



## wwPDB EM Validation Summary Report ⓘ

Jan 7, 2025 – 10:25 PM EST

PDB ID : 9CL3  
EMDB ID : EMD-45660  
Title : Particulate methane monooxygenase in unwashed native membranes  
Authors : Tucci, F.J.; Rosenzweig, A.C.  
Deposited on : 2024-07-10  
Resolution : 2.59 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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>.

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

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

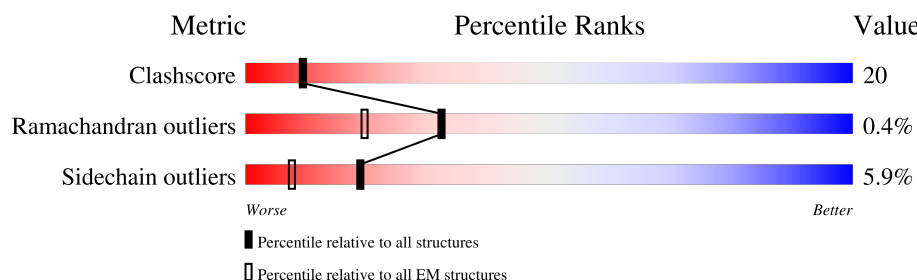
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.59 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	Ba	239	
1	Bb	239	
1	Bc	239	
2	Ca	241	
2	Cb	241	
2	Cc	241	
3	Aa	382	
3	Ab	382	

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Mol	Chain	Length	Quality of chain
3	Ac	382	 A horizontal bar chart showing the quality of chain 3. The bar is green for 89% and yellow for 10%. A small red dot is at the end of the bar. The text '89%' and '10%' are placed below the bar.

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28437 atoms, of which 4161 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 Particulate methane monooxygenase gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ba	239	Total 1993	C 1352	N 302	O 334	S 5	0	0
1	Bb	239	Total 1993	C 1352	N 302	O 334	S 5	0	0
1	Bc	239	Total 1993	C 1352	N 302	O 334	S 5	0	0

- Molecule 2 is a protein called Particulate methane monooxygenase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ca	241	Total 1976	C 1328	N 315	O 322	S 11	0	0
2	Cb	241	Total 1976	C 1328	N 315	O 322	S 11	0	0
2	Cc	241	Total 1976	C 1328	N 315	O 322	S 11	0	0

- Molecule 3 is a protein called Particulate methane monooxygenase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Aa	382	Total 3017	C 1938	N 513	O 551	S 15	0	0
3	Ab	382	Total 3017	C 1938	N 513	O 551	S 15	0	0
3	Ac	382	Total 3017	C 1938	N 513	O 551	S 15	0	0

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

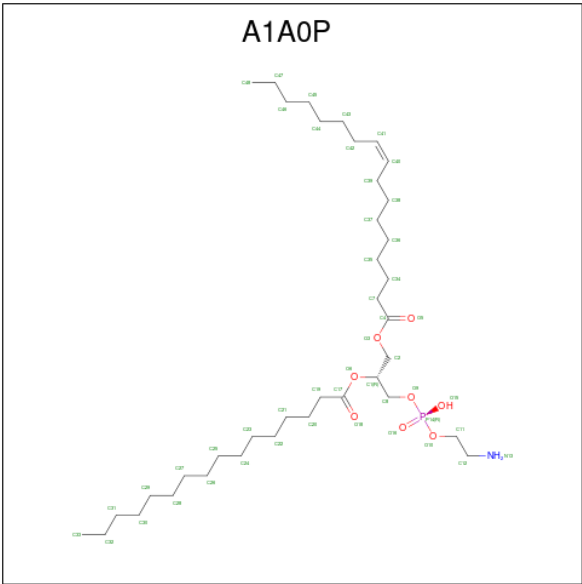
Mol	Chain	Residues	Atoms		AltConf
4	Ba	1	Total 1	Cu 1	0

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Mol	Chain	Residues	Atoms		AltConf
4	Aa	2	Total	Cu	0
			2	2	
4	Ab	2	Total	Cu	0
			2	2	
4	Ac	2	Total	Cu	0
			2	2	
4	Bb	1	Total	Cu	0
			1	1	
4	Bc	1	Total	Cu	0
			1	1	

- Molecule 5 is (2R)-3-[[[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(hexadecanoyloxy)propyl (9Z)-heptadec-9-enoate (three-letter code: A1A0P) (formula: C<sub>38</sub>H<sub>74</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms						AltConf
5	Ba	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
5	Ba	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
5	Ba	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
5	Ba	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
5	Ba	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
5	Ba	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	

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Mol	Chain	Residues	Atoms						AltConf
5	Ba	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ba	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ca	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ca	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ca	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ca	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ca	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ca	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ca	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ca	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Aa	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Aa	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Aa	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms						AltConf
5	Cc	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cc	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cc	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cc	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cc	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cc	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cc	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Cc	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ab	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ab	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ab	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ac	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ac	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Ac	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Bb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Bb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Bb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Bb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Bb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Bb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0
5	Bb	1	Total 121	C 38	H 73	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms						AltConf
5	Bb	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
5	Bc	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
5	Bc	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
5	Bc	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
5	Bc	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
5	Bc	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
5	Bc	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
5	Bc	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	

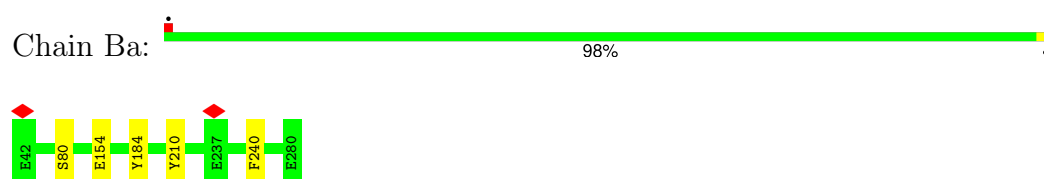
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	Ba	25	Total	O	0
			25	25	
6	Ca	47	Total	O	0
			47	47	
6	Aa	120	Total	O	0
			120	120	
6	Cb	46	Total	O	0
			46	46	
6	Cc	47	Total	O	0
			47	47	
6	Ab	119	Total	O	0
			119	119	
6	Ac	117	Total	O	0
			117	117	
6	Bb	26	Total	O	0
			26	26	
6	Bc	26	Total	O	0
			26	26	

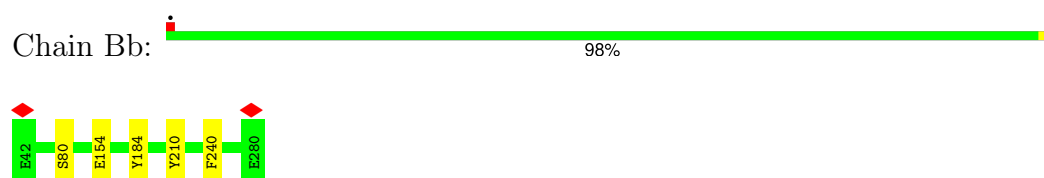
### 3 Residue-property plots [i](#)

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.

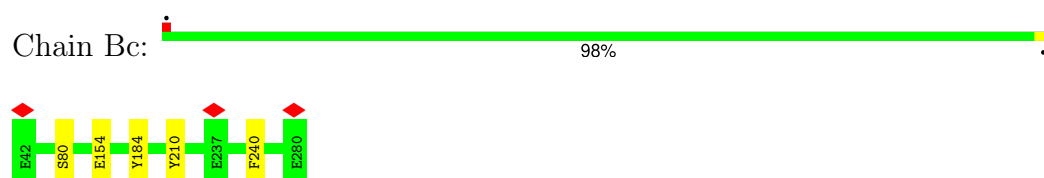
- Molecule 1: Particulate methane monooxygenase gamma subunit



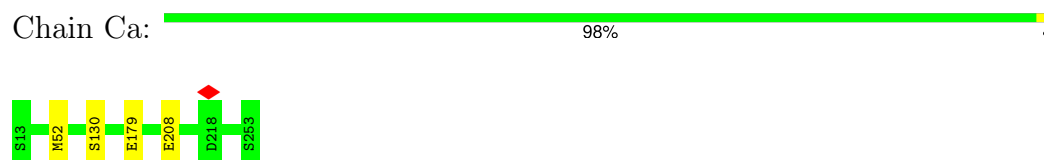
- Molecule 1: Particulate methane monooxygenase gamma subunit



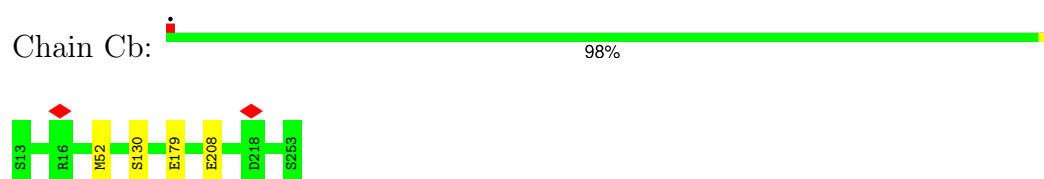
- Molecule 1: Particulate methane monooxygenase gamma subunit



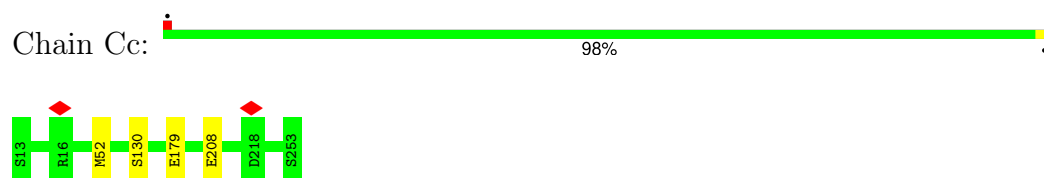
- Molecule 2: Particulate methane monooxygenase beta subunit



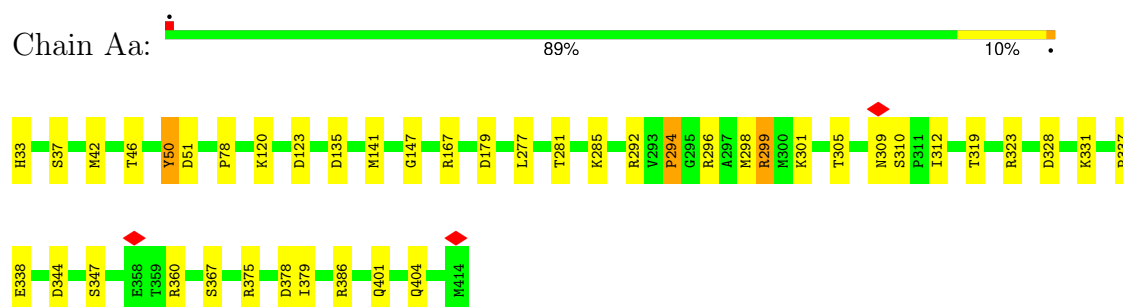
- Molecule 2: Particulate methane monooxygenase beta subunit



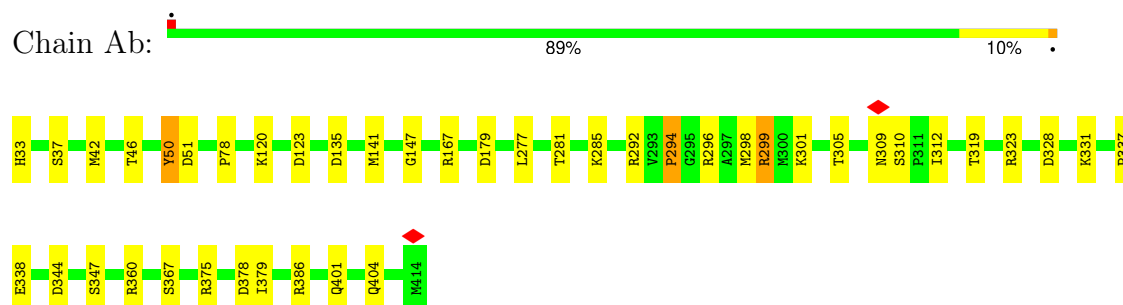
- Molecule 2: Particulate methane monooxygenase beta subunit



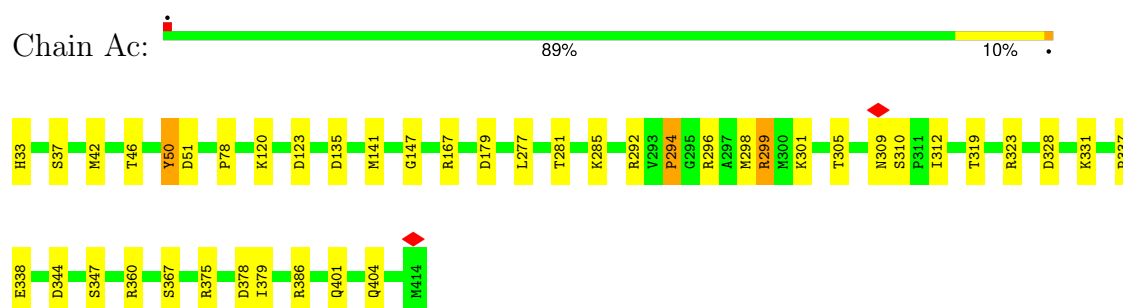
- Molecule 3: Particulate methane monooxygenase alpha subunit



- Molecule 3: Particulate methane monooxygenase alpha subunit



- Molecule 3: Particulate methane monooxygenase alpha subunit



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86073	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.711	Depositor
Minimum map value	-0.300	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.127	Depositor
Map size (Å)	332.0, 332.0, 332.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1A0P, CU

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	Ba	0.27	0/2073	0.45	0/2841
1	Bb	0.27	0/2073	0.45	0/2841
1	Bc	0.27	0/2073	0.45	0/2841
2	Ca	0.26	0/2052	0.47	0/2808
2	Cb	0.26	0/2052	0.48	0/2808
2	Cc	0.26	0/2052	0.48	0/2808
3	Aa	0.44	0/3099	0.64	2/4215 (0.0%)
3	Ab	0.44	0/3099	0.64	2/4215 (0.0%)
3	Ac	0.44	0/3099	0.64	2/4215 (0.0%)
All	All	0.35	0/21672	0.55	6/29592 (0.0%)

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
3	Aa	0	8
3	Ab	0	8
3	Ac	0	8
All	All	0	24

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Ab	50	TYR	N-CA-CB	6.72	122.69	110.60
3	Ac	50	TYR	N-CA-CB	6.71	122.67	110.60
3	Aa	50	TYR	N-CA-CB	6.69	122.64	110.60
3	Aa	50	TYR	CA-CB-CG	6.35	125.47	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Ab	50	TYR	CA-CB-CG	6.34	125.45	113.40

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	Aa	292	ARG	Sidechain
3	Aa	294	PRO	Peptide
3	Aa	296	ARG	Sidechain
3	Aa	299	ARG	Sidechain
3	Aa	323	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ba	1993	0	1922	0	0
1	Bb	1993	0	1922	0	0
1	Bc	1993	0	1922	0	0
2	Ca	1976	0	1934	0	0
2	Cb	1976	0	1934	0	0
2	Cc	1976	0	1934	0	0
3	Aa	3017	0	2980	0	0
3	Ab	3017	0	2980	0	0
3	Ac	3017	0	2980	0	0
4	Aa	2	0	0	0	0
4	Ab	2	0	0	0	0
4	Ac	2	0	0	0	0
4	Ba	1	0	0	0	0
4	Bb	1	0	0	0	0
4	Bc	1	0	0	0	0
5	Aa	144	219	0	0	0
5	Ab	144	219	0	0	0
5	Ac	144	219	0	0	0
5	Ba	384	584	0	0	0
5	Bb	384	584	0	0	0
5	Bc	384	584	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Ca	384	584	0	0	0
5	Cb	384	584	0	0	0
5	Cc	384	584	0	0	0
6	Aa	120	0	0	0	0
6	Ab	119	0	0	0	0
6	Ac	117	0	0	0	0
6	Ba	25	0	0	0	0
6	Bb	26	0	0	0	0
6	Bc	26	0	0	0	0
6	Ca	47	0	0	0	0
6	Cb	46	0	0	0	0
6	Cc	47	0	0	0	0
All	All	24276	4161	20508	0	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 20.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	Ba	237/239 (99%)	228 (96%)	9 (4%)	0	100	100
1	Bb	237/239 (99%)	228 (96%)	9 (4%)	0	100	100
1	Bc	237/239 (99%)	228 (96%)	9 (4%)	0	100	100
2	Ca	239/241 (99%)	229 (96%)	10 (4%)	0	100	100
2	Cb	239/241 (99%)	229 (96%)	10 (4%)	0	100	100
2	Cc	239/241 (99%)	229 (96%)	10 (4%)	0	100	100
3	Aa	380/382 (100%)	359 (94%)	18 (5%)	3 (1%)	16	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ab	380/382 (100%)	358 (94%)	19 (5%)	3 (1%)	16	34
3	Ac	380/382 (100%)	359 (94%)	18 (5%)	3 (1%)	16	34
All	All	2568/2586 (99%)	2447 (95%)	112 (4%)	9 (0%)	32	52

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Aa	281	THR
3	Aa	294	PRO
3	Ab	281	THR
3	Ab	294	PRO
3	Ac	281	THR

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	Ba	202/202 (100%)	197 (98%)	5 (2%)	42	68
1	Bb	202/202 (100%)	197 (98%)	5 (2%)	42	68
1	Bc	202/202 (100%)	197 (98%)	5 (2%)	42	68
2	Ca	206/206 (100%)	202 (98%)	4 (2%)	52	75
2	Cb	206/206 (100%)	202 (98%)	4 (2%)	52	75
2	Cc	206/206 (100%)	202 (98%)	4 (2%)	52	75
3	Aa	323/323 (100%)	289 (90%)	34 (10%)	5	11
3	Ab	323/323 (100%)	289 (90%)	34 (10%)	5	11
3	Ac	323/323 (100%)	289 (90%)	34 (10%)	5	11
All	All	2193/2193 (100%)	2064 (94%)	129 (6%)	19	35

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Ac	378	ASP

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Mol	Chain	Res	Type
1	Bb	80	SER
2	Cc	130	SER
2	Cc	52	MET
1	Bb	184	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	Bc	173	HIS
1	Bb	173	HIS
3	Ac	306	ASN
3	Ab	309	ASN
3	Ac	309	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 9 are monoatomic - leaving 57 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	A1A0P	Cb	307	-	47,47,47	0.41	0	50,52,52	0.82	2 (4%)
5	A1A0P	Cc	304	-	47,47,47	0.31	0	50,52,52	0.34	0
5	A1A0P	Ba	302	-	47,47,47	0.31	0	50,52,52	0.33	0
5	A1A0P	Bb	308	-	47,47,47	0.31	0	50,52,52	0.43	0
5	A1A0P	Ba	306	-	47,47,47	0.31	0	50,52,52	0.42	0
5	A1A0P	Ba	305	-	47,47,47	0.32	0	50,52,52	0.50	1 (2%)
5	A1A0P	Aa	504	-	47,47,47	0.39	0	50,52,52	0.51	1 (2%)
5	A1A0P	Cc	307	-	47,47,47	0.39	0	50,52,52	0.63	1 (2%)
5	A1A0P	Cb	303	-	47,47,47	0.30	0	50,52,52	0.34	0
5	A1A0P	Ca	302	-	47,47,47	0.45	0	50,52,52	0.73	1 (2%)
5	A1A0P	Cb	306	-	47,47,47	0.39	0	50,52,52	0.63	1 (2%)
5	A1A0P	Ca	307	-	47,47,47	0.41	0	50,52,52	0.82	2 (4%)
5	A1A0P	Ba	309	-	47,47,47	0.81	3 (6%)	50,52,52	1.24	6 (12%)
5	A1A0P	Bb	301	-	47,47,47	0.82	3 (6%)	50,52,52	1.24	6 (12%)
5	A1A0P	Cb	304	-	47,47,47	0.31	0	50,52,52	0.49	0
5	A1A0P	Bc	304	-	47,47,47	0.31	0	50,52,52	0.33	0
5	A1A0P	Bc	308	-	47,47,47	0.31	0	50,52,52	0.42	0
5	A1A0P	Ba	304	-	47,47,47	0.37	0	50,52,52	0.46	0
5	A1A0P	Aa	505	-	47,47,47	0.30	0	50,52,52	0.35	0
5	A1A0P	Bb	304	-	47,47,47	0.30	0	50,52,52	0.33	0
5	A1A0P	Ba	308	-	47,47,47	0.77	0	50,52,52	1.22	2 (4%)
5	A1A0P	Ca	301	-	47,47,47	0.36	0	50,52,52	0.77	3 (6%)
5	A1A0P	Cc	308	-	47,47,47	0.41	0	50,52,52	0.83	2 (4%)
5	A1A0P	Bb	305	-	47,47,47	0.34	0	50,52,52	0.52	0
5	A1A0P	Bb	307	-	47,47,47	0.32	0	50,52,52	0.50	1 (2%)
5	A1A0P	Ab	502	-	47,47,47	0.39	0	50,52,52	0.51	1 (2%)
5	A1A0P	Cc	303	-	47,47,47	0.46	0	50,52,52	0.73	1 (2%)
5	A1A0P	Ca	305	-	47,47,47	0.33	0	50,52,52	0.37	0
5	A1A0P	Cb	302	-	47,47,47	0.45	0	50,52,52	0.73	1 (2%)
5	A1A0P	Ac	504	-	47,47,47	0.32	0	50,52,52	0.51	1 (2%)
5	A1A0P	Bb	309	-	47,47,47	0.33	0	50,52,52	0.45	0
5	A1A0P	Bb	302	-	47,47,47	0.77	0	50,52,52	1.22	2 (4%)
5	A1A0P	Bc	309	-	47,47,47	0.33	0	50,52,52	0.45	0
5	A1A0P	Bc	301	-	47,47,47	0.81	3 (6%)	50,52,52	1.24	6 (12%)
5	A1A0P	Bc	302	-	47,47,47	0.76	0	50,52,52	1.22	2 (4%)
5	A1A0P	Ab	501	-	47,47,47	0.30	0	50,52,52	0.35	0
5	A1A0P	Ac	505	-	47,47,47	0.30	0	50,52,52	0.35	0
5	A1A0P	Ca	304	-	47,47,47	0.31	0	50,52,52	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	A1A0P	Ac	501	-	47,47,47	0.39	0	50,52,52	0.51	1 (2%)
5	A1A0P	Bb	306	-	47,47,47	0.37	0	50,52,52	0.45	0
5	A1A0P	Cb	305	-	47,47,47	0.33	0	50,52,52	0.37	0
5	A1A0P	Ca	308	-	47,47,47	0.68	1 (2%)	50,52,52	0.44	0
5	A1A0P	Cc	302	-	47,47,47	0.36	0	50,52,52	0.77	3 (6%)
5	A1A0P	Cc	305	-	47,47,47	0.30	0	50,52,52	0.49	0
5	A1A0P	Cb	301	-	47,47,47	0.36	0	50,52,52	0.77	3 (6%)
5	A1A0P	Ba	303	-	47,47,47	0.34	0	50,52,52	0.52	0
5	A1A0P	Ca	306	-	47,47,47	0.39	0	50,52,52	0.63	1 (2%)
5	A1A0P	Bc	306	-	47,47,47	0.37	0	50,52,52	0.46	0
5	A1A0P	Bc	305	-	47,47,47	0.34	0	50,52,52	0.52	0
5	A1A0P	Ab	505	-	47,47,47	0.32	0	50,52,52	0.51	1 (2%)
5	A1A0P	Ca	303	-	47,47,47	0.31	0	50,52,52	0.34	0
5	A1A0P	Cc	301	-	47,47,47	0.68	1 (2%)	50,52,52	0.44	0
5	A1A0P	Bc	307	-	47,47,47	0.32	0	50,52,52	0.50	1 (2%)
5	A1A0P	Cc	306	-	47,47,47	0.33	0	50,52,52	0.37	0
5	A1A0P	Ba	307	-	47,47,47	0.33	0	50,52,52	0.45	0
5	A1A0P	Aa	503	-	47,47,47	0.32	0	50,52,52	0.51	1 (2%)
5	A1A0P	Cb	308	-	47,47,47	0.68	1 (2%)	50,52,52	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1A0P	Cb	307	-	-	26/51/51/51	-
5	A1A0P	Cc	304	-	-	24/51/51/51	-
5	A1A0P	Ba	302	-	-	17/51/51/51	-
5	A1A0P	Bb	308	-	-	22/51/51/51	-
5	A1A0P	Ba	306	-	-	22/51/51/51	-
5	A1A0P	Ba	305	-	-	21/51/51/51	-
5	A1A0P	Aa	504	-	-	25/51/51/51	-
5	A1A0P	Cc	307	-	-	25/51/51/51	-
5	A1A0P	Cb	303	-	-	23/51/51/51	-
5	A1A0P	Ca	302	-	-	25/51/51/51	-
5	A1A0P	Cb	306	-	-	25/51/51/51	-
5	A1A0P	Ca	307	-	-	26/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1A0P	Ba	309	-	-	28/51/51/51	-
5	A1A0P	Bb	301	-	-	28/51/51/51	-
5	A1A0P	Cb	304	-	-	27/51/51/51	-
5	A1A0P	Bc	304	-	-	17/51/51/51	-
5	A1A0P	Bc	308	-	-	22/51/51/51	-
5	A1A0P	Ba	304	-	-	25/51/51/51	-
5	A1A0P	Aa	505	-	-	23/51/51/51	-
5	A1A0P	Bb	304	-	-	17/51/51/51	-
5	A1A0P	Ba	308	-	-	26/51/51/51	-
5	A1A0P	Ca	301	-	-	28/51/51/51	-
5	A1A0P	Cc	308	-	-	26/51/51/51	-
5	A1A0P	Bb	305	-	-	26/51/51/51	-
5	A1A0P	Bb	307	-	-	21/51/51/51	-
5	A1A0P	Ab	502	-	-	25/51/51/51	-
5	A1A0P	Cc	303	-	-	25/51/51/51	-
5	A1A0P	Ca	305	-	-	16/51/51/51	-
5	A1A0P	Cb	302	-	-	25/51/51/51	-
5	A1A0P	Ac	504	-	-	21/51/51/51	-
5	A1A0P	Bb	309	-	-	24/51/51/51	-
5	A1A0P	Bb	302	-	-	26/51/51/51	-
5	A1A0P	Bc	309	-	-	24/51/51/51	-
5	A1A0P	Bc	301	-	-	28/51/51/51	-
5	A1A0P	Bc	302	-	-	26/51/51/51	-
5	A1A0P	Ab	501	-	-	23/51/51/51	-
5	A1A0P	Ac	505	-	-	23/51/51/51	-
5	A1A0P	Ca	304	-	-	27/51/51/51	-
5	A1A0P	Ac	501	-	-	25/51/51/51	-
5	A1A0P	Bb	306	-	-	25/51/51/51	-
5	A1A0P	Cb	305	-	-	16/51/51/51	-
5	A1A0P	Ca	308	-	-	22/51/51/51	-
5	A1A0P	Cc	302	-	-	28/51/51/51	-
5	A1A0P	Cc	305	-	-	27/51/51/51	-
5	A1A0P	Cb	301	-	-	28/51/51/51	-
5	A1A0P	Ba	303	-	-	26/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1A0P	Ca	306	-	-	25/51/51/51	-
5	A1A0P	Bc	306	-	-	25/51/51/51	-
5	A1A0P	Bc	305	-	-	26/51/51/51	-
5	A1A0P	Ab	505	-	-	21/51/51/51	-
5	A1A0P	Ca	303	-	-	24/51/51/51	-
5	A1A0P	Cc	301	-	-	22/51/51/51	-
5	A1A0P	Bc	307	-	-	21/51/51/51	-
5	A1A0P	Cc	306	-	-	16/51/51/51	-
5	A1A0P	Ba	307	-	-	24/51/51/51	-
5	A1A0P	Aa	503	-	-	21/51/51/51	-
5	A1A0P	Cb	308	-	-	22/51/51/51	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Bb	301	A1A0P	P14-O10	3.42	1.72	1.59
5	Ba	309	A1A0P	P14-O10	3.41	1.72	1.59
5	Bc	301	A1A0P	P14-O10	3.37	1.72	1.59
5	Bc	301	A1A0P	O10-C11	2.74	1.55	1.44
5	Bb	301	A1A0P	O10-C11	2.73	1.55	1.44

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Bc	302	A1A0P	O3-C2-C1	-5.13	93.62	108.40
5	Ba	308	A1A0P	O3-C2-C1	-5.12	93.63	108.40
5	Bb	302	A1A0P	O3-C2-C1	-5.11	93.66	108.40
5	Bb	302	A1A0P	C8-C1-C2	-4.23	101.93	111.78
5	Ba	308	A1A0P	C8-C1-C2	-4.22	101.94	111.78

There are no chirality outliers.

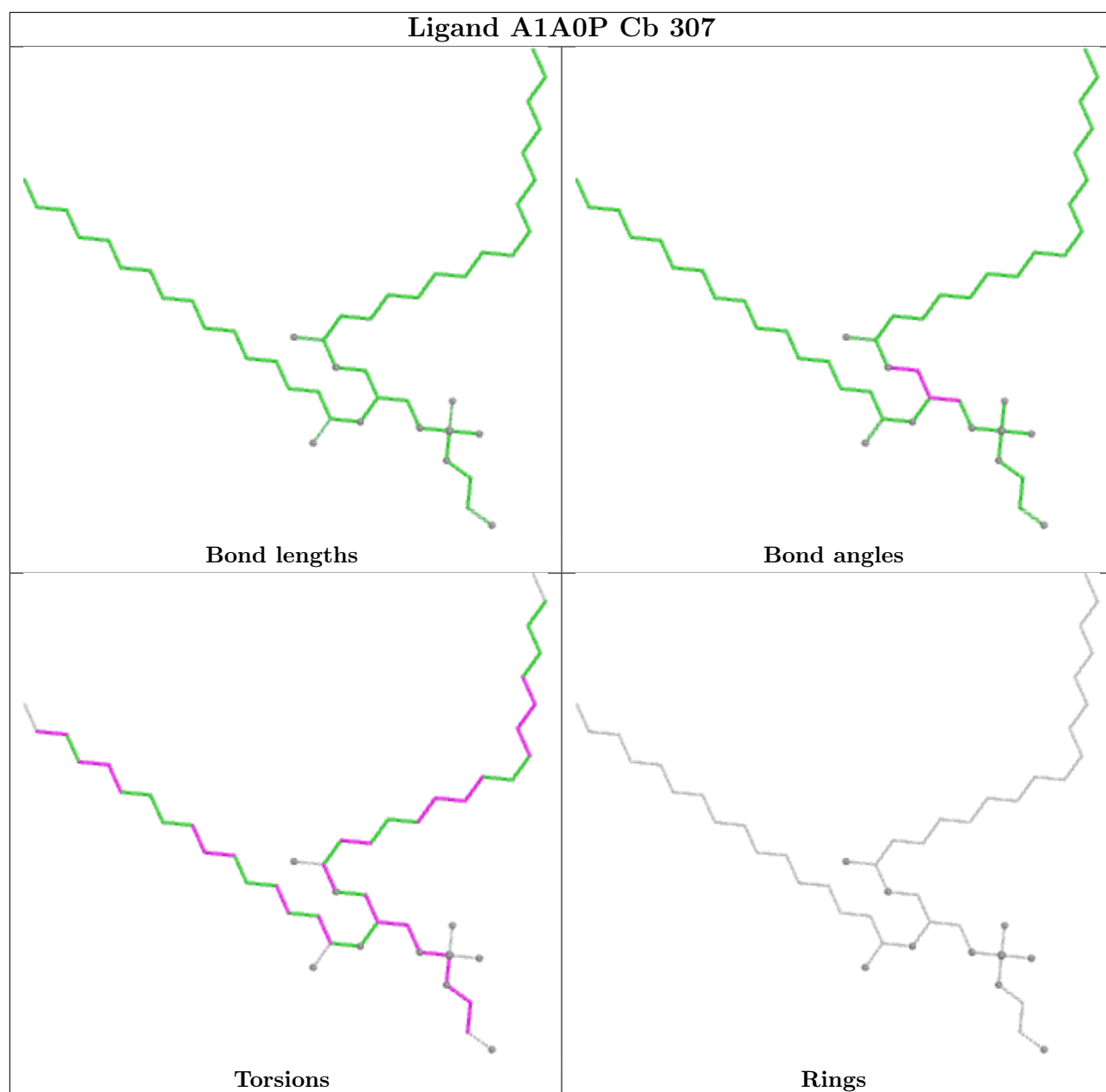
5 of 1352 torsion outliers are listed below:

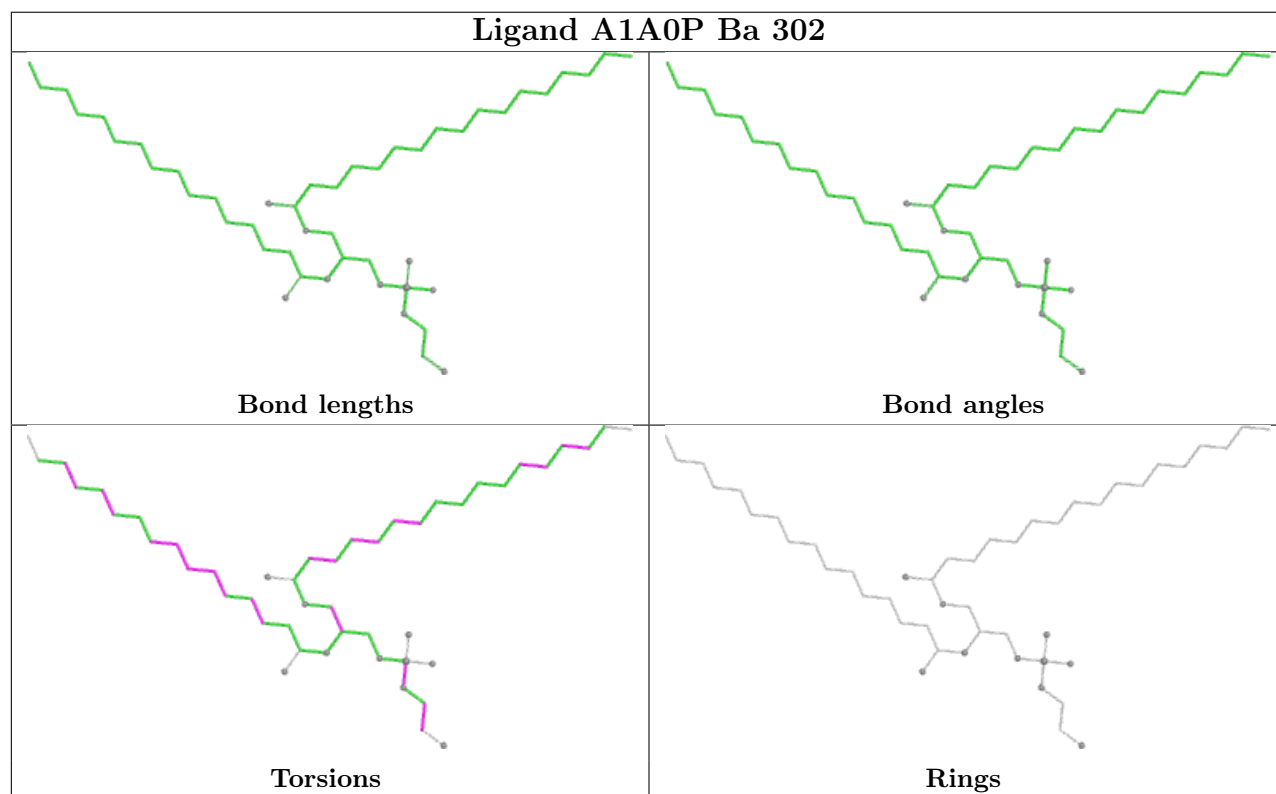
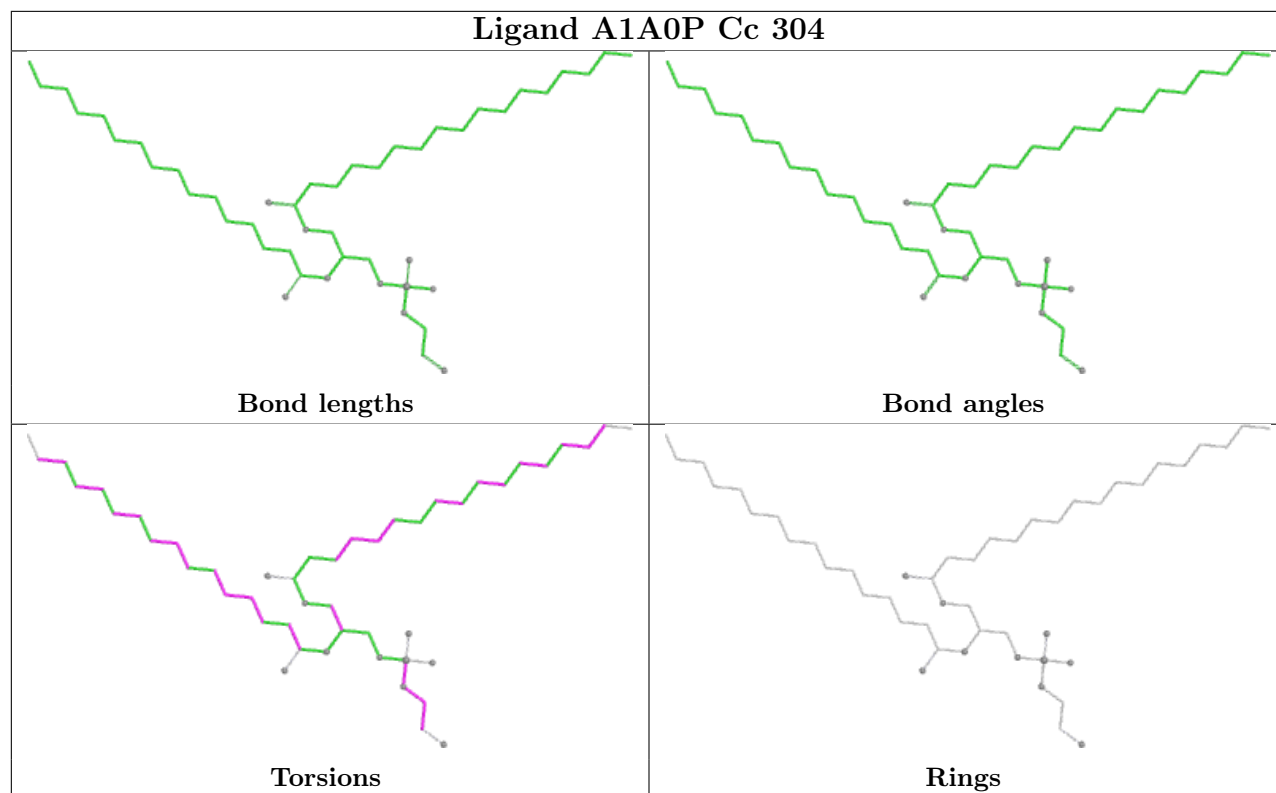
Mol	Chain	Res	Type	Atoms
5	Ba	302	A1A0P	C11-O10-P14-O9
5	Ba	302	A1A0P	C11-O10-P14-O15
5	Ba	302	A1A0P	O10-C11-C12-N13
5	Ba	303	A1A0P	O5-C4-O3-C2
5	Ba	303	A1A0P	C7-C4-O3-C2

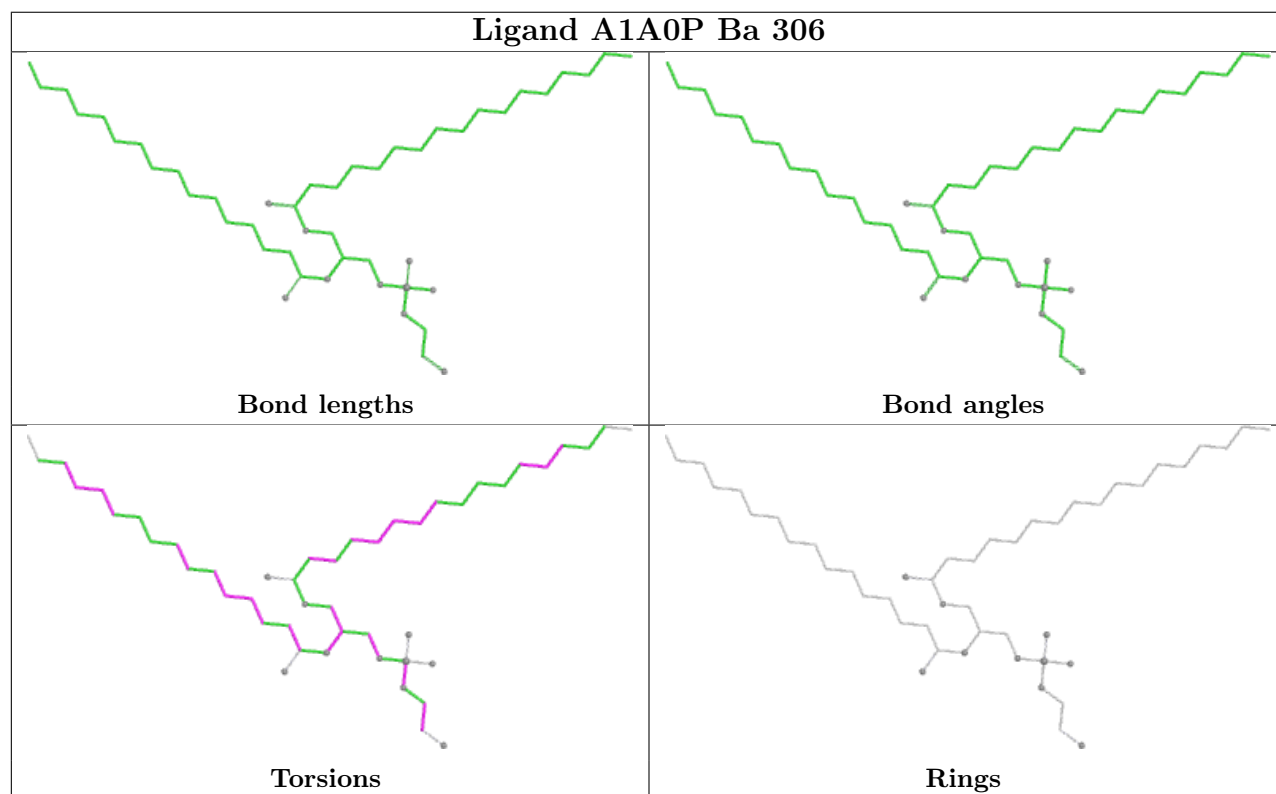
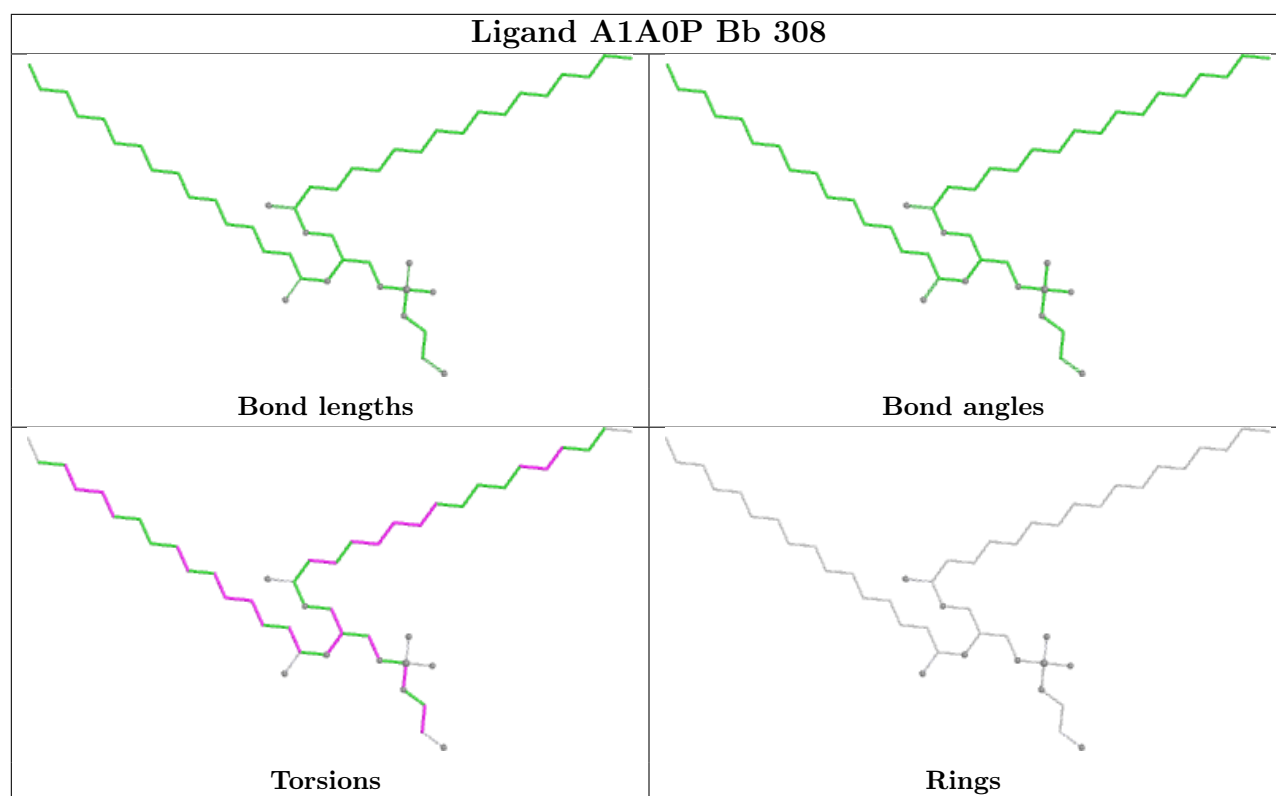
There are no ring outliers.

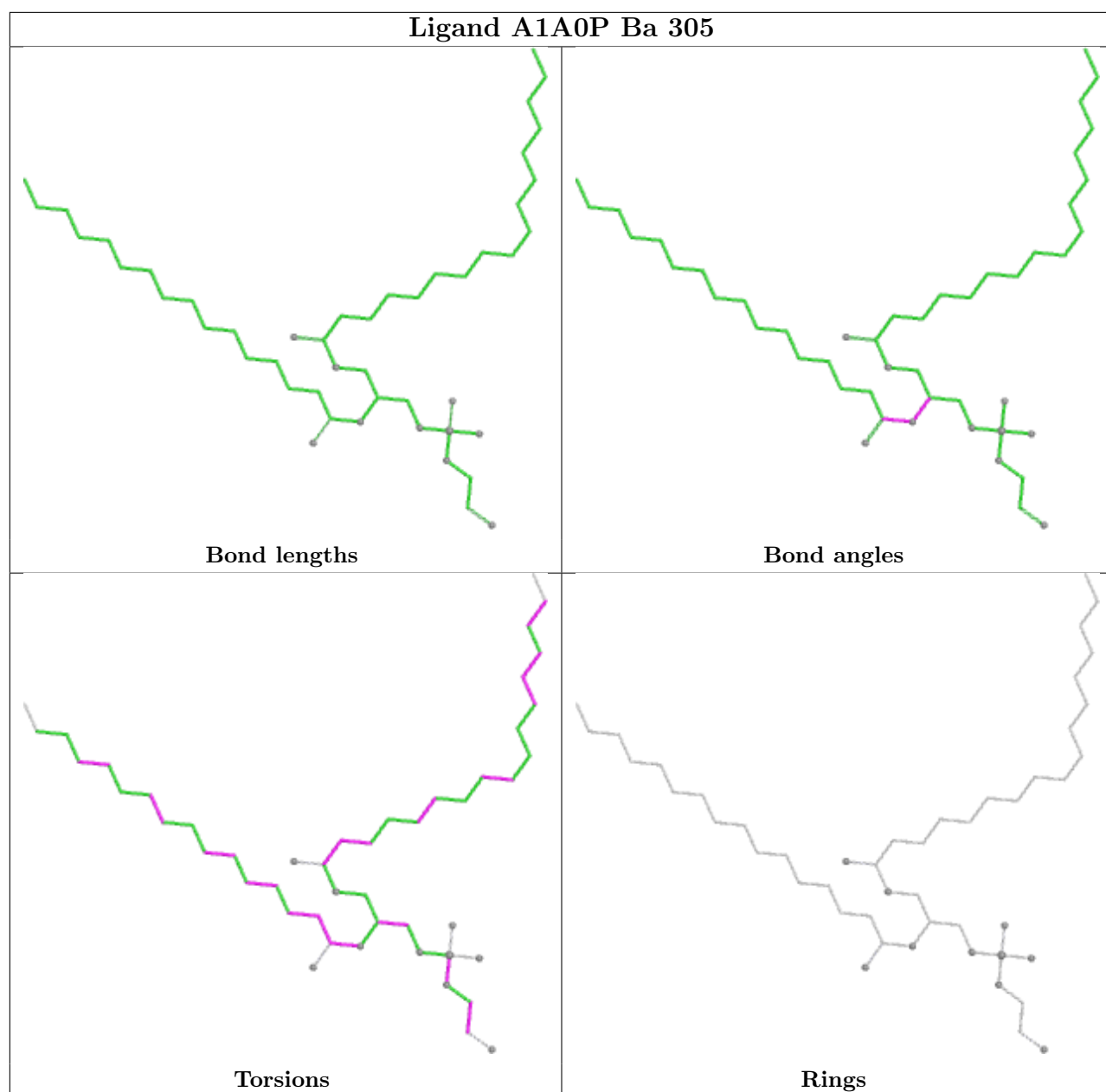
No monomer is involved in short contacts.

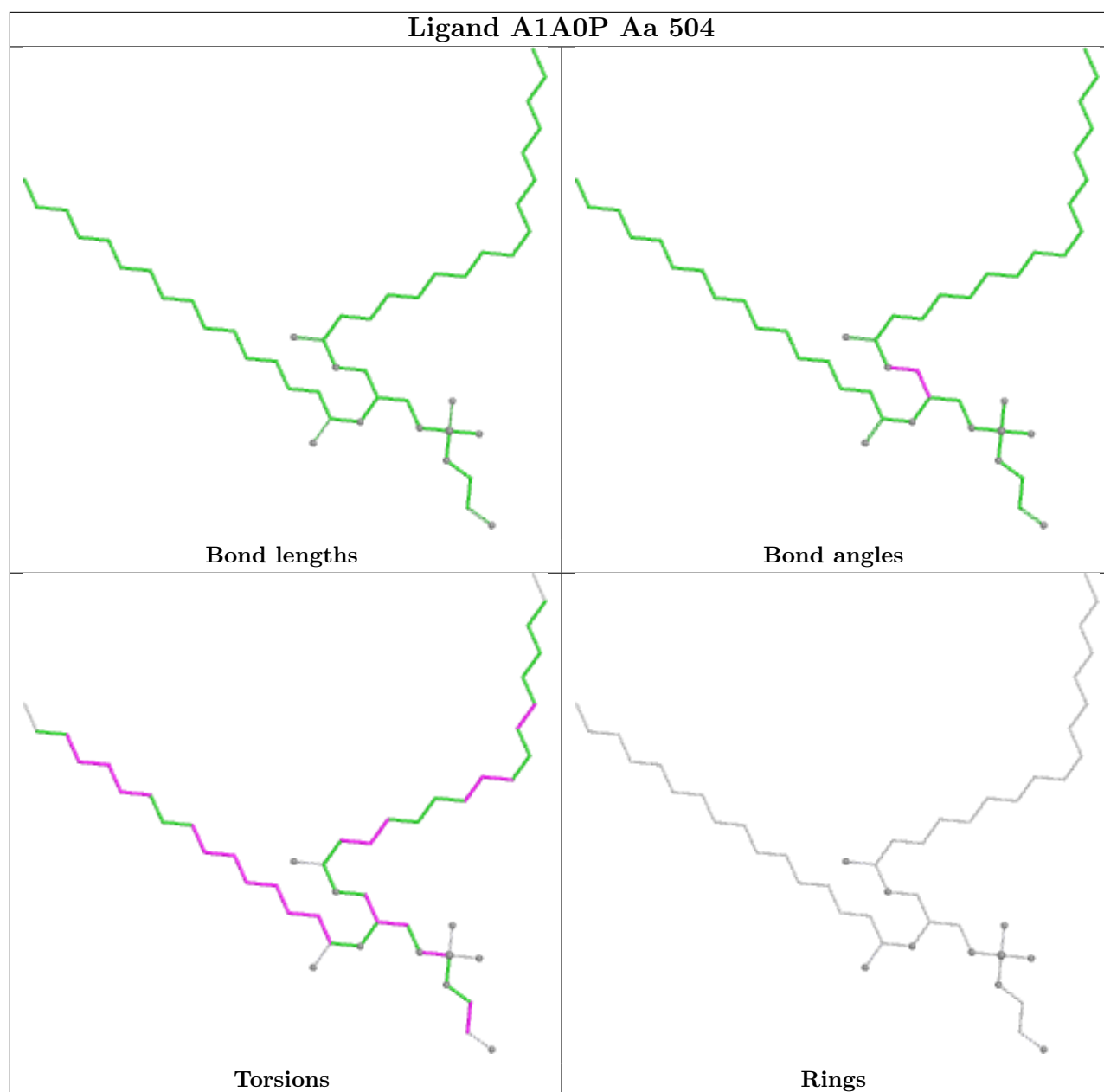
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

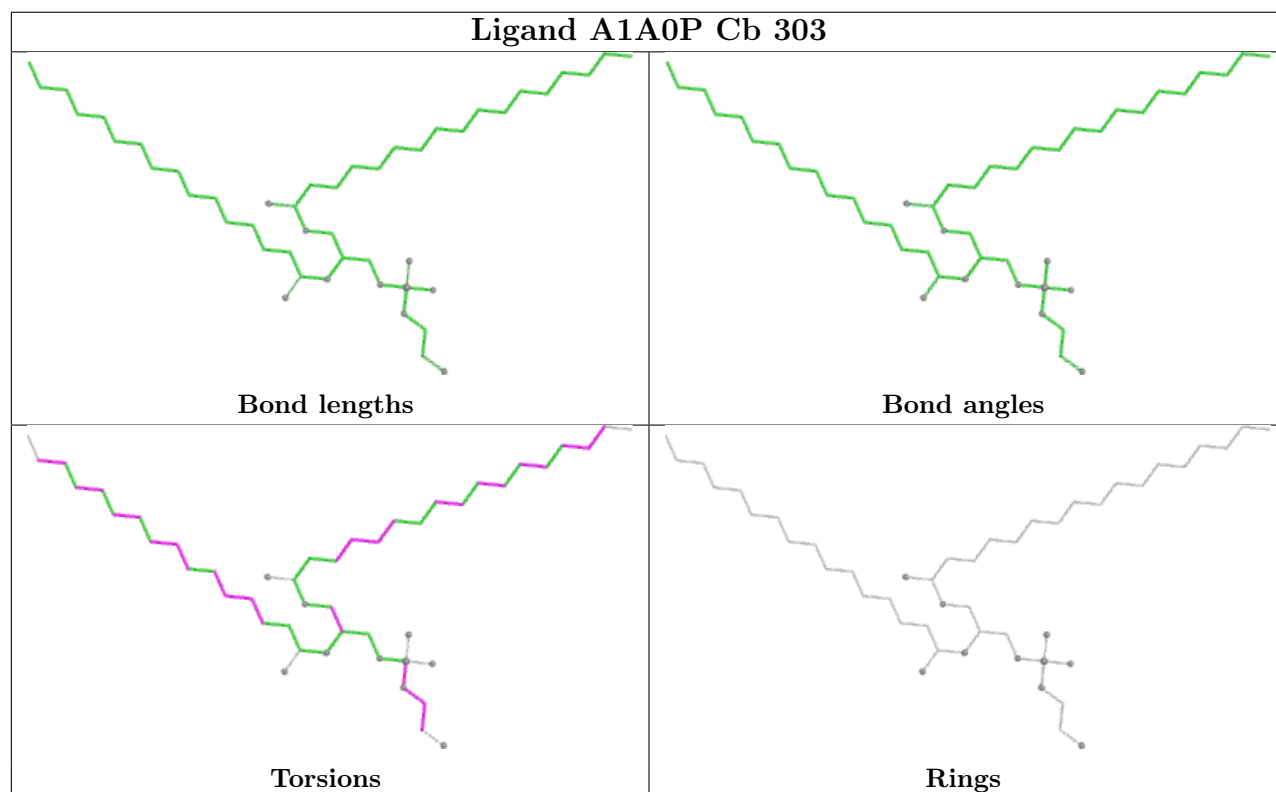
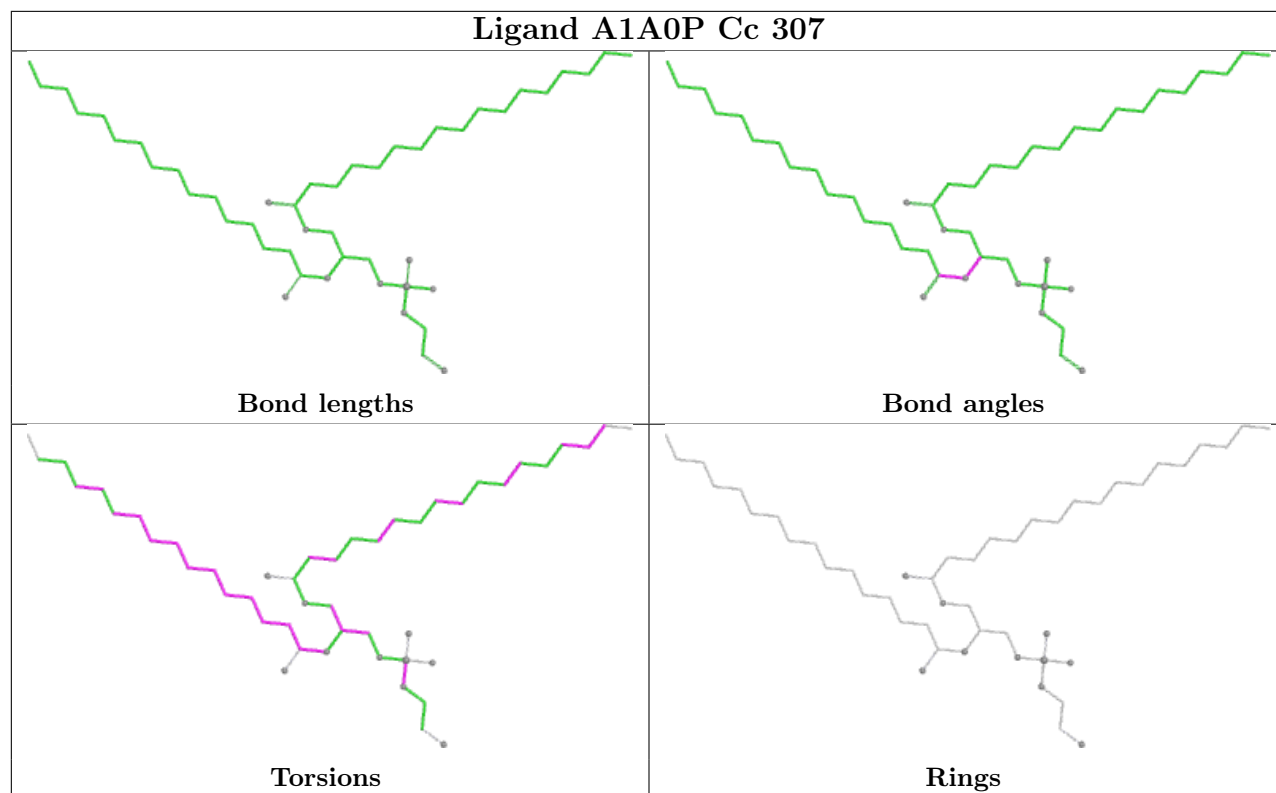


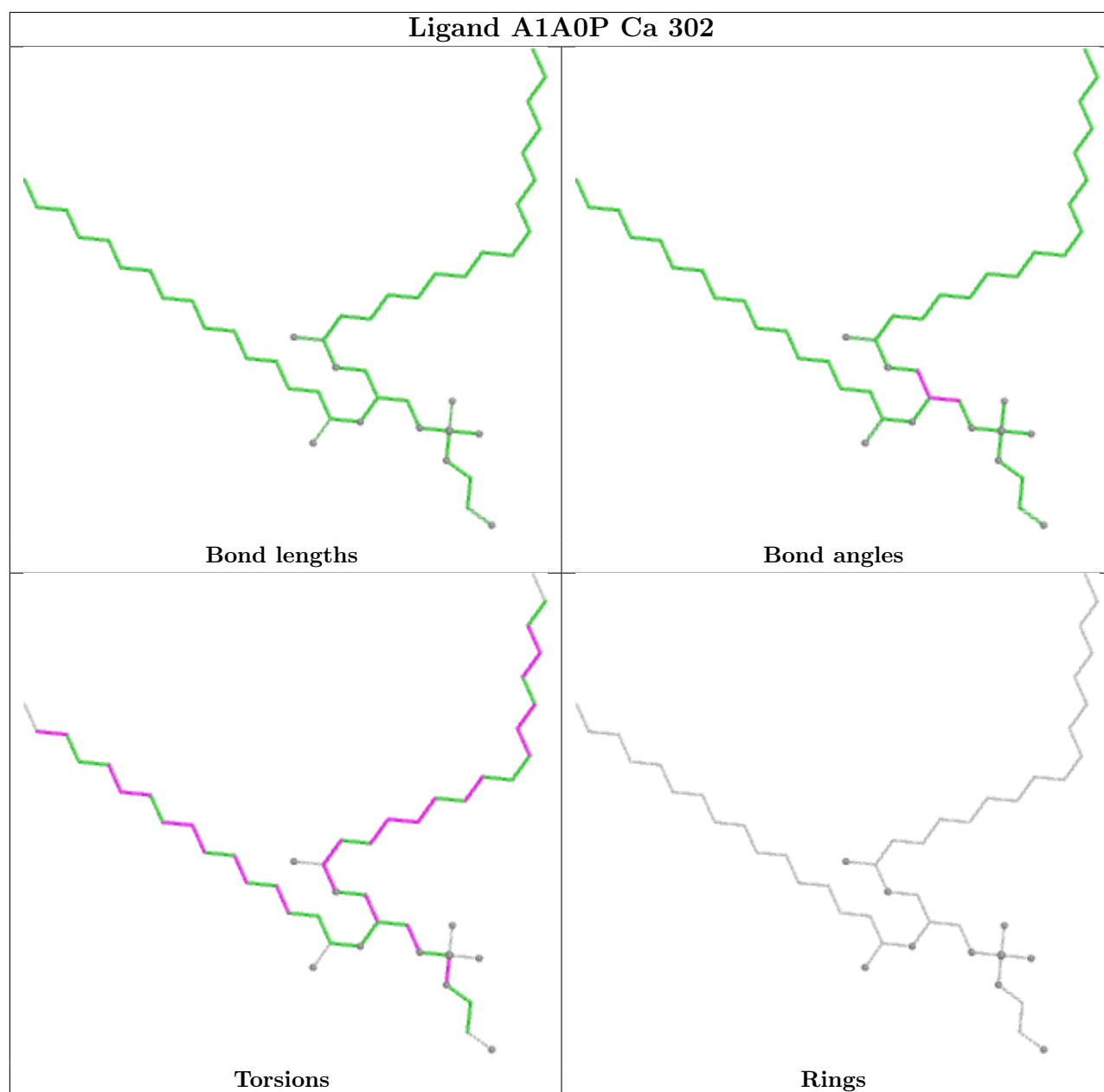


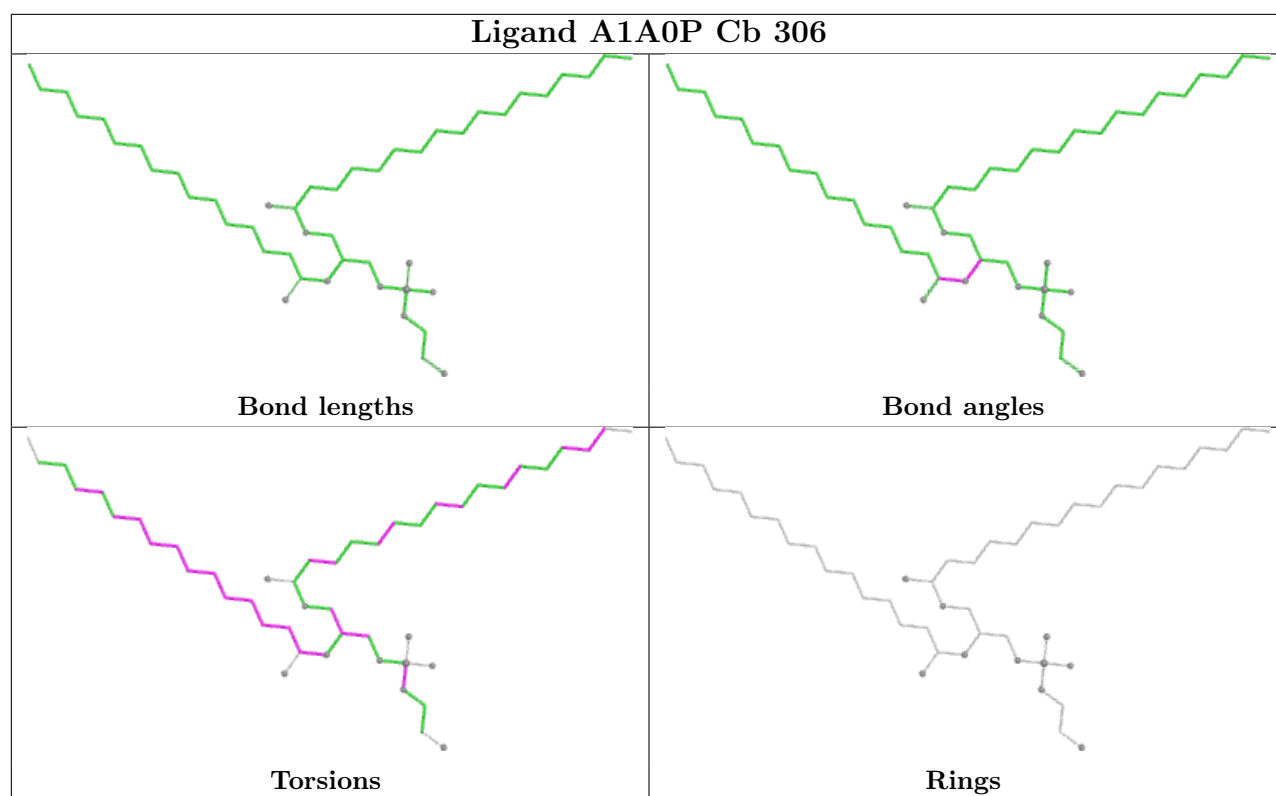


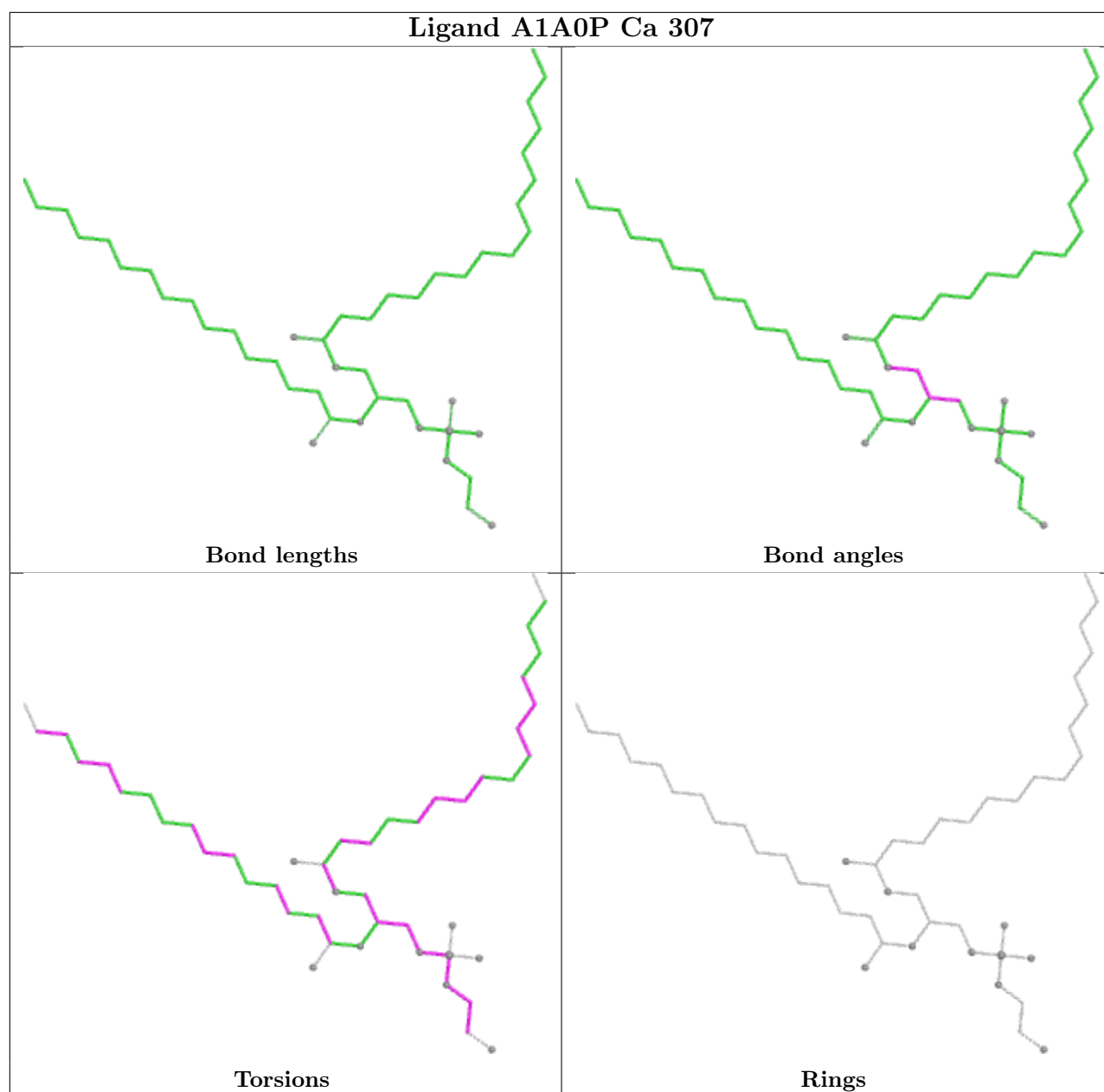


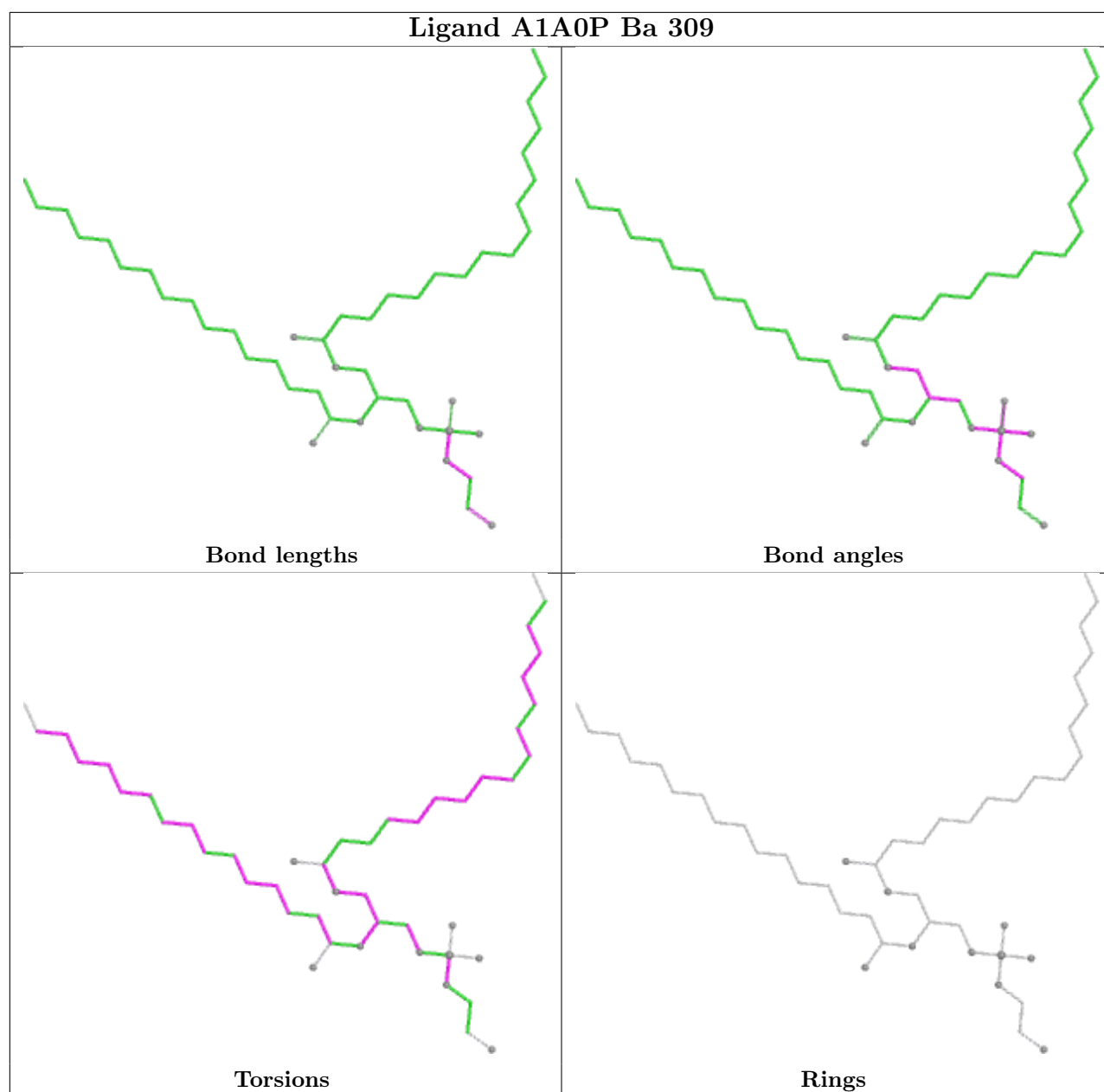


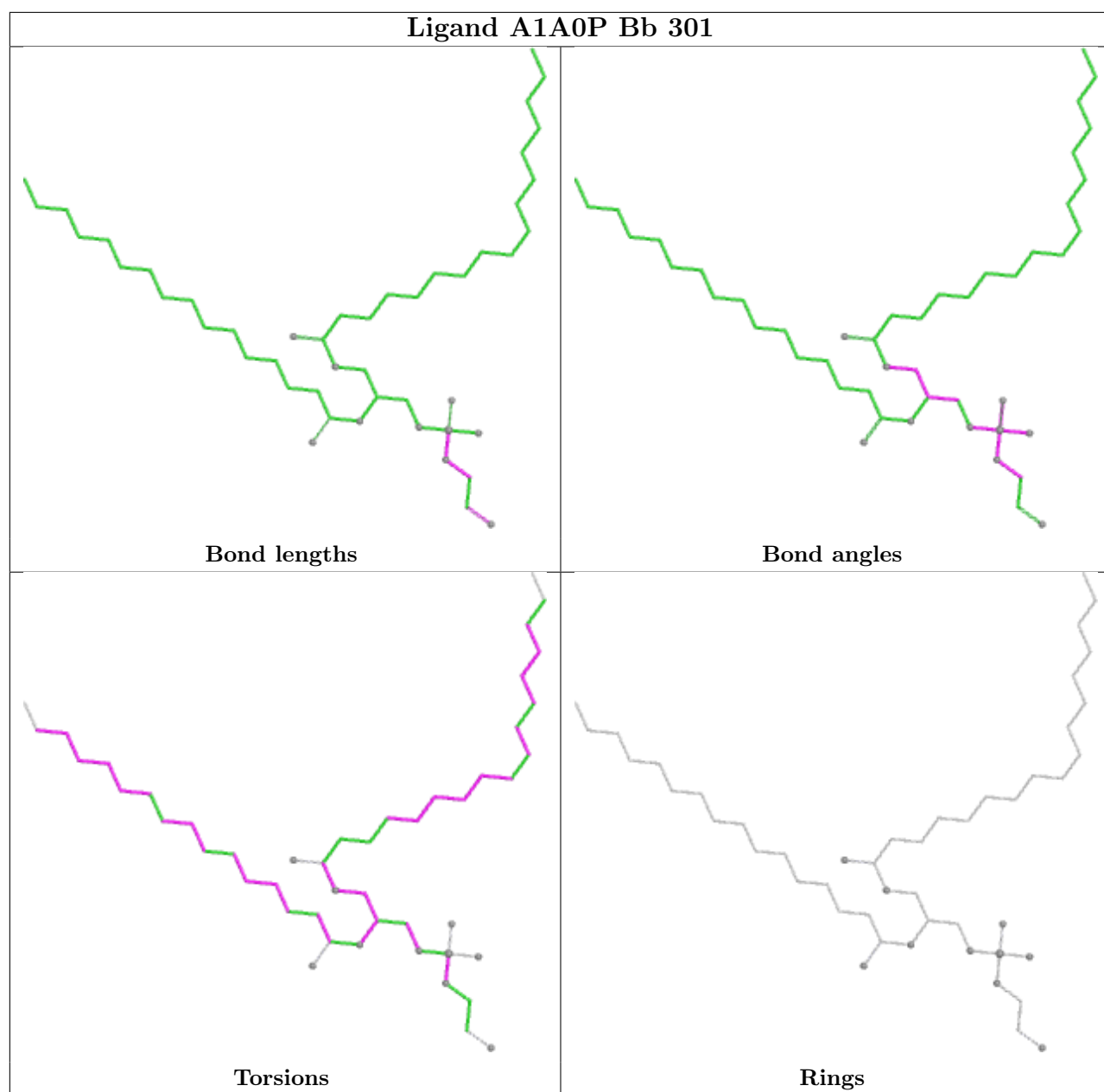


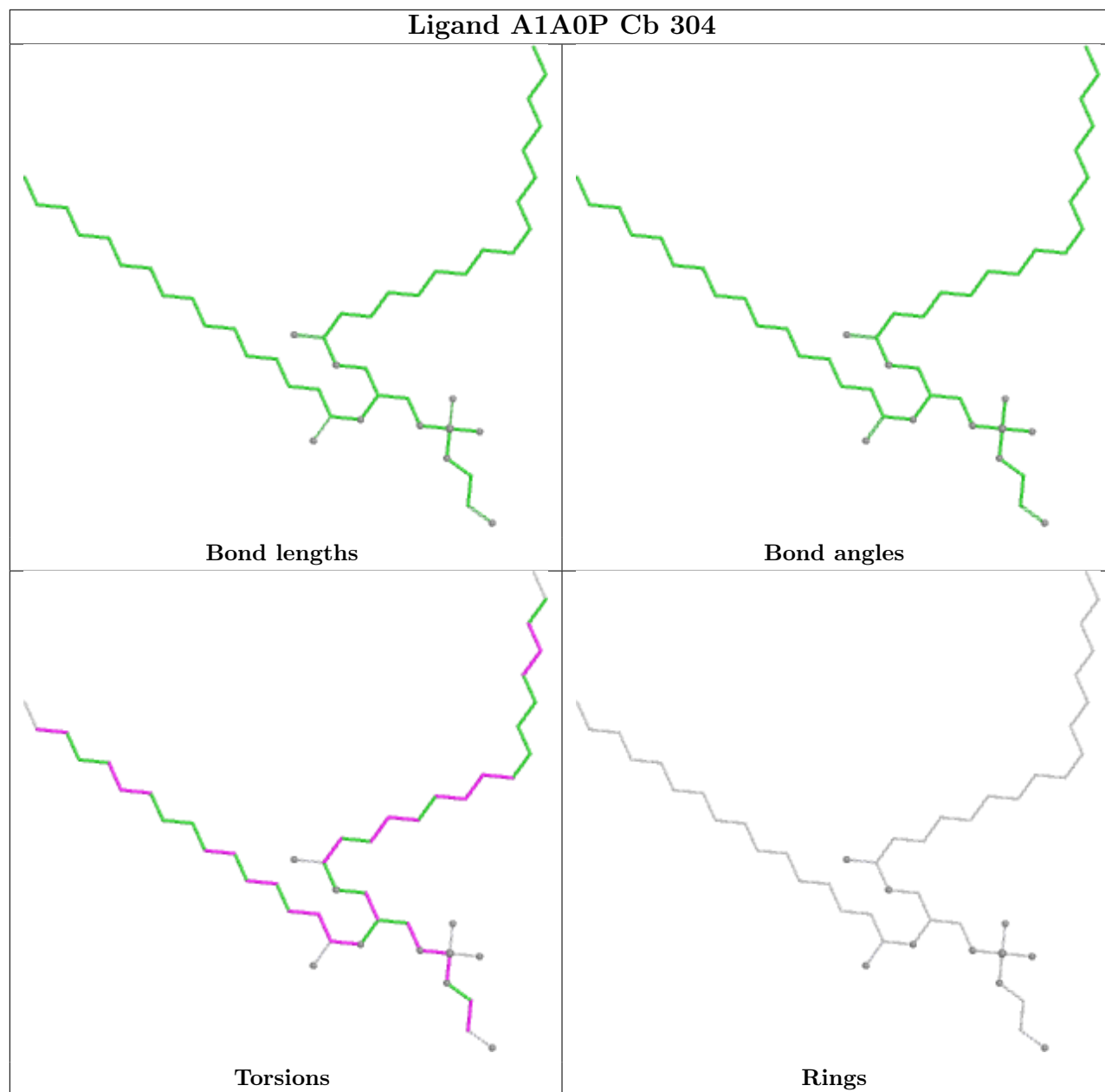


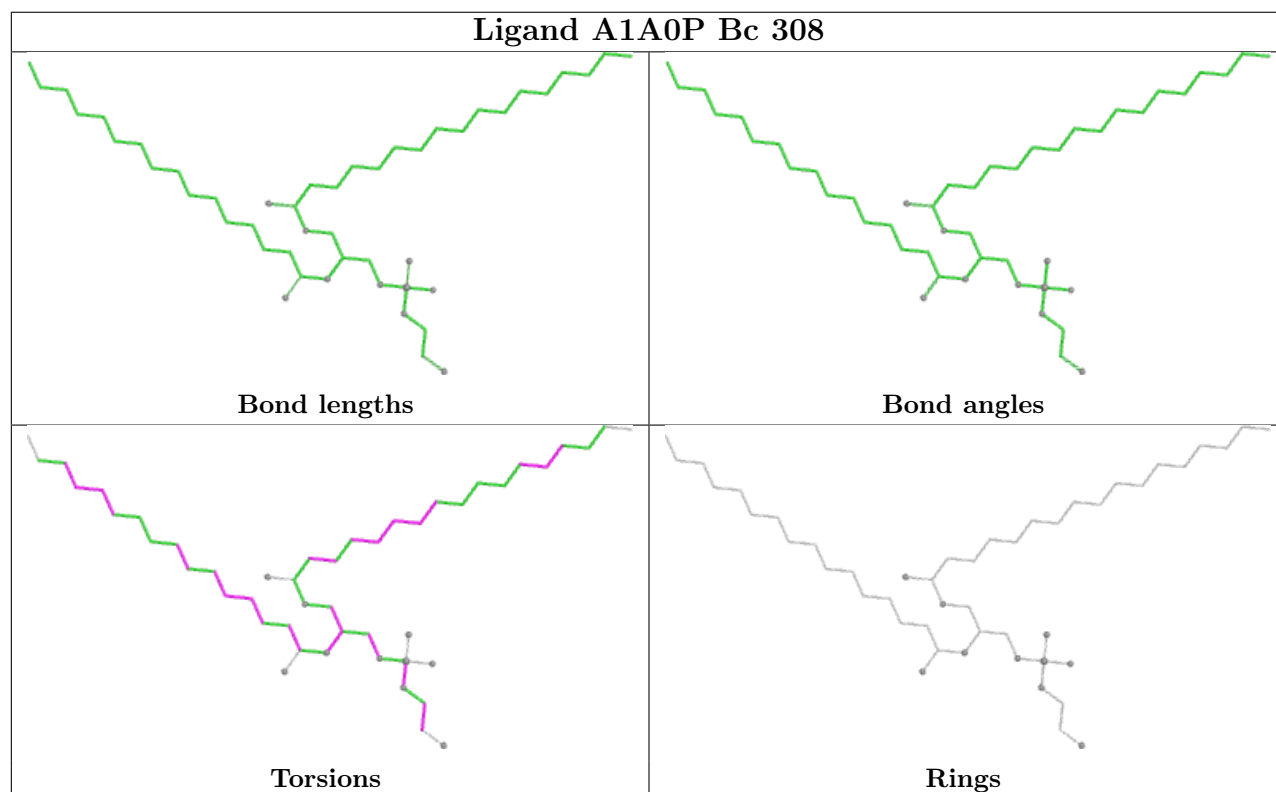
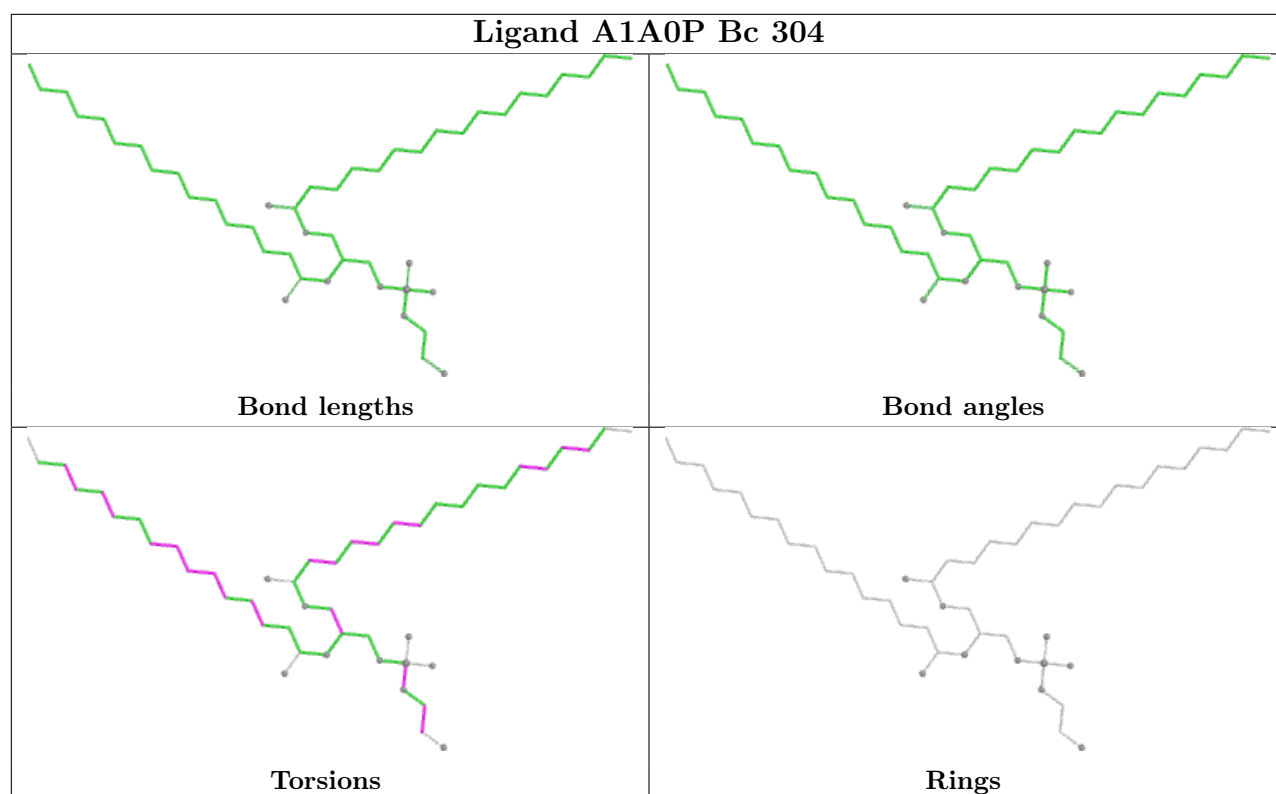


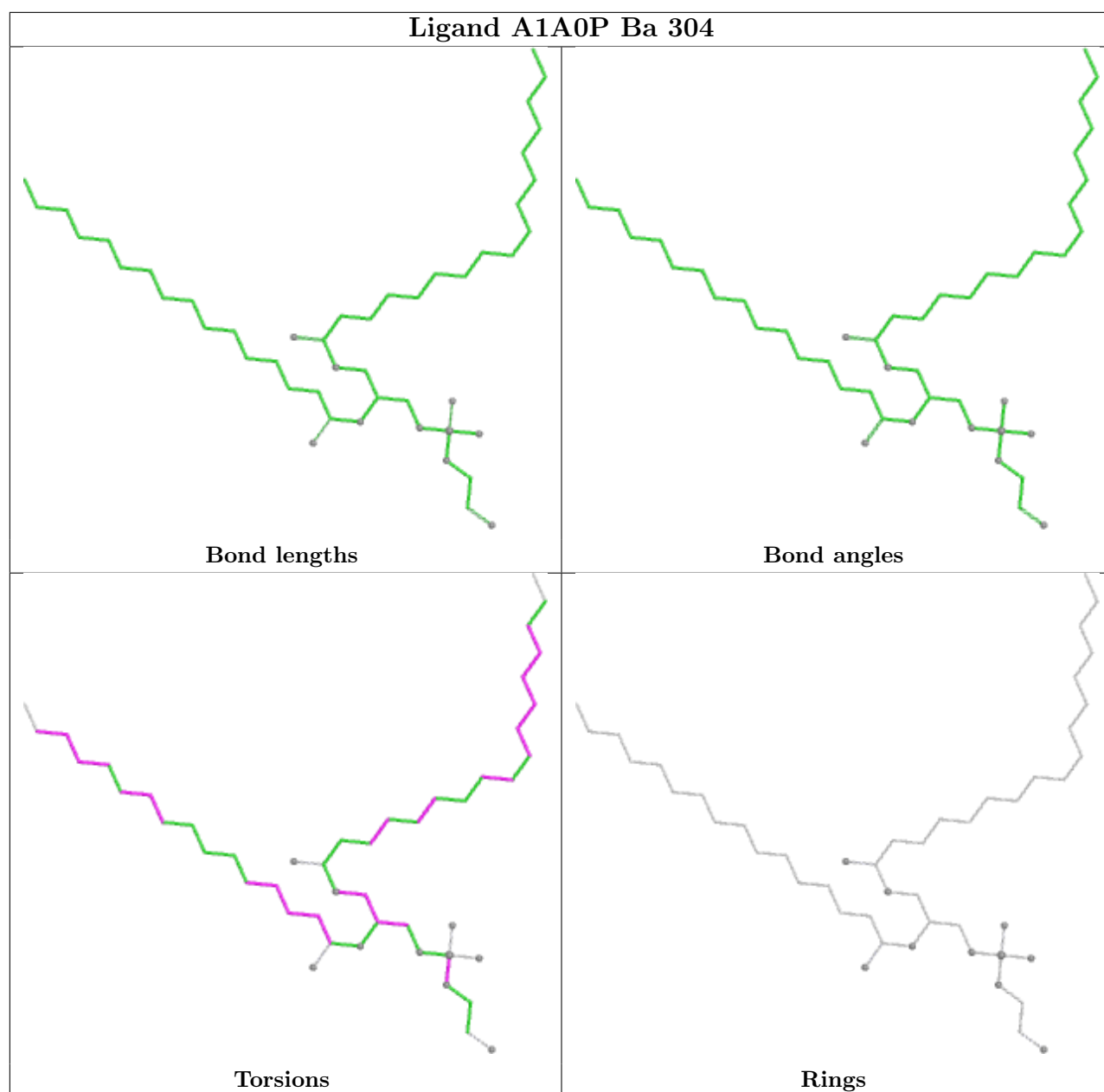


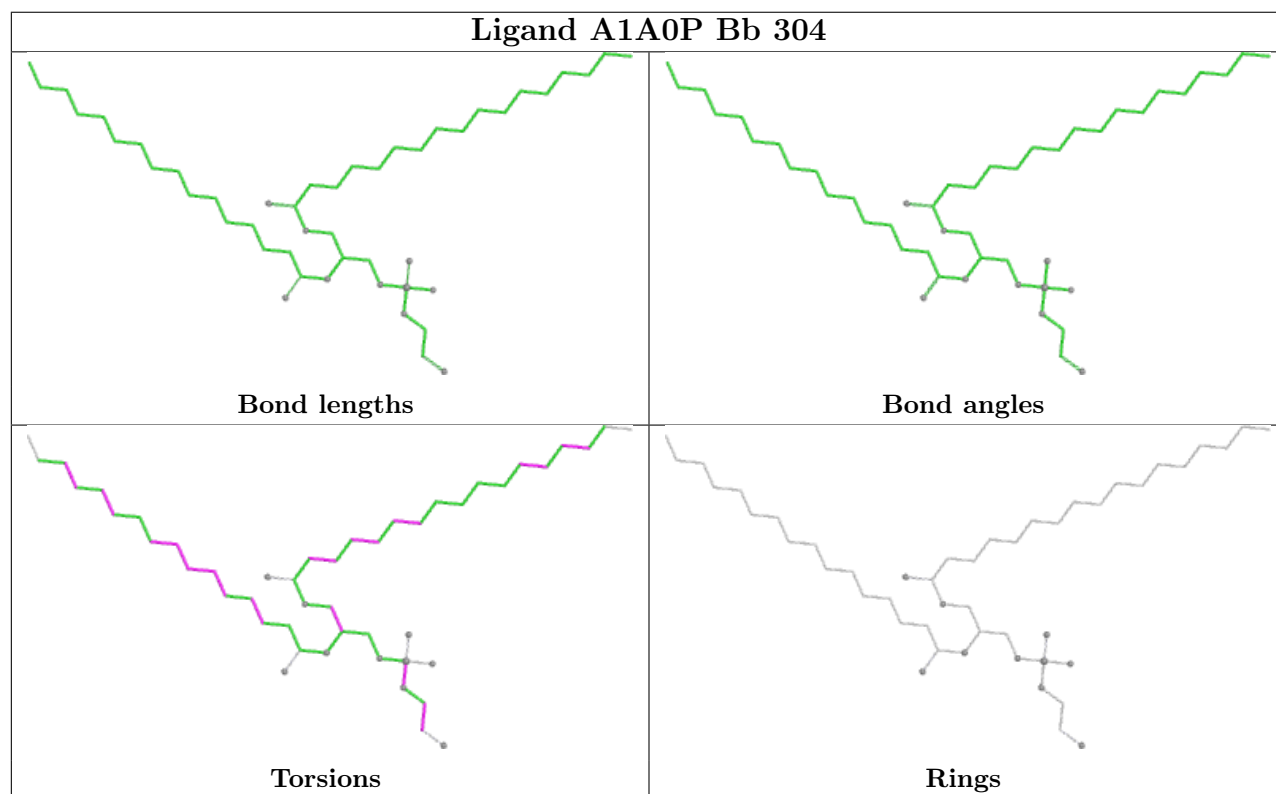
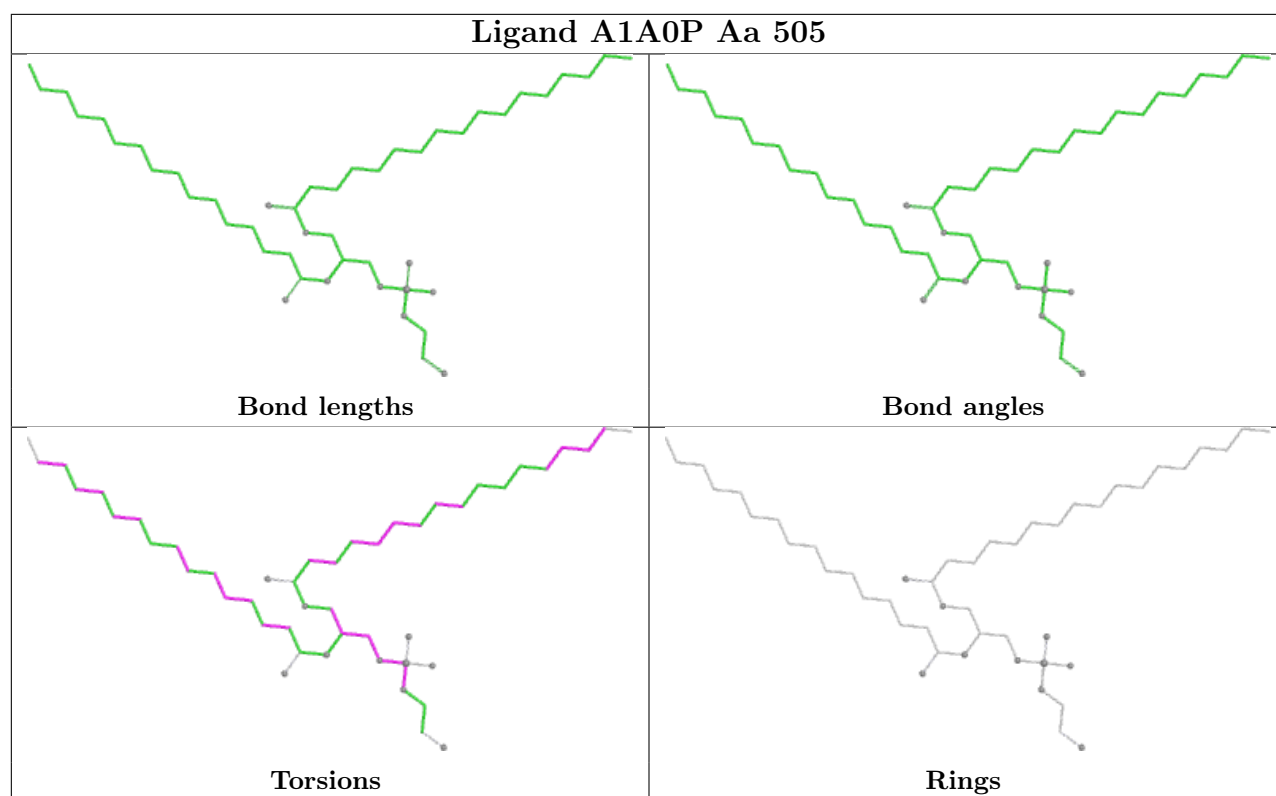


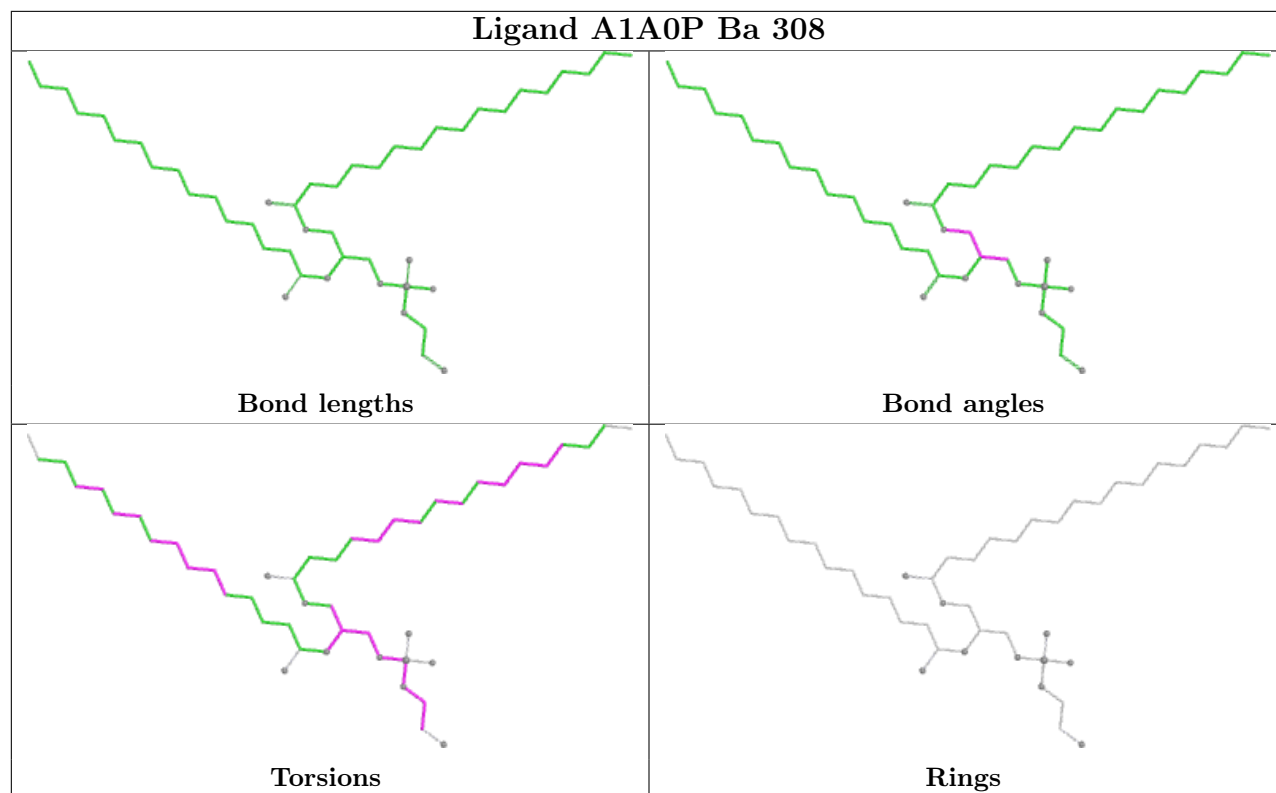


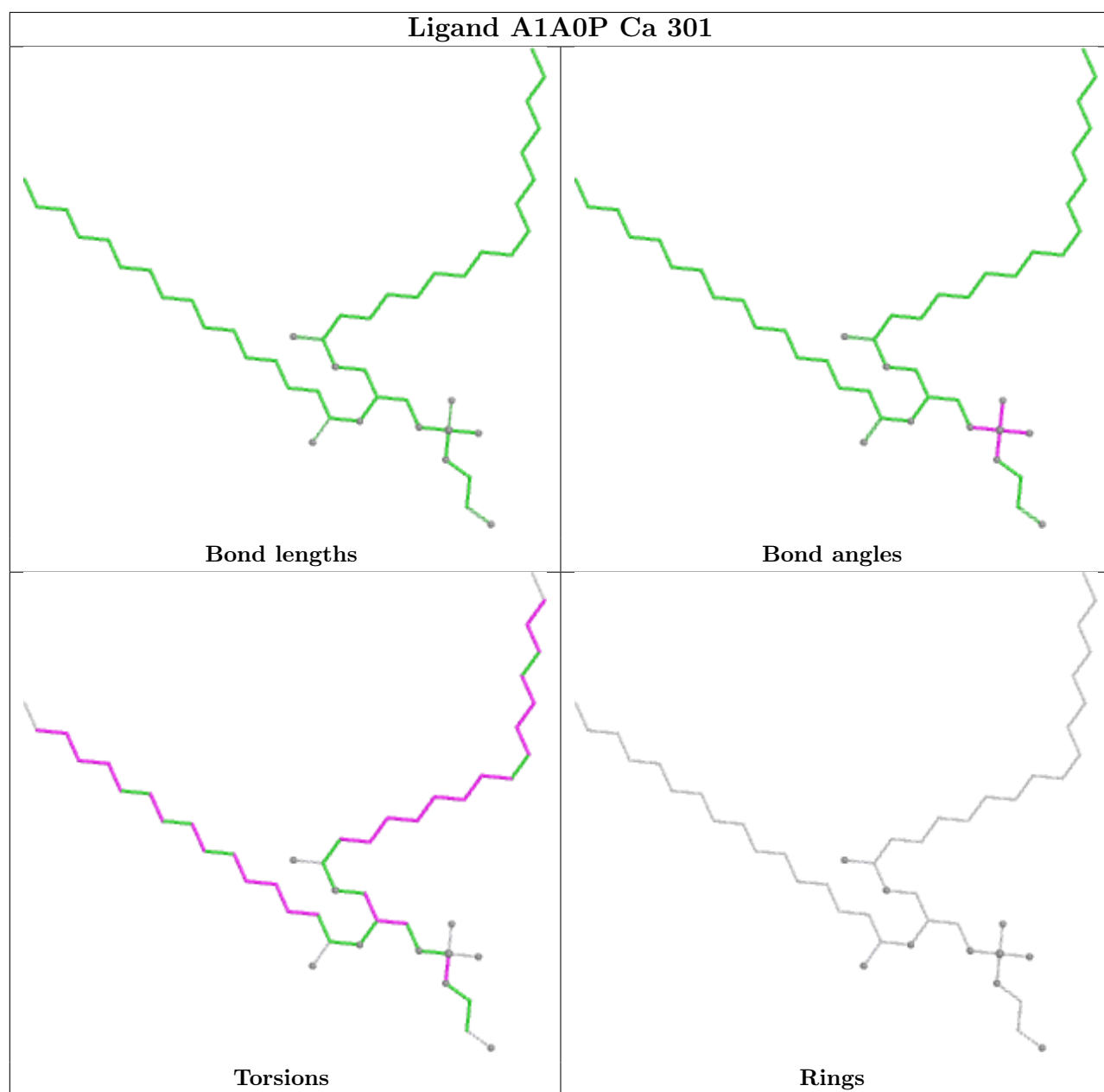


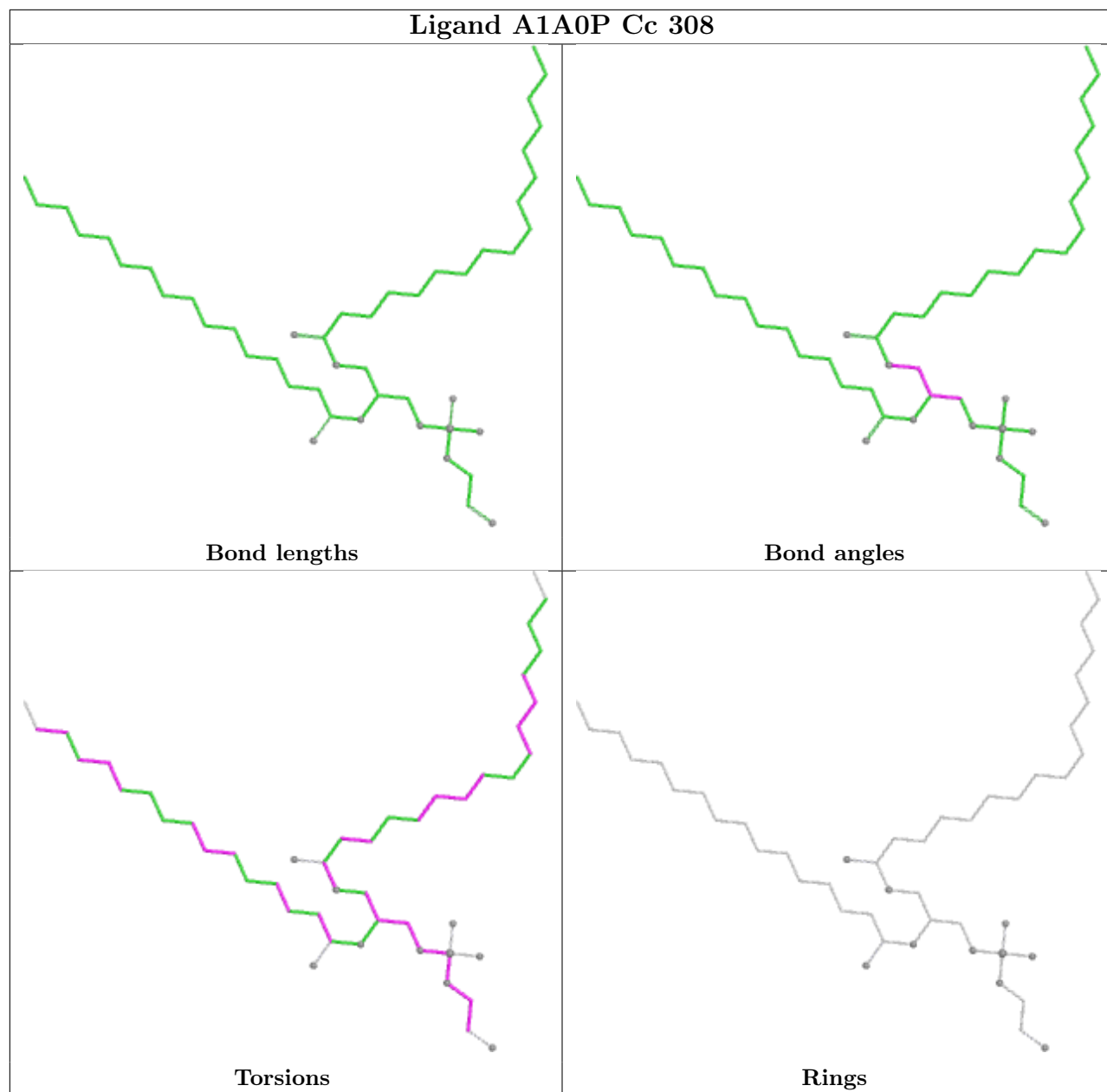


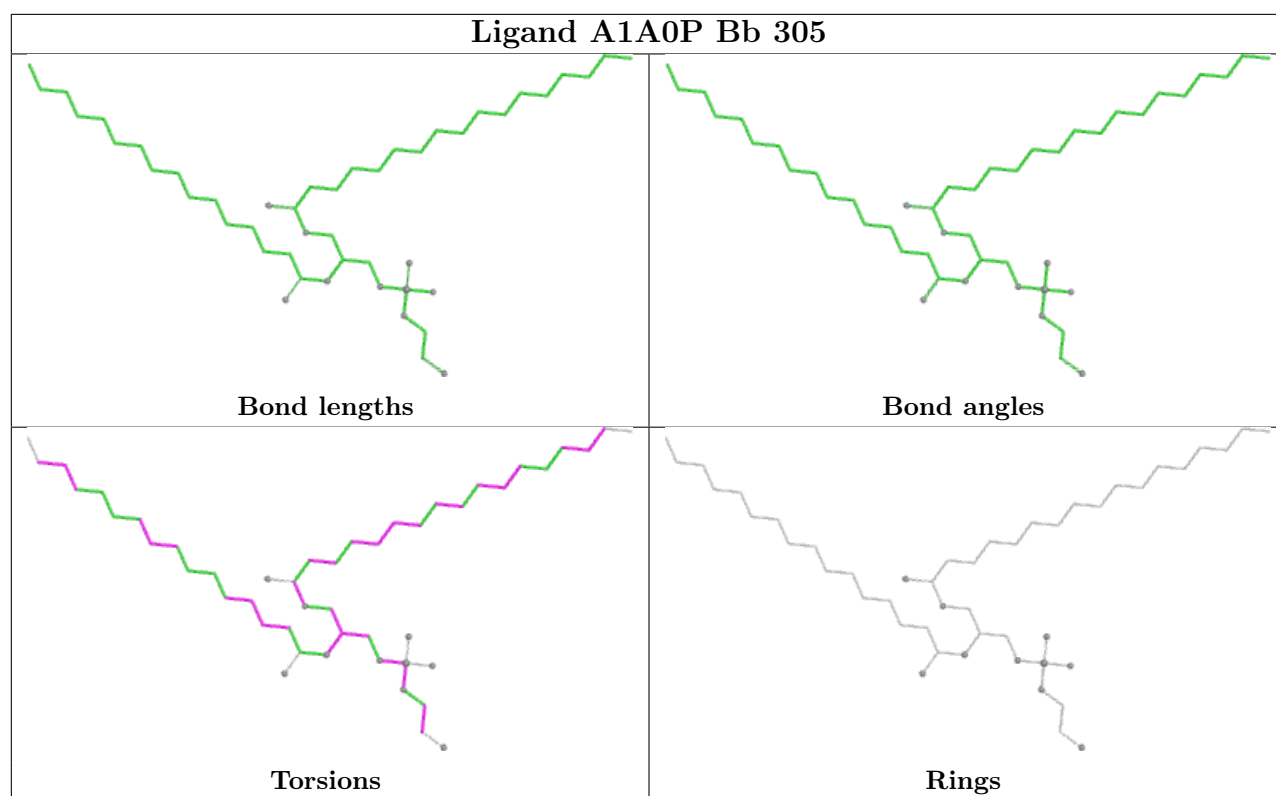


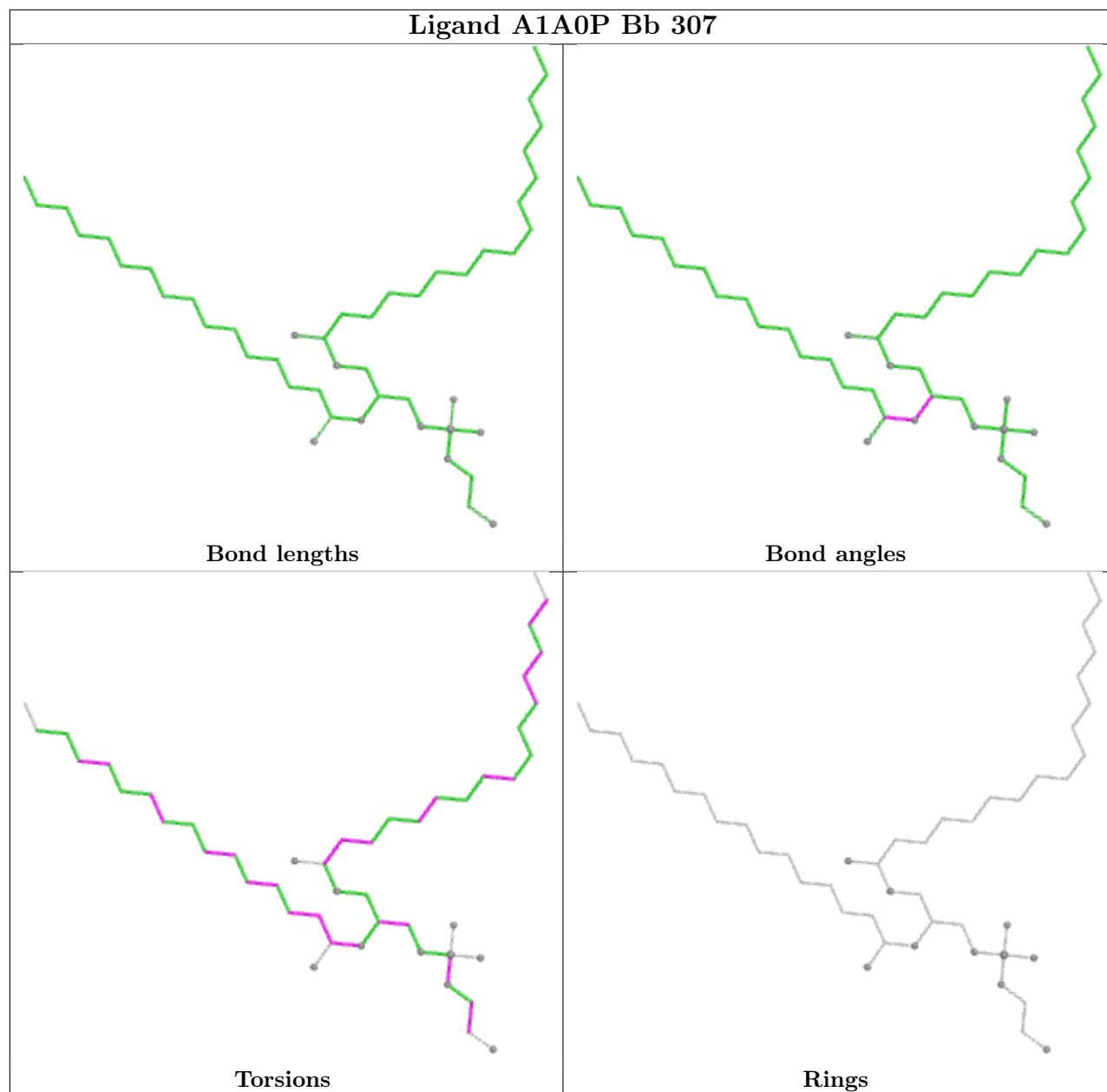




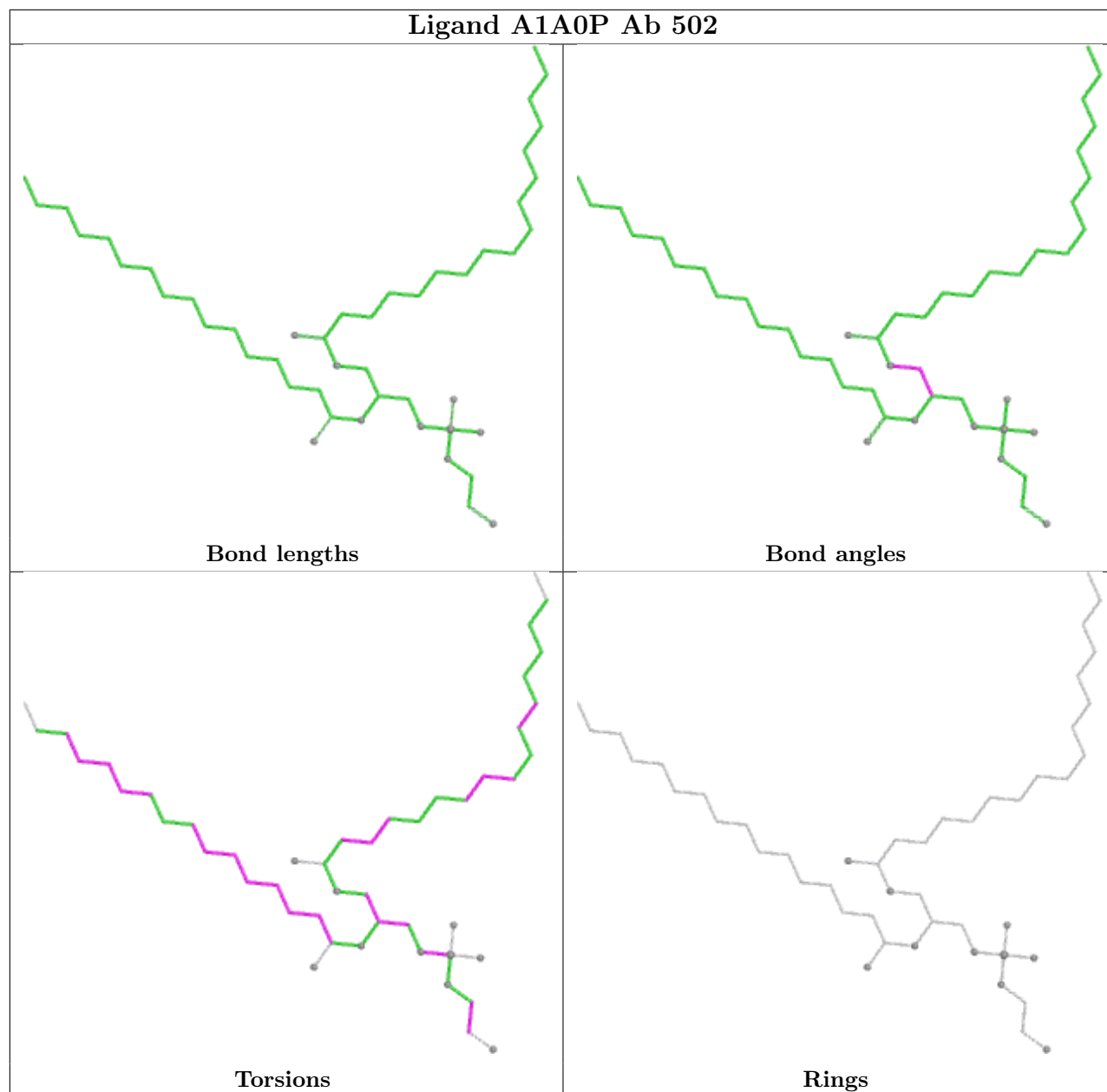


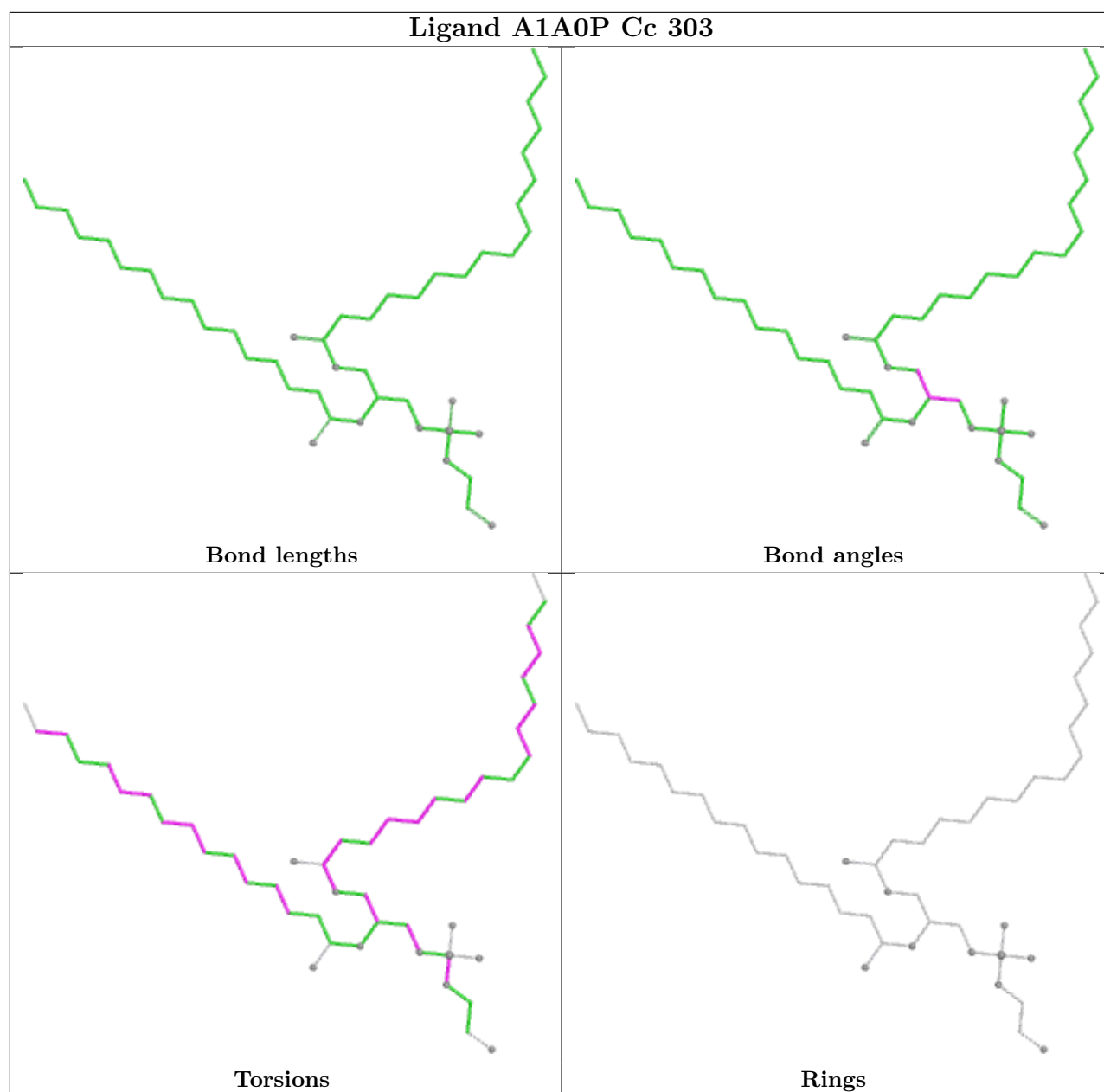


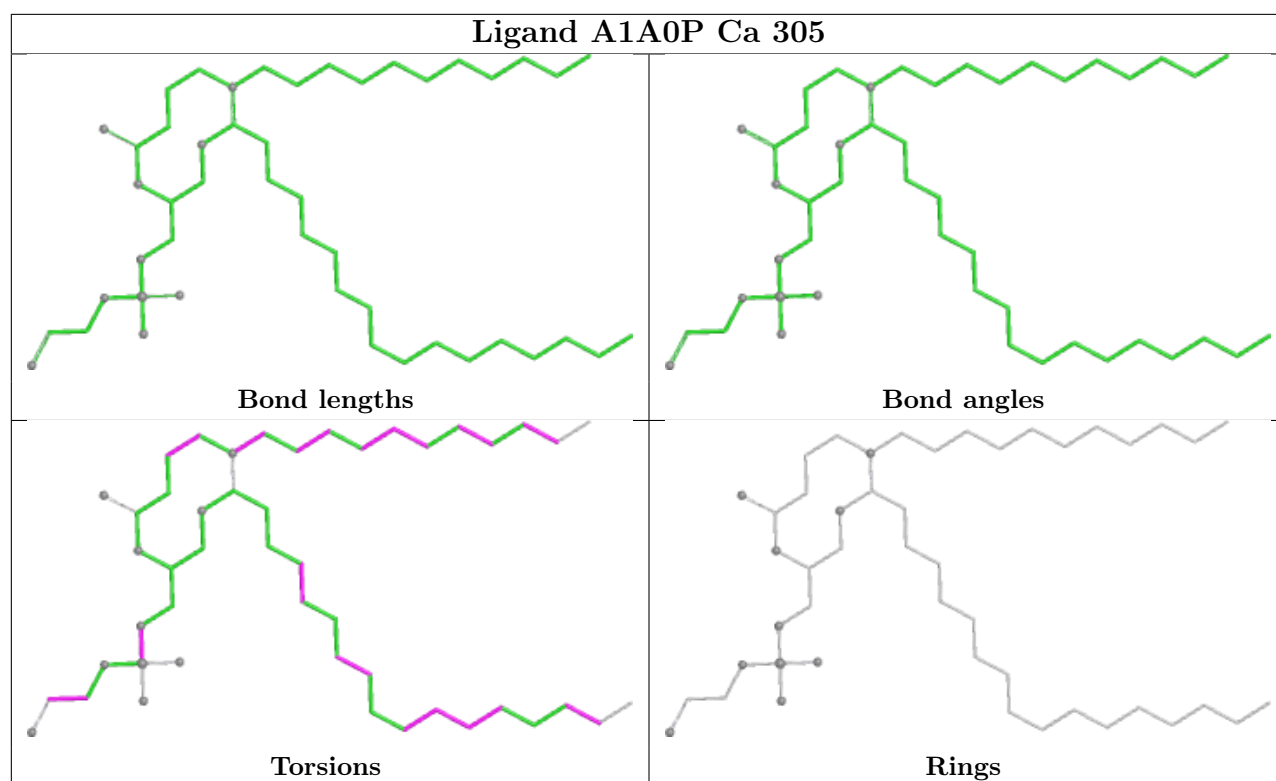


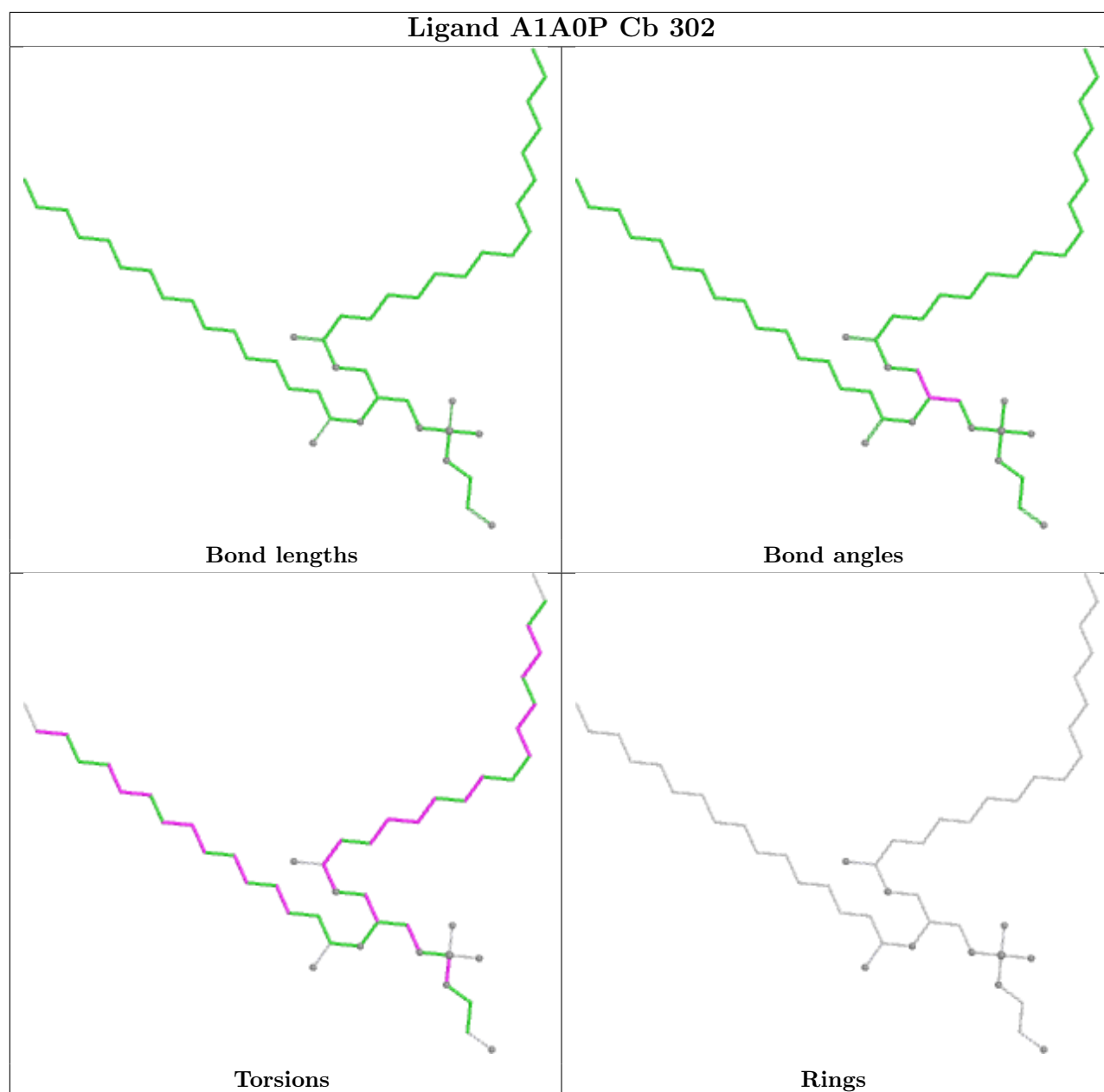


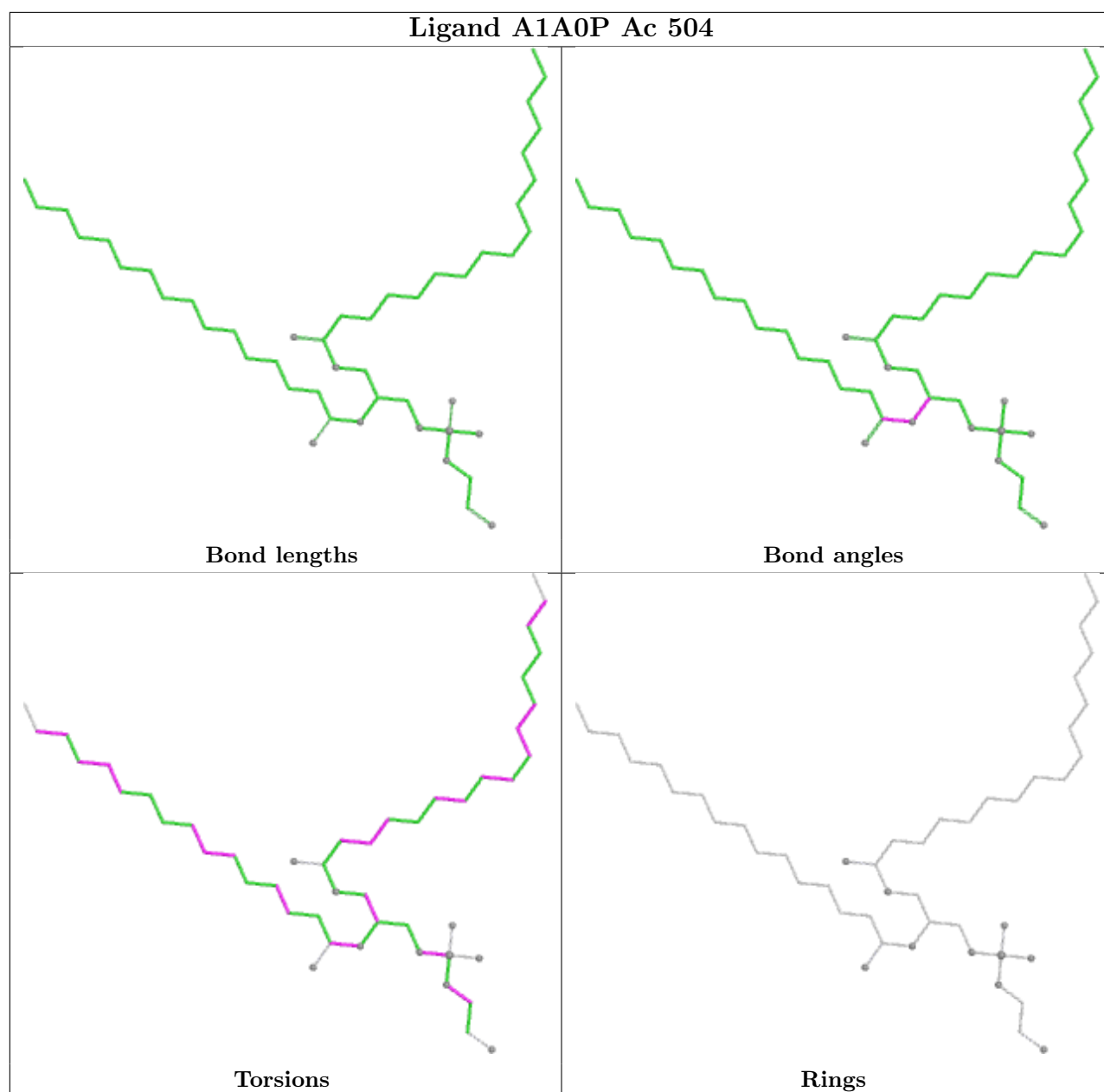
## Ligand A1A0P Ab 502

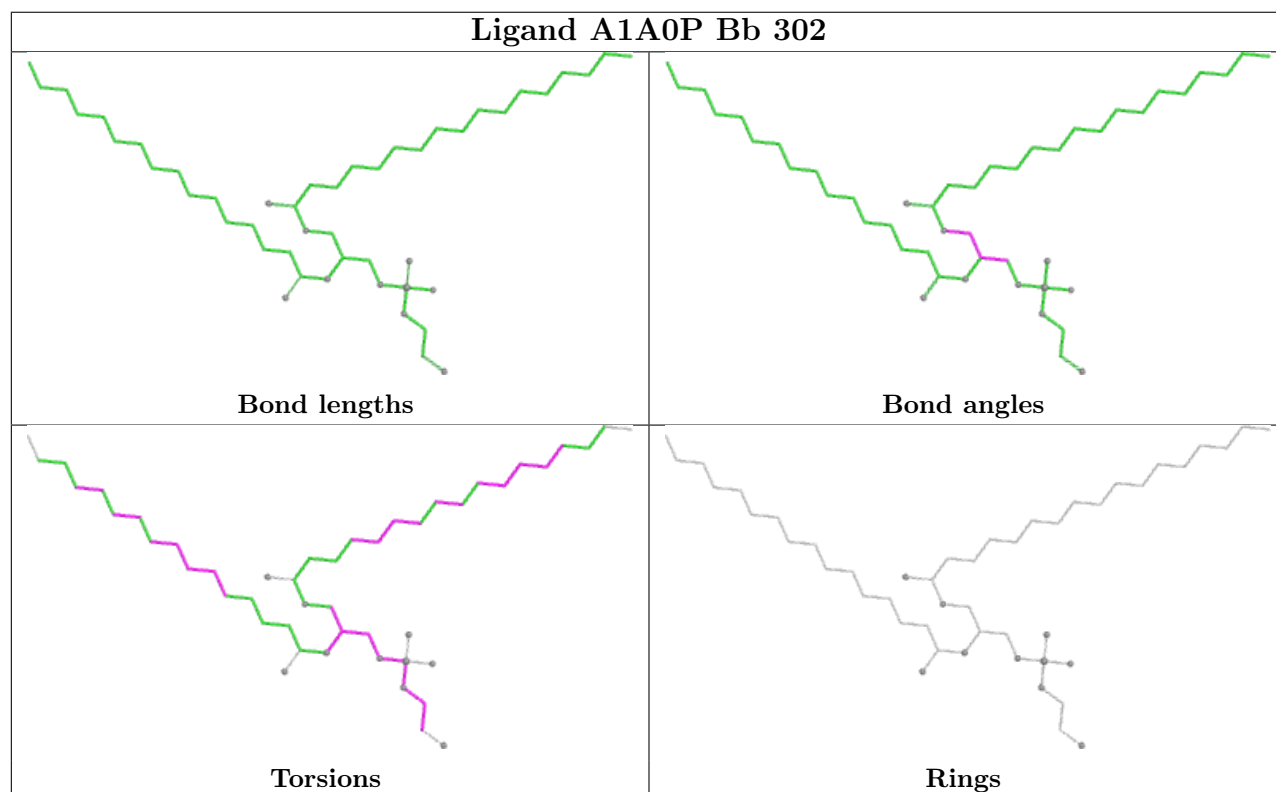
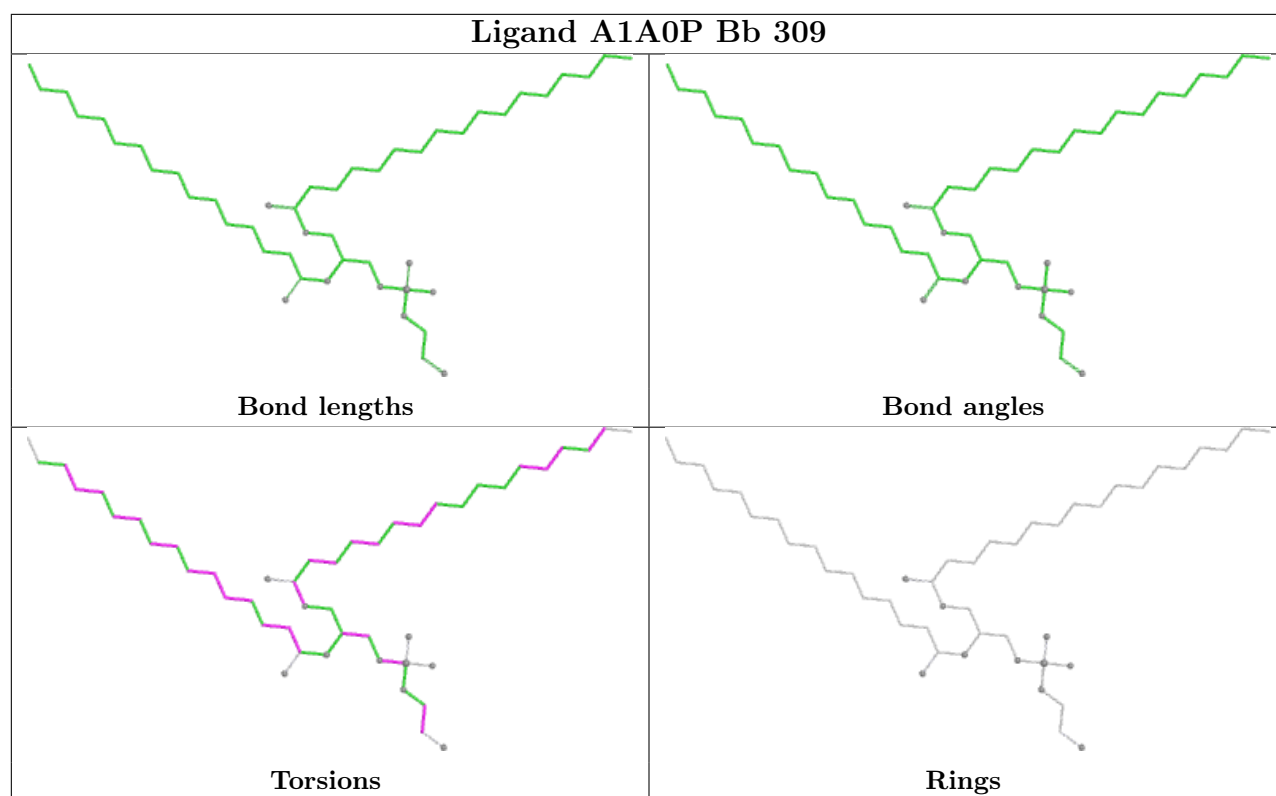


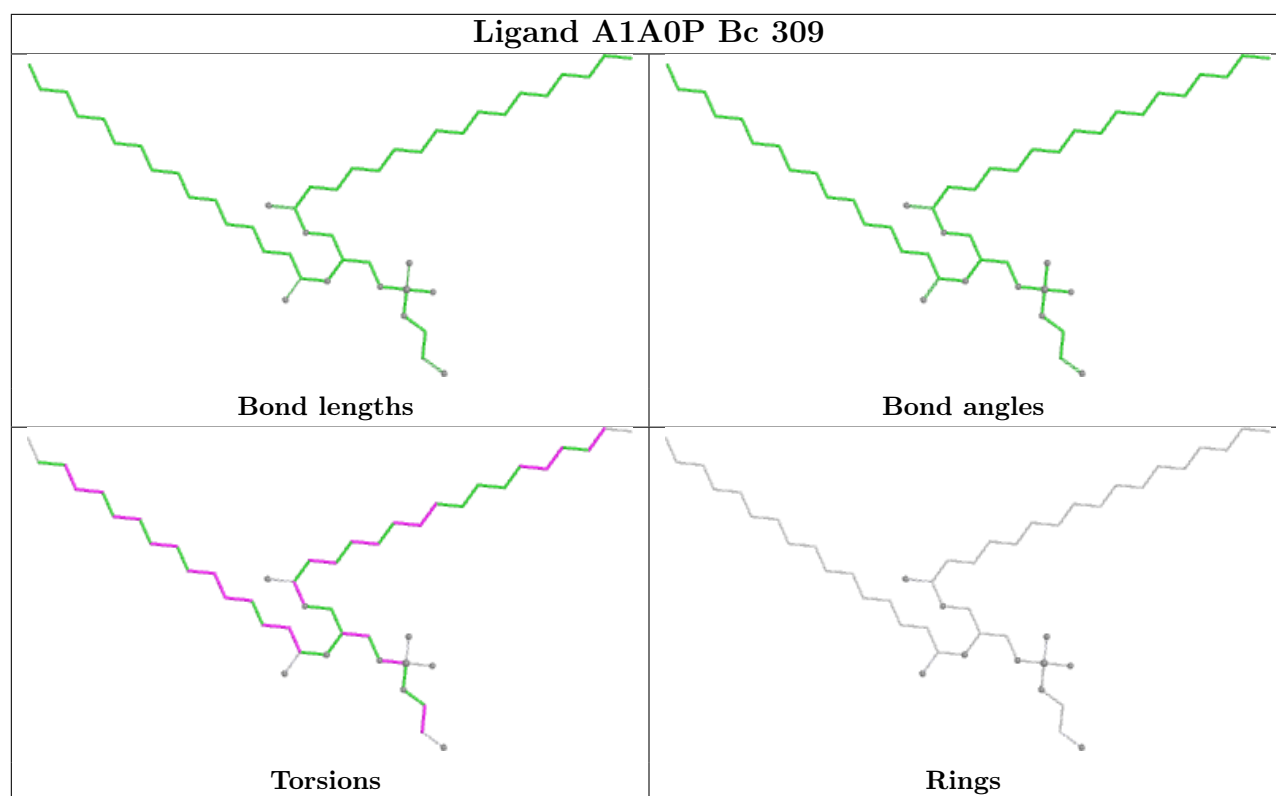


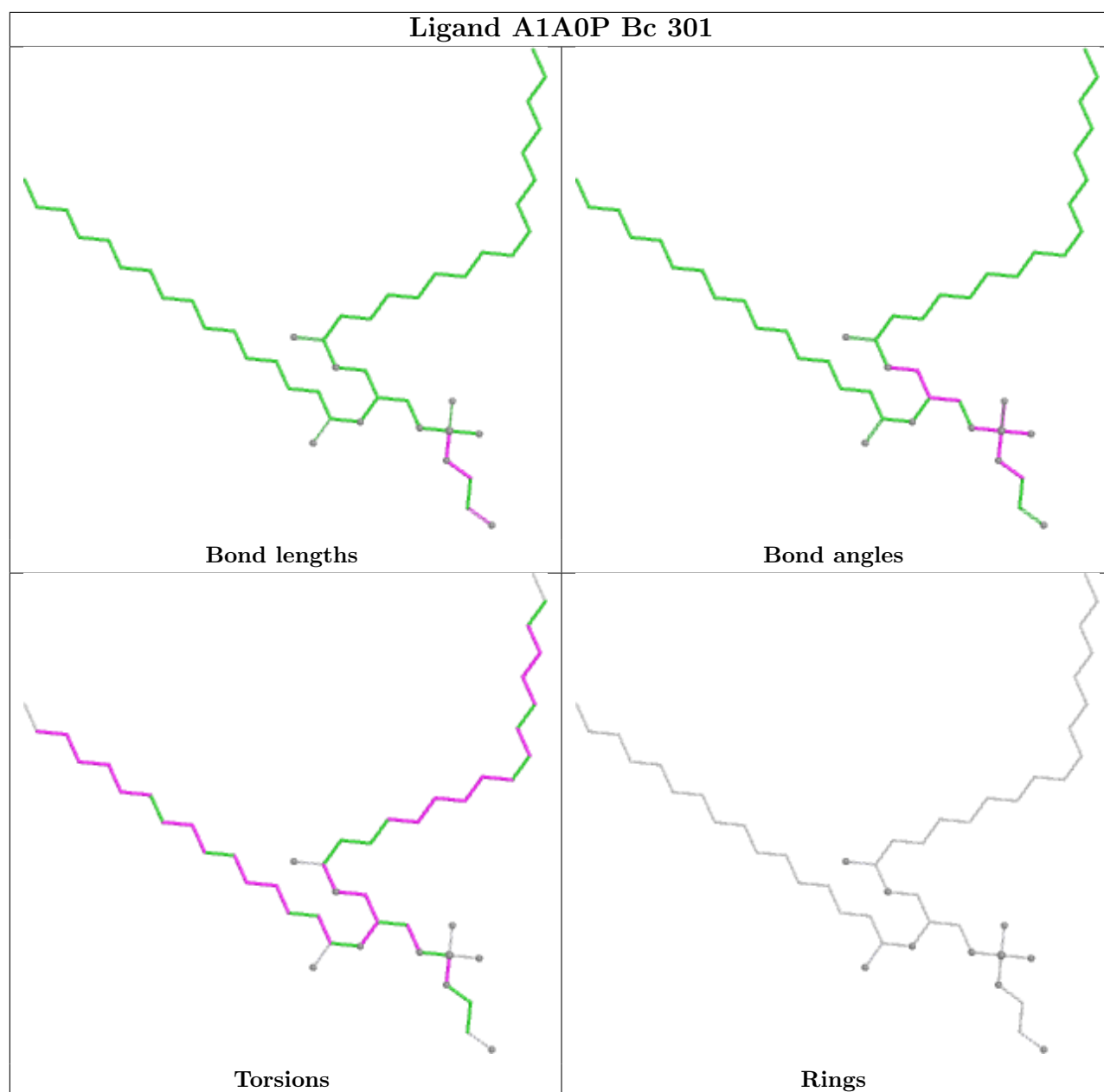


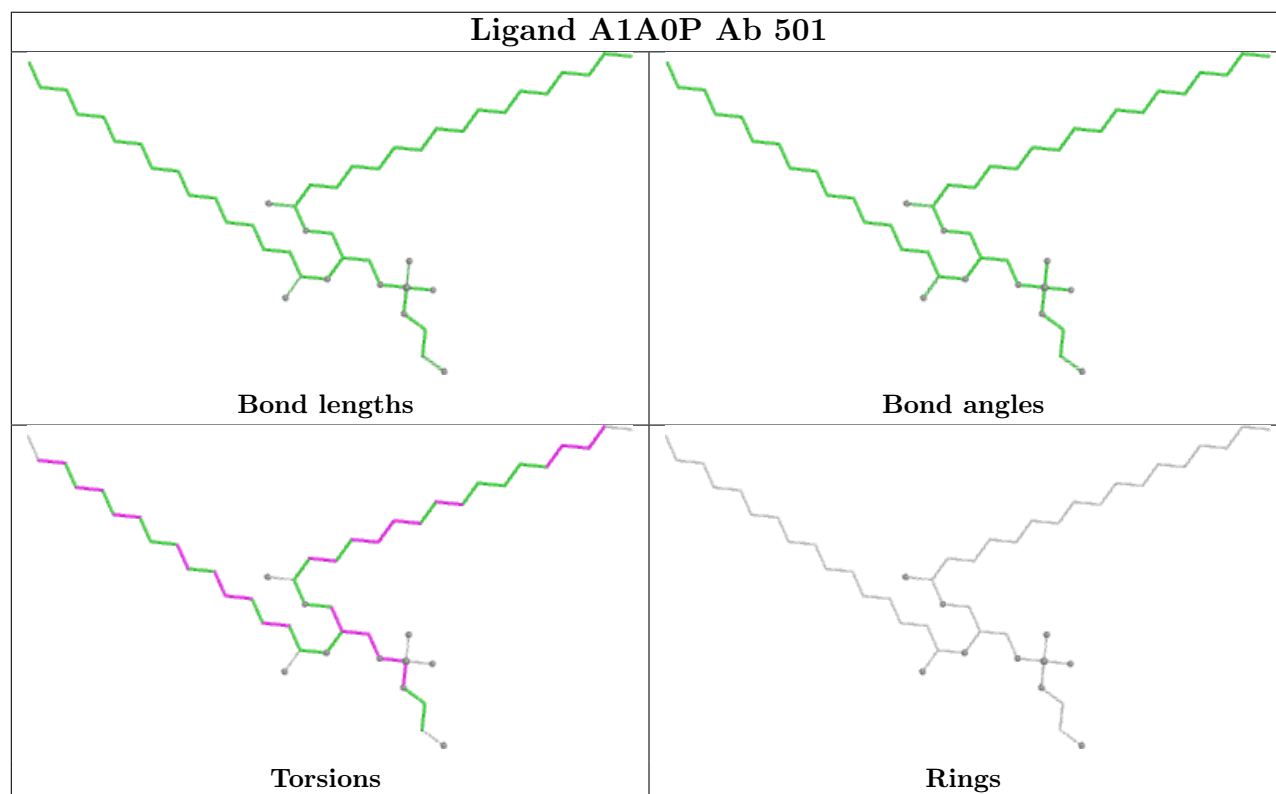
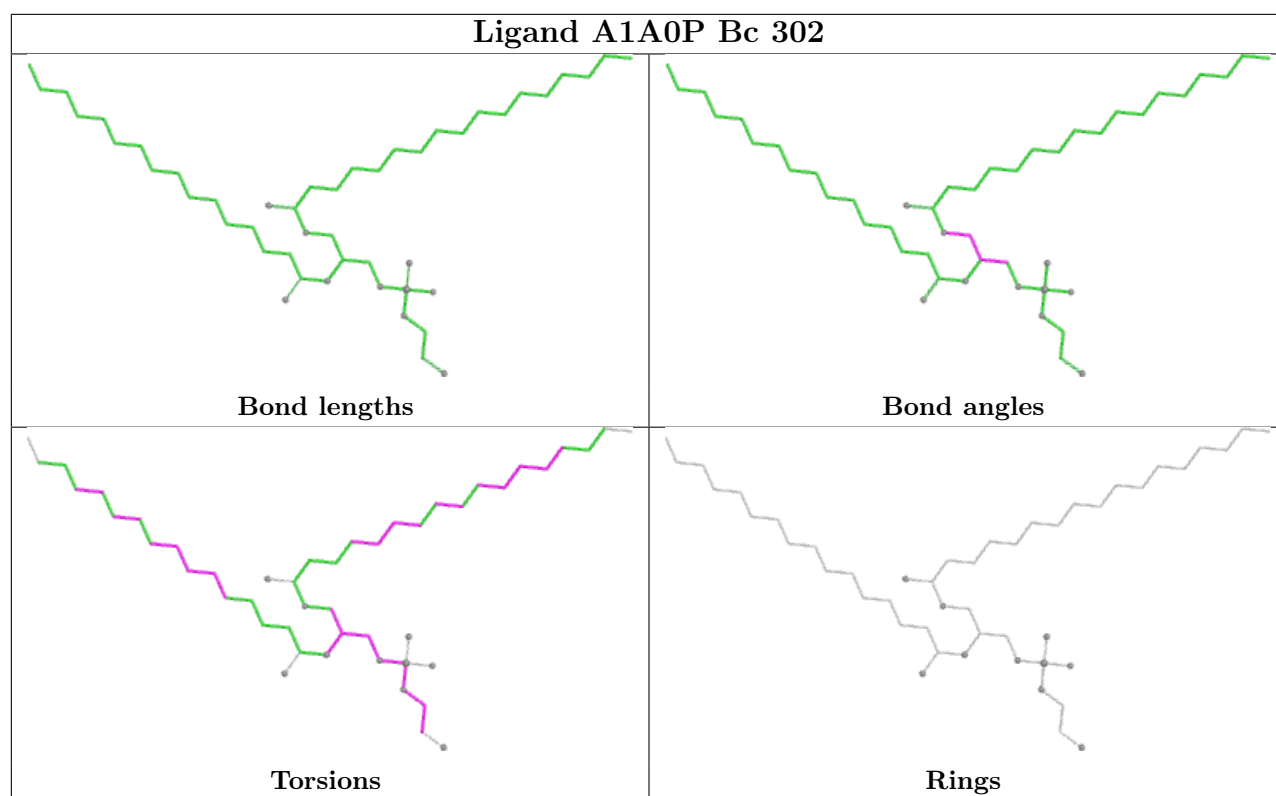


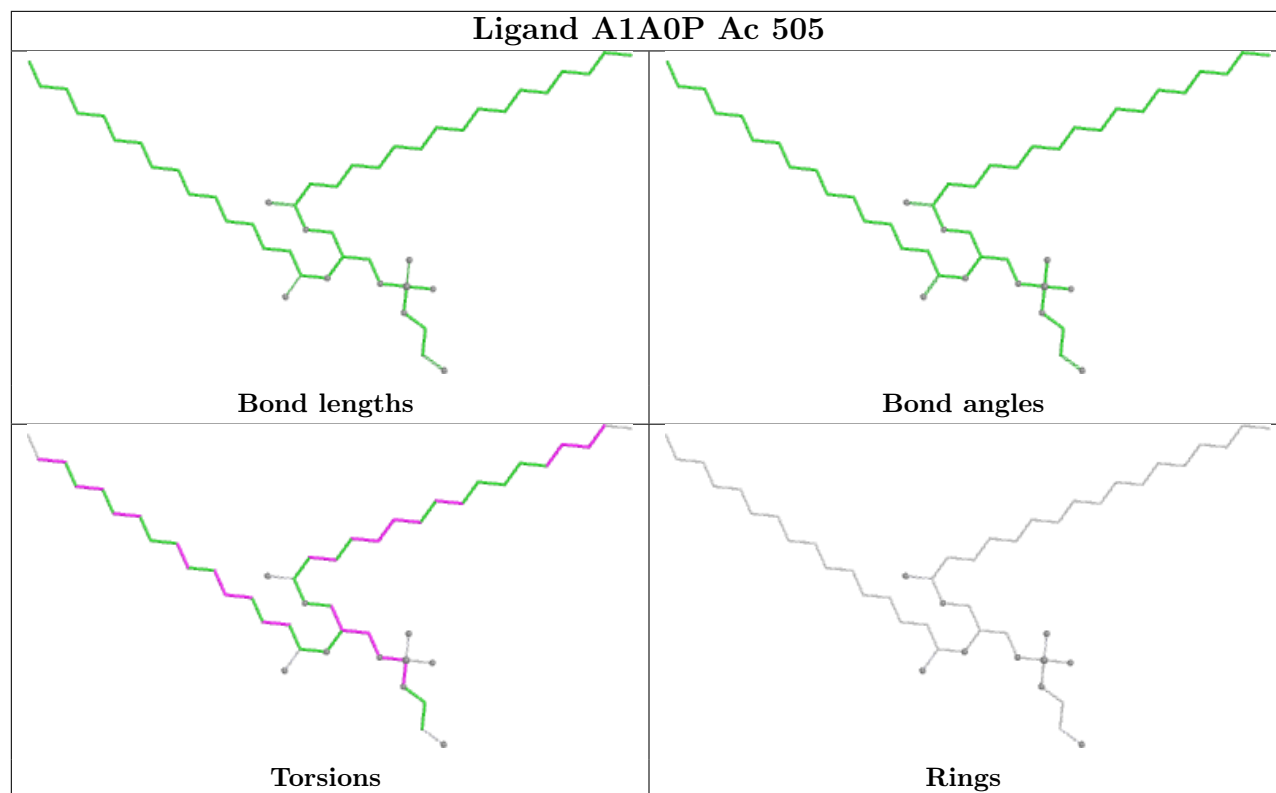


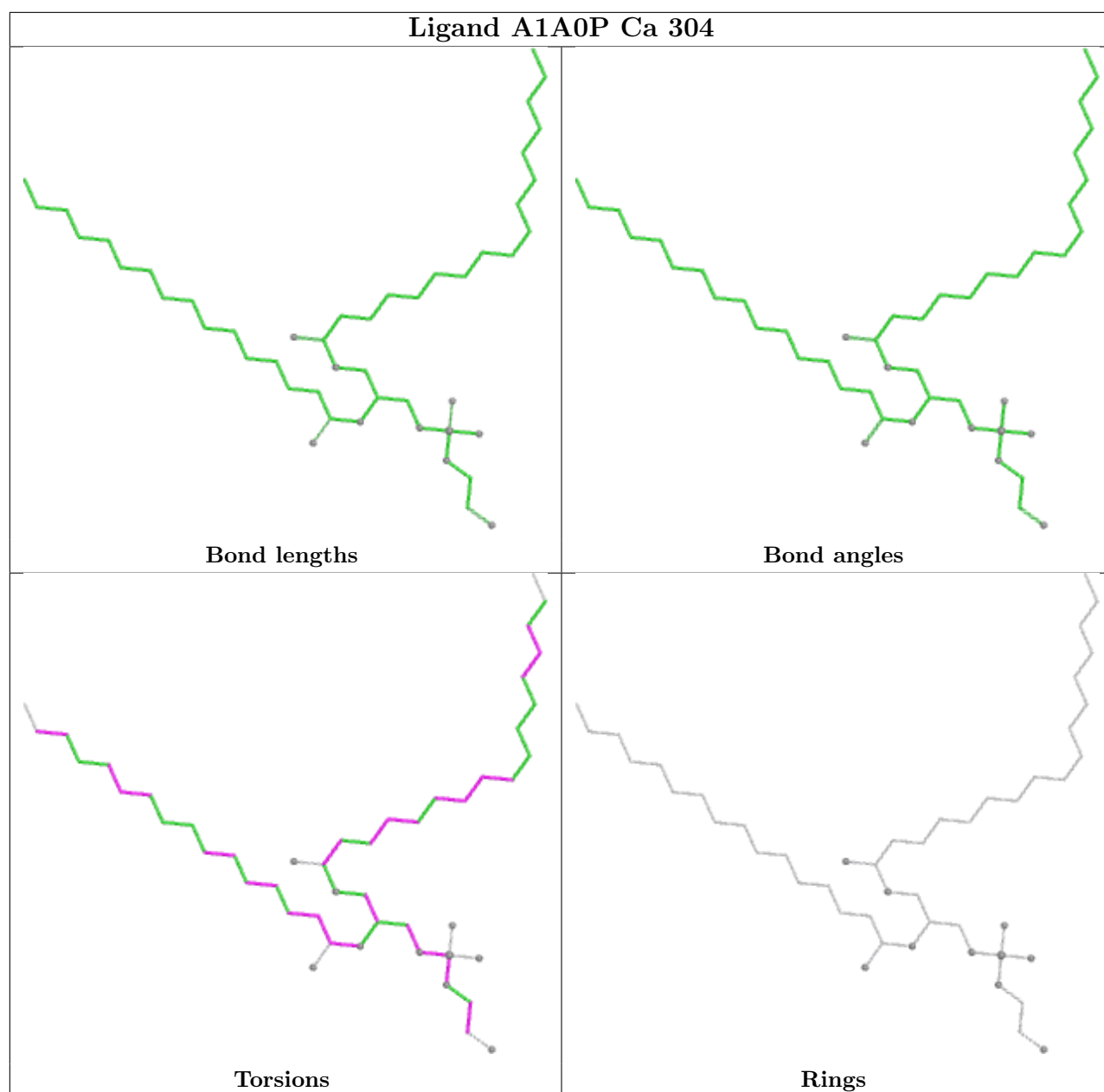


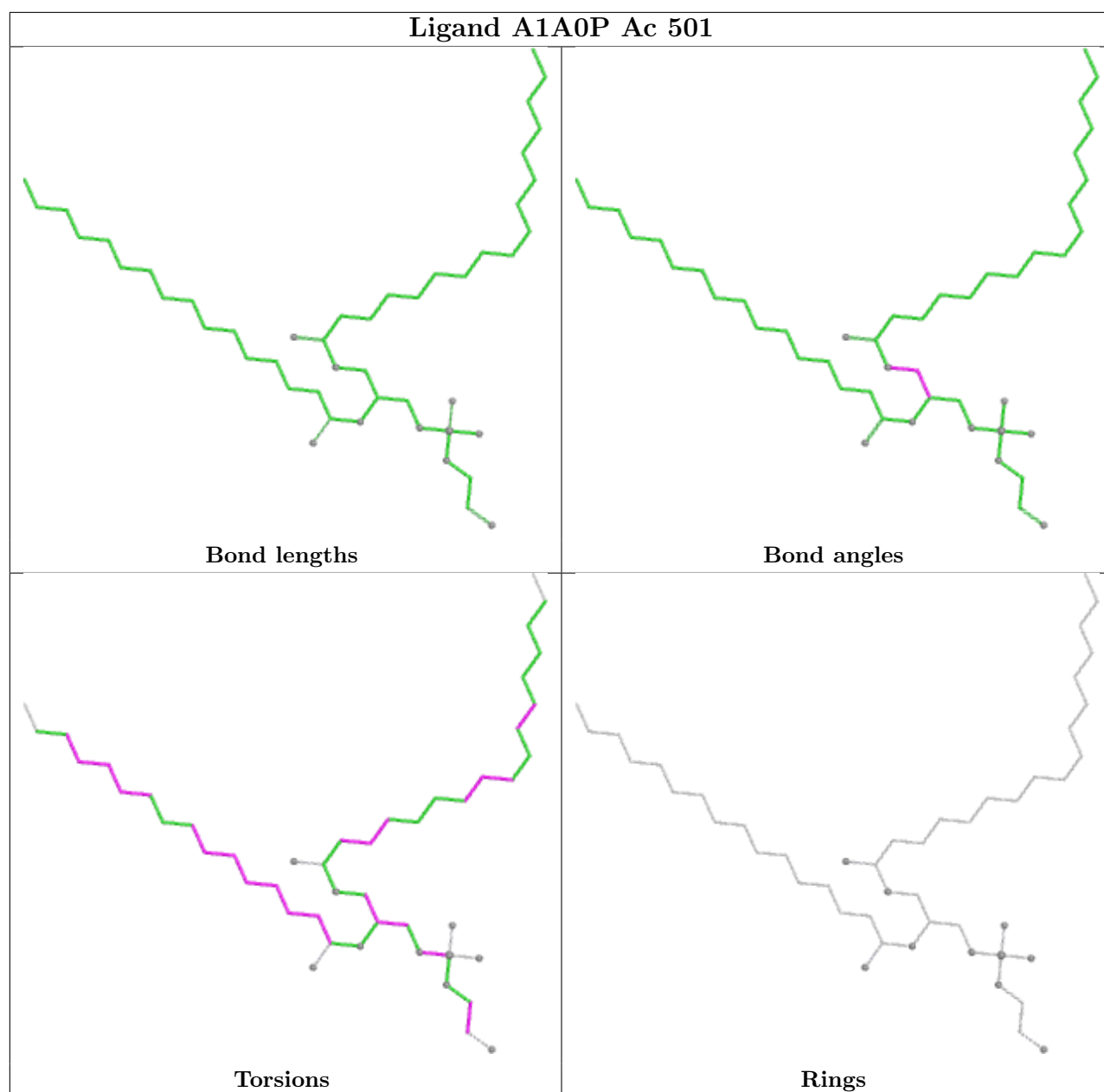


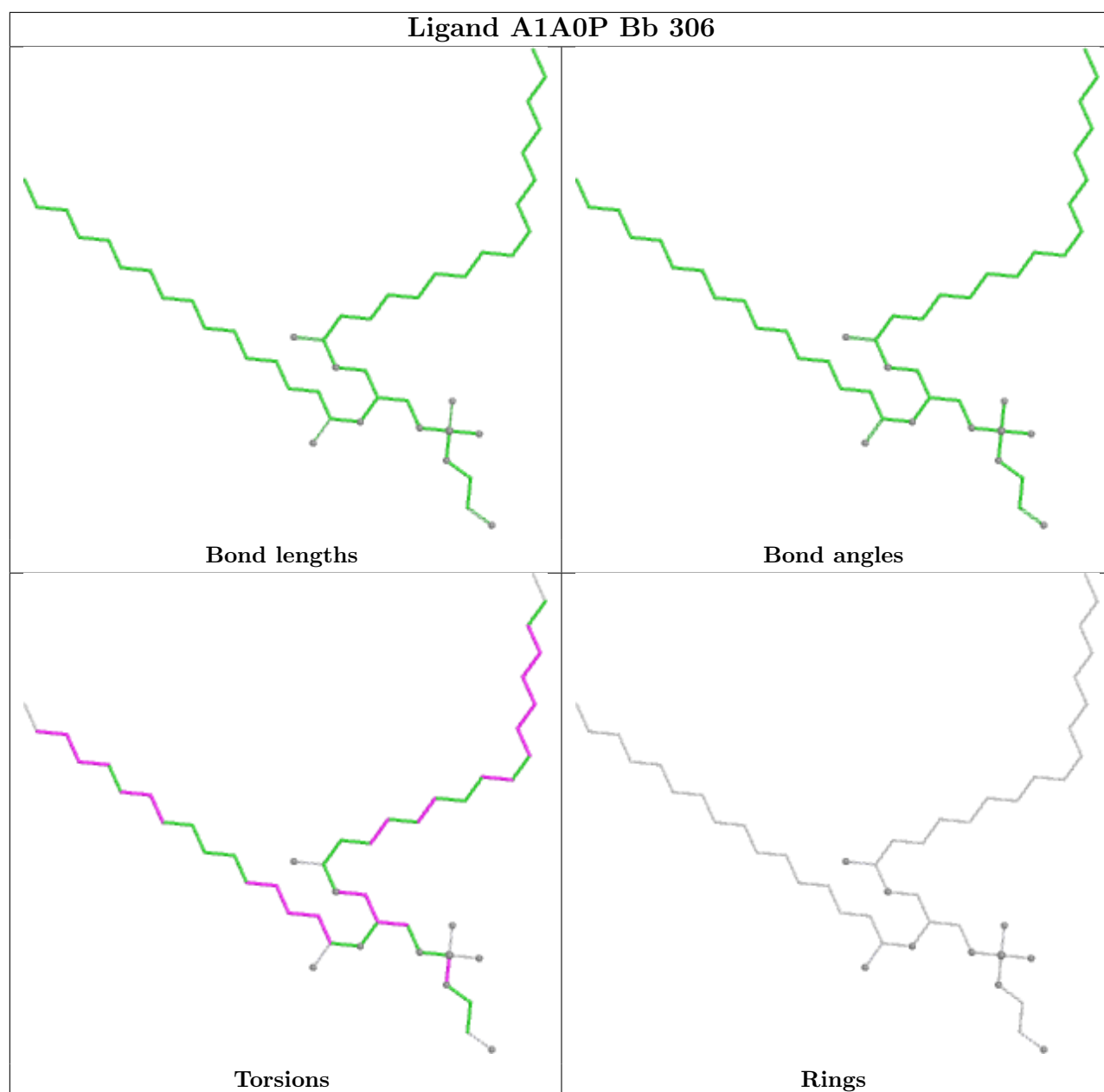


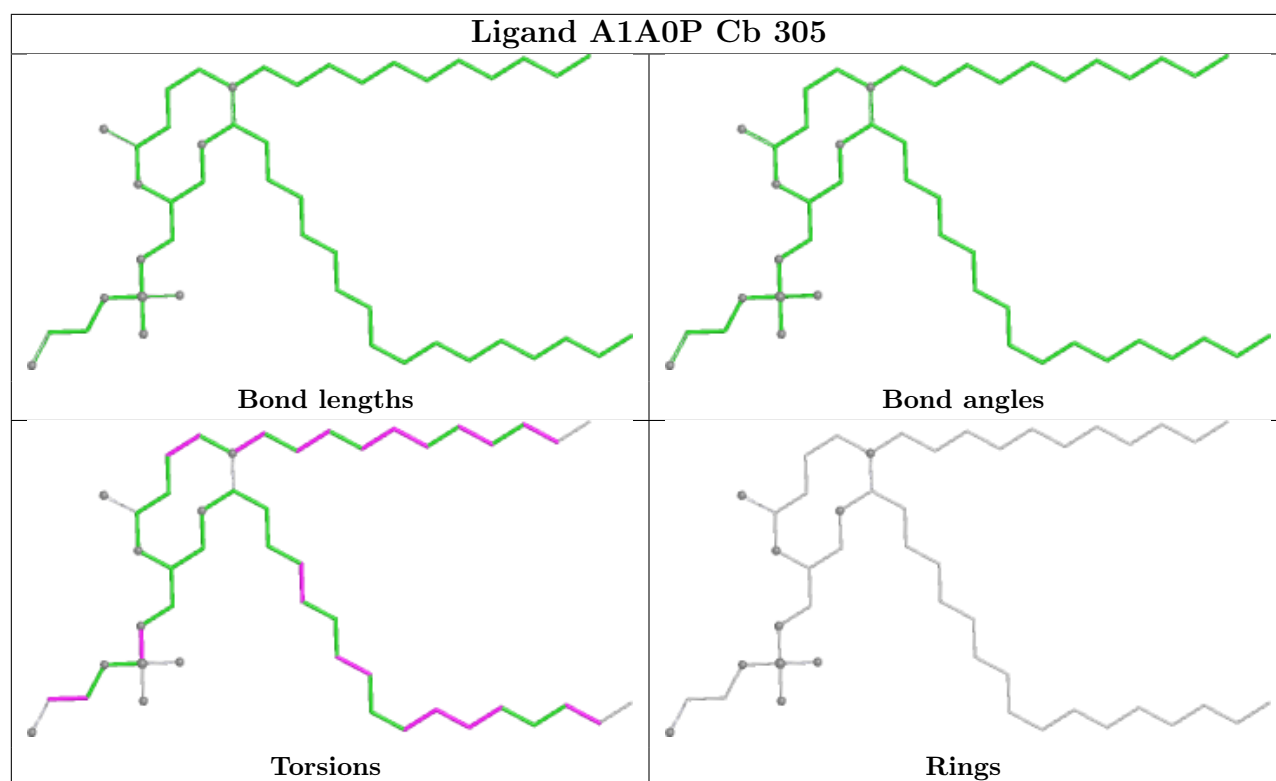


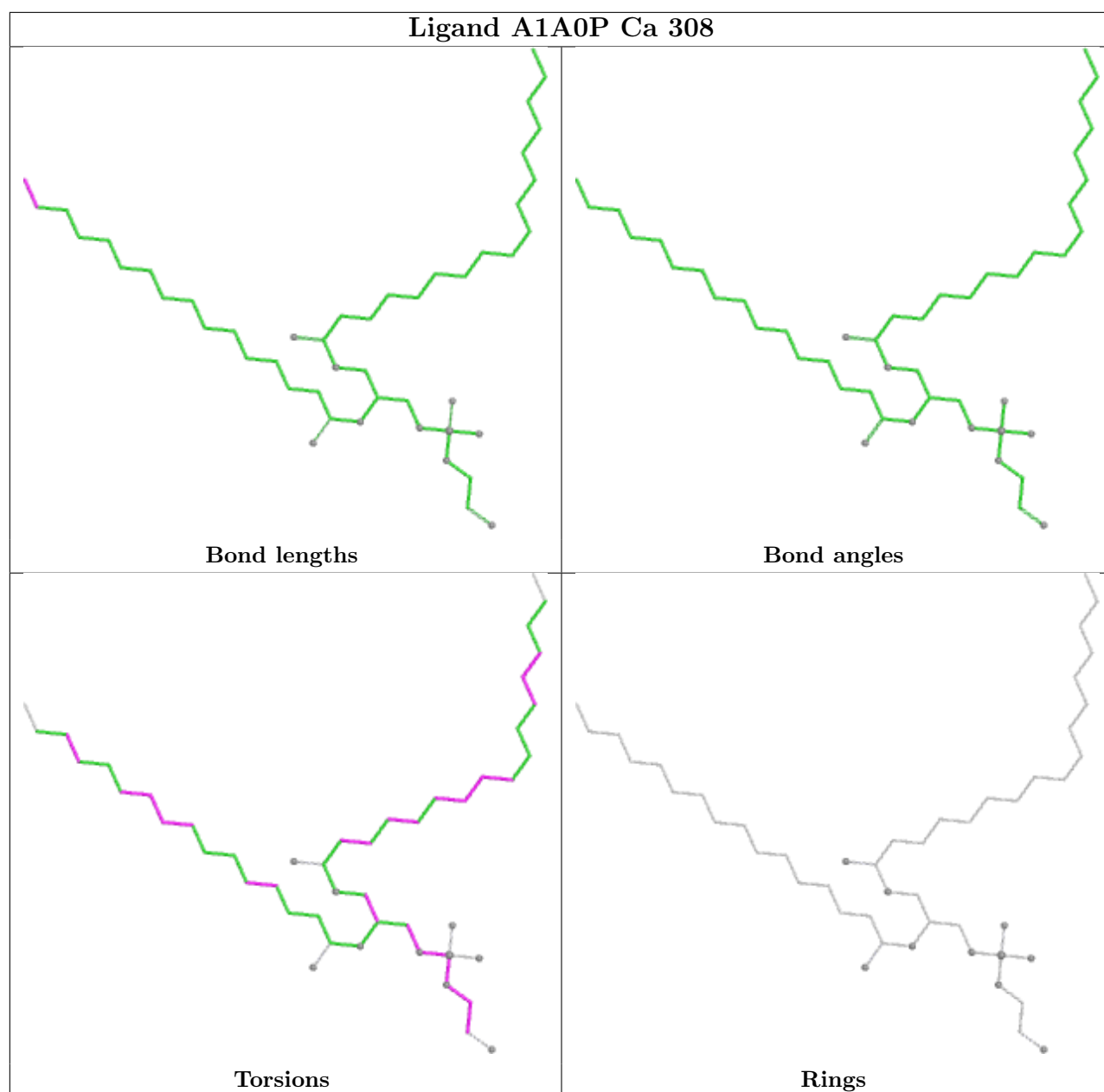


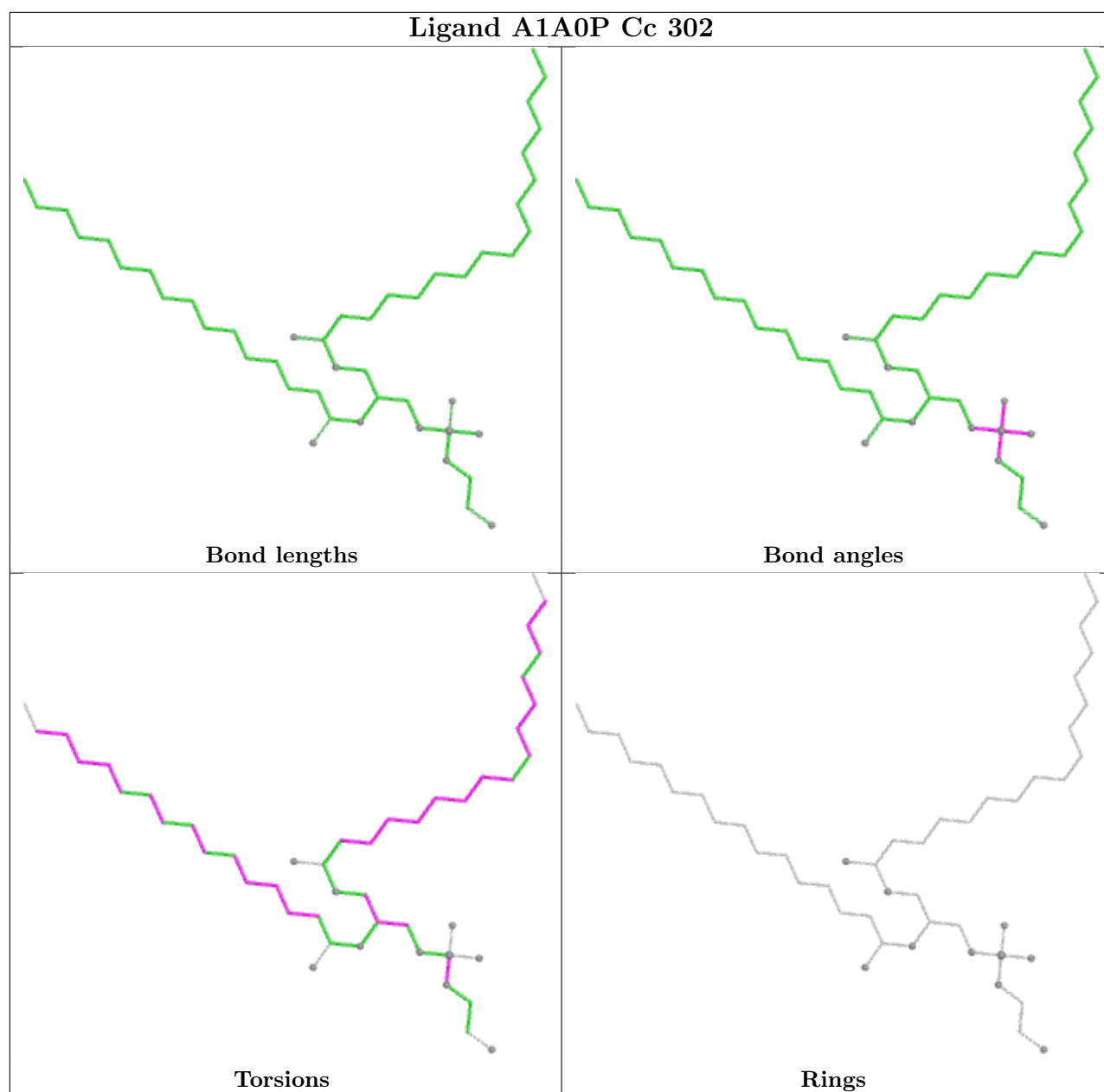


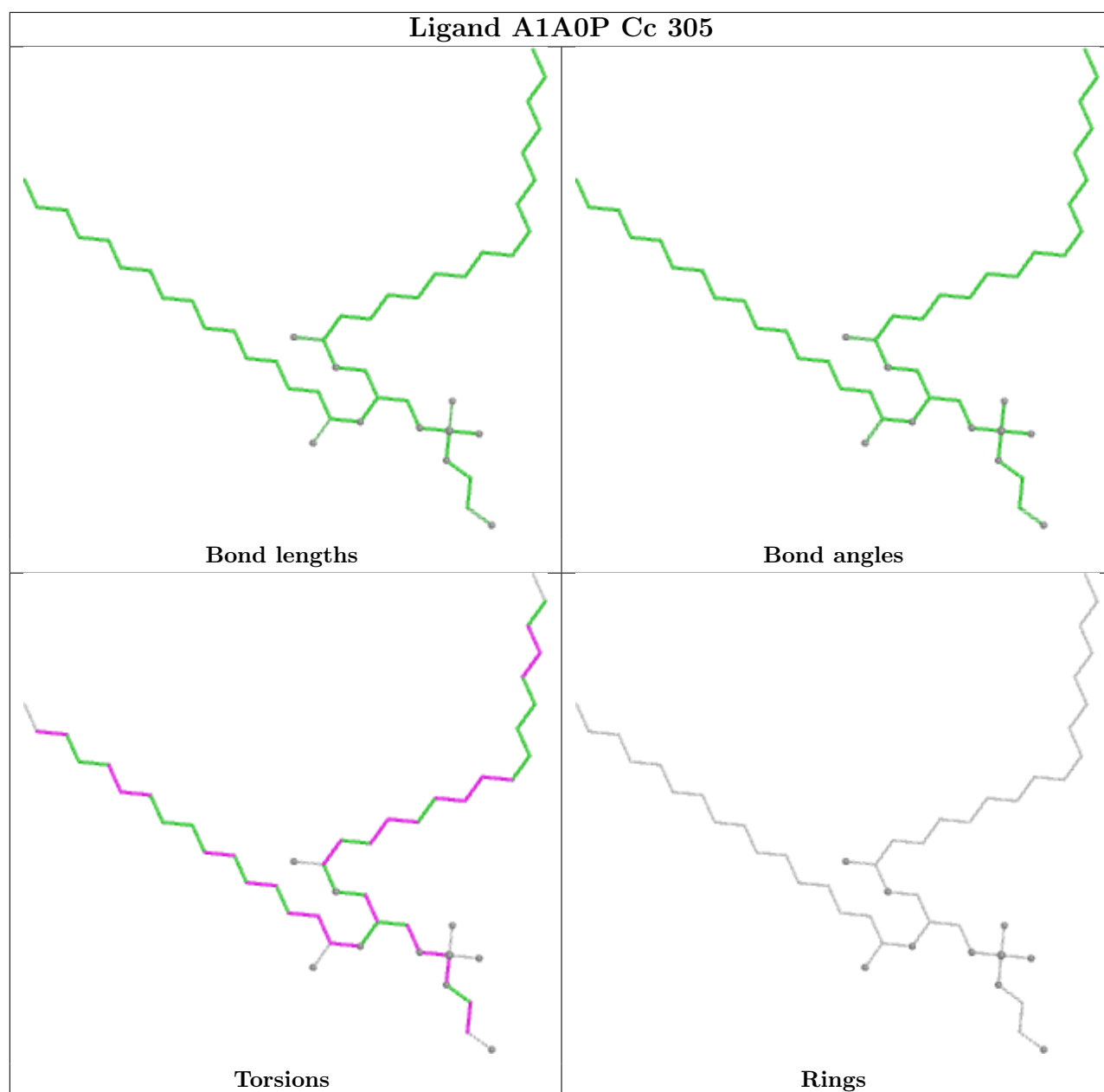


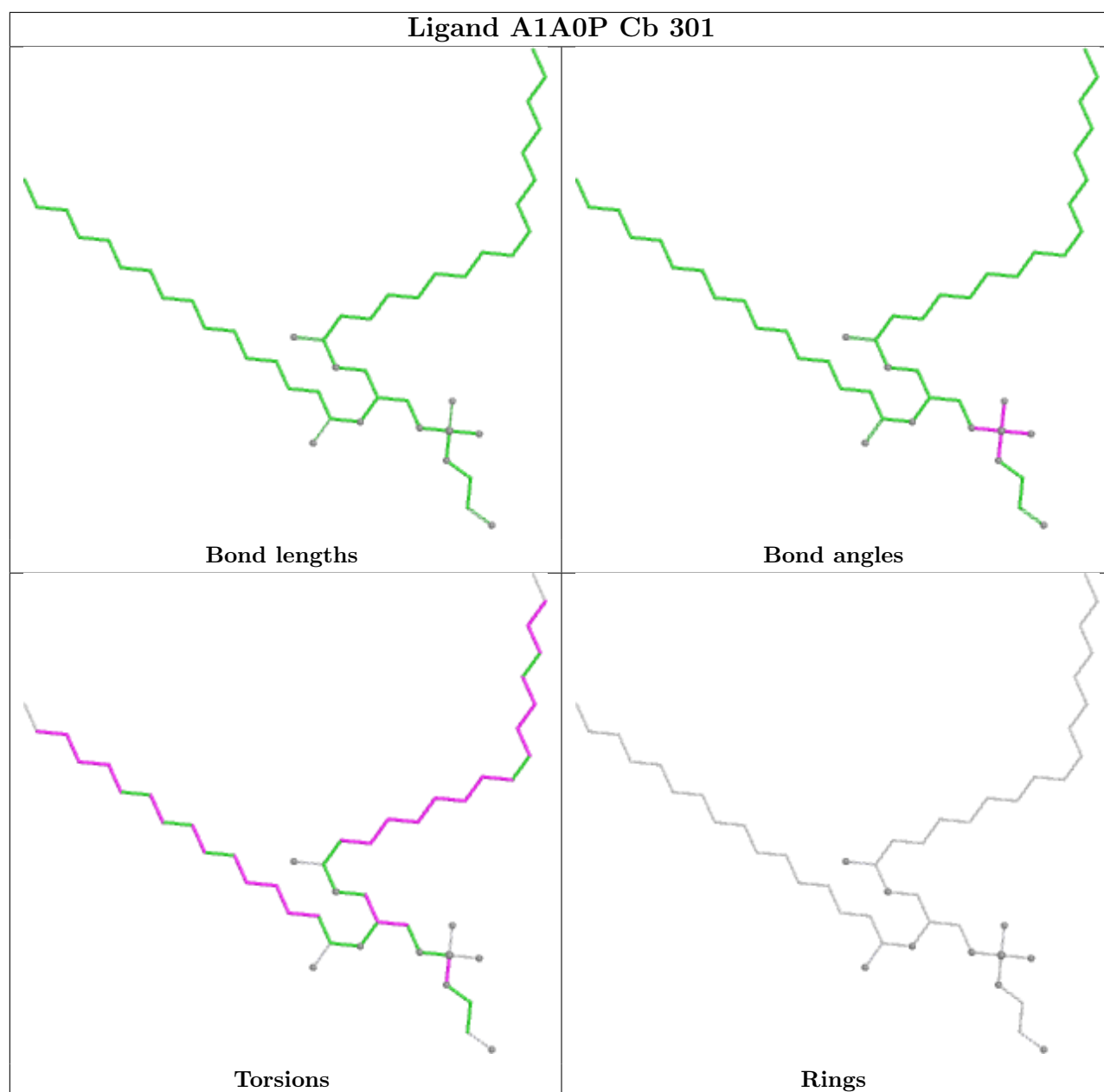


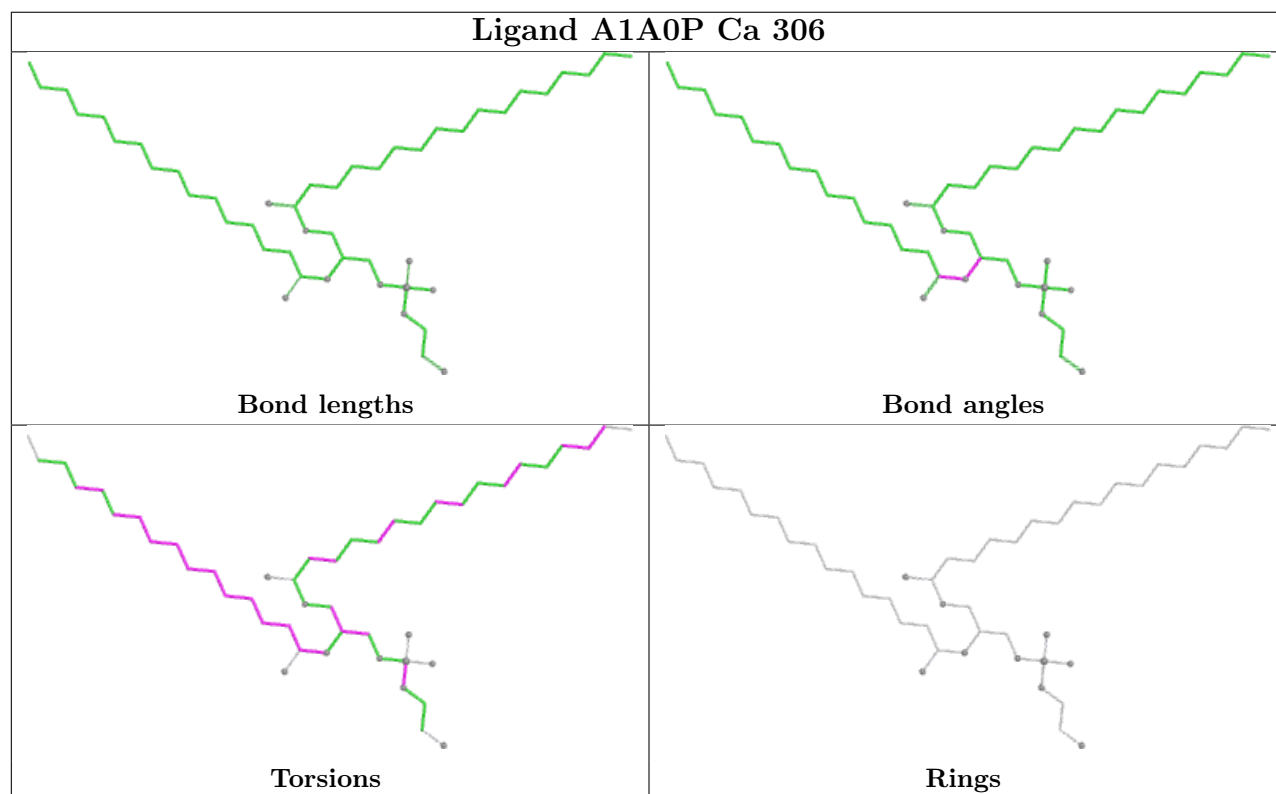
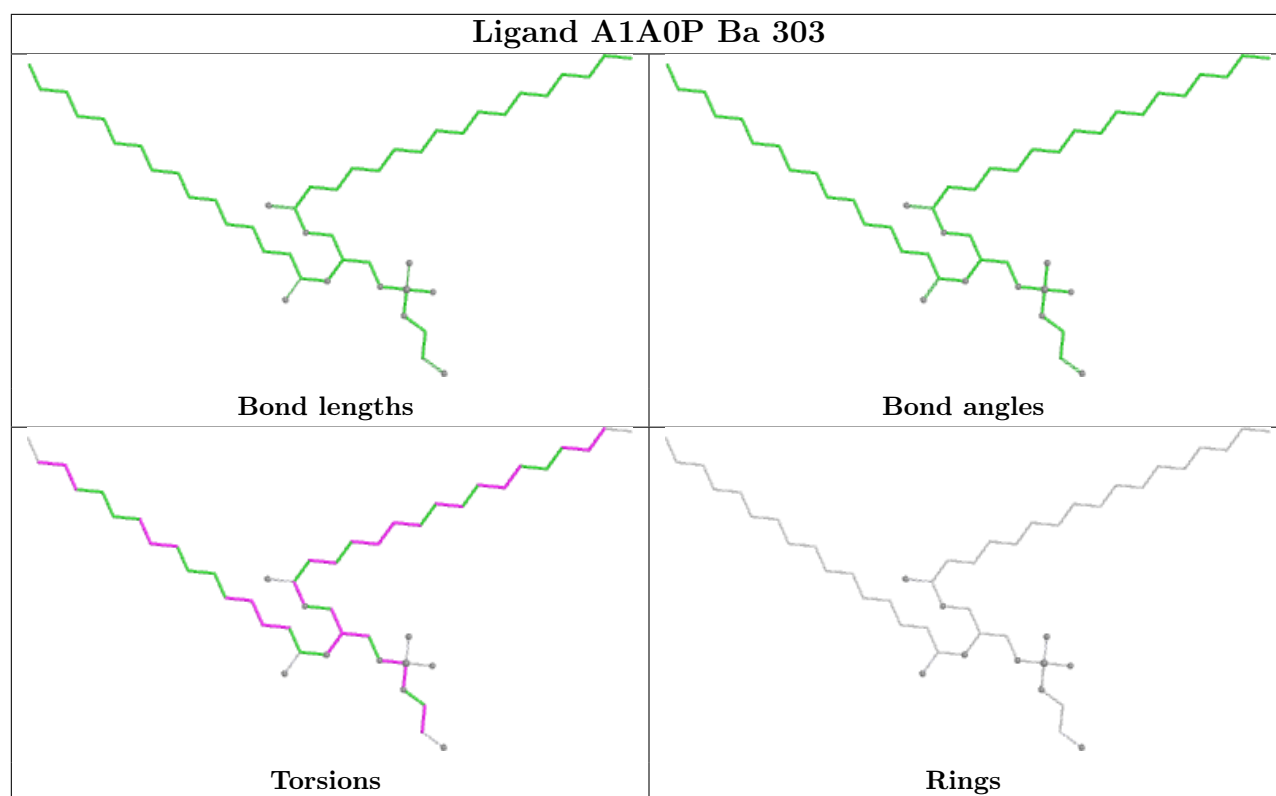


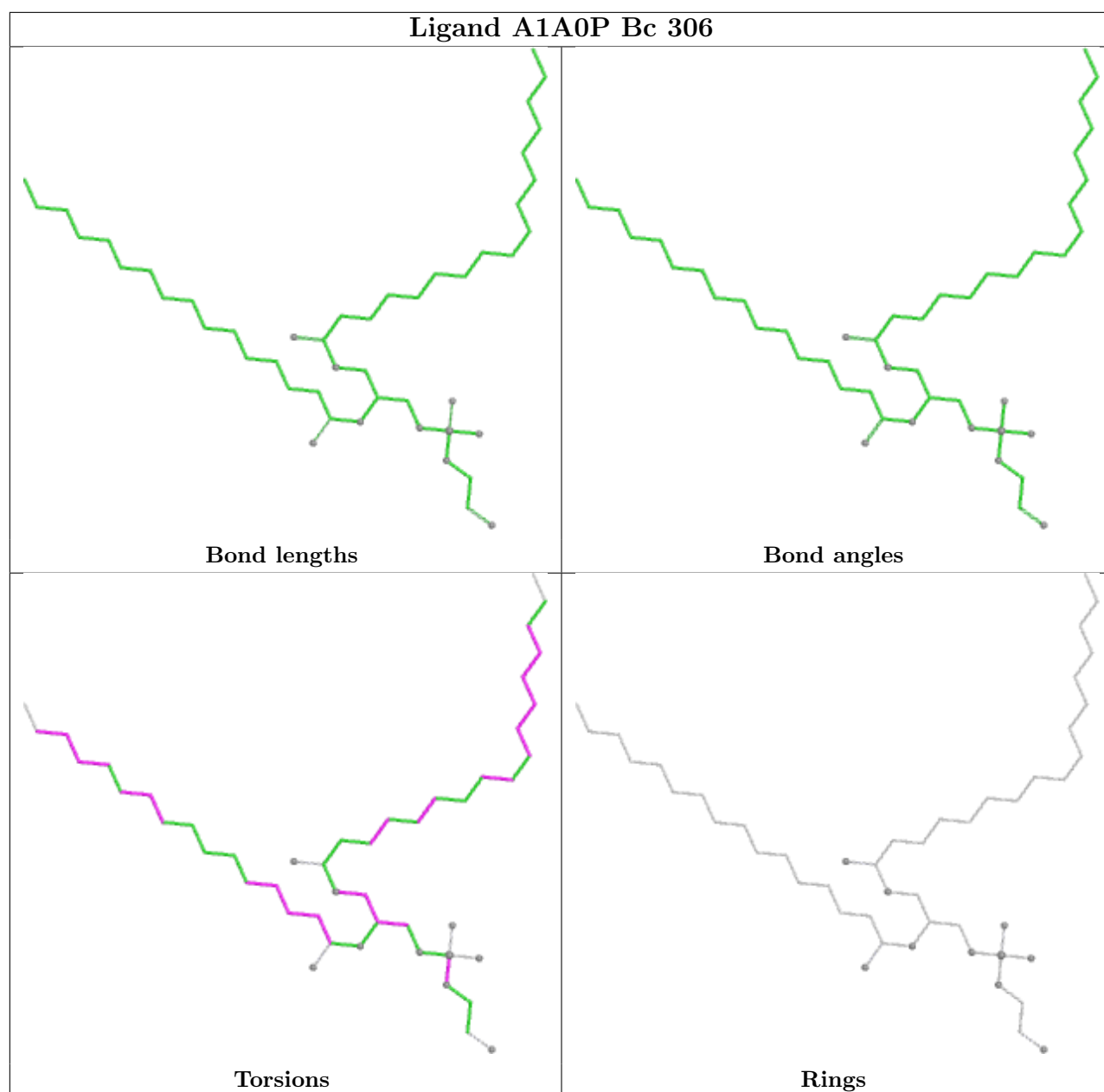


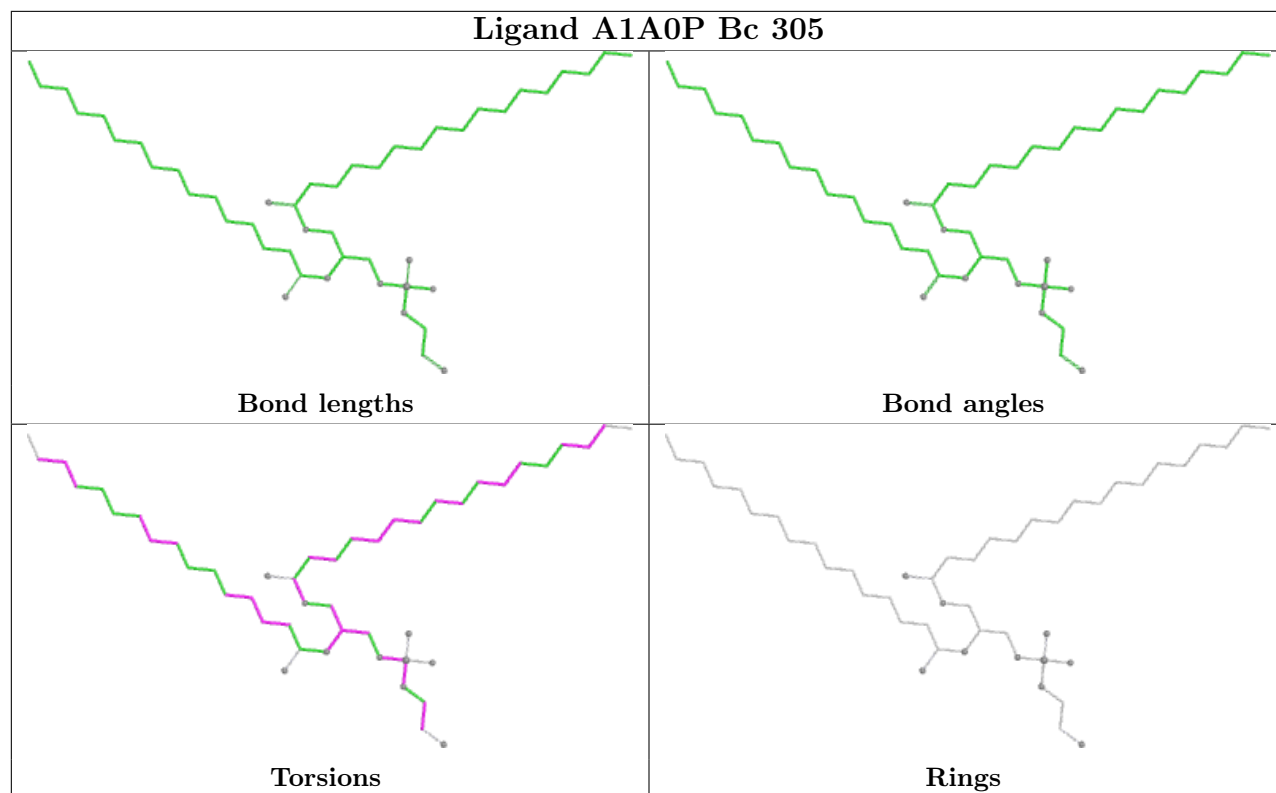


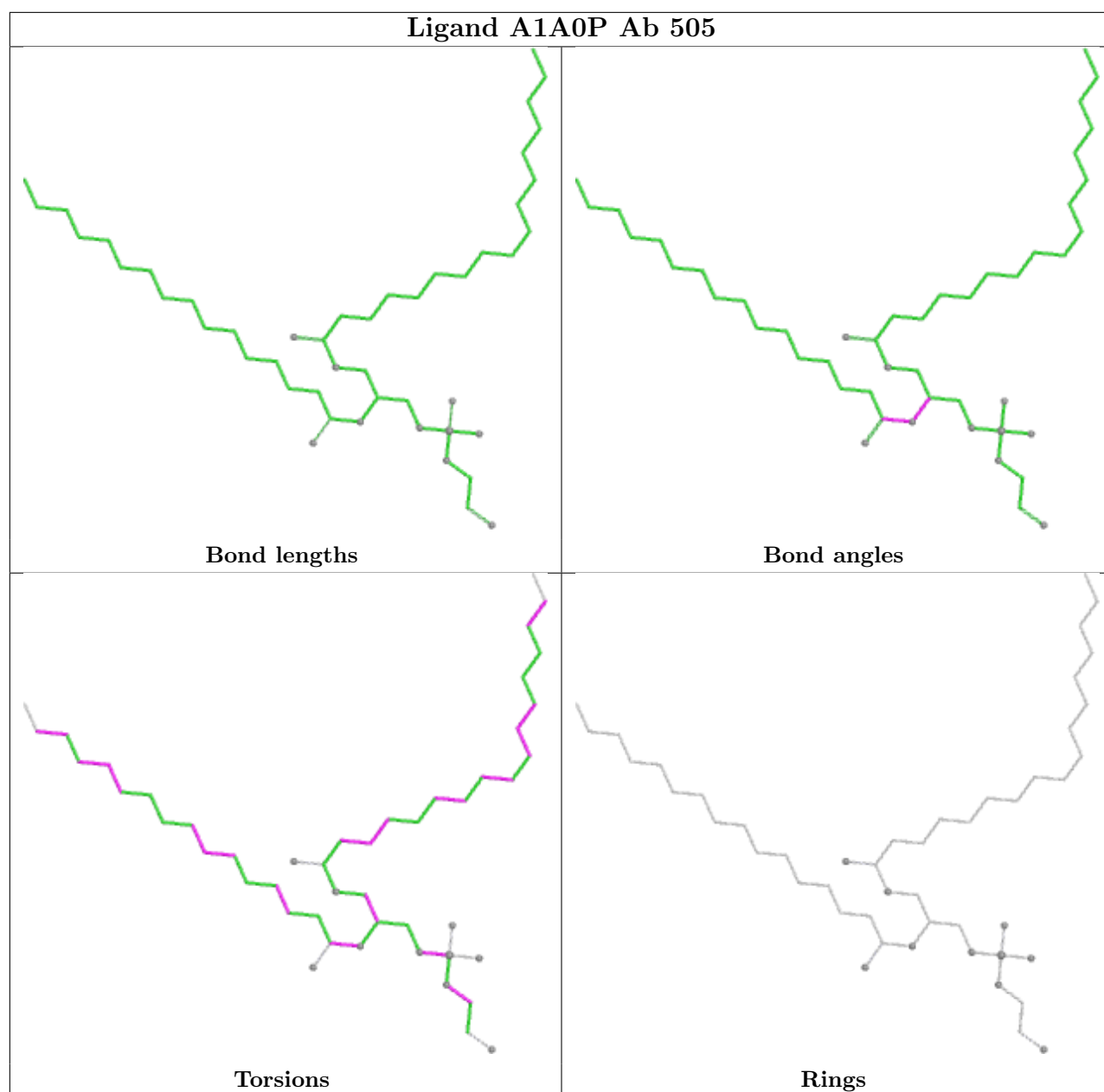


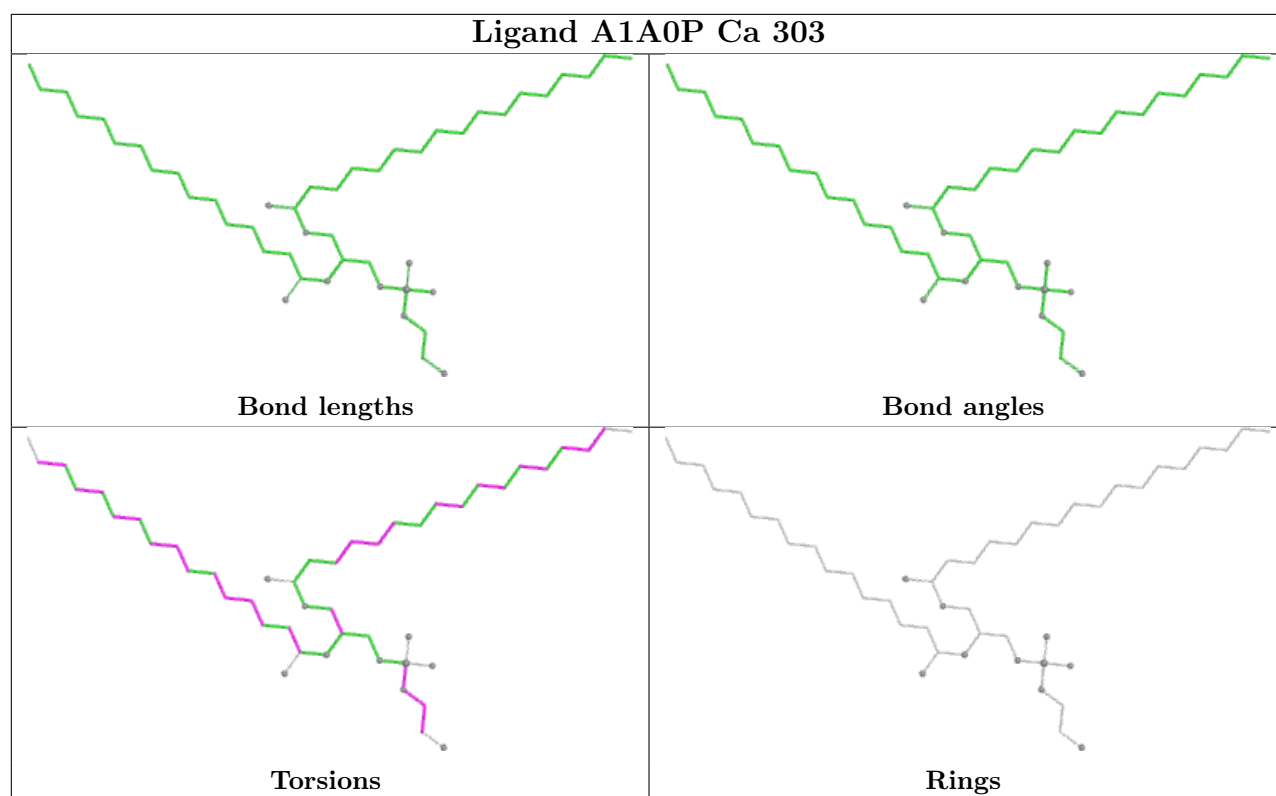


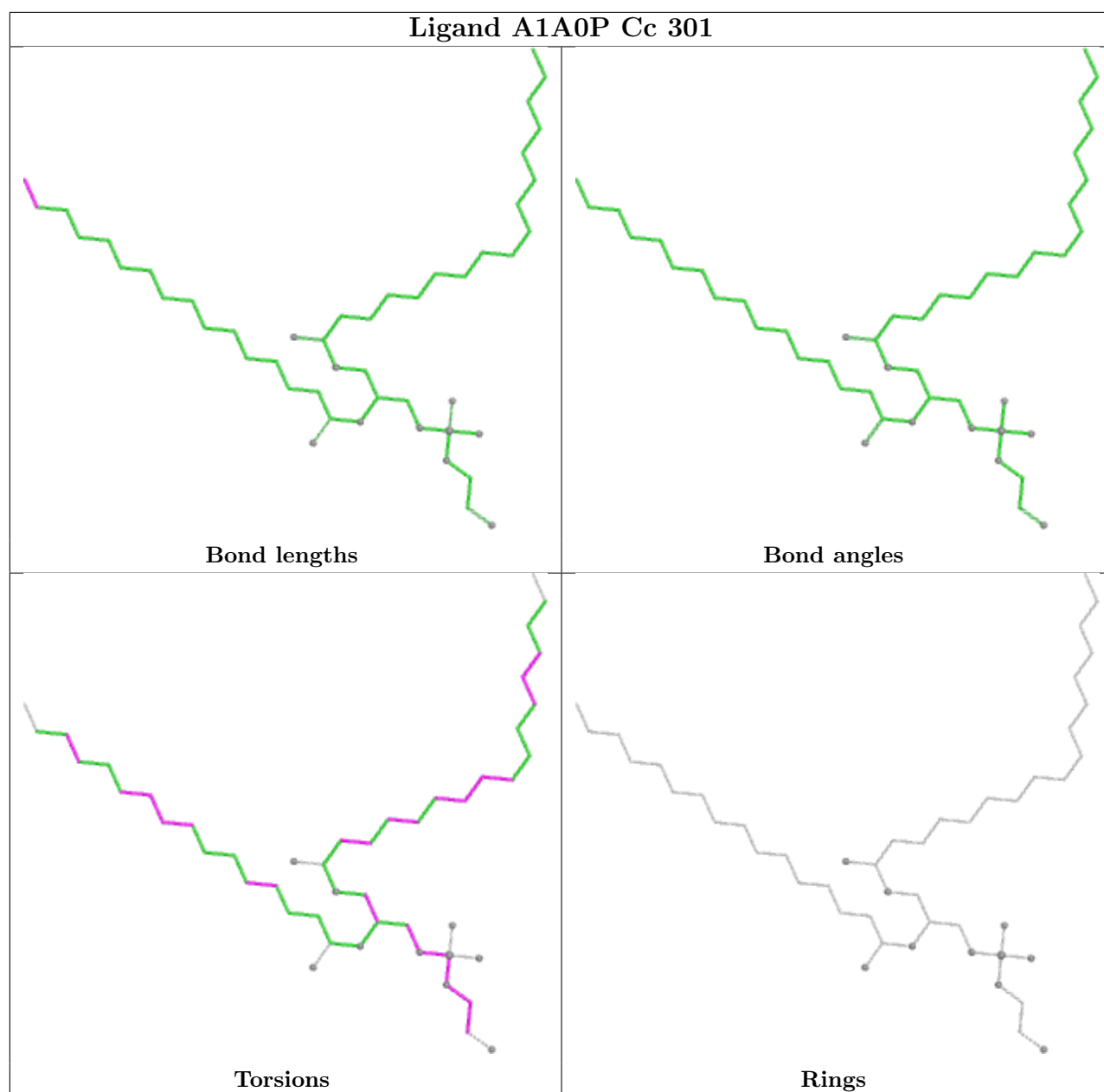




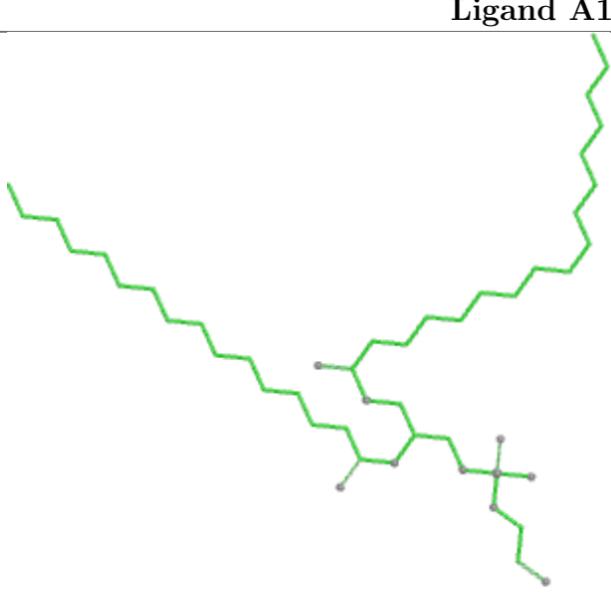
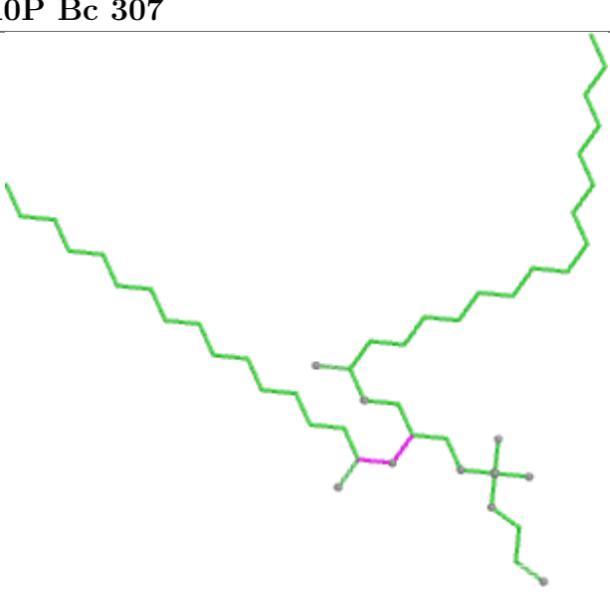
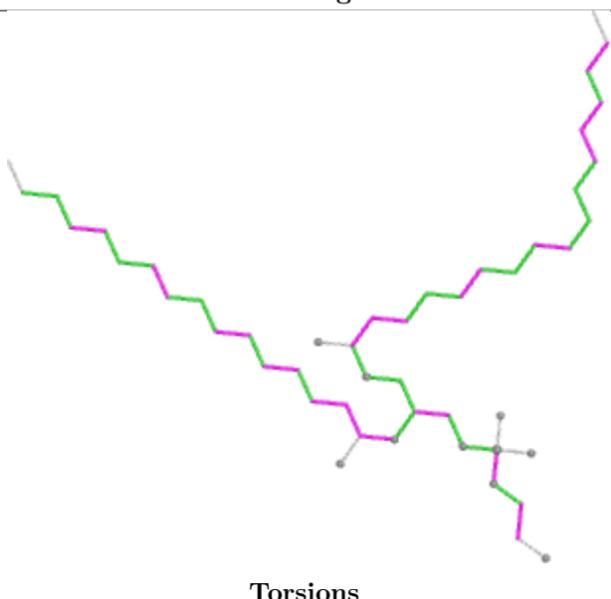
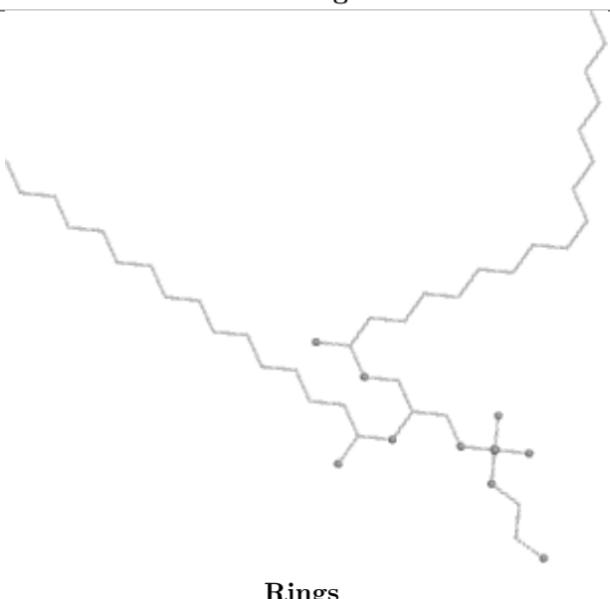


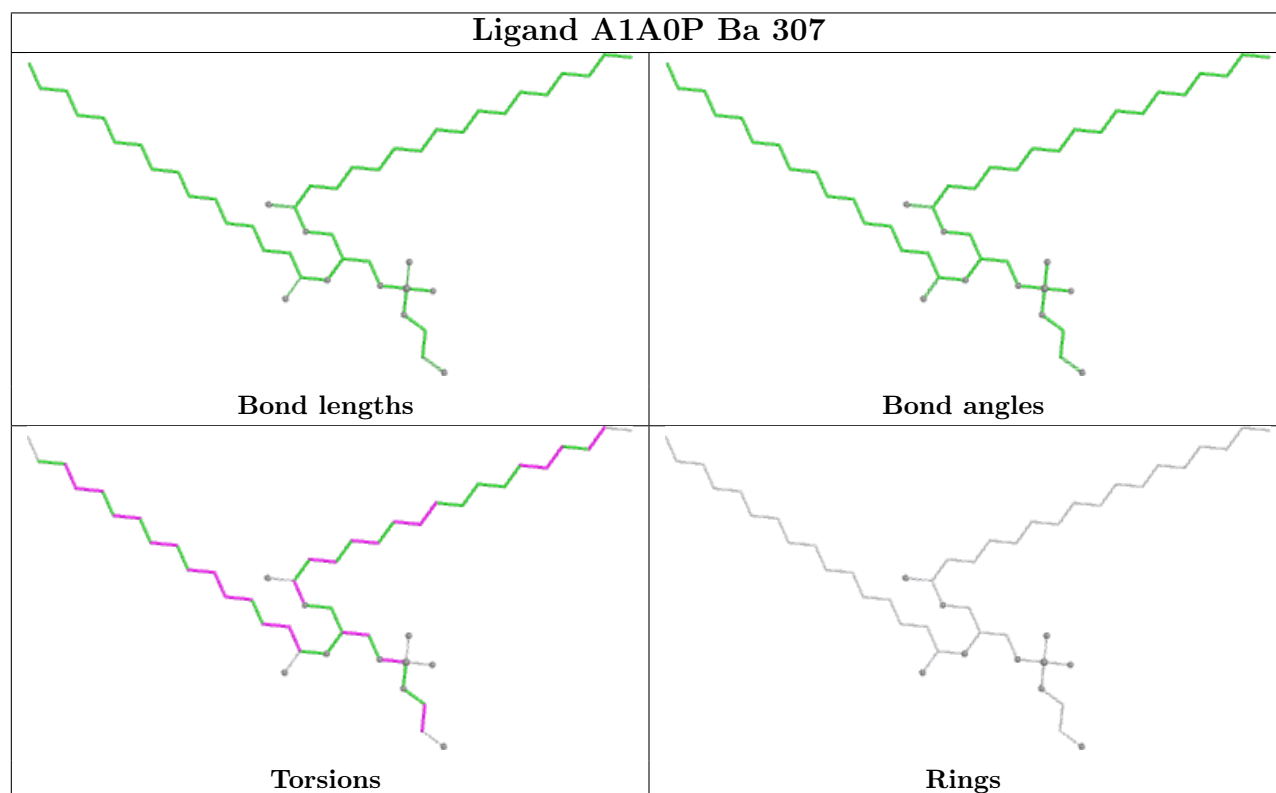
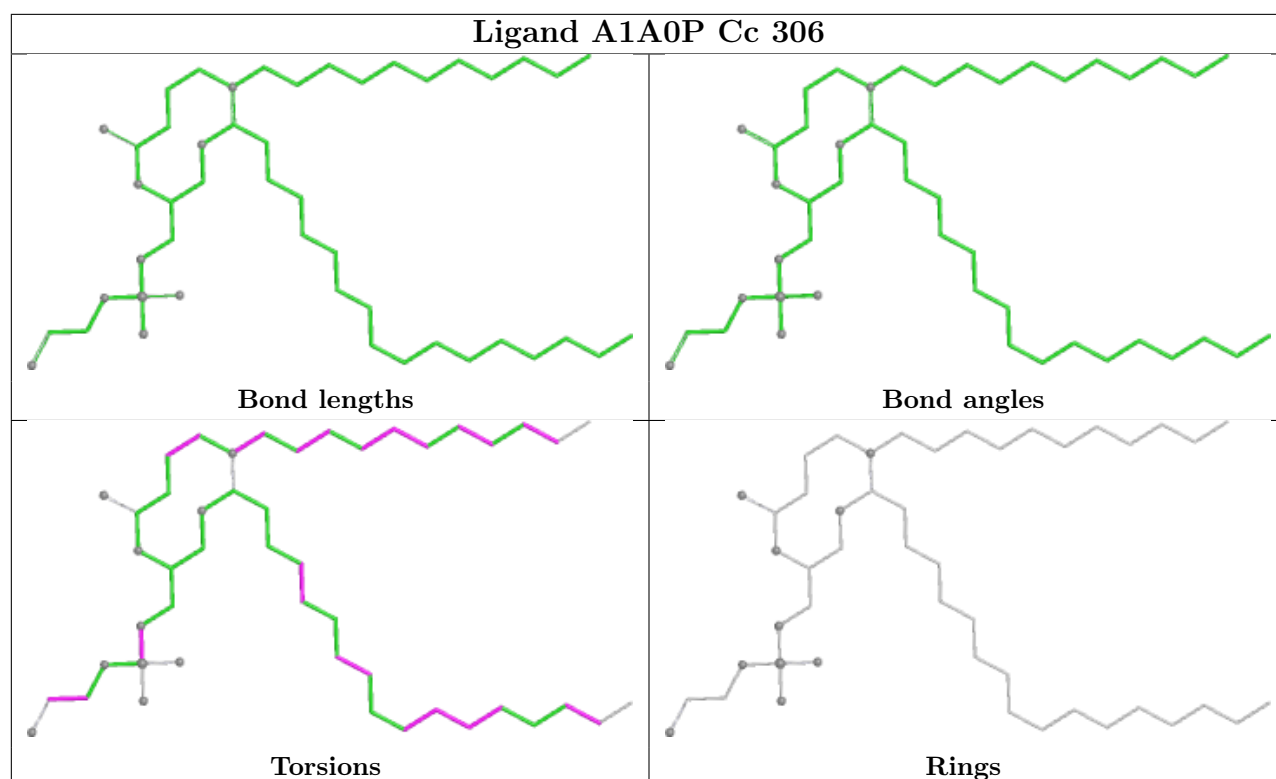


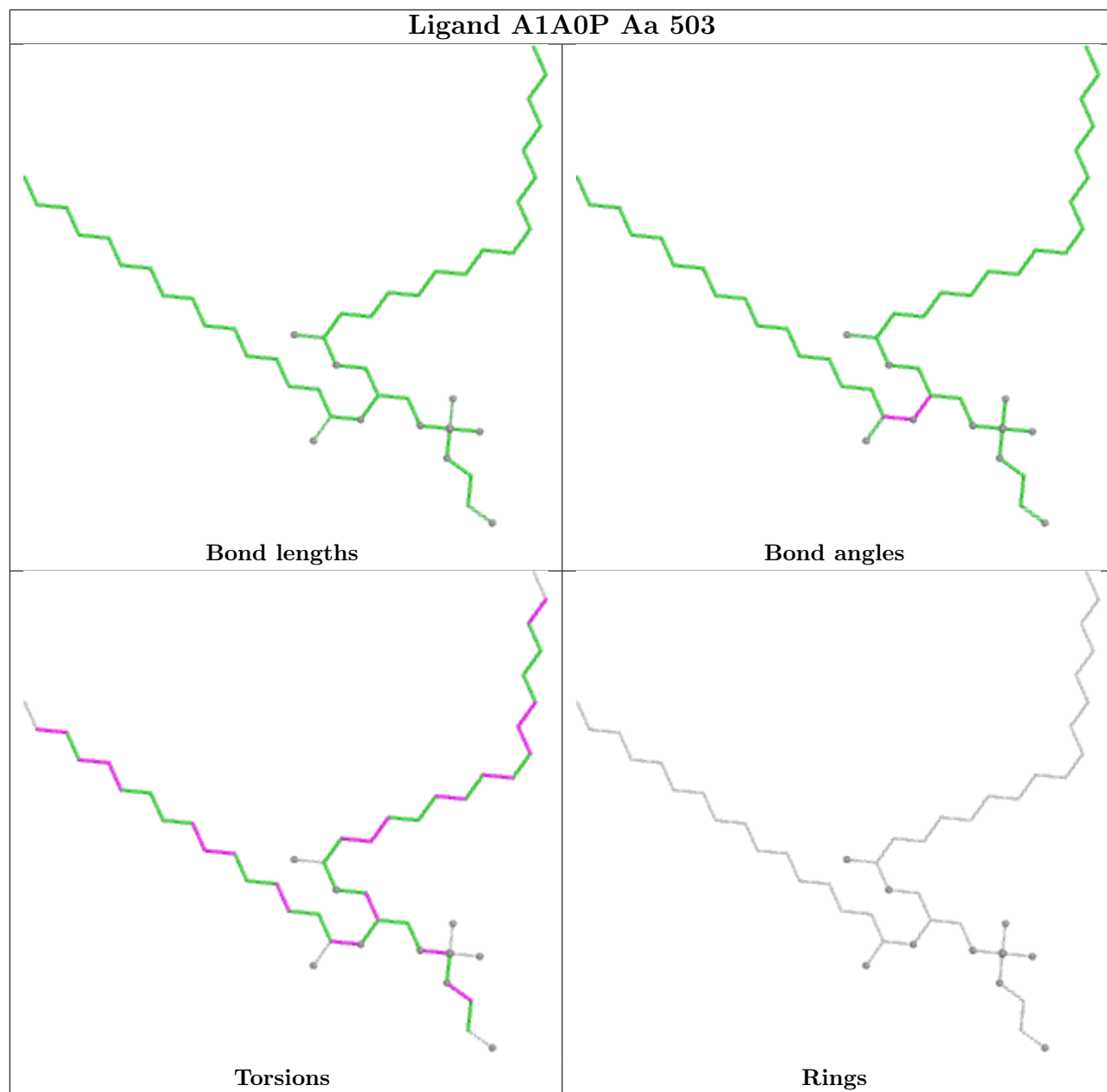


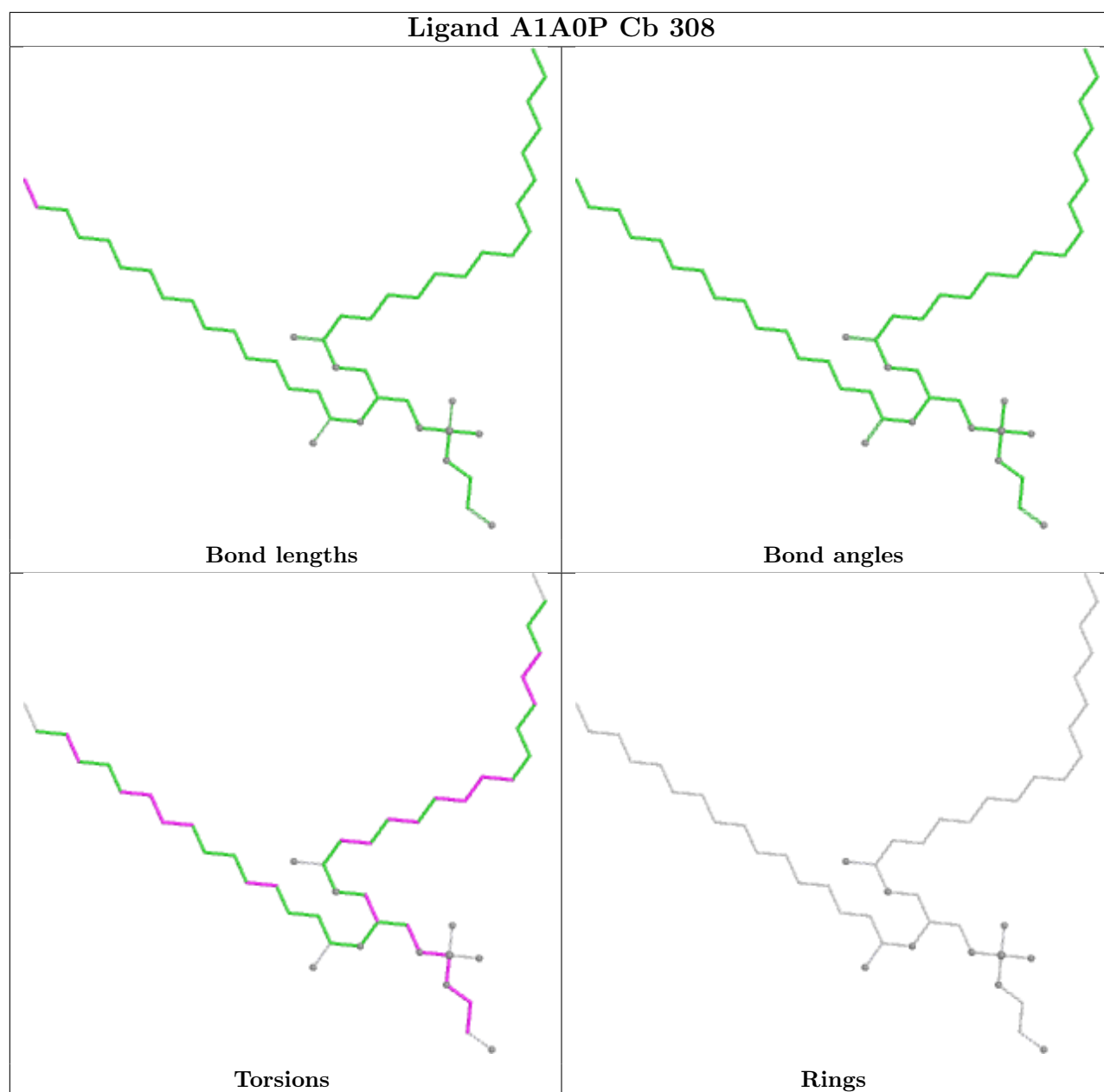


Ligand A1A0P Bc 307

 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>







## 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.

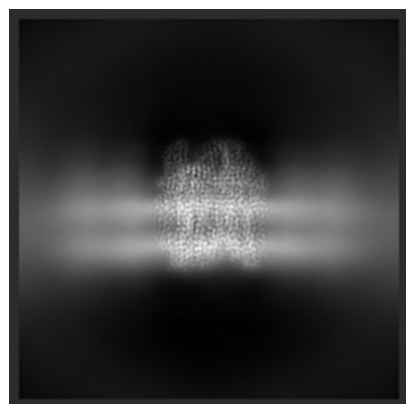
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45660. These allow visual inspection of the internal detail of the map and identification of artifacts.

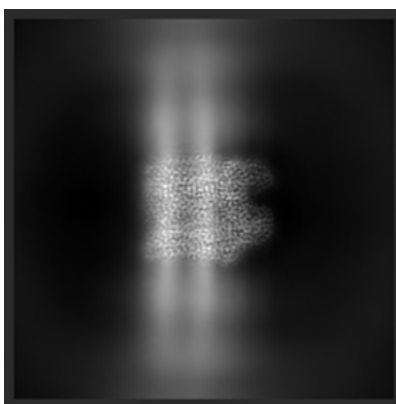
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

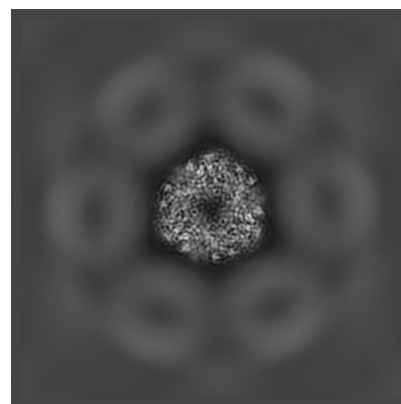
#### 6.1.1 Primary map



X

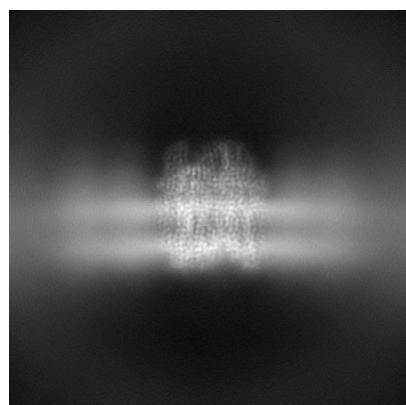


Y

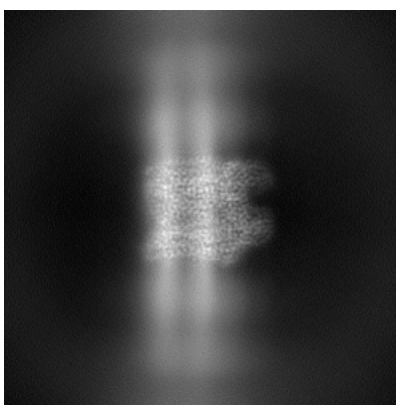


Z

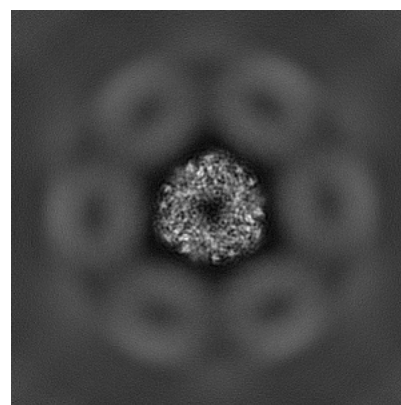
#### 6.1.2 Raw map



X



Y

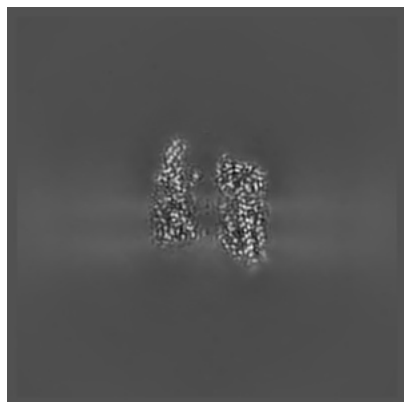


Z

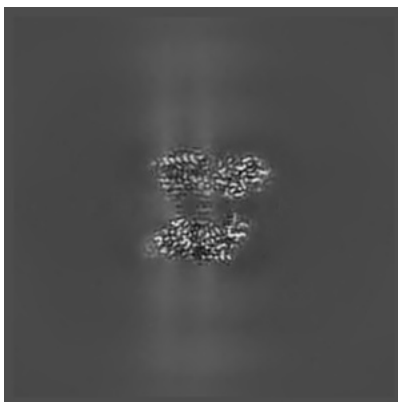
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

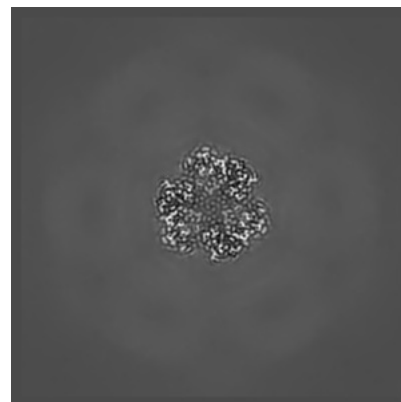
### 6.2.1 Primary map



X Index: 200

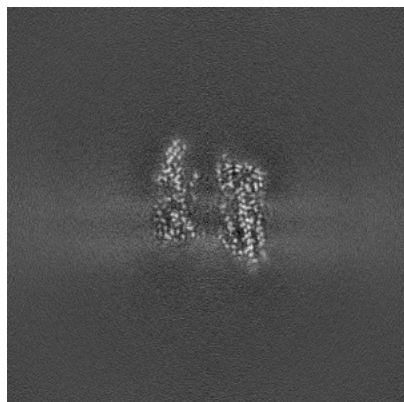


Y Index: 200

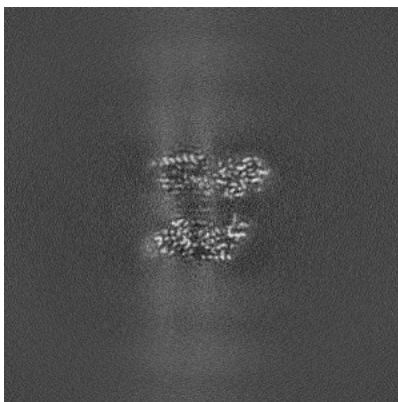


Z Index: 200

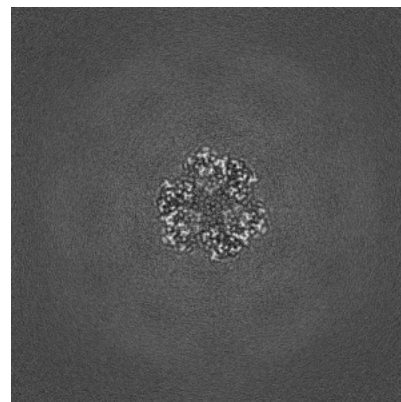
### 6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

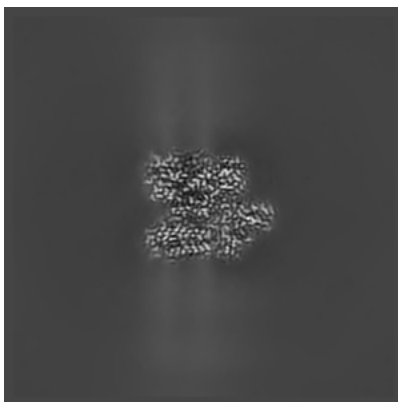
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

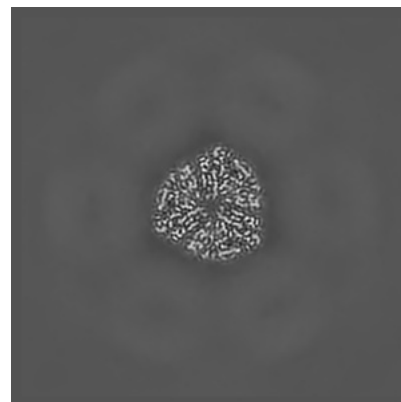
### 6.3.1 Primary map



X Index: 225

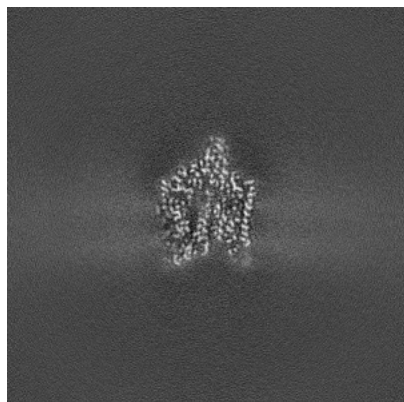


Y Index: 172

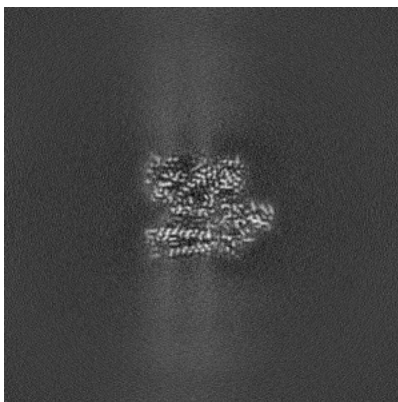


Z Index: 225

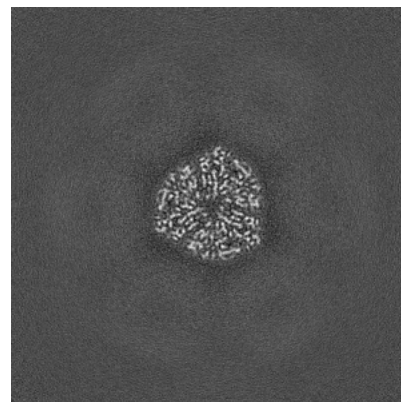
### 6.3.2 Raw map



X Index: 226



Y Index: 171

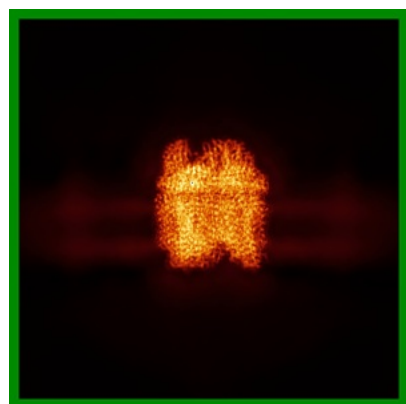


Z Index: 225

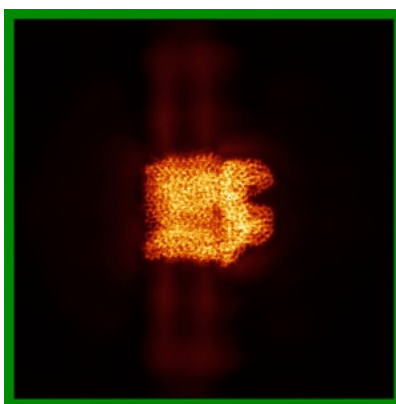
The images above show the largest variance slices of the map in three orthogonal directions.

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

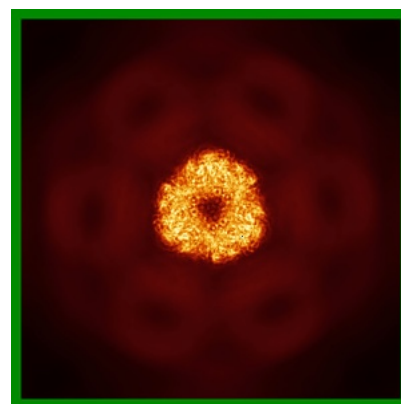
### 6.4.1 Primary map



X

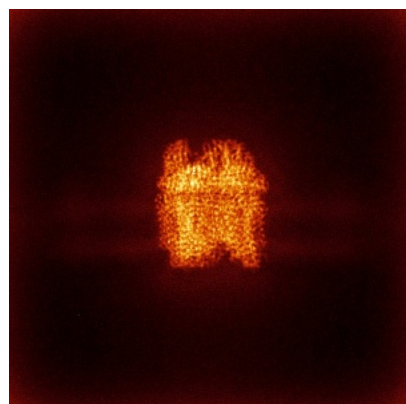


Y

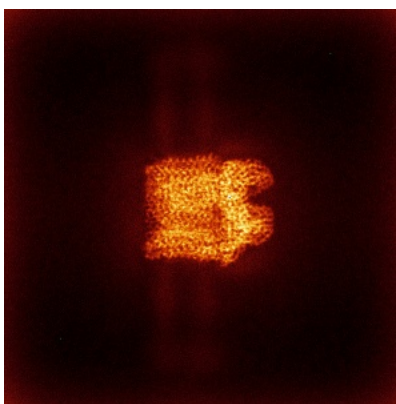


Z

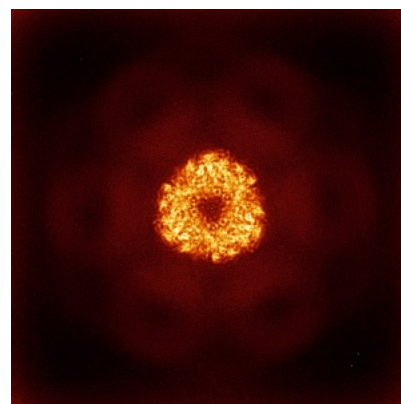
### 6.4.2 Raw map



X



Y

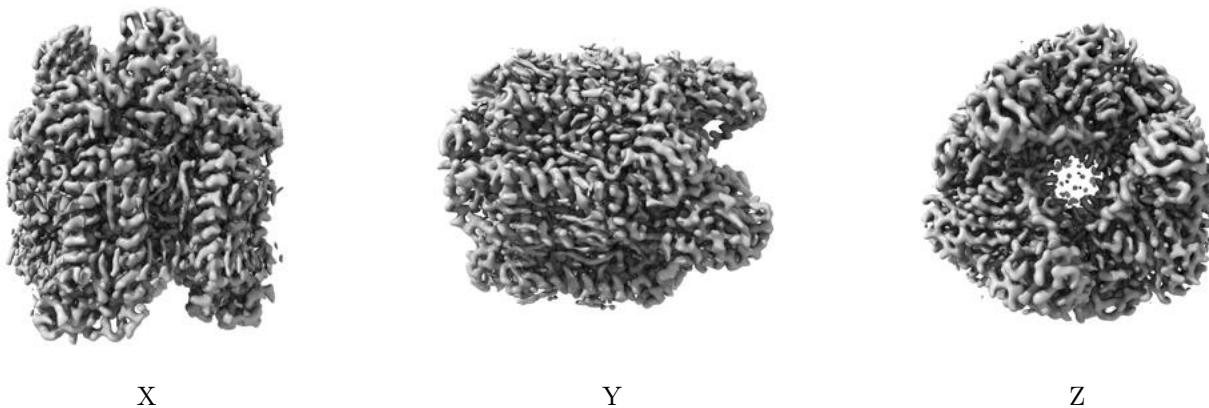


Z

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.

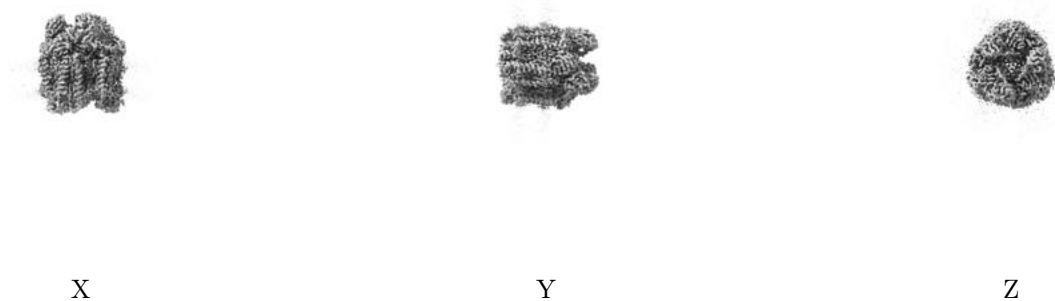
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.127. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

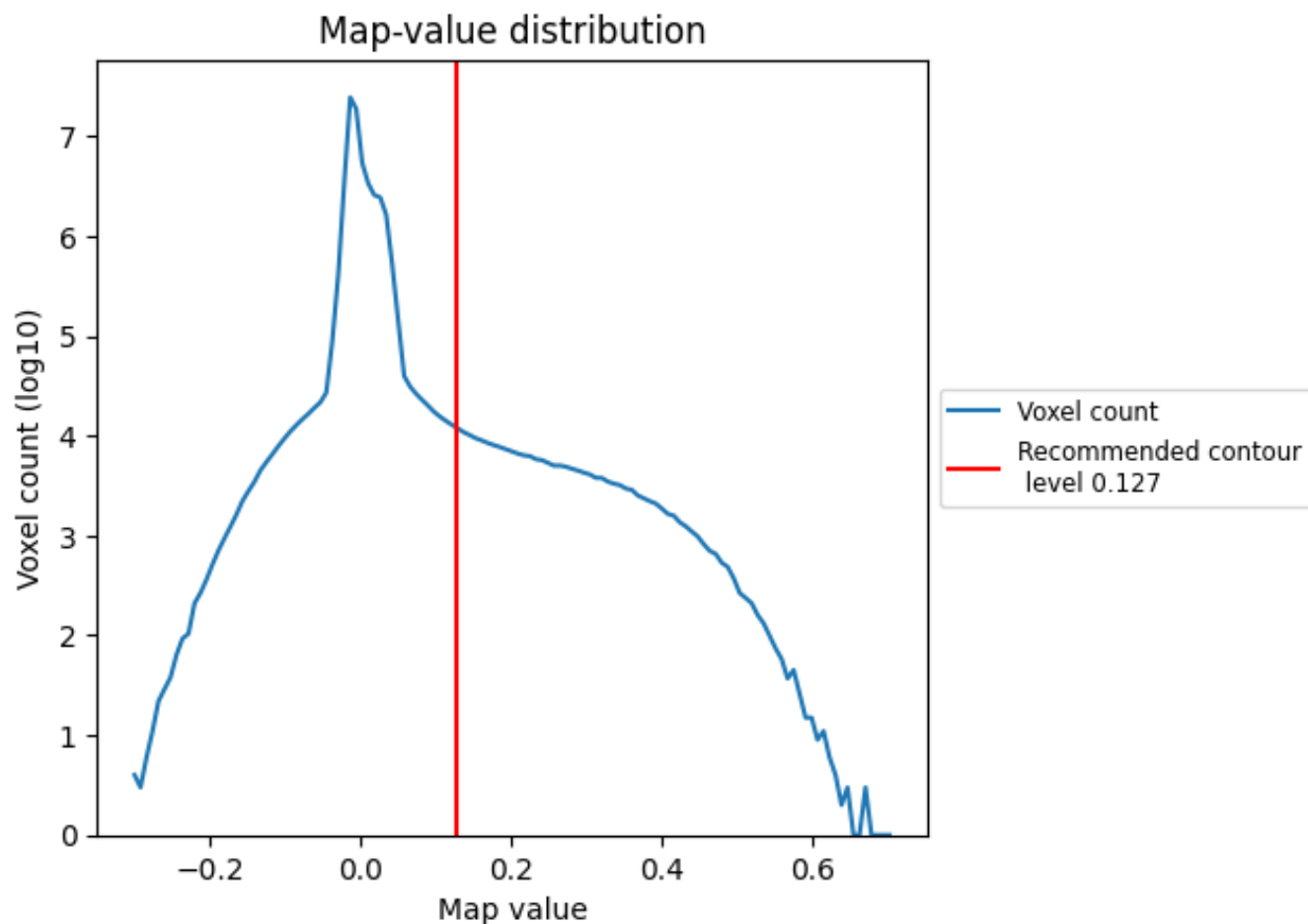
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

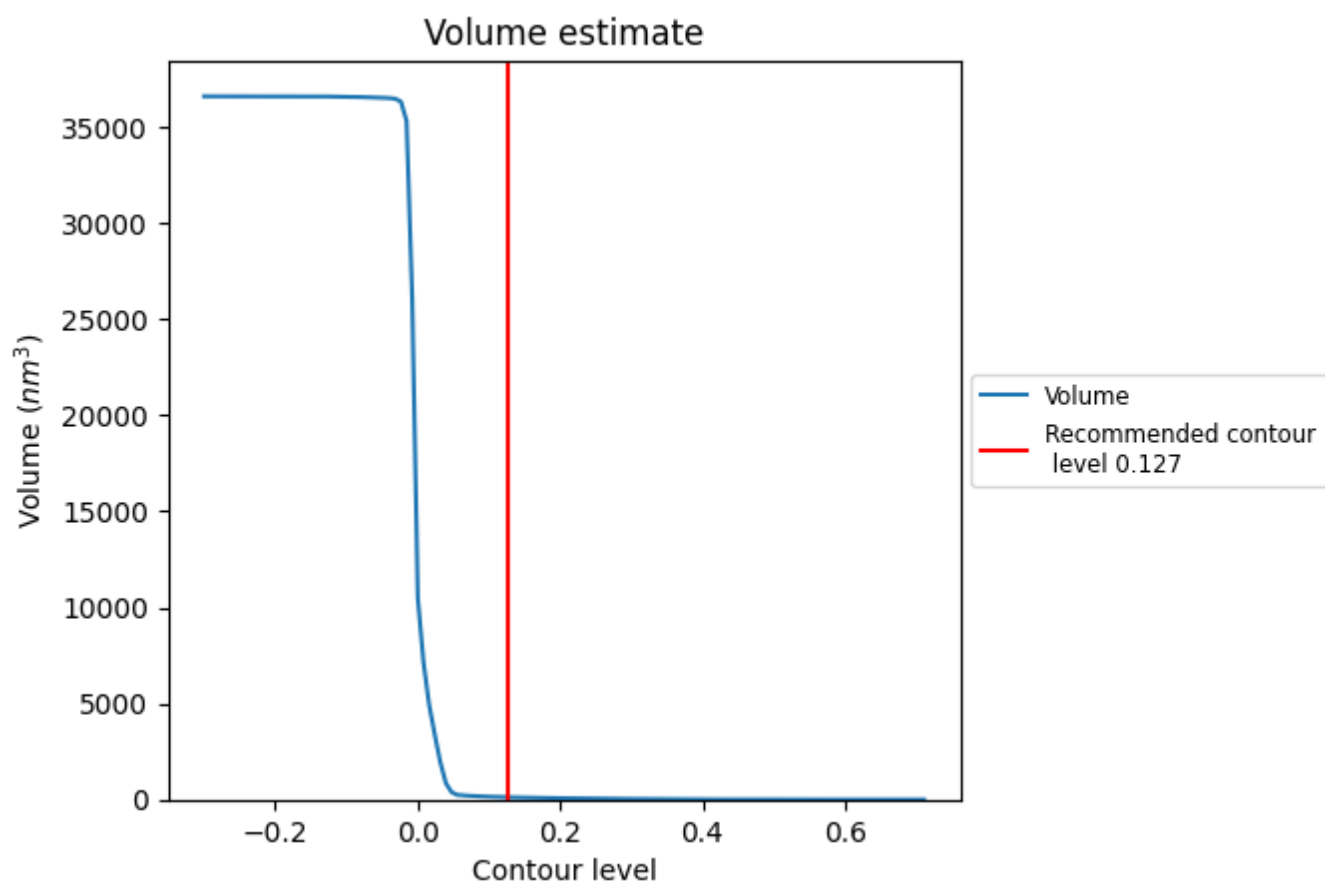
This section contains the results of statistical analysis of the map.

### 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.

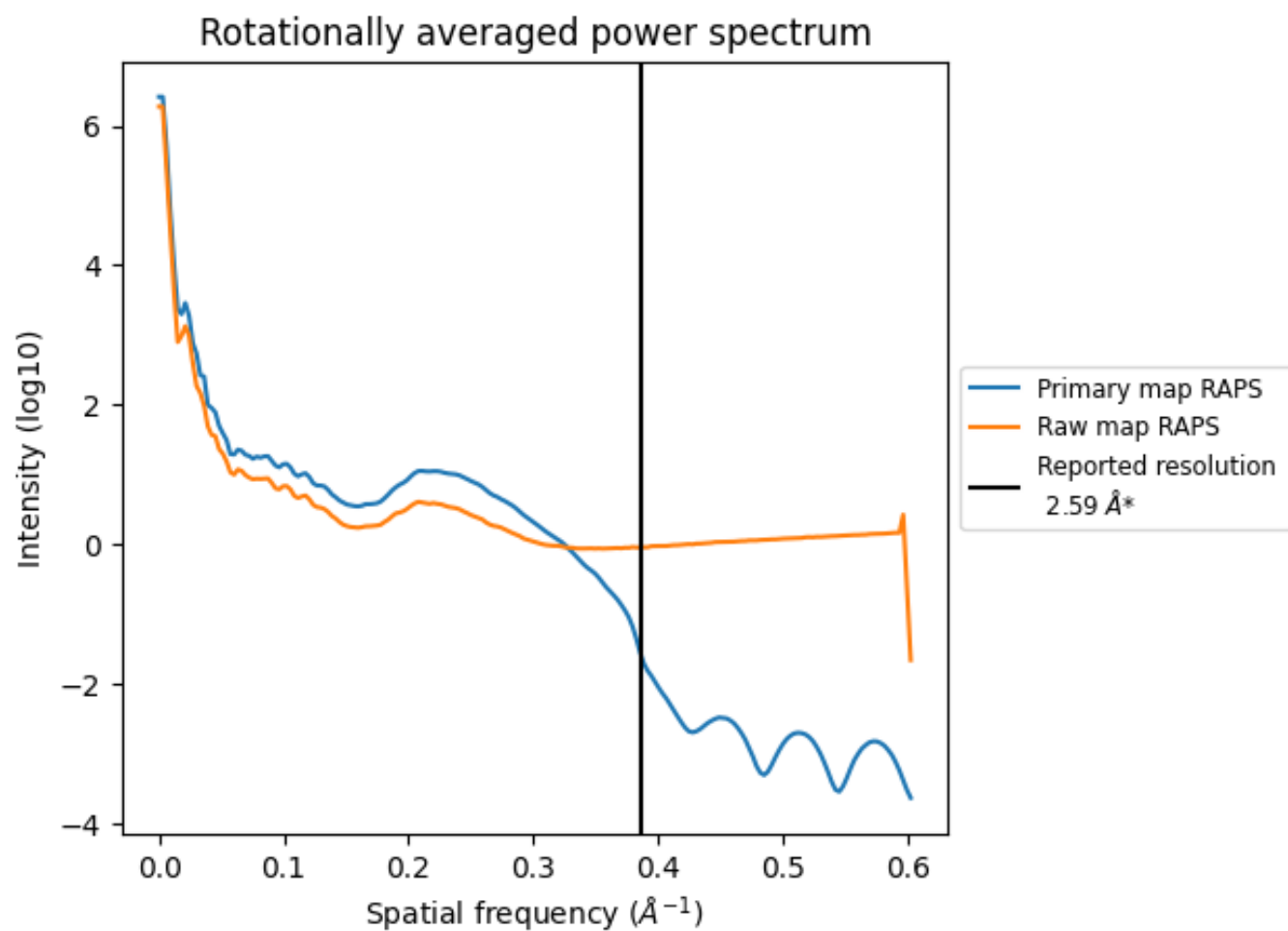
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 120  $\text{nm}^3$ ; this corresponds to an approximate mass of 108 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 ⓘ

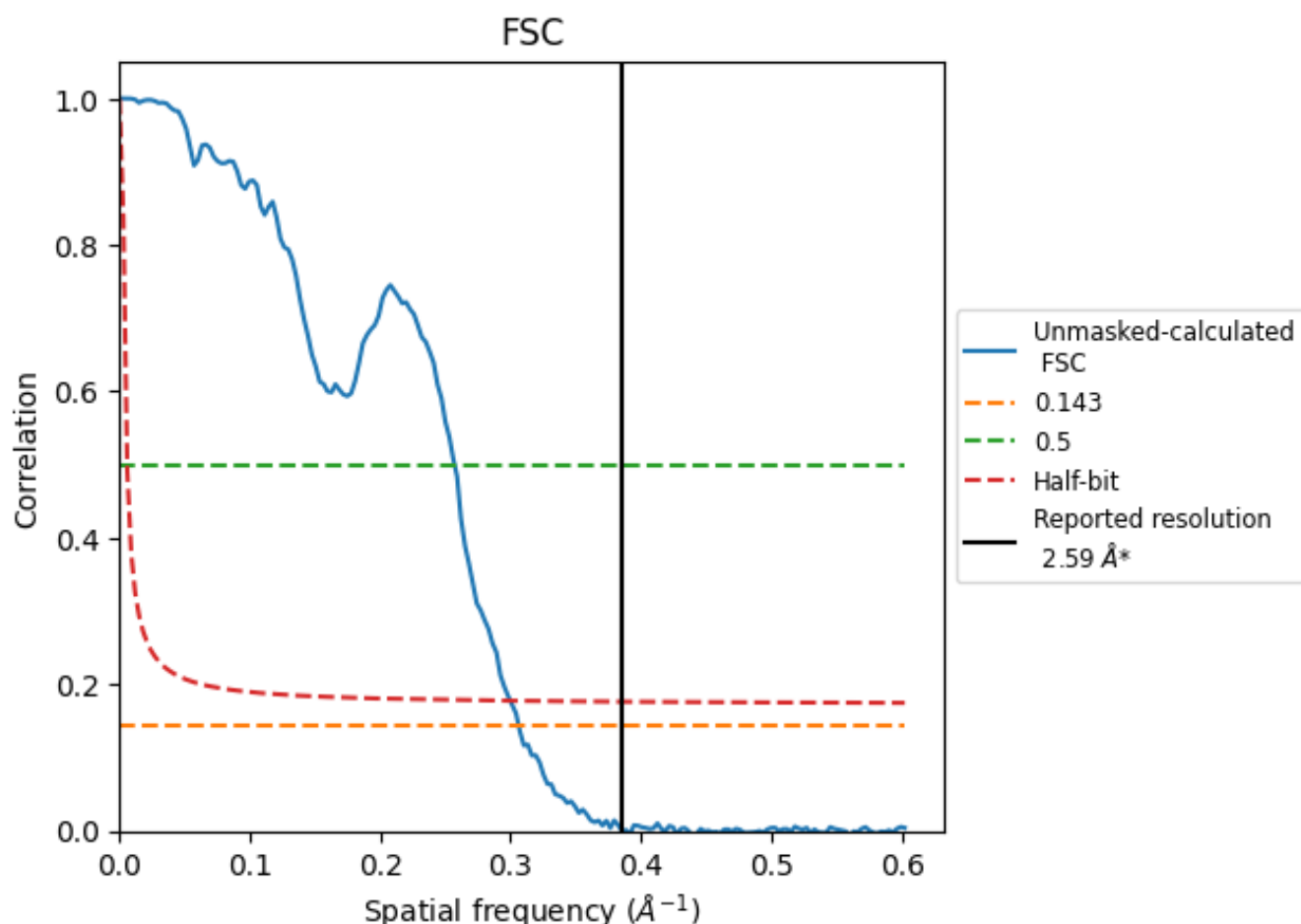


\*Reported resolution corresponds to spatial frequency of 0.386 Å<sup>-1</sup>

## 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 0.386 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

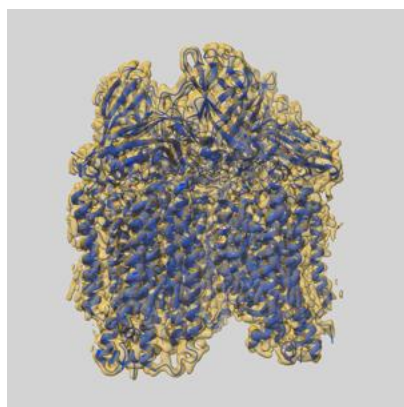
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.26	3.89	3.34

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.26 differs from the reported value 2.59 by more than 10 %

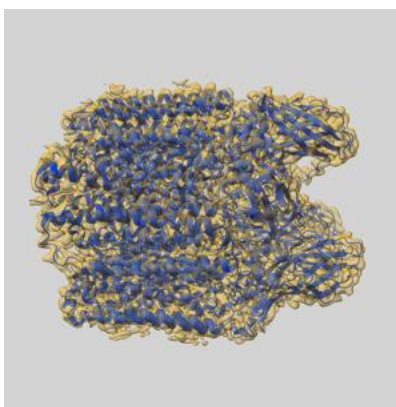
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45660 and PDB model 9CL3. Per-residue inclusion information can be found in section [3](#) on page [9](#).

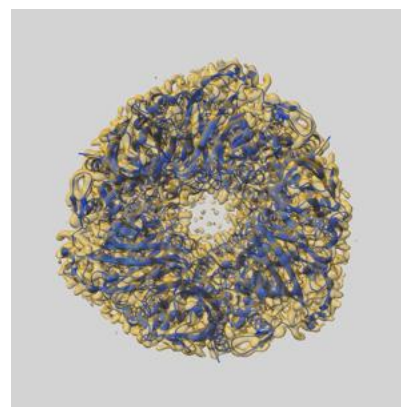
### 9.1 Map-model overlay [i](#)



X



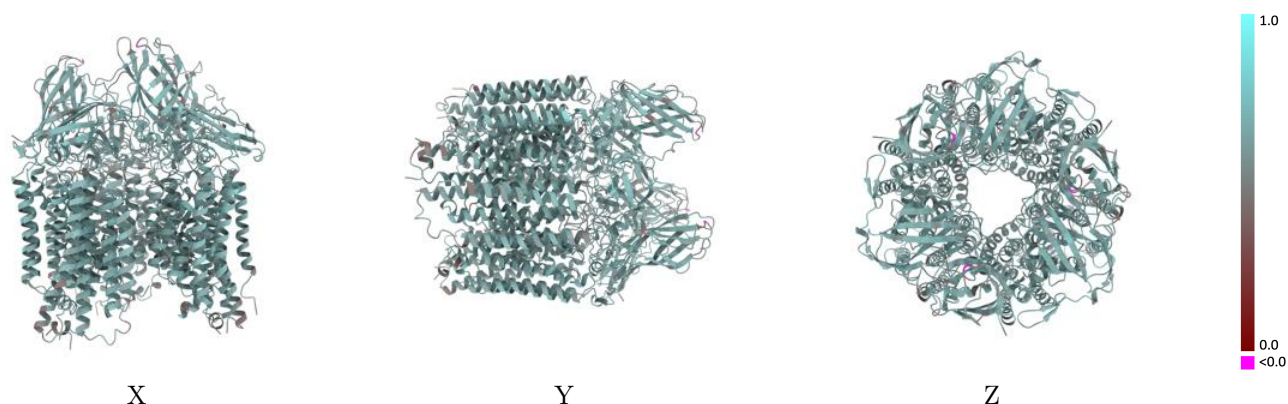
Y



Z

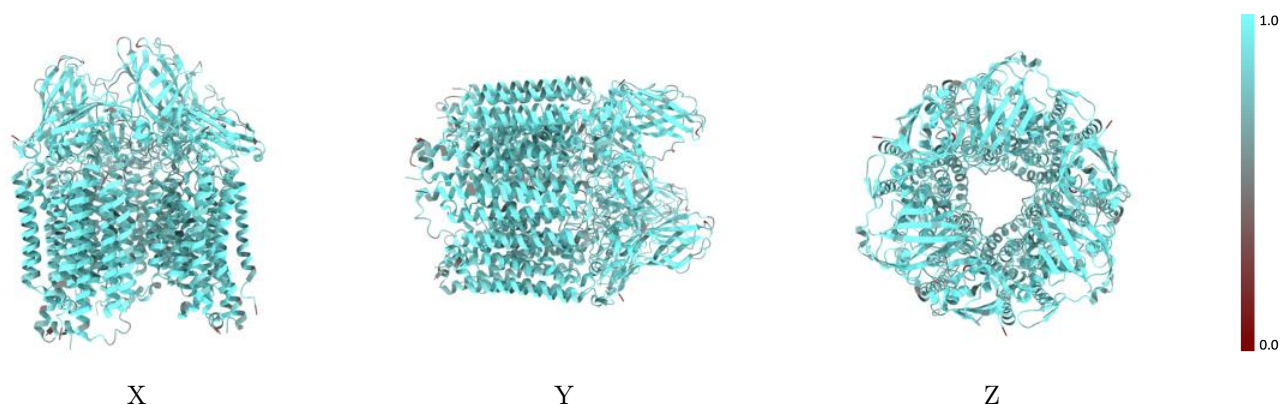
The images above show the 3D surface view of the map at the recommended contour level 0.127 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



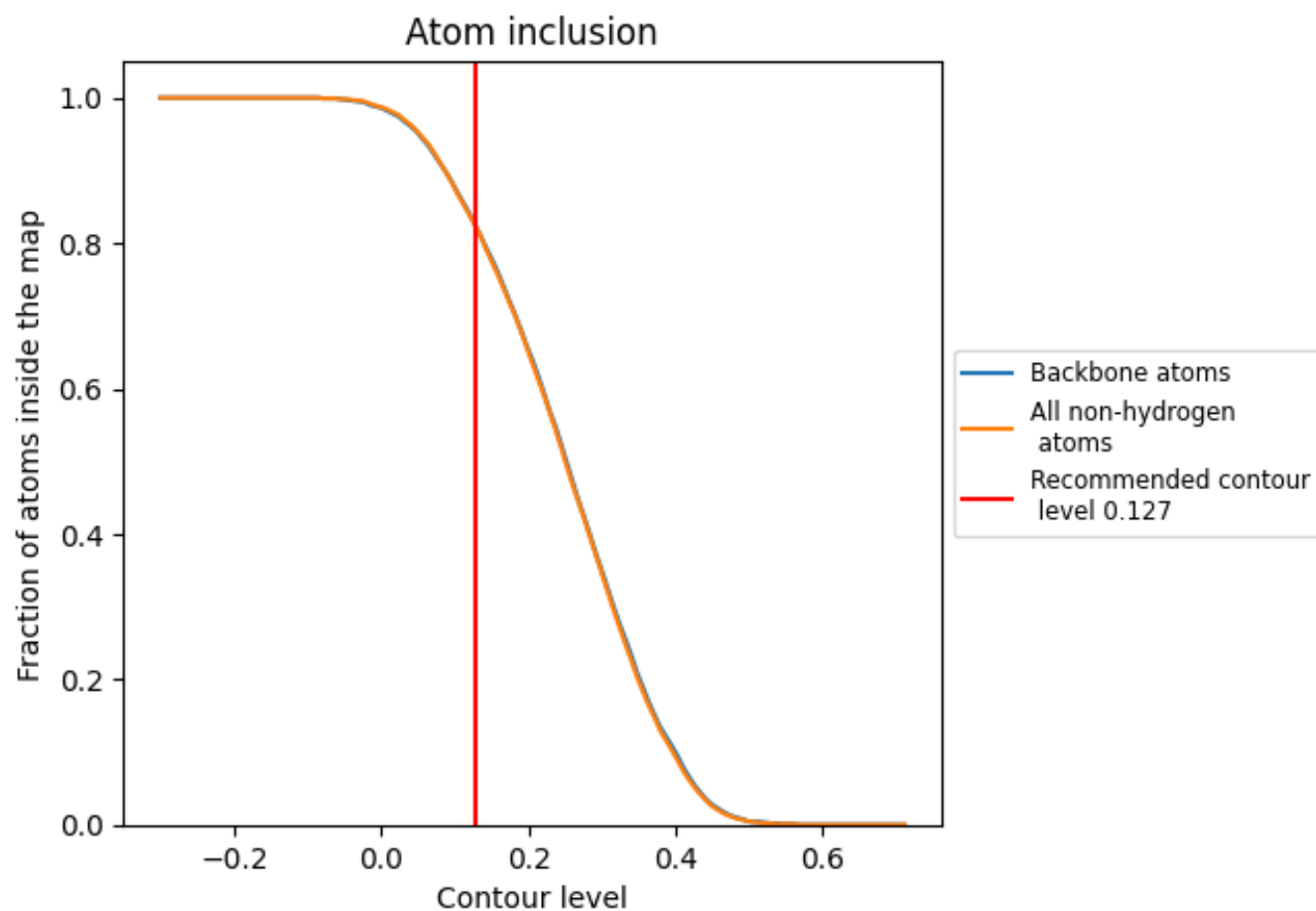
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.127).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.127) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8250	<div><div></div></div> 0.5760
Aa	<div><div></div></div> 0.8600	<div><div></div></div> 0.5960
Ab	<div><div></div></div> 0.8610	<div><div></div></div> 0.5950
Ac	<div><div></div></div> 0.8630	<div><div></div></div> 0.5950
Ba	<div><div></div></div> 0.7900	<div><div></div></div> 0.5600
Bb	<div><div></div></div> 0.7890	<div><div></div></div> 0.5580
Bc	<div><div></div></div> 0.7920	<div><div></div></div> 0.5580
Ca	<div><div></div></div> 0.8160	<div><div></div></div> 0.5690
Cb	<div><div></div></div> 0.8190	<div><div></div></div> 0.5690
Cc	<div><div></div></div> 0.8170	<div><div></div></div> 0.5690

1.0

0.0

<0.0