



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2026 – 12:30 PM JST

PDB ID : 9XK6 / pdb_00009xk6
EMDB ID : EMD-66949
Title : In situ C2S2M2L4-type PSII-LHCII supercomplex, strongly bound (S-) LHCII trimer with CP26, protomer 1
Authors : Li, J.; Elias, E.; Zhang, K.; Croce, R.; Zhu, J.
Deposited on : 2025-11-05
Resolution : 3.27 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

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:

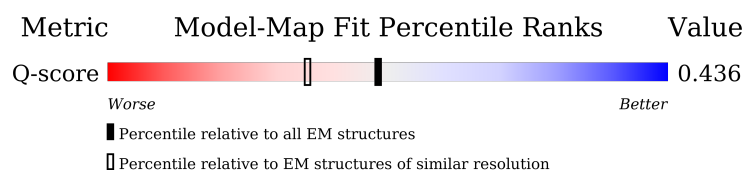
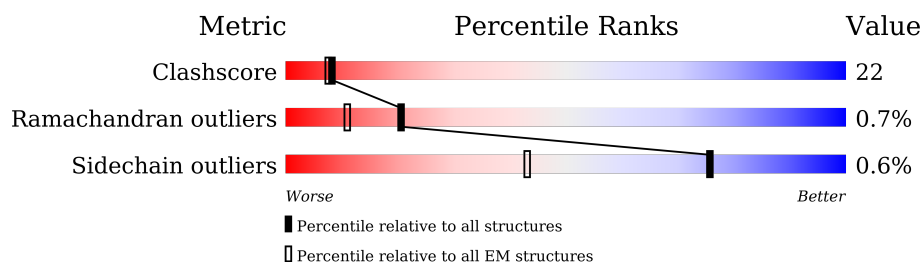
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.51

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 3.27 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	14508 (2.77 - 3.77)

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	00	219	
1	1G	219	
1	1N	219	
2	1S	218	

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	CLA	00	301	X	-	-	-
3	CLA	00	302	X	-	-	-
3	CLA	00	309	X	-	-	-
3	CLA	00	310	X	-	-	-
3	CLA	00	311	X	-	-	-
3	CLA	00	319	X	-	-	-
3	CLA	1G	602	X	-	-	-
3	CLA	1G	603	X	-	-	-
3	CLA	1G	610	X	-	-	-
3	CLA	1G	612	X	-	-	-
3	CLA	1N	602	X	-	-	-
3	CLA	1N	603	X	-	-	-
3	CLA	1N	613	X	-	-	-
3	CLA	1S	308	X	-	-	-
3	CLA	1S	309	X	-	-	-
3	CLA	1S	311	X	-	-	-
4	CHL	00	306	X	-	-	-
4	CHL	00	307	X	-	-	-
4	CHL	00	308	X	-	-	-
4	CHL	1G	601	X	-	X	-
4	CHL	1G	607	X	-	X	-
4	CHL	1G	609	X	-	-	-
4	CHL	1N	601	X	-	X	-
4	CHL	1N	607	X	-	-	-
4	CHL	1N	609	X	-	-	-
5	LUT	1G	616	-	-	X	-

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 10406 atoms, of which 0 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.

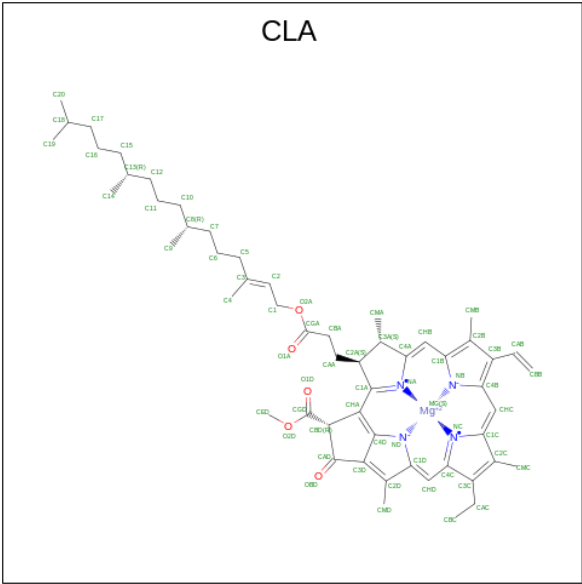
- Molecule 1 is a protein called Chlorophyll a-b binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	00	219	Total	C	N	O	S	0	0
			1659	1079	269	306	5		
1	1G	219	Total	C	N	O	S	0	0
			1659	1079	269	306	5		
1	1N	219	Total	C	N	O	S	0	0
			1652	1073	269	305	5		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1S	218	Total	C	N	O	S	0	0
			1661	1079	269	308	5		

- Molecule 3 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



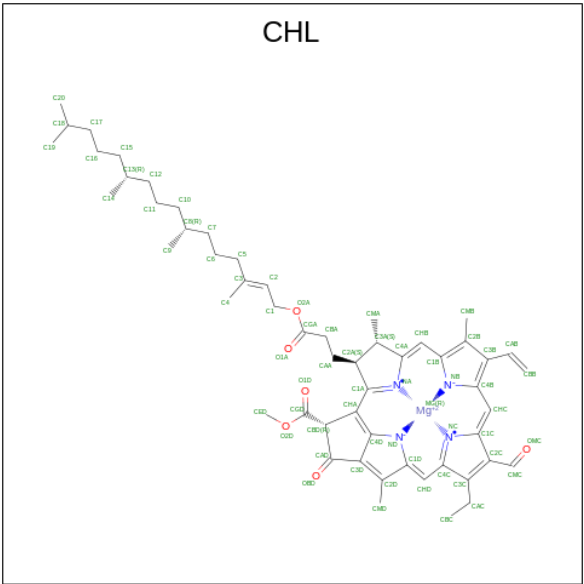
Mol	Chain	Residues	Atoms					AltConf
3	00	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	00	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	00	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
3	00	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	00	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	00	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	00	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
3	00	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
3	1G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	1G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	1G	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
3	1G	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
3	1G	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
3	1G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	1G	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
3	1G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
3	1N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	1N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
3	1N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
3	1N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
3	1N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
3	1N	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
3	1N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	1N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
3	1S	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
3	1S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
3	1S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	1S	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
3	1S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
3	1S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	1S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
3	1S	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	1S	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

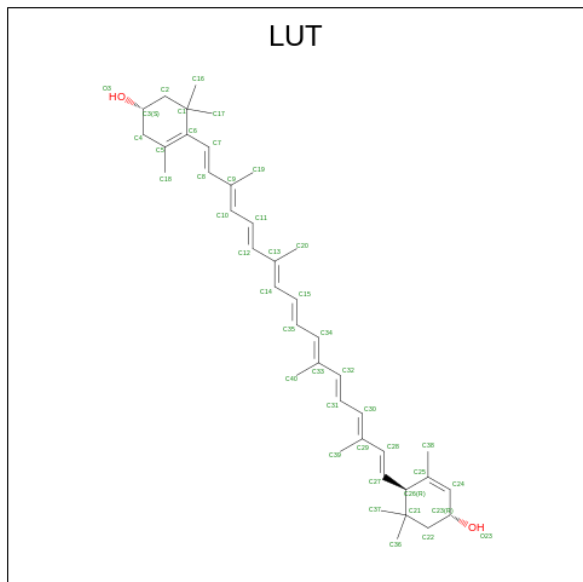
- Molecule 4 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	00	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
4	00	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
4	00	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	00	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	00	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	1G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	1G	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
4	1G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	1G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	1G	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
4	1G	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
4	1N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	1N	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
4	1N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	1N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	1N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
4	1N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
4	1S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	1S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	1S	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
4	1S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 5 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTE

NE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	00	1	Total	C	O	0
			42	40	2	
5	00	1	Total	C	O	0
			42	40	2	
5	1G	1	Total	C	O	0
			42	40	2	
5	1G	1	Total	C	O	0
			42	40	2	
5	1N	1	Total	C	O	0
			42	40	2	
5	1S	1	Total	C	O	0
			42	40	2	
5	1S	1	Total	C	O	0
			42	40	2	

- Molecule 6 is (2R)-2,5,7,8-TETRAMETHYL-2-[(4R,8R)-4,8,12-TRIMETHYLTRIDECYL]CHROMAN-6-OL (CCD ID: VIV) (formula: $C_{29}H_{50}O_2$).



Mol	Chain	Residues	Atoms			AltConf
6	00	1	Total	C	O	0
			27	25	2	

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



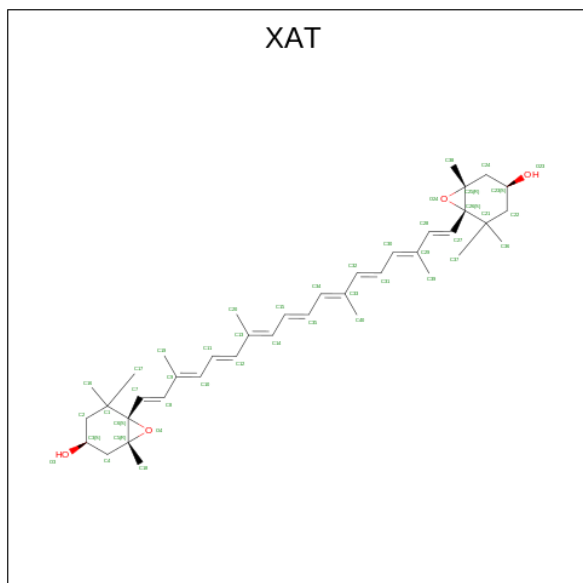
Mol	Chain	Residues	Atoms				AltConf
7	00	1	Total 33	C 24	O 8	P 1	0
7	00	1	Total 49	C 38	O 10	P 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
7	00	1	Total	C	O	P	0
			49	38	10	1	
7	00	1	Total	C	O	P	0
			49	38	10	1	
7	1G	1	Total	C	O	P	0
			41	30	10	1	
7	1N	1	Total	C	O	P	0
			43	32	10	1	
7	1N	1	Total	C	O	P	0
			48	37	10	1	
7	1S	1	Total	C	O		0
			29	24	5		
7	1S	1	Total	C	O	P	0
			31	20	10	1	
7	1S	1	Total	C	O	P	0
			40	31	8	1	
7	1S	1	Total	C	O	P	0
			32	23	8	1	

- Molecule 8 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



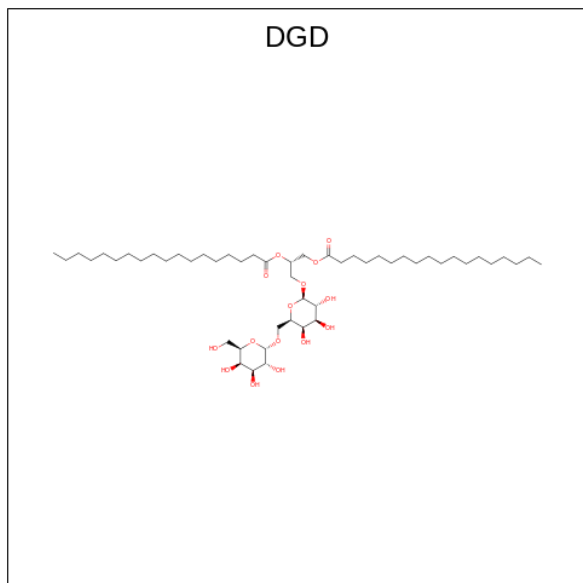
Mol	Chain	Residues	Atoms				AltConf
8	1G	1	Total	C	O		0
			44	40	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	1G	1	44	40	4	0

- Molecule 9 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

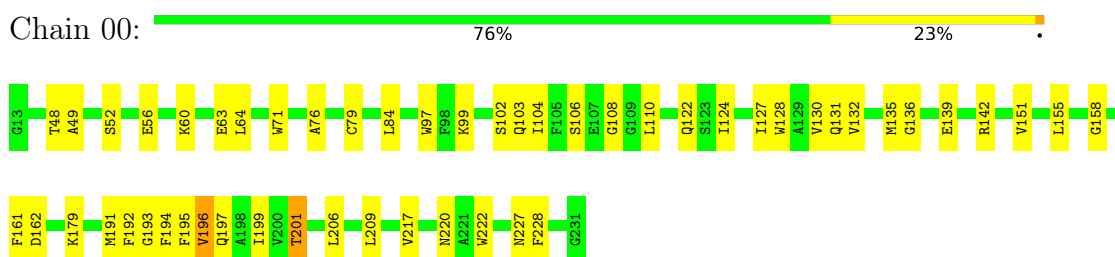


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
9	1S	1	46	31	15	0

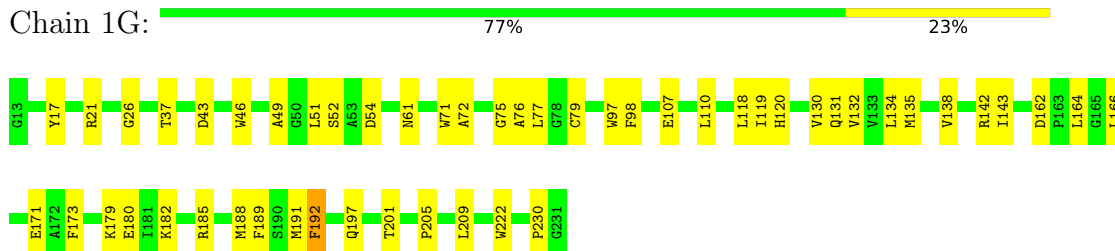
3 Residue-property plots

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.

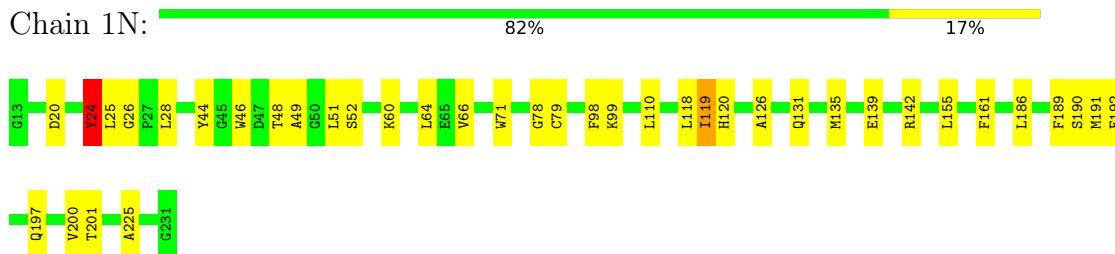
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



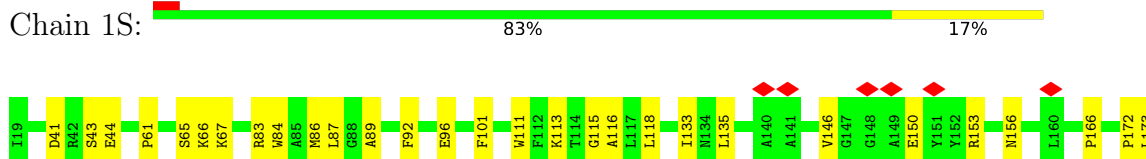
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



E189	M200	Q206	L218	L230	L231	T232	S235	G236
	L201							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	172752	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 ($e^-/\text{\AA}^2$)	1.375	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.794	Depositor
Minimum map value	-0.533	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.012	Depositor
Map size ($\text{\AA}$)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: VIV, CLA, DGD, CHL, LHG, XAT, LUT

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	00	0.24	0/1710	0.46	0/2332
1	1G	0.22	0/1710	0.45	0/2332
1	1N	0.25	0/1702	0.52	2/2321 (0.1%)
2	1S	0.22	0/1706	0.47	0/2322
All	All	0.23	0/6828	0.48	2/9307 (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
1	1G	0	1
1	1N	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1N	24	TYR	CA-C-N	-5.48	111.08	121.54
1	1N	24	TYR	C-N-CA	-5.48	111.08	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1G	192	PHE	Peptide
1	1N	192	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	1N	24	TYR	Peptide

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	00	1659	0	1598	57	0
1	1G	1659	0	1598	71	0
1	1N	1652	0	1589	49	0
2	1S	1661	0	1612	44	0
3	00	471	0	459	26	0
3	1G	422	0	382	23	0
3	1N	405	0	360	19	0
3	1S	447	0	361	12	0
4	00	296	0	280	69	0
4	1G	324	0	284	79	0
4	1N	331	0	299	85	0
4	1S	180	0	120	25	0
5	00	84	0	112	33	0
5	1G	84	0	112	42	0
5	1N	42	0	56	20	0
5	1S	84	0	112	33	0
6	00	27	0	38	5	0
7	00	180	0	259	5	0
7	1G	41	0	55	8	0
7	1N	91	0	128	7	0
7	1S	132	0	162	2	0
8	1G	88	0	112	36	0
9	1S	46	0	50	1	0
All	All	10406	0	10138	447	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 22.

The worst 5 of 447 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)
4:1S:305:CHL:HBB1	5:1S:316:LUT:H161	1.39	1.03
4:00:305:CHL:HBB1	5:00:314:LUT:H161	1.36	1.02
4:1N:606:CHL:HBB1	5:1N:615:LUT:H161	1.43	0.97
4:1G:609:CHL:HBB1	4:1N:601:CHL:H51	1.47	0.95
2:1S:218:LEU:HD13	5:1S:315:LUT:H163	1.47	0.95

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	00	217/219 (99%)	195 (90%)	22 (10%)	0	100	100
1	1G	217/219 (99%)	196 (90%)	18 (8%)	3 (1%)	9	34
1	1N	217/219 (99%)	189 (87%)	27 (12%)	1 (0%)	24	55
2	1S	216/218 (99%)	185 (86%)	29 (13%)	2 (1%)	14	43
All	All	867/875 (99%)	765 (88%)	96 (11%)	6 (1%)	20	48

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1S	66	LYS
1	1G	17	TYR
2	1S	156	ASN
1	1G	54	ASP
1	1N	119	ILE

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	00	166/166 (100%)	163 (98%)	3 (2%)	51	70
1	1G	166/166 (100%)	165 (99%)	1 (1%)	78	82
1	1N	165/166 (99%)	165 (100%)	0	100	100
2	1S	169/173 (98%)	169 (100%)	0	100	100
All	All	666/671 (99%)	662 (99%)	4 (1%)	76	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	00	97	TRP
1	00	196	VAL
1	00	201	THR
1	1G	173	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	00	103	GLN
1	1G	122	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](#)

76 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	$\# Z > 2$
9	DGD	1S	318	-	47,47,67	1.02	3 (6%)	61,61,81	0.98	3 (4%)
3	CLA	00	309	1	64,68,73	2.24	19 (29%)	77,107,113	2.97	28 (36%)
4	CHL	1N	607	-	70,74,74	1.91	18 (25%)	80,114,114	2.73	25 (31%)
4	CHL	1S	307	-	50,54,74	2.24	15 (30%)	56,90,114	3.17	21 (37%)
3	CLA	1G	604	-	45,49,73	2.64	19 (42%)	54,84,113	3.34	26 (48%)
7	LHG	1G	618	3	40,40,48	0.29	0	43,46,54	0.40	0
4	CHL	00	304	1	52,56,74	2.20	17 (32%)	58,92,114	3.15	24 (41%)
4	CHL	00	305	-	54,58,74	2.15	16 (29%)	59,94,114	3.12	24 (40%)
4	CHL	00	308	1	70,74,74	1.88	17 (24%)	80,114,114	2.73	26 (32%)
3	CLA	1S	309	7	60,64,73	2.26	20 (33%)	72,102,113	3.10	32 (44%)
4	CHL	1G	607	-	70,74,74	1.92	18 (25%)	80,114,114	2.73	26 (32%)
4	CHL	1N	605	1	46,50,74	2.37	19 (41%)	51,85,114	3.35	25 (49%)
4	CHL	1G	608	-	47,51,74	2.23	17 (36%)	52,86,114	3.28	25 (48%)
3	CLA	1N	612	-	46,50,73	2.54	19 (41%)	55,85,113	3.42	28 (50%)
7	LHG	1N	616	3	42,42,48	0.28	0	45,48,54	0.37	0
3	CLA	00	310	7	64,68,73	2.23	19 (29%)	77,107,113	2.98	28 (36%)
4	CHL	1G	601	-	70,74,74	1.89	16 (22%)	80,114,114	2.77	25 (31%)
3	CLA	00	311	-	64,68,73	2.21	19 (29%)	77,107,113	2.98	28 (36%)
4	CHL	1N	601	1	70,74,74	1.91	15 (21%)	80,114,114	2.72	26 (32%)
4	CHL	1S	305	-	50,54,74	2.26	16 (32%)	56,90,114	3.16	23 (41%)
3	CLA	1G	614	7	46,50,73	2.52	19 (41%)	55,85,113	3.39	26 (47%)
8	XAT	1G	619	-	39,47,47	0.89	0	54,74,74	3.13	23 (42%)
3	CLA	1N	604	-	54,58,73	2.42	20 (37%)	65,95,113	3.11	28 (43%)
3	CLA	1G	611	-	47,52,73	2.56	20 (42%)	56,88,113	3.37	25 (44%)
3	CLA	1S	314	-	50,54,73	2.51	20 (40%)	60,90,113	3.29	26 (43%)
7	LHG	1S	317	3	30,30,48	0.34	0	33,36,54	0.54	0
8	XAT	1G	617	-	39,47,47	0.79	0	54,74,74	3.13	25 (46%)
3	CLA	1G	602	1	69,73,73	2.14	21 (30%)	83,113,113	2.83	29 (34%)
4	CHL	1G	606	-	50,54,74	2.24	19 (38%)	56,90,114	3.17	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CHL	1G	609	1	65,69,74	1.97	17 (26%)	74,108,114	2.84	25 (33%)
5	LUT	00	313	-	42,43,43	1.67	8 (19%)	51,60,60	1.50	12 (23%)
5	LUT	1S	316	-	42,43,43	1.66	8 (19%)	51,60,60	1.56	10 (19%)
7	LHG	1S	301	-	28,28,48	0.32	0	30,30,54	1.11	2 (6%)
3	CLA	00	319	1	67,71,73	2.14	19 (28%)	80,110,113	2.89	26 (32%)
4	CHL	1S	302	2	50,54,74	2.27	17 (34%)	56,90,114	3.18	23 (41%)
3	CLA	1N	613	1	64,68,73	2.20	20 (31%)	77,107,113	2.84	29 (37%)
7	LHG	1S	319	-	39,39,48	0.35	0	42,44,54	1.01	2 (4%)
3	CLA	1G	613	1	52,56,73	2.46	19 (36%)	62,92,113	3.33	29 (46%)
3	CLA	1S	304	-	54,58,73	2.42	20 (37%)	65,95,113	3.11	29 (44%)
4	CHL	1N	608	-	49,53,74	2.18	17 (34%)	53,88,114	3.25	23 (43%)
4	CHL	1S	306	-	46,50,74	2.32	17 (36%)	51,85,114	3.28	22 (43%)
3	CLA	1G	610	1	66,70,73	2.23	20 (30%)	79,109,113	2.91	29 (36%)
3	CLA	00	301	1	69,73,73	2.13	19 (27%)	83,113,113	2.92	28 (33%)
4	CHL	1G	605	1	46,50,74	2.33	16 (34%)	51,85,114	3.30	22 (43%)
5	LUT	1G	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.95	10 (19%)
7	LHG	00	318	-	48,48,48	0.28	0	51,54,54	0.32	0
5	LUT	00	314	-	42,43,43	1.64	8 (19%)	51,60,60	1.53	11 (21%)
7	LHG	1S	320	-	31,31,48	0.42	0	35,36,54	0.71	2 (5%)
3	CLA	1N	611	7	45,49,73	2.64	20 (44%)	54,84,113	3.45	26 (48%)
3	CLA	1N	614	1	45,49,73	2.62	20 (44%)	54,84,113	3.44	26 (48%)
5	LUT	1S	315	-	42,43,43	1.63	8 (19%)	51,60,60	1.48	11 (21%)
3	CLA	1G	612	1	59,63,73	2.32	20 (33%)	71,101,113	3.03	30 (42%)
3	CLA	1N	602	-	69,73,73	2.13	19 (27%)	83,113,113	2.87	29 (34%)
4	CHL	1N	606	-	50,54,74	2.23	18 (36%)	56,90,114	3.11	24 (42%)
3	CLA	1S	311	2	59,63,73	2.30	19 (32%)	71,101,113	3.03	29 (40%)
4	CHL	1N	609	1	70,74,74	1.90	19 (27%)	80,114,114	2.67	26 (32%)
4	CHL	00	307	-	70,74,74	1.88	18 (25%)	80,114,114	2.73	26 (32%)
3	CLA	1N	603	-	69,73,73	2.13	21 (30%)	83,113,113	2.88	30 (36%)
7	LHG	00	316	3	32,32,48	0.32	0	35,37,54	0.40	0
3	CLA	1S	303	2	45,49,73	2.63	20 (44%)	54,84,113	3.44	27 (50%)
6	VIV	00	315	-	28,28,32	0.55	1 (3%)	36,40,45	0.87	2 (5%)
7	LHG	00	317	-	48,48,48	0.27	0	51,54,54	1.04	3 (5%)
7	LHG	00	320	-	48,48,48	0.27	0	51,54,54	0.39	0
3	CLA	00	303	-	54,58,73	2.40	20 (37%)	65,95,113	3.08	28 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLA	1S	312	2	53,57,73	2.46	20 (37%)	62,93,113	3.25	28 (45%)
3	CLA	00	302	-	69,73,73	2.15	20 (28%)	83,113,113	2.91	28 (33%)
3	CLA	1G	603	-	69,73,73	2.15	20 (28%)	83,113,113	2.83	29 (34%)
3	CLA	00	312	1	50,54,73	2.48	19 (38%)	60,90,113	3.28	27 (45%)
3	CLA	1S	308	2	59,63,73	2.34	19 (32%)	71,101,113	3.00	29 (40%)
4	CHL	00	306	-	70,74,74	1.89	19 (27%)	80,114,114	2.79	24 (30%)
5	LUT	1G	615	-	42,43,43	1.71	8 (19%)	51,60,60	1.56	9 (17%)
5	LUT	1N	615	-	42,43,43	1.60	8 (19%)	51,60,60	1.46	9 (17%)
7	LHG	1N	617	-	47,47,48	0.28	0	50,53,54	0.48	1 (2%)
3	CLA	1N	610	1	45,49,73	2.60	19 (42%)	54,84,113	3.35	25 (46%)
3	CLA	1S	313	2	50,54,73	2.60	21 (42%)	60,90,113	3.40	25 (41%)
3	CLA	1S	310	2	53,57,73	2.46	20 (37%)	62,93,113	3.30	26 (41%)

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
9	DGD	1S	318	-	-	11/35/75/95	0/2/2/2
3	CLA	00	309	1	1/1/14/20	10/33/109/115	-
4	CHL	1S	307	-	-	9/17/93/117	-
3	CLA	1G	604	-	-	4/10/86/115	-
7	LHG	1G	618	3	-	6/45/45/53	-
4	CHL	00	304	1	-	12/20/96/117	-
4	CHL	00	308	1	1/1/15/21	17/41/117/117	-
4	CHL	00	305	-	-	8/22/98/117	-
3	CLA	1S	309	7	1/1/13/20	12/29/105/115	-
4	CHL	1N	605	1	-	8/12/88/117	-
4	CHL	1G	608	-	-	6/14/90/117	-
3	CLA	1N	612	-	-	3/12/88/115	-
7	LHG	1N	616	3	-	2/47/47/53	-
3	CLA	00	310	7	1/1/14/20	9/33/109/115	-
4	CHL	1G	601	-	1/1/15/21	22/41/117/117	-
3	CLA	00	311	-	1/1/14/20	9/33/109/115	-
4	CHL	1N	601	1	1/1/15/21	20/41/117/117	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHL	1S	305	-	-	9/17/93/117	-
3	CLA	1G	614	7	-	2/12/88/115	-
8	XAT	1G	619	-	-	7/31/93/93	0/4/4/4
3	CLA	1N	604	-	-	4/21/97/115	-
3	CLA	1G	611	-	-	2/13/89/115	-
3	CLA	1S	314	-	-	2/17/93/115	-
7	LHG	1S	317	3	-	8/35/35/53	-
8	XAT	1G	617	-	-	7/31/93/93	0/4/4/4
3	CLA	1G	602	1	1/1/15/20	15/39/115/115	-
4	CHL	1G	606	-	-	5/17/93/117	-
4	CHL	1G	609	1	1/1/14/21	19/35/111/117	-
5	LUT	00	313	-	-	2/29/67/67	0/2/2/2
5	LUT	1S	316	-	-	2/29/67/67	0/2/2/2
7	LHG	1S	301	-	-	5/30/30/53	-
3	CLA	00	319	1	1/1/15/20	13/33/109/115	-
4	CHL	1S	302	2	-	11/17/93/117	-
3	CLA	1N	613	1	1/1/14/20	9/33/109/115	-
7	LHG	1S	319	-	-	6/43/43/53	-
3	CLA	1G	613	1	-	7/19/95/115	-
3	CLA	1S	304	-	-	8/21/97/115	-
4	CHL	1N	608	-	-	4/15/92/117	-
4	CHL	1S	306	-	-	6/12/88/117	-
3	CLA	1G	610	1	1/1/14/20	9/36/112/115	-
3	CLA	00	301	1	1/1/15/20	8/39/115/115	-
4	CHL	1G	605	1	-	6/12/88/117	-
5	LUT	1G	616	-	-	0/29/67/67	0/2/2/2
7	LHG	00	318	-	-	21/53/53/53	-
5	LUT	00	314	-	-	2/29/67/67	0/2/2/2
7	LHG	1S	320	-	-	10/33/33/53	-
3	CLA	1N	611	7	-	3/10/86/115	-
3	CLA	1N	614	1	-	3/10/86/115	-
5	LUT	1S	315	-	-	3/29/67/67	0/2/2/2
3	CLA	1S	313	2	-	0/17/93/115	-
3	CLA	1G	612	1	1/1/13/20	12/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	1N	602	-	1/1/15/20	7/39/115/115	-
4	CHL	1N	609	1	1/1/15/21	18/41/117/117	-
3	CLA	1S	311	2	1/1/13/20	10/27/103/115	-
4	CHL	1N	606	-	-	6/17/93/117	-
4	CHL	00	307	-	1/1/15/21	20/41/117/117	-
3	CLA	1N	603	-	1/1/15/20	20/39/115/115	-
7	LHG	00	316	3	-	2/36/36/53	-
3	CLA	1S	303	2	-	2/10/86/115	-
6	VIV	00	315	-	-	9/15/26/30	0/2/2/2
7	LHG	00	317	-	-	9/53/53/53	-
7	LHG	00	320	-	-	11/53/53/53	-
3	CLA	00	303	-	-	4/21/97/115	-
3	CLA	1S	312	2	-	6/20/96/115	-
3	CLA	00	302	-	1/1/15/20	13/39/115/115	-
3	CLA	1G	603	-	1/1/15/20	8/39/115/115	-
3	CLA	1S	308	2	1/1/13/20	4/27/103/115	-
4	CHL	00	306	-	1/1/15/21	27/41/117/117	-
3	CLA	00	312	1	-	5/17/93/115	-
5	LUT	1G	615	-	-	2/29/67/67	0/2/2/2
5	LUT	1N	615	-	-	2/29/67/67	0/2/2/2
3	CLA	1S	310	2	-	5/20/96/115	-
7	LHG	1N	617	-	-	15/52/52/53	-
3	CLA	1N	610	1	-	3/10/86/115	-
4	CHL	1N	607	-	1/1/15/21	21/41/117/117	-
4	CHL	1G	607	-	1/1/15/21	22/41/117/117	-

The worst 5 of 1070 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1G	612	CLA	C1D-ND	8.66	1.48	1.37
3	1S	313	CLA	C1D-ND	8.65	1.48	1.37
3	1S	310	CLA	C1D-ND	8.60	1.48	1.37
3	1N	611	CLA	C1D-ND	8.54	1.48	1.37
3	1N	612	CLA	C1D-ND	8.48	1.48	1.37

The worst 5 of 1558 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1N	605	CHL	C2B-C1B-NB	10.65	117.37	110.23
3	1S	313	CLA	C1D-ND-C4D	-10.63	98.78	106.33
4	00	307	CHL	C2B-C1B-NB	10.55	117.30	110.23
3	1N	602	CLA	C1D-ND-C4D	-10.50	98.88	106.33
4	1S	302	CHL	C2B-C1B-NB	10.48	117.26	110.23

5 of 25 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	00	301	CLA	C8
3	00	302	CLA	C8
3	00	309	CLA	C8
3	00	310	CLA	C8
3	00	311	CLA	C8

5 of 649 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	00	303	CLA	CBD-CGD-O2D-CED
3	00	303	CLA	O1D-CGD-O2D-CED
3	00	310	CLA	CBA-CGA-O2A-C1
3	00	319	CLA	CHA-CBD-CGD-O1D
3	00	319	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

63 monomers are involved in 392 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	1S	318	DGD	1	0
3	00	309	CLA	3	0
4	1N	607	CHL	14	0
4	1S	307	CHL	4	0
3	1G	604	CLA	2	0
7	1G	618	LHG	8	0
4	00	304	CHL	4	0
4	00	305	CHL	20	0
4	00	308	CHL	17	0
4	1G	607	CHL	23	0
4	1N	605	CHL	7	0
4	1G	608	CHL	3	0
7	1N	616	LHG	4	0
4	1G	601	CHL	30	0
3	00	311	CLA	1	0

Continued on next page...

Continued from previous page...

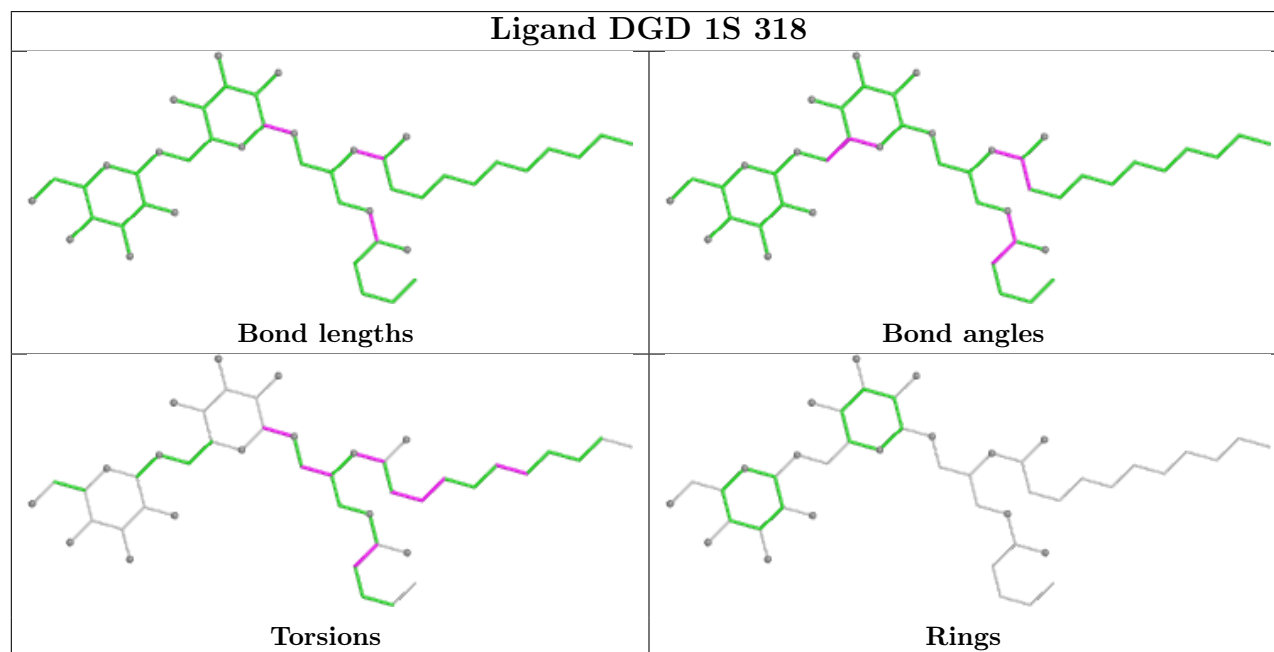
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	1N	601	CHL	33	0
4	1S	305	CHL	10	0
3	1G	614	CLA	1	0
8	1G	619	XAT	16	0
3	1N	604	CLA	1	0
3	1G	611	CLA	1	0
3	1S	314	CLA	3	0
7	1S	317	LHG	2	0
8	1G	617	XAT	20	0
3	1G	602	CLA	6	0
4	1G	606	CHL	11	0
4	1G	609	CHL	14	0
5	00	313	LUT	13	0
5	1S	316	LUT	16	0
3	00	319	CLA	3	0
4	1S	302	CHL	3	0
3	1S	304	CLA	1	0
4	1N	608	CHL	4	0
4	1S	306	CHL	9	0
3	1G	610	CLA	4	0
3	00	301	CLA	4	0
4	1G	605	CHL	2	0
5	1G	616	LUT	24	0
7	00	318	LHG	4	0
5	00	314	LUT	20	0
3	1N	611	CLA	1	0
5	1S	315	LUT	17	0
3	1G	612	CLA	7	0
3	1N	602	CLA	8	0
4	1N	606	CHL	17	0
3	1S	311	CLA	1	0
4	1N	609	CHL	15	0
4	00	307	CHL	16	0
3	1N	603	CLA	8	0
3	1S	303	CLA	1	0
6	00	315	VIV	5	0
7	00	320	LHG	1	0
3	00	303	CLA	4	0
3	00	302	CLA	8	0
3	1G	603	CLA	2	0
3	00	312	CLA	4	0
3	1S	308	CLA	5	0

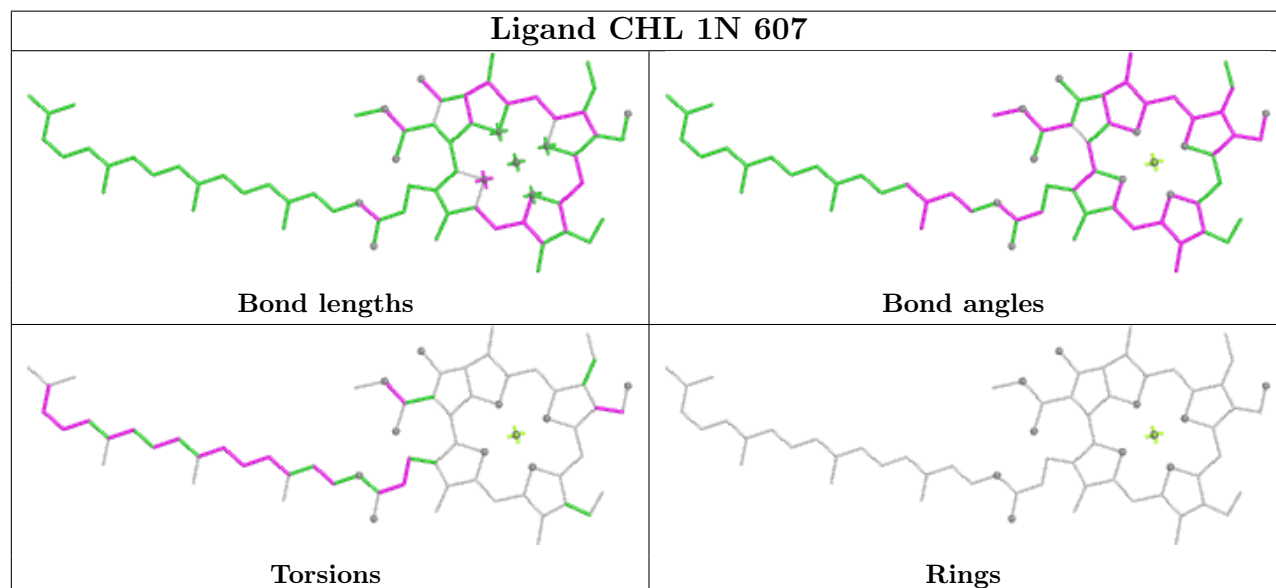
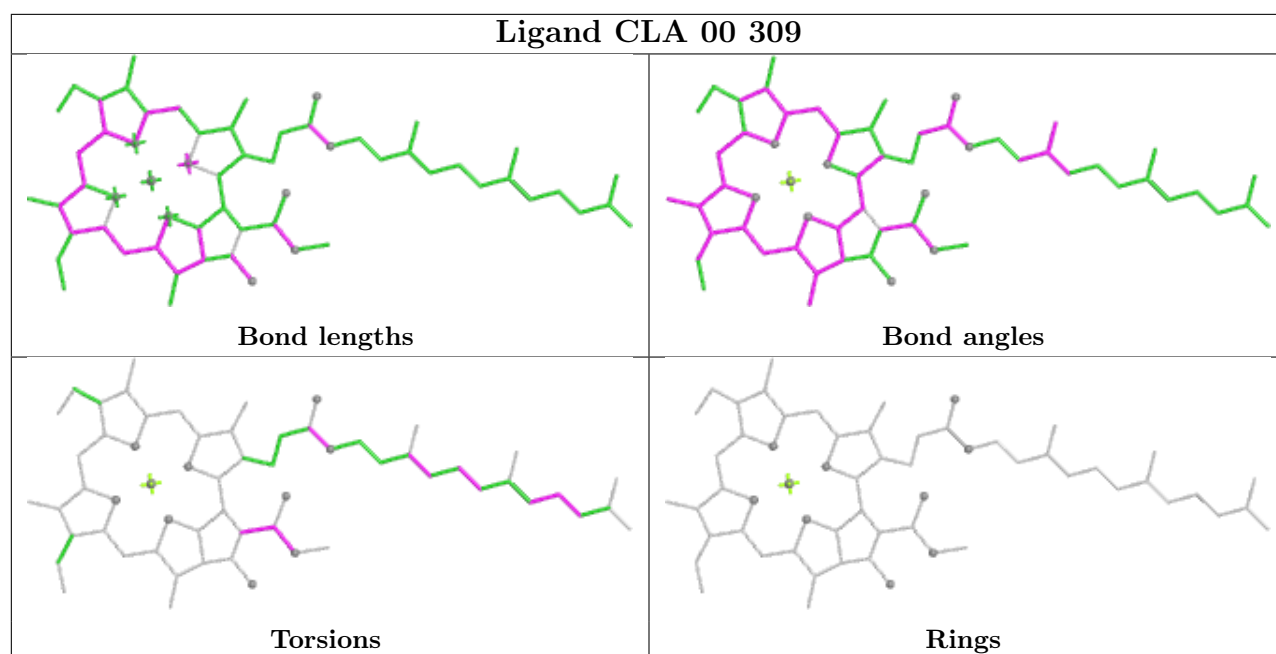
Continued on next page...

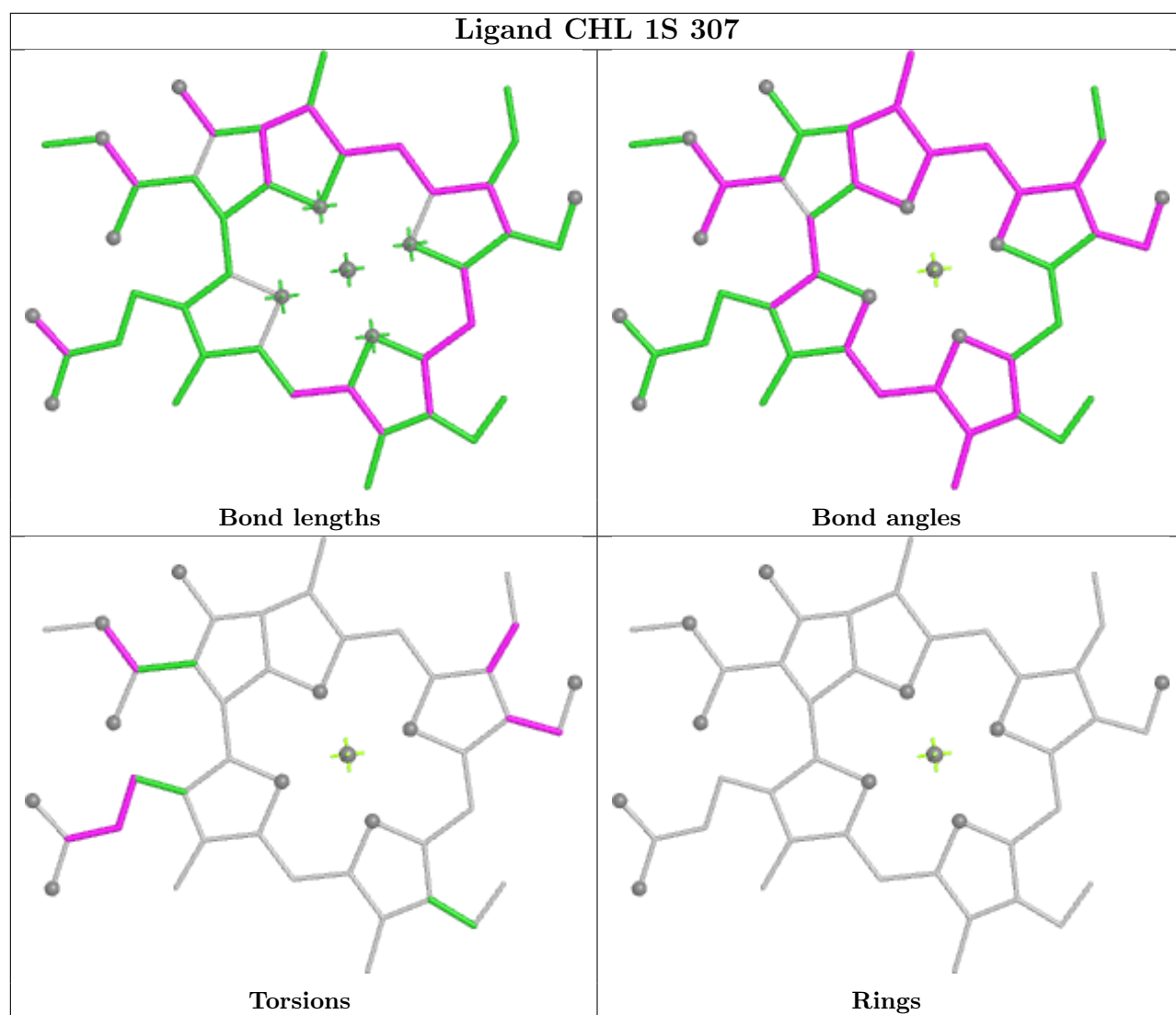
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	00	306	CHL	19	0
5	1G	615	LUT	18	0
5	1N	615	LUT	20	0
7	1N	617	LHG	3	0
3	1N	610	CLA	1	0
3	1S	310	CLA	2	0

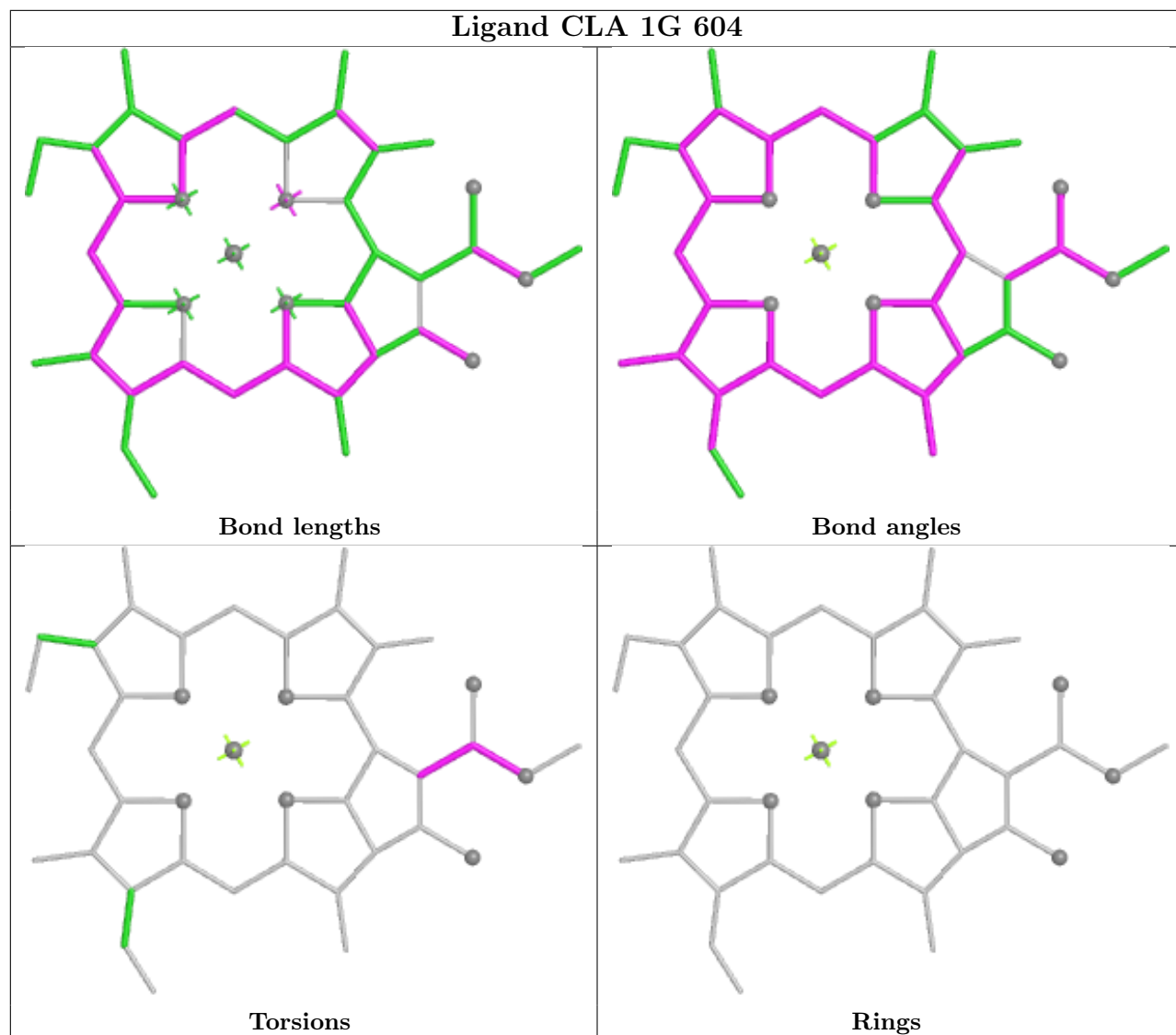
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

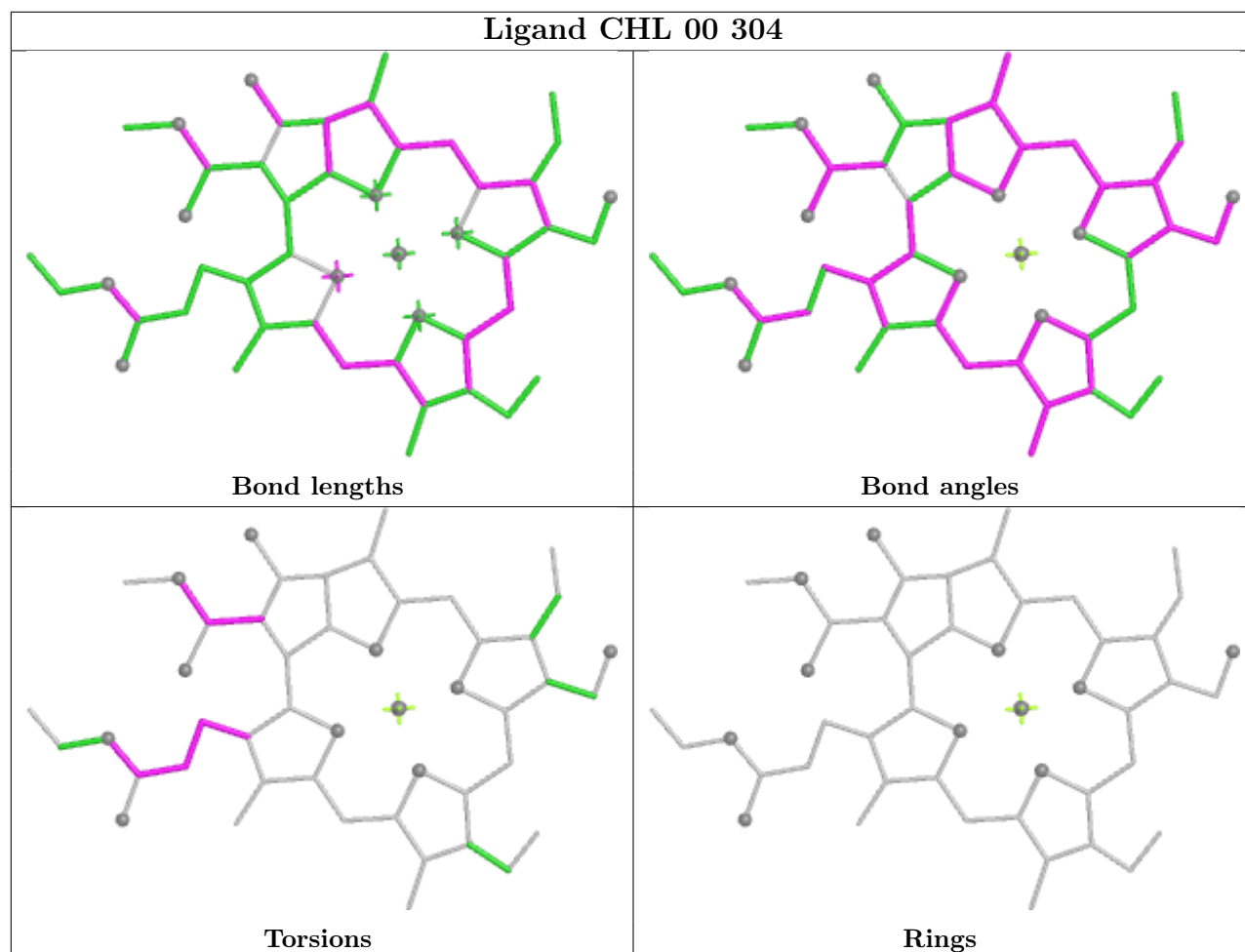
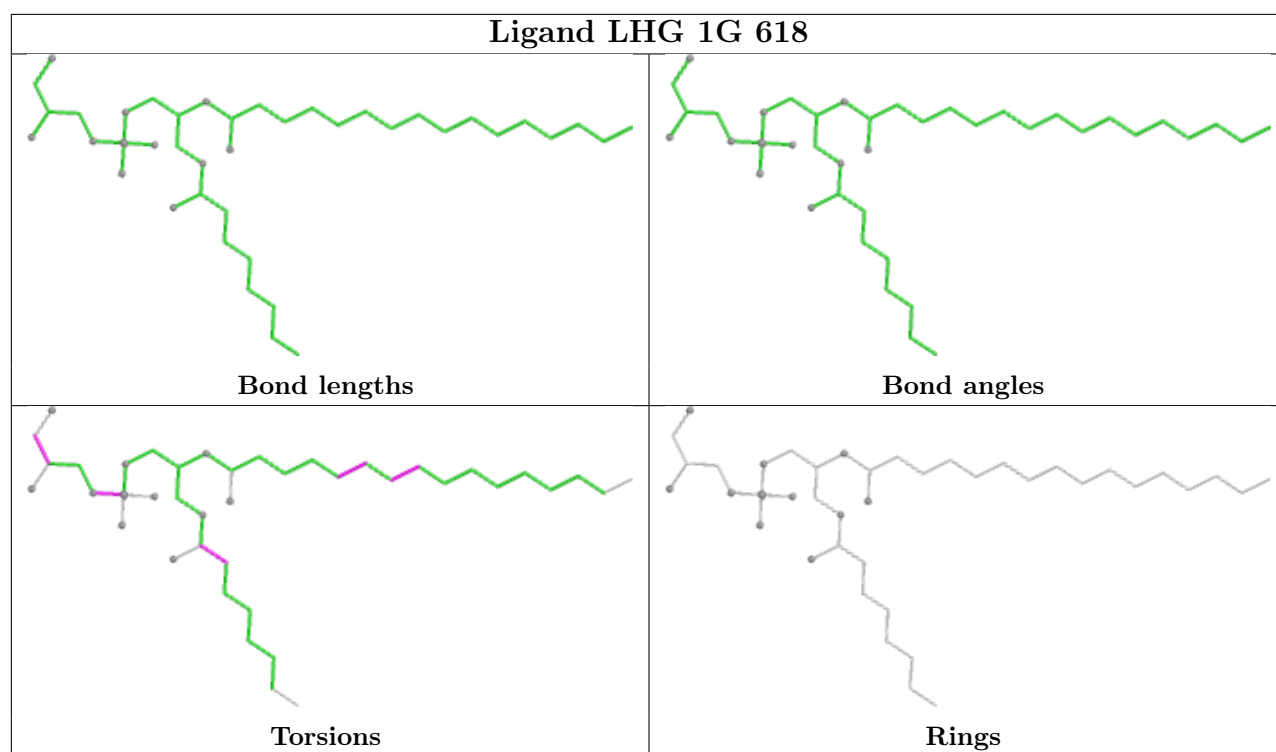


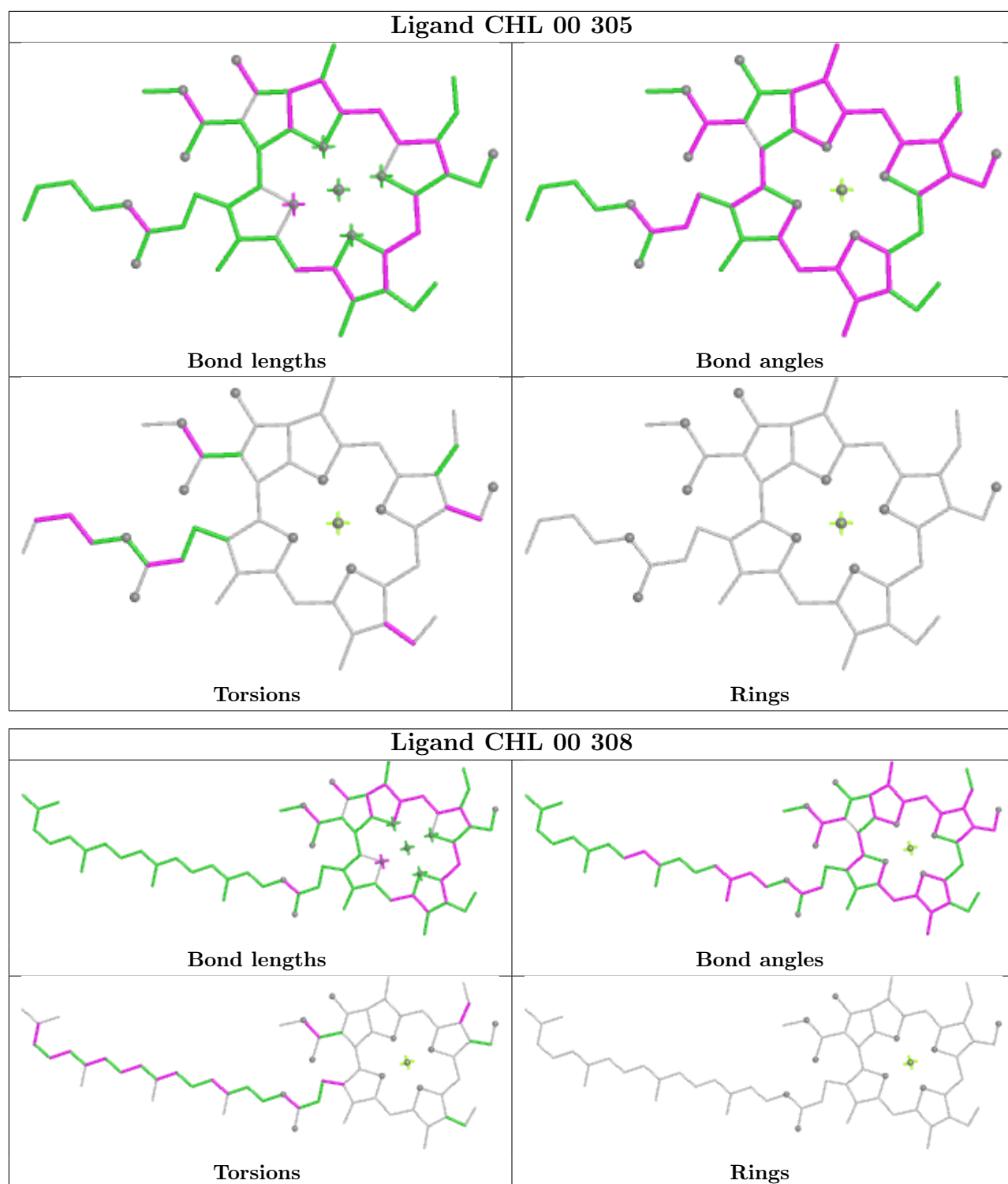


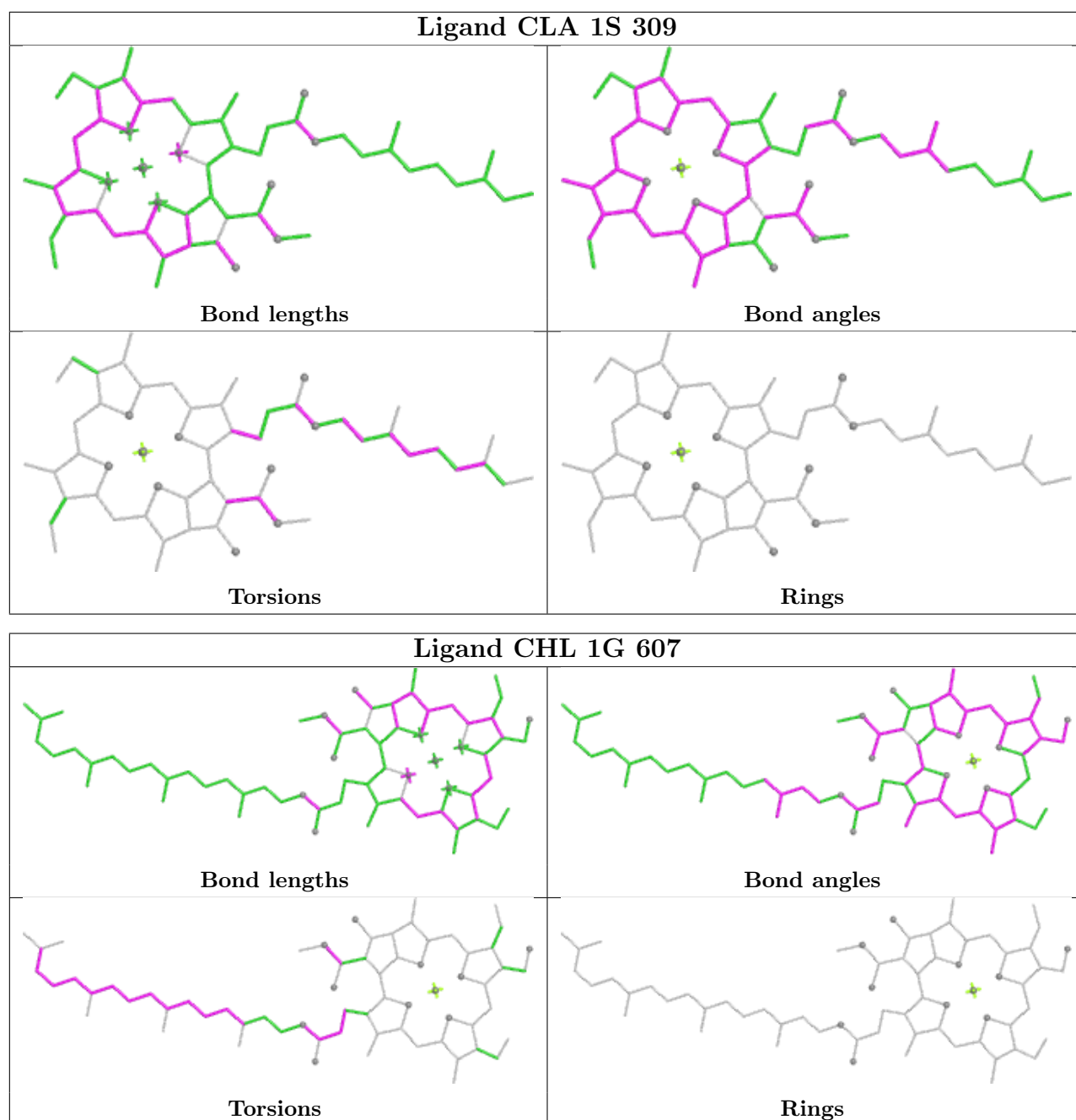


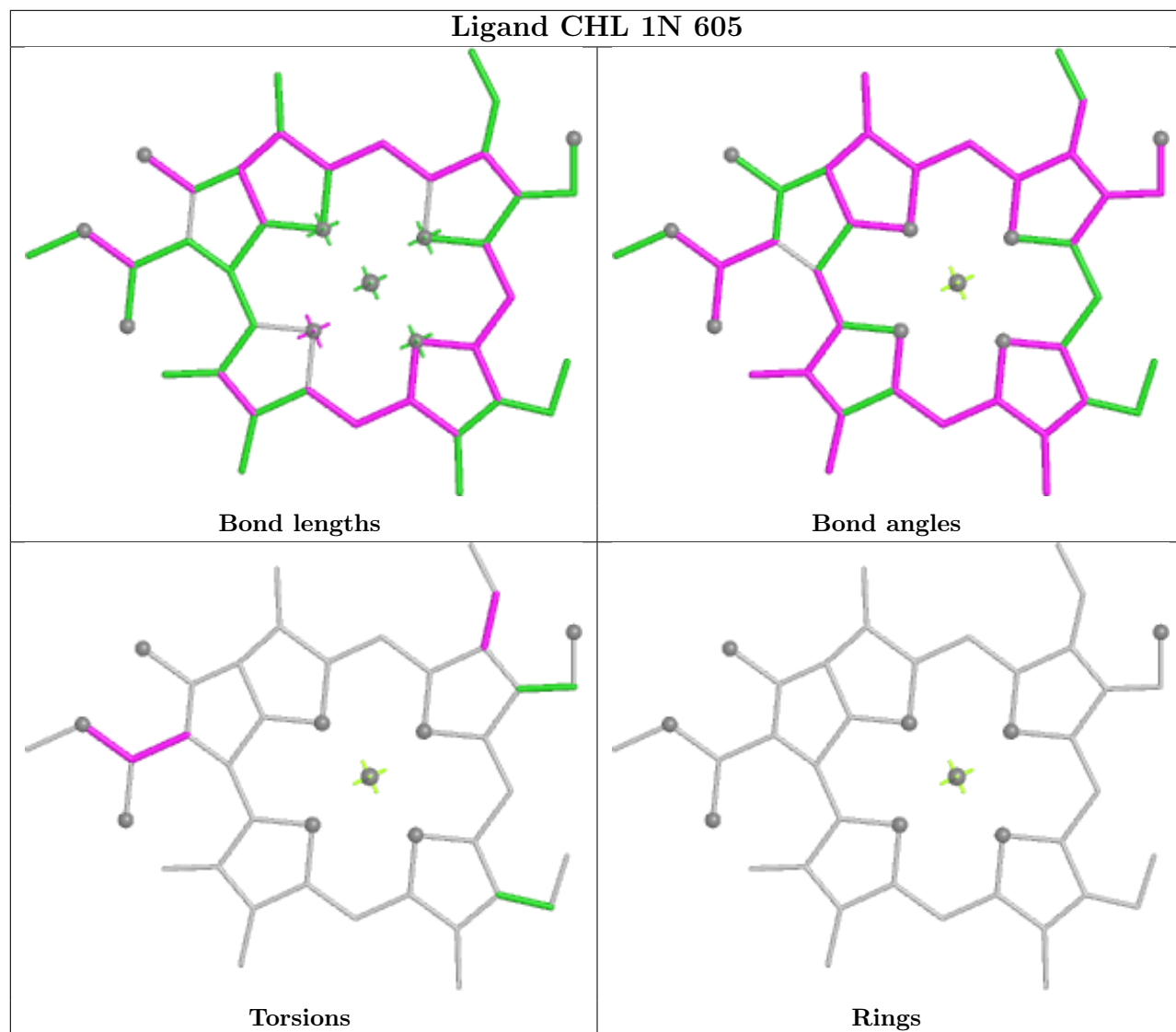
Ligand CLA 1G 604

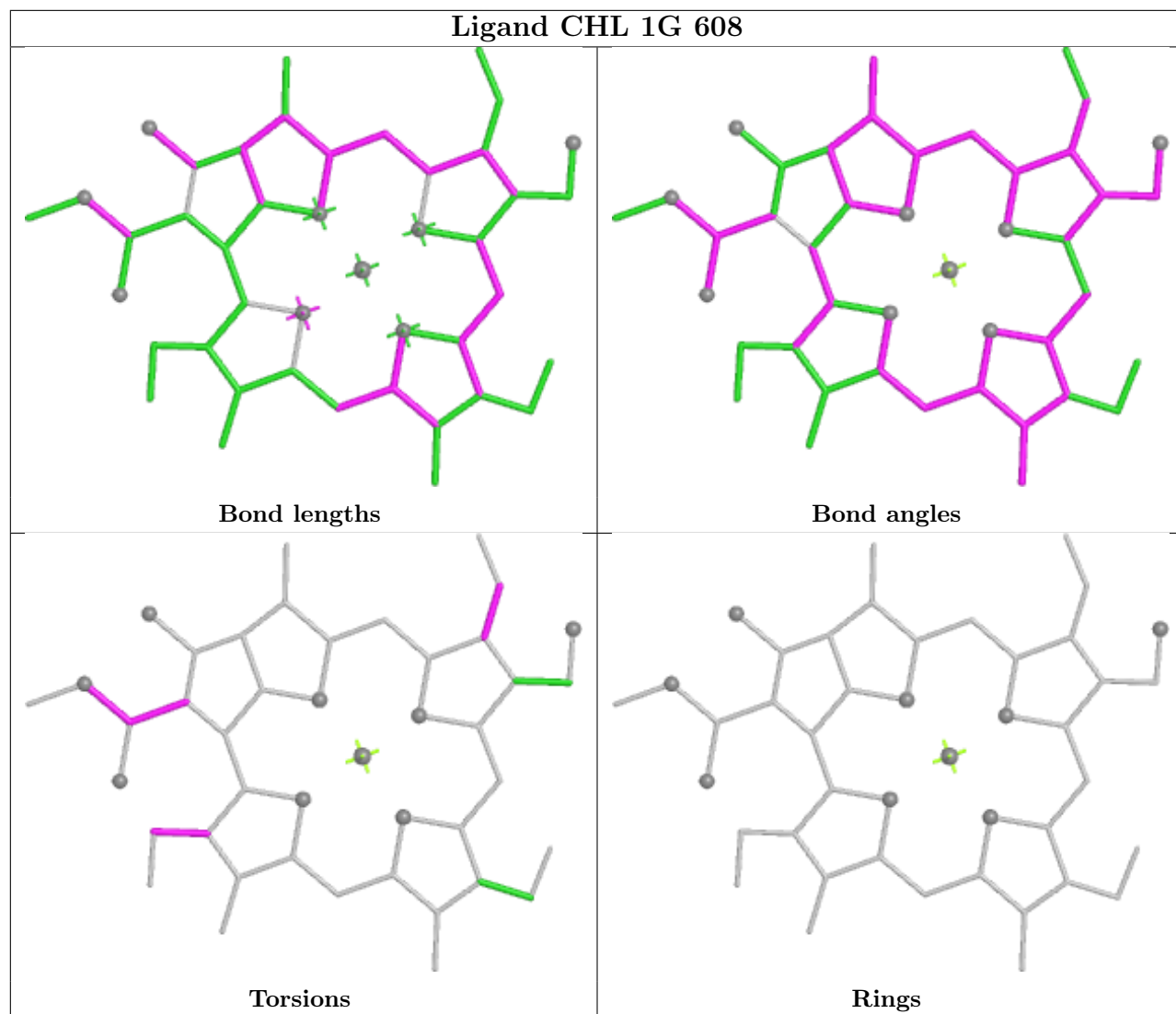


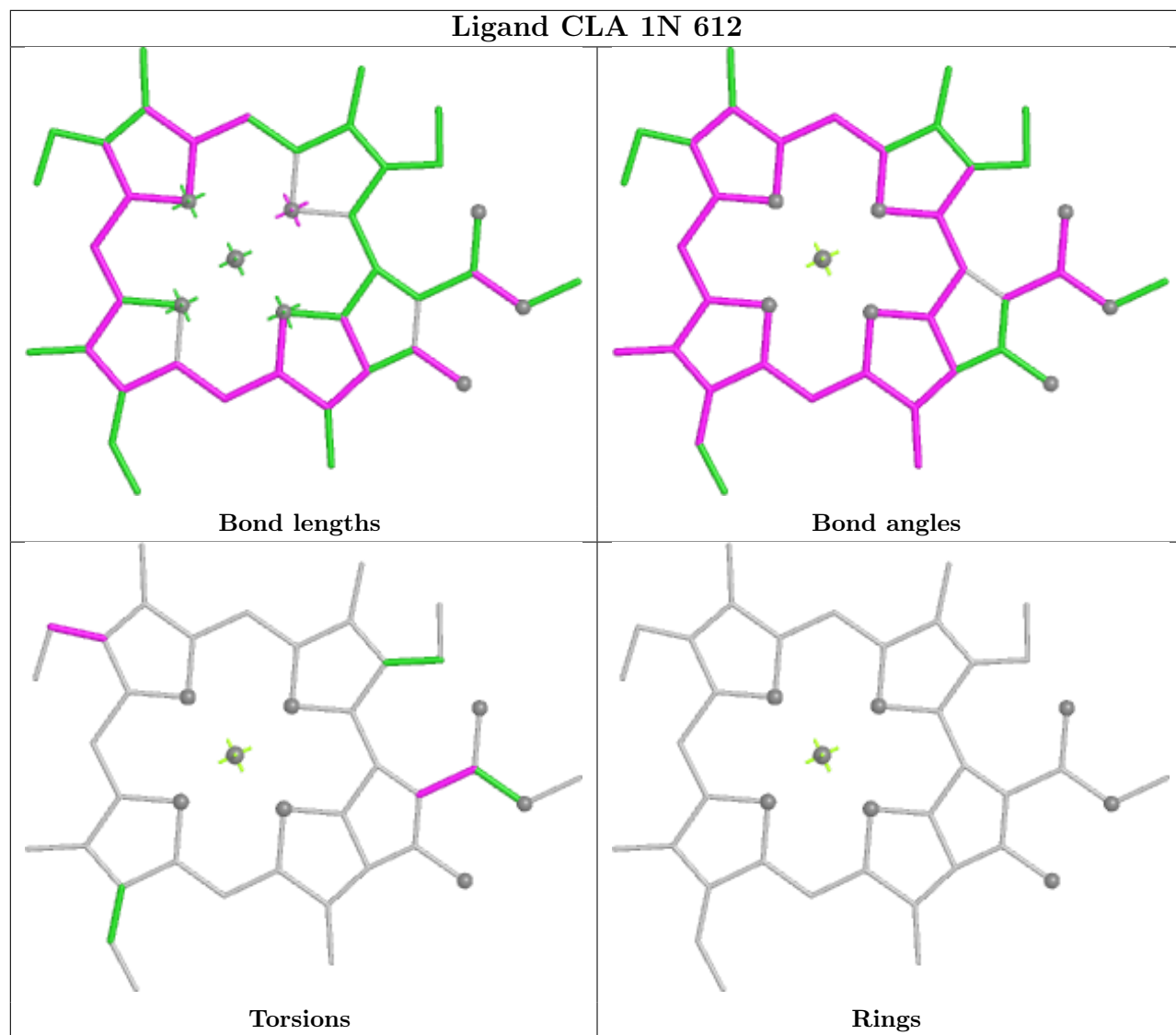


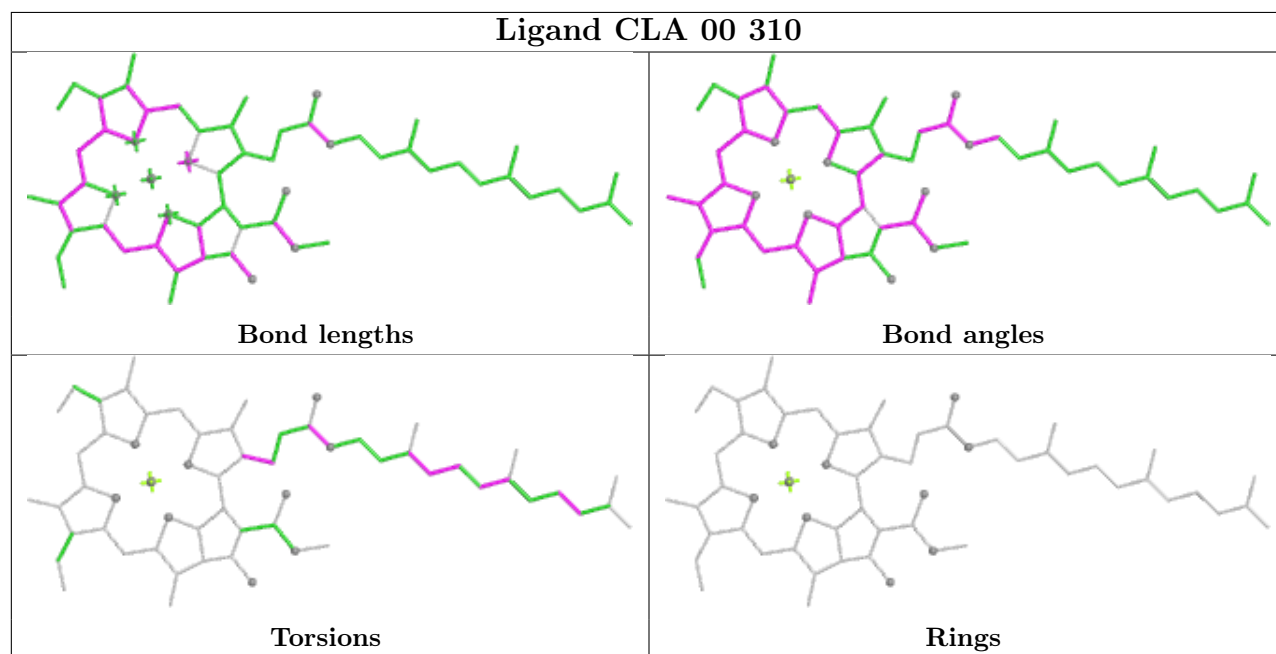
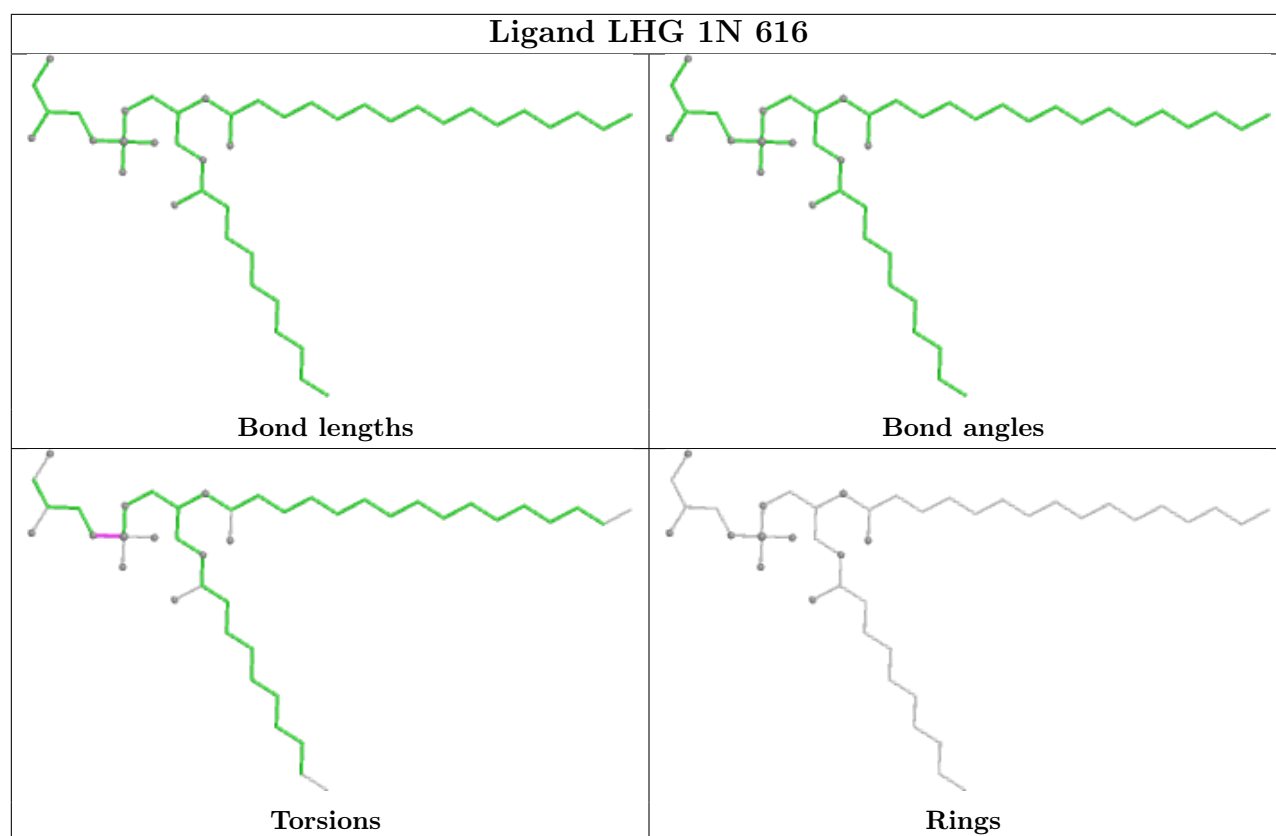


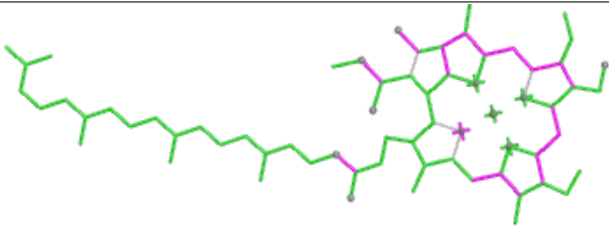
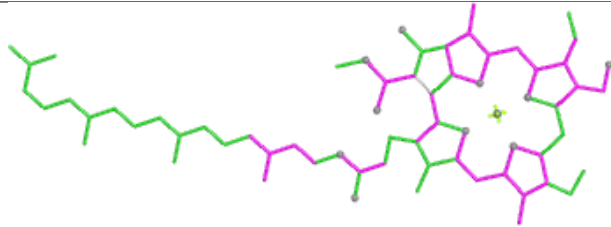
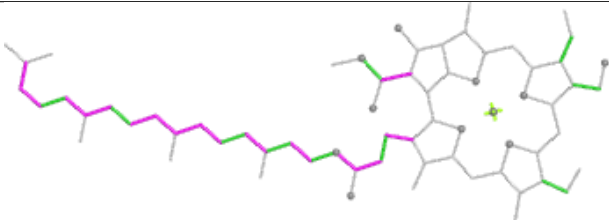
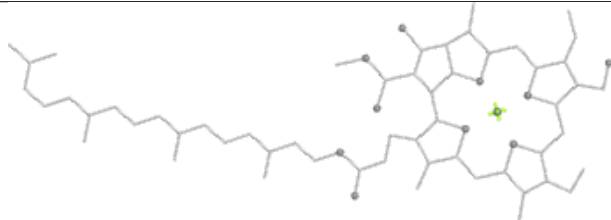
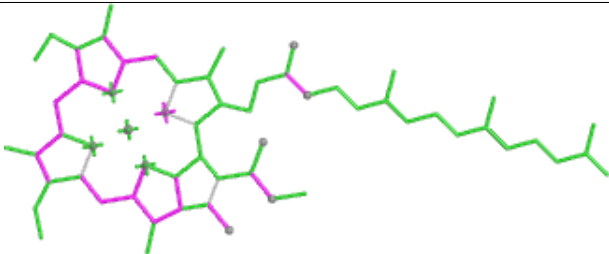
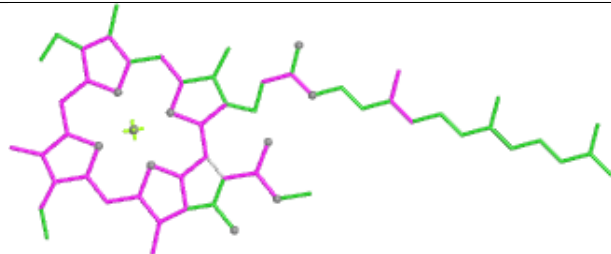
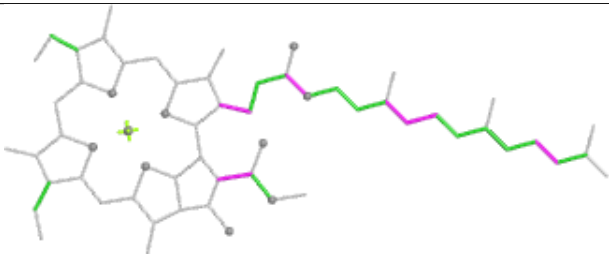
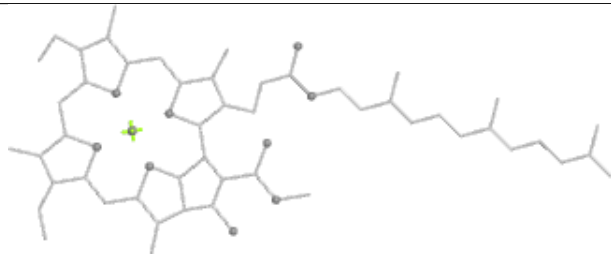


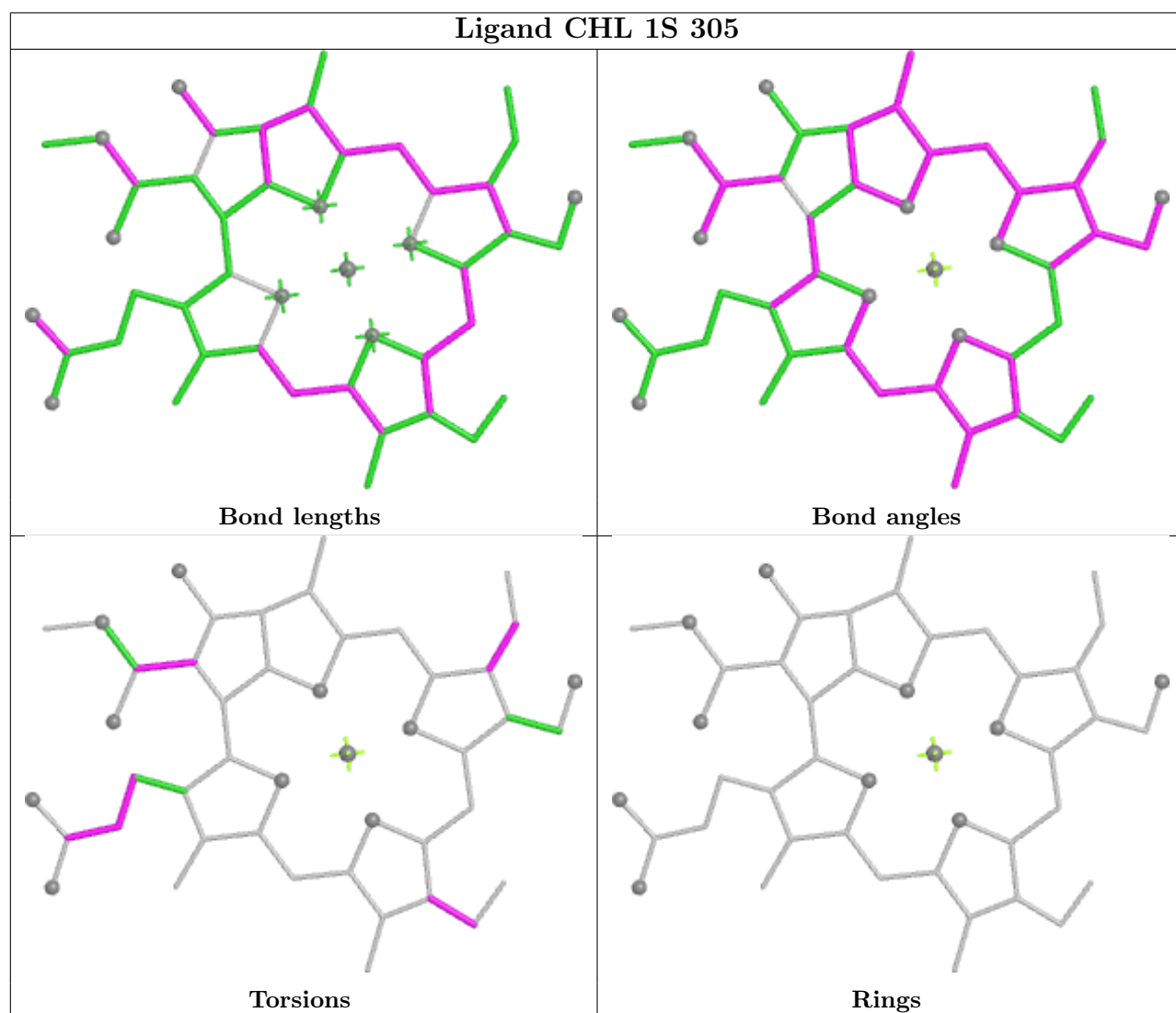
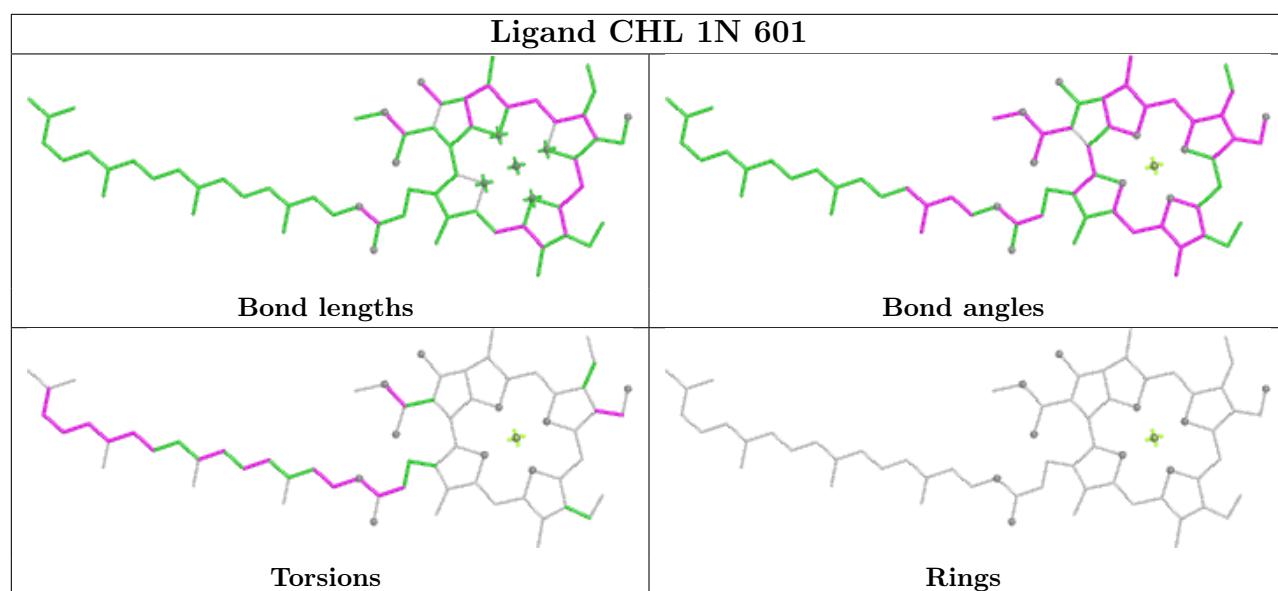




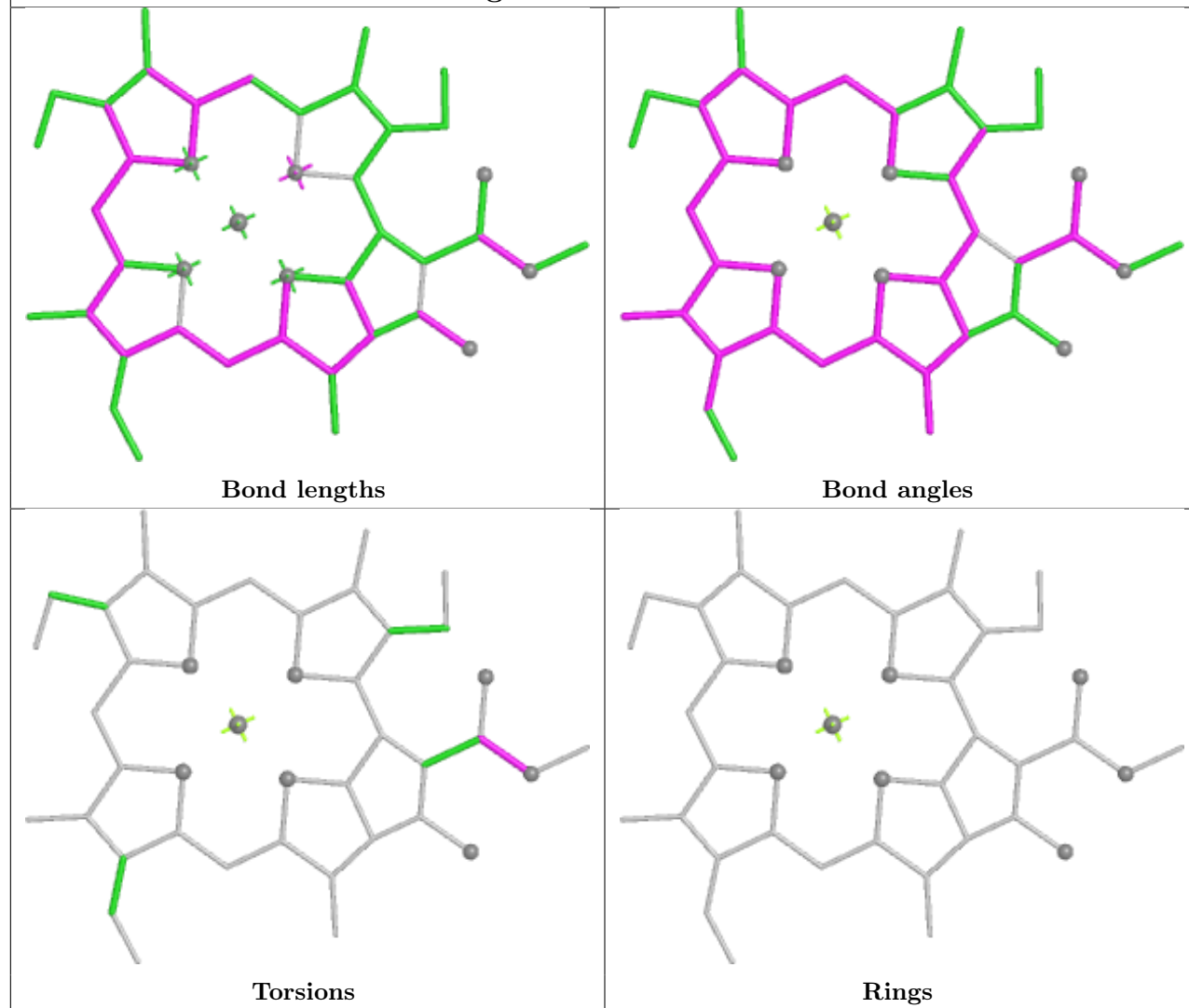




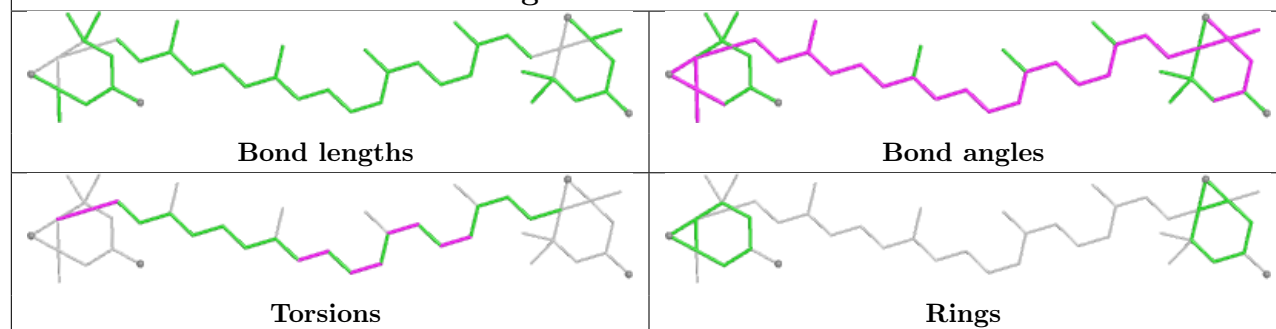
Ligand CHL 1G 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 00 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

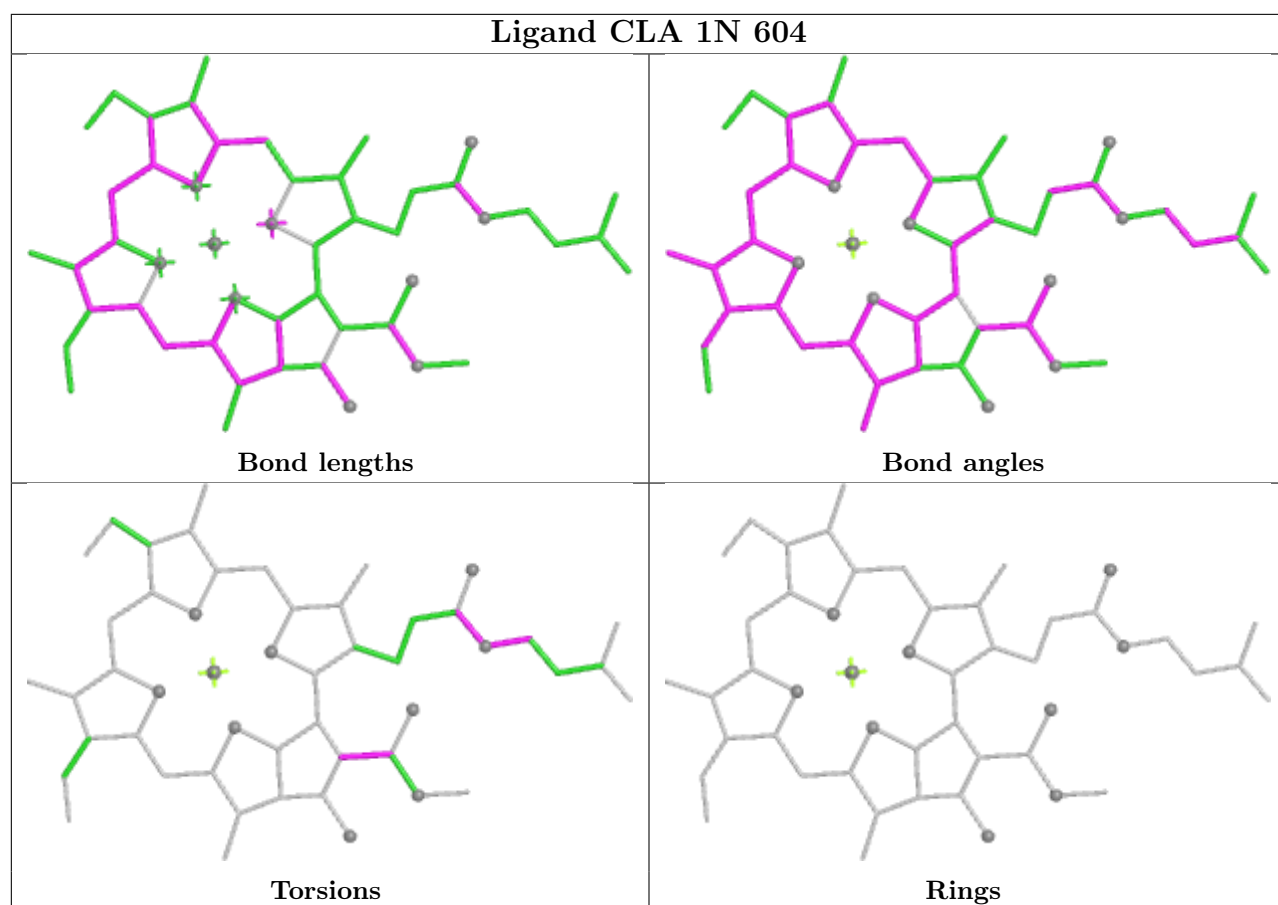


Ligand CLA 1G 614

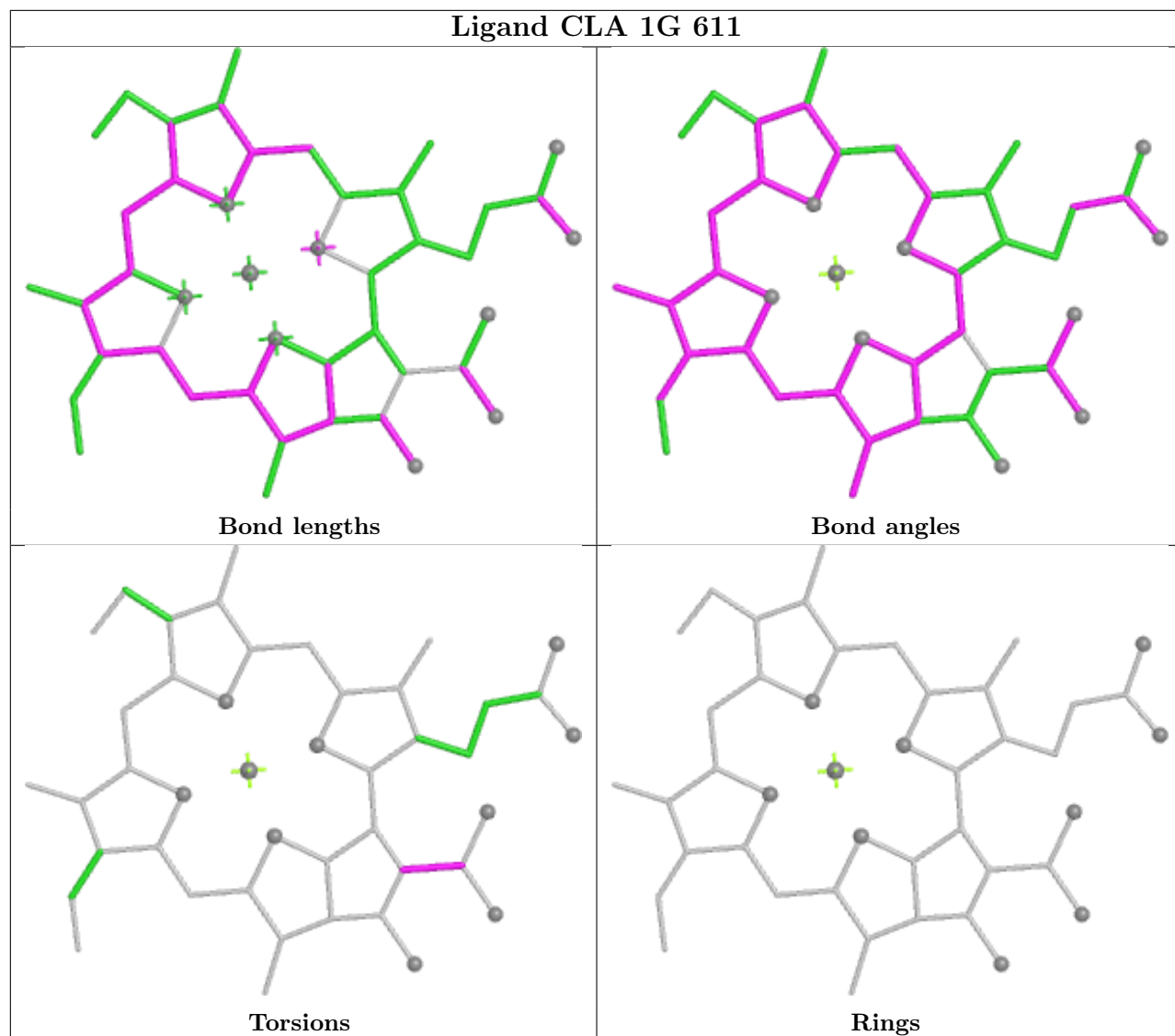


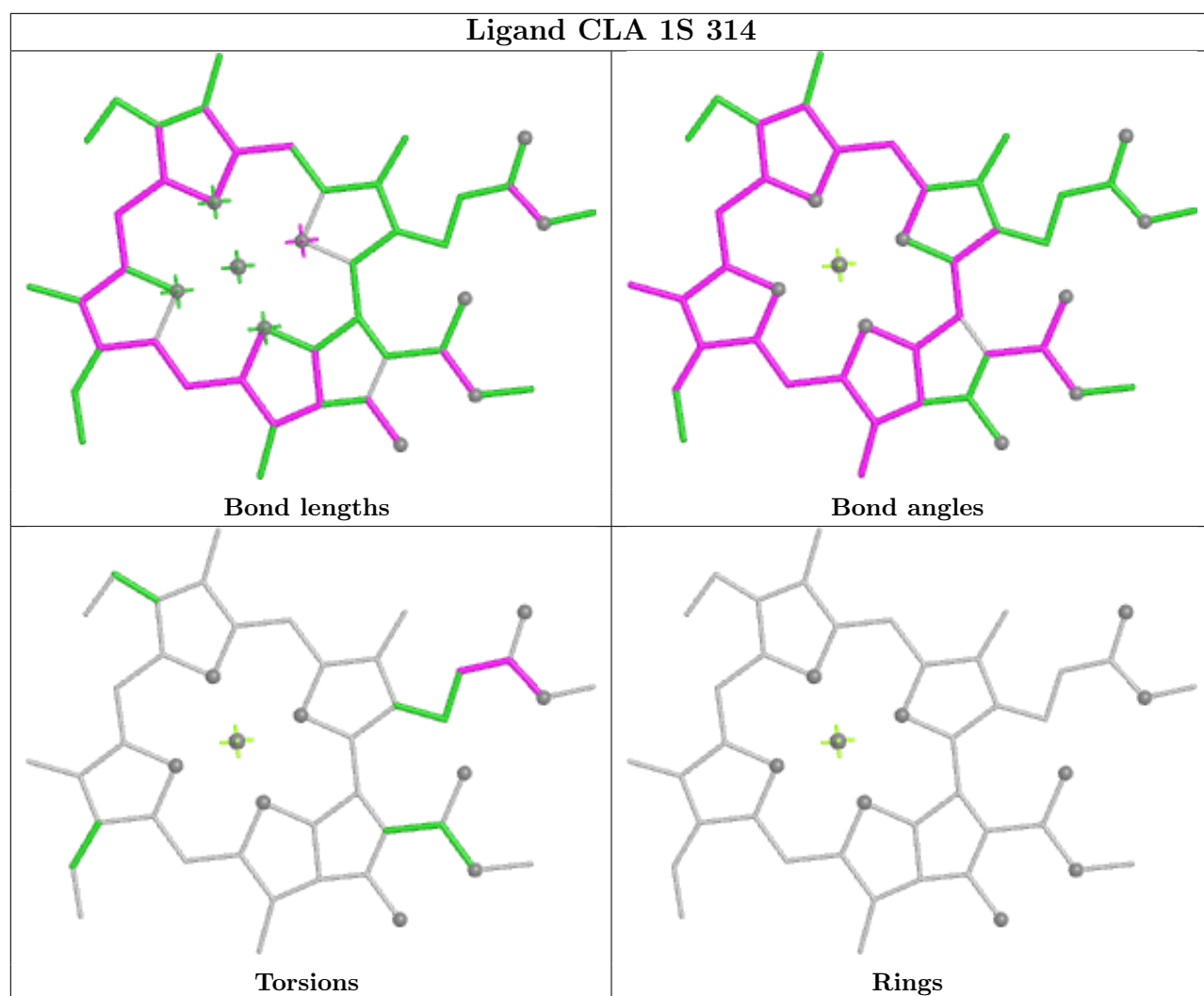
Ligand XAT 1G 619

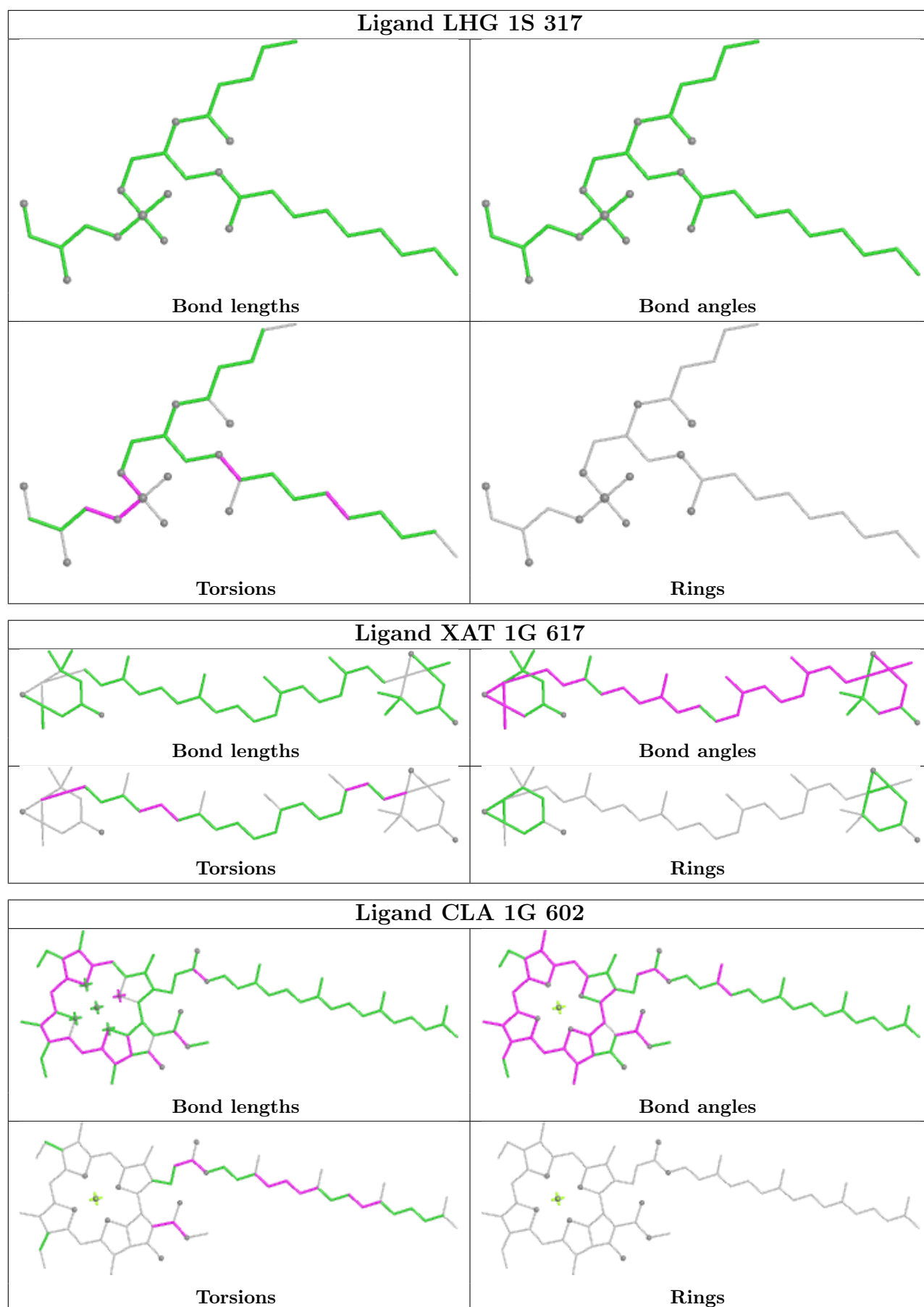




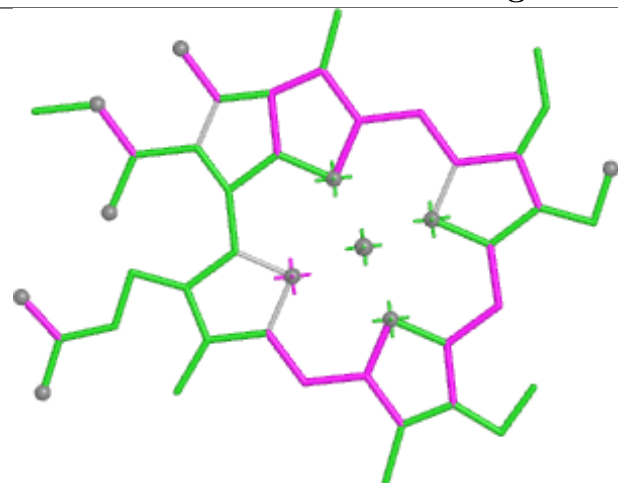
Ligand CLA 1G 611



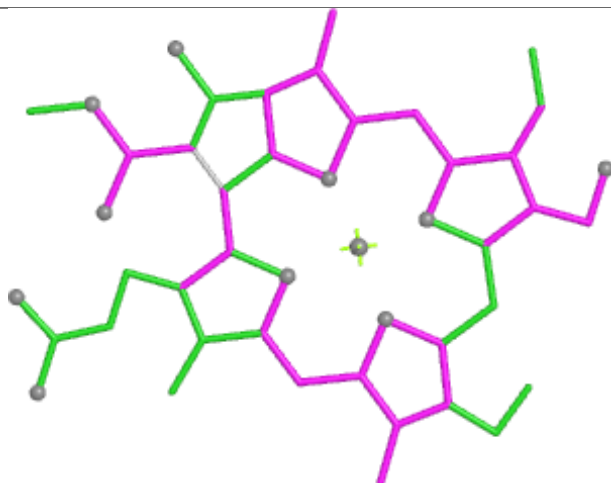




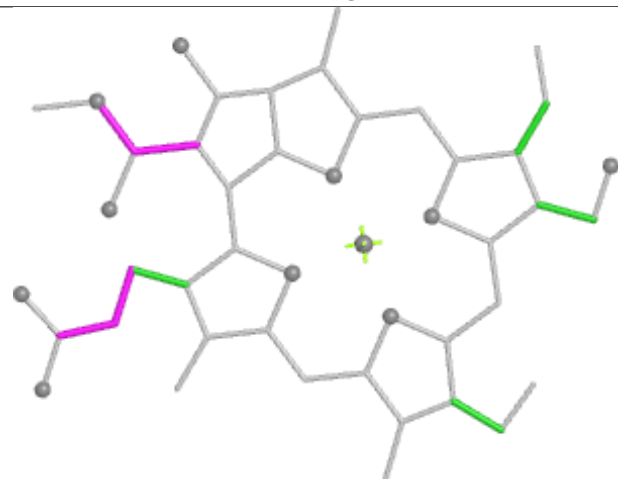
Ligand CHL 1G 606



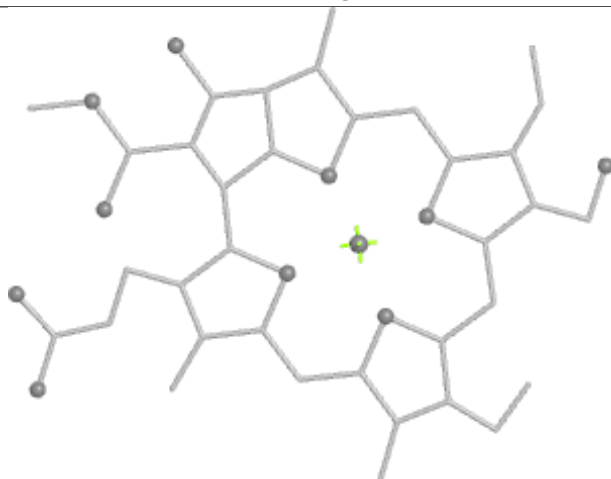
Bond lengths



Bond angles

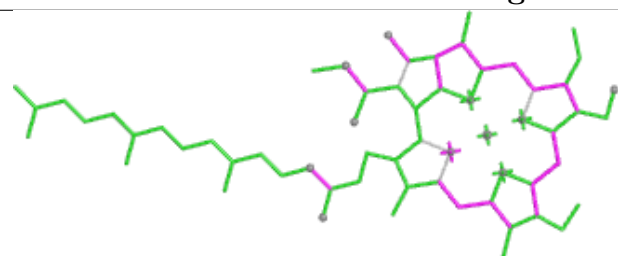


Torsions

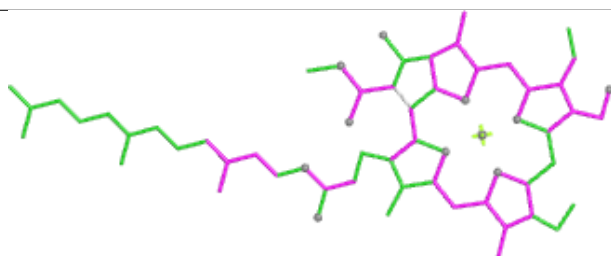


Rings

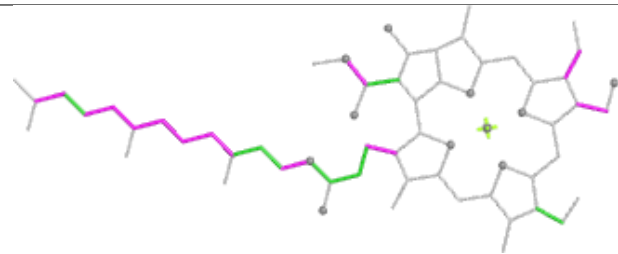
Ligand CHL 1G 609



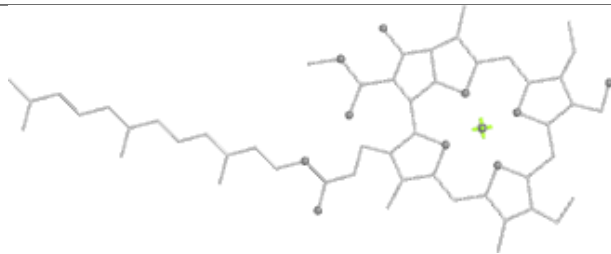
Bond lengths



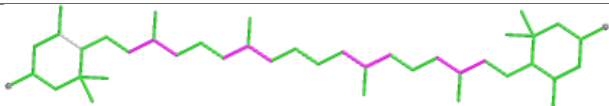
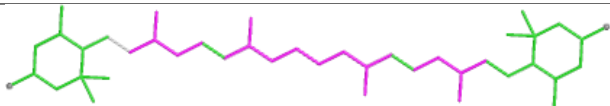
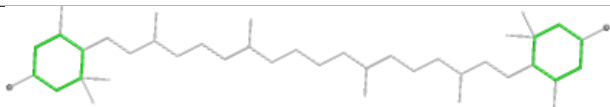
Bond angles

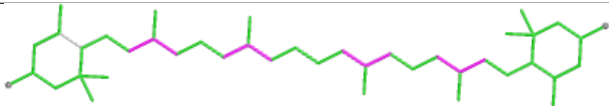
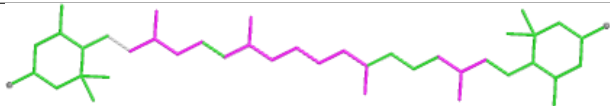
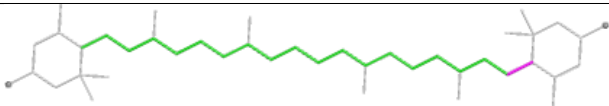
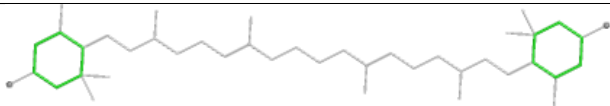


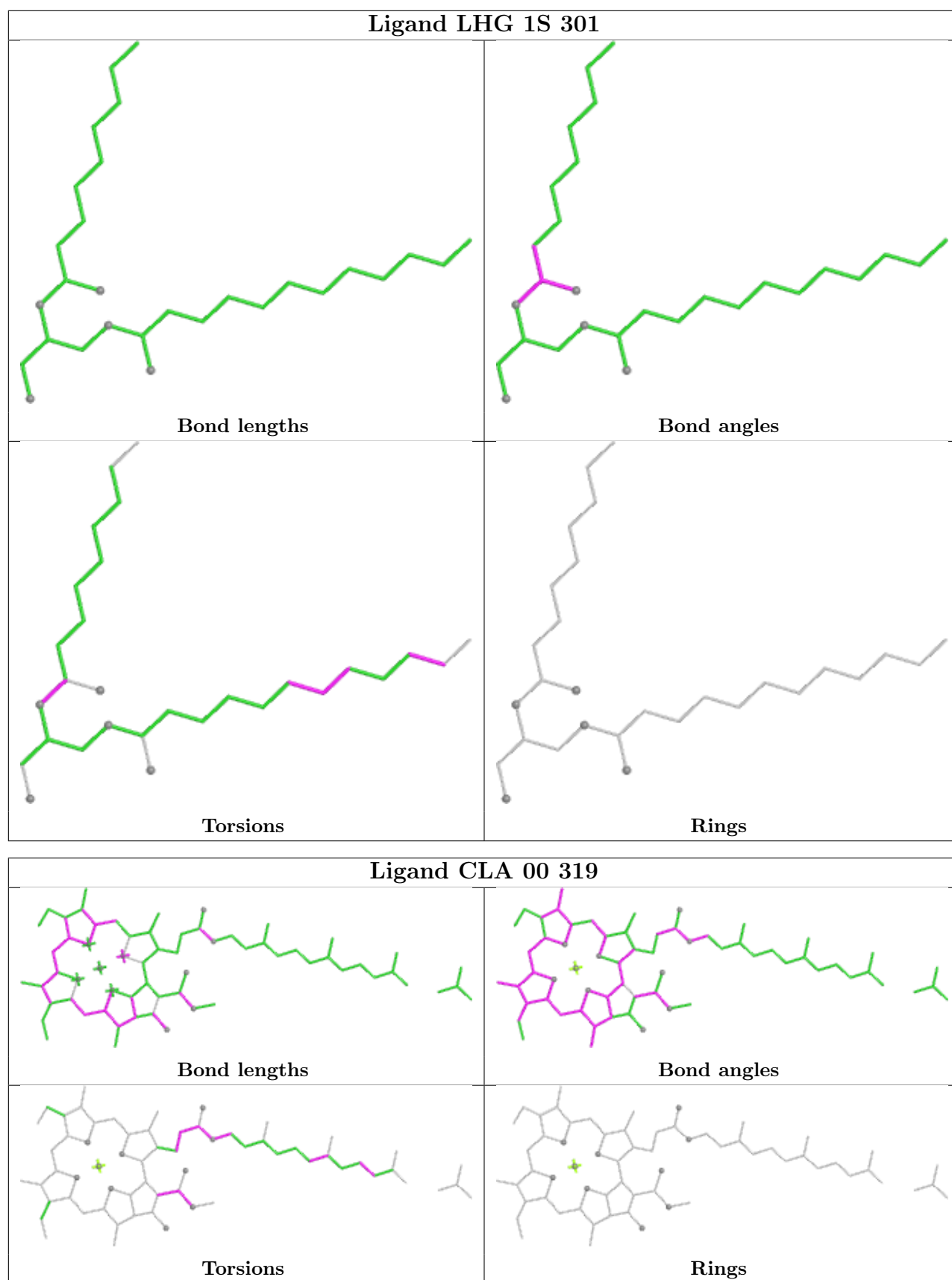
Torsions

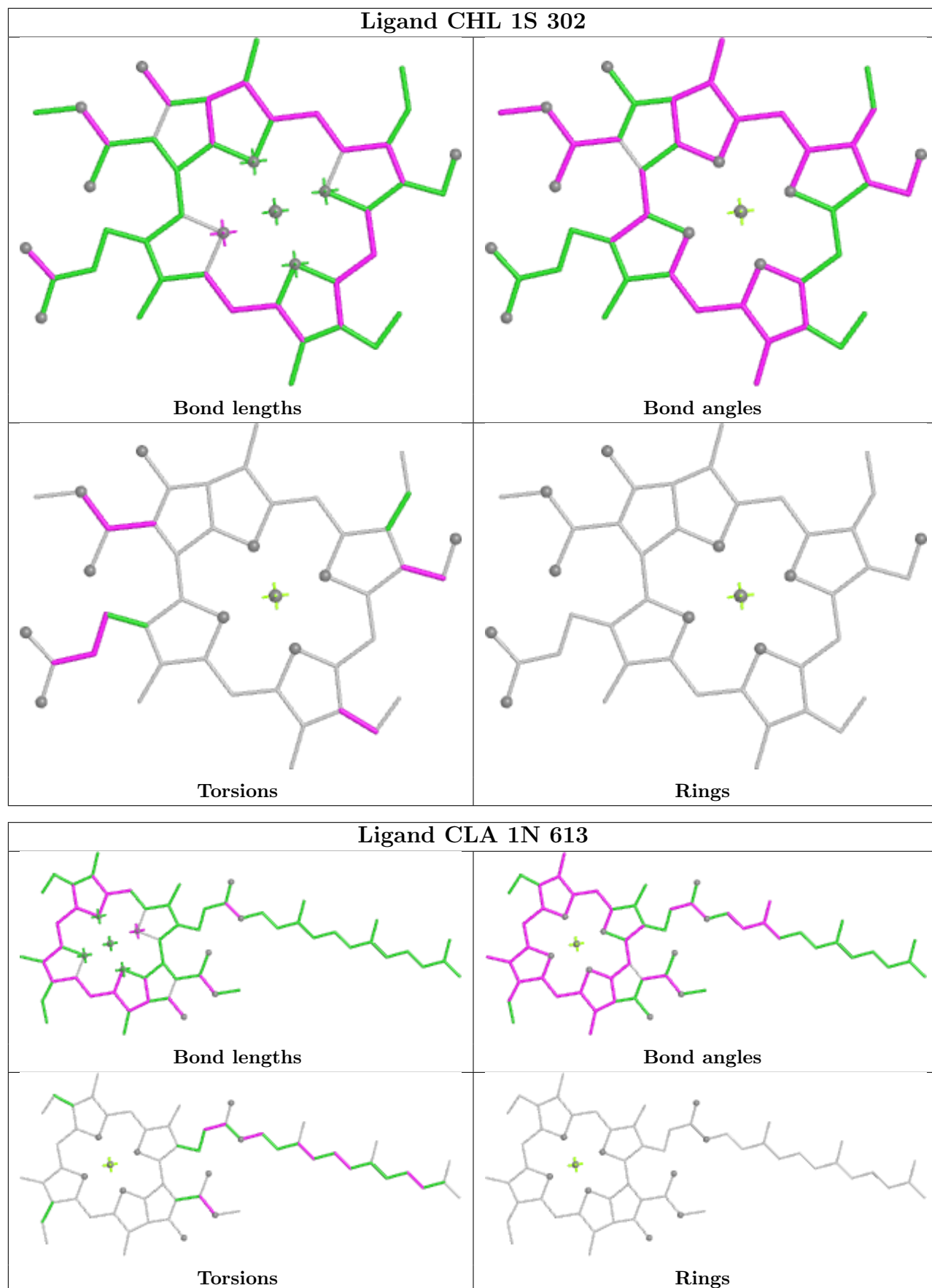


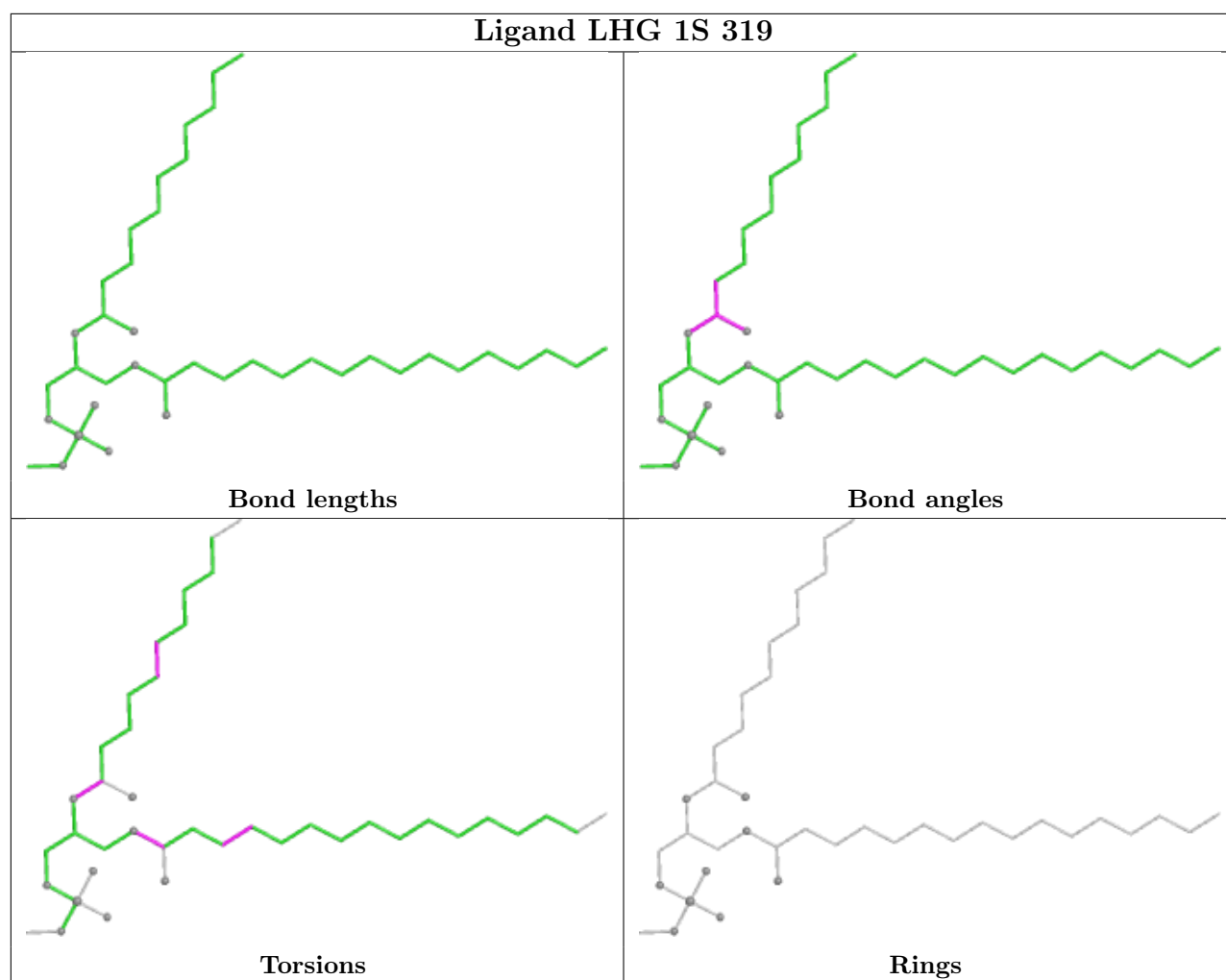
Rings

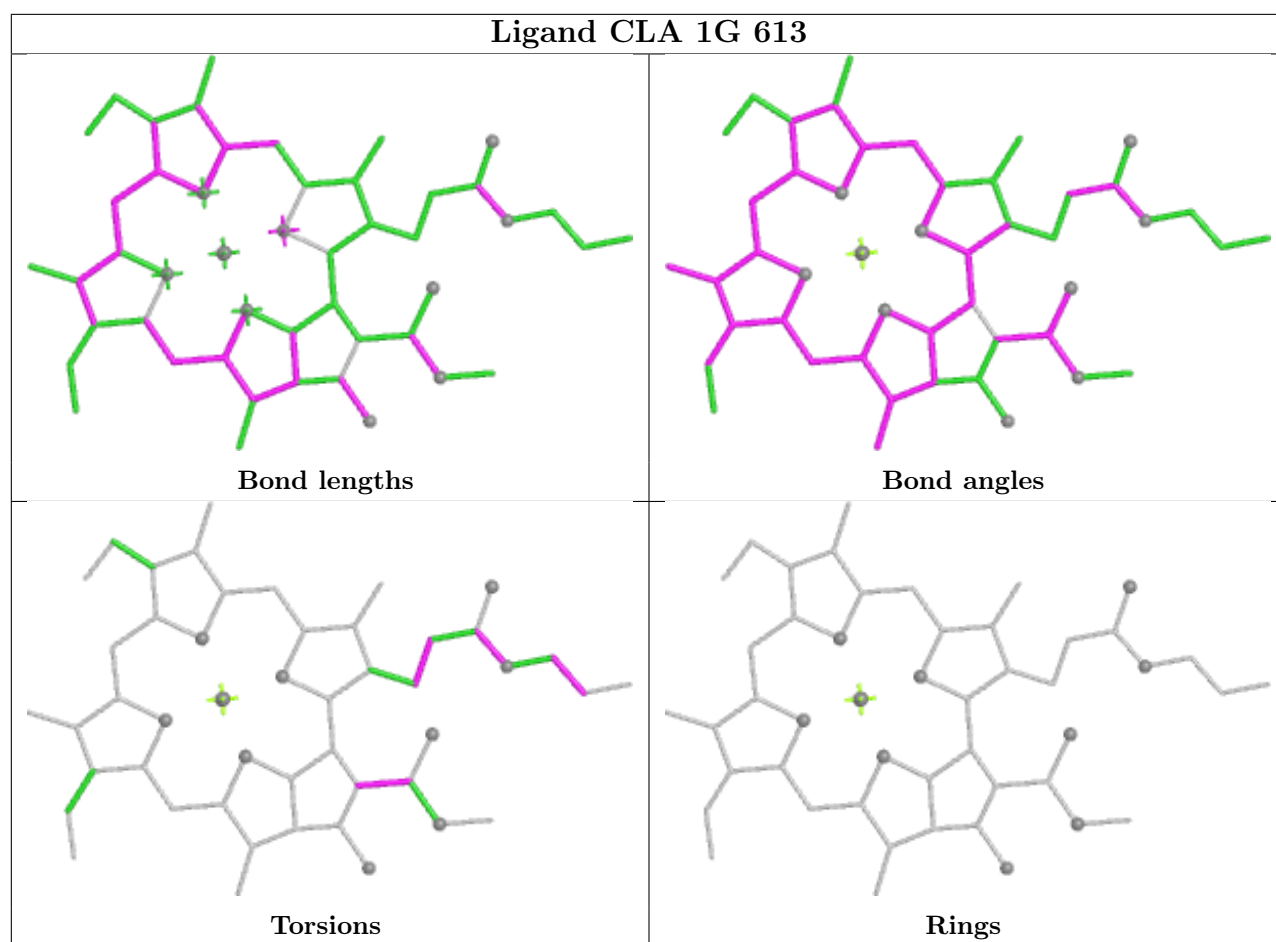
Ligand LUT 00 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

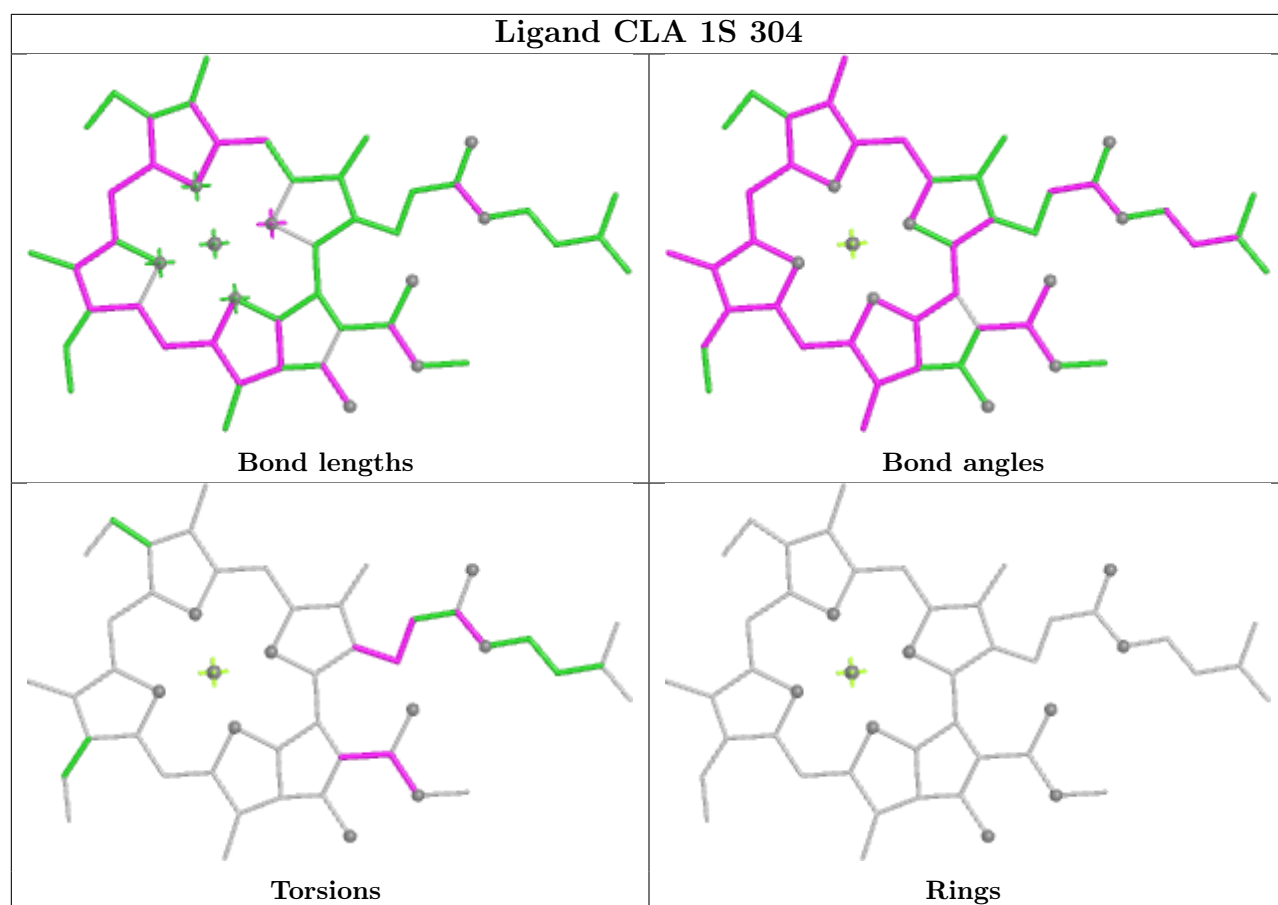
Ligand LUT 1S 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

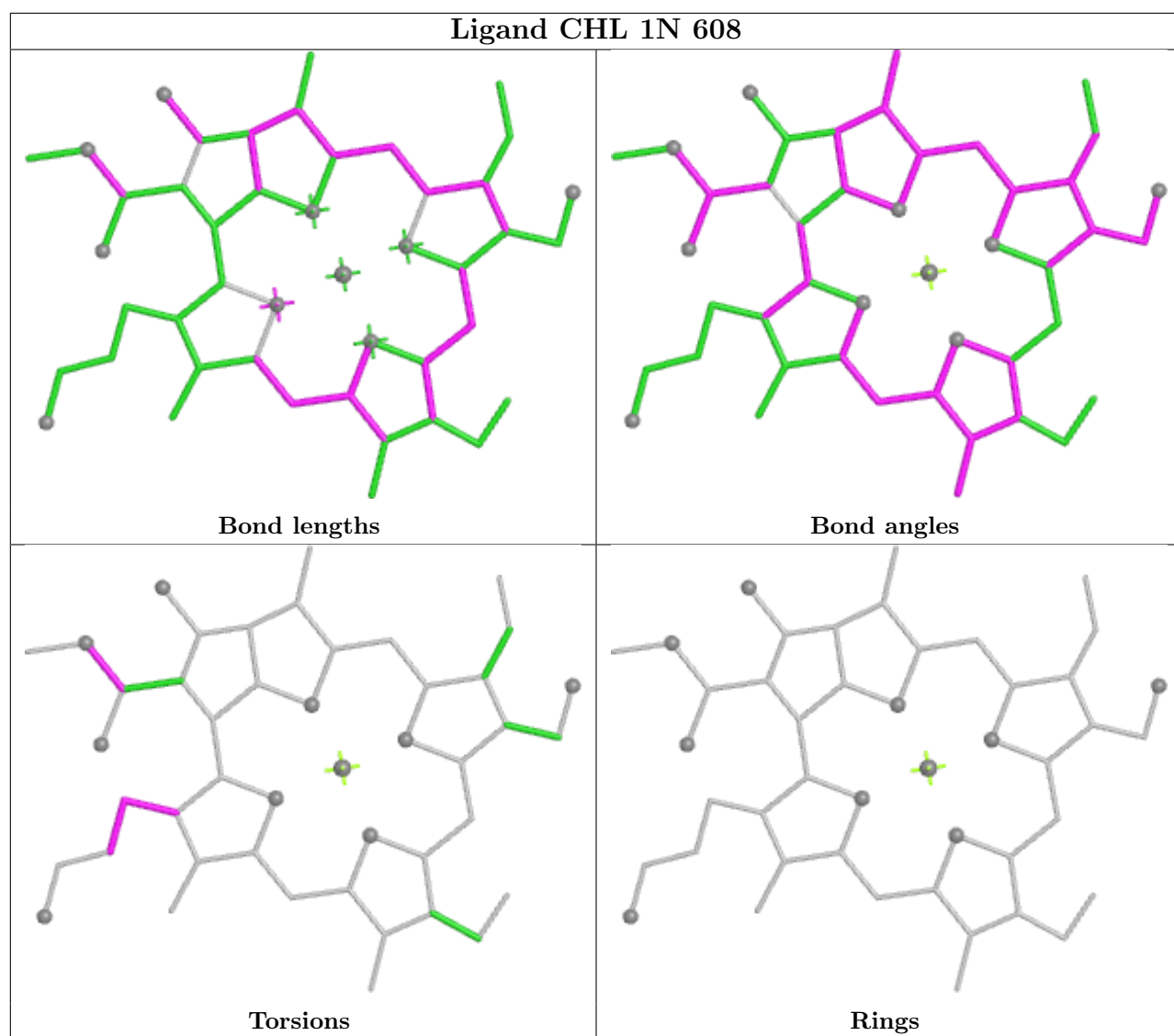


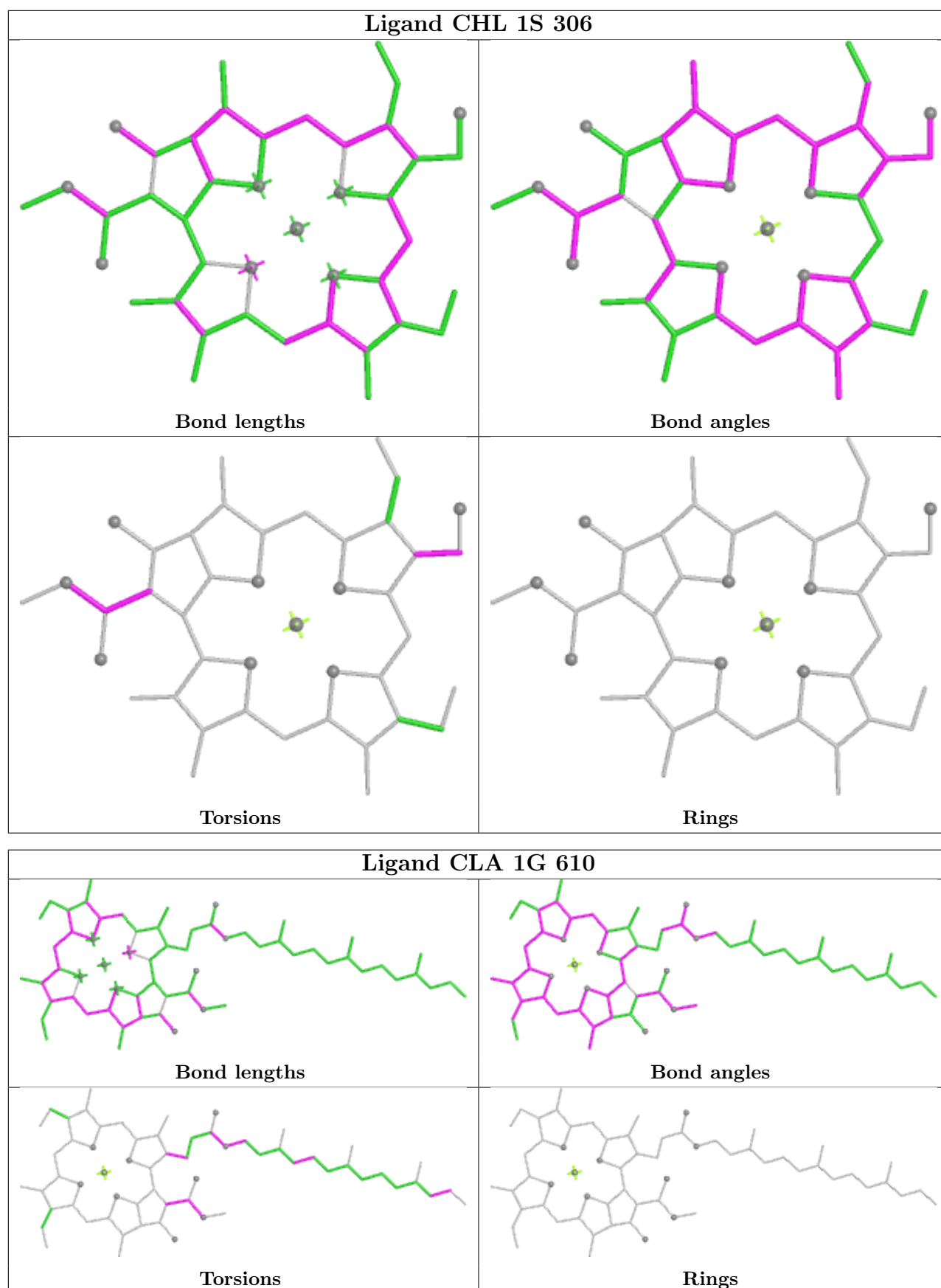


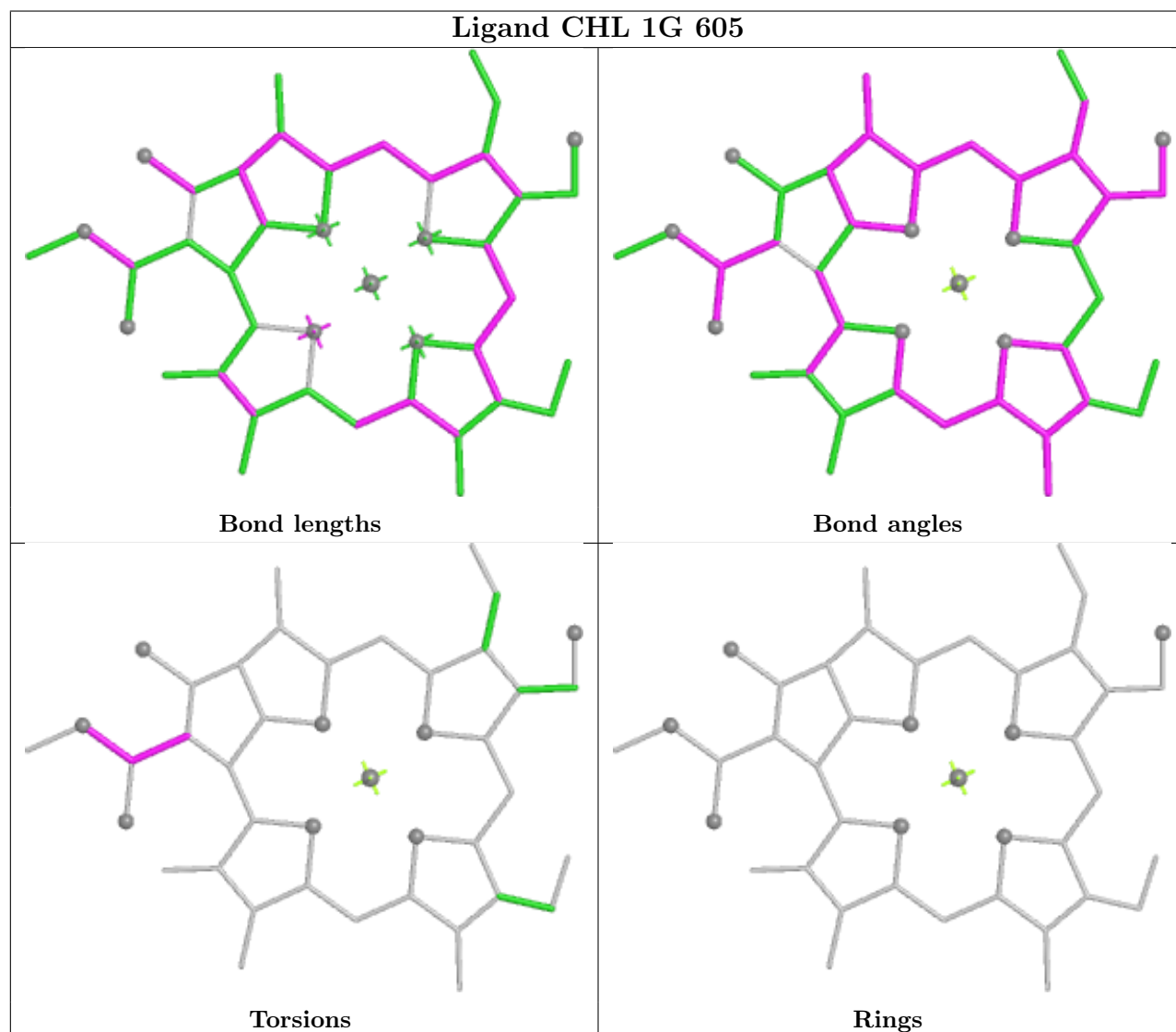
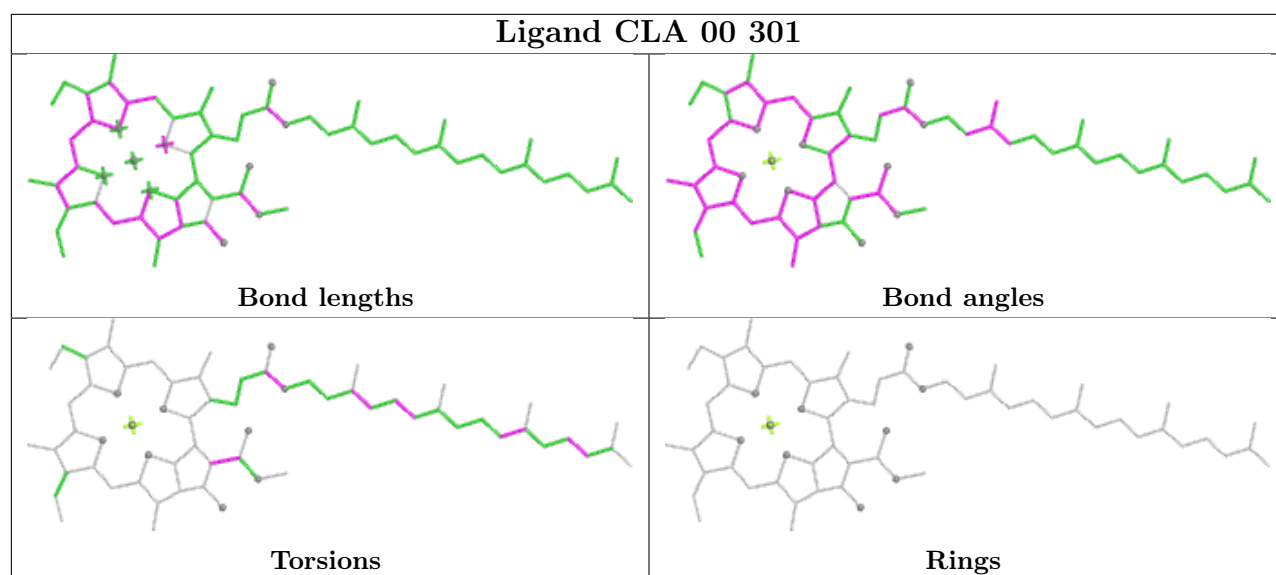


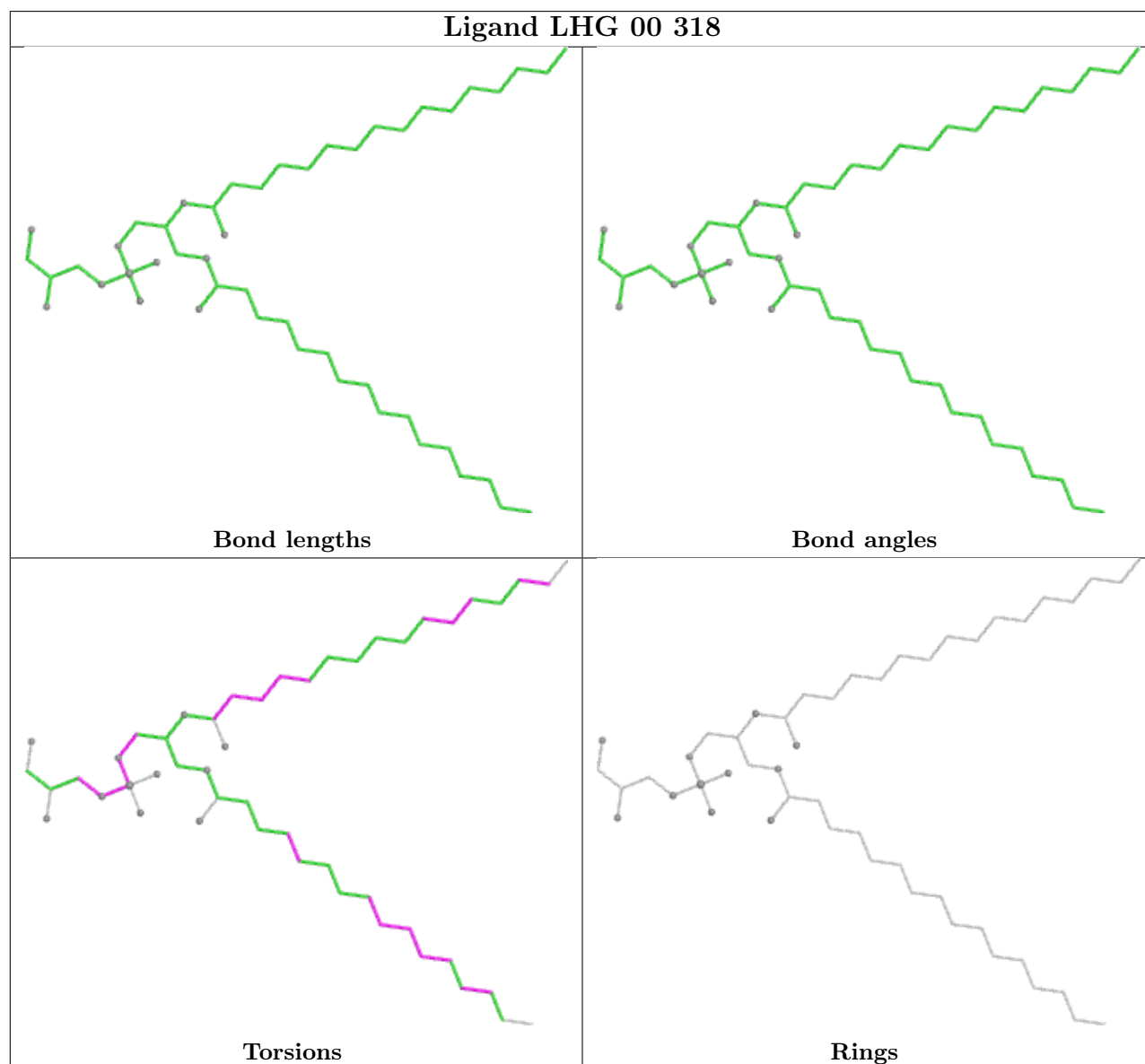
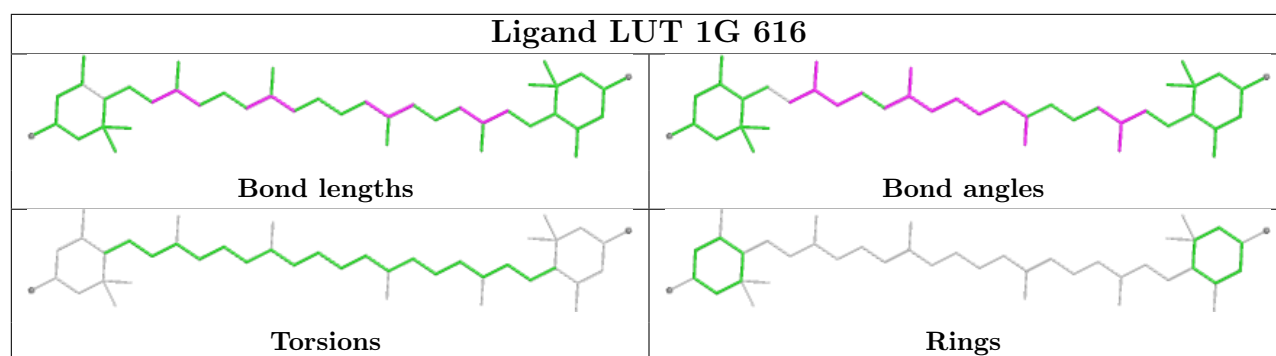


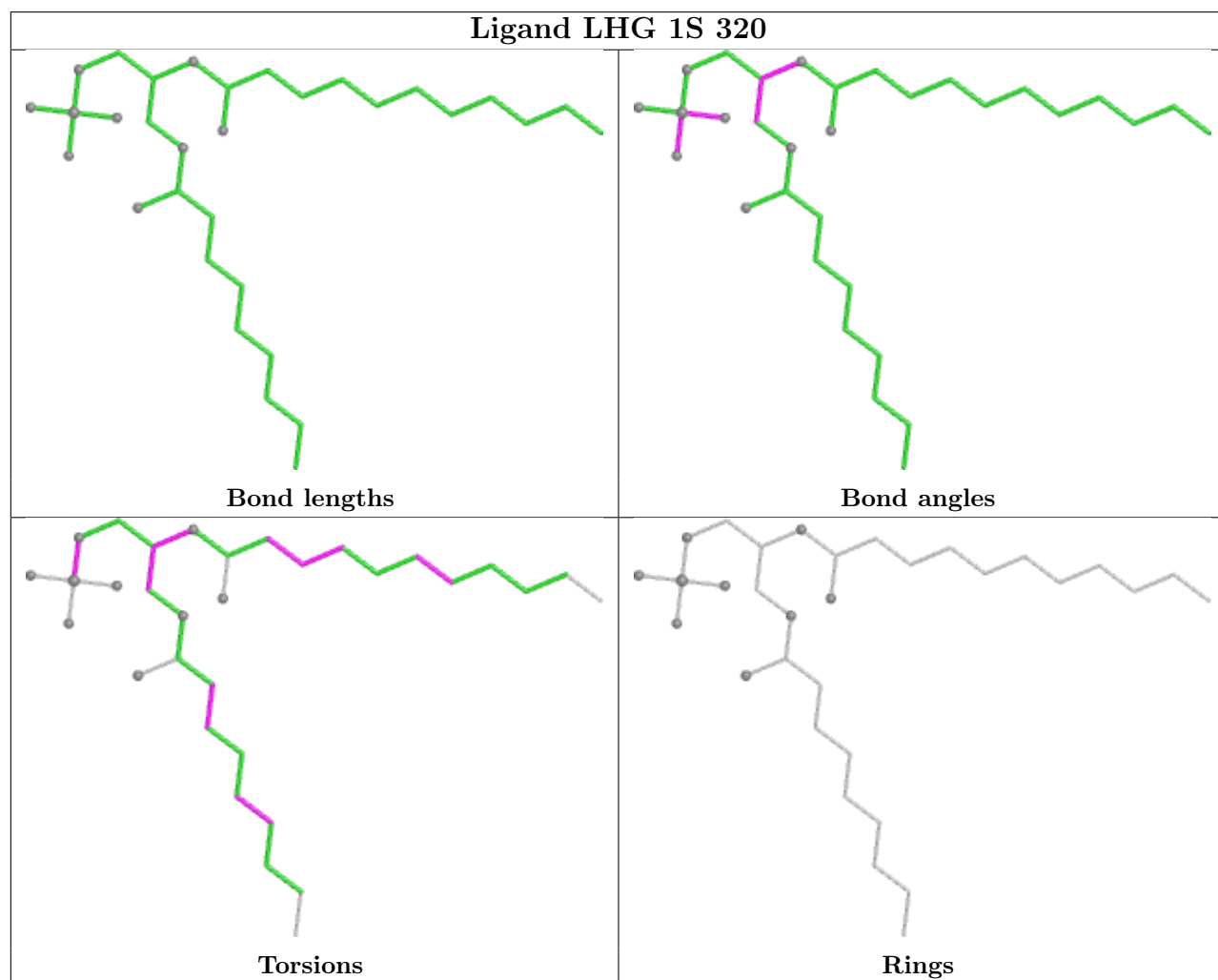
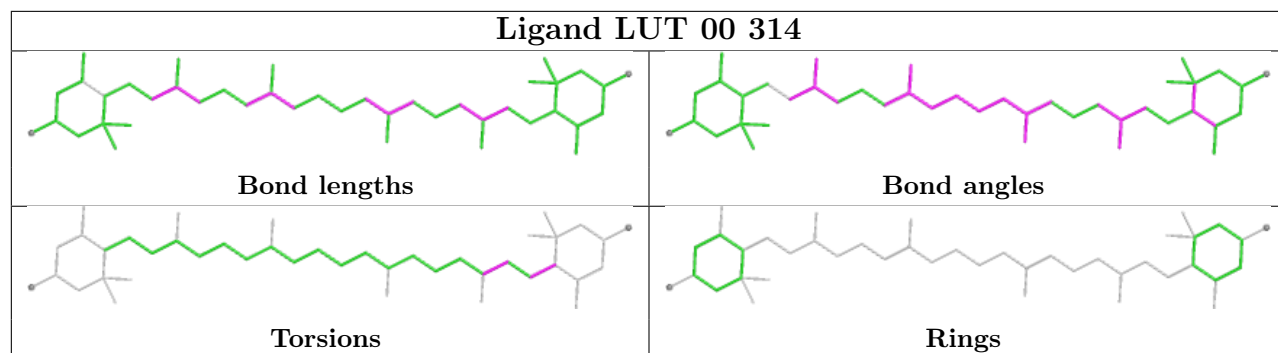




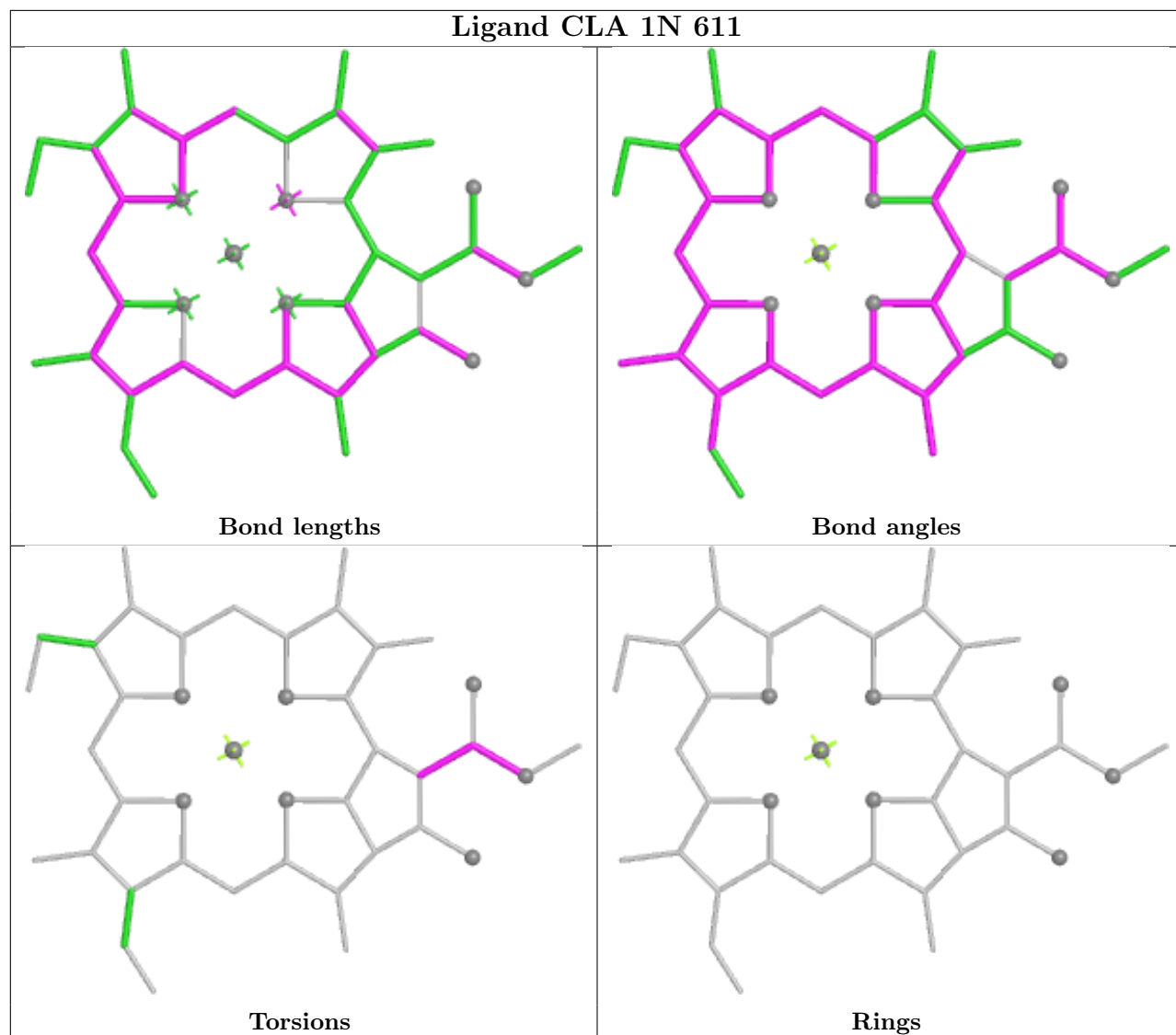




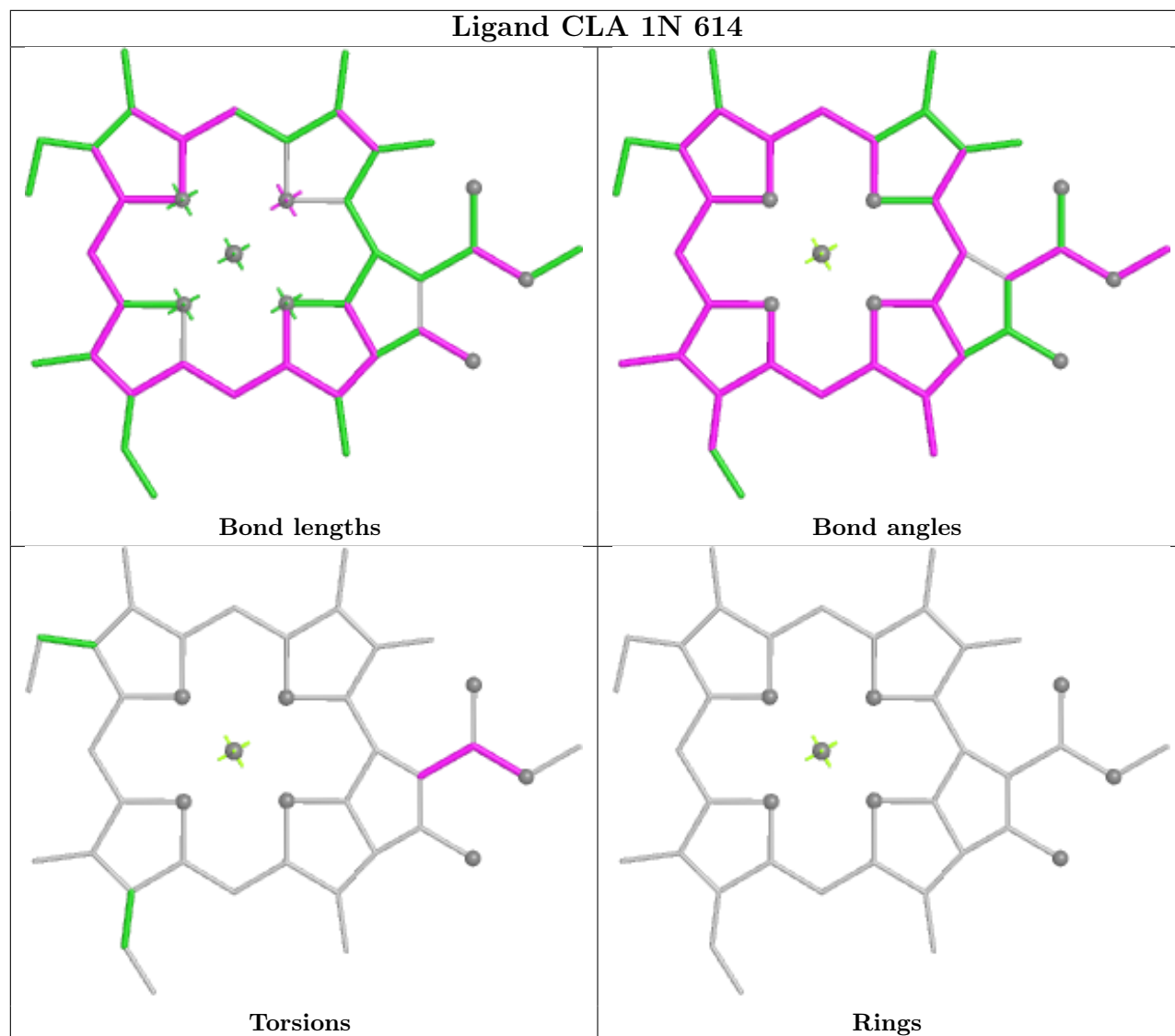




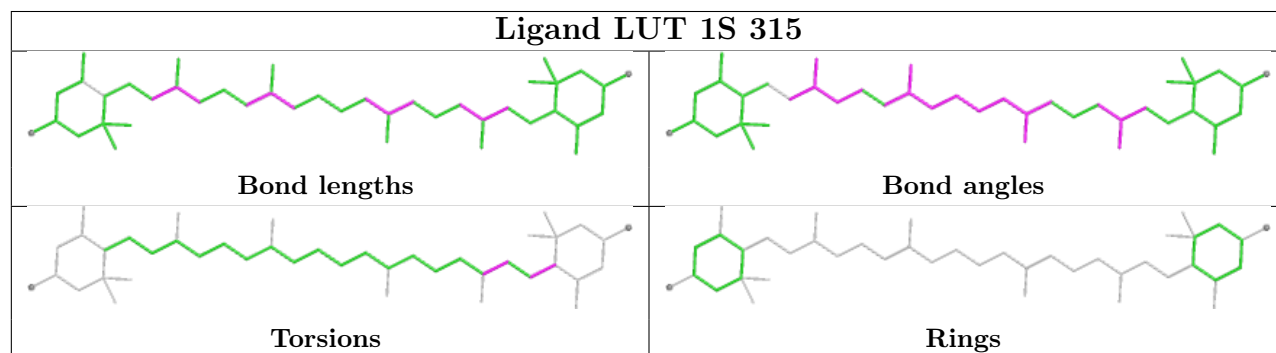
Ligand CLA 1N 611

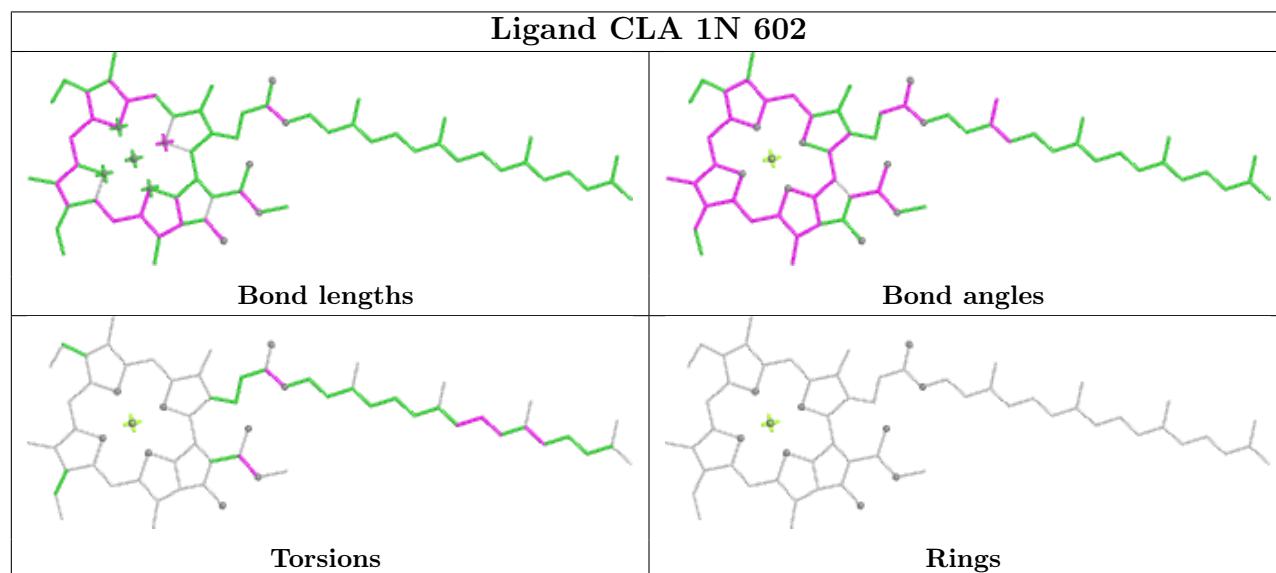
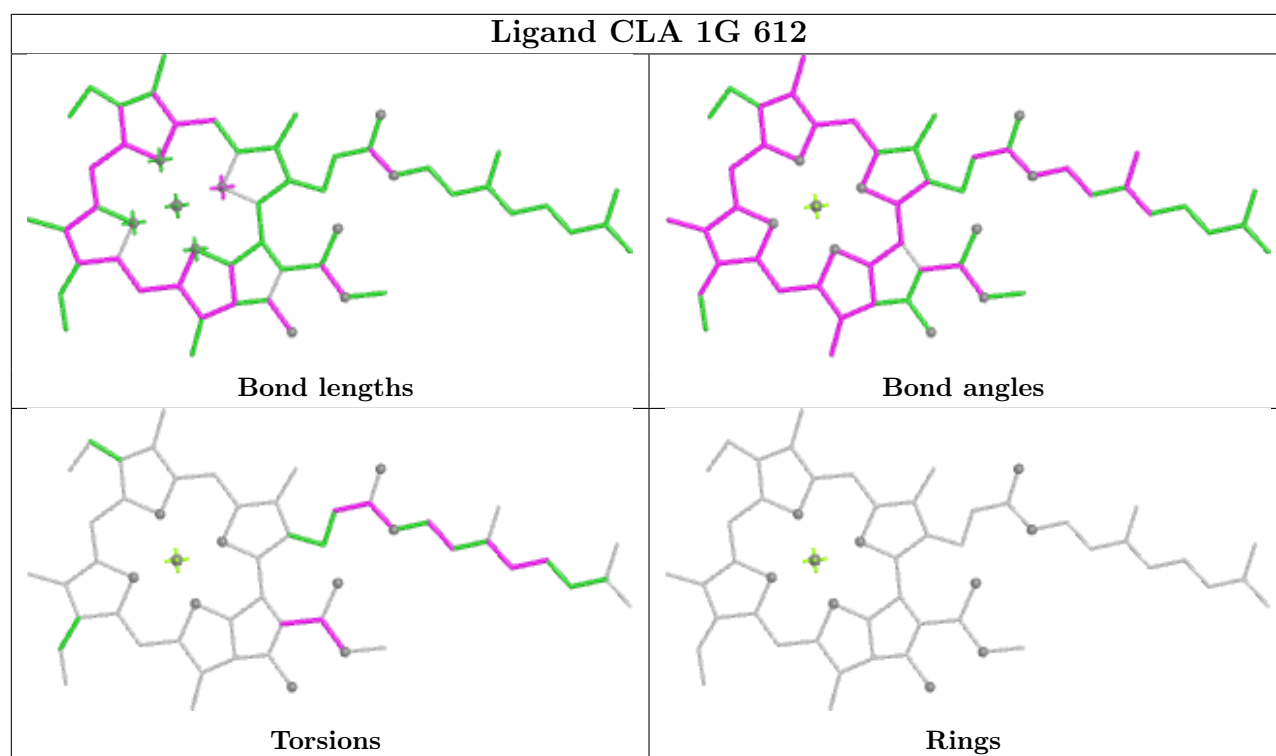


Ligand CLA 1N 614

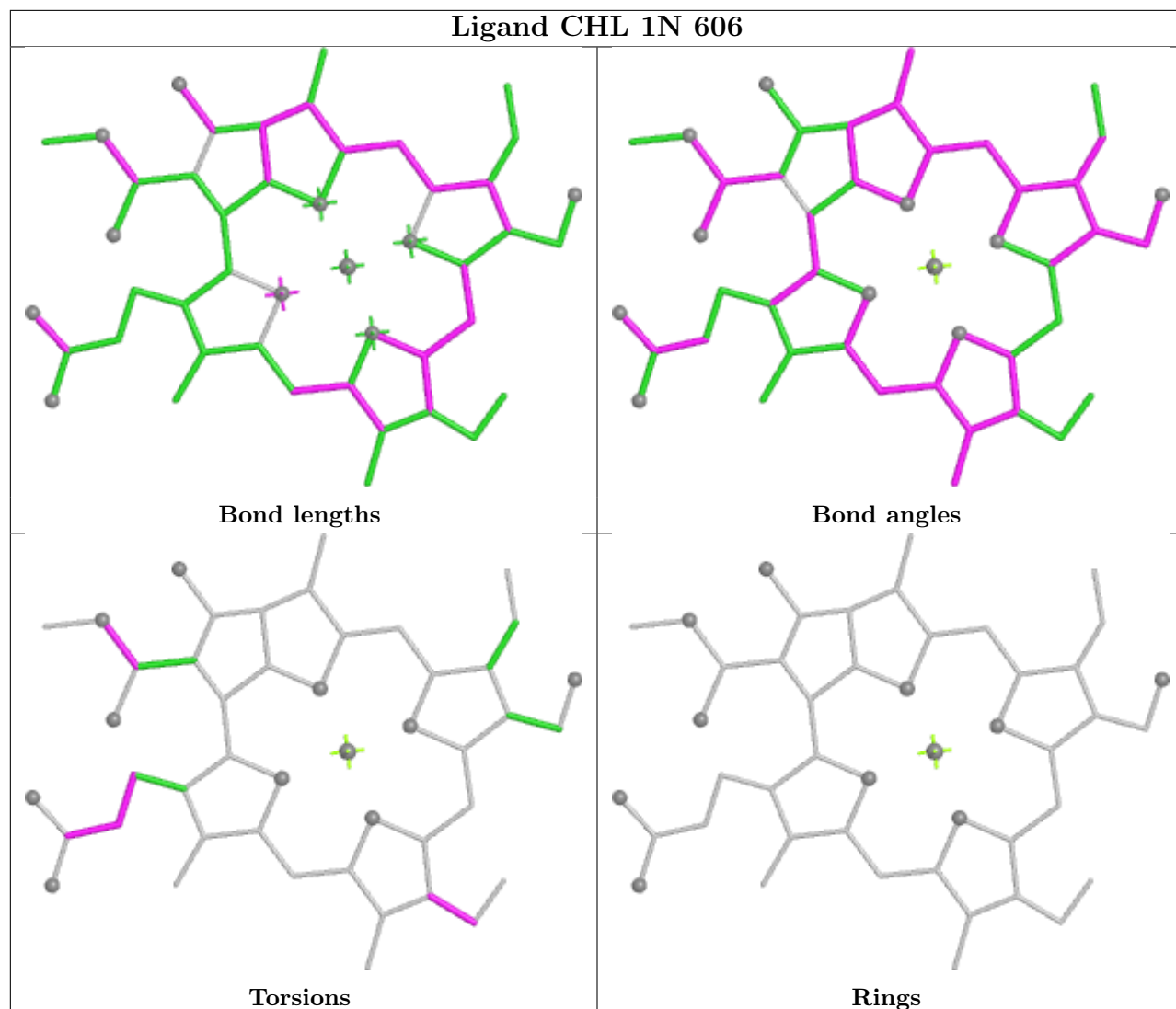


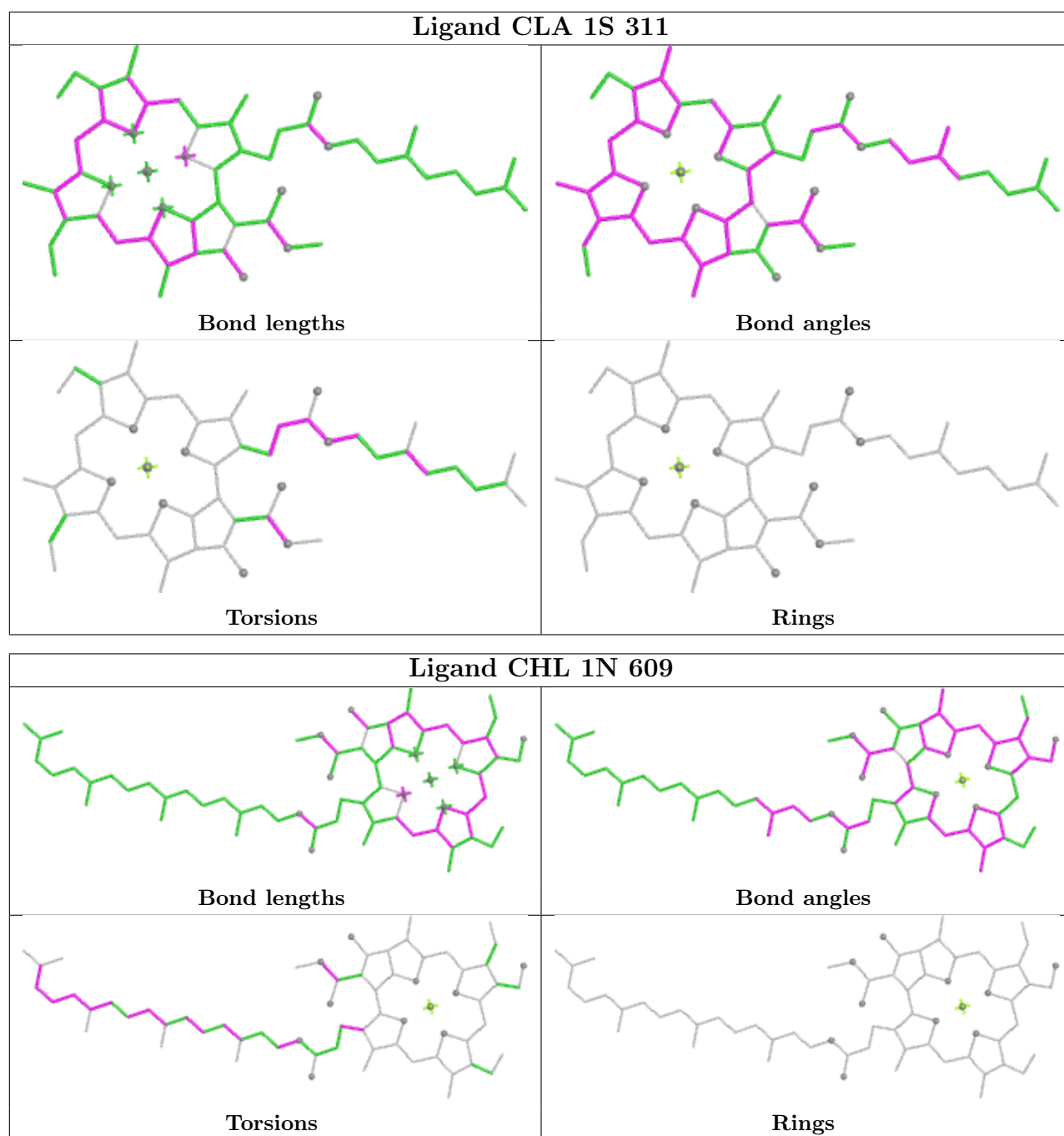
Ligand LUT 1S 315

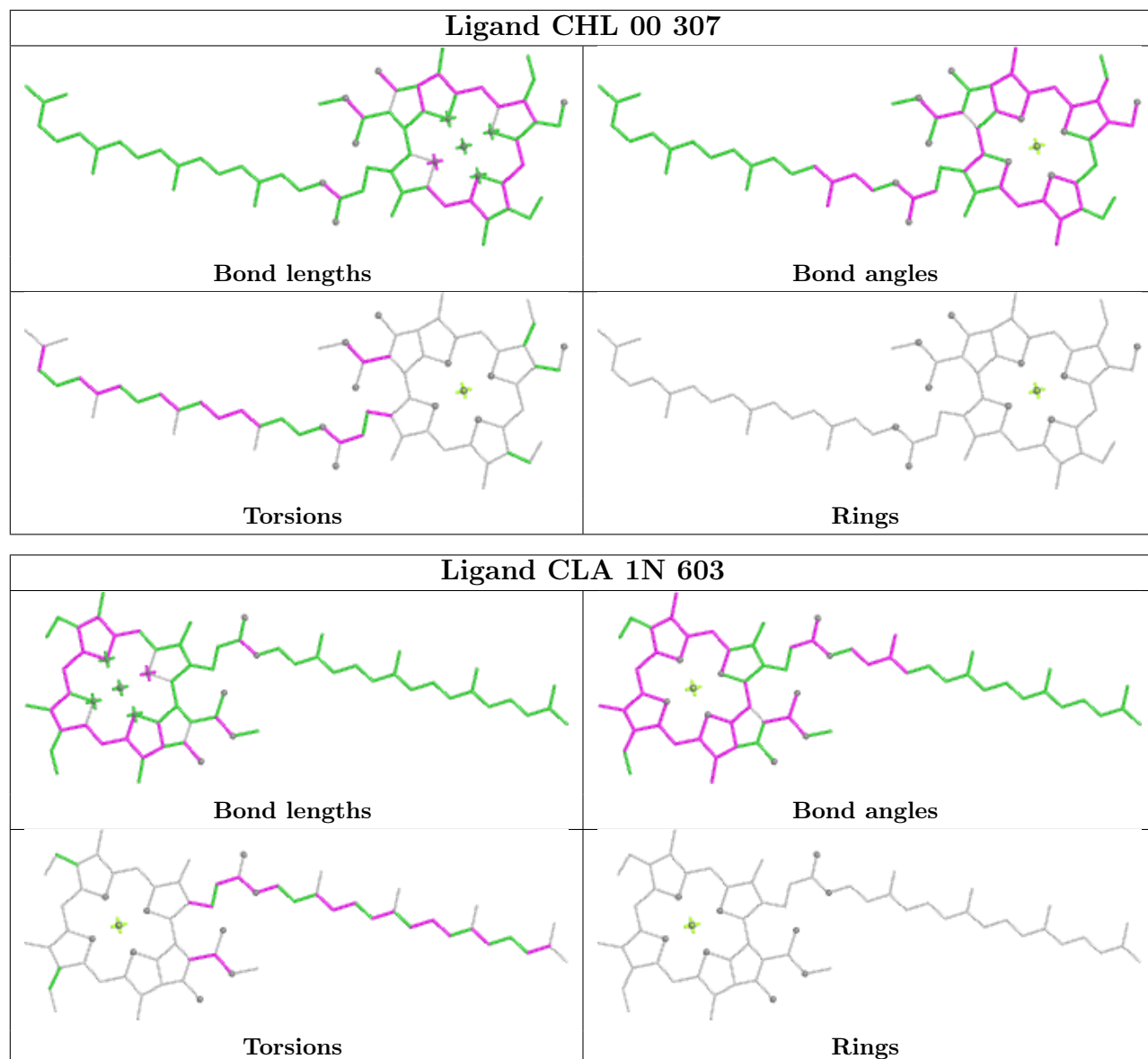


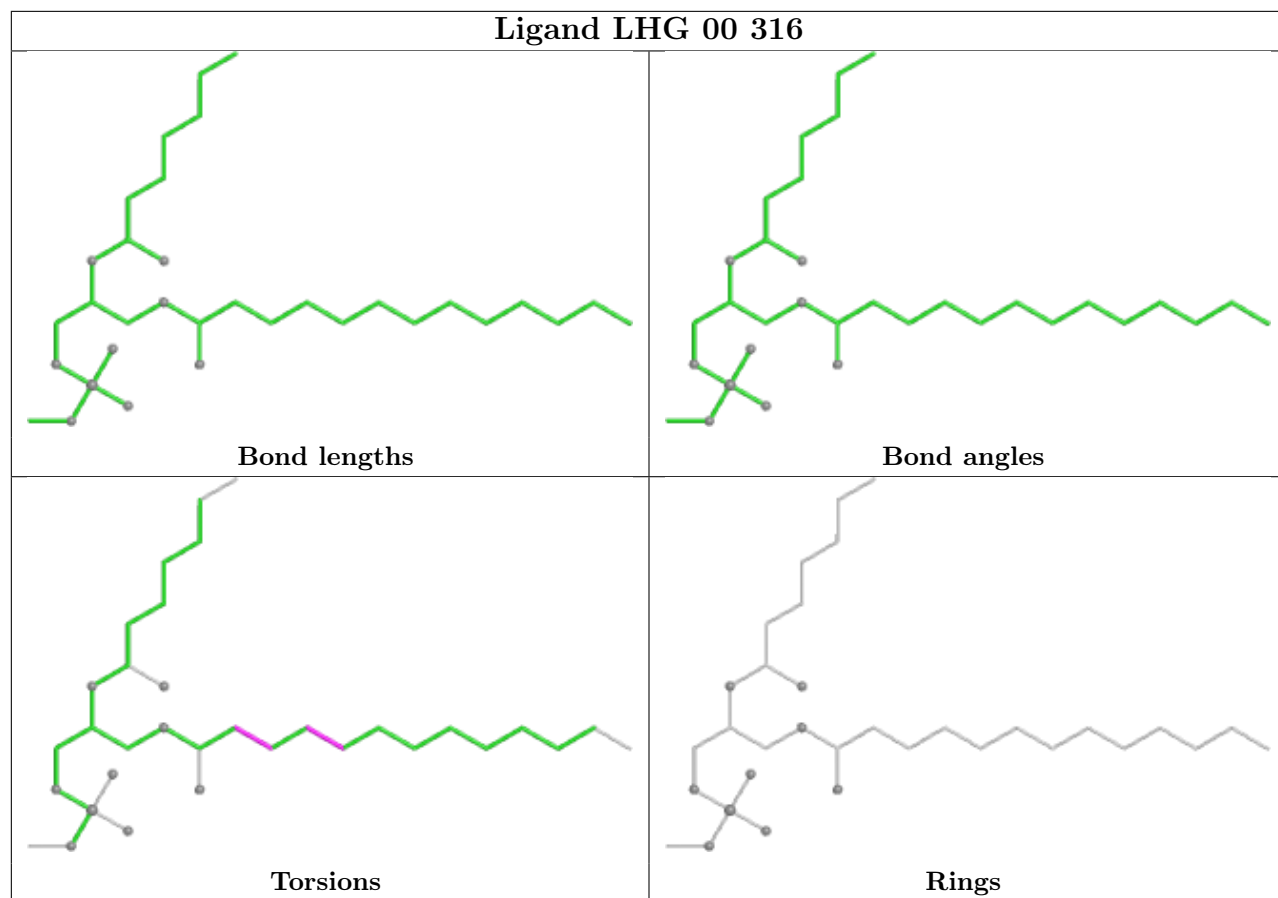


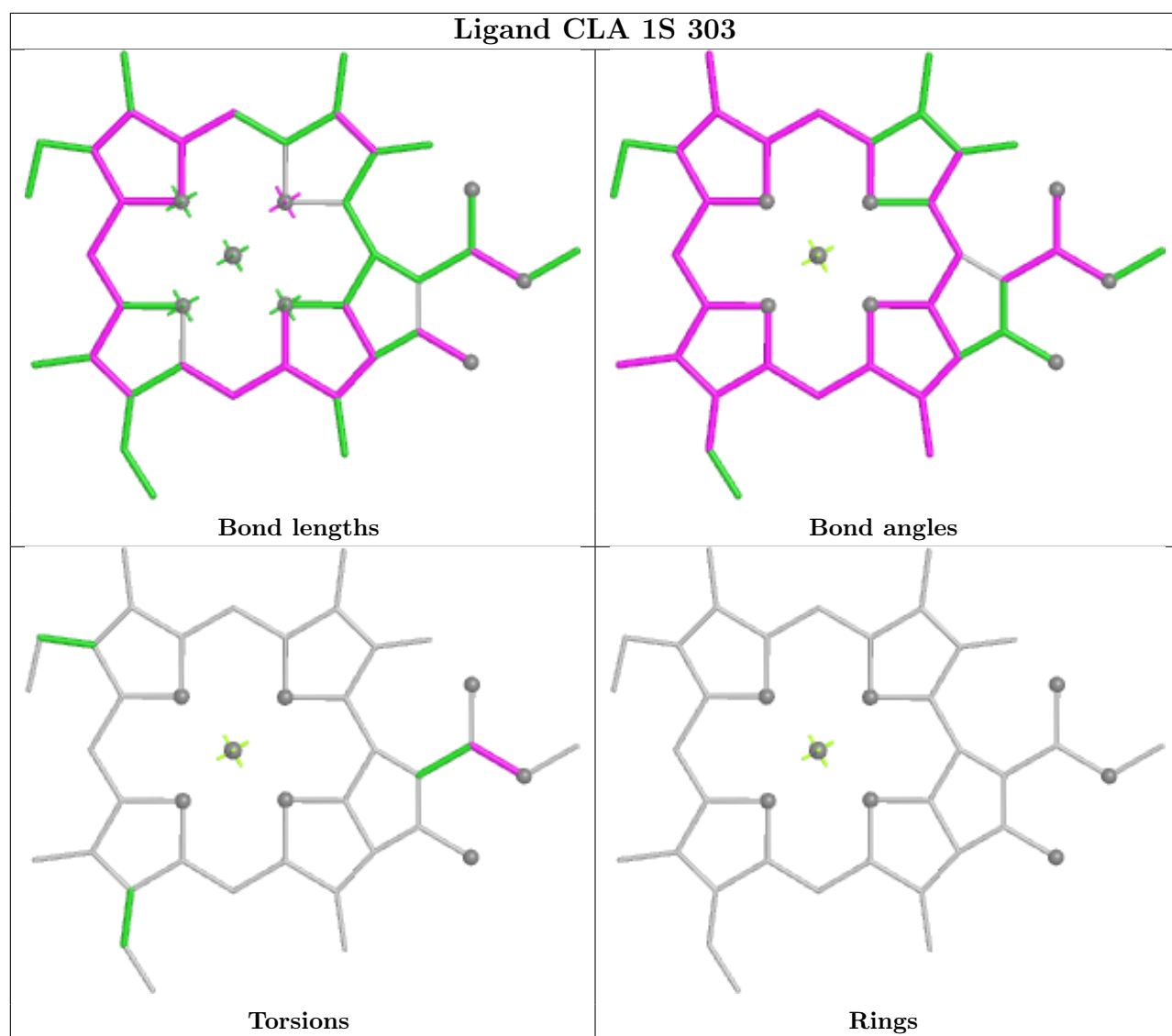
Ligand CHL 1N 606

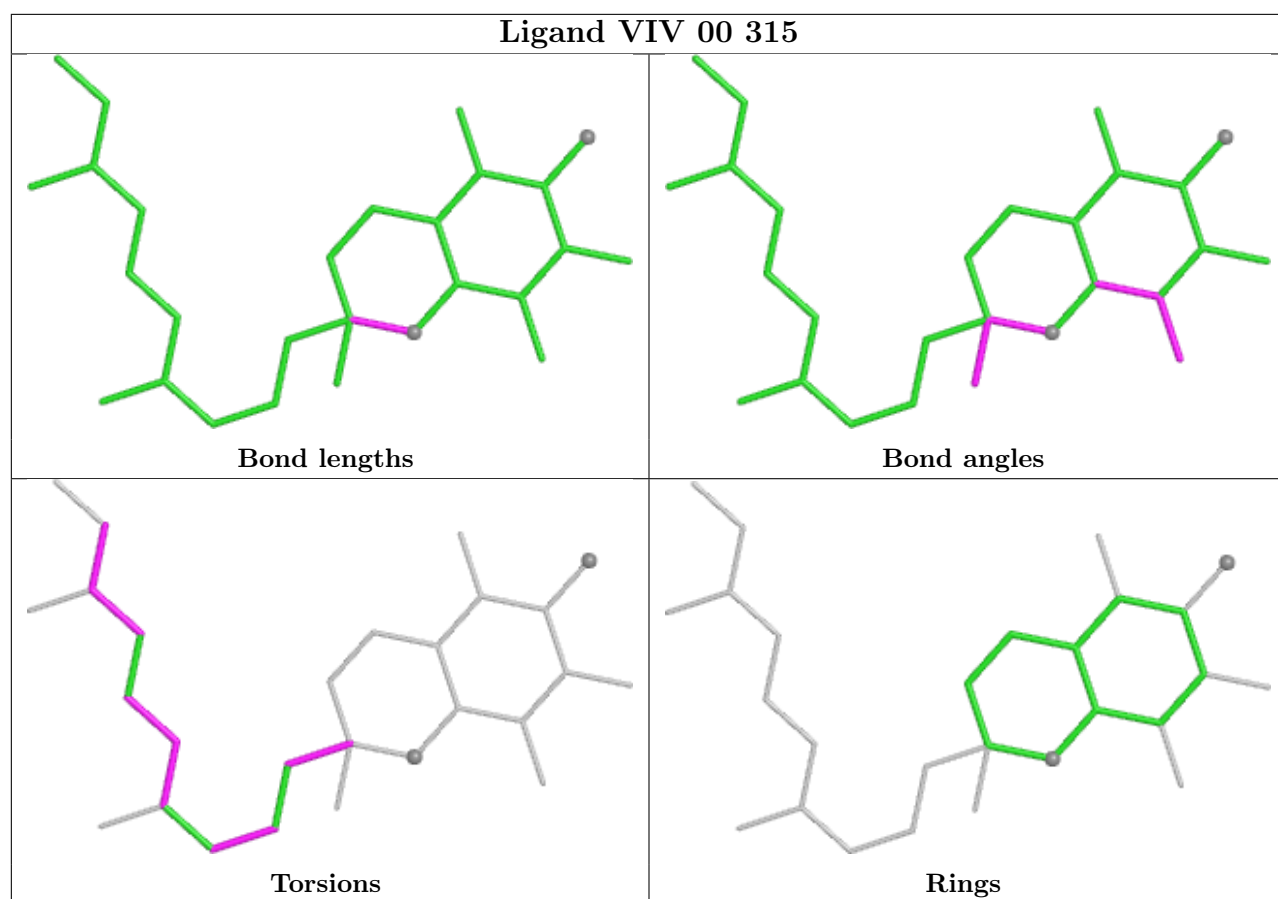


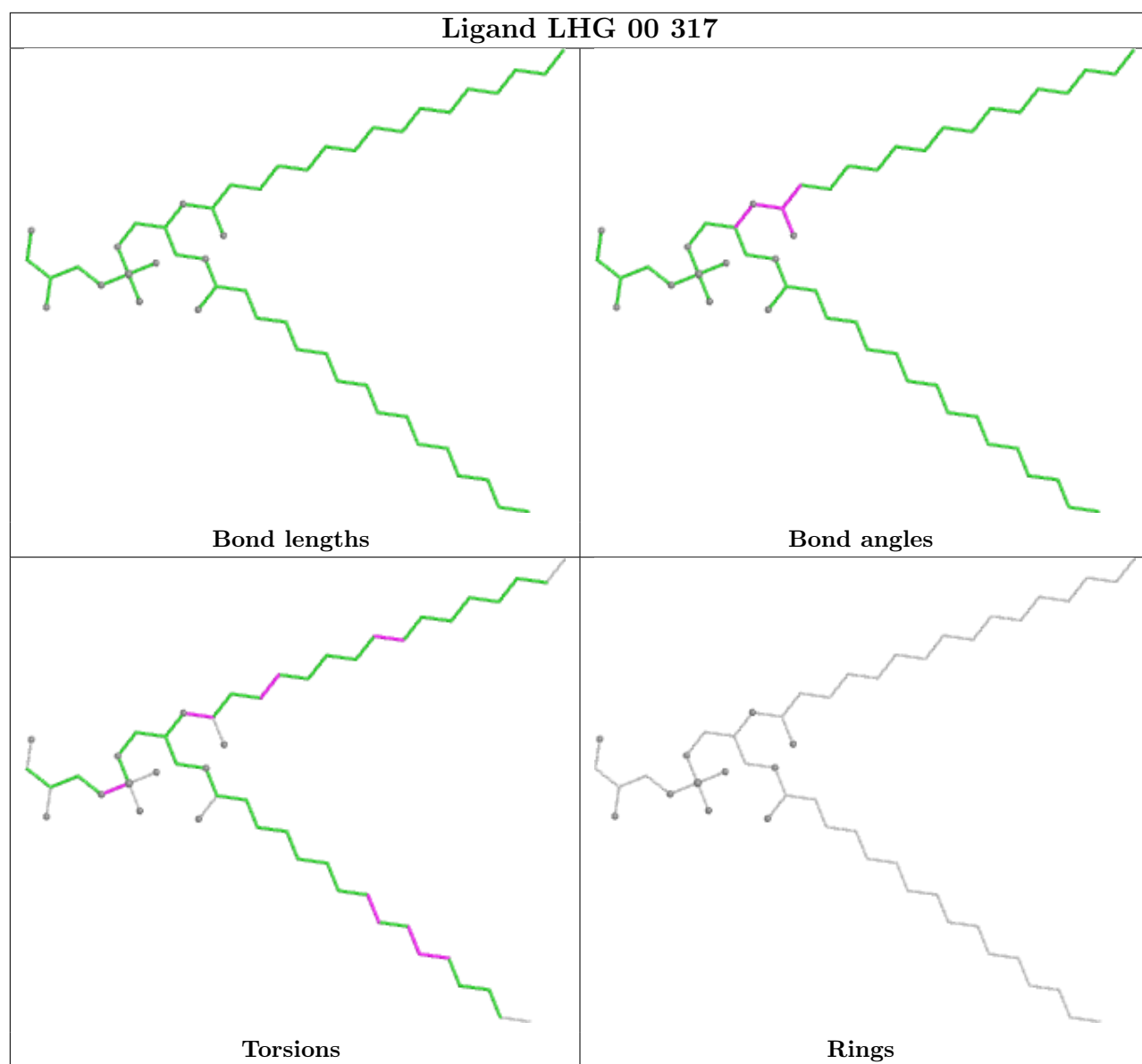


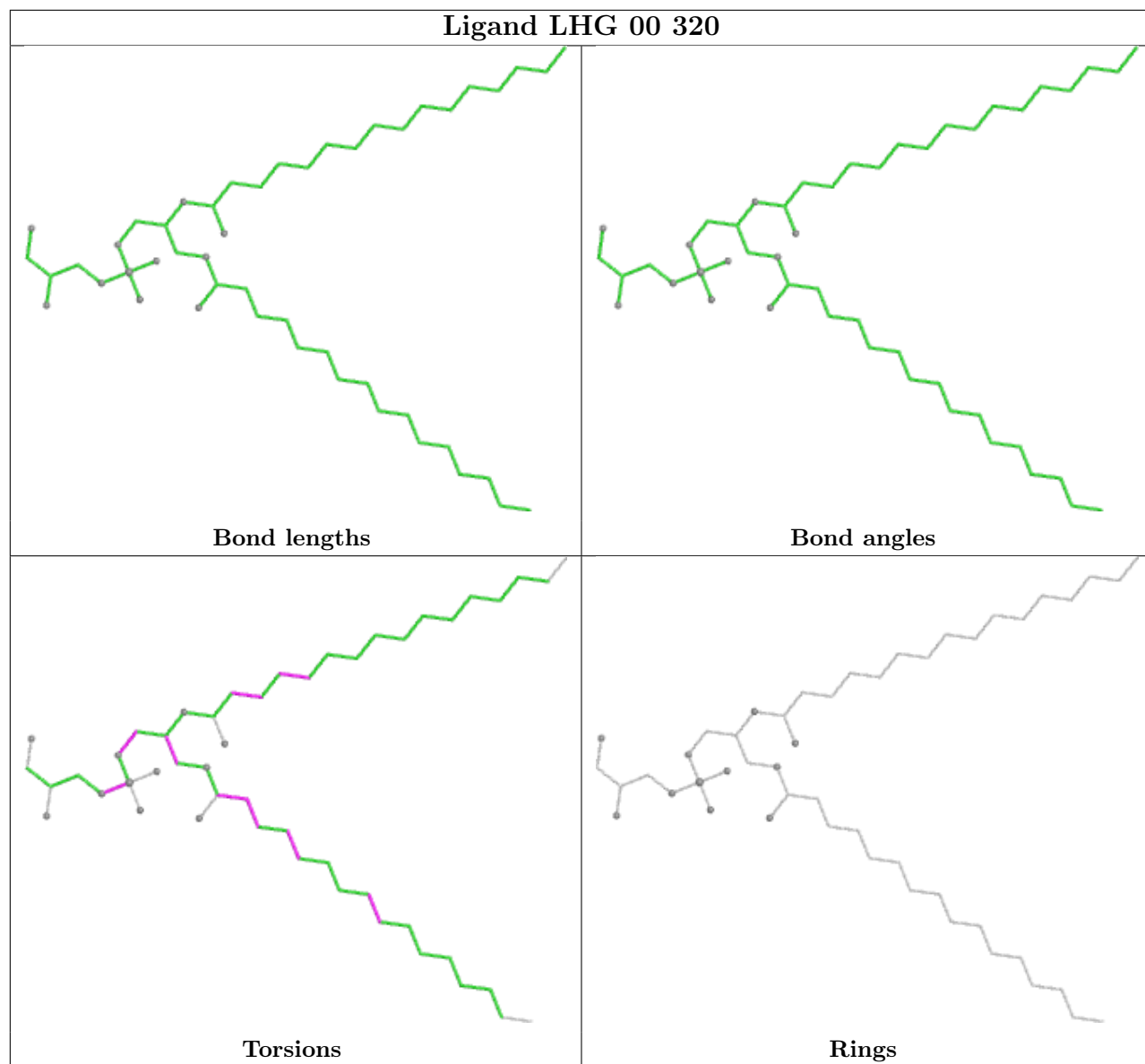


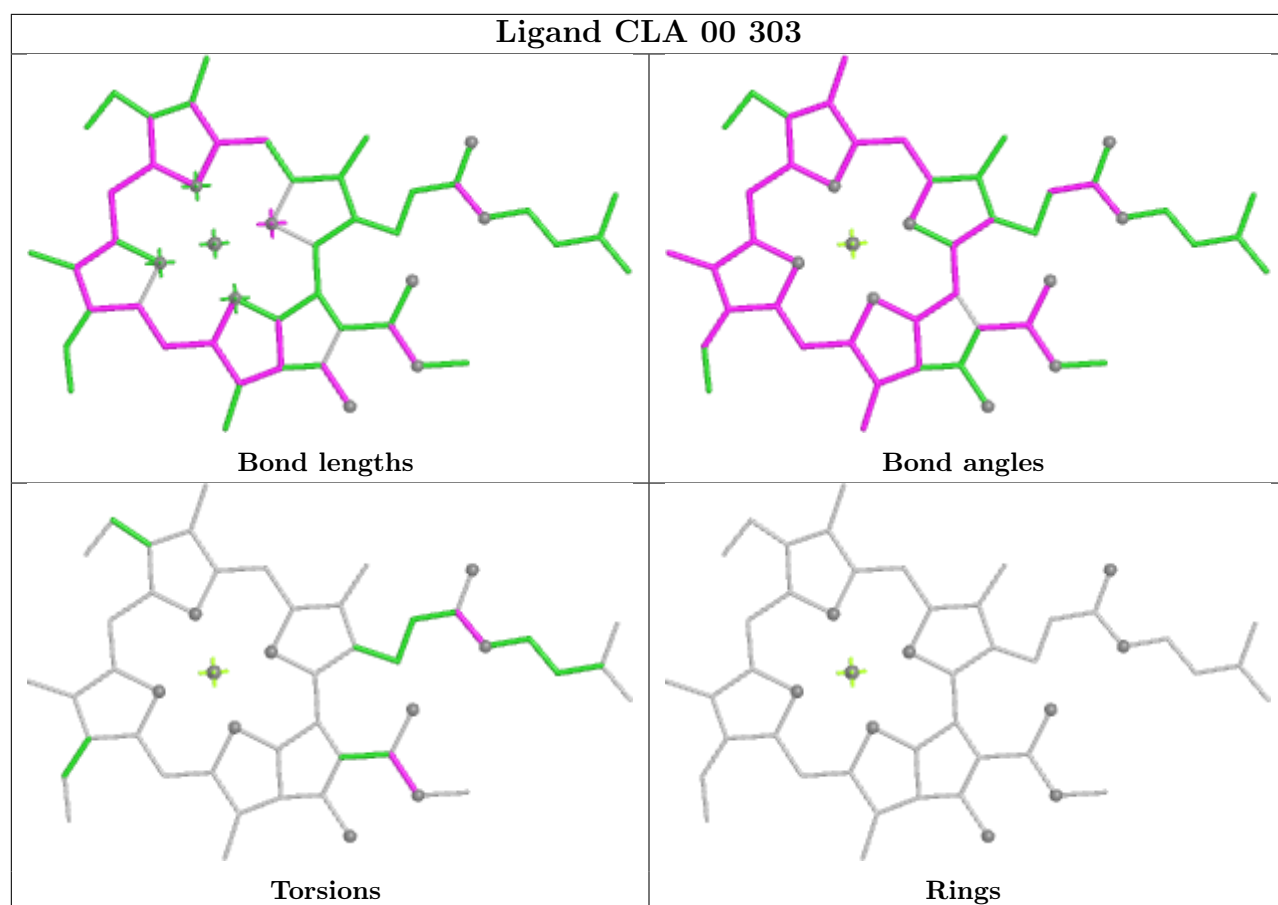


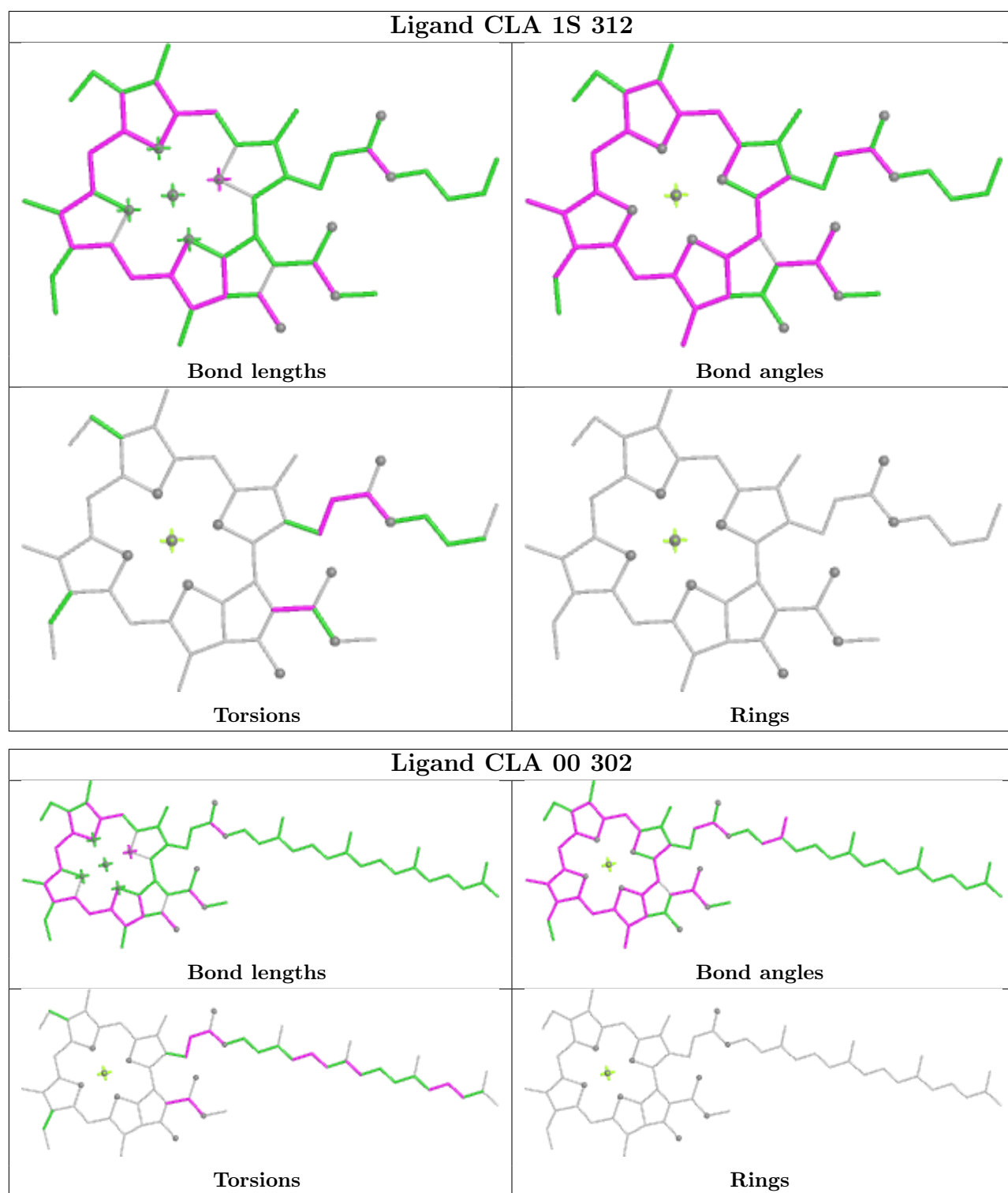


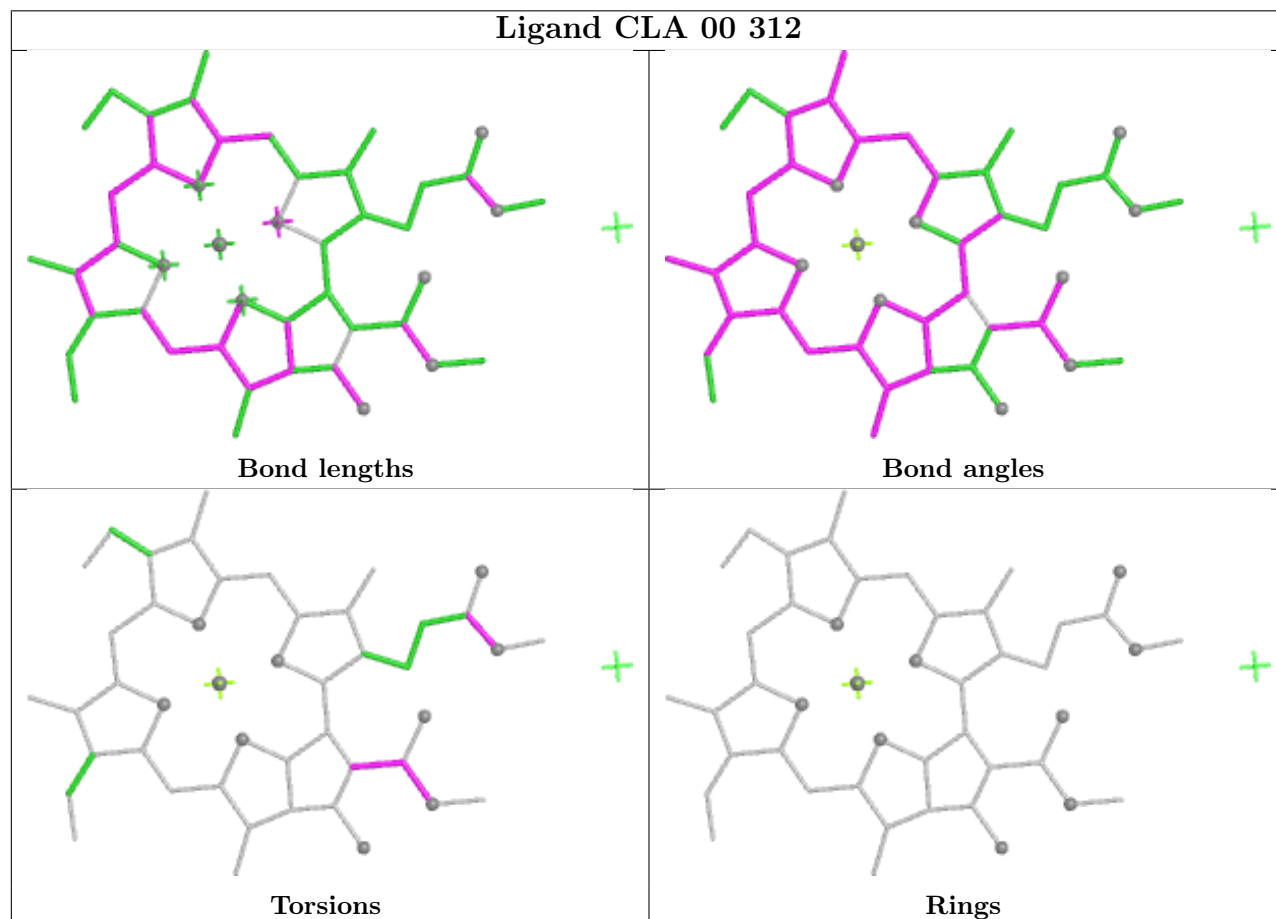
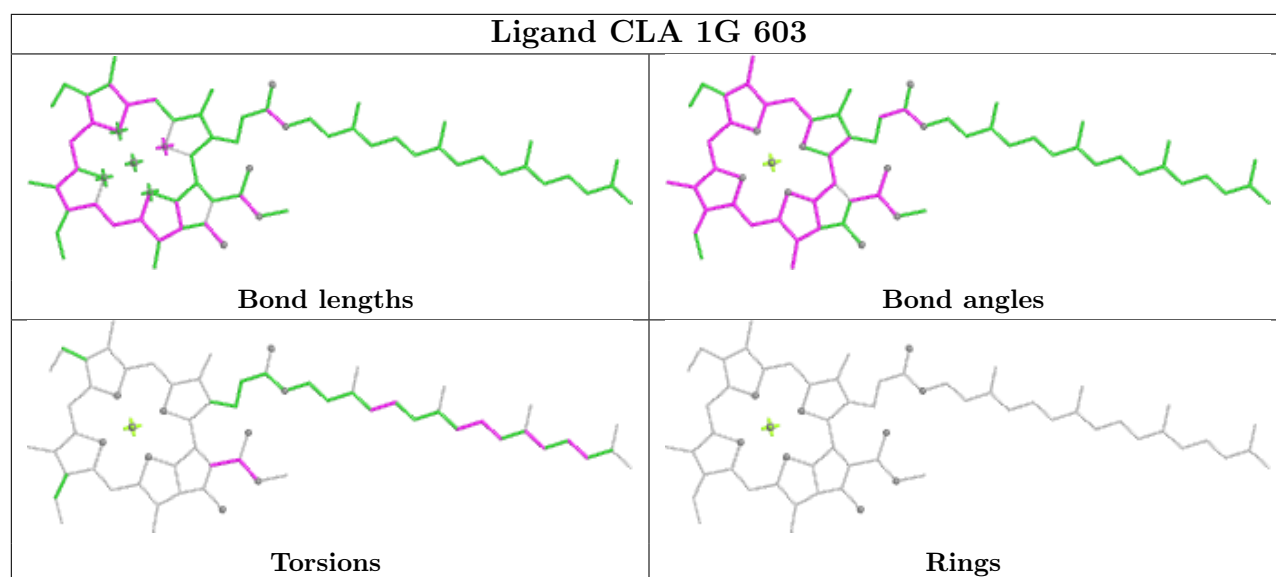


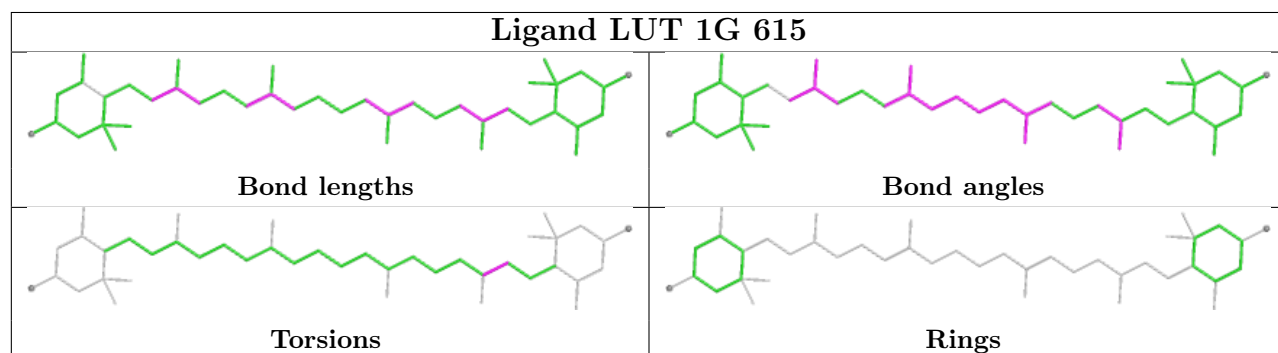
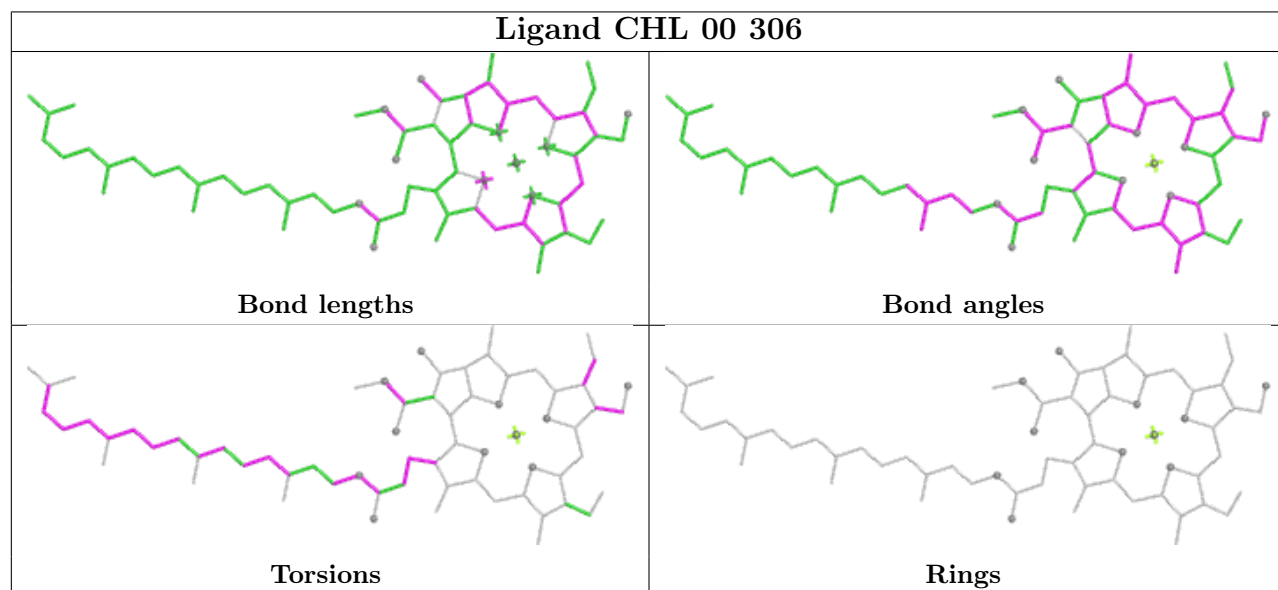
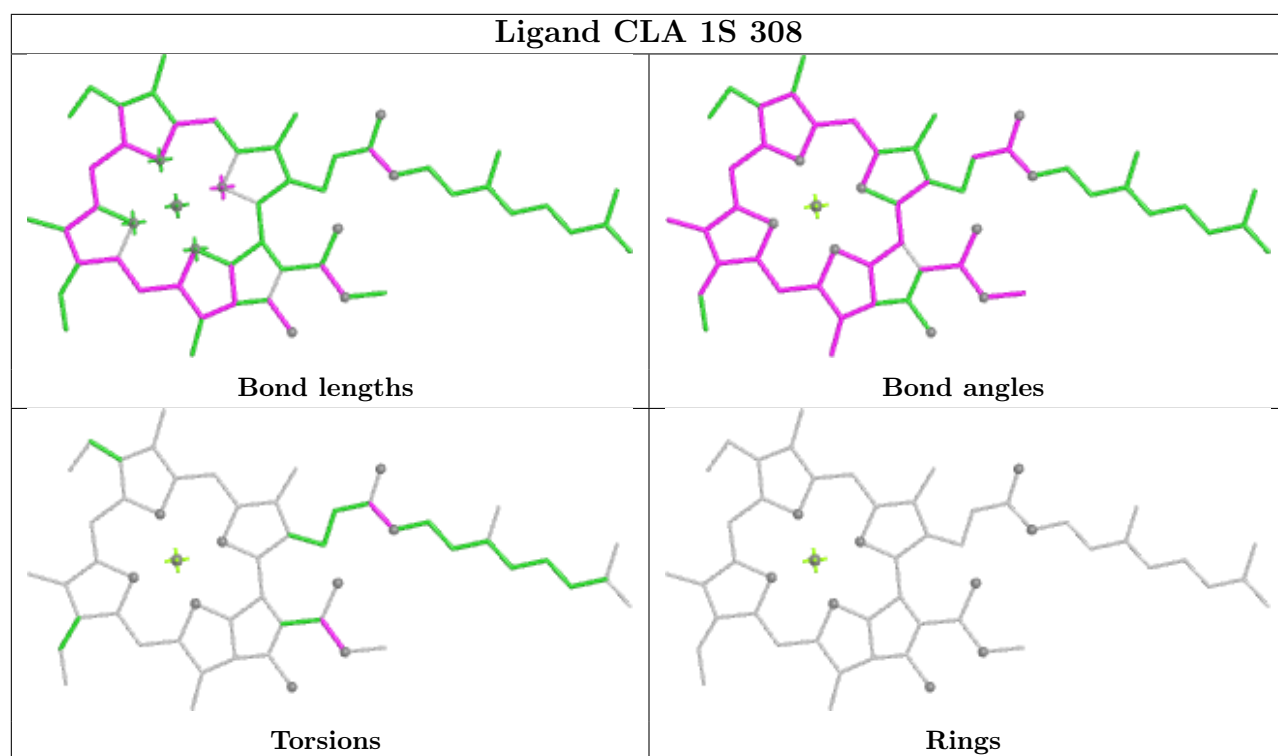


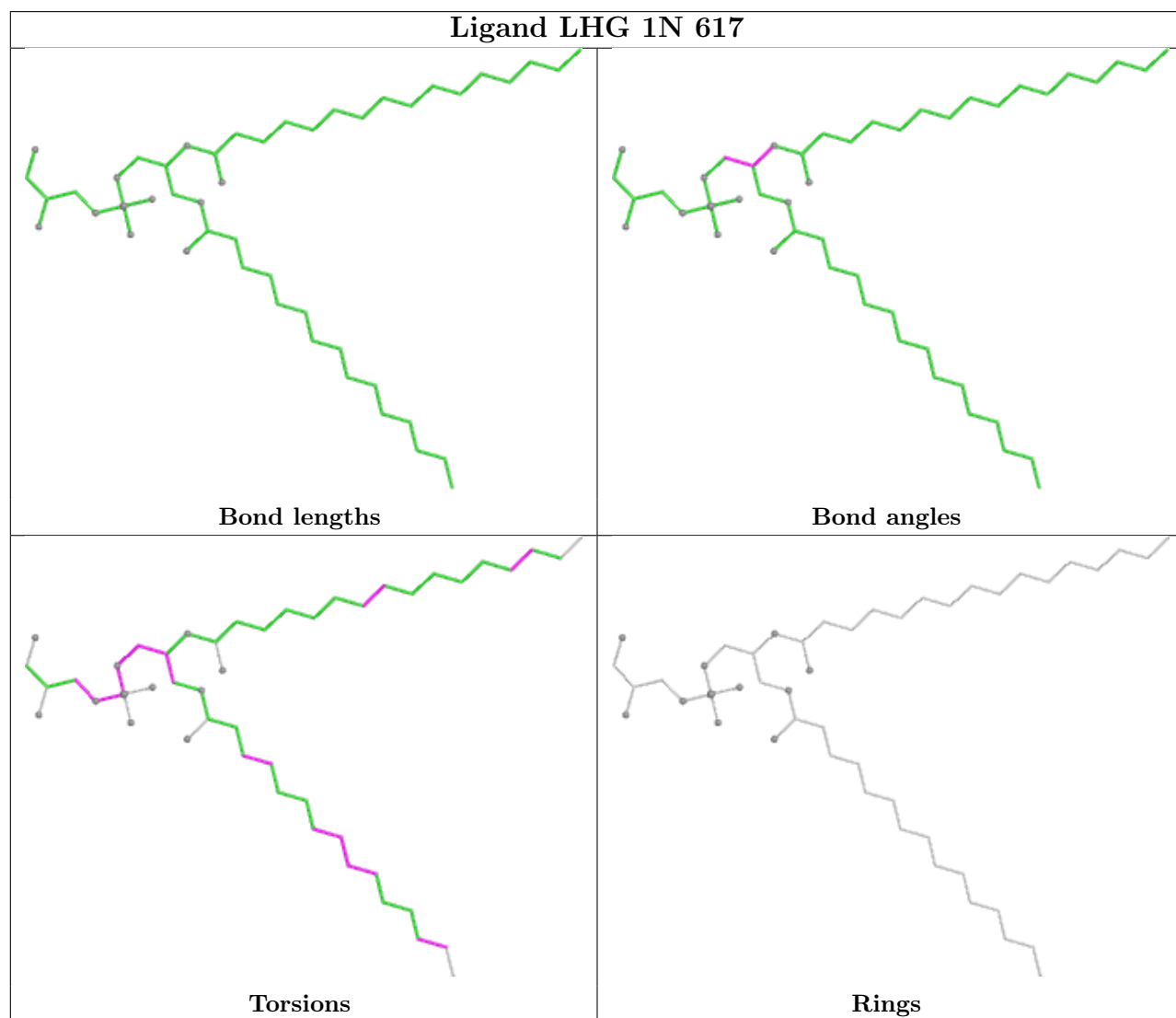
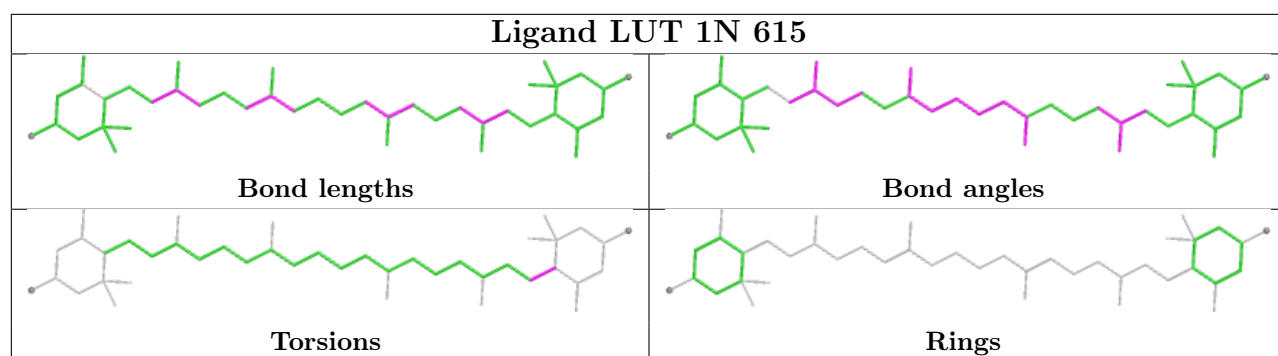


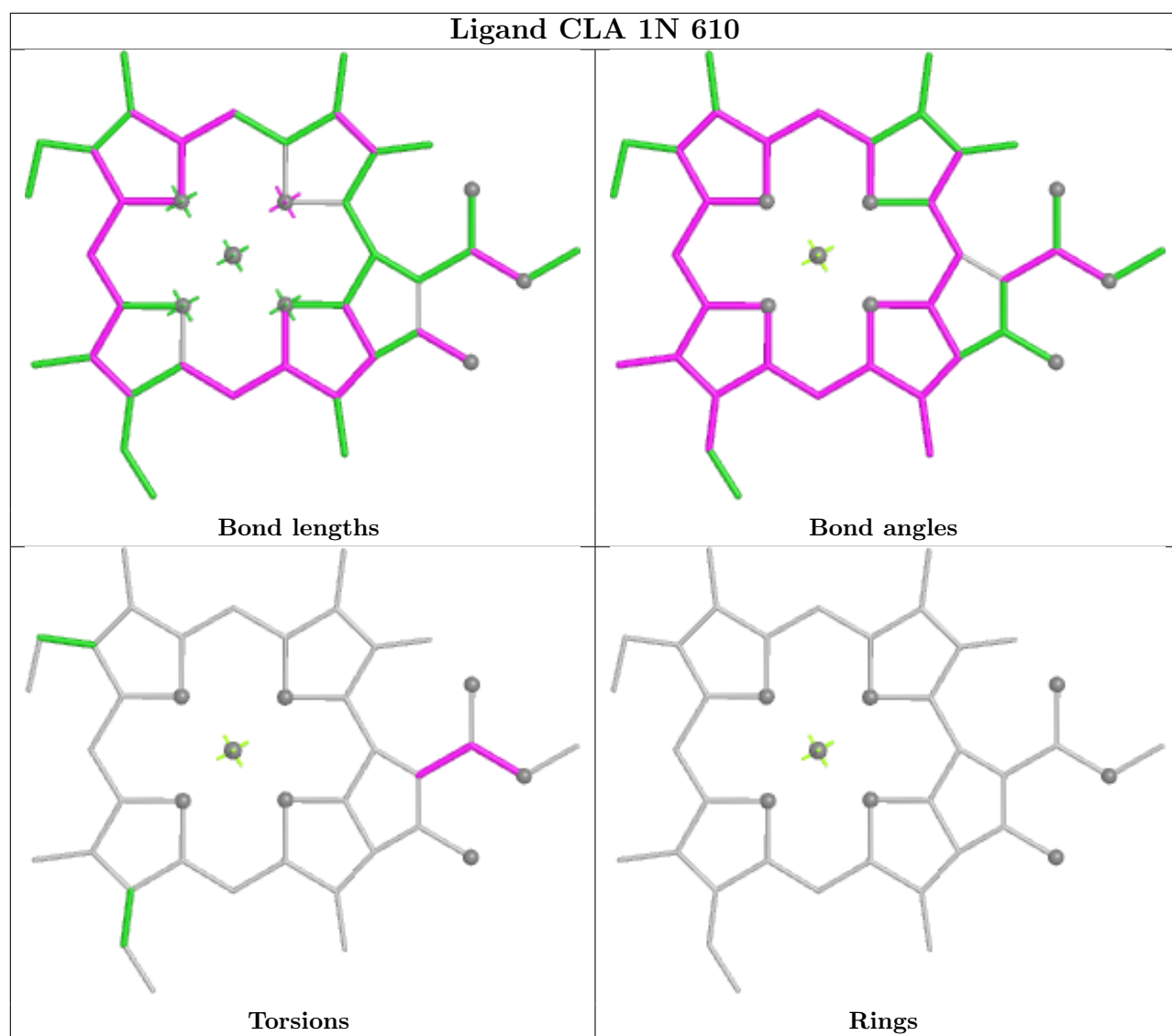


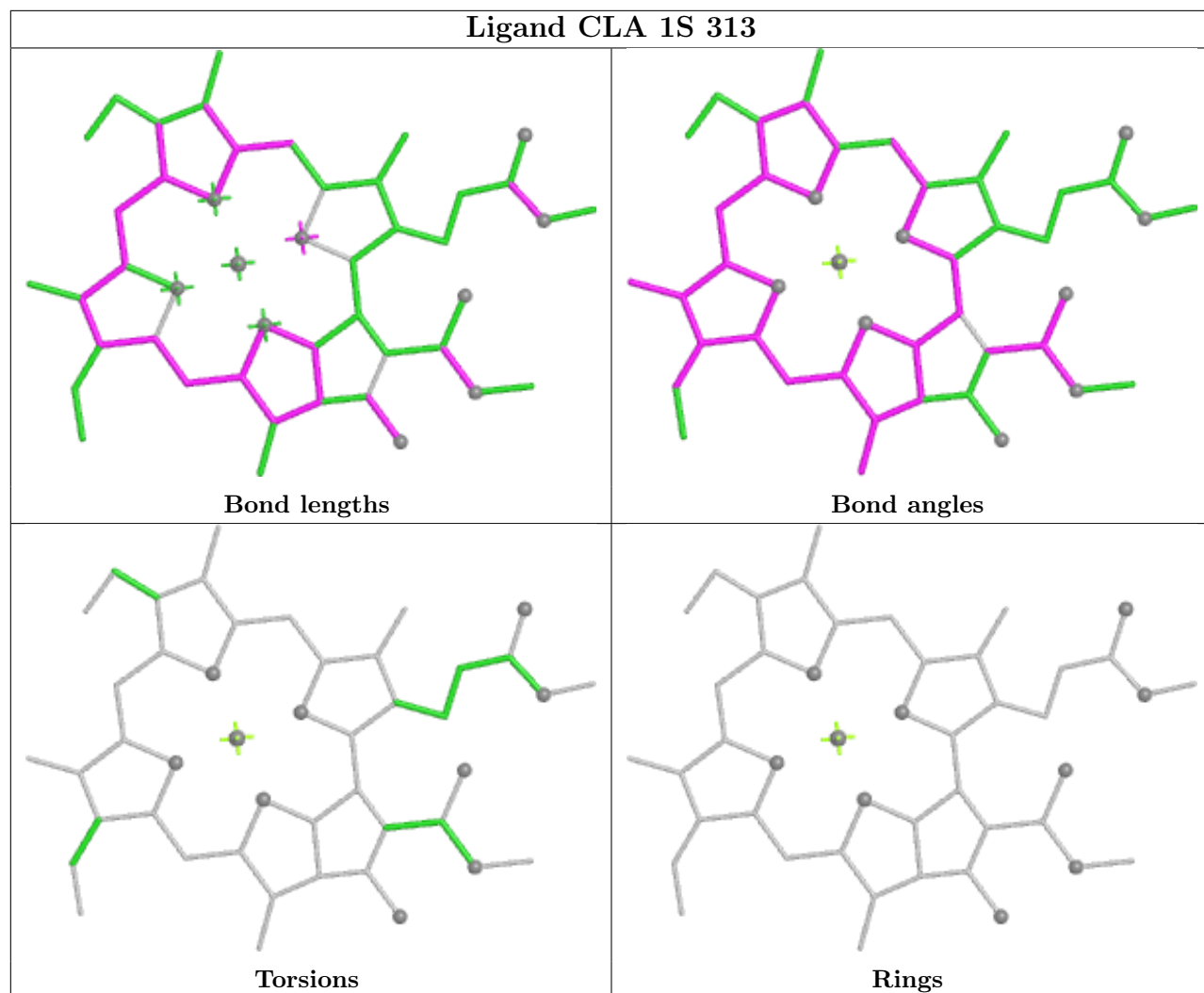


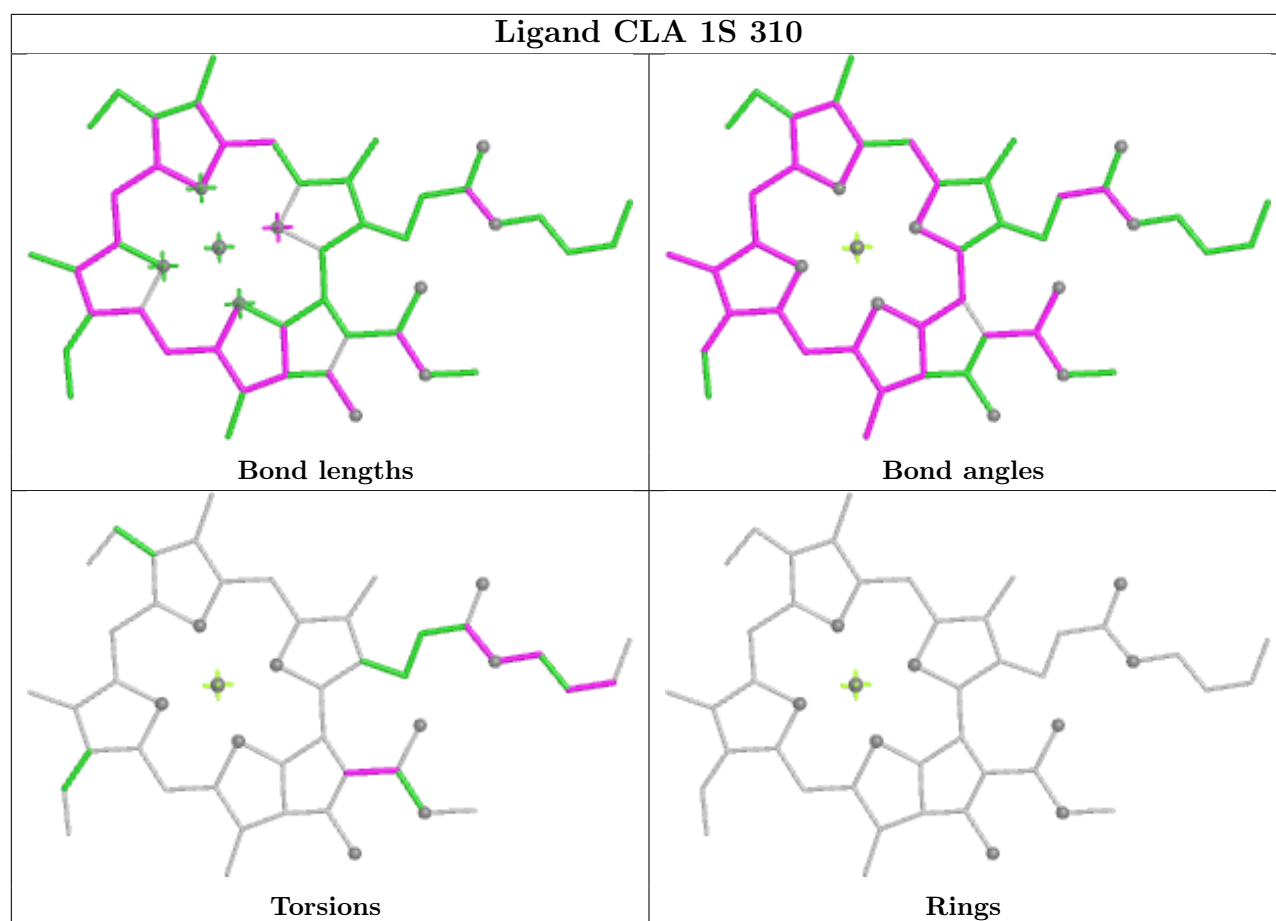












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

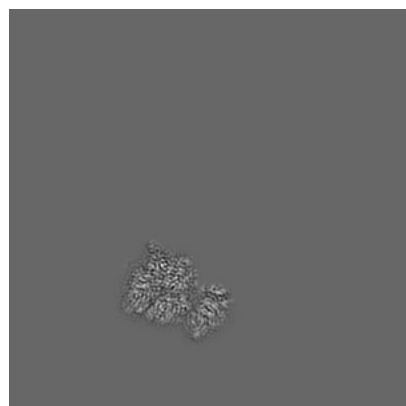
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66949. These allow visual inspection of the internal detail of the map and identification of artifacts.

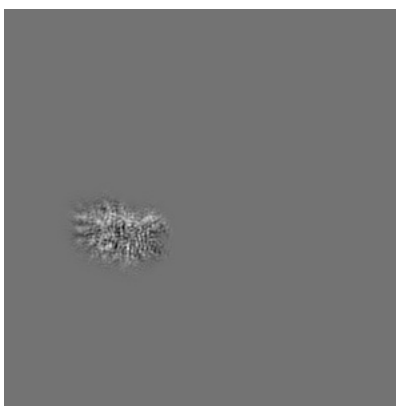
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

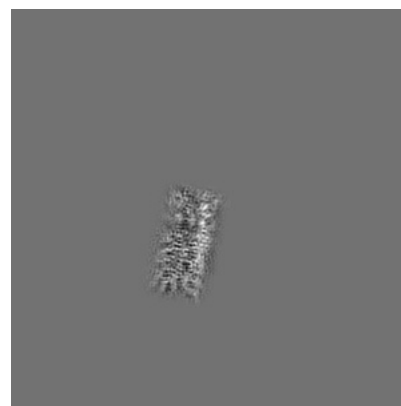
6.1.1 Primary map



X

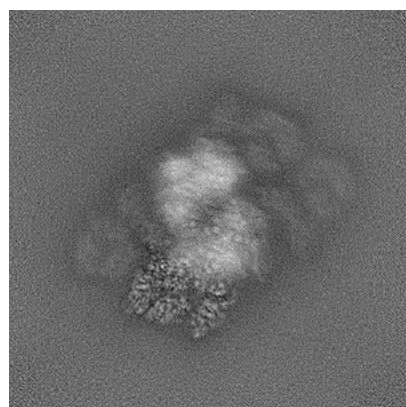


Y

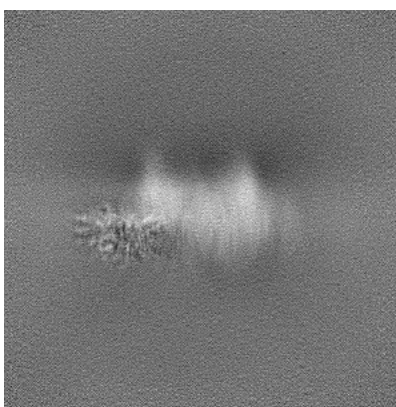


Z

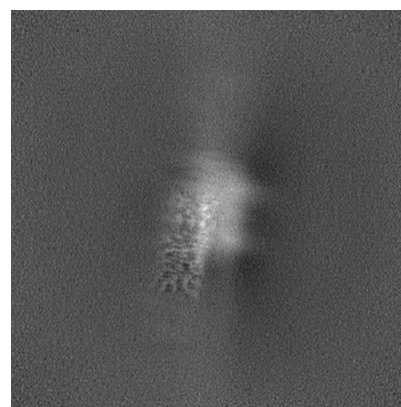
6.1.2 Raw map



X



Y

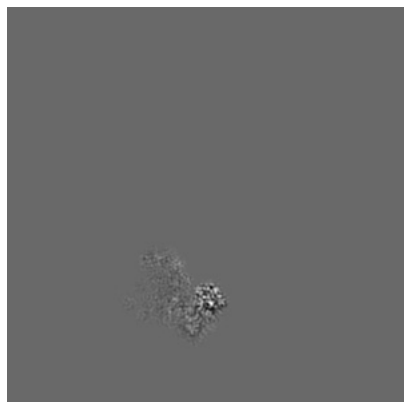


Z

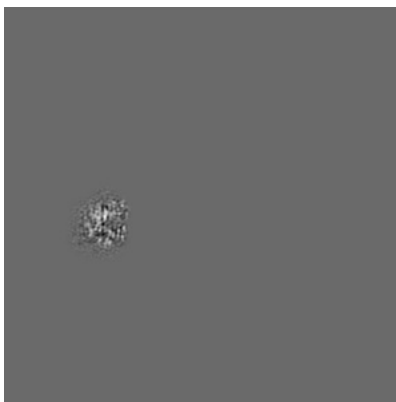
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

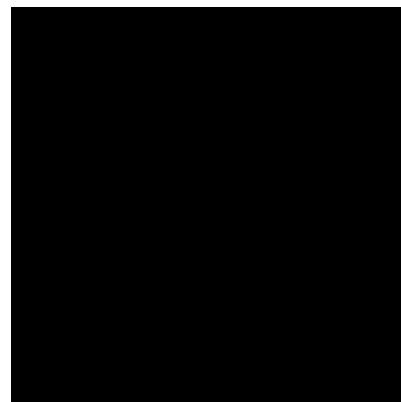
6.2.1 Primary map



X Index: 256

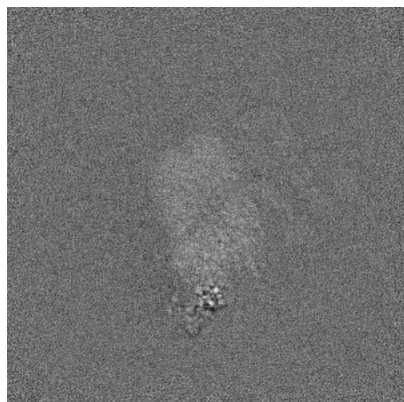


Y Index: 256

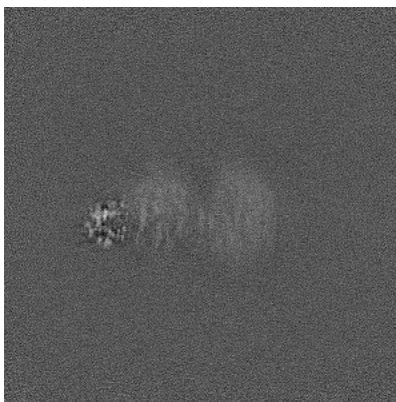


Z Index: 256

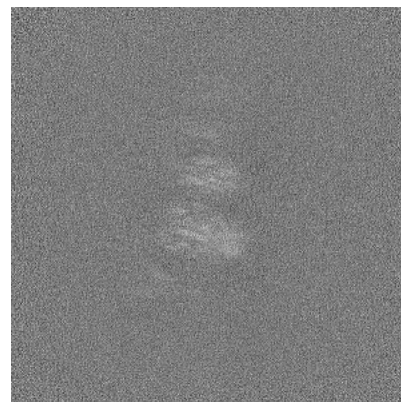
6.2.2 Raw map



X Index: 256



Y Index: 256

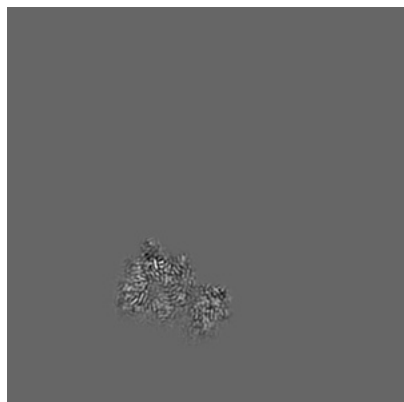


Z Index: 256

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

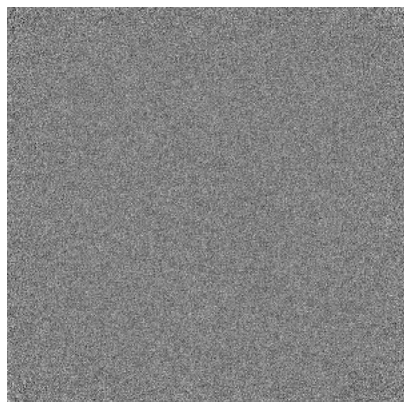


Y Index: 212

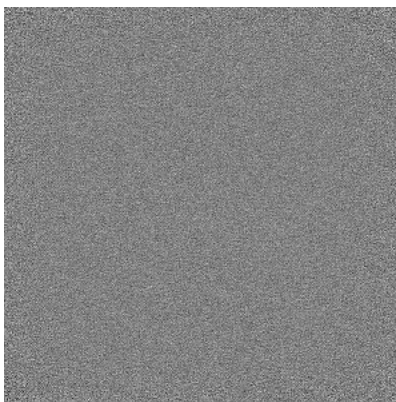


Z Index: 140

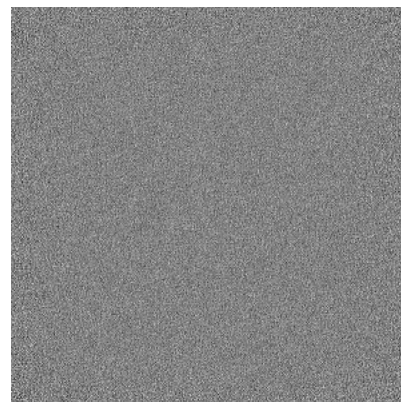
6.3.2 Raw map



X Index: 0



Y Index: 0

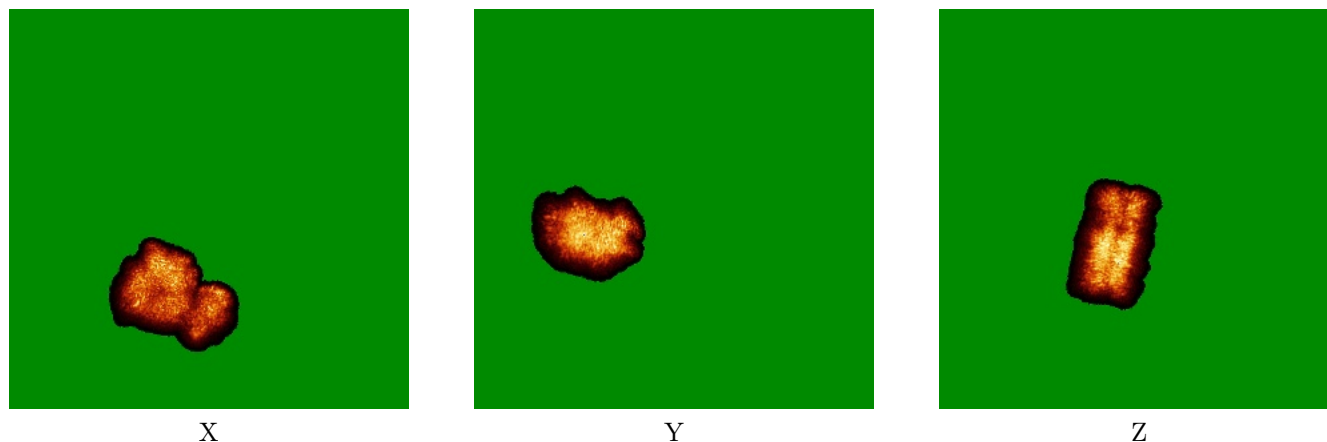


Z Index: 0

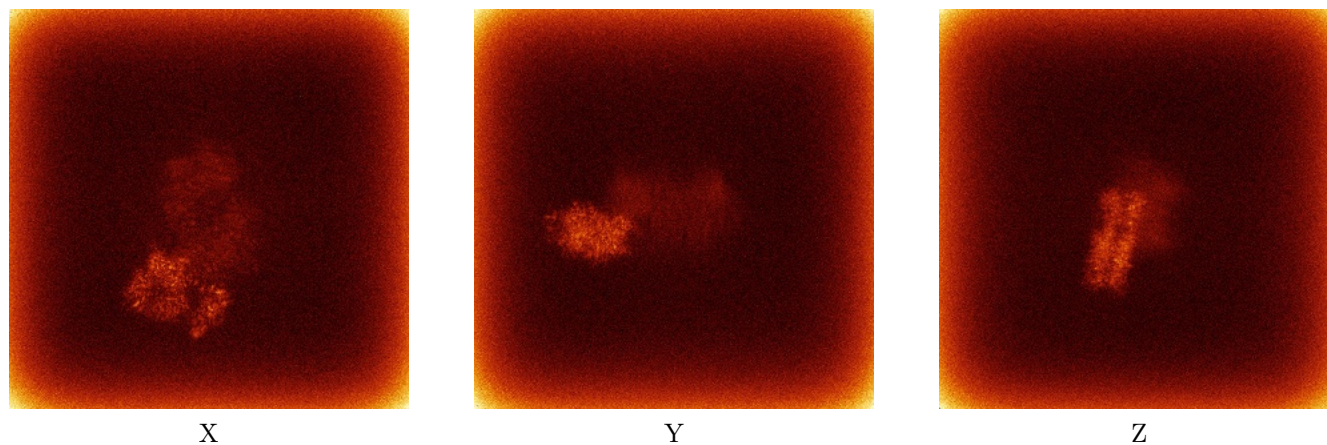
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



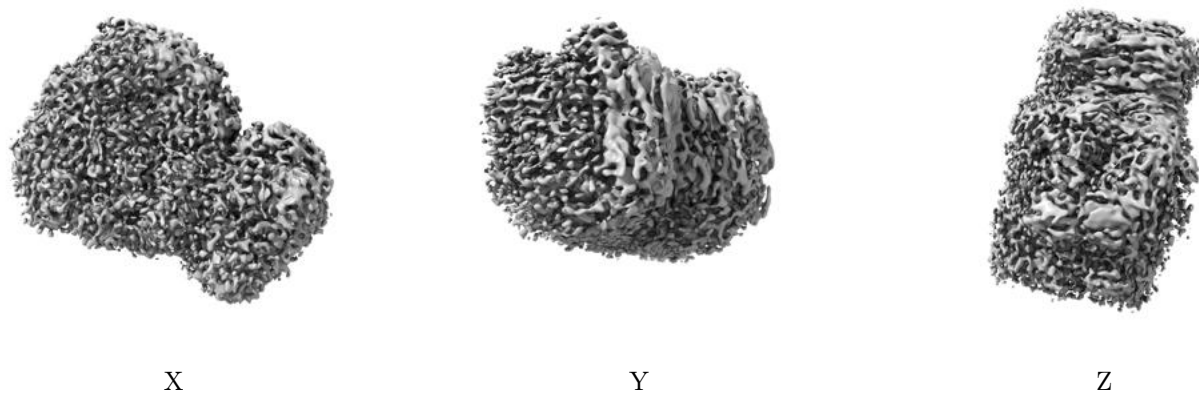
6.4.2 Raw map



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.

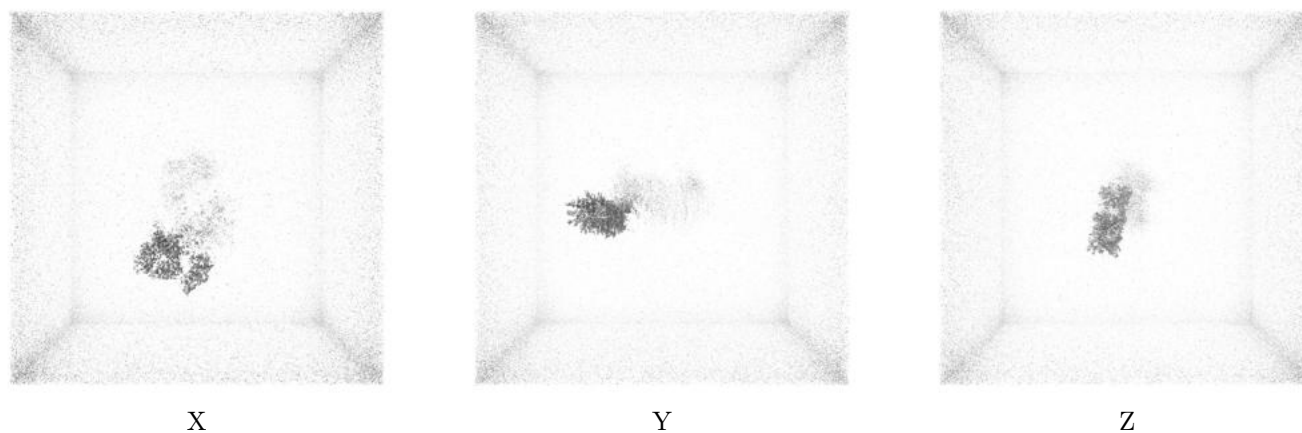
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

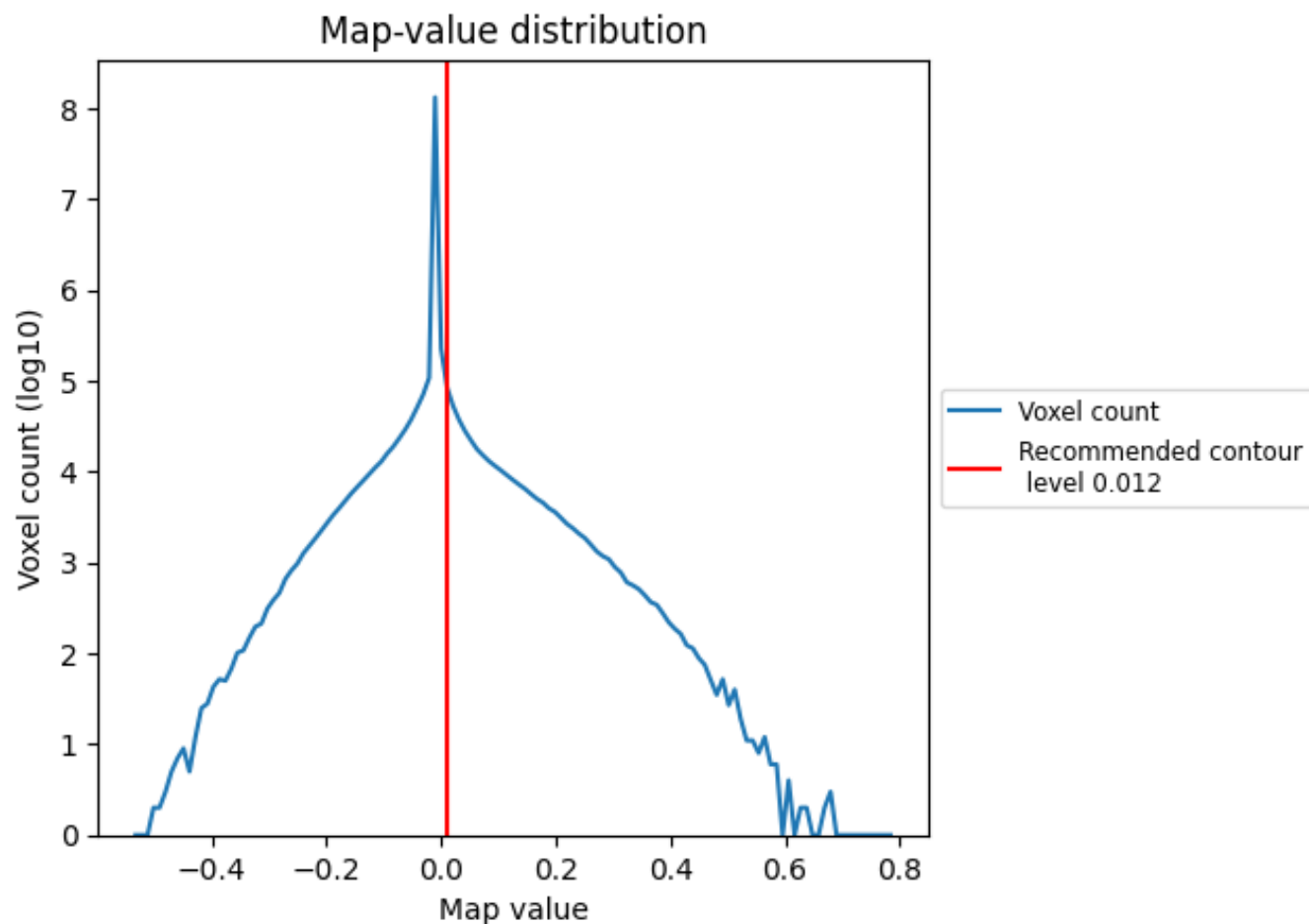
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

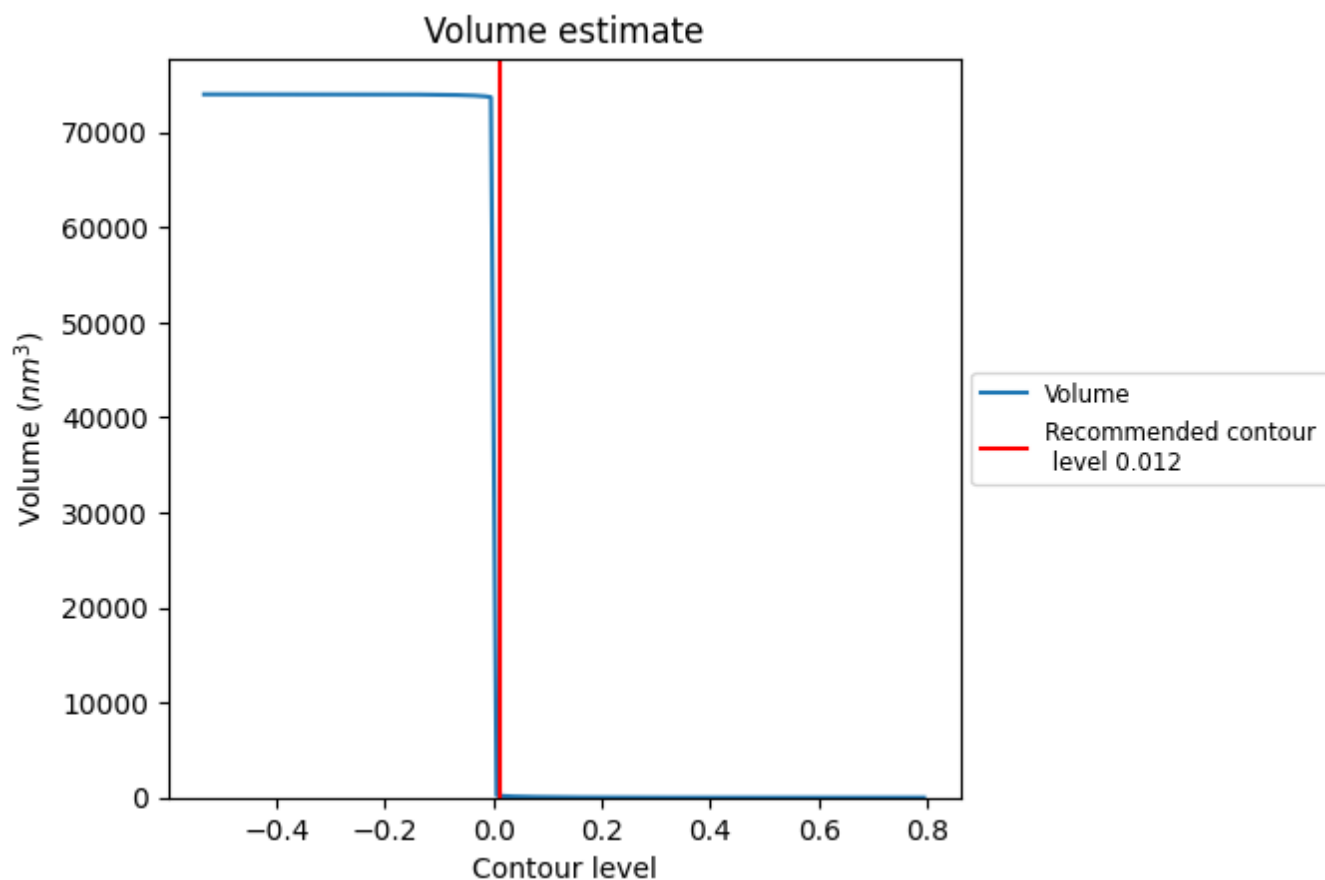
This section contains the results of statistical analysis of the map.

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.

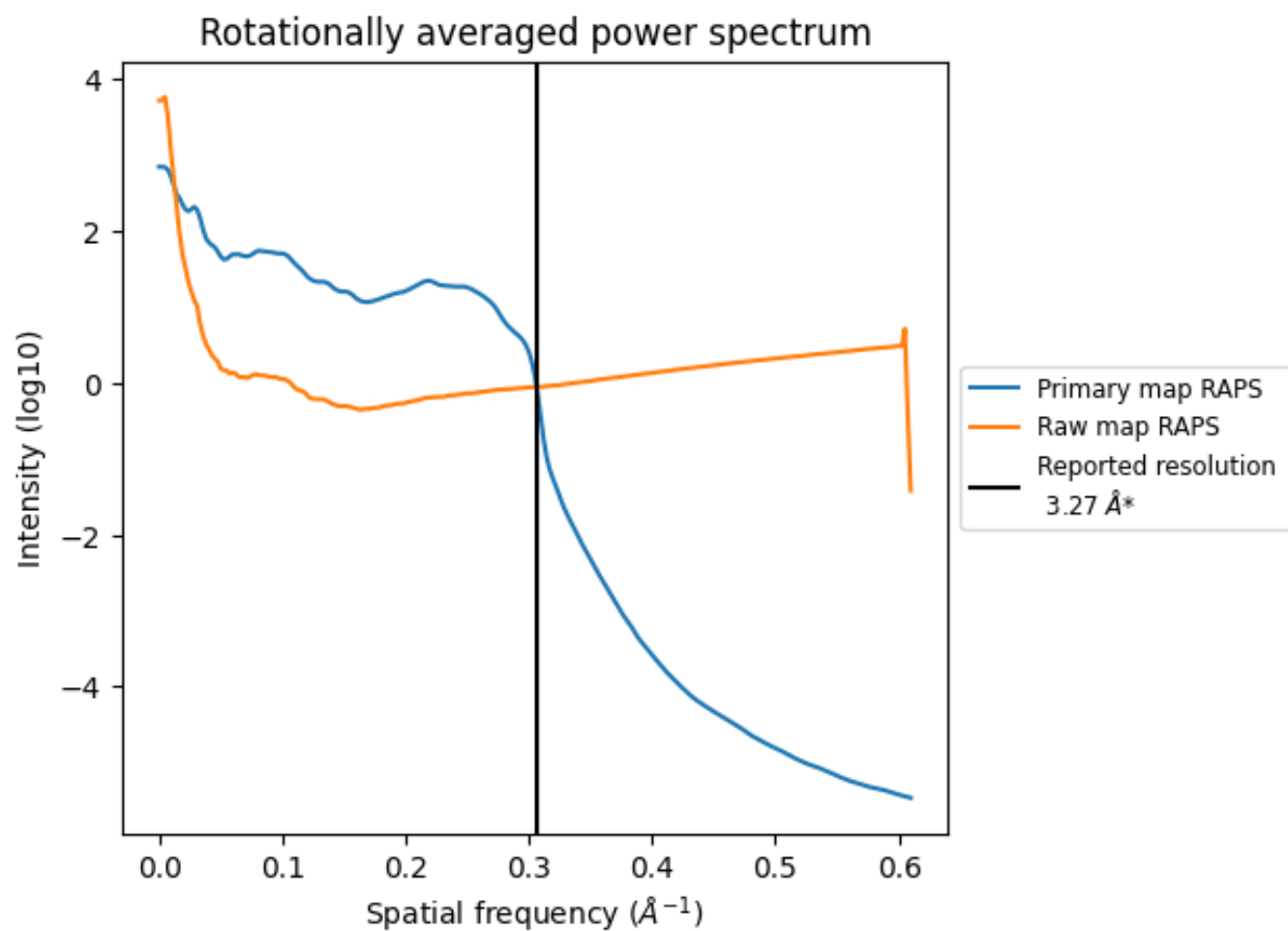
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 202 nm³; this corresponds to an approximate mass of 182 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 ⓘ

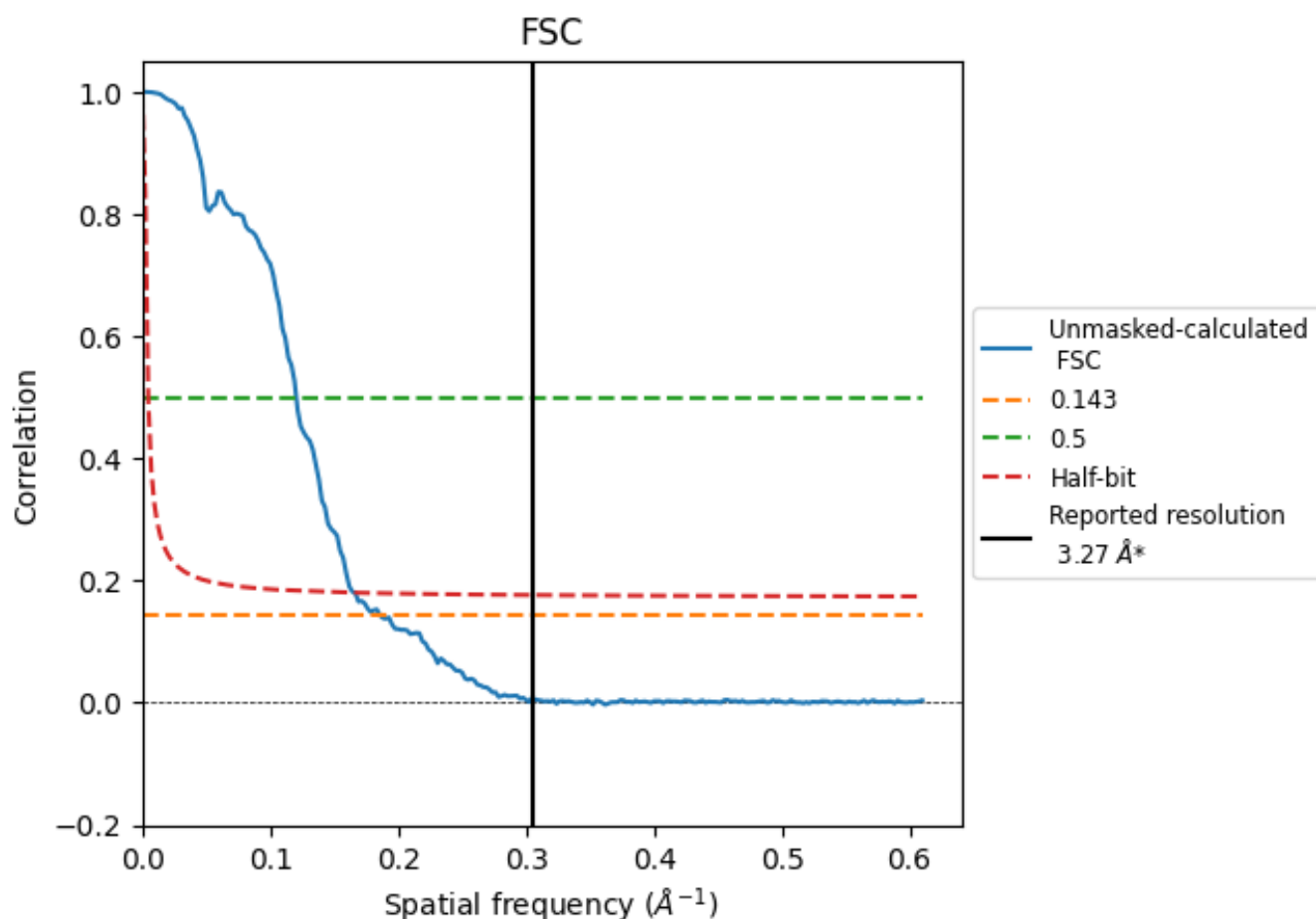


*Reported resolution corresponds to spatial frequency of 0.306 Å⁻¹

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 0.306 Å⁻¹

8.2 Resolution estimates [i](#)

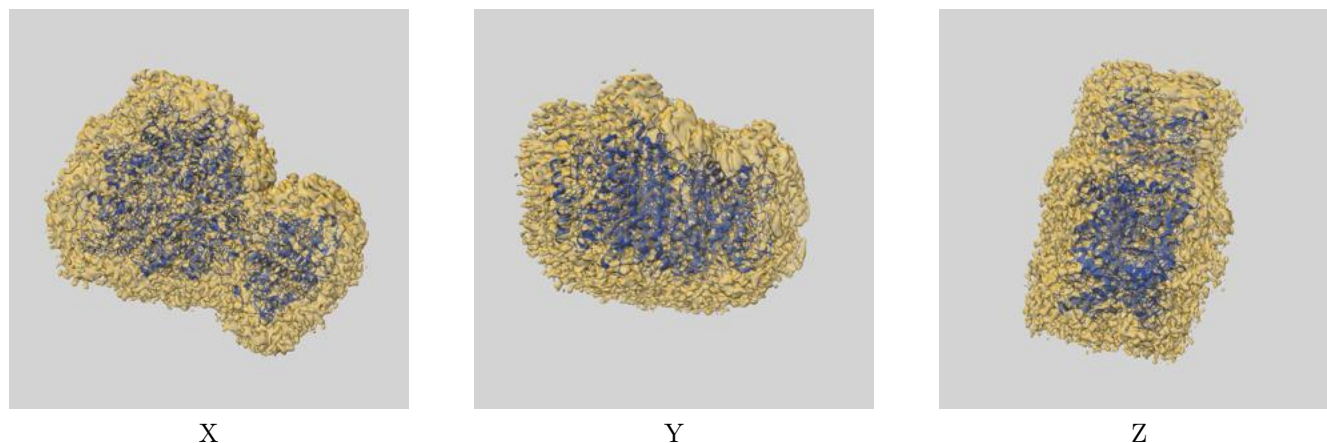
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.38	8.31	6.03

*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 5.38 differs from the reported value 3.27 by more than 10 %

9 Map-model fit [i](#)

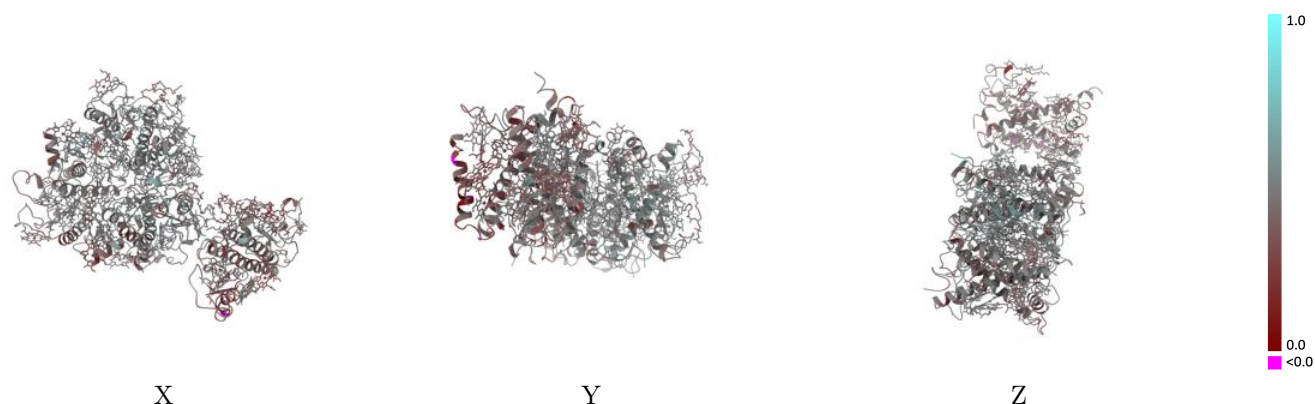
This section contains information regarding the fit between EMDB map EMD-66949 and PDB model 9XK6. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



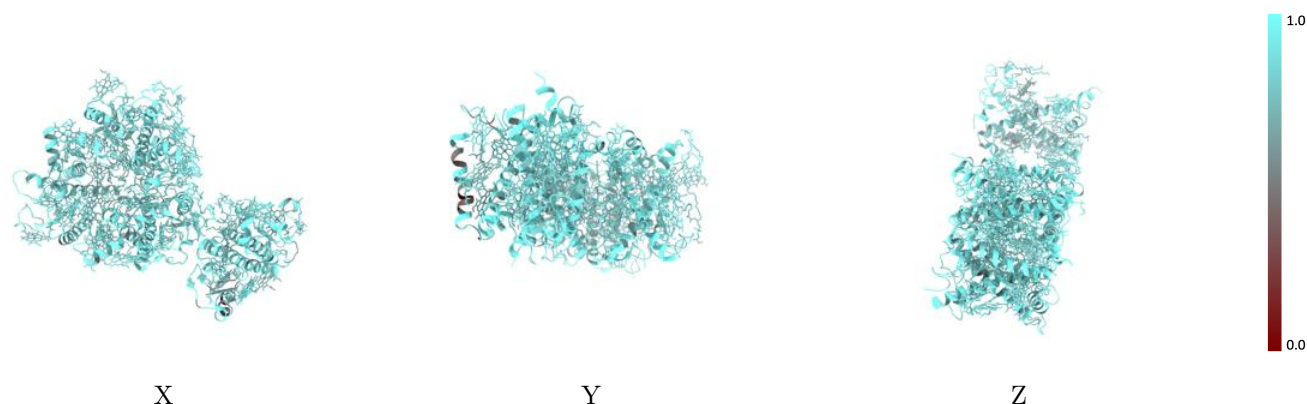
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



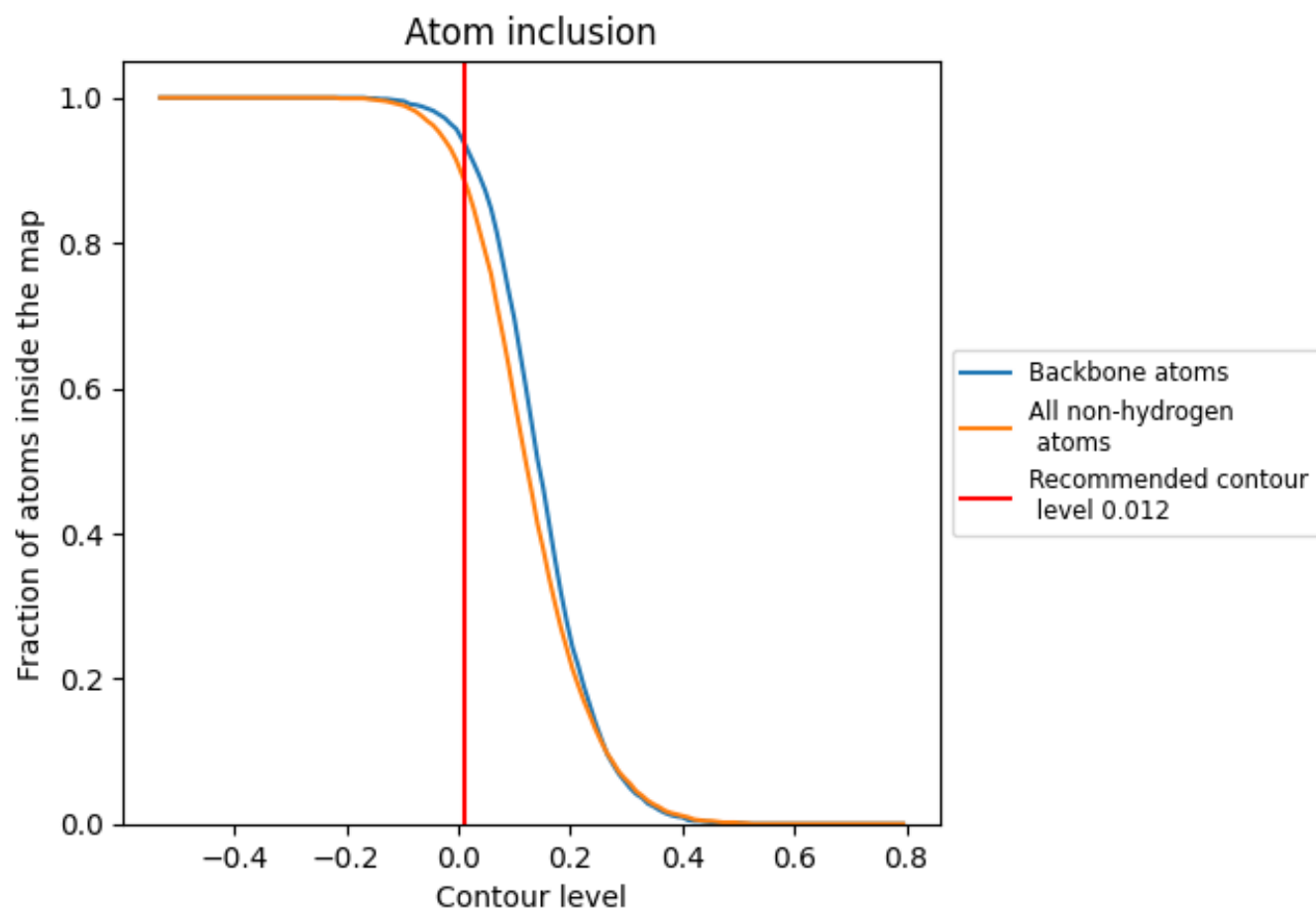
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8830	0.4360
00	0.8940	0.4710
1G	0.8880	0.4360
1N	0.9050	0.4500
1S	0.8420	0.3840

