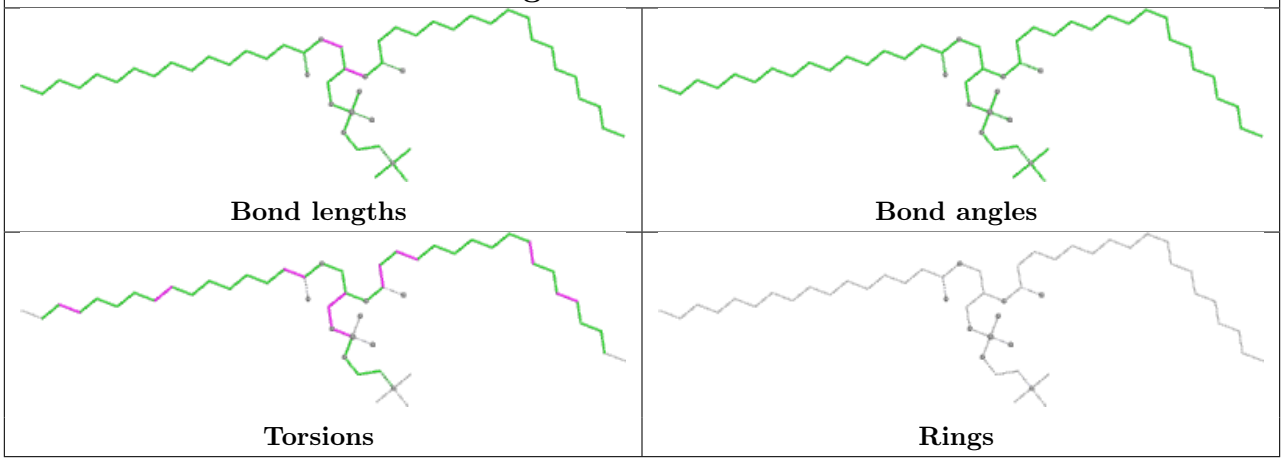
Ligand POV A 387



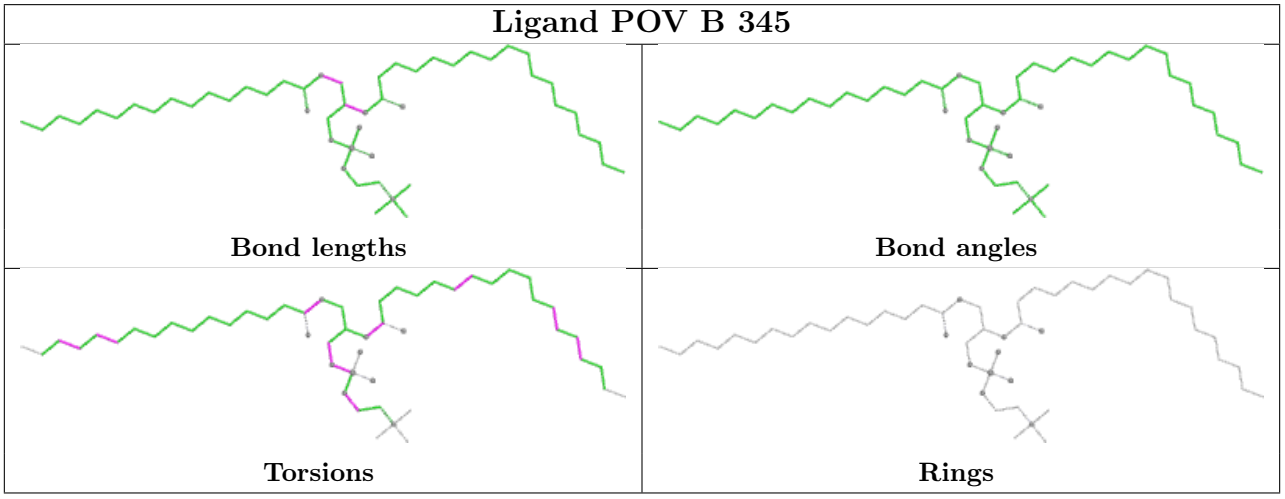
Ligand POV A 305



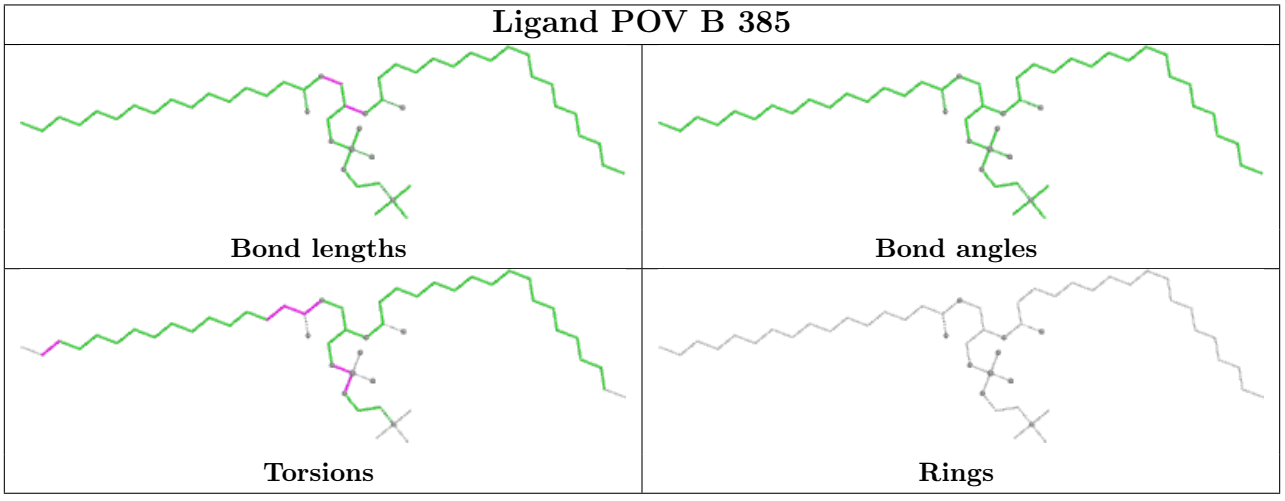
Ligand POV A 394



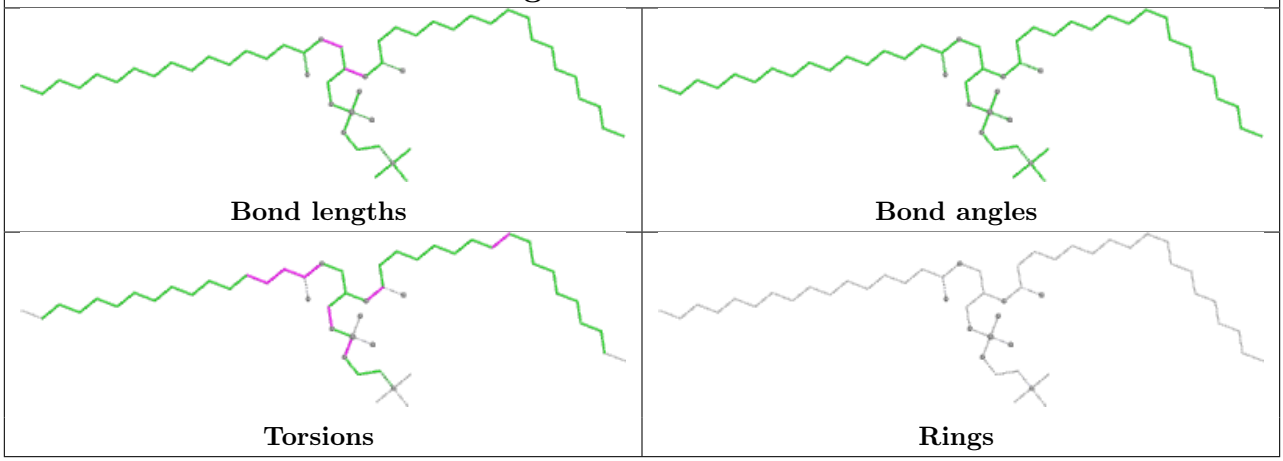
Ligand POV B 345



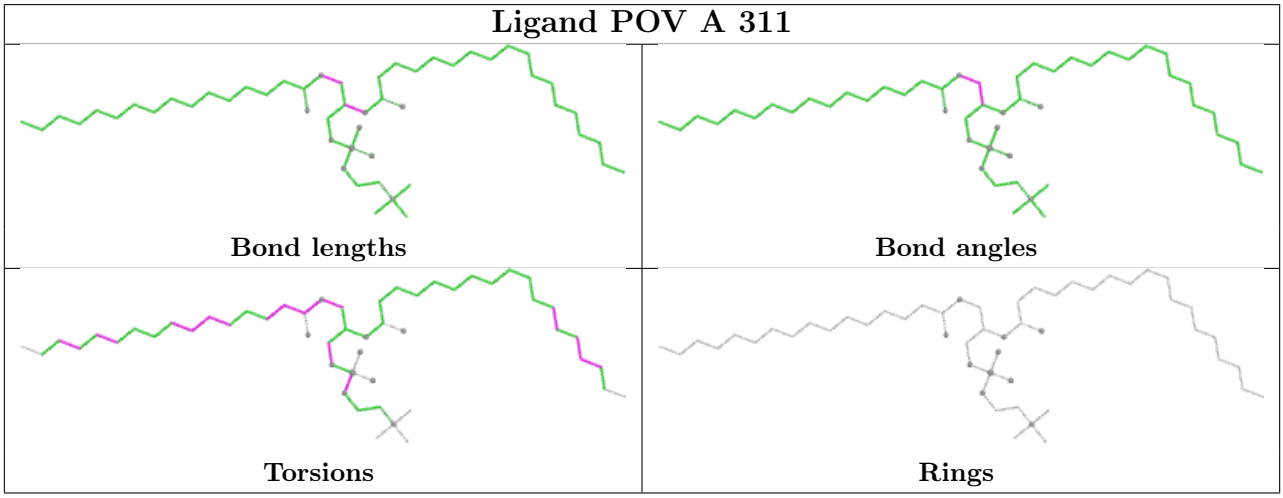
Ligand POV B 385



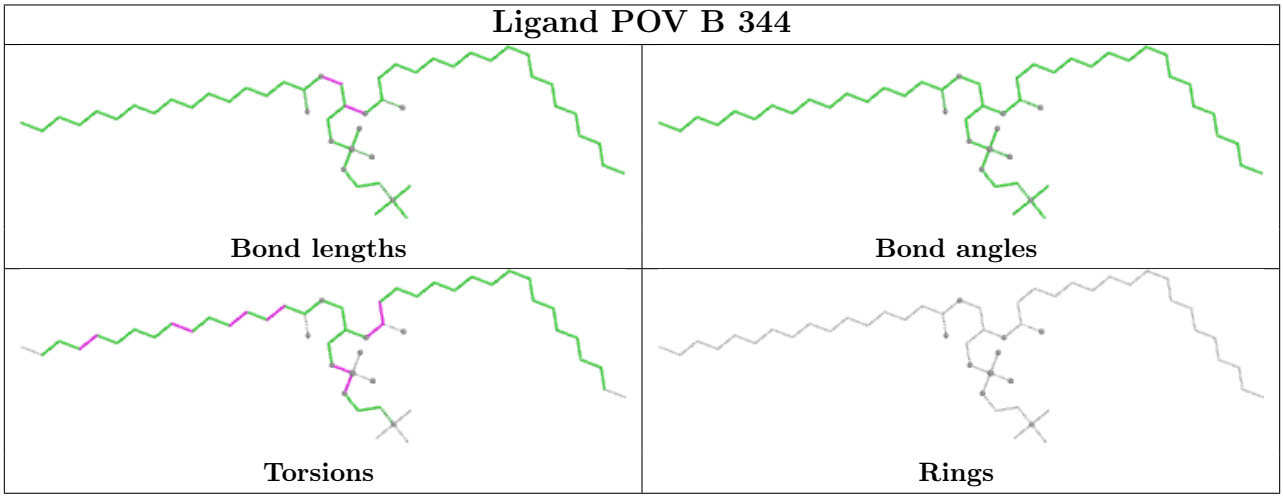
Ligand POV B 387



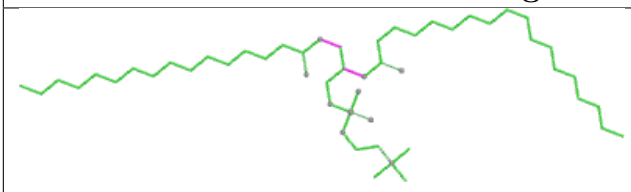
Ligand POV A 311



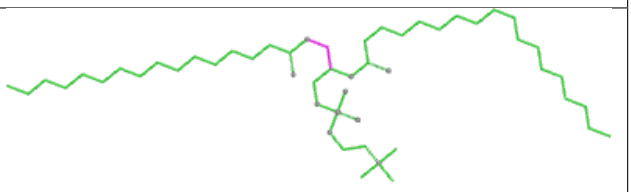
Ligand POV B 344



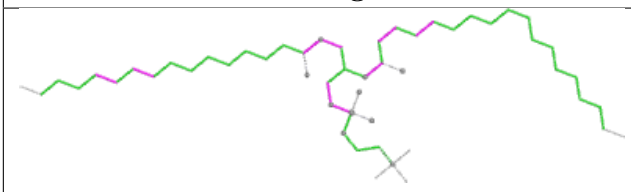
Ligand POV A 362



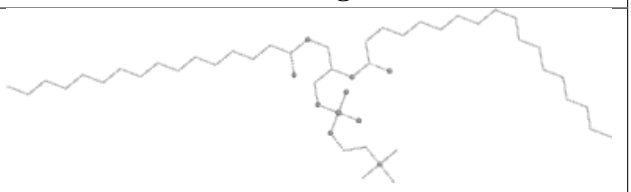
Bond lengths



Bond angles

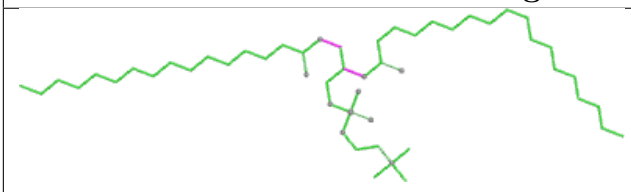


Torsions

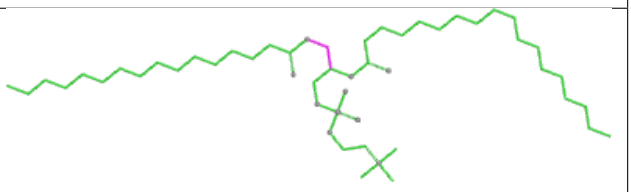


Rings

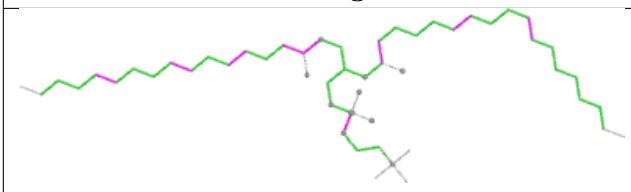
Ligand POV B 383



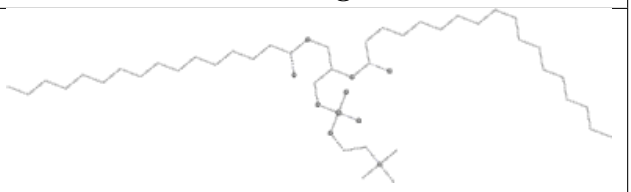
Bond lengths



Bond angles

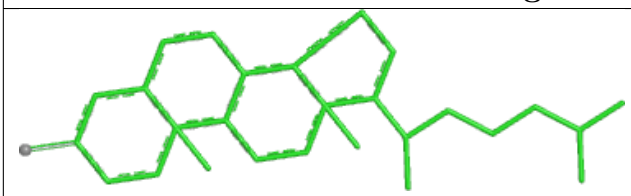


Torsions

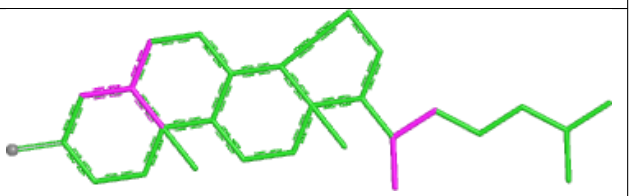


Rings

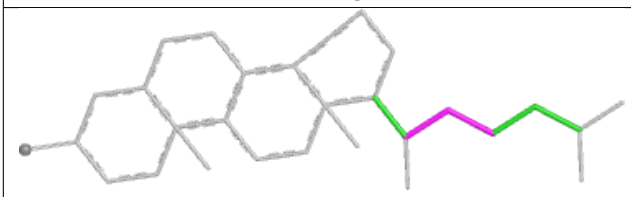
Ligand CLR A 421



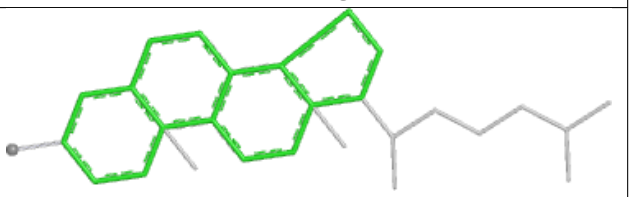
Bond lengths



Bond angles

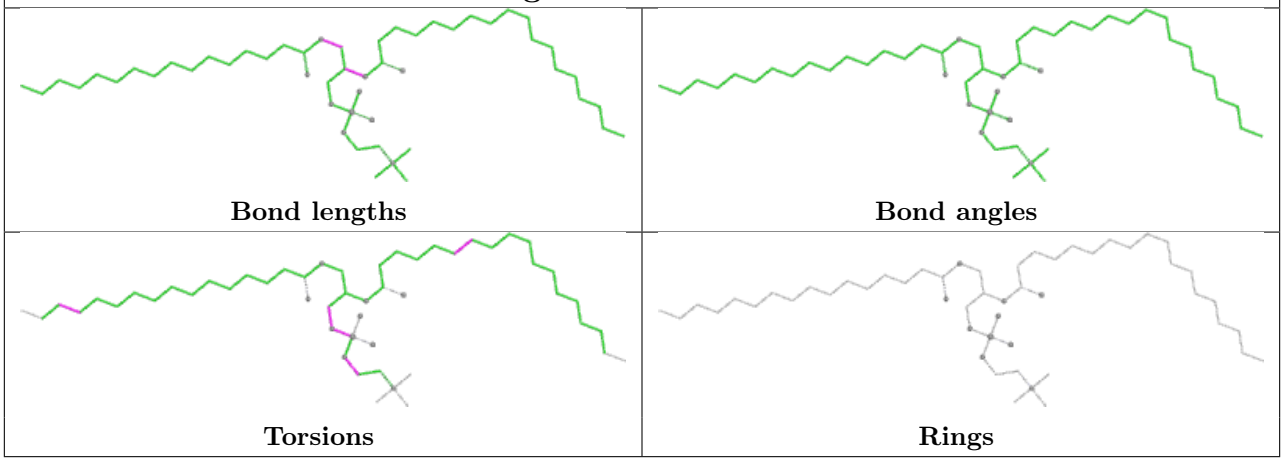


Torsions

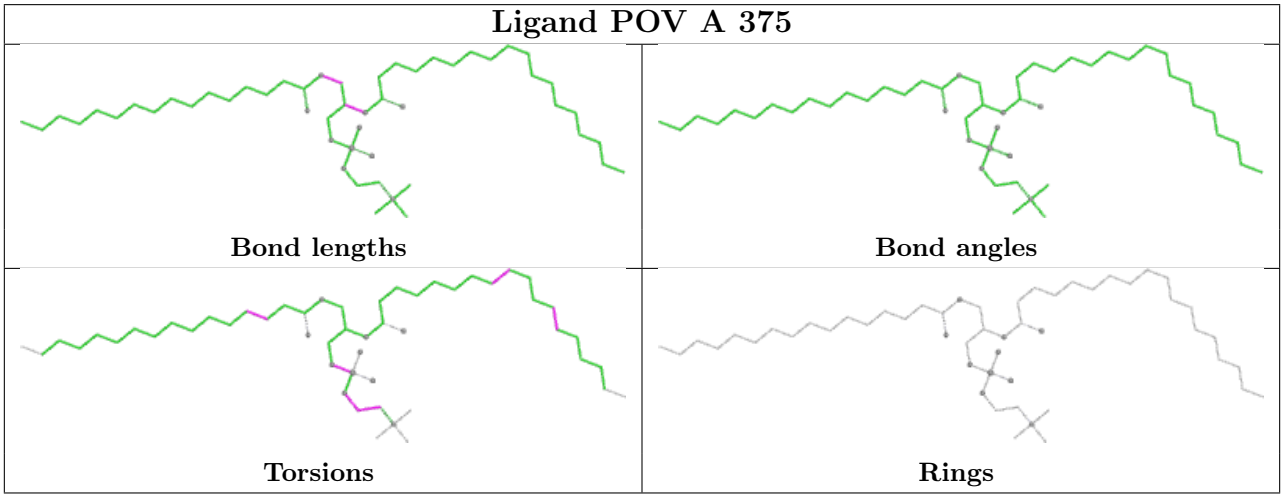


Rings

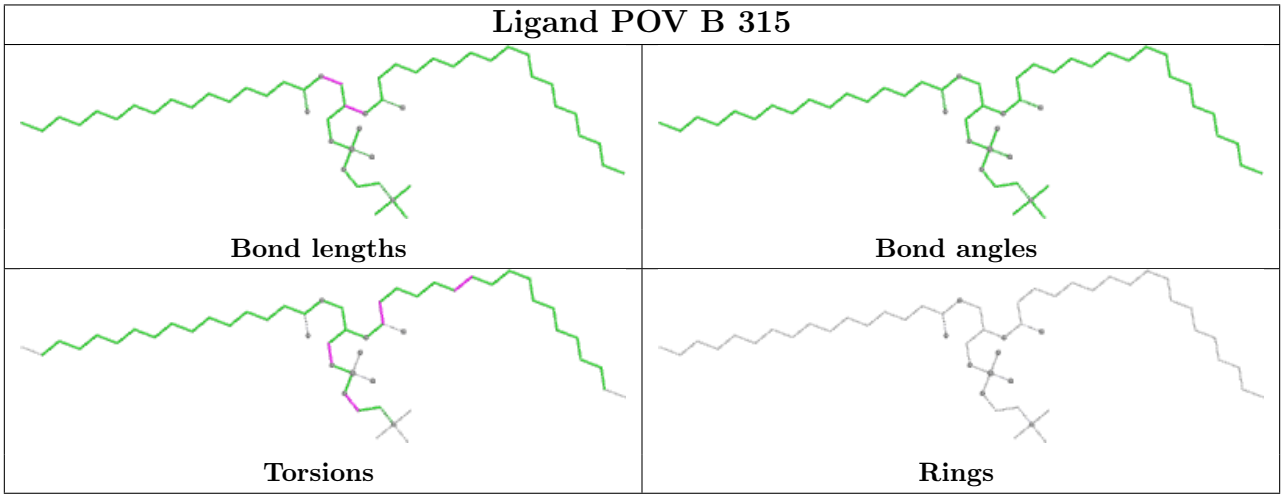
Ligand POV A 414



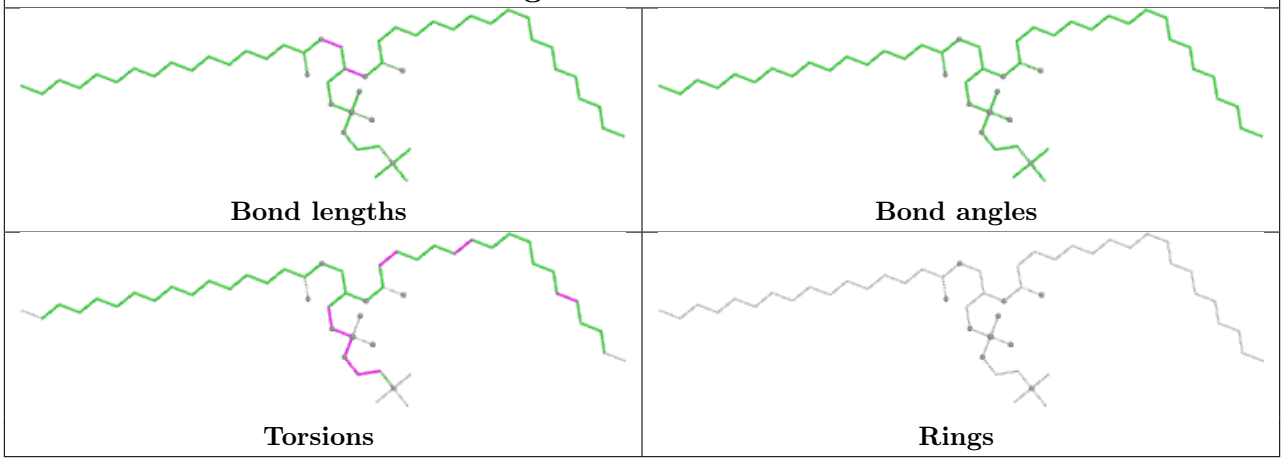
Ligand POV A 375



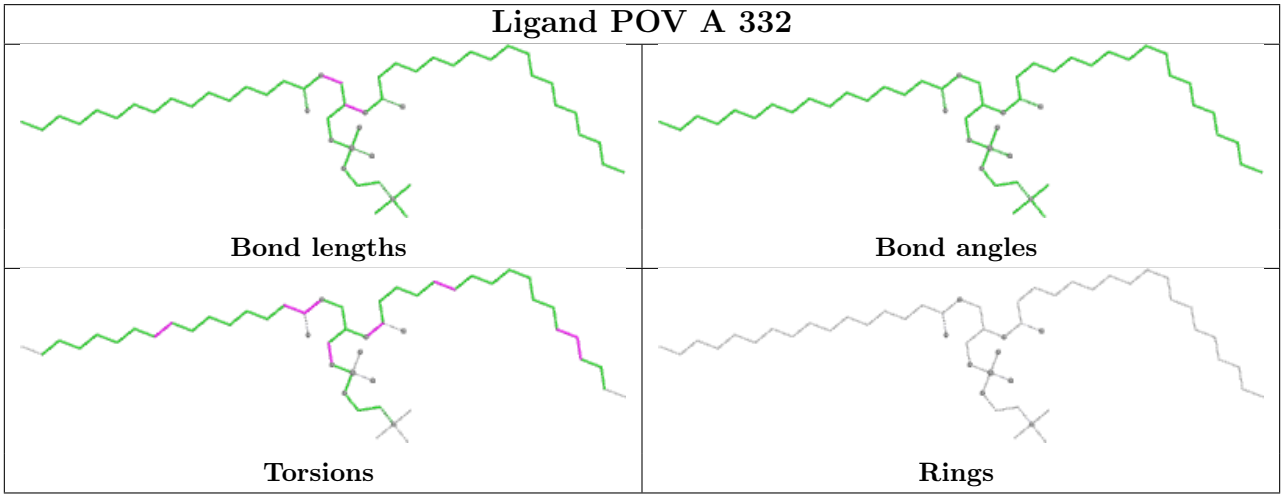
Ligand POV B 315



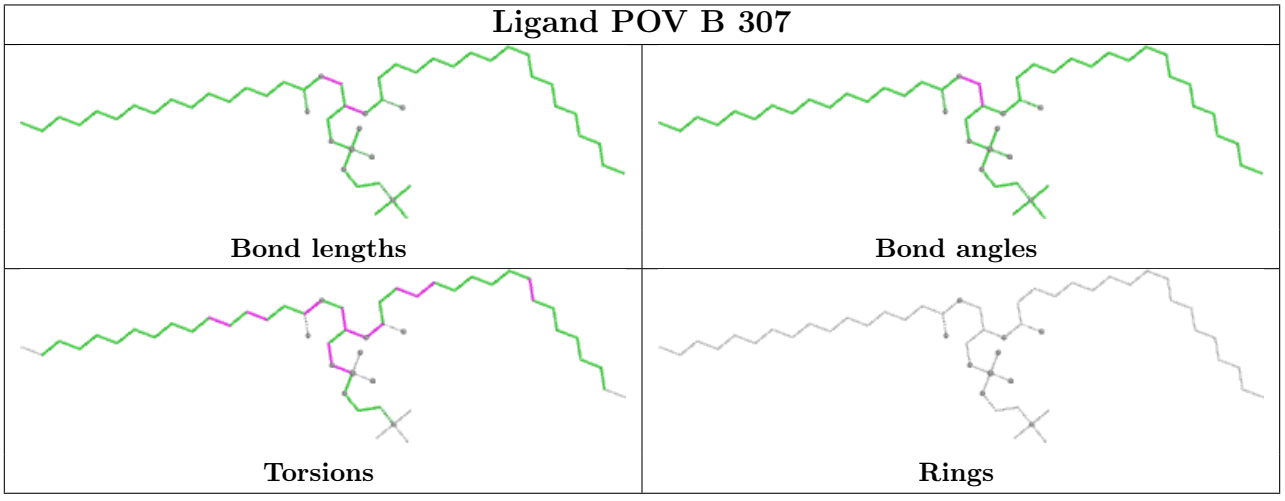
Ligand POV B 364



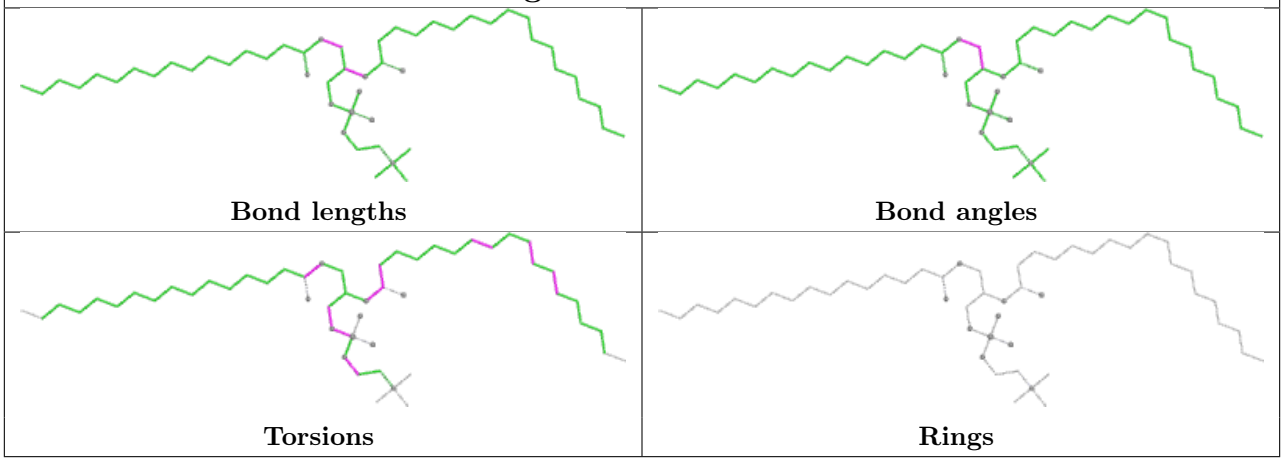
Ligand POV A 332



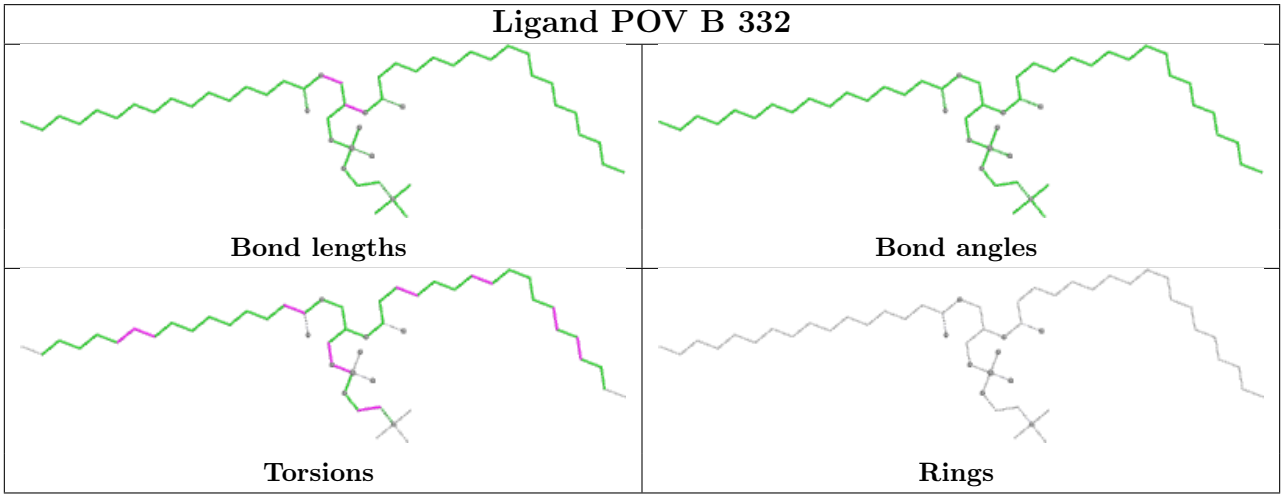
Ligand POV B 307



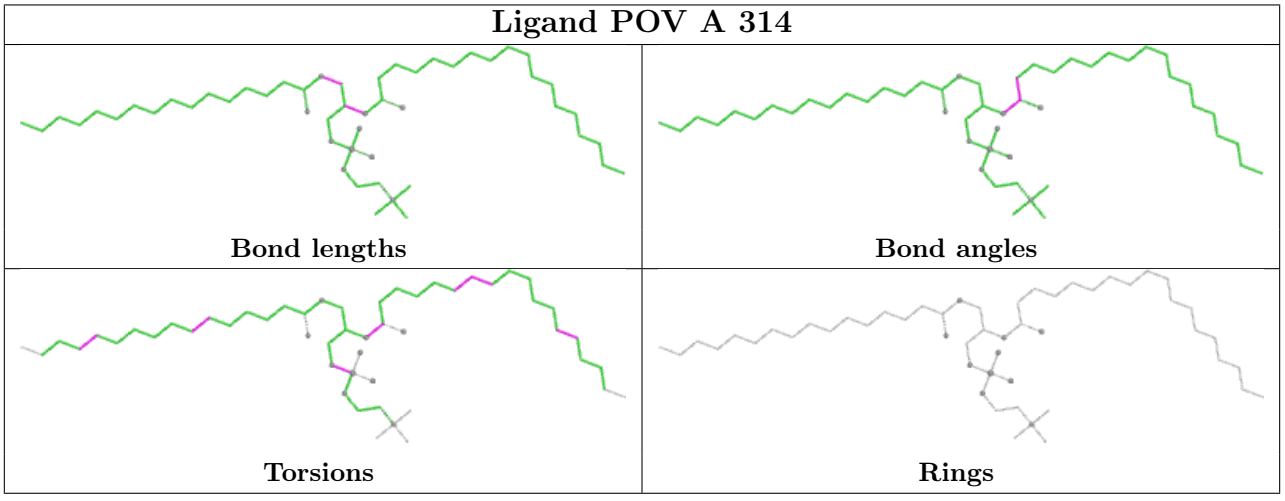
Ligand POV B 318



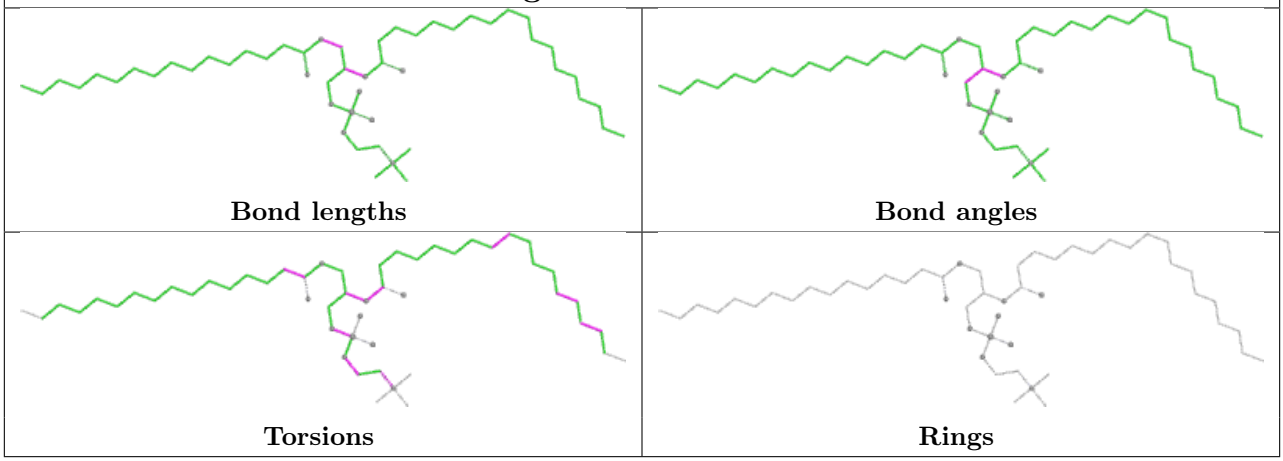
Ligand POV B 332



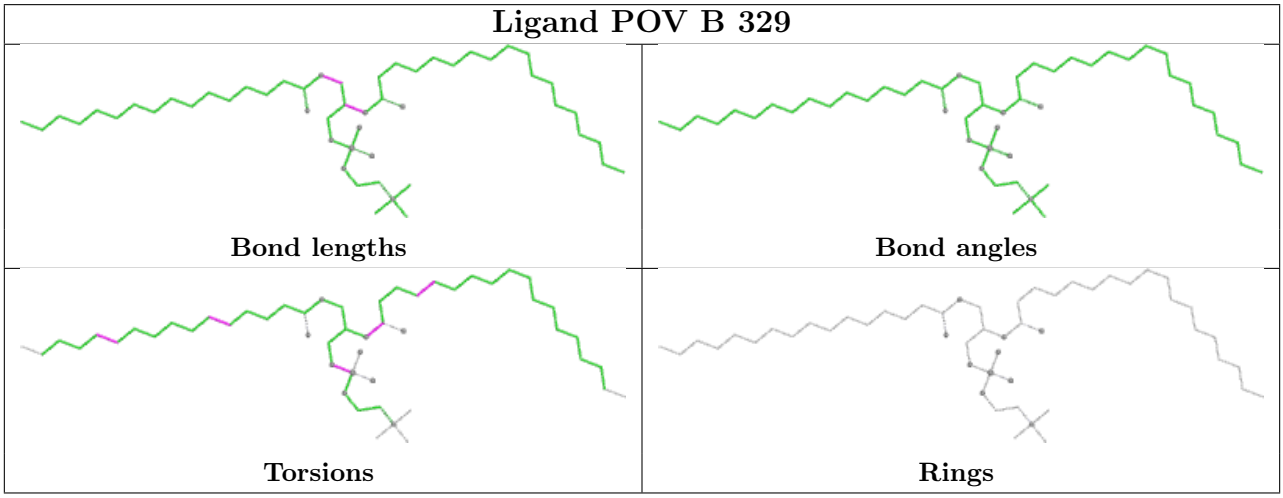
Ligand POV A 314



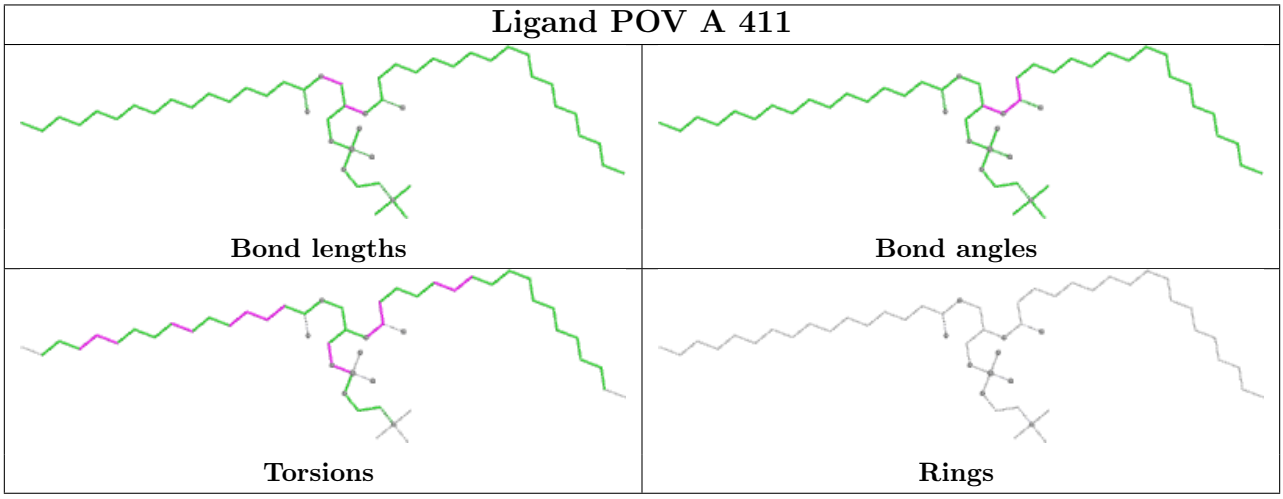
Ligand POV A 327



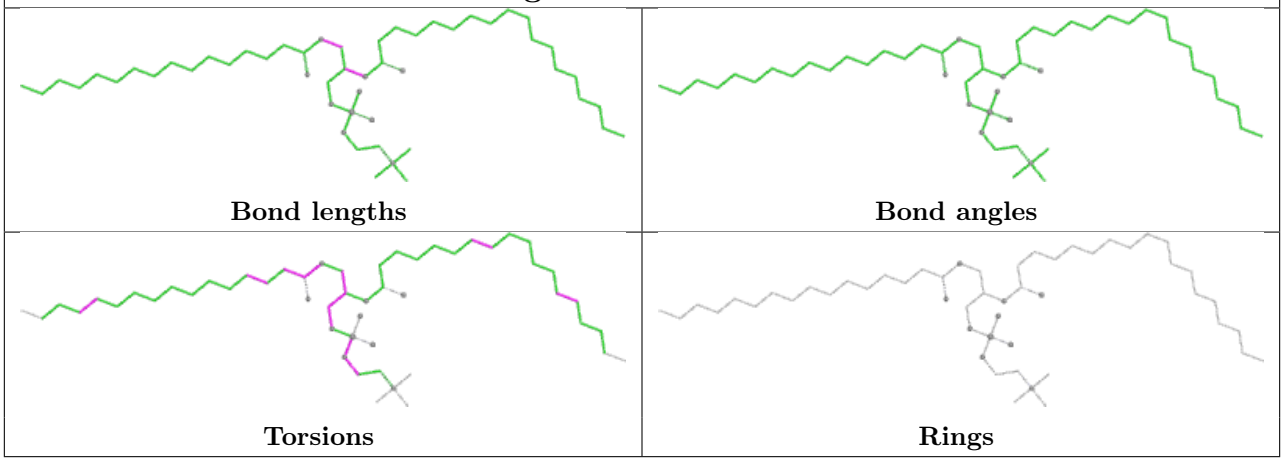
Ligand POV B 329



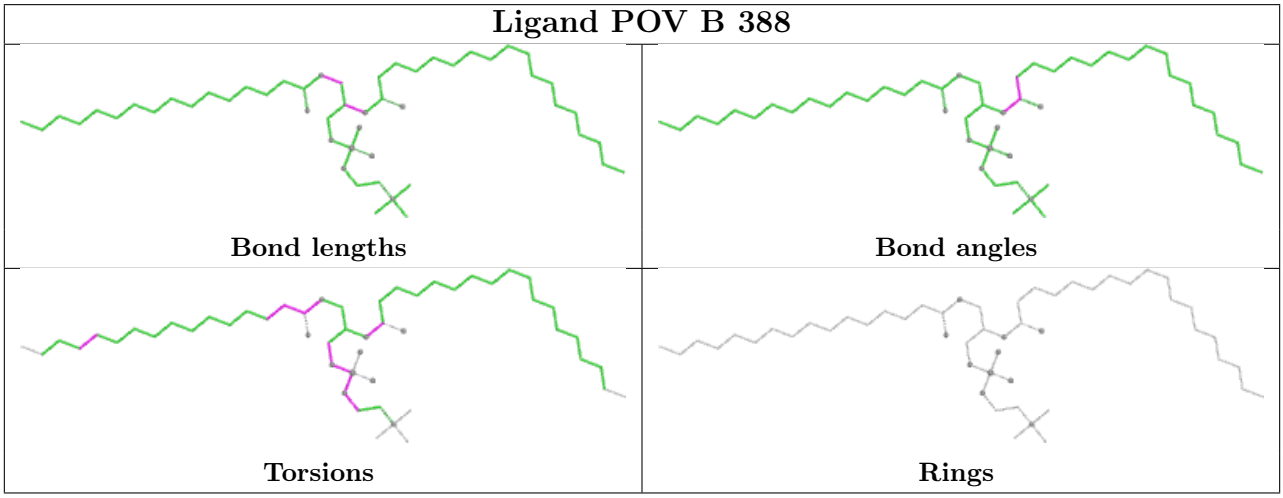
Ligand POV A 411



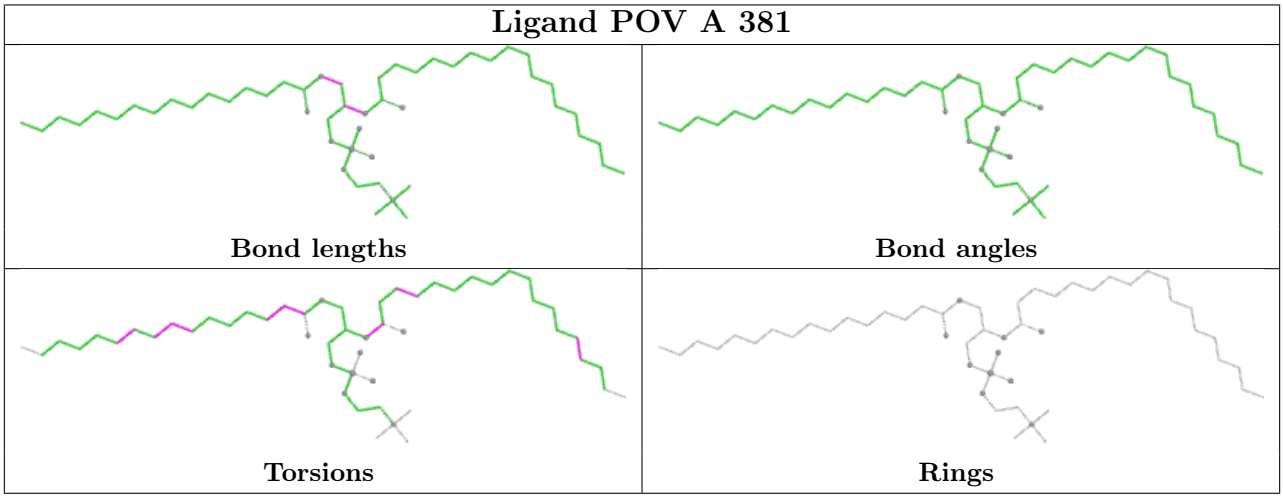
Ligand POV B 381



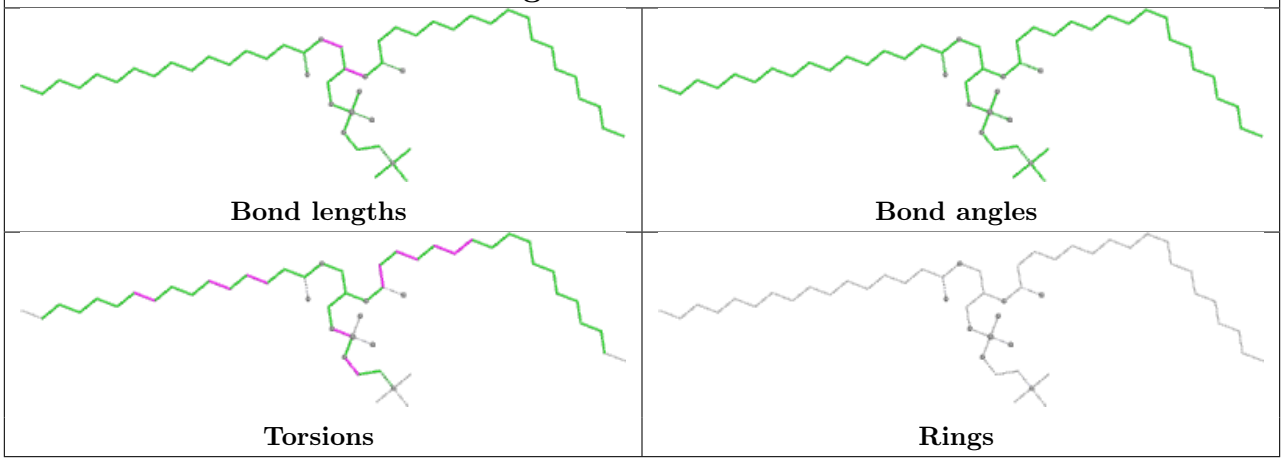
Ligand POV B 388



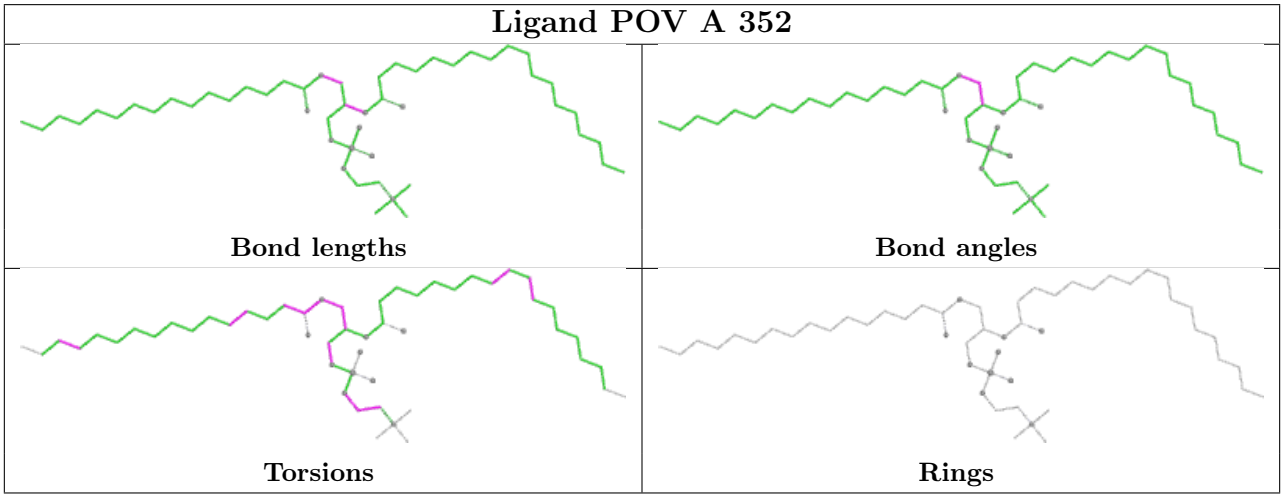
Ligand POV A 381



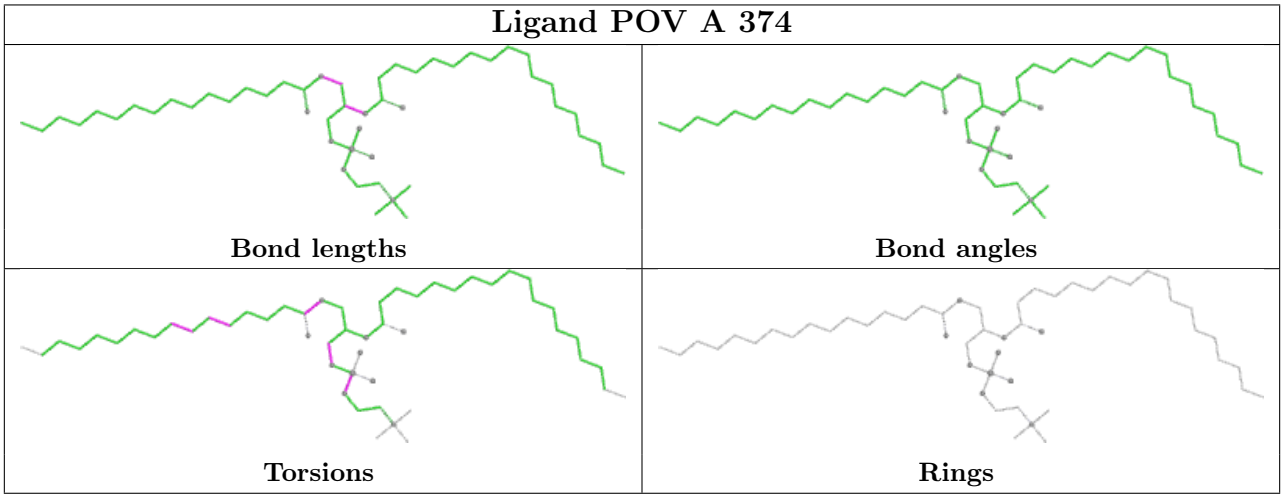
Ligand POV A 324



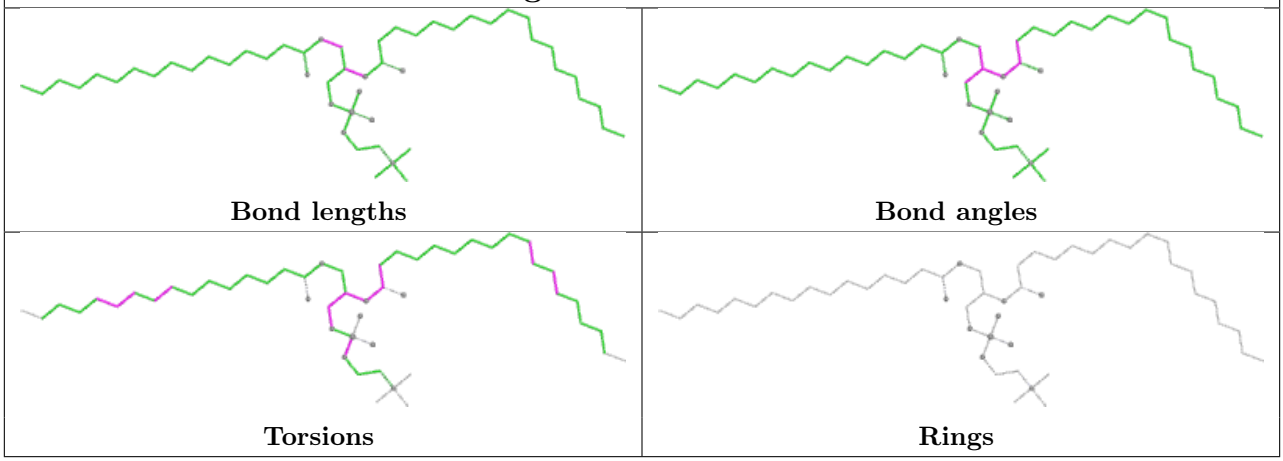
Ligand POV A 352



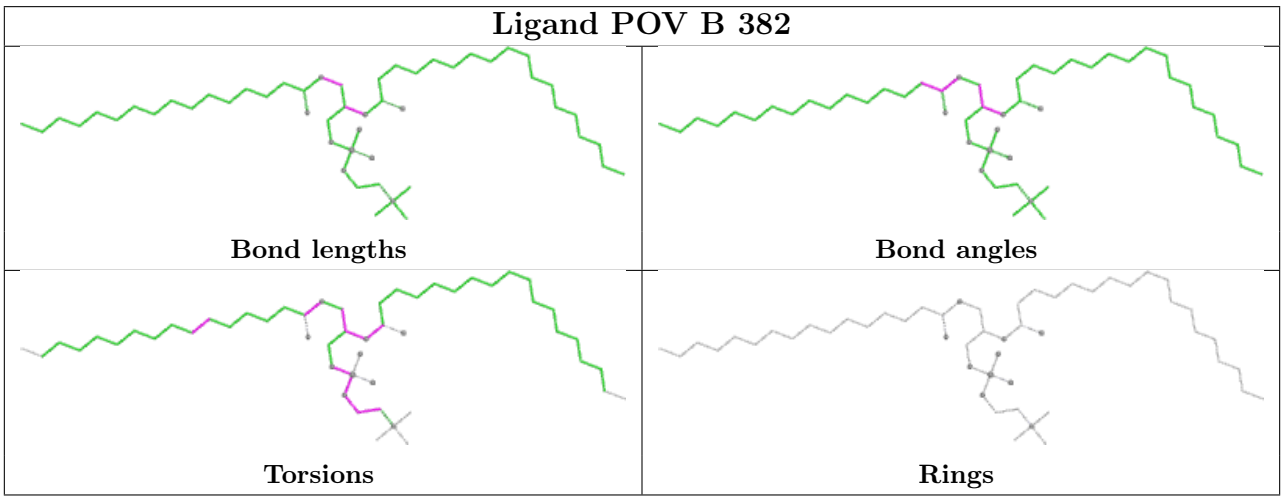
Ligand POV A 374



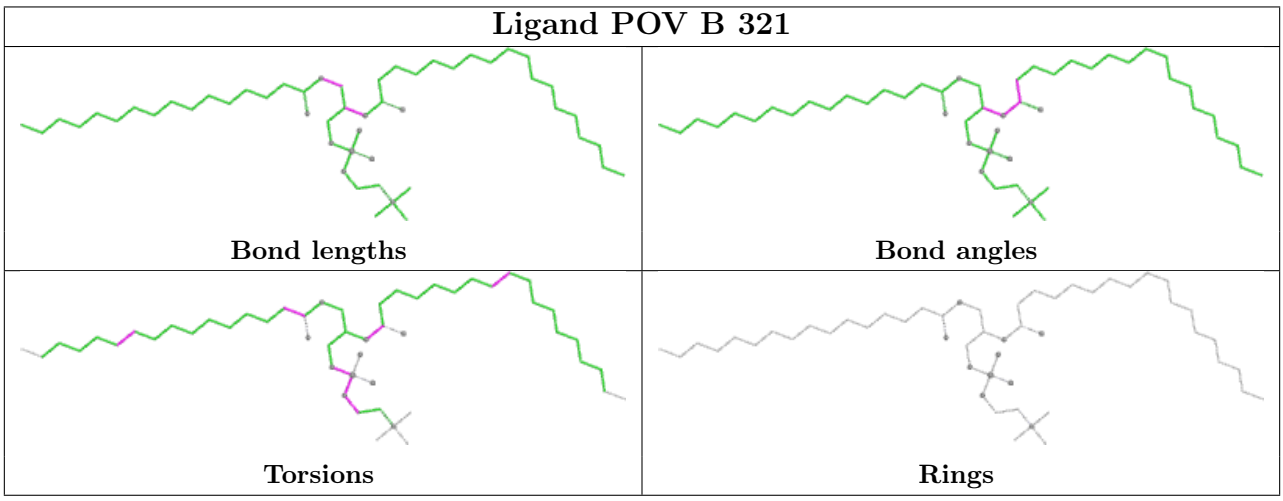
Ligand POV B 331



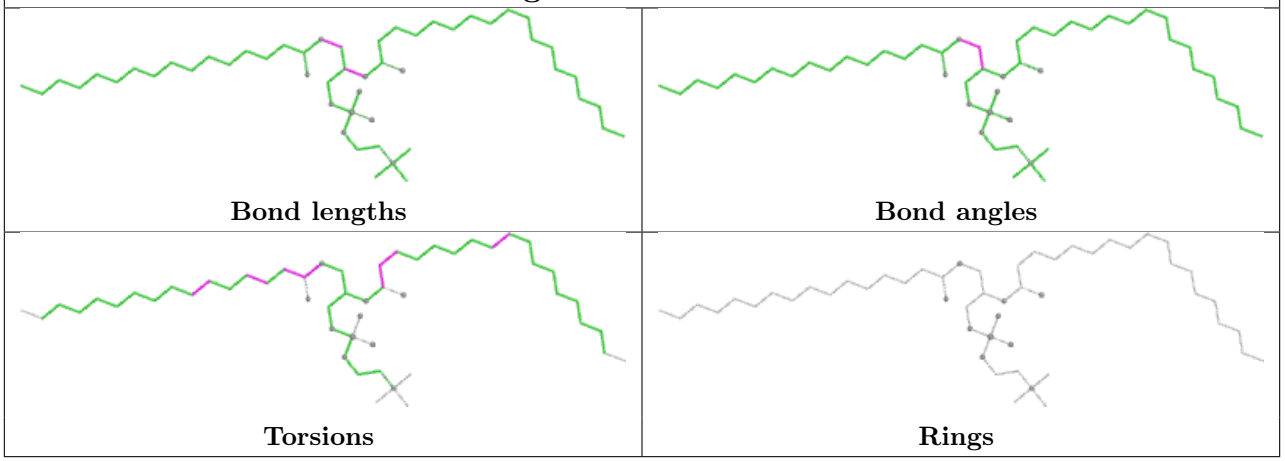
Ligand POV B 382



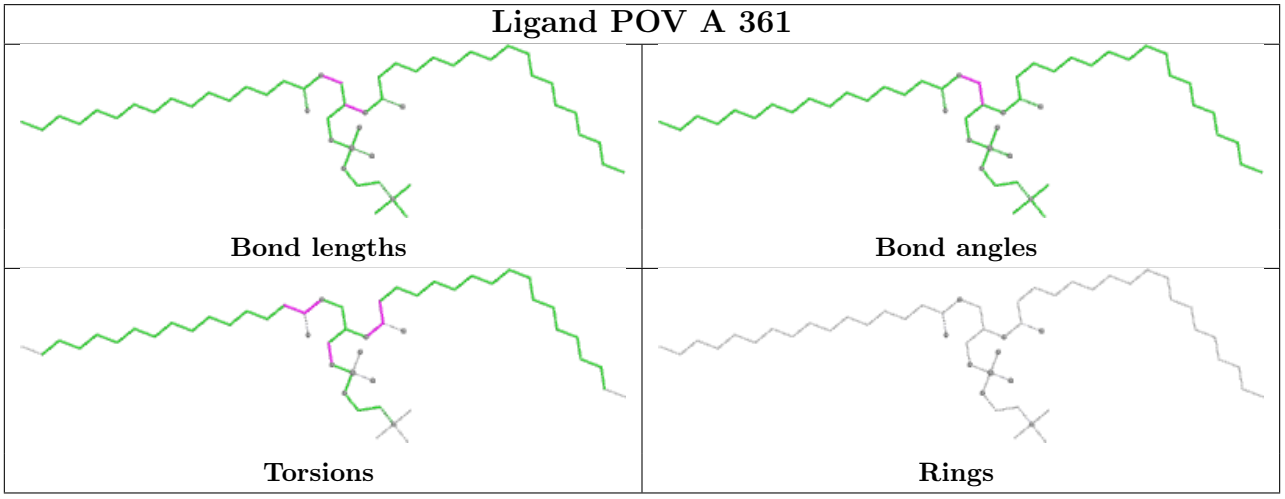
Ligand POV B 321



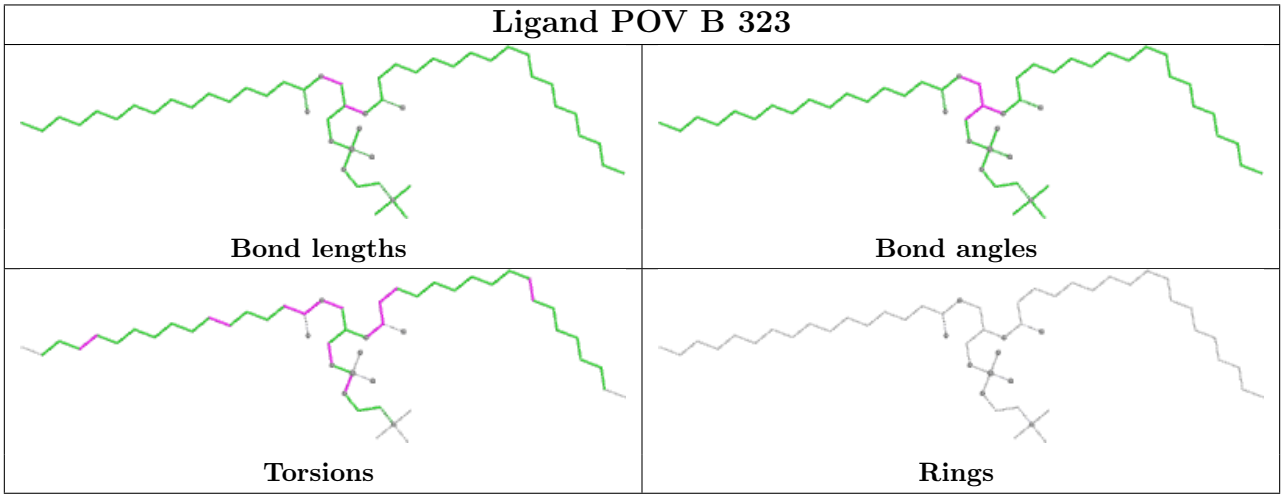
Ligand POV A 329



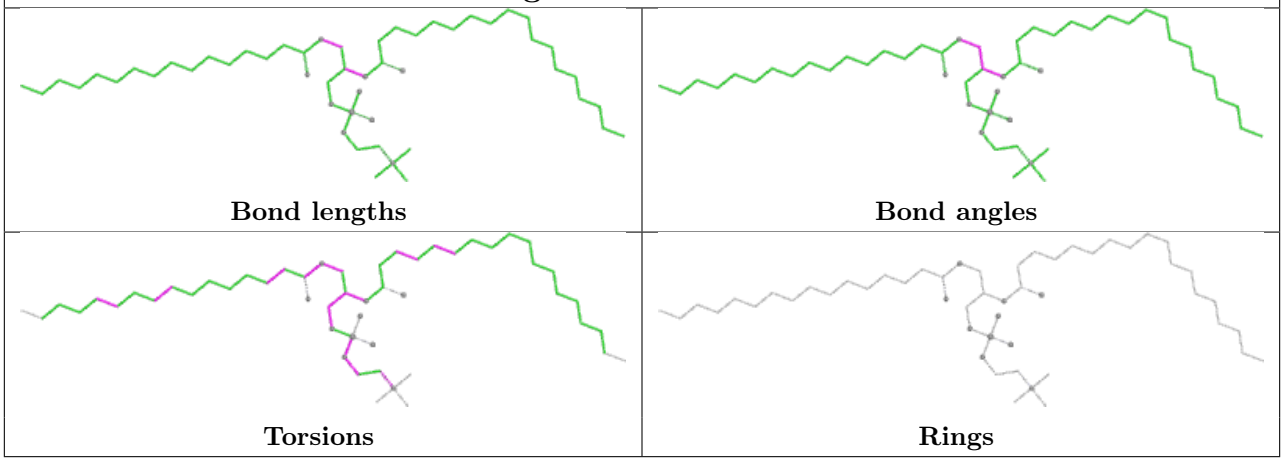
Ligand POV A 361



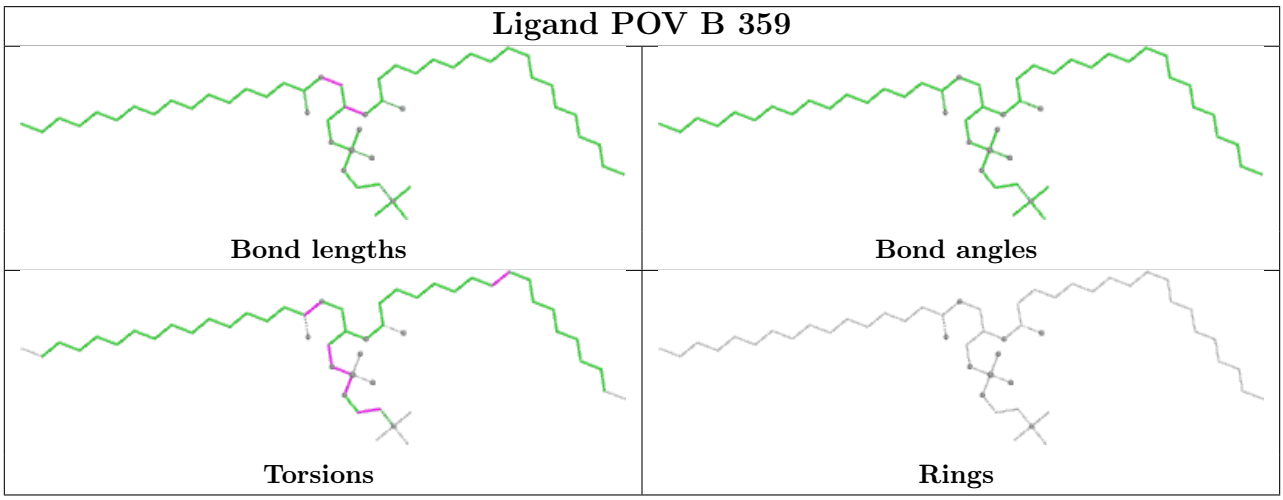
Ligand POV B 323



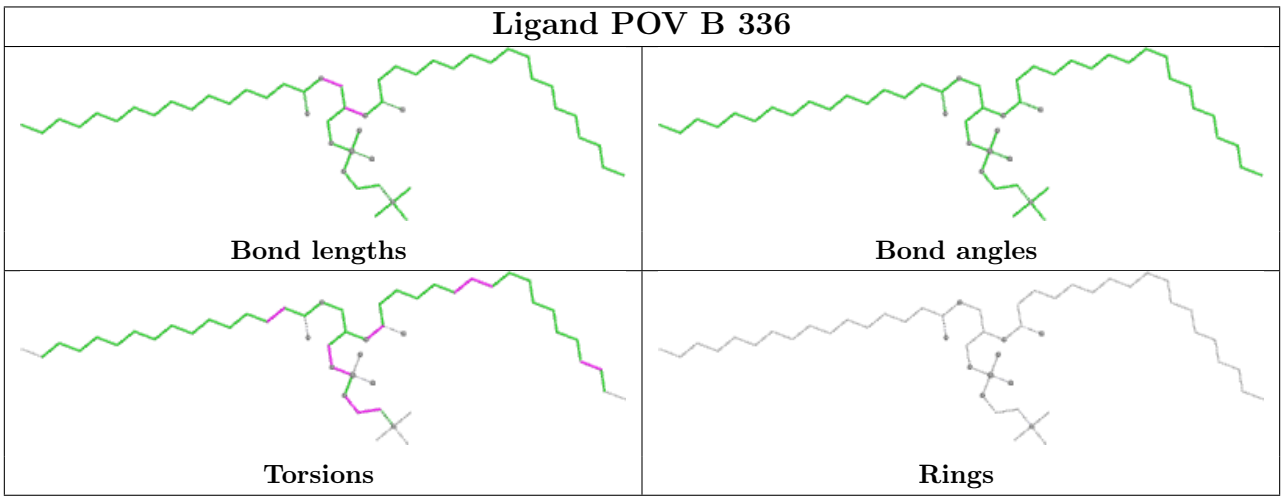
Ligand POV A 359



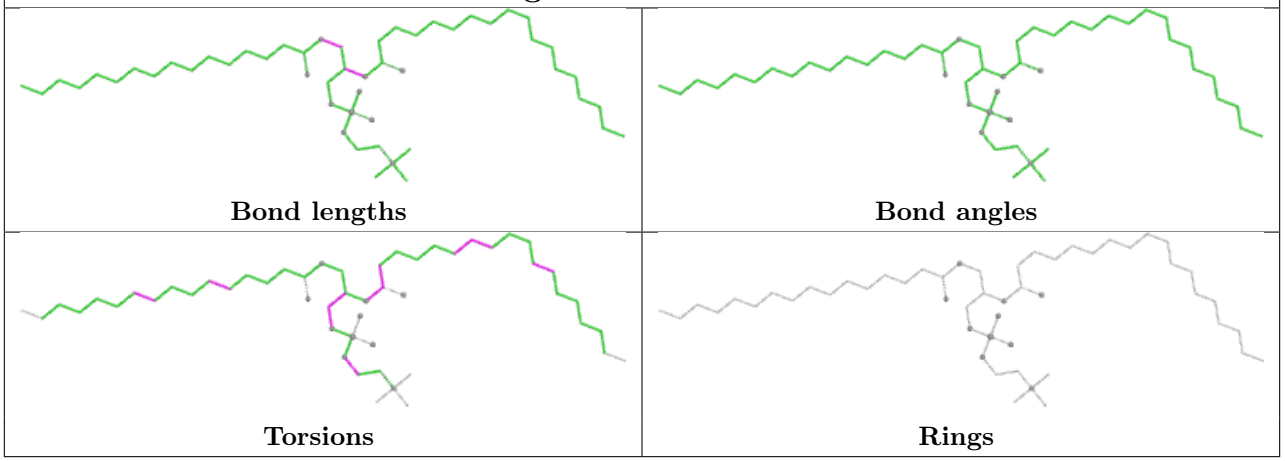
Ligand POV B 359



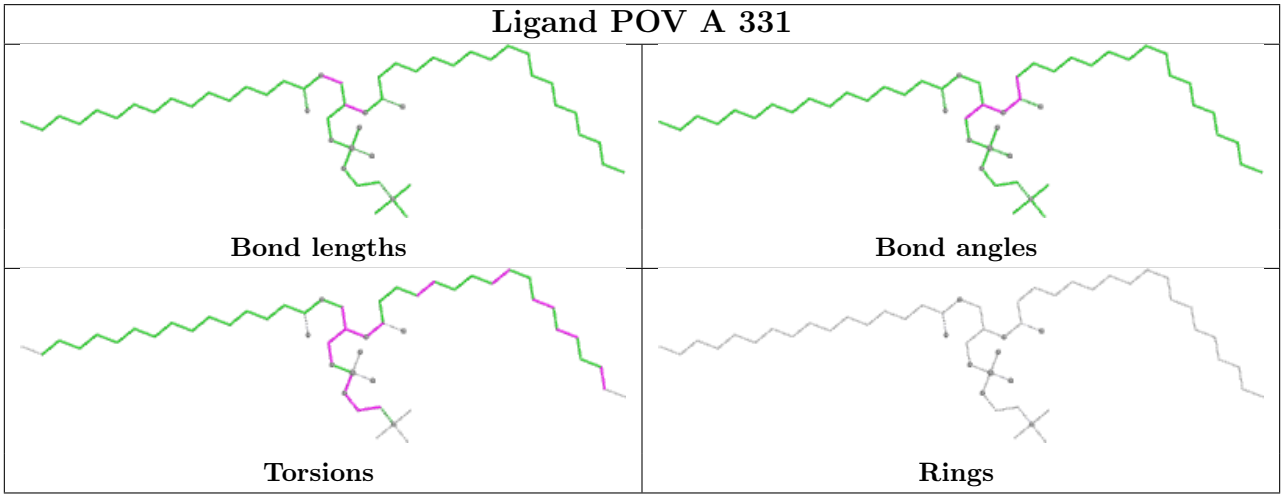
Ligand POV B 336



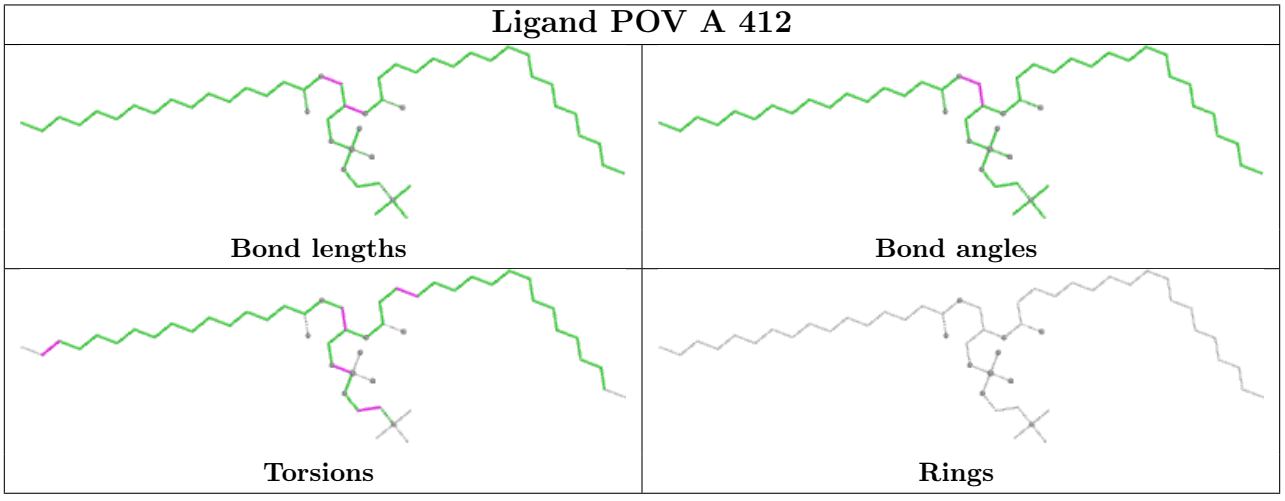
Ligand POV B 354



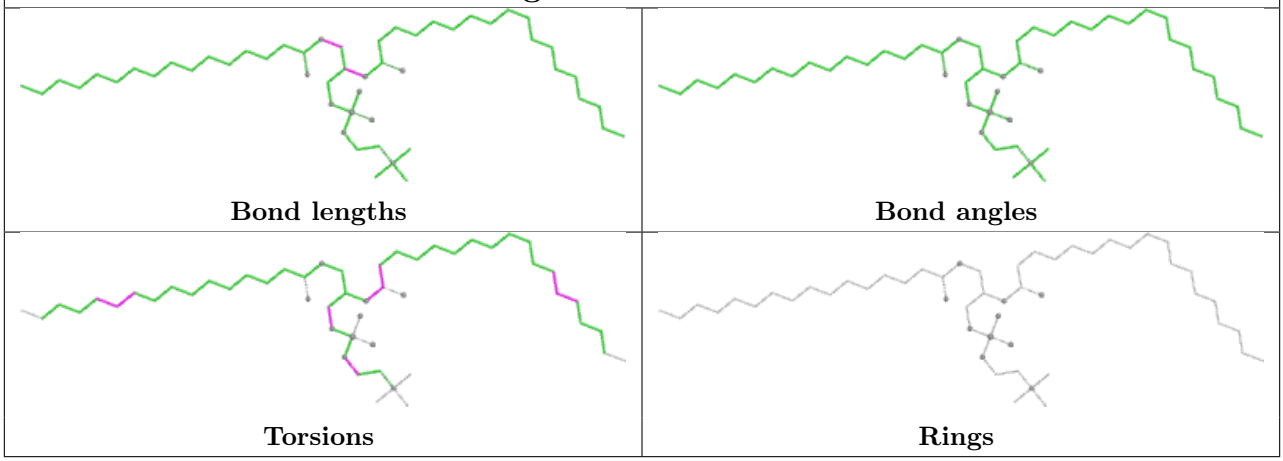
Ligand POV A 331



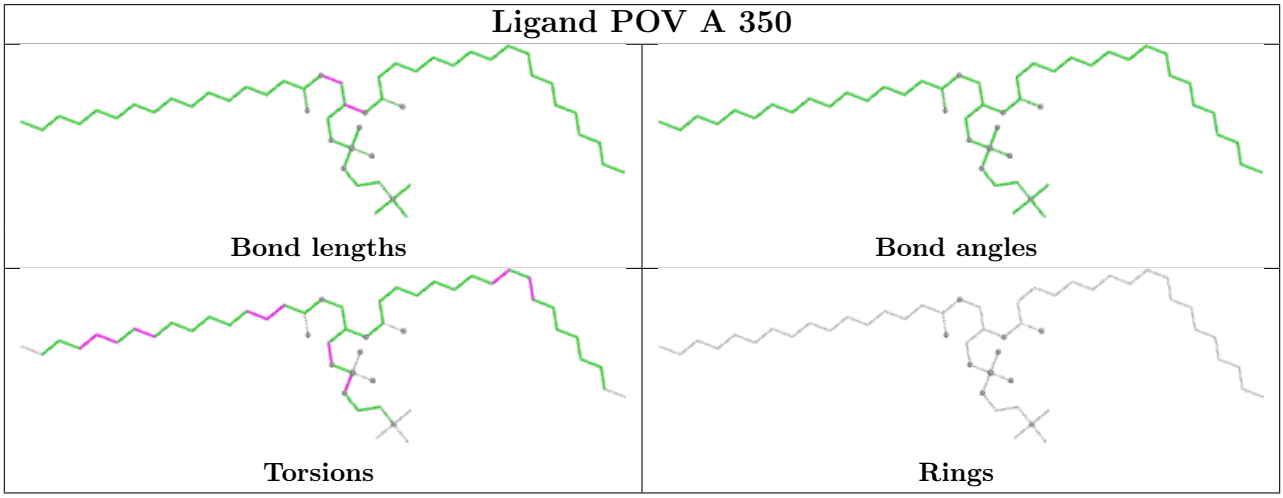
Ligand POV A 412



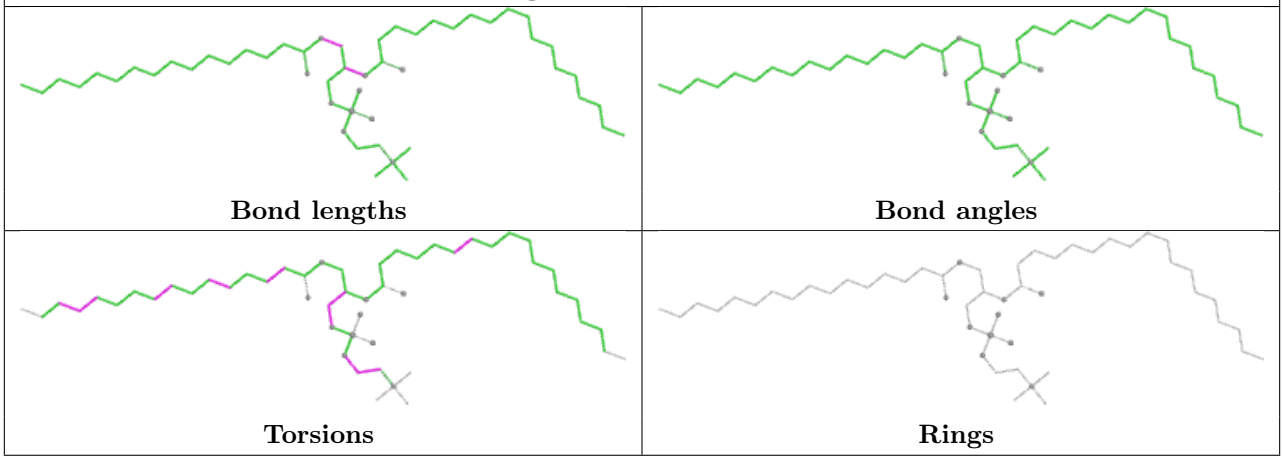
Ligand POV A 328



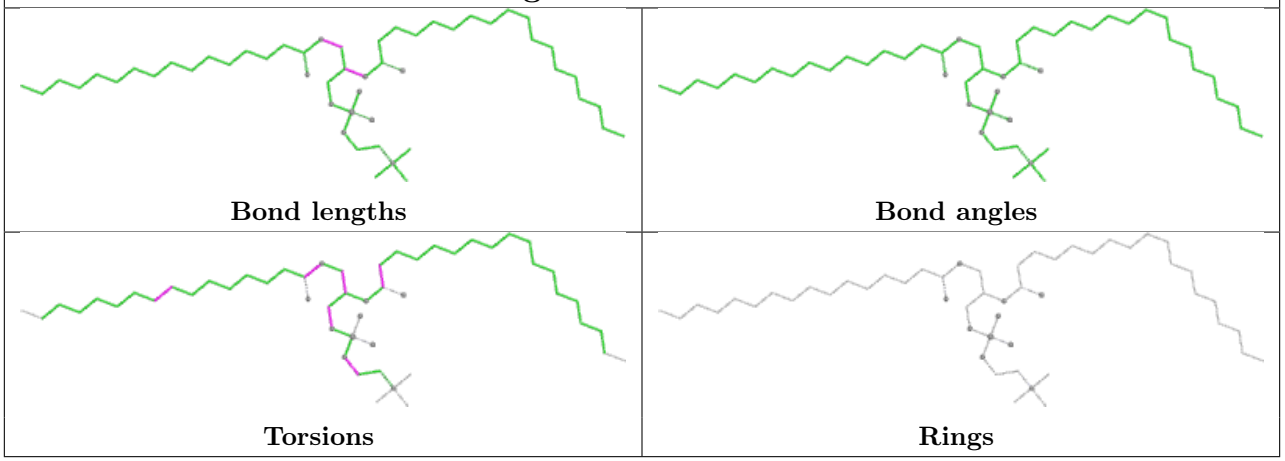
Ligand POV A 350



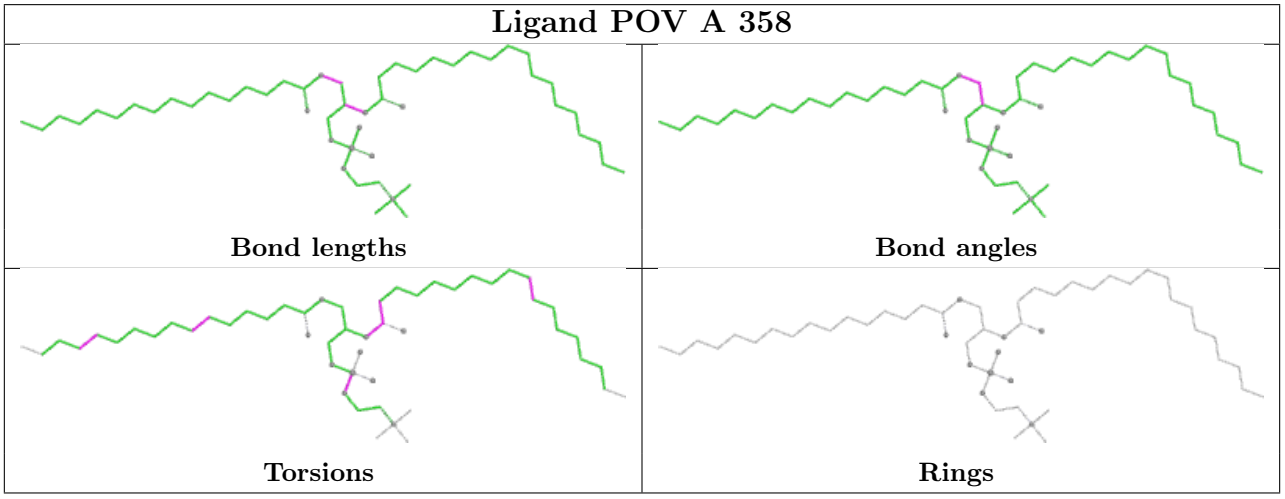
Ligand POV A 370



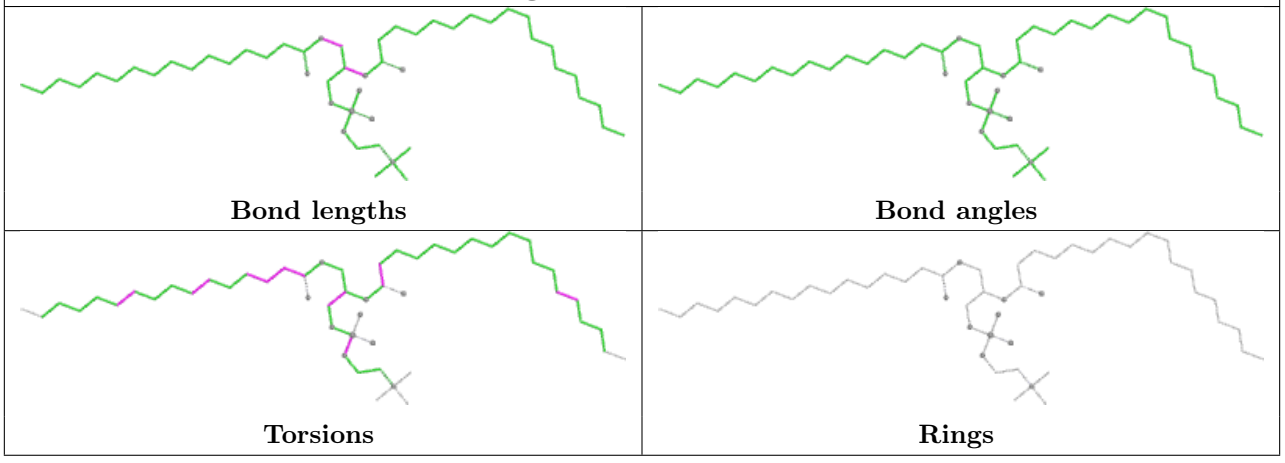
Ligand POV A 398



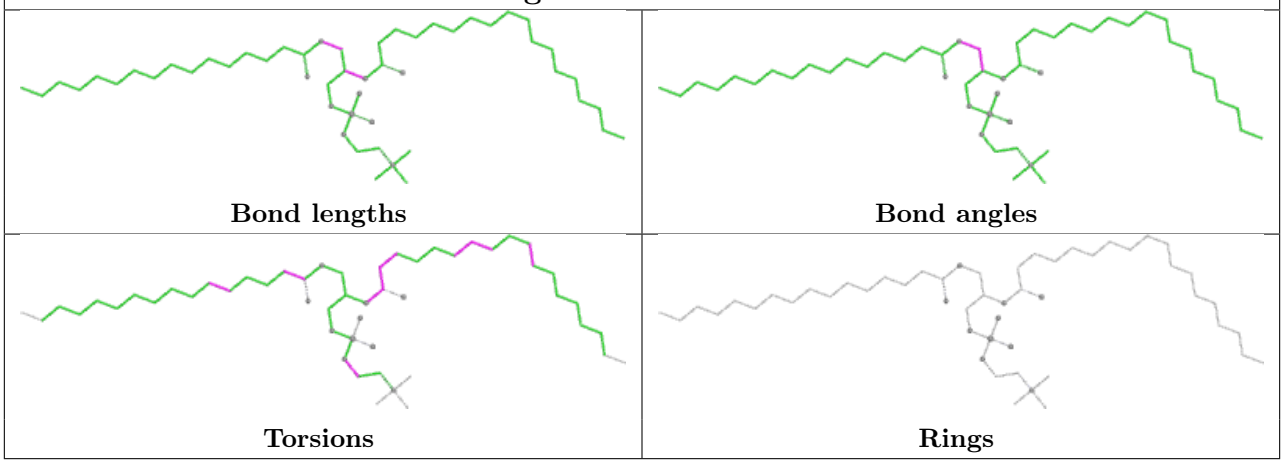
Ligand POV A 358



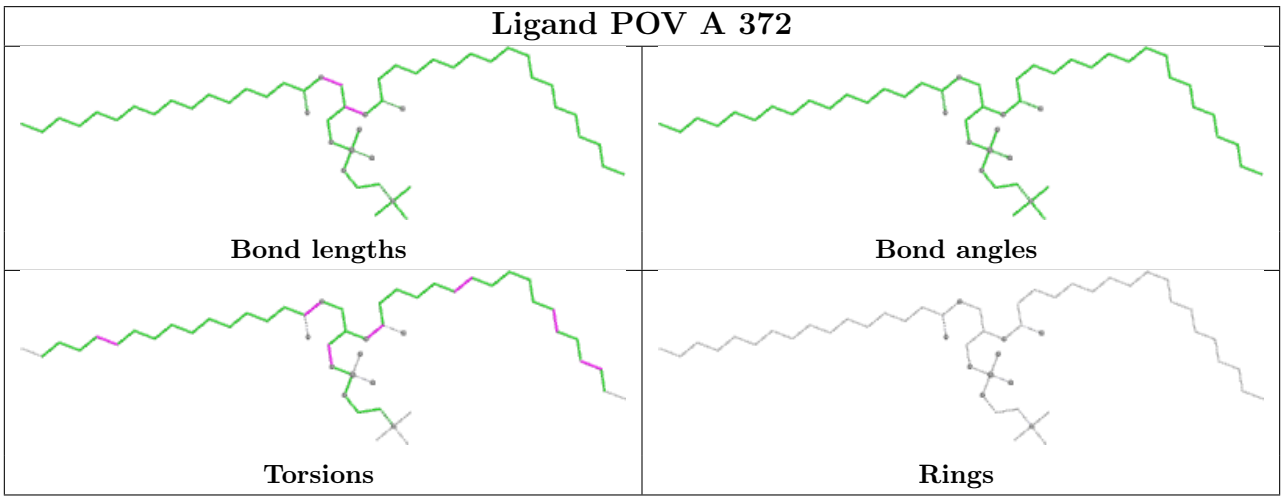
Ligand POV A 382



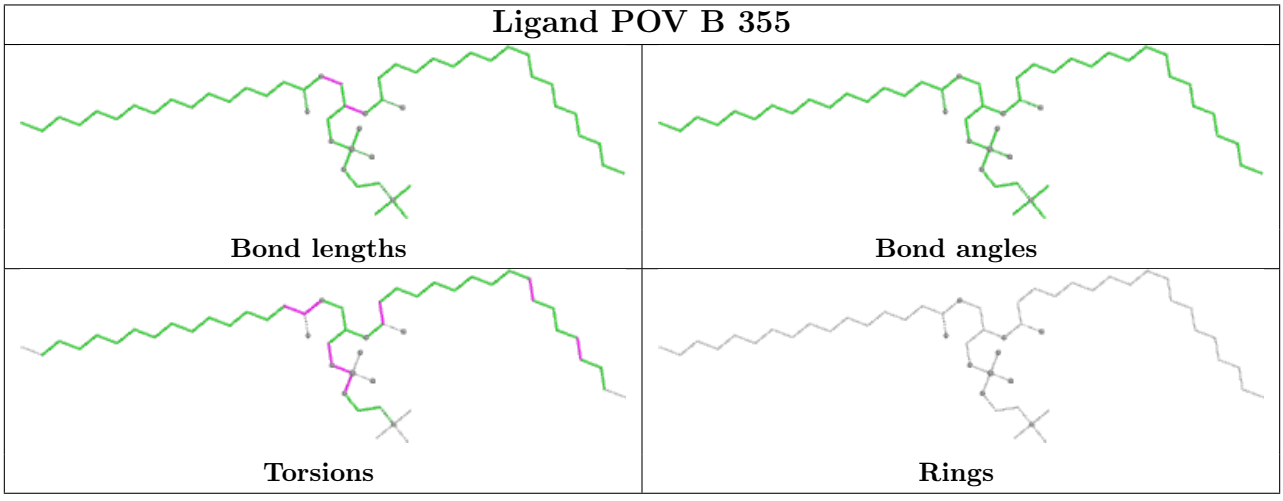
Ligand POV B 367



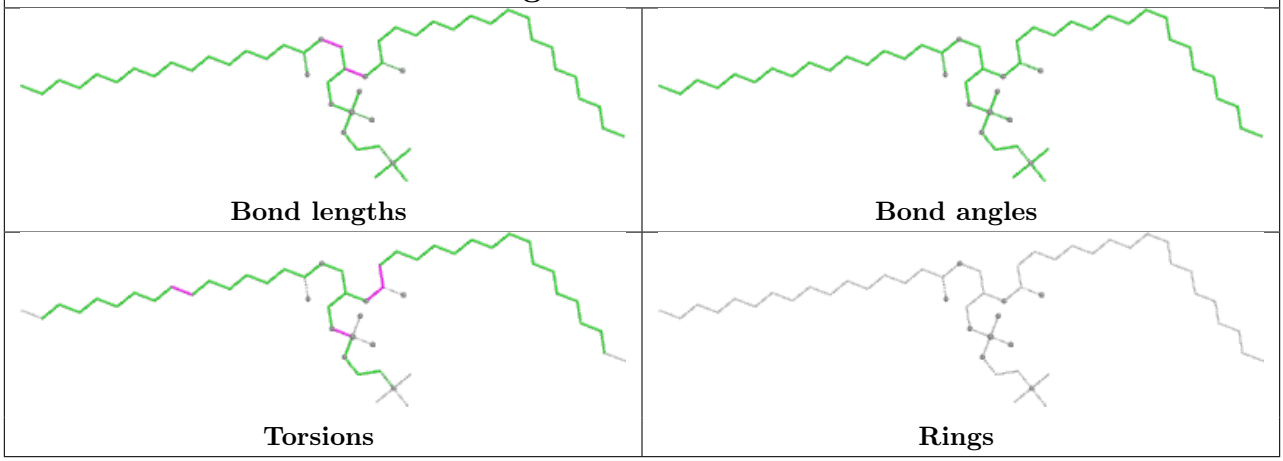
Ligand POV A 372



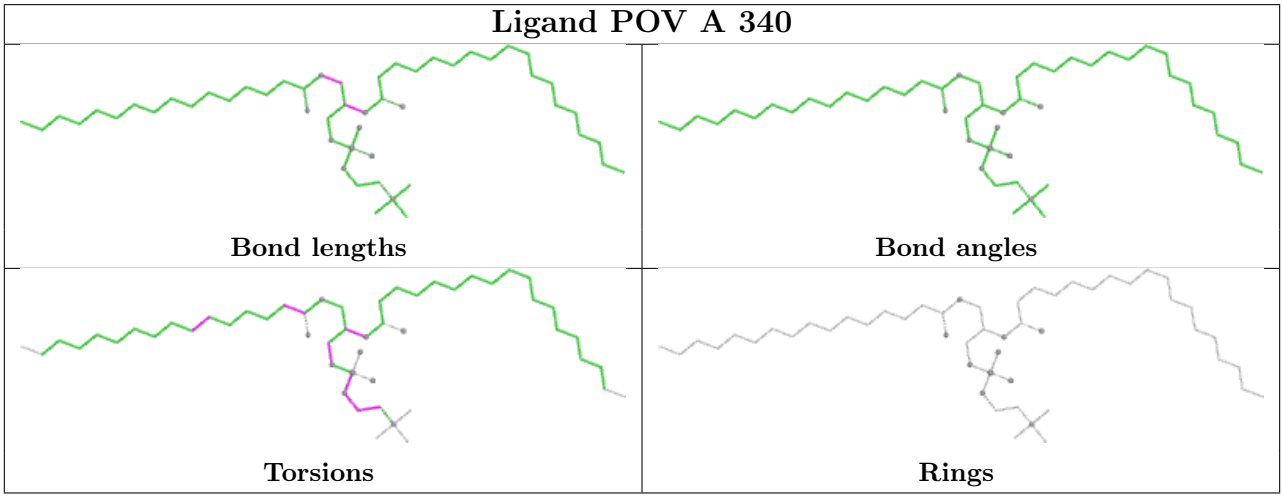
Ligand POV B 355



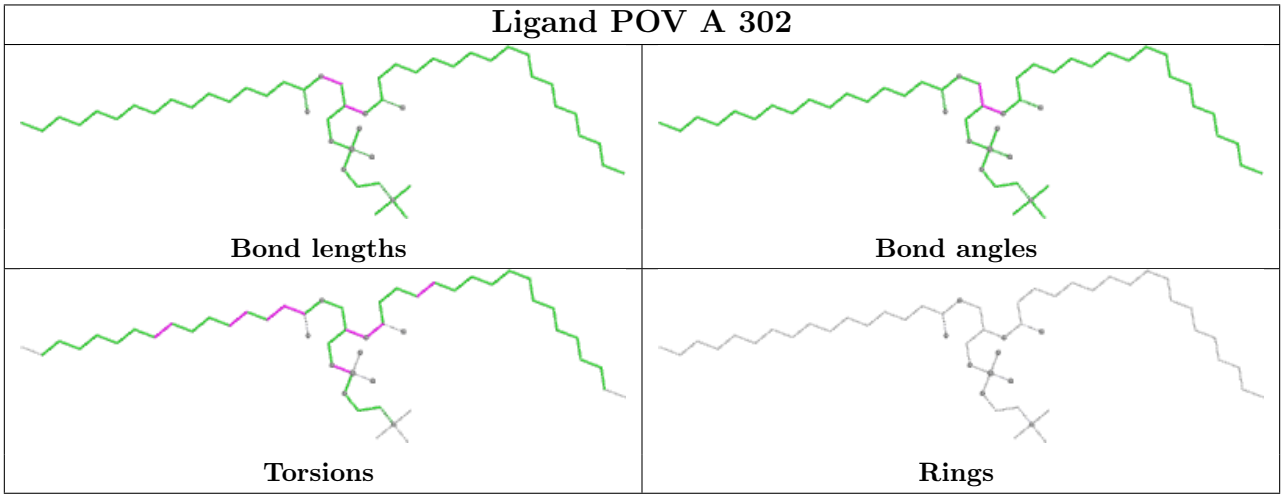
Ligand POV A 377



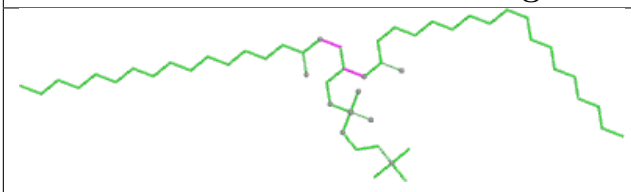
Ligand POV A 340



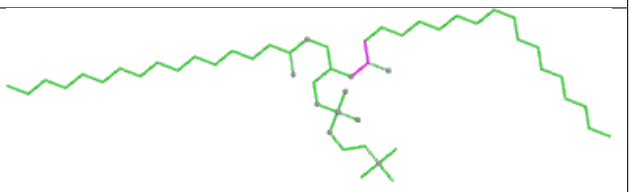
Ligand POV A 302



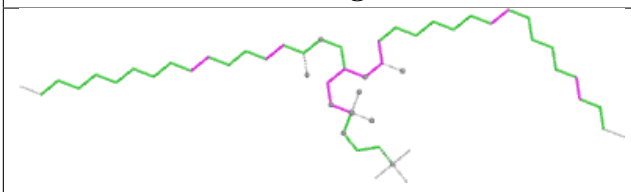
Ligand POV A 319



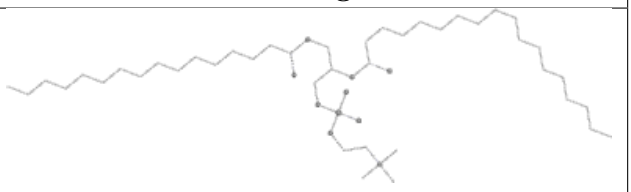
Bond lengths



Bond angles

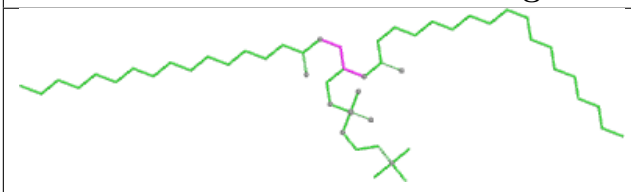


Torsions

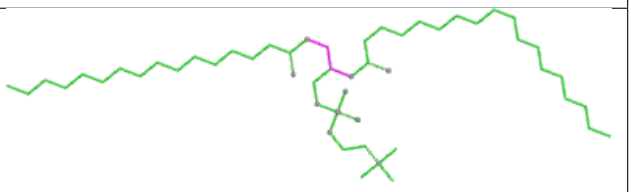


Rings

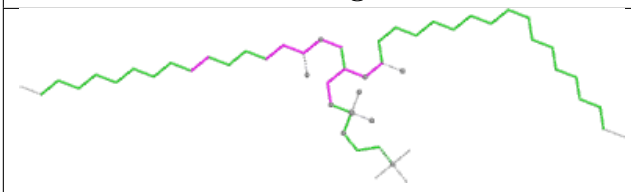
Ligand POV B 340



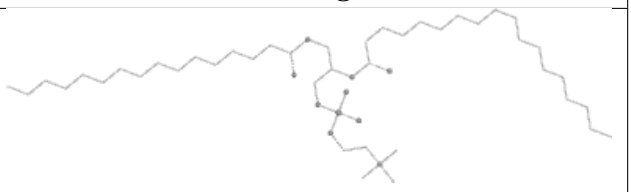
Bond lengths



Bond angles

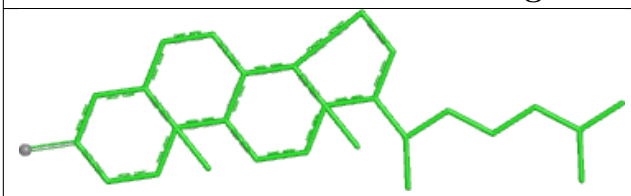


Torsions

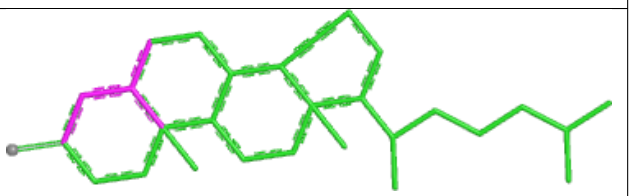


Rings

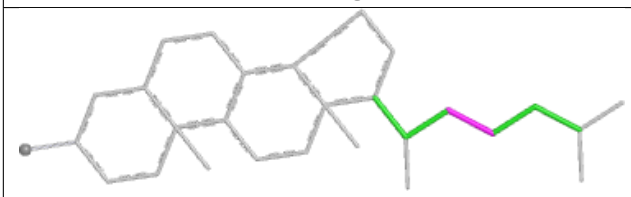
Ligand CLR B 398



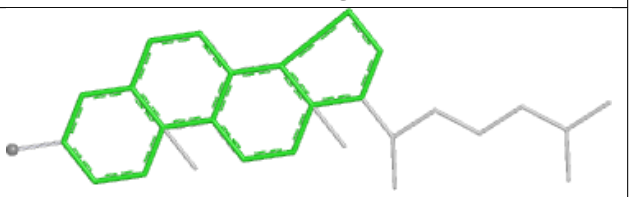
Bond lengths



Bond angles

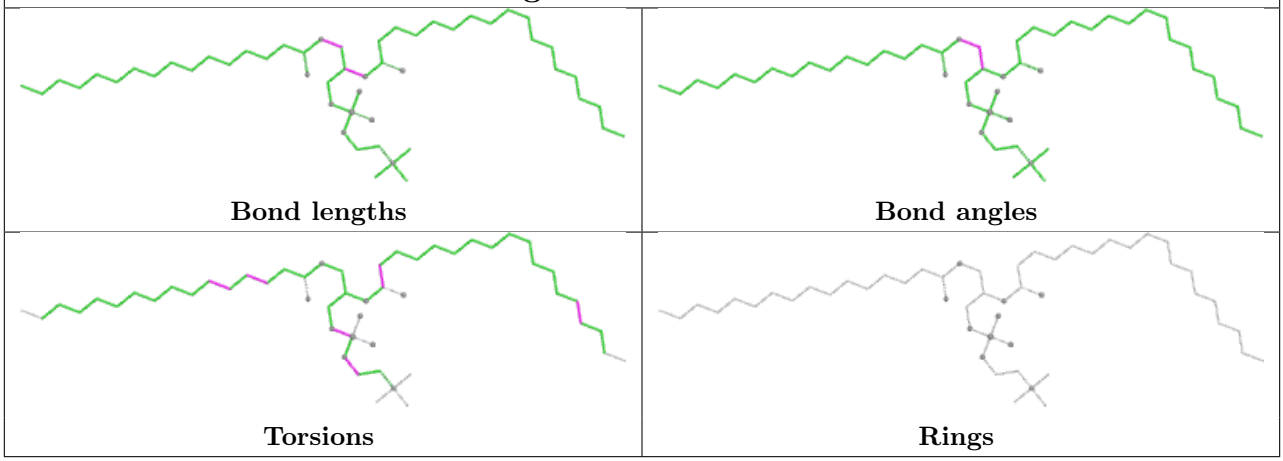


Torsions

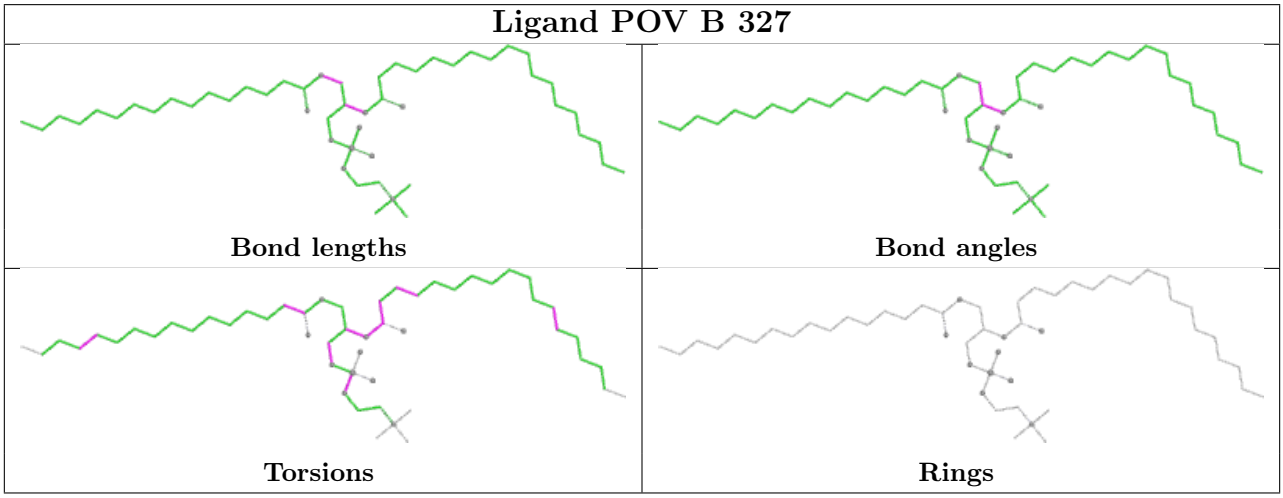


Rings

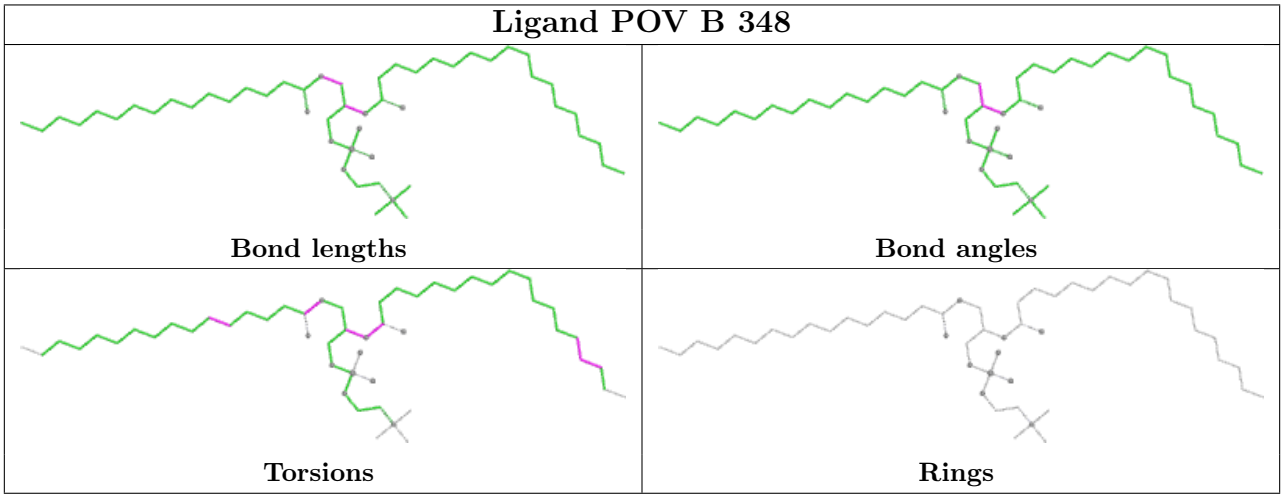
Ligand POV A 312



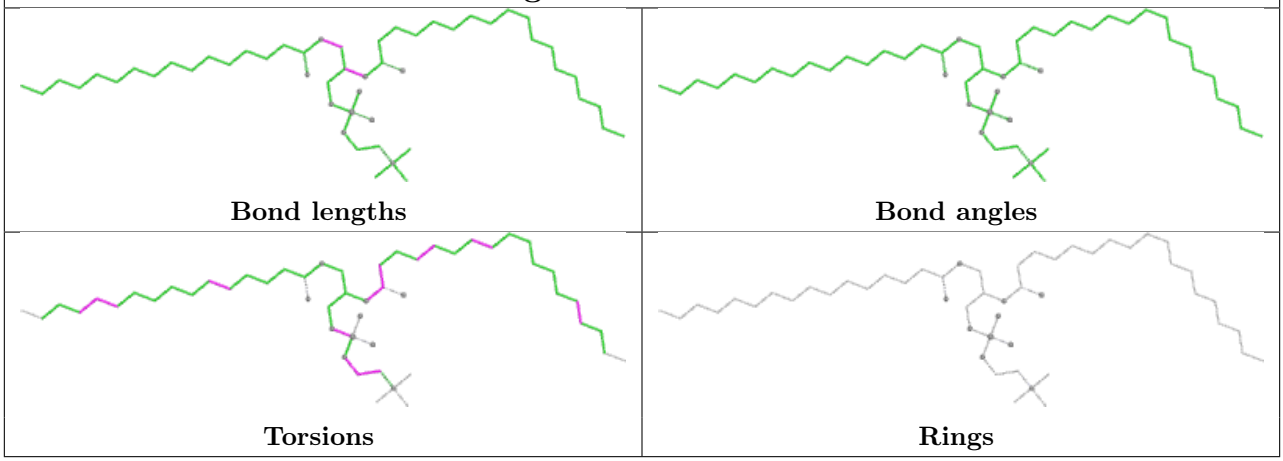
Ligand POV B 327



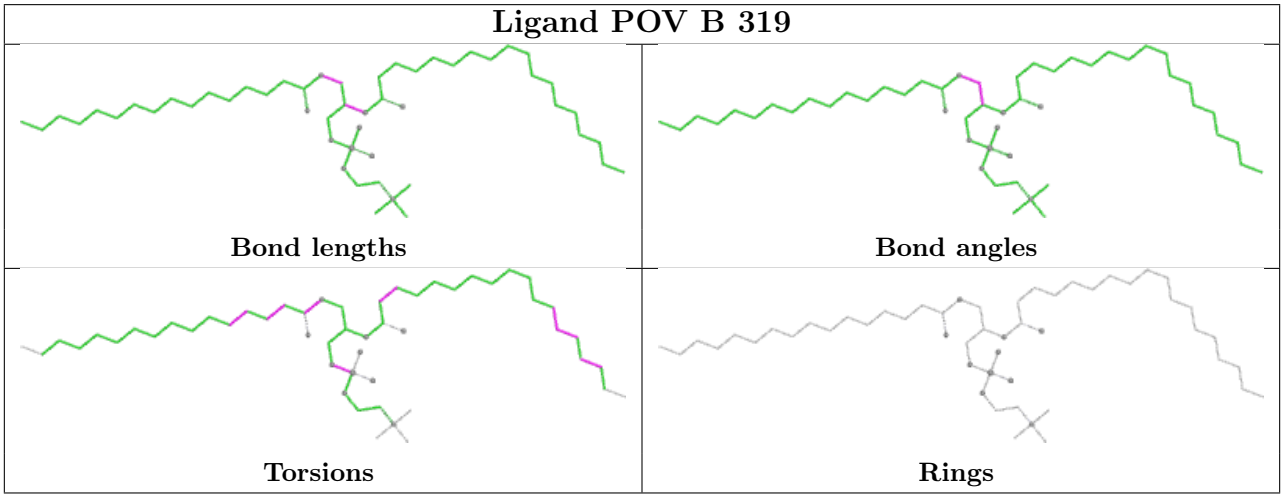
Ligand POV B 348



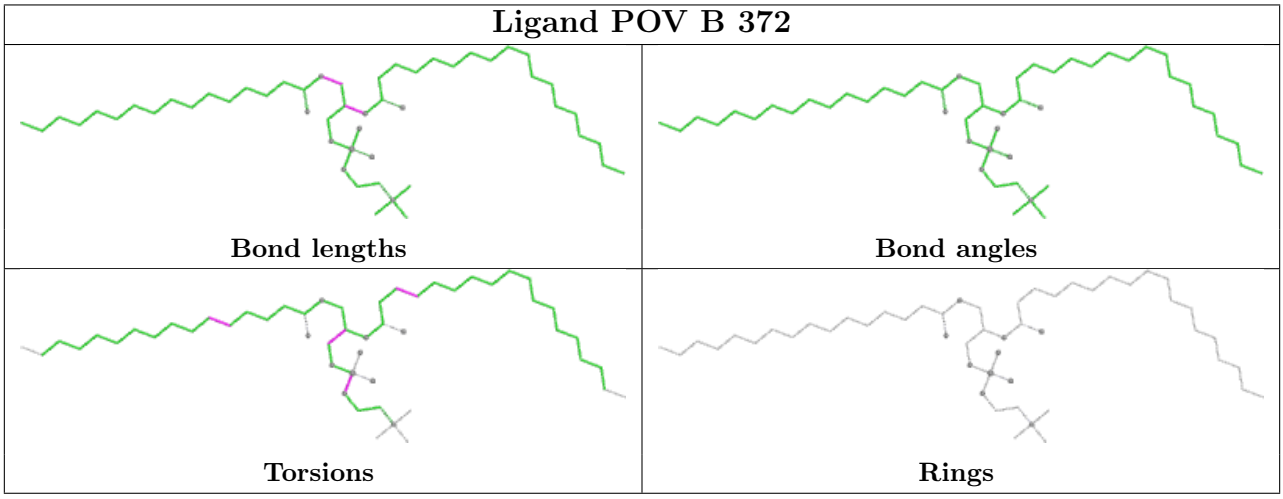
Ligand POV B 369



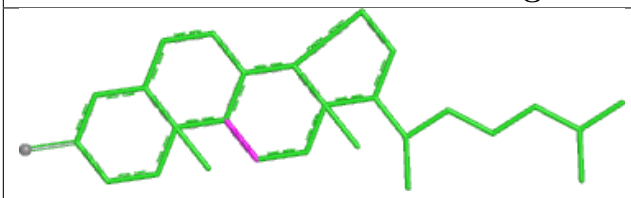
Ligand POV B 319



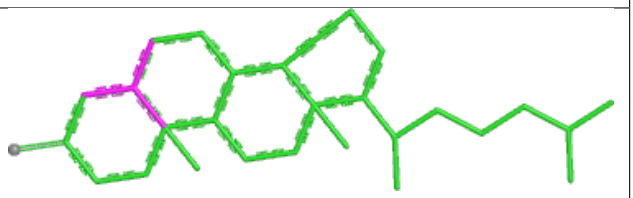
Ligand POV B 372



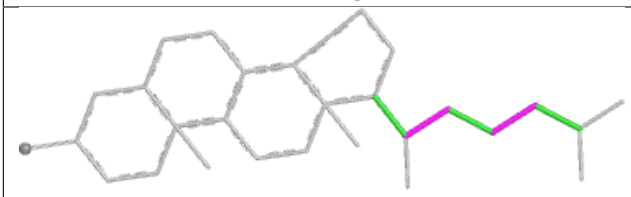
Ligand CLR A 404



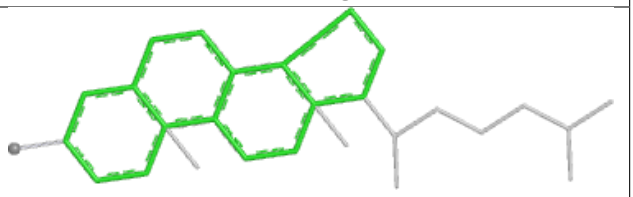
Bond lengths



Bond angles

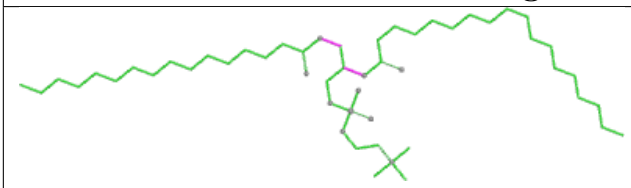


Torsions

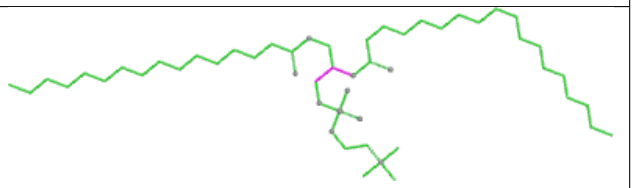


Rings

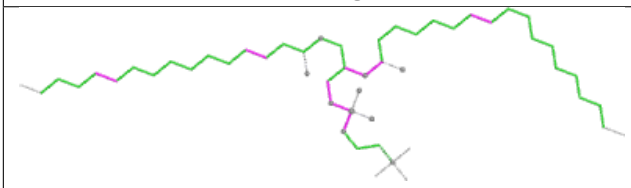
Ligand POV A 315



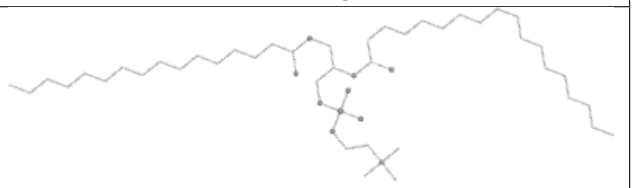
Bond lengths



Bond angles

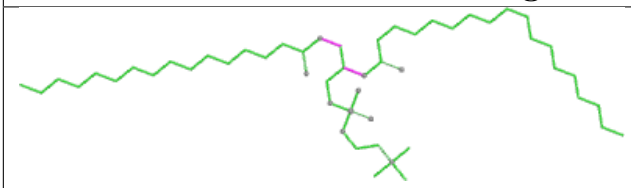


Torsions

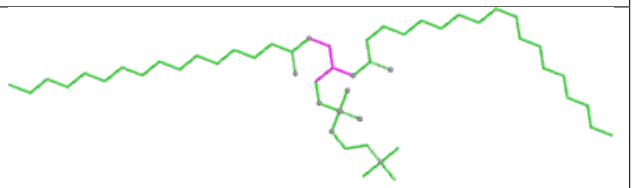


Rings

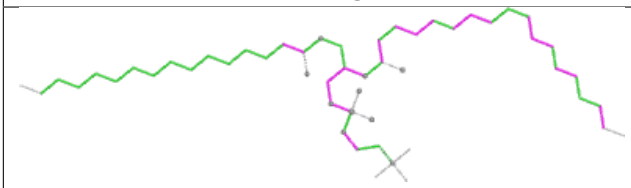
Ligand POV A 384



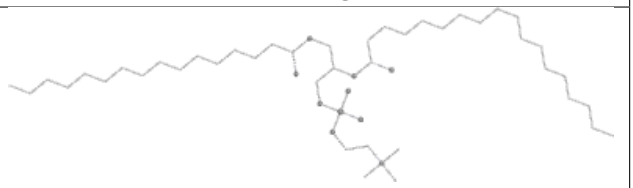
Bond lengths



Bond angles

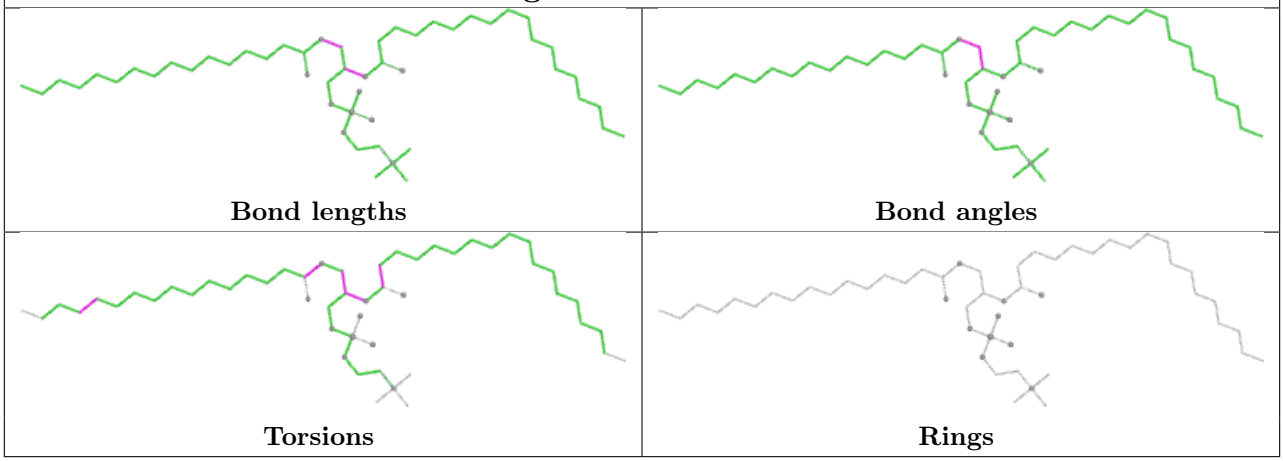


Torsions

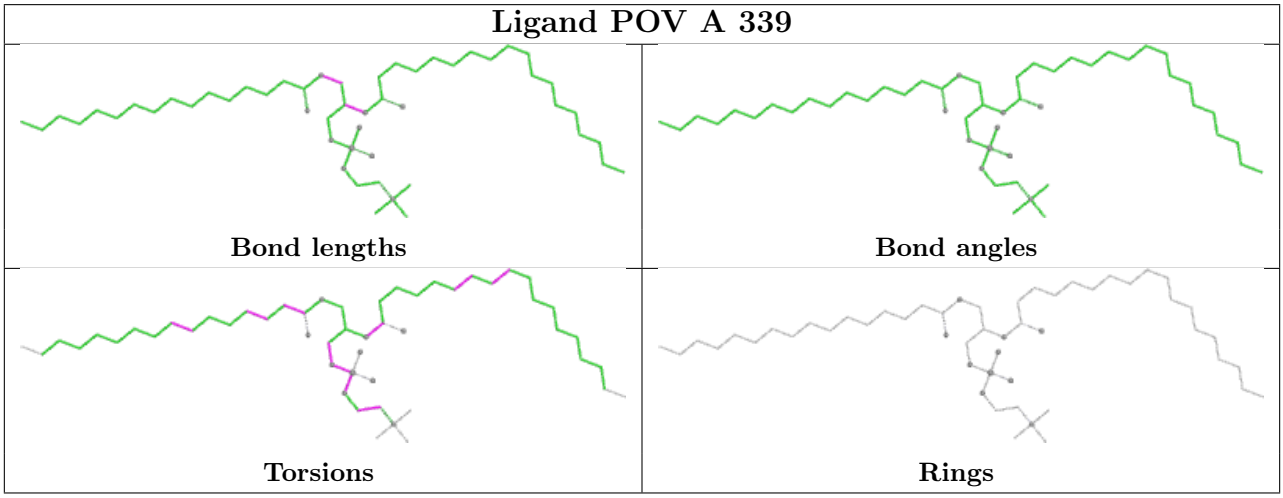


Rings

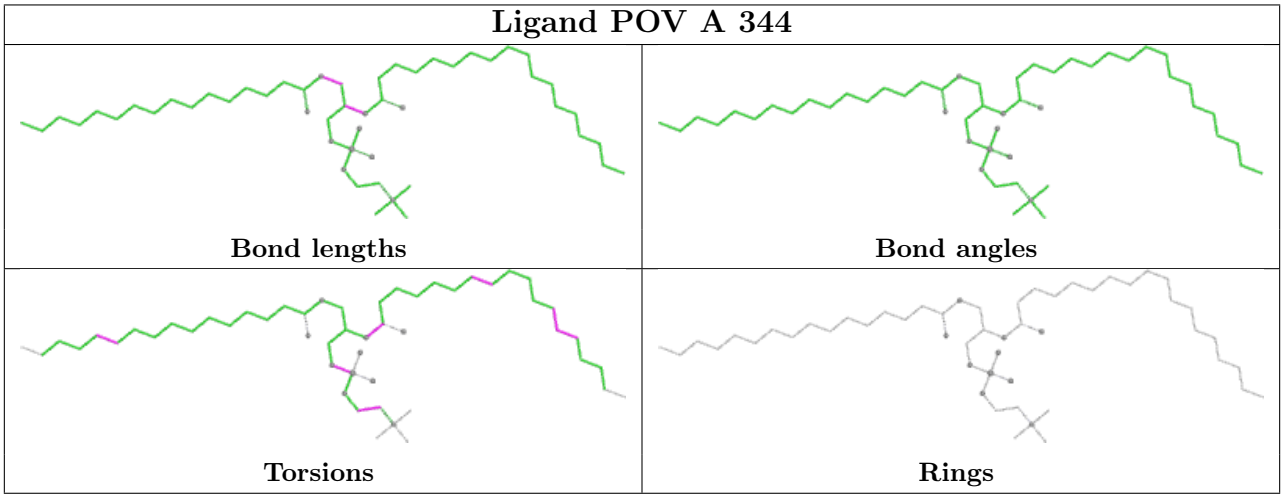
Ligand POV A 355



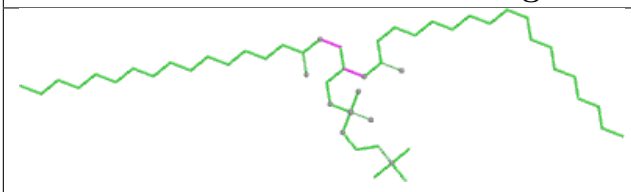
Ligand POV A 339



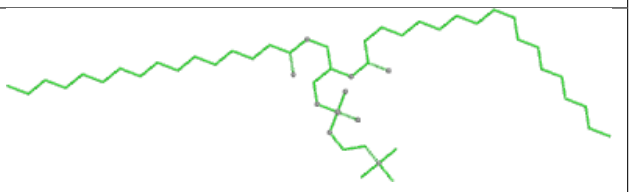
Ligand POV A 344



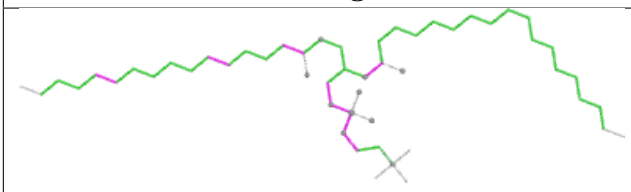
Ligand POV A 380



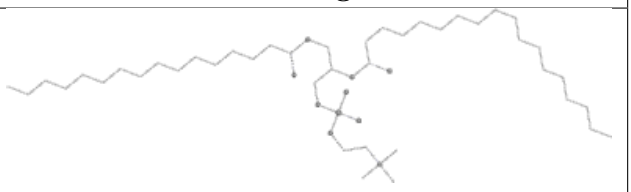
Bond lengths



Bond angles

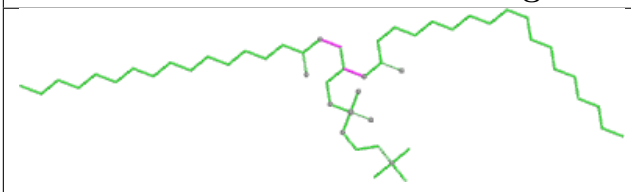


Torsions

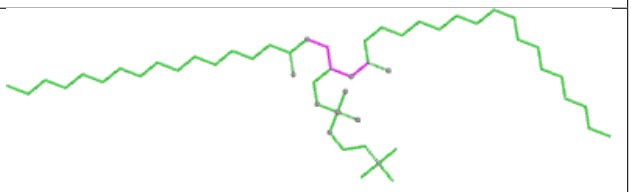


Rings

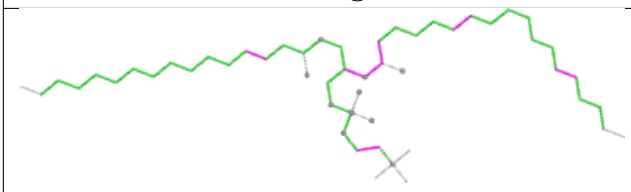
Ligand POV B 380



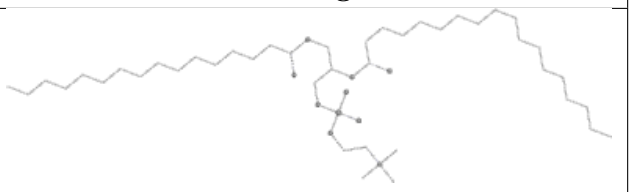
Bond lengths



Bond angles

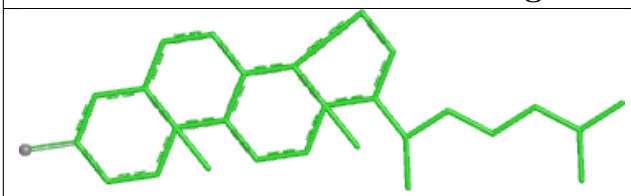


Torsions

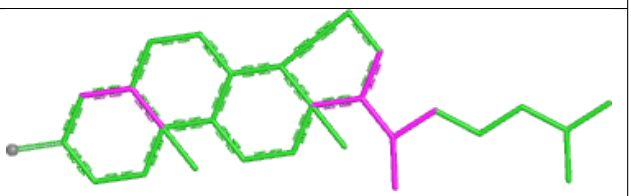


Rings

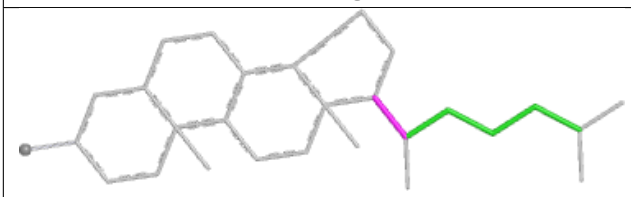
Ligand CLR B 392



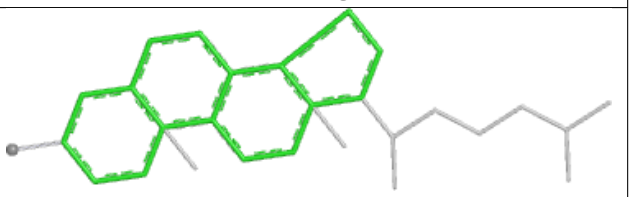
Bond lengths



Bond angles

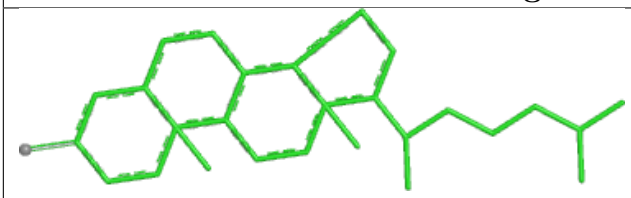


Torsions

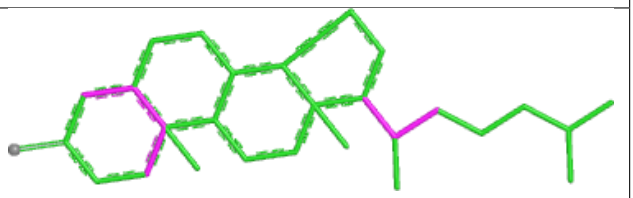


Rings

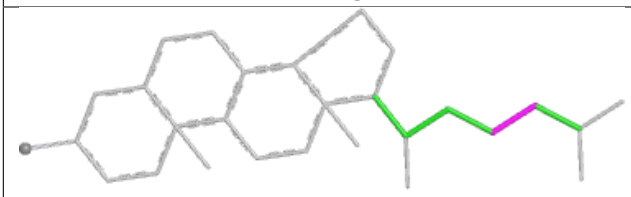
Ligand CLR A 420



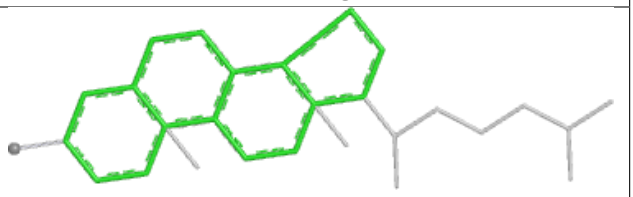
Bond lengths



Bond angles

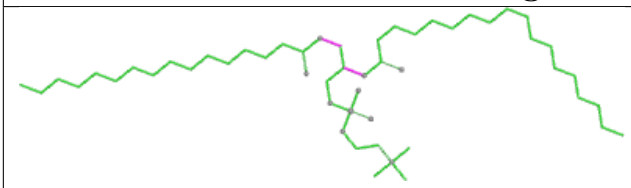


Torsions

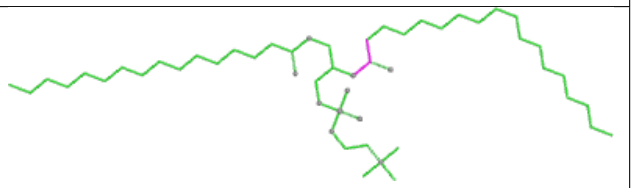


Rings

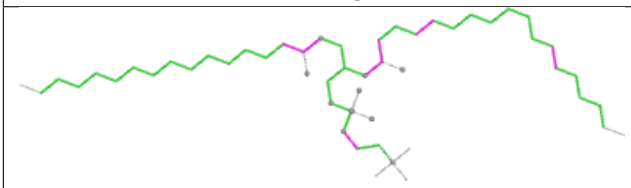
Ligand POV A 369



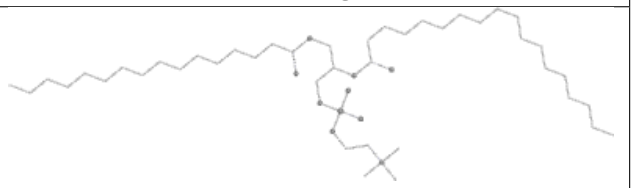
Bond lengths



Bond angles

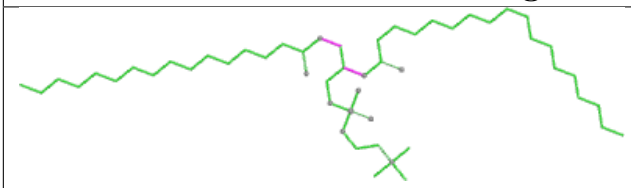


Torsions

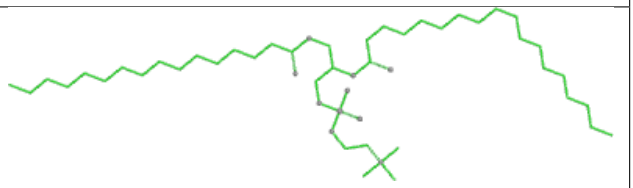


Rings

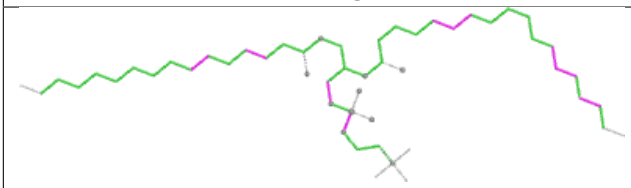
Ligand POV A 304



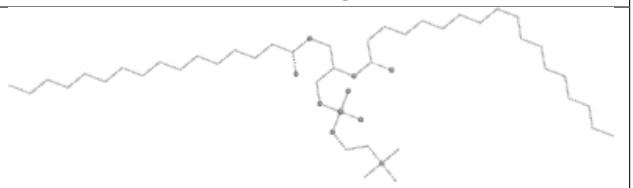
Bond lengths



Bond angles

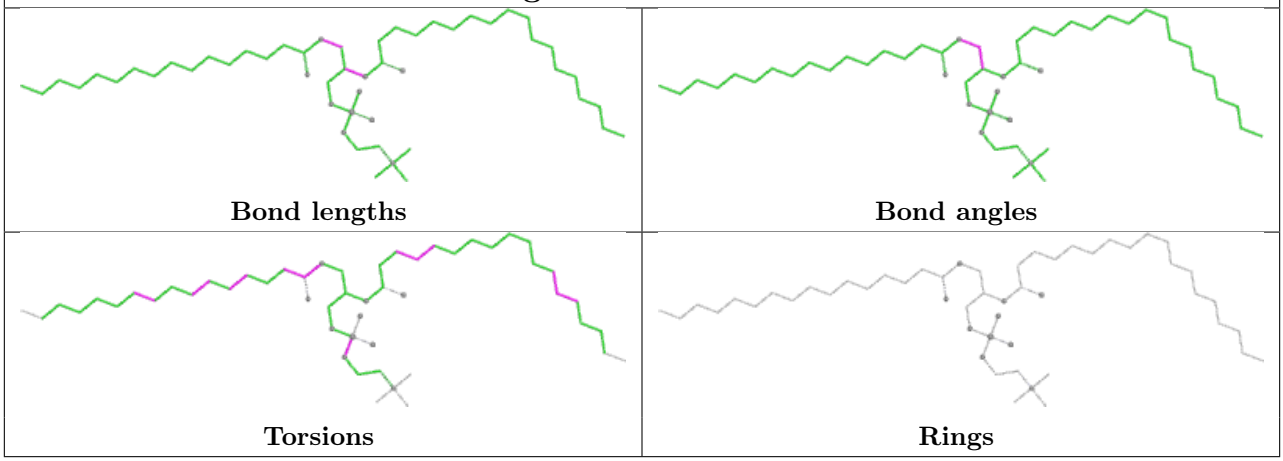


Torsions

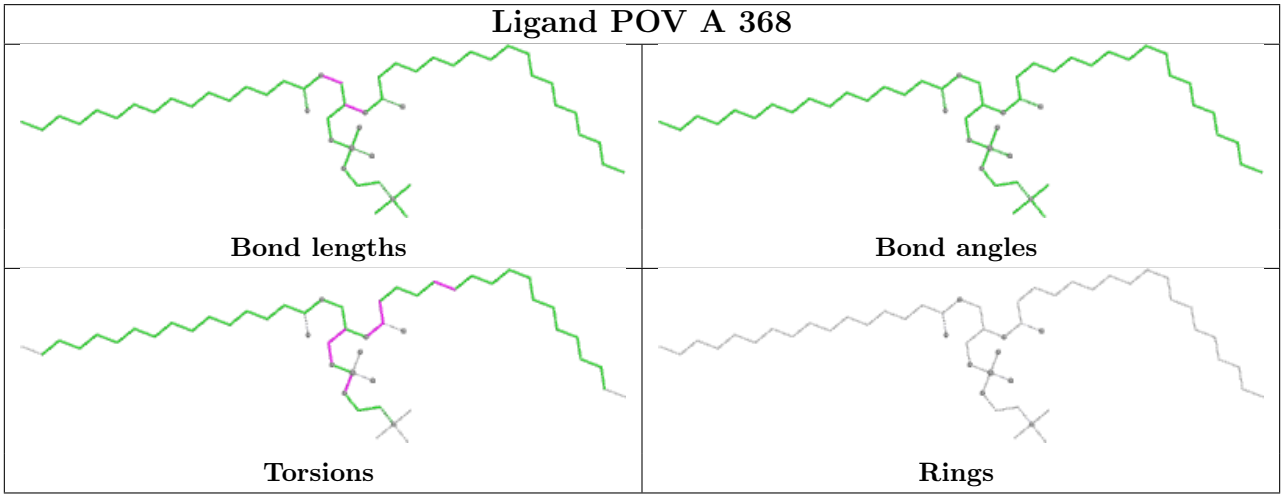


Rings

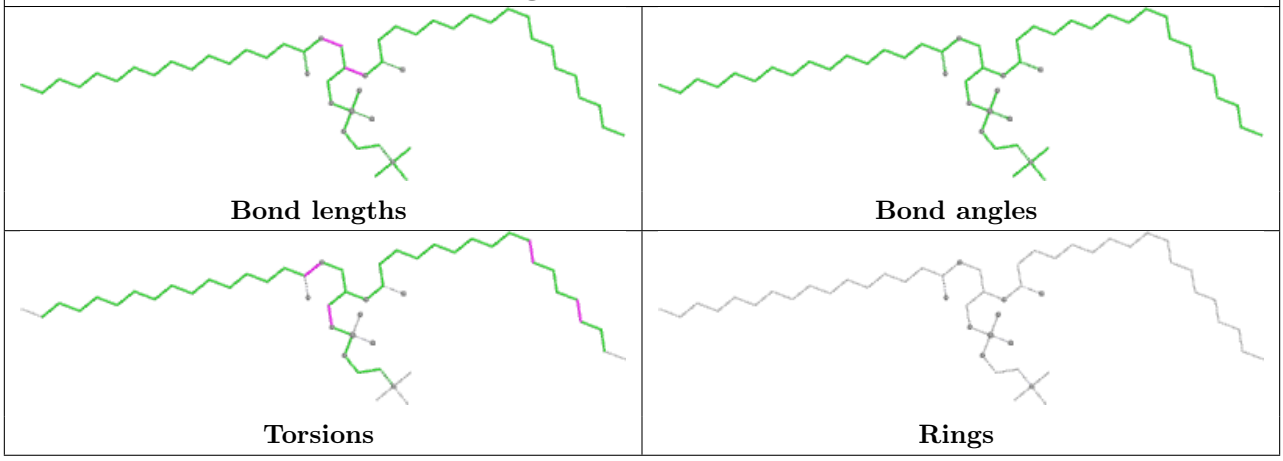
Ligand POV A 376



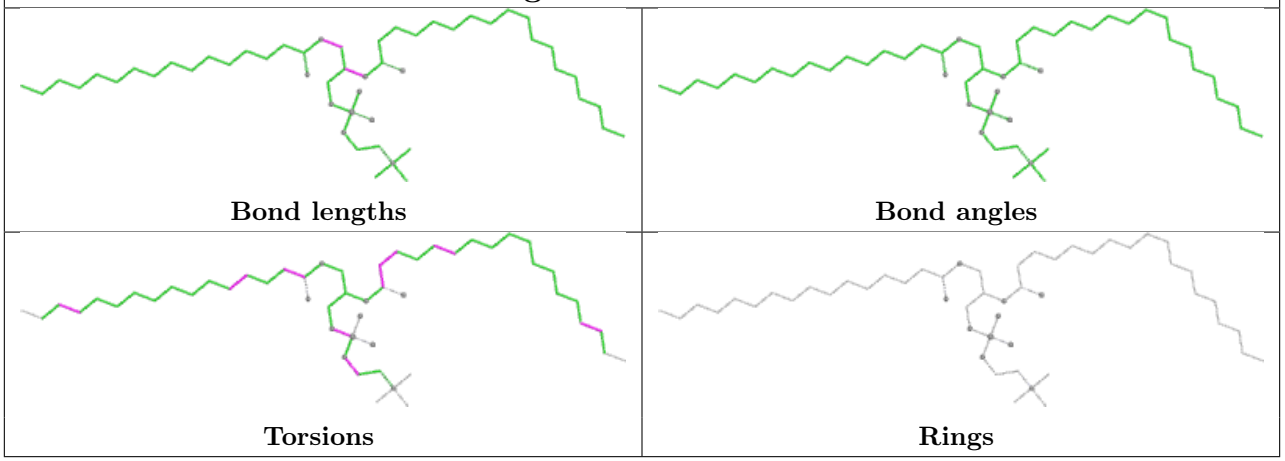
Ligand POV A 368



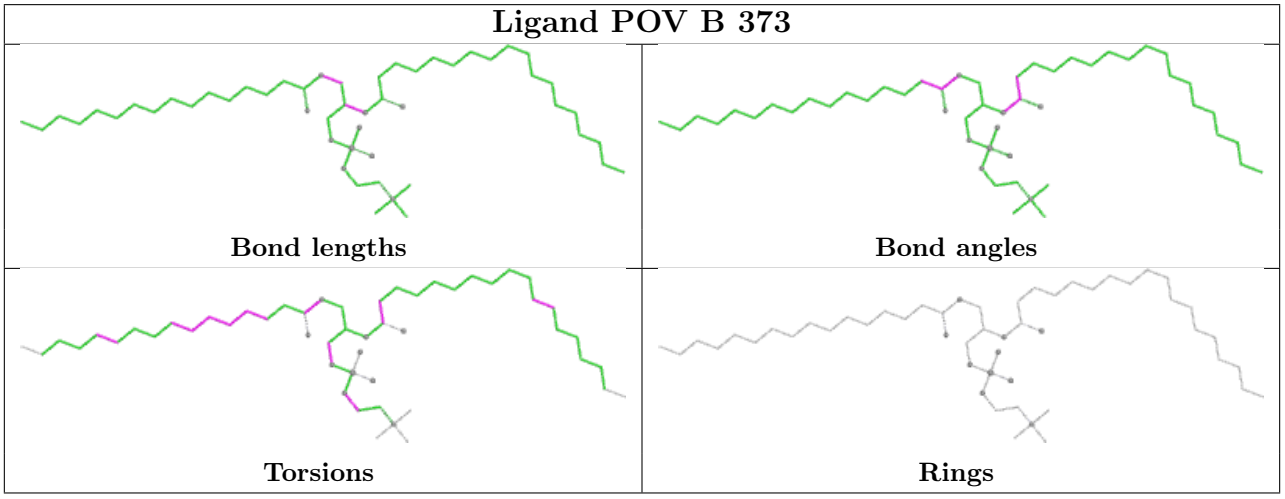
Ligand POV A 367



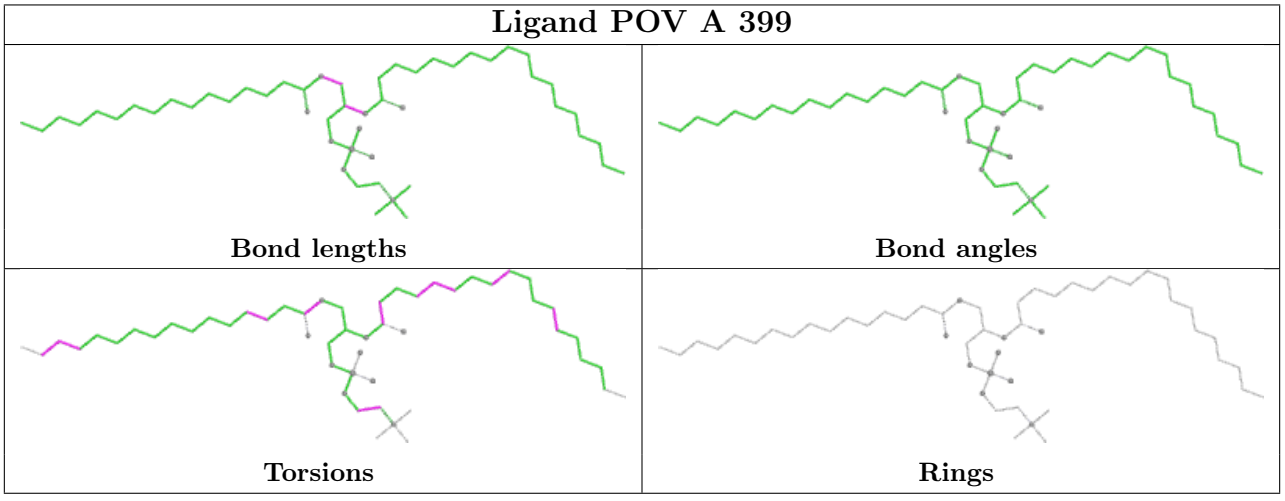
Ligand POV B 338



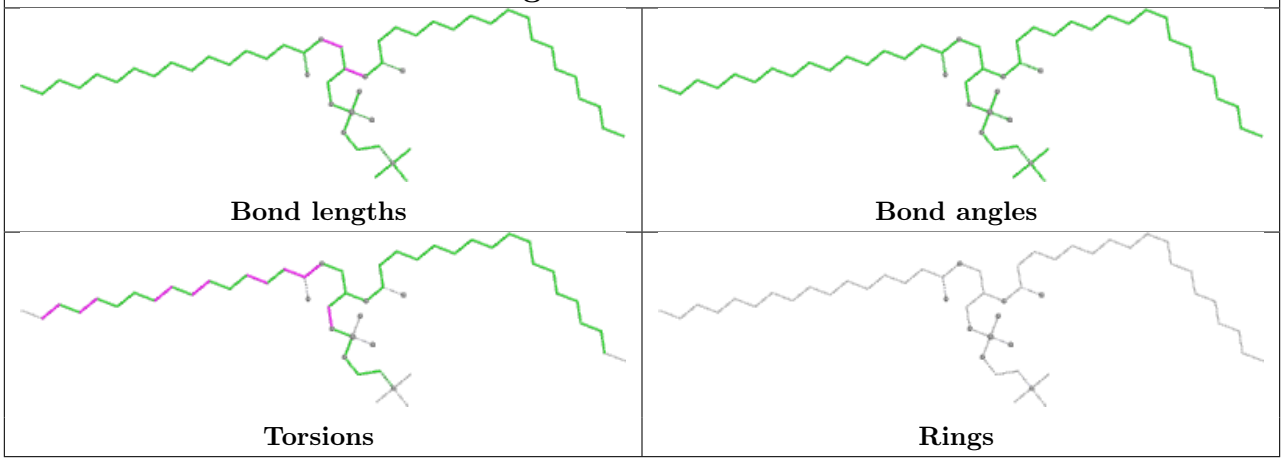
Ligand POV B 373



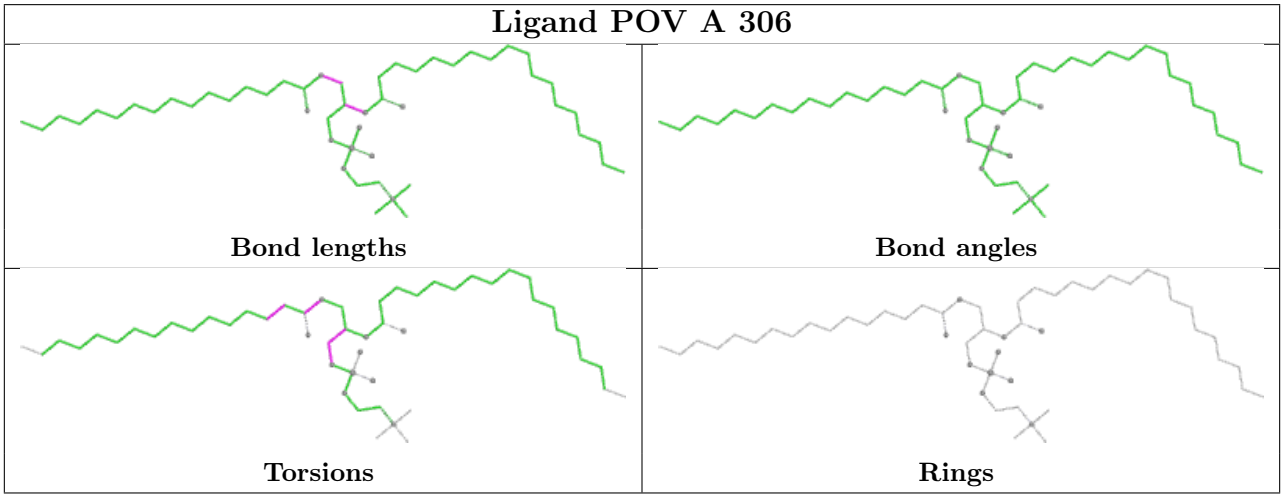
Ligand POV A 399



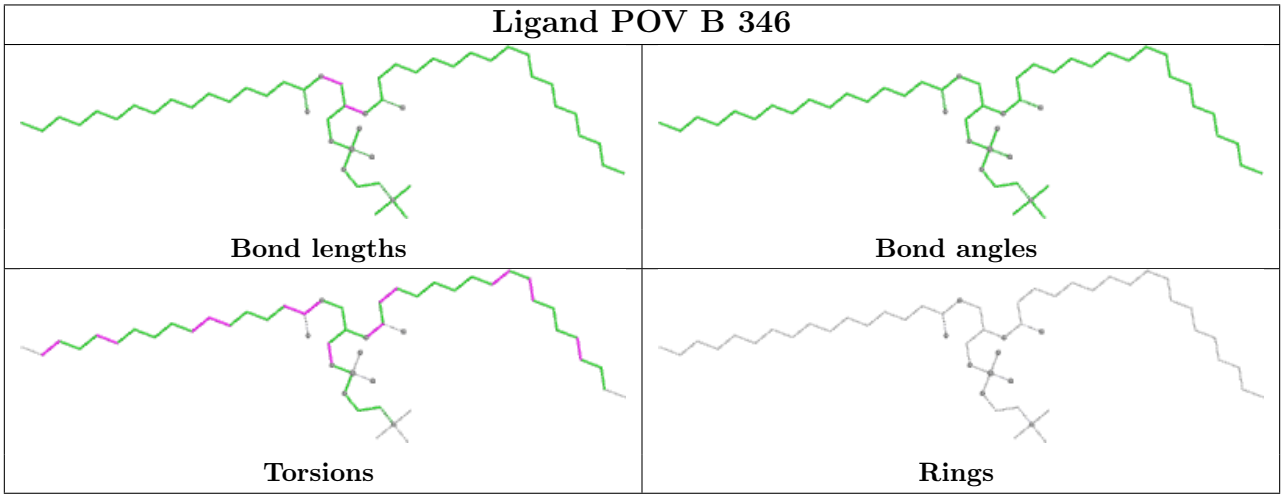
Ligand POV A 416



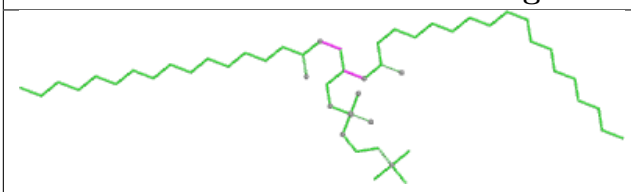
Ligand POV A 306



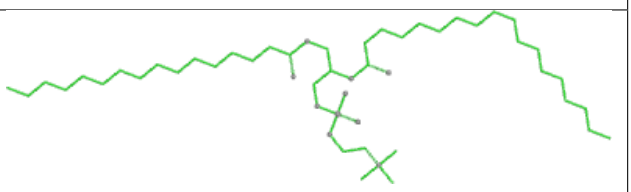
Ligand POV B 346



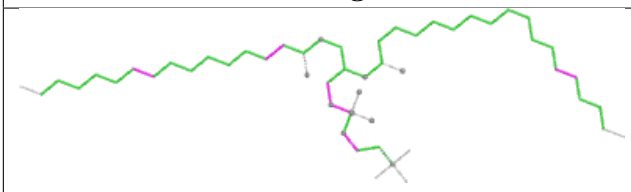
Ligand POV B 316



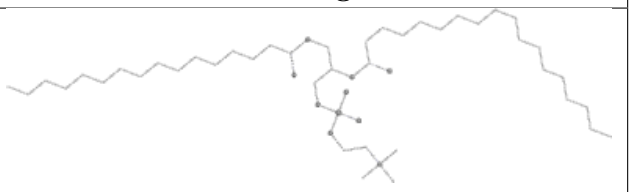
Bond lengths



Bond angles

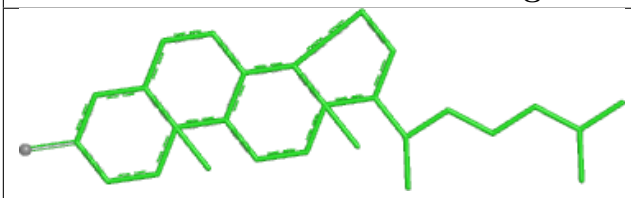


Torsions

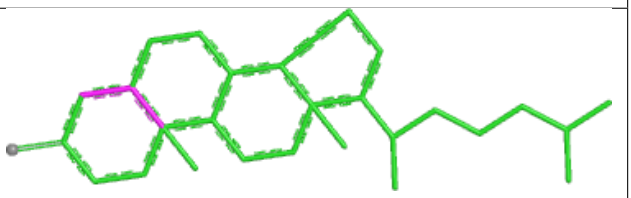


Rings

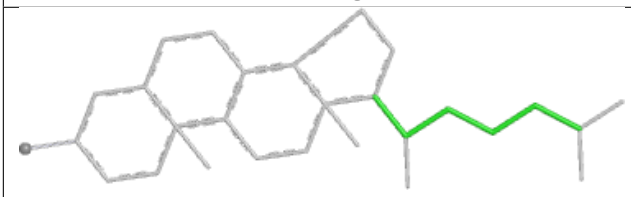
Ligand CLR A 401



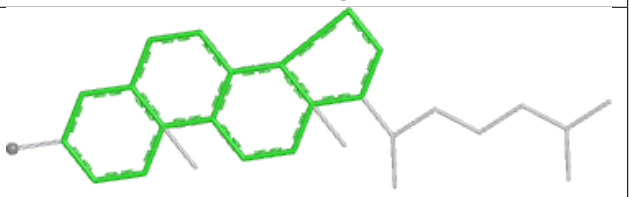
Bond lengths



Bond angles

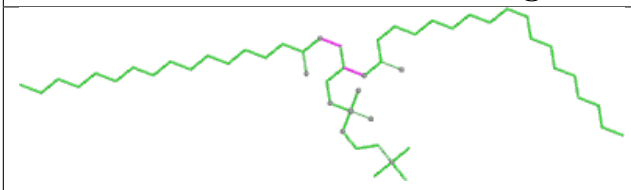


Torsions

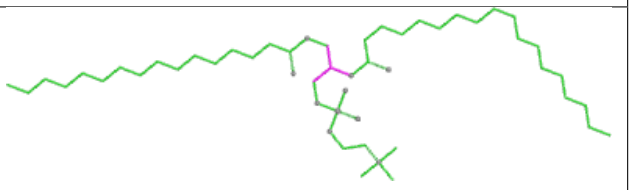


Rings

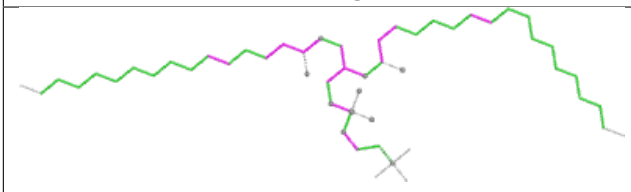
Ligand POV B 360



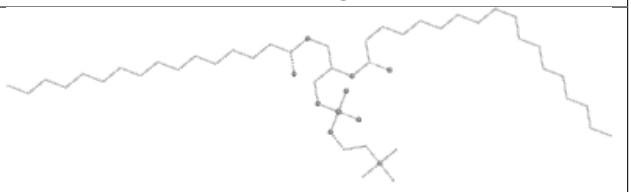
Bond lengths



Bond angles

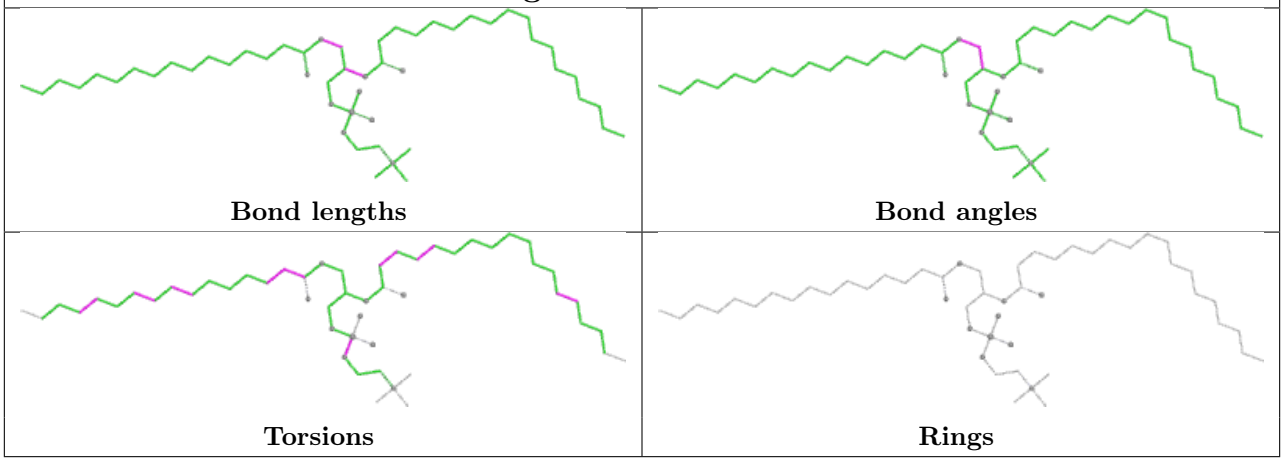


Torsions

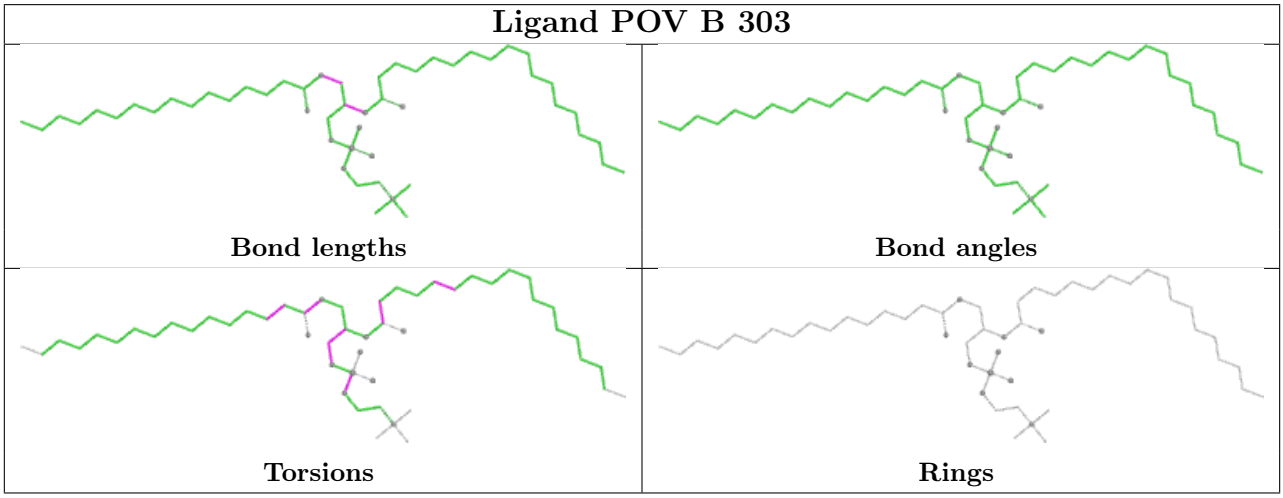


Rings

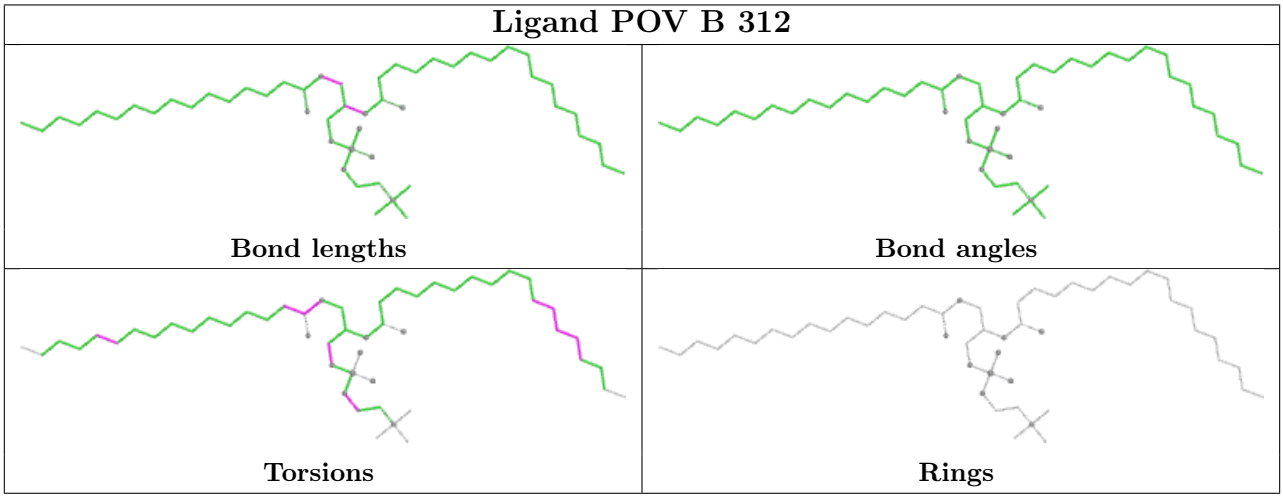
Ligand POV A 303



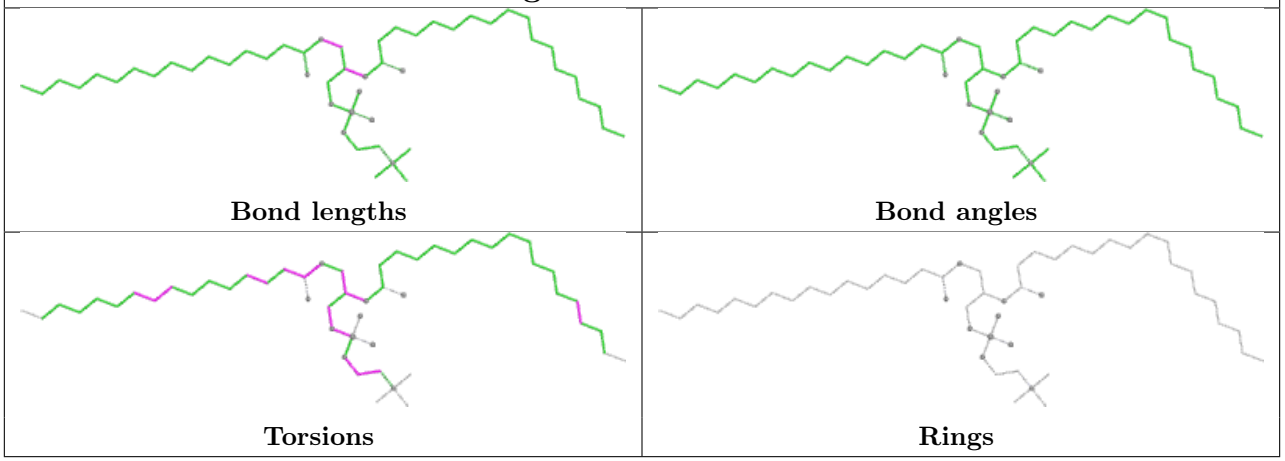
Ligand POV B 303



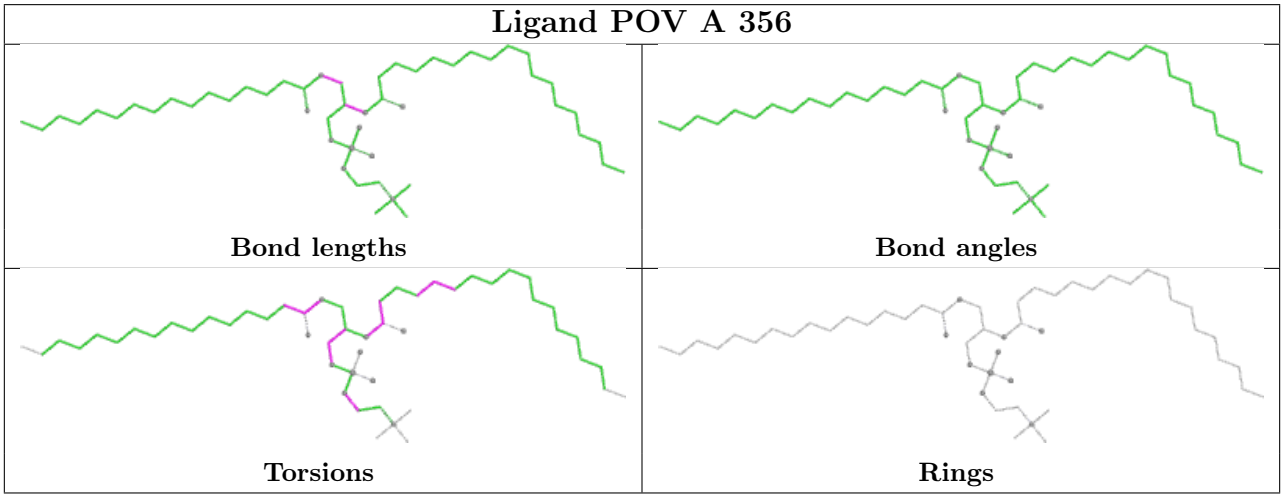
Ligand POV B 312



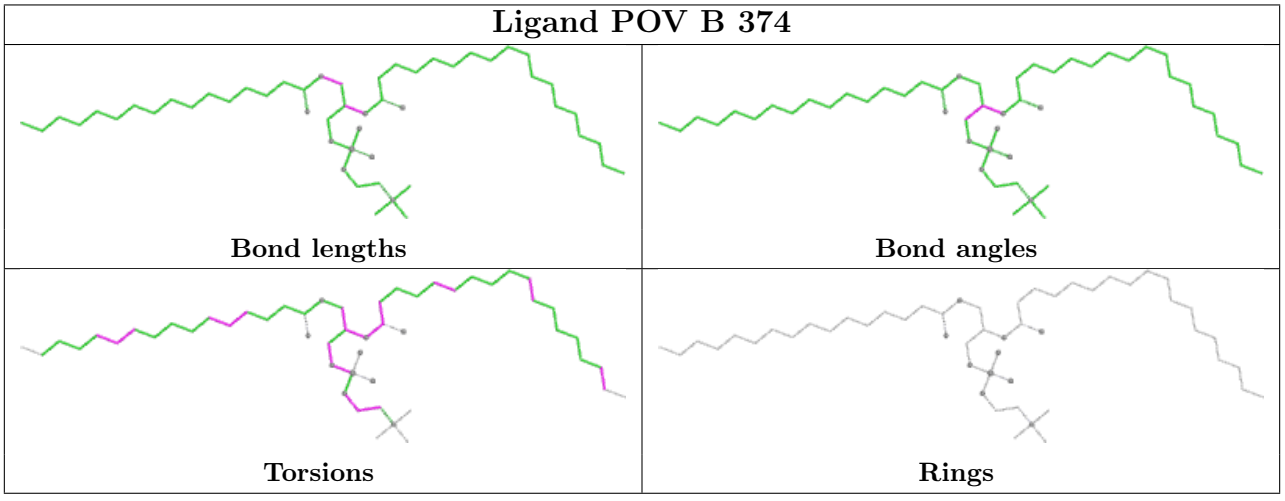
Ligand POV A 354



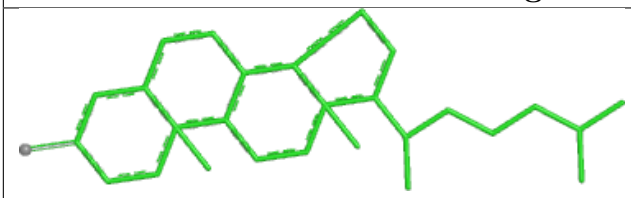
Ligand POV A 356



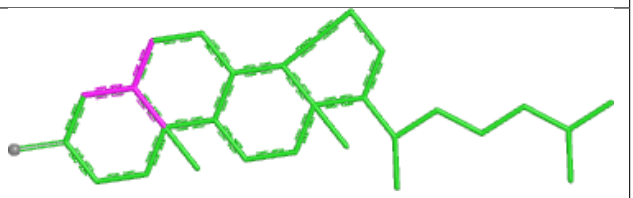
Ligand POV B 374



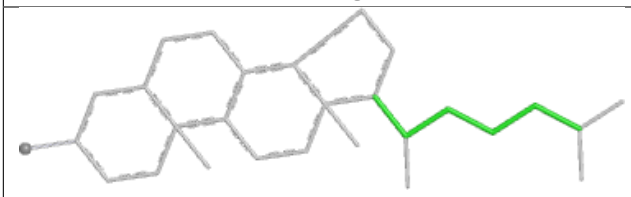
Ligand CLR B 397



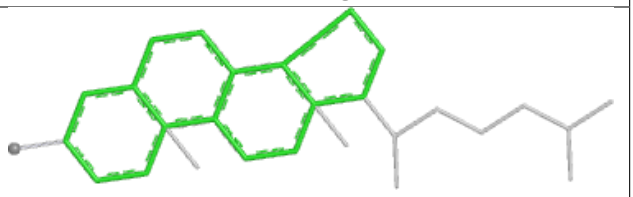
Bond lengths



Bond angles

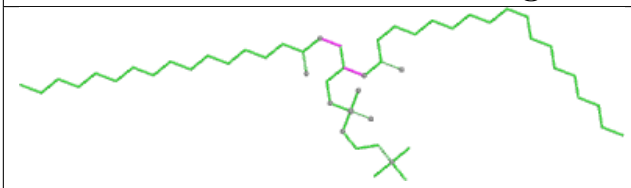


Torsions

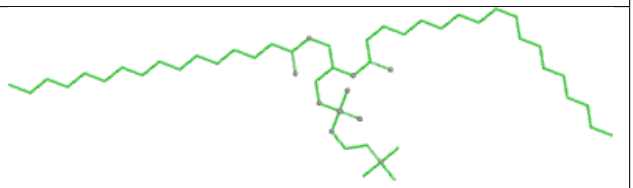


Rings

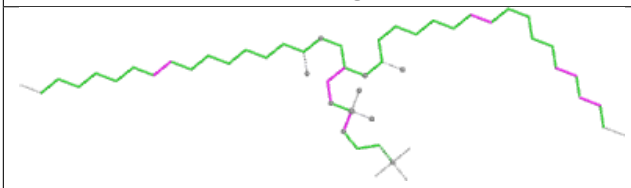
Ligand POV A 342



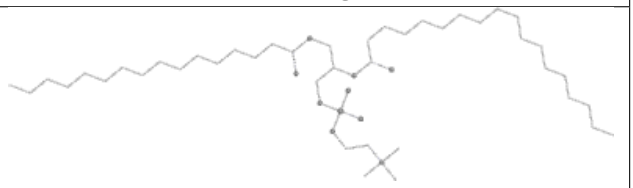
Bond lengths



Bond angles

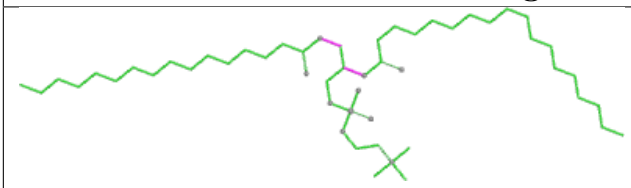


Torsions

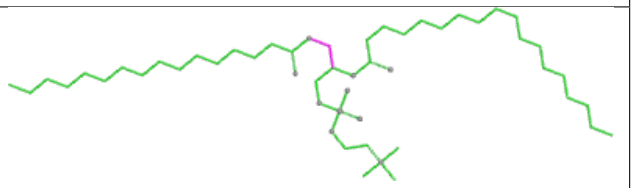


Rings

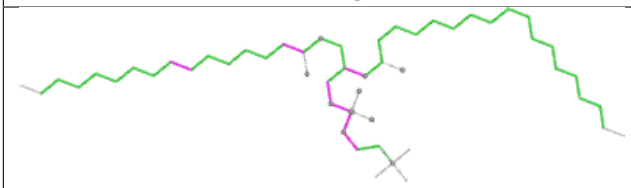
Ligand POV A 407



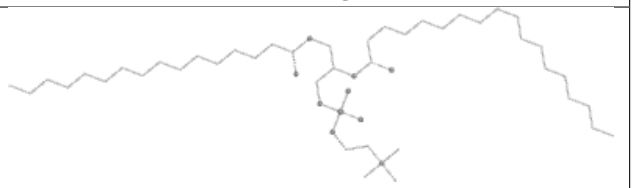
Bond lengths



Bond angles

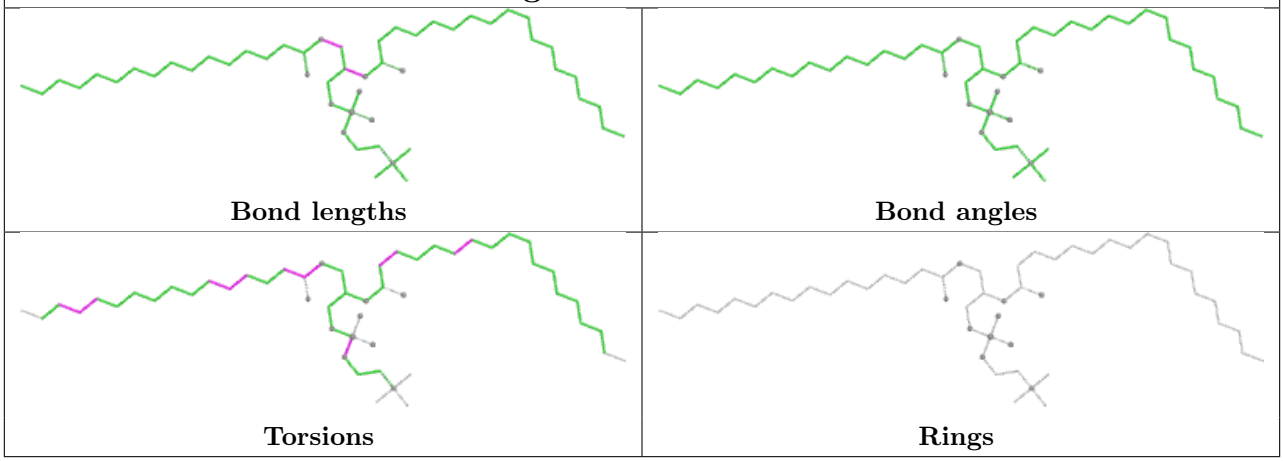


Torsions

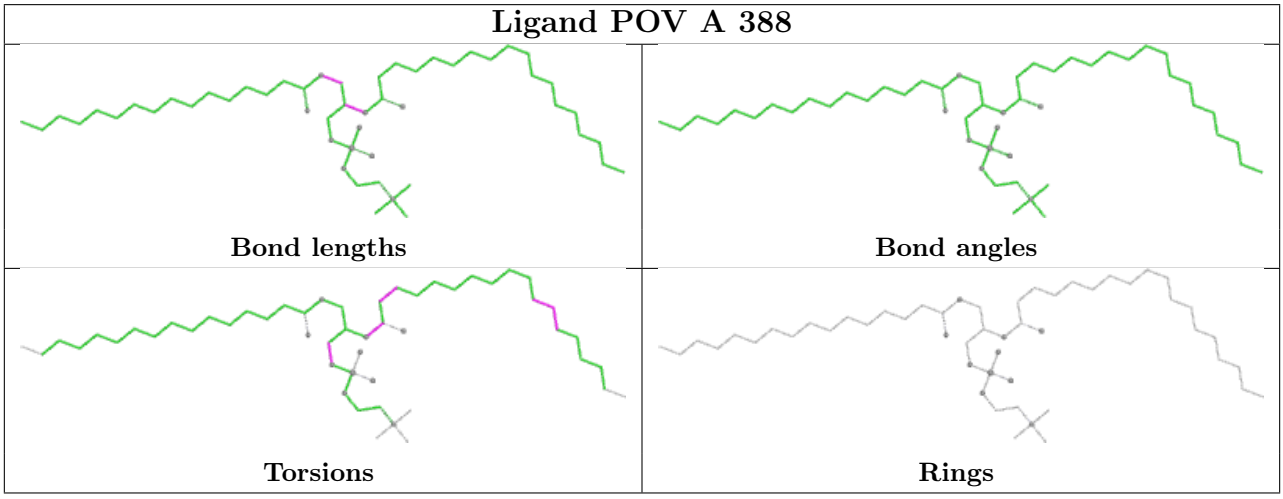


Rings

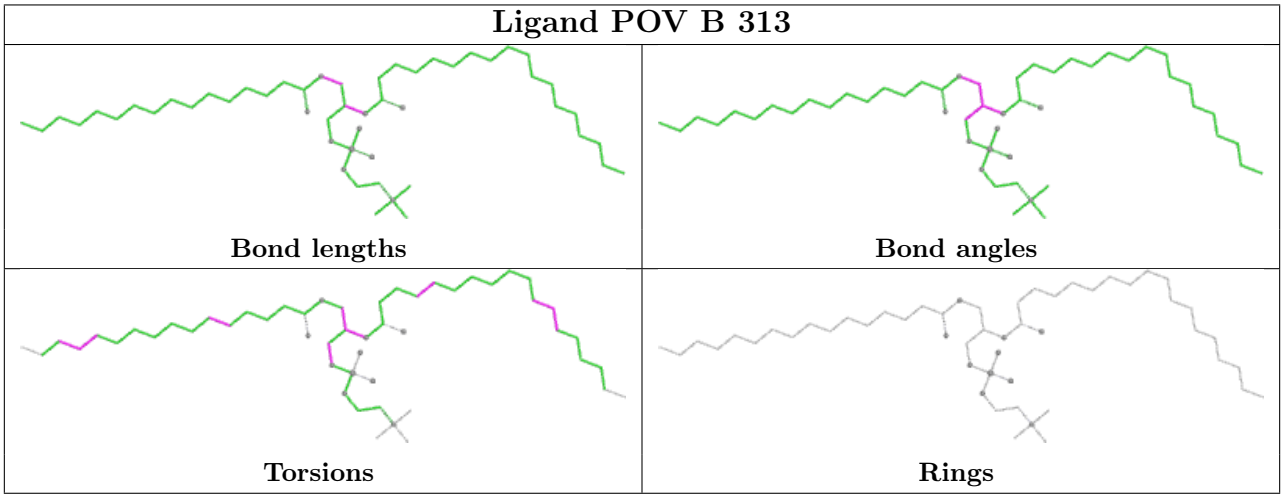
Ligand POV A 346



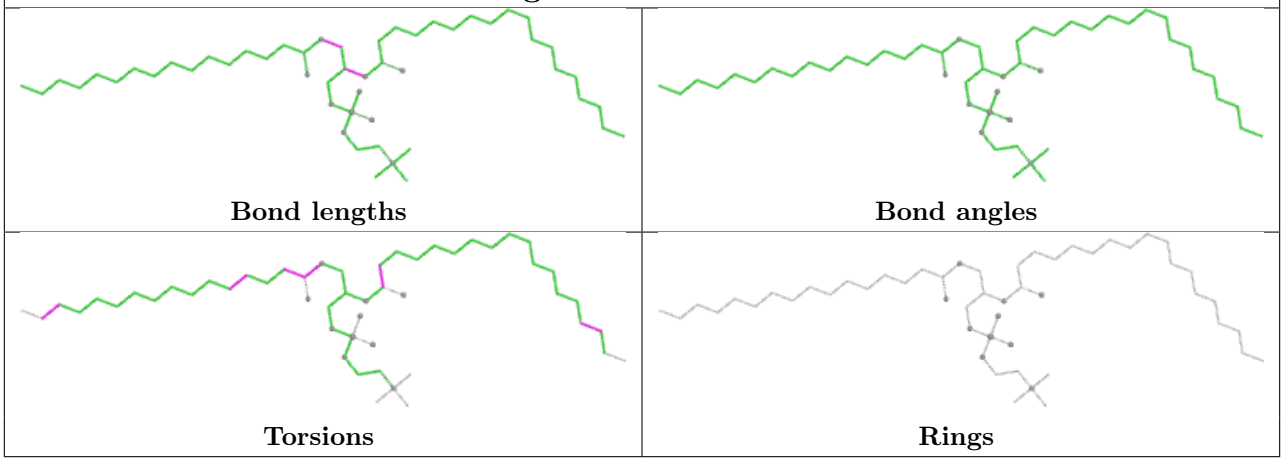
Ligand POV A 388



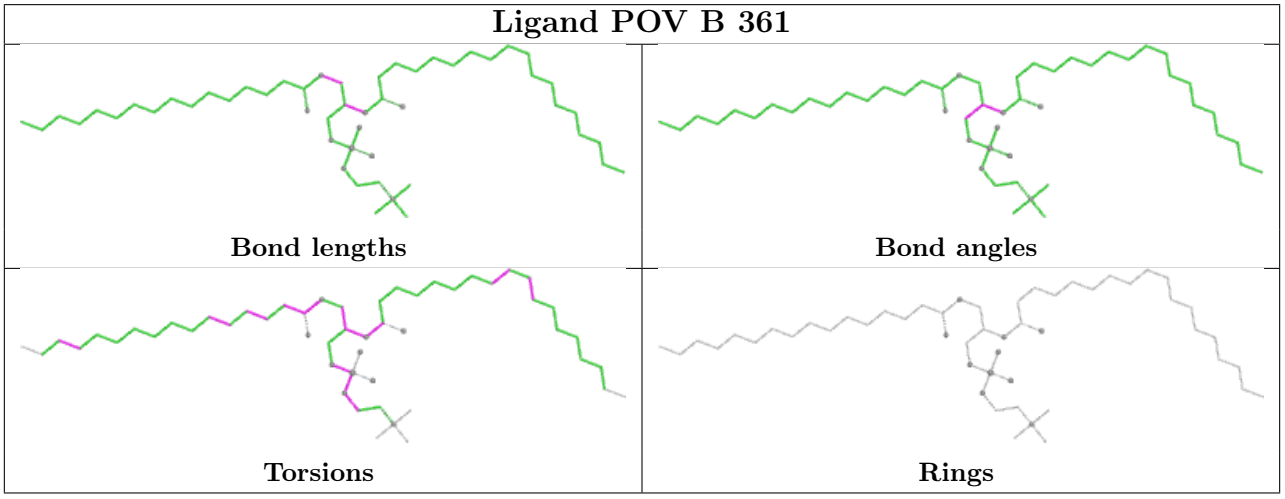
Ligand POV B 313



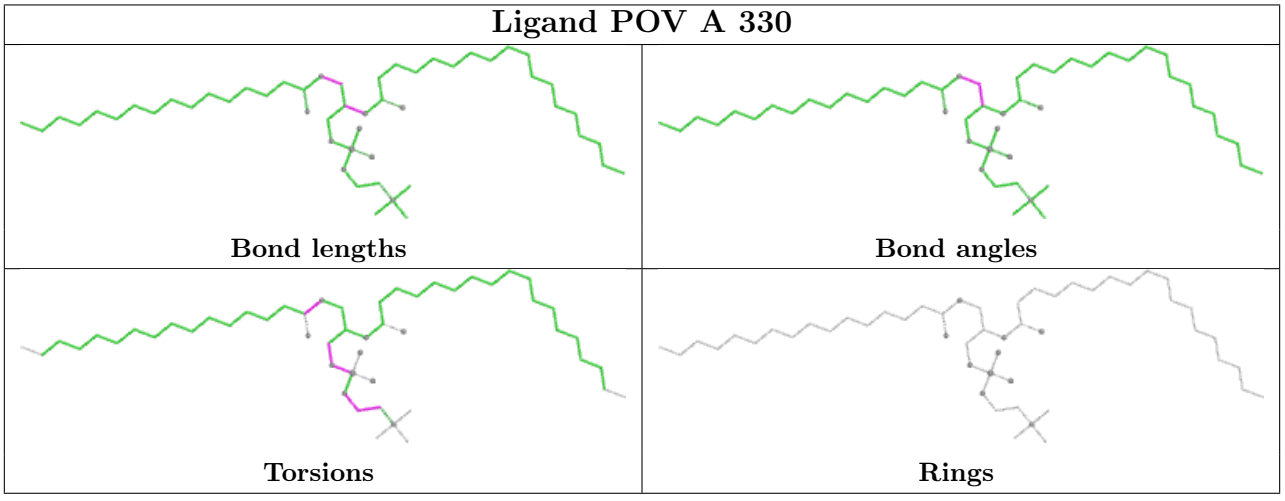
Ligand POV A 410



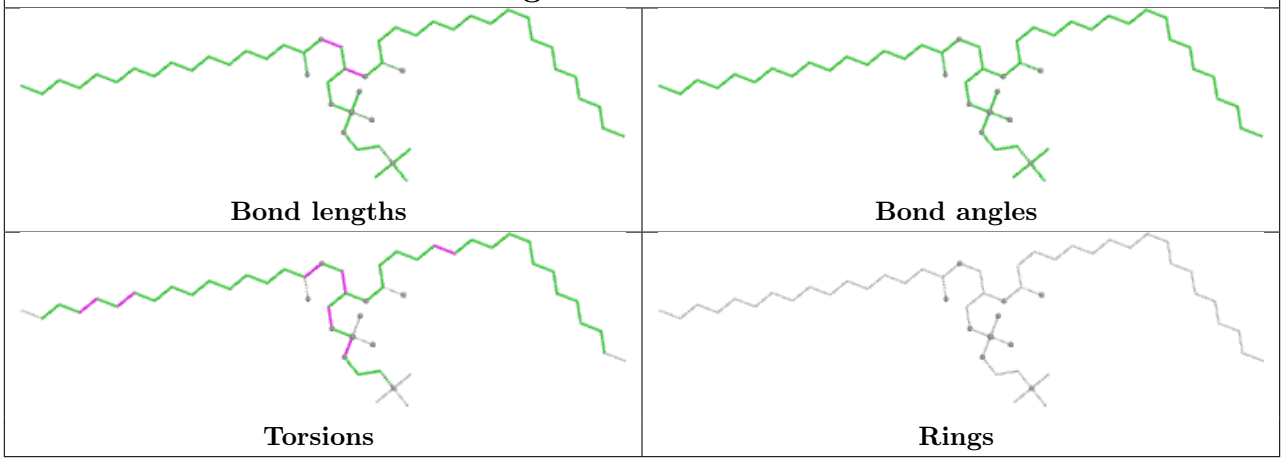
Ligand POV B 361



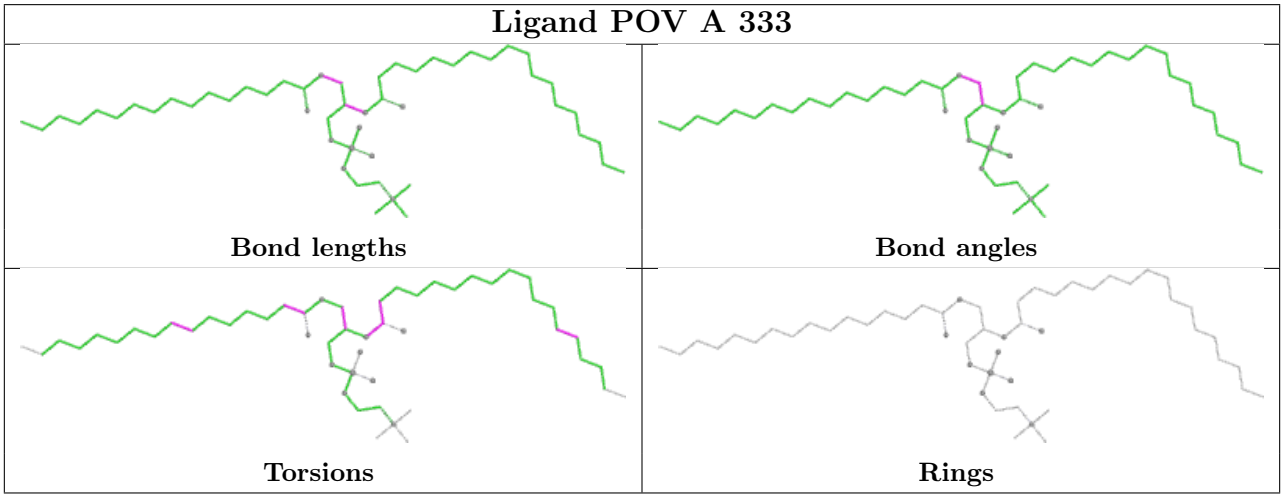
Ligand POV A 330



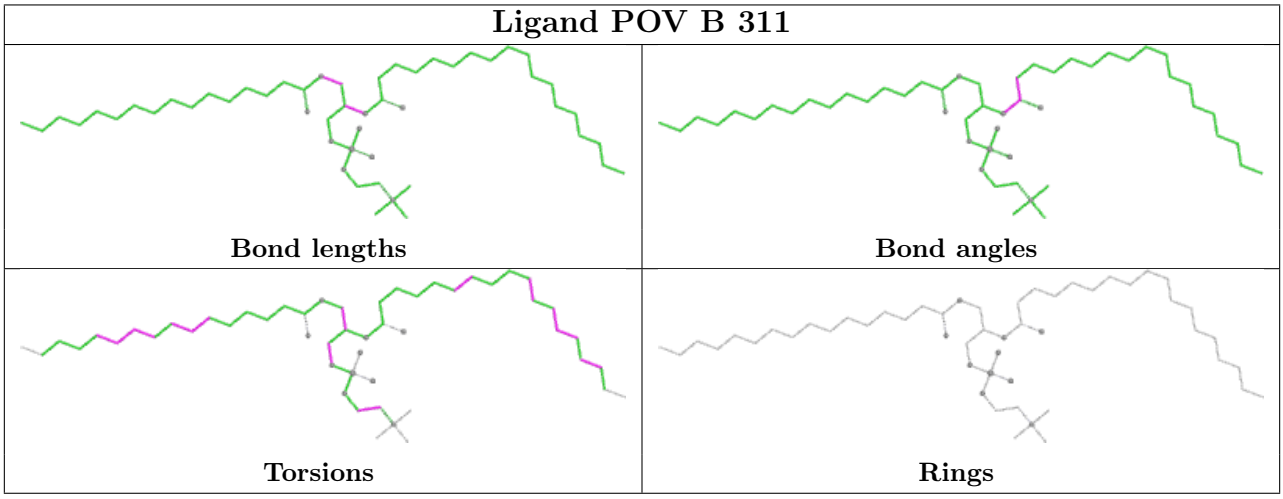
Ligand POV A 320



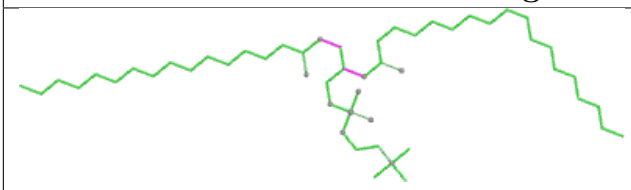
Ligand POV A 333

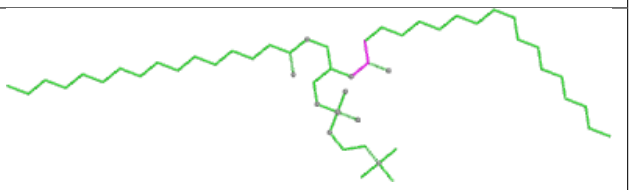


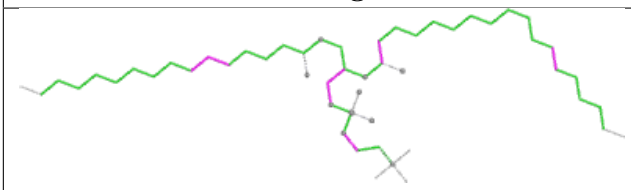
Ligand POV B 311

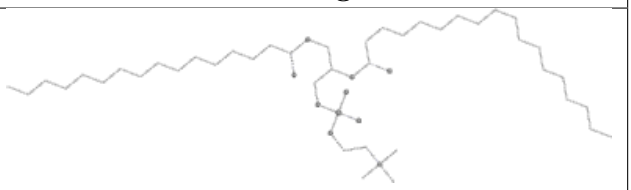


Ligand POV A 413

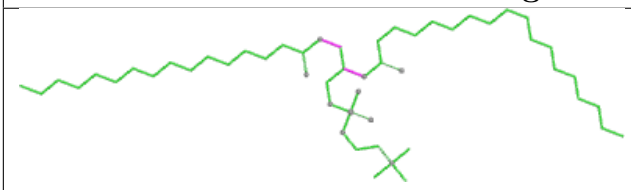

Bond lengths

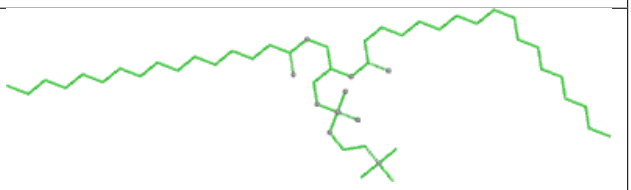

Bond angles

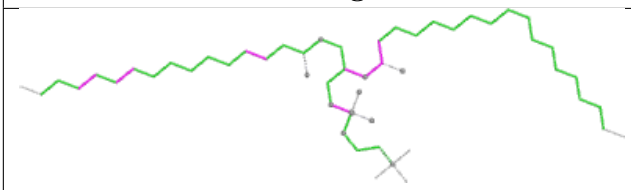

Torsions

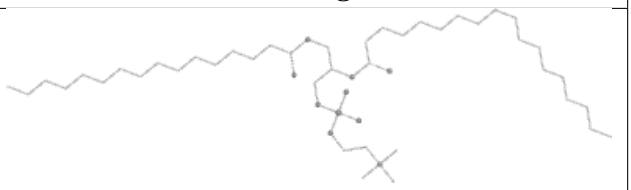

Rings

Ligand POV A 360

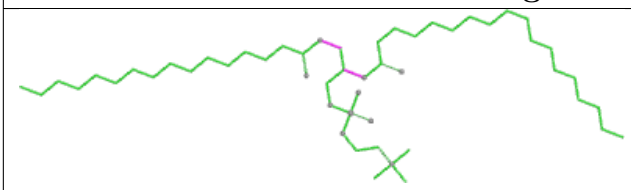

Bond lengths

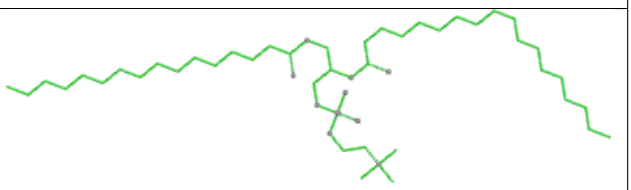

Bond angles

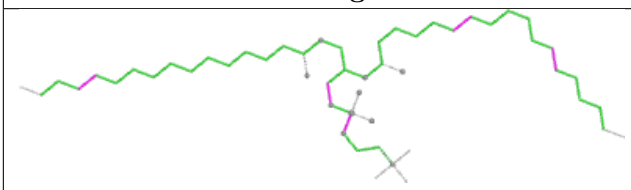

Torsions

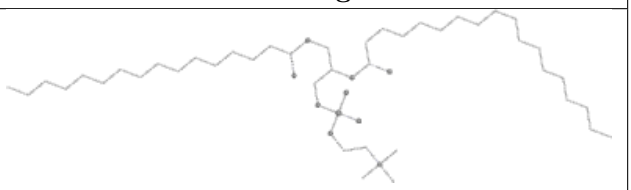

Rings

Ligand POV B 308

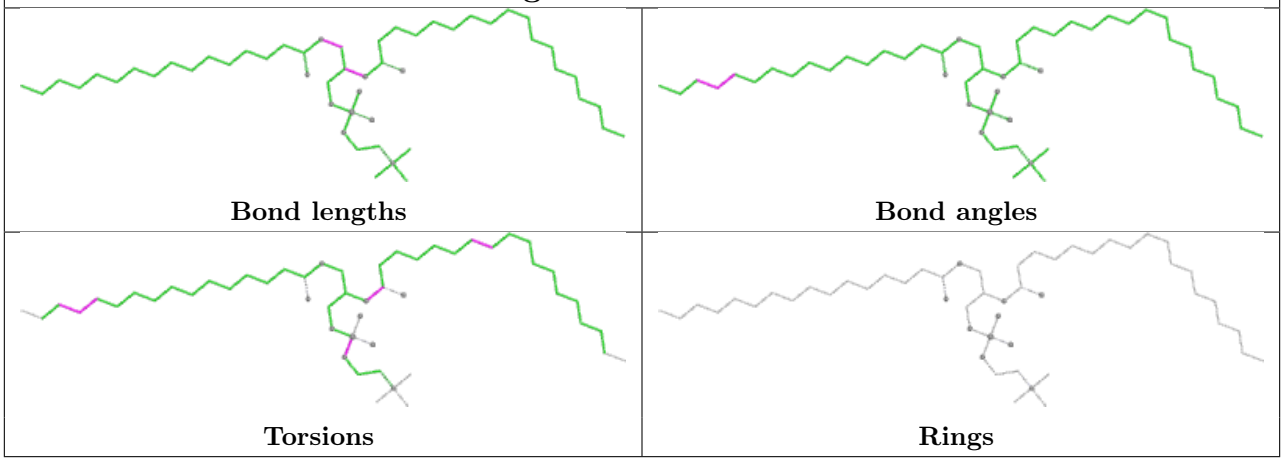

Bond lengths


Bond angles

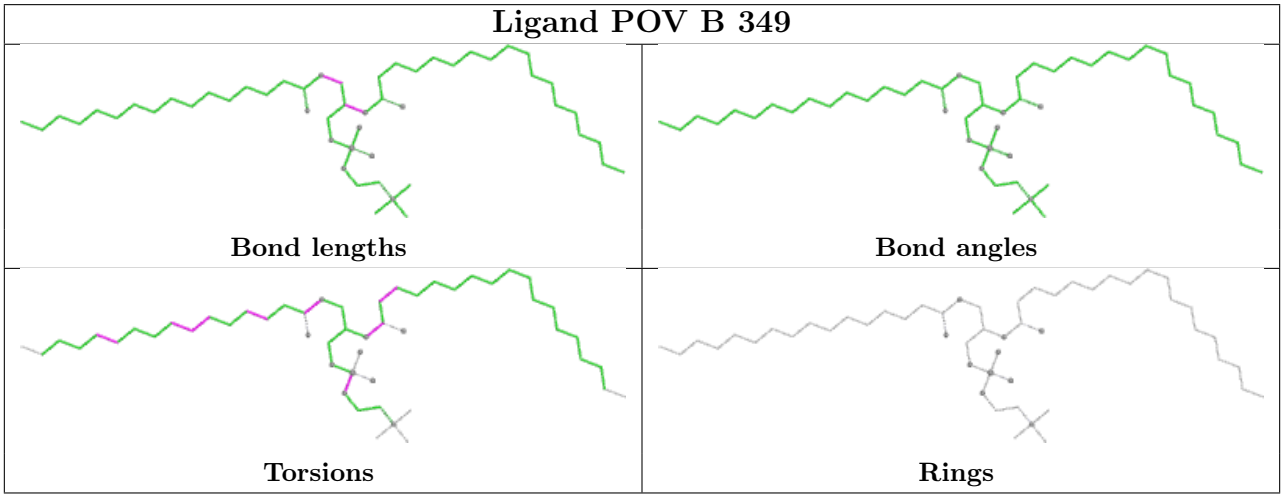

Torsions


Rings

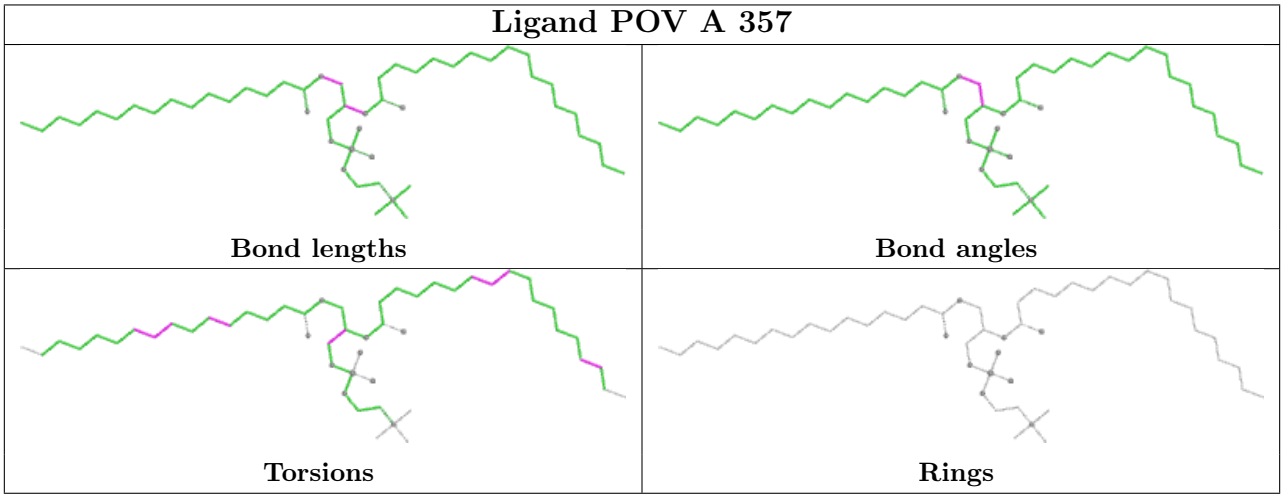
Ligand POV A 417



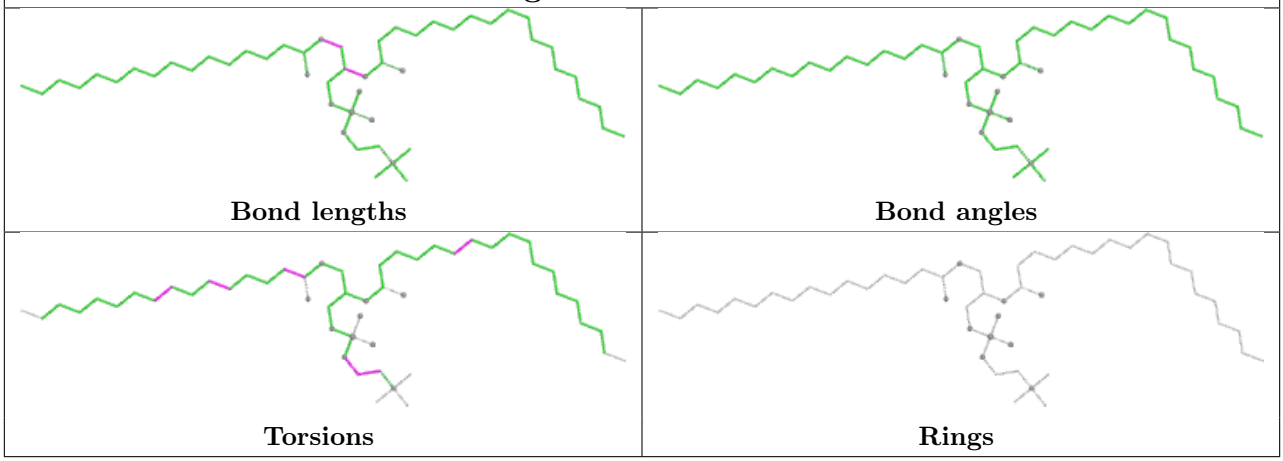
Ligand POV B 349



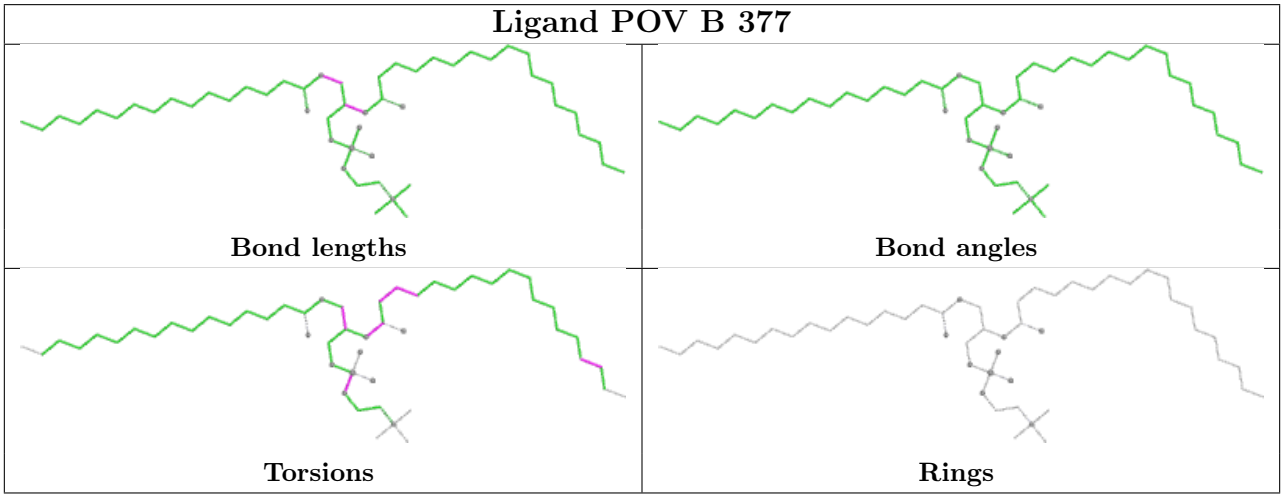
Ligand POV A 357



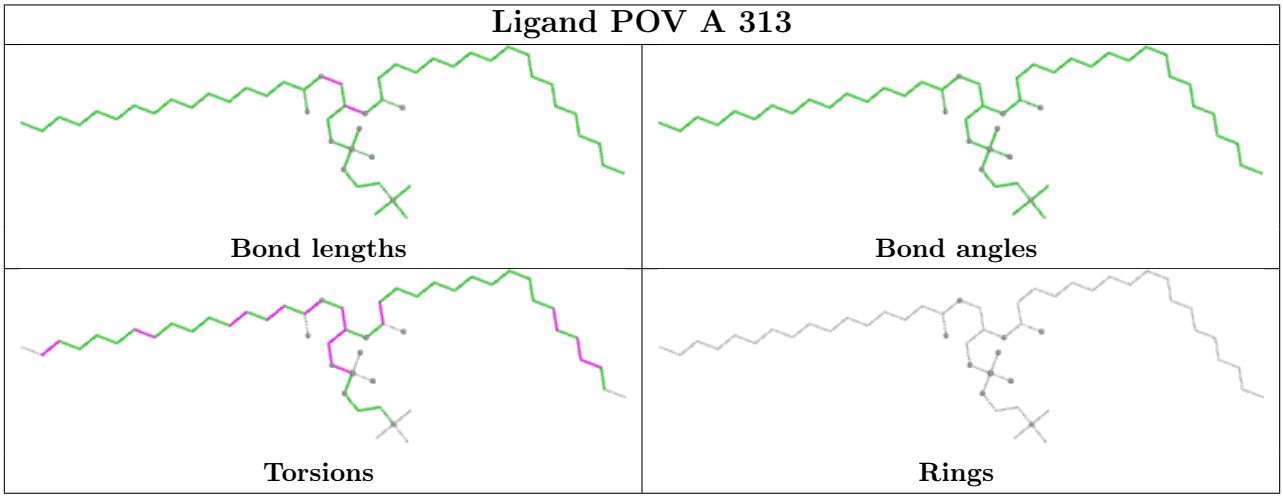
Ligand POV B 335



Ligand POV B 377



Ligand POV A 313



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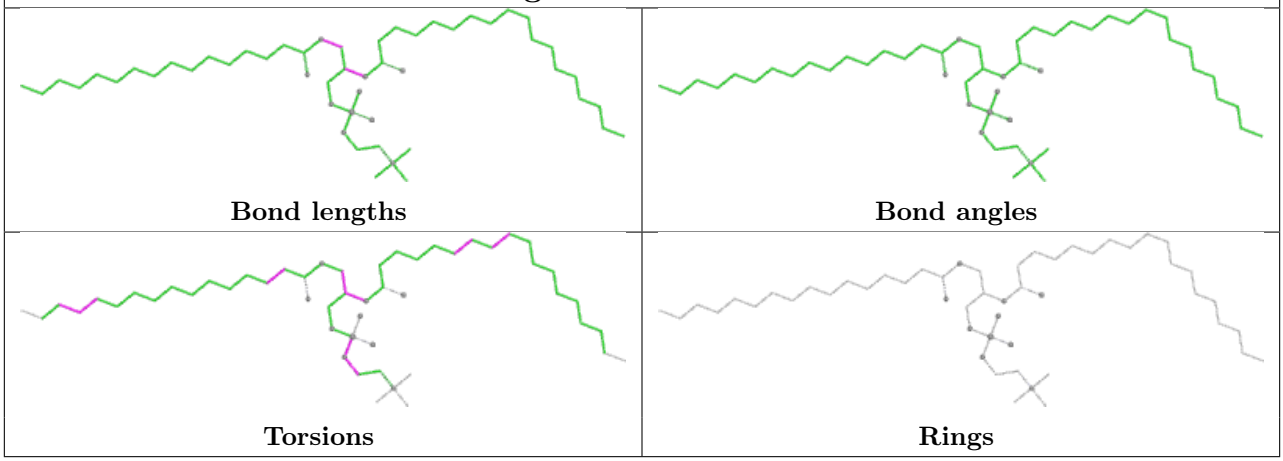
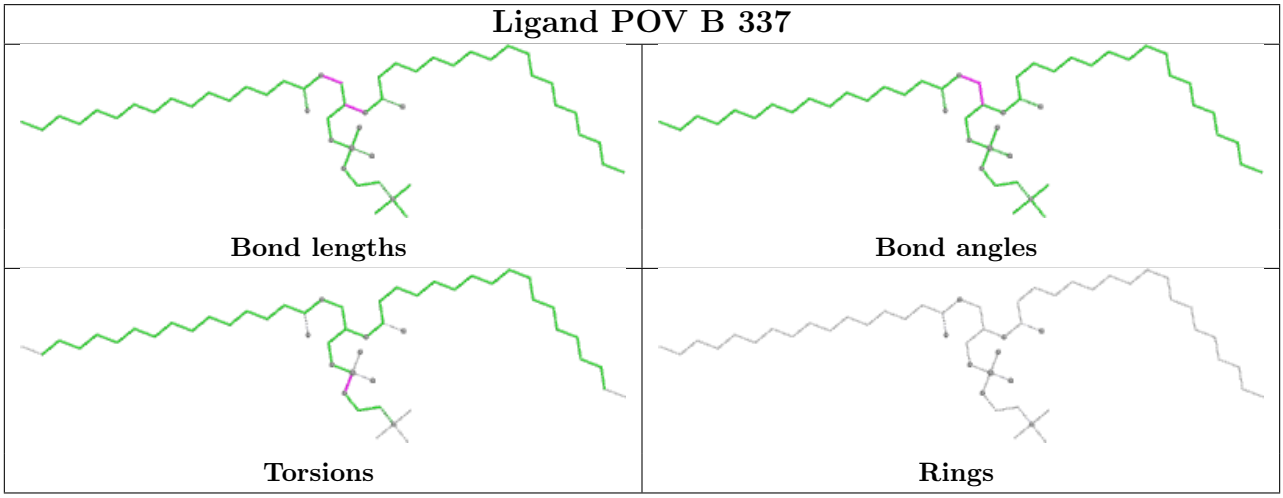
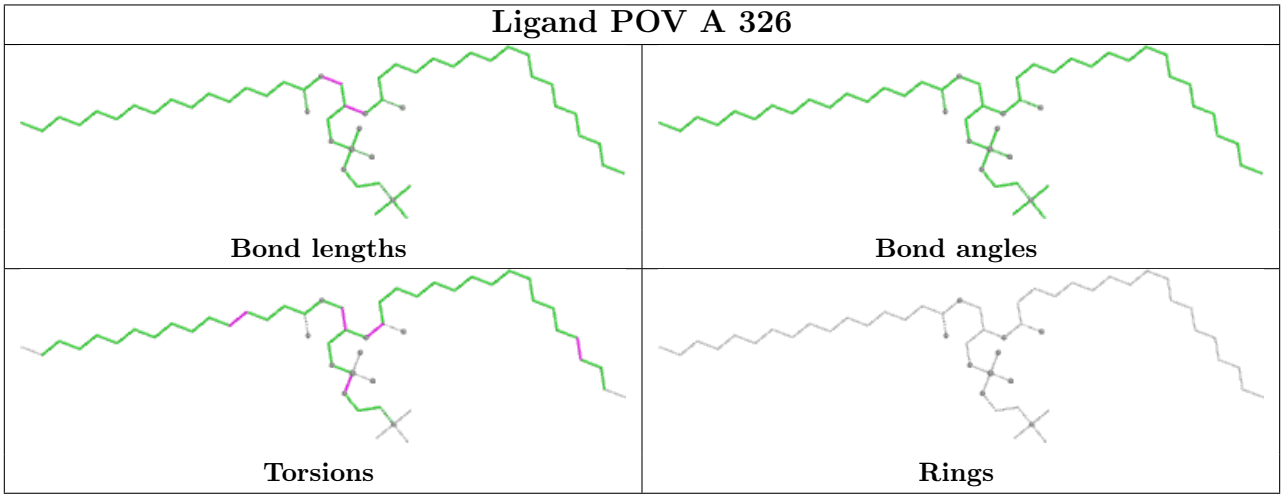


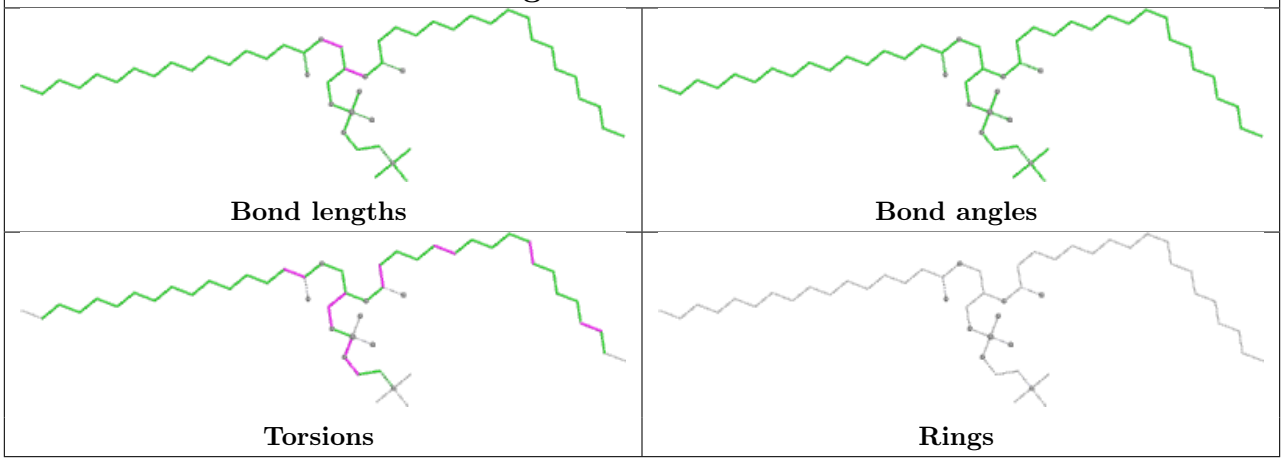
Ligand POV B 337



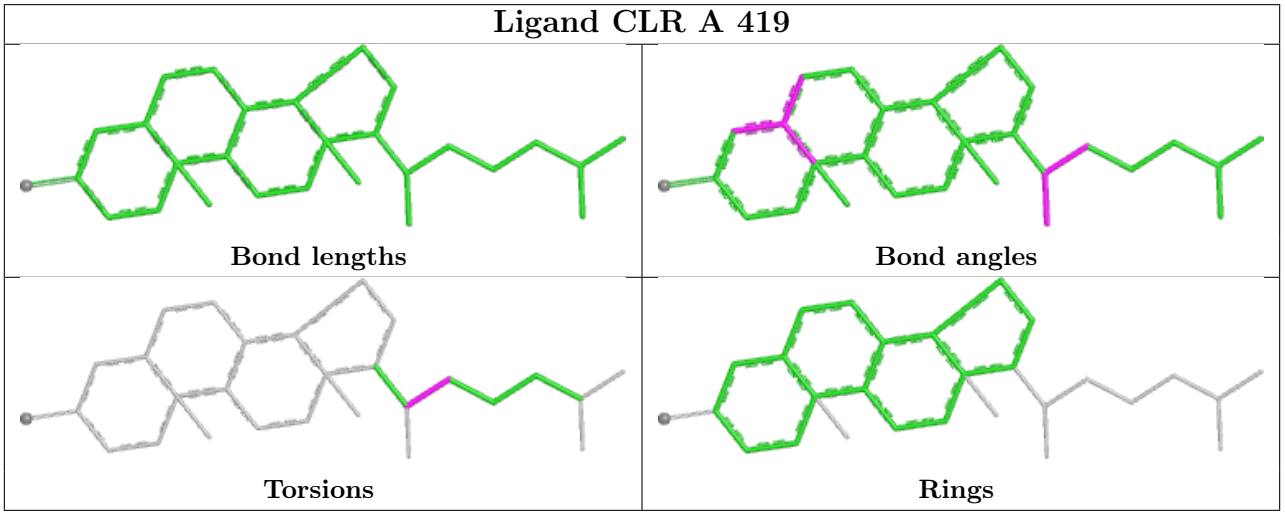
Ligand POV A 326



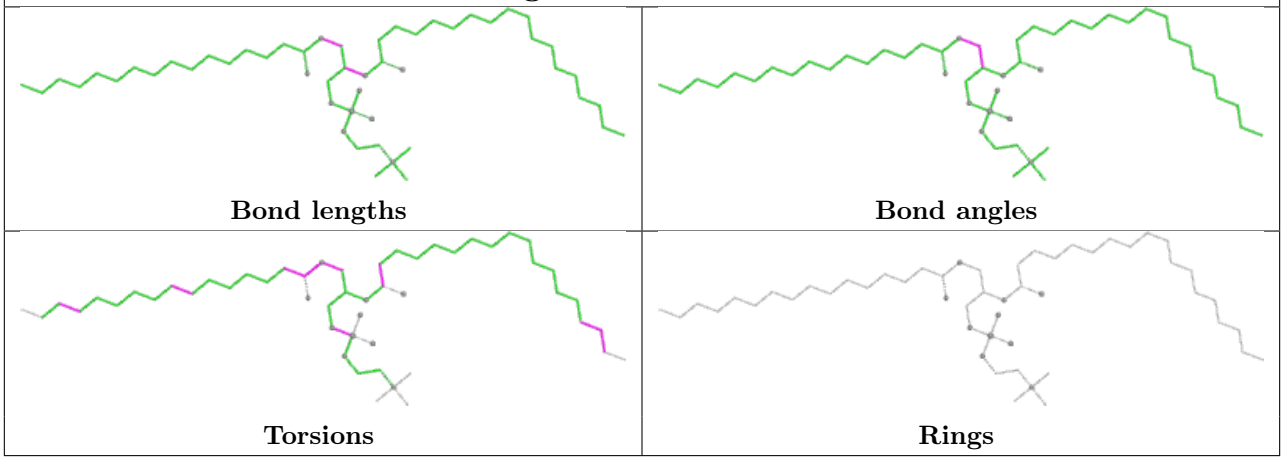
Ligand POV A 364



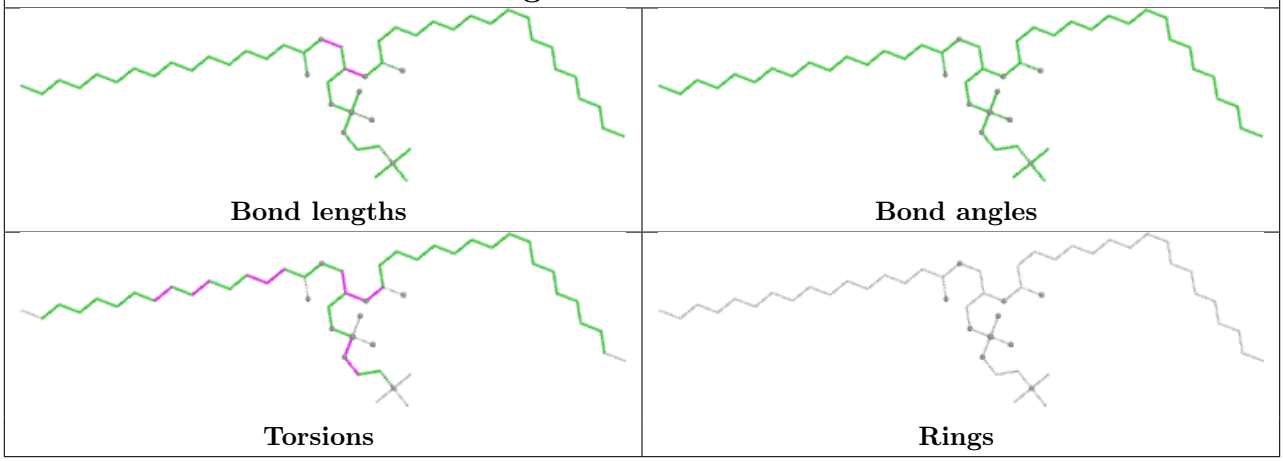
Ligand CLR A 419



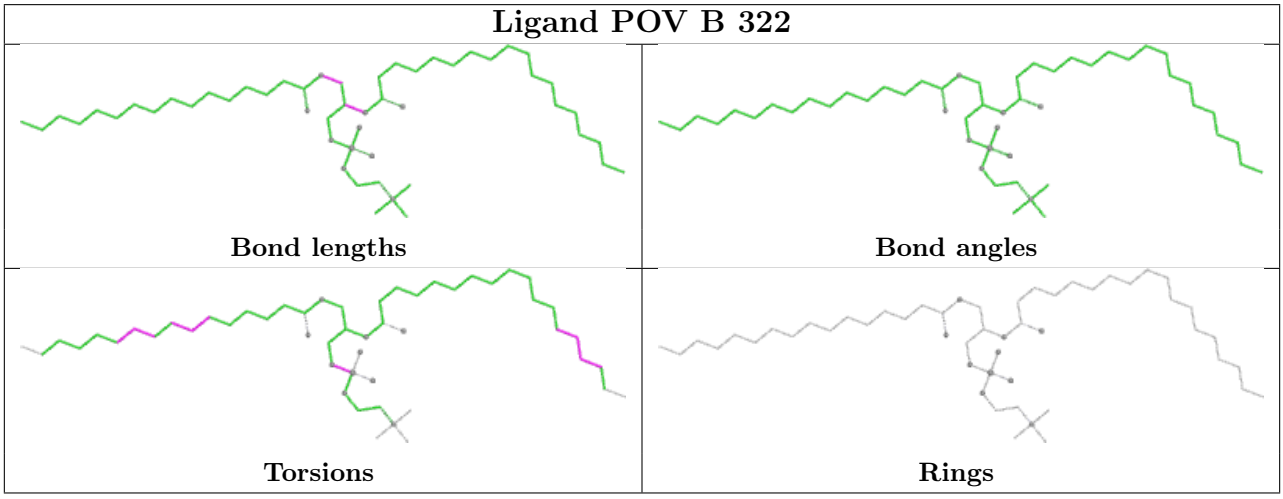
Ligand POV A 318



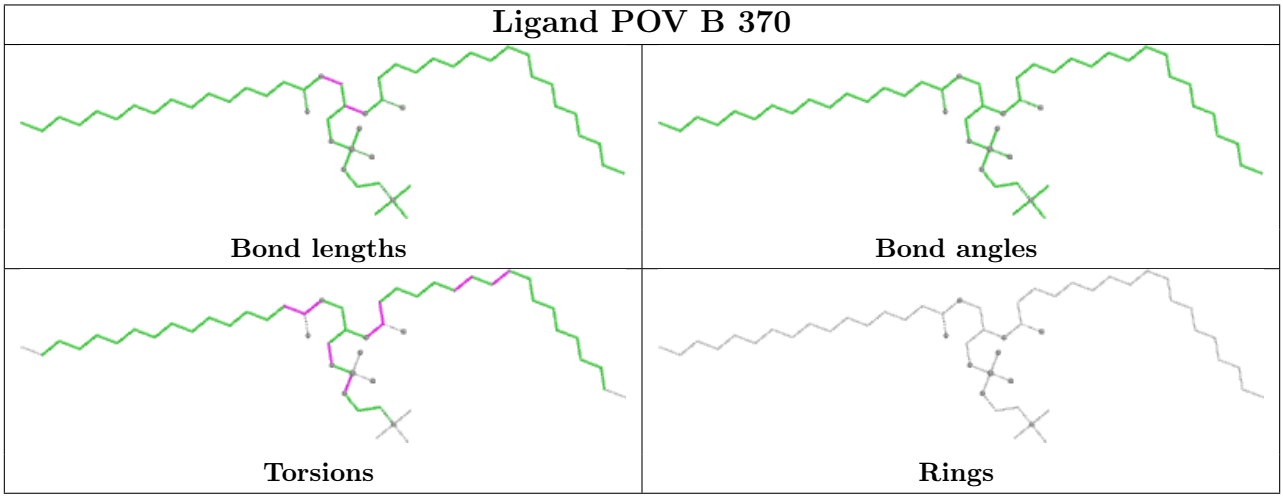
Ligand POV A 389



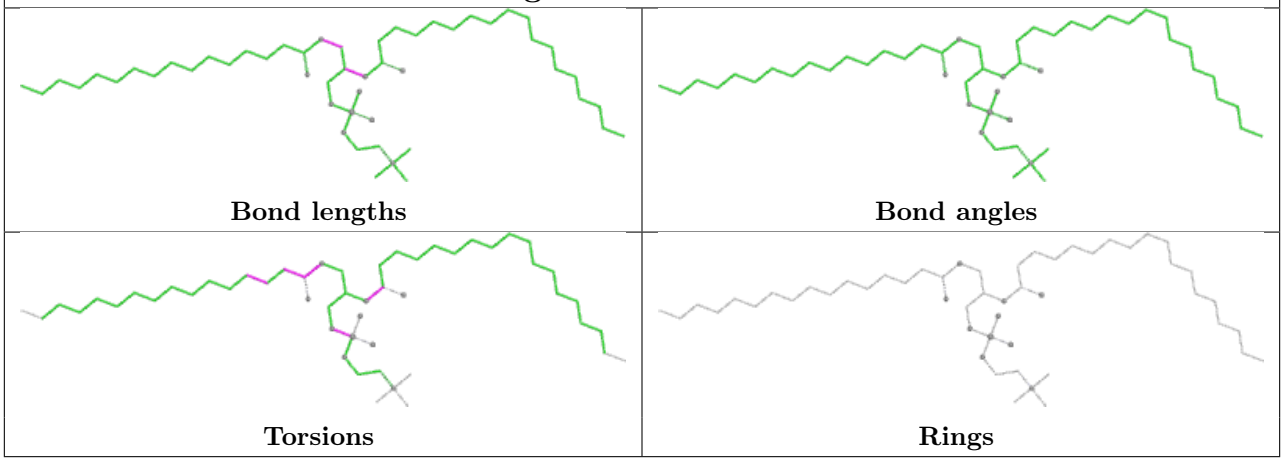
Ligand POV B 322



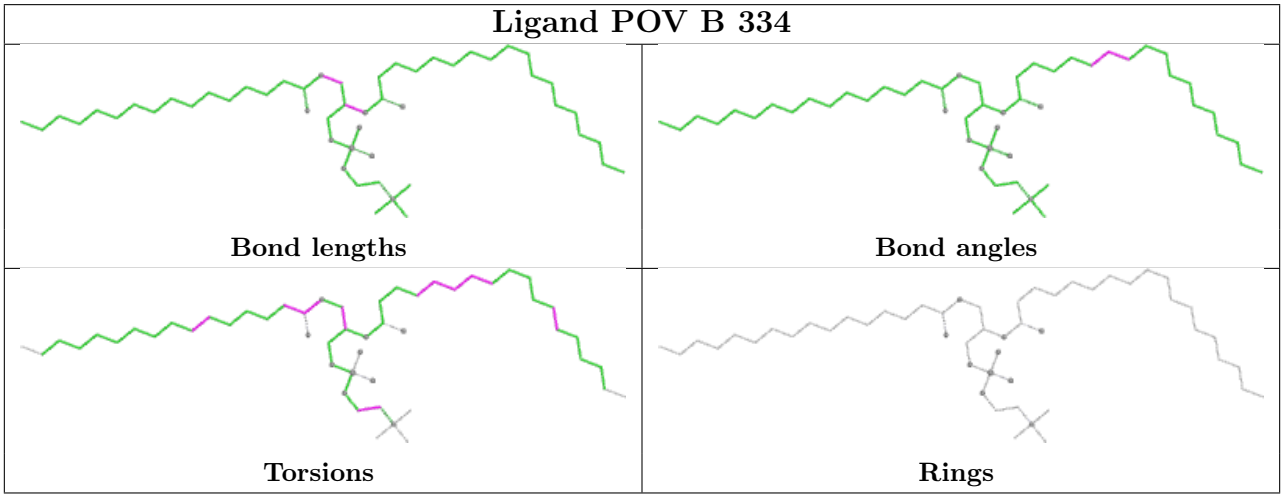
Ligand POV B 370



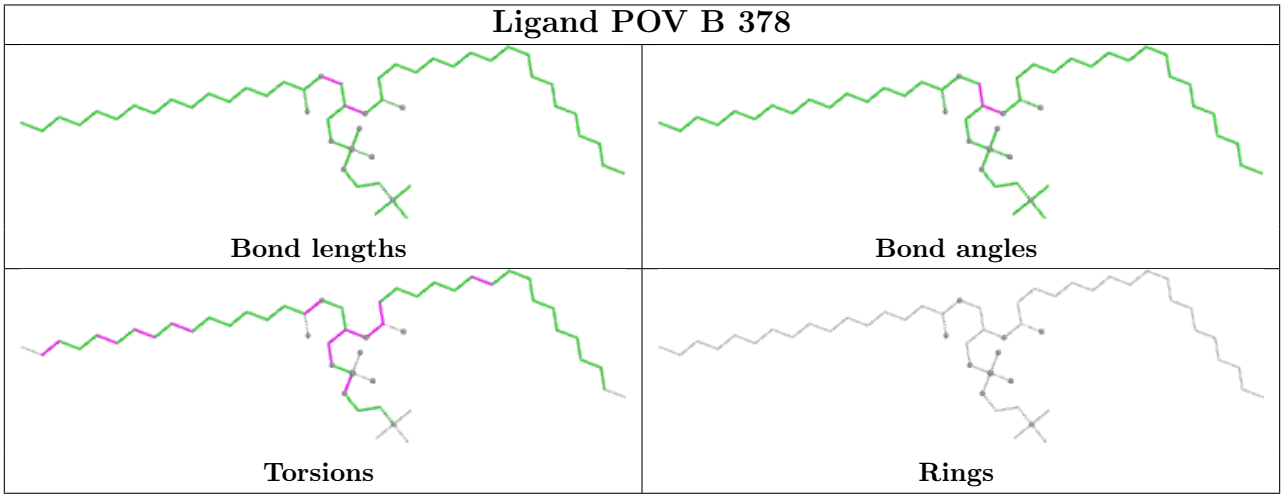
Ligand POV B 386



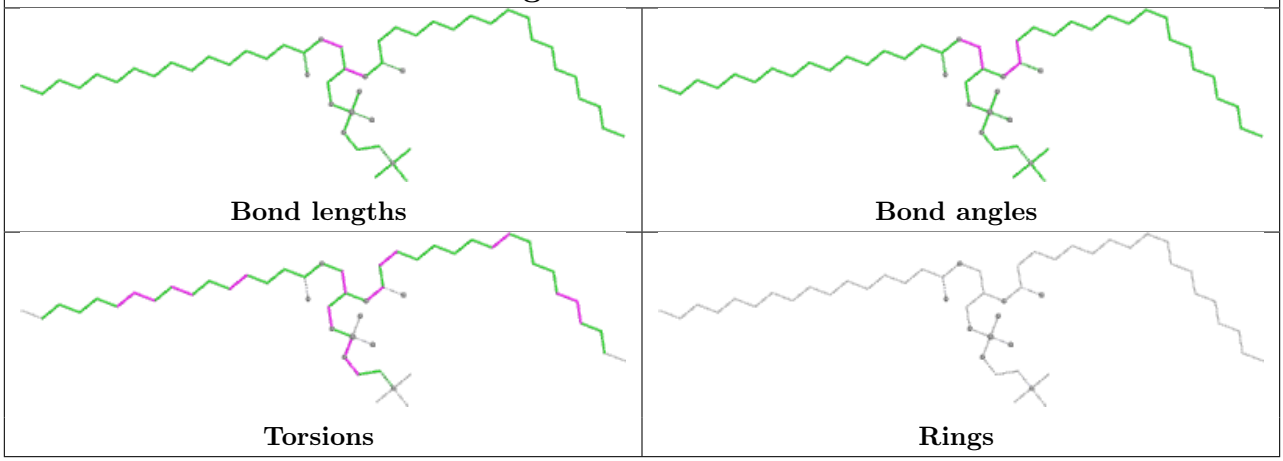
Ligand POV B 334



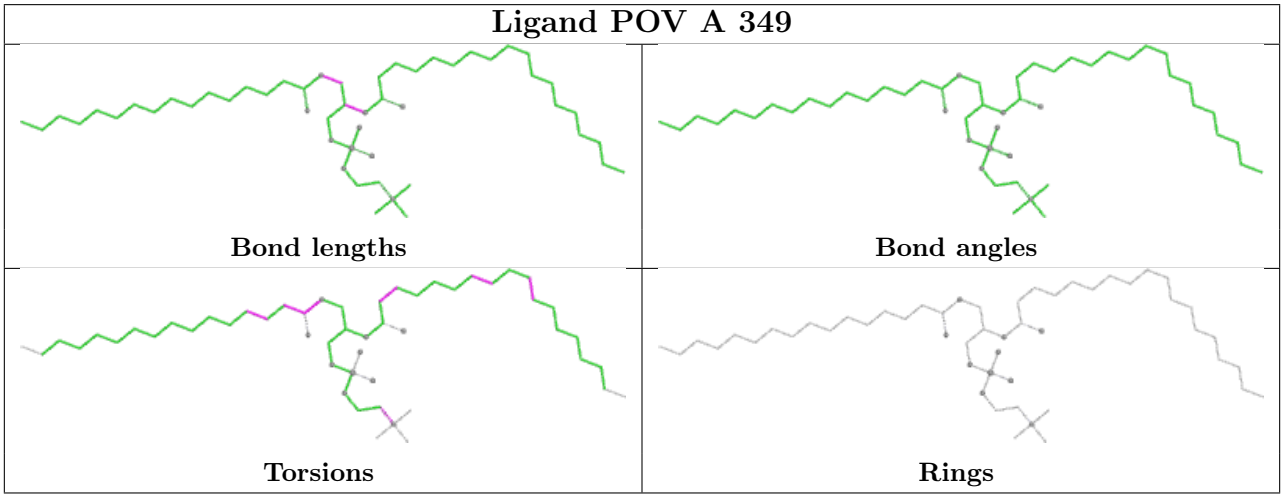
Ligand POV B 378



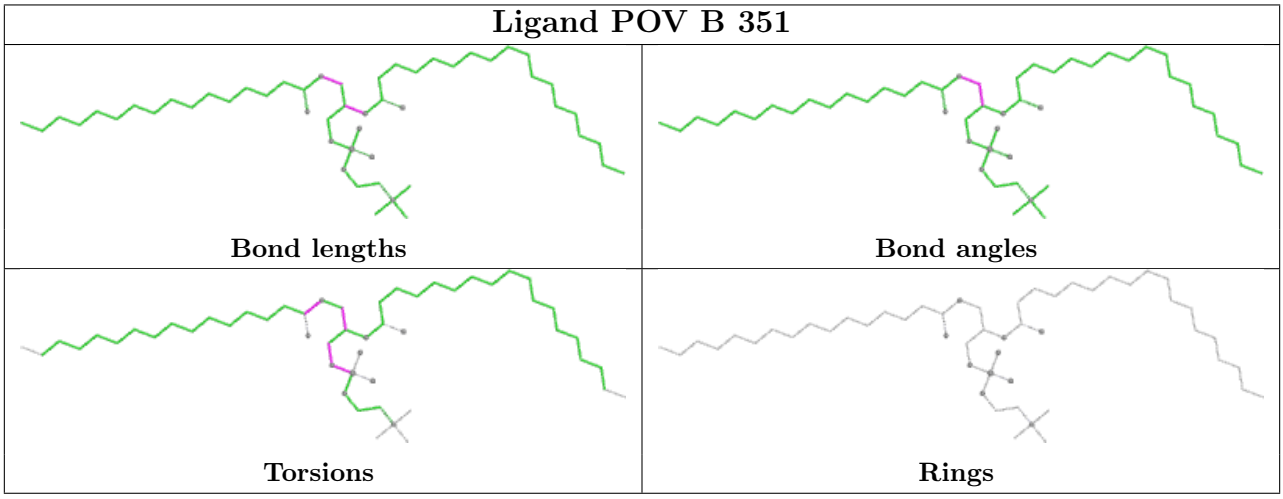
Ligand POV A 378



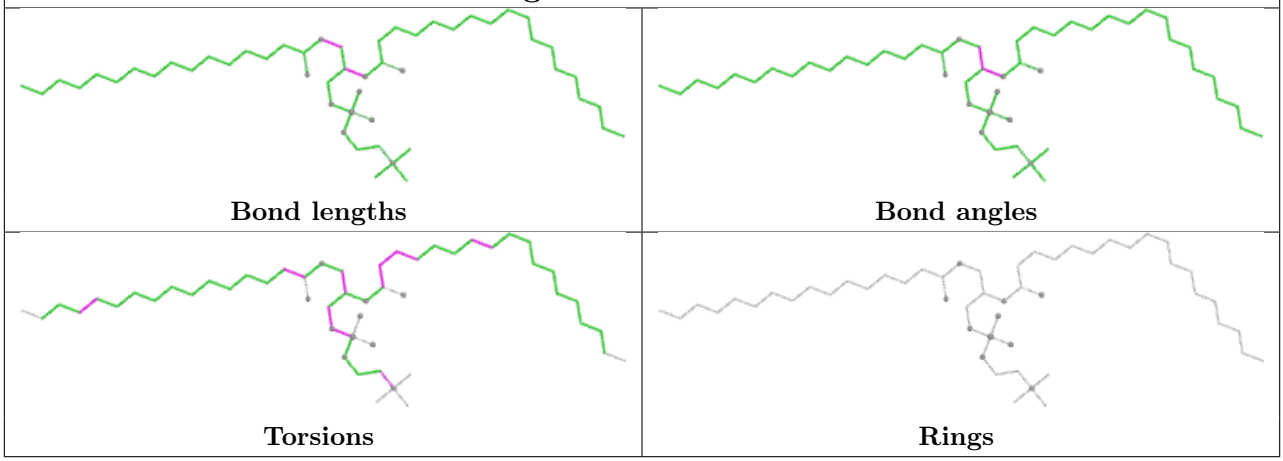
Ligand POV A 349



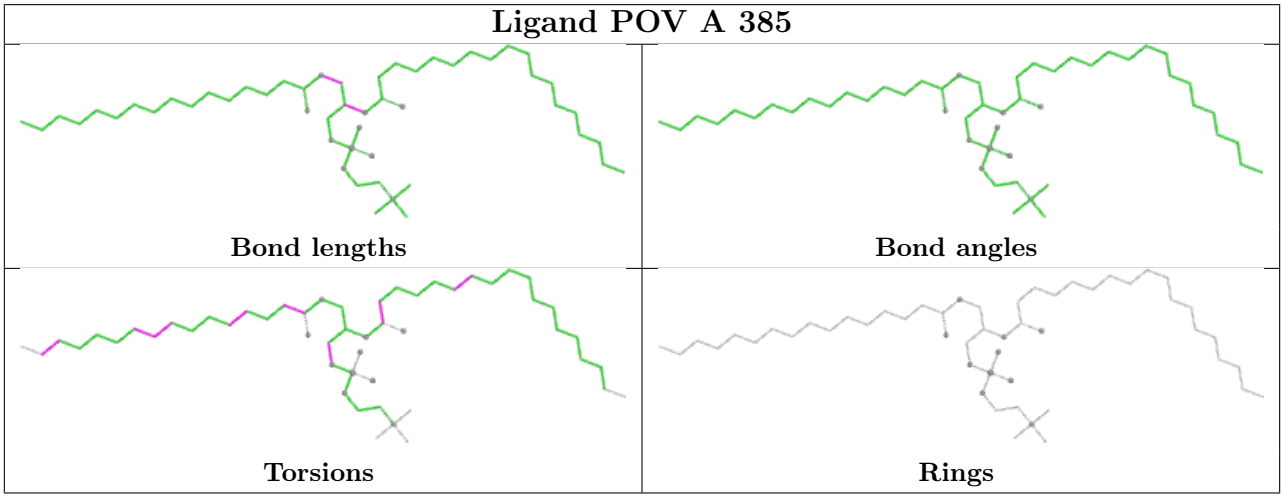
Ligand POV B 351



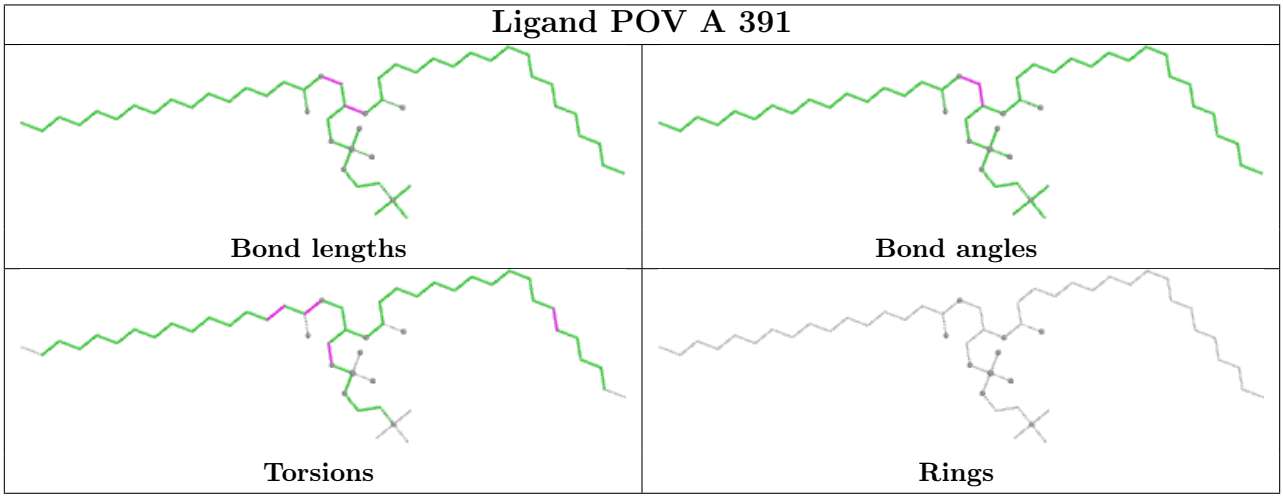
Ligand POV A 336



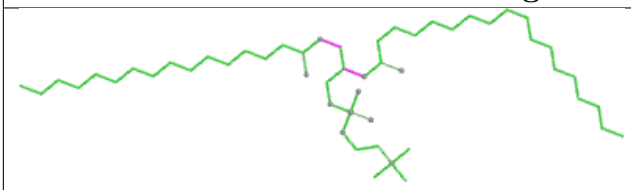
Ligand POV A 385



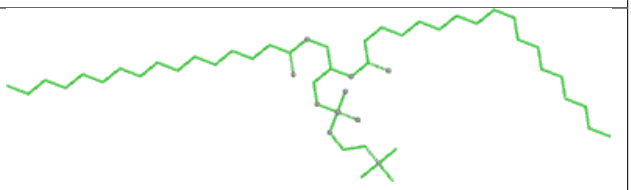
Ligand POV A 391



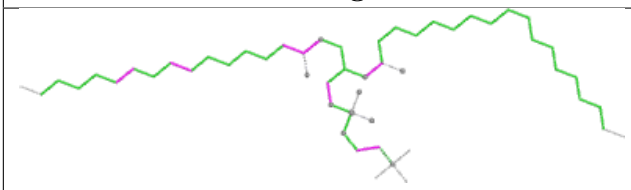
Ligand POV A 400



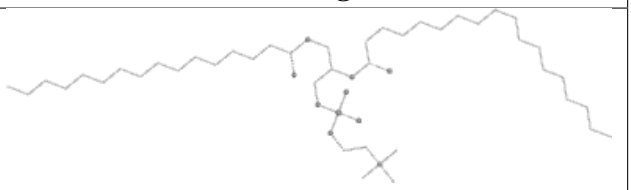
Bond lengths



Bond angles

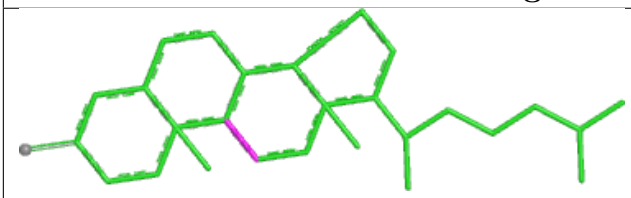


Torsions

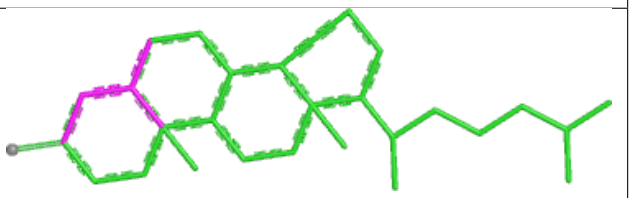


Rings

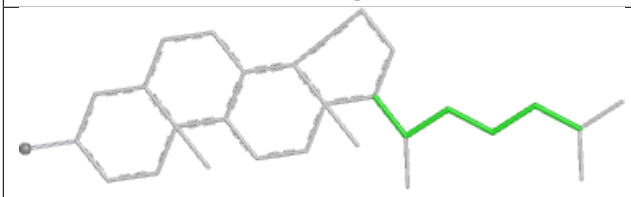
Ligand CLR A 406



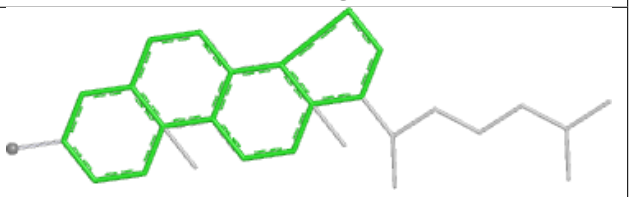
Bond lengths



Bond angles

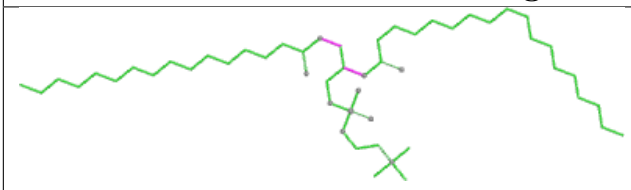


Torsions

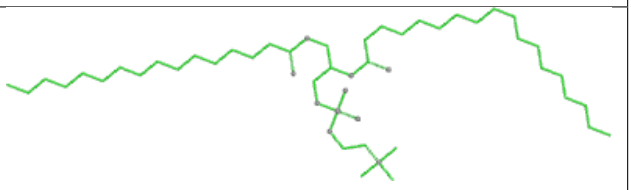


Rings

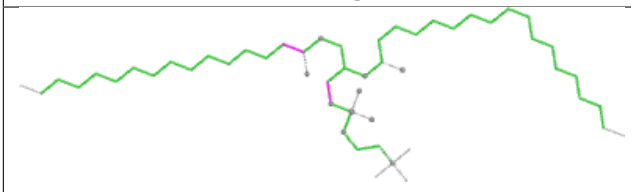
Ligand POV B 363



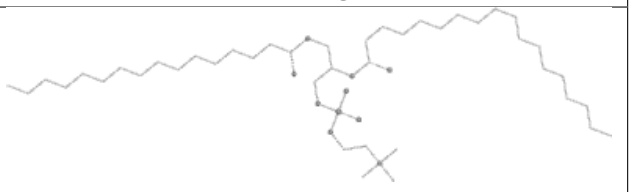
Bond lengths



Bond angles

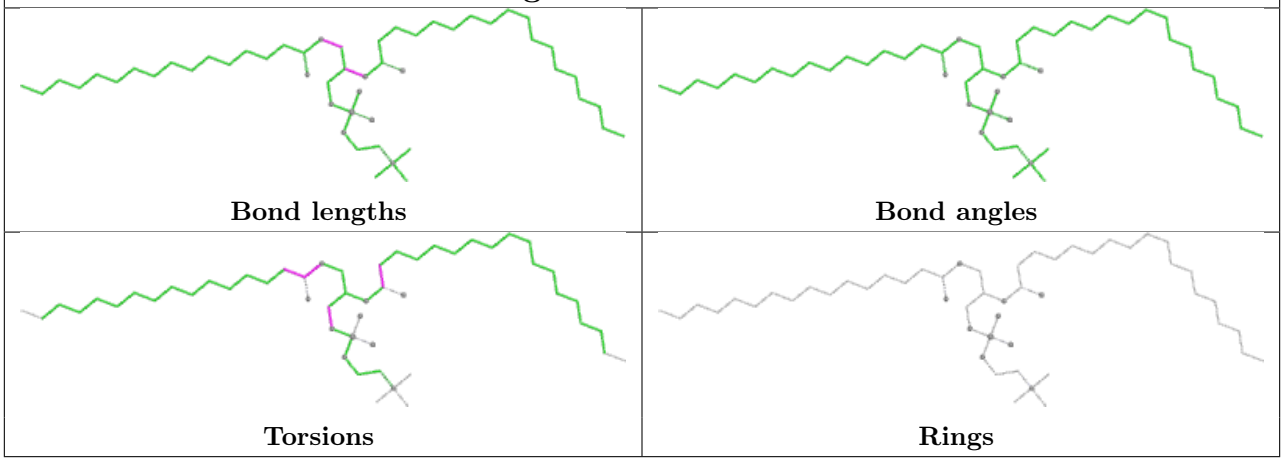


Torsions

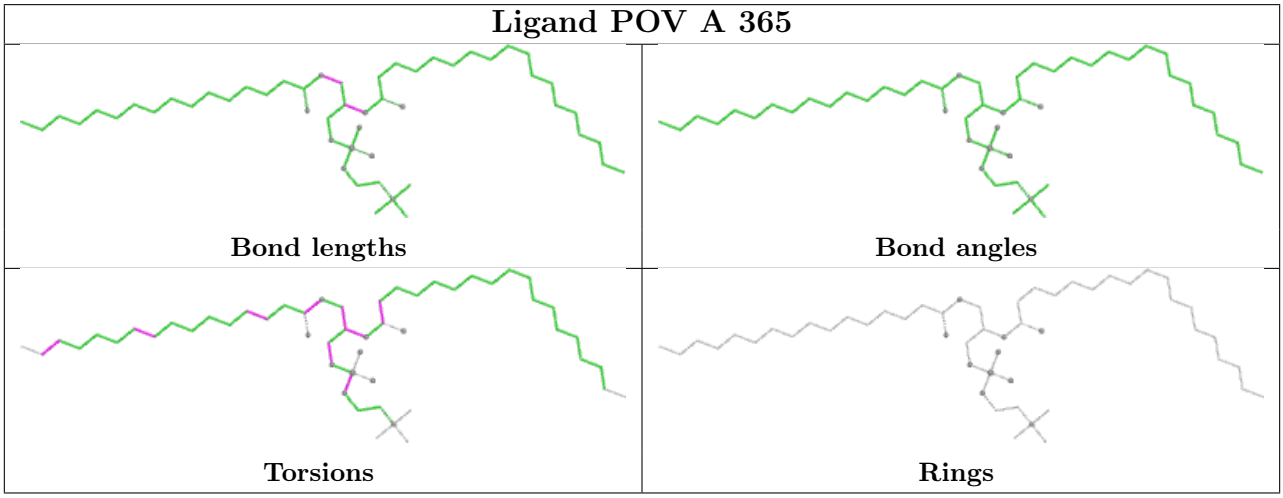


Rings

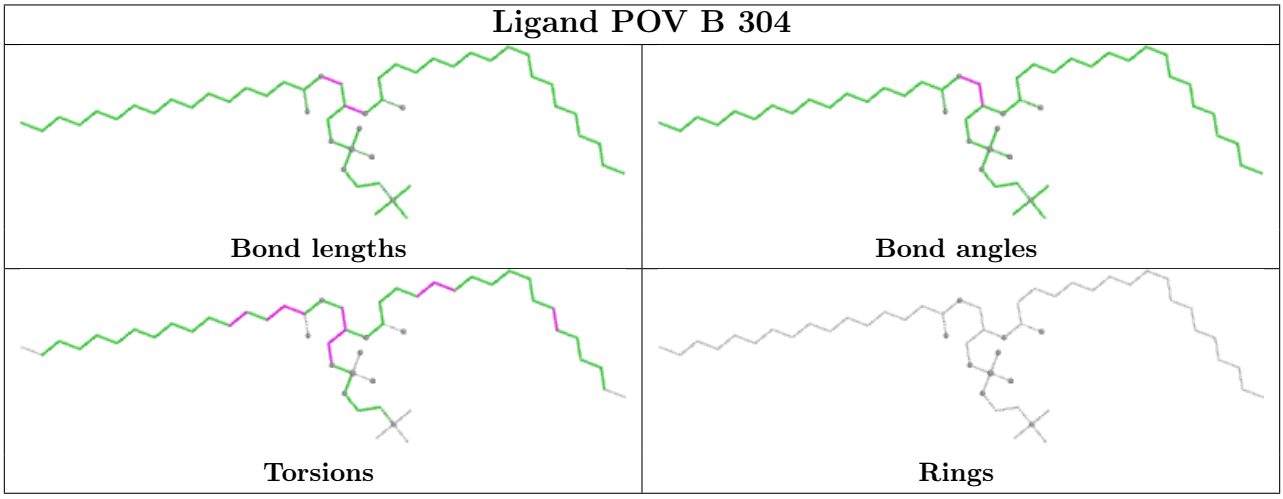
Ligand POV A 307



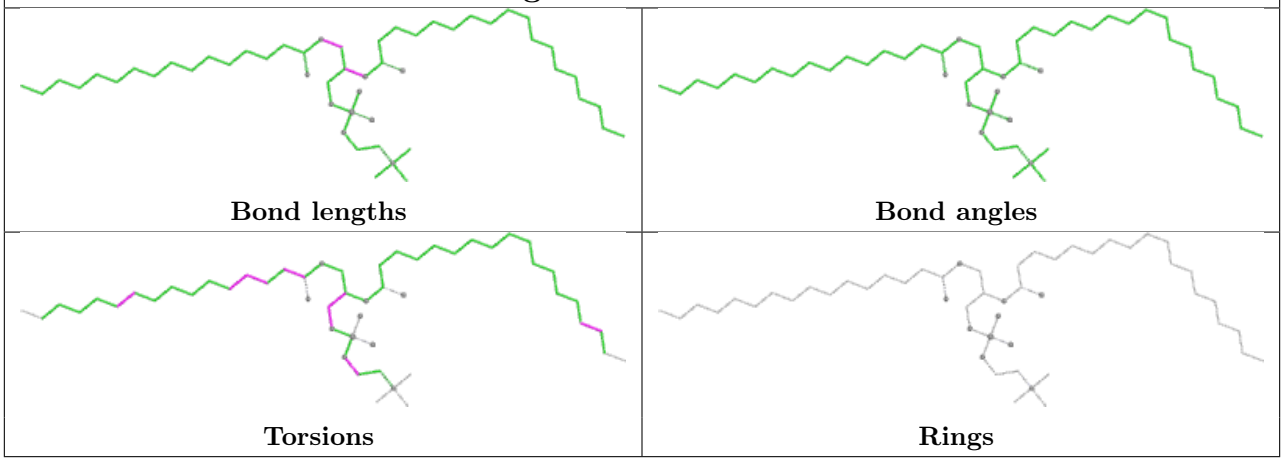
Ligand POV A 365



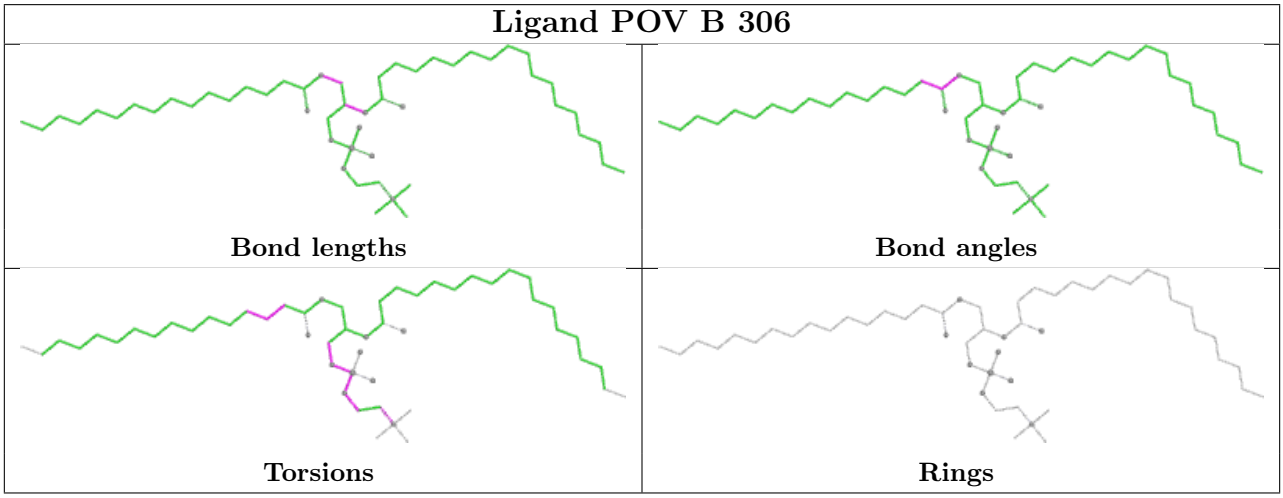
Ligand POV B 304



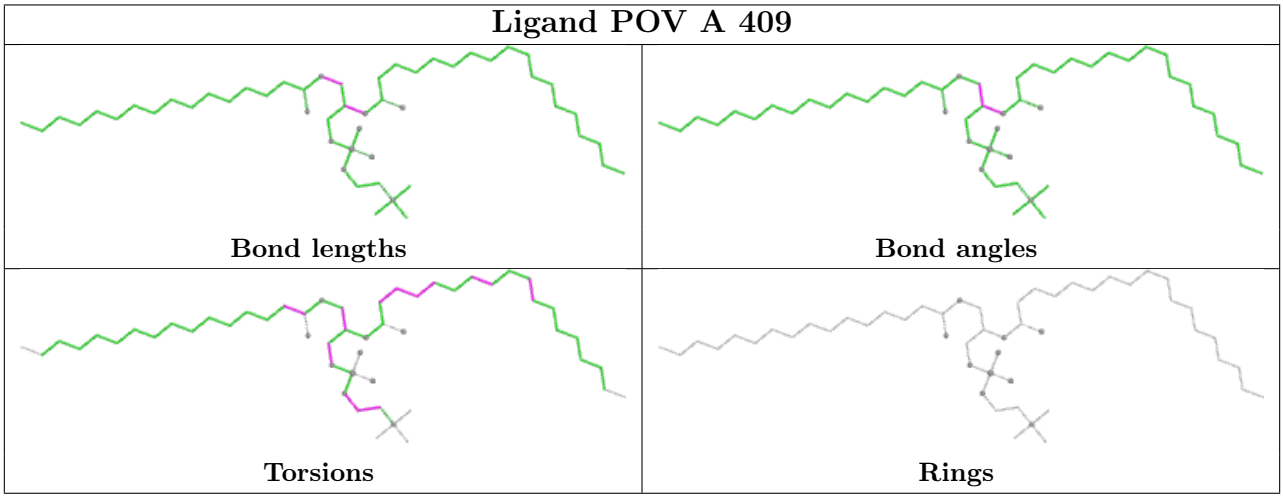
Ligand POV A 351



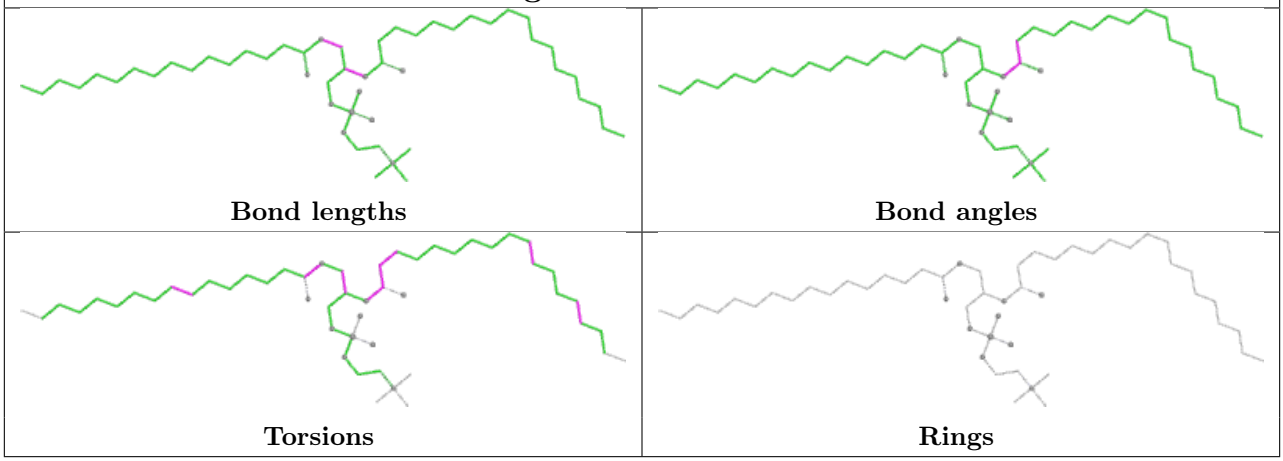
Ligand POV B 306



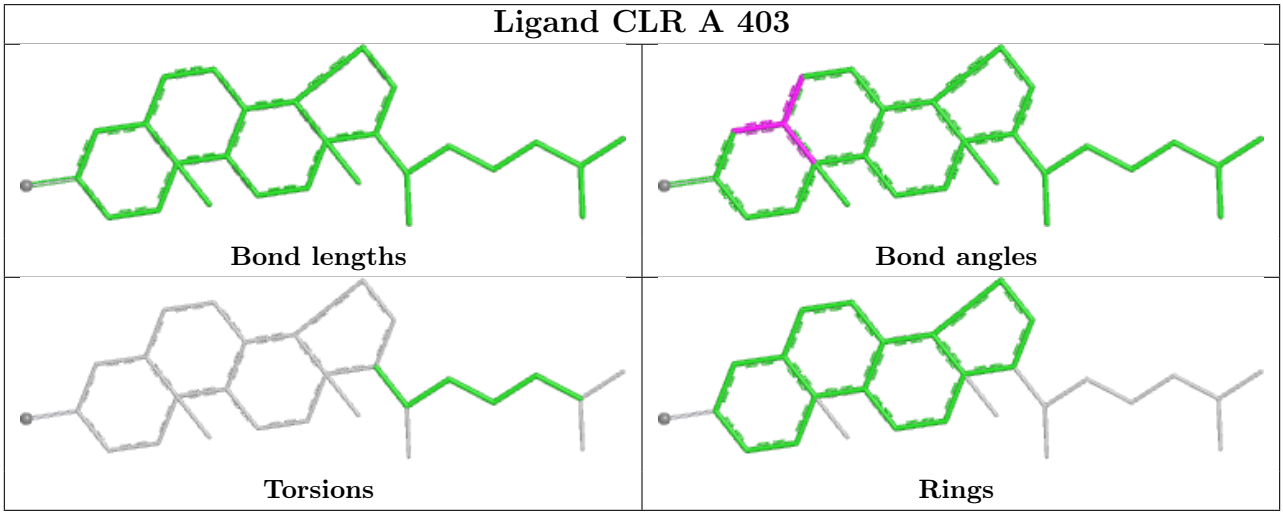
Ligand POV A 409



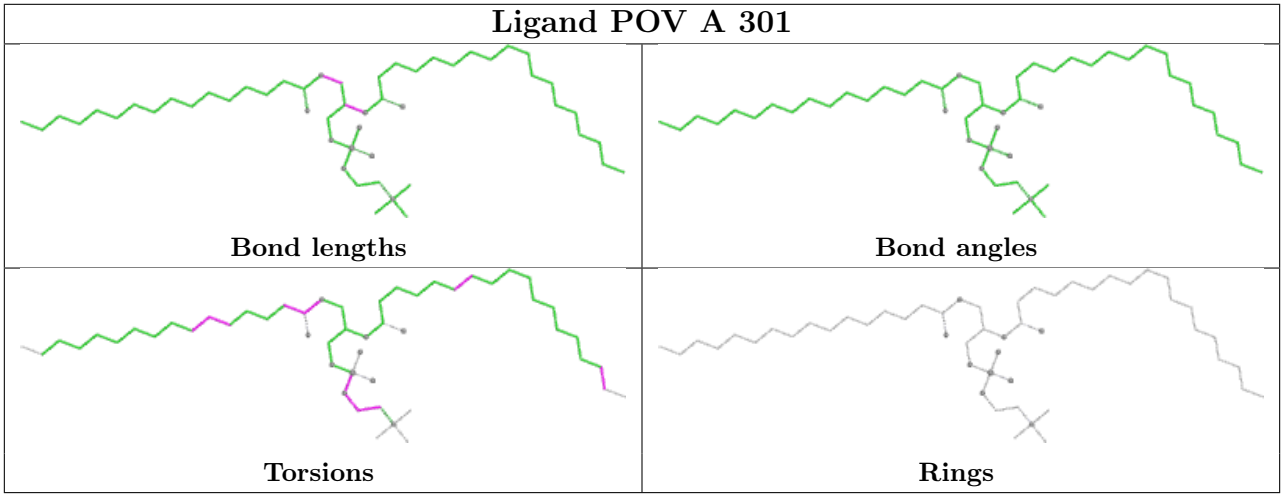
Ligand POV B 365



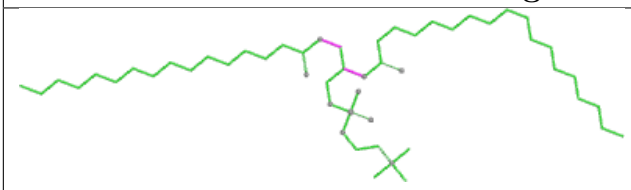
Ligand CLR A 403



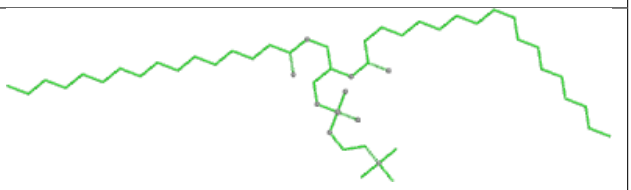
Ligand POV A 301



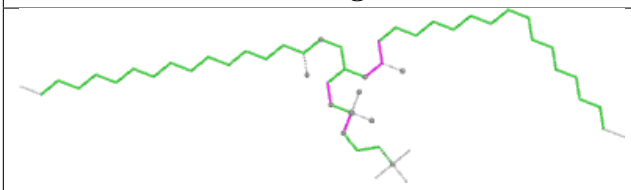
Ligand POV B 301



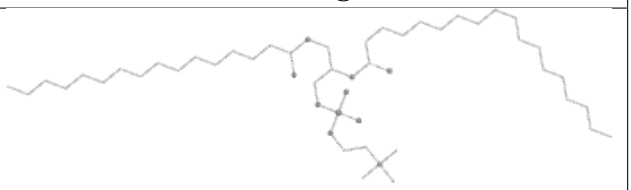
Bond lengths



Bond angles

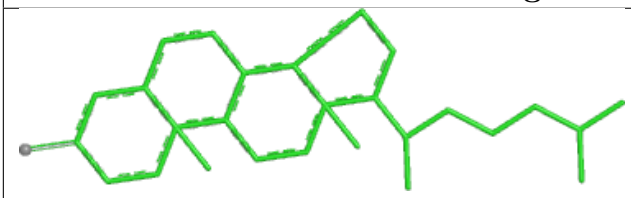


Torsions

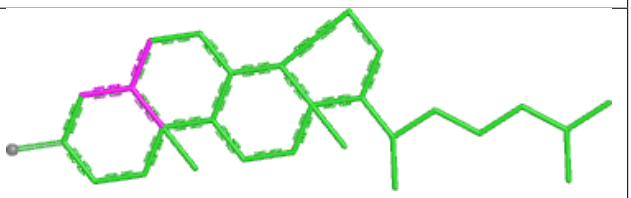


Rings

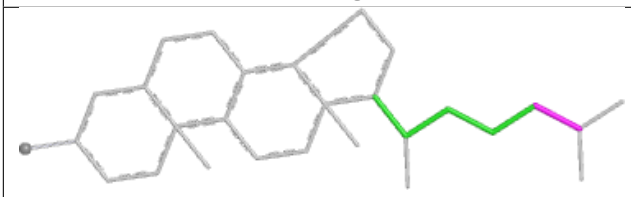
Ligand CLR A 418



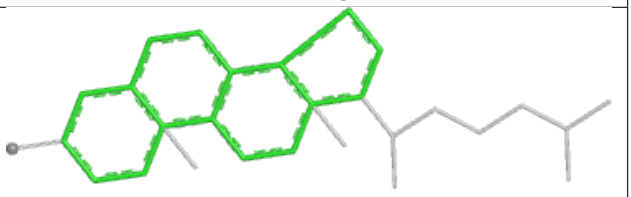
Bond lengths



Bond angles

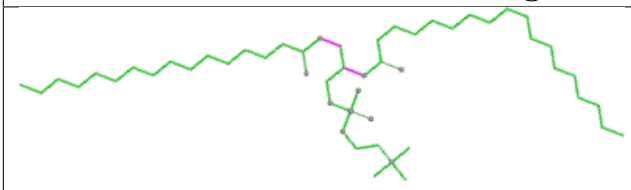


Torsions

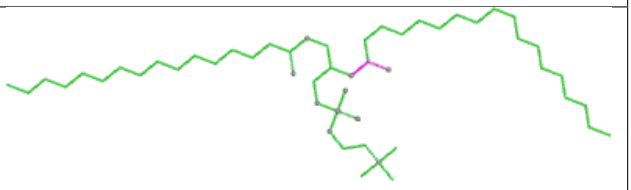


Rings

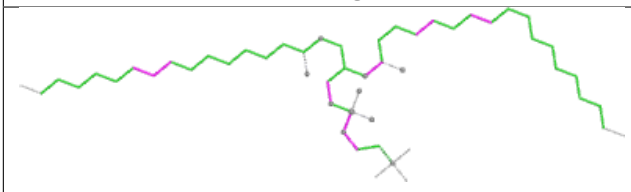
Ligand POV B 324



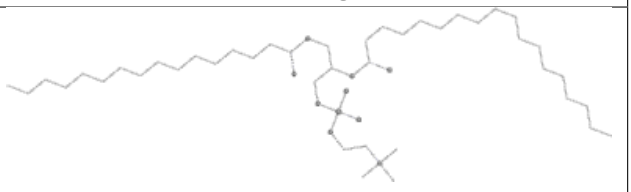
Bond lengths



Bond angles

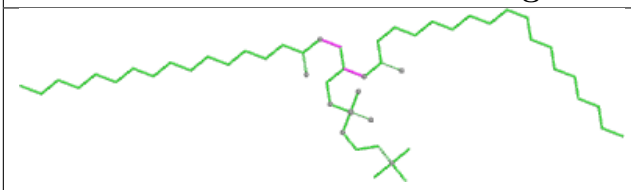


Torsions

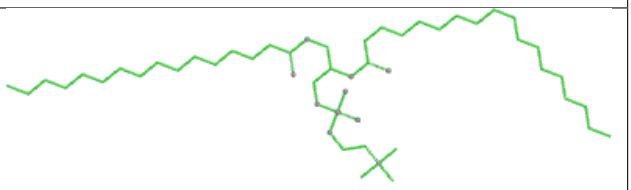


Rings

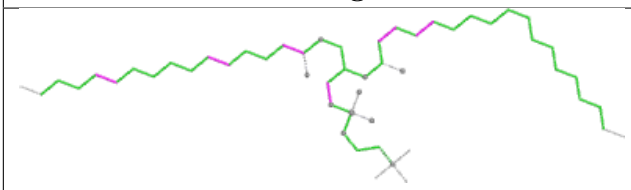
Ligand POV A 373



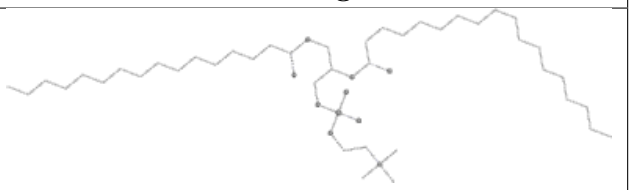
Bond lengths



Bond angles

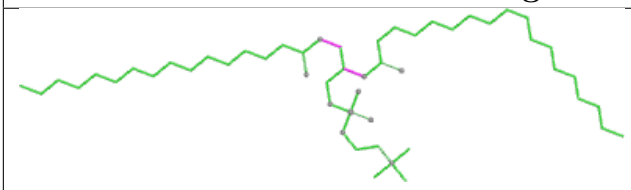


Torsions

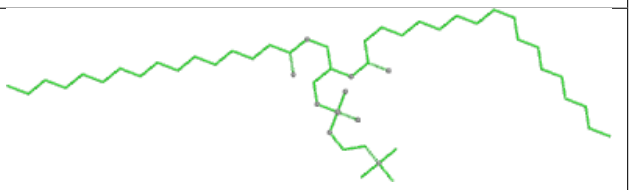


Rings

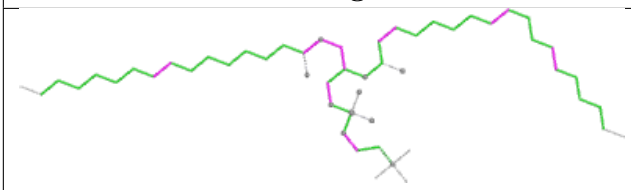
Ligand POV A 321



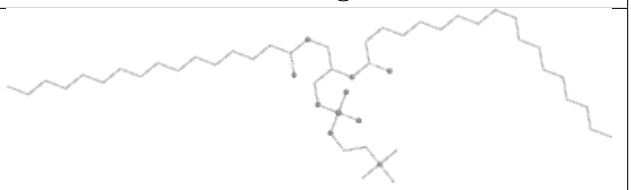
Bond lengths



Bond angles

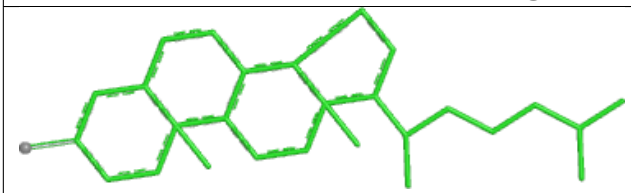


Torsions

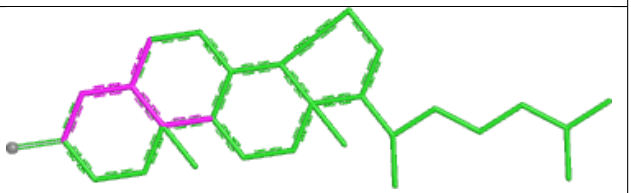


Rings

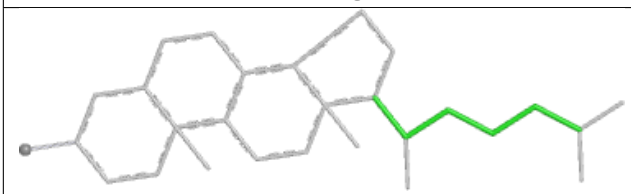
Ligand CLR B 395



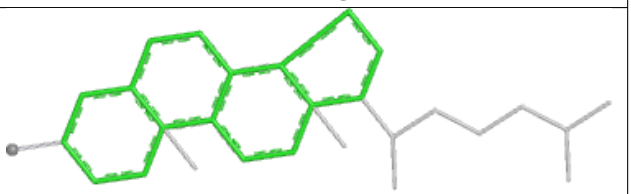
Bond lengths



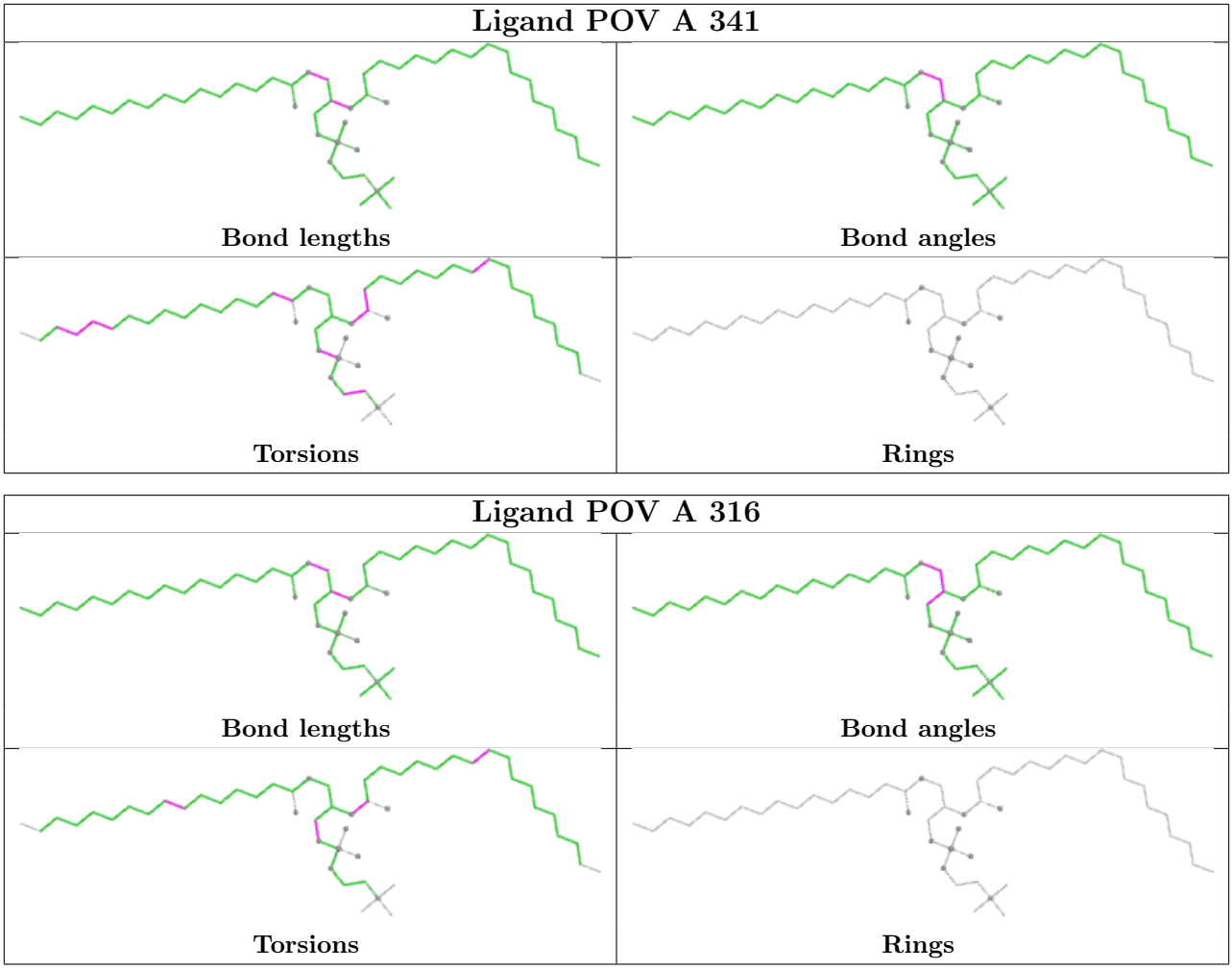
Bond angles



Torsions



Rings



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.