



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:28 AM UTC

PDB ID : 9MXZ / pdb_00009mxz
EMDB ID : EMD-48724
Title : Lecithin:Cholesterol Acyltransferase Bound to Apolipoprotein A-I dimer in HDL
Authors : Coleman, B.; Bedi, S.; Hill, J.H.; Morris, J.; Manthei, K.A.; Hart, R.C.; He, Y.; Shah, A.S.; Jerome, W.G.; Vaisar, T.; Bornfeldt, K.E.; Song, H.; Segrest, J.P.; Heinecke, J.W.; Aller, S.G.; Tesmer, J.J.G.; Davidson, S.
Deposited on : 2025-01-21
Resolution : 9.80 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

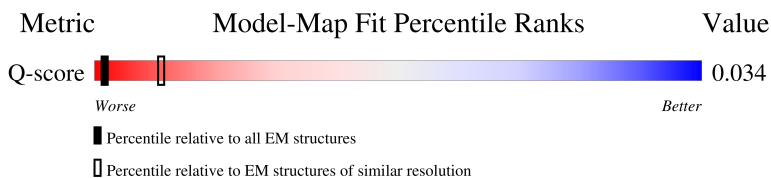
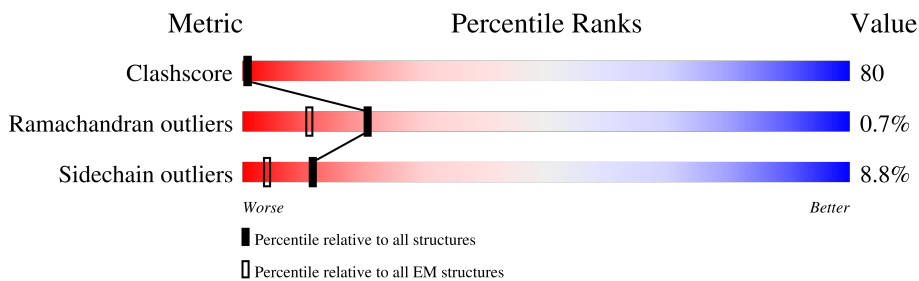
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



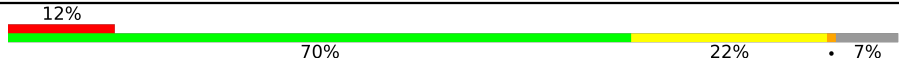
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	157 (9.30 - 10.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	243	 5% 72% 26%
1	E	243	 14% 66% 31%
2	B	396	 71% 21% 7%

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Mol	Chain	Length	Quality of chain
2	C	396	

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
3	6PL	A	502	-	-	X	-
3	6PL	A	503	-	-	X	-
3	6PL	A	504	-	-	X	-
3	6PL	A	505	-	-	X	-
3	6PL	A	506	-	-	X	-
3	6PL	A	508	-	-	X	-
3	6PL	A	509	-	-	X	-
3	6PL	A	510	-	-	X	-
3	6PL	A	511	-	-	X	-
3	6PL	A	512	-	-	X	-
3	6PL	A	513	-	-	X	-
3	6PL	A	515	-	-	X	-
3	6PL	A	516	-	-	X	-
3	6PL	A	517	-	-	X	-
3	6PL	A	518	-	-	X	-
3	6PL	A	519	-	-	X	-
3	6PL	A	520	-	-	X	-
3	6PL	A	521	-	-	X	-
3	6PL	A	522	-	-	X	-
3	6PL	A	523	-	-	X	-
3	6PL	A	524	-	-	X	-
3	6PL	A	525	-	-	X	-
3	6PL	A	526	-	-	X	-
3	6PL	A	527	-	-	X	-
3	6PL	A	528	-	-	X	-
3	6PL	A	529	-	-	X	-
3	6PL	A	530	-	-	X	-
3	6PL	A	531	-	-	X	-
3	6PL	A	532	-	-	X	-
3	6PL	A	533	-	-	X	-
3	6PL	A	534	-	-	X	-
3	6PL	A	535	-	-	X	-
3	6PL	A	536	-	-	X	-
3	6PL	A	537	-	-	X	-
3	6PL	A	538	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	6PL	A	539	-	-	X	-
3	6PL	A	540	-	-	X	-
3	6PL	A	541	-	-	X	-
3	6PL	A	542	-	-	X	-
3	6PL	A	543	-	-	X	-
3	6PL	A	544	-	-	X	-
3	6PL	A	546	-	-	X	-
3	6PL	A	548	-	-	X	-
3	6PL	A	549	-	-	X	-
3	6PL	A	550	-	-	X	-
3	6PL	A	552	-	-	X	-
3	6PL	A	554	-	-	X	-
3	6PL	A	555	-	-	X	-
3	6PL	A	556	-	-	X	-
3	6PL	A	557	-	-	X	-
3	6PL	A	558	-	-	X	-
3	6PL	A	559	-	-	X	-
3	6PL	A	560	-	-	X	-
3	6PL	A	562	-	-	X	-
3	6PL	A	563	-	-	X	-
3	6PL	A	564	-	-	X	-
3	6PL	A	565	-	-	X	-
3	6PL	A	566	-	-	X	-
3	6PL	A	567	-	-	X	-
3	6PL	A	570	-	-	X	-
3	6PL	A	571	-	-	X	-
3	6PL	A	572	-	-	X	-
3	6PL	A	573	-	-	X	-
3	6PL	A	574	-	-	X	-
3	6PL	A	575	-	-	X	-
3	6PL	A	576	-	-	X	-
3	6PL	A	578	-	-	X	-
3	6PL	A	579	-	-	X	-
3	6PL	A	580	-	-	X	-
3	6PL	A	581	-	-	X	-
3	6PL	A	582	-	-	X	-
3	6PL	A	584	-	-	X	-
3	6PL	A	587	-	-	X	-
3	6PL	A	588	-	-	X	-
3	6PL	C	501	-	-	X	-
3	6PL	E	301	-	-	X	-
3	6PL	E	302	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	6PL	E	304	-	-	X	-
3	6PL	E	306	-	-	X	-
3	6PL	E	308	-	-	X	-
3	6PL	E	309	-	-	X	-
3	6PL	E	310	-	-	X	-
3	6PL	E	312	-	-	X	-
3	6PL	E	315	-	-	X	-
3	6PL	E	317	-	-	X	-
3	6PL	E	318	-	-	X	-
3	6PL	E	320	-	-	X	-
3	6PL	E	321	-	-	X	-
3	6PL	E	322	-	-	X	-
3	6PL	E	323	-	-	X	-
3	6PL	E	324	-	-	X	-
3	6PL	E	325	-	-	X	-
3	6PL	E	326	-	-	X	-
3	6PL	E	328	-	-	X	-
3	6PL	E	329	-	-	X	-
3	6PL	E	330	-	-	X	-
3	6PL	E	331	-	-	X	-
3	6PL	E	332	-	-	X	-
3	6PL	E	333	-	-	X	-
3	6PL	E	335	-	-	X	-
3	6PL	E	337	-	-	X	-
3	6PL	E	339	-	-	X	-
3	6PL	E	340	-	-	X	-
3	6PL	E	341	-	-	X	-
3	6PL	E	344	-	-	X	-
3	6PL	E	345	-	-	X	-
3	6PL	E	346	-	-	X	-
3	6PL	E	347	-	-	X	-
3	6PL	E	348	-	-	X	-
3	6PL	E	350	-	-	X	-
3	6PL	E	351	-	-	X	-
3	6PL	E	353	-	-	X	-
3	6PL	E	355	-	-	X	-
3	6PL	E	356	-	-	X	-
3	6PL	E	357	-	-	X	-
3	6PL	E	358	-	-	X	-
3	6PL	E	359	-	-	X	-
3	6PL	E	360	-	-	X	-
3	6PL	E	361	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	6PL	E	362	-	-	X	-
3	6PL	E	363	-	-	X	-
3	6PL	E	364	-	-	X	-
3	6PL	E	365	-	-	X	-
3	6PL	E	366	-	-	X	-
3	6PL	E	367	-	-	X	-
3	6PL	E	368	-	-	X	-
3	6PL	E	369	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20264 atoms, of which 2138 are hydrogens and 0 are deuteriums.

In the tables below, 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						AltConf	Trace
			Total	C	H	N	O	S		
1	E	243	Total	C	H	N	O	S	0	0
			2438	1241	459	347	388	3		
1	A	243	Total	C	H	N	O	S	0	0
			2438	1241	459	347	388	3		

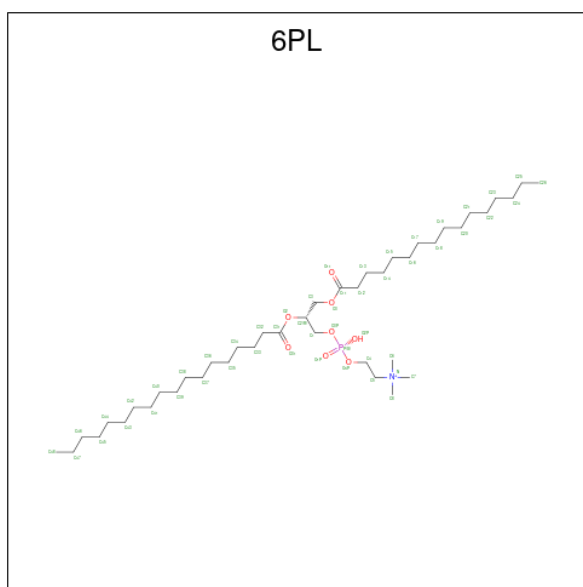
- Molecule 2 is a protein called Phosphatidylcholine-sterol acyltransferase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	369	Total	C	H	N	O	S	0	0
			3586	1930	610	501	532	13		
2	C	369	Total	C	H	N	O	S	0	0
			3586	1930	610	501	532	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	31	TYR	CYS	conflict	UNP P04180
C	31	TYR	CYS	conflict	UNP P04180

- Molecule 3 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: 6PL) (formula: C₄₂H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	E	1	52	42	1	8	1	0
3	E	1	52	42	1	8	1	0
3	E	1	52	42	1	8	1	0
3	E	1	52	42	1	8	1	0
3	E	1	52	42	1	8	1	0
3	E	1	52	42	1	8	1	0
3	E	1	52	42	1	8	1	0
3	E	1	52	42	1	8	1	0
3	E	1	52	42	1	8	1	0
3	E	1	52	42	1	8	1	0
3	E	1	52	42	1	8	1	0
3	E	1	52	42	1	8	1	0
3	E	1	52	42	1	8	1	0
3	E	1	52	42	1	8	1	0

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

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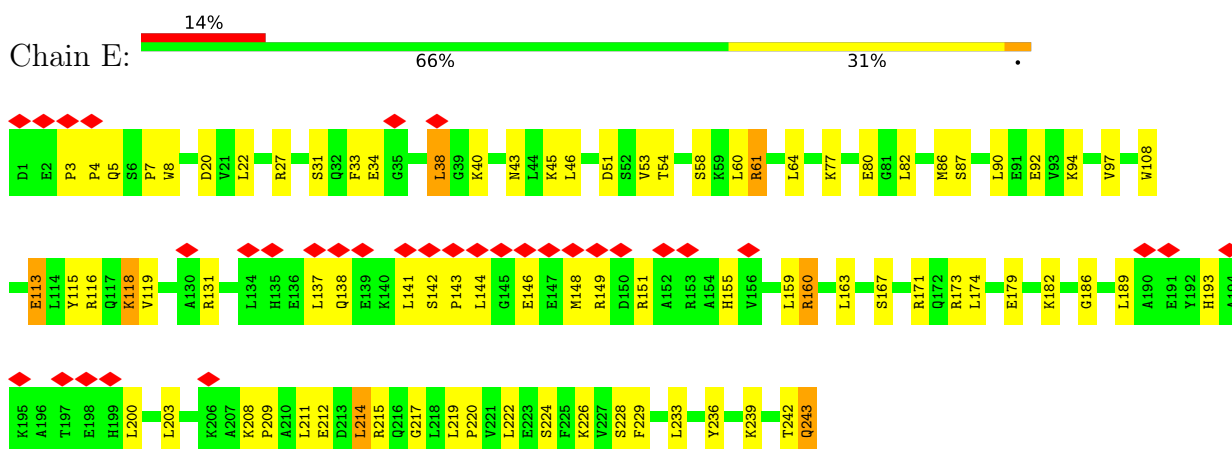
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	52	42	1	8	1	0
3	A	1	52	42	1	8	1	0
3	A	1	52	42	1	8	1	0
3	A	1	52	42	1	8	1	0
3	A	1	52	42	1	8	1	0
3	A	1	52	42	1	8	1	0
3	A	1	52	42	1	8	1	0
3	A	1	52	42	1	8	1	0
3	A	1	52	42	1	8	1	0
3	A	1	52	42	1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

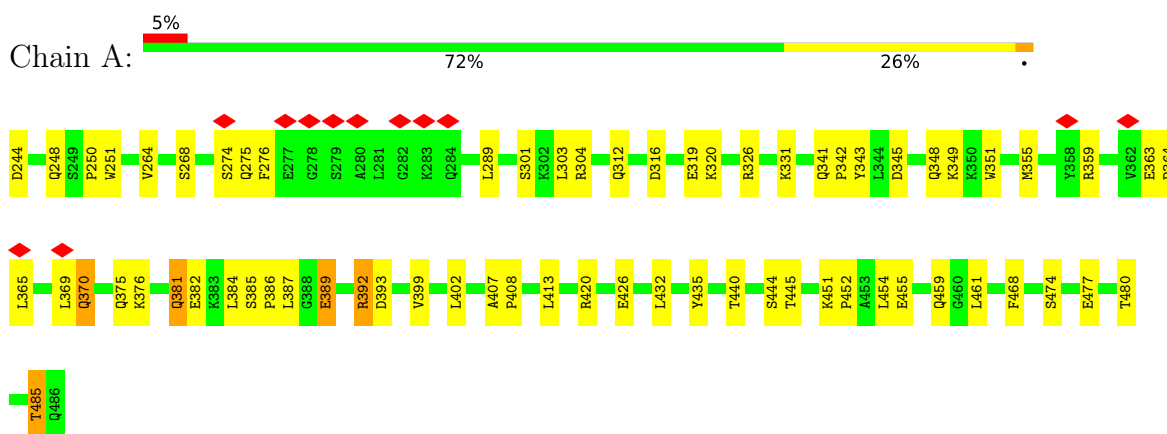
3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

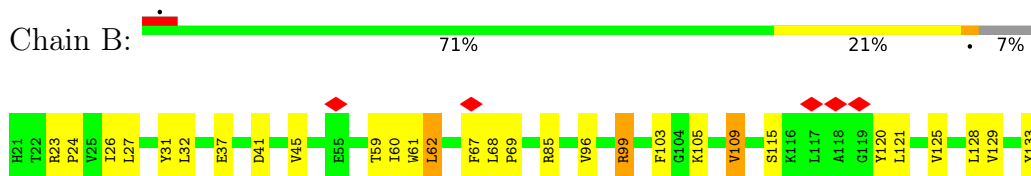
- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



- Molecule 2: Phosphatidylcholine-sterol acyltransferase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.599	Depositor
Minimum map value	-0.233	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	246.96, 246.96, 246.96	wwPDB
Map dimensions	126, 126, 126	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.96, 1.96, 1.96	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6PL

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	0.41	0/2014	0.77	0/2714
1	E	0.41	0/2014	0.77	0/2714
2	B	0.40	0/3070	0.81	0/4187
2	C	0.39	0/3070	0.80	0/4187
All	All	0.40	0/10168	0.79	0/13802

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	E	1	0
2	B	2	0
2	C	1	0
All	All	4	0

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	38	LEU	CA
2	B	61	TRP	CA
2	B	62	LEU	CA
2	C	62	LEU	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1979	459	1965	82	0
1	E	1979	459	1968	98	0
2	B	2976	610	2884	45	0
2	C	2976	610	2884	43	0
3	A	4576	0	7392	1949	0
3	C	52	0	84	45	0
3	E	3588	0	5796	1433	0
All	All	18126	2138	22973	3281	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 80.

The worst 5 of 3281 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)
3:E:306:6PL:H351	3:E:306:6PL:C16	1.60	1.31
3:E:306:6PL:H162	3:E:306:6PL:C35	1.59	1.30
3:A:525:6PL:H51	3:A:583:6PL:H321	1.21	1.19
3:A:549:6PL:C41	3:A:555:6PL:H262	1.71	1.19
3:A:541:6PL:H402	3:A:541:6PL:H441	1.23	1.18

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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	241/243 (99%)	238 (99%)	3 (1%)	0	100	100
1	E	241/243 (99%)	237 (98%)	3 (1%)	1 (0%)	30	67
2	B	365/396 (92%)	341 (93%)	20 (6%)	4 (1%)	11	46
2	C	365/396 (92%)	341 (93%)	21 (6%)	3 (1%)	16	54
All	All	1212/1278 (95%)	1157 (96%)	47 (4%)	8 (1%)	20	56

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	38	LEU
2	B	62	LEU
2	C	62	LEU
2	B	41	ASP
2	C	243	GLN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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	214/214 (100%)	194 (91%)	20 (9%)	8	26
1	E	214/214 (100%)	192 (90%)	22 (10%)	7	23
2	B	319/342 (93%)	295 (92%)	24 (8%)	12	33
2	C	319/342 (93%)	291 (91%)	28 (9%)	9	28
All	All	1066/1112 (96%)	972 (91%)	94 (9%)	11	28

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	201	ARG
2	C	60	ILE
2	B	241	GLU
2	B	346	ASP
2	C	99	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	370	GLN
1	A	381	GLN
2	B	34	ASN
1	E	162	HIS
1	A	284	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

158 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
3	6PL	A	552	-	51,51,51	0.84	3 (5%)	57,59,59	1.57	8 (14%)
3	6PL	A	580	-	51,51,51	0.84	3 (5%)	57,59,59	1.08	4 (7%)
3	6PL	A	512	-	51,51,51	0.84	3 (5%)	57,59,59	0.96	3 (5%)
3	6PL	A	514	-	51,51,51	0.84	3 (5%)	57,59,59	1.60	9 (15%)
3	6PL	E	366	-	51,51,51	0.84	3 (5%)	57,59,59	1.53	9 (15%)
3	6PL	A	551	-	51,51,51	0.84	3 (5%)	57,59,59	1.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6PL	E	302	-	51,51,51	0.84	3 (5%)	57,59,59	1.12	4 (7%)
3	6PL	A	517	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	E	332	-	51,51,51	0.84	3 (5%)	57,59,59	1.50	9 (15%)
3	6PL	A	583	-	51,51,51	0.84	3 (5%)	57,59,59	1.54	9 (15%)
3	6PL	E	324	-	51,51,51	0.84	3 (5%)	57,59,59	1.51	8 (14%)
3	6PL	A	560	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	3 (5%)
3	6PL	E	351	-	51,51,51	0.84	3 (5%)	57,59,59	0.95	1 (1%)
3	6PL	E	323	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	10 (17%)
3	6PL	E	361	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	5 (8%)
3	6PL	A	568	-	51,51,51	0.84	3 (5%)	57,59,59	1.04	4 (7%)
3	6PL	A	581	-	51,51,51	0.84	3 (5%)	57,59,59	1.57	9 (15%)
3	6PL	E	344	-	51,51,51	0.83	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	A	585	-	51,51,51	0.84	3 (5%)	57,59,59	1.06	5 (8%)
3	6PL	E	303	-	51,51,51	0.84	3 (5%)	57,59,59	1.56	8 (14%)
3	6PL	E	345	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	4 (7%)
3	6PL	A	544	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	9 (15%)
3	6PL	A	516	-	51,51,51	0.84	3 (5%)	57,59,59	1.52	8 (14%)
3	6PL	E	364	-	51,51,51	0.83	3 (5%)	57,59,59	1.03	4 (7%)
3	6PL	A	563	-	51,51,51	0.84	3 (5%)	57,59,59	1.49	8 (14%)
3	6PL	A	555	-	51,51,51	0.84	3 (5%)	57,59,59	1.49	8 (14%)
3	6PL	E	312	-	51,51,51	0.85	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	E	330	-	51,51,51	0.84	3 (5%)	57,59,59	1.08	4 (7%)
3	6PL	A	507	-	51,51,51	0.83	3 (5%)	57,59,59	1.07	4 (7%)
3	6PL	A	531	-	51,51,51	0.83	3 (5%)	57,59,59	1.63	9 (15%)
3	6PL	A	502	-	51,51,51	0.83	3 (5%)	57,59,59	1.06	4 (7%)
3	6PL	E	307	-	51,51,51	0.84	3 (5%)	57,59,59	1.05	3 (5%)
3	6PL	A	540	-	51,51,51	0.84	3 (5%)	57,59,59	0.93	3 (5%)
3	6PL	A	536	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	3 (5%)
3	6PL	E	329	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	3 (5%)
3	6PL	A	556	-	51,51,51	0.84	3 (5%)	57,59,59	0.95	3 (5%)
3	6PL	A	527	-	51,51,51	0.84	3 (5%)	57,59,59	1.57	8 (14%)
3	6PL	A	508	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)
3	6PL	A	520	-	51,51,51	0.84	3 (5%)	57,59,59	1.51	8 (14%)
3	6PL	A	521	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	10 (17%)
3	6PL	E	341	-	51,51,51	0.84	3 (5%)	57,59,59	1.59	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6PL	E	359	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	A	577	-	51,51,51	0.84	3 (5%)	57,59,59	1.51	9 (15%)
3	6PL	E	310	-	51,51,51	0.84	3 (5%)	57,59,59	1.08	4 (7%)
3	6PL	A	550	-	51,51,51	0.84	3 (5%)	57,59,59	1.51	8 (14%)
3	6PL	A	565	-	51,51,51	0.84	3 (5%)	57,59,59	1.00	3 (5%)
3	6PL	A	515	-	51,51,51	0.83	3 (5%)	57,59,59	1.05	3 (5%)
3	6PL	A	546	-	51,51,51	0.84	3 (5%)	57,59,59	1.06	3 (5%)
3	6PL	A	569	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)
3	6PL	A	542	-	51,51,51	0.84	3 (5%)	57,59,59	0.95	3 (5%)
3	6PL	A	525	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	8 (14%)
3	6PL	A	573	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	4 (7%)
3	6PL	A	548	-	51,51,51	0.84	3 (5%)	57,59,59	0.99	3 (5%)
3	6PL	E	317	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	3 (5%)
3	6PL	E	363	-	51,51,51	0.84	3 (5%)	57,59,59	1.10	4 (7%)
3	6PL	A	519	-	51,51,51	0.84	3 (5%)	57,59,59	1.20	6 (10%)
3	6PL	A	584	-	51,51,51	0.84	3 (5%)	57,59,59	1.60	8 (14%)
3	6PL	E	358	-	51,51,51	0.84	3 (5%)	57,59,59	1.61	10 (17%)
3	6PL	A	513	-	51,51,51	0.84	3 (5%)	57,59,59	1.52	8 (14%)
3	6PL	E	342	-	51,51,51	0.84	3 (5%)	57,59,59	0.99	2 (3%)
3	6PL	E	338	-	51,51,51	0.84	3 (5%)	57,59,59	1.56	8 (14%)
3	6PL	E	350	-	51,51,51	0.83	3 (5%)	57,59,59	1.14	5 (8%)
3	6PL	A	524	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	4 (7%)
3	6PL	E	339	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	3 (5%)
3	6PL	E	325	-	51,51,51	0.84	3 (5%)	57,59,59	1.10	4 (7%)
3	6PL	A	562	-	51,51,51	0.84	3 (5%)	57,59,59	0.96	4 (7%)
3	6PL	A	576	-	51,51,51	0.84	3 (5%)	57,59,59	1.57	9 (15%)
3	6PL	A	578	-	51,51,51	0.84	3 (5%)	57,59,59	1.21	8 (14%)
3	6PL	E	354	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	3 (5%)
3	6PL	A	506	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	A	574	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	8 (14%)
3	6PL	A	535	-	51,51,51	0.84	3 (5%)	57,59,59	0.95	4 (7%)
3	6PL	A	582	-	51,51,51	0.84	3 (5%)	57,59,59	0.98	4 (7%)
3	6PL	E	326	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	4 (7%)
3	6PL	E	328	-	51,51,51	0.84	3 (5%)	57,59,59	1.07	4 (7%)
3	6PL	E	327	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6PL	A	557	-	51,51,51	0.84	3 (5%)	57,59,59	1.05	4 (7%)
3	6PL	A	501	-	51,51,51	0.84	3 (5%)	57,59,59	0.97	3 (5%)
3	6PL	A	570	-	51,51,51	0.84	3 (5%)	57,59,59	1.05	4 (7%)
3	6PL	E	311	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	3 (5%)
3	6PL	A	588	-	51,51,51	0.84	3 (5%)	57,59,59	1.04	4 (7%)
3	6PL	A	572	-	51,51,51	0.84	3 (5%)	57,59,59	1.09	3 (5%)
3	6PL	E	362	-	51,51,51	0.84	3 (5%)	57,59,59	1.05	3 (5%)
3	6PL	A	554	-	51,51,51	0.84	3 (5%)	57,59,59	1.54	10 (17%)
3	6PL	E	305	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	E	306	-	51,51,51	0.84	3 (5%)	57,59,59	1.63	9 (15%)
3	6PL	E	315	-	51,51,51	0.84	3 (5%)	57,59,59	0.96	4 (7%)
3	6PL	E	367	-	51,51,51	0.84	3 (5%)	57,59,59	1.52	8 (14%)
3	6PL	E	349	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	10 (17%)
3	6PL	A	505	-	51,51,51	0.83	3 (5%)	57,59,59	1.46	7 (12%)
3	6PL	E	348	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)
3	6PL	E	347	-	51,51,51	0.84	3 (5%)	57,59,59	1.05	3 (5%)
3	6PL	A	566	-	51,51,51	0.83	3 (5%)	57,59,59	1.53	8 (14%)
3	6PL	E	309	-	51,51,51	0.84	3 (5%)	57,59,59	1.00	3 (5%)
3	6PL	A	523	-	51,51,51	0.83	3 (5%)	57,59,59	1.01	3 (5%)
3	6PL	E	368	-	51,51,51	0.84	3 (5%)	57,59,59	0.99	4 (7%)
3	6PL	E	336	-	51,51,51	0.84	3 (5%)	57,59,59	1.60	9 (15%)
3	6PL	E	357	-	51,51,51	0.84	3 (5%)	57,59,59	1.01	4 (7%)
3	6PL	E	353	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)
3	6PL	A	522	-	51,51,51	0.84	3 (5%)	57,59,59	1.00	5 (8%)
3	6PL	A	529	-	51,51,51	0.84	3 (5%)	57,59,59	1.29	9 (15%)
3	6PL	E	352	-	51,51,51	0.84	3 (5%)	57,59,59	1.09	5 (8%)
3	6PL	A	533	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	3 (5%)
3	6PL	E	355	-	51,51,51	0.84	3 (5%)	57,59,59	1.00	4 (7%)
3	6PL	A	503	-	51,51,51	0.84	3 (5%)	57,59,59	0.95	2 (3%)
3	6PL	A	532	-	51,51,51	0.84	3 (5%)	57,59,59	0.93	2 (3%)
3	6PL	E	316	-	51,51,51	0.84	3 (5%)	57,59,59	1.59	9 (15%)
3	6PL	E	365	-	51,51,51	0.84	3 (5%)	57,59,59	1.63	8 (14%)
3	6PL	E	340	-	51,51,51	0.84	3 (5%)	57,59,59	1.57	8 (14%)
3	6PL	A	567	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	5 (8%)
3	6PL	E	346	-	51,51,51	0.84	3 (5%)	57,59,59	0.96	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6PL	E	333	-	51,51,51	0.84	3 (5%)	57,59,59	1.54	8 (14%)
3	6PL	A	571	-	51,51,51	0.84	3 (5%)	57,59,59	0.90	3 (5%)
3	6PL	A	543	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	3 (5%)
3	6PL	E	356	-	51,51,51	0.84	3 (5%)	57,59,59	1.56	10 (17%)
3	6PL	E	369	-	51,51,51	0.84	3 (5%)	57,59,59	1.06	3 (5%)
3	6PL	A	559	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	3 (5%)
3	6PL	E	320	-	51,51,51	0.84	3 (5%)	57,59,59	0.95	3 (5%)
3	6PL	E	318	-	51,51,51	0.84	3 (5%)	57,59,59	1.60	9 (15%)
3	6PL	A	575	-	51,51,51	0.84	3 (5%)	57,59,59	1.09	3 (5%)
3	6PL	A	549	-	51,51,51	0.83	3 (5%)	57,59,59	1.10	3 (5%)
3	6PL	E	337	-	51,51,51	0.84	3 (5%)	57,59,59	1.04	5 (8%)
3	6PL	A	534	-	51,51,51	0.84	3 (5%)	57,59,59	1.09	3 (5%)
3	6PL	E	313	-	51,51,51	0.84	3 (5%)	57,59,59	1.25	8 (14%)
3	6PL	A	511	-	51,51,51	0.83	3 (5%)	57,59,59	1.09	4 (7%)
3	6PL	E	335	-	51,51,51	0.84	3 (5%)	57,59,59	0.99	3 (5%)
3	6PL	A	586	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)
3	6PL	E	314	-	51,51,51	0.84	3 (5%)	57,59,59	1.53	8 (14%)
3	6PL	A	510	-	51,51,51	0.83	3 (5%)	57,59,59	1.76	10 (17%)
3	6PL	A	509	-	51,51,51	0.84	3 (5%)	57,59,59	1.50	8 (14%)
3	6PL	A	558	-	51,51,51	0.84	3 (5%)	57,59,59	1.13	6 (10%)
3	6PL	A	561	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	3 (5%)
3	6PL	A	579	-	51,51,51	0.84	3 (5%)	57,59,59	1.55	8 (14%)
3	6PL	C	501	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	3 (5%)
3	6PL	A	553	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	5 (8%)
3	6PL	E	360	-	51,51,51	0.84	3 (5%)	57,59,59	0.89	3 (5%)
3	6PL	A	587	-	51,51,51	0.84	3 (5%)	57,59,59	1.02	4 (7%)
3	6PL	E	334	-	51,51,51	0.84	3 (5%)	57,59,59	1.04	3 (5%)
3	6PL	A	541	-	51,51,51	0.84	3 (5%)	57,59,59	1.04	5 (8%)
3	6PL	E	308	-	51,51,51	0.84	3 (5%)	57,59,59	1.00	3 (5%)
3	6PL	E	304	-	51,51,51	0.83	3 (5%)	57,59,59	1.01	3 (5%)
3	6PL	A	564	-	51,51,51	0.84	3 (5%)	57,59,59	1.03	3 (5%)
3	6PL	A	537	-	51,51,51	0.84	3 (5%)	57,59,59	1.61	8 (14%)
3	6PL	A	528	-	51,51,51	0.83	3 (5%)	57,59,59	1.07	4 (7%)
3	6PL	A	547	-	51,51,51	0.84	3 (5%)	57,59,59	1.28	8 (14%)
3	6PL	E	331	-	51,51,51	0.84	3 (5%)	57,59,59	1.59	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6PL	E	322	-	51,51,51	0.83	3 (5%)	57,59,59	1.16	3 (5%)
3	6PL	A	539	-	51,51,51	0.84	3 (5%)	57,59,59	1.54	9 (15%)
3	6PL	E	301	-	51,51,51	0.84	3 (5%)	57,59,59	1.06	3 (5%)
3	6PL	A	504	-	51,51,51	0.84	3 (5%)	57,59,59	1.57	9 (15%)
3	6PL	A	545	-	51,51,51	0.84	3 (5%)	57,59,59	1.59	8 (14%)
3	6PL	E	321	-	51,51,51	0.84	3 (5%)	57,59,59	1.52	8 (14%)
3	6PL	E	319	-	51,51,51	0.84	3 (5%)	57,59,59	1.60	9 (15%)
3	6PL	E	343	-	51,51,51	0.84	3 (5%)	57,59,59	1.56	8 (14%)
3	6PL	A	518	-	51,51,51	0.84	3 (5%)	57,59,59	0.92	3 (5%)
3	6PL	A	530	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)
3	6PL	A	538	-	51,51,51	0.84	3 (5%)	57,59,59	1.59	9 (15%)
3	6PL	A	526	-	51,51,51	0.84	3 (5%)	57,59,59	1.58	9 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6PL	A	552	-	-	5/55/55/55	-
3	6PL	A	580	-	-	8/55/55/55	-
3	6PL	A	512	-	-	7/55/55/55	-
3	6PL	A	514	-	-	9/55/55/55	-
3	6PL	E	366	-	-	6/55/55/55	-
3	6PL	A	551	-	-	13/55/55/55	-
3	6PL	E	302	-	-	8/55/55/55	-
3	6PL	A	517	-	-	9/55/55/55	-
3	6PL	E	332	-	-	5/55/55/55	-
3	6PL	A	583	-	-	3/55/55/55	-
3	6PL	E	324	-	-	7/55/55/55	-
3	6PL	A	560	-	-	8/55/55/55	-
3	6PL	E	351	-	-	13/55/55/55	-
3	6PL	E	323	-	-	5/55/55/55	-
3	6PL	E	361	-	-	8/55/55/55	-
3	6PL	A	568	-	-	6/55/55/55	-
3	6PL	A	581	-	-	11/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6PL	E	344	-	-	9/55/55/55	-
3	6PL	A	585	-	-	3/55/55/55	-
3	6PL	E	303	-	-	7/55/55/55	-
3	6PL	E	345	-	-	8/55/55/55	-
3	6PL	A	544	-	-	1/55/55/55	-
3	6PL	A	516	-	-	10/55/55/55	-
3	6PL	E	364	-	-	8/55/55/55	-
3	6PL	A	563	-	-	14/55/55/55	-
3	6PL	A	555	-	-	9/55/55/55	-
3	6PL	E	312	-	-	14/55/55/55	-
3	6PL	E	330	-	-	5/55/55/55	-
3	6PL	A	507	-	-	6/55/55/55	-
3	6PL	A	531	-	-	9/55/55/55	-
3	6PL	A	502	-	-	5/55/55/55	-
3	6PL	E	307	-	-	12/55/55/55	-
3	6PL	A	540	-	-	9/55/55/55	-
3	6PL	A	536	-	-	7/55/55/55	-
3	6PL	E	329	-	-	6/55/55/55	-
3	6PL	A	556	-	-	8/55/55/55	-
3	6PL	A	527	-	-	3/55/55/55	-
3	6PL	A	508	-	-	7/55/55/55	-
3	6PL	A	520	-	-	11/55/55/55	-
3	6PL	A	521	-	-	5/55/55/55	-
3	6PL	E	341	-	-	5/55/55/55	-
3	6PL	E	359	-	-	6/55/55/55	-
3	6PL	A	577	-	-	10/55/55/55	-
3	6PL	E	310	-	-	7/55/55/55	-
3	6PL	A	550	-	-	7/55/55/55	-
3	6PL	A	565	-	-	10/55/55/55	-
3	6PL	A	515	-	-	7/55/55/55	-
3	6PL	A	546	-	-	10/55/55/55	-
3	6PL	A	569	-	-	7/55/55/55	-
3	6PL	A	542	-	-	10/55/55/55	-
3	6PL	A	525	-	-	6/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6PL	A	573	-	-	4/55/55/55	-
3	6PL	A	548	-	-	11/55/55/55	-
3	6PL	E	317	-	-	6/55/55/55	-
3	6PL	E	363	-	-	7/55/55/55	-
3	6PL	A	519	-	-	6/55/55/55	-
3	6PL	A	584	-	-	11/55/55/55	-
3	6PL	E	358	-	-	7/55/55/55	-
3	6PL	A	513	-	-	8/55/55/55	-
3	6PL	E	342	-	-	12/55/55/55	-
3	6PL	E	338	-	-	2/55/55/55	-
3	6PL	E	350	-	-	6/55/55/55	-
3	6PL	A	524	-	-	7/55/55/55	-
3	6PL	E	339	-	-	6/55/55/55	-
3	6PL	E	325	-	-	12/55/55/55	-
3	6PL	A	562	-	-	6/55/55/55	-
3	6PL	A	576	-	-	10/55/55/55	-
3	6PL	A	578	-	-	8/55/55/55	-
3	6PL	E	354	-	-	4/55/55/55	-
3	6PL	A	506	-	-	12/55/55/55	-
3	6PL	A	574	-	-	7/55/55/55	-
3	6PL	A	535	-	-	10/55/55/55	-
3	6PL	A	582	-	-	9/55/55/55	-
3	6PL	E	326	-	-	14/55/55/55	-
3	6PL	E	328	-	-	6/55/55/55	-
3	6PL	E	327	-	-	5/55/55/55	-
3	6PL	A	557	-	-	5/55/55/55	-
3	6PL	A	501	-	-	7/55/55/55	-
3	6PL	A	570	-	-	9/55/55/55	-
3	6PL	E	311	-	-	3/55/55/55	-
3	6PL	A	588	-	-	8/55/55/55	-
3	6PL	A	572	-	-	5/55/55/55	-
3	6PL	E	362	-	-	6/55/55/55	-
3	6PL	A	554	-	-	4/55/55/55	-
3	6PL	E	305	-	-	10/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6PL	E	306	-	-	6/55/55/55	-
3	6PL	E	315	-	-	11/55/55/55	-
3	6PL	E	367	-	-	14/55/55/55	-
3	6PL	E	349	-	-	9/55/55/55	-
3	6PL	A	505	-	-	6/55/55/55	-
3	6PL	E	348	-	-	12/55/55/55	-
3	6PL	E	347	-	-	4/55/55/55	-
3	6PL	A	566	-	-	6/55/55/55	-
3	6PL	E	309	-	-	4/55/55/55	-
3	6PL	A	523	-	-	8/55/55/55	-
3	6PL	E	368	-	-	9/55/55/55	-
3	6PL	E	336	-	-	5/55/55/55	-
3	6PL	E	357	-	-	5/55/55/55	-
3	6PL	E	353	-	-	14/55/55/55	-
3	6PL	A	522	-	-	15/55/55/55	-
3	6PL	A	529	-	-	7/55/55/55	-
3	6PL	E	352	-	-	10/55/55/55	-
3	6PL	A	533	-	-	9/55/55/55	-
3	6PL	E	355	-	-	6/55/55/55	-
3	6PL	A	503	-	-	8/55/55/55	-
3	6PL	A	532	-	-	6/55/55/55	-
3	6PL	E	316	-	-	10/55/55/55	-
3	6PL	E	365	-	-	10/55/55/55	-
3	6PL	E	340	-	-	7/55/55/55	-
3	6PL	A	567	-	-	4/55/55/55	-
3	6PL	E	346	-	-	2/55/55/55	-
3	6PL	E	333	-	-	12/55/55/55	-
3	6PL	A	571	-	-	10/55/55/55	-
3	6PL	A	543	-	-	5/55/55/55	-
3	6PL	E	356	-	-	4/55/55/55	-
3	6PL	E	369	-	-	11/55/55/55	-
3	6PL	A	559	-	-	15/55/55/55	-
3	6PL	E	320	-	-	7/55/55/55	-
3	6PL	E	318	-	-	6/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6PL	A	575	-	-	11/55/55/55	-
3	6PL	A	549	-	-	7/55/55/55	-
3	6PL	E	337	-	-	6/55/55/55	-
3	6PL	A	534	-	-	9/55/55/55	-
3	6PL	E	313	-	-	9/55/55/55	-
3	6PL	A	511	-	-	12/55/55/55	-
3	6PL	E	335	-	-	11/55/55/55	-
3	6PL	A	586	-	-	10/55/55/55	-
3	6PL	E	314	-	-	10/55/55/55	-
3	6PL	A	510	-	-	8/55/55/55	-
3	6PL	A	509	-	-	12/55/55/55	-
3	6PL	A	558	-	-	8/55/55/55	-
3	6PL	A	561	-	-	7/55/55/55	-
3	6PL	A	579	-	-	8/55/55/55	-
3	6PL	C	501	-	-	5/55/55/55	-
3	6PL	A	553	-	-	6/55/55/55	-
3	6PL	E	360	-	-	11/55/55/55	-
3	6PL	A	587	-	-	6/55/55/55	-
3	6PL	E	334	-	-	5/55/55/55	-
3	6PL	A	541	-	-	6/55/55/55	-
3	6PL	E	308	-	-	5/55/55/55	-
3	6PL	E	304	-	-	6/55/55/55	-
3	6PL	A	564	-	-	9/55/55/55	-
3	6PL	A	537	-	-	11/55/55/55	-
3	6PL	A	528	-	-	10/55/55/55	-
3	6PL	A	547	-	-	9/55/55/55	-
3	6PL	E	331	-	-	7/55/55/55	-
3	6PL	E	322	-	-	10/55/55/55	-
3	6PL	A	539	-	-	3/55/55/55	-
3	6PL	E	301	-	-	7/55/55/55	-
3	6PL	A	504	-	-	6/55/55/55	-
3	6PL	A	545	-	-	6/55/55/55	-
3	6PL	E	321	-	-	11/55/55/55	-
3	6PL	E	319	-	-	7/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6PL	E	343	-	-	8/55/55/55	-
3	6PL	A	518	-	-	11/55/55/55	-
3	6PL	A	530	-	-	3/55/55/55	-
3	6PL	A	538	-	-	4/55/55/55	-
3	6PL	A	526	-	-	10/55/55/55	-

The worst 5 of 474 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	306	6PL	C40-C39	-2.58	1.39	1.51
3	A	523	6PL	C40-C39	-2.56	1.39	1.51
3	E	369	6PL	C40-C39	-2.56	1.39	1.51
3	A	553	6PL	C41-C40	-2.55	1.39	1.51
3	A	507	6PL	C40-C39	-2.54	1.39	1.51

The worst 5 of 909 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	510	6PL	C2-O2-C31	-5.12	105.54	117.80
3	A	569	6PL	C6-N-C8	-4.92	96.05	108.98
3	A	531	6PL	C6-N-C8	-4.92	96.07	108.98
3	A	508	6PL	C6-N-C8	-4.91	96.07	108.98
3	A	579	6PL	C6-N-C8	-4.90	96.10	108.98

There are no chirality outliers.

5 of 1232 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	302	6PL	C1-O3P-P-O1P
3	E	302	6PL	C1-O3P-P-O2P
3	E	302	6PL	C1-O3P-P-O4P
3	E	302	6PL	C5-C4-O4P-P
3	E	303	6PL	C1-O3P-P-O1P

There are no ring outliers.

158 monomers are involved in 3165 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	552	6PL	28	0
3	A	580	6PL	72	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	512	6PL	41	0
3	A	514	6PL	20	0
3	E	366	6PL	34	0
3	A	551	6PL	18	0
3	E	302	6PL	30	0
3	A	517	6PL	31	0
3	E	332	6PL	26	0
3	A	583	6PL	17	0
3	E	324	6PL	47	0
3	A	560	6PL	33	0
3	E	351	6PL	34	0
3	E	323	6PL	24	0
3	E	361	6PL	23	0
3	A	568	6PL	14	0
3	A	581	6PL	34	0
3	E	344	6PL	48	0
3	A	585	6PL	14	0
3	E	303	6PL	9	0
3	E	345	6PL	35	0
3	A	544	6PL	31	0
3	A	516	6PL	22	0
3	E	364	6PL	45	0
3	A	563	6PL	32	0
3	A	555	6PL	33	0
3	E	312	6PL	22	0
3	E	330	6PL	32	0
3	A	507	6PL	10	0
3	A	531	6PL	32	0
3	A	502	6PL	33	0
3	E	307	6PL	16	0
3	A	540	6PL	43	0
3	A	536	6PL	36	0
3	E	329	6PL	31	0
3	A	556	6PL	36	0
3	A	527	6PL	31	0
3	A	508	6PL	34	0
3	A	520	6PL	52	0
3	A	521	6PL	26	0
3	E	341	6PL	23	0
3	E	359	6PL	32	0
3	A	577	6PL	16	0
3	E	310	6PL	34	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	550	6PL	39	0
3	A	565	6PL	42	0
3	A	515	6PL	28	0
3	A	546	6PL	34	0
3	A	569	6PL	9	0
3	A	542	6PL	69	0
3	A	525	6PL	26	0
3	A	573	6PL	28	0
3	A	548	6PL	34	0
3	E	317	6PL	41	0
3	E	363	6PL	50	0
3	A	519	6PL	31	0
3	A	584	6PL	24	0
3	E	358	6PL	41	0
3	A	513	6PL	43	0
3	E	342	6PL	15	0
3	E	338	6PL	17	0
3	E	350	6PL	38	0
3	A	524	6PL	38	0
3	E	339	6PL	22	0
3	E	325	6PL	37	0
3	A	562	6PL	40	0
3	A	576	6PL	23	0
3	A	578	6PL	33	0
3	E	354	6PL	12	0
3	A	506	6PL	41	0
3	A	574	6PL	24	0
3	A	535	6PL	43	0
3	A	582	6PL	29	0
3	E	326	6PL	42	0
3	E	328	6PL	24	0
3	E	327	6PL	17	0
3	A	557	6PL	46	0
3	A	501	6PL	12	0
3	A	570	6PL	29	0
3	E	311	6PL	15	0
3	A	588	6PL	58	0
3	A	572	6PL	35	0
3	E	362	6PL	28	0
3	A	554	6PL	32	0
3	E	305	6PL	11	0
3	E	306	6PL	49	0

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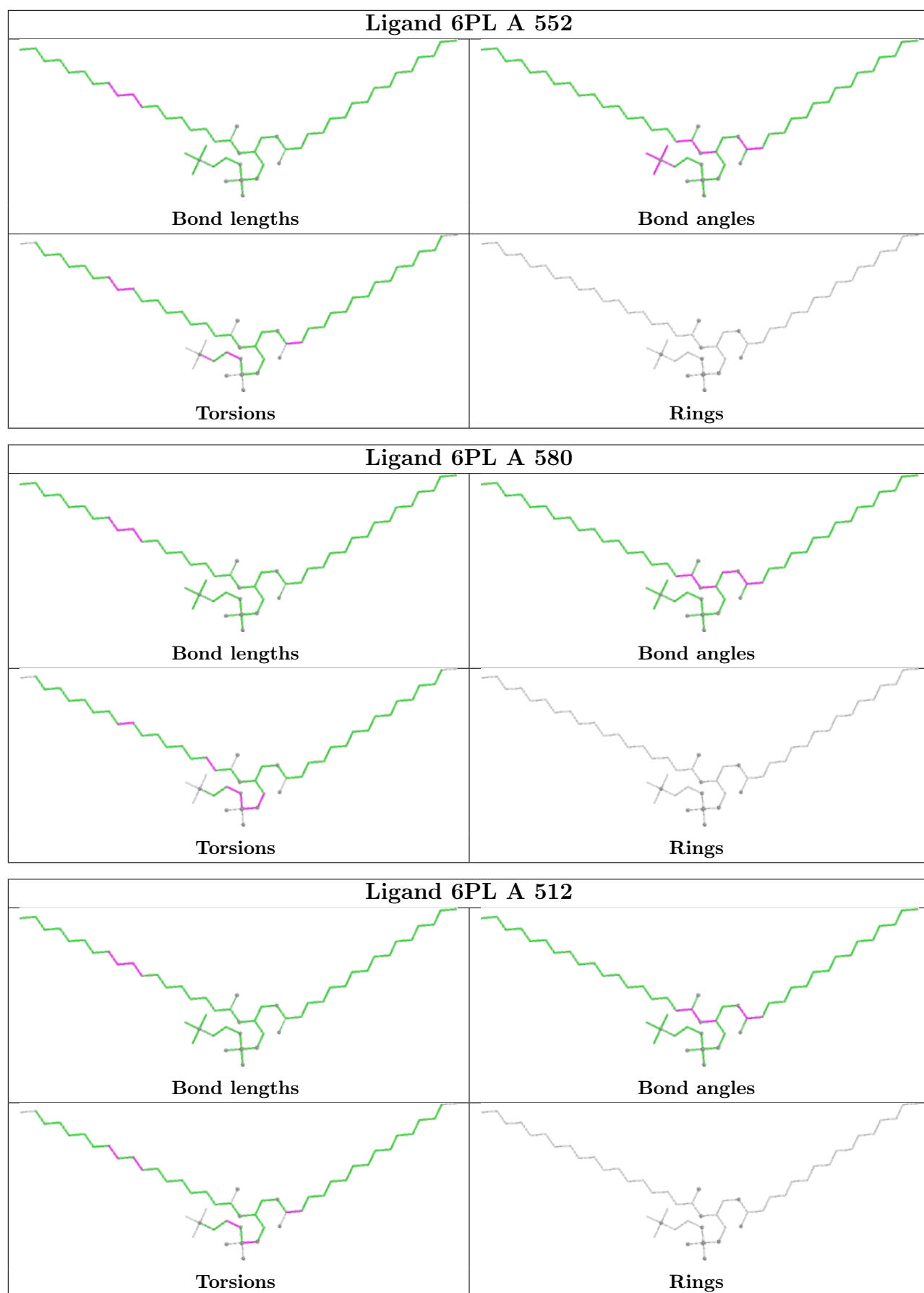
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	315	6PL	31	0
3	E	367	6PL	21	0
3	E	349	6PL	14	0
3	A	505	6PL	51	0
3	E	348	6PL	26	0
3	E	347	6PL	28	0
3	A	566	6PL	58	0
3	E	309	6PL	40	0
3	A	523	6PL	25	0
3	E	368	6PL	31	0
3	E	336	6PL	13	0
3	E	357	6PL	42	0
3	E	353	6PL	34	0
3	A	522	6PL	37	0
3	A	529	6PL	34	0
3	E	352	6PL	15	0
3	A	533	6PL	38	0
3	E	355	6PL	50	0
3	A	503	6PL	43	0
3	A	532	6PL	46	0
3	E	316	6PL	15	0
3	E	365	6PL	36	0
3	E	340	6PL	32	0
3	A	567	6PL	29	0
3	E	346	6PL	28	0
3	E	333	6PL	45	0
3	A	571	6PL	40	0
3	A	543	6PL	53	0
3	E	356	6PL	24	0
3	E	369	6PL	42	0
3	A	559	6PL	23	0
3	E	320	6PL	25	0
3	E	318	6PL	34	0
3	A	575	6PL	39	0
3	A	549	6PL	48	0
3	E	337	6PL	26	0
3	A	534	6PL	34	0
3	E	313	6PL	19	0
3	A	511	6PL	28	0
3	E	335	6PL	34	0
3	A	586	6PL	17	0
3	E	314	6PL	14	0

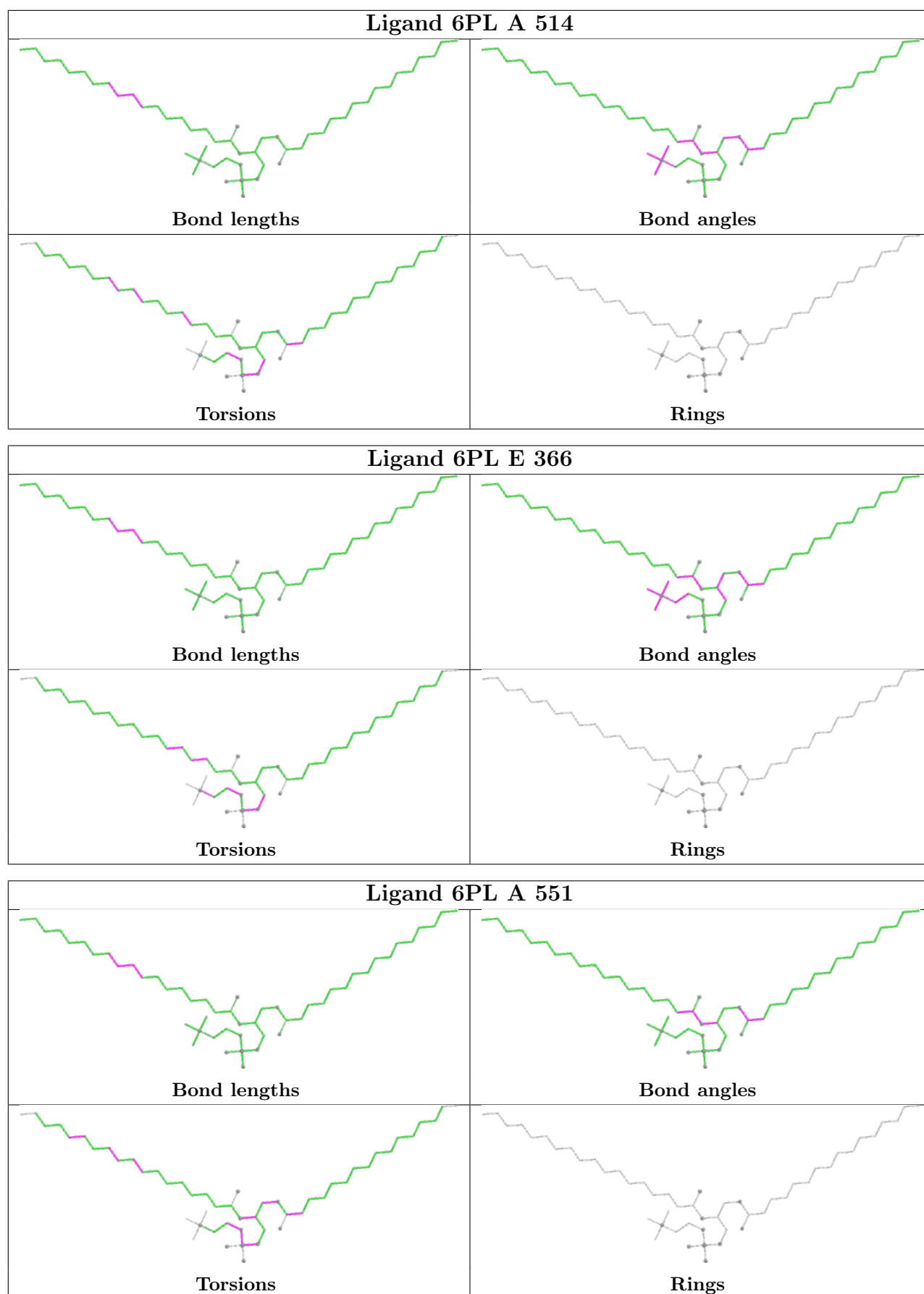
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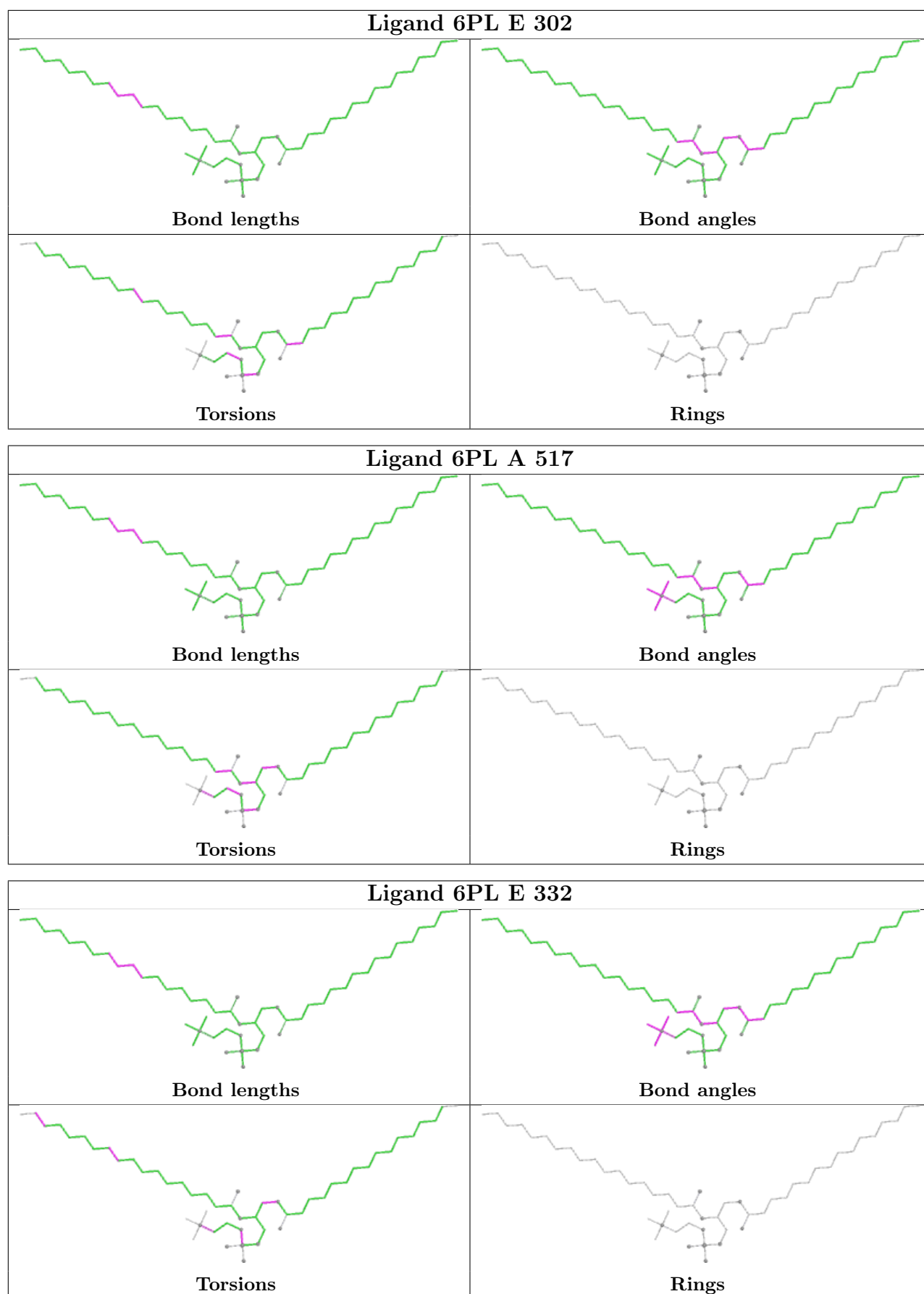
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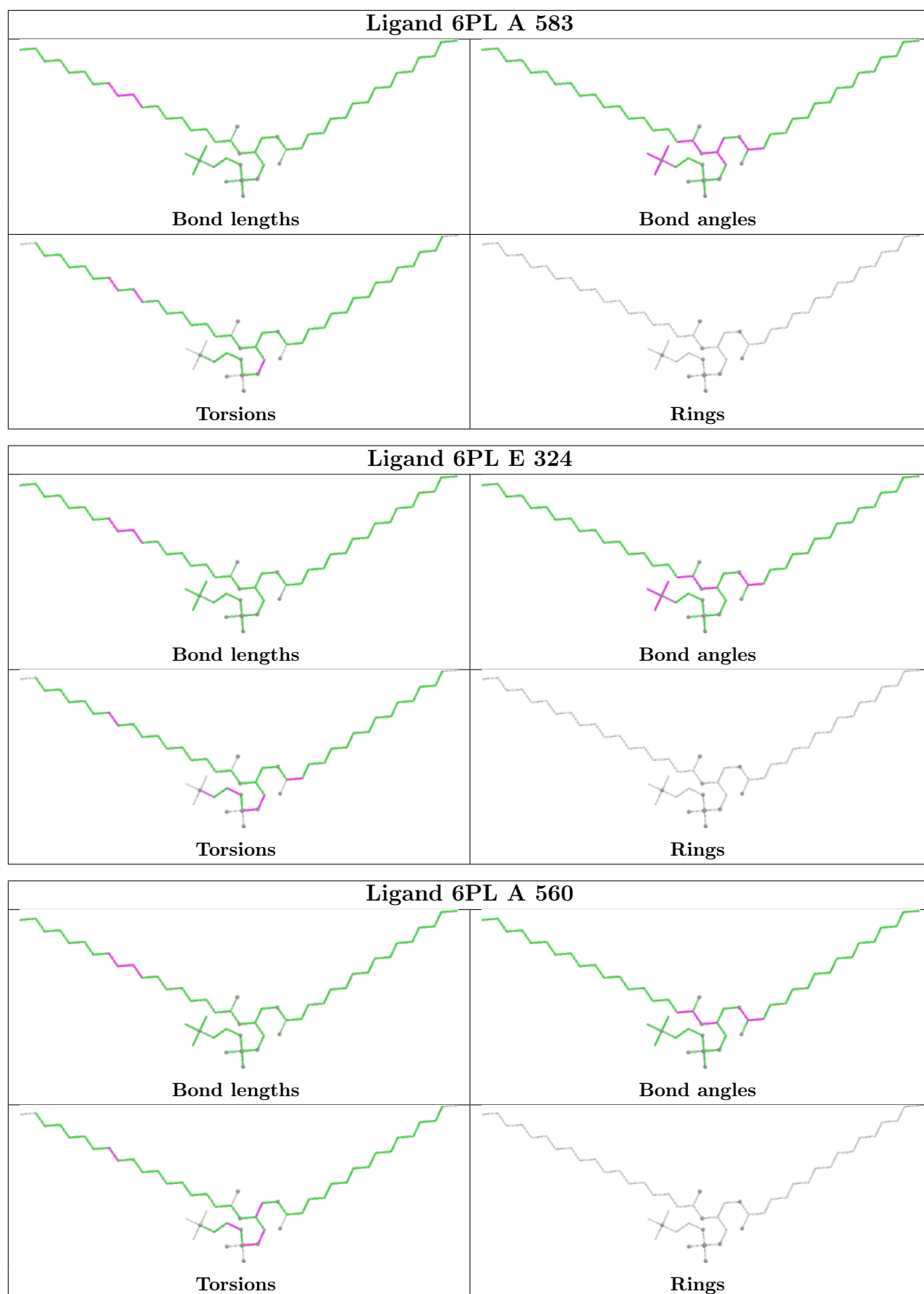
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	510	6PL	31	0
3	A	509	6PL	35	0
3	A	558	6PL	27	0
3	A	561	6PL	16	0
3	A	579	6PL	34	0
3	C	501	6PL	45	0
3	A	553	6PL	20	0
3	E	360	6PL	28	0
3	A	587	6PL	28	0
3	E	334	6PL	8	0
3	A	541	6PL	51	0
3	E	308	6PL	44	0
3	E	304	6PL	46	0
3	A	564	6PL	38	0
3	A	537	6PL	41	0
3	A	528	6PL	36	0
3	A	547	6PL	14	0
3	E	331	6PL	54	0
3	E	322	6PL	27	0
3	A	539	6PL	21	0
3	E	301	6PL	24	0
3	A	504	6PL	30	0
3	A	545	6PL	10	0
3	E	321	6PL	53	0
3	E	319	6PL	17	0
3	E	343	6PL	13	0
3	A	518	6PL	58	0
3	A	530	6PL	25	0
3	A	538	6PL	34	0
3	A	526	6PL	30	0

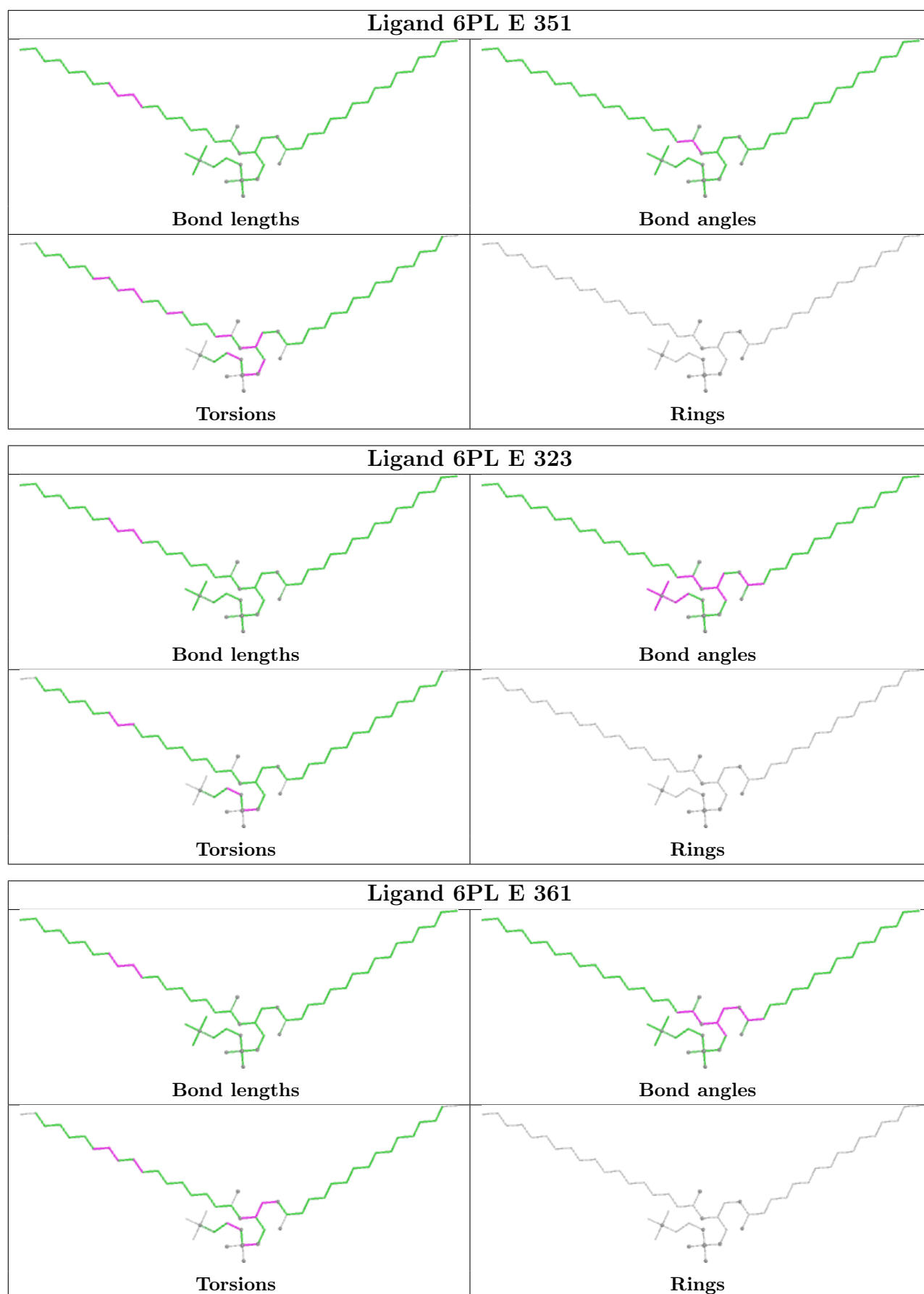
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

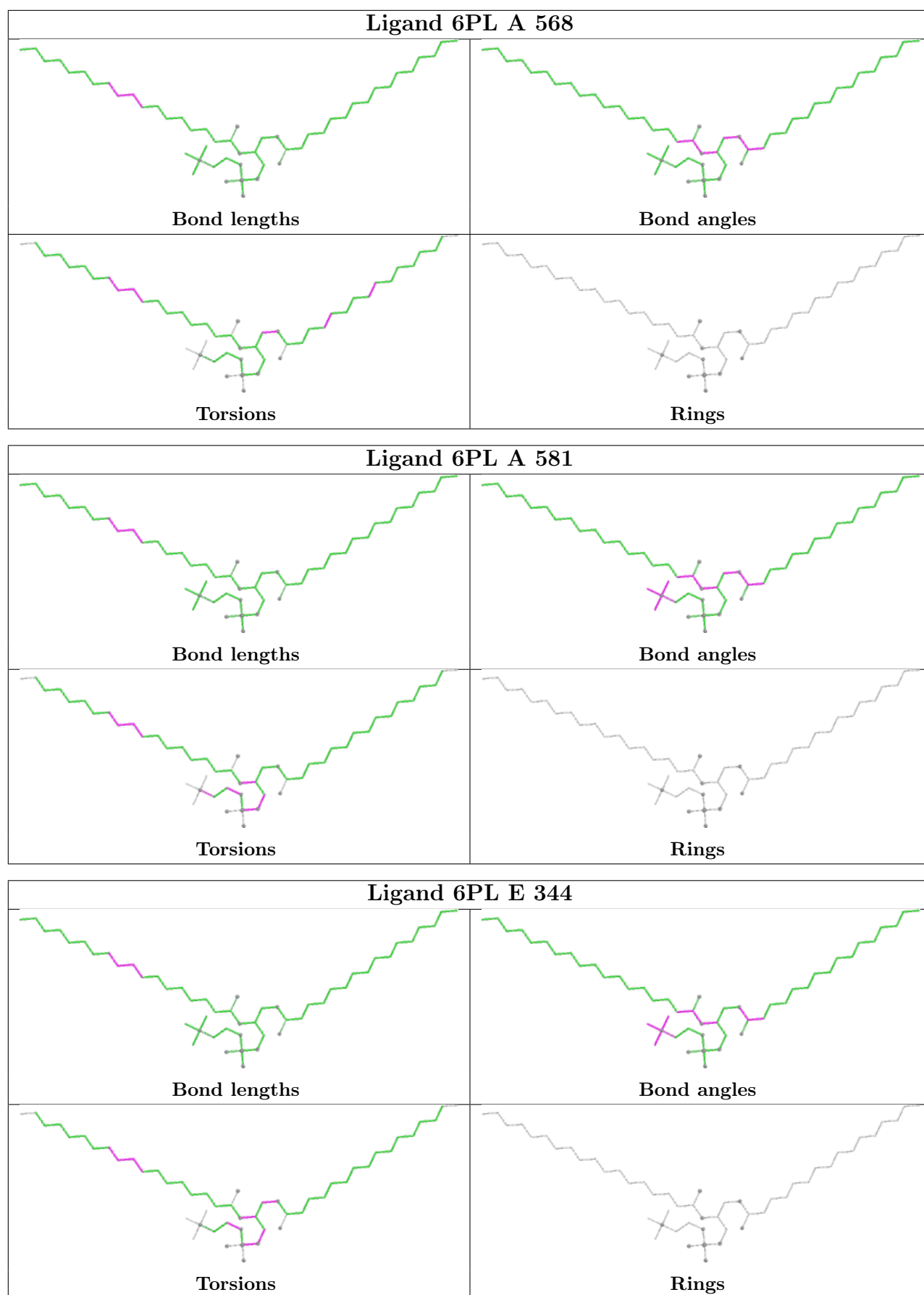


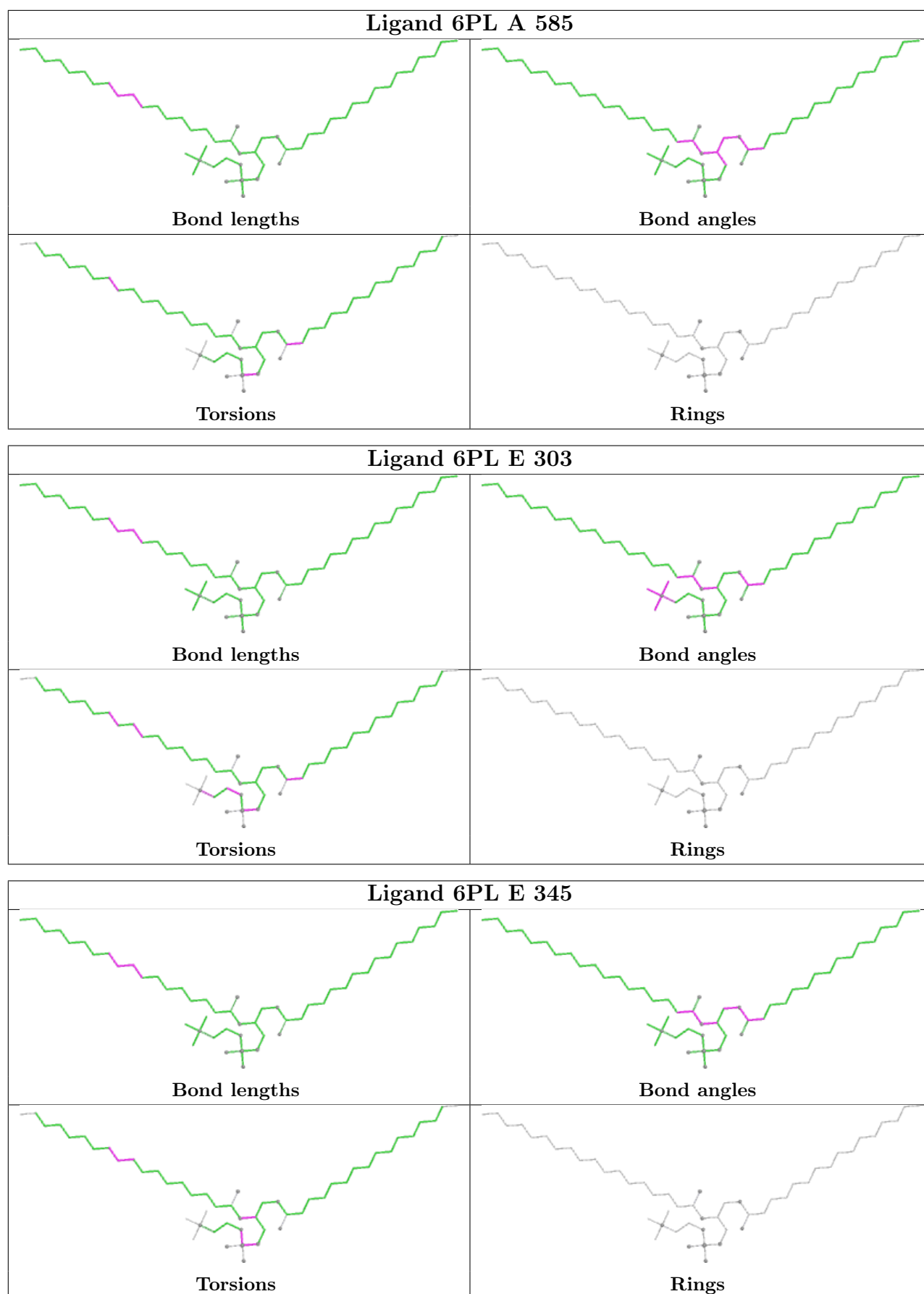


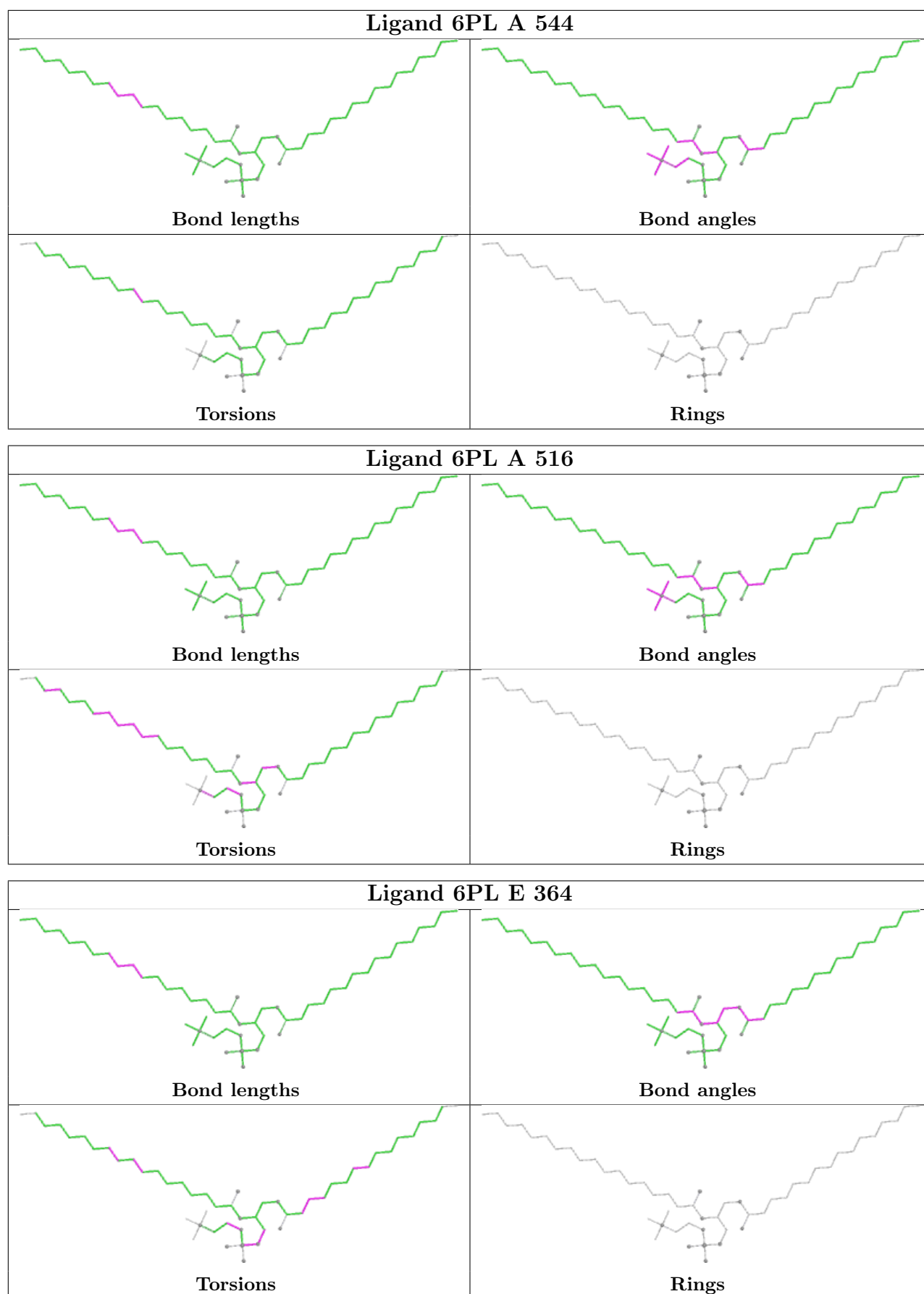


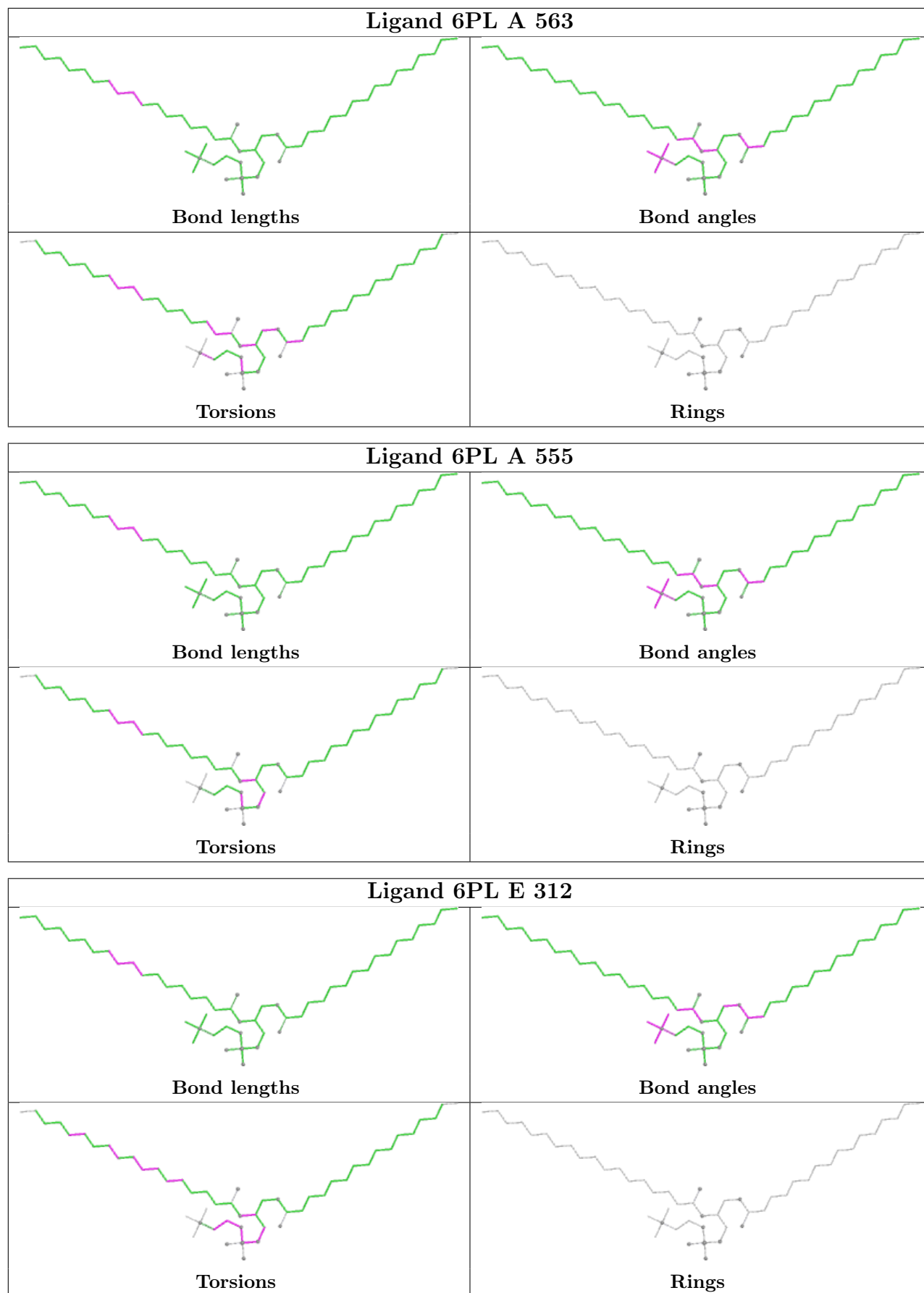


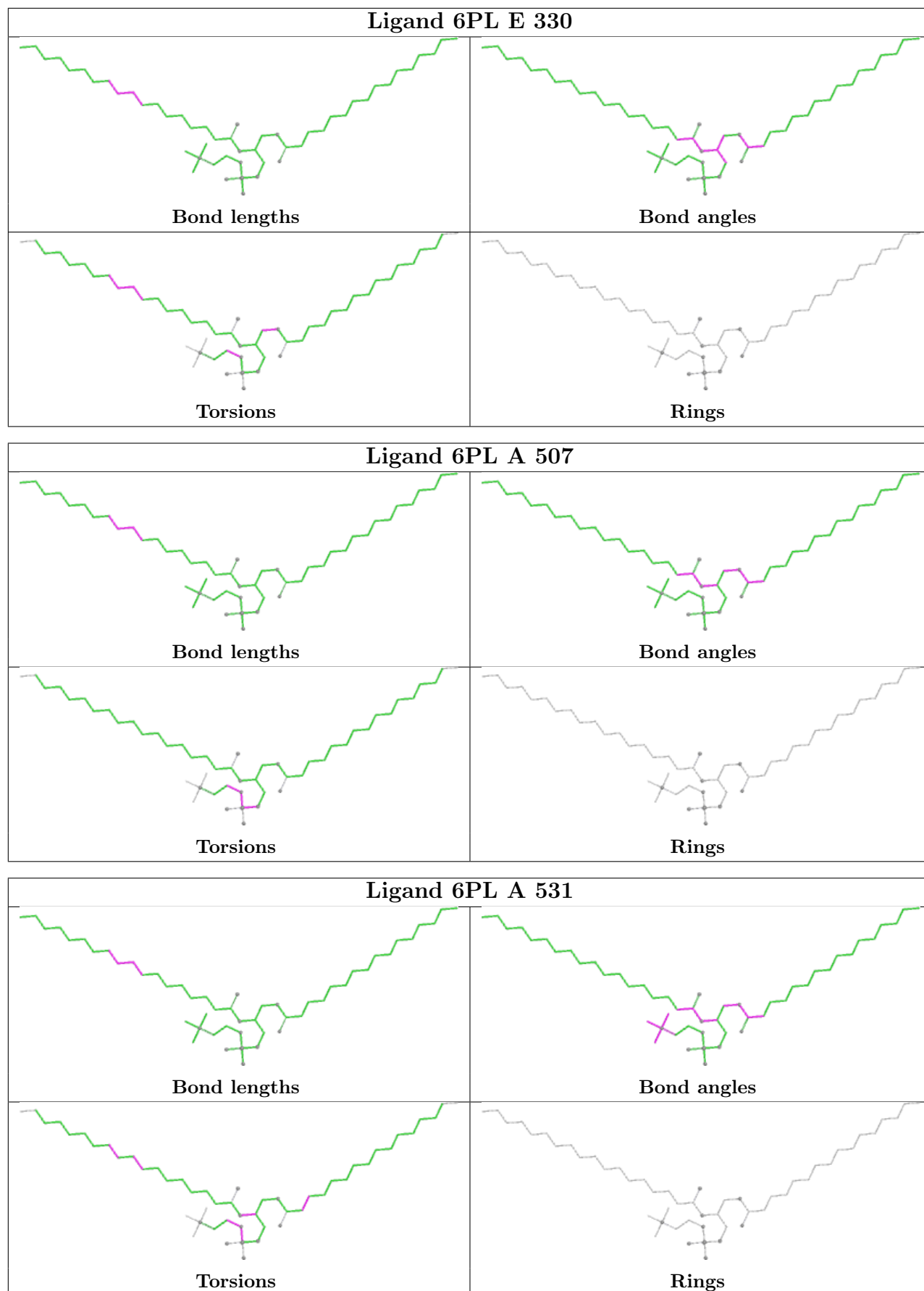


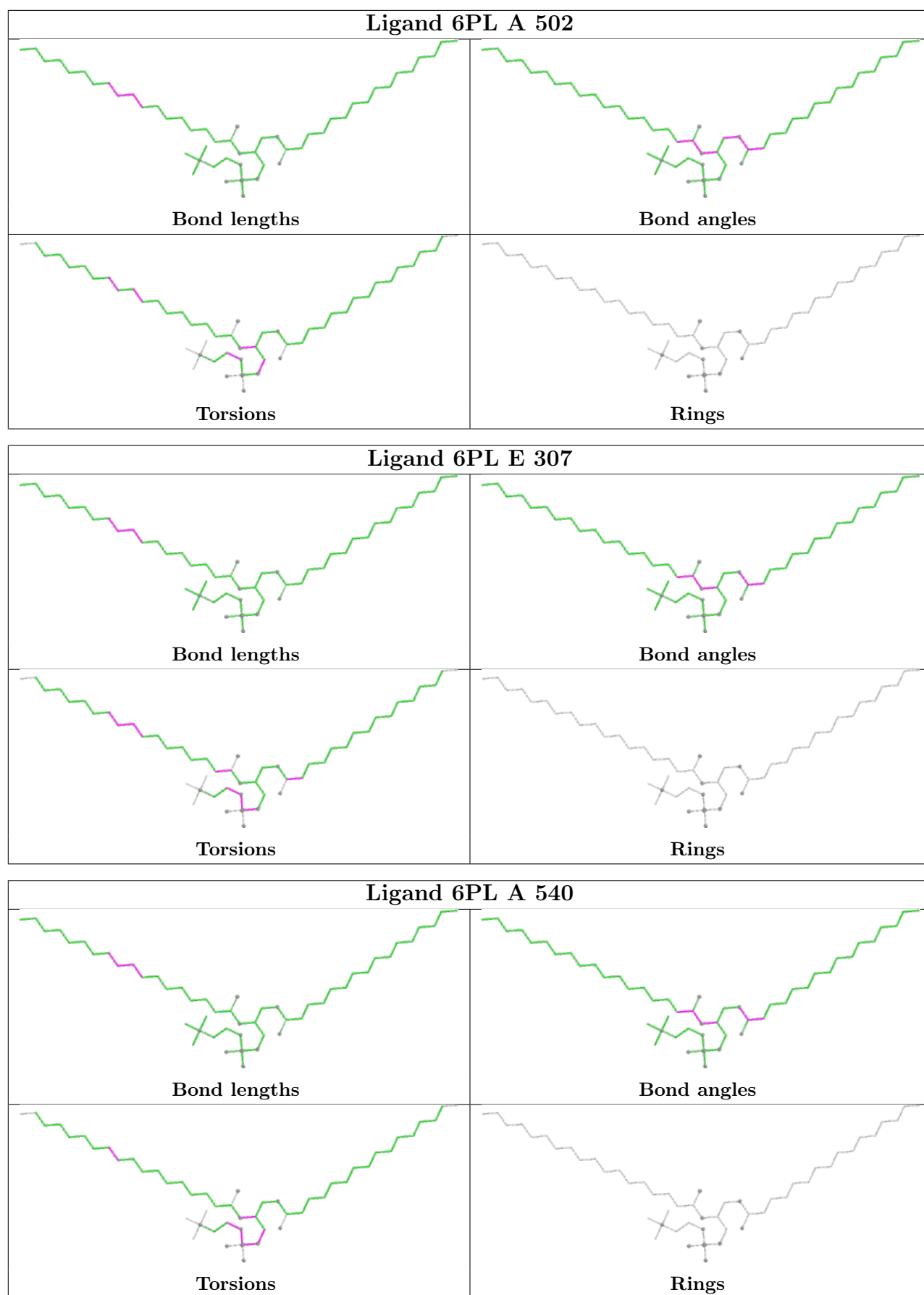


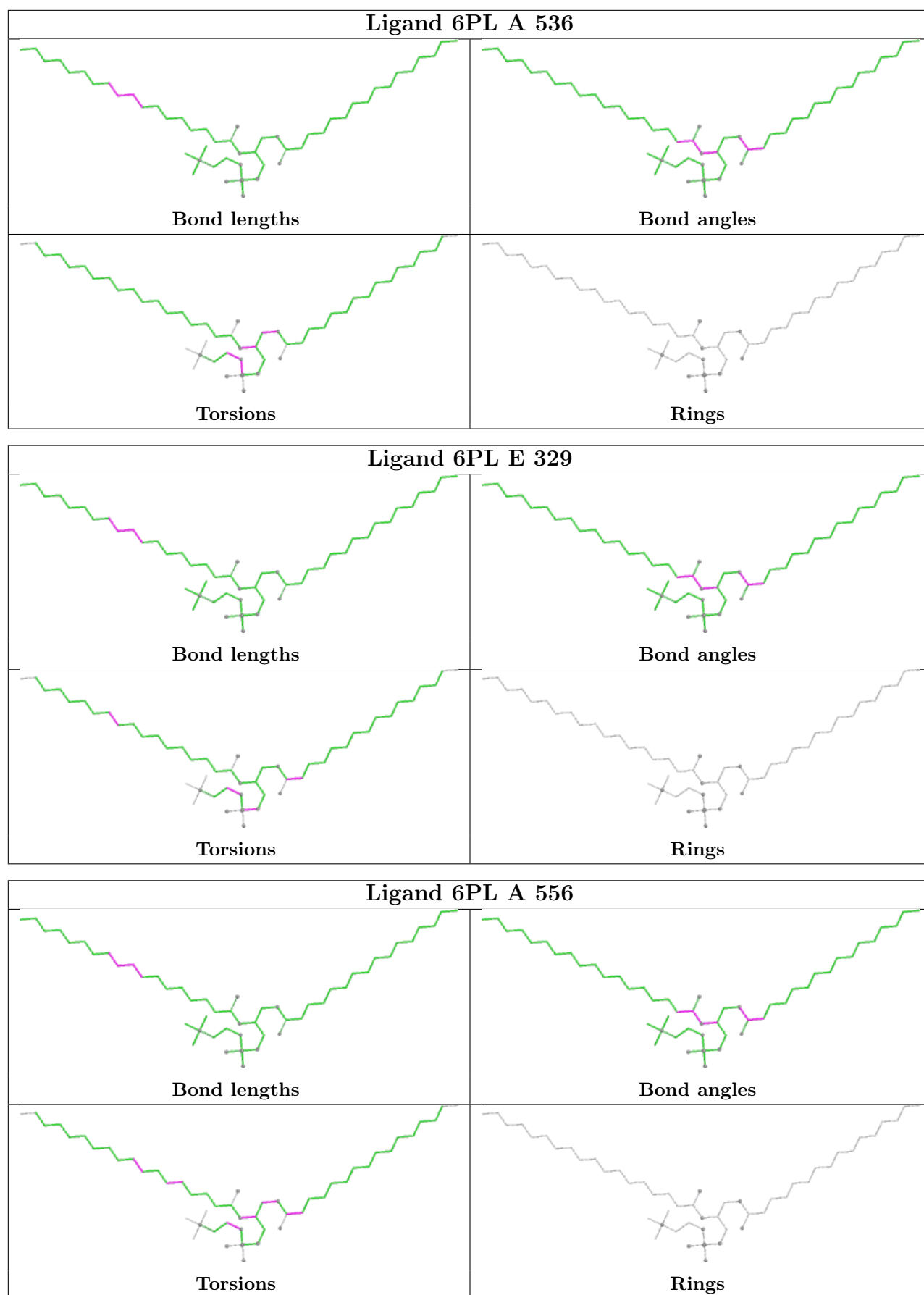


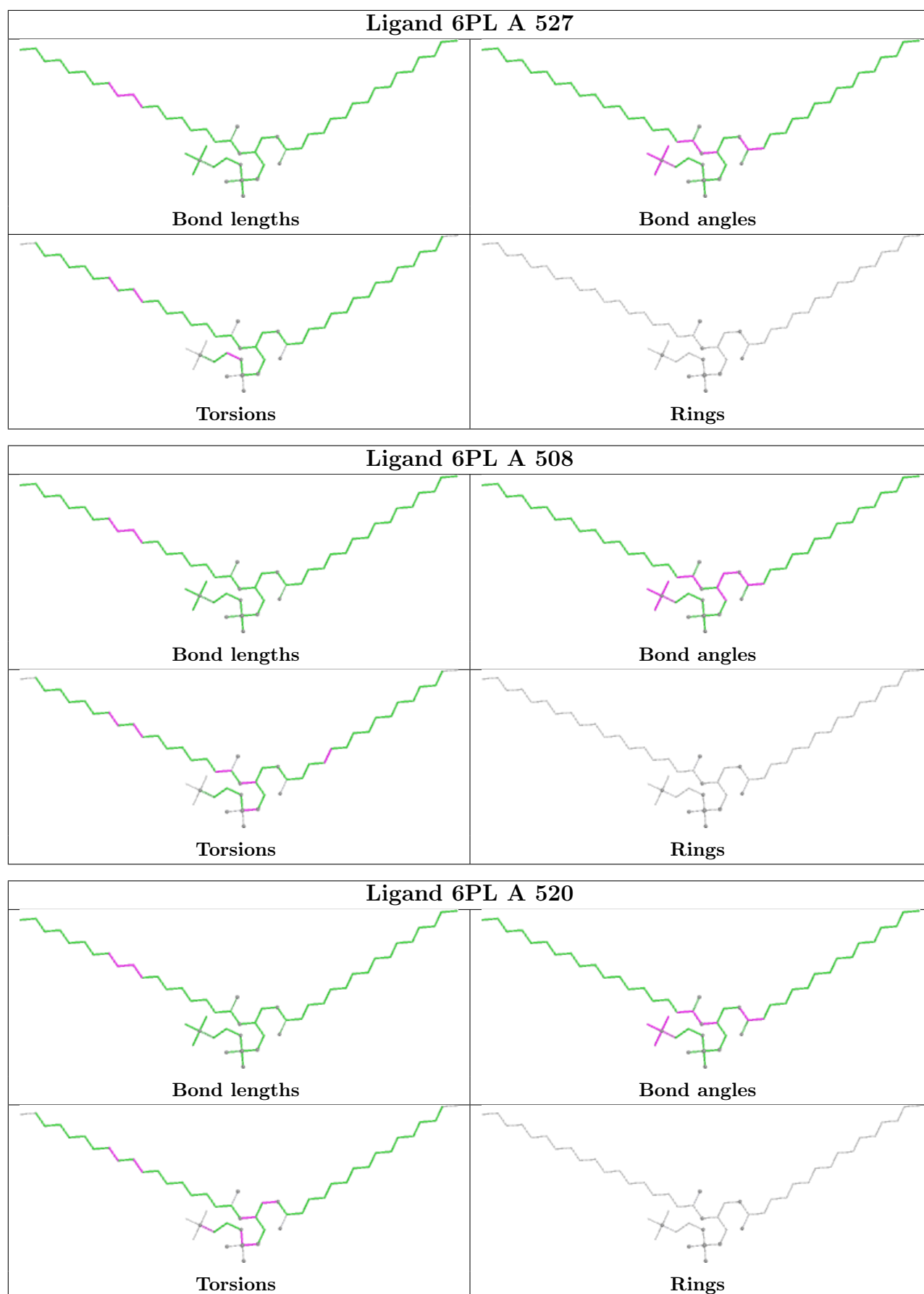


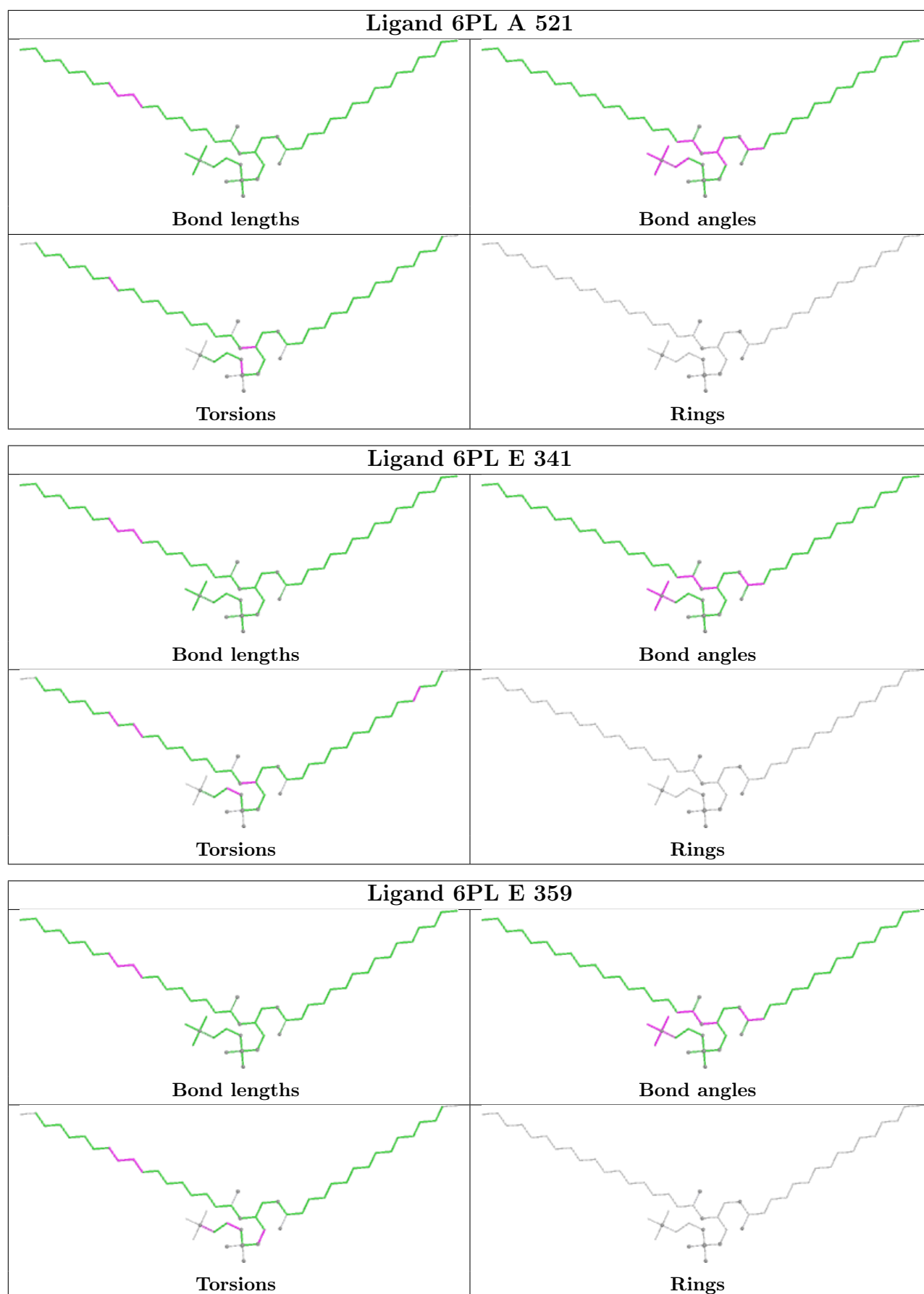


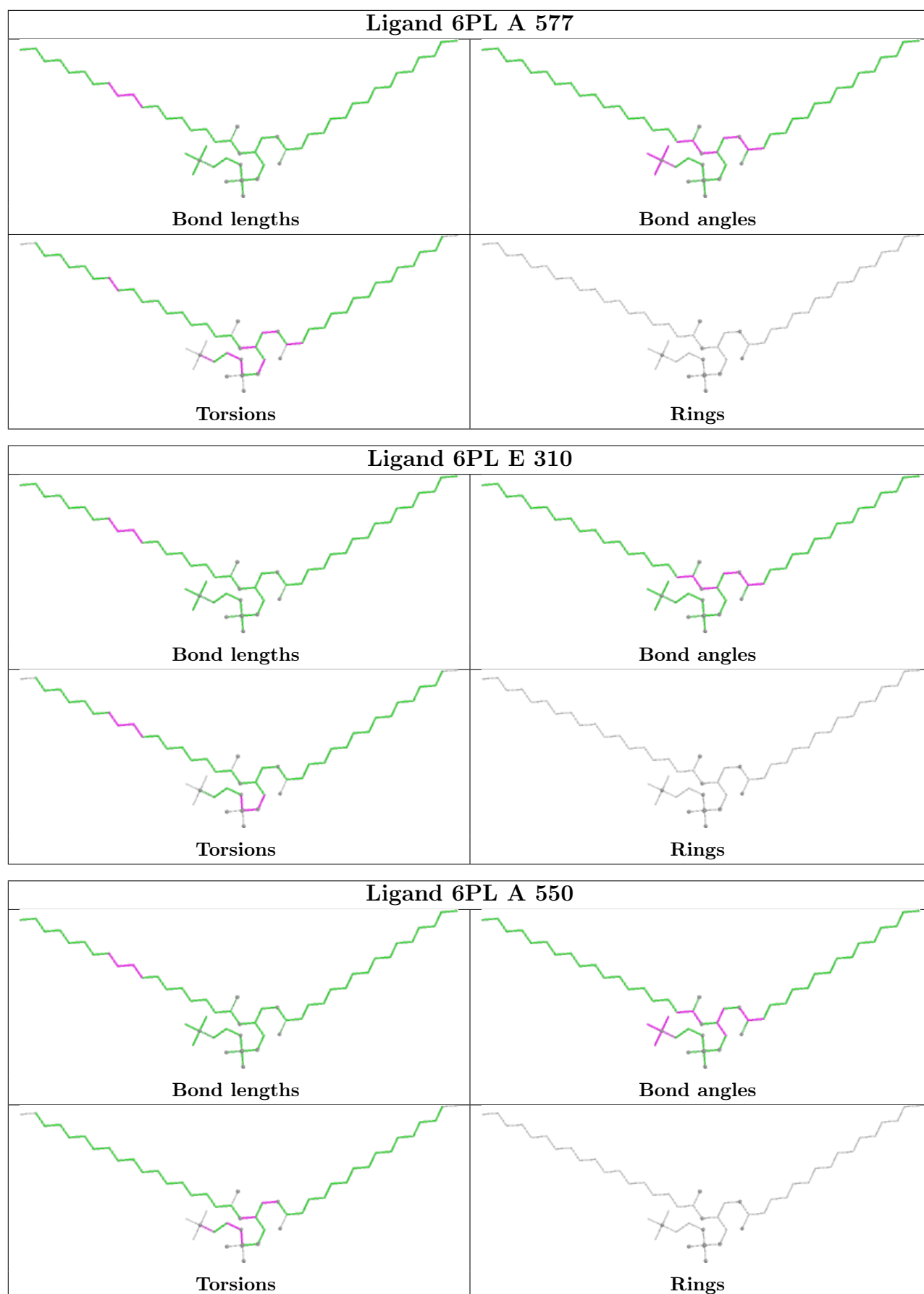


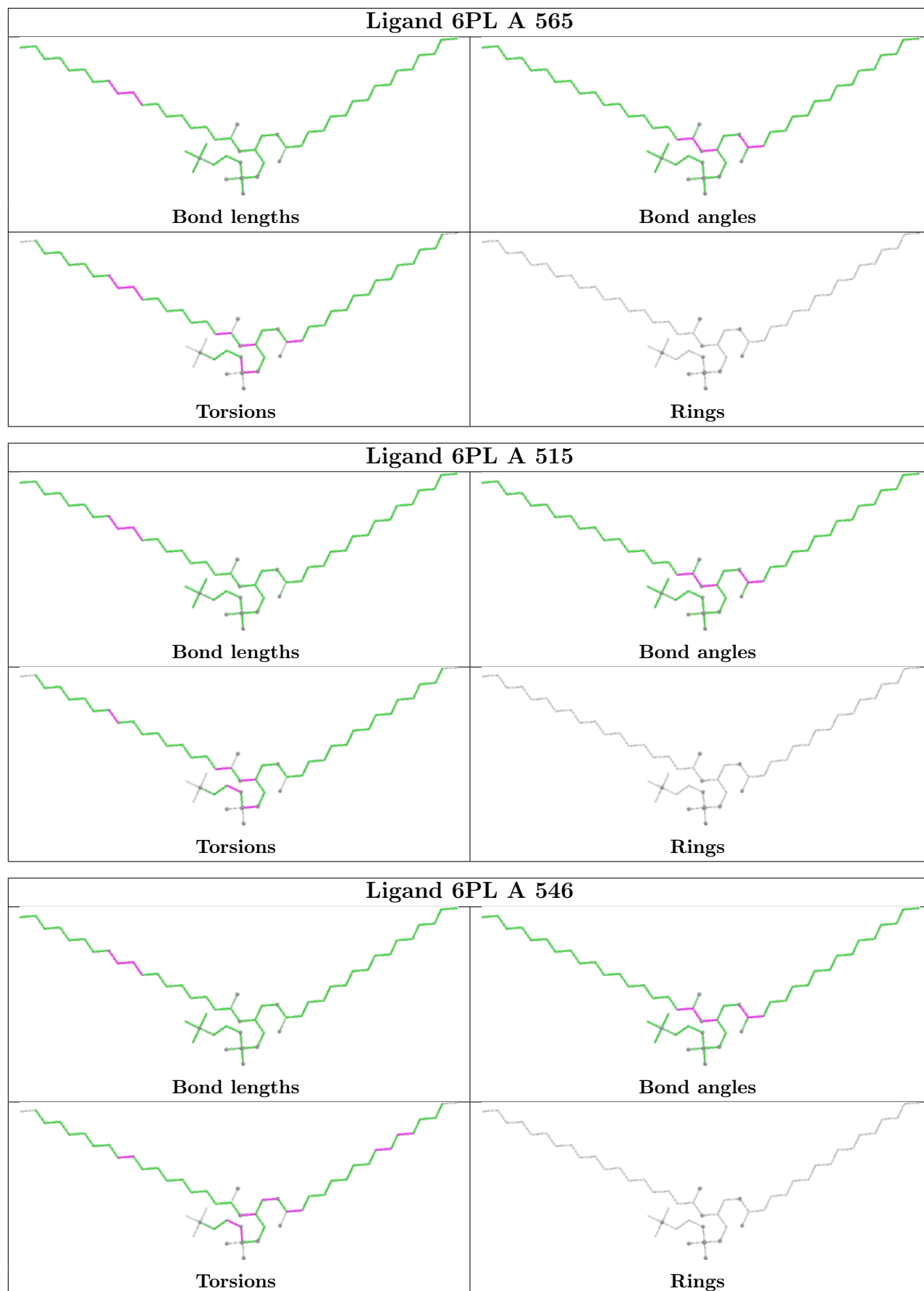


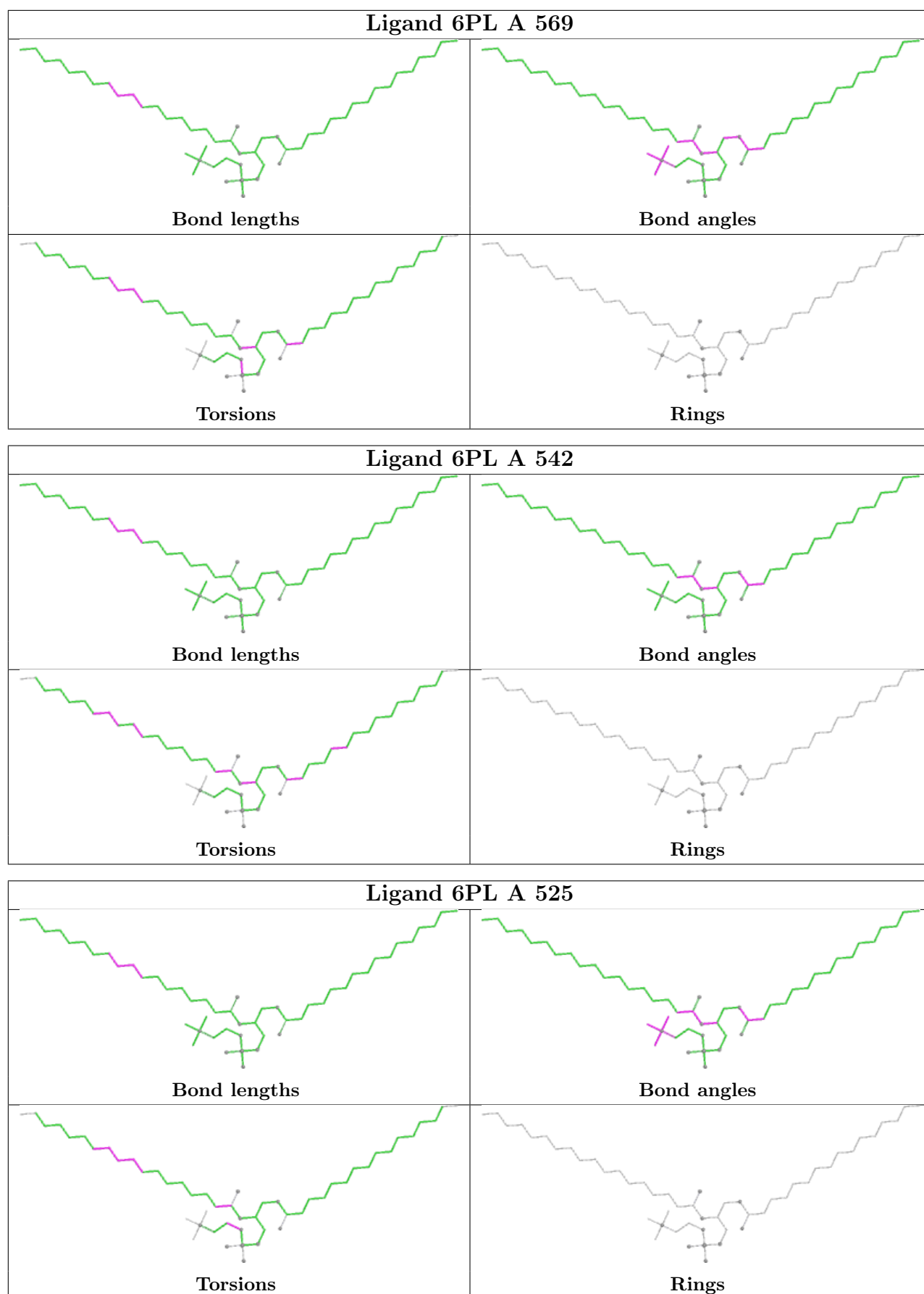


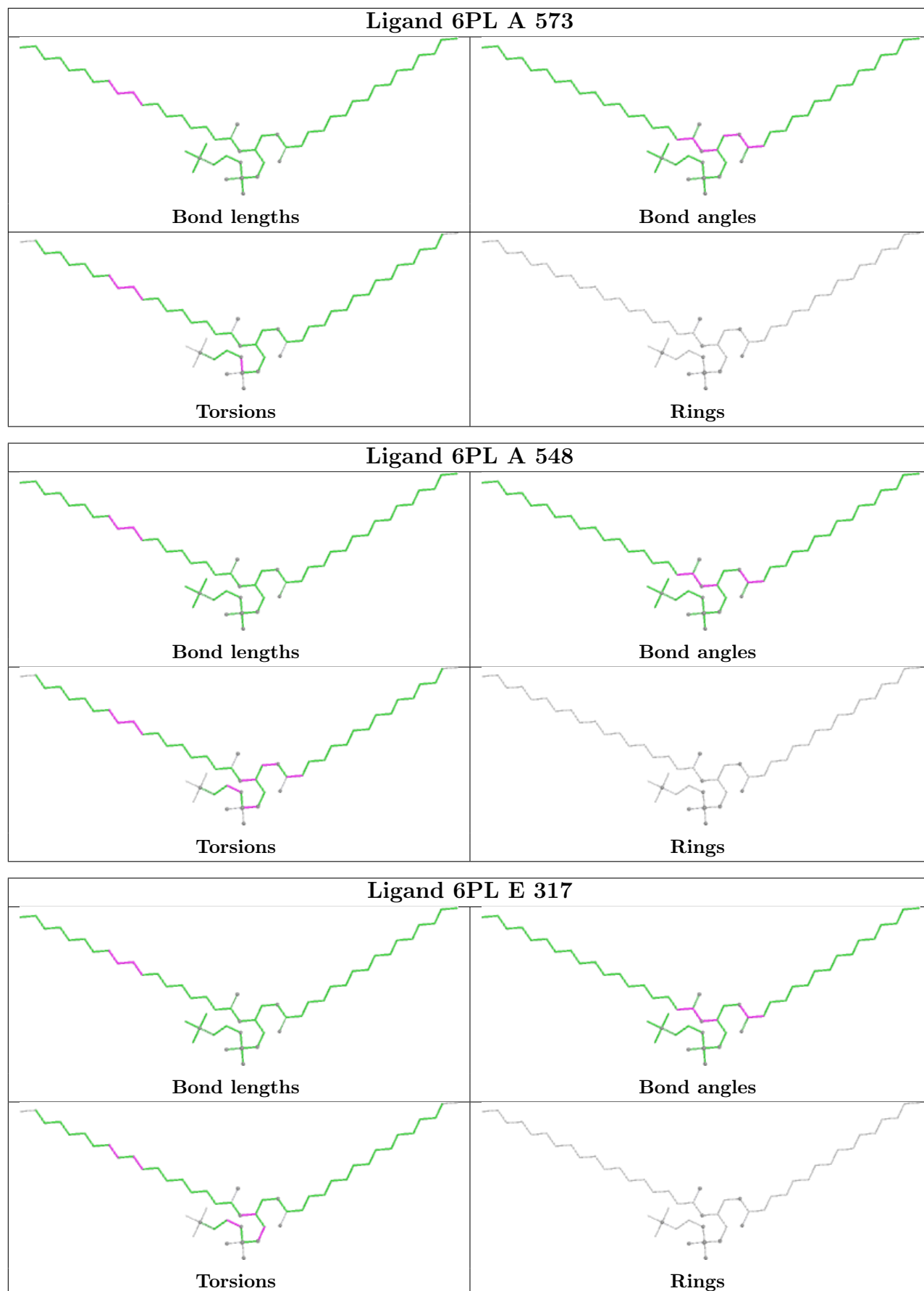


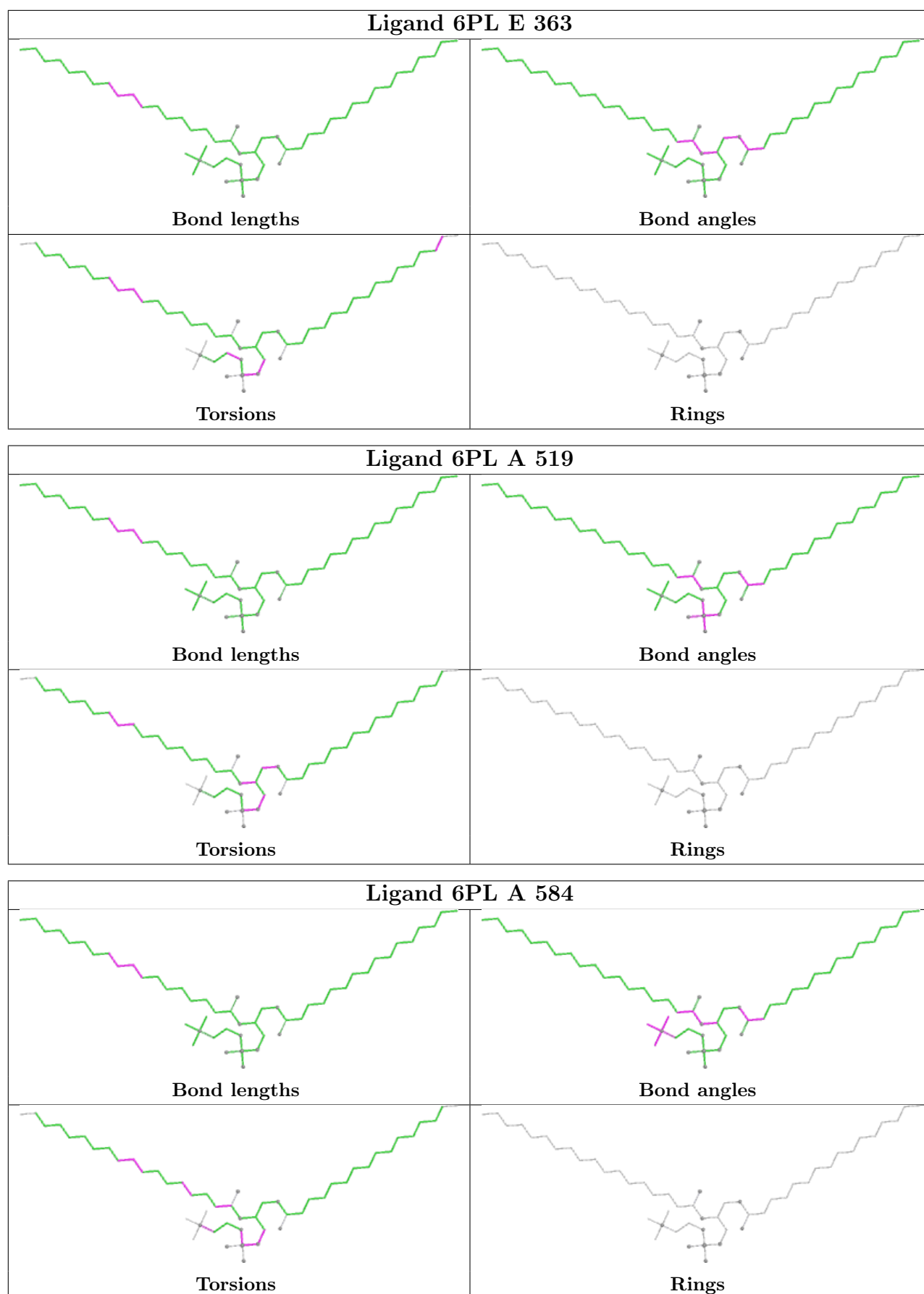


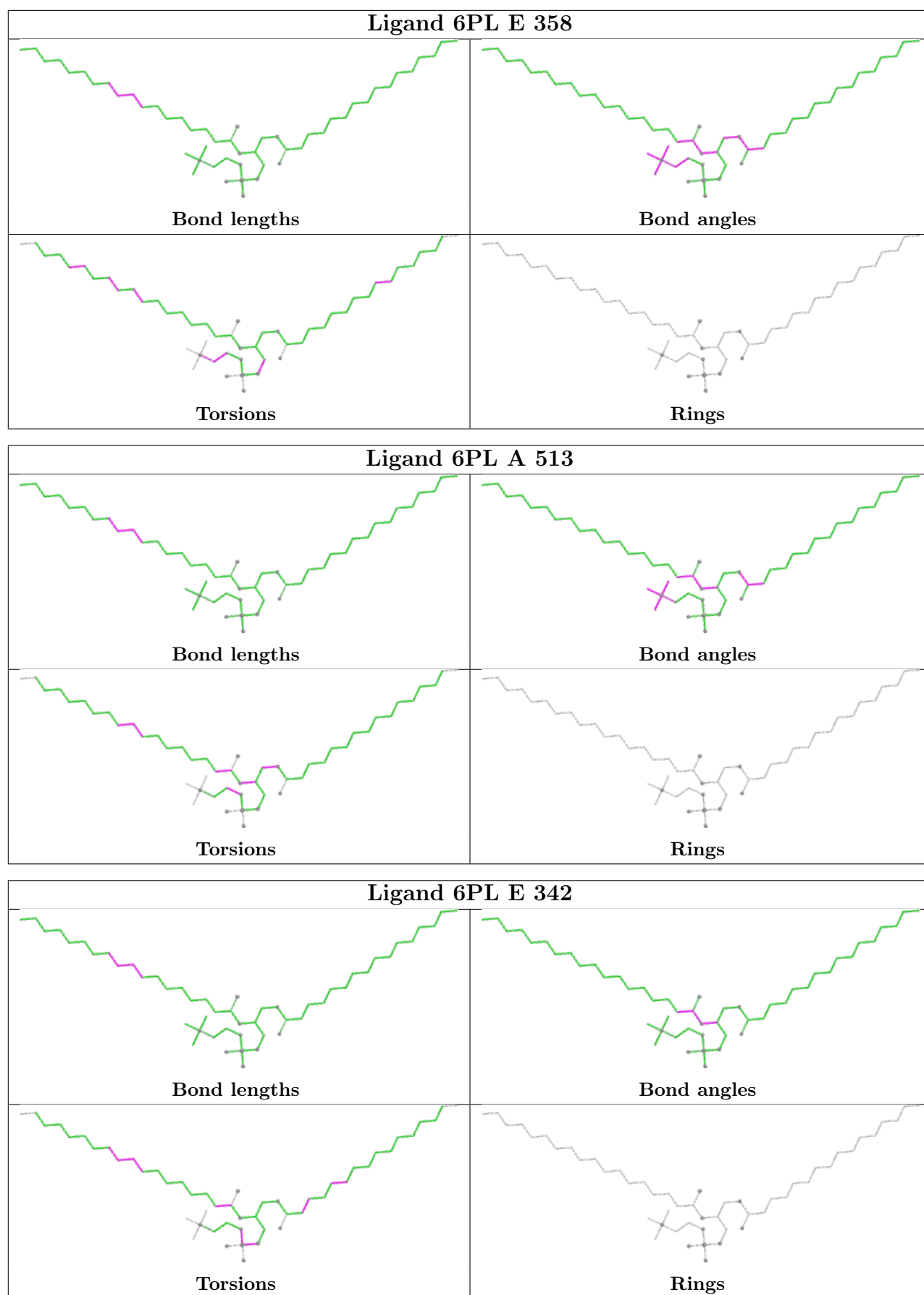


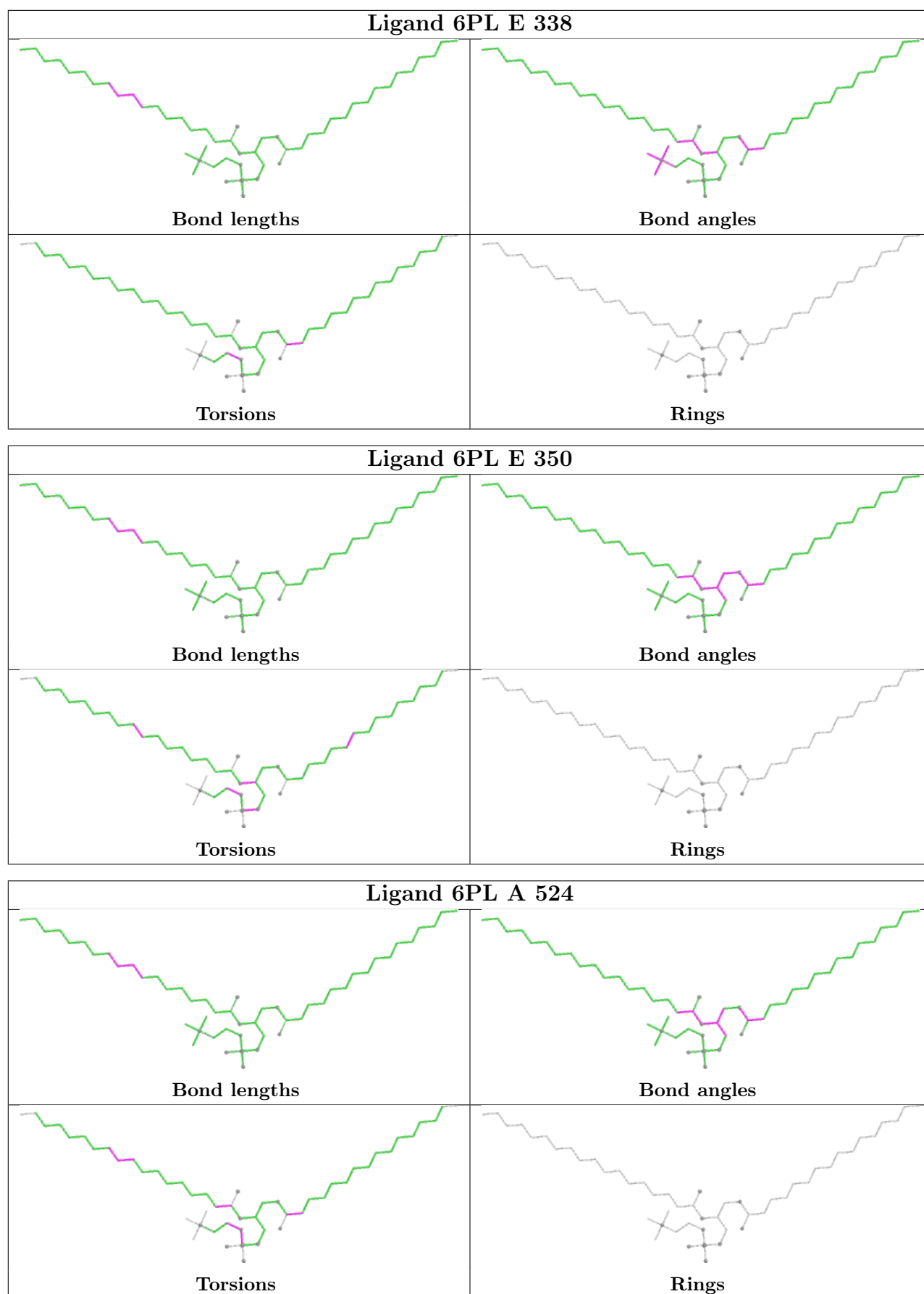


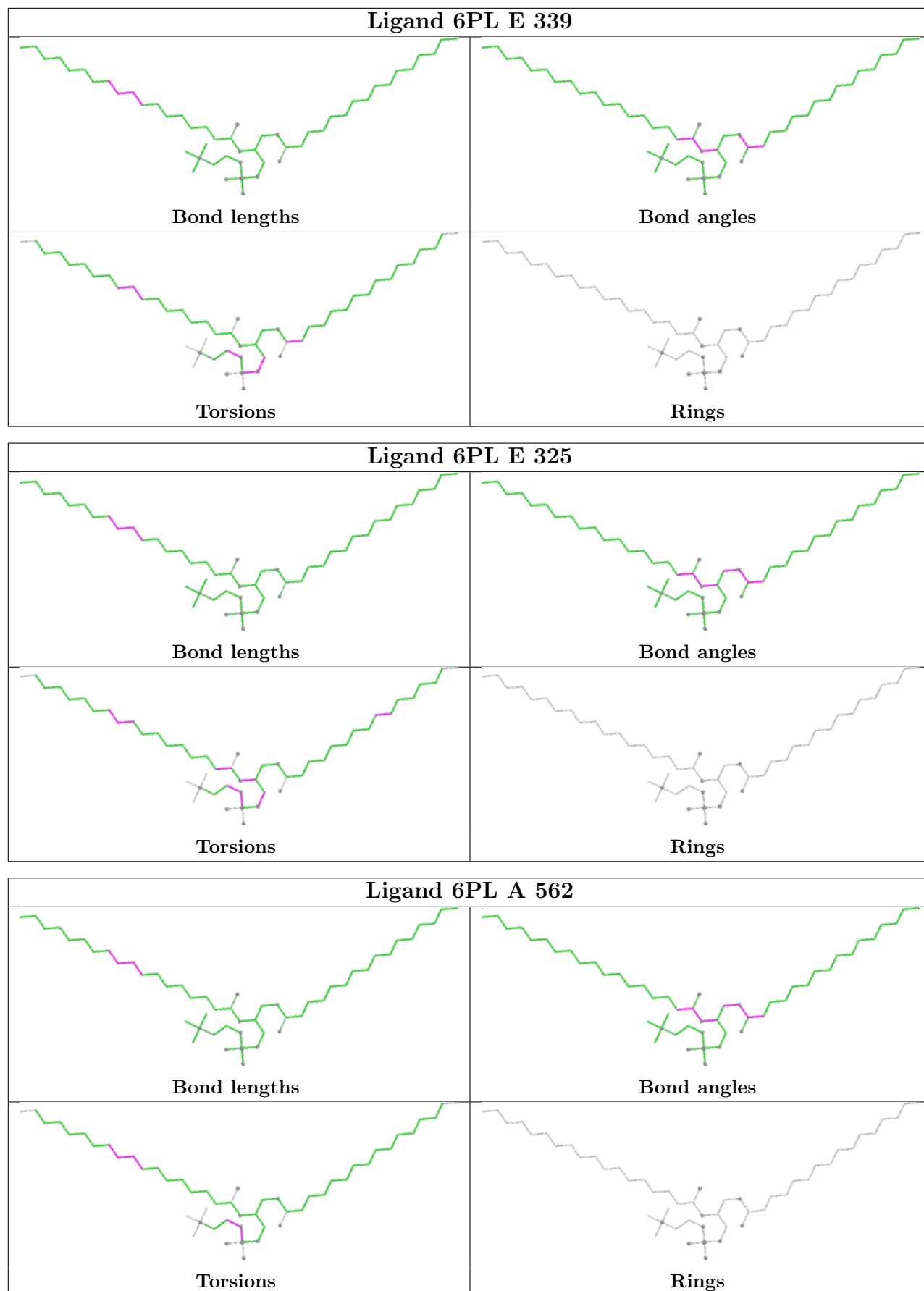


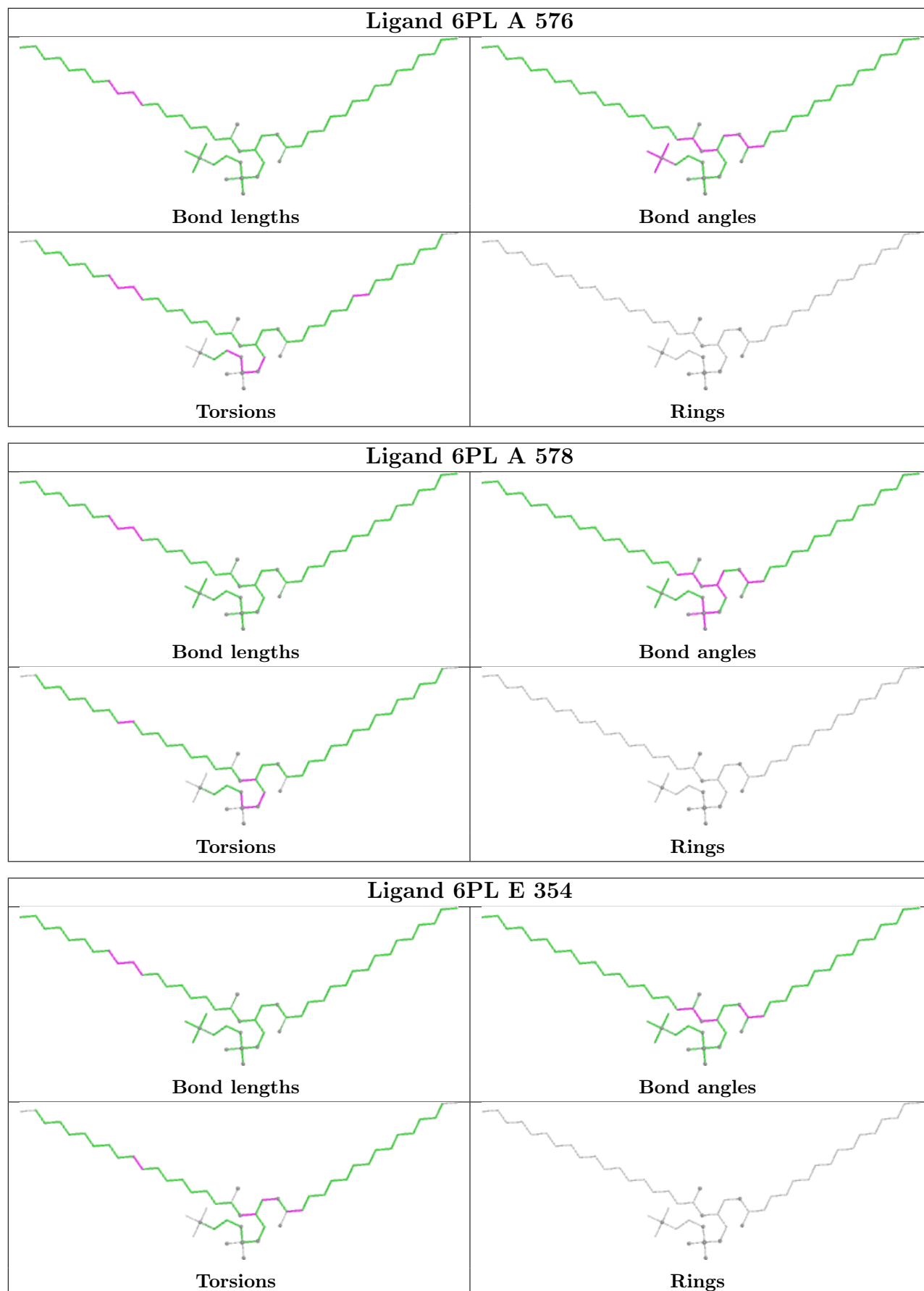


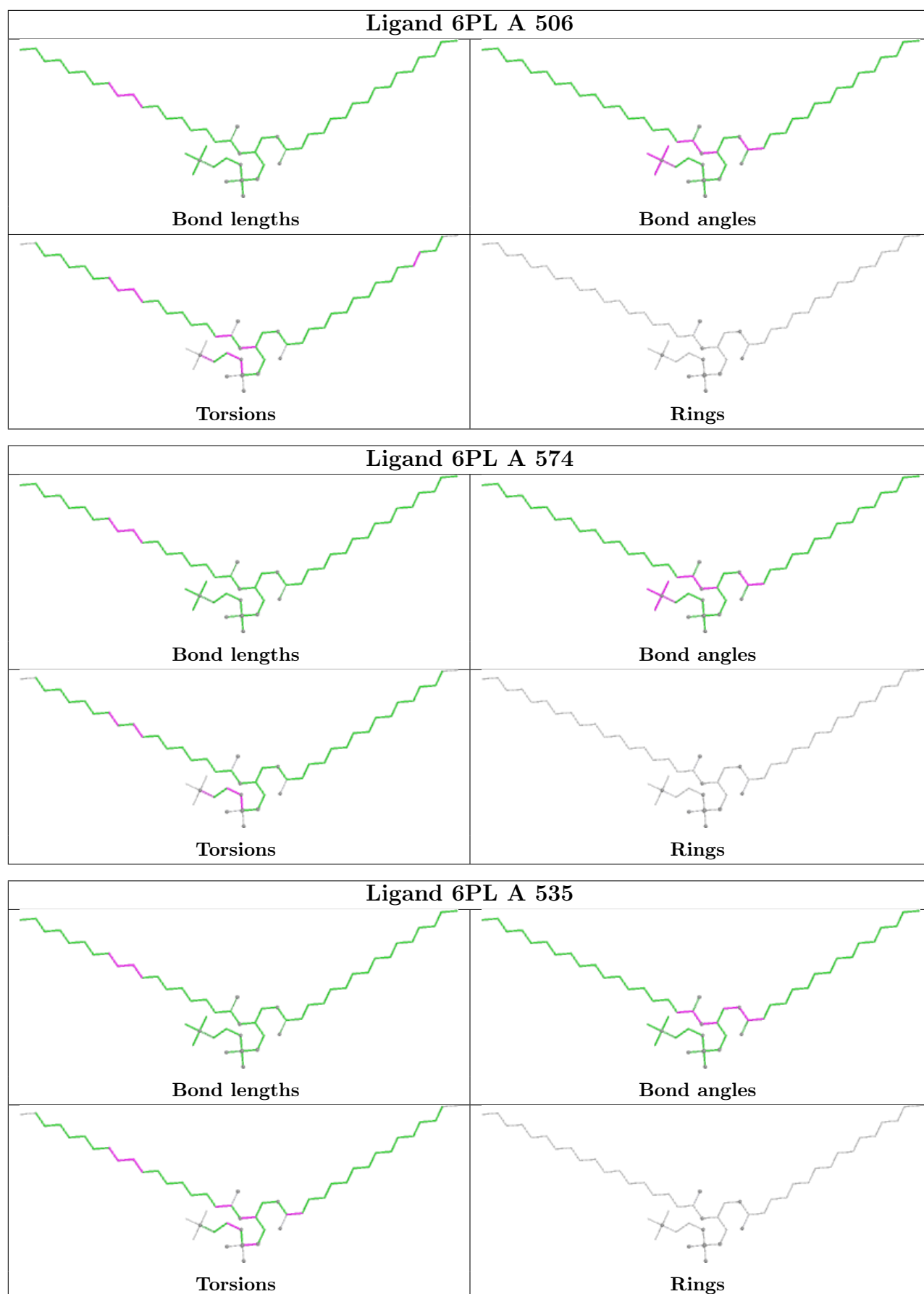


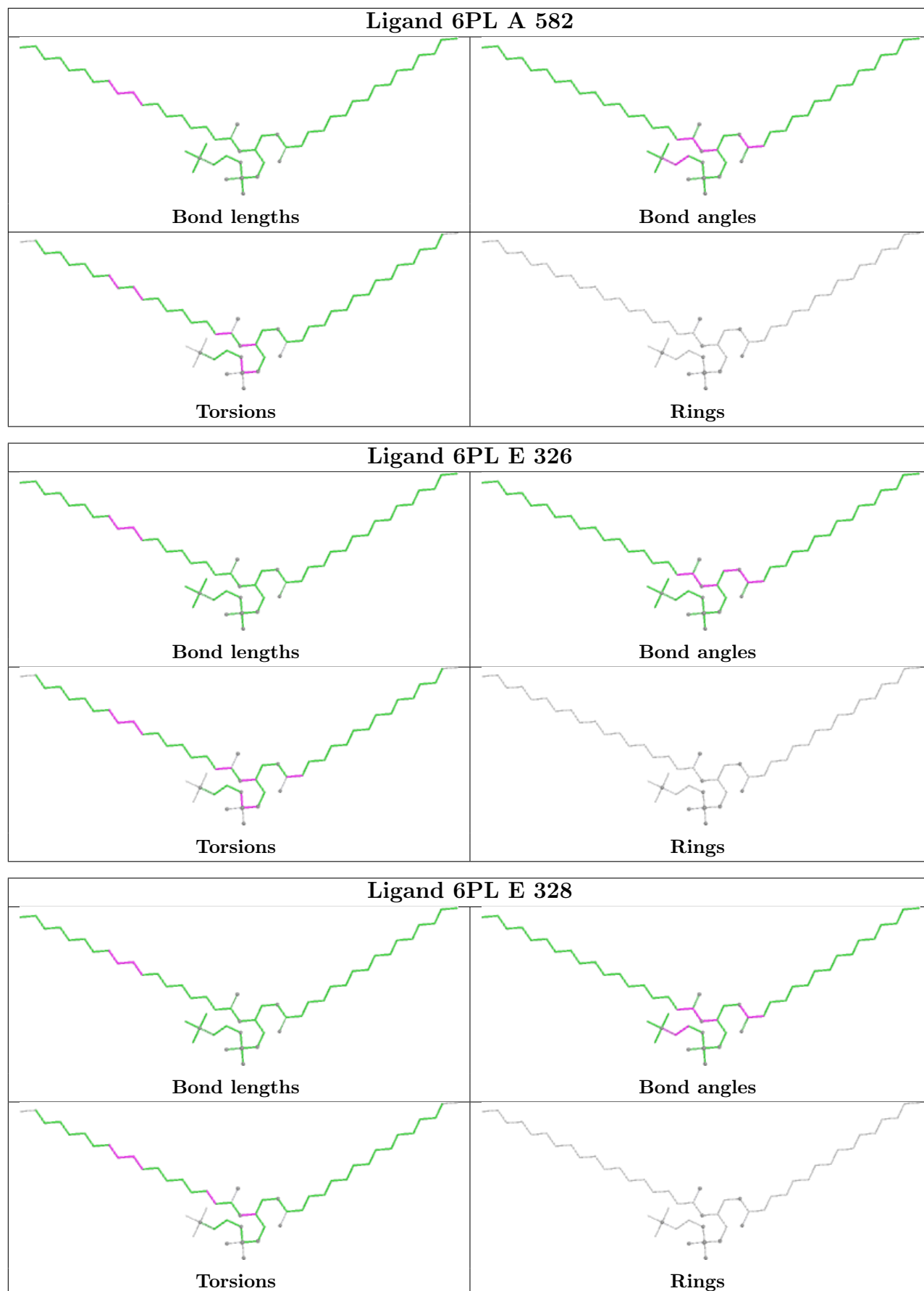


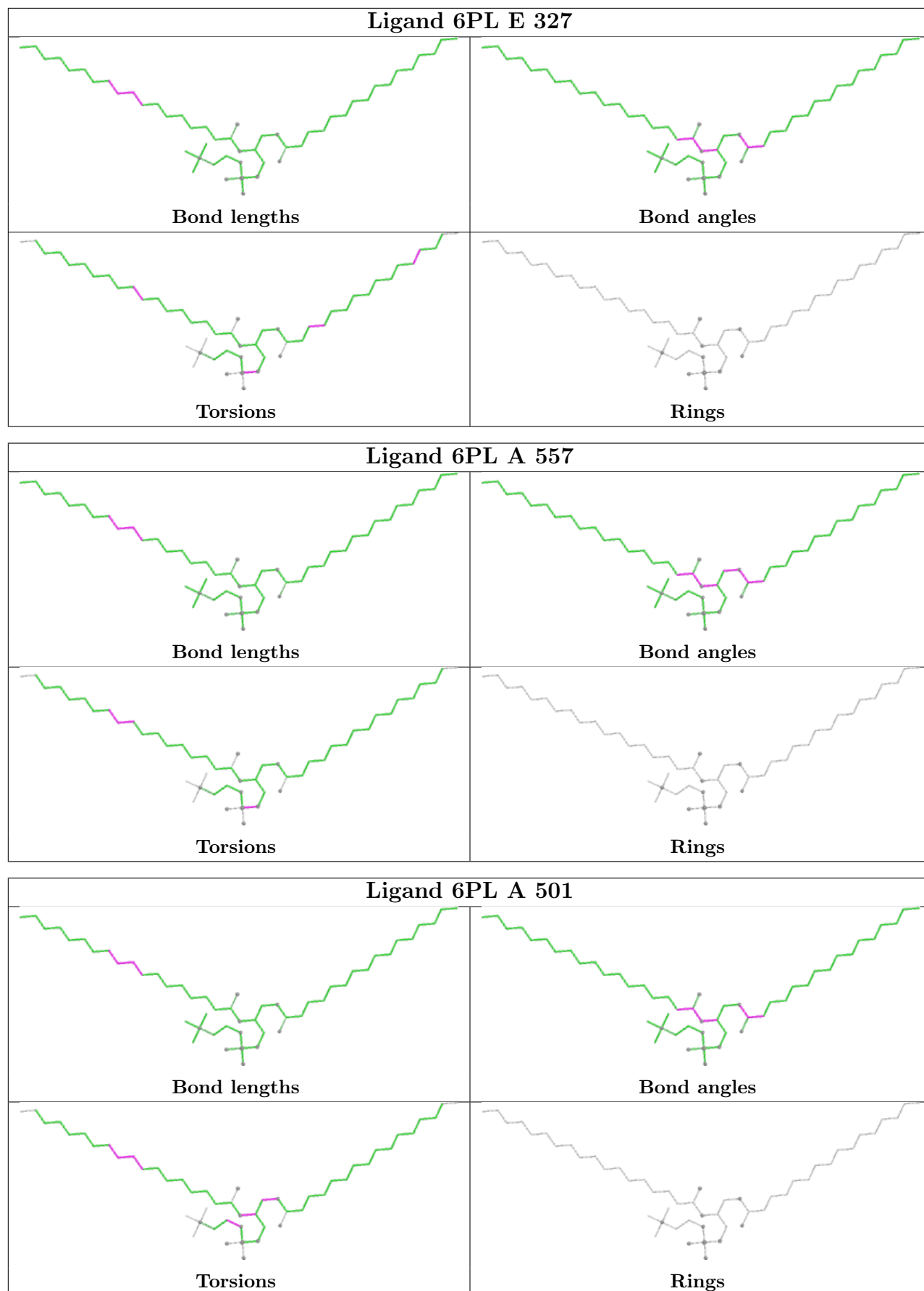


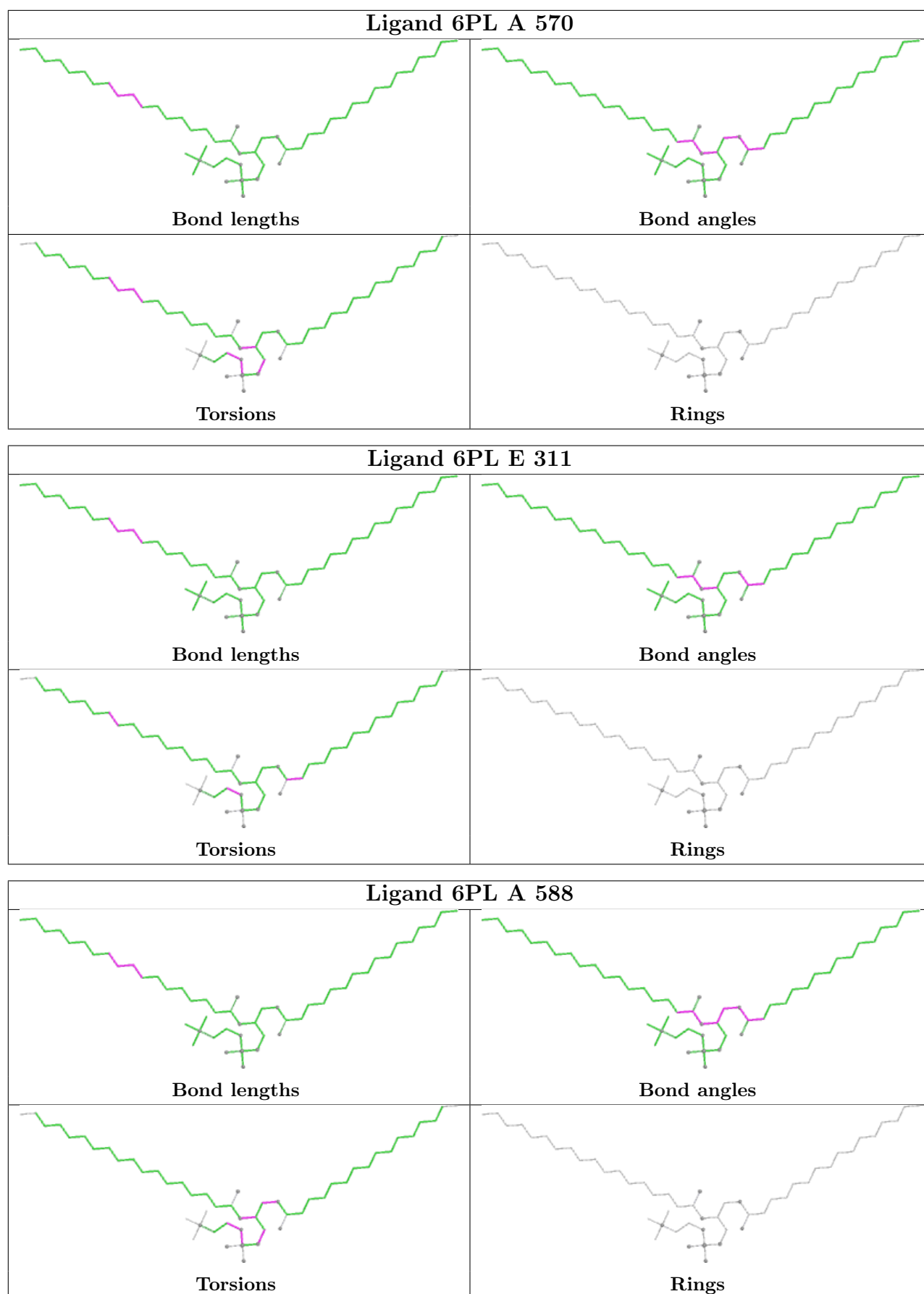


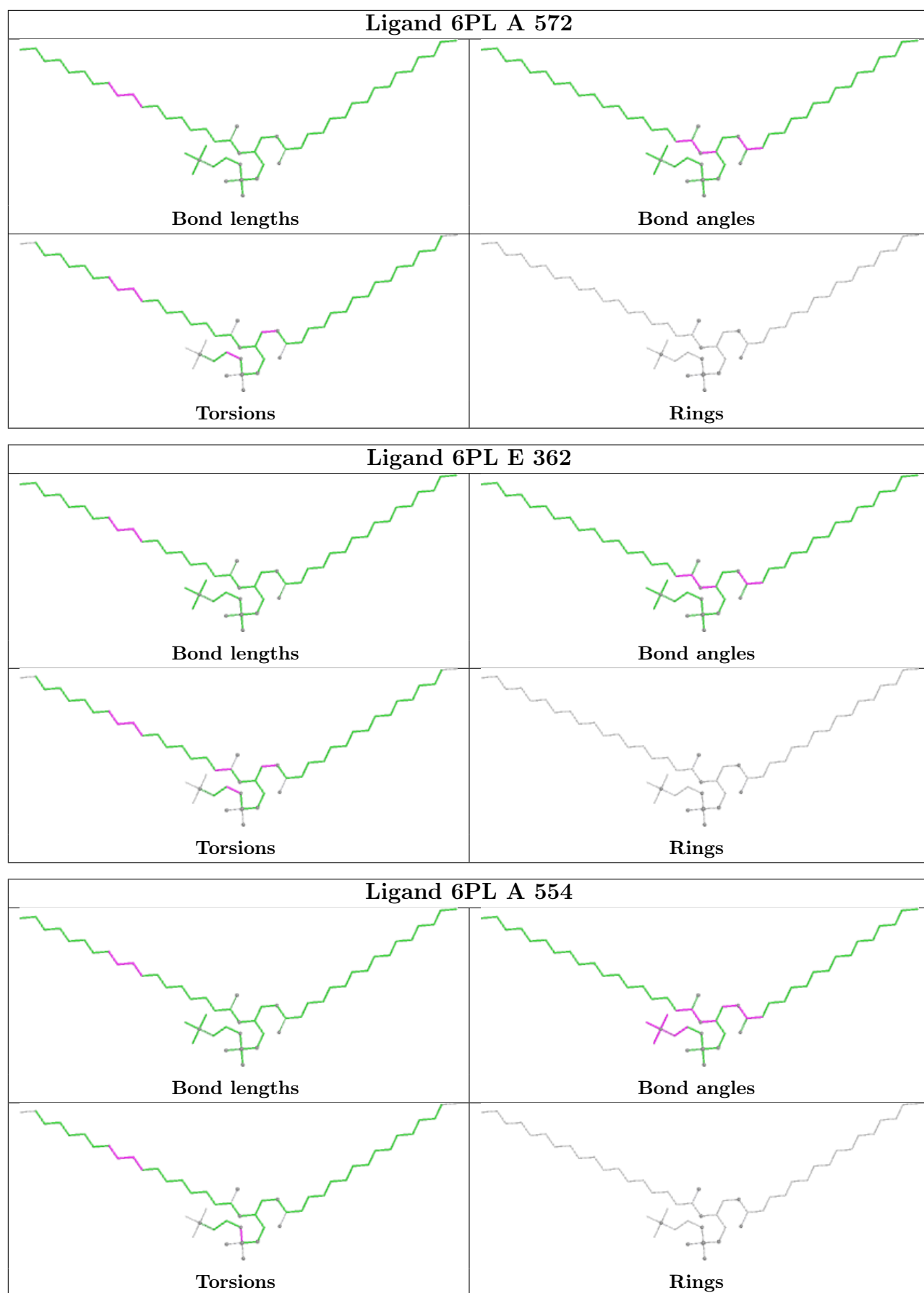


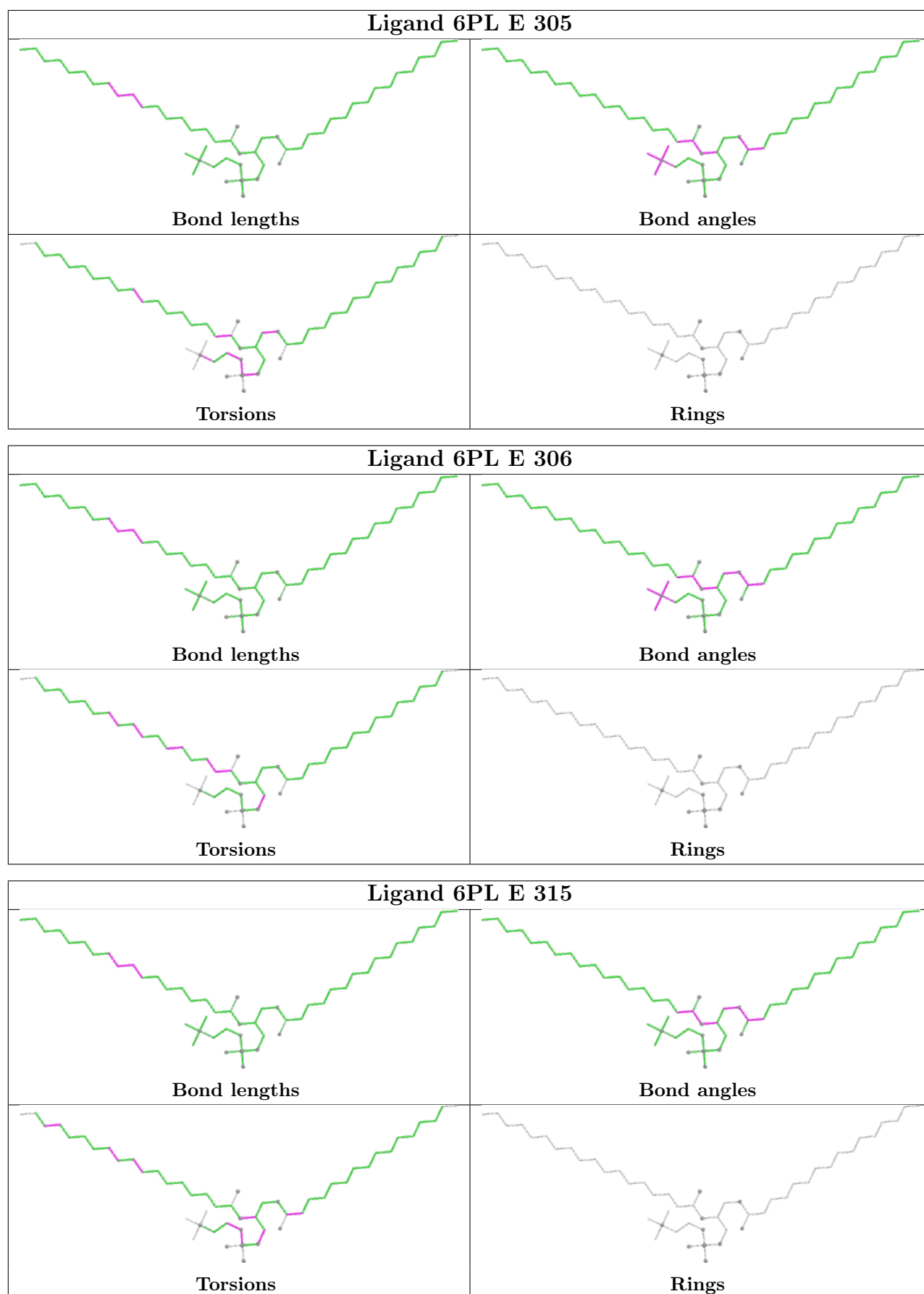


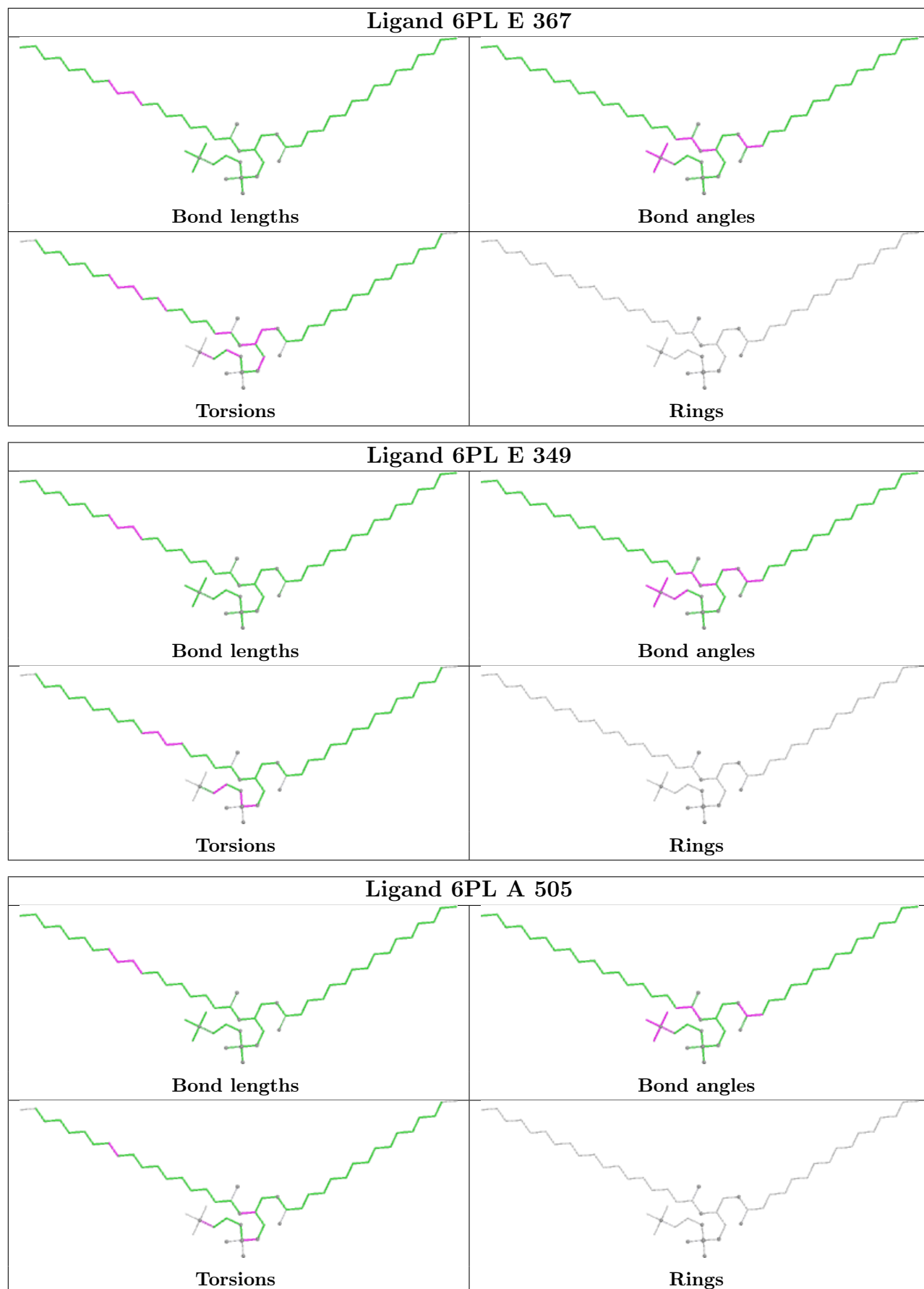


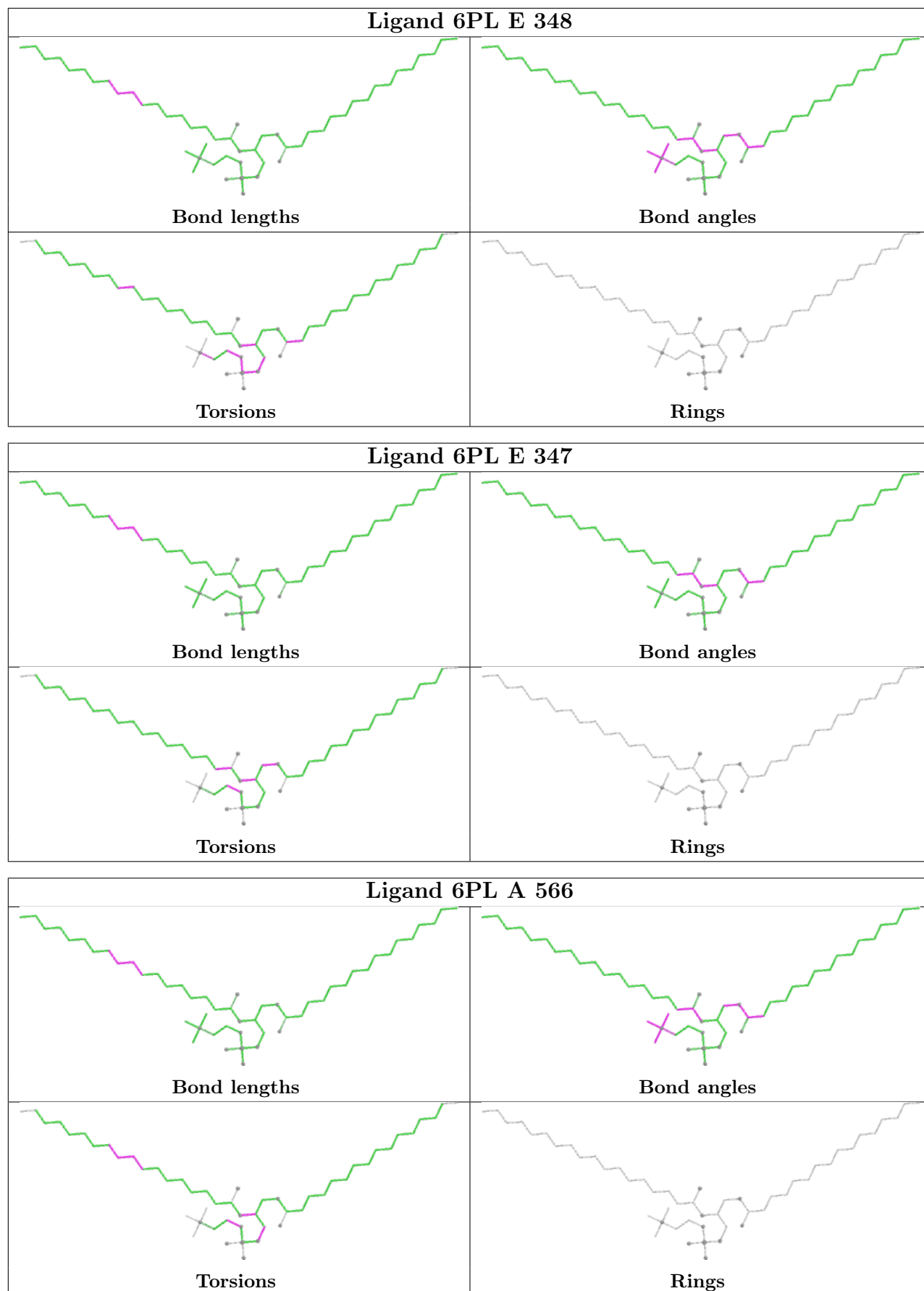


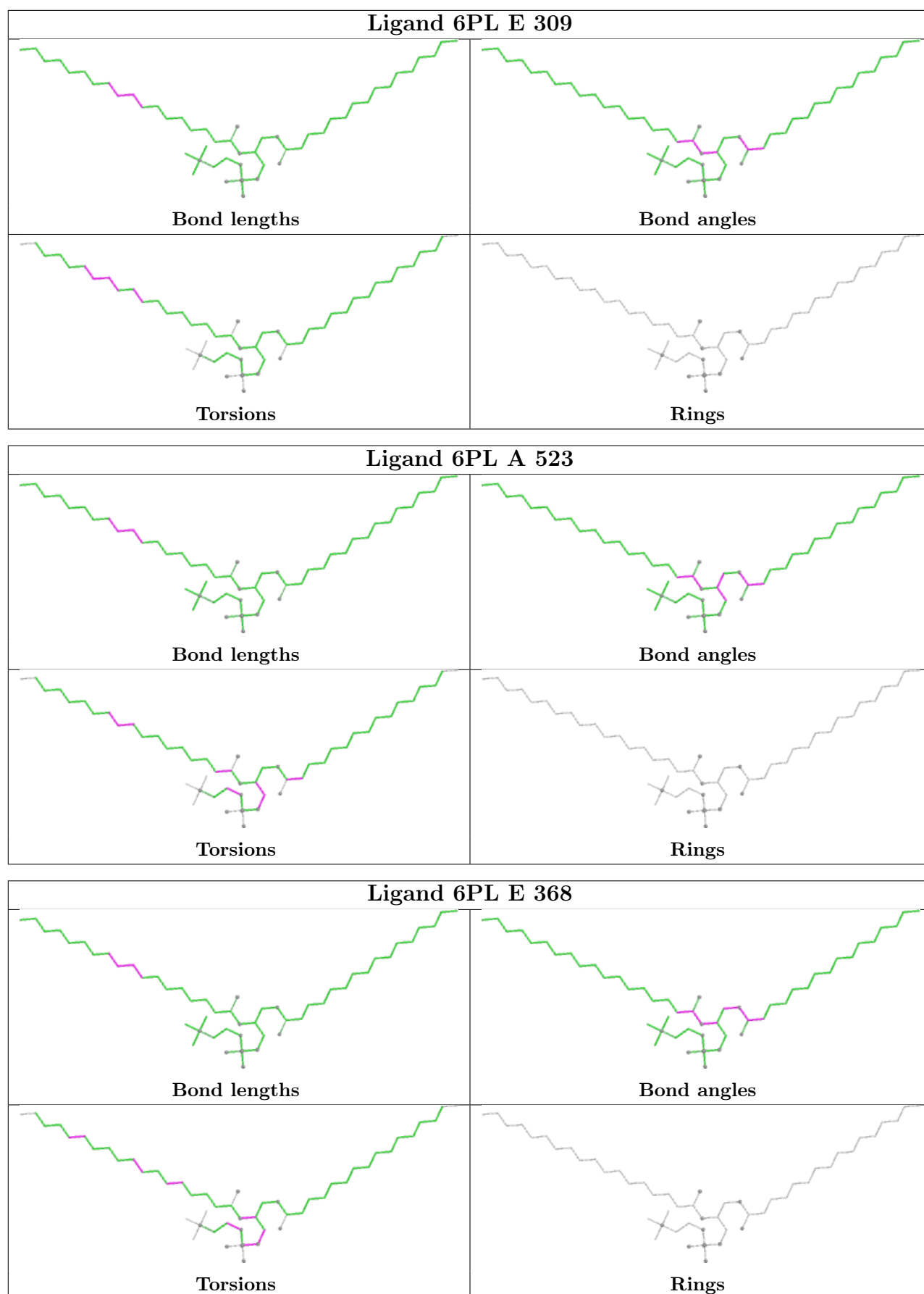


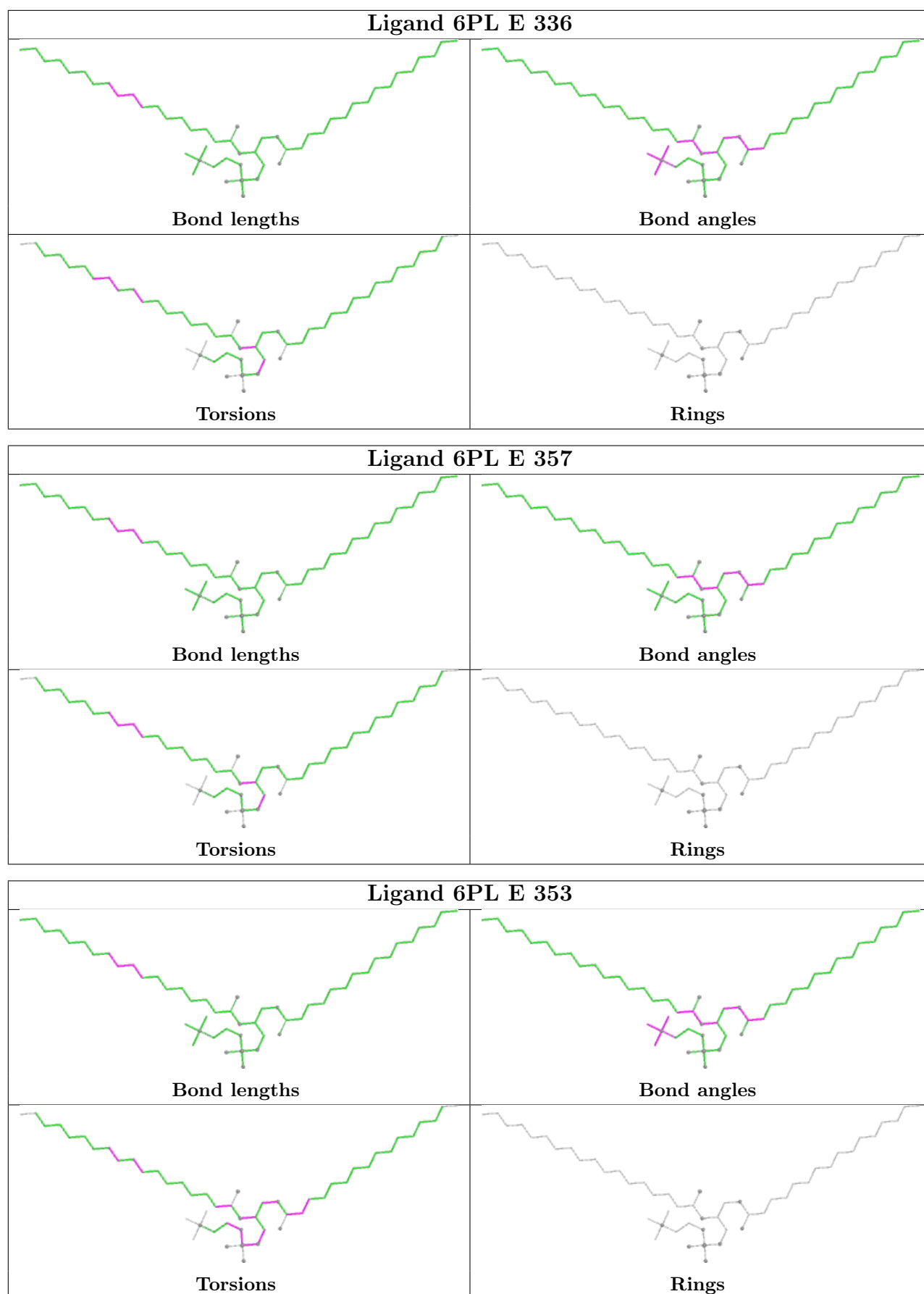


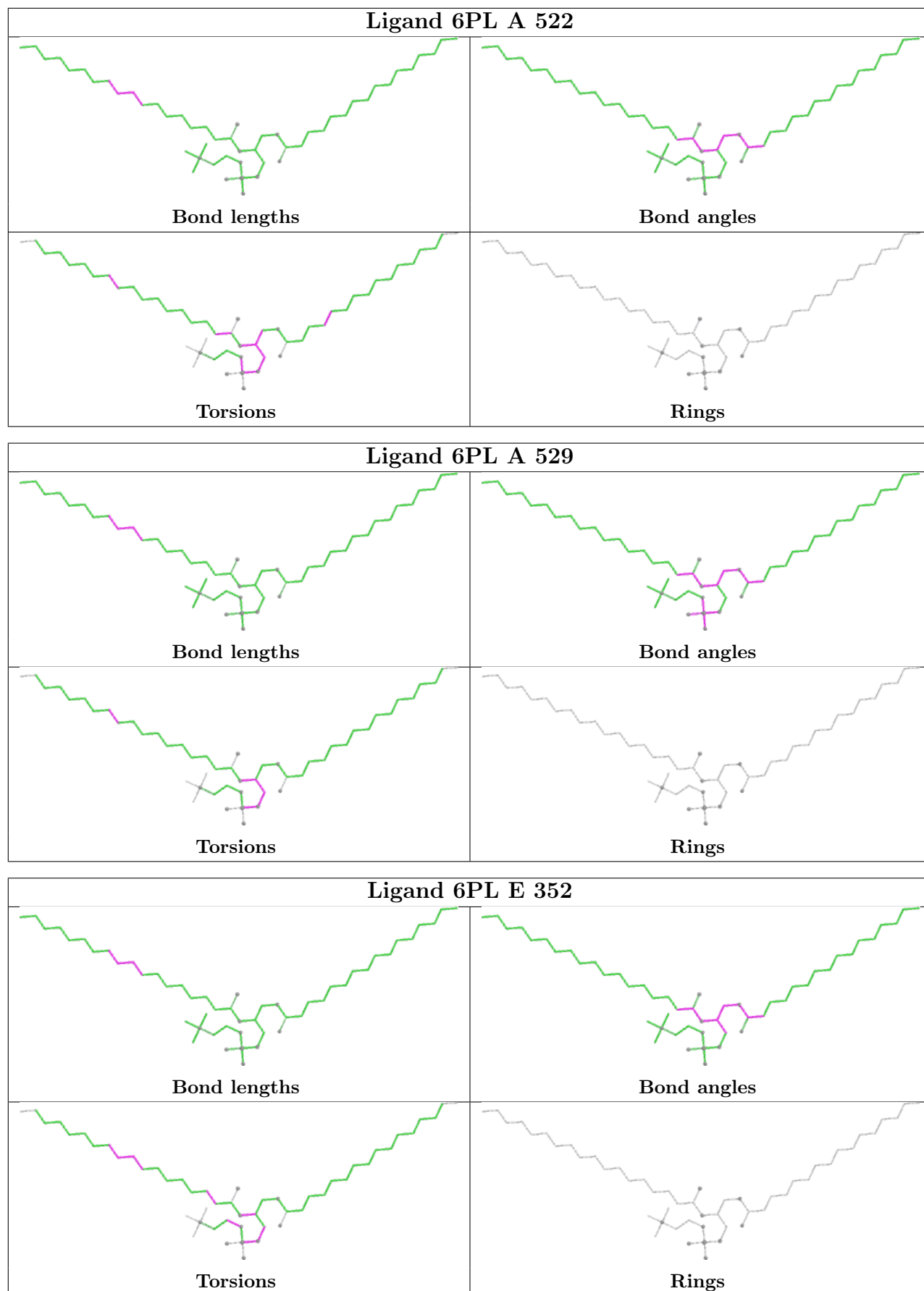


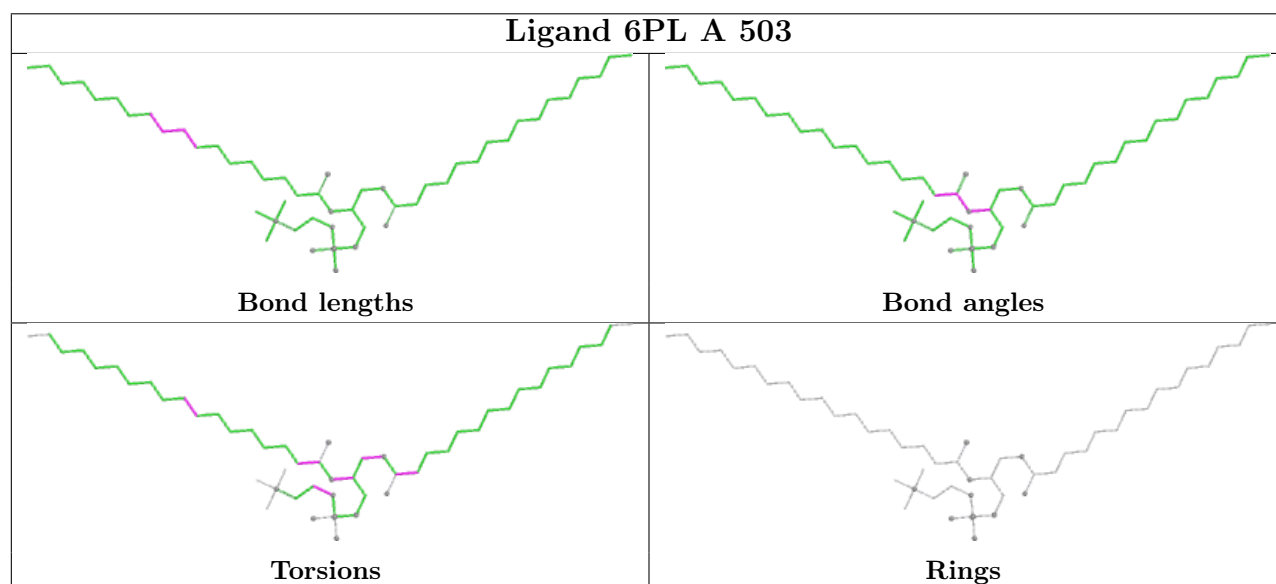
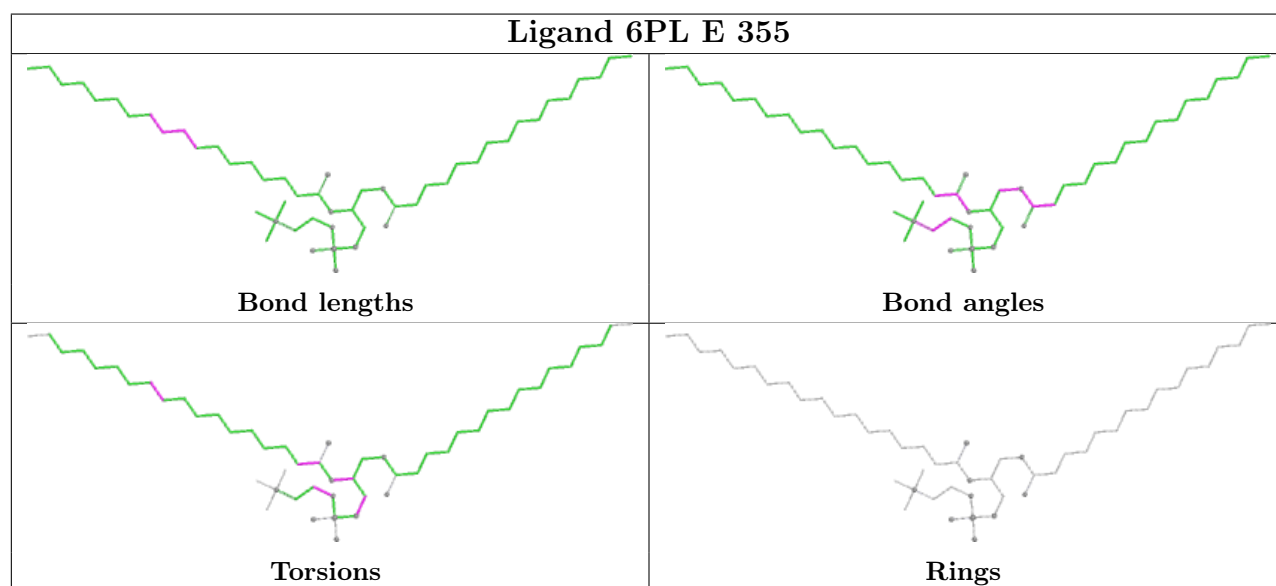
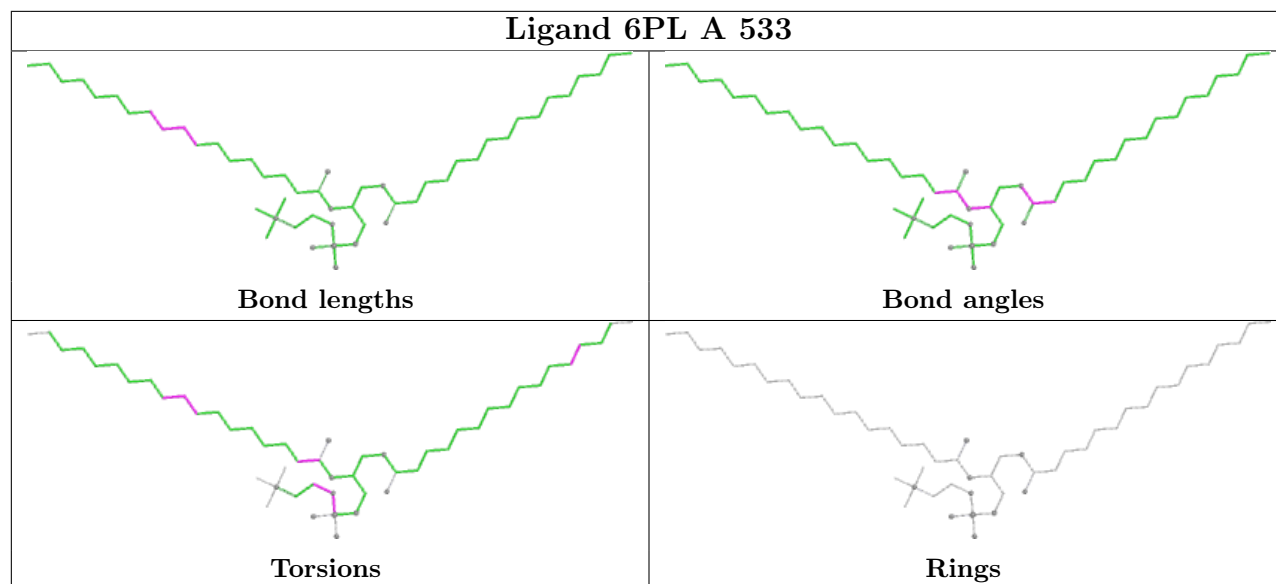


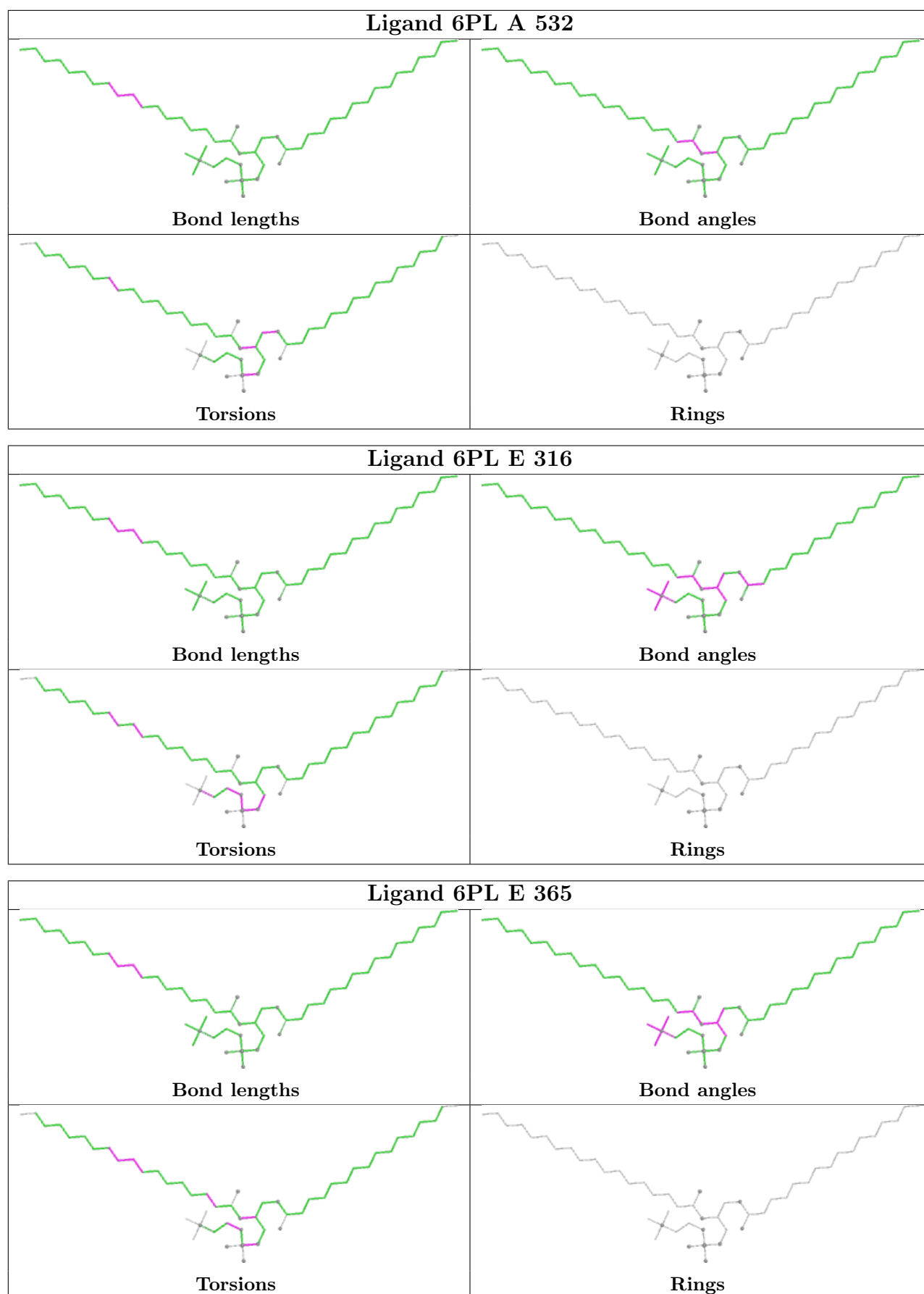


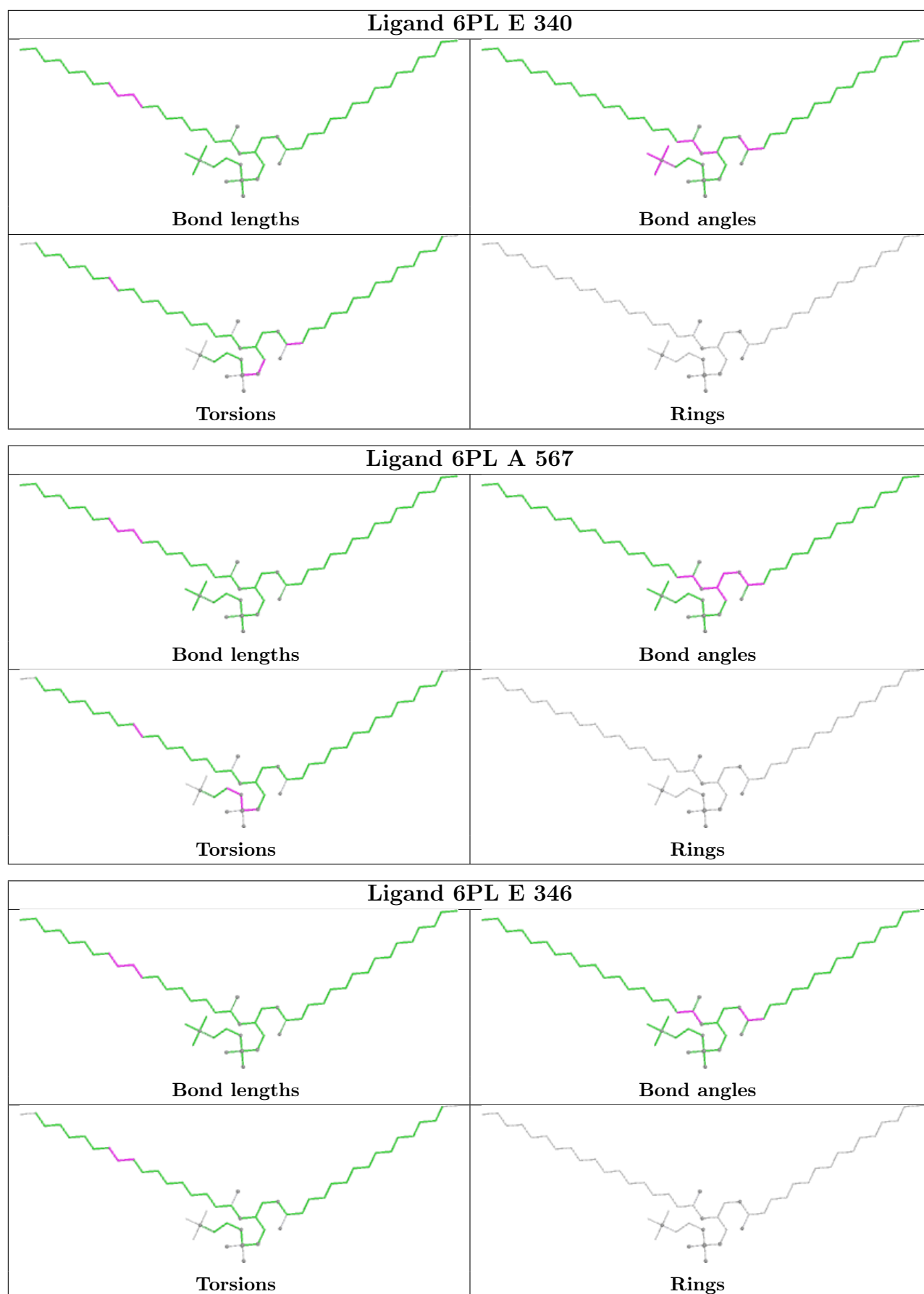


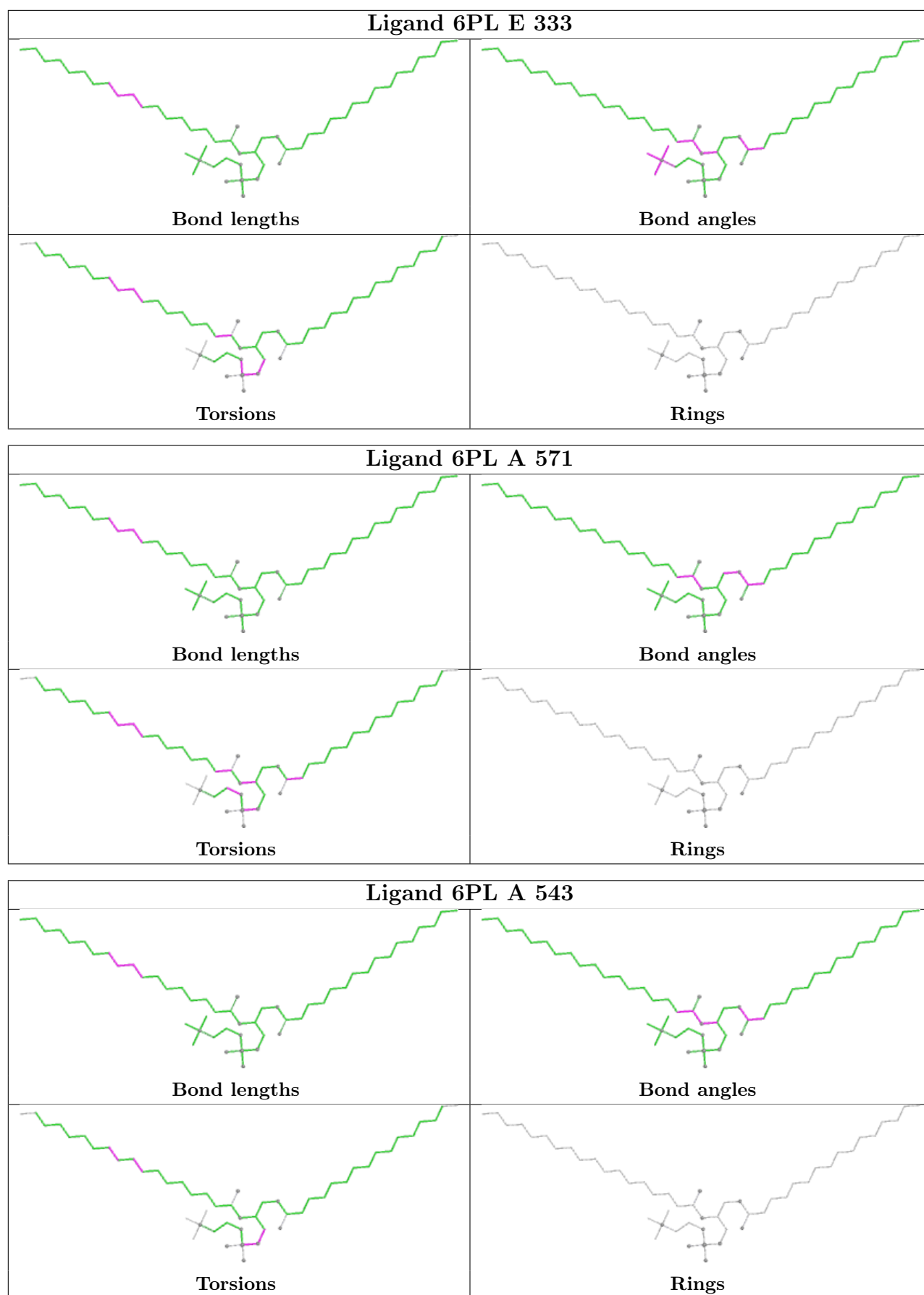


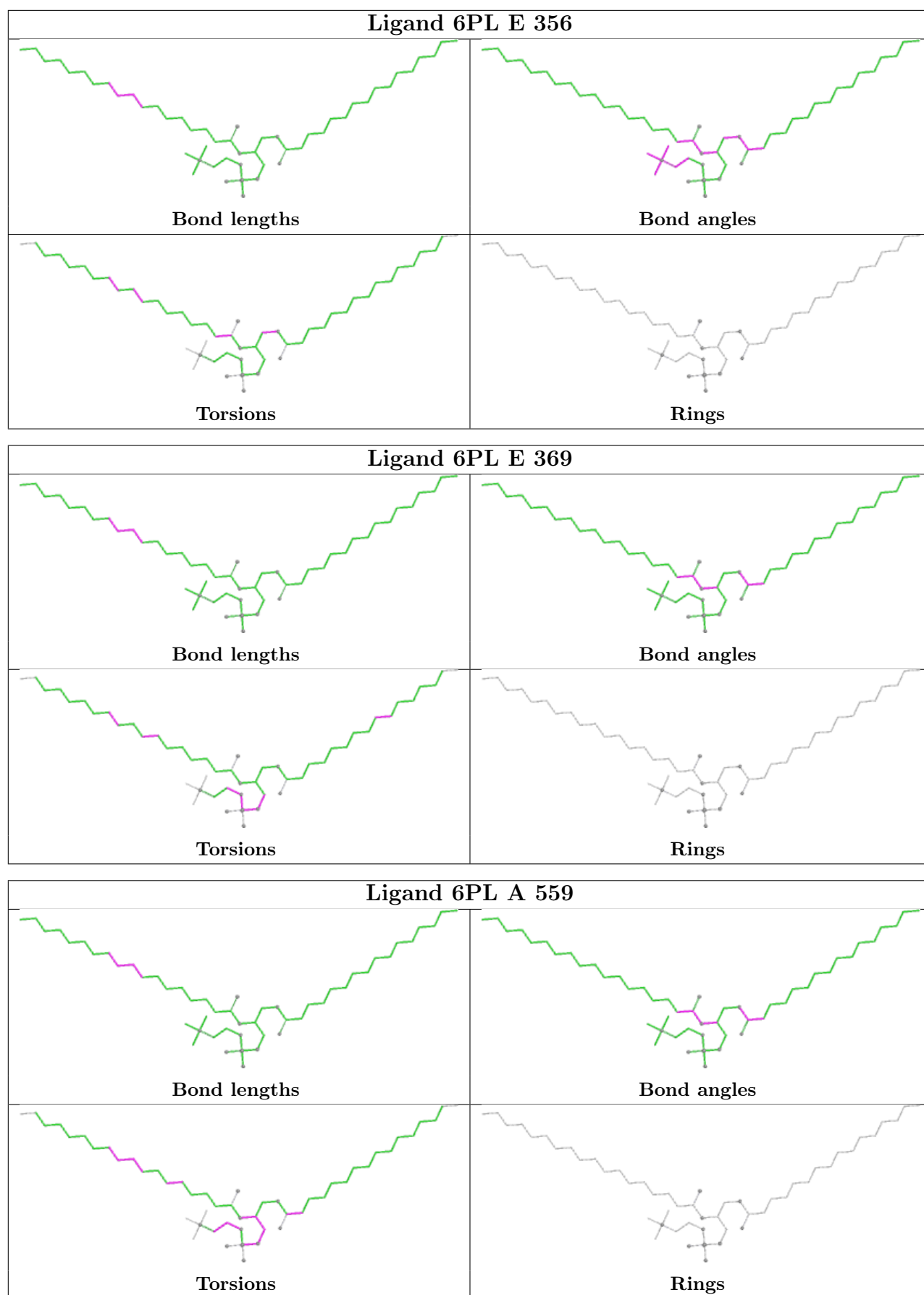


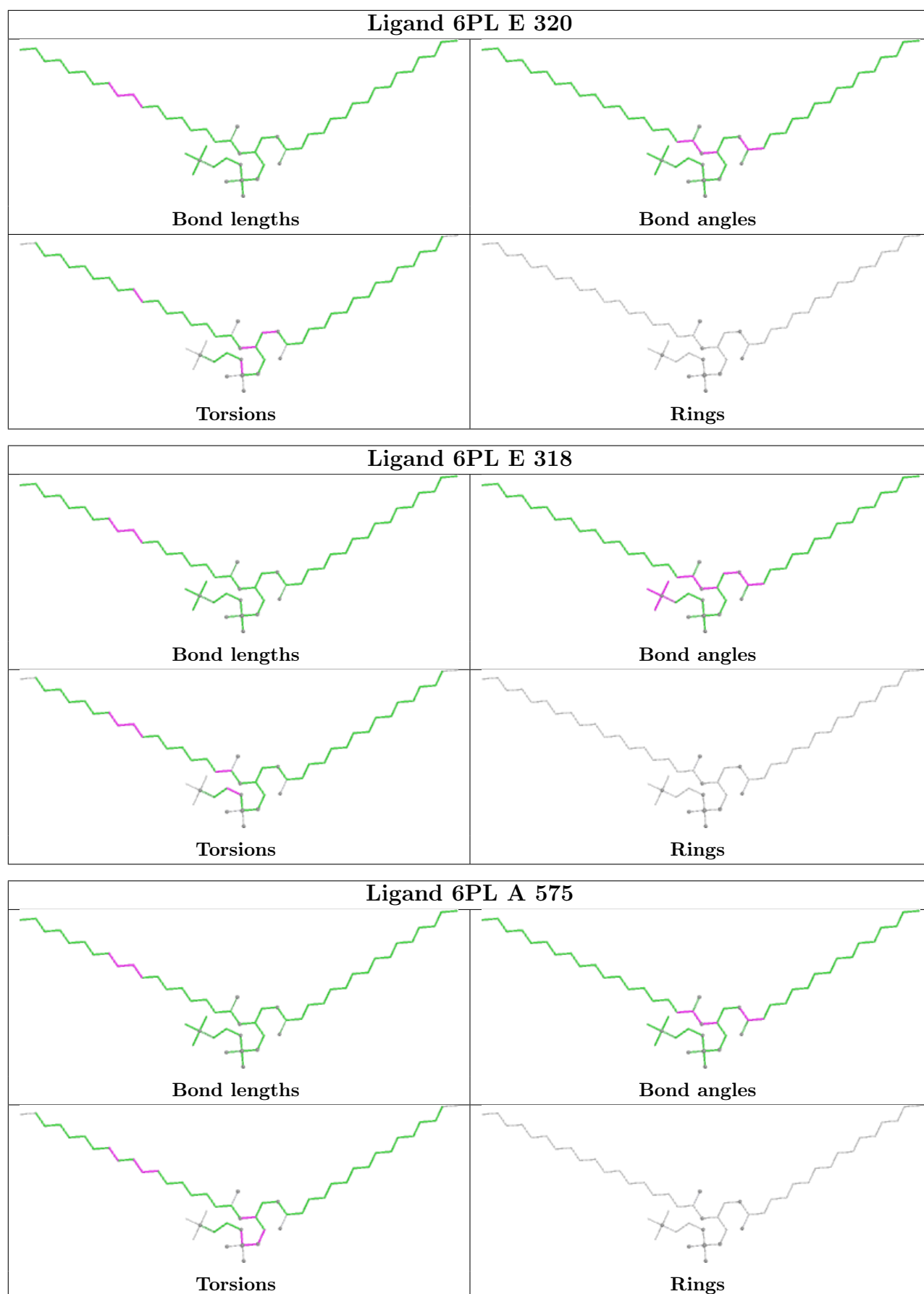


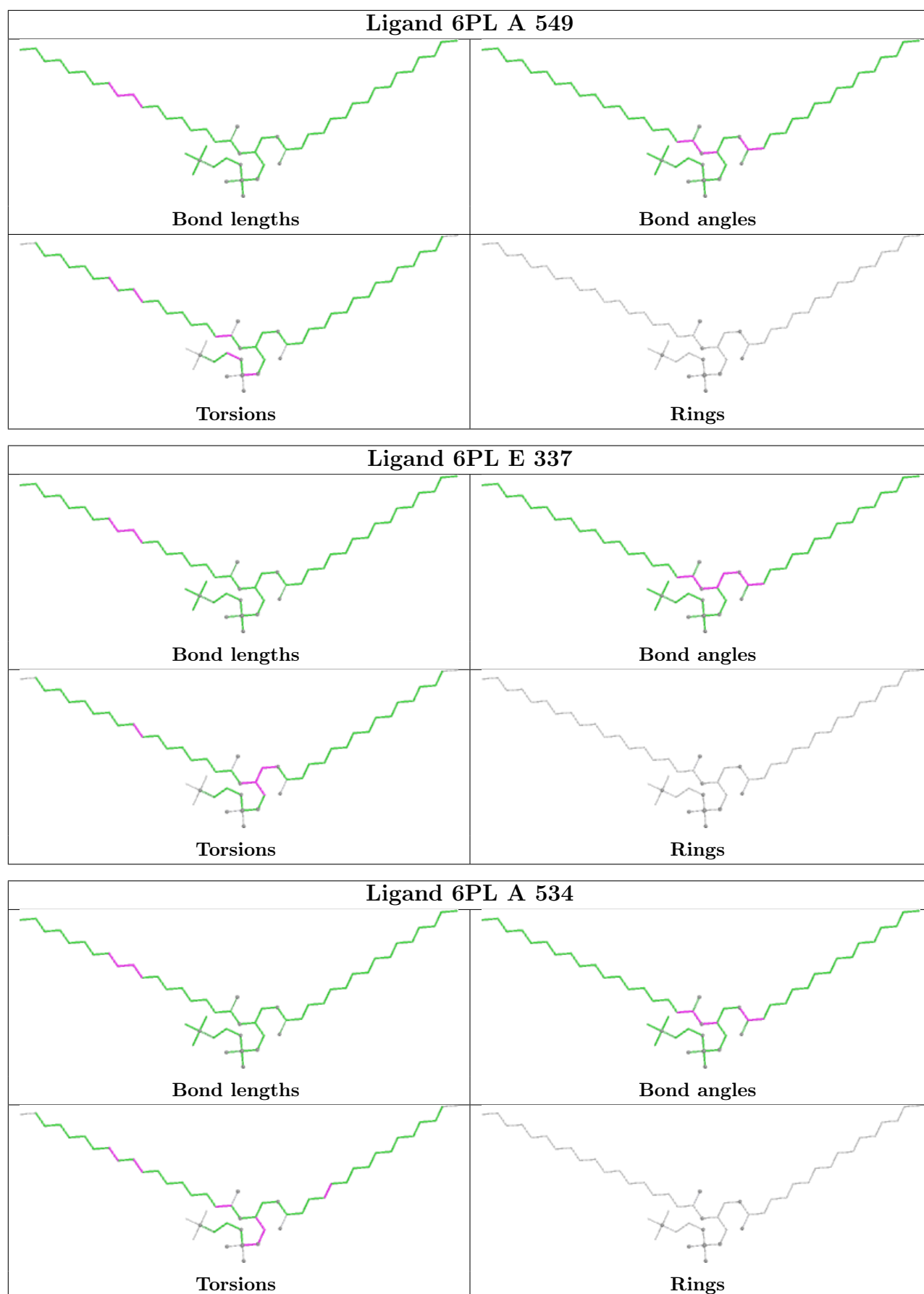


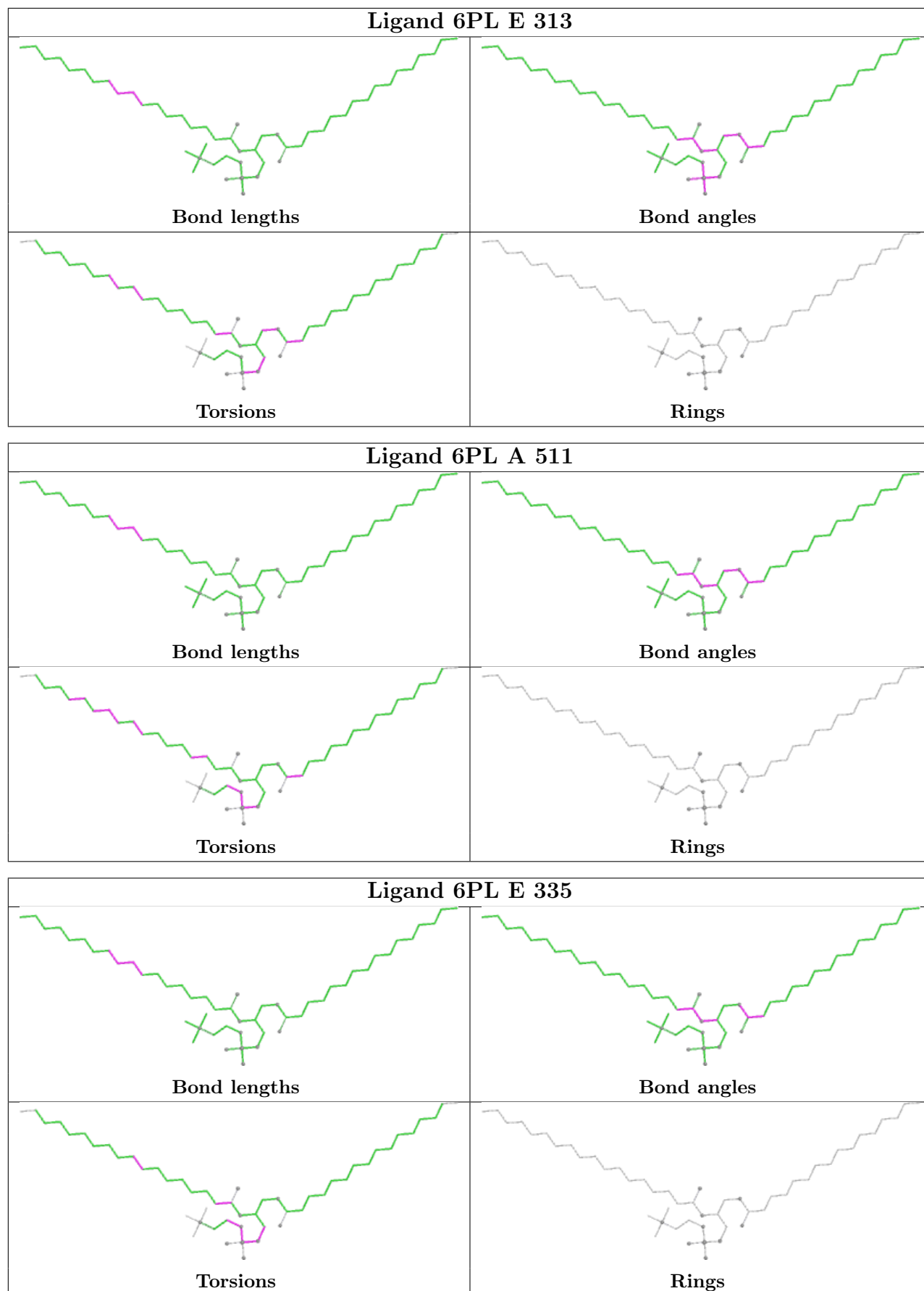


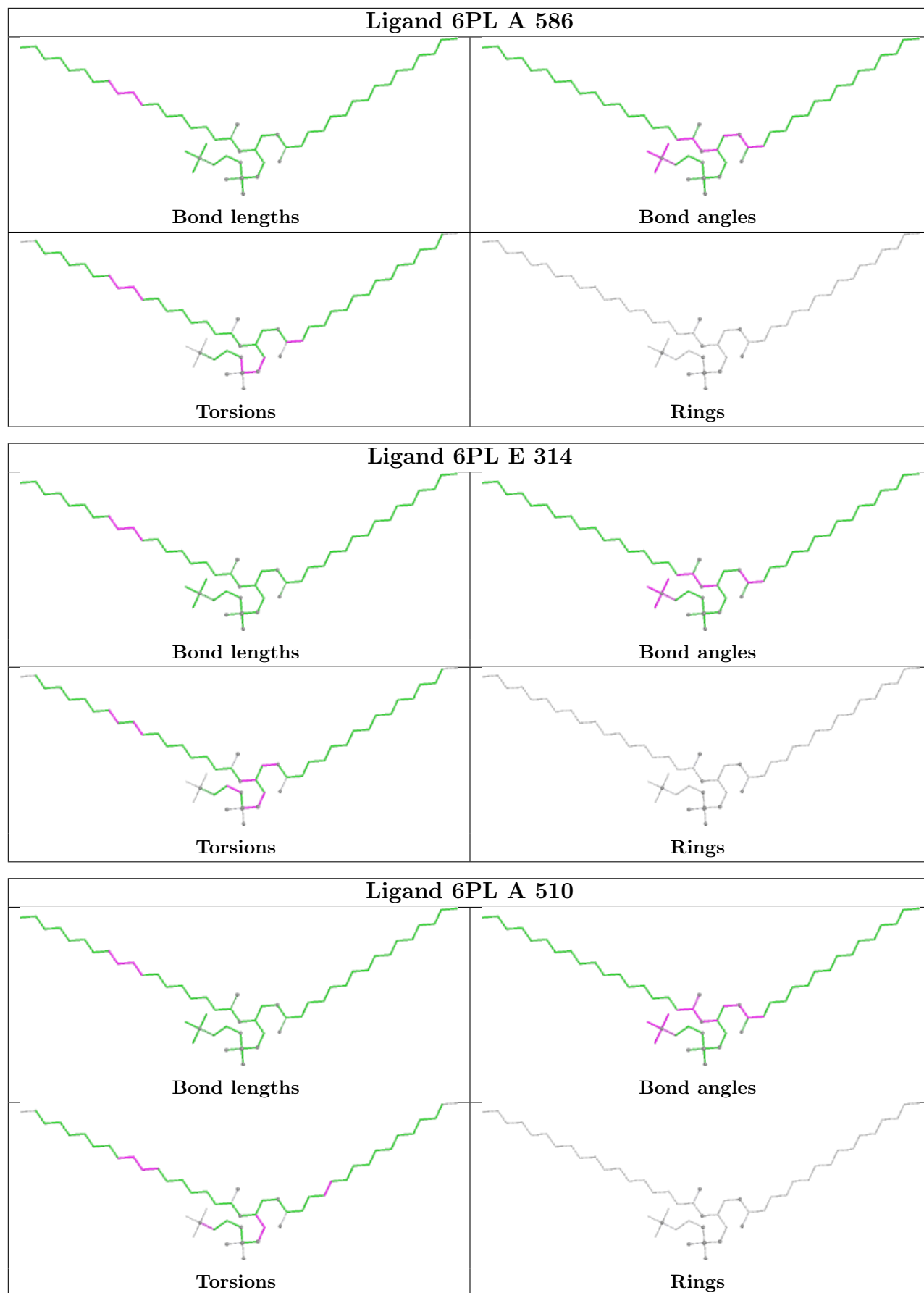


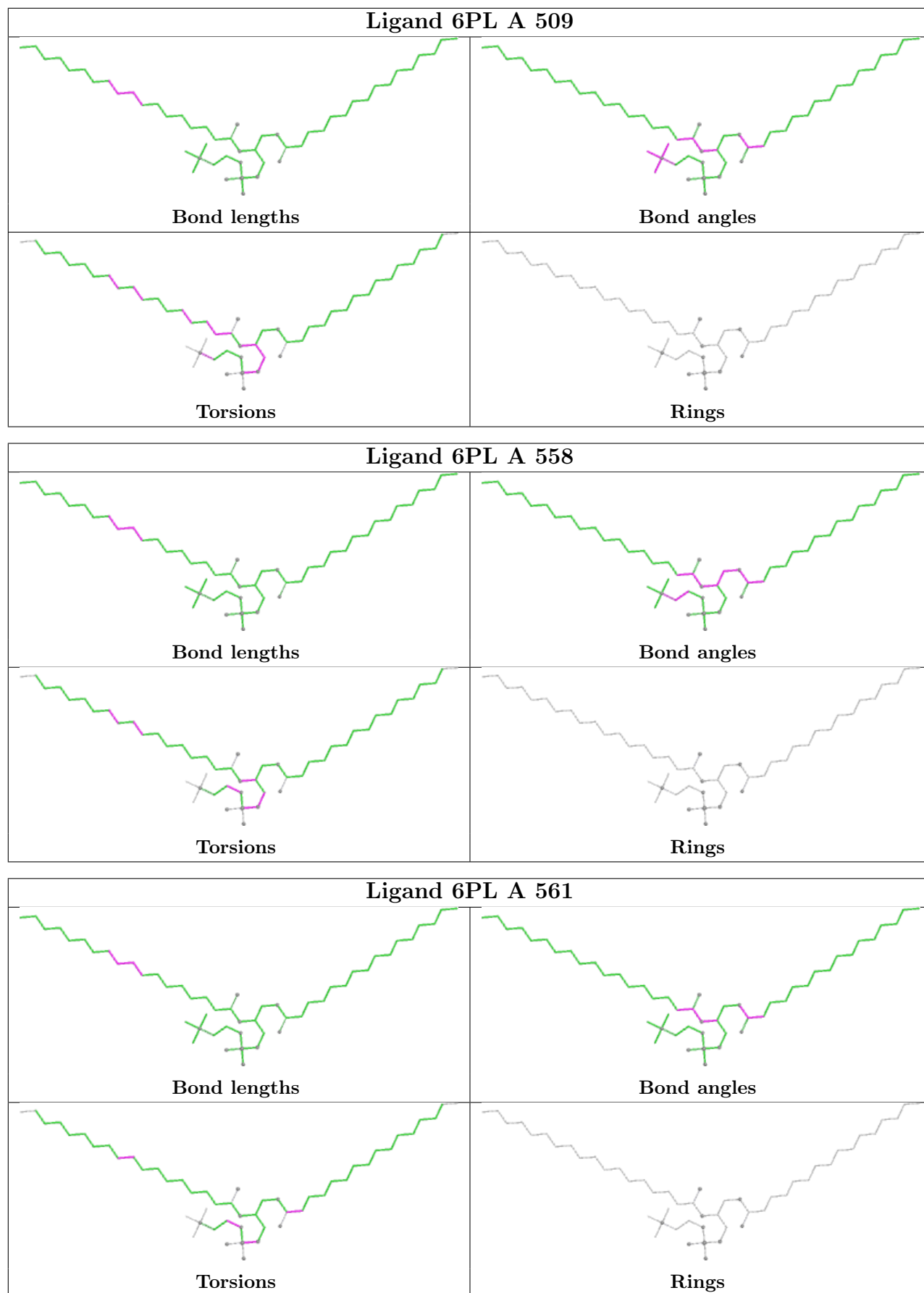


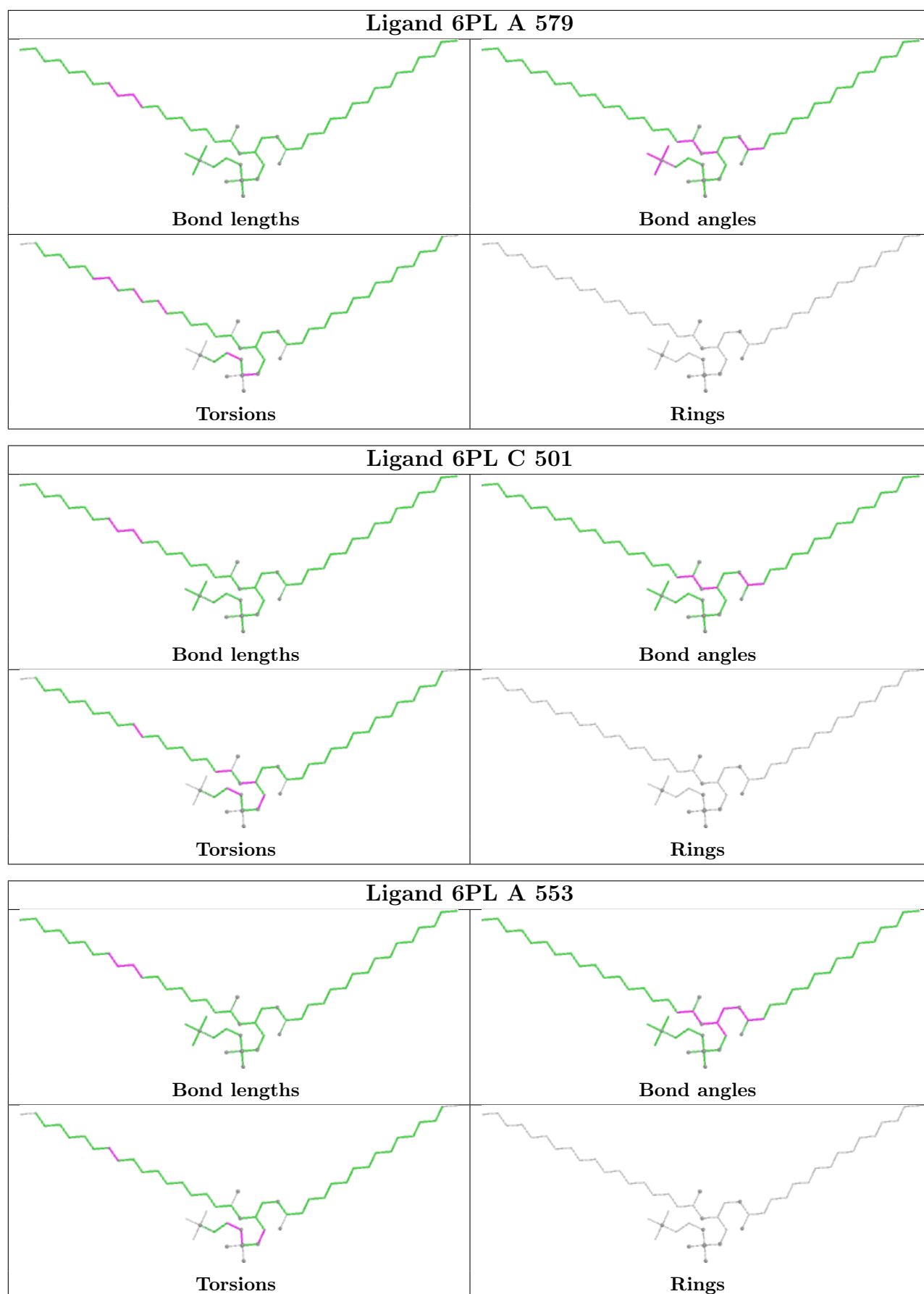


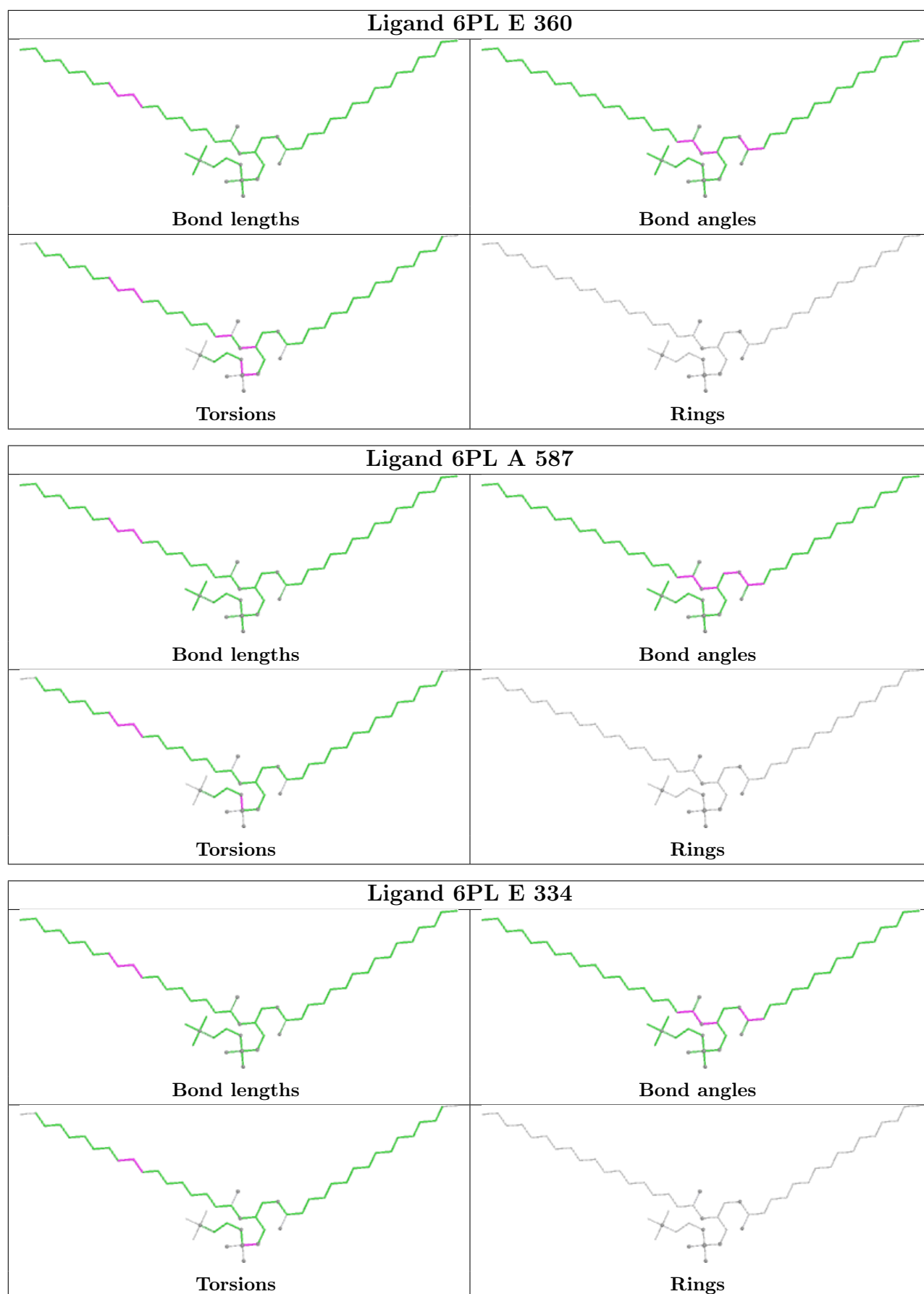


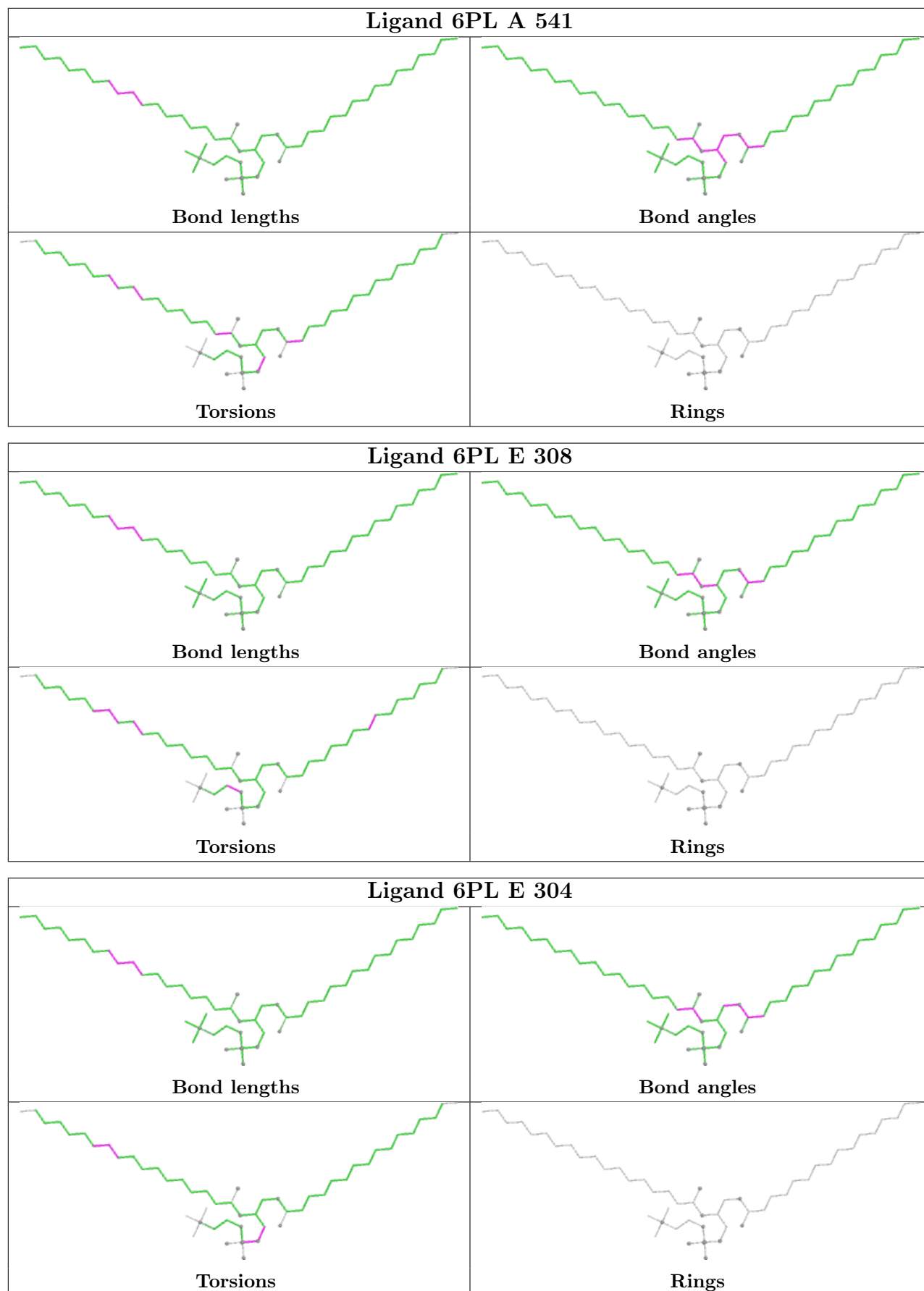


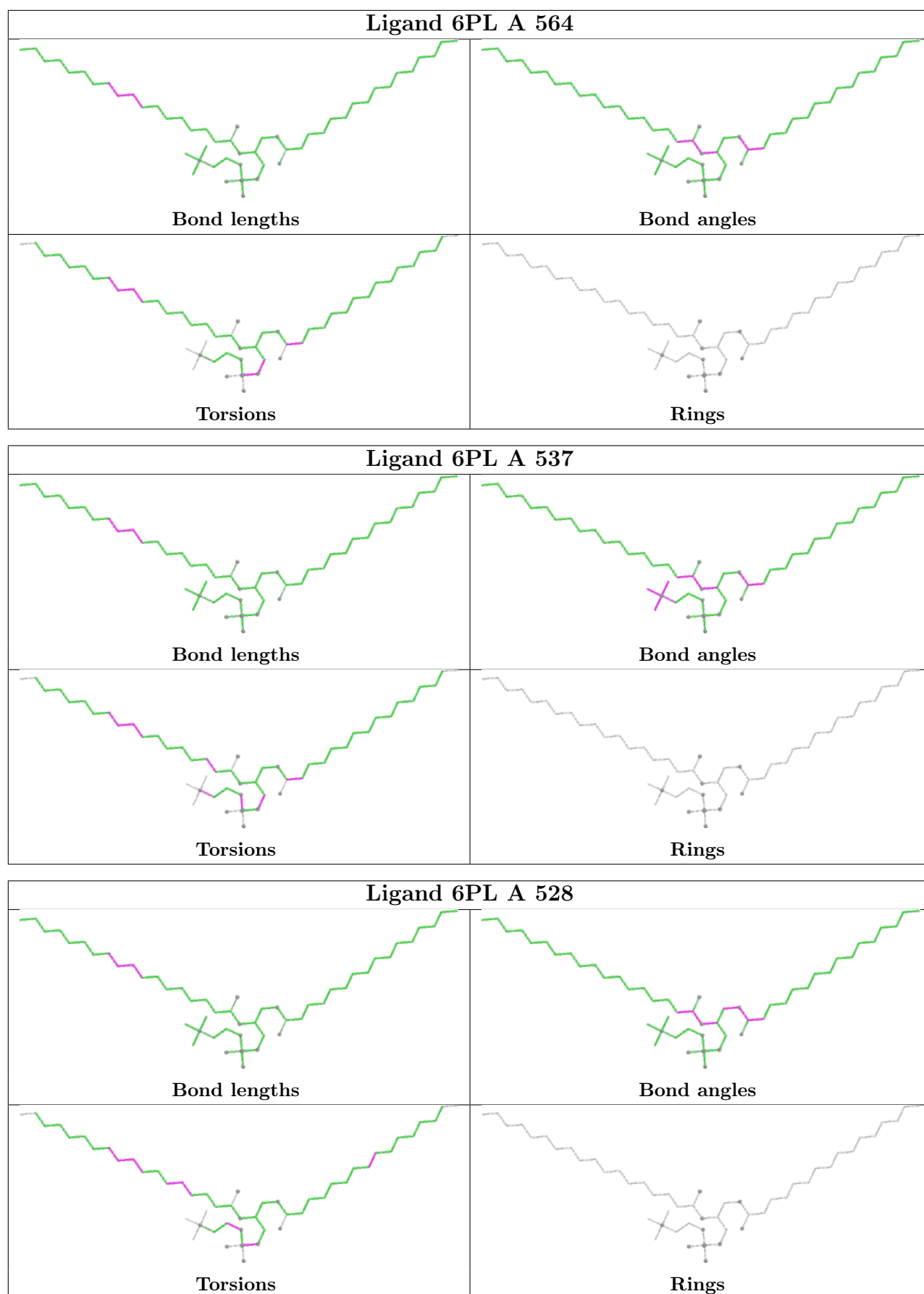


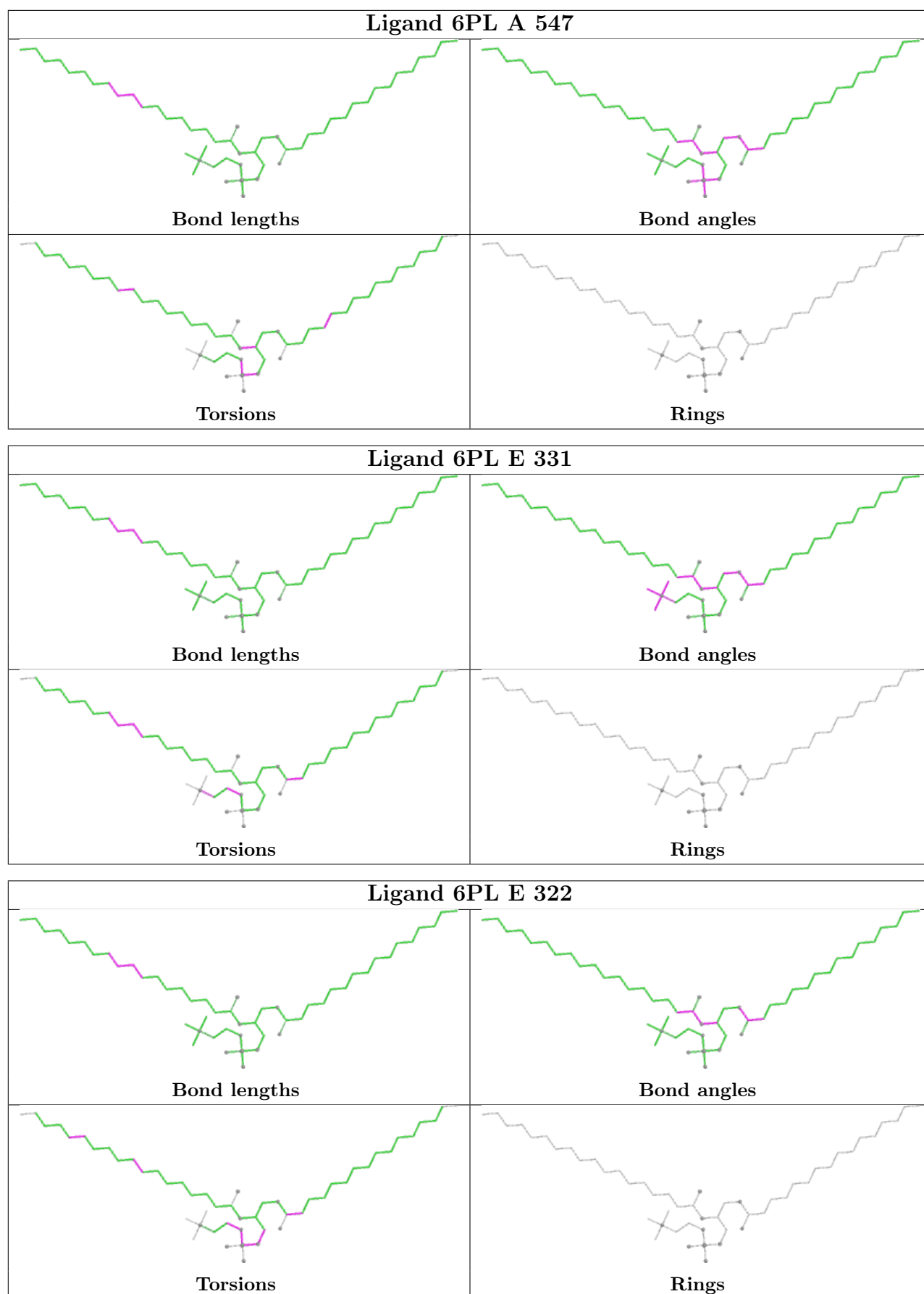


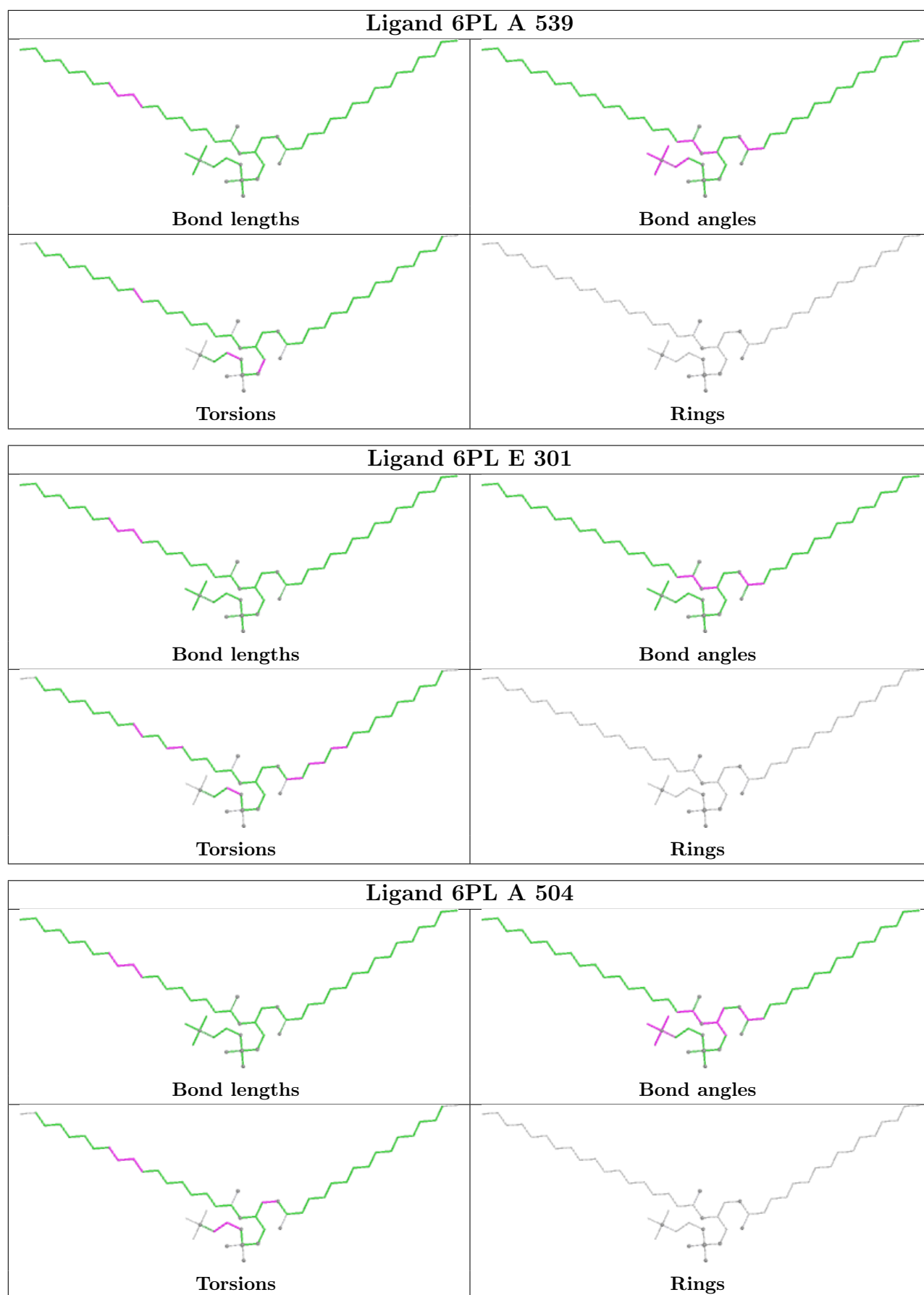


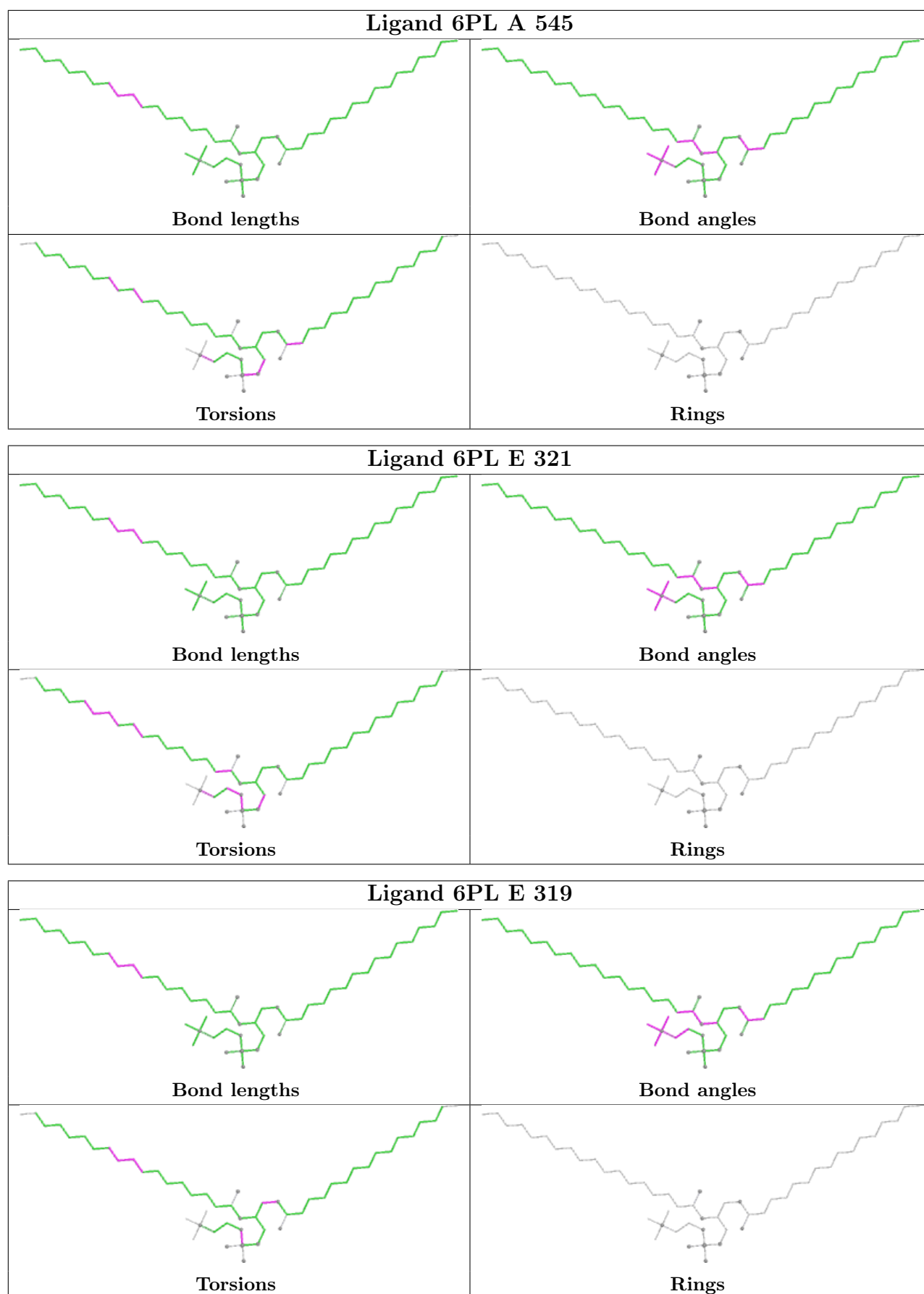


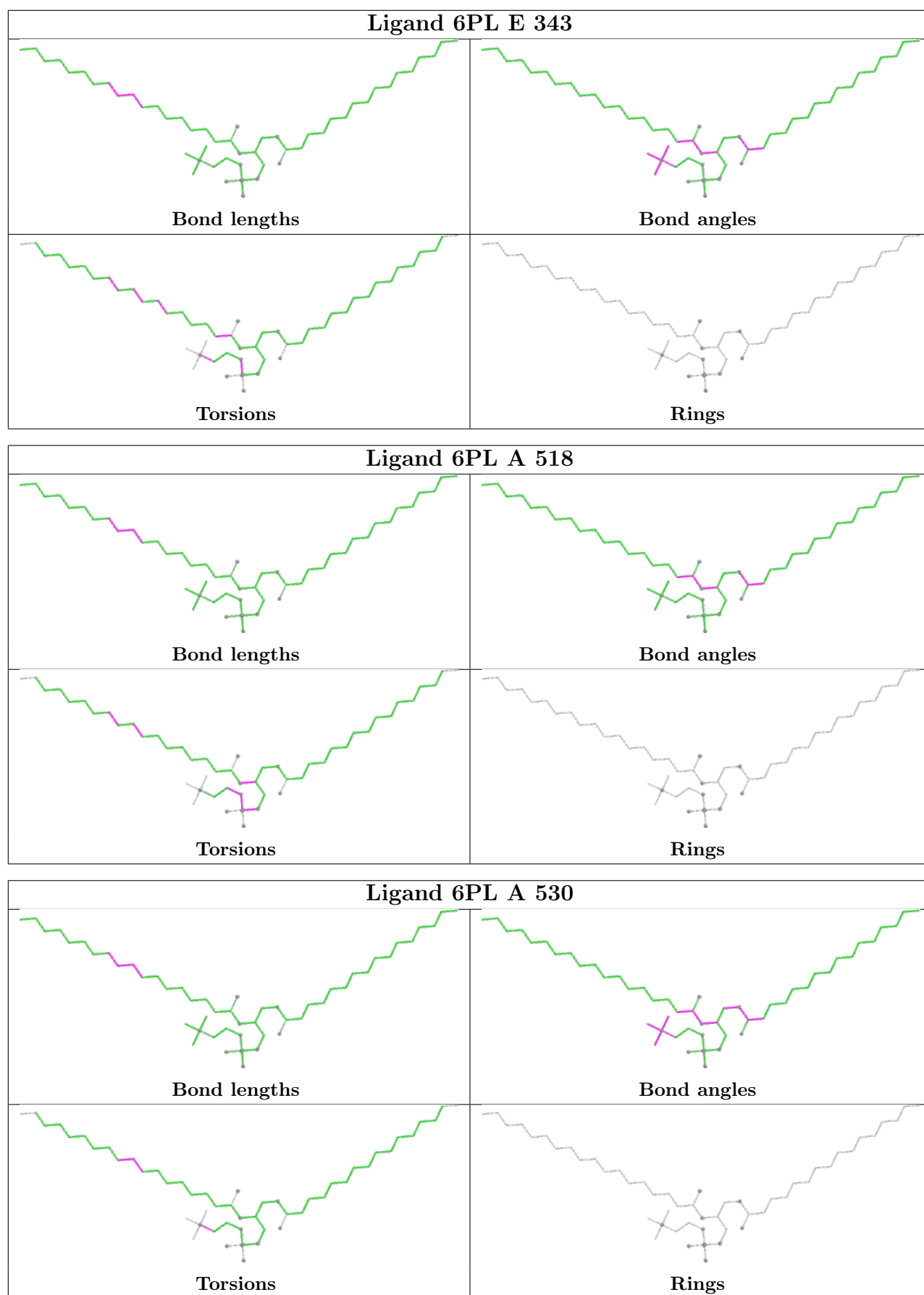


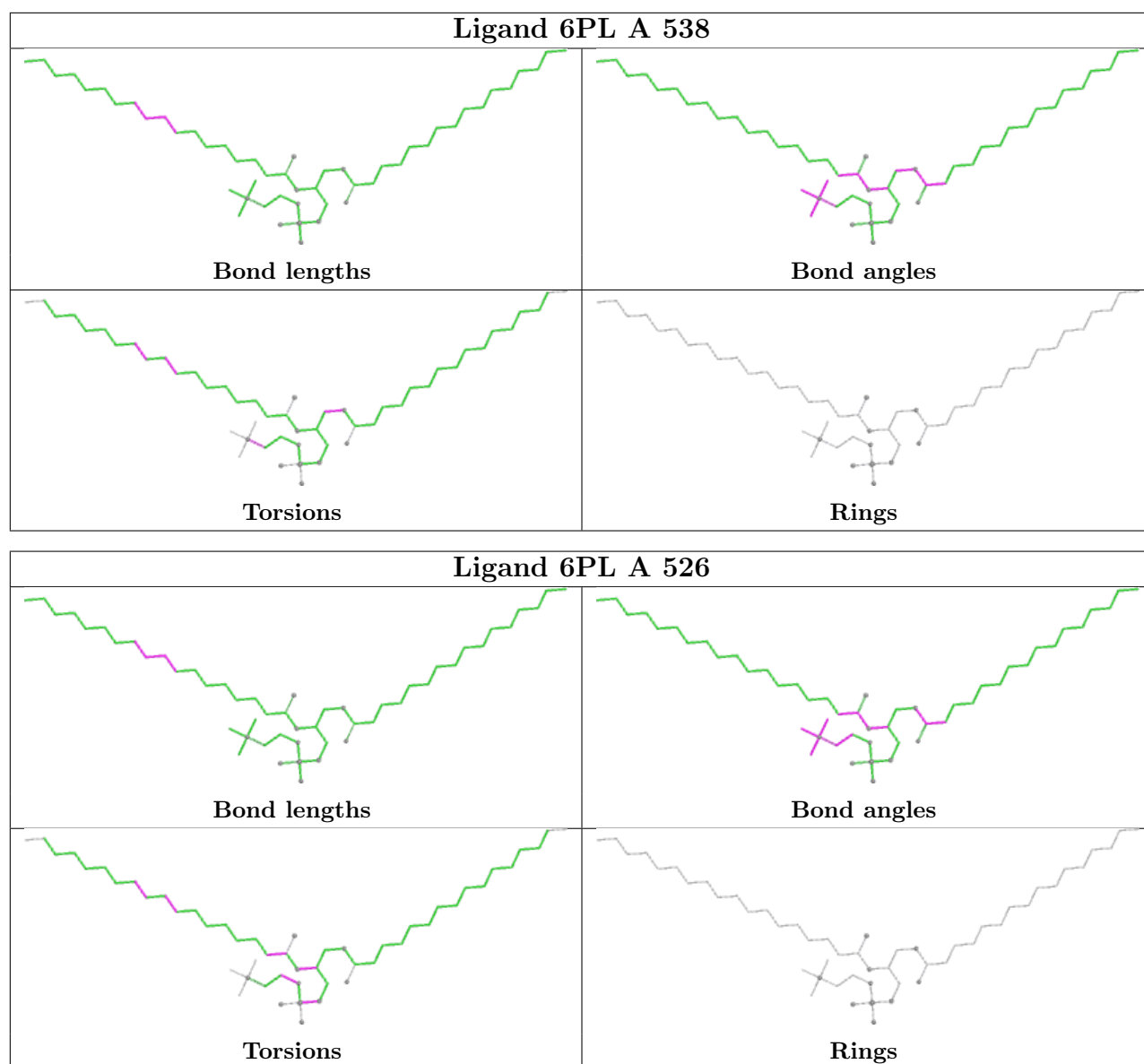












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

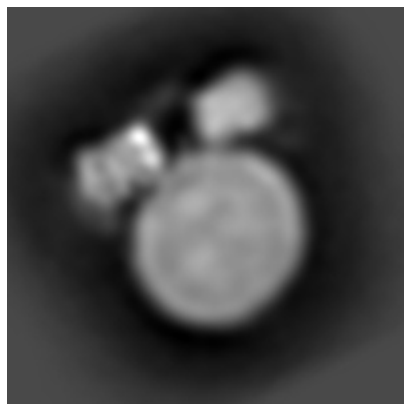
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48724. These allow visual inspection of the internal detail of the map and identification of artifacts.

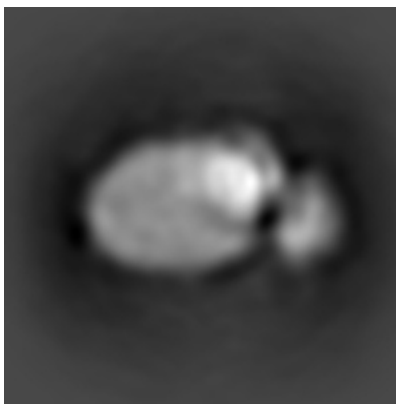
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

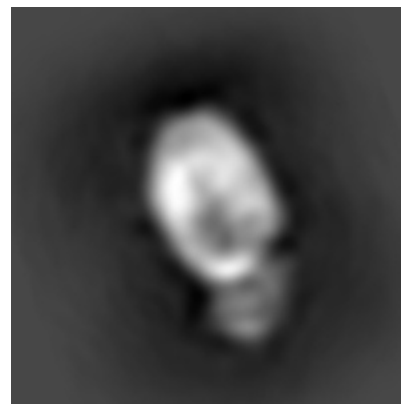
6.1.1 Primary map



X

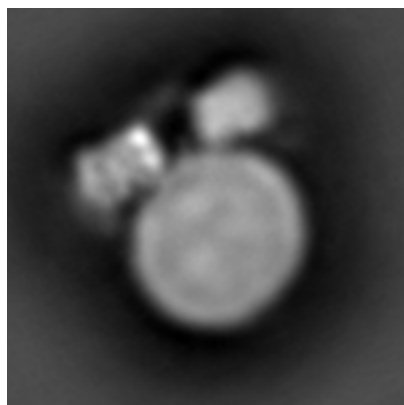


Y

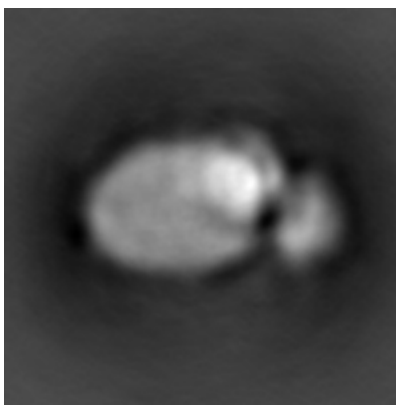


Z

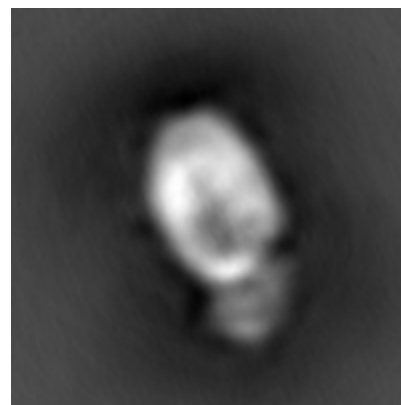
6.1.2 Raw map



X



Y

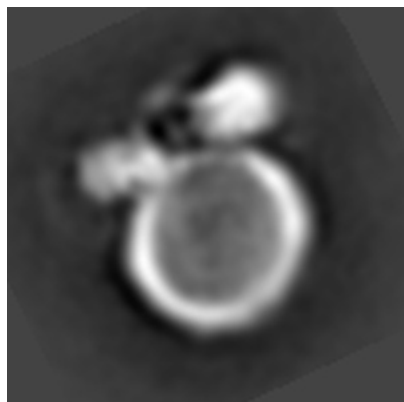


Z

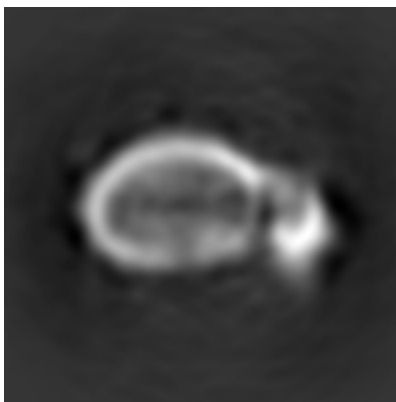
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

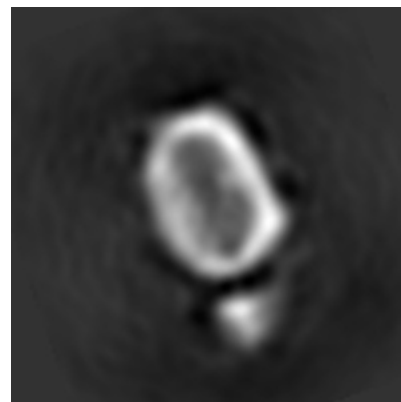
6.2.1 Primary map



X Index: 63

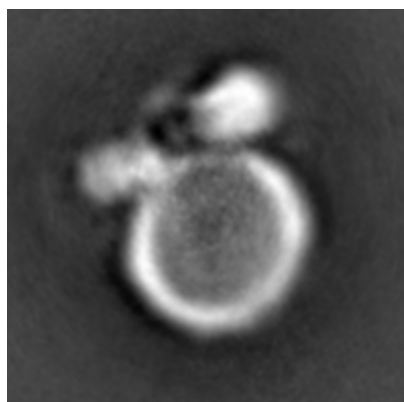


Y Index: 63

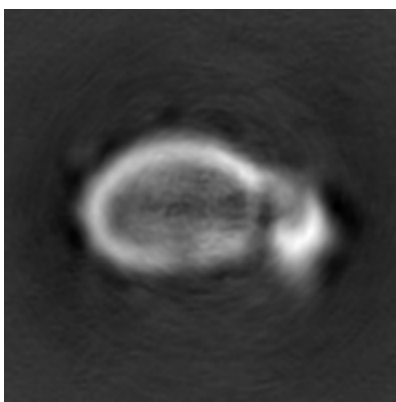


Z Index: 63

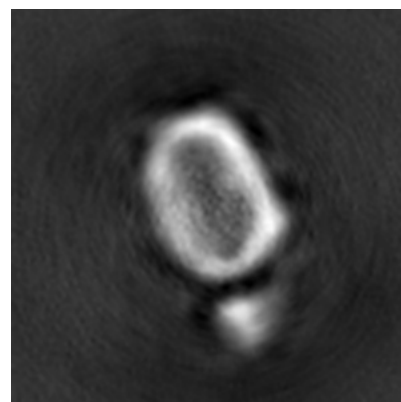
6.2.2 Raw map



X Index: 63



Y Index: 63

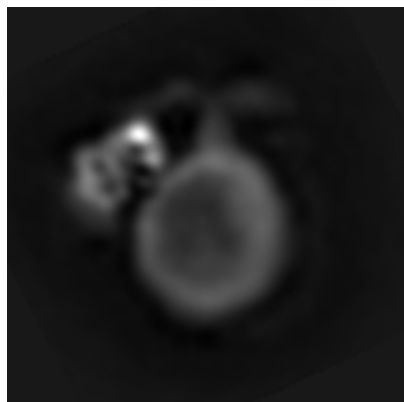


Z Index: 63

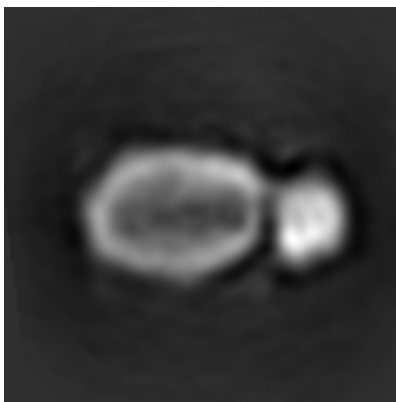
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 72

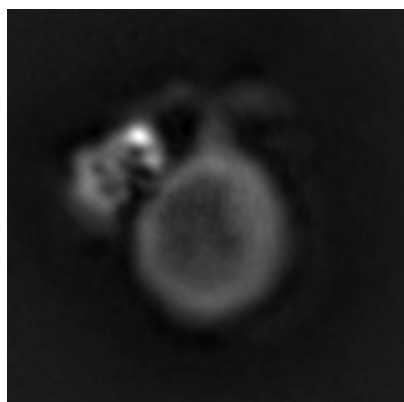


Y Index: 73

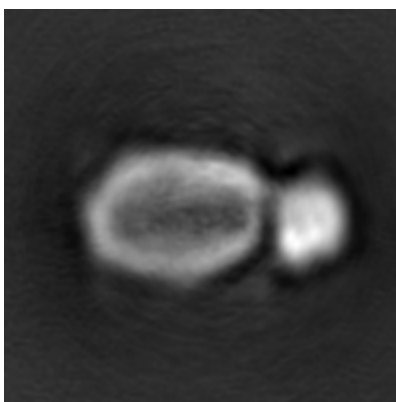


Z Index: 73

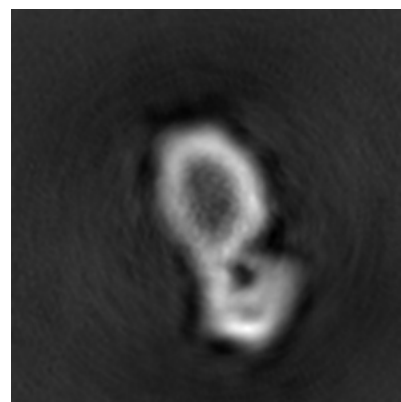
6.3.2 Raw map



X Index: 72



Y Index: 73

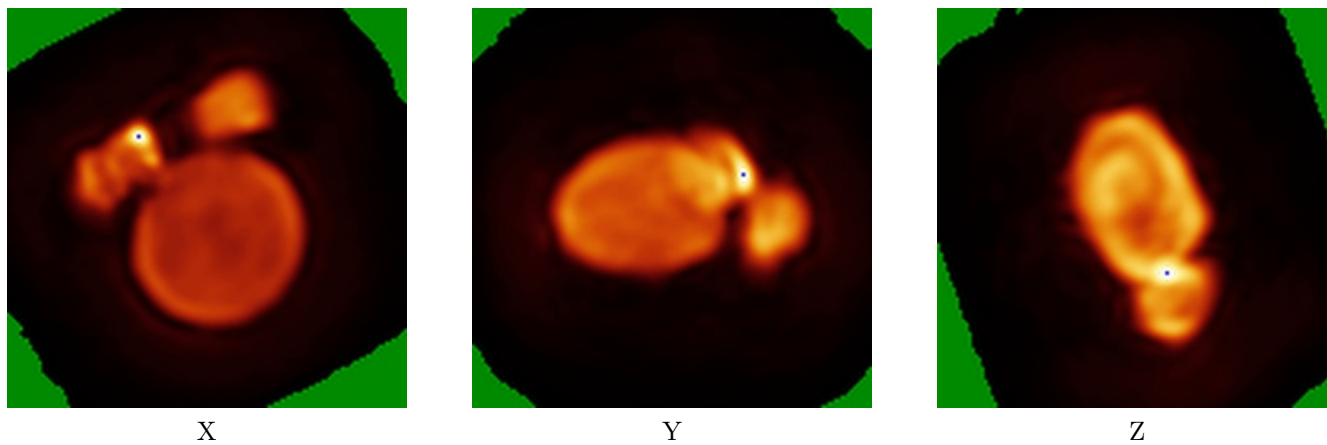


Z Index: 73

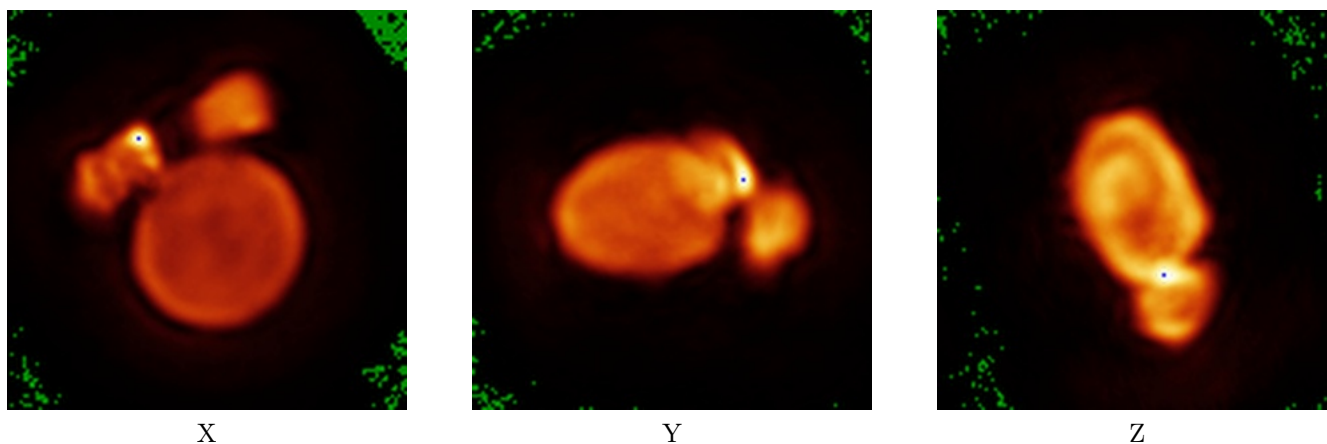
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

This section was not generated.

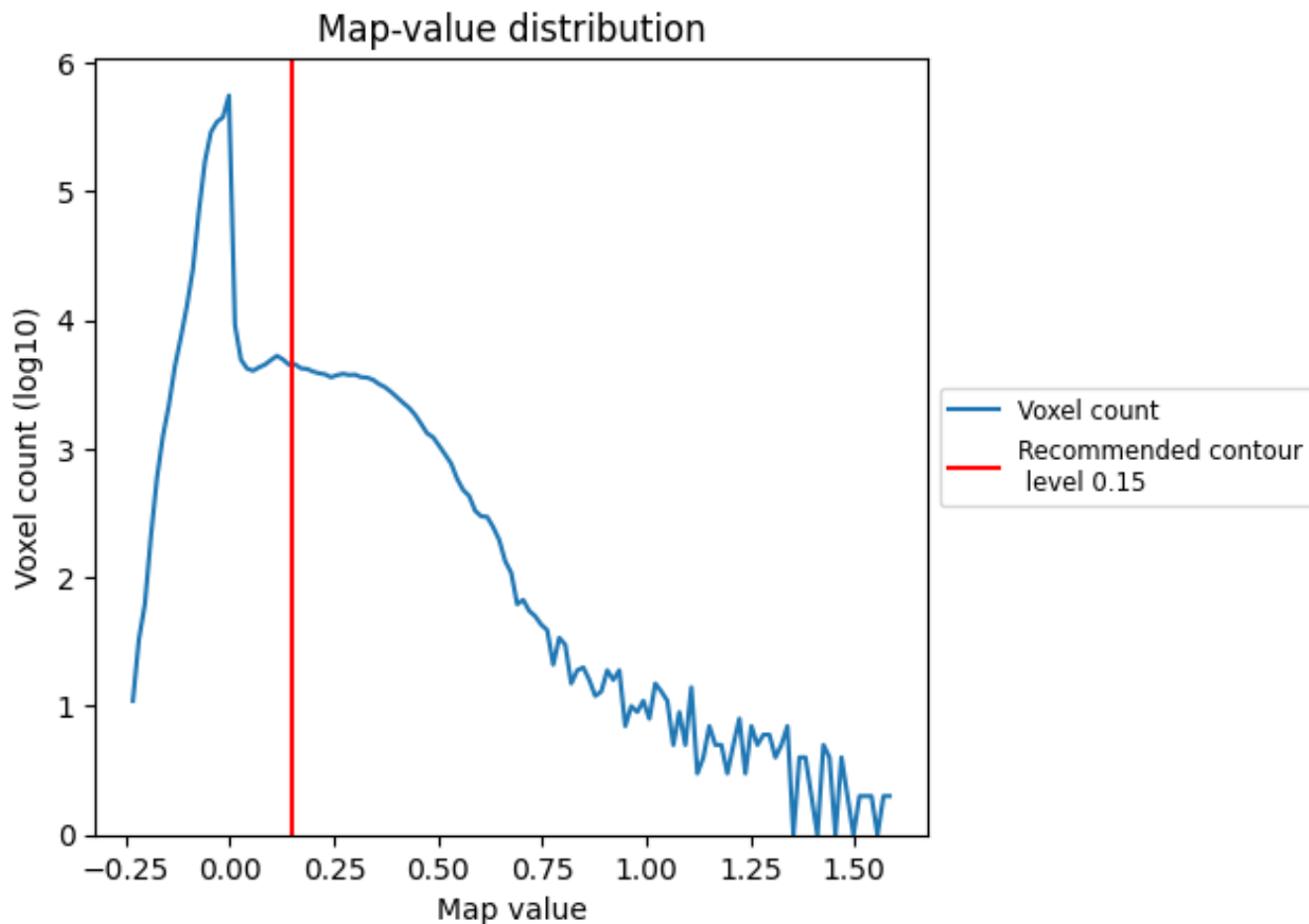
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

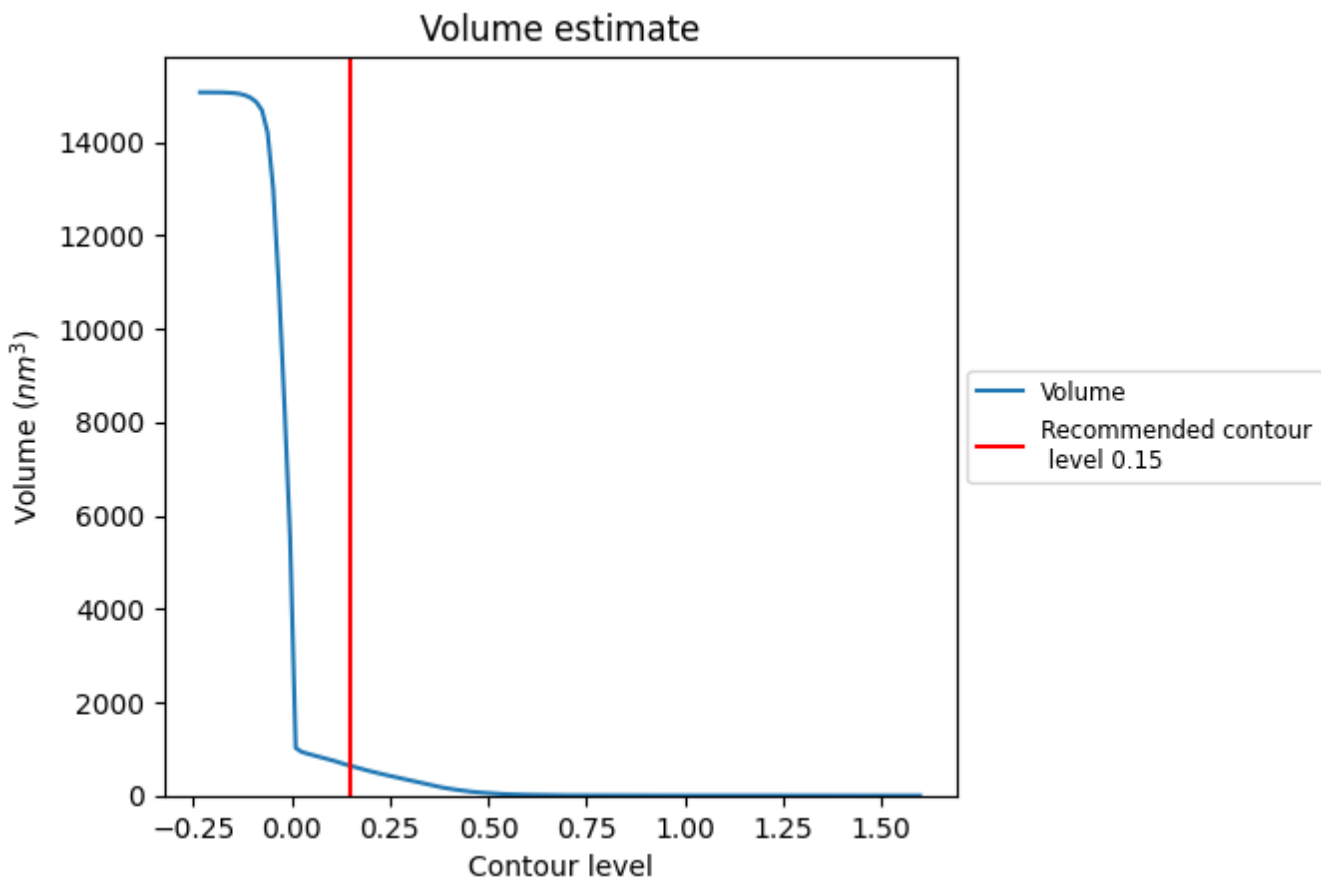
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

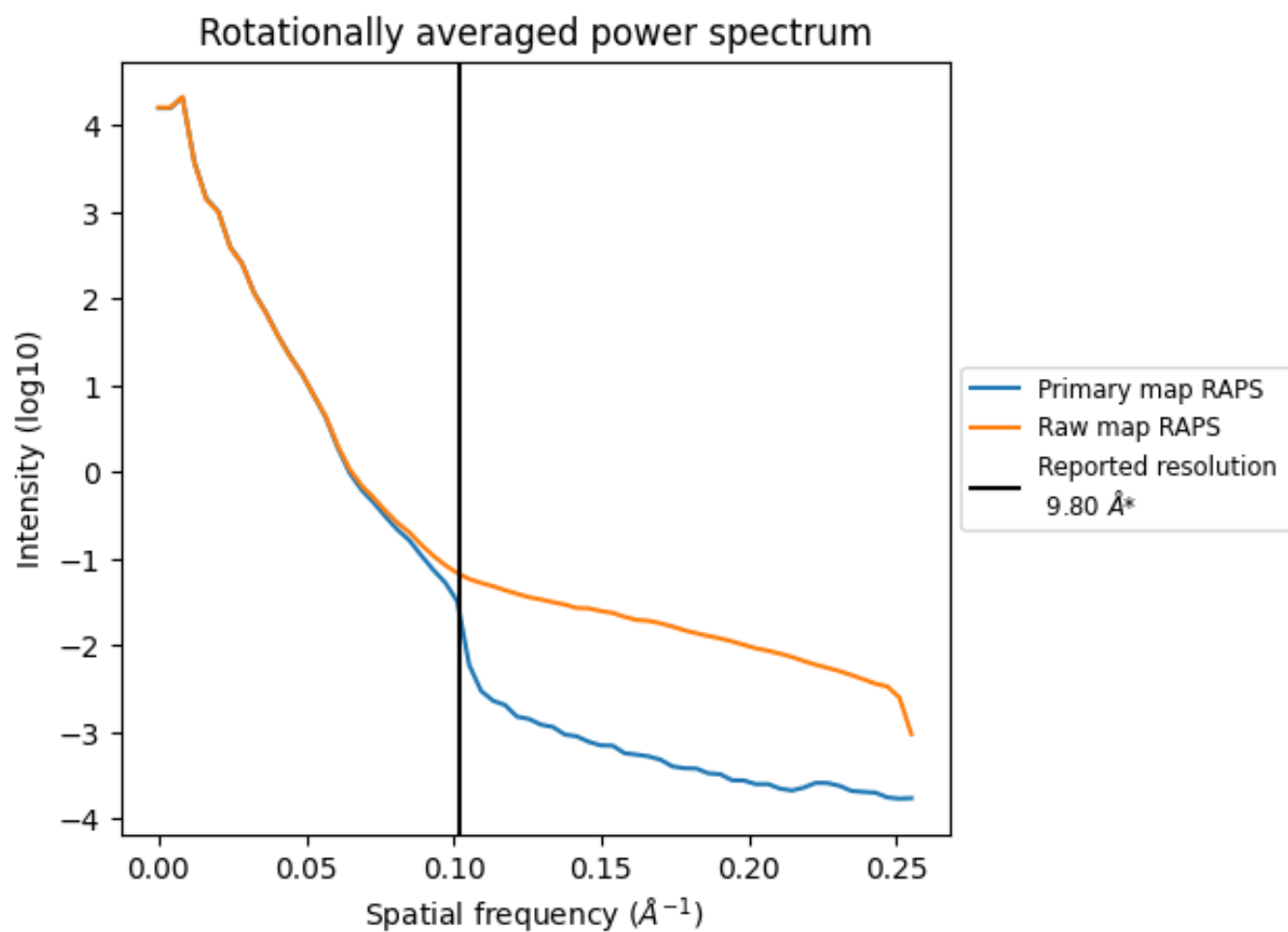
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 634 nm³; this corresponds to an approximate mass of 573 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

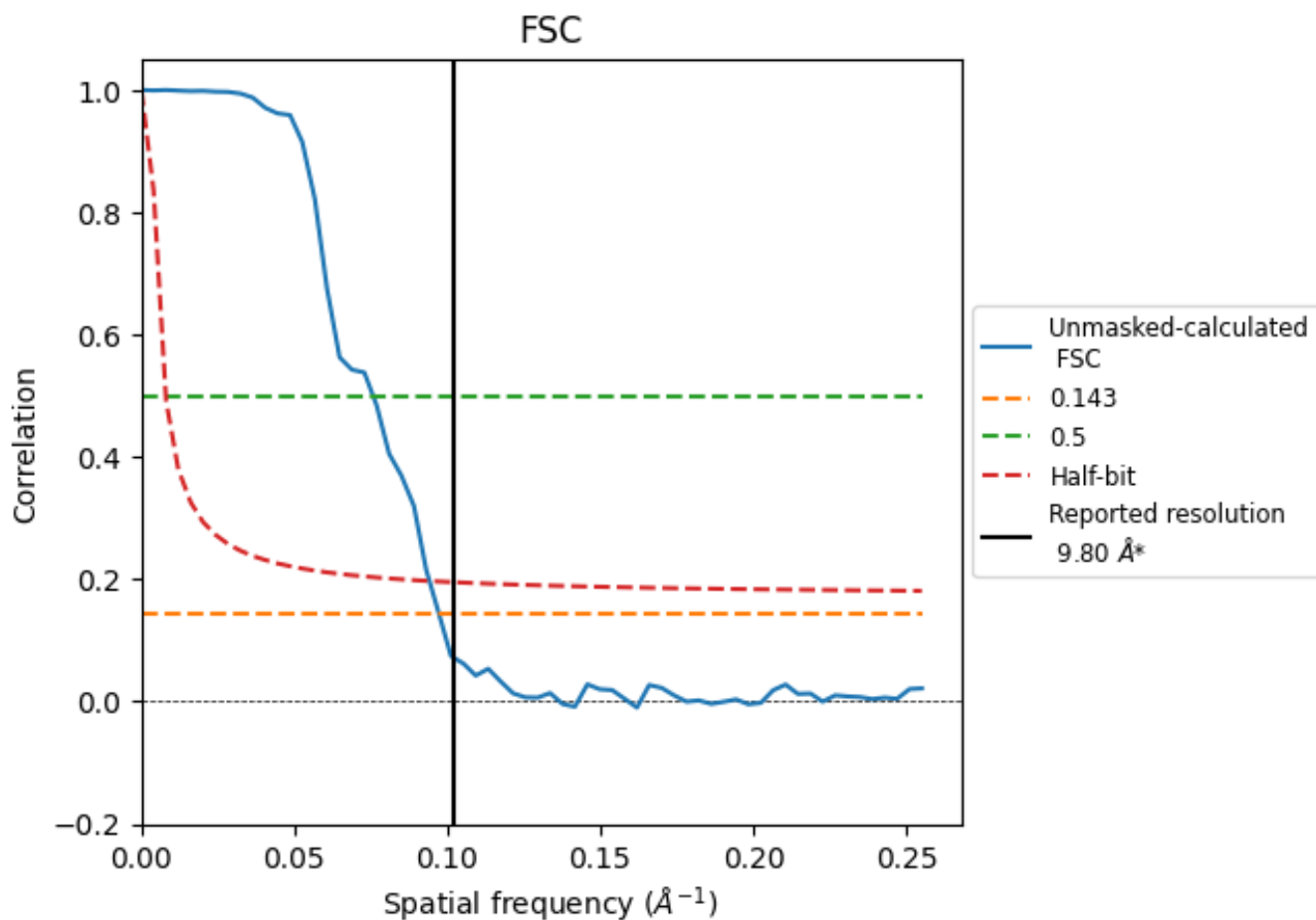


*Reported resolution corresponds to spatial frequency of 0.102 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.102 Å⁻¹

8.2 Resolution estimates [i](#)

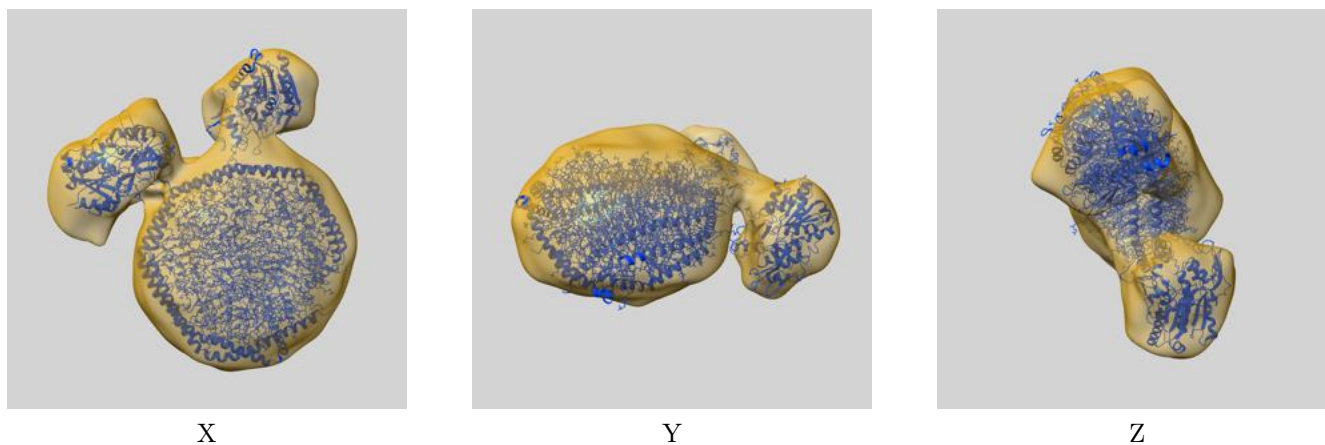
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.28	13.21	10.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

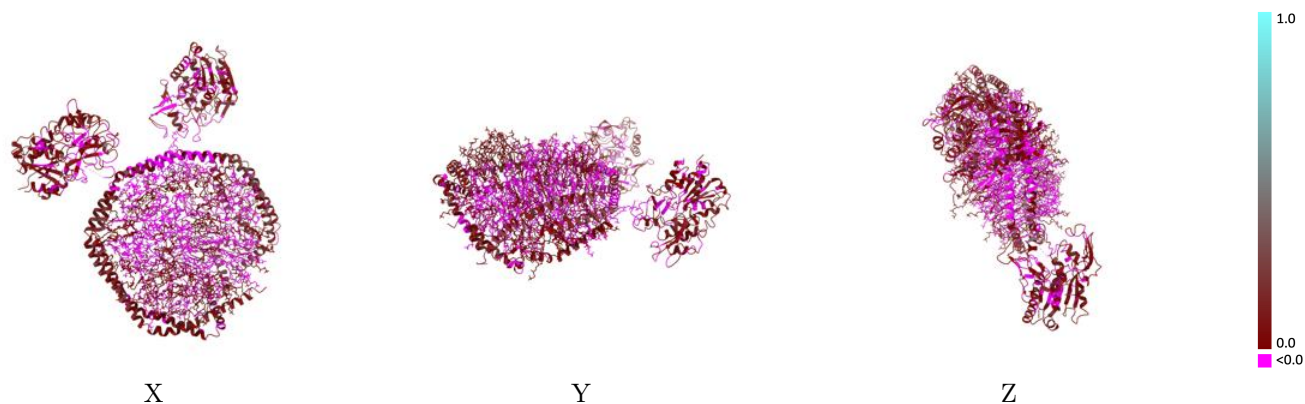
This section contains information regarding the fit between EMDB map EMD-48724 and PDB model 9MXZ. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



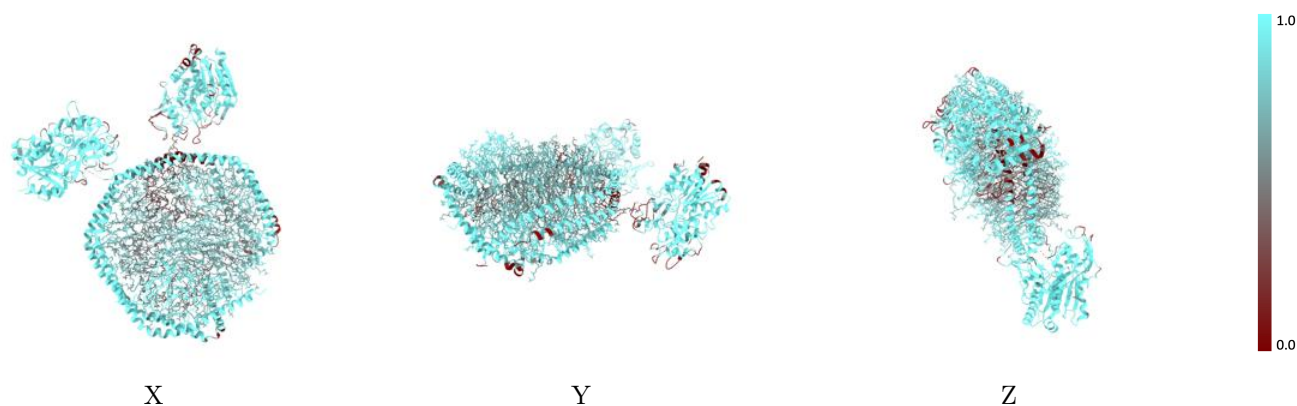
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



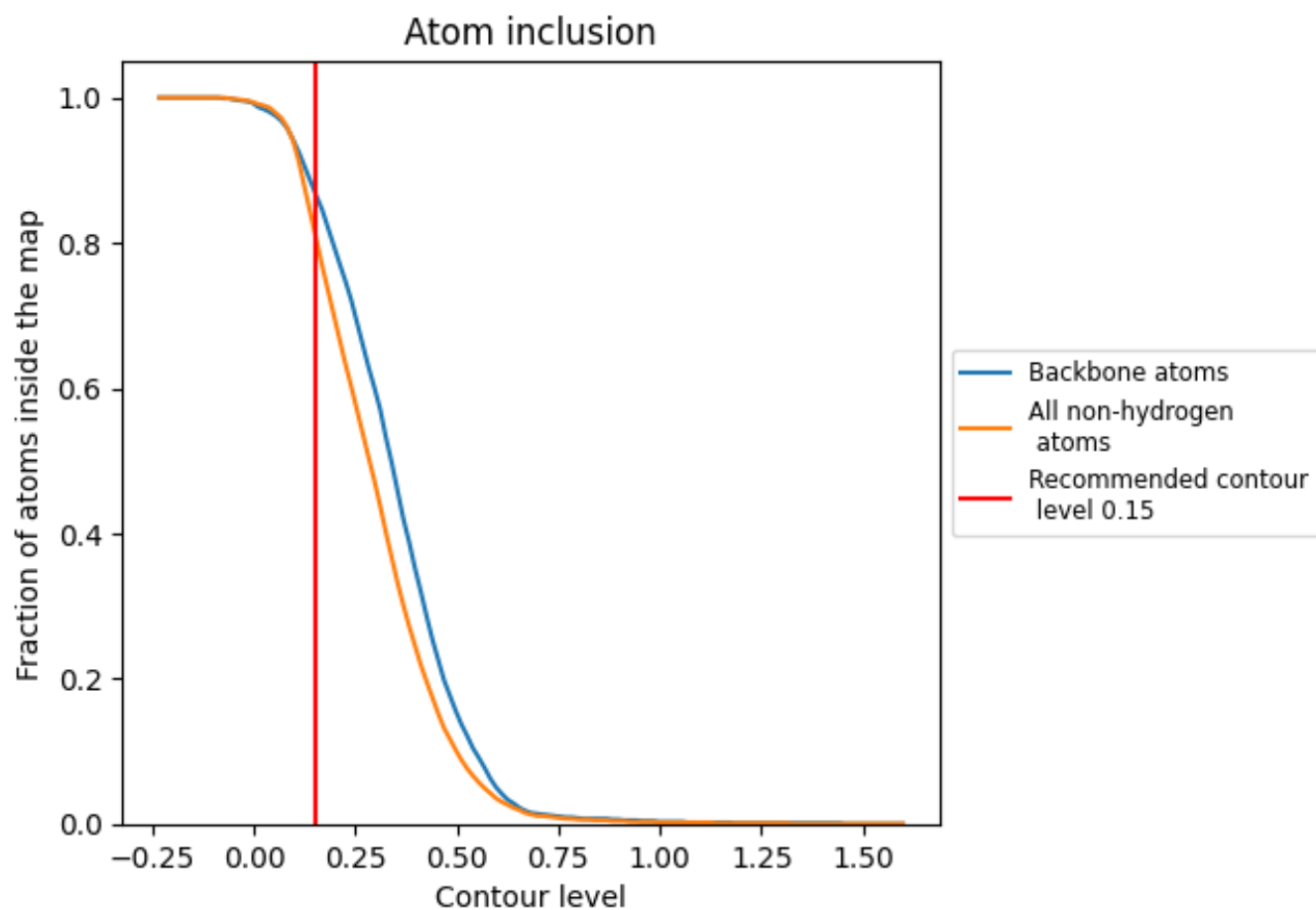
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).











9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8140	 0.0340
A	 0.8240	 0.0370
B	 0.9360	 0.0490
C	 0.8290	 0.0470
E	 0.7540	 0.0150

