wwPDB NMR Structure Validation Summary Report (i)

Apr 21, 2024 – 11:45 AM EDT

PDB ID	:	2MLS
BMRB ID	:	7089
Title	:	Membrane Bilayer complex with Matrix Metalloproteinase-12 at its Beta-face
Authors	:	Koppisetti, R.K.; Fulcher, Y.G.; Prior, S.H.; Lenoir, M.; Overduin, M.; Van Doren, S.R.
Deposited on	:	2014-03-04

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
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:

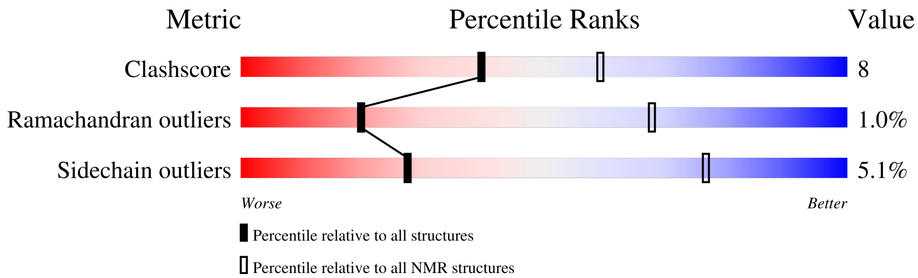
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (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 NMR

The overall completeness of chemical shifts assignment is 82%.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

Mol	Chain	Length	Quality of chain
1	A	164	

2 Ensemble composition and analysis

This entry contains 14 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:101-A:262 (162)	0.69	8

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 5 single-model clusters were found.

Cluster number	Models
1	5, 8, 10, 13
2	11, 12, 14
3	1, 2
Single-model clusters	3; 4; 6; 7; 9

3 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8263 atoms, of which 1221 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	164	2508	824	1221	225	234	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	ALA	GLU	engineered mutation	UNP P39900

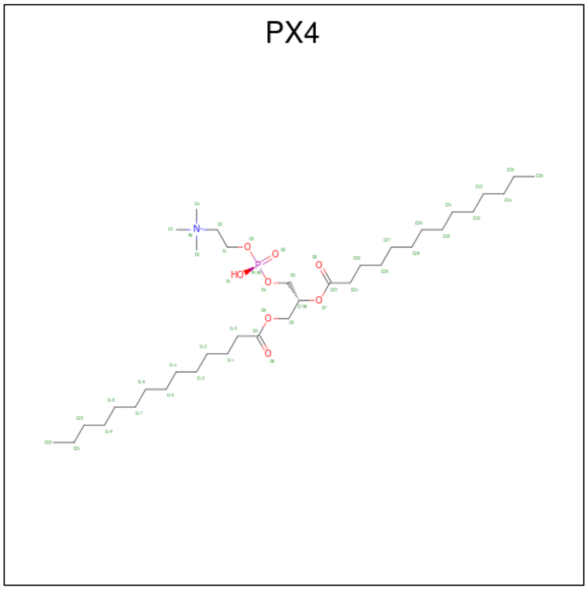
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
			Total	Ca
3	A	3	3	3

- Molecule 4 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: $C_{36}H_{73}NO_8P$).



Mol	Chain	Residues	Atoms
4	A	1	Total C N O P 46 36 1 8 1
4	A	1	Total C N O P 46 36 1 8 1
4	A	1	Total C N O P 46 36 1 8 1
4	A	1	Total C N O P 46 36 1 8 1
4	A	1	Total C N O P 46 36 1 8 1
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Mol	Chain	Residues	Atoms				
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4	A	1	Total	C	N	O	P
			46	36	1	8	1
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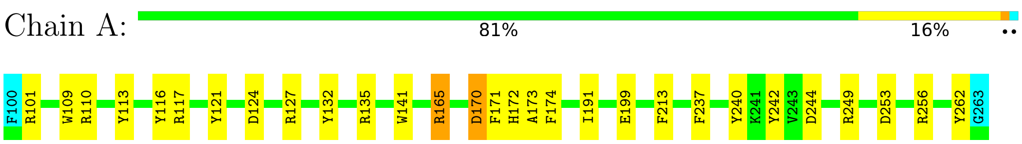
4	A	1	Total 46	C 36	N 1	O 8	P 1

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

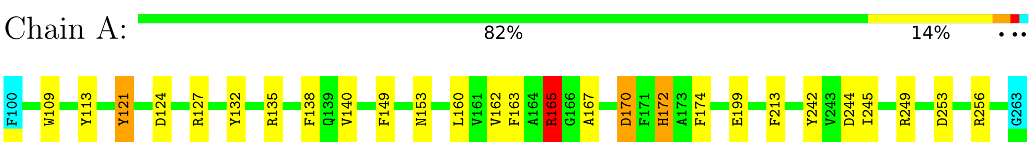
- Molecule 1: Macrophage metalloelastase



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: Macrophage metalloelastase



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics*.

Of the 14 calculated structures, 14 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
GROMACS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1762
Number of shifts mapped to atoms	1762
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, PX4

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 (average) 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	0.57±0.00	0±0/1311 (0.0± 0.0%)	2.03±0.06	38±6/1779 (2.2± 0.4%)
All	All	0.57	0/18354 (0.0%)	2.03	537/24906 (2.2%)

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	Planarity
1	A	0.0±0.0	4.9±2.3
All	All	0	68

There are no bond-length outliers.

5 of 232 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	110	ARG	NE-CZ-NH1	19.82	130.21	120.30	10	5
1	A	170	ASP	CB-CG-OD1	16.29	132.96	118.30	7	14
1	A	256	ARG	NE-CZ-NH1	16.04	128.32	120.30	5	9
1	A	101	ARG	NE-CZ-NH1	-15.89	112.36	120.30	6	7
1	A	197	PHE	CB-CG-CD1	15.56	131.69	120.80	5	3

There are no chirality outliers.

5 of 31 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	174	PHE	Peptide,Sidechain	11

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	121	TYR	Sidechain	6
1	A	262	TYR	Sidechain	5
1	A	171	PHE	Sidechain	4
1	A	132	TYR	Sidechain,Mainchain	4

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1271	1207	1207	2±1
4	A	5750	0	9000	132±12
All	All	98364	16898	142898	1849

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 8.

5 of 1767 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:423:PX4:H16	4:A:424:PX4:H24	1.02	1.23	7	1
4:A:347:PX4:H56	4:A:355:PX4:H25	0.99	1.33	11	1
4:A:321:PX4:H51	4:A:354:PX4:H34	0.93	1.41	10	1
4:A:306:PX4:H23	4:A:360:PX4:H44	0.91	1.42	1	1
4:A:408:PX4:H15	4:A:409:PX4:H2	0.90	1.44	10	2

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	162/164 (99%)	151±2 (93±1%)	10±2 (6±1%)	2±1 (1±1%)	20	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2268/2296 (99%)	2109 (93%)	136 (6%)	23 (1%)	20	68

5 of 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	173	ALA	11
1	A	179	GLY	4
1	A	172	HIS	2
1	A	170	ASP	2
1	A	109	TRP	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	130/131 (99%)	123±1 (95±1%)	7±1 (5±1%)	27	77
All	All	1820/1834 (99%)	1728 (95%)	92 (5%)	27	77

5 of 26 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	165	ARG	14
1	A	199	GLU	14
1	A	170	ASP	12
1	A	172	HIS	11
1	A	244	ASP	6

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 130 ligands modelled in this entry, 5 are monoatomic - leaving 125 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	348	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	380	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	352	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	307	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	376	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	410	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	414	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	338	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	413	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	426	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	306	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	366	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	311	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	330	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	356	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	418	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	342	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	389	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	419	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	429	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	337	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	365	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	367	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	388	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.64±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	361	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	396	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	362	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	335	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	378	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	383	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	391	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	340	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	310	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	374	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	322	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	379	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	346	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	315	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	371	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	427	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	347	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	402	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	392	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	390	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	363	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	411	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	372	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	314	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	398	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	400	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	370	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	394	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	405	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	368	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	353	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	415	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	349	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	397	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	326	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	399	-	45,45,45	0.64±0.02	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	334	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	328	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	336	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	381	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	343	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	319	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	354	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	385	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	428	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	341	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	393	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	351	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	401	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	333	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	416	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	404	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	329	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	412	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	323	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	375	-	45,45,45	0.64±0.03	0±0 (0±0%)
4	PX4	A	327	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	345	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	369	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	312	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	423	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	406	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	421	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	403	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	395	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	332	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.63±0.01	0±0 (0±0%)
4	PX4	A	387	-	45,45,45	0.63±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	382	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	384	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	331	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	373	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	320	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	422	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	424	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	318	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	430	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	317	-	45,45,45	0.63±0.02	0±0 (0±0%)
4	PX4	A	355	-	45,45,45	0.63±0.01	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	348	-	51,53,53	1.42±0.17	8±2 (15±4%)
4	PX4	A	380	-	51,53,53	1.50±0.16	10±2 (19±4%)
4	PX4	A	352	-	51,53,53	1.48±0.16	9±2 (16±3%)
4	PX4	A	307	-	51,53,53	1.44±0.19	8±3 (16±5%)
4	PX4	A	376	-	51,53,53	1.48±0.15	10±2 (18±4%)
4	PX4	A	410	-	51,53,53	1.44±0.16	9±2 (17±3%)
4	PX4	A	414	-	51,53,53	1.51±0.15	9±2 (17±4%)
4	PX4	A	338	-	51,53,53	1.46±0.11	9±2 (16±4%)
4	PX4	A	413	-	51,53,53	1.55±0.15	10±2 (19±4%)
4	PX4	A	420	-	51,53,53	1.53±0.16	10±2 (19±4%)
4	PX4	A	426	-	51,53,53	1.48±0.14	9±2 (18±4%)
4	PX4	A	306	-	51,53,53	1.42±0.13	8±3 (14±4%)
4	PX4	A	366	-	51,53,53	1.55±0.16	9±2 (18±4%)
4	PX4	A	311	-	51,53,53	1.51±0.14	9±2 (18±3%)
4	PX4	A	330	-	51,53,53	1.41±0.16	8±3 (14±5%)
4	PX4	A	356	-	51,53,53	1.46±0.13	8±2 (16±4%)

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					Counts	RMSZ	#Z>2
4	PX4	A	409	-	51,53,53	1.45±0.17	8±2 (16±4%)
4	PX4	A	418	-	51,53,53	1.48±0.12	8±2 (16±3%)
4	PX4	A	342	-	51,53,53	1.46±0.14	9±2 (17±3%)
4	PX4	A	389	-	51,53,53	1.49±0.09	8±2 (16±4%)
4	PX4	A	419	-	51,53,53	1.44±0.10	9±2 (16±3%)
4	PX4	A	429	-	51,53,53	1.45±0.15	8±3 (16±5%)
4	PX4	A	337	-	51,53,53	1.43±0.12	8±2 (14±4%)
4	PX4	A	365	-	51,53,53	1.41±0.09	8±3 (14±4%)
4	PX4	A	367	-	51,53,53	1.46±0.10	8±2 (16±3%)
4	PX4	A	388	-	51,53,53	1.52±0.11	10±2 (19±4%)
4	PX4	A	359	-	51,53,53	1.47±0.12	9±2 (17±3%)
4	PX4	A	361	-	51,53,53	1.58±0.14	10±2 (20±4%)
4	PX4	A	396	-	51,53,53	1.44±0.15	7±2 (14±4%)
4	PX4	A	362	-	51,53,53	1.45±0.12	8±2 (16±4%)
4	PX4	A	335	-	51,53,53	1.52±0.15	9±2 (18±3%)
4	PX4	A	378	-	51,53,53	1.55±0.14	9±2 (18±4%)
4	PX4	A	377	-	51,53,53	1.43±0.13	8±2 (16±4%)
4	PX4	A	383	-	51,53,53	1.42±0.12	8±2 (16±4%)
4	PX4	A	391	-	51,53,53	1.48±0.14	8±3 (16±5%)
4	PX4	A	364	-	51,53,53	1.47±0.13	8±3 (15±5%)
4	PX4	A	308	-	51,53,53	1.53±0.12	9±2 (18±3%)
4	PX4	A	340	-	51,53,53	1.44±0.13	8±2 (16±4%)
4	PX4	A	310	-	51,53,53	1.48±0.12	9±2 (17±3%)
4	PX4	A	386	-	51,53,53	1.51±0.14	9±2 (17±4%)
4	PX4	A	374	-	51,53,53	1.45±0.14	8±3 (15±5%)
4	PX4	A	407	-	51,53,53	1.52±0.11	9±2 (17±4%)
4	PX4	A	322	-	51,53,53	1.47±0.10	9±2 (18±4%)
4	PX4	A	379	-	51,53,53	1.62±0.17	10±3 (19±5%)
4	PX4	A	346	-	51,53,53	1.46±0.12	9±2 (16±4%)
4	PX4	A	425	-	51,53,53	1.48±0.14	8±2 (16±4%)
4	PX4	A	315	-	51,53,53	1.41±0.09	8±2 (15±3%)
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4	PX4	A	427	-	51,53,53	1.57±0.12	9±2 (17±3%)
4	PX4	A	347	-	51,53,53	1.49±0.18	9±3 (17±5%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	402	-	51,53,53	1.57±0.15	9±2 (18±4%)
4	PX4	A	392	-	51,53,53	1.46±0.10	9±2 (17±3%)
4	PX4	A	390	-	51,53,53	1.47±0.11	8±2 (16±4%)
4	PX4	A	363	-	51,53,53	1.56±0.08	10±1 (20±2%)
4	PX4	A	411	-	51,53,53	1.54±0.23	10±4 (19±7%)
4	PX4	A	372	-	51,53,53	1.43±0.20	8±4 (15±7%)
4	PX4	A	314	-	51,53,53	1.56±0.12	9±1 (17±2%)
4	PX4	A	398	-	51,53,53	1.53±0.16	9±3 (18±5%)
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4	PX4	A	370	-	51,53,53	1.51±0.17	9±2 (16±4%)
4	PX4	A	394	-	51,53,53	1.42±0.14	8±2 (14±3%)
4	PX4	A	405	-	51,53,53	1.39±0.14	7±2 (14±3%)
4	PX4	A	368	-	51,53,53	1.46±0.14	8±2 (16±4%)
4	PX4	A	353	-	51,53,53	1.49±0.11	9±2 (18±3%)
4	PX4	A	415	-	51,53,53	1.53±0.14	9±3 (18±5%)
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4	PX4	A	381	-	51,53,53	1.49±0.15	9±2 (18±4%)
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4	PX4	A	319	-	51,53,53	1.41±0.10	8±2 (15±3%)
4	PX4	A	354	-	51,53,53	1.60±0.11	10±3 (20±6%)
4	PX4	A	385	-	51,53,53	1.48±0.13	9±2 (17±4%)
4	PX4	A	428	-	51,53,53	1.49±0.13	9±2 (17±4%)
4	PX4	A	341	-	51,53,53	1.44±0.12	7±2 (13±4%)
4	PX4	A	344	-	51,53,53	1.54±0.10	8±2 (16±4%)
4	PX4	A	393	-	51,53,53	1.43±0.13	8±2 (15±4%)
4	PX4	A	351	-	51,53,53	1.44±0.12	8±2 (16±3%)
4	PX4	A	401	-	51,53,53	1.43±0.16	8±2 (16±4%)
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4	PX4	A	345	-	51,53,53	1.34±0.09	7±1 (13±2%)
4	PX4	A	309	-	51,53,53	1.52±0.14	10±3 (18±5%)
4	PX4	A	369	-	51,53,53	1.51±0.09	9±1 (17±2%)
4	PX4	A	312	-	51,53,53	1.49±0.12	8±2 (16±3%)
4	PX4	A	313	-	51,53,53	1.48±0.13	9±3 (16±5%)
4	PX4	A	423	-	51,53,53	1.50±0.11	8±2 (16±3%)
4	PX4	A	406	-	51,53,53	1.45±0.13	8±2 (15±3%)
4	PX4	A	421	-	51,53,53	1.50±0.16	9±3 (18±5%)
4	PX4	A	403	-	51,53,53	1.51±0.16	9±2 (18±4%)
4	PX4	A	395	-	51,53,53	1.43±0.11	8±2 (16±3%)
4	PX4	A	358	-	51,53,53	1.36±0.10	7±2 (14±4%)
4	PX4	A	332	-	51,53,53	1.49±0.14	9±2 (18±4%)
4	PX4	A	357	-	51,53,53	1.52±0.08	9±2 (17±3%)
4	PX4	A	316	-	51,53,53	1.38±0.12	8±2 (14±3%)
4	PX4	A	321	-	51,53,53	1.55±0.14	9±2 (18±4%)
4	PX4	A	387	-	51,53,53	1.45±0.19	8±3 (16±5%)
4	PX4	A	382	-	51,53,53	1.51±0.12	10±2 (19±4%)
4	PX4	A	384	-	51,53,53	1.44±0.13	8±2 (15±4%)
4	PX4	A	331	-	51,53,53	1.45±0.12	8±2 (16±3%)
4	PX4	A	373	-	51,53,53	1.48±0.11	8±2 (16±3%)
4	PX4	A	320	-	51,53,53	1.50±0.12	9±2 (18±4%)
4	PX4	A	422	-	51,53,53	1.48±0.16	9±3 (17±5%)
4	PX4	A	424	-	51,53,53	1.45±0.15	8±2 (14±3%)
4	PX4	A	360	-	51,53,53	1.50±0.12	9±2 (16±3%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	318	-	51,53,53	1.44±0.14	8±2 (16±3%)
4	PX4	A	430	-	51,53,53	1.49±0.11	9±2 (17±3%)
4	PX4	A	317	-	51,53,53	1.45±0.11	8±1 (15±2%)
4	PX4	A	355	-	51,53,53	1.47±0.17	8±3 (16±5%)

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
4	PX4	A	418	-	-	0±0,49,49,49	-
4	PX4	A	342	-	-	0±0,49,49,49	-
4	PX4	A	362	-	-	0±0,49,49,49	-
4	PX4	A	352	-	-	0±0,49,49,49	-
4	PX4	A	330	-	-	0±0,49,49,49	-
4	PX4	A	340	-	-	0±0,49,49,49	-
4	PX4	A	349	-	-	0±0,49,49,49	-
4	PX4	A	390	-	-	0±0,49,49,49	-
4	PX4	A	347	-	-	0±0,49,49,49	-
4	PX4	A	416	-	-	0±0,49,49,49	-
4	PX4	A	380	-	-	0±0,49,49,49	-
4	PX4	A	379	-	-	0±0,49,49,49	-
4	PX4	A	314	-	-	0±0,49,49,49	-
4	PX4	A	411	-	-	0±0,49,49,49	-
4	PX4	A	325	-	-	0±0,49,49,49	-
4	PX4	A	392	-	-	0±0,49,49,49	-
4	PX4	A	324	-	-	0±0,49,49,49	-
4	PX4	A	429	-	-	0±0,49,49,49	-
4	PX4	A	402	-	-	0±0,49,49,49	-
4	PX4	A	382	-	-	0±0,49,49,49	-
4	PX4	A	384	-	-	0±0,49,49,49	-
4	PX4	A	391	-	-	0±0,49,49,49	-
4	PX4	A	345	-	-	0±0,49,49,49	-
4	PX4	A	419	-	-	0±0,49,49,49	-
4	PX4	A	393	-	-	0±0,49,49,49	-
4	PX4	A	398	-	-	0±0,49,49,49	-
4	PX4	A	423	-	-	0±0,49,49,49	-
4	PX4	A	311	-	-	0±0,49,49,49	-
4	PX4	A	331	-	-	0±0,49,49,49	-
4	PX4	A	406	-	-	0±0,49,49,49	-
4	PX4	A	378	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	401	-	-	0±0,49,49,49	-
4	PX4	A	365	-	-	0±0,49,49,49	-
4	PX4	A	346	-	-	0±0,49,49,49	-
4	PX4	A	373	-	-	0±0,49,49,49	-
4	PX4	A	410	-	-	0±0,49,49,49	-
4	PX4	A	376	-	-	0±0,49,49,49	-
4	PX4	A	377	-	-	0±0,49,49,49	-
4	PX4	A	413	-	-	0±0,49,49,49	-
4	PX4	A	322	-	-	0±0,49,49,49	-
4	PX4	A	426	-	-	0±0,49,49,49	-
4	PX4	A	361	-	-	0±0,49,49,49	-
4	PX4	A	417	-	-	0±0,49,49,49	-
4	PX4	A	422	-	-	0±0,49,49,49	-
4	PX4	A	338	-	-	0±0,49,49,49	-
4	PX4	A	425	-	-	0±0,49,49,49	-
4	PX4	A	348	-	-	0±0,49,49,49	-
4	PX4	A	399	-	-	0±0,49,49,49	-
4	PX4	A	403	-	-	0±0,49,49,49	-
4	PX4	A	310	-	-	0±0,49,49,49	-
4	PX4	A	381	-	-	0±0,49,49,49	-
4	PX4	A	404	-	-	0±0,49,49,49	-
4	PX4	A	388	-	-	0±0,49,49,49	-
4	PX4	A	353	-	-	0±0,49,49,49	-
4	PX4	A	420	-	-	0±0,49,49,49	-
4	PX4	A	374	-	-	0±0,49,49,49	-
4	PX4	A	359	-	-	0±0,49,49,49	-
4	PX4	A	397	-	-	0±0,49,49,49	-
4	PX4	A	326	-	-	0±0,49,49,49	-
4	PX4	A	313	-	-	0±0,49,49,49	-
4	PX4	A	415	-	-	0±0,49,49,49	-
4	PX4	A	395	-	-	0±0,49,49,49	-
4	PX4	A	421	-	-	0±0,49,49,49	-
4	PX4	A	341	-	-	0±0,49,49,49	-
4	PX4	A	386	-	-	0±0,49,49,49	-
4	PX4	A	364	-	-	0±0,49,49,49	-
4	PX4	A	328	-	-	0±0,49,49,49	-
4	PX4	A	334	-	-	0±0,49,49,49	-
4	PX4	A	428	-	-	0±0,49,49,49	-
4	PX4	A	367	-	-	0±0,49,49,49	-
4	PX4	A	356	-	-	0±0,49,49,49	-
4	PX4	A	383	-	-	0±0,49,49,49	-
4	PX4	A	368	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	371	-	-	0±0,49,49,49	-
4	PX4	A	414	-	-	0±0,49,49,49	-
4	PX4	A	319	-	-	0±0,49,49,49	-
4	PX4	A	332	-	-	0±0,49,49,49	-
4	PX4	A	336	-	-	0±0,49,49,49	-
4	PX4	A	396	-	-	0±0,49,49,49	-
4	PX4	A	343	-	-	0±0,49,49,49	-
4	PX4	A	339	-	-	0±0,49,49,49	-
4	PX4	A	430	-	-	0±0,49,49,49	-
4	PX4	A	408	-	-	0±0,49,49,49	-
4	PX4	A	309	-	-	0±0,49,49,49	-
4	PX4	A	335	-	-	0±0,49,49,49	-
4	PX4	A	363	-	-	0±0,49,49,49	-
4	PX4	A	354	-	-	0±0,49,49,49	-
4	PX4	A	405	-	-	0±0,49,49,49	-
4	PX4	A	400	-	-	0±0,49,49,49	-
4	PX4	A	337	-	-	0±0,49,49,49	-
4	PX4	A	350	-	-	0±0,49,49,49	-
4	PX4	A	333	-	-	0±0,49,49,49	-
4	PX4	A	307	-	-	0±0,49,49,49	-
4	PX4	A	329	-	-	0±0,49,49,49	-
4	PX4	A	412	-	-	0±0,49,49,49	-
4	PX4	A	308	-	-	0±0,49,49,49	-
4	PX4	A	427	-	-	0±0,49,49,49	-
4	PX4	A	358	-	-	0±0,49,49,49	-
4	PX4	A	389	-	-	0±0,49,49,49	-
4	PX4	A	407	-	-	0±0,49,49,49	-
4	PX4	A	327	-	-	0±0,49,49,49	-
4	PX4	A	344	-	-	0±0,49,49,49	-
4	PX4	A	321	-	-	0±0,49,49,49	-
4	PX4	A	387	-	-	0±0,49,49,49	-
4	PX4	A	369	-	-	0±0,49,49,49	-
4	PX4	A	375	-	-	0±0,49,49,49	-
4	PX4	A	394	-	-	0±0,49,49,49	-
4	PX4	A	320	-	-	0±0,49,49,49	-
4	PX4	A	312	-	-	0±0,49,49,49	-
4	PX4	A	409	-	-	0±0,49,49,49	-
4	PX4	A	315	-	-	0±0,49,49,49	-
4	PX4	A	372	-	-	0±0,49,49,49	-
4	PX4	A	355	-	-	0±0,49,49,49	-
4	PX4	A	306	-	-	0±0,49,49,49	-
4	PX4	A	357	-	-	0±0,49,49,49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	323	-	-	0±0,49,49,49	-
4	PX4	A	366	-	-	0±0,49,49,49	-
4	PX4	A	360	-	-	0±0,49,49,49	-
4	PX4	A	317	-	-	0±0,49,49,49	-
4	PX4	A	351	-	-	0±0,49,49,49	-
4	PX4	A	385	-	-	0±0,49,49,49	-
4	PX4	A	318	-	-	0±0,49,49,49	-
4	PX4	A	370	-	-	0±0,49,49,49	-
4	PX4	A	316	-	-	0±0,49,49,49	-
4	PX4	A	424	-	-	0±0,49,49,49	-

There are no bond-length outliers.

5 of 4497 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
4	A	307	PX4	C8-C7-C6	7.73	93.49	111.79	5	5
4	A	314	PX4	C8-C7-C6	7.54	93.95	111.79	11	10
4	A	378	PX4	C8-C7-C6	7.49	94.07	111.79	2	10
4	A	341	PX4	C7-O7-C23	7.48	136.20	117.79	2	9
4	A	371	PX4	C8-C7-C6	7.35	94.42	111.79	3	12

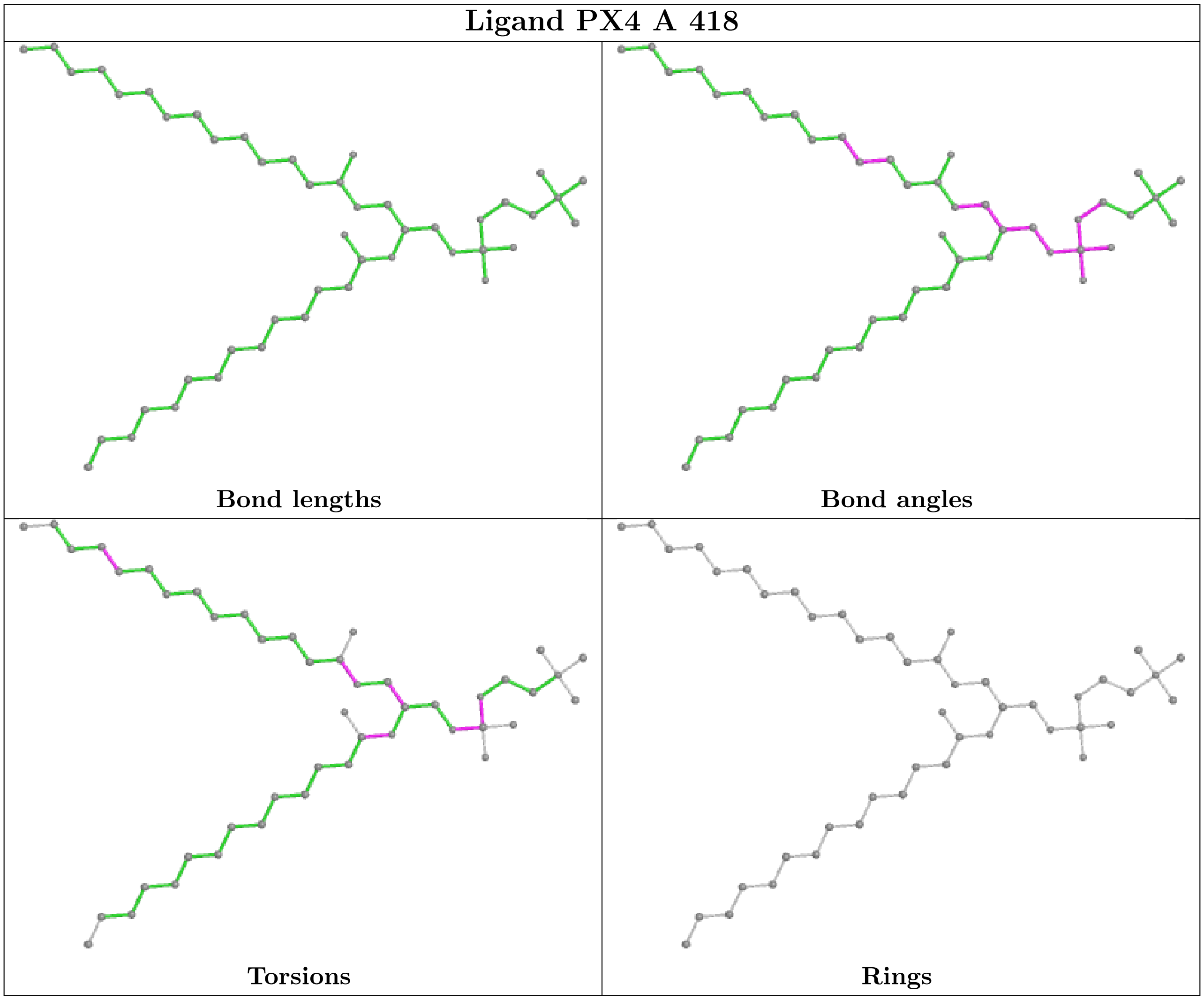
There are no chirality outliers.

All unique torsion outliers are listed below.

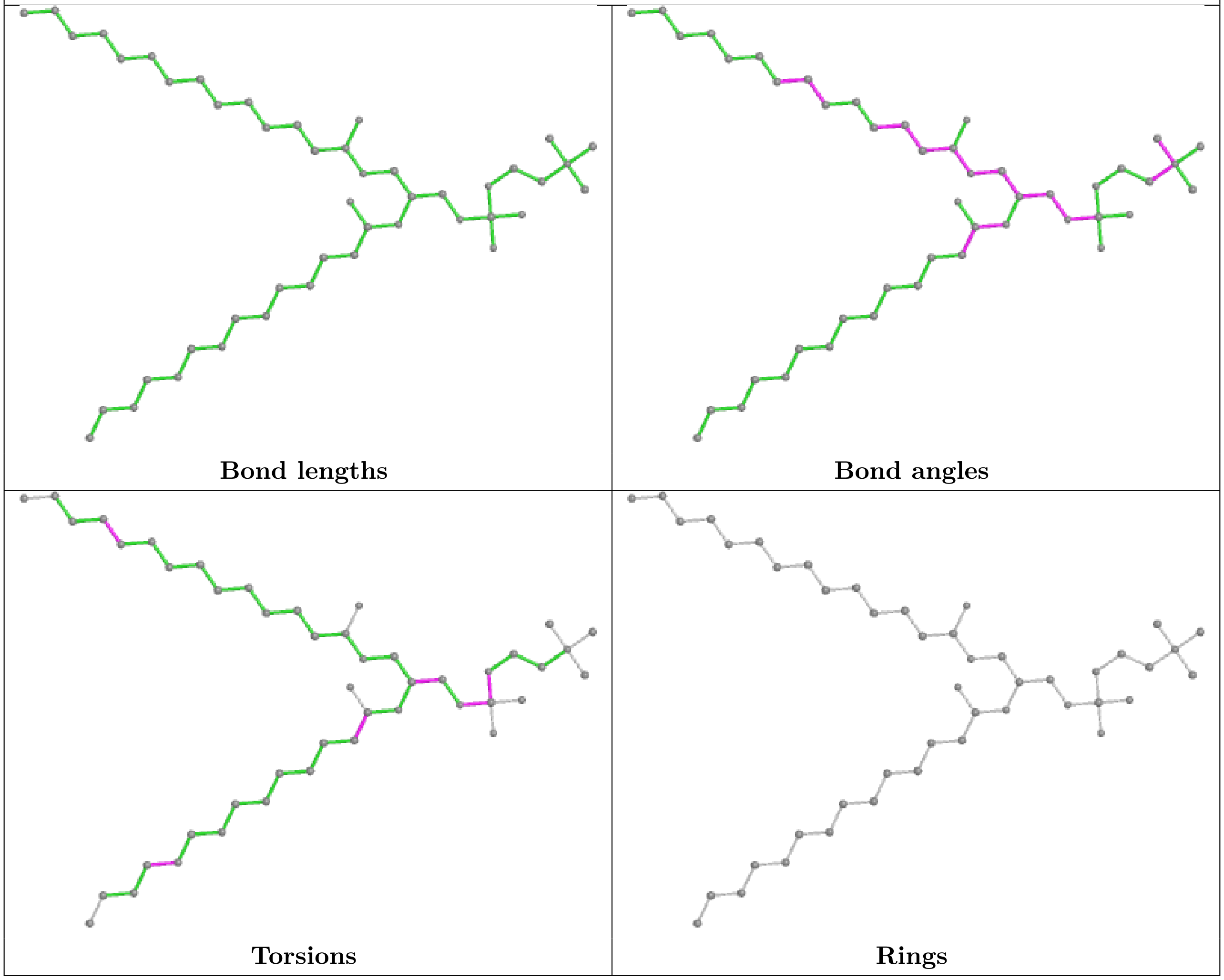
Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	335	PX4	O8-C23-O7-C7	2

There are no ring outliers.

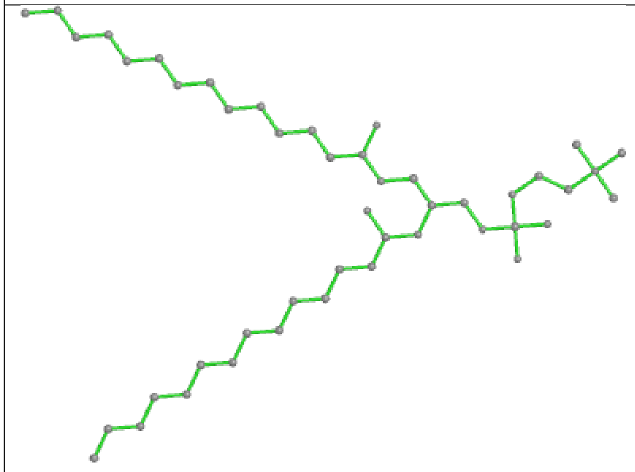
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



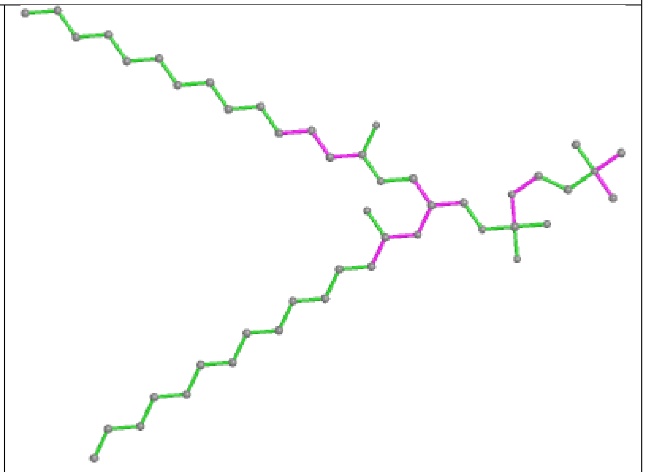
Ligand PX4 A 342



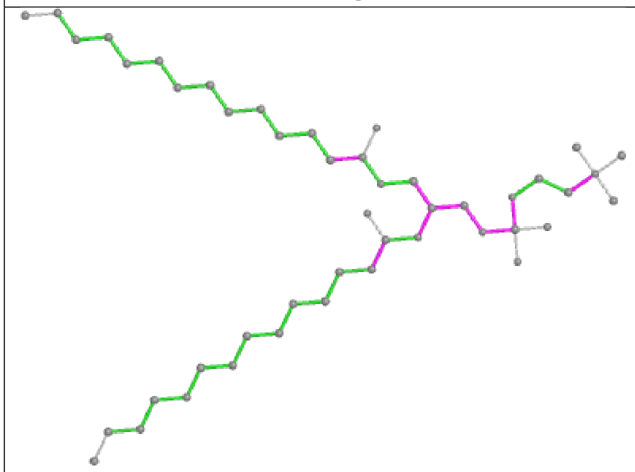
Ligand PX4 A 362



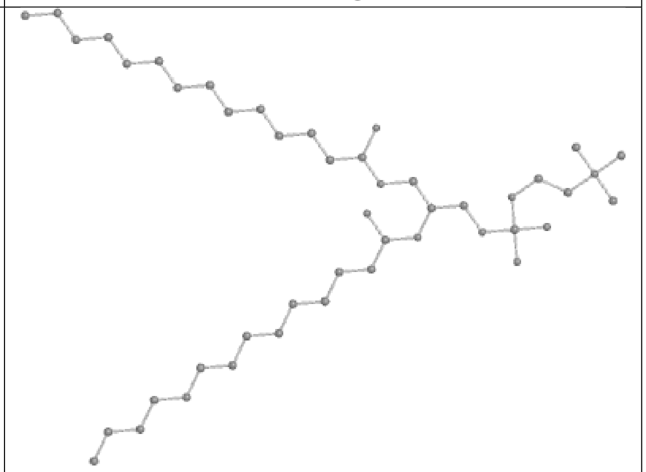
Bond lengths



Bond angles

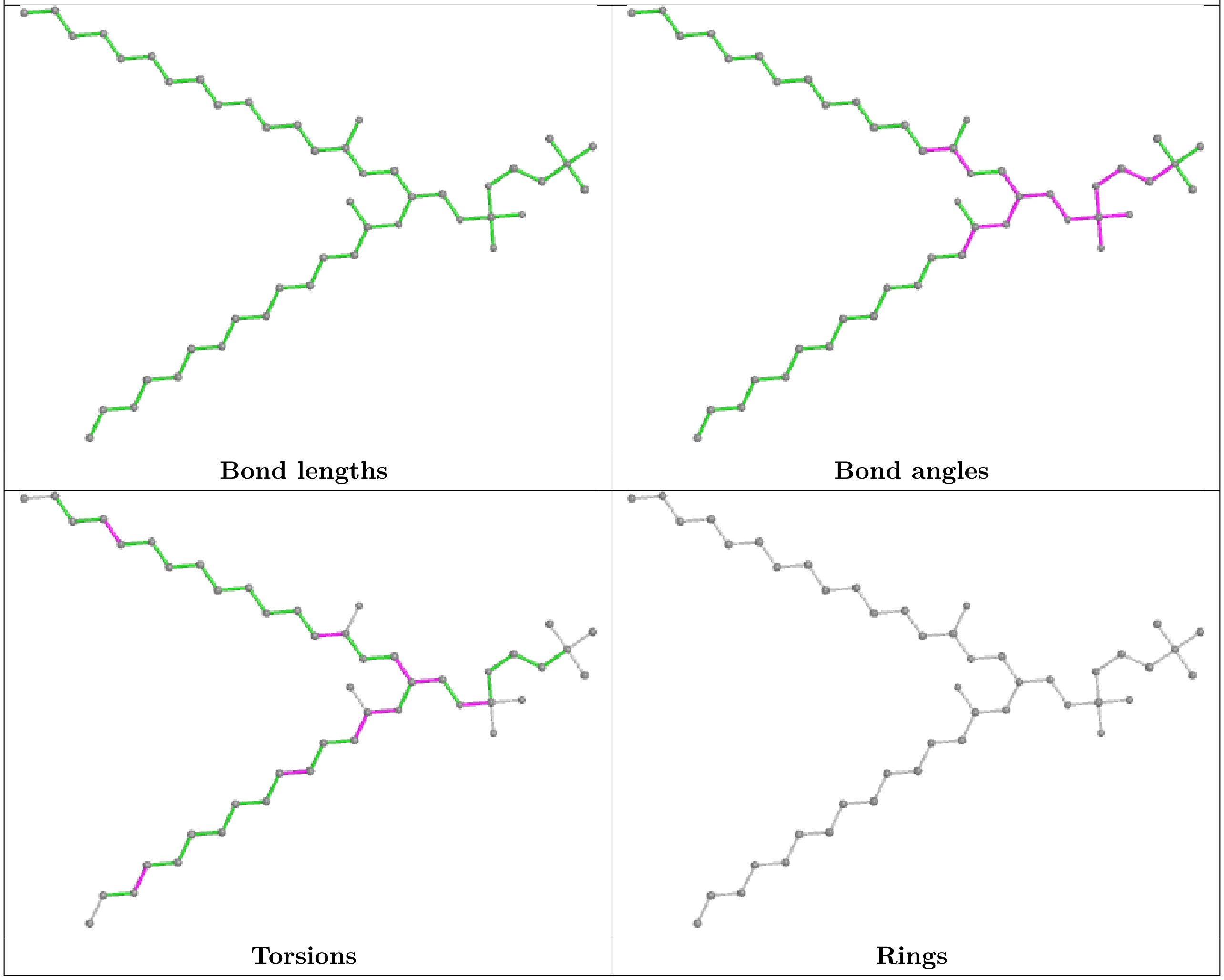


Torsions

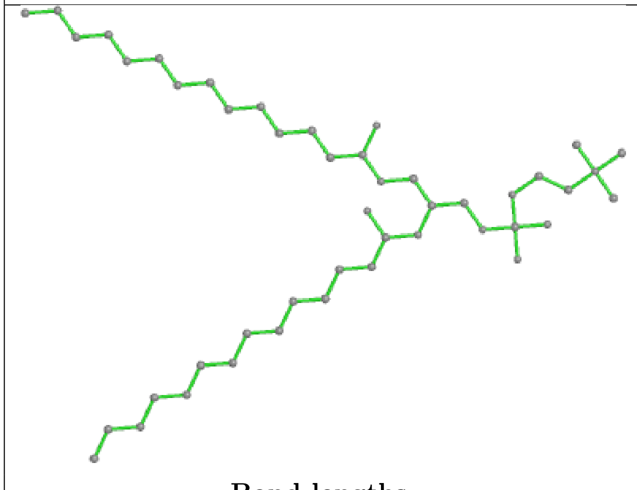


Rings

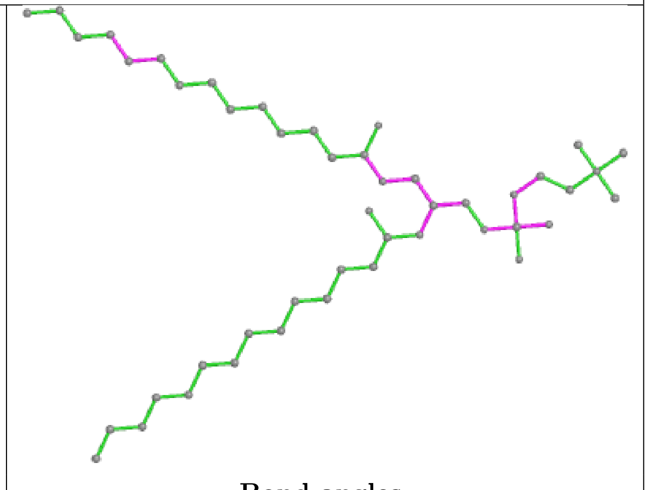
Ligand PX4 A 352



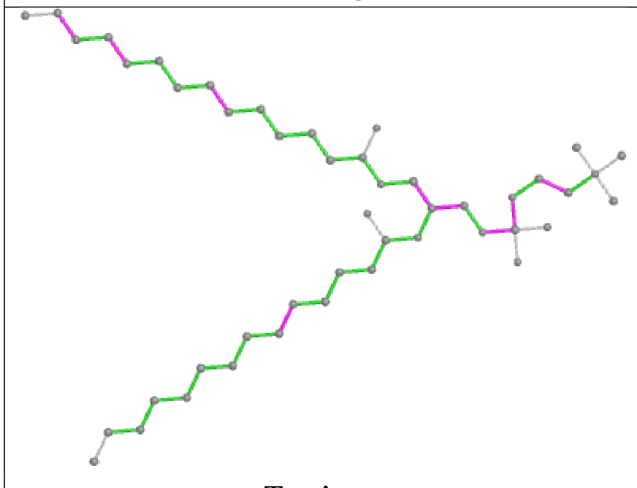
Ligand PX4 A 330



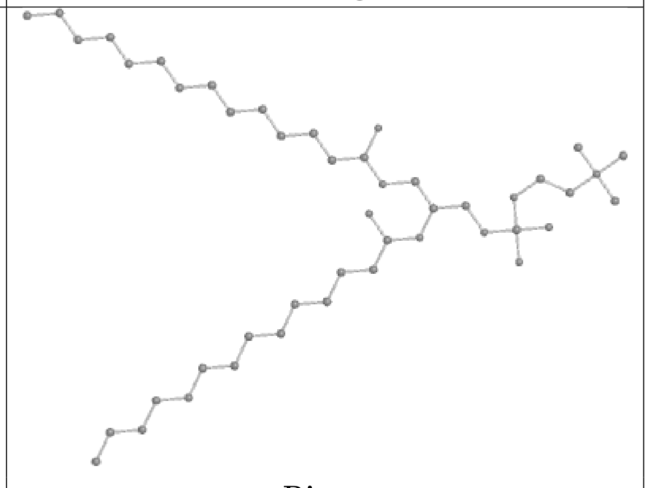
Bond lengths



Bond angles

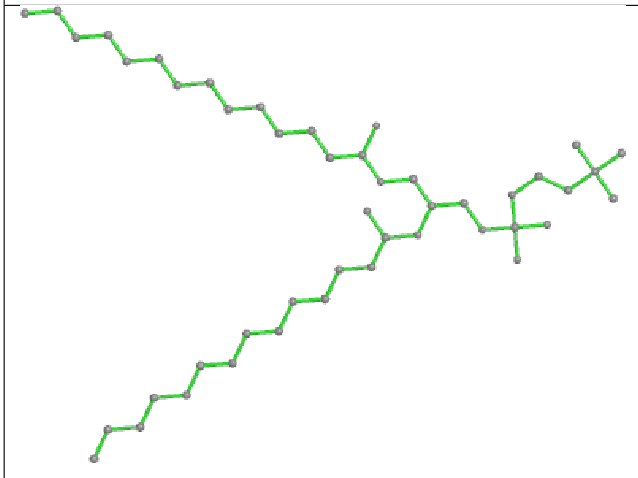


Torsions

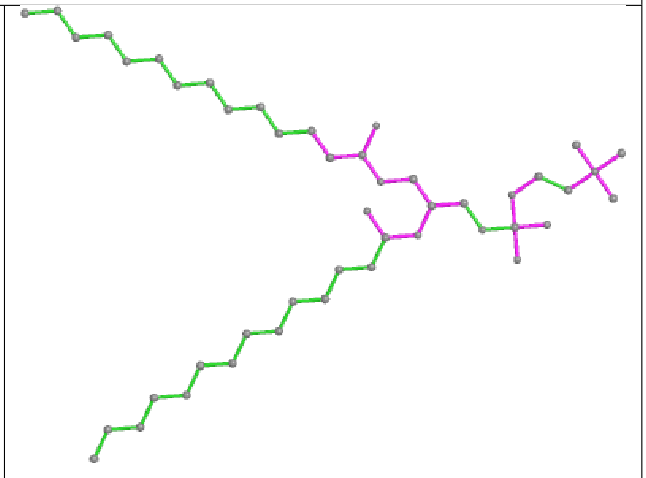


Rings

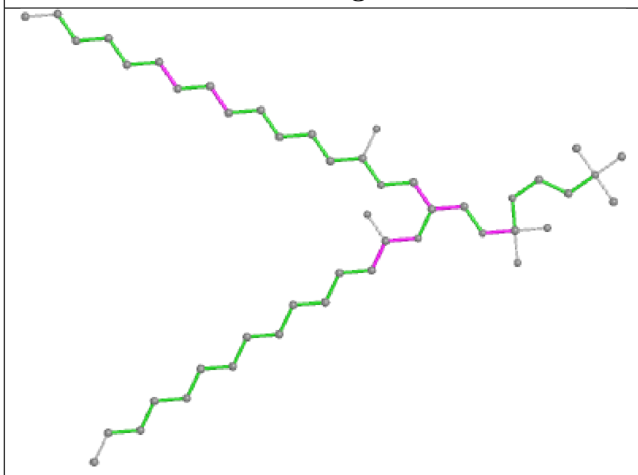
Ligand PX4 A 340



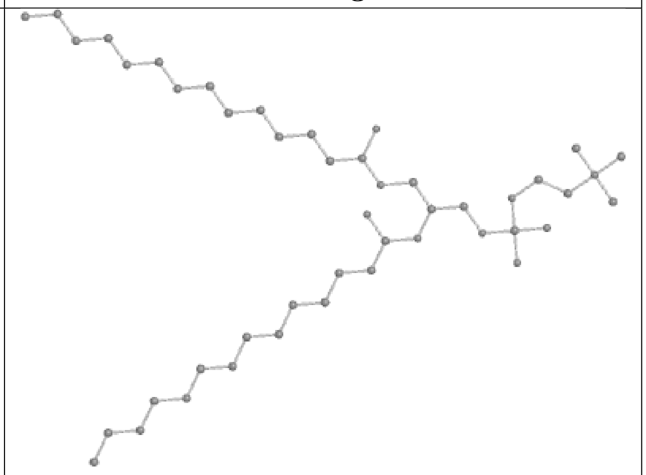
Bond lengths



Bond angles

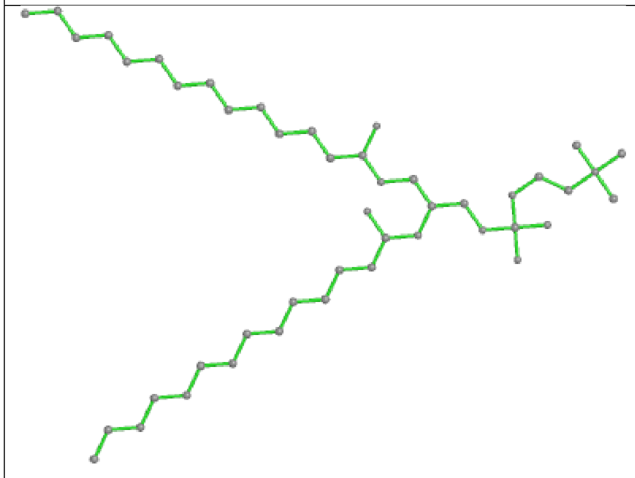


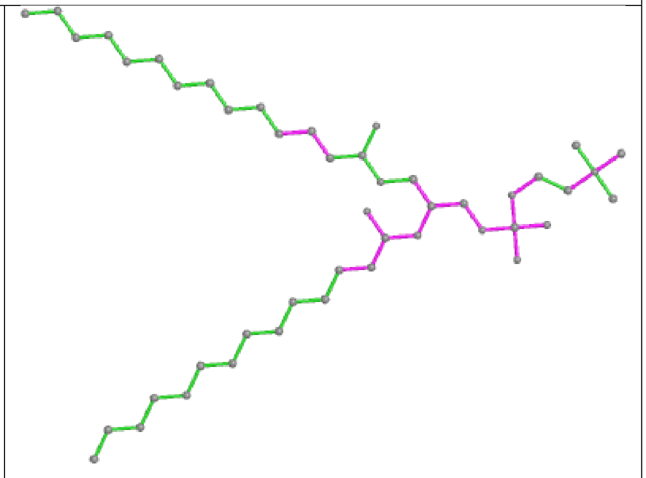
Torsions

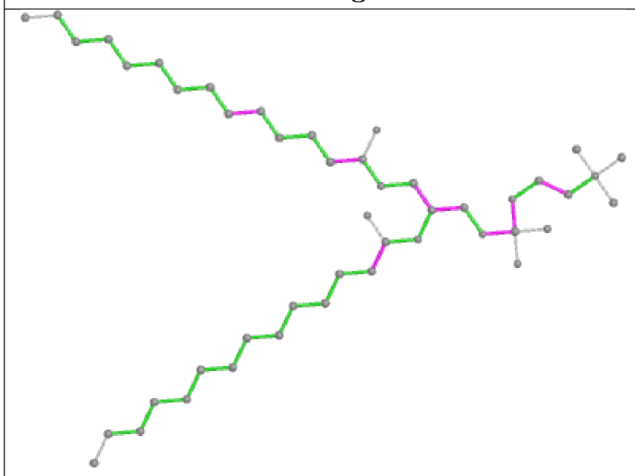


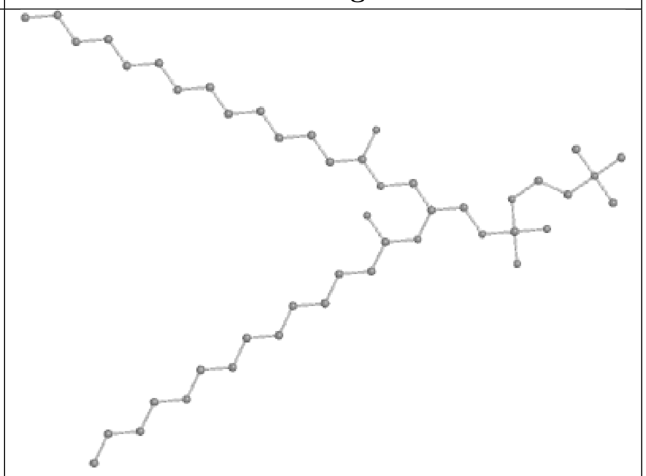
Rings

Ligand PX4 A 349

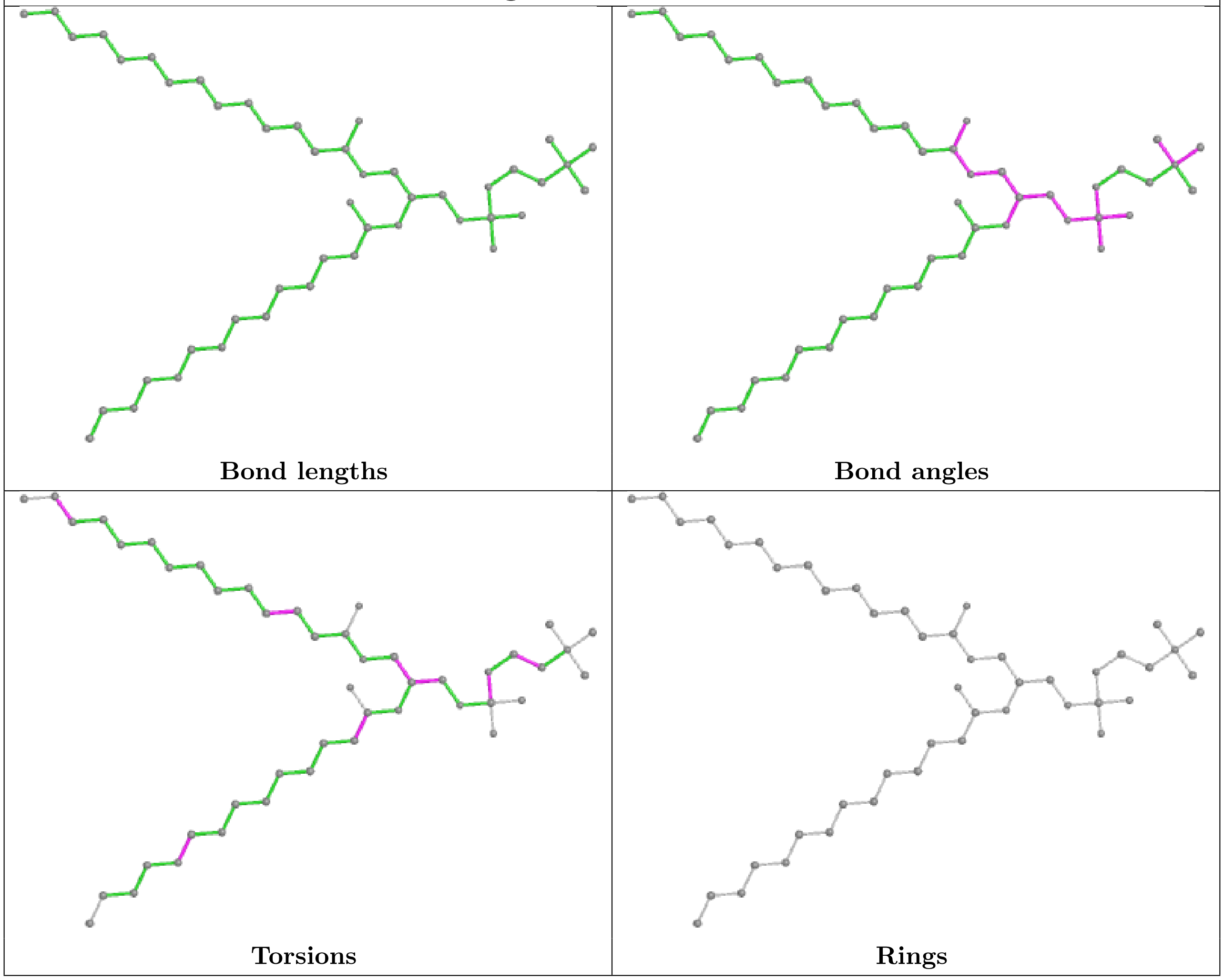

Bond lengths

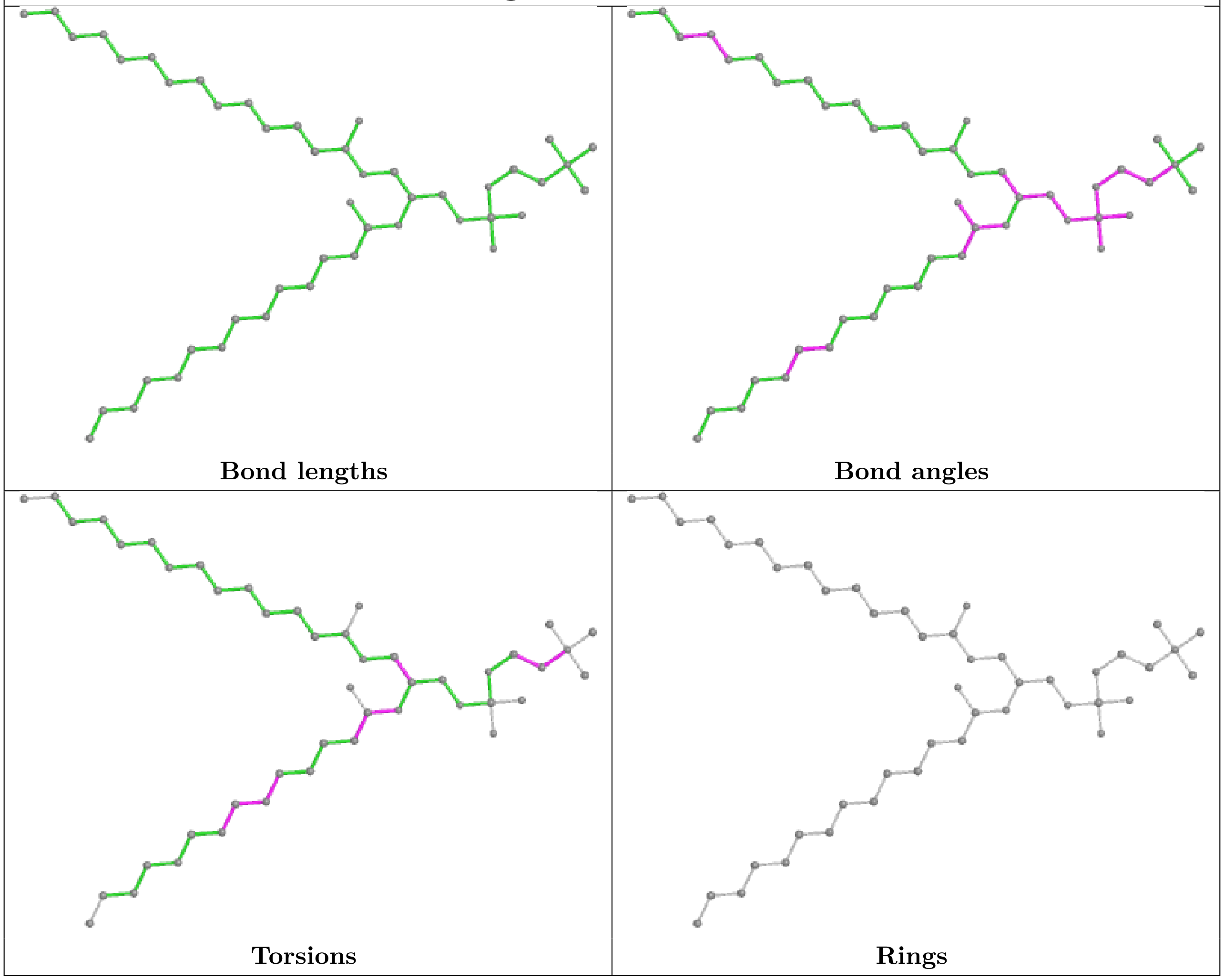

Bond angles


Torsions

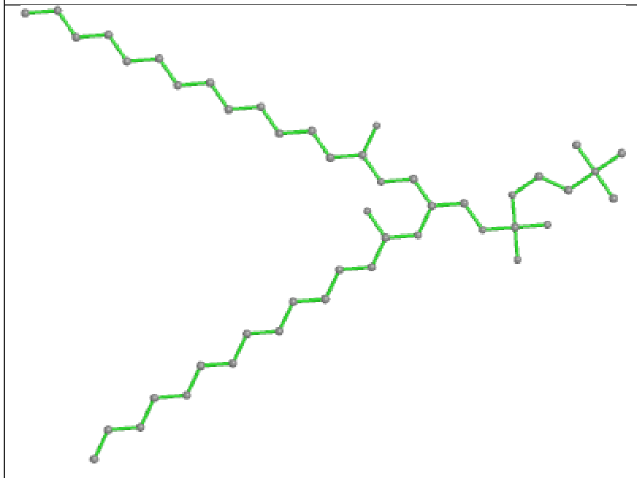

Rings

Ligand PX4 A 390

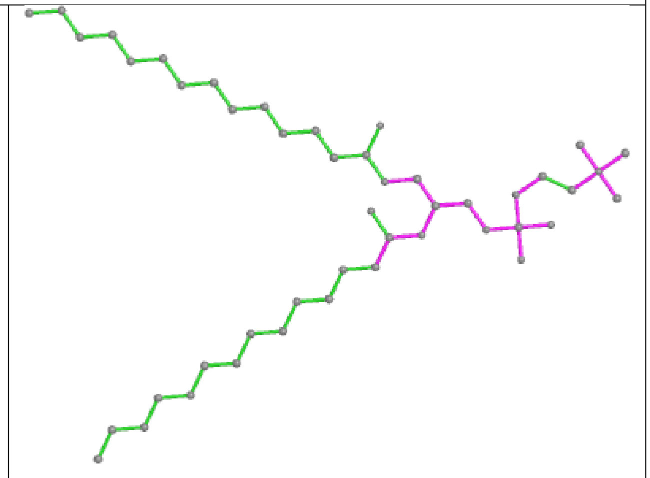


Ligand PX4 A 347	
	
Bond lengths	Bond angles
Torsions	Rings

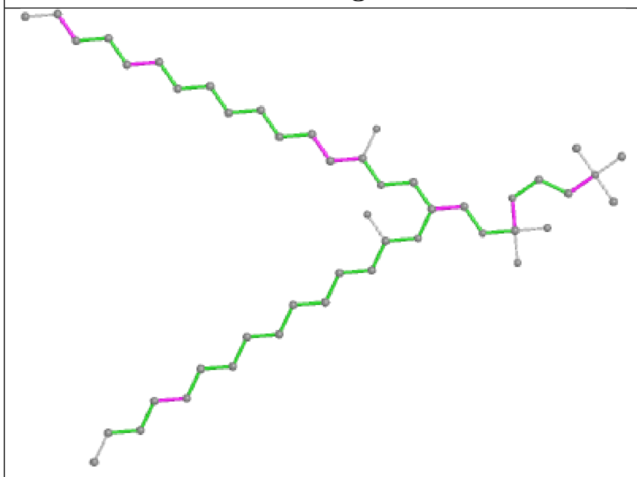
Ligand PX4 A 416



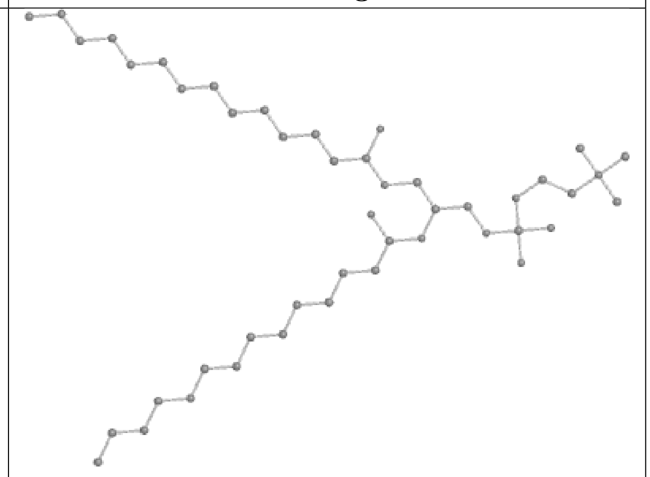
Bond lengths



Bond angles

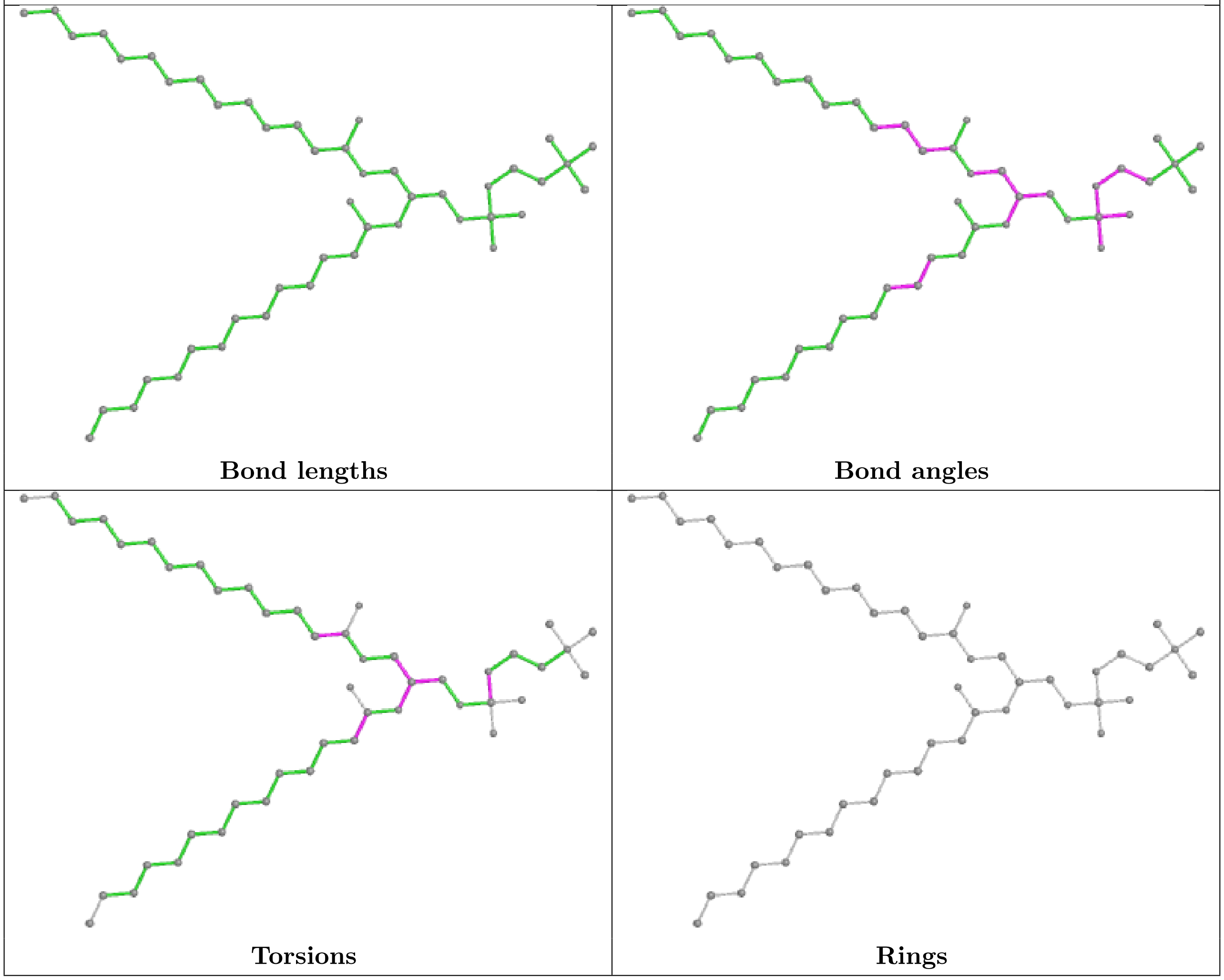


Torsions

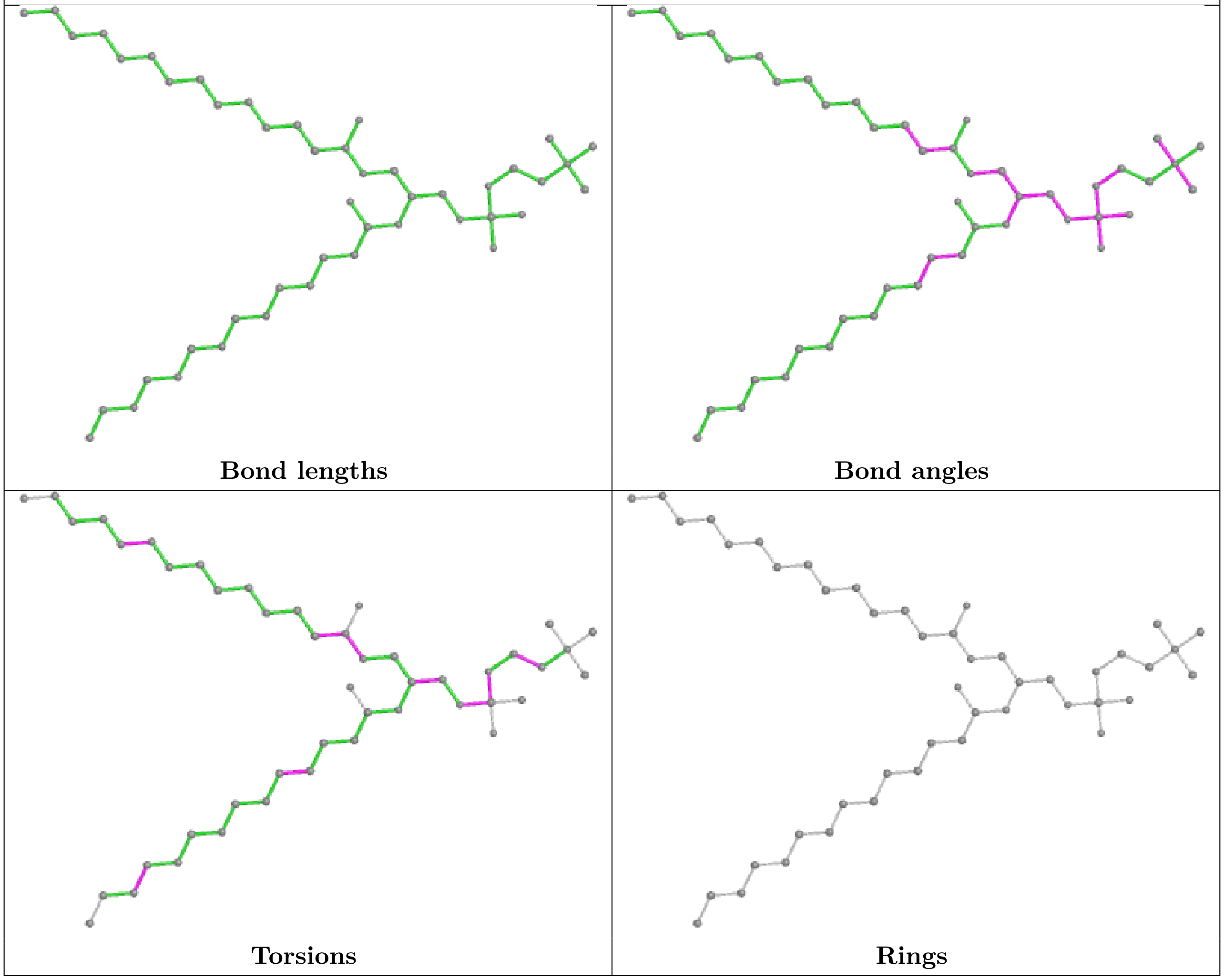


Rings

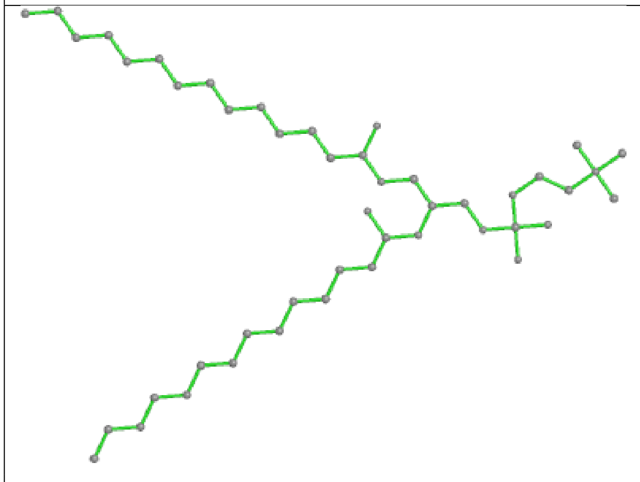
Ligand PX4 A 380



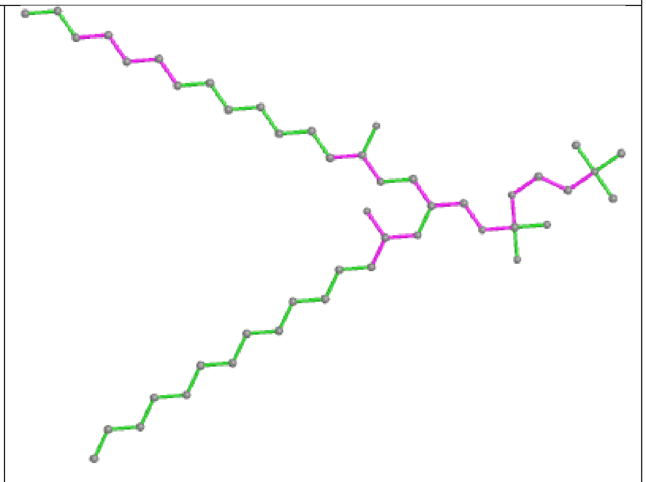
Ligand PX4 A 379



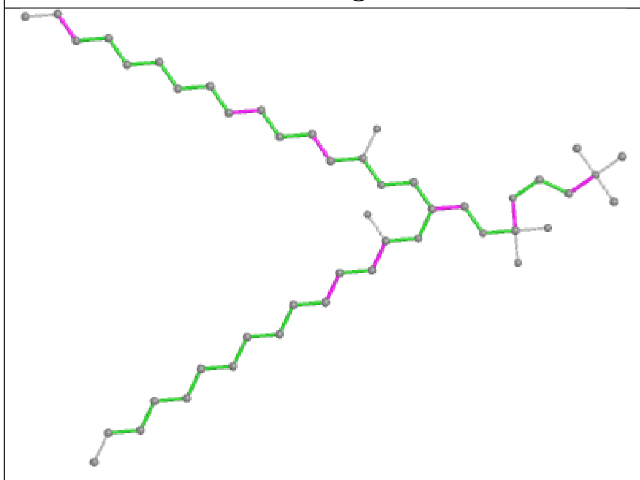
Ligand PX4 A 314



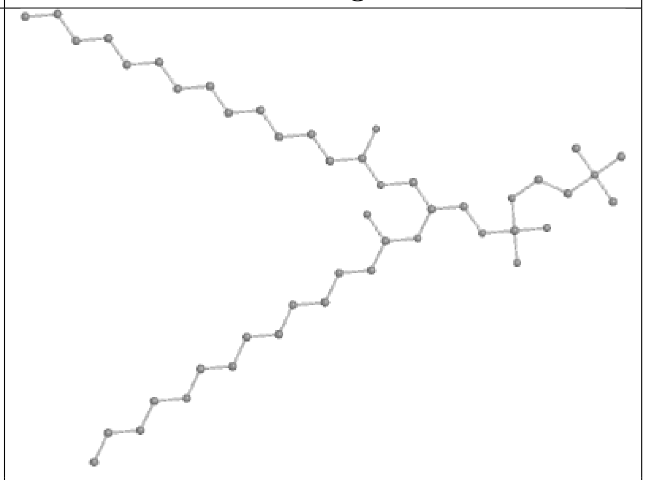
Bond lengths



Bond angles

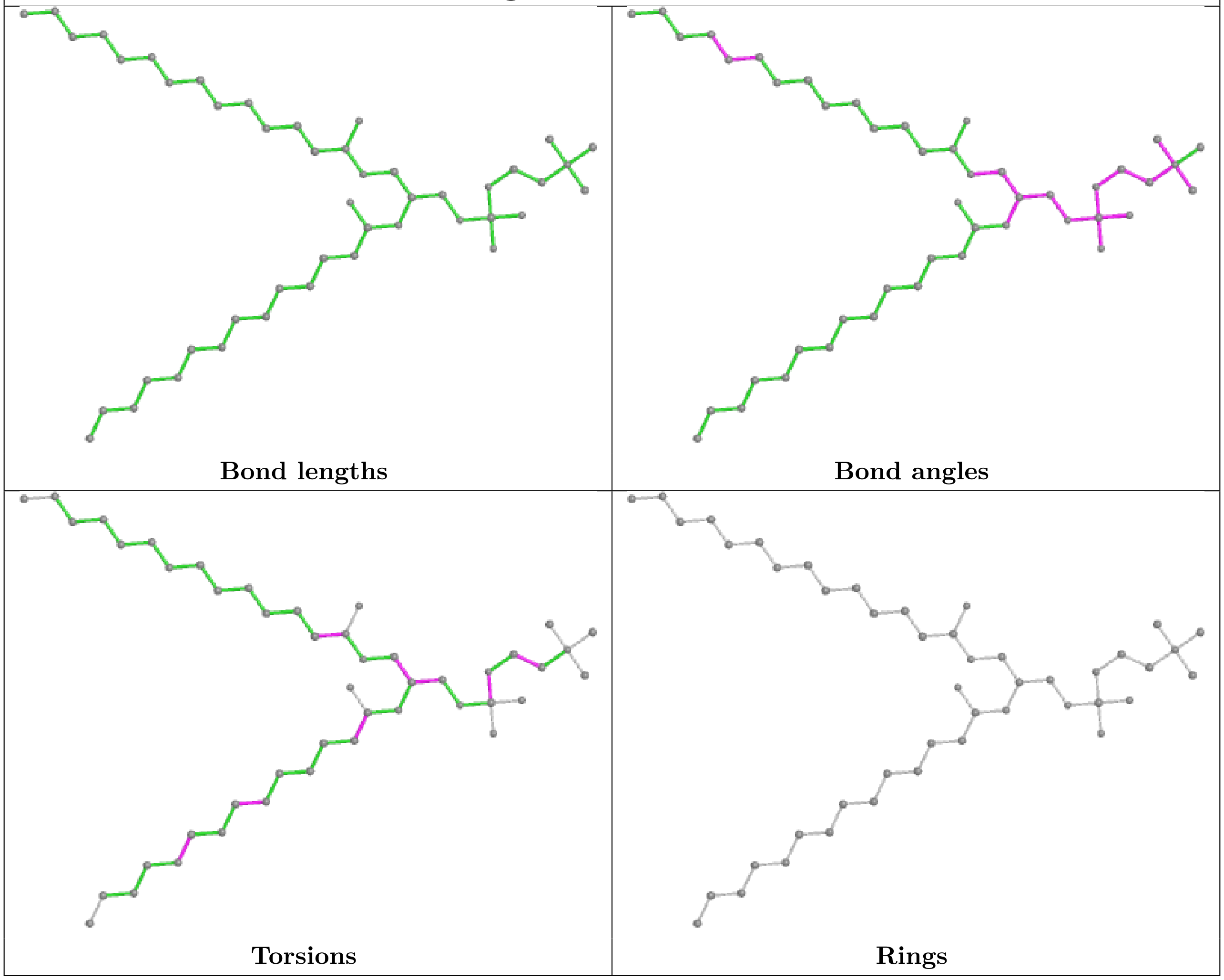


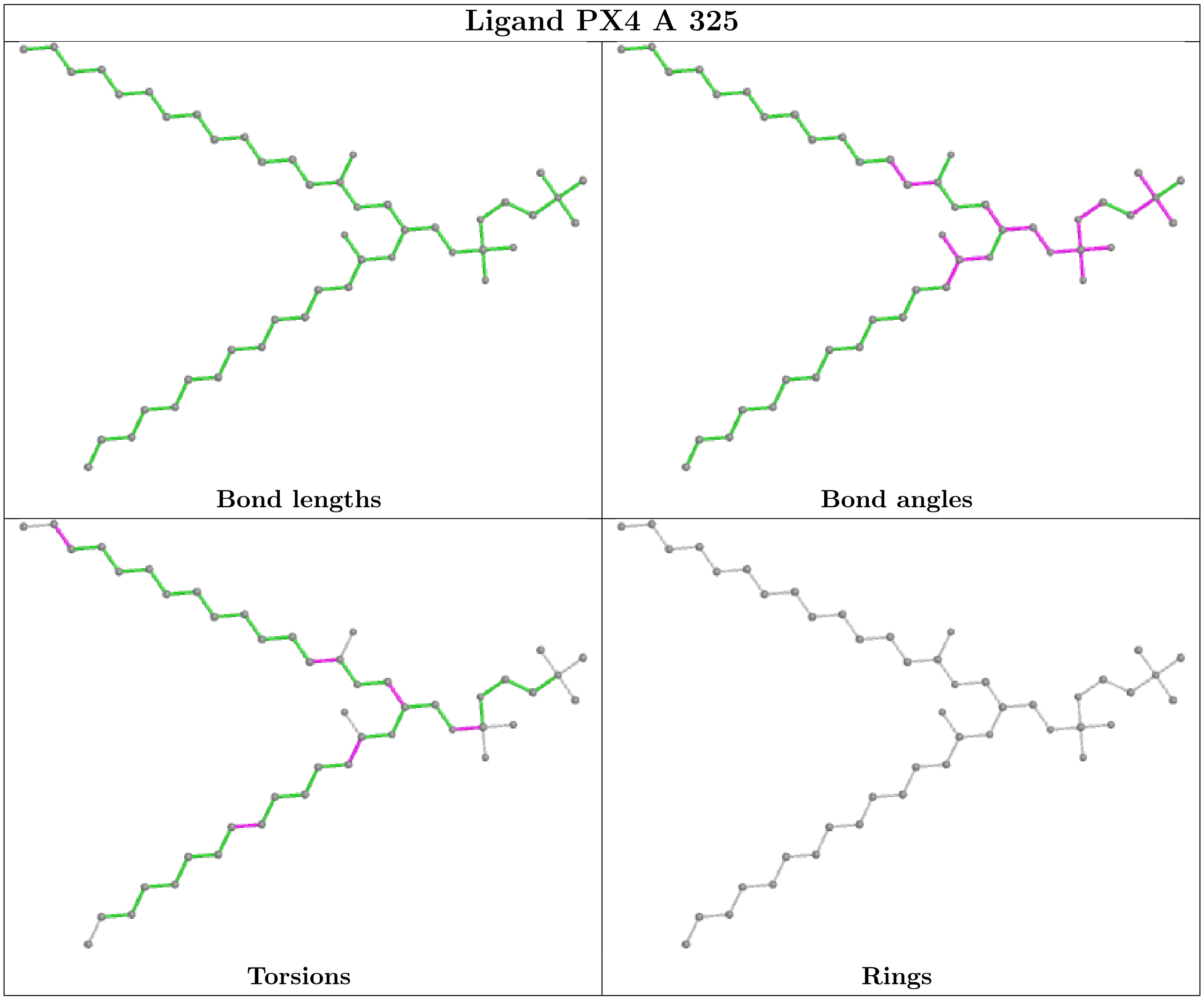
Torsions



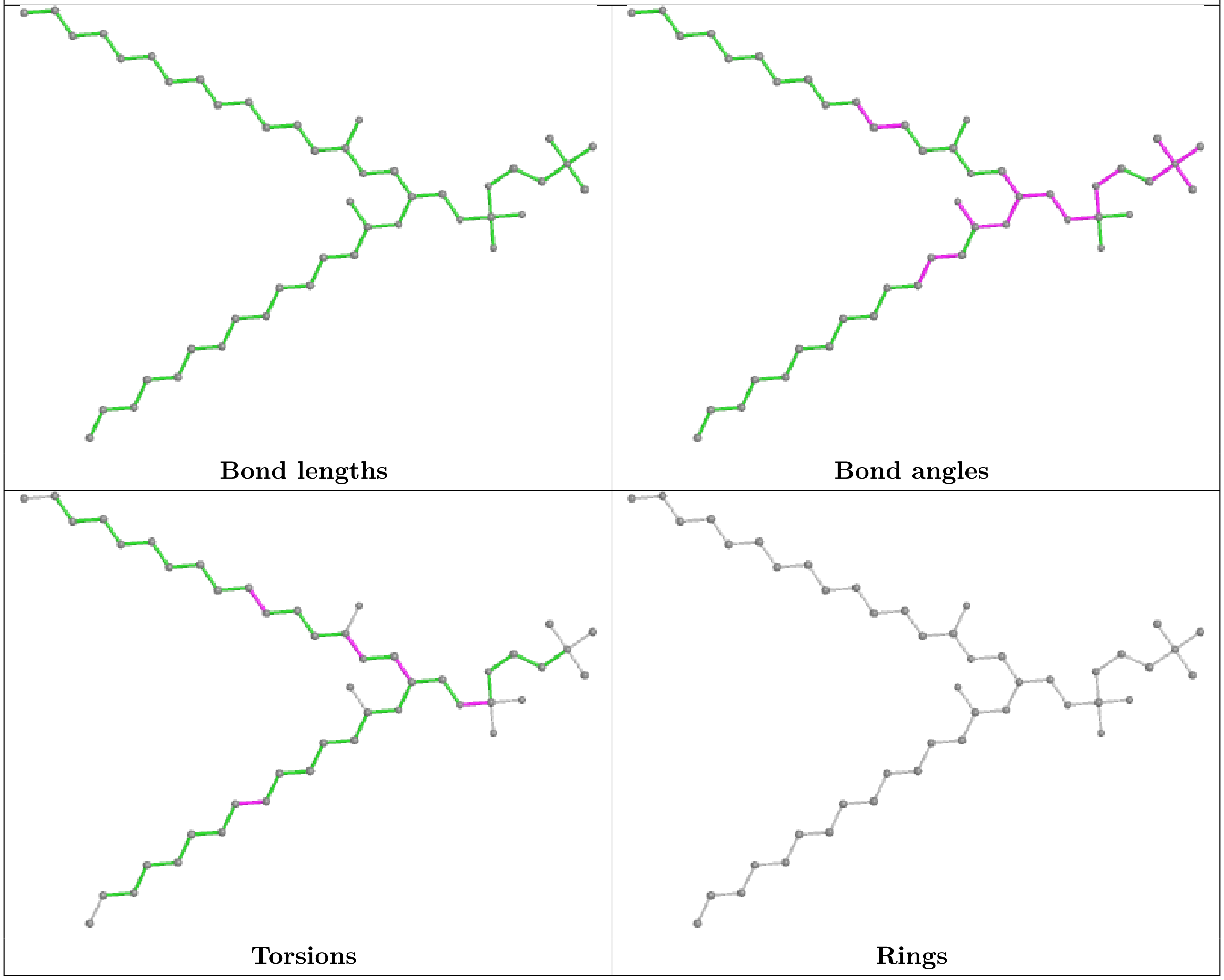
Rings

Ligand PX4 A 411

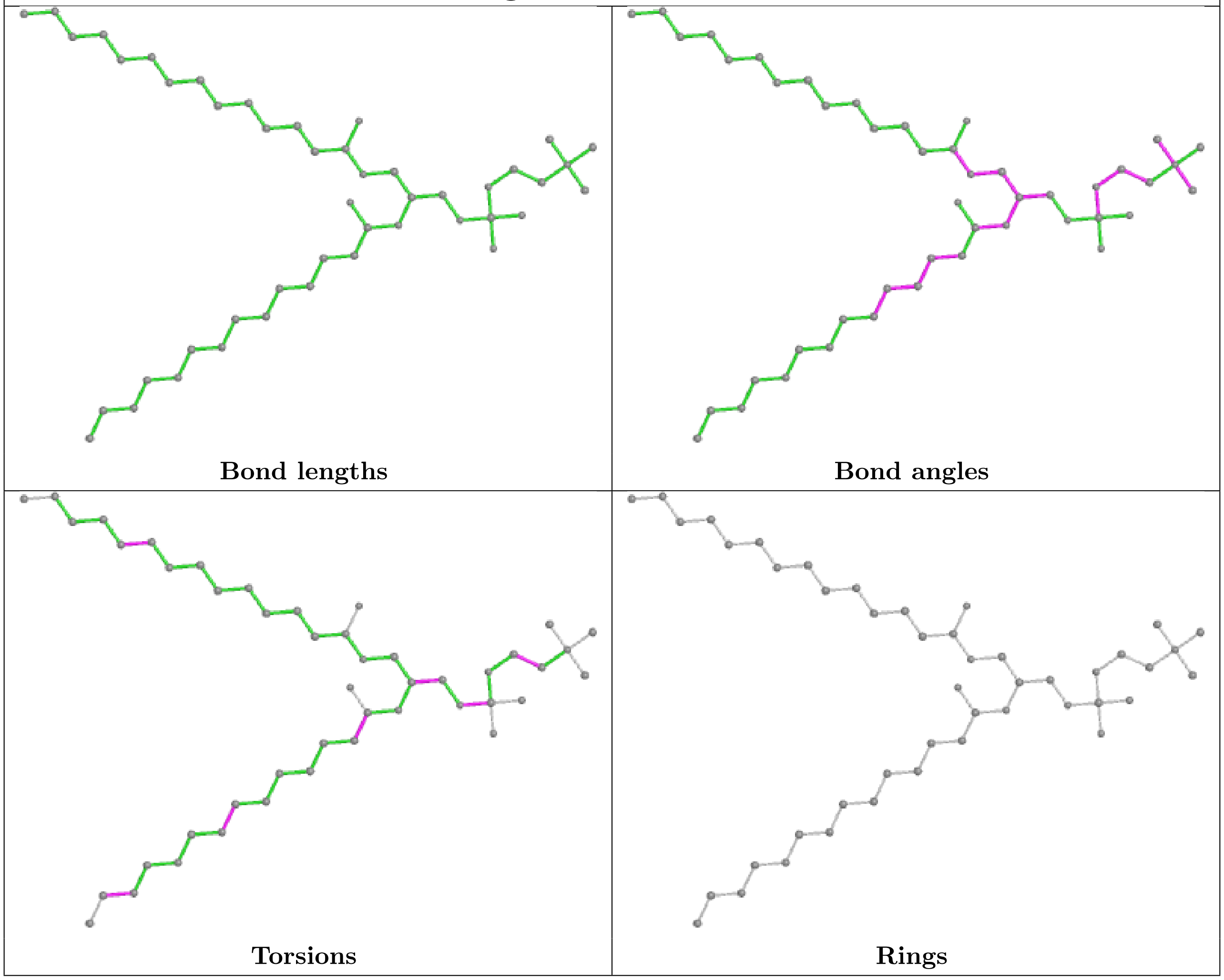



Ligand PX4 A 325
Bond lengths
Bond angles
Torsions
Rings

Ligand PX4 A 392



Ligand PX4 A 324



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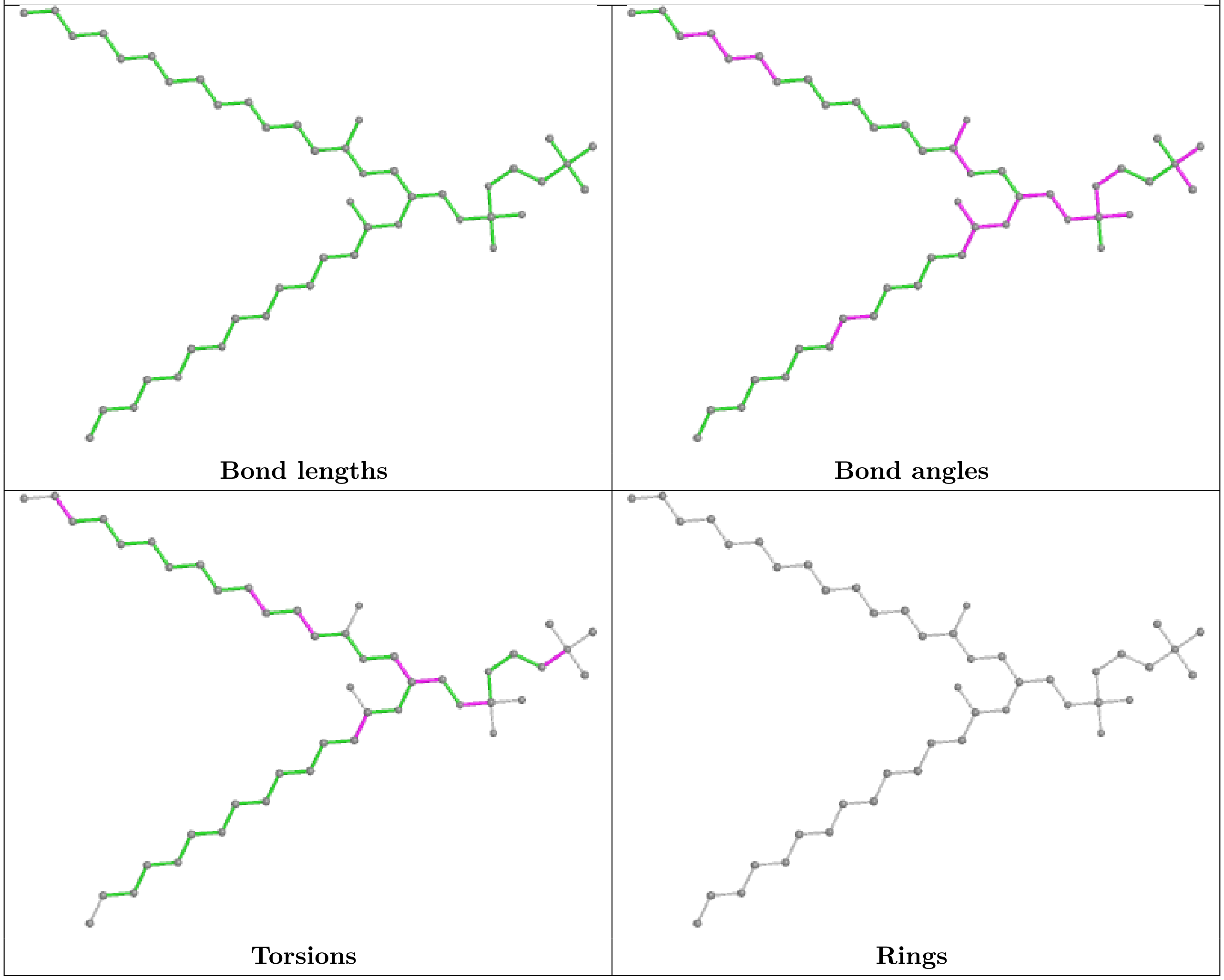
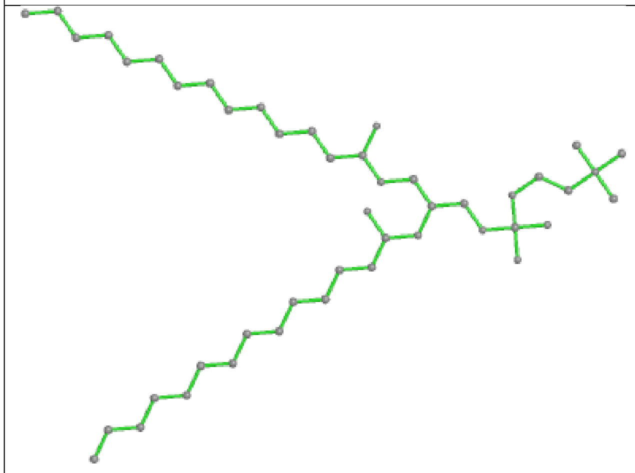
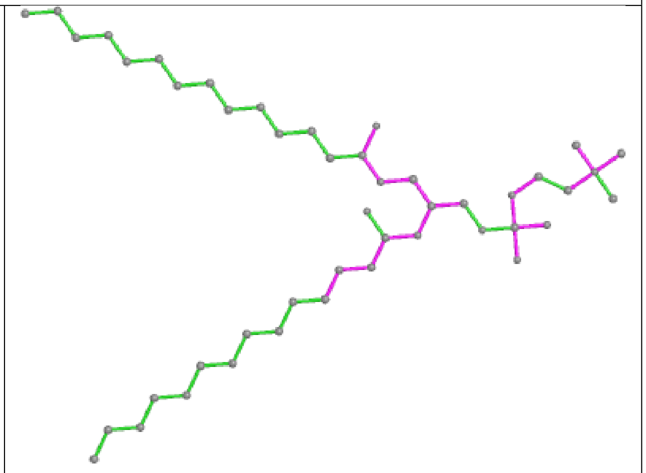


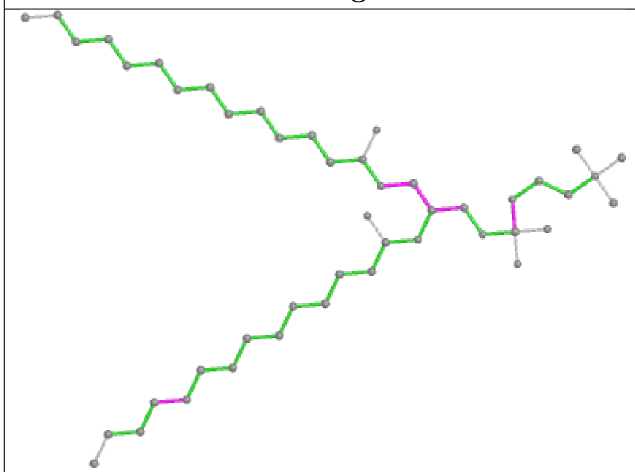
Ligand PX4 A 402



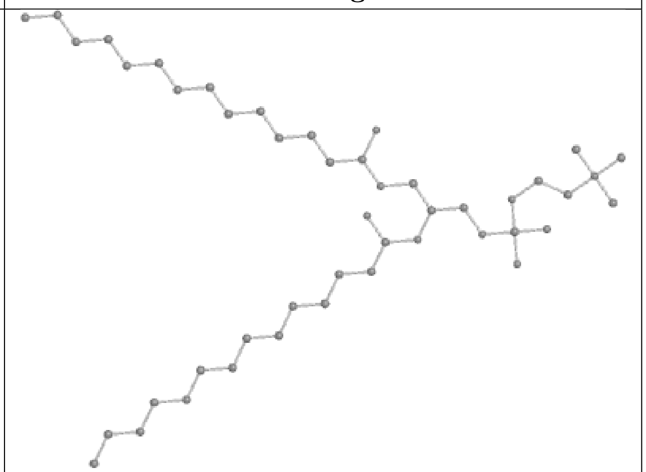
Bond lengths



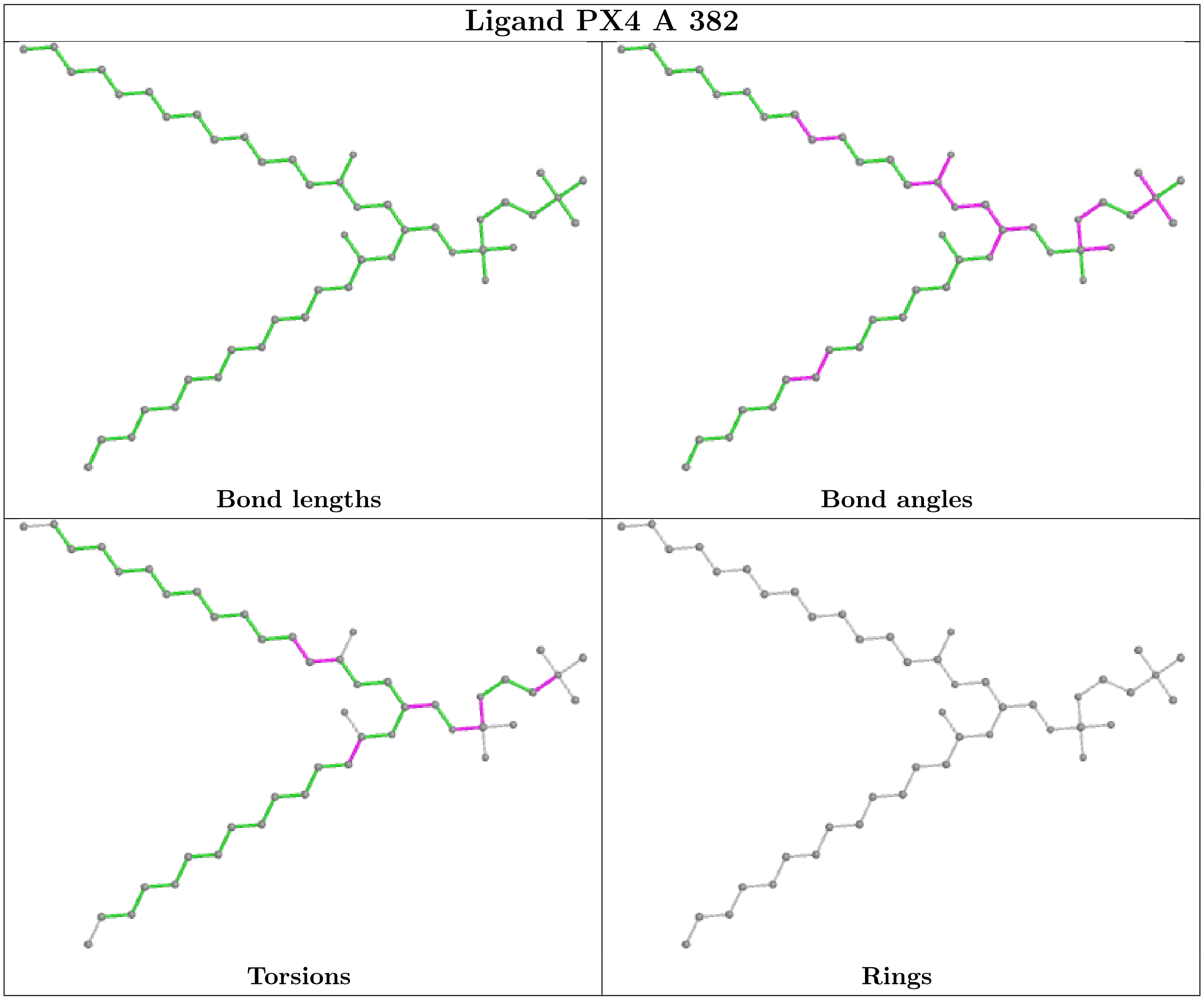
Bond angles

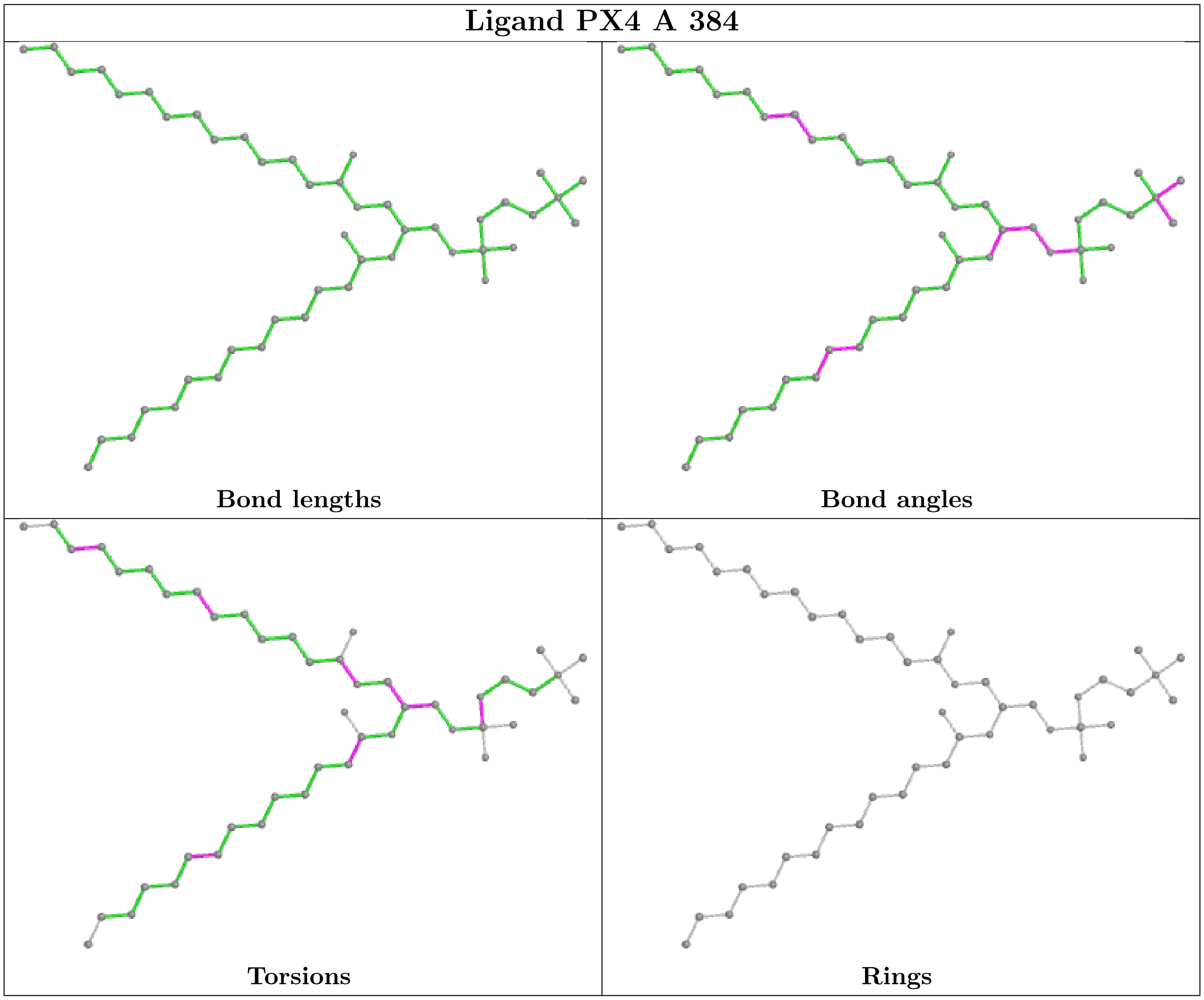


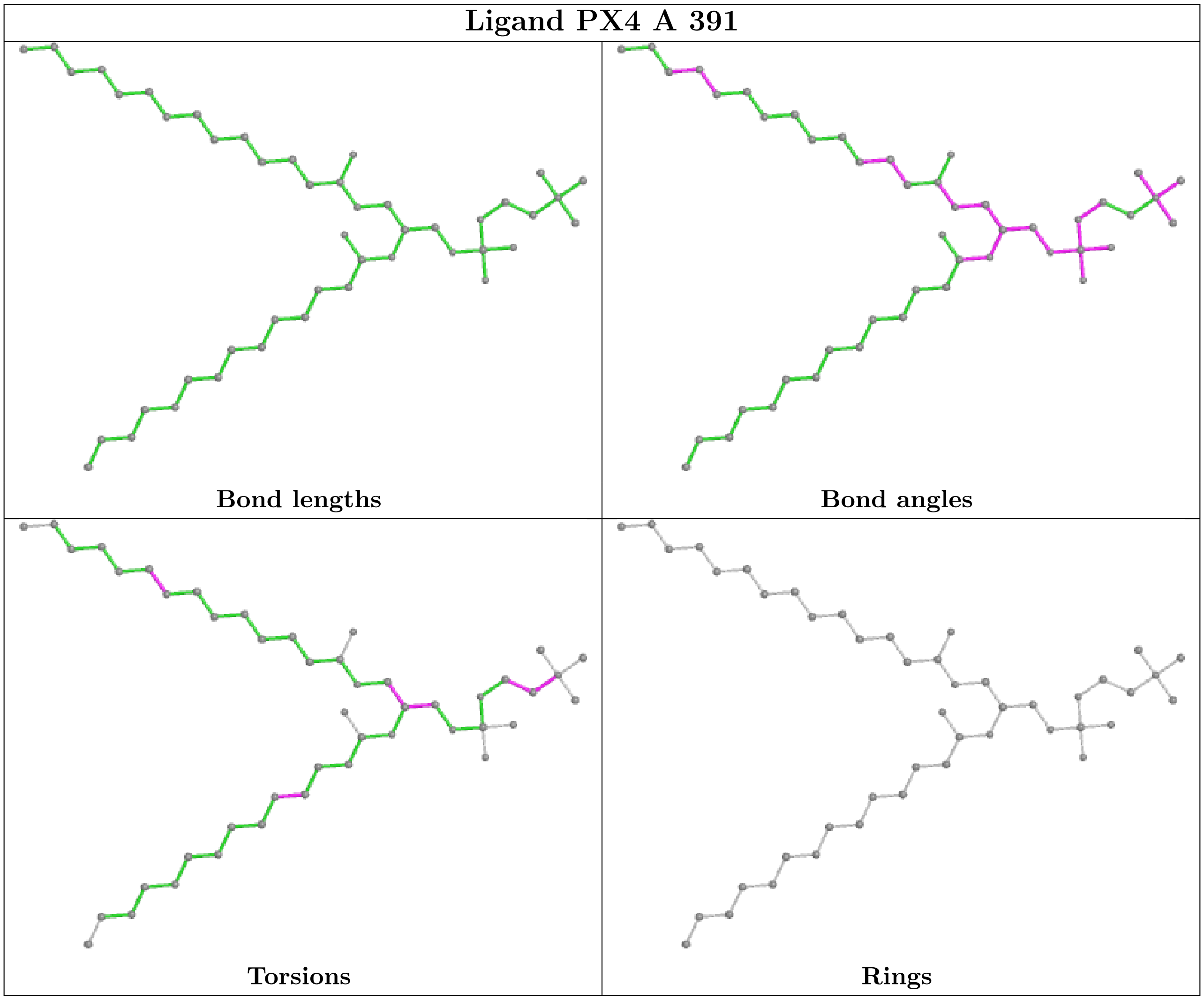
Torsions



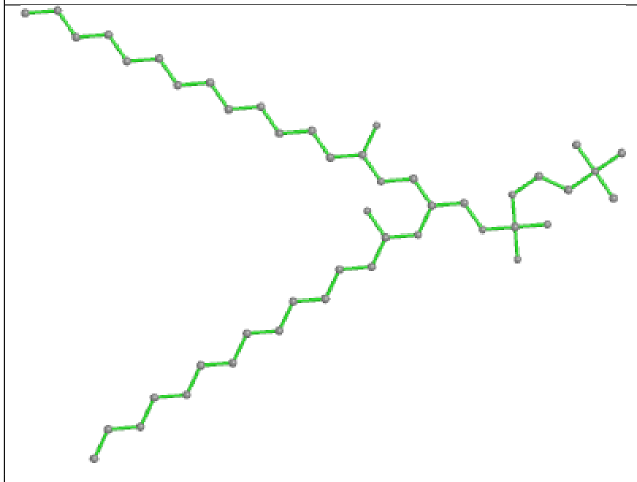
Rings


Ligand PX4 A 382
Bond lengths
Bond angles
Torsions
Rings

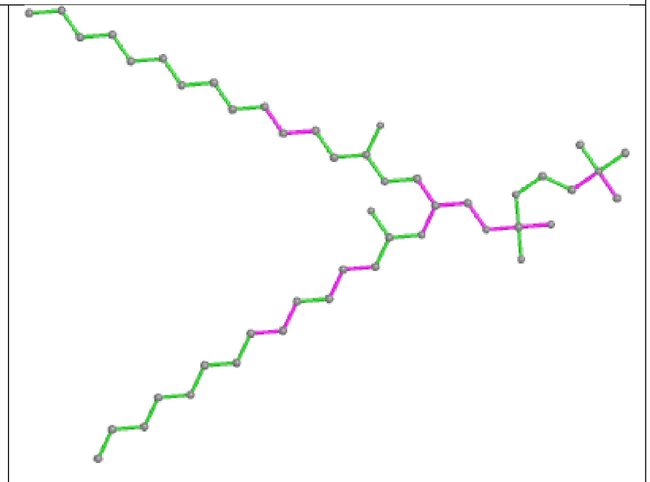

Ligand PX4 A 384
Bond lengths
Bond angles
Torsions
Rings


Ligand PX4 A 391
Bond lengths
Bond angles
Torsions
Rings

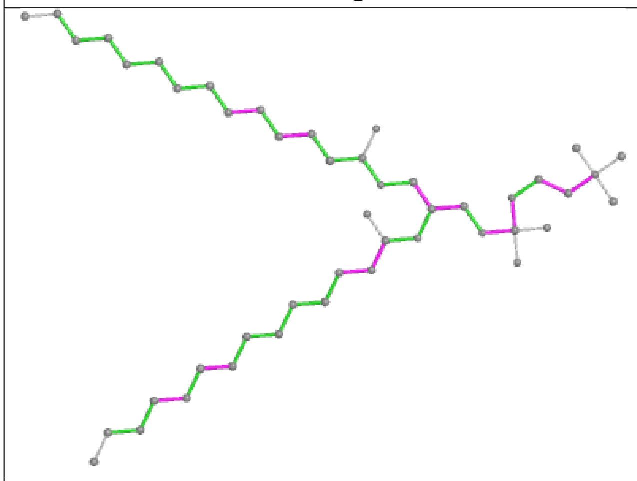
Ligand PX4 A 345



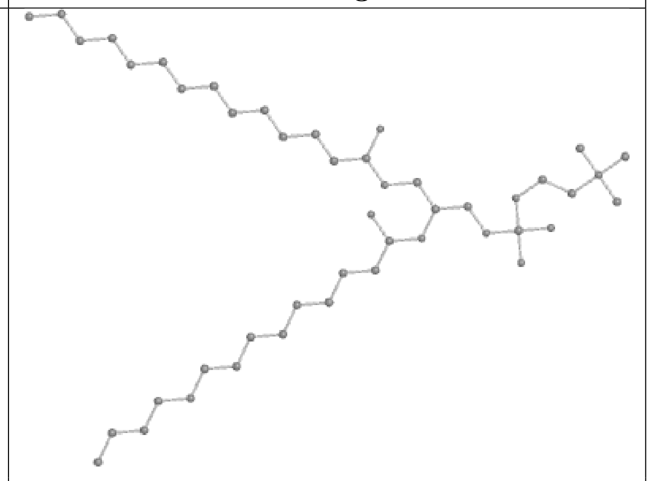
Bond lengths



Bond angles

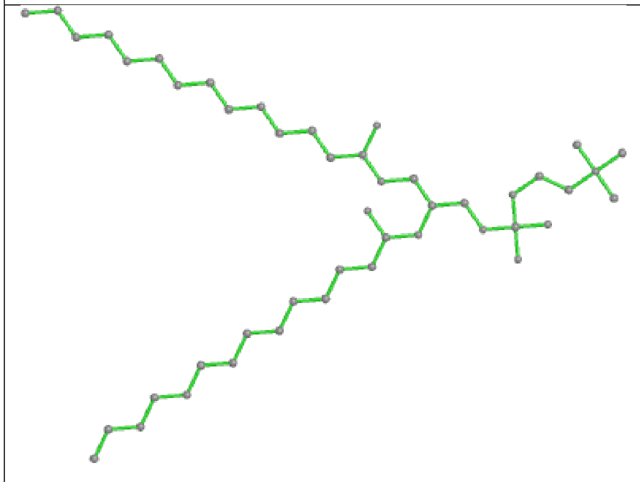


Torsions

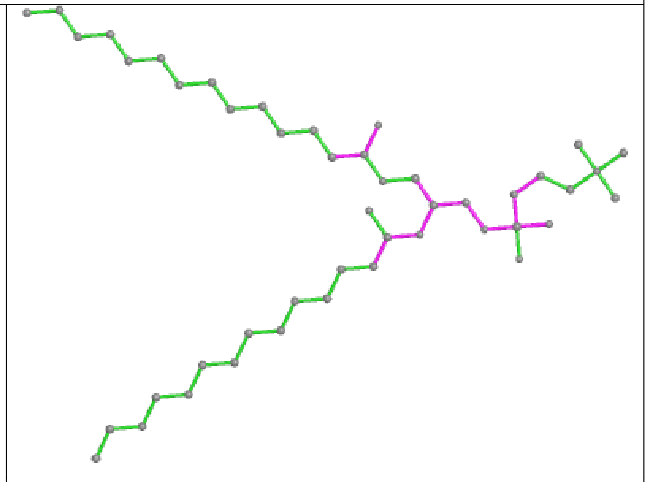


Rings

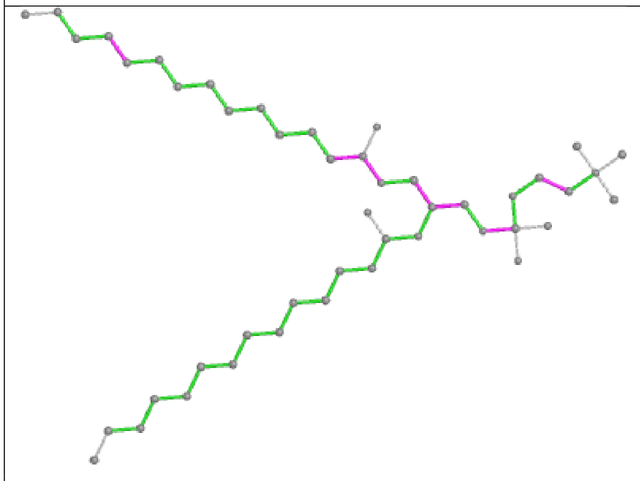
Ligand PX4 A 419



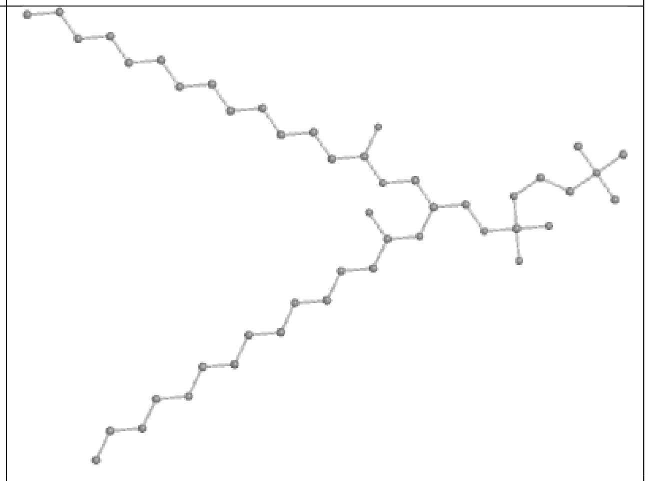
Bond lengths



Bond angles

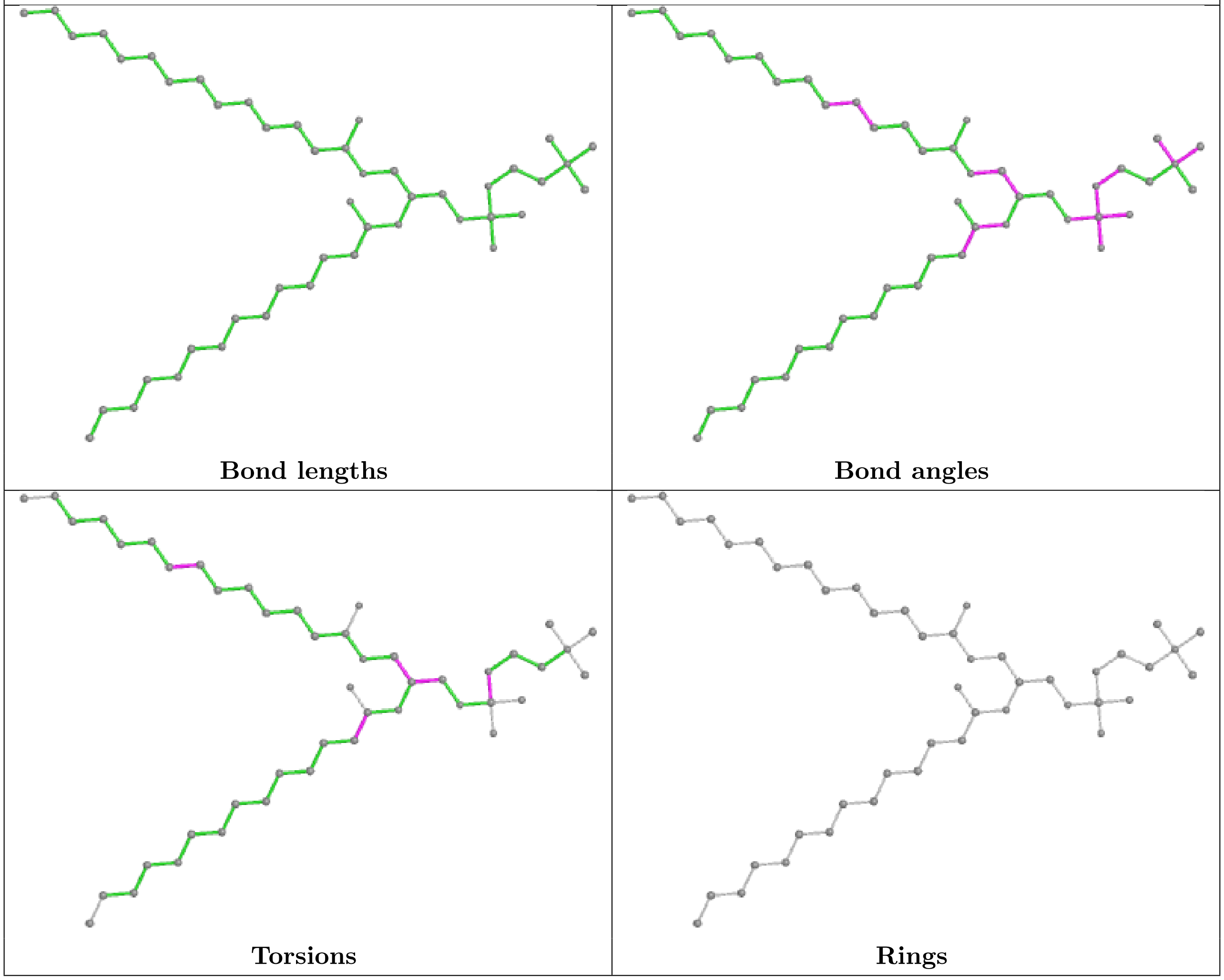


Torsions

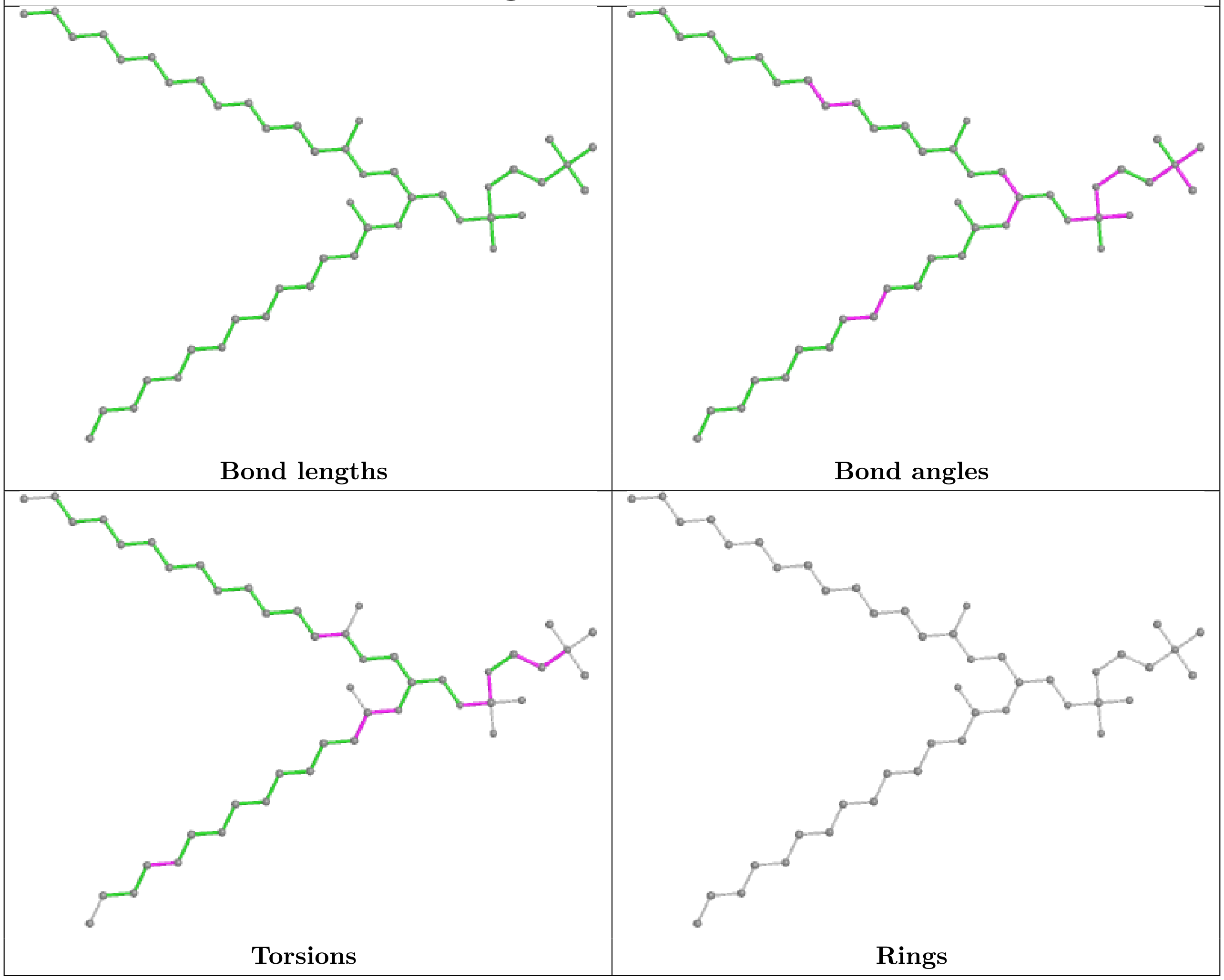


Rings

Ligand PX4 A 393



Ligand PX4 A 398



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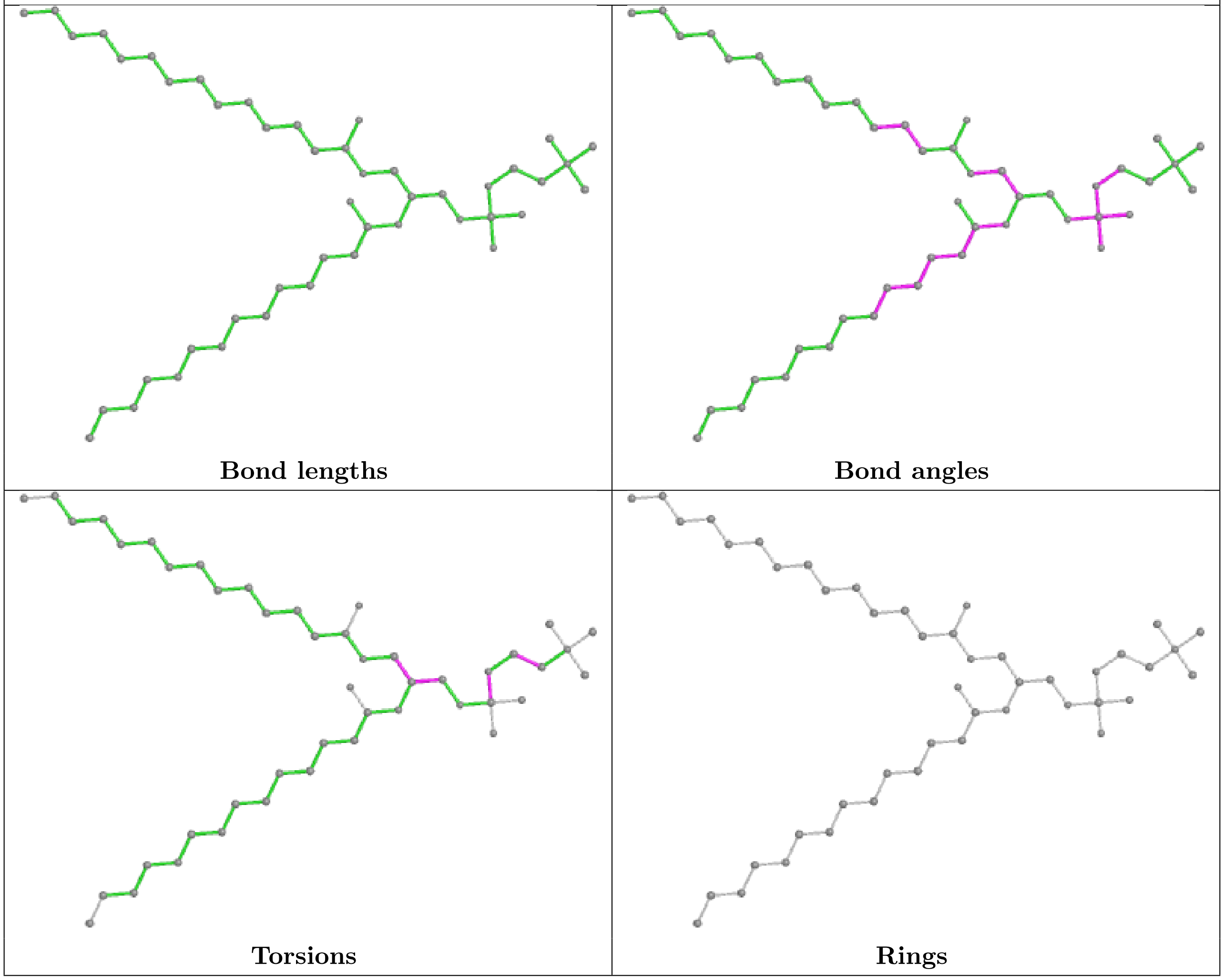
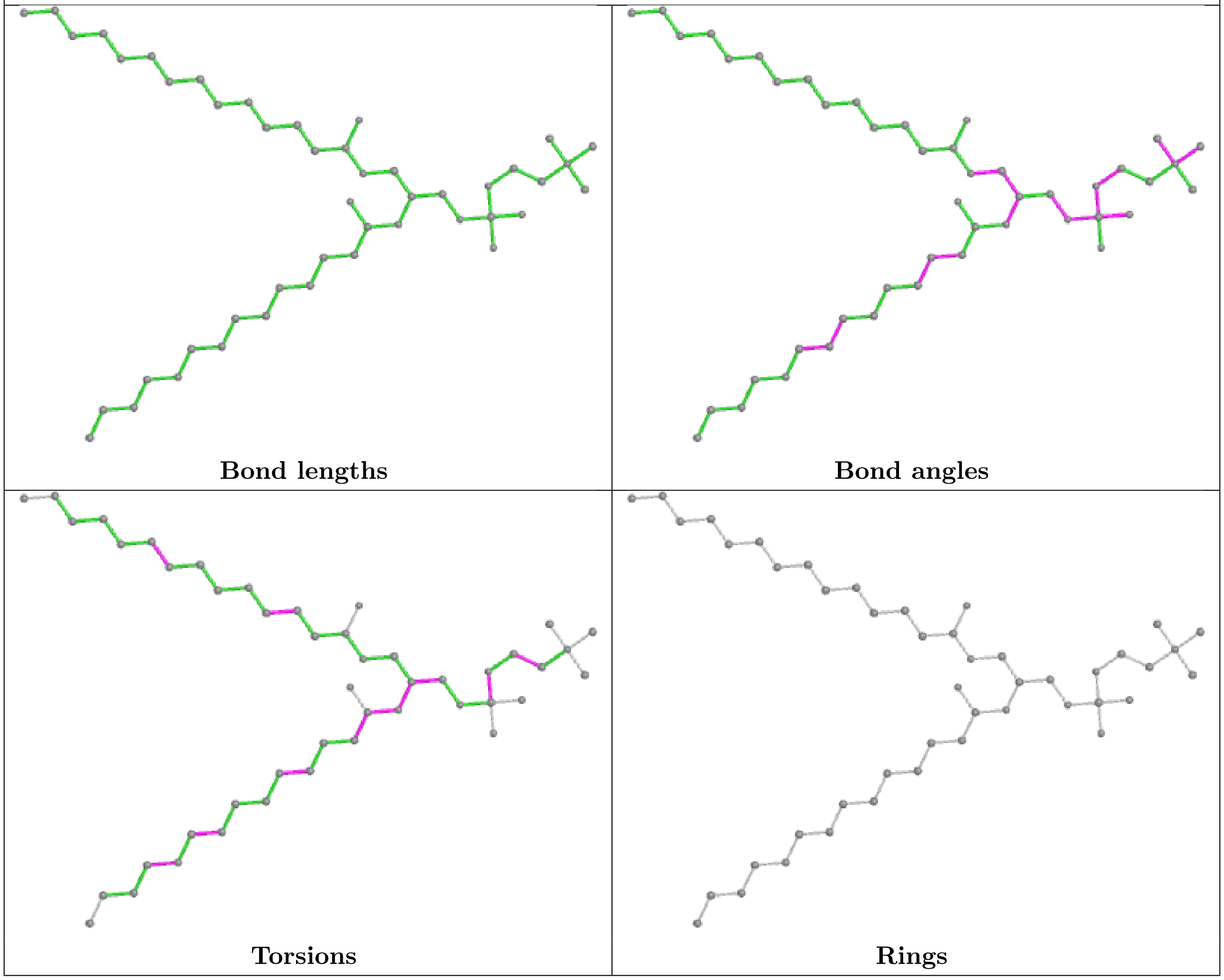
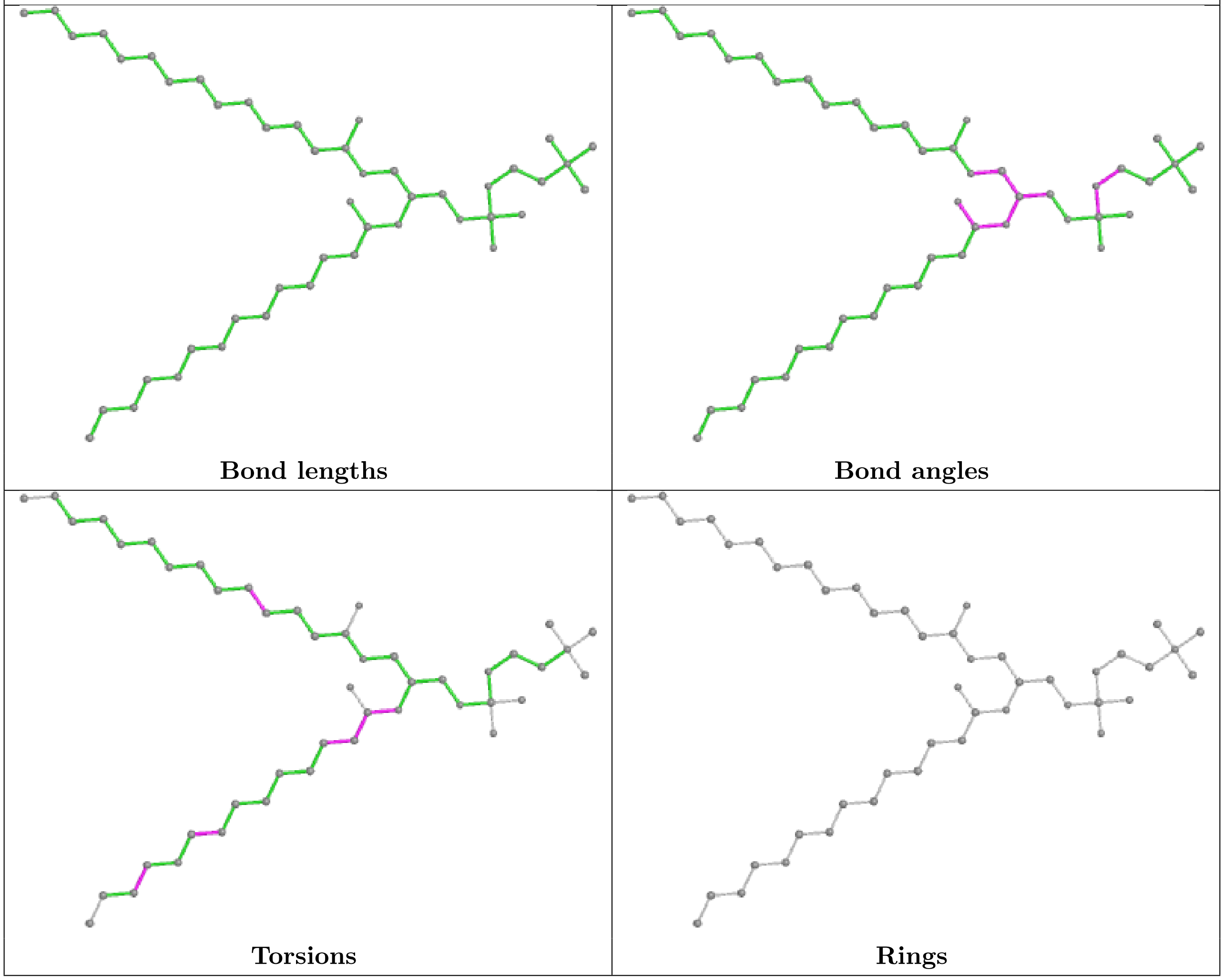


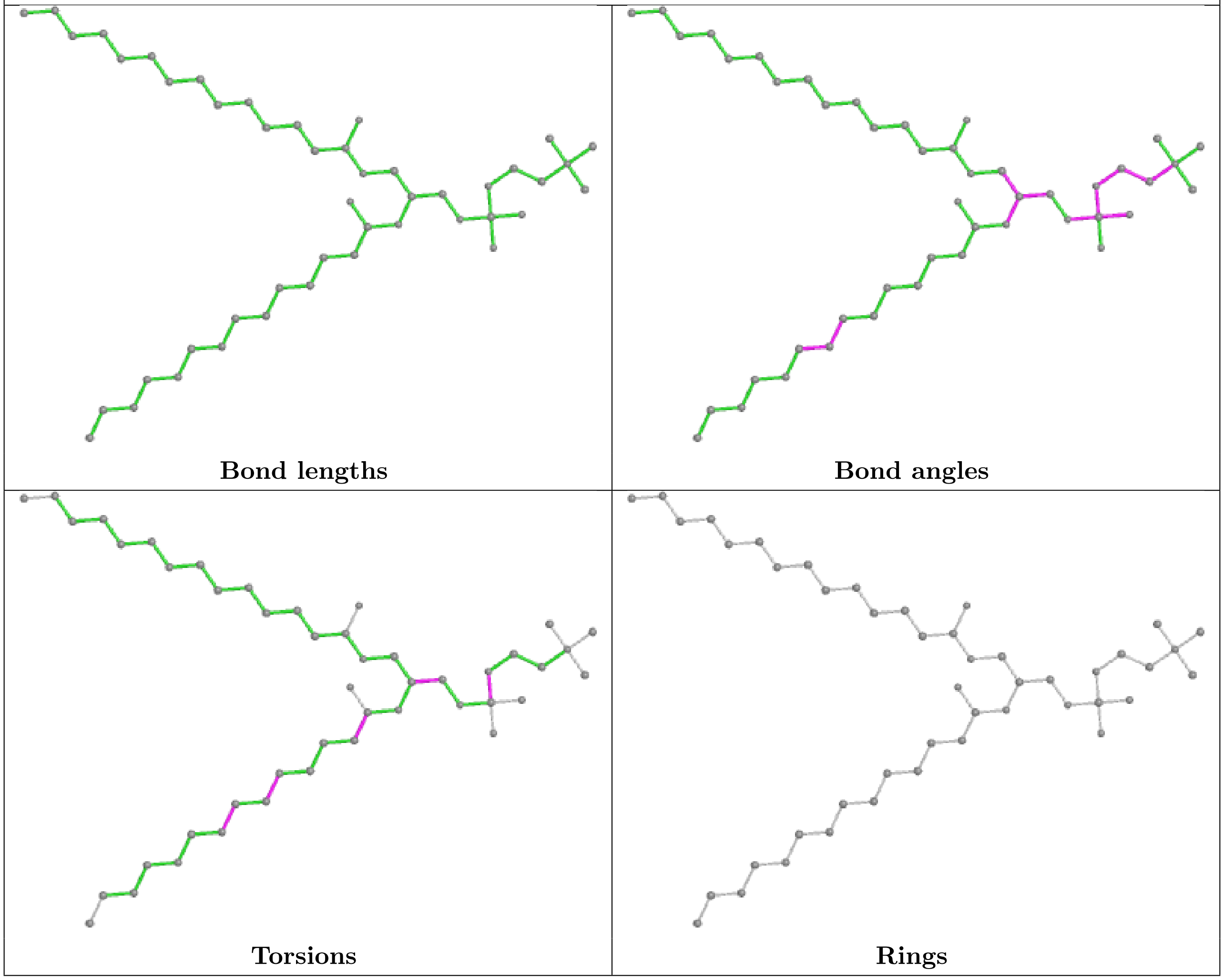
Ligand PX4 A 311

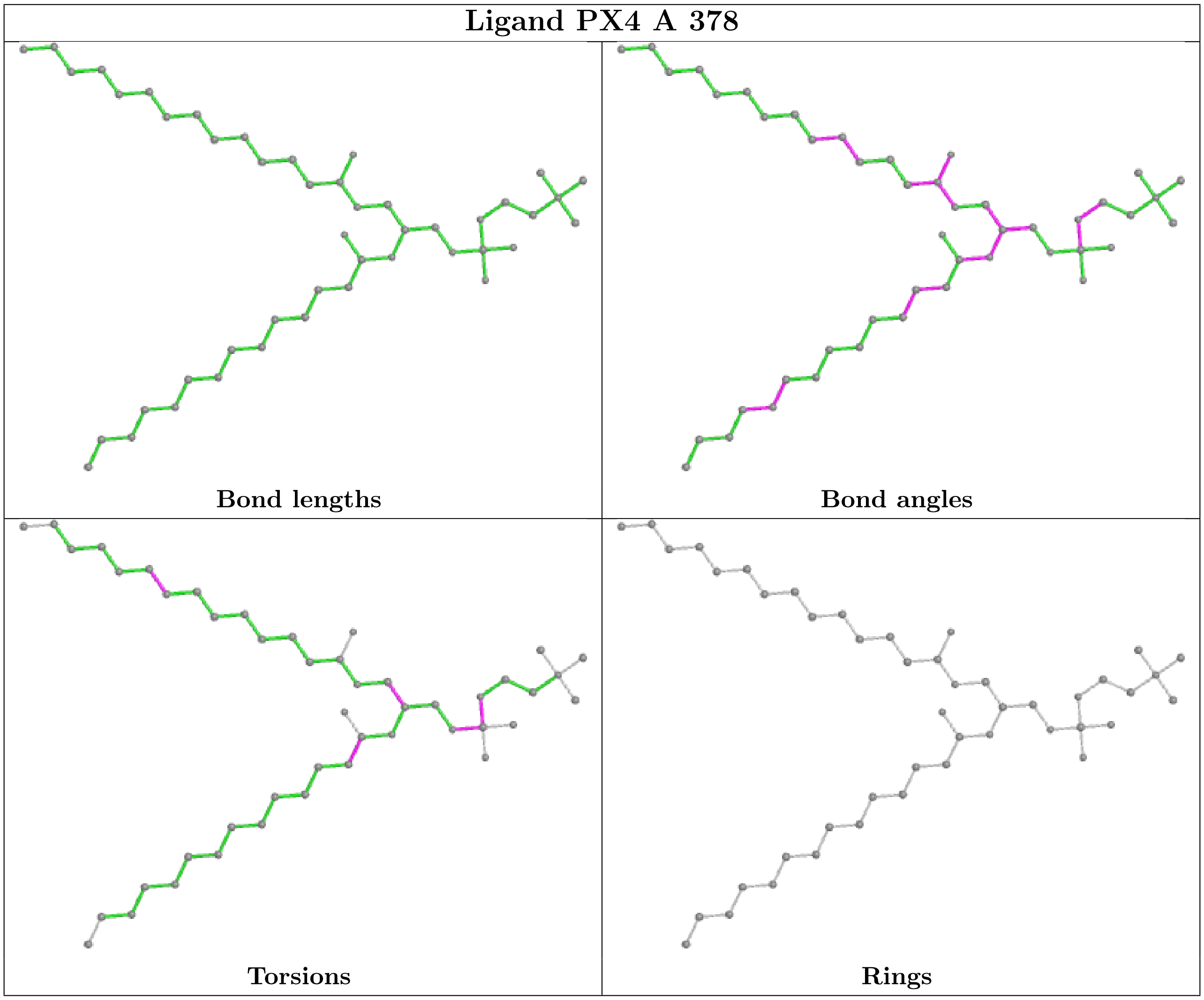


Ligand PX4 A 331

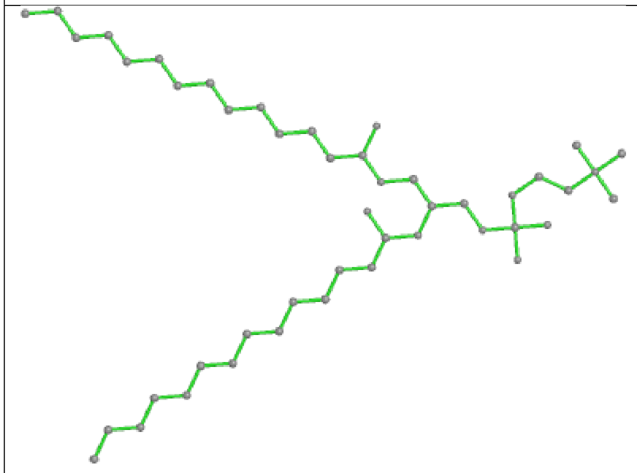


Ligand PX4 A 406

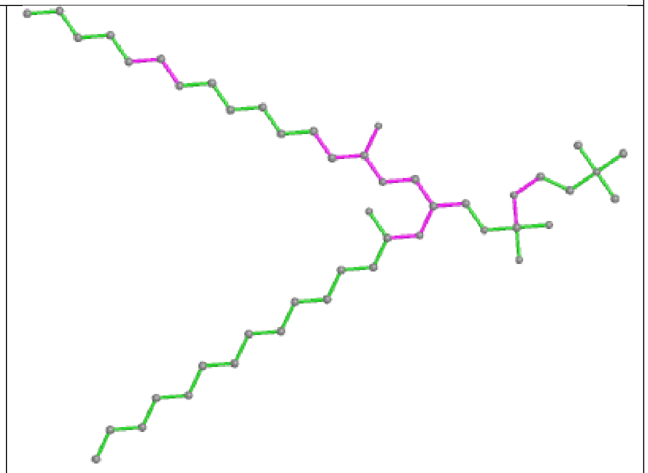



Ligand PX4 A 378
Bond lengths
Bond angles
Torsions
Rings

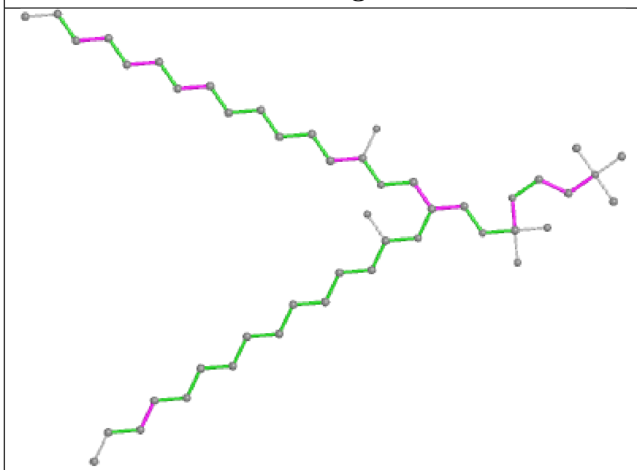
Ligand PX4 A 401



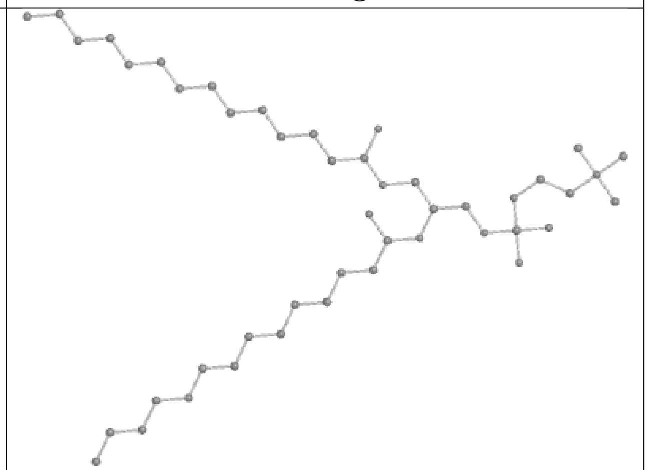
Bond lengths



Bond angles

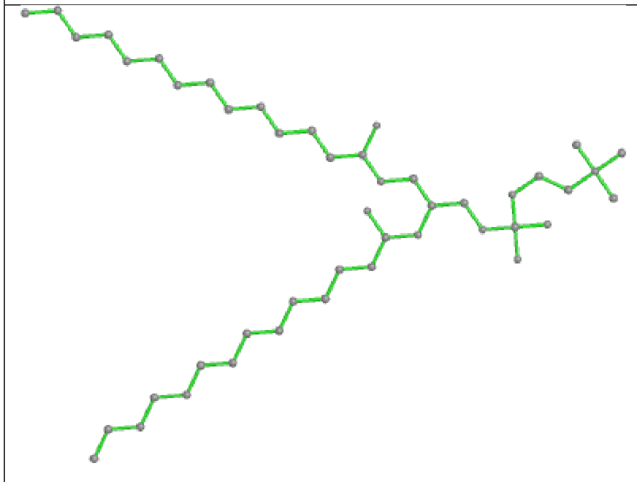


Torsions

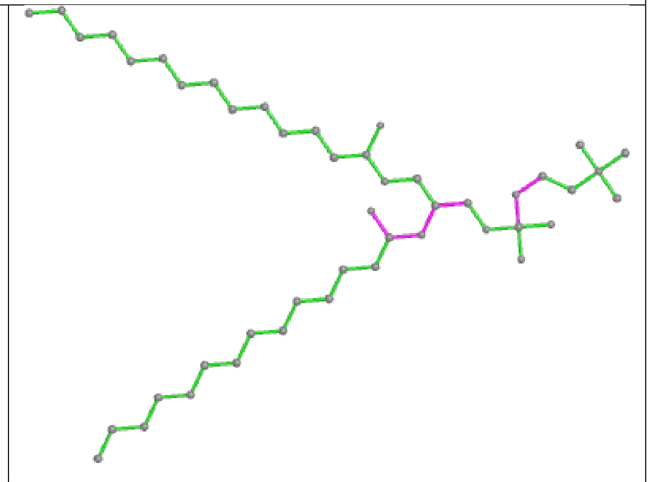


Rings

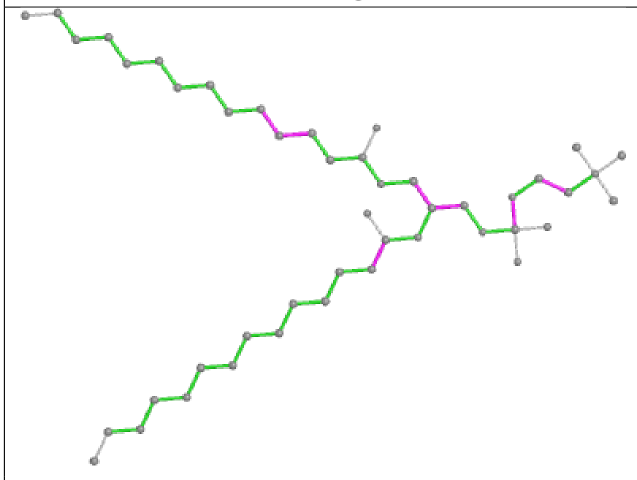
Ligand PX4 A 365



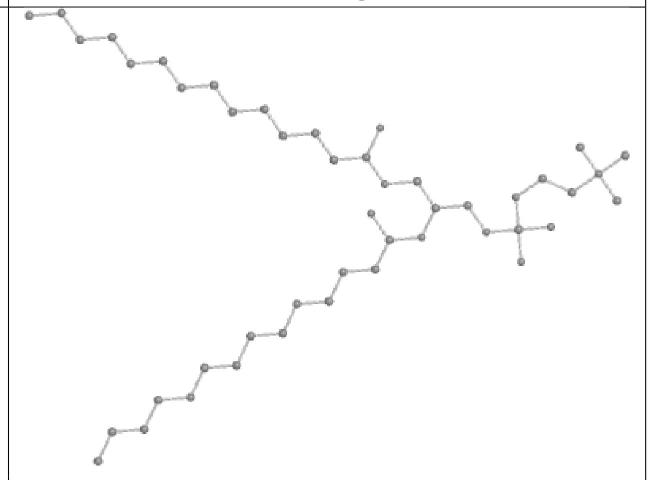
Bond lengths



Bond angles

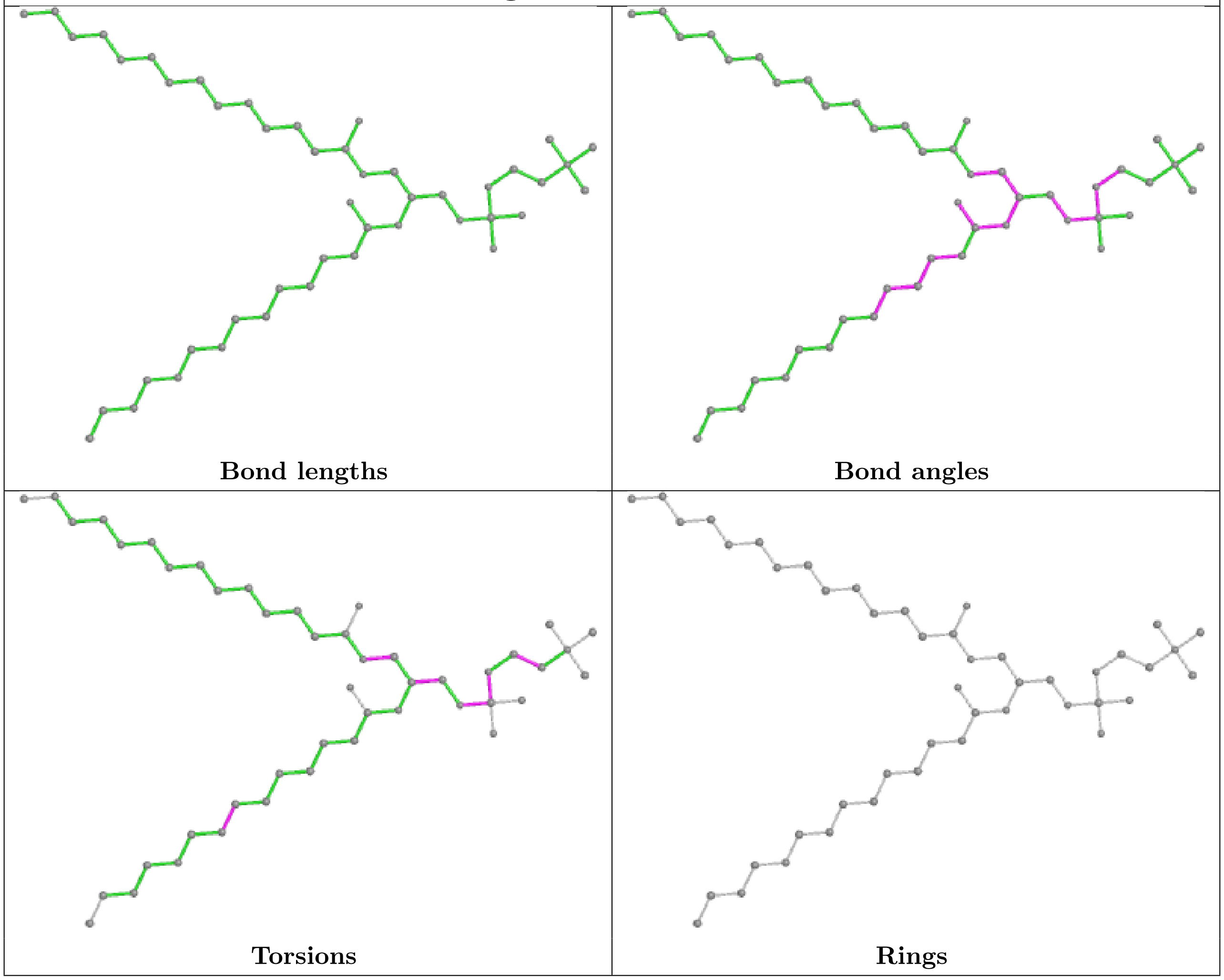


Torsions

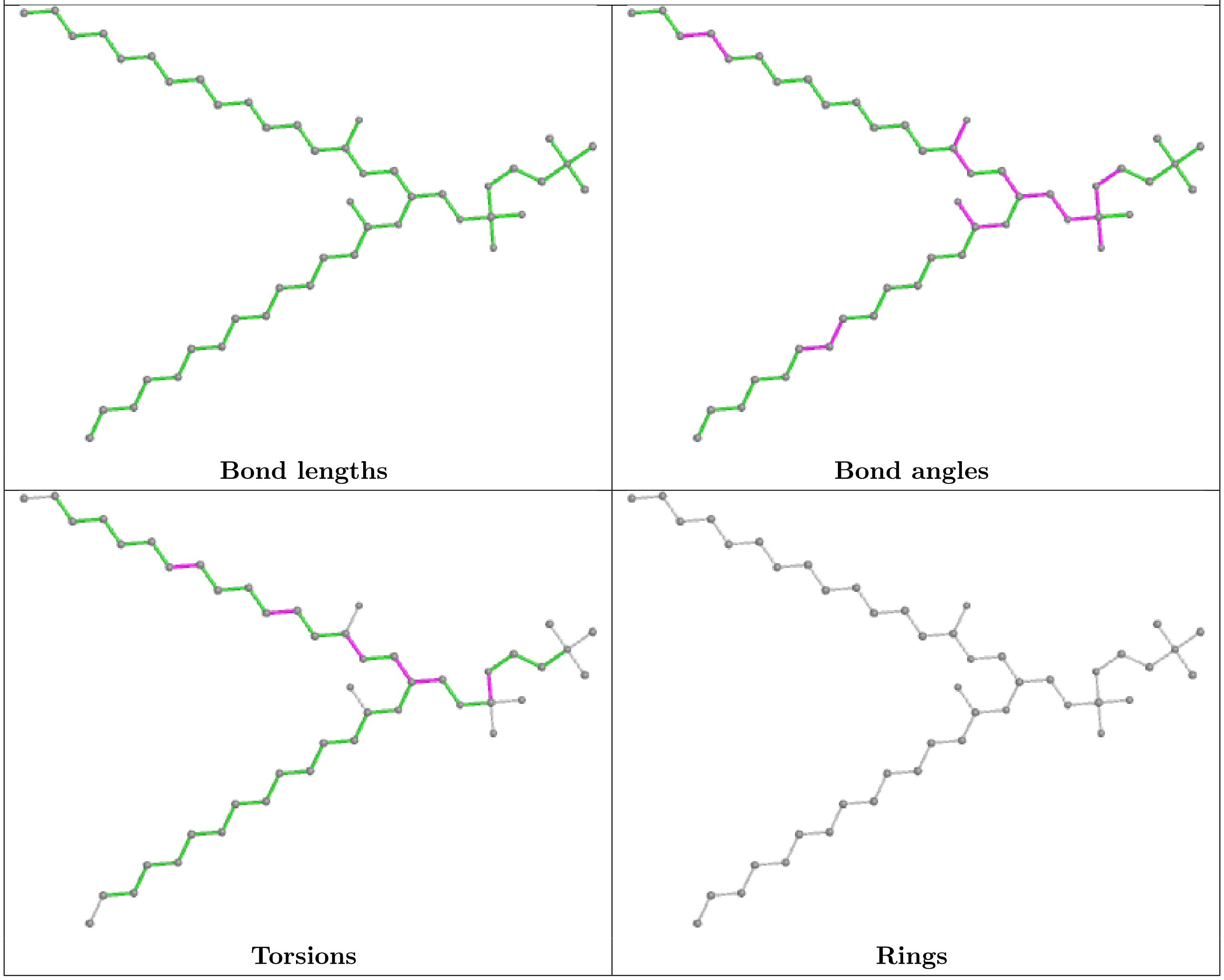


Rings

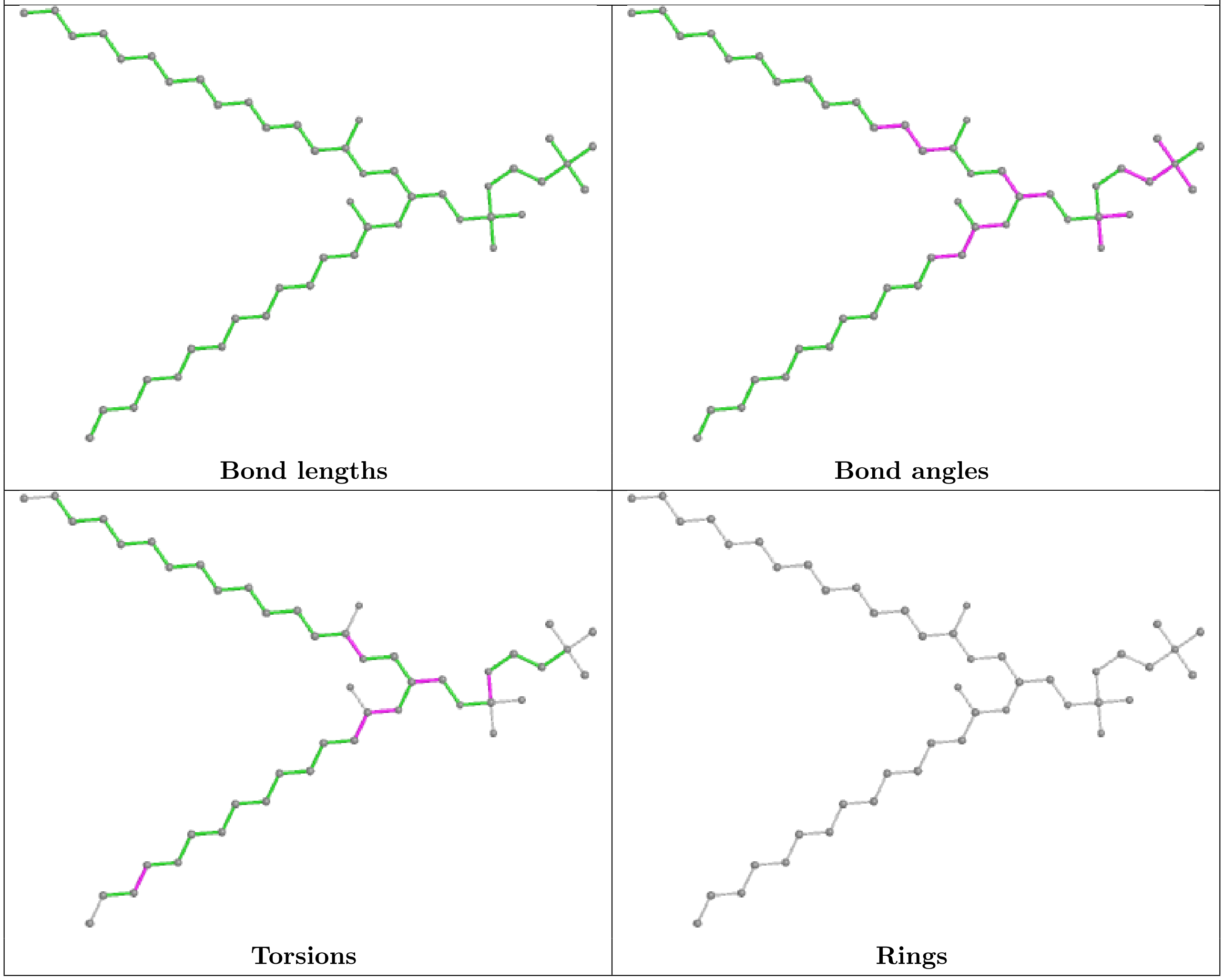
Ligand PX4 A 346



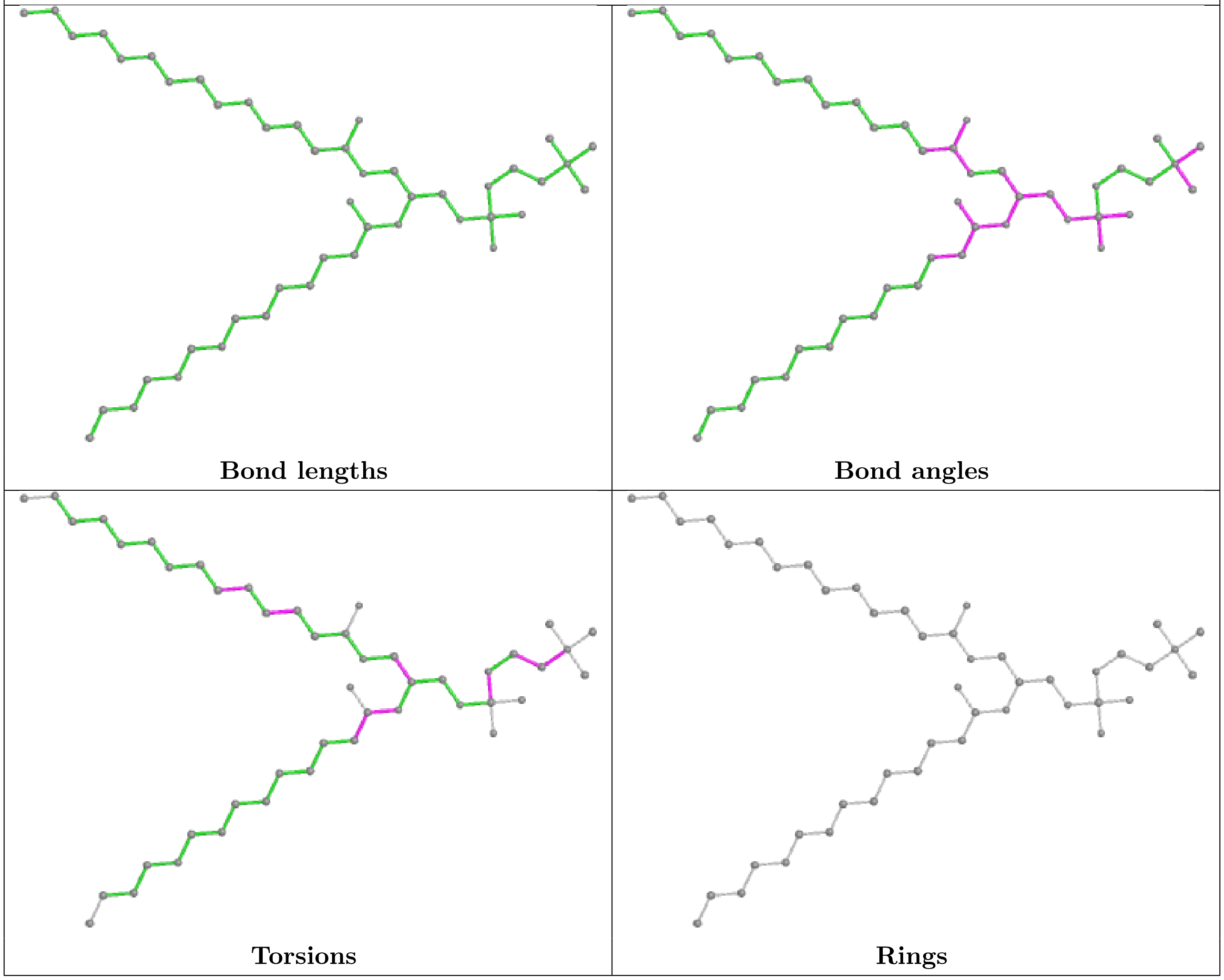
Ligand PX4 A 373



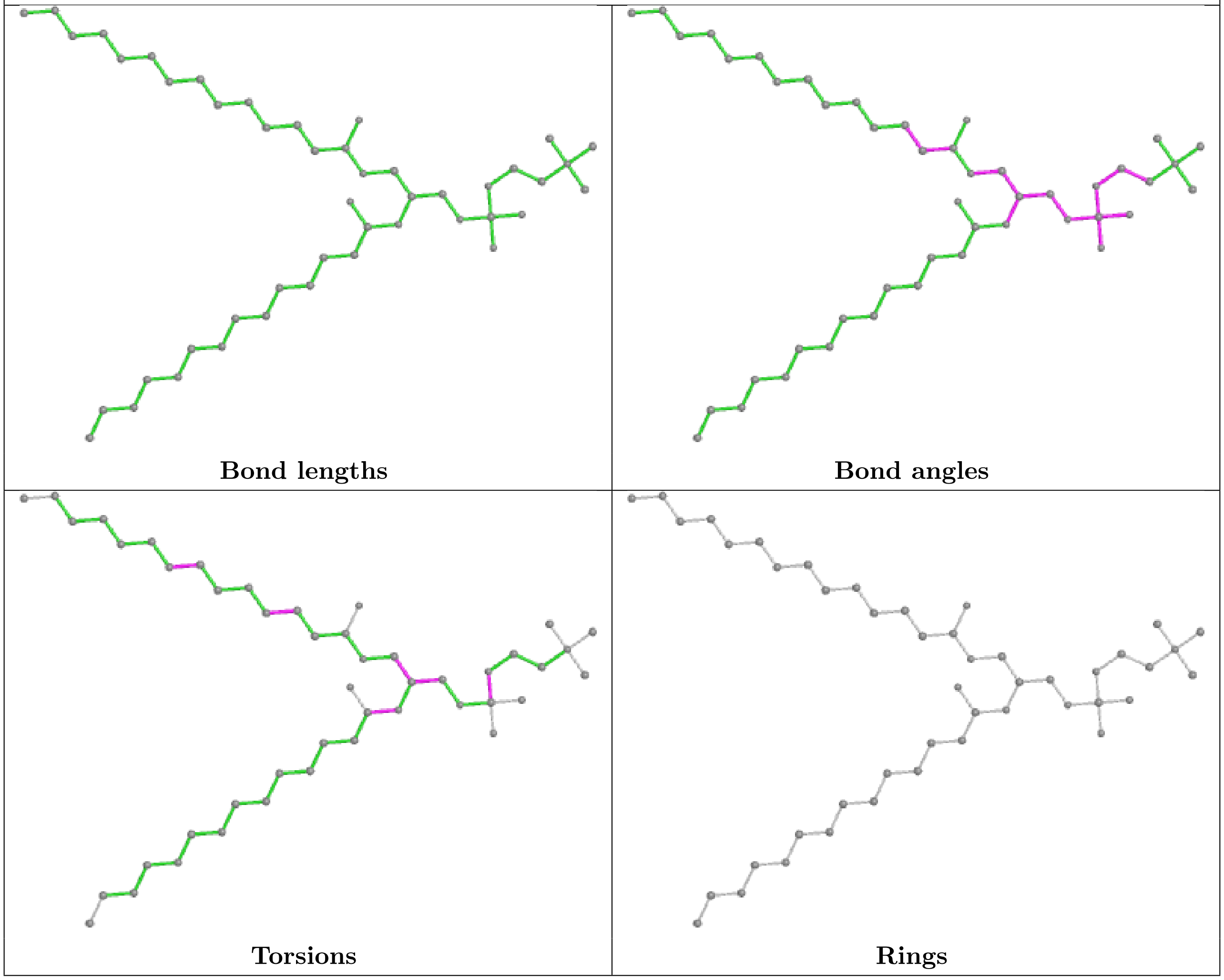
Ligand PX4 A 410



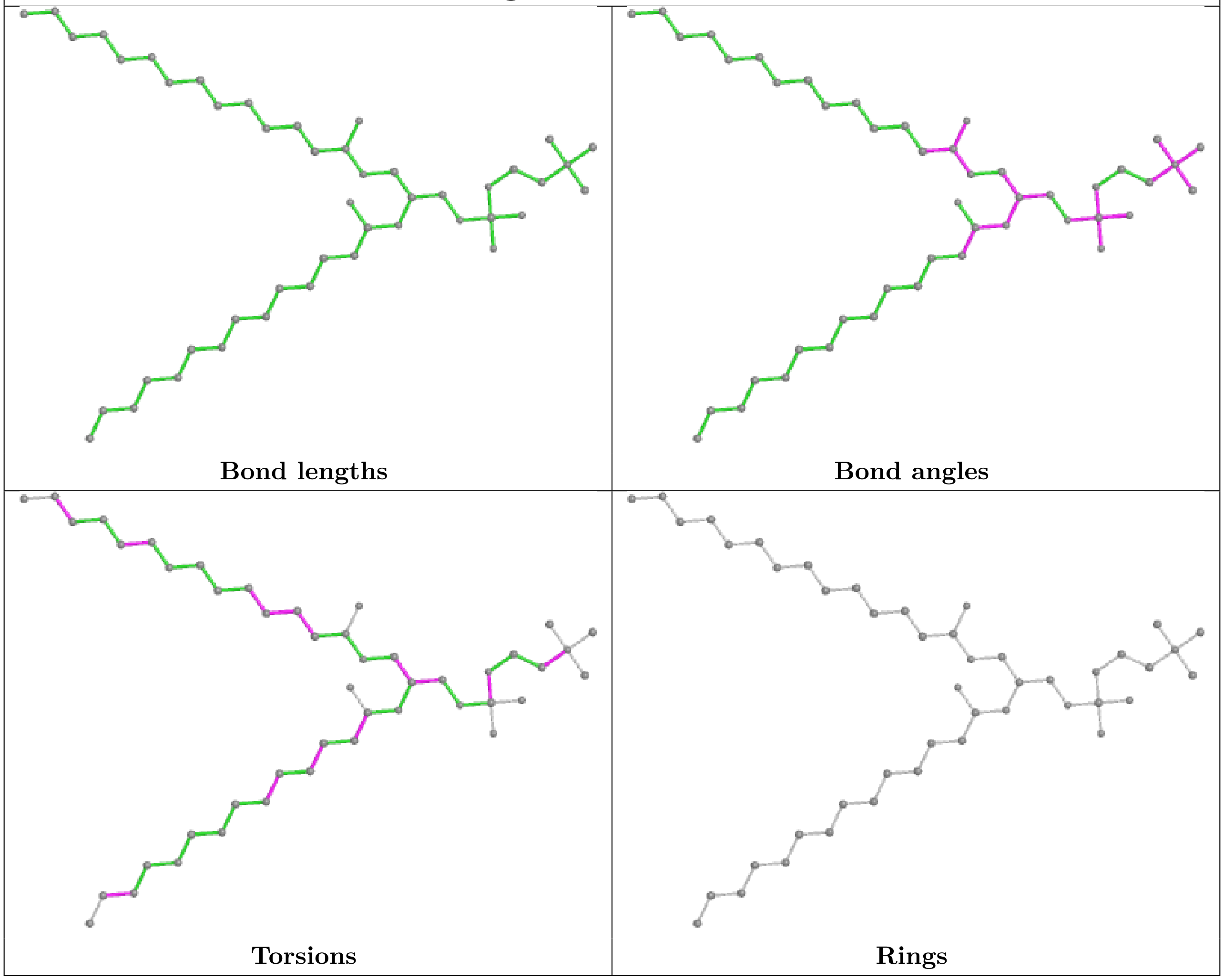
Ligand PX4 A 376



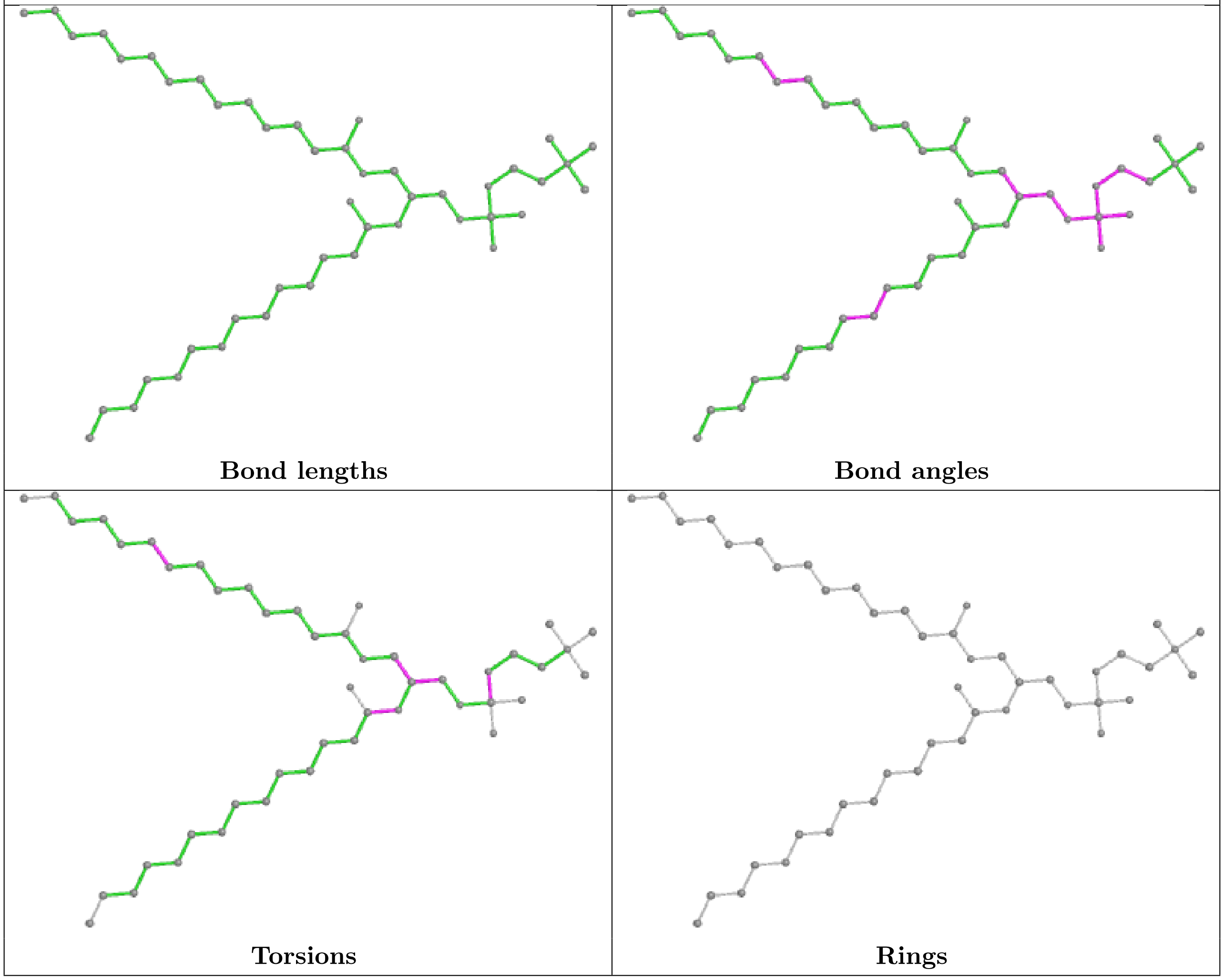
Ligand PX4 A 377



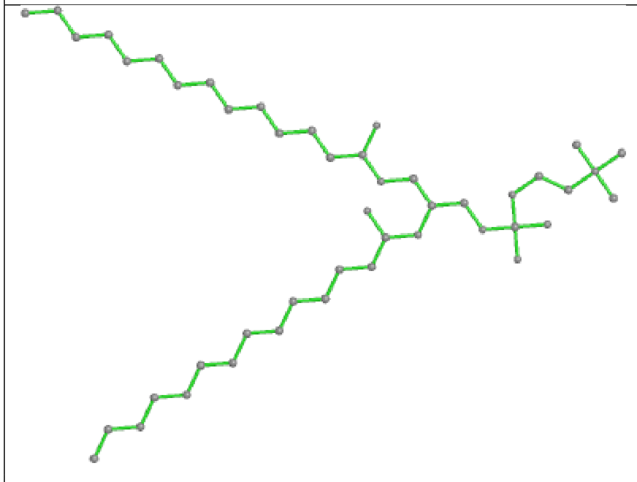
Ligand PX4 A 413



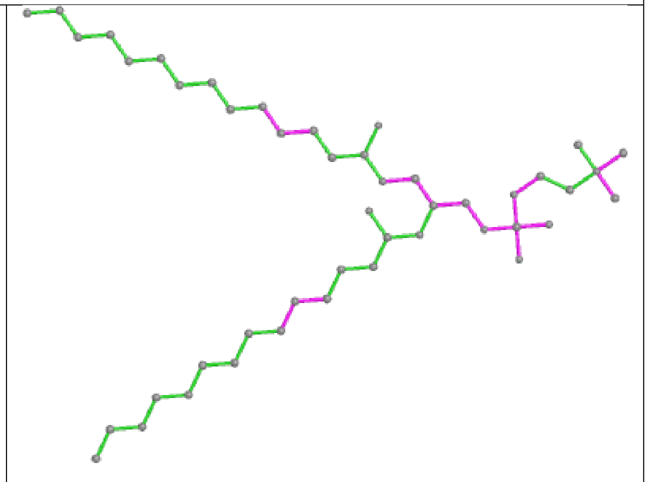
Ligand PX4 A 322



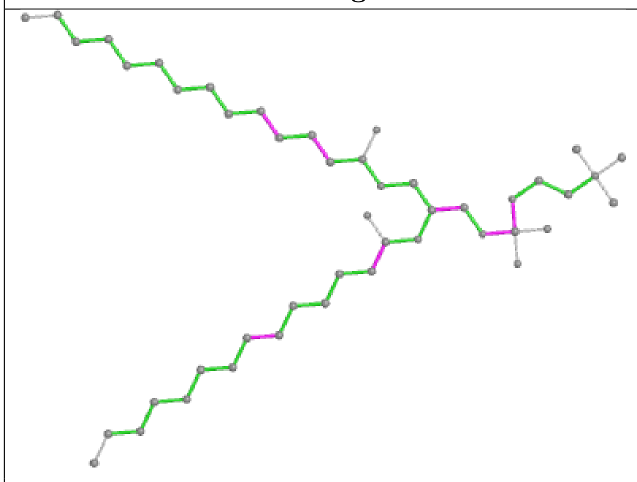
Ligand PX4 A 426



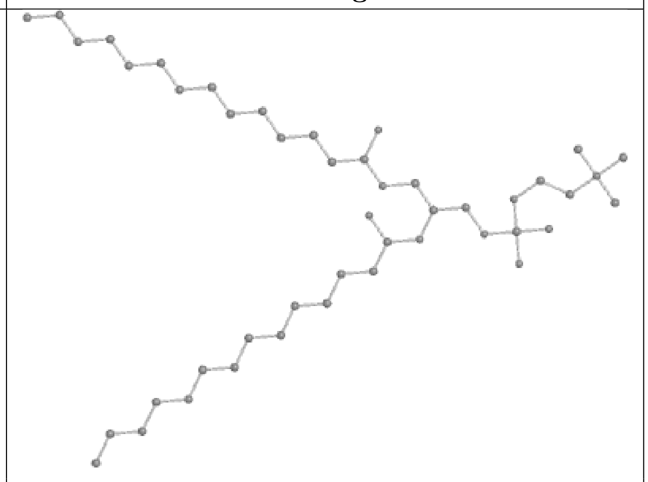
Bond lengths



Bond angles

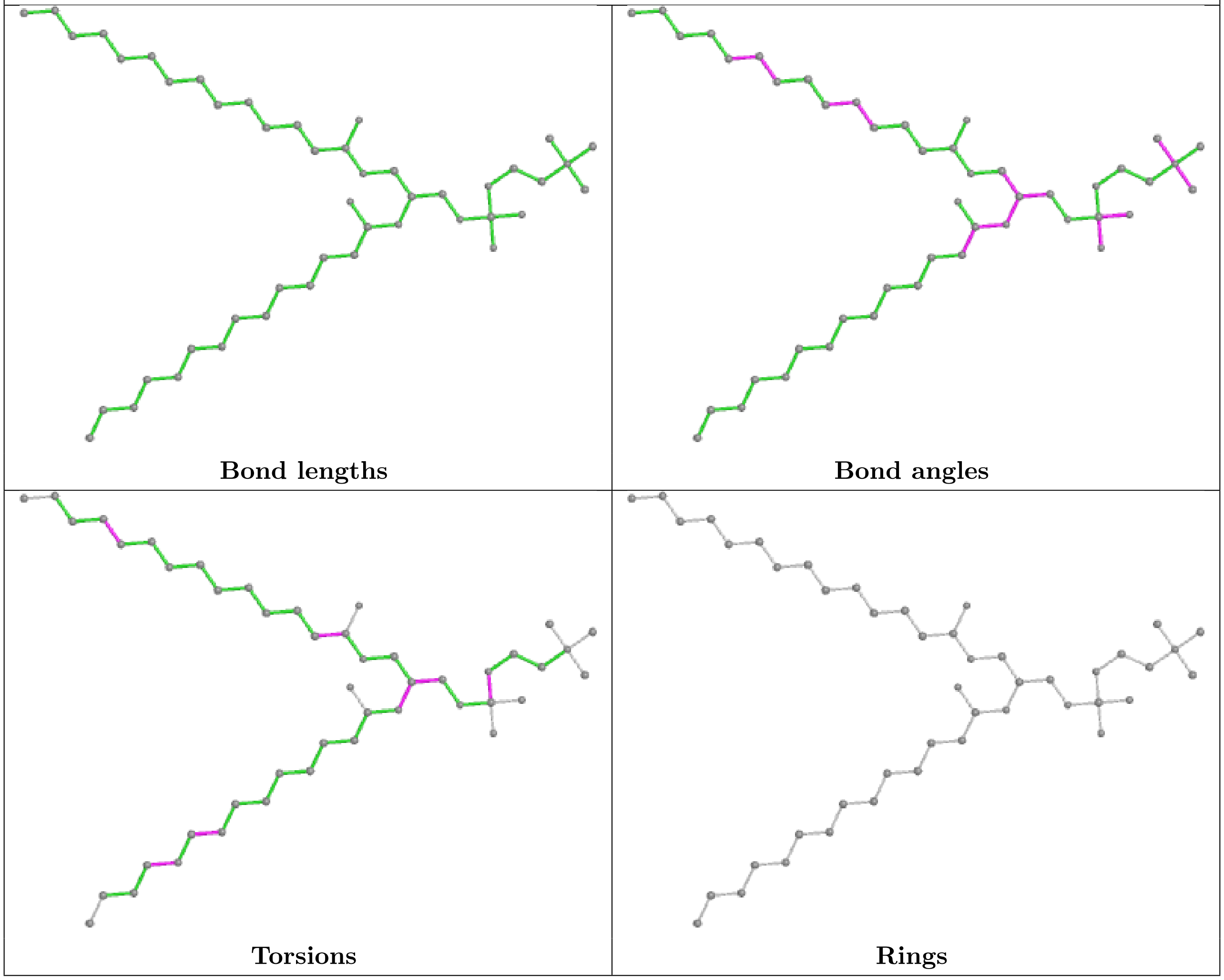


Torsions

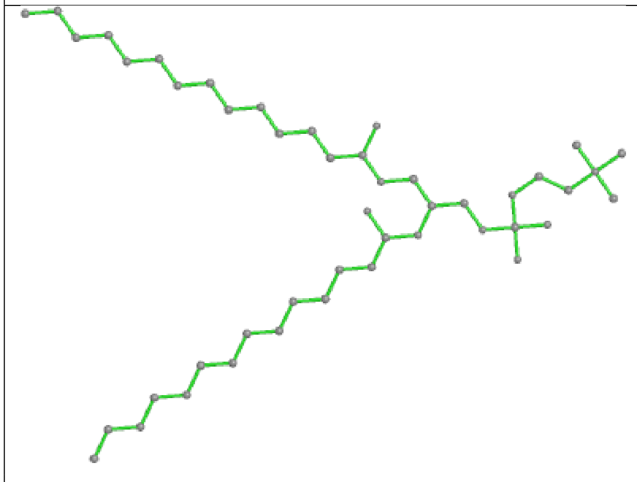


Rings

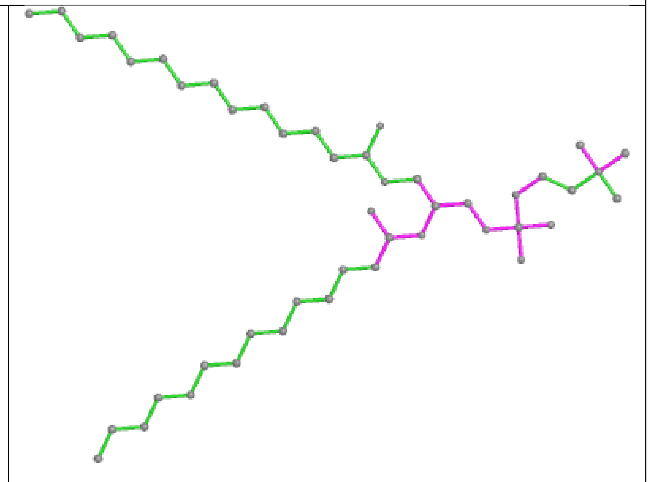
Ligand PX4 A 361



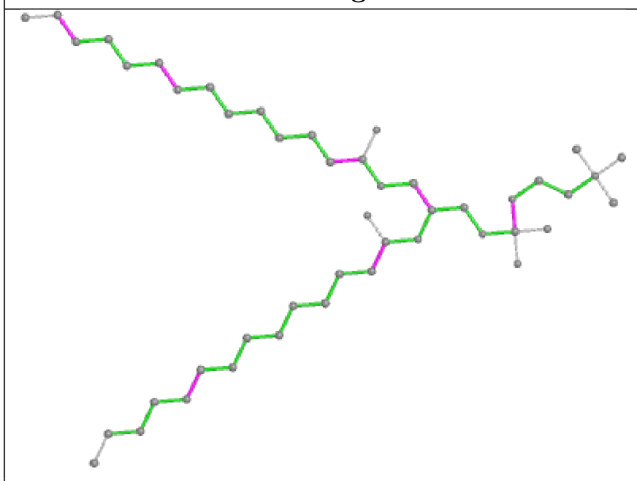
Ligand PX4 A 417



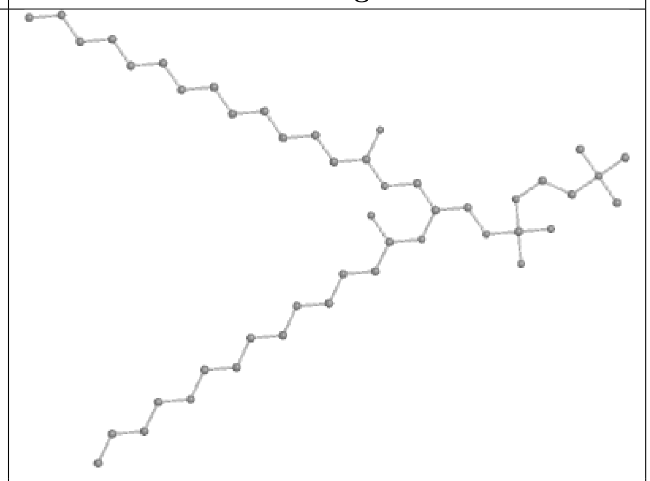
Bond lengths



Bond angles

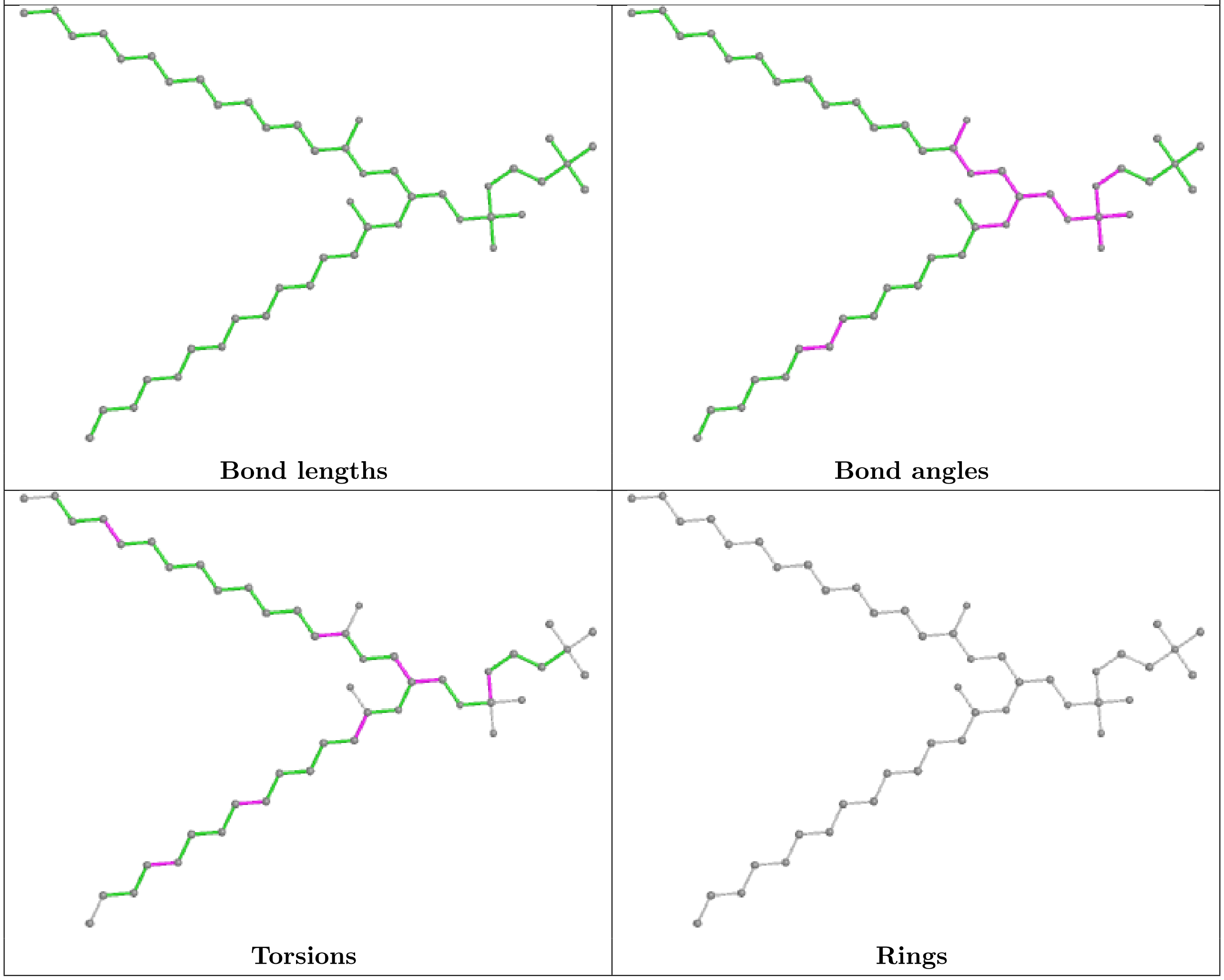


Torsions

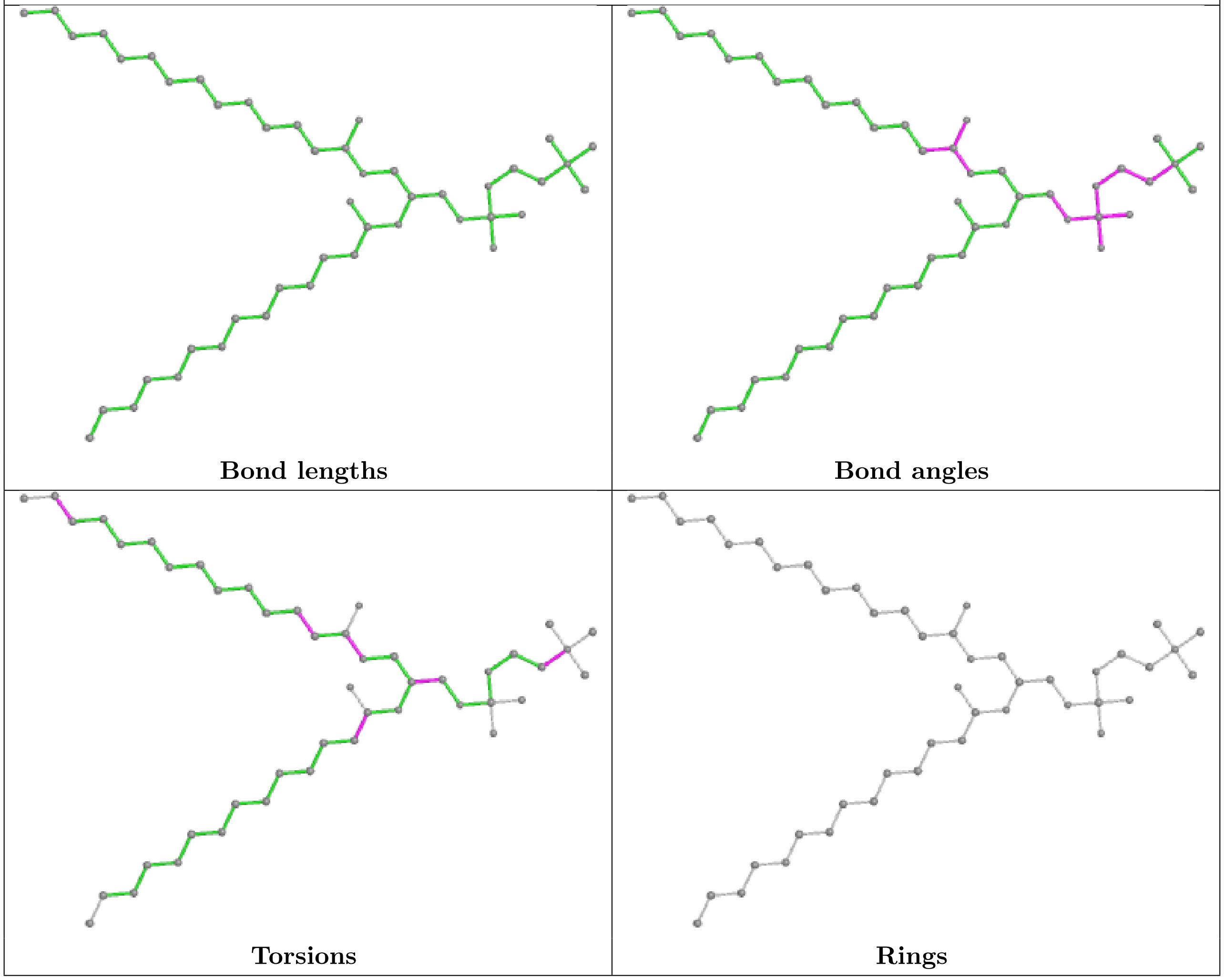


Rings

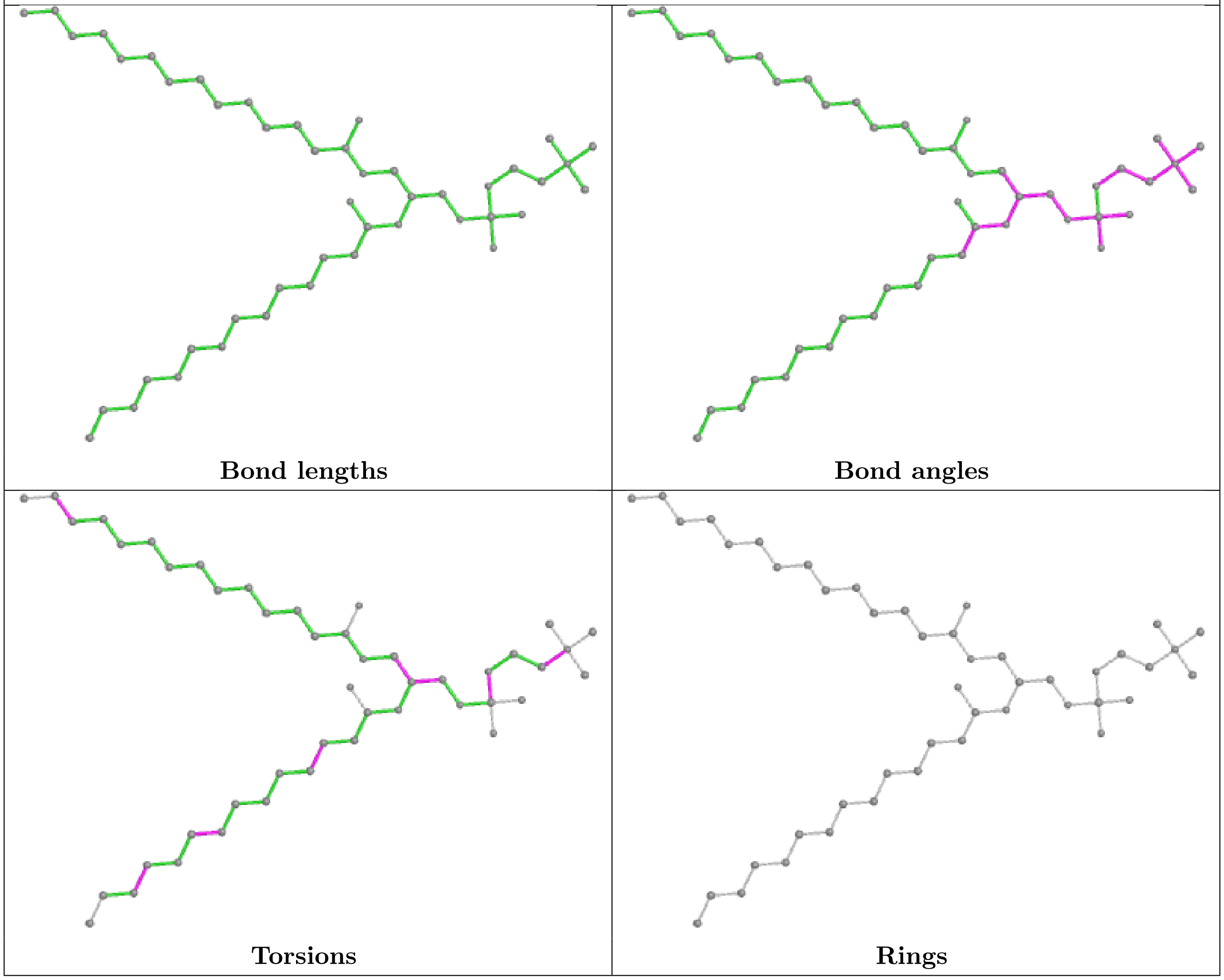
Ligand PX4 A 422



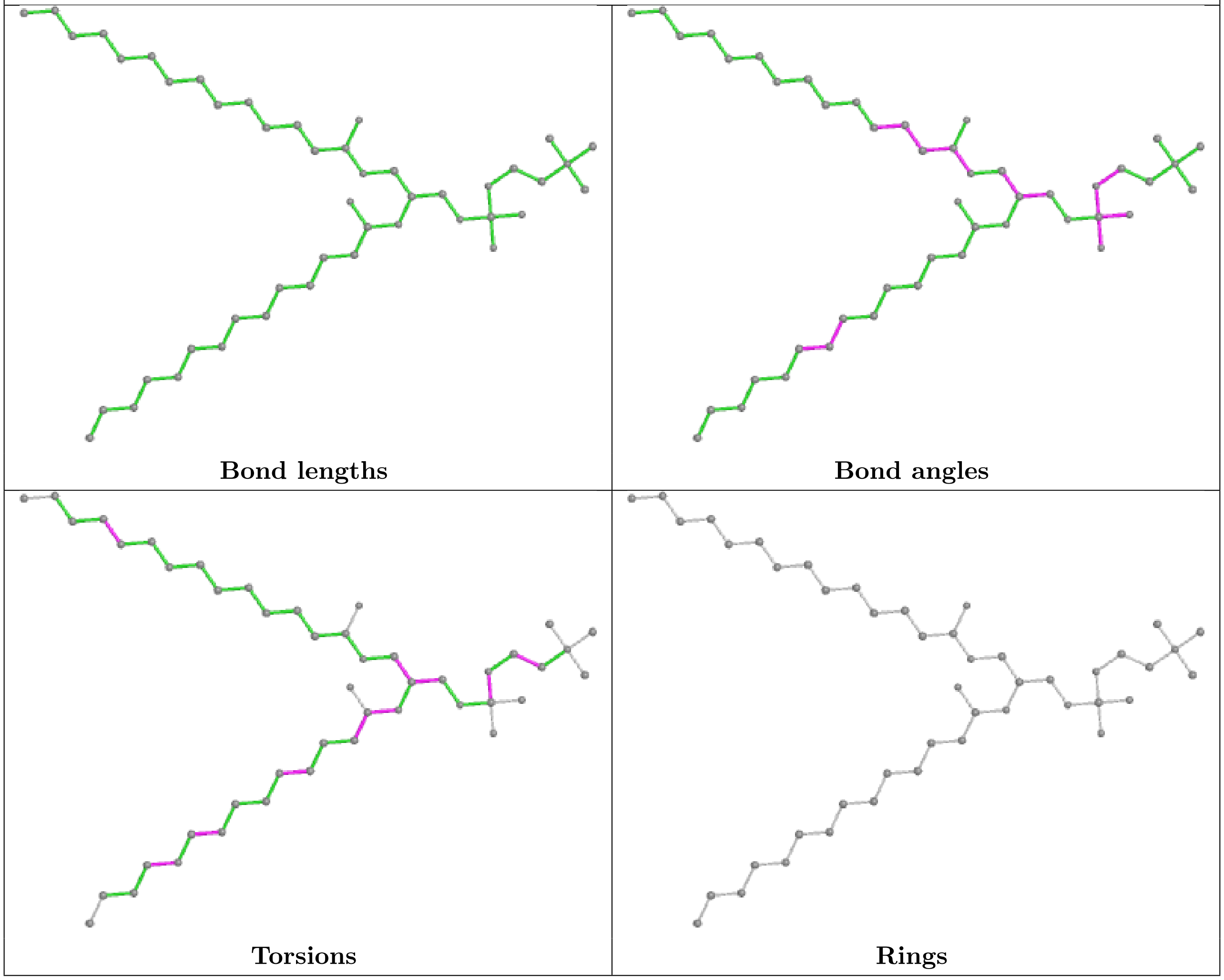
Ligand PX4 A 338



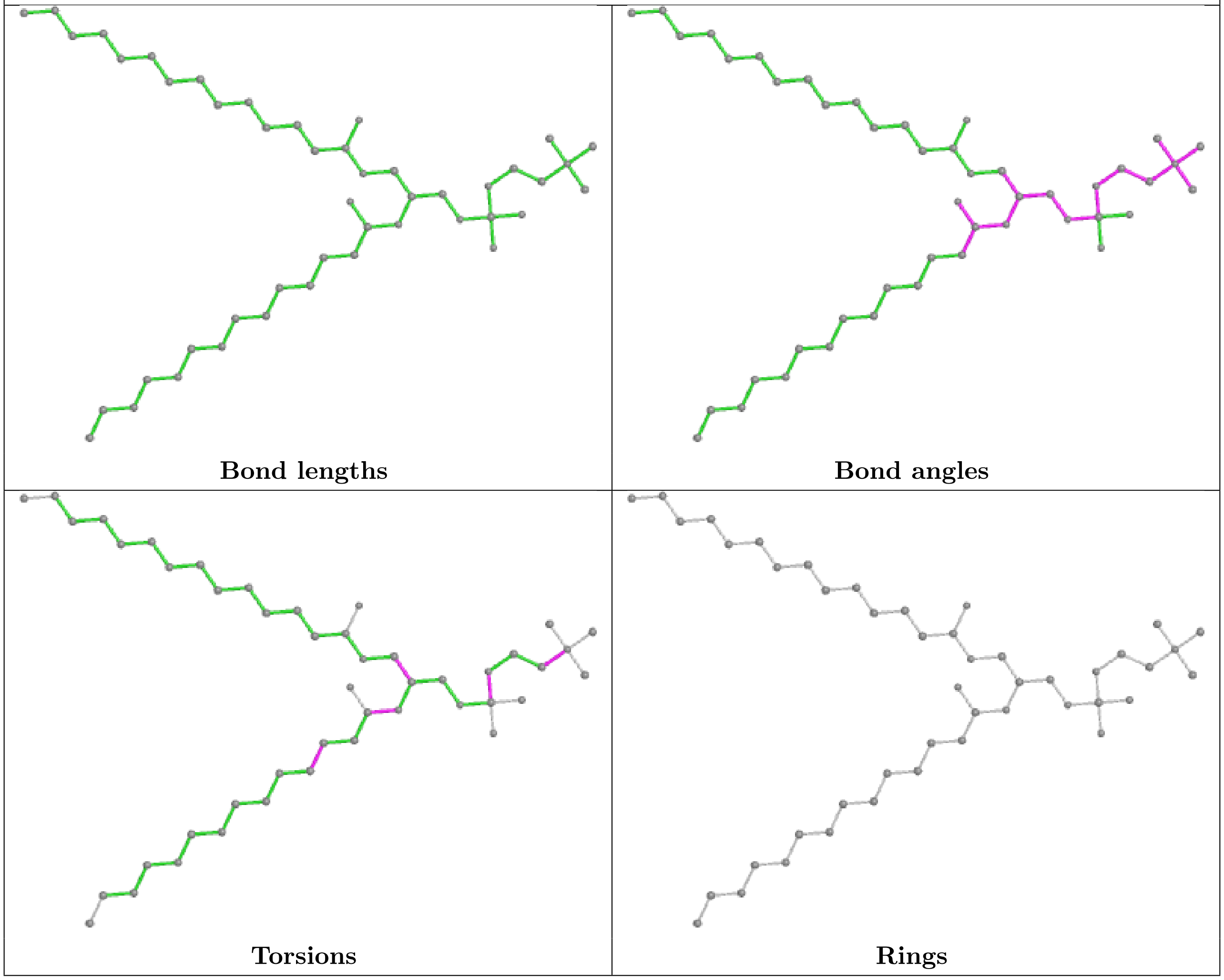
Ligand PX4 A 425



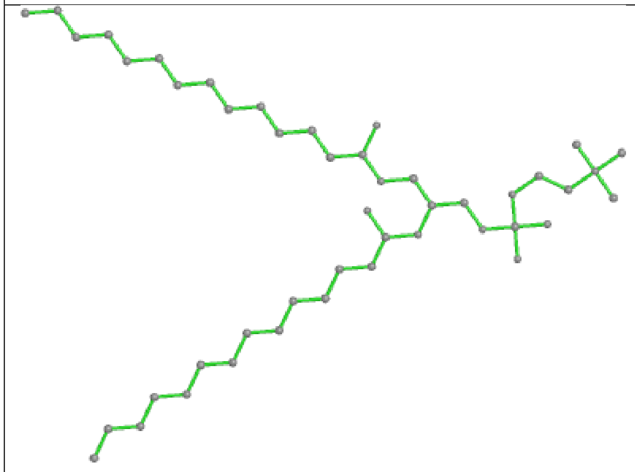
Ligand PX4 A 348



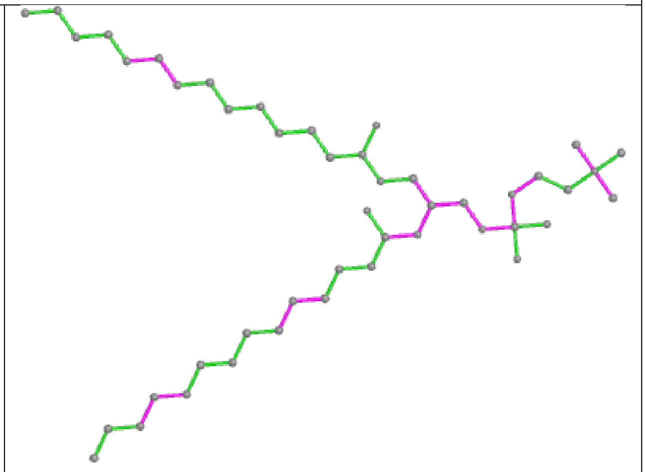
Ligand PX4 A 399



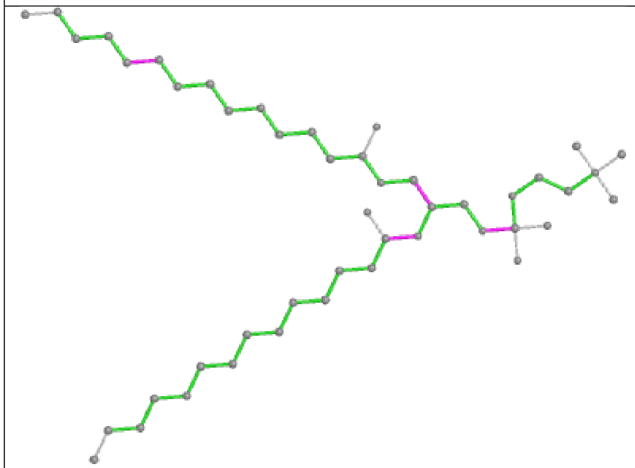
Ligand PX4 A 403



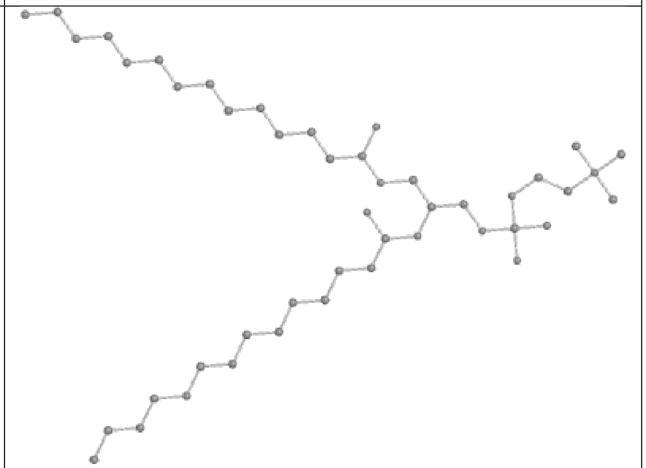
Bond lengths



Bond angles

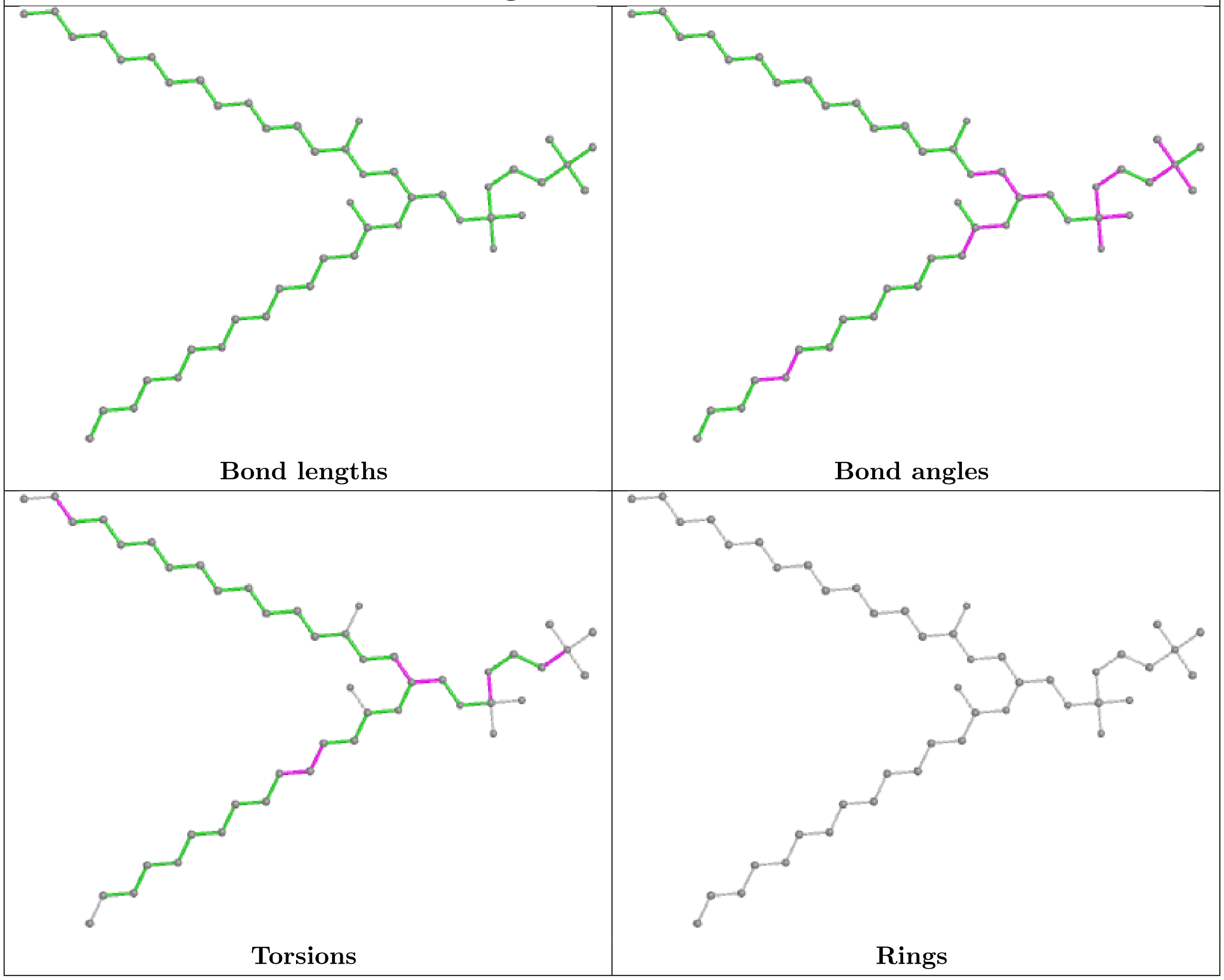


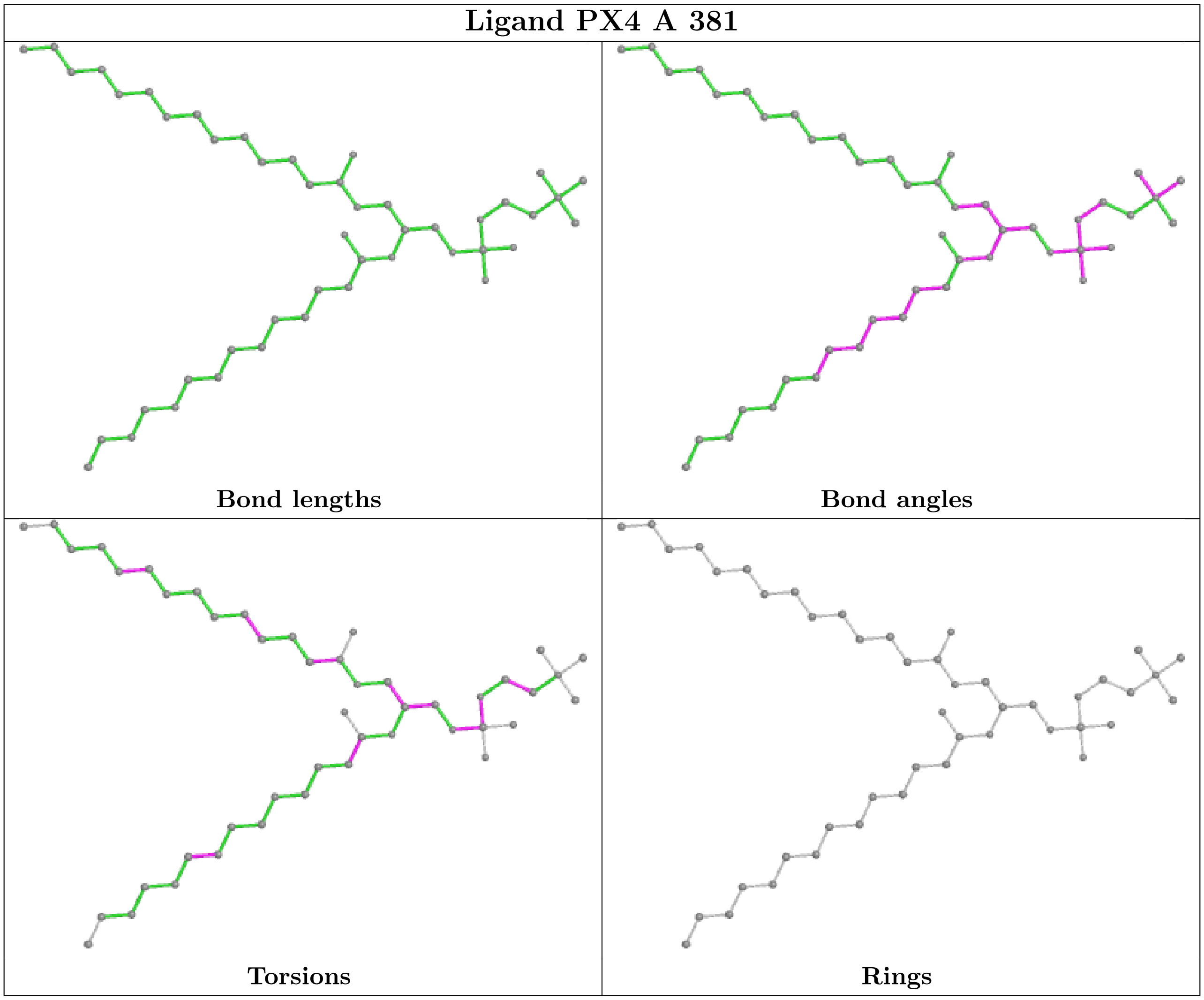
Torsions



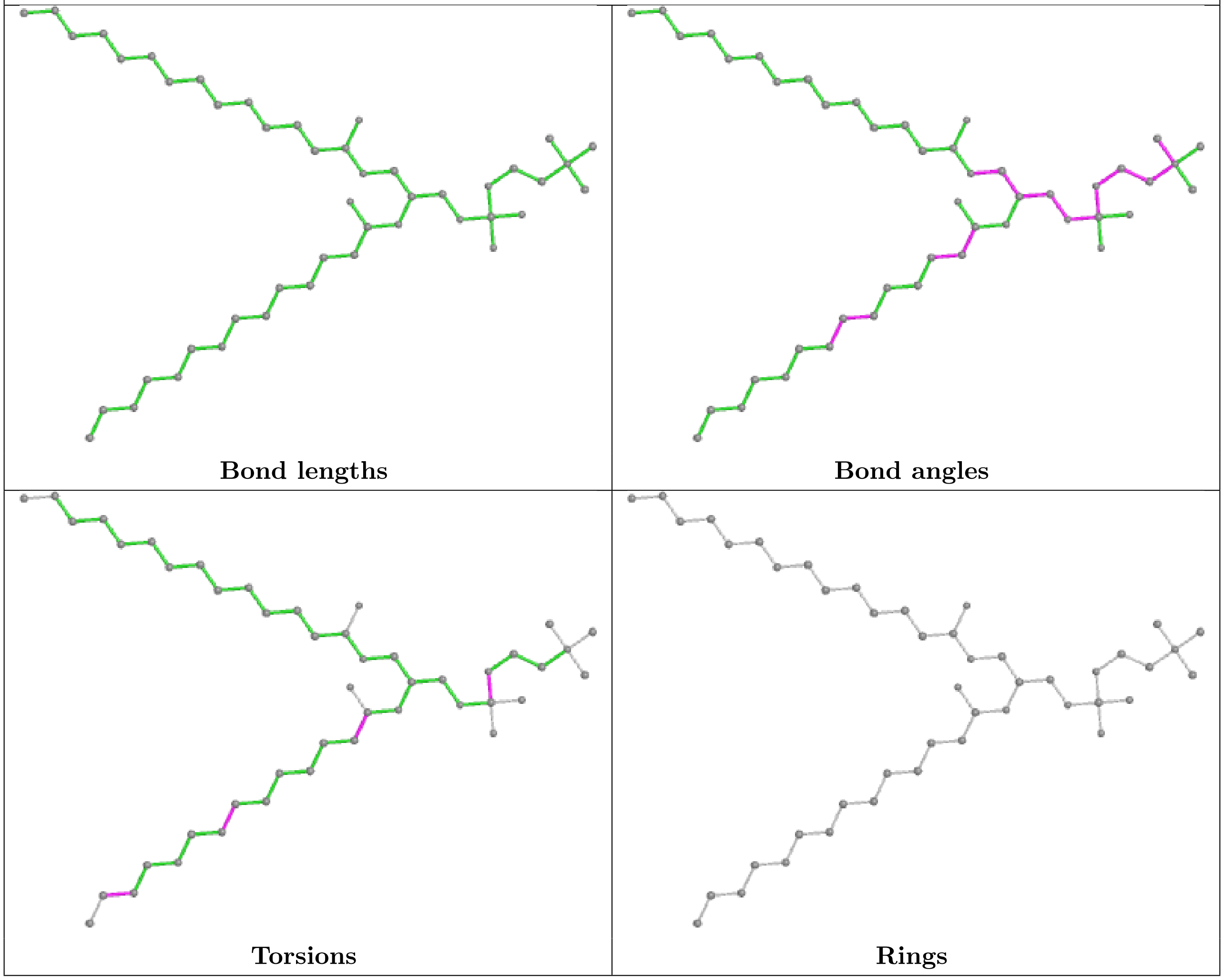
Rings

Ligand PX4 A 310

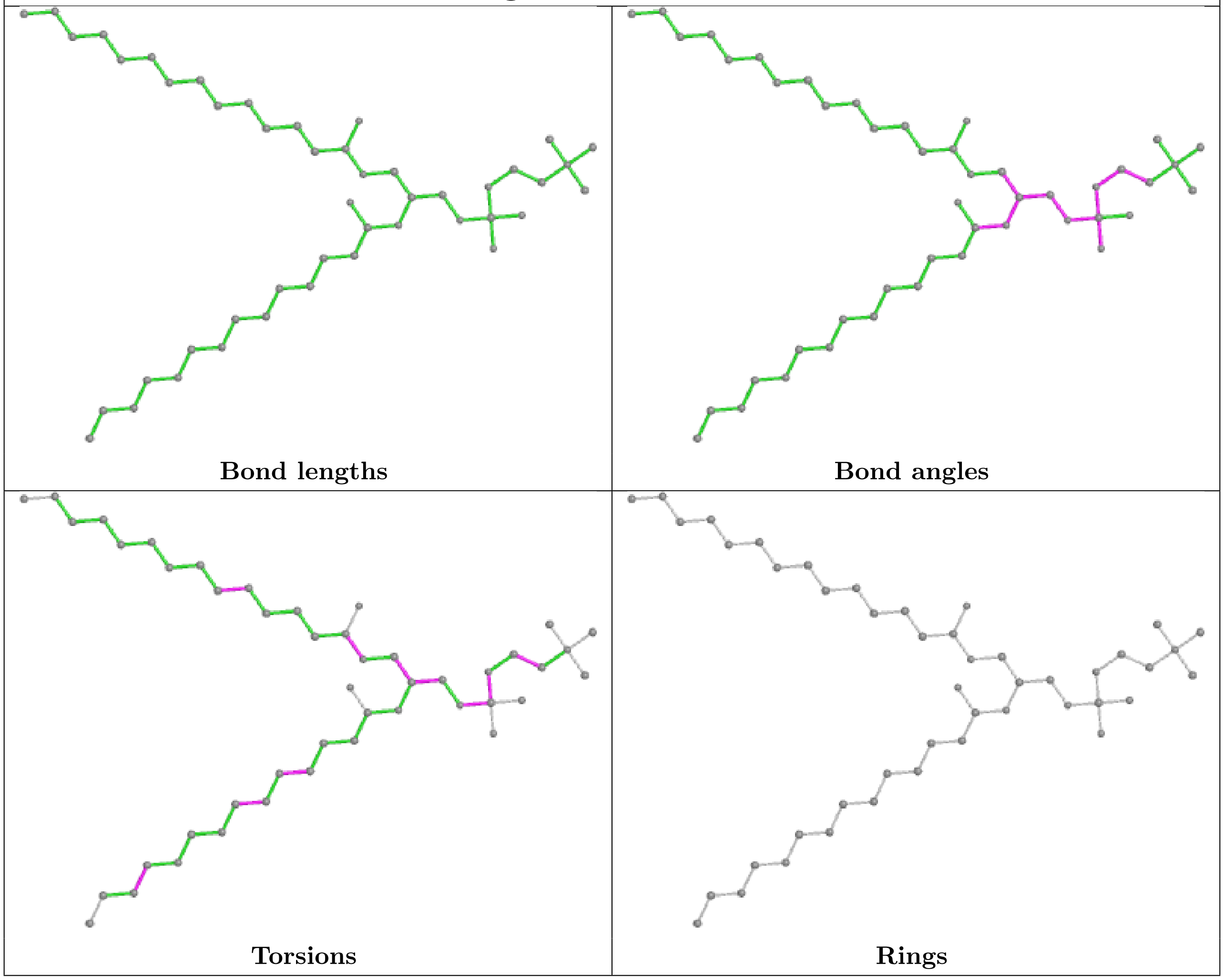



Ligand PX4 A 381
Bond lengths
Bond angles
Torsions
Rings

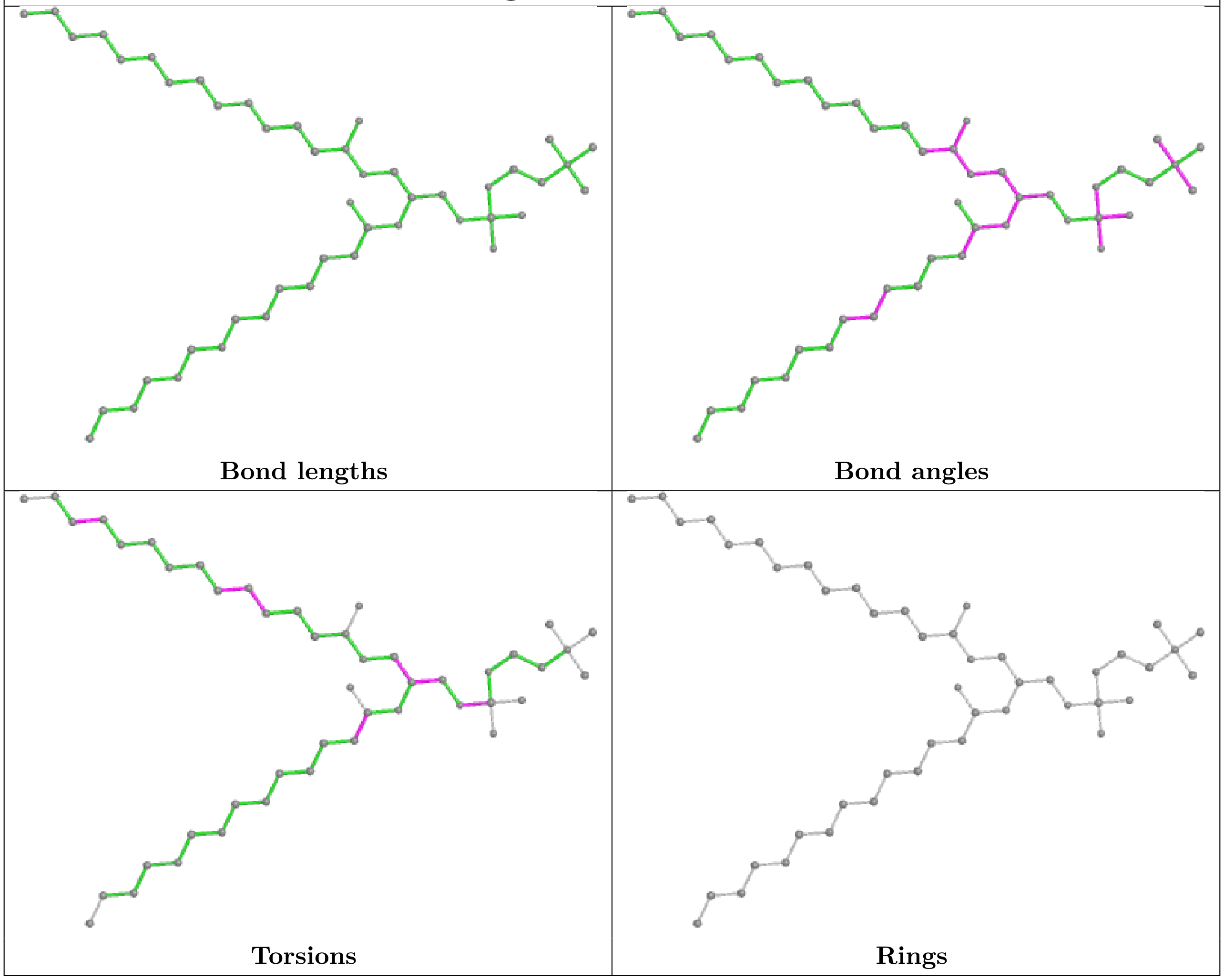
Ligand PX4 A 404



Ligand PX4 A 388

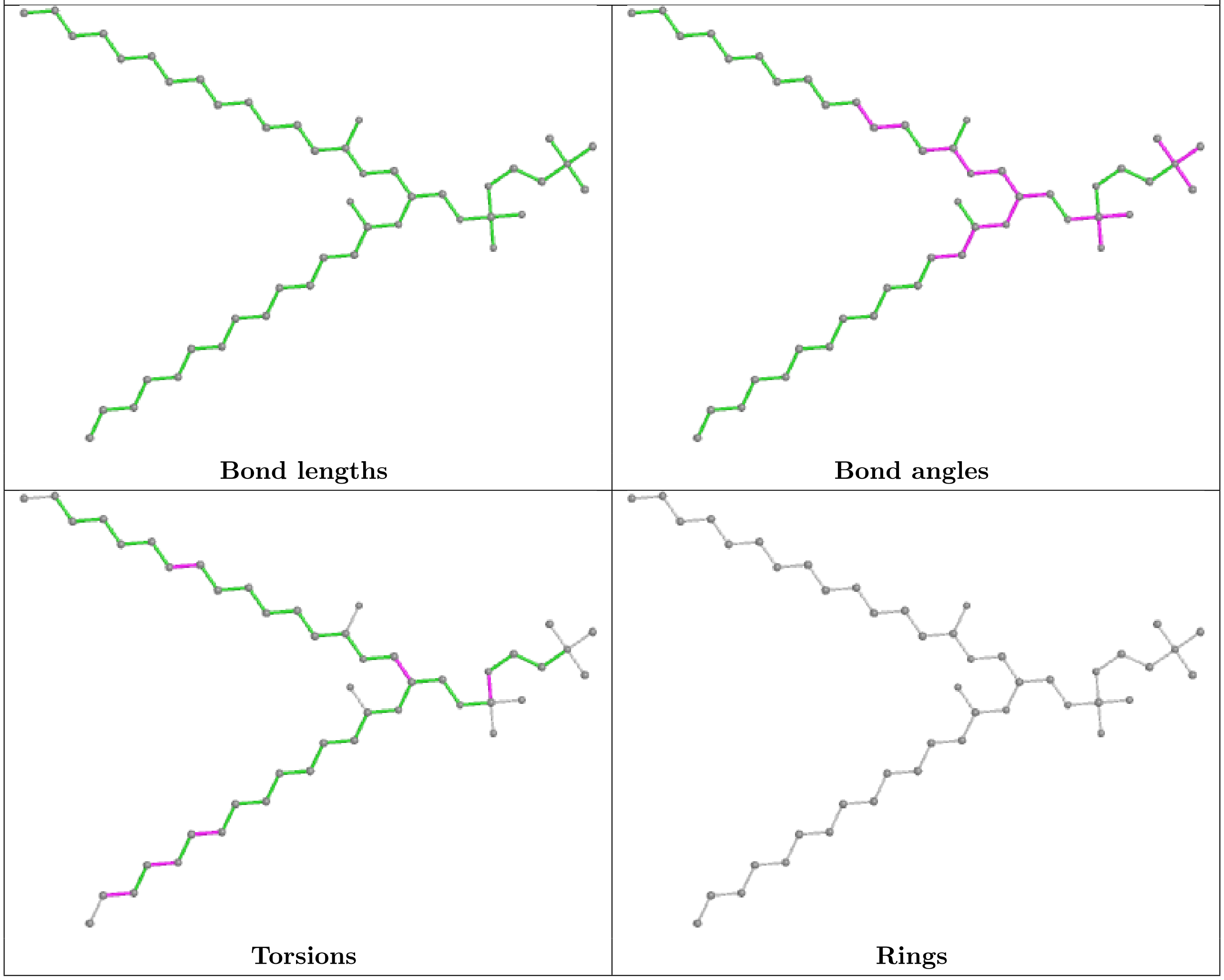


Ligand PX4 A 353

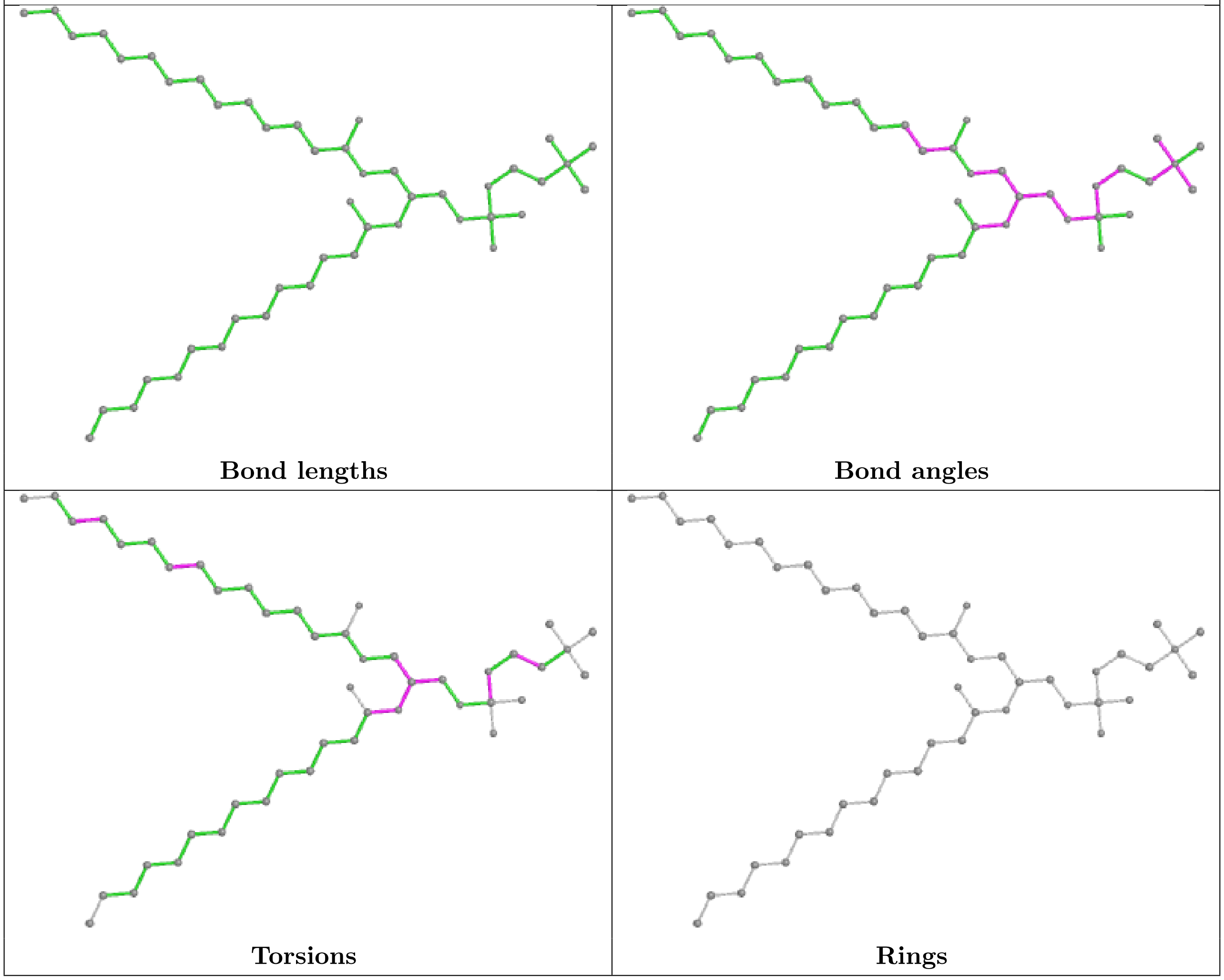


Bond lengths | Bond angles | Torsions | Rings

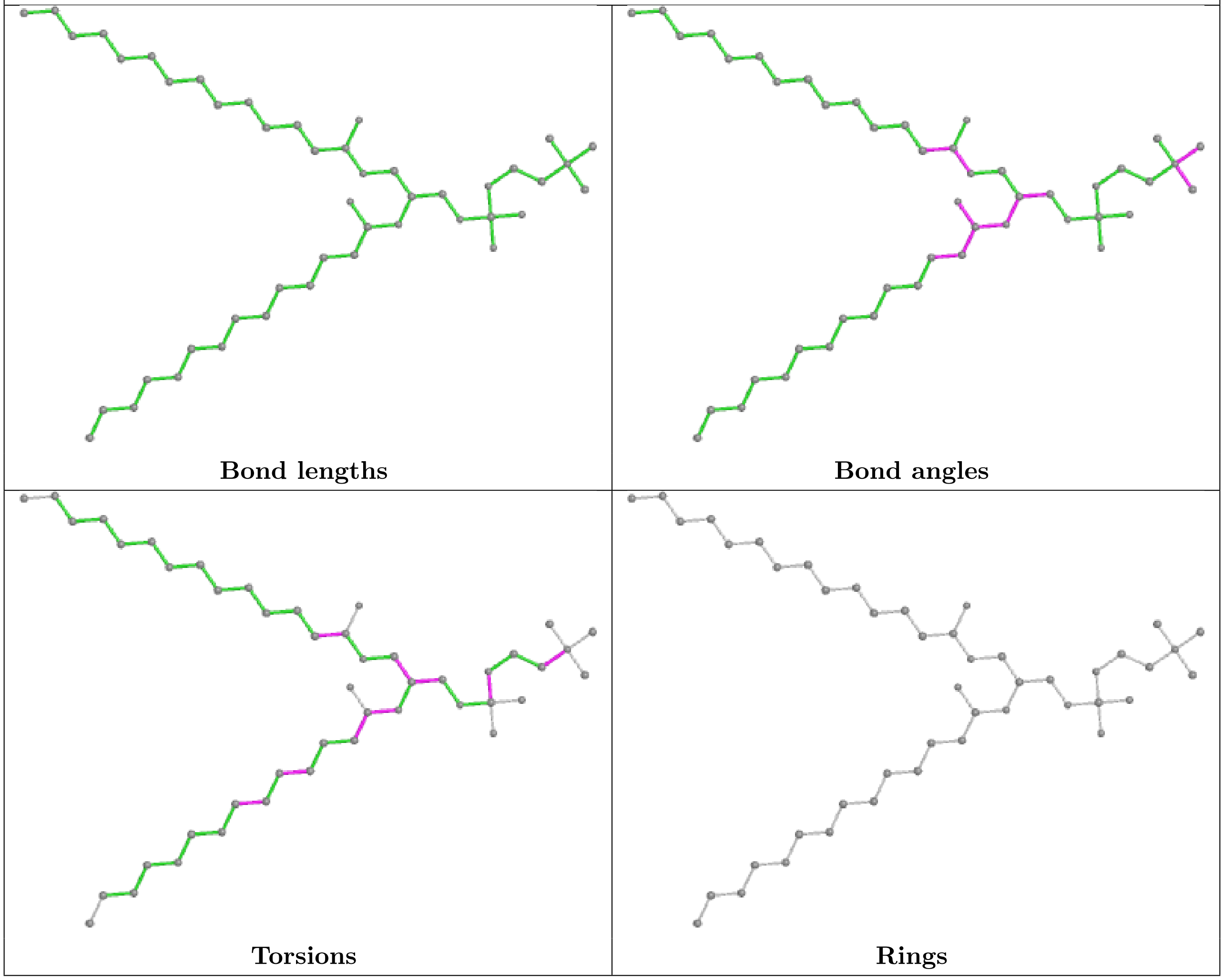
Ligand PX4 A 420



Ligand PX4 A 374



Ligand PX4 A 359



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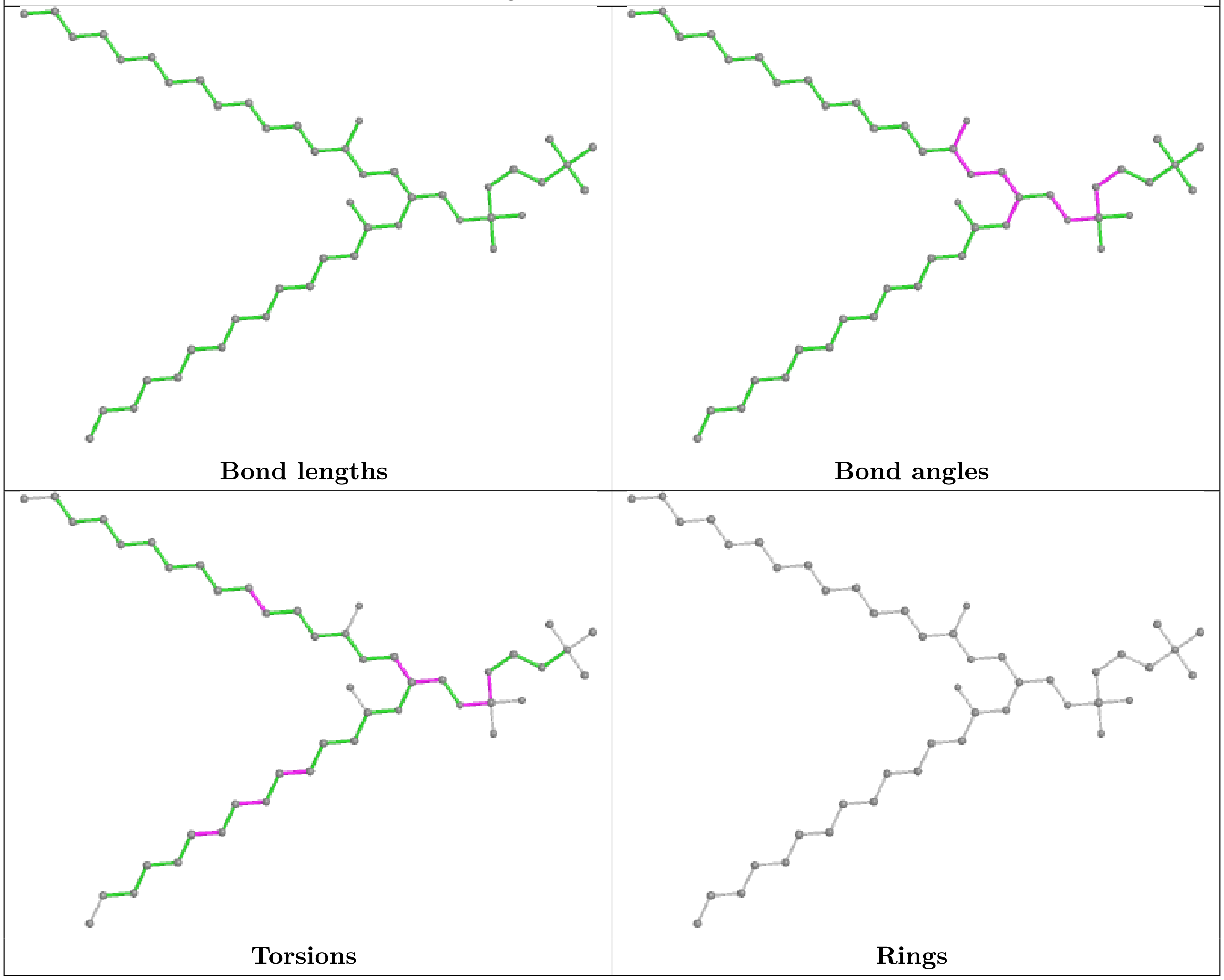
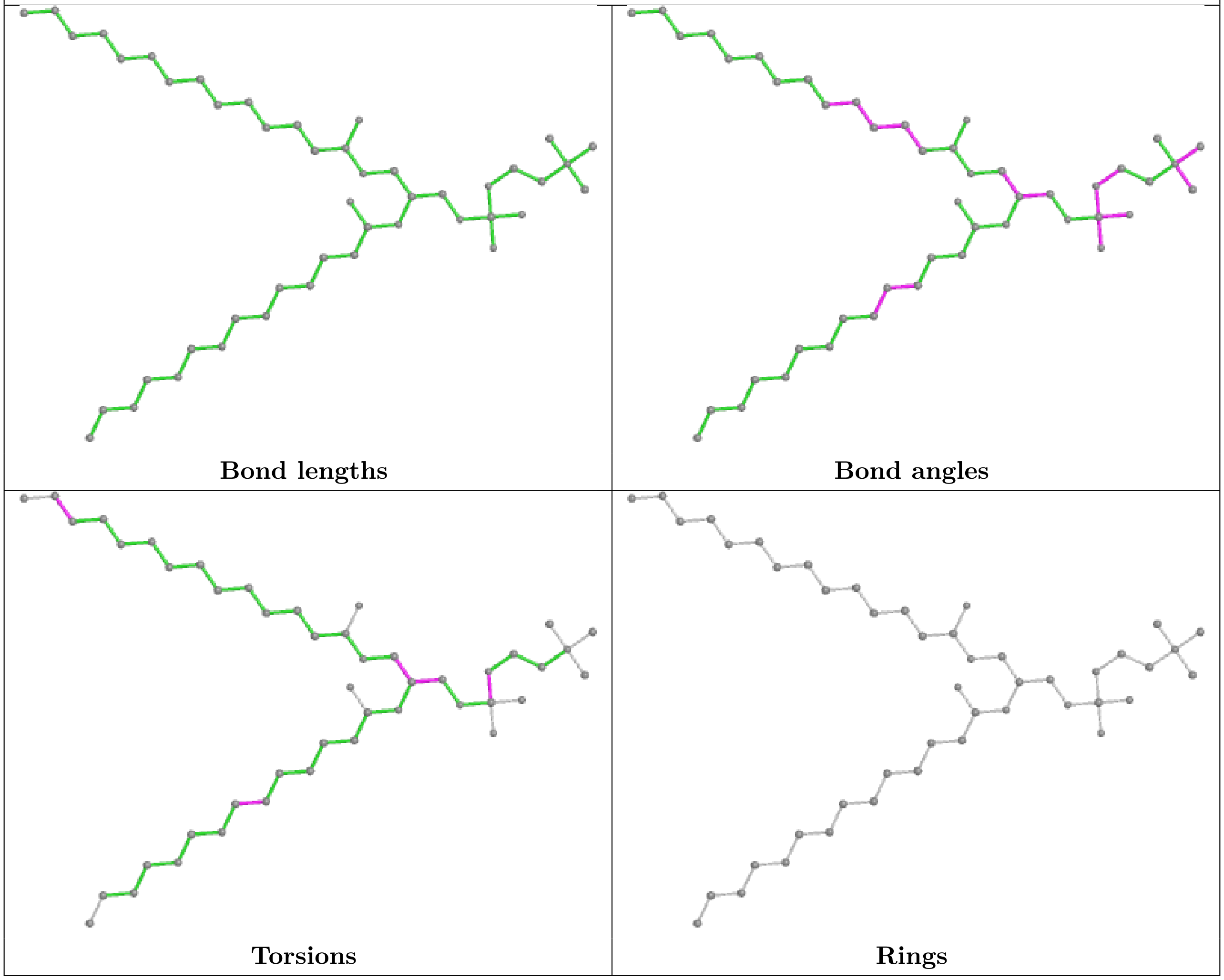
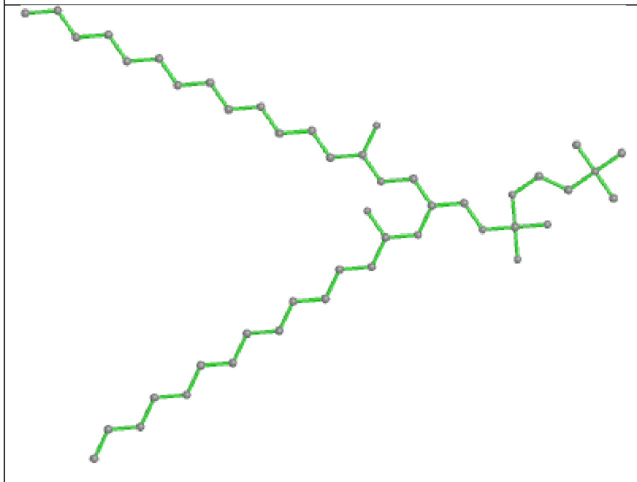


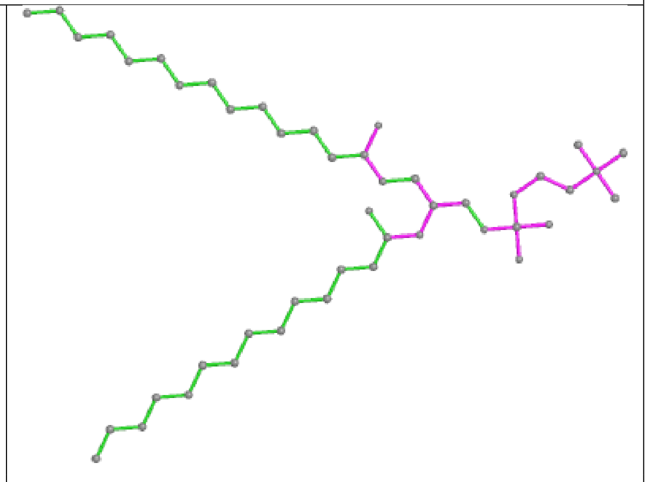
Ligand PX4 A 326



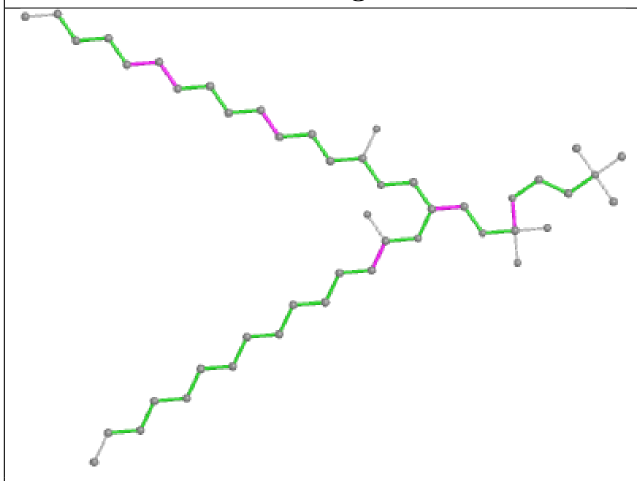
Ligand PX4 A 313



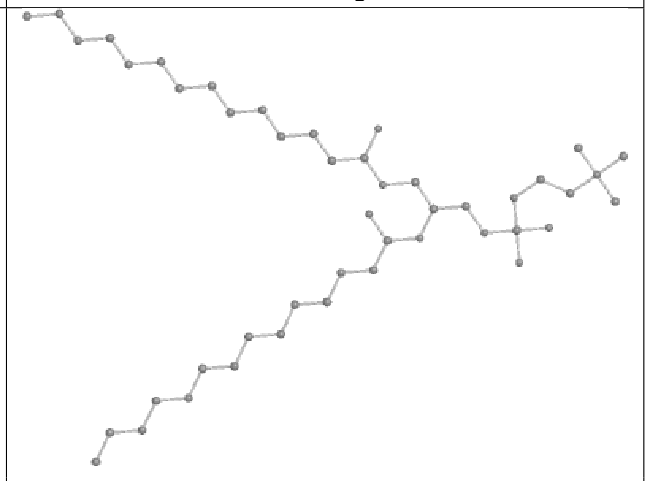
Bond lengths



Bond angles

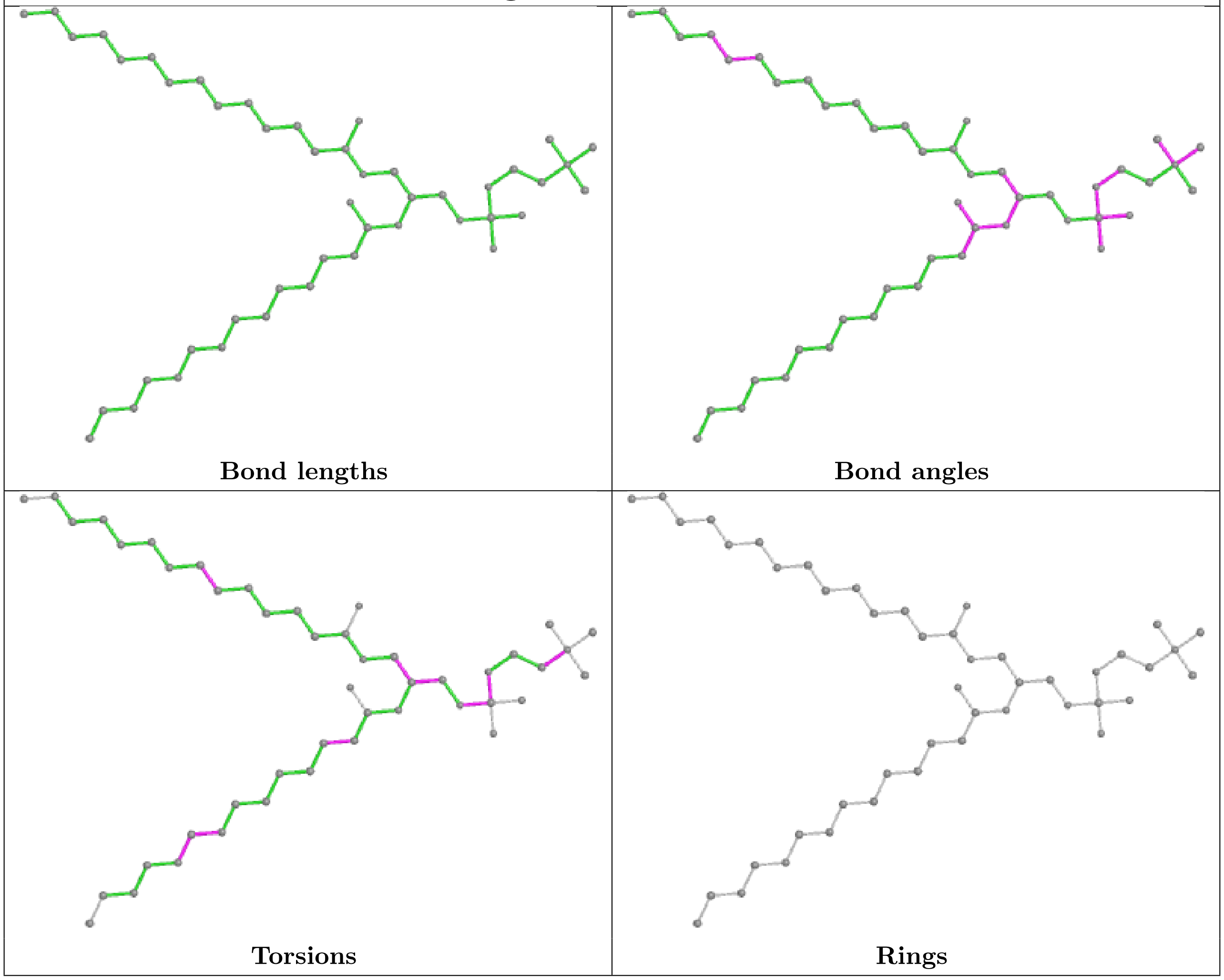


Torsions

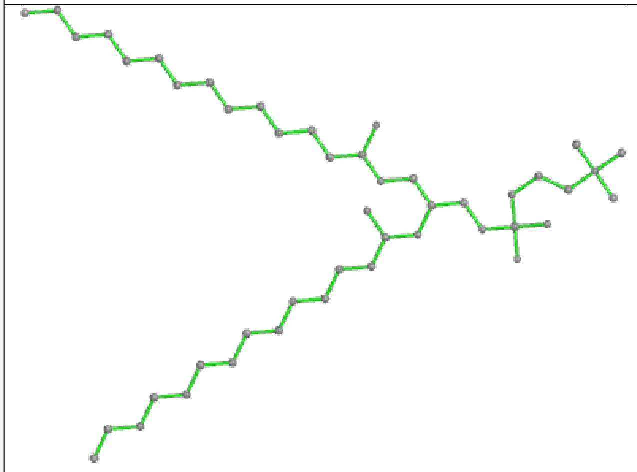


Rings

Ligand PX4 A 415



Ligand PX4 A 395



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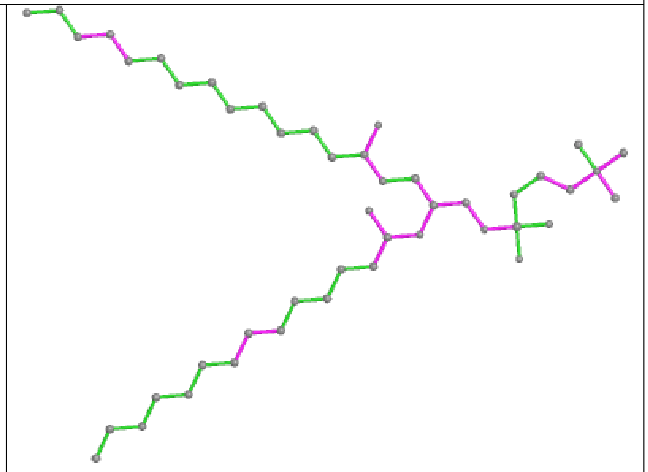
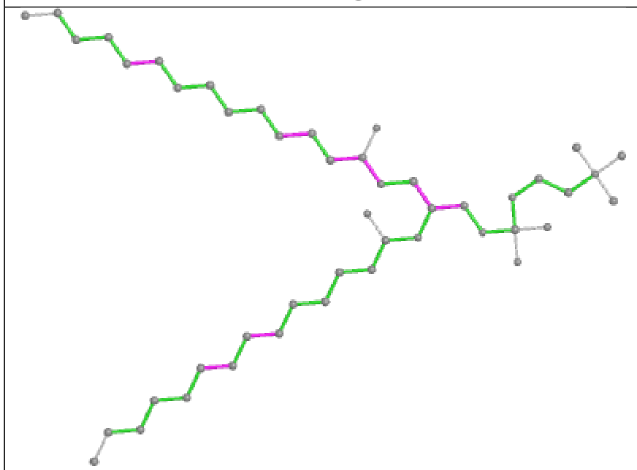
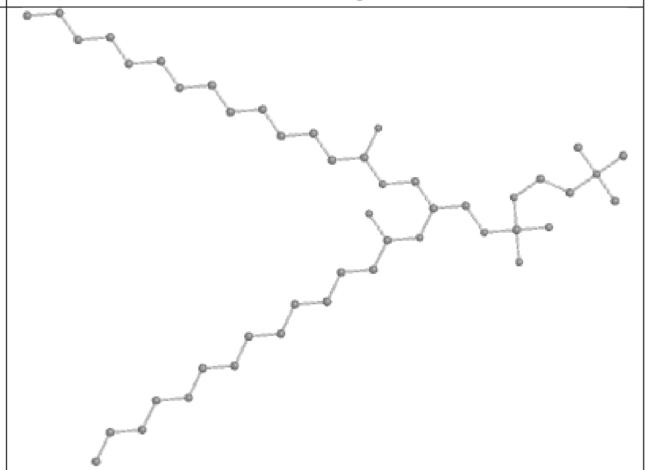


Bond angles

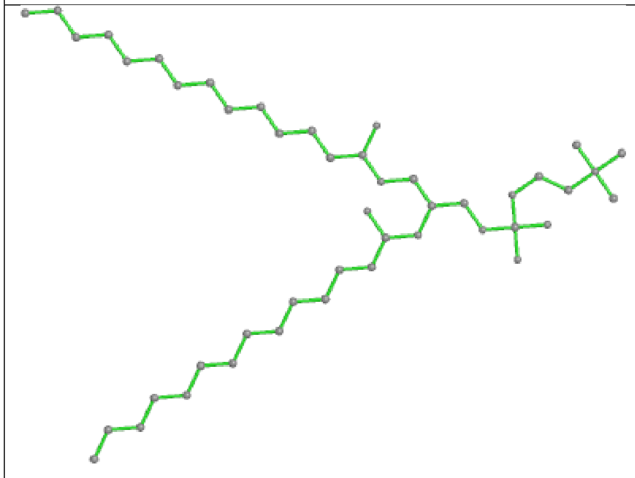


Torsions



Rings

Ligand PX4 A 421



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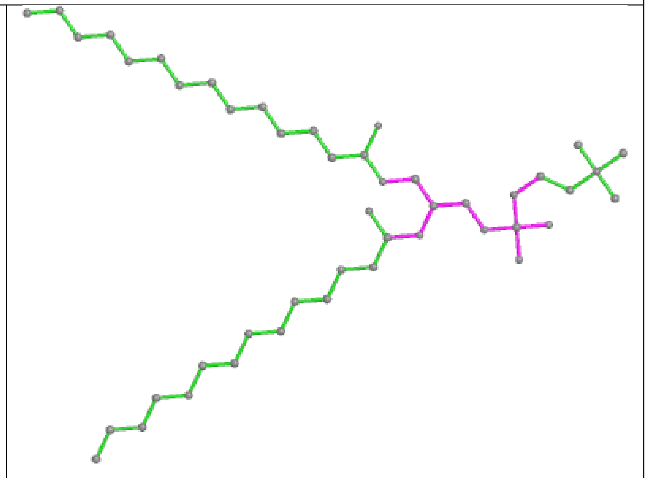
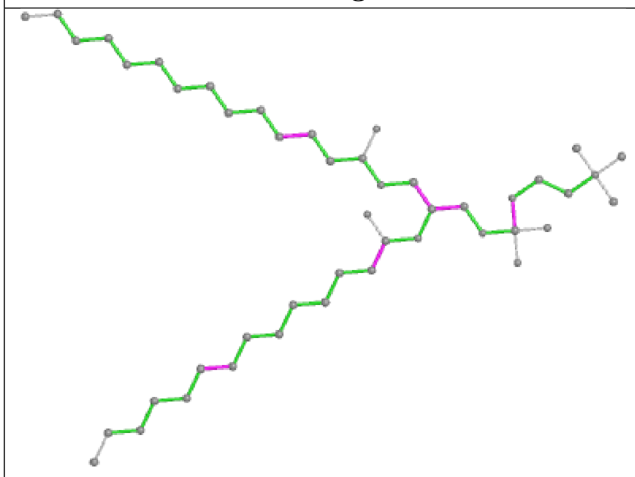


Bond angles



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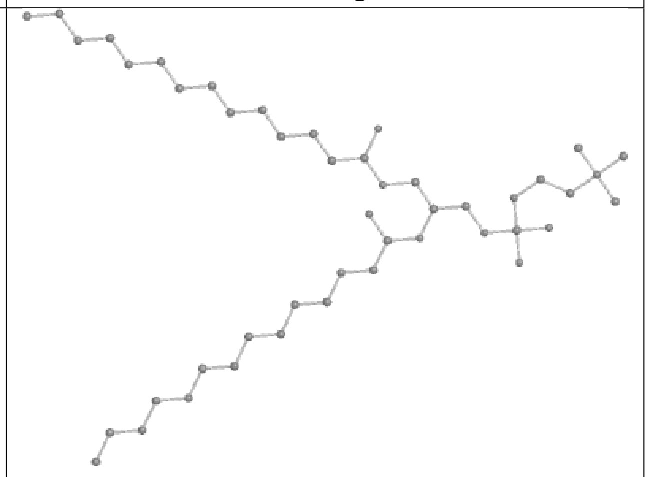
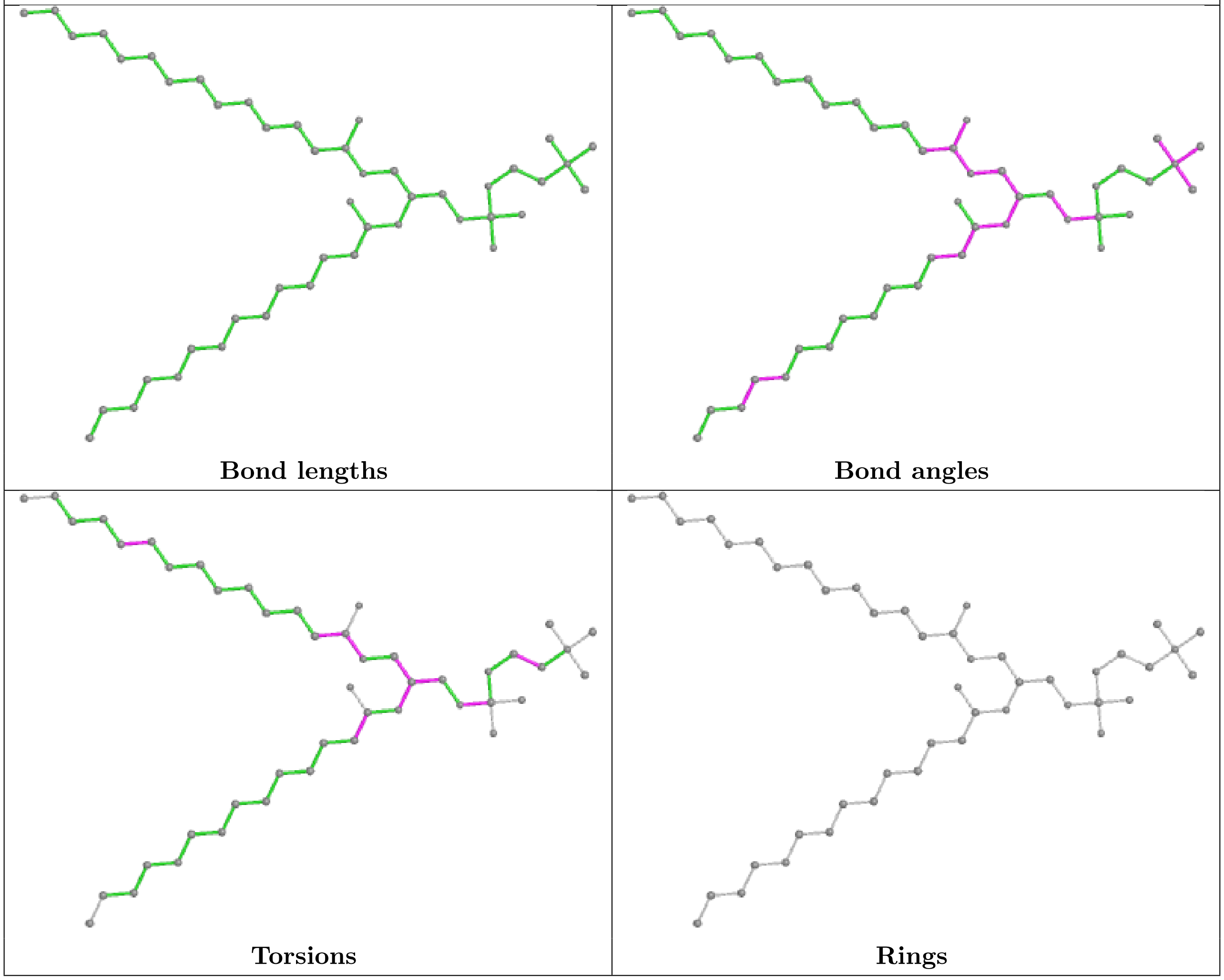
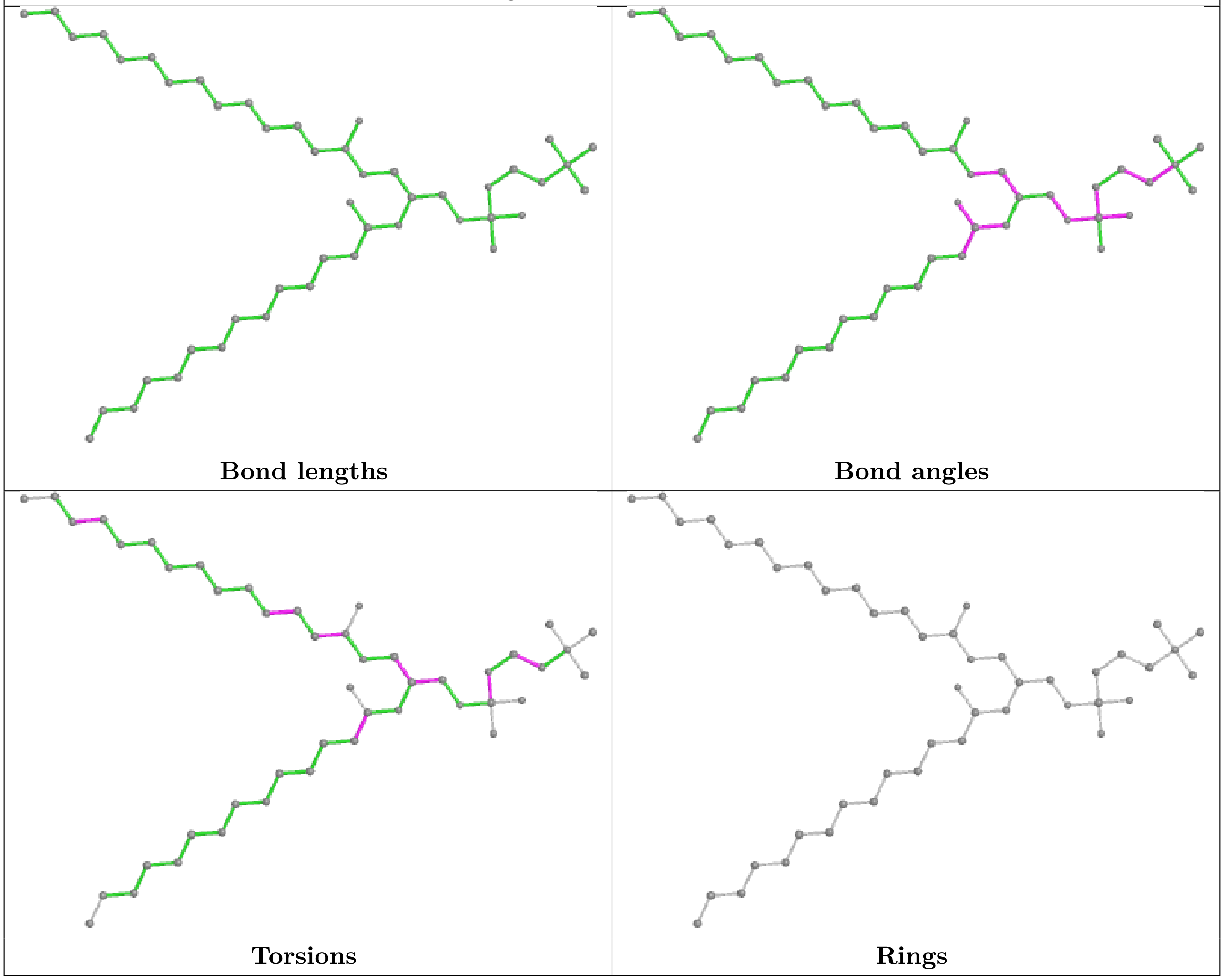


Rings

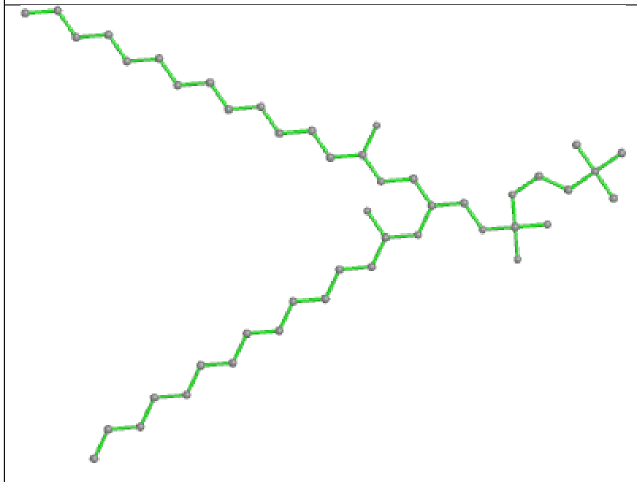
Ligand PX4 A 341



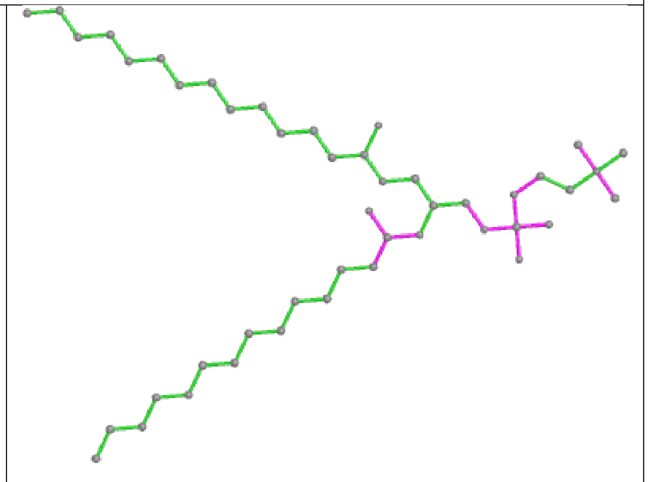
Ligand PX4 A 386



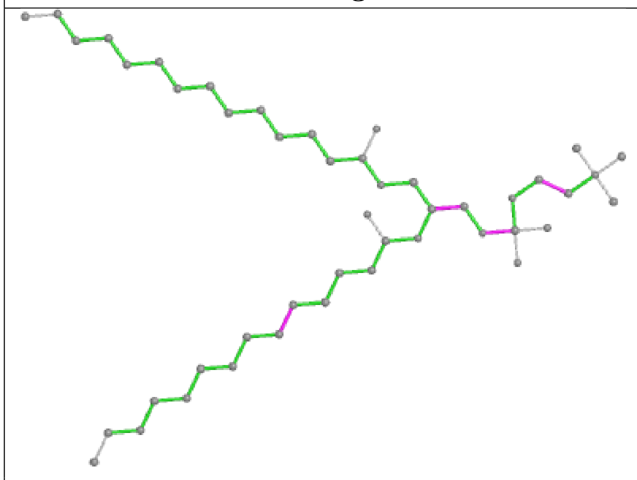
Ligand PX4 A 364



Bond lengths



Bond angles



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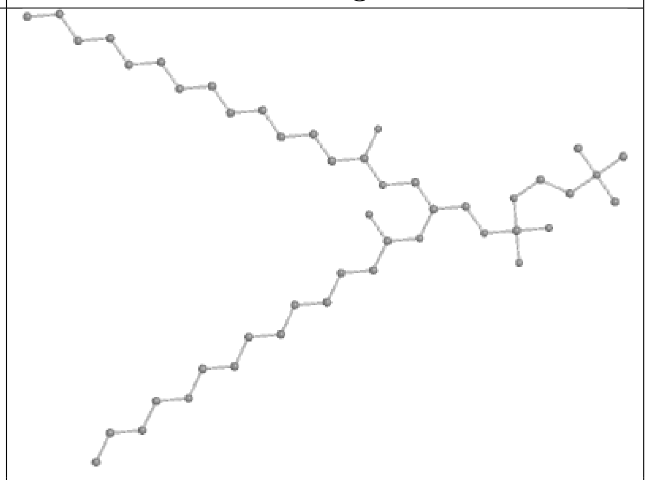
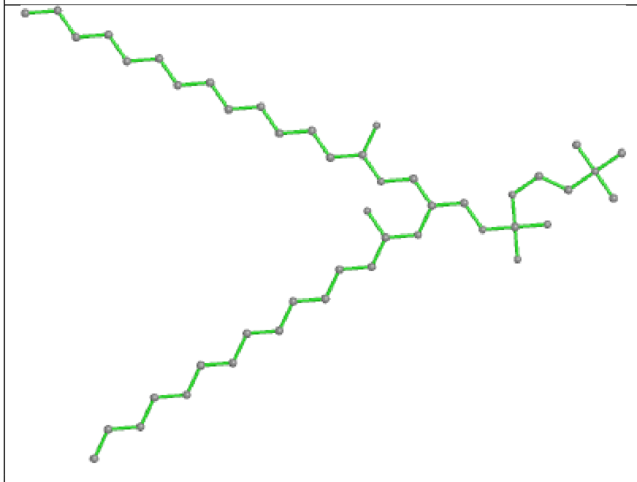
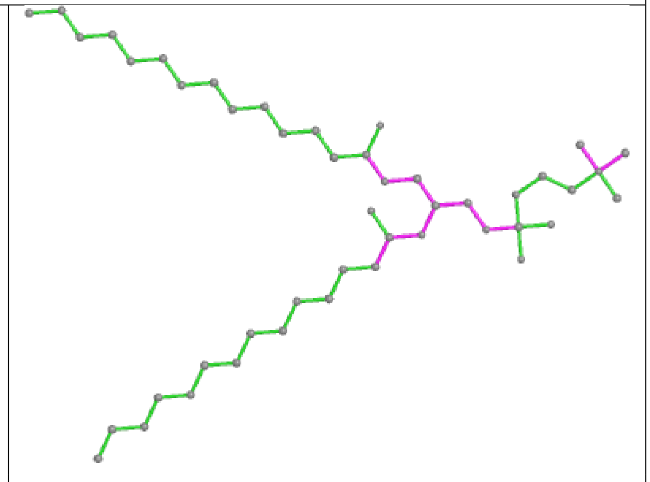


Rings

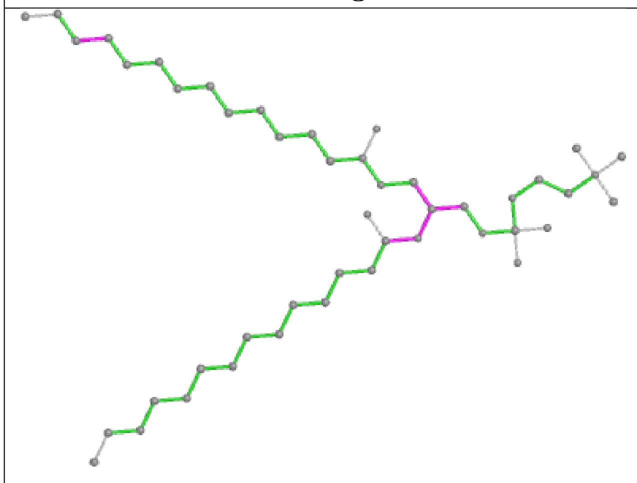
Ligand PX4 A 328



Bond lengths



Bond angles



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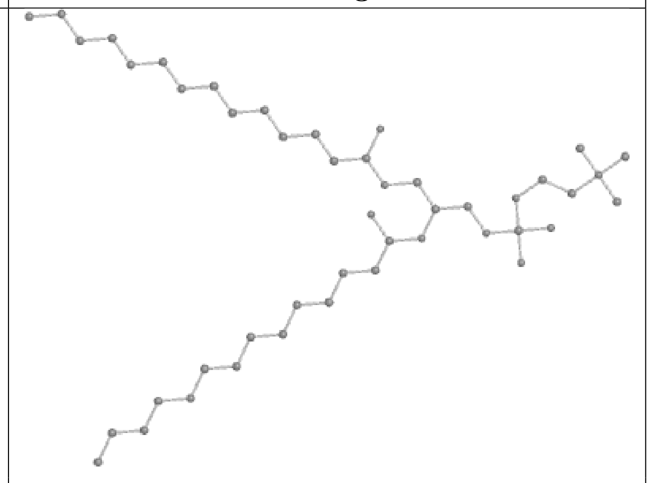
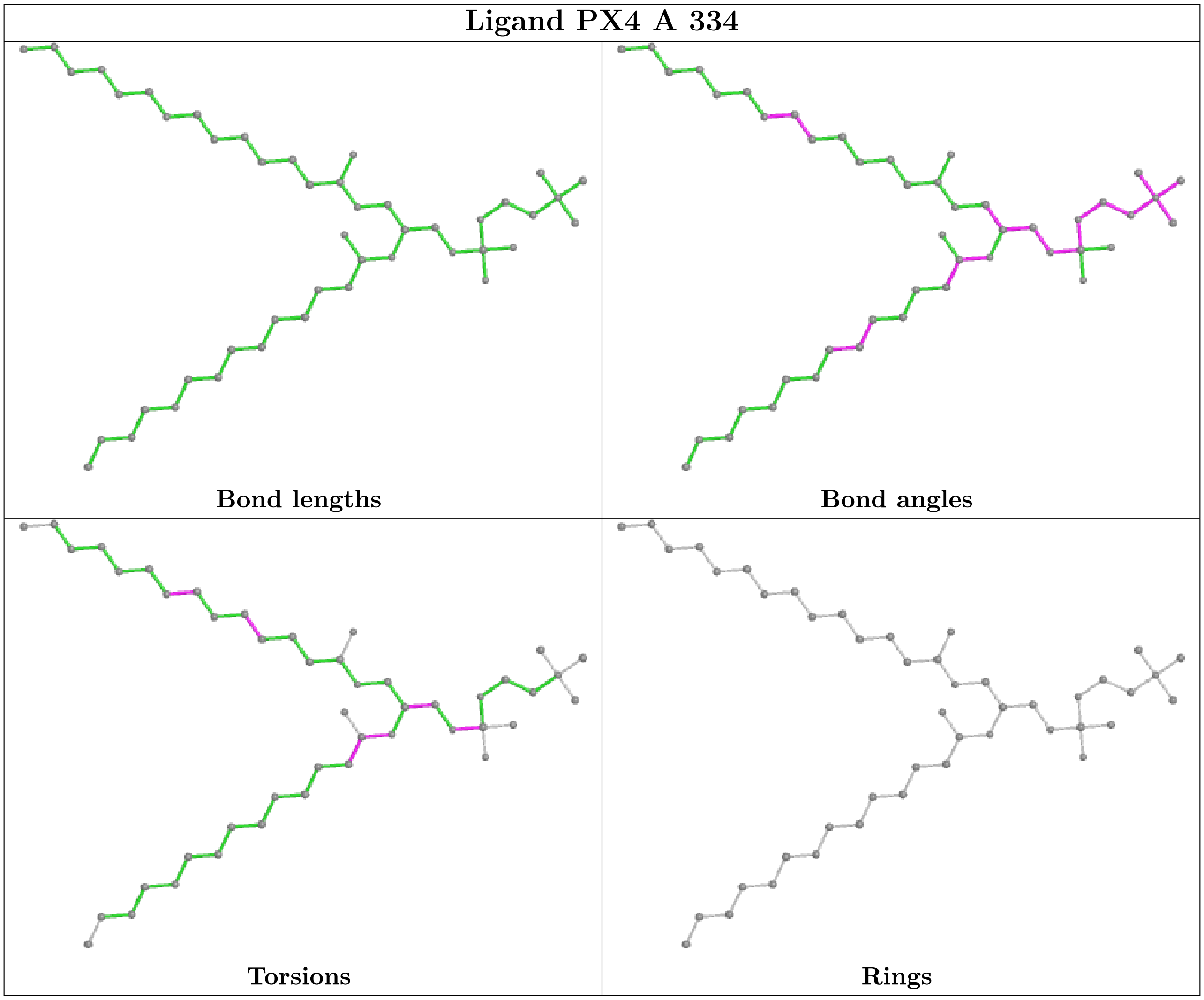
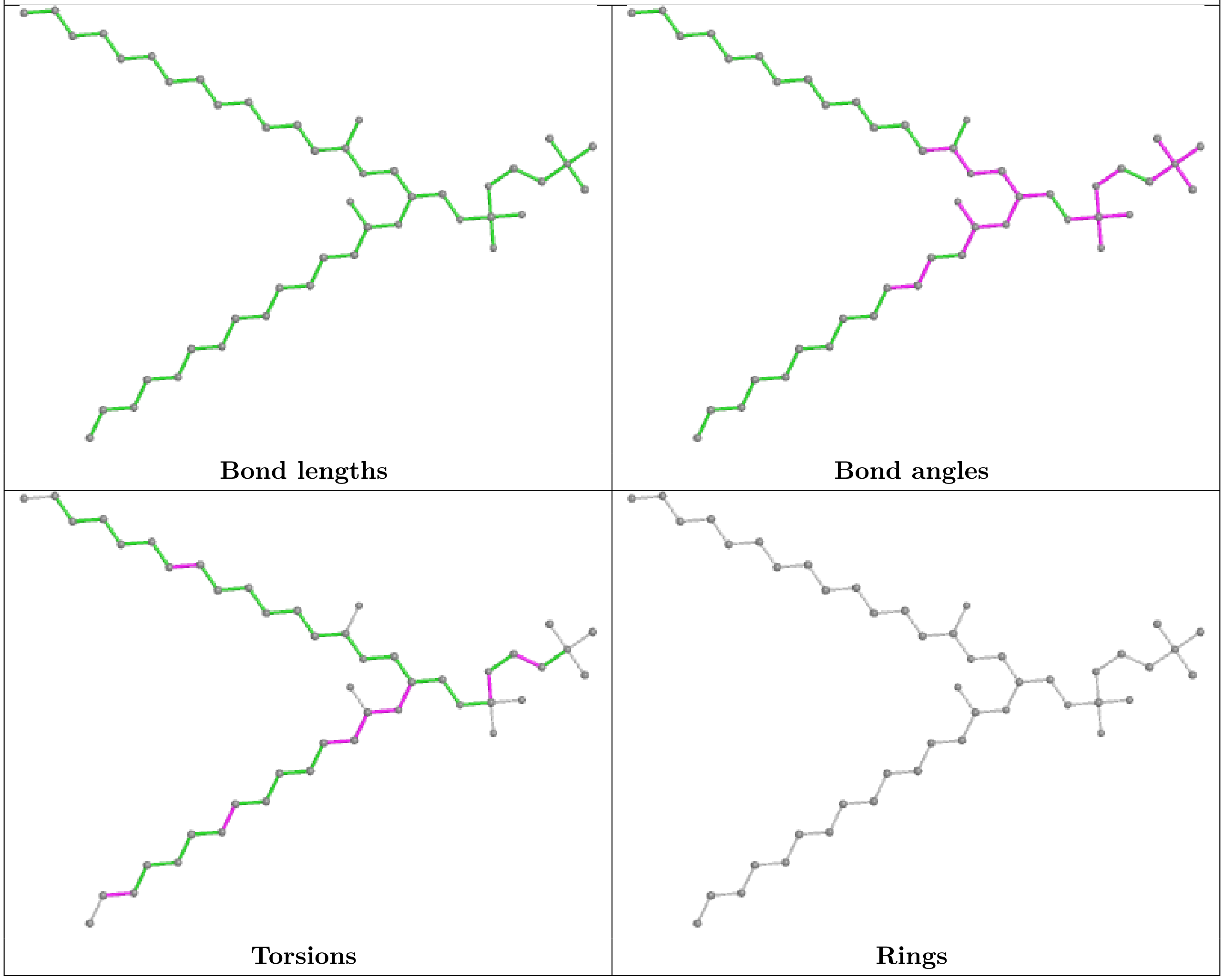


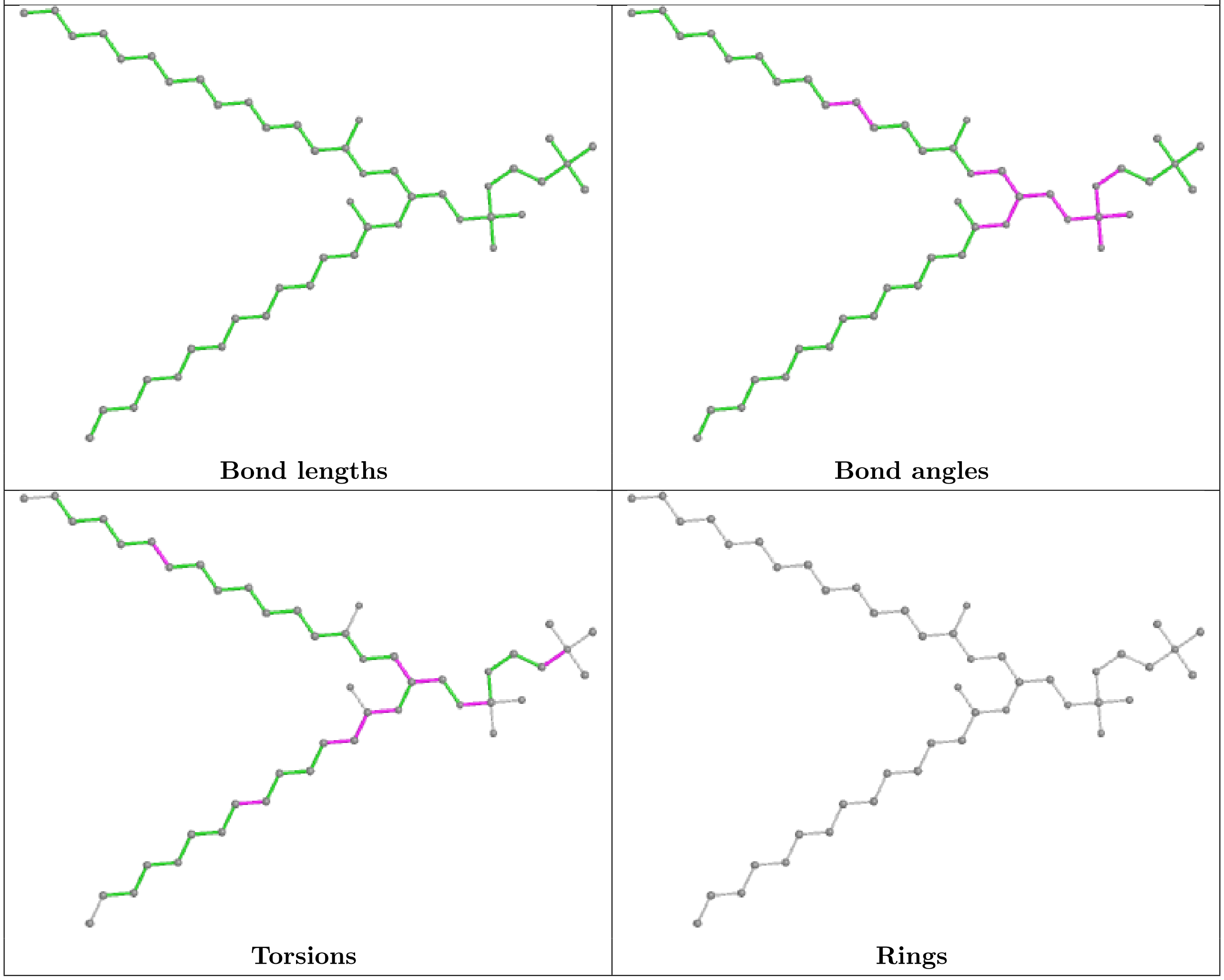
Rings


Ligand PX4 A 334
Bond lengths
Bond angles
Torsions
Rings

Ligand PX4 A 428



Ligand PX4 A 367



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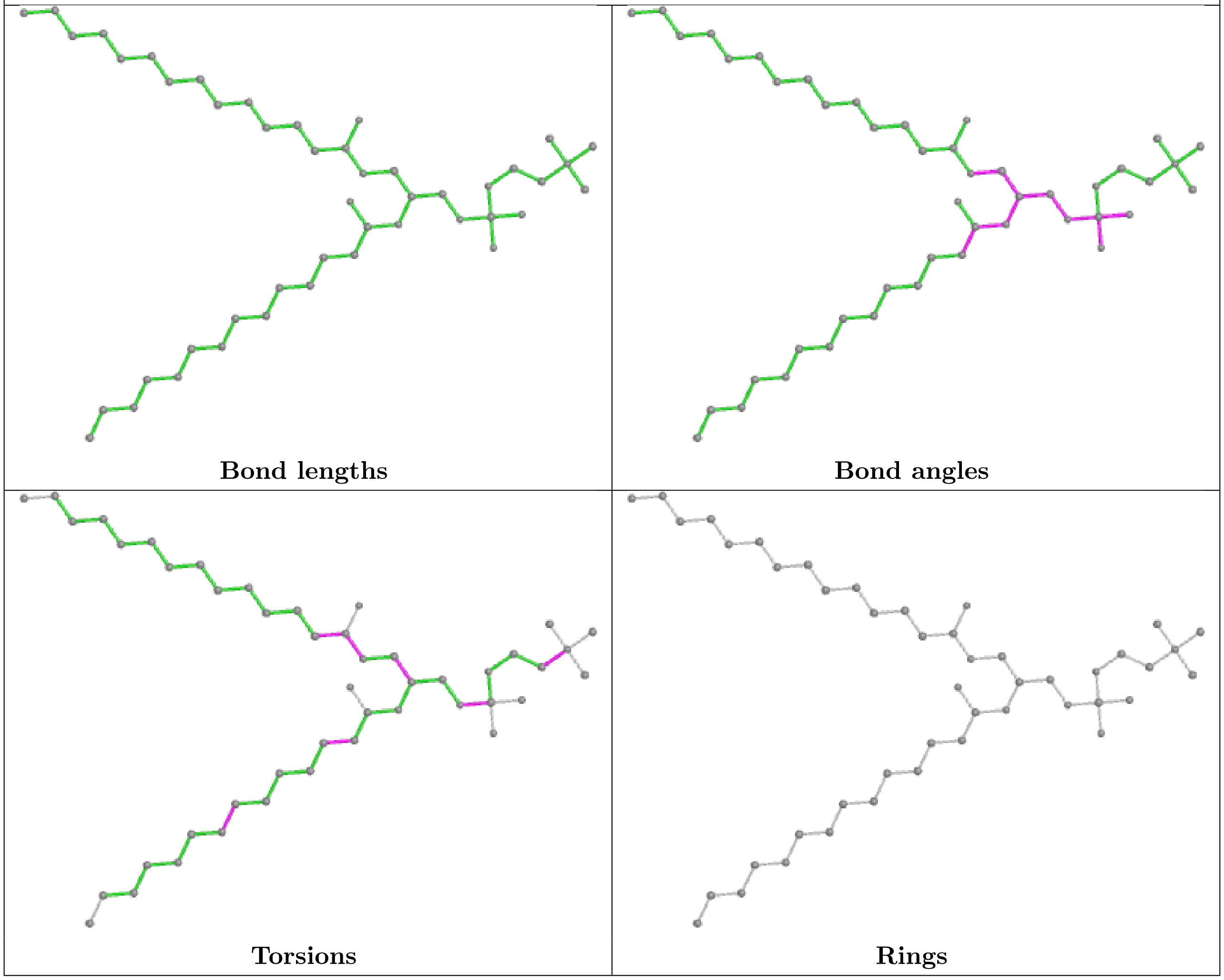

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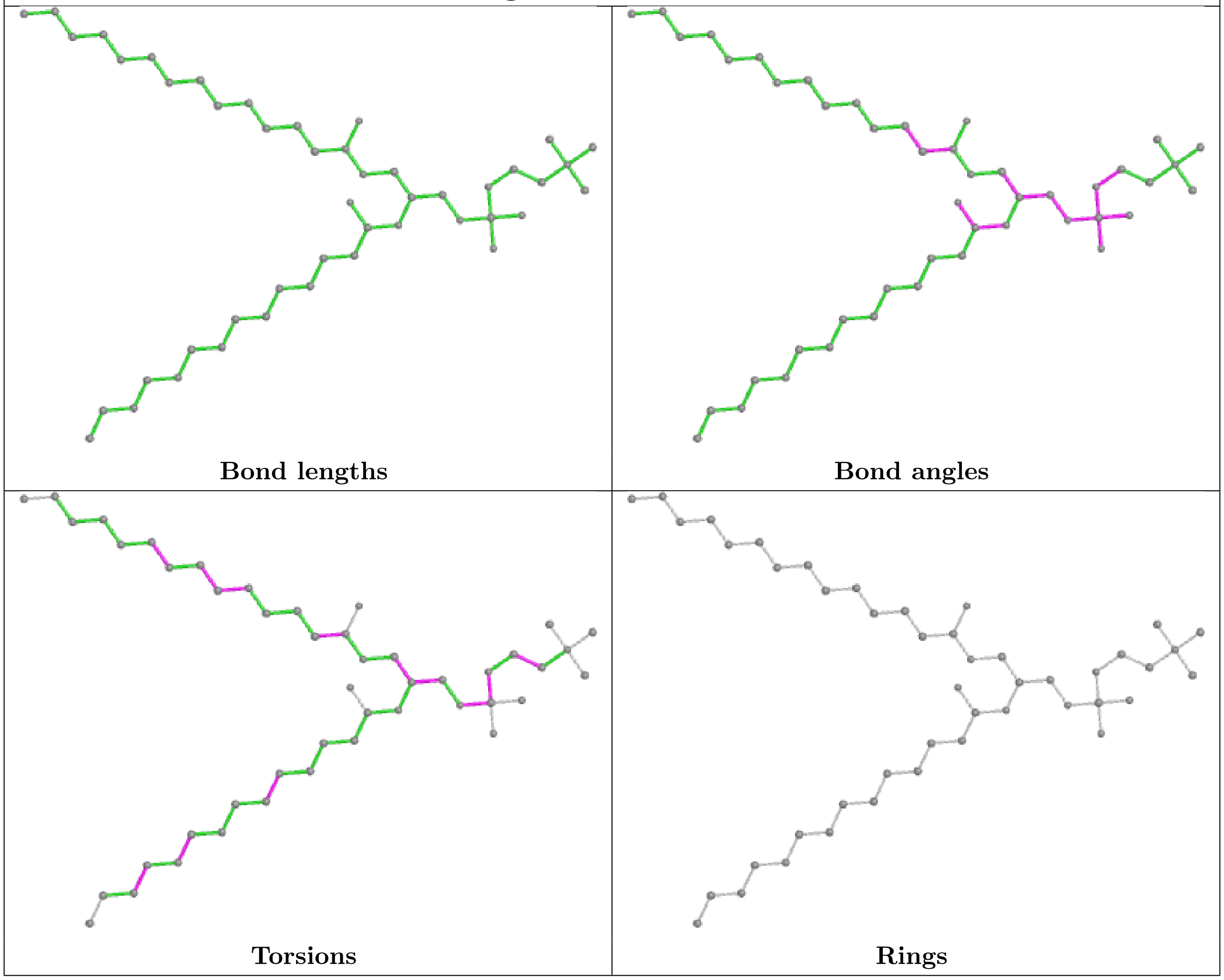

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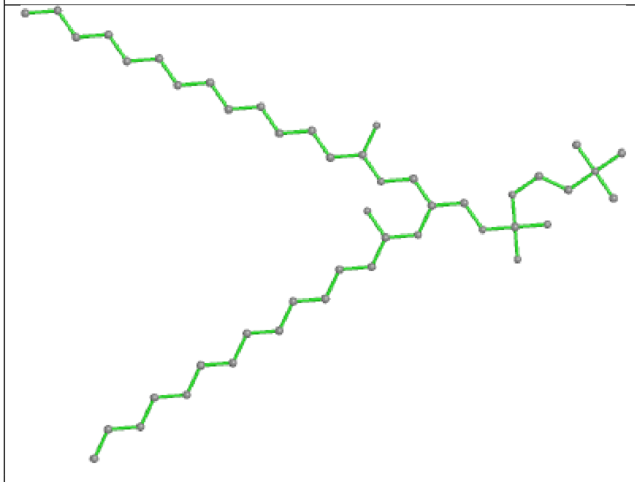
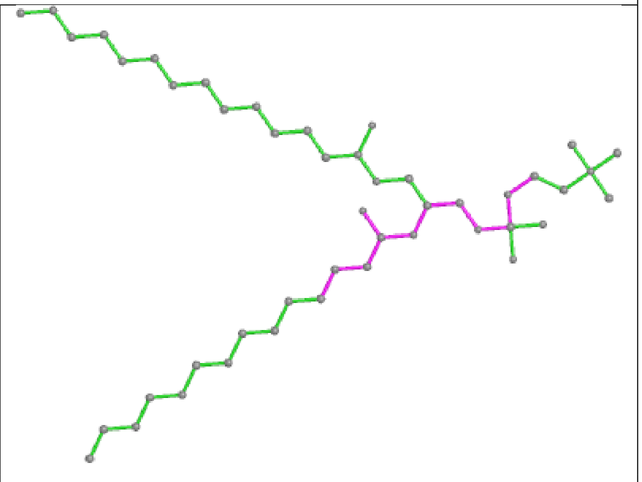
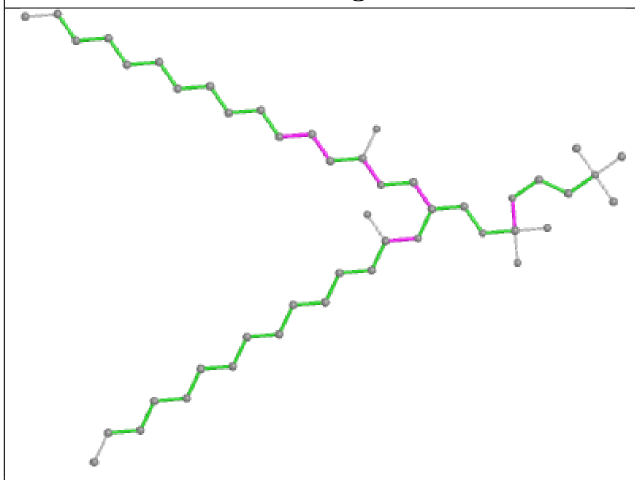


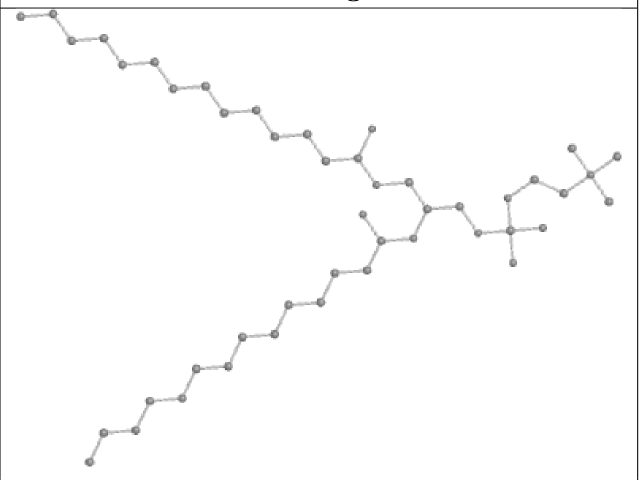
Bond lengths



Bond angles

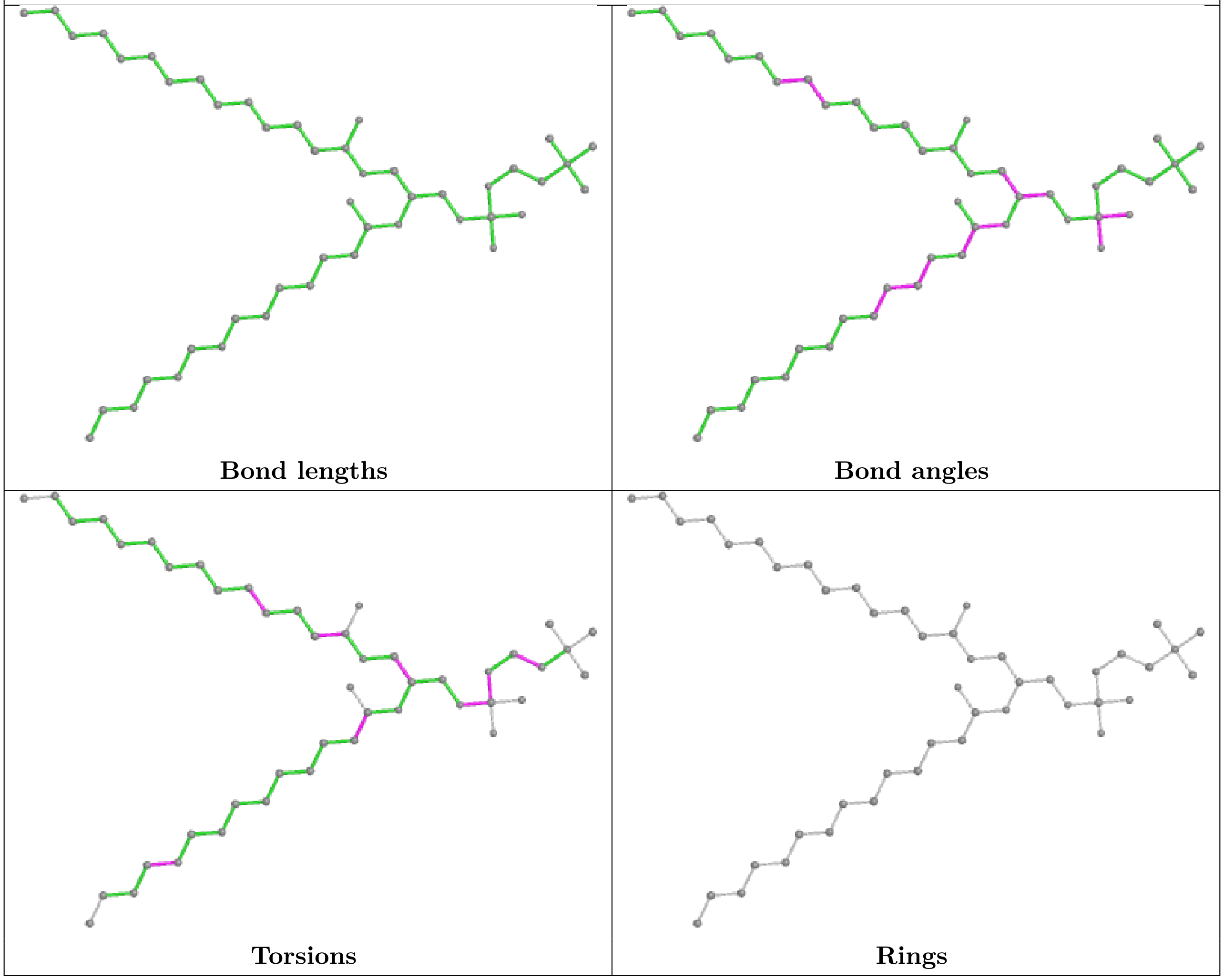


Torsions

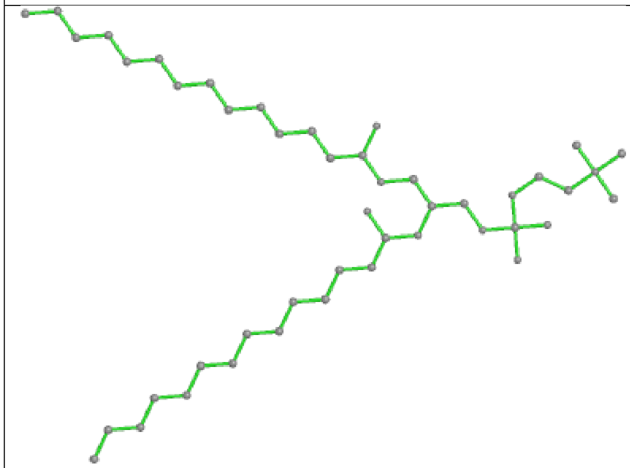


Rings

Ligand PX4 A 371



Ligand PX4 A 414



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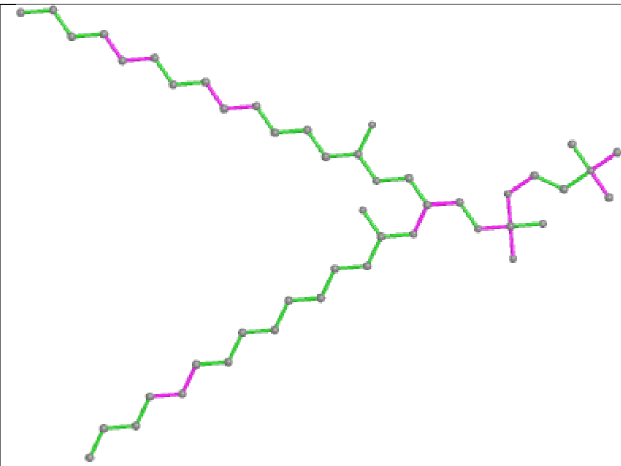
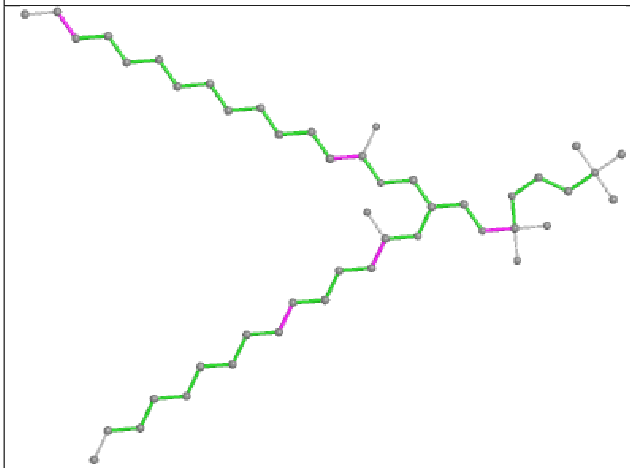


Bond angles



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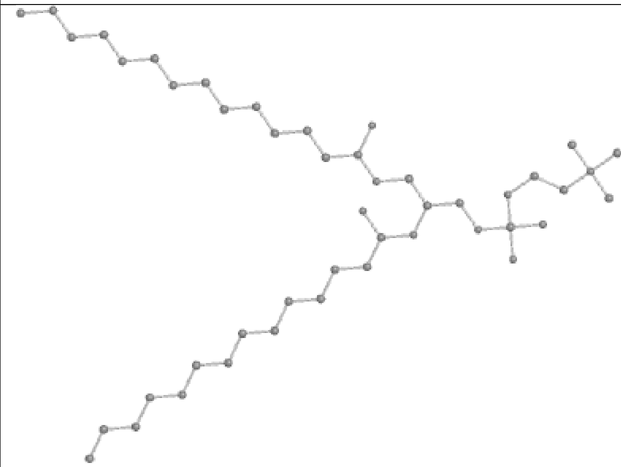
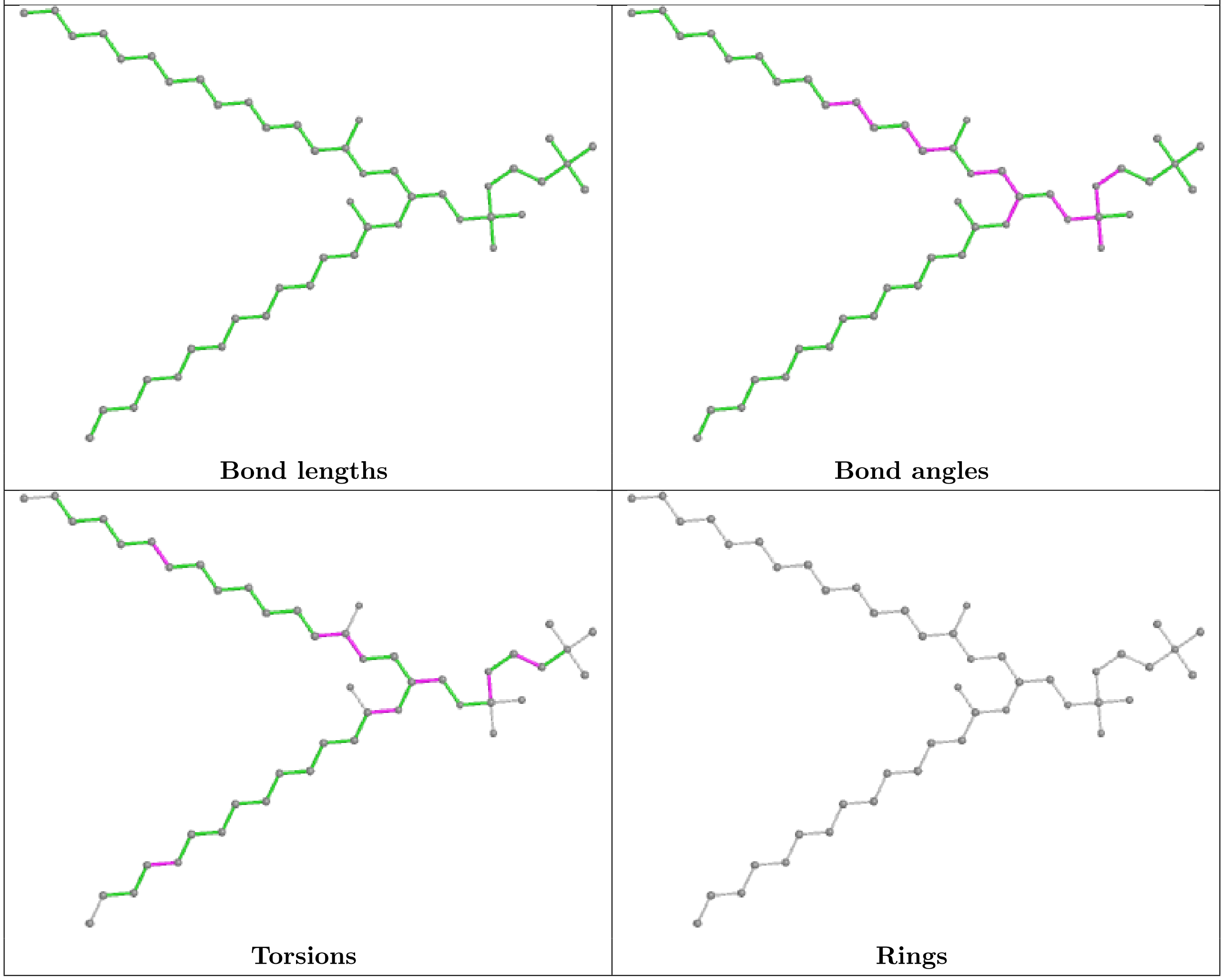


Rings

Ligand PX4 A 319



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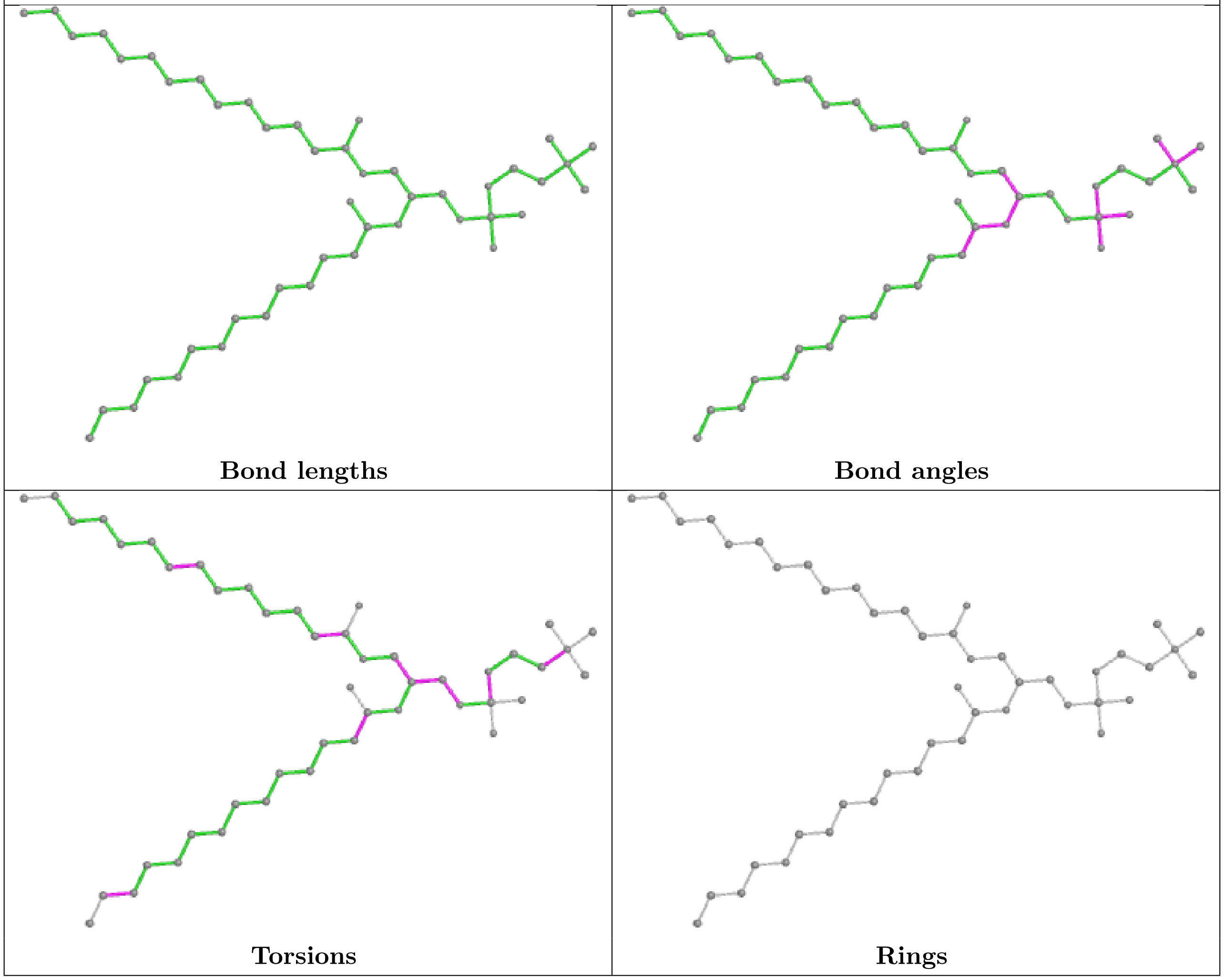
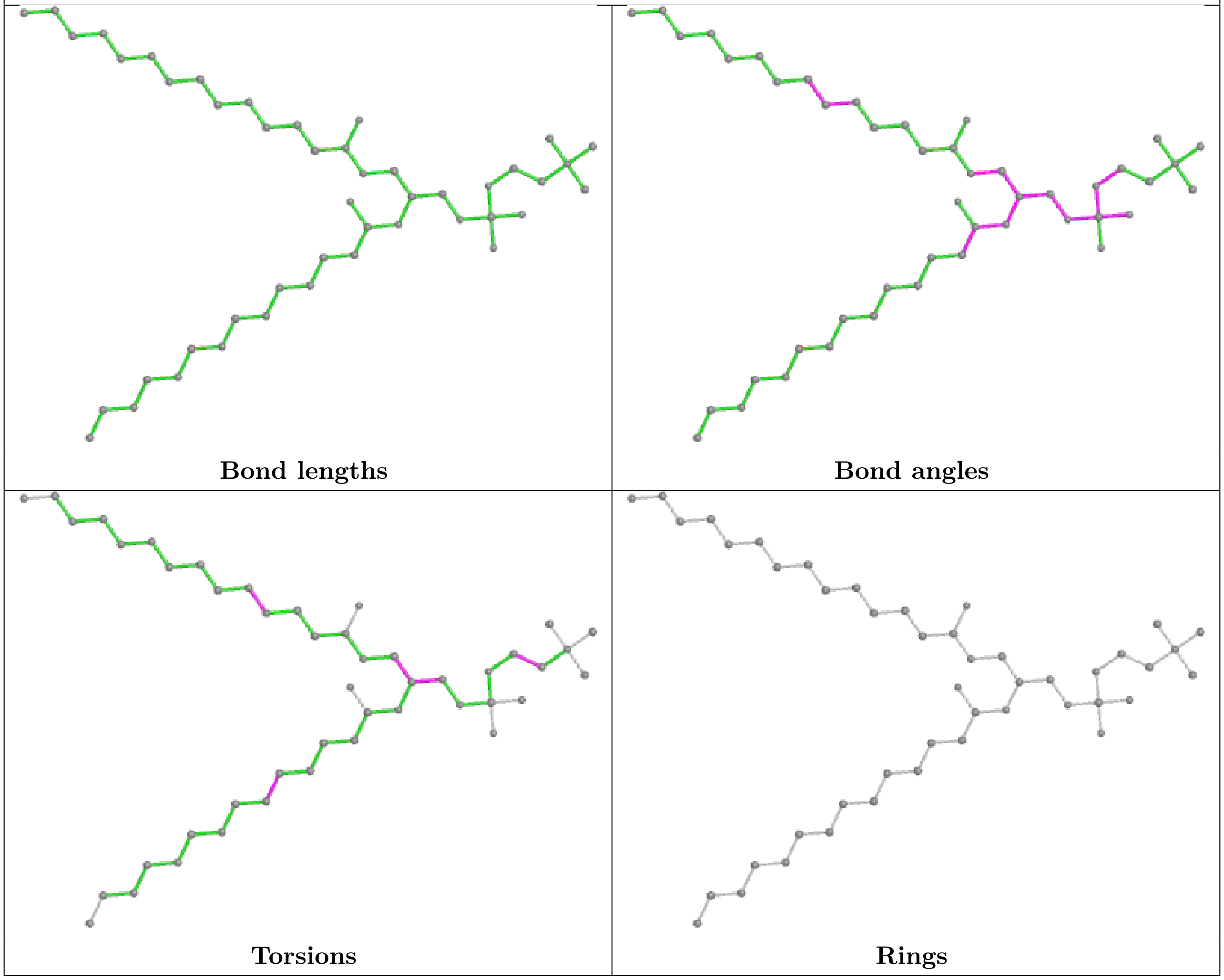
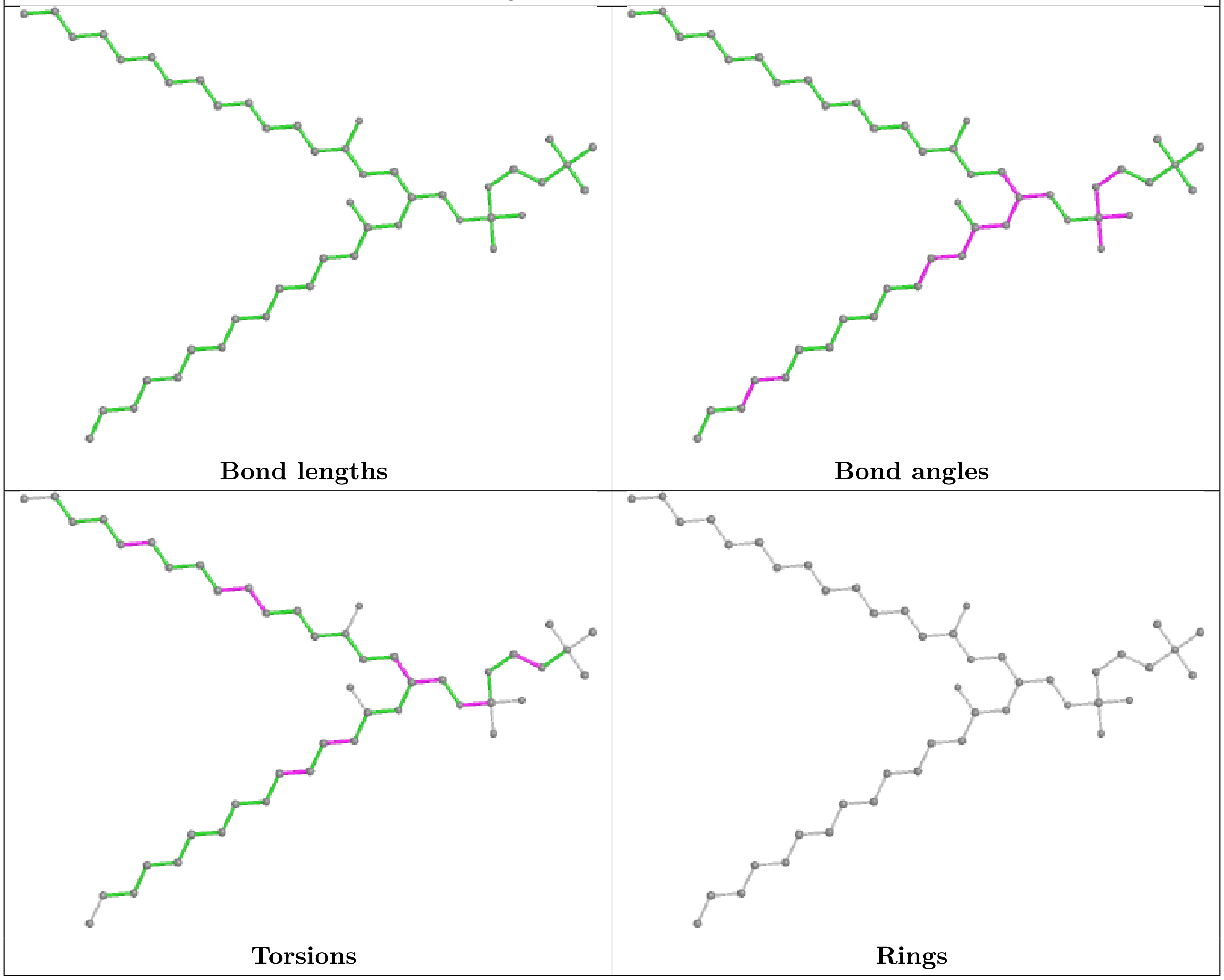


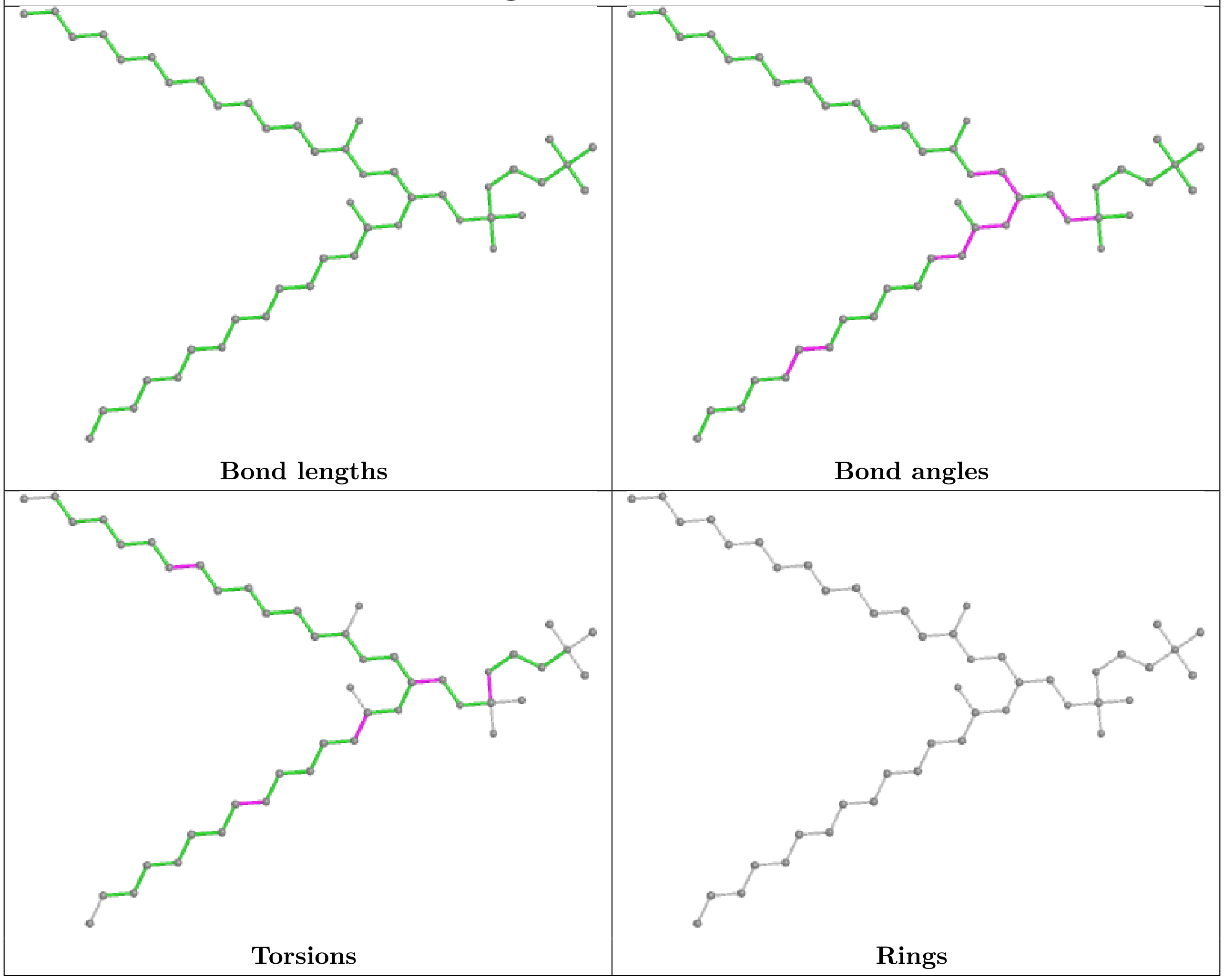
Ligand PX4 A 336



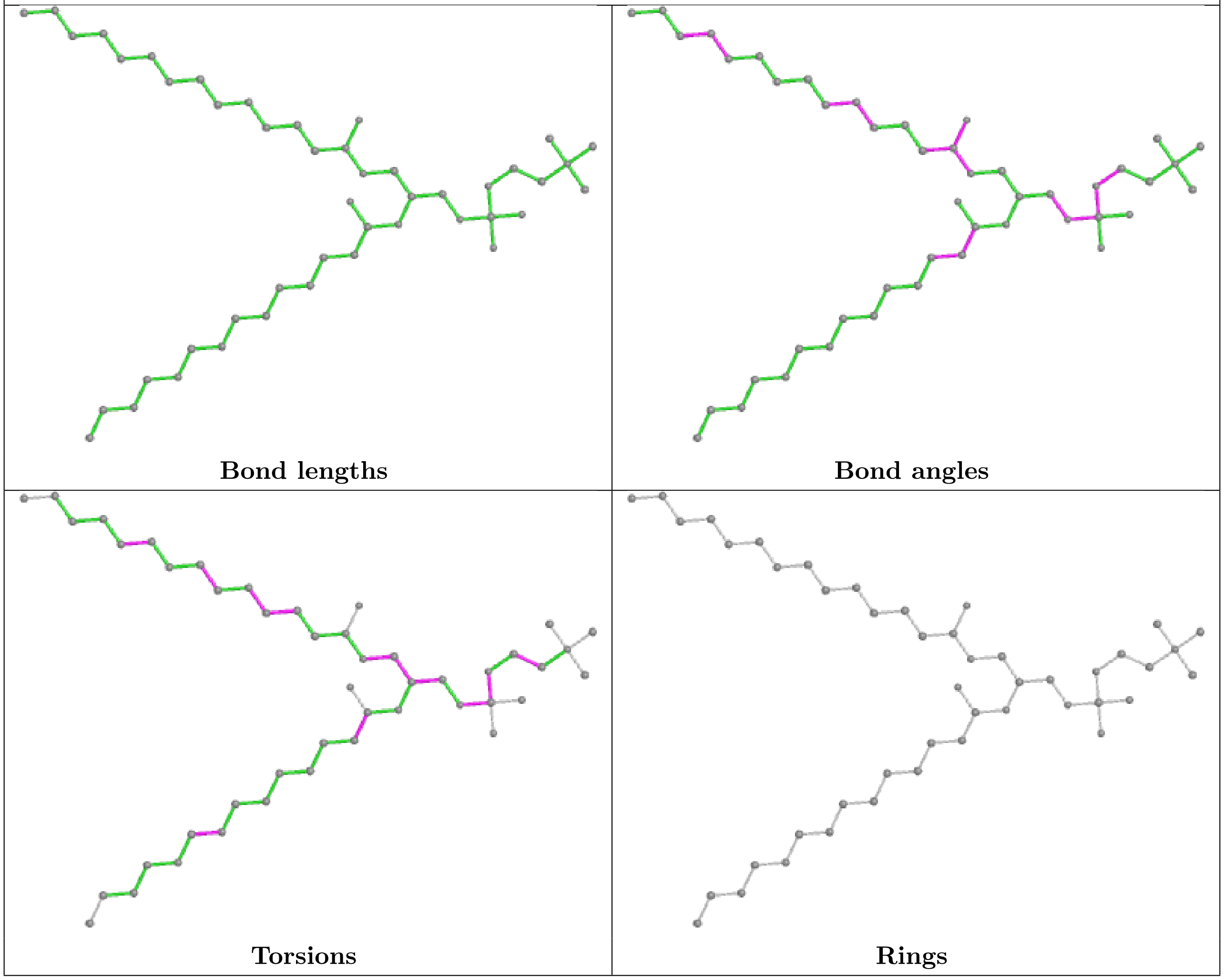
Ligand PX4 A 396



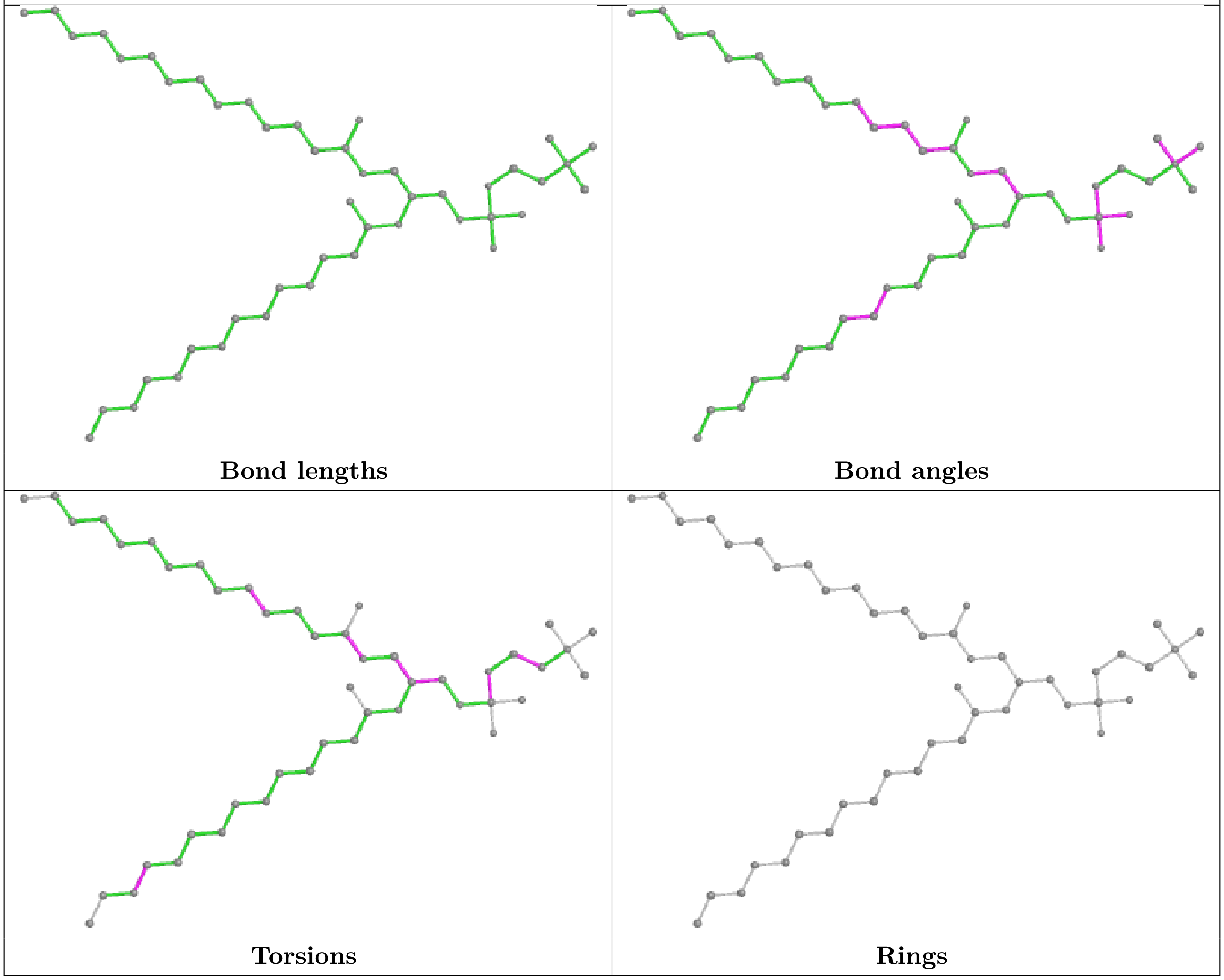
Ligand PX4 A 343



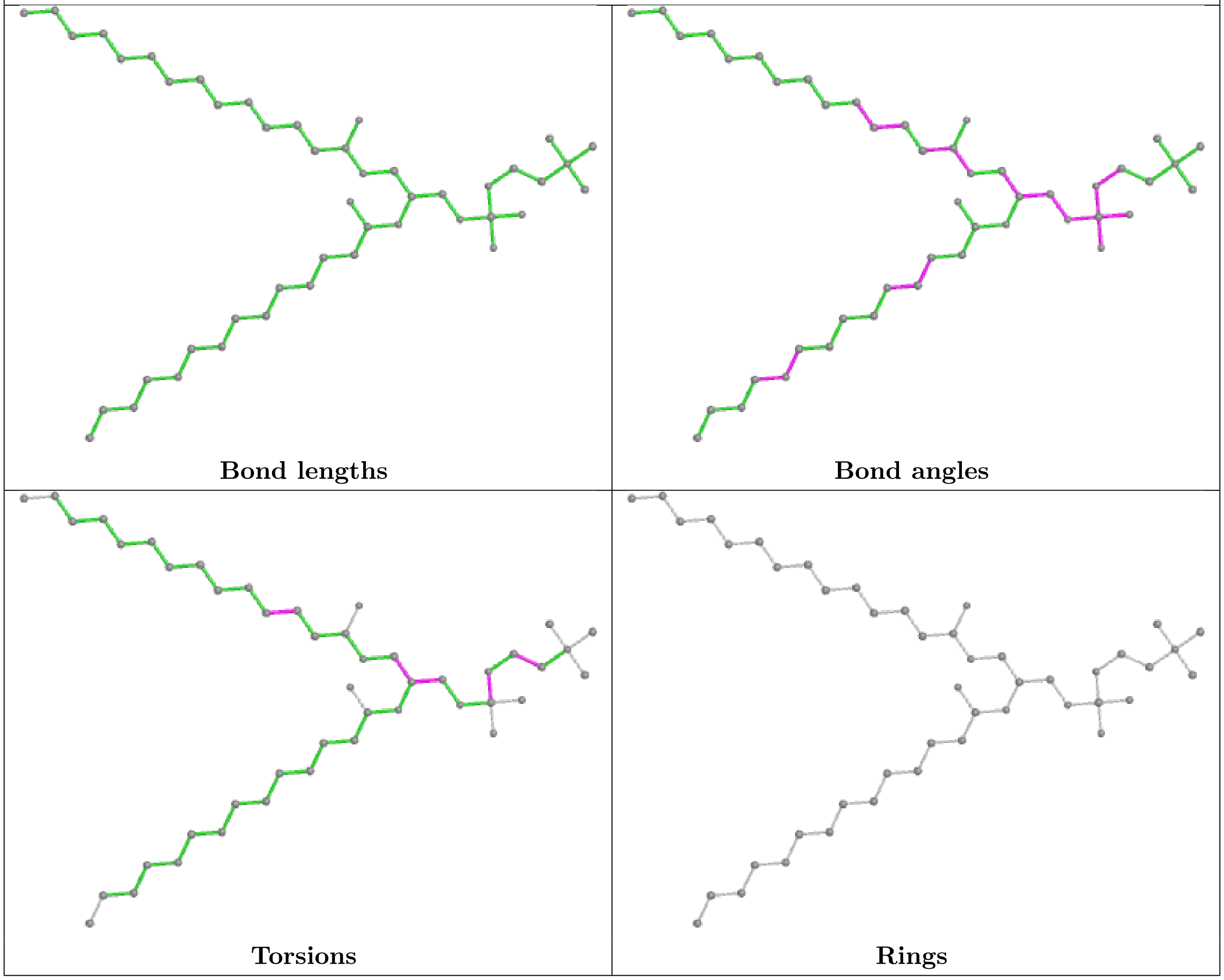
Ligand PX4 A 339

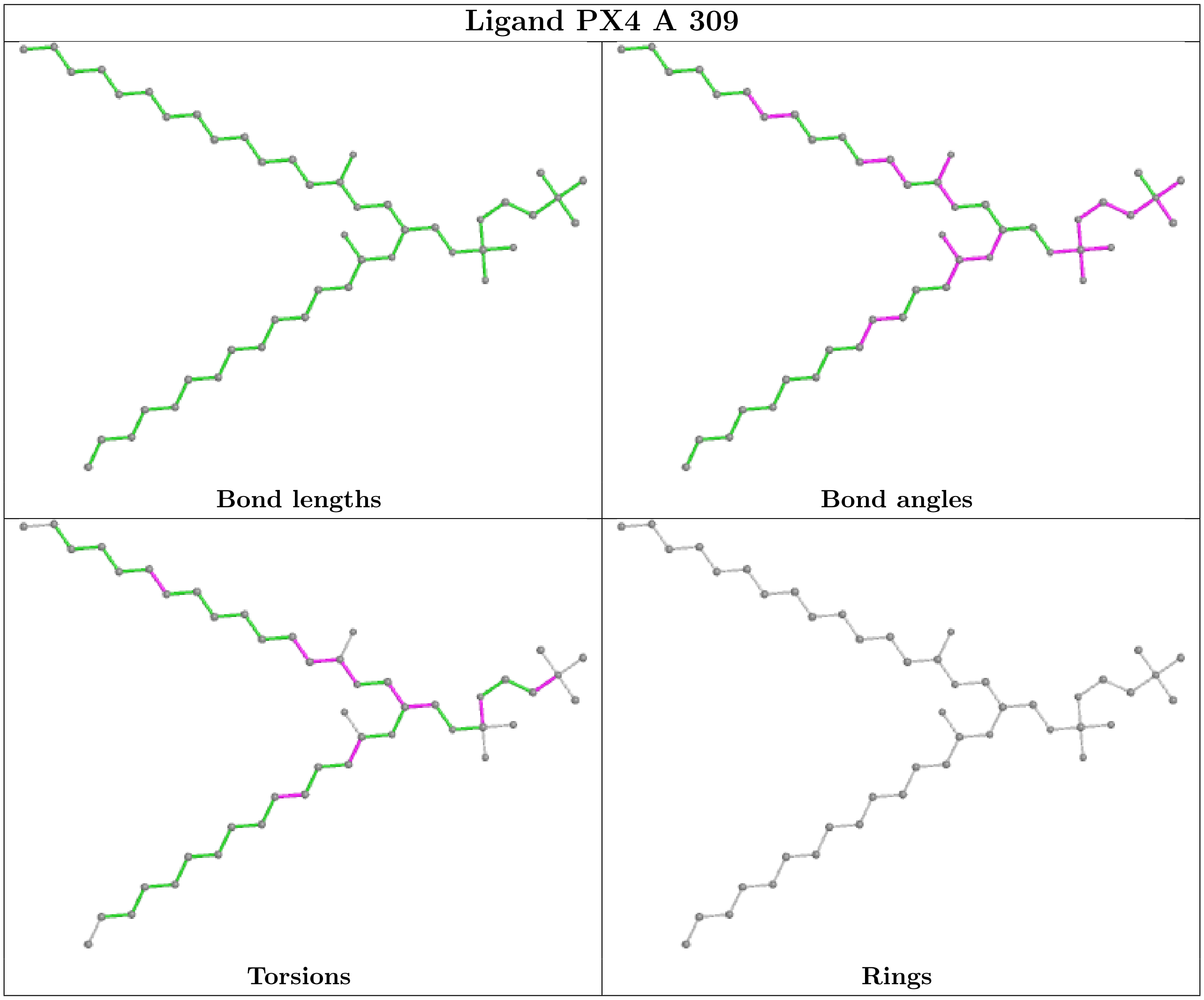


Ligand PX4 A 430

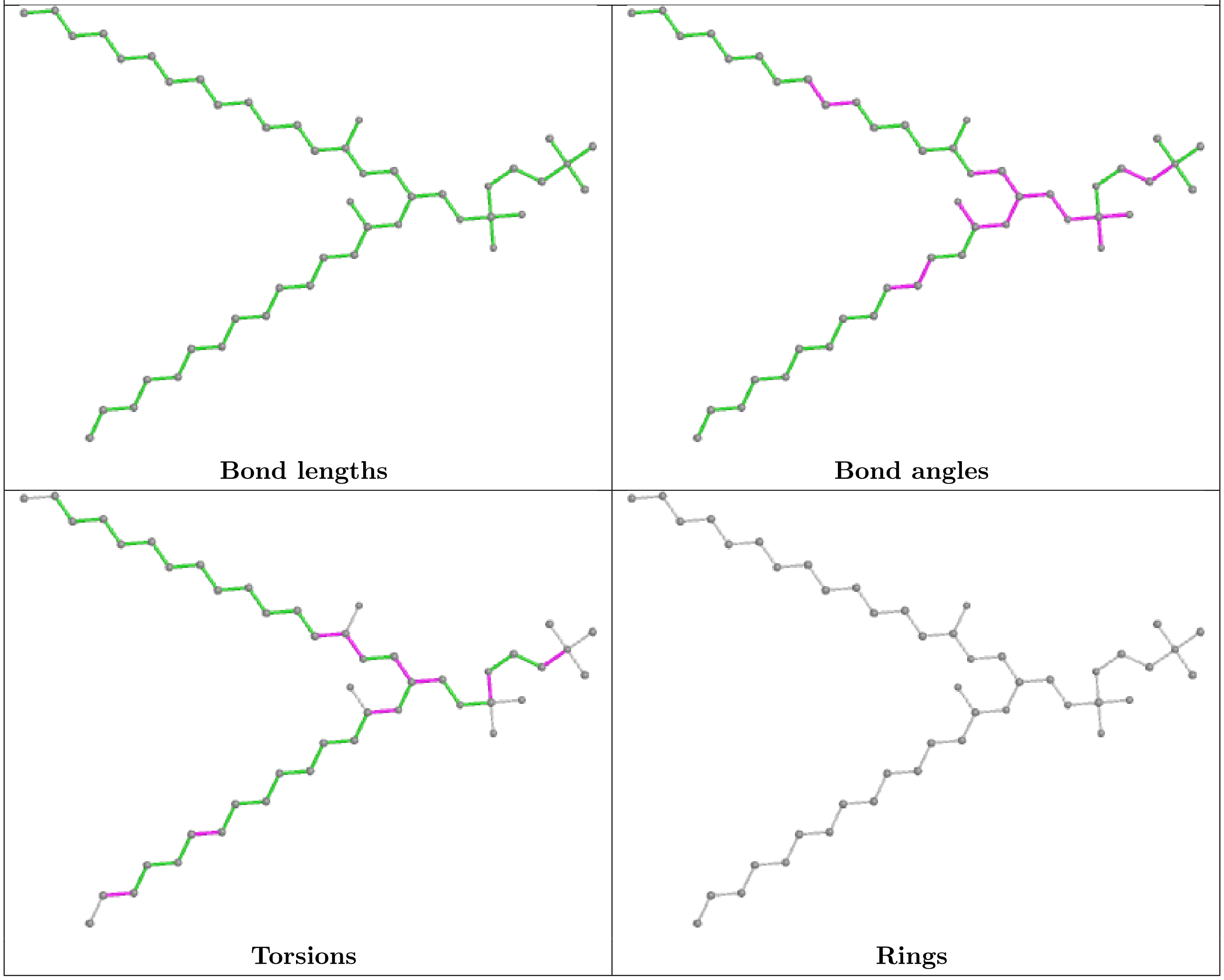


Ligand PX4 A 408

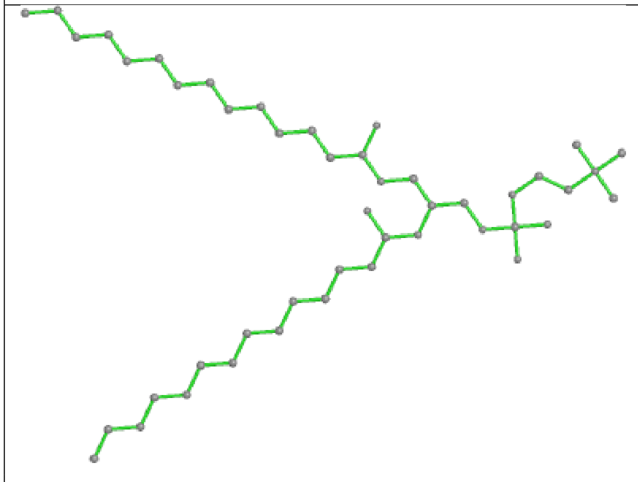



Ligand PX4 A 309
Bond lengths
Bond angles
Torsions
Rings

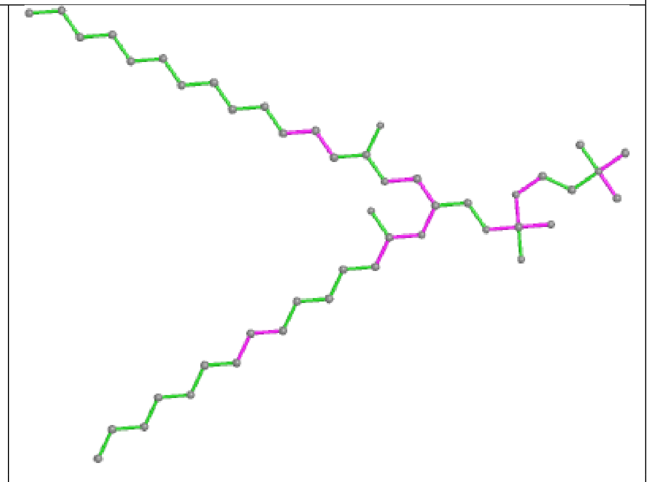
Ligand PX4 A 335



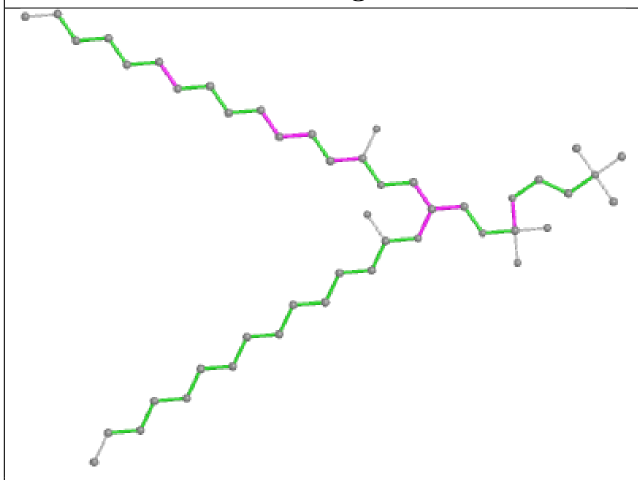
Ligand PX4 A 363



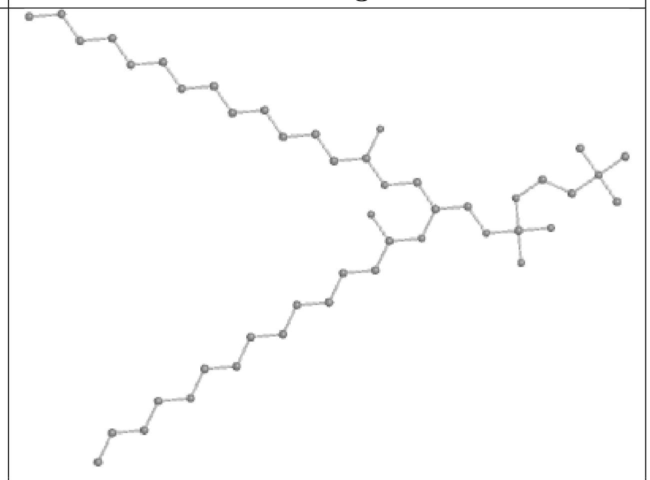
Bond lengths



Bond angles

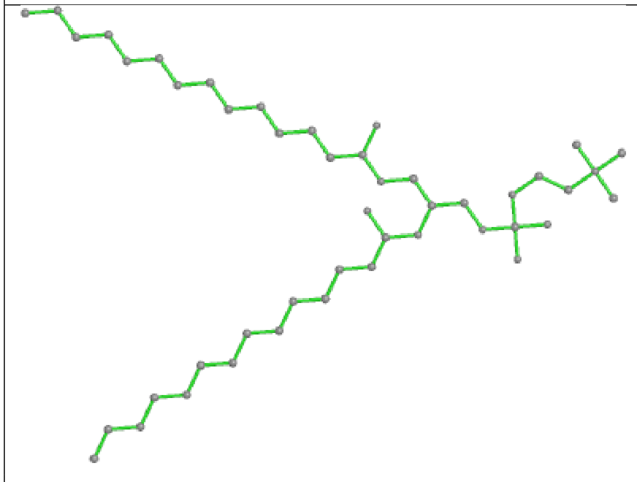


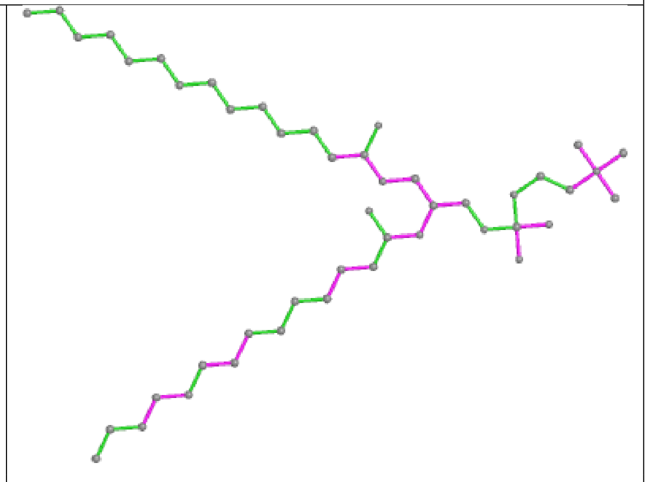
Torsions

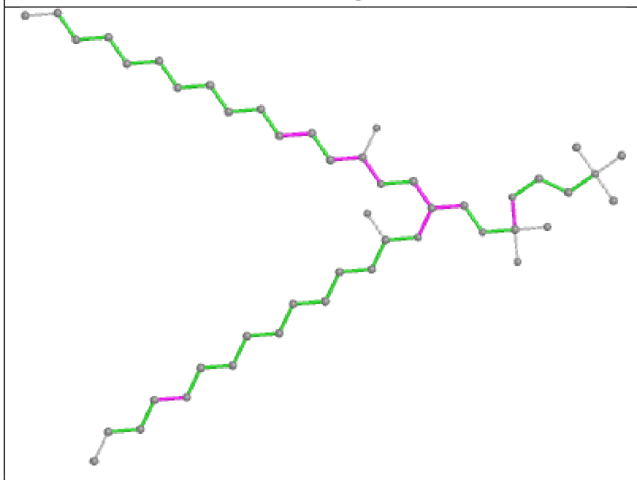


Rings

Ligand PX4 A 354


Bond lengths


Bond angles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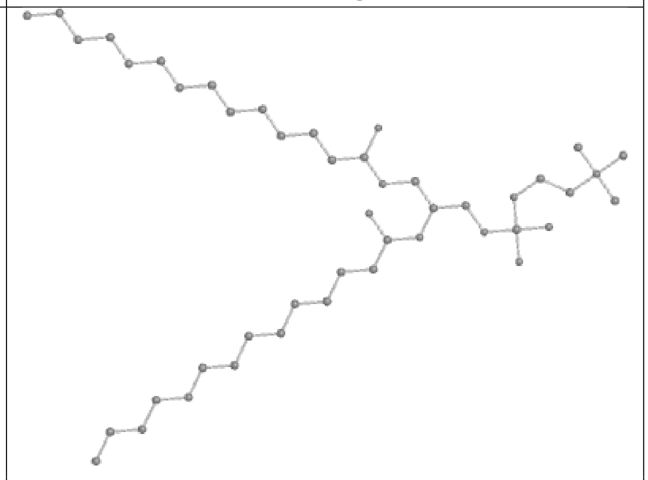
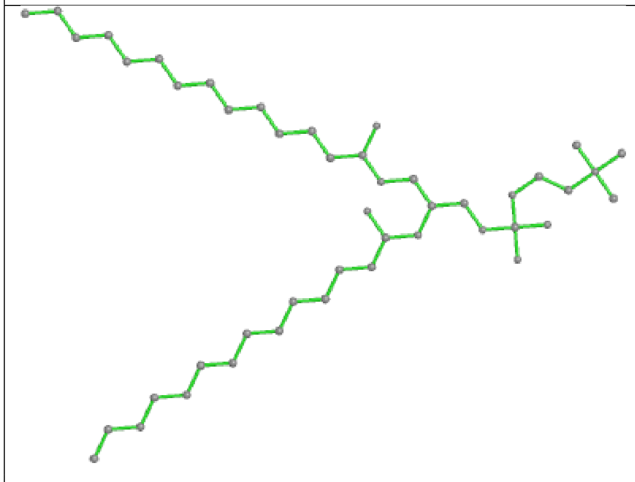
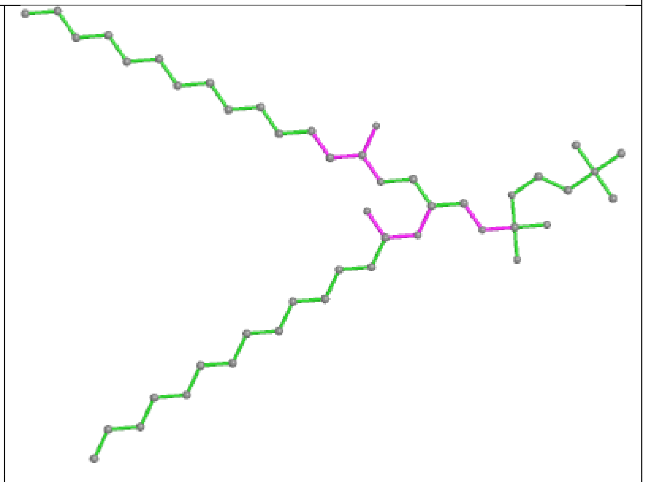

Rings

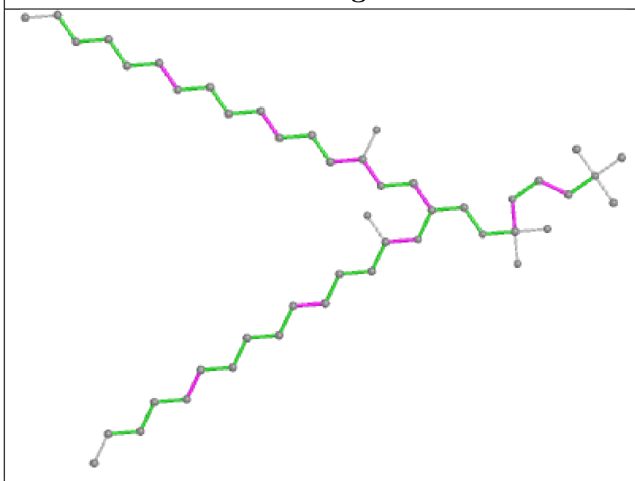
Ligand PX4 A 405



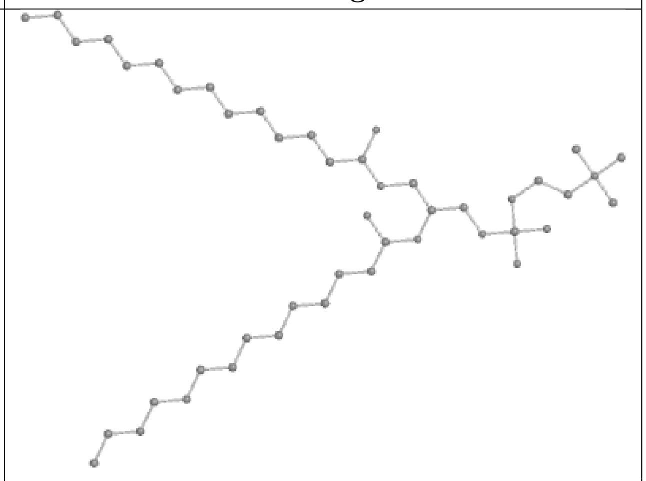
Bond lengths



Bond angles

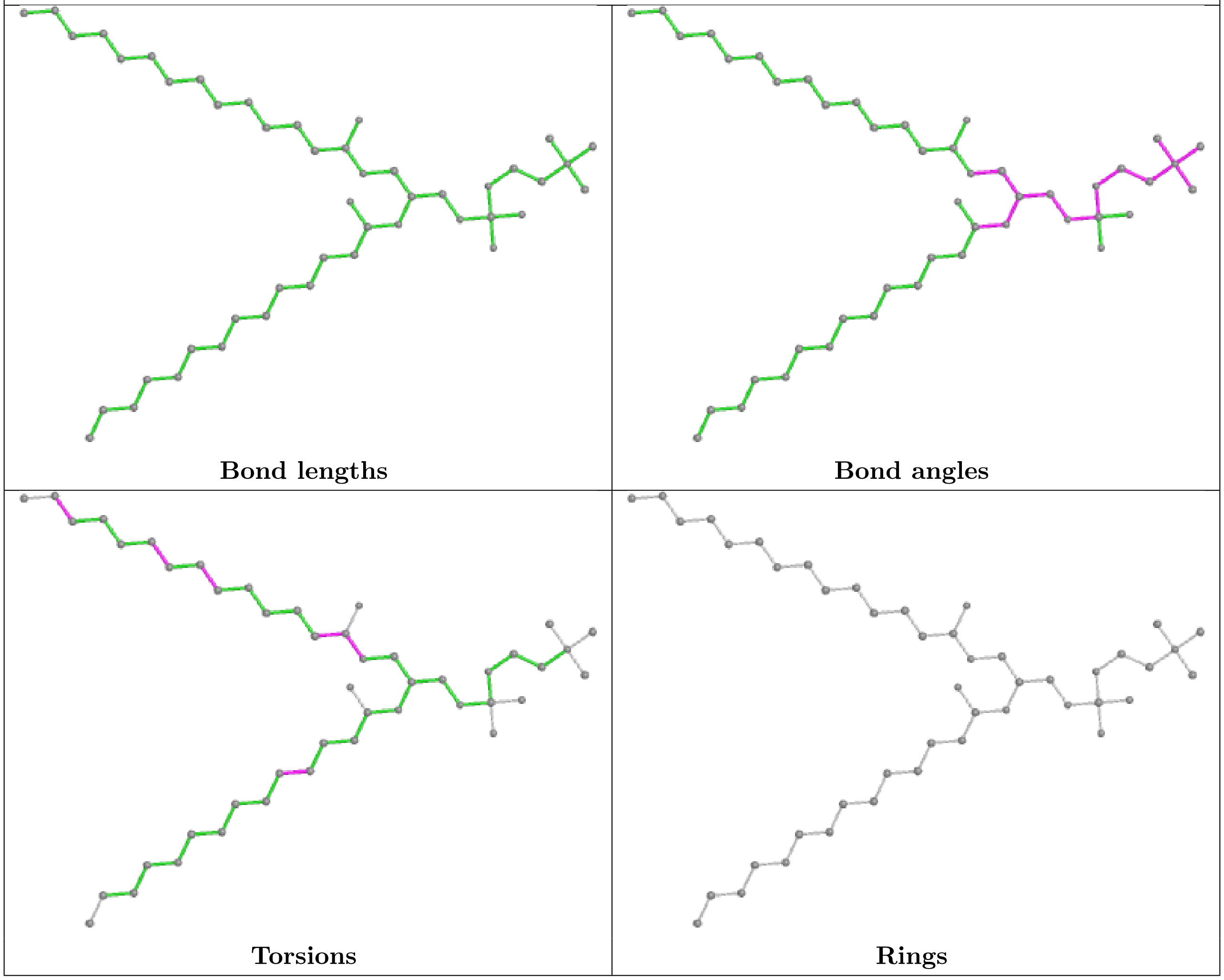


Torsions

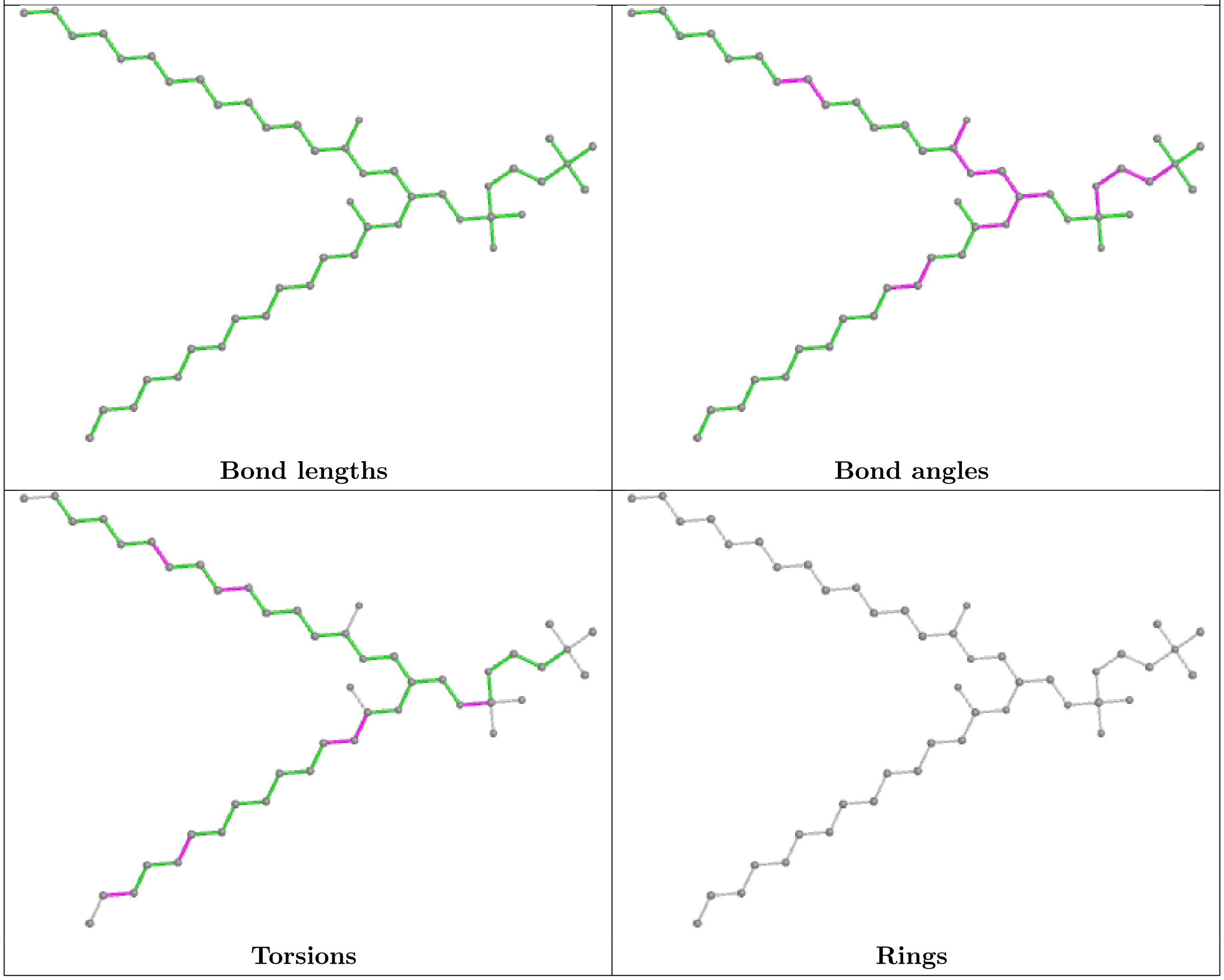


Rings

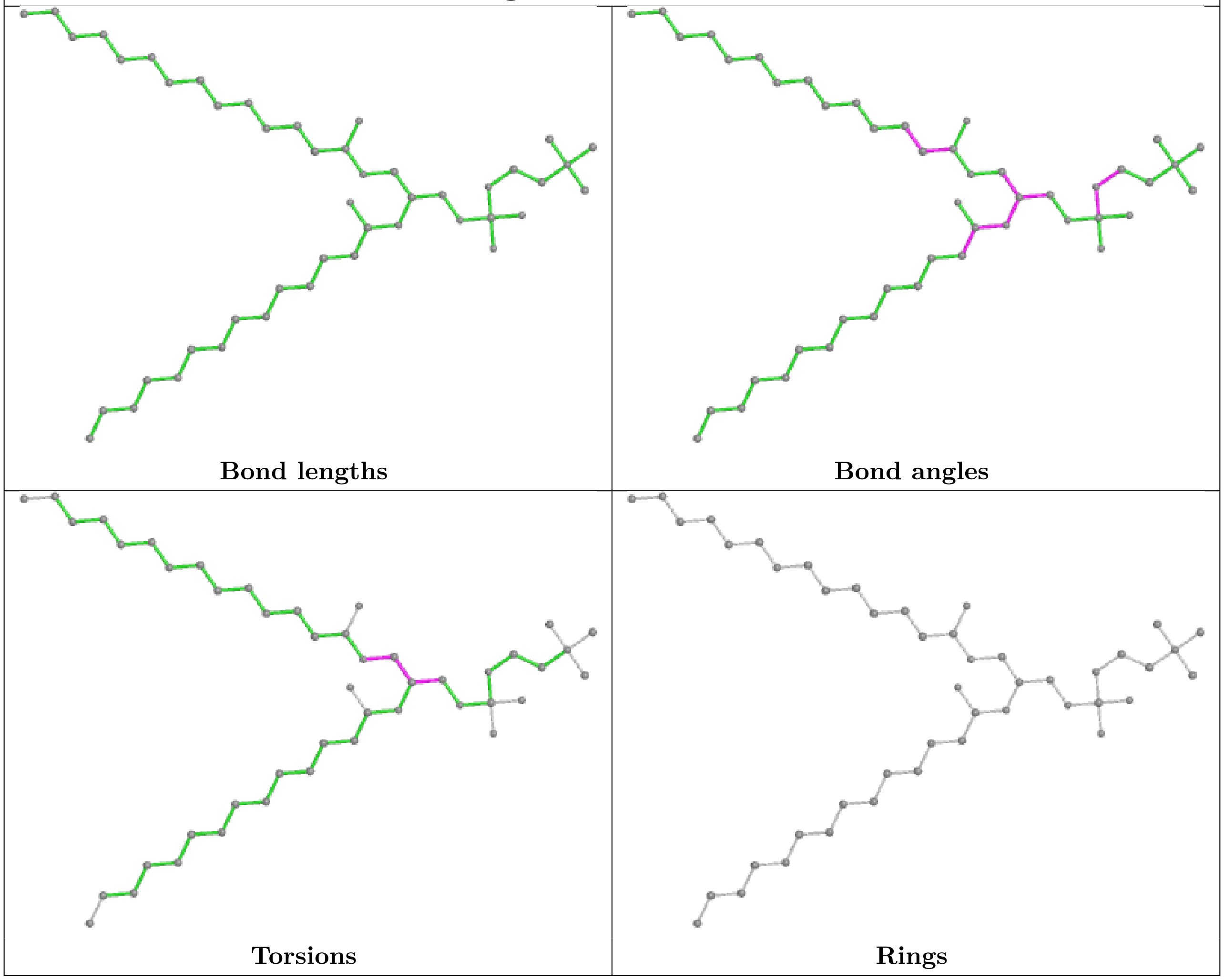
Ligand PX4 A 400



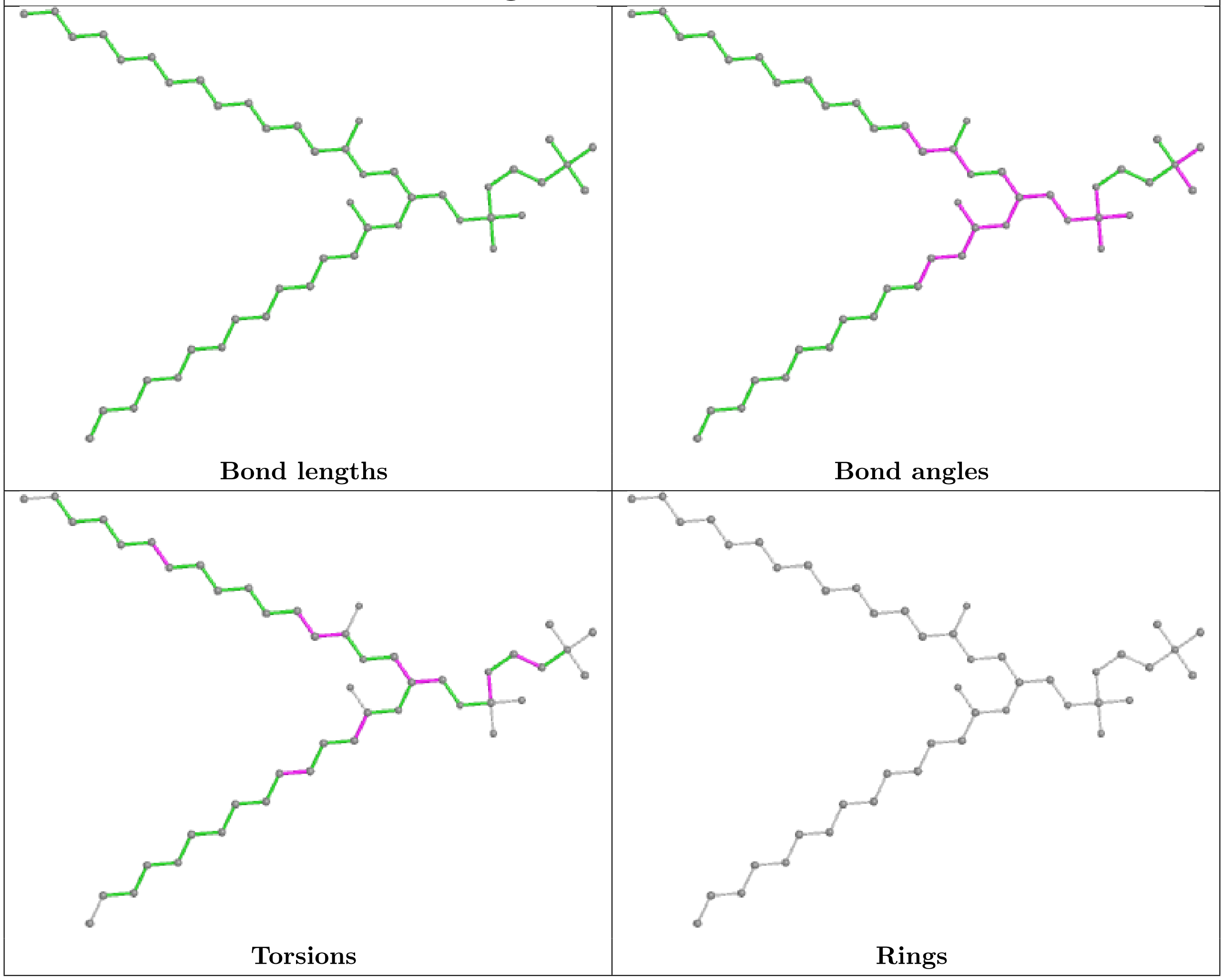
Ligand PX4 A 337



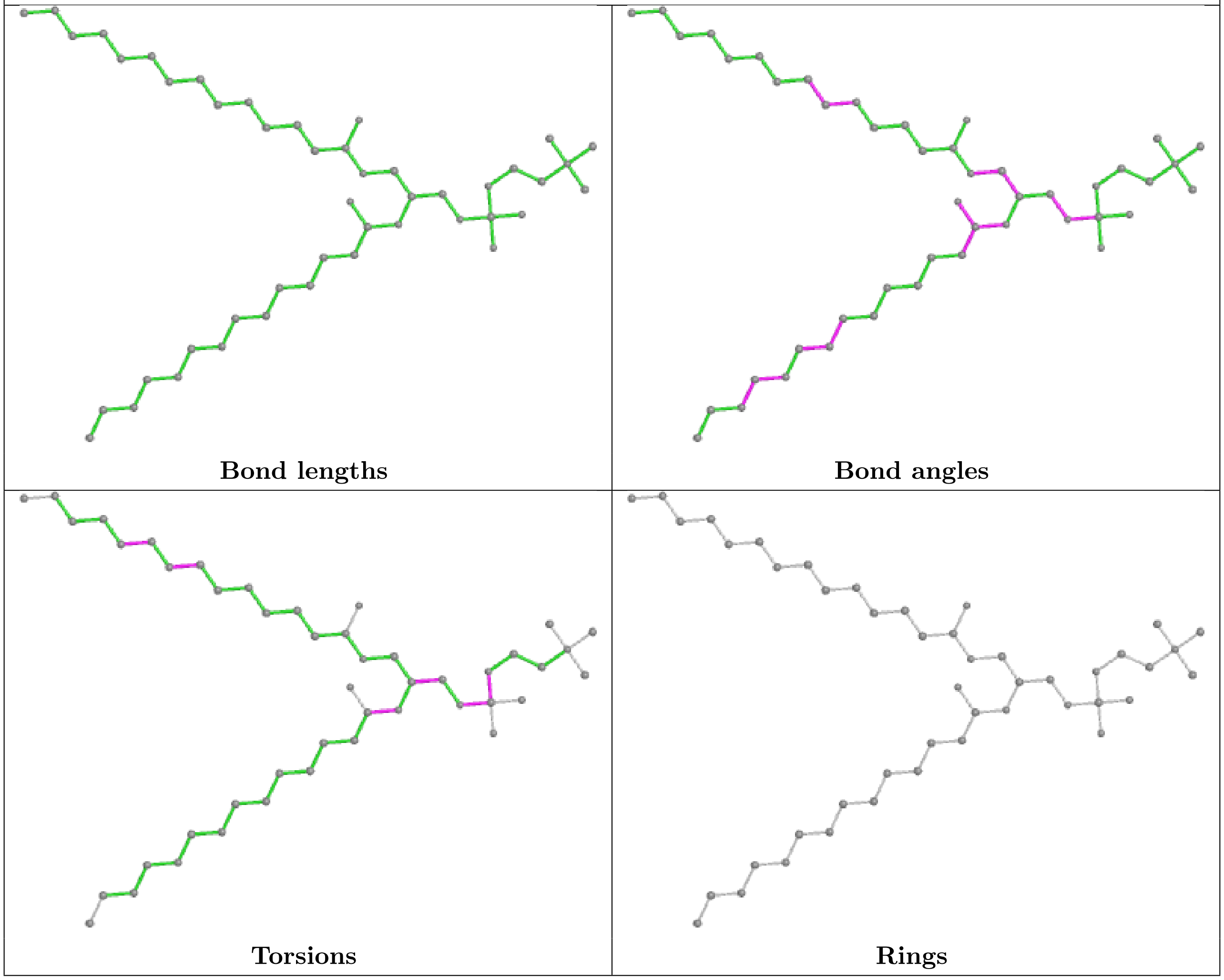
Ligand PX4 A 350



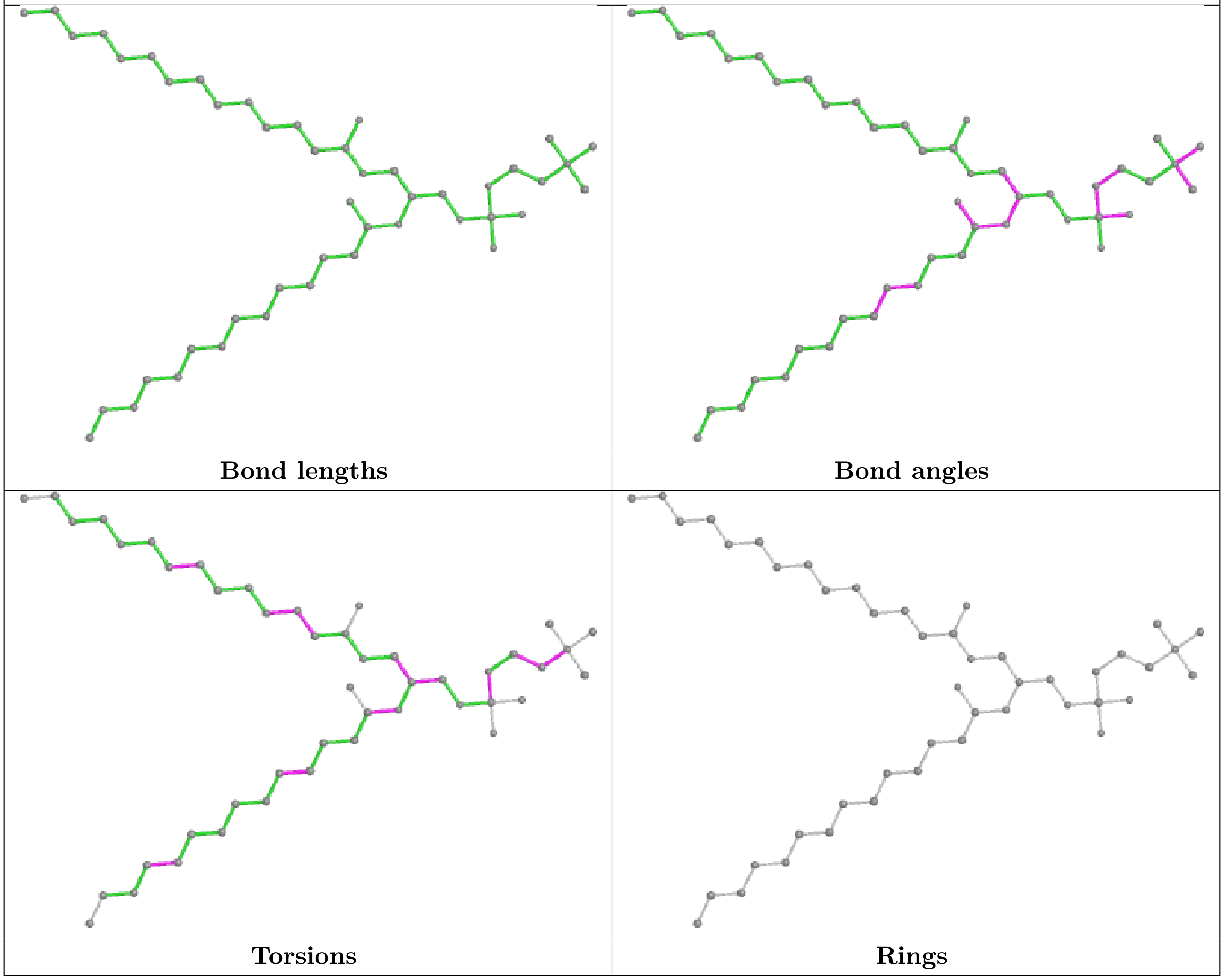
Ligand PX4 A 333



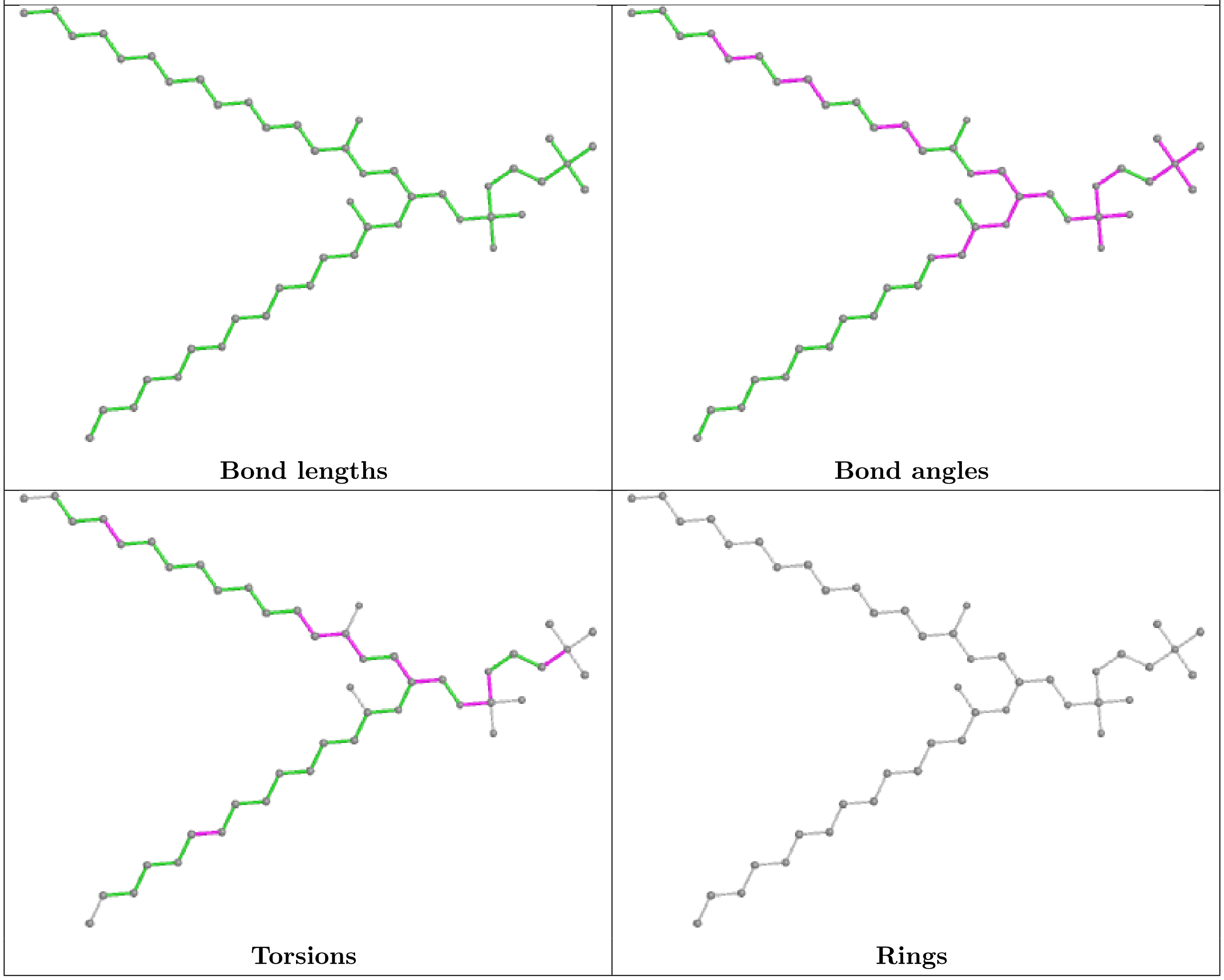
Ligand PX4 A 307



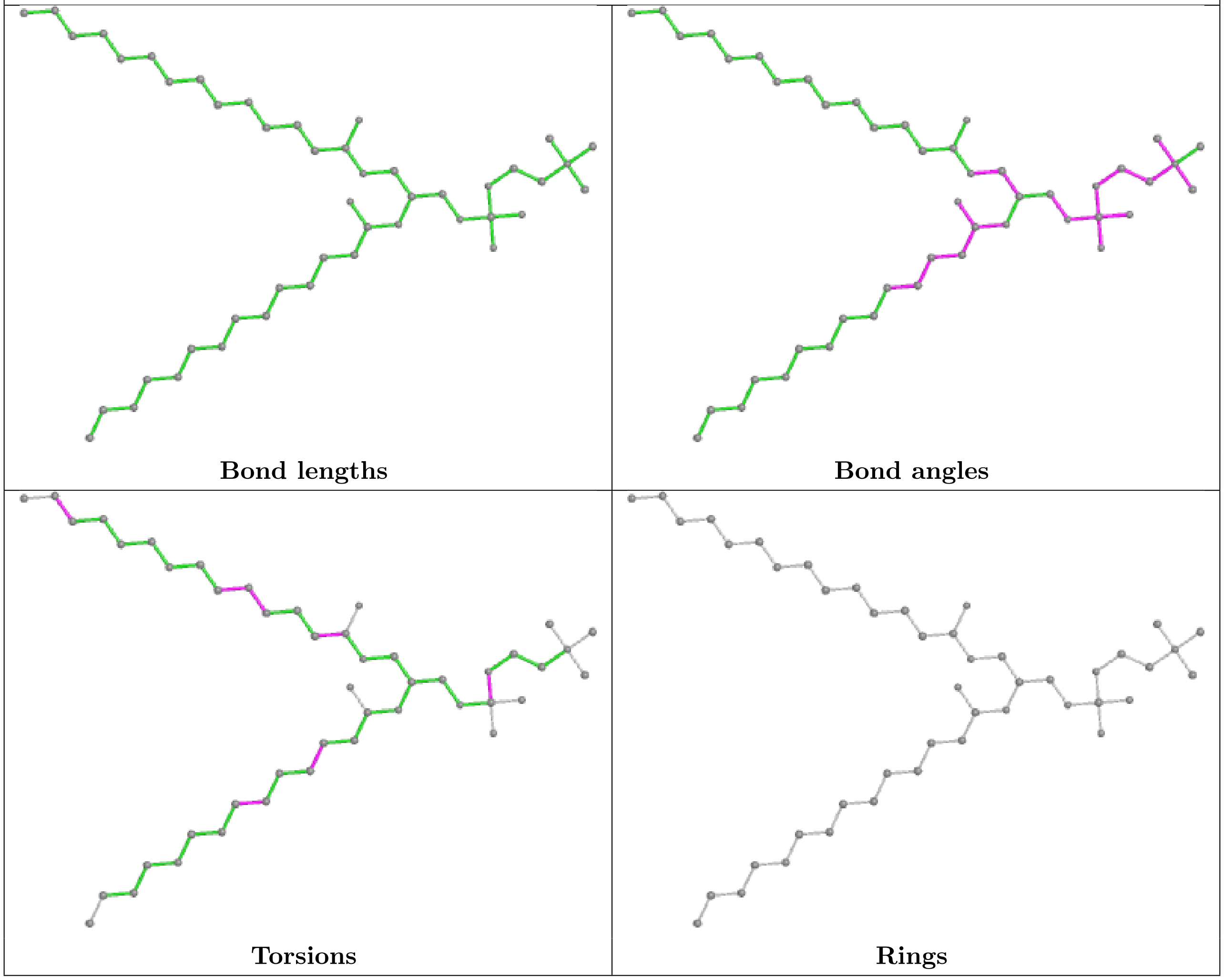
Ligand PX4 A 329



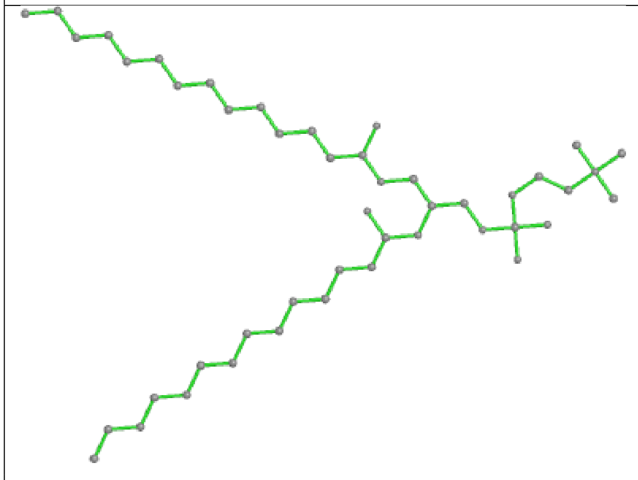
Ligand PX4 A 412



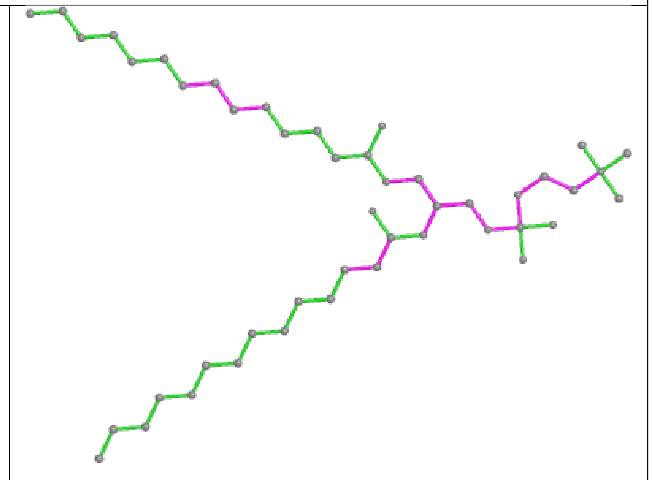
Ligand PX4 A 308



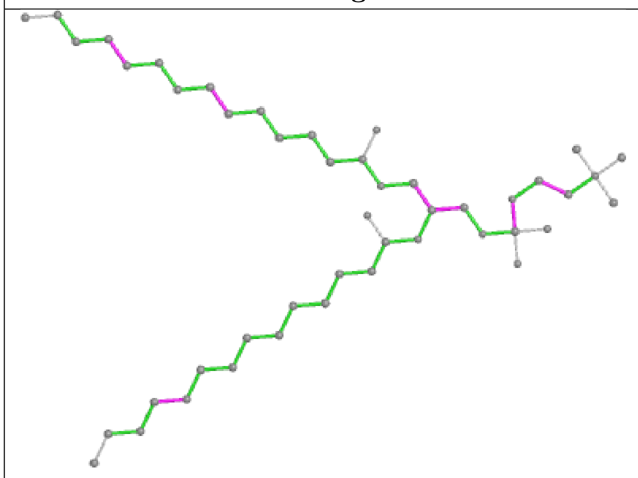
Ligand PX4 A 427



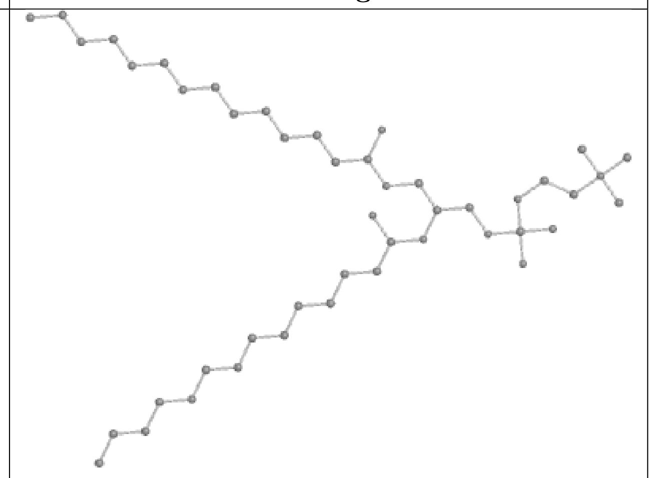
Bond lengths



Bond angles

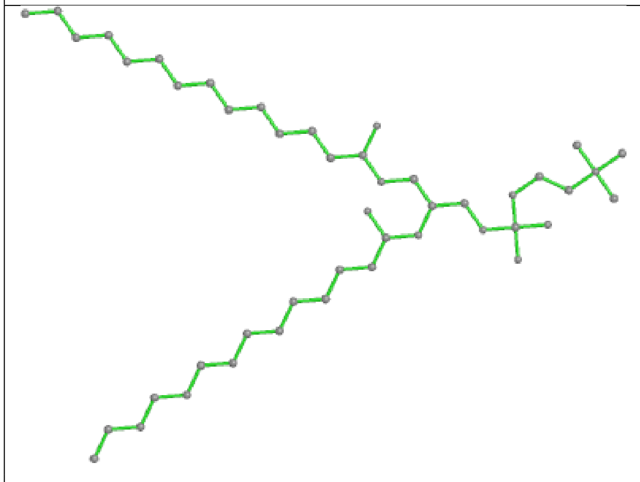


Torsions

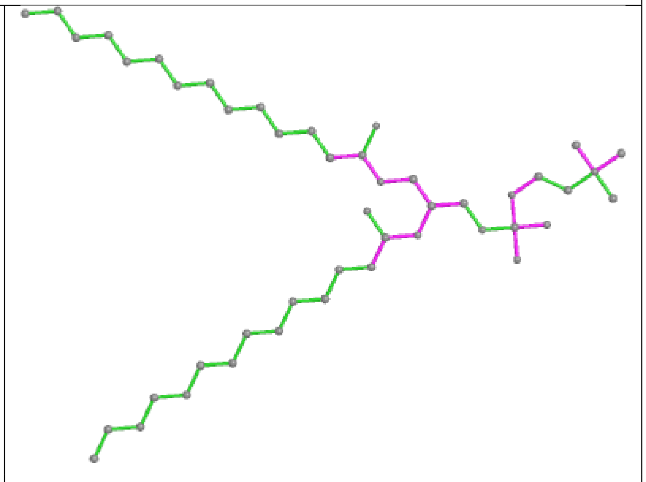


Rings

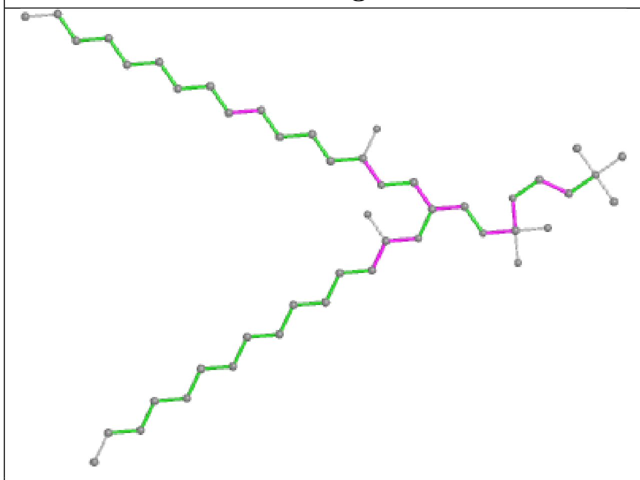
Ligand PX4 A 358



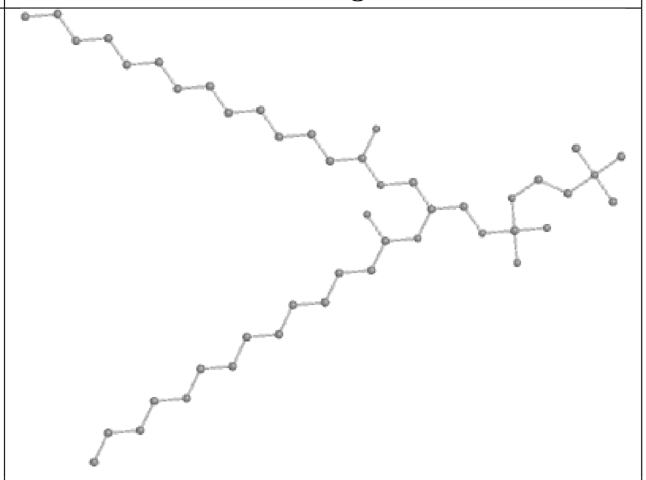
Bond lengths



Bond angles

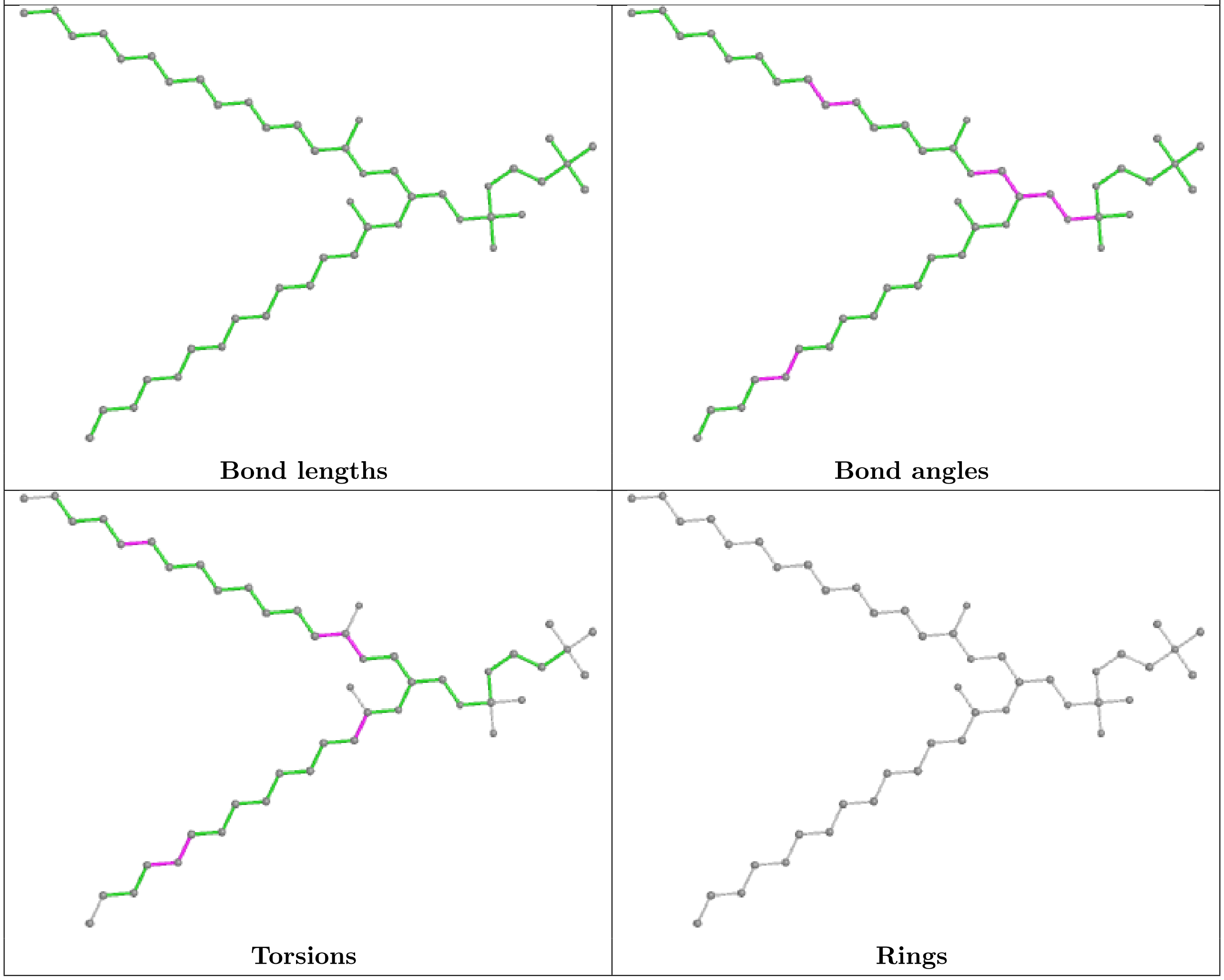


Torsions



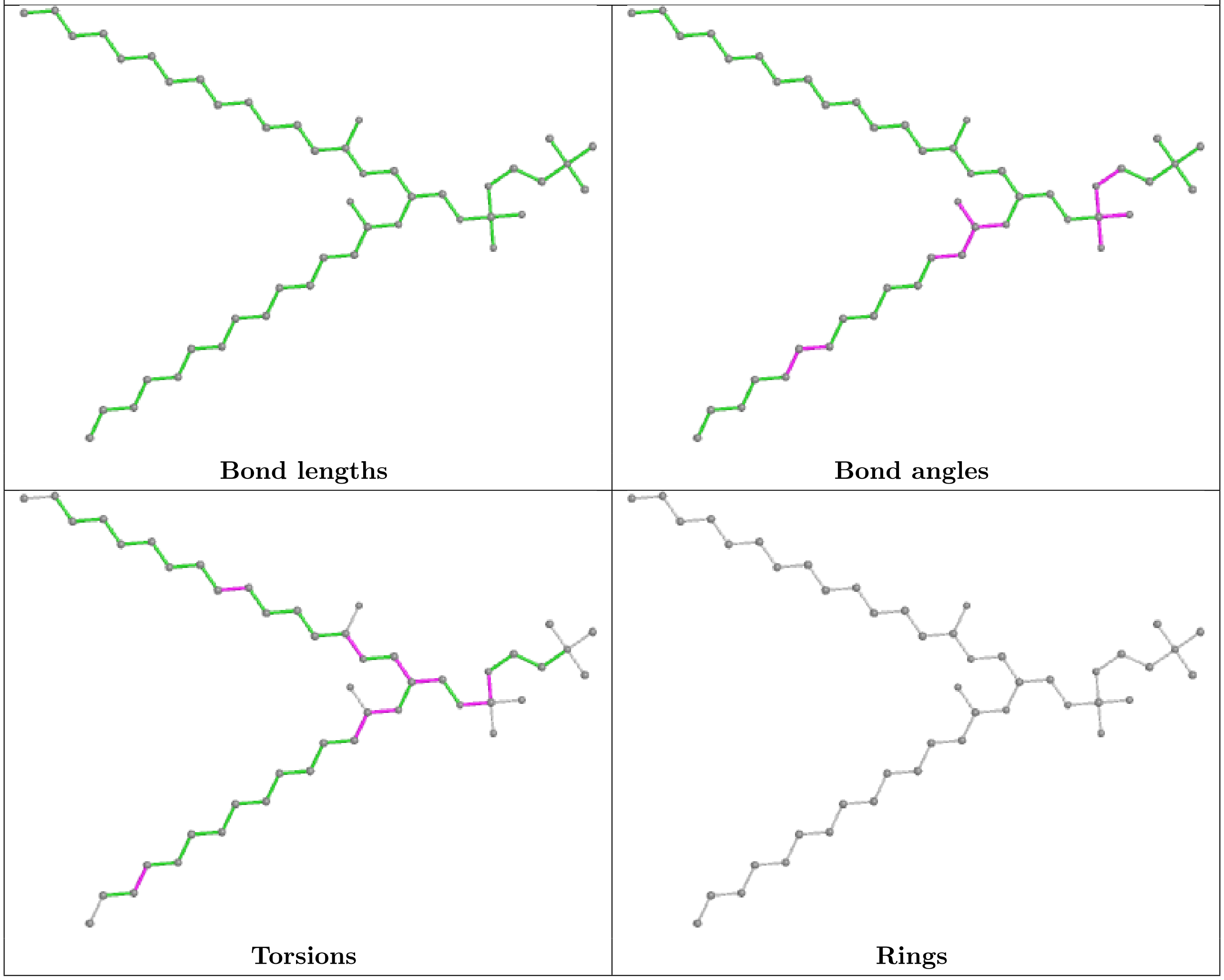
Rings

Ligand PX4 A 389

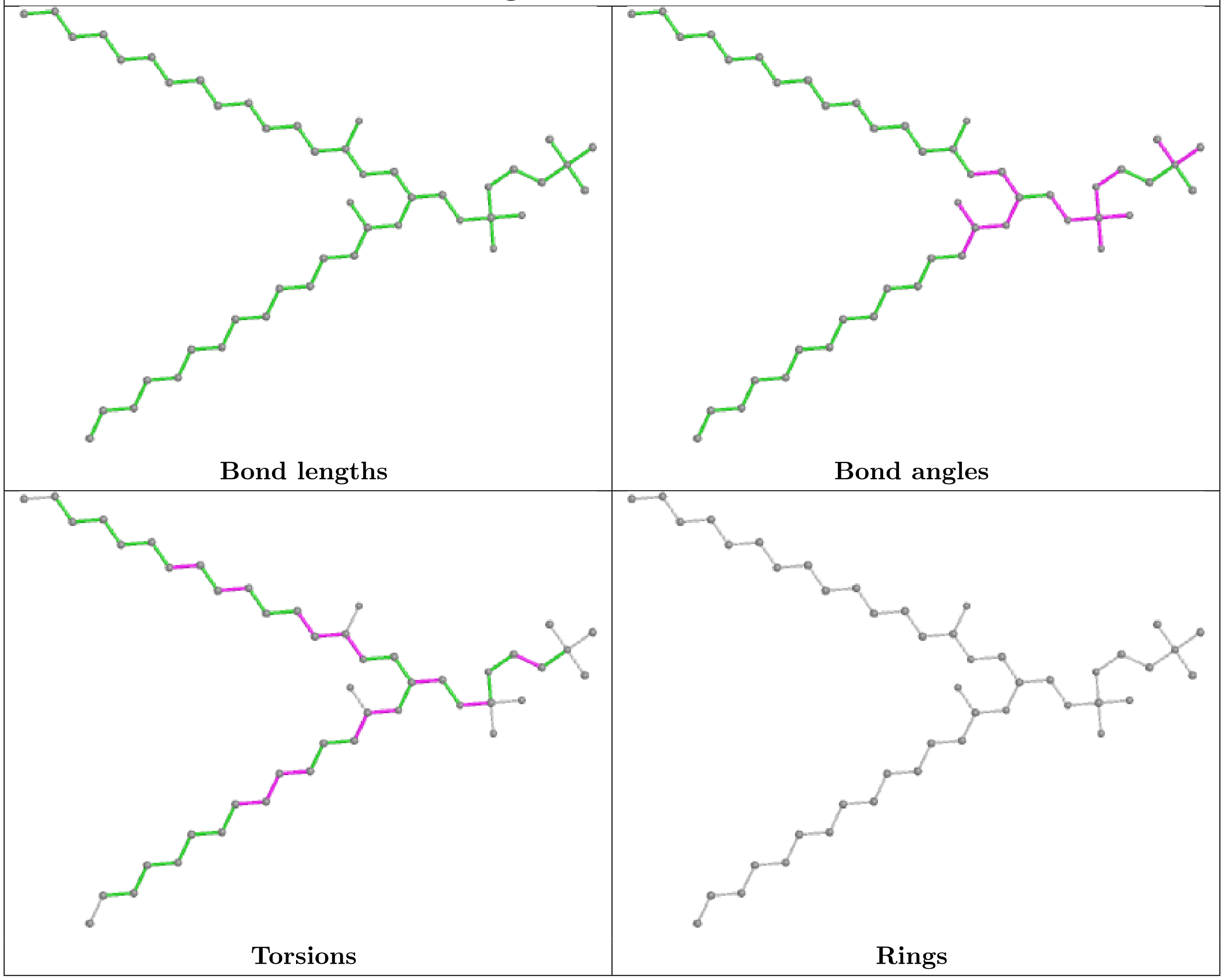


Bond lengths | Bond angles | Torsions | Rings

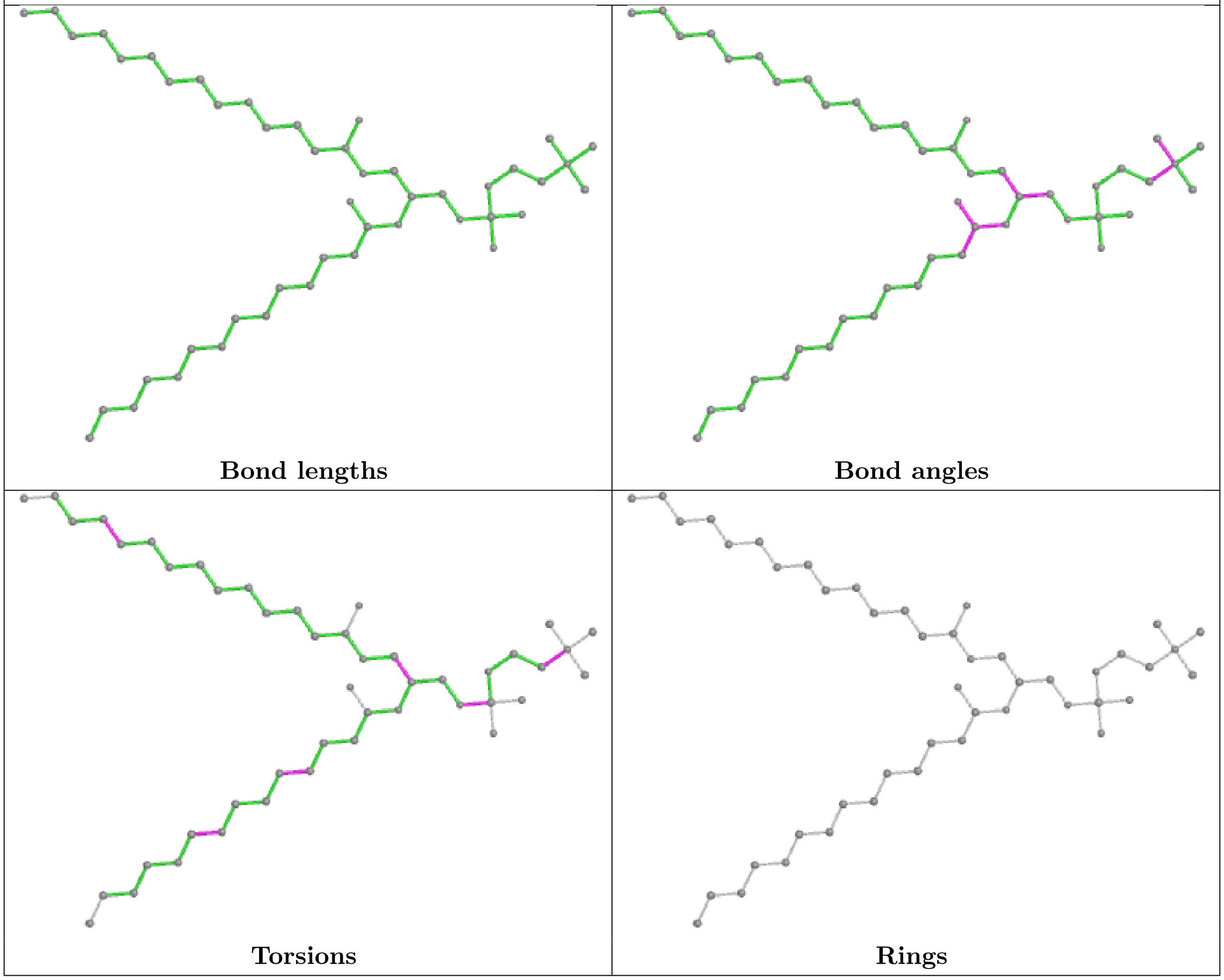
Ligand PX4 A 407



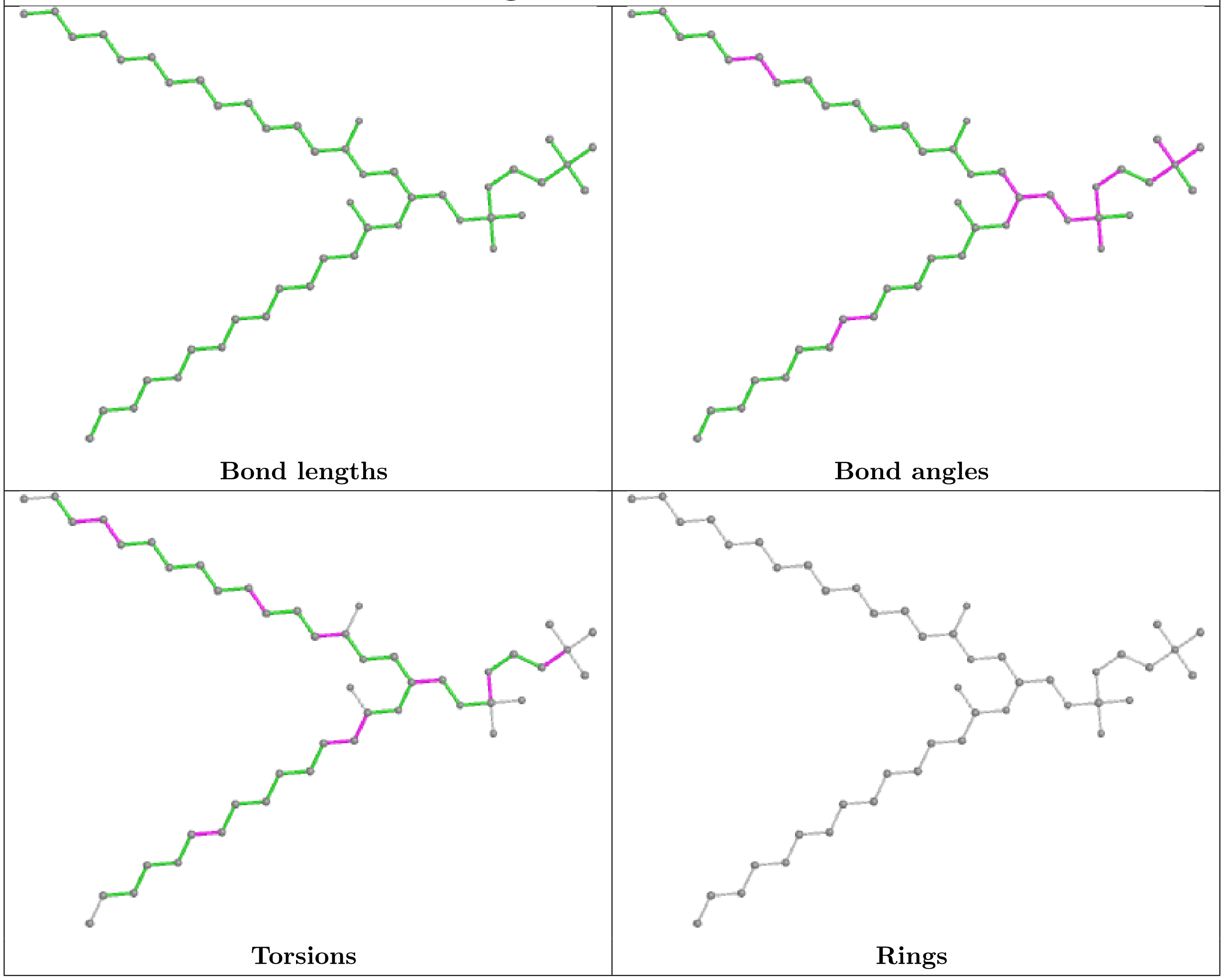
Ligand PX4 A 327



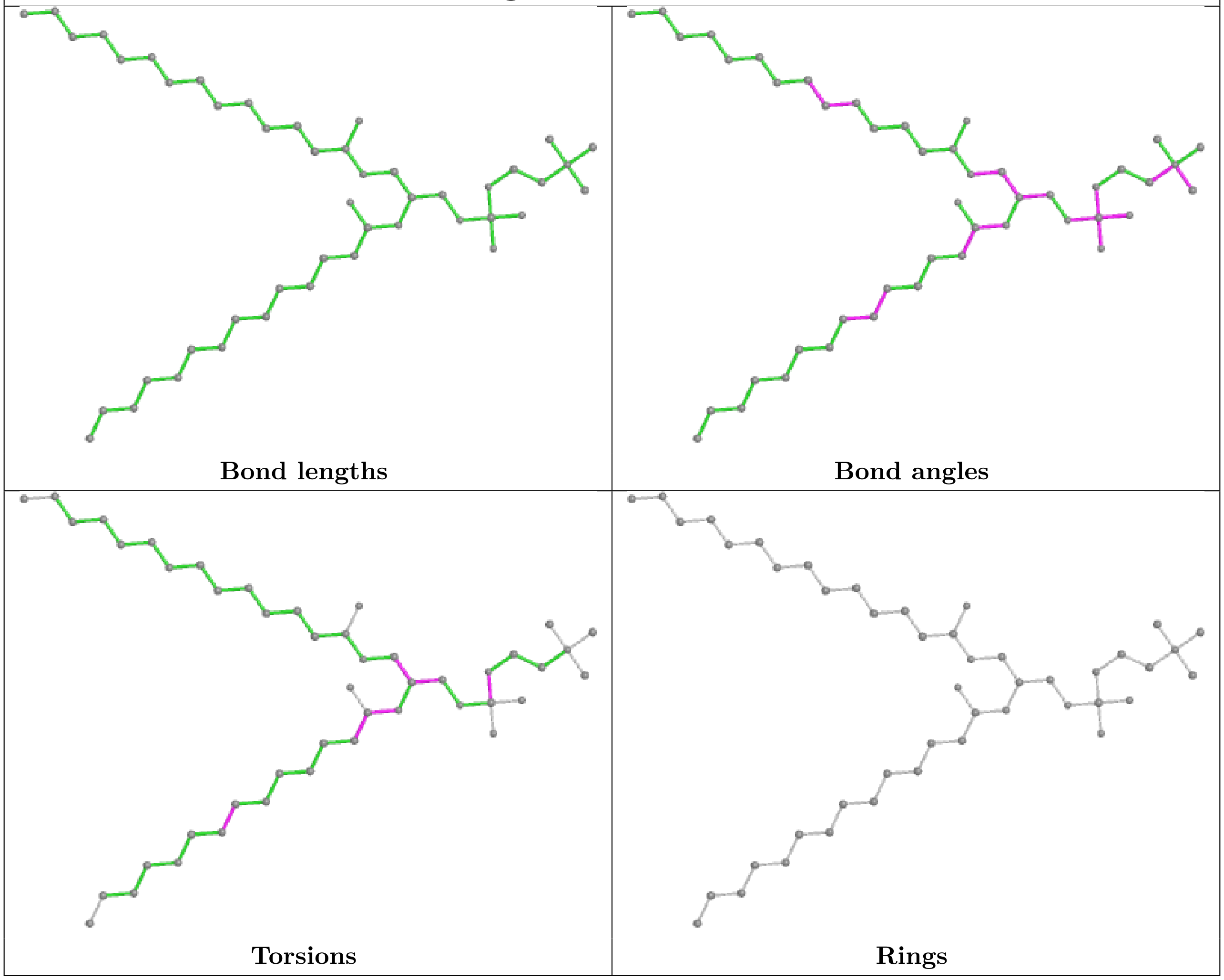
Ligand PX4 A 344

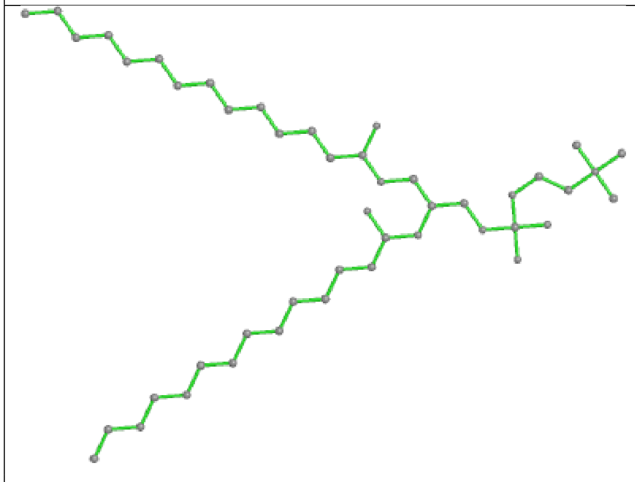
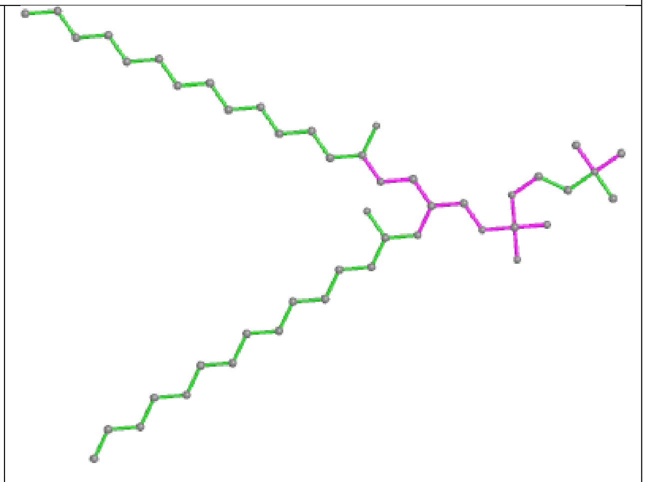
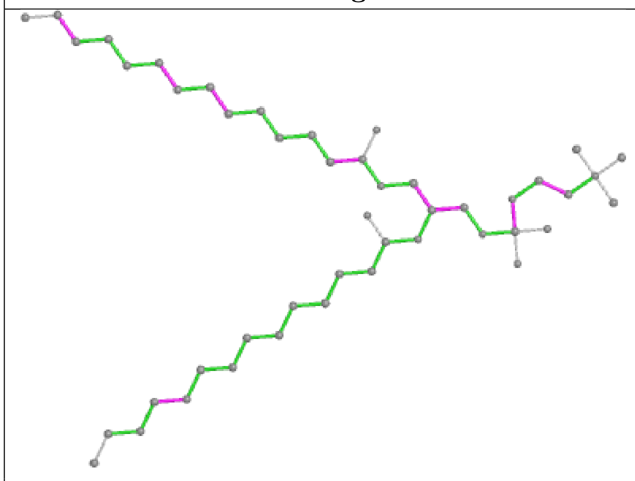
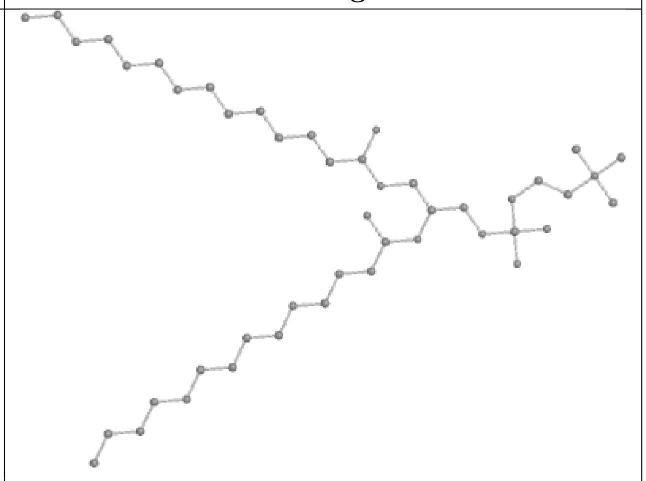


Ligand PX4 A 321

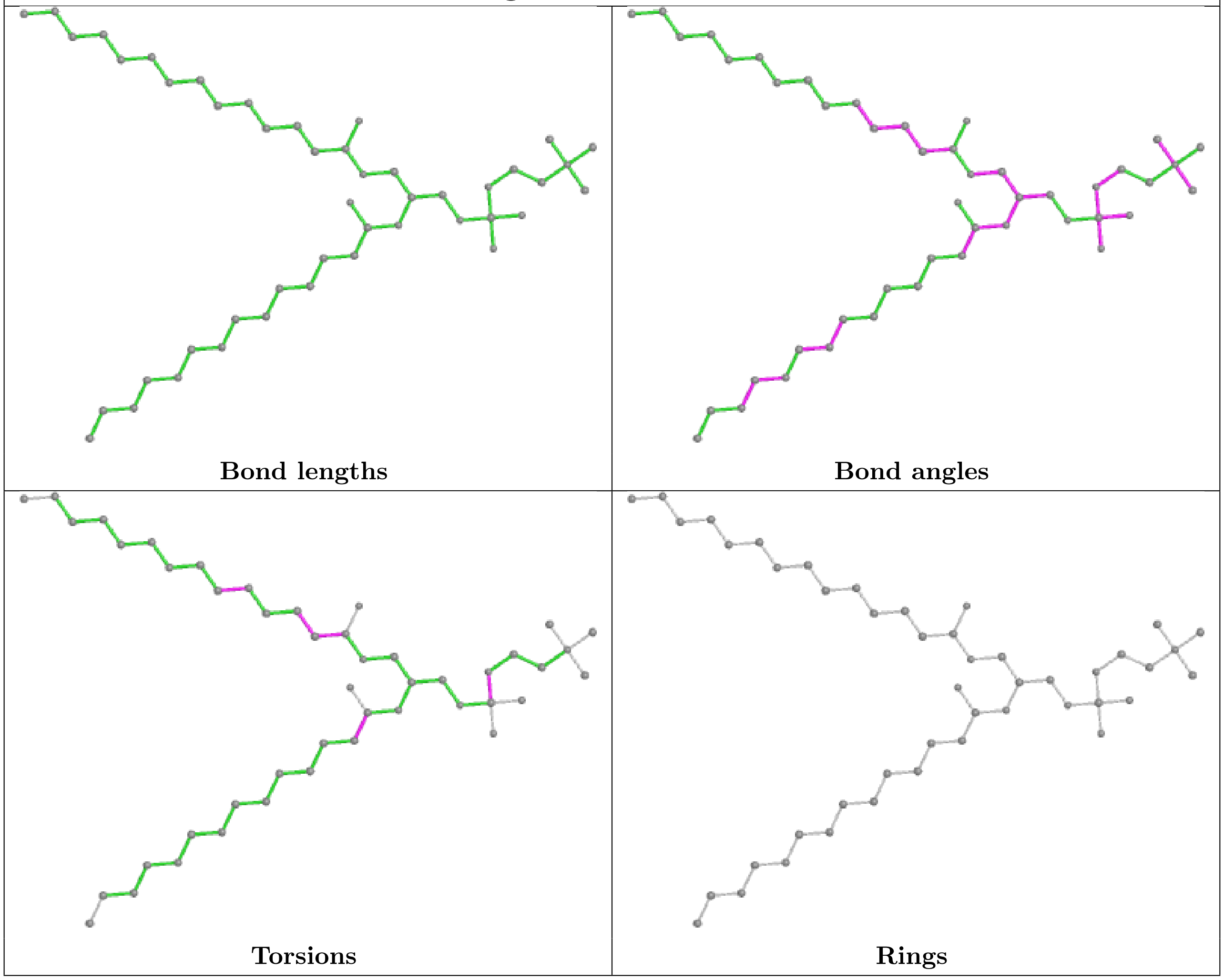


Ligand PX4 A 387

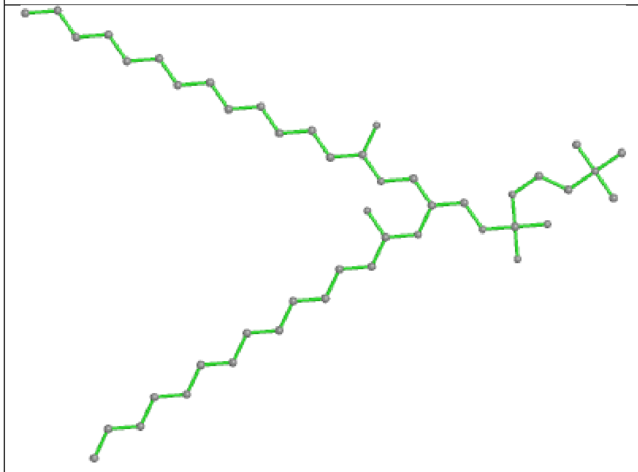


Ligand PX4 A 369	
 Bond lengths	 Bond angles
 Torsions	 Rings

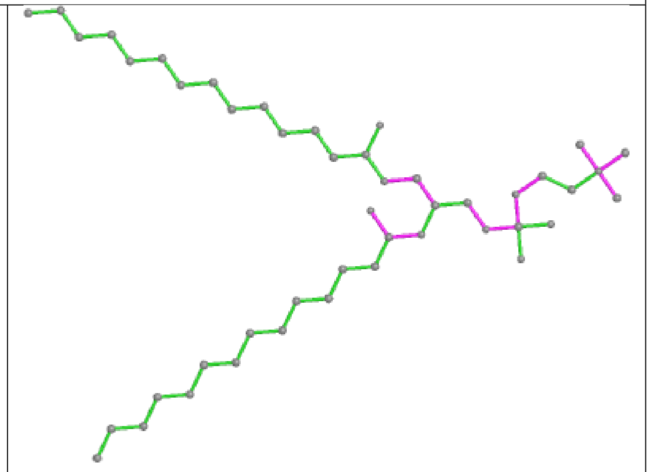
Ligand PX4 A 375



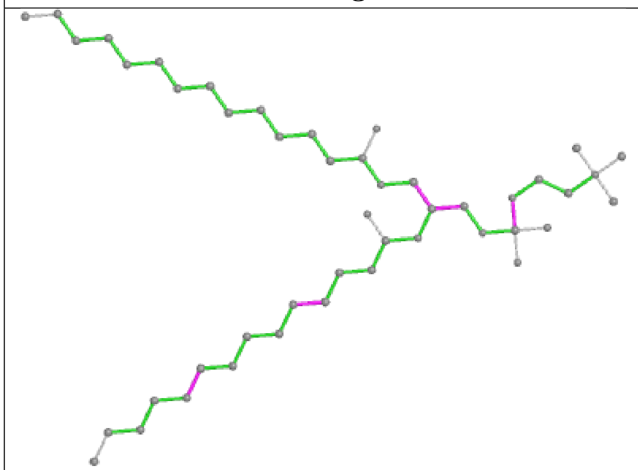
Ligand PX4 A 394



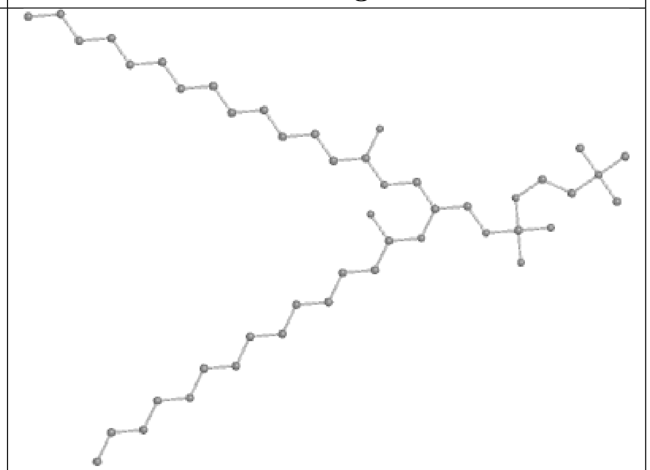
Bond lengths



Bond angles

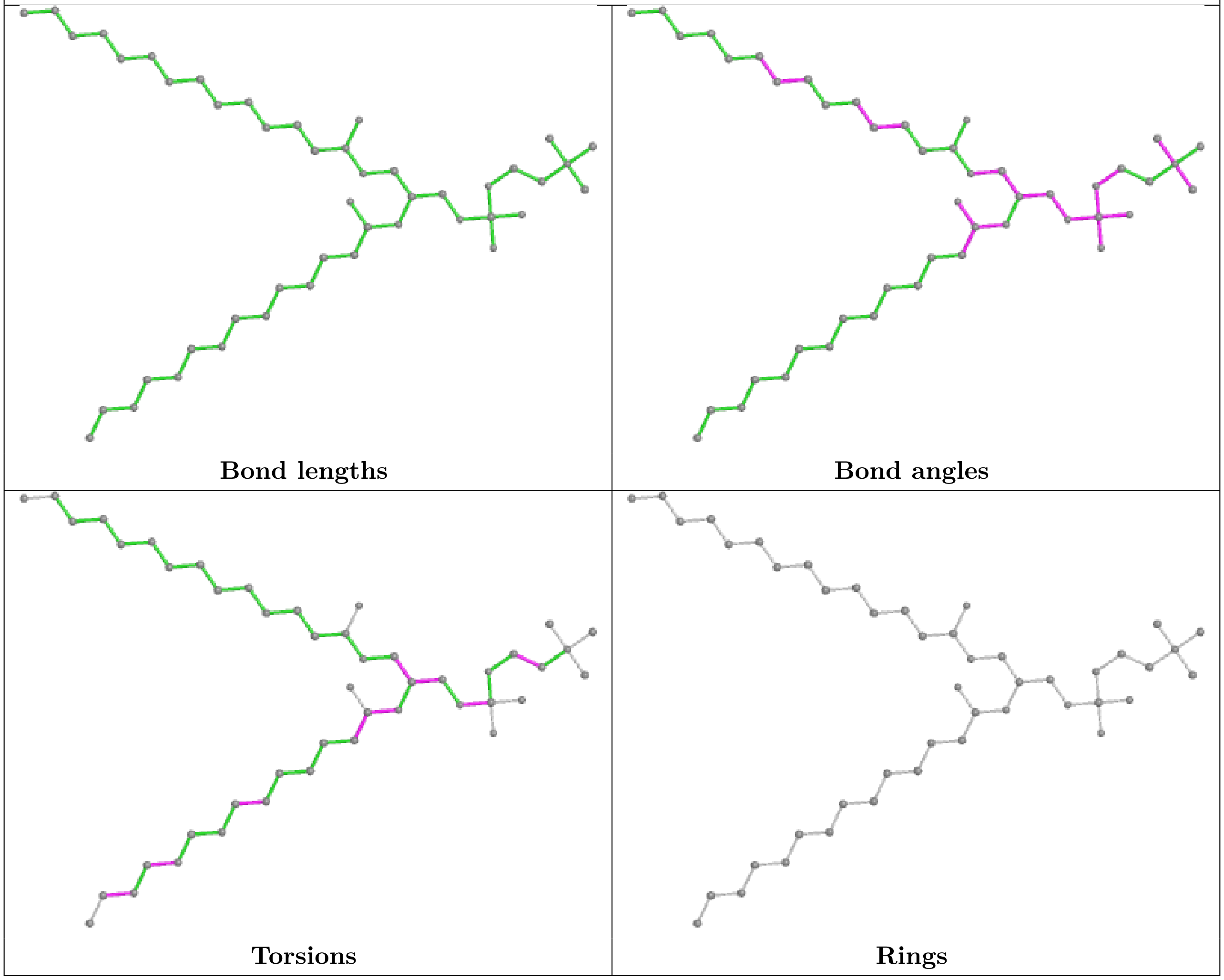


Torsions

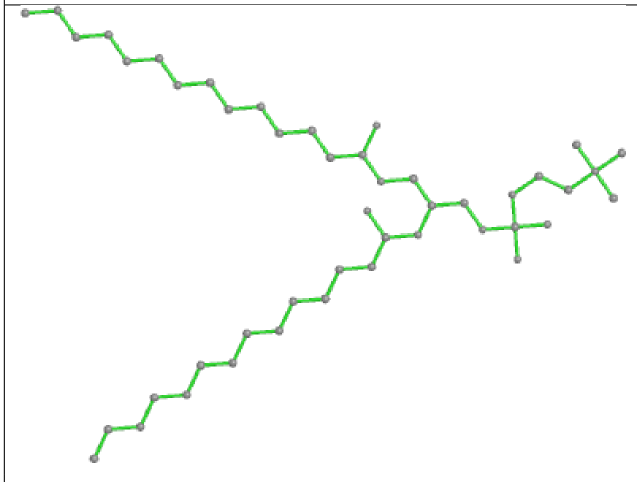


Rings

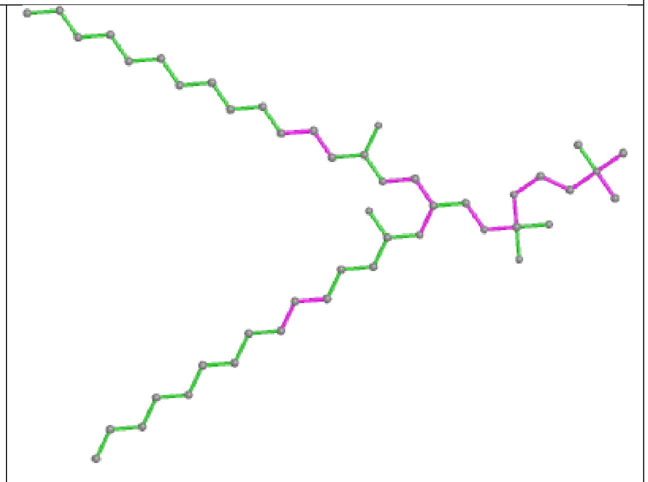
Ligand PX4 A 320



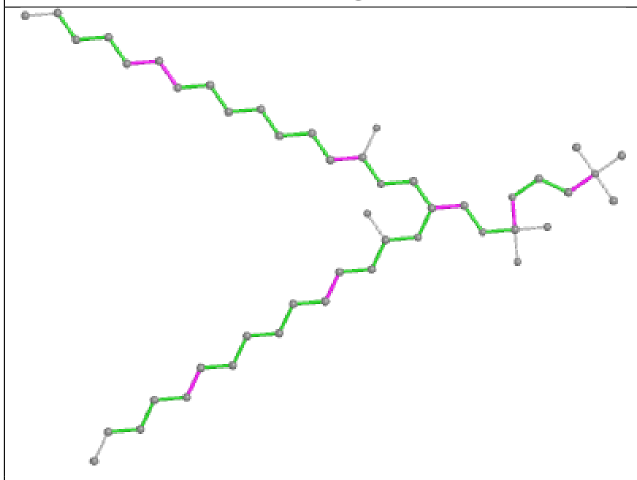
Ligand PX4 A 312



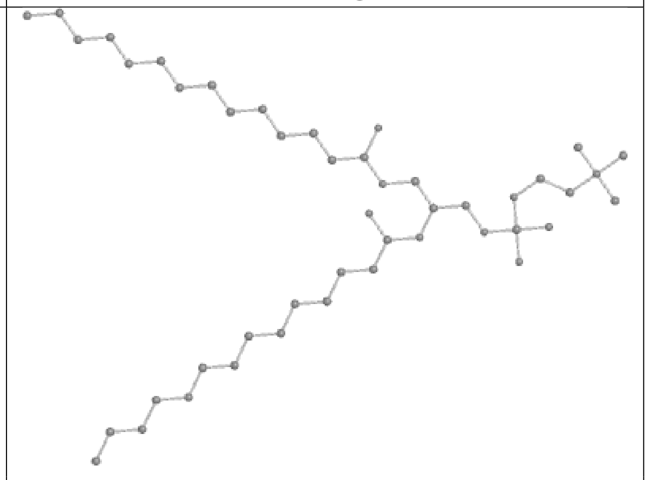
Bond lengths



Bond angles

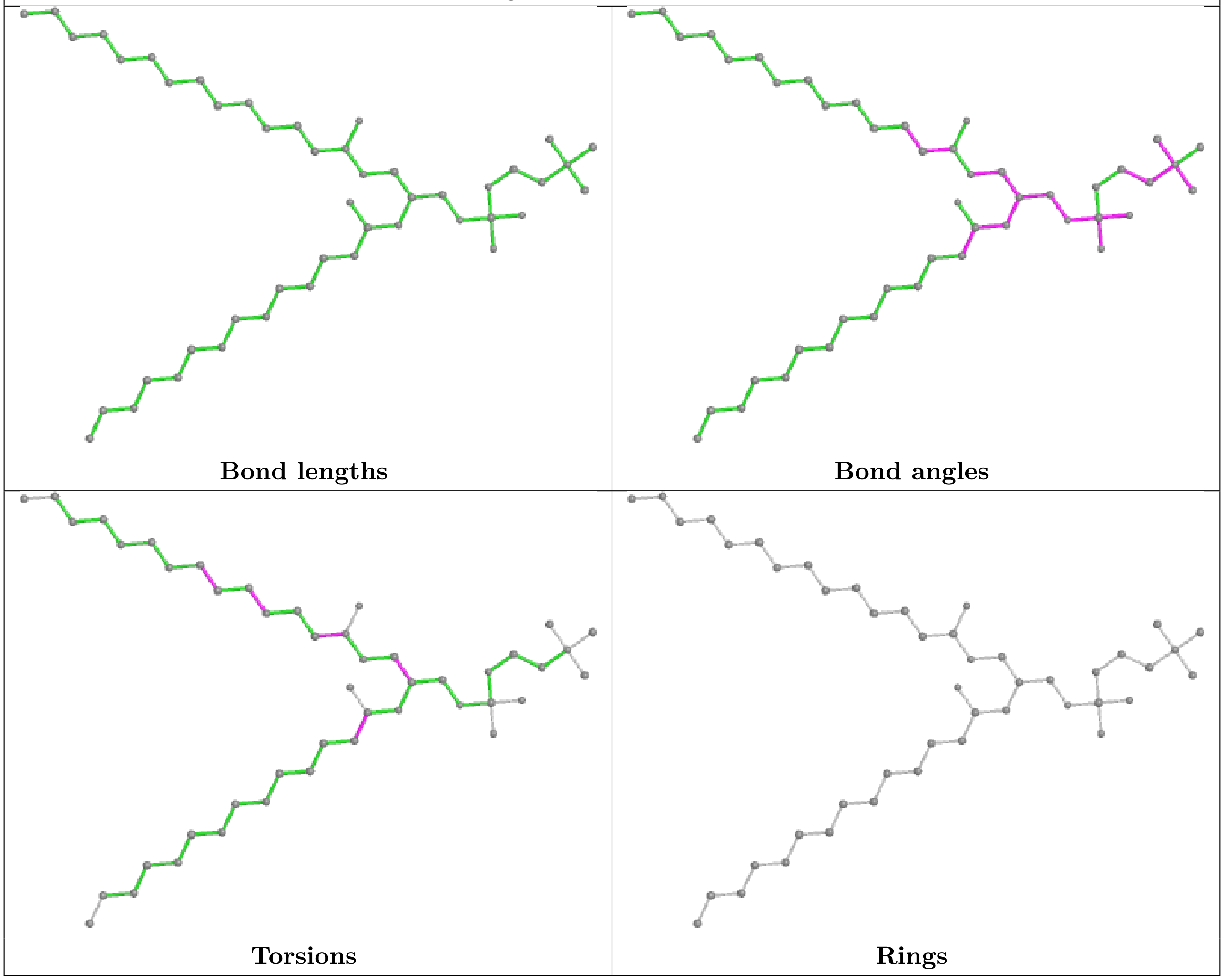


Torsions

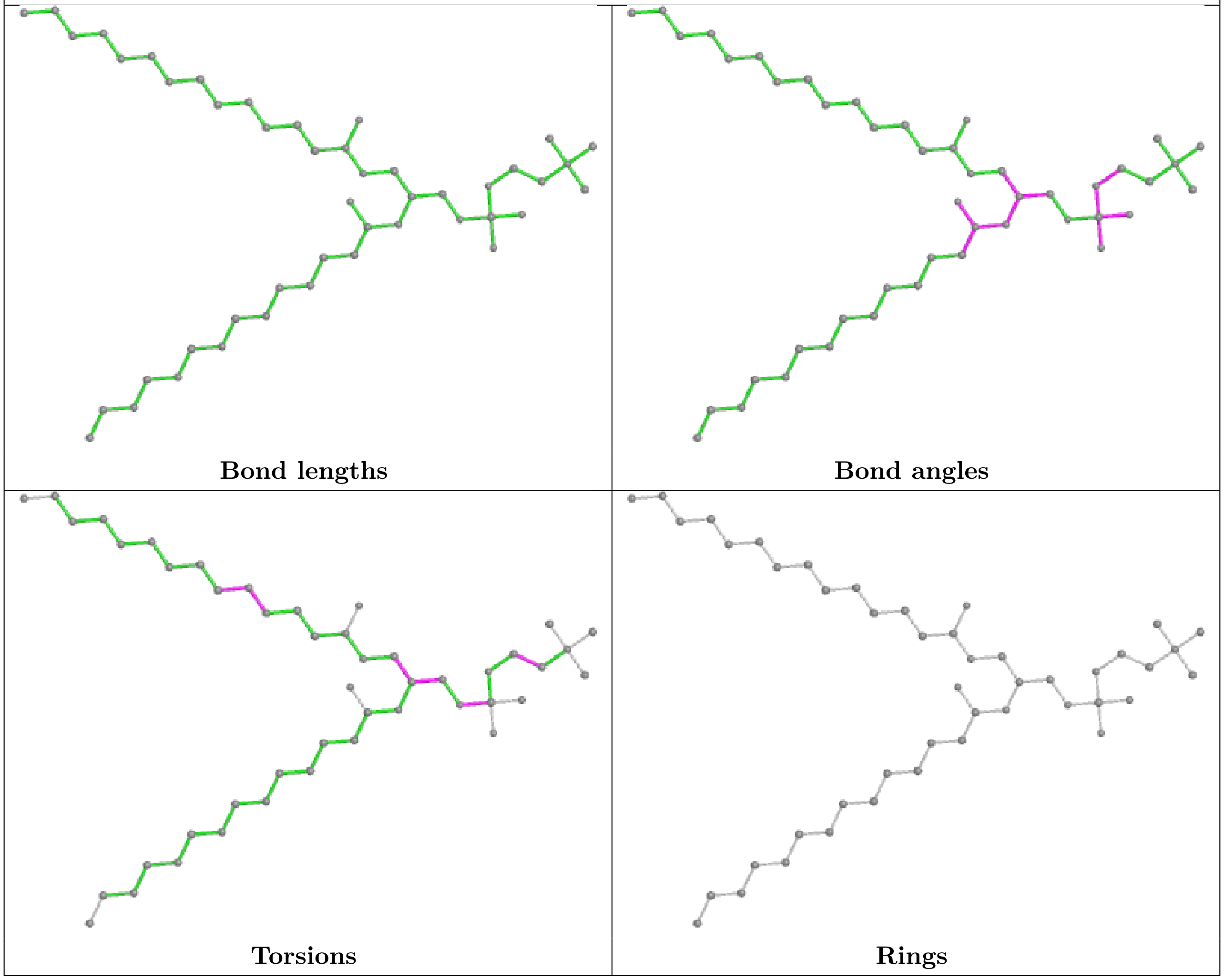


Rings

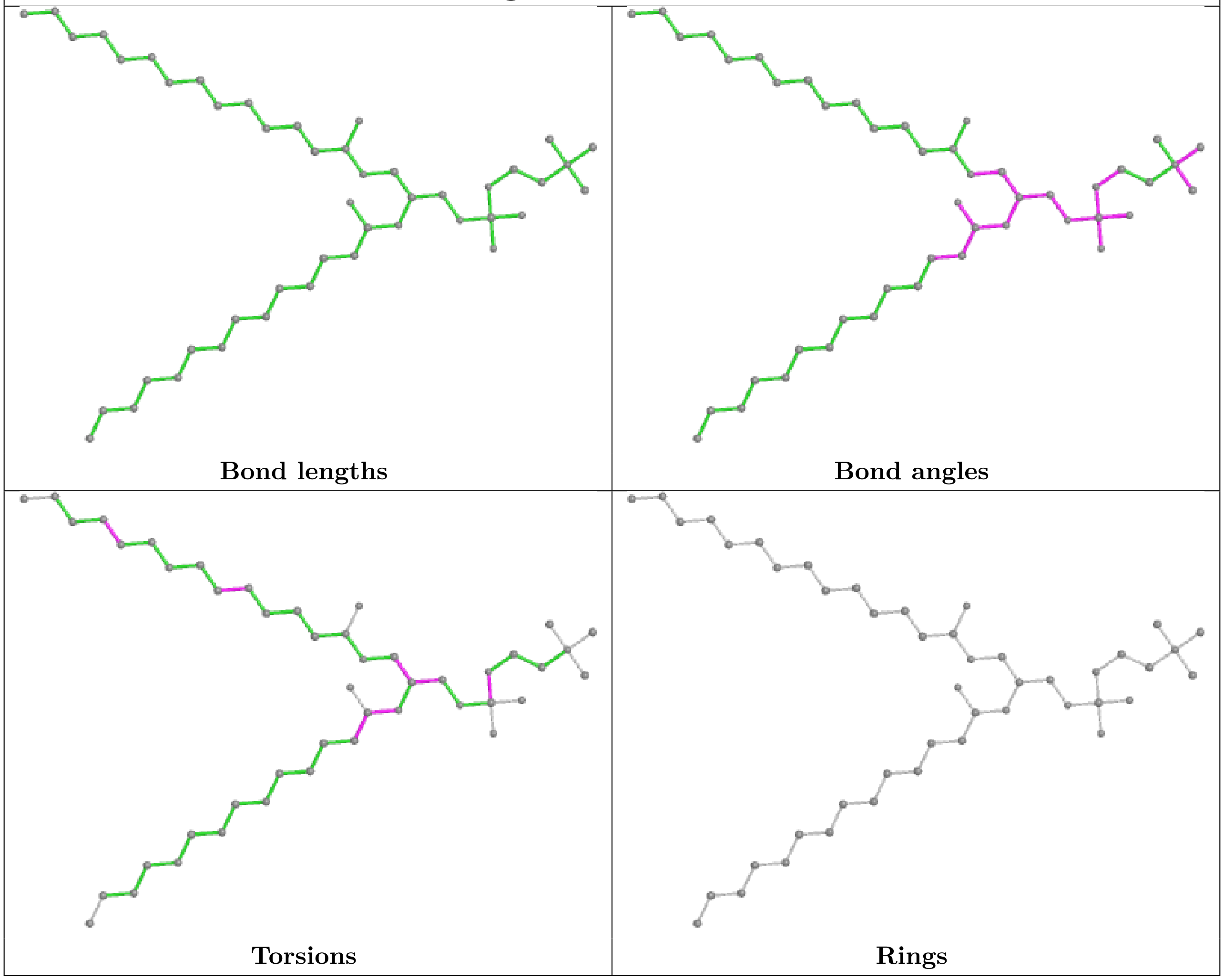
Ligand PX4 A 409



Ligand PX4 A 315



Ligand PX4 A 372



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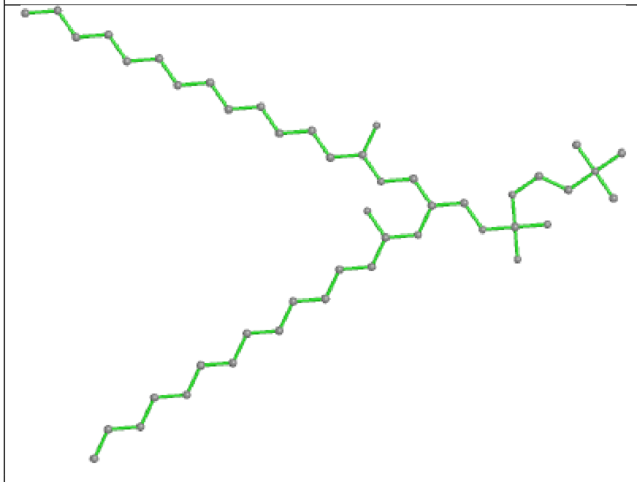
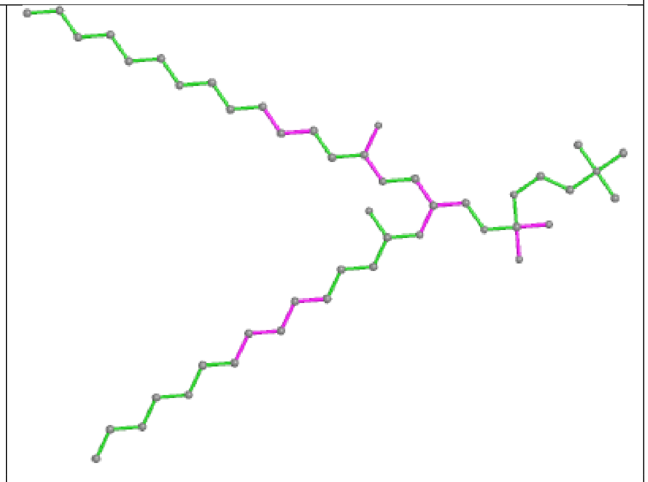
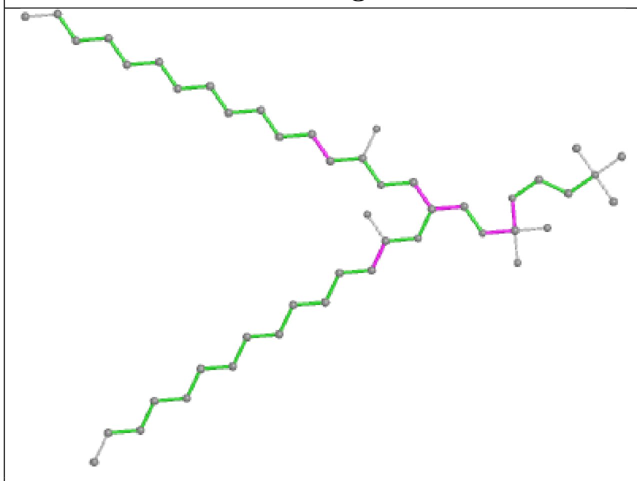


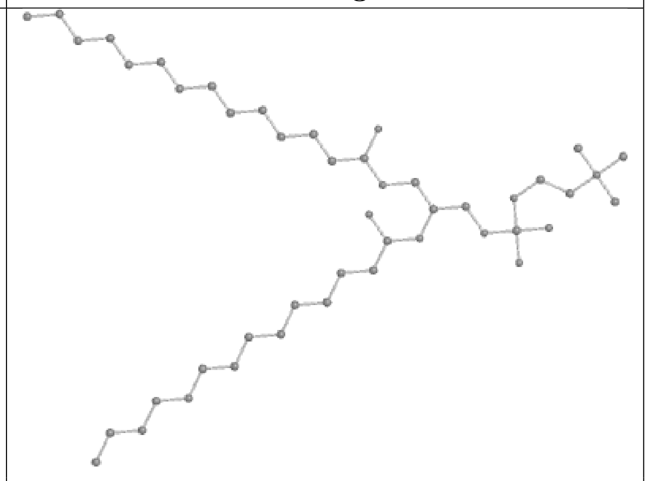
Bond lengths



Bond angles

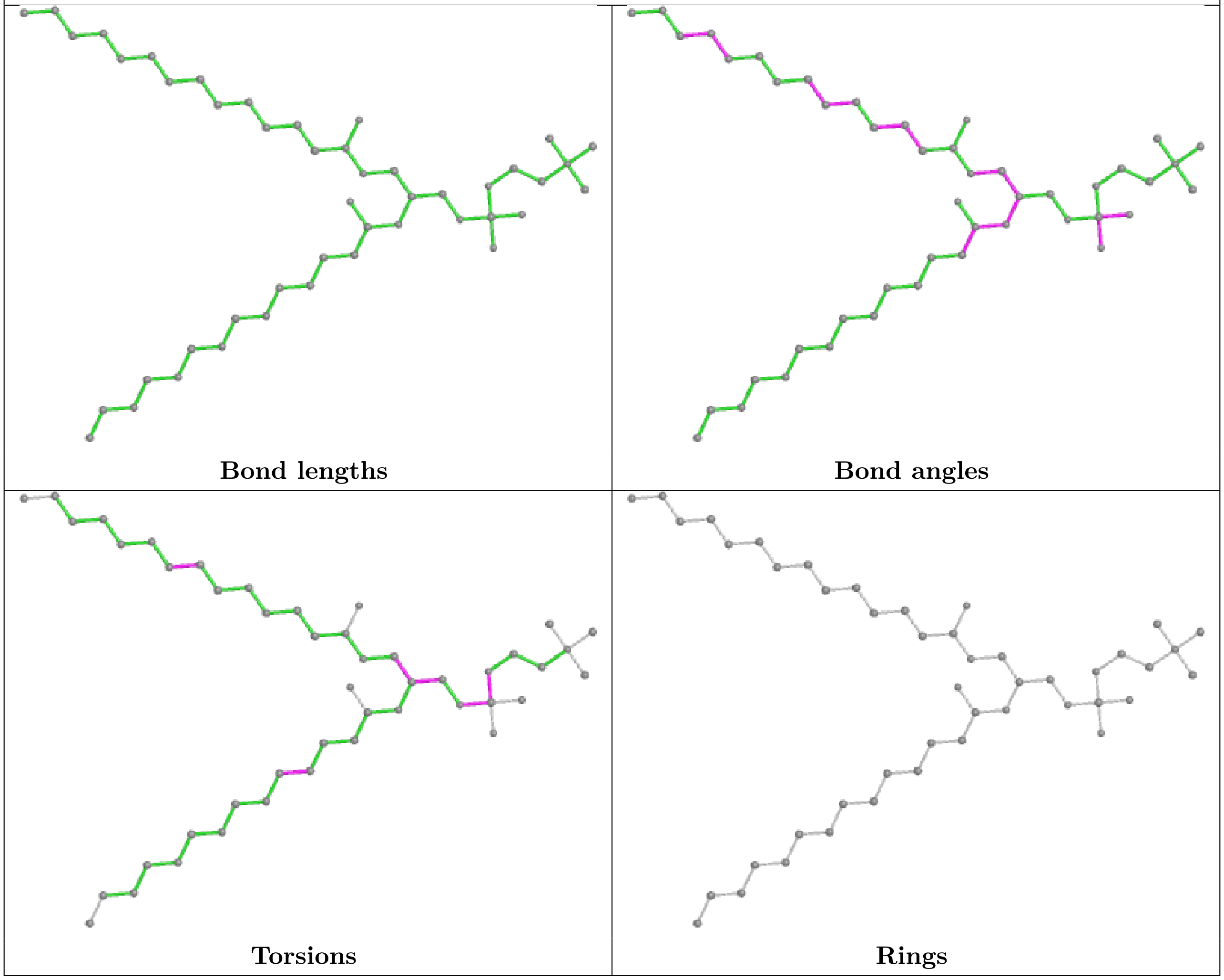


Torsions



Rings

Ligand PX4 A 306



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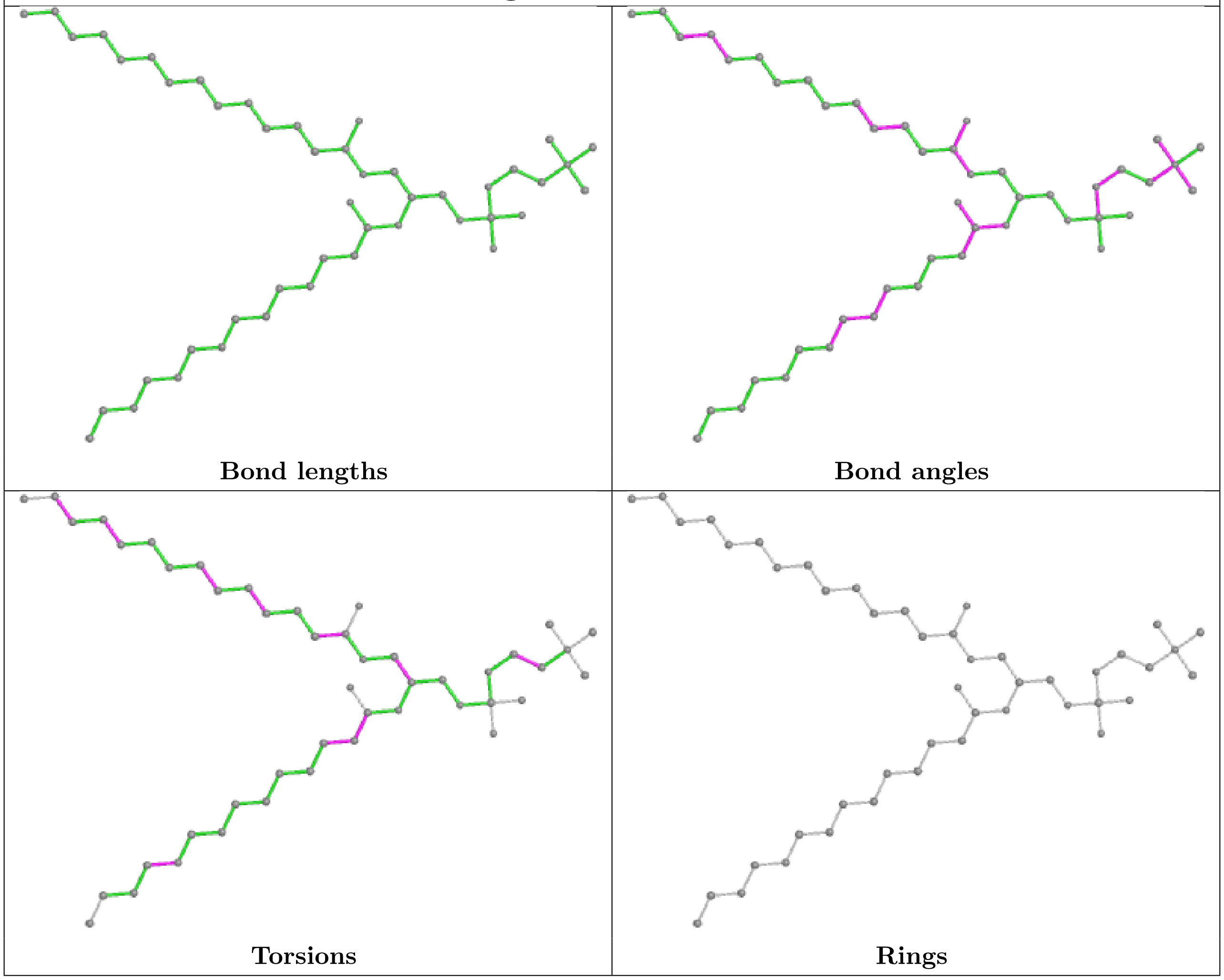
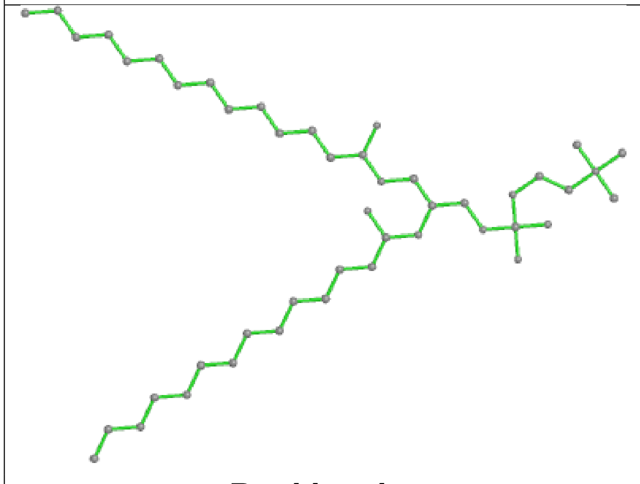
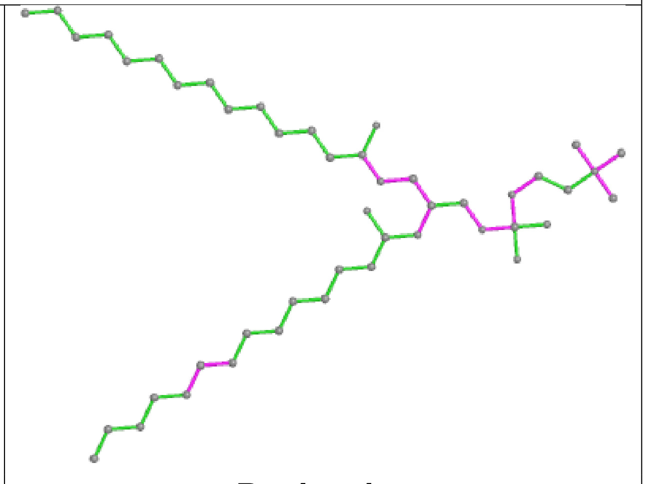
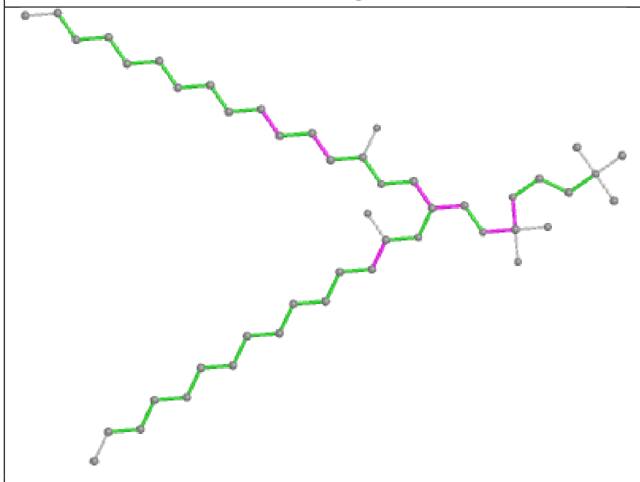
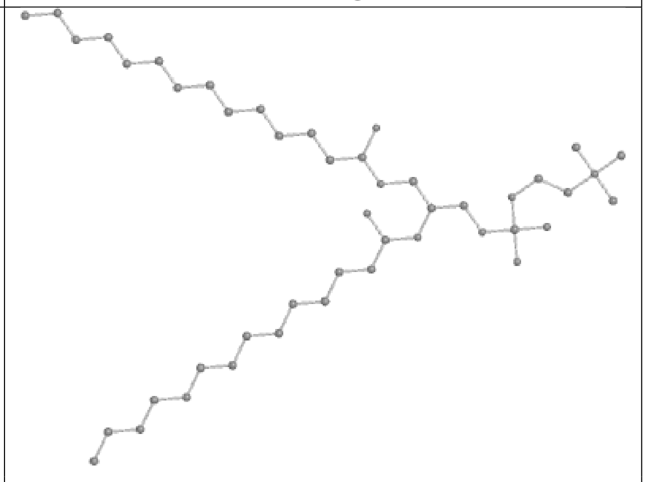
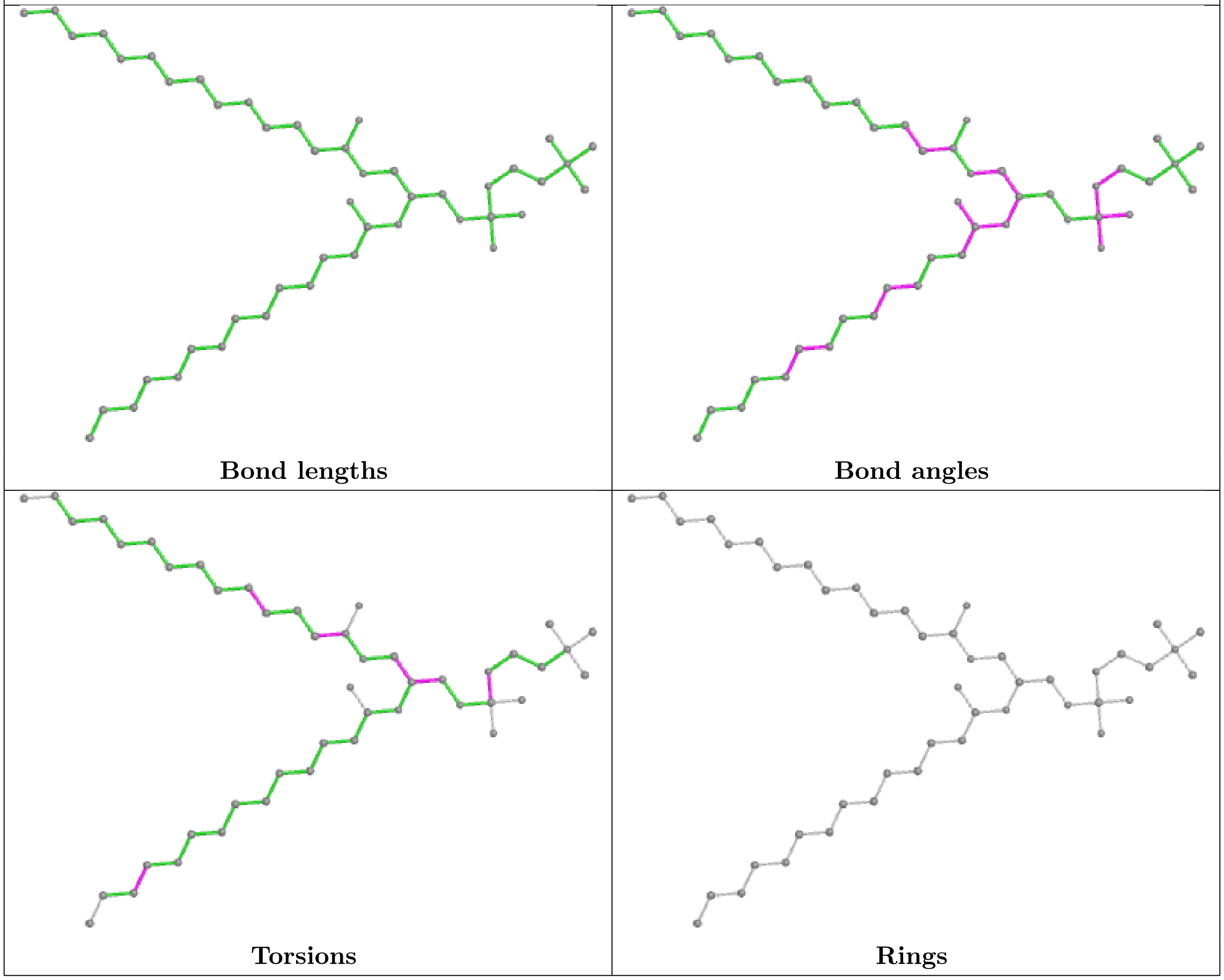
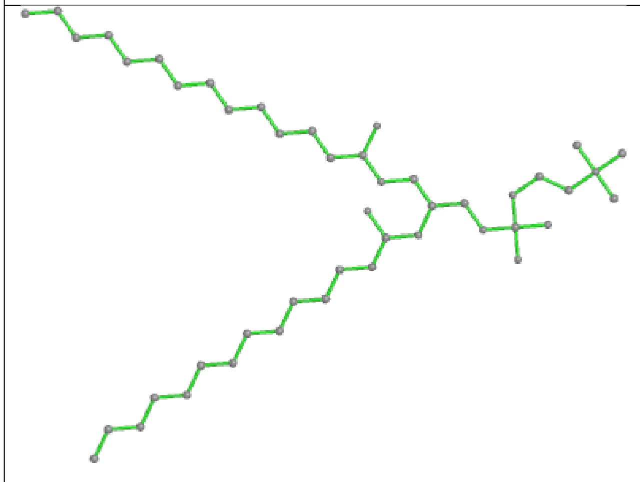


Ligand PX4 A 323	
 Bond lengths	 Bond angles
 Torsions	 Rings

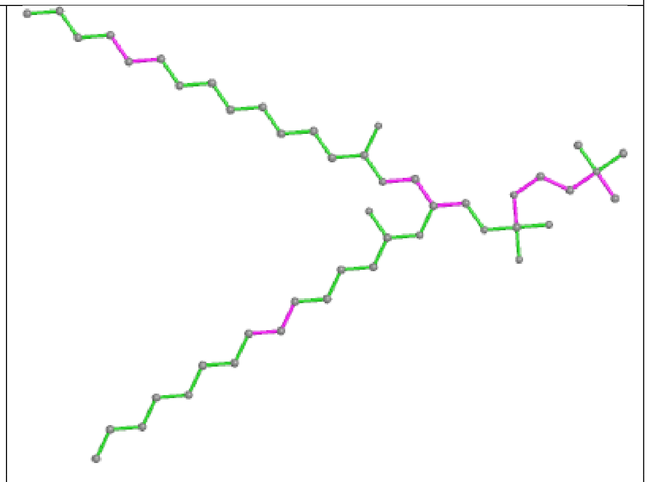
Ligand PX4 A 366



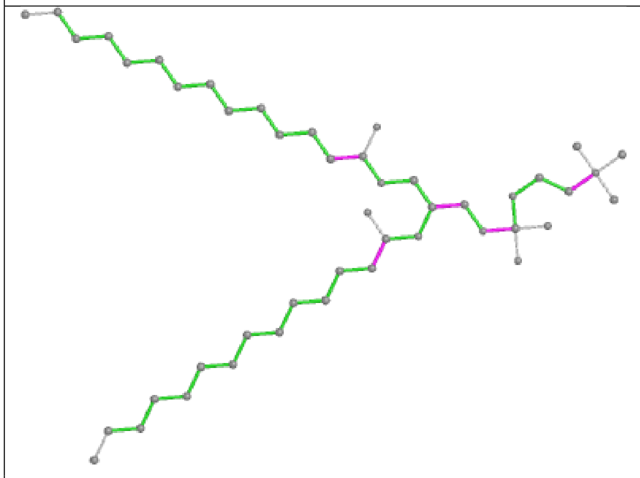
Ligand PX4 A 360



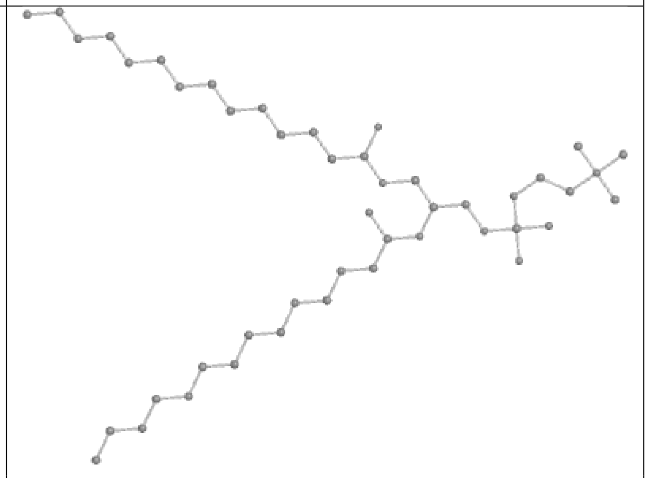
Bond lengths



Bond angles

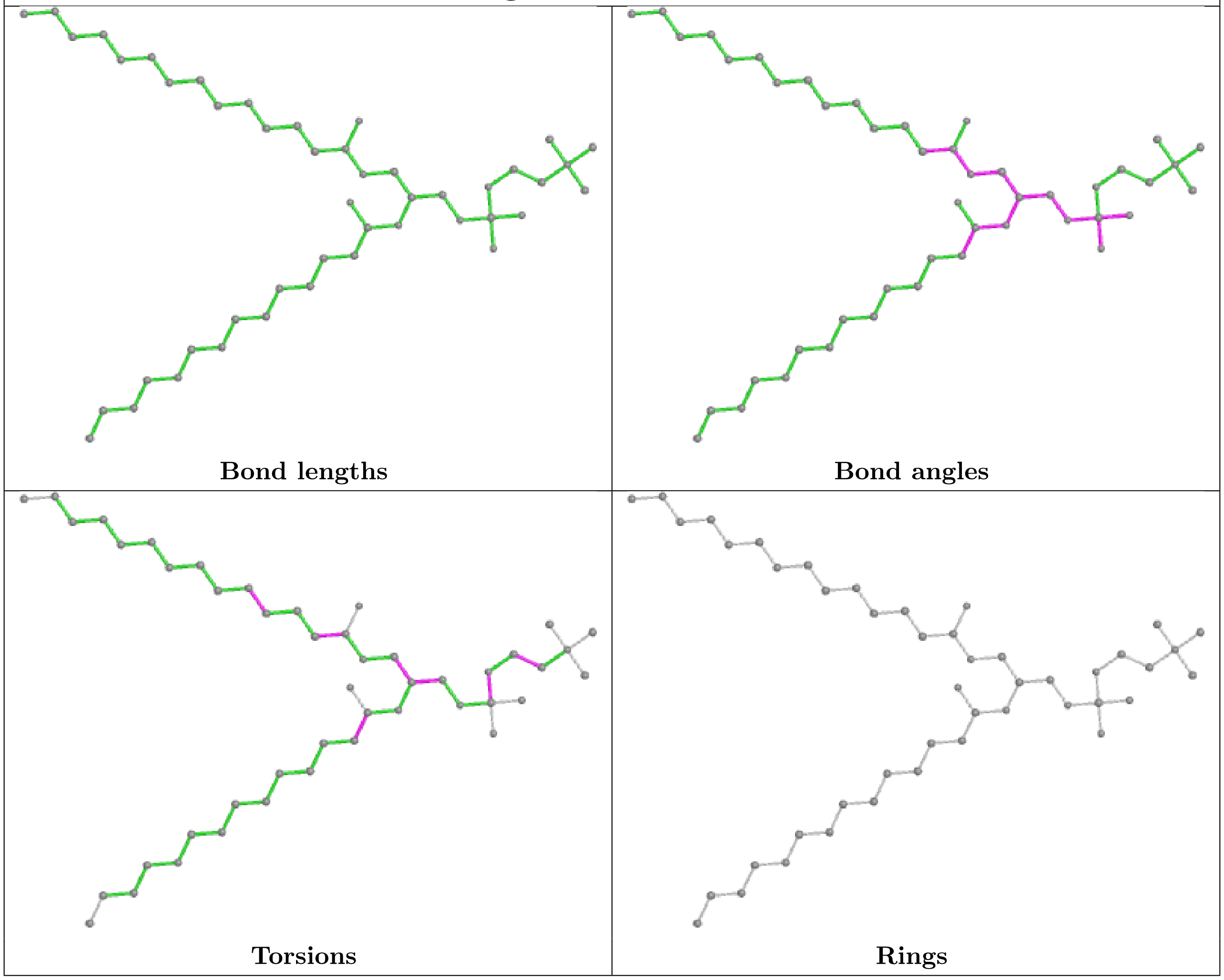


Torsions

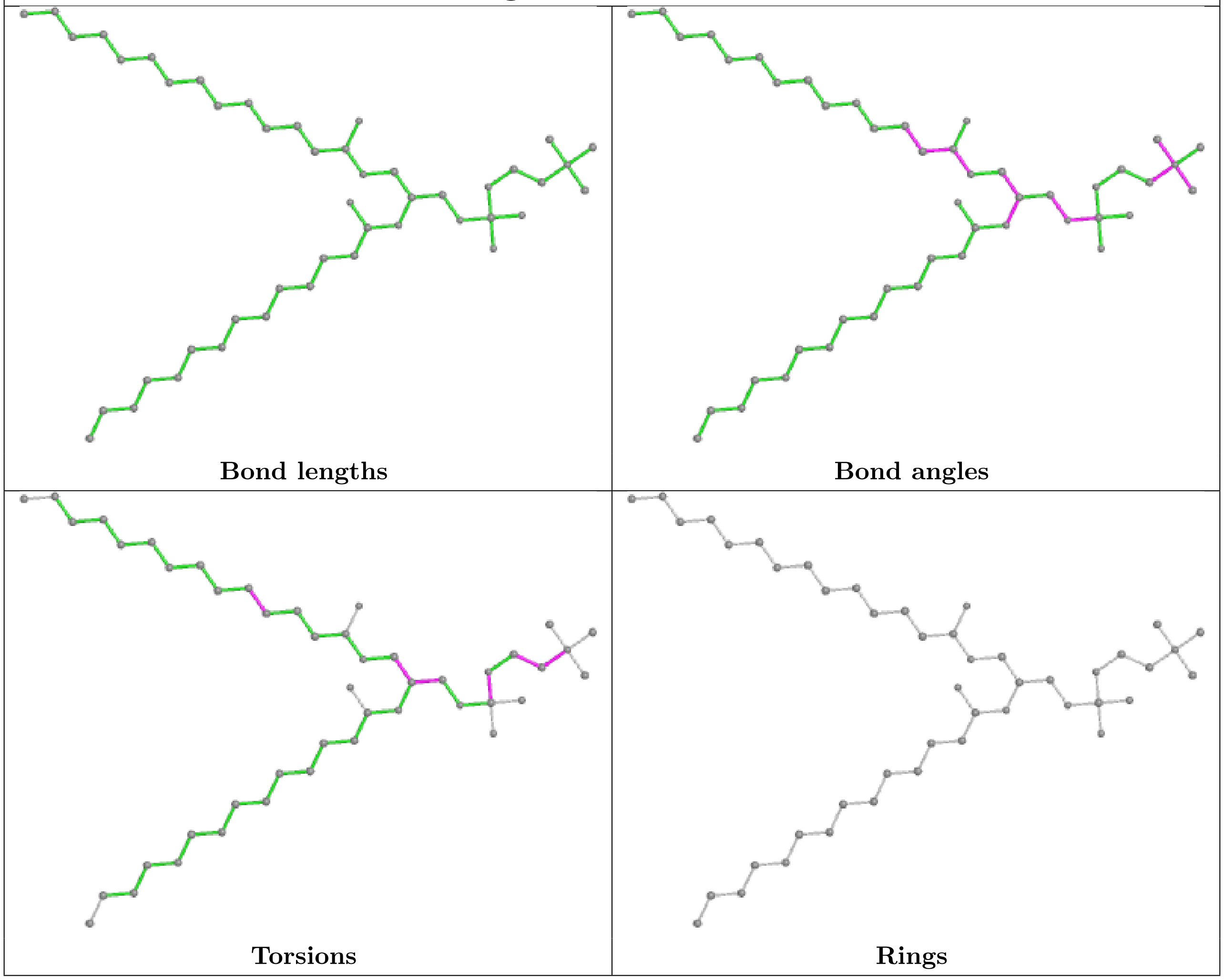


Rings

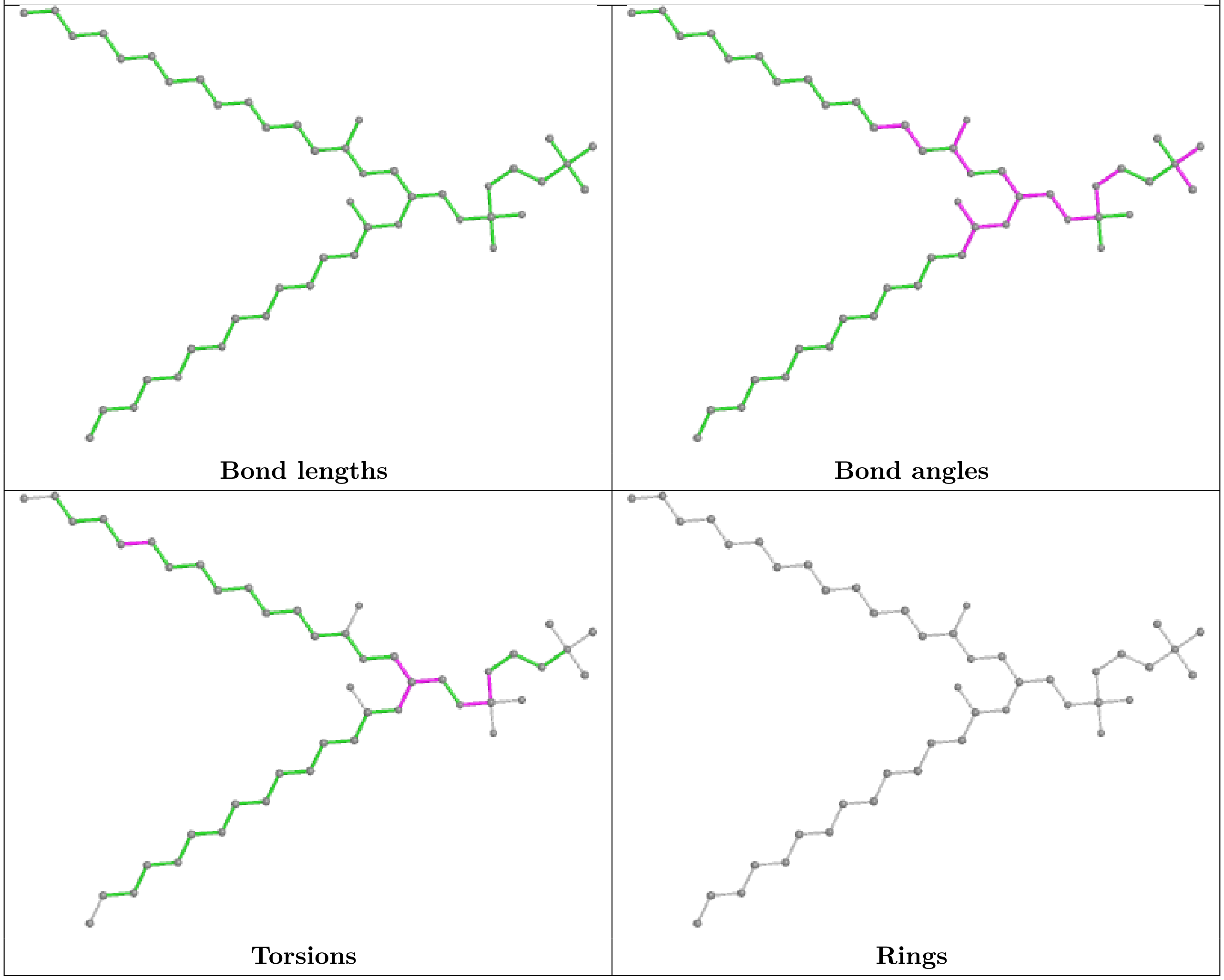
Ligand PX4 A 317



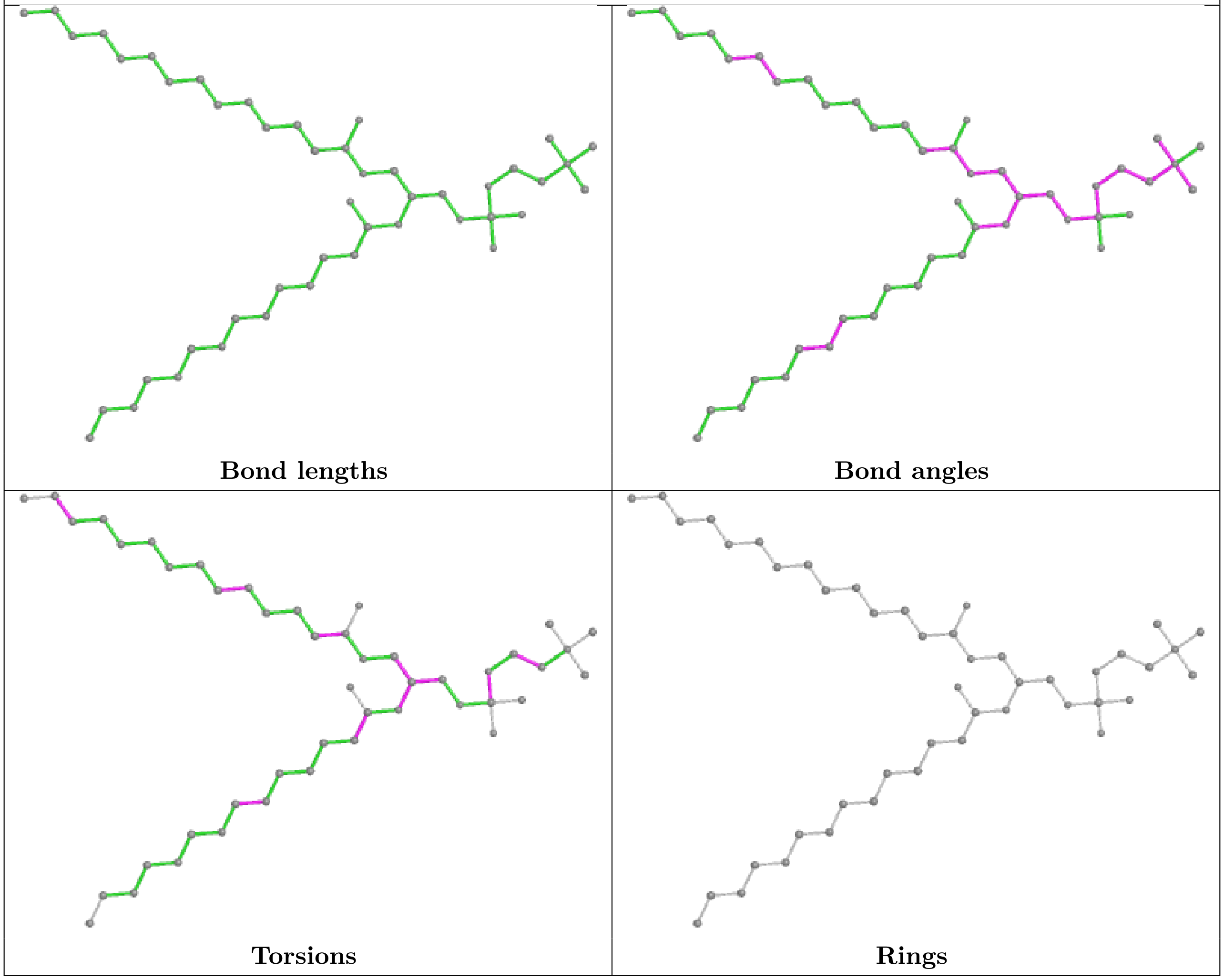
Ligand PX4 A 351



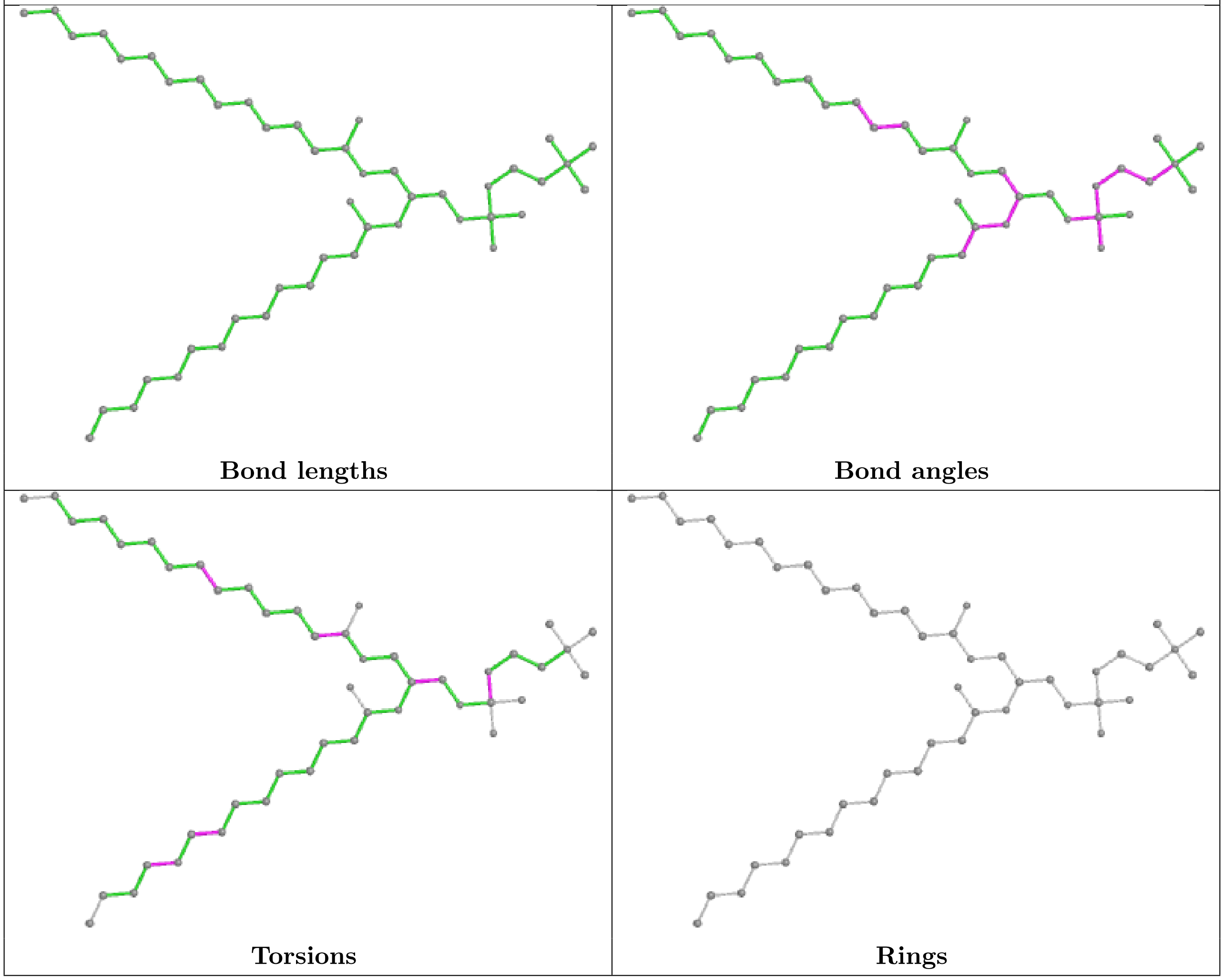
Ligand PX4 A 385



Ligand PX4 A 318



Ligand PX4 A 370



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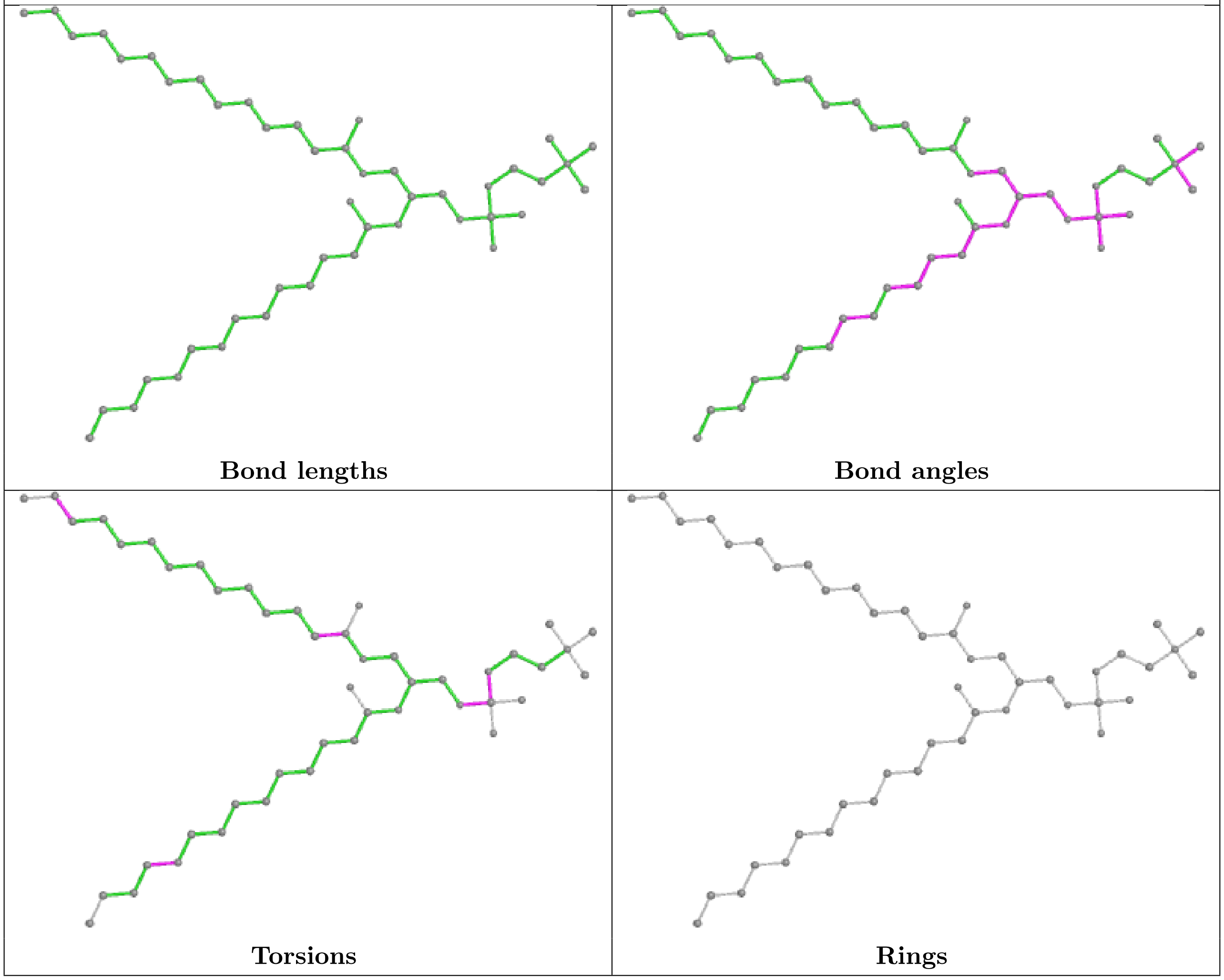

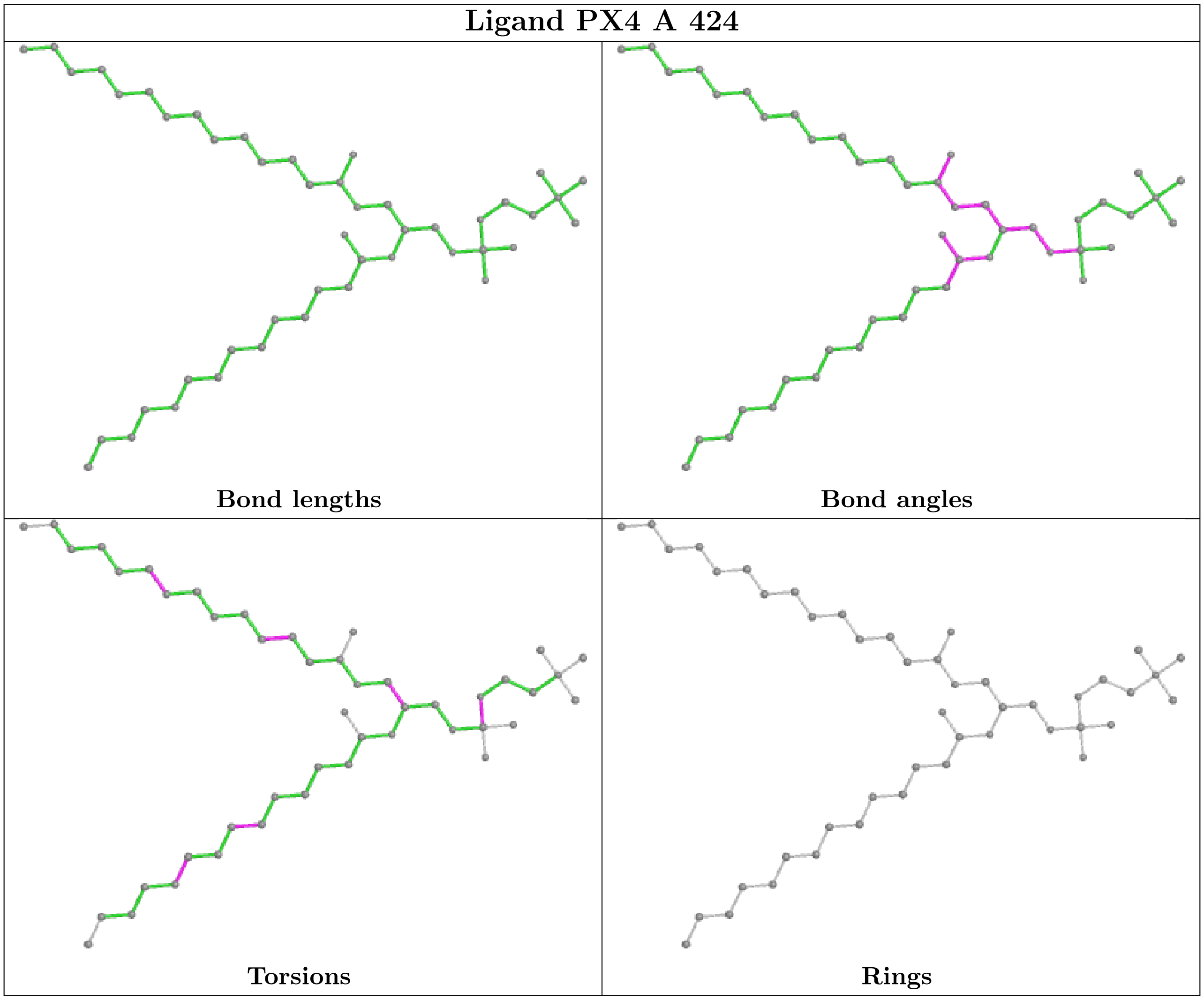

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1762
Number of shifts mapped to atoms	1762
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	160	-0.25 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	138	0.12 ± 0.15	None needed (< 0.5 ppm)
$^{13}C'$	129	-0.17 ± 0.12	None needed (< 0.5 ppm)
^{15}N	154	-0.67 ± 0.35	None needed (imprecise)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 1756 atoms were assigned a chemical shift out of a possible 2153. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	769/815 (94%)	329/336 (98%)	287/324 (89%)	153/155 (99%)
Sidechain	829/1066 (78%)	547/696 (79%)	273/330 (83%)	9/40 (22%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	158/272 (58%)	79/137 (58%)	76/123 (62%)	3/12 (25%)
Overall	1756/2153 (82%)	955/1169 (82%)	636/777 (82%)	165/207 (80%)

7.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	214	LEU	CG	33.00	21.37 – 32.19	5.8
1	A	226	LEU	CG	33.00	21.37 – 32.19	5.8
1	A	224	LEU	CG	32.30	21.37 – 32.19	5.1

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: