



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2026 – 12:31 PM JST

PDB ID : 9XK7 / pdb_00009xk7
EMDB ID : EMD-66950
Title : In situ C2S2M2L4-type PSII-LHCII supercomplex, strongly bound (S-) LHCII trimer with CP26, protomer 2
Authors : Li, J.; Elias, E.; Zhang, K.; Croce, R.; Zhu, J.
Deposited on : 2025-11-05
Resolution : 3.25 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

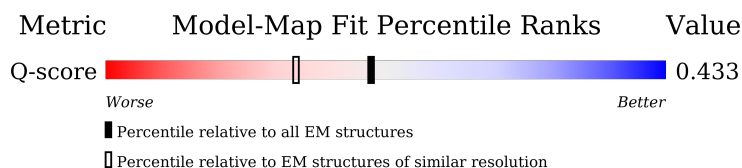
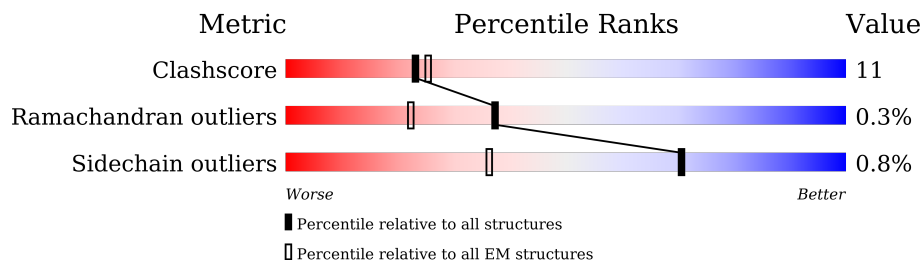
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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	14599 (2.75 - 3.75)

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	09	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	09	301	X	-	-	-
3	CLA	09	302	X	-	-	-
3	CLA	1g	602	X	-	-	-
3	CLA	1g	610	X	-	-	-
3	CLA	1g	611	X	-	-	-
3	CLA	1g	612	X	-	-	-
3	CLA	1n	602	X	-	-	-
3	CLA	1n	603	X	-	-	-
3	CLA	1n	610	X	-	-	-
3	CLA	1n	611	X	-	-	-
3	CLA	1n	613	X	-	-	-
3	CLA	1s	308	X	-	-	-
3	CLA	1s	311	X	-	-	-
4	CHL	09	308	X	-	-	-
4	CHL	1g	601	X	-	-	-
4	CHL	1g	609	X	-	-	-
4	CHL	1n	601	X	-	-	-
4	CHL	1n	607	X	-	-	-
4	CHL	1n	609	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9950 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.

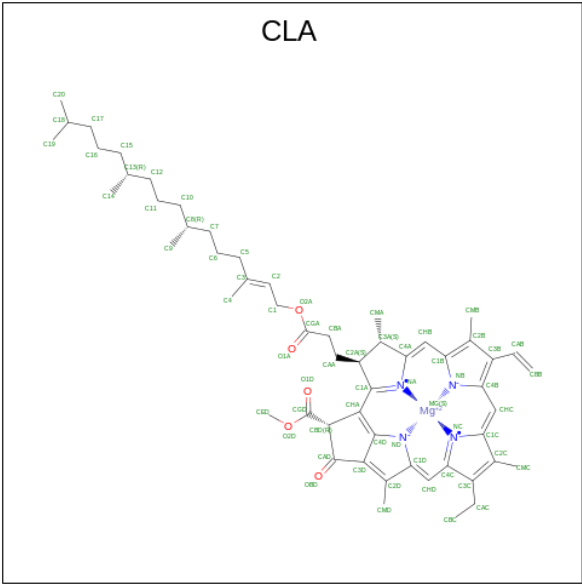
- Molecule 1 is a protein called Chlorophyll a-b binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	09	219	Total	C	N	O	S	0	0
			1659	1079	269	306	5		
1	1g	219	Total	C	N	O	S	0	0
			1655	1076	268	306	5		
1	1n	219	Total	C	N	O	S	0	0
			1653	1073	269	306	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1s	217	Total	C	N	O	S	0	0
			1658	1075	270	308	5		

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



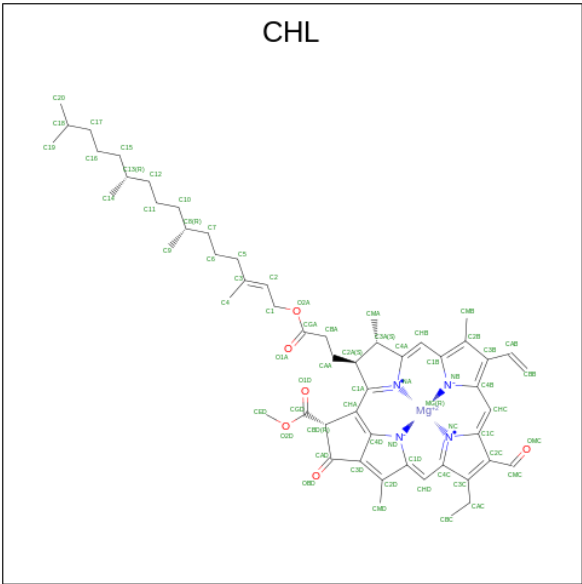
Mol	Chain	Residues	Atoms					AltConf
3	09	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	09	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
3	09	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
3	09	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
3	09	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
3	09	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
3	09	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
3	09	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
3	1g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
3	1g	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
3	1g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
3	1g	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
3	1g	1	Total	C	Mg	N	O	0
			60	50	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
			45	35	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
			56	46	1	4	5	
3	1n	1	Total	C	Mg	N	O	0
			57	47	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
			58	48	1	4	5	
3	1n	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
3	1n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
3	1n	1	Total	C	Mg	N	O	0
			57	47	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
			45	35	1	4	5	
3	1s	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
3	1s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
3	1s	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
3	1s	1	Total	C	Mg	N	O	0
			44	34	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
			46	36	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
			42	34	1	4	3	

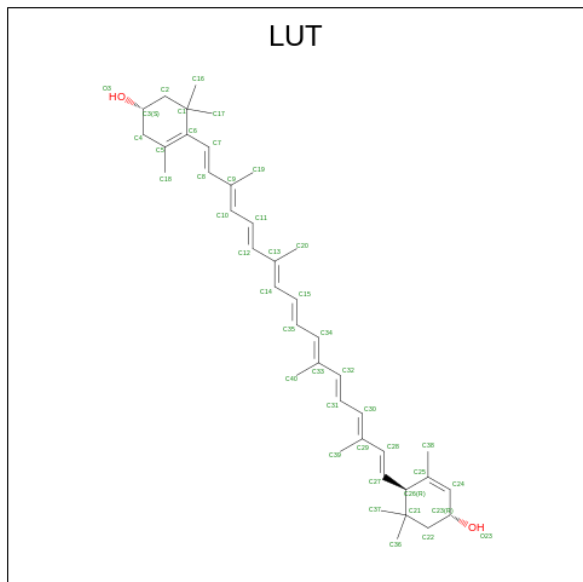
- Molecule 4 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	09	1	Total 41	C 32	Mg 1	N 4	O 4	0
4	09	1	Total 43	C 34	Mg 1	N 4	O 4	0
4	09	1	Total 43	C 34	Mg 1	N 4	O 4	0
4	09	1	Total 43	C 34	Mg 1	N 4	O 4	0
4	09	1	Total 61	C 50	Mg 1	N 4	O 6	0
4	1g	1	Total 58	C 47	Mg 1	N 4	O 6	0
4	1g	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	1g	1	Total 50	C 39	Mg 1	N 4	O 6	0
4	1g	1	Total 47	C 36	Mg 1	N 4	O 6	0
4	1g	1	Total 43	C 34	Mg 1	N 4	O 4	0
4	1g	1	Total 61	C 50	Mg 1	N 4	O 6	0
4	1n	1	Total 62	C 51	Mg 1	N 4	O 6	0
4	1n	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	1n	1	Total 47	C 36	Mg 1	N 4	O 6	0
4	1n	1	Total 66	C 55	Mg 1	N 4	O 6	0
4	1n	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	1n	1	Total 61	C 50	Mg 1	N 4	O 6	0
4	1s	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	1s	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	1s	1	Total 42	C 33	Mg 1	N 4	O 4	0
4	1s	1	Total 42	C 33	Mg 1	N 4	O 4	0

- 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	09	1	Total	C	O	0
			42	40	2	
5	09	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: $C_{29}H_{50}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	09	1	Total	C	O	0
			31	29	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).



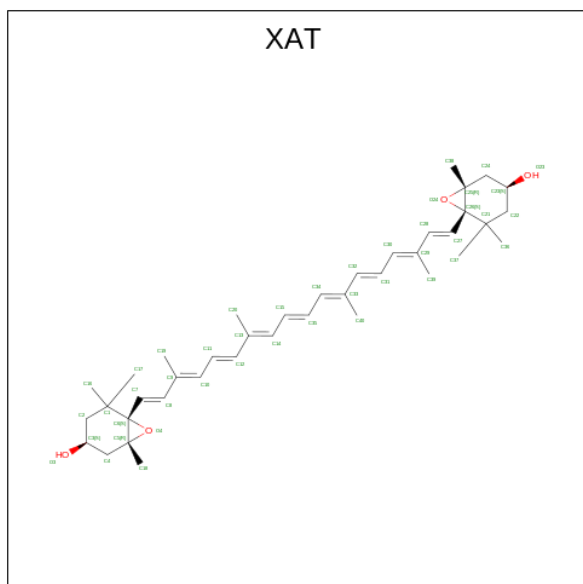
Mol	Chain	Residues	Atoms				AltConf
7	09	1	Total 37	C 26	O 10	P 1	0
7	09	1	Total 49	C 38	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
7	1g	1	Total	C	O	P	0
			36	25	10	1	
7	1n	1	Total	C	O	P	0
			43	32	10	1	
7	1n	1	Total	C	O	P	0
			38	32	5	1	
7	1s	1	Total	C	O		0
			29	24	5		
7	1s	1	Total	C	O		0
			27	22	5		

- 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).

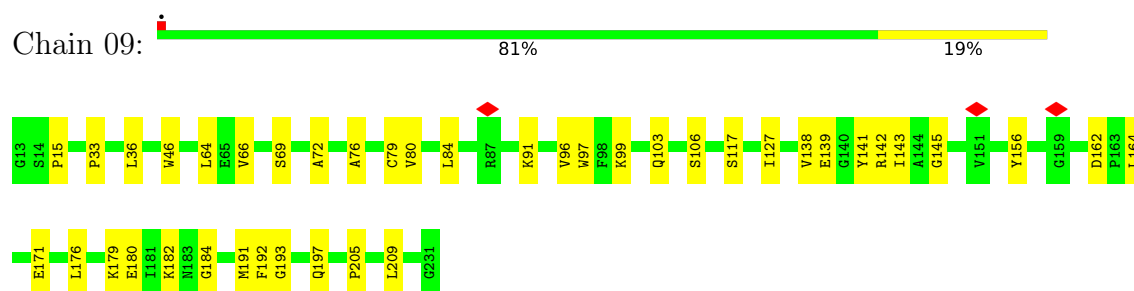


Mol	Chain	Residues	Atoms				AltConf
8	1g	1	Total	C	O		0
			44	40	4		
8	1g	1	Total	C	O		0
			44	40	4		

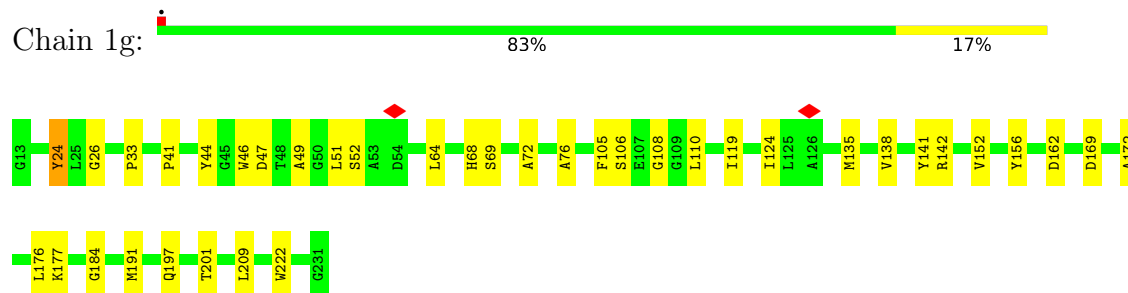
3 Residue-property plots [i](#)

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.

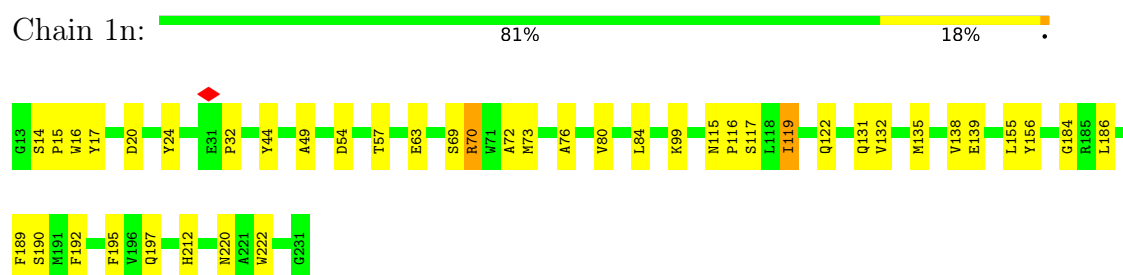
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



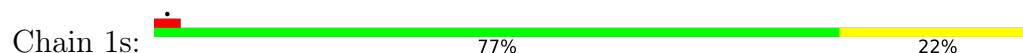
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



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



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





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	0.799	Depositor
Minimum map value	-0.515	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 [i](#)

5.1 Standard geometry [i](#)

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

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	09	0.25	0/1710	0.64	3/2332 (0.1%)
1	1g	0.25	1/1706 (0.1%)	0.60	4/2328 (0.2%)
1	1n	0.20	0/1703	0.54	1/2323 (0.0%)
2	1s	0.21	0/1702	0.57	0/2313
All	All	0.23	1/6821 (0.0%)	0.59	8/9296 (0.1%)

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	1n	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1g	24	TYR	C-N	5.18	1.40	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	09	15	PRO	CA-N-CD	-11.63	95.72	112.00
1	1n	32	PRO	CA-N-CD	-7.53	101.46	112.00
1	1g	24	TYR	CA-C-N	-7.24	112.27	125.02
1	1g	24	TYR	C-N-CA	-7.24	112.27	125.02
1	09	180	GLU	CA-CB-CG	5.64	125.37	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1n	192	PHE	Peptide
1	1n	70	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	09	1659	0	1597	35	0
1	1g	1655	0	1586	32	0
1	1n	1653	0	1591	30	0
2	1s	1658	0	1620	41	0
3	09	372	0	291	16	0
3	1g	414	0	354	19	0
3	1n	412	0	356	17	0
3	1s	415	0	316	14	0
4	09	231	0	168	11	0
4	1g	305	0	236	11	0
4	1n	328	0	279	22	0
4	1s	176	0	115	4	0
5	09	84	0	112	14	0
5	1g	84	0	112	9	0
5	1n	42	0	56	4	0
5	1s	84	0	112	20	0
6	09	31	0	49	0	0
7	09	86	0	118	9	0
7	1g	36	0	42	0	0
7	1n	81	0	114	6	0
7	1s	56	0	74	4	0
8	1g	88	0	111	9	0
All	All	9950	0	9409	214	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 11.

The worst 5 of 214 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:09:191:MET:HG2	5:09:314:LUT:H12	1.68	0.75
1:09:145:GLY:HA2	4:09:307:CHL:HMC	1.69	0.74
2:1s:200:MET:HE1	5:1s:316:LUT:H12	1.70	0.71
3:1g:602:CLA:H52	3:1g:602:CLA:HBB1	1.76	0.68
1:1n:69:SER:HB2	1:1n:184:GLY:HA3	1.76	0.66

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	09	217/219 (99%)	199 (92%)	18 (8%)	0	100	100
1	1g	217/219 (99%)	197 (91%)	19 (9%)	1 (0%)	24	55
1	1n	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	55
2	1s	215/218 (99%)	189 (88%)	25 (12%)	1 (0%)	24	55
All	All	866/875 (99%)	784 (90%)	79 (9%)	3 (0%)	37	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1s	66	LYS
1	1n	119	ILE
1	1g	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	09	166/166 (100%)	165 (99%)	1 (1%)	78	81
1	1g	165/166 (99%)	165 (100%)	0	100	100
1	1n	165/166 (99%)	164 (99%)	1 (1%)	78	81
2	1s	170/173 (98%)	167 (98%)	3 (2%)	51	69
All	All	666/671 (99%)	661 (99%)	5 (1%)	70	78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	09	143	ILE
1	1n	139	GLU
2	1s	86	MET
2	1s	160	LEU
2	1s	180	ASP

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

Mol	Chain	Res	Type
1	1n	218	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

71 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	$\# Z > 2$
4	CHL	1n	605	1	50,54,74	2.23	17 (34%)	56,90,114	3.21	21 (37%)
3	CLA	1n	604	-	45,49,73	2.64	19 (42%)	54,84,113	3.40	29 (53%)
4	CHL	1g	607	-	51,55,74	2.18	19 (37%)	57,91,114	3.07	20 (35%)
3	CLA	1g	612	-	59,63,73	2.26	19 (32%)	71,101,113	3.06	29 (40%)
3	CLA	1g	602	1	64,68,73	2.19	19 (29%)	77,107,113	3.02	31 (40%)
4	CHL	09	306	-	47,51,74	2.20	17 (36%)	52,86,114	3.32	21 (40%)
3	CLA	1s	310	-	47,52,73	2.53	19 (40%)	56,88,113	3.36	26 (46%)
4	CHL	1g	606	-	54,58,74	2.15	20 (37%)	59,94,114	3.01	23 (38%)
4	CHL	1n	608	-	50,54,74	2.23	18 (36%)	56,90,114	3.17	24 (42%)
4	CHL	09	305	-	47,51,74	2.19	16 (34%)	52,86,114	3.17	23 (44%)
3	CLA	1n	602	1	60,64,73	2.26	19 (31%)	72,102,113	2.99	31 (43%)
4	CHL	1g	605	1	50,54,74	2.23	17 (34%)	56,90,114	3.21	23 (41%)
5	LUT	09	314	-	42,43,43	1.63	8 (19%)	51,60,60	1.58	11 (21%)
5	LUT	1g	616	-	42,43,43	1.79	8 (19%)	51,60,60	2.36	14 (27%)
7	LHG	09	316	3	36,36,48	0.32	0	39,42,54	0.37	0
8	XAT	1g	619	-	39,47,47	1.00	1 (2%)	54,74,74	3.97	29 (53%)
3	CLA	1s	311	2	59,63,73	2.27	19 (32%)	71,101,113	3.04	30 (42%)
3	CLA	09	302	-	60,64,73	2.24	19 (31%)	72,102,113	3.11	31 (43%)
3	CLA	1s	309	-	45,49,73	2.60	20 (44%)	54,84,113	3.47	28 (51%)
3	CLA	09	310	7	45,49,73	2.59	20 (44%)	54,84,113	3.40	30 (55%)
4	CHL	1n	601	-	66,70,74	1.95	18 (27%)	75,109,114	2.82	26 (34%)
3	CLA	1s	304	-	45,49,73	2.59	20 (44%)	54,84,113	3.39	28 (51%)
7	LHG	1n	616	3	42,42,48	0.29	0	45,48,54	0.43	0
3	CLA	1s	303	2	49,53,73	2.45	19 (38%)	59,89,113	3.29	27 (45%)
3	CLA	1s	314	-	46,50,73	2.53	19 (41%)	55,85,113	3.44	27 (49%)
6	VIV	09	315	-	32,32,32	0.49	1 (3%)	41,45,45	0.80	2 (4%)
3	CLA	1g	613	1	49,53,73	2.51	20 (40%)	59,89,113	3.36	27 (45%)
3	CLA	1g	614	7	46,50,73	2.49	18 (39%)	55,85,113	3.34	27 (49%)
3	CLA	1s	312	2	50,54,73	2.49	19 (38%)	60,90,113	3.25	29 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	LHG	1n	617	-	36,37,48	0.29	0	38,39,54	1.47	4 (10%)
3	CLA	09	312	1	47,52,73	2.55	20 (42%)	56,88,113	3.33	26 (46%)
4	CHL	1g	608	-	47,51,74	2.20	17 (36%)	52,86,114	3.26	24 (46%)
5	LUT	1n	615	-	42,43,43	1.68	8 (19%)	51,60,60	1.71	11 (21%)
3	CLA	1n	613	1	61,65,73	2.26	20 (32%)	73,103,113	3.01	31 (42%)
3	CLA	1g	604	-	54,58,73	2.36	18 (33%)	65,95,113	3.11	31 (47%)
4	CHL	09	307	-	47,51,74	2.19	16 (34%)	52,86,114	3.25	25 (48%)
3	CLA	1g	603	-	50,54,73	2.45	18 (36%)	60,90,113	3.28	28 (46%)
3	CLA	09	311	-	45,49,73	2.60	19 (42%)	54,84,113	3.49	28 (51%)
4	CHL	1s	305	-	50,54,74	2.20	17 (34%)	56,90,114	3.14	22 (39%)
3	CLA	1g	610	1	60,64,73	2.26	19 (31%)	72,102,113	2.97	29 (40%)
3	CLA	09	303	-	43,48,73	2.60	19 (44%)	51,83,113	3.32	25 (49%)
4	CHL	1n	607	-	70,74,74	1.88	18 (25%)	80,114,114	2.75	24 (30%)
3	CLA	1g	611	-	64,68,73	2.21	19 (29%)	77,107,113	3.02	29 (37%)
7	LHG	1s	301	-	28,28,48	0.31	0	30,30,54	0.85	2 (6%)
3	CLA	1n	603	-	61,65,73	2.23	19 (31%)	73,103,113	3.00	31 (42%)
3	CLA	1n	611	7	61,65,73	2.26	20 (32%)	73,103,113	3.06	30 (41%)
3	CLA	1n	614	1	45,49,73	2.62	20 (44%)	54,84,113	3.40	27 (50%)
8	XAT	1g	617	-	39,47,47	0.84	0	54,74,74	3.11	24 (44%)
7	LHG	1g	618	3	35,35,48	0.31	0	38,41,54	0.47	0
4	CHL	09	308	1	65,69,74	1.94	18 (27%)	74,108,114	2.67	25 (33%)
3	CLA	09	301	1	59,63,73	2.28	19 (32%)	71,101,113	3.10	30 (42%)
3	CLA	1n	610	1	62,66,73	2.20	19 (30%)	74,104,113	3.05	29 (39%)
4	CHL	1n	606	-	51,55,74	2.18	17 (33%)	57,91,114	3.01	22 (38%)
4	CHL	1s	302	2	50,54,74	2.25	18 (36%)	56,90,114	3.13	22 (39%)
3	CLA	09	309	1	45,49,73	2.58	18 (40%)	54,84,113	3.37	29 (53%)
3	CLA	1s	308	2	59,63,73	2.31	20 (33%)	71,101,113	3.01	31 (43%)
3	CLA	09	317	1	58,62,73	2.29	20 (34%)	69,99,113	3.10	32 (46%)
4	CHL	1g	601	1	62,66,74	2.00	15 (24%)	70,104,114	2.94	25 (35%)
4	CHL	1s	307	-	45,50,74	2.25	16 (35%)	49,85,114	3.26	22 (44%)
5	LUT	09	313	-	42,43,43	1.75	8 (19%)	51,60,60	1.70	11 (21%)
5	LUT	1s	315	-	42,43,43	1.69	8 (19%)	51,60,60	1.65	13 (25%)
4	CHL	09	304	1	44,49,74	2.33	17 (38%)	48,84,114	3.37	22 (45%)
3	CLA	1n	612	-	49,53,73	2.50	19 (38%)	59,89,113	3.34	27 (45%)
4	CHL	1g	609	1	65,69,74	1.98	18 (27%)	74,108,114	2.75	26 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	LUT	1g	615	-	42,43,43	1.69	8 (19%)	51,60,60	1.60	11 (21%)
5	LUT	1s	316	-	42,43,43	1.78	8 (19%)	51,60,60	2.03	17 (33%)
7	LHG	09	318	-	48,48,48	0.29	0	51,54,54	0.40	0
4	CHL	1s	306	-	46,50,74	2.33	19 (41%)	51,85,114	3.34	23 (45%)
4	CHL	1n	609	1	65,69,74	1.96	16 (24%)	74,108,114	2.79	25 (33%)
7	LHG	1s	317	-	26,26,48	0.31	0	28,28,54	0.32	0
3	CLA	1s	313	2	50,54,73	2.55	20 (40%)	60,90,113	3.34	27 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHL	1n	605	1	-	12/17/93/117	-
3	CLA	1n	604	-	-	6/10/86/115	-
4	CHL	1g	607	-	-	9/19/95/117	-
3	CLA	1g	612	-	1/1/13/20	13/27/103/115	-
3	CLA	1g	602	1	1/1/14/20	14/33/109/115	-
4	CHL	09	306	-	-	8/14/90/117	-
3	CLA	1s	310	-	-	4/13/89/115	-
4	CHL	1g	606	-	-	9/22/98/117	-
4	CHL	1n	608	-	-	6/17/93/117	-
4	CHL	09	305	-	-	4/14/90/117	-
3	CLA	1n	602	1	1/1/13/20	5/29/105/115	-
4	CHL	1g	605	1	-	12/17/93/117	-
5	LUT	09	314	-	-	0/29/67/67	0/2/2/2
5	LUT	1g	616	-	-	4/29/67/67	0/2/2/2
7	LHG	09	316	3	-	5/41/41/53	-
8	XAT	1g	619	-	-	8/31/93/93	0/4/4/4
3	CLA	1s	311	2	1/1/13/20	13/27/103/115	-
3	CLA	09	302	-	1/1/13/20	6/29/105/115	-
3	CLA	1s	309	-	-	1/10/86/115	-
3	CLA	09	310	7	-	5/10/86/115	-
4	CHL	1n	601	-	1/1/14/21	9/37/113/117	-
3	CLA	1s	304	-	-	4/10/86/115	-
7	LHG	1n	616	3	-	6/47/47/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	1s	303	2	-	8/15/91/115	-
3	CLA	1s	314	-	-	1/12/88/115	-
6	VIV	09	315	-	-	11/19/30/30	0/2/2/2
3	CLA	1g	613	1	-	11/15/91/115	-
3	CLA	1g	614	7	-	4/12/88/115	-
3	CLA	1s	312	2	-	5/17/93/115	-
7	LHG	1n	617	-	-	9/38/39/53	-
3	CLA	09	312	1	-	3/13/89/115	-
4	CHL	1g	608	-	-	3/14/90/117	-
5	LUT	1n	615	-	-	3/29/67/67	0/2/2/2
3	CLA	1n	613	1	1/1/13/20	14/30/106/115	-
3	CLA	1g	604	-	-	6/21/97/115	-
4	CHL	09	307	-	-	2/14/90/117	-
3	CLA	1g	603	-	-	5/17/93/115	-
3	CLA	09	311	-	-	0/10/86/115	-
4	CHL	1s	305	-	-	13/17/93/117	-
3	CLA	1g	610	1	1/1/13/20	11/29/105/115	-
4	CHL	1n	607	-	1/1/15/21	25/41/117/117	-
3	CLA	09	303	-	-	2/8/84/115	-
3	CLA	1g	611	-	1/1/14/20	5/33/109/115	-
7	LHG	1s	301	-	-	7/30/30/53	-
3	CLA	1n	603	-	1/1/13/20	11/30/106/115	-
3	CLA	1n	611	7	1/1/13/20	7/30/106/115	-
3	CLA	1n	614	1	-	4/10/86/115	-
8	XAT	1g	617	-	-	8/31/93/93	0/4/4/4
7	LHG	1g	618	3	-	12/40/40/53	-
4	CHL	09	308	1	1/1/14/21	13/35/111/117	-
3	CLA	09	301	1	1/1/13/20	10/27/103/115	-
3	CLA	1n	610	1	1/1/13/20	11/31/107/115	-
4	CHL	1n	606	-	-	5/19/95/117	-
4	CHL	1s	302	2	-	10/17/93/117	-
4	CHL	1g	601	1	1/1/13/21	12/32/108/117	-
3	CLA	1s	308	2	1/1/13/20	9/27/103/115	-
3	CLA	09	309	1	-	3/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLA	09	317	1	-	11/26/102/115	-
4	CHL	1s	307	-	-	4/12/88/117	-
5	LUT	09	313	-	-	0/29/67/67	0/2/2/2
5	LUT	1s	315	-	-	6/29/67/67	0/2/2/2
4	CHL	09	304	1	-	6/10/86/117	-
3	CLA	1n	612	-	-	6/15/91/115	-
4	CHL	1g	609	1	1/1/14/21	11/35/111/117	-
5	LUT	1g	615	-	-	0/29/67/67	0/2/2/2
5	LUT	1s	316	-	-	4/29/67/67	0/2/2/2
7	LHG	09	318	-	-	13/53/53/53	-
4	CHL	1s	306	-	-	10/12/88/117	-
4	CHL	1n	609	1	1/1/14/21	21/35/111/117	-
7	LHG	1s	317	-	-	3/28/28/53	-
3	CLA	1s	313	2	-	1/17/93/115	-

The worst 5 of 1056 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1s	313	CLA	C1D-ND	8.76	1.48	1.37
3	09	312	CLA	C1D-ND	8.58	1.48	1.37
3	1n	611	CLA	C1D-ND	8.57	1.48	1.37
3	1s	312	CLA	C1D-ND	8.56	1.48	1.37
3	09	317	CLA	C1D-ND	8.56	1.48	1.37

The worst 5 of 1587 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1g	601	CHL	C2B-C1B-NB	11.22	117.76	110.23
4	1g	607	CHL	C2B-C1B-NB	10.70	117.41	110.23
4	1n	607	CHL	C2B-C1B-NB	10.66	117.38	110.23
4	1n	608	CHL	C2B-C1B-NB	10.63	117.36	110.23
4	09	306	CHL	C2B-C1B-NB	10.56	117.31	110.23

5 of 19 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	09	301	CLA	C8
3	09	302	CLA	C8
3	1g	602	CLA	C8

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Mol	Chain	Res	Type	Atom
3	1g	610	CLA	C8
3	1g	611	CLA	C8

5 of 522 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	09	301	CLA	C2-C3-C5-C6
3	09	301	CLA	C4-C3-C5-C6
3	09	302	CLA	C2B-C3B-CAB-CBB
3	09	302	CLA	C4B-C3B-CAB-CBB
3	09	303	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

55 monomers are involved in 149 short contacts:

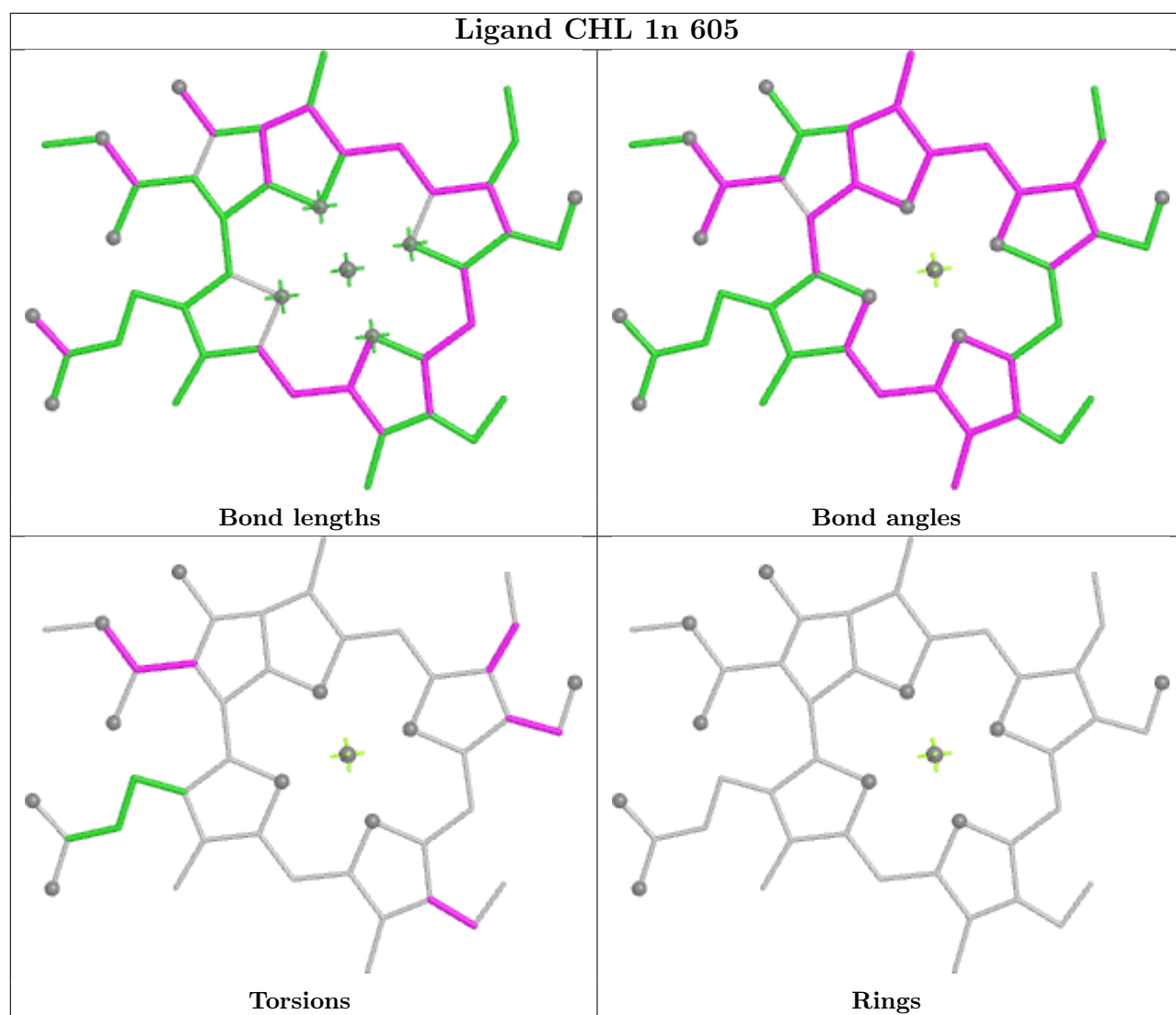
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	1n	605	CHL	3	0
4	1g	607	CHL	3	0
3	1g	602	CLA	10	0
4	09	306	CHL	3	0
4	1g	606	CHL	3	0
4	09	305	CHL	3	0
3	1n	602	CLA	4	0
5	09	314	LUT	6	0
5	1g	616	LUT	6	0
7	09	316	LHG	2	0
8	1g	619	XAT	5	0
3	1s	311	CLA	1	0
3	09	302	CLA	6	0
3	1s	309	CLA	1	0
4	1n	601	CHL	5	0
7	1n	616	LHG	4	0
3	1s	303	CLA	4	0
3	1s	312	CLA	1	0
7	1n	617	LHG	2	0
3	09	312	CLA	1	0
4	1g	608	CHL	1	0
5	1n	615	LUT	4	0
3	1n	613	CLA	4	0
3	1g	604	CLA	2	0
4	09	307	CHL	2	0
3	1g	603	CLA	1	0

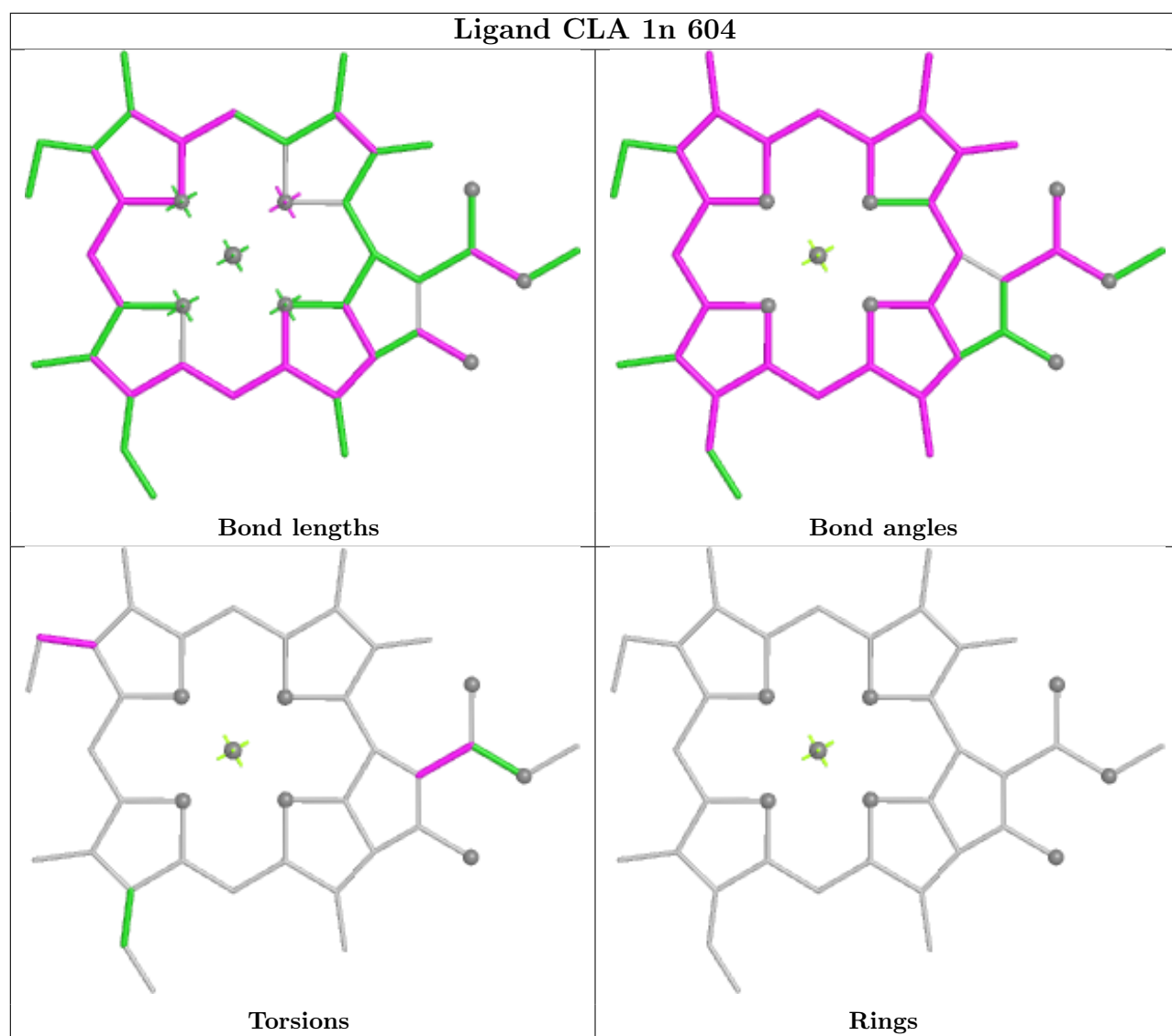
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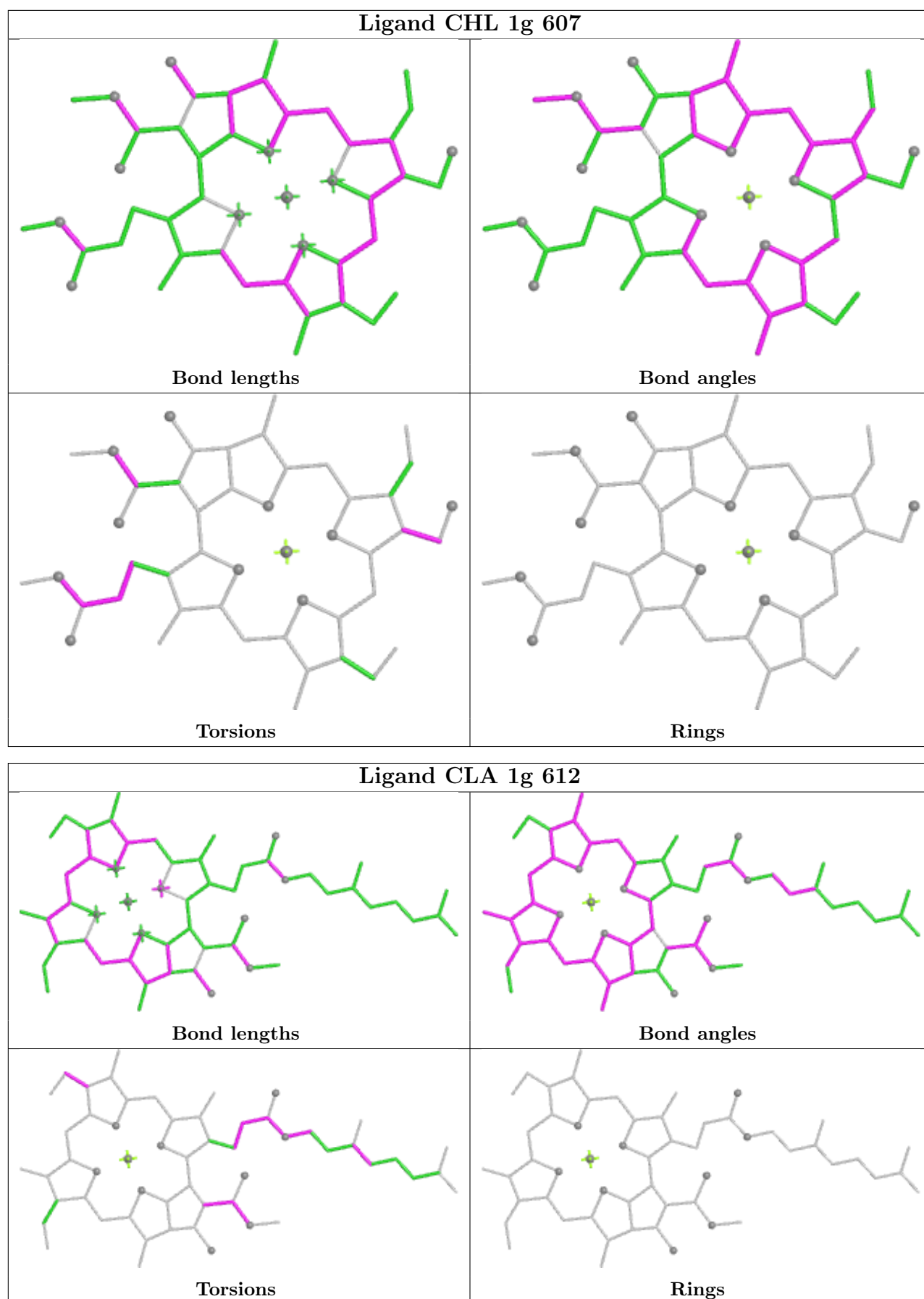
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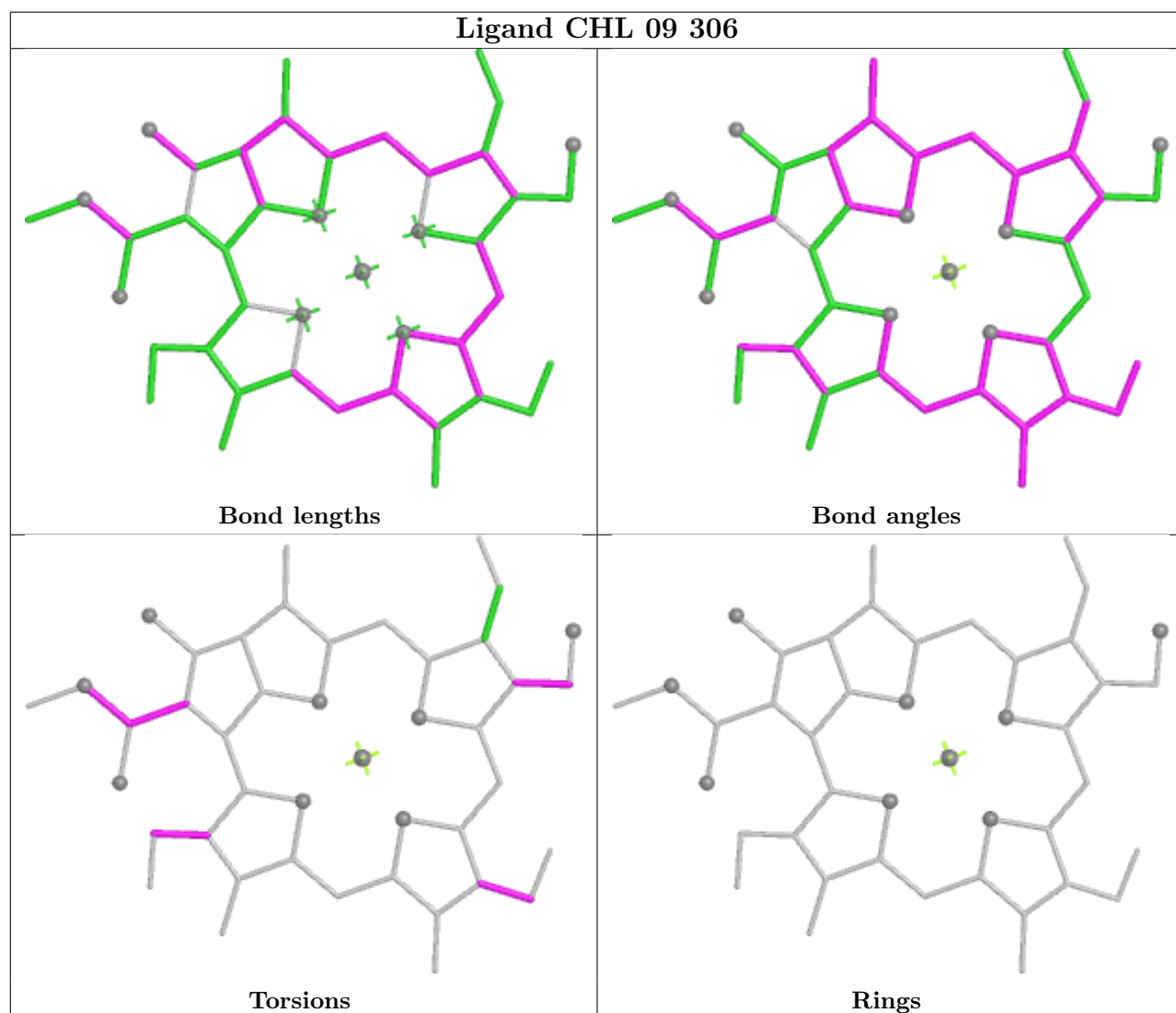
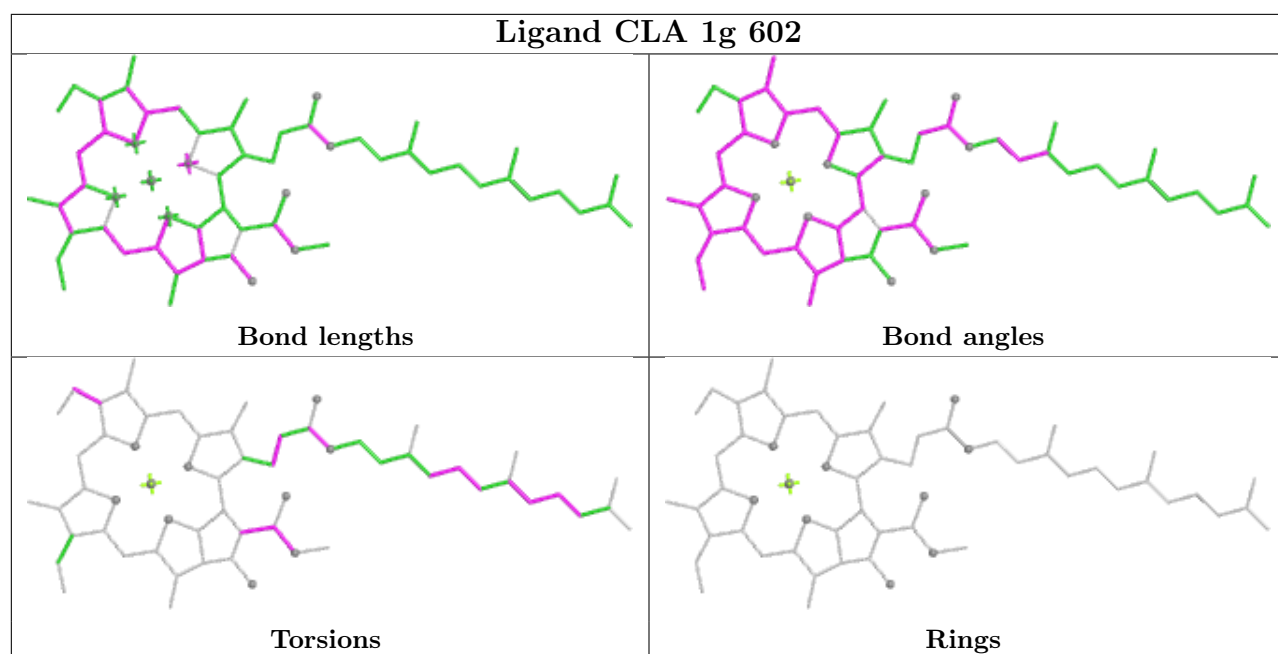
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	1s	305	CHL	1	0
3	1g	610	CLA	5	0
4	1n	607	CHL	6	0
3	1g	611	CLA	3	0
7	1s	301	LHG	2	0
3	1n	603	CLA	4	0
3	1n	611	CLA	1	0
3	1n	614	CLA	2	0
8	1g	617	XAT	4	0
4	09	308	CHL	4	0
3	09	301	CLA	3	0
3	1n	610	CLA	3	0
4	1n	606	CHL	4	0
4	1s	302	CHL	2	0
3	09	309	CLA	2	0
3	1s	308	CLA	6	0
3	09	317	CLA	5	0
4	1g	601	CHL	2	0
5	09	313	LUT	8	0
5	1s	315	LUT	7	0
4	09	304	CHL	1	0
4	1g	609	CHL	2	0
5	1g	615	LUT	3	0
5	1s	316	LUT	13	0
7	09	318	LHG	7	0
4	1s	306	CHL	2	0
4	1n	609	CHL	5	0
7	1s	317	LHG	2	0
3	1s	313	CLA	1	0

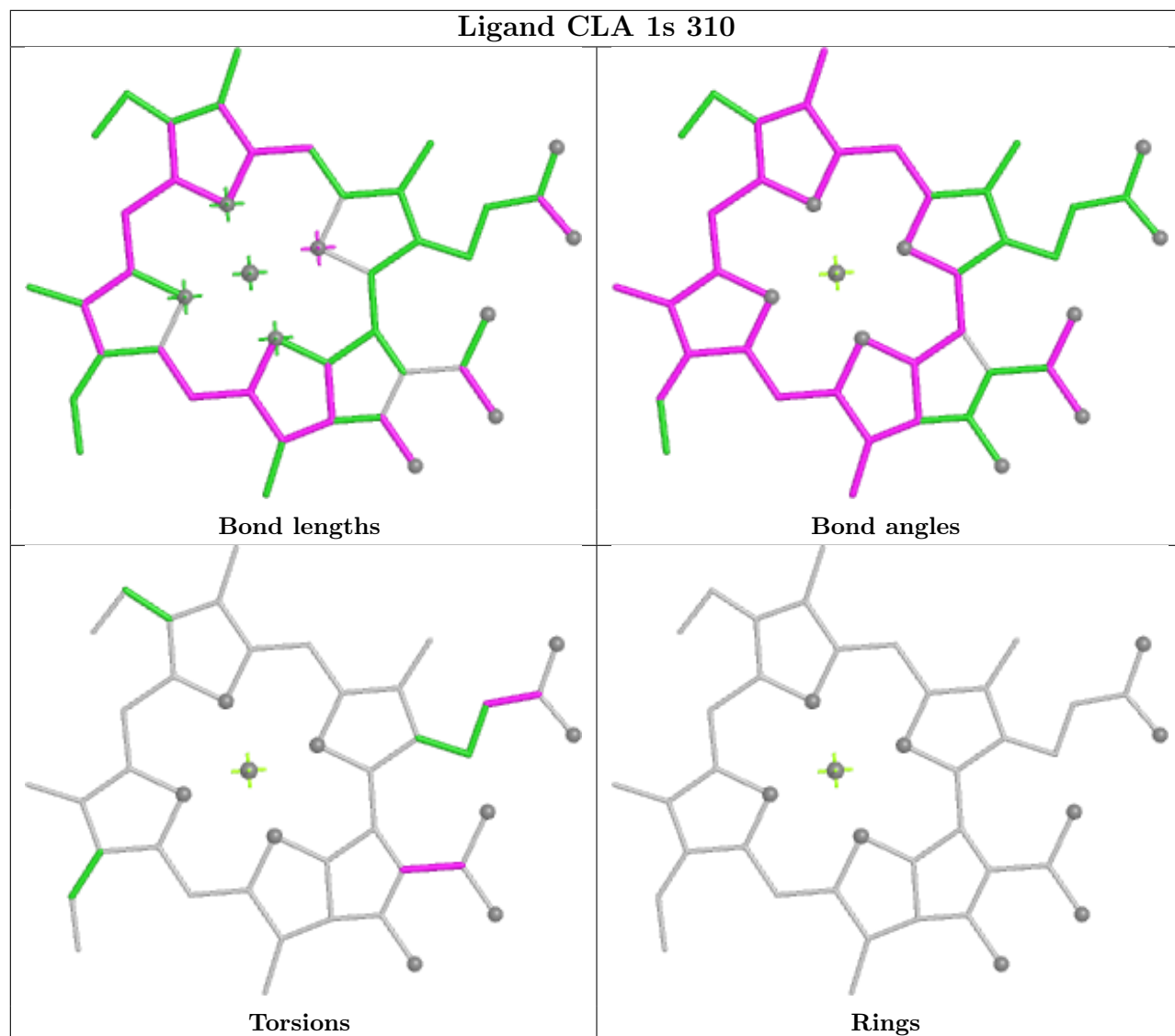
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

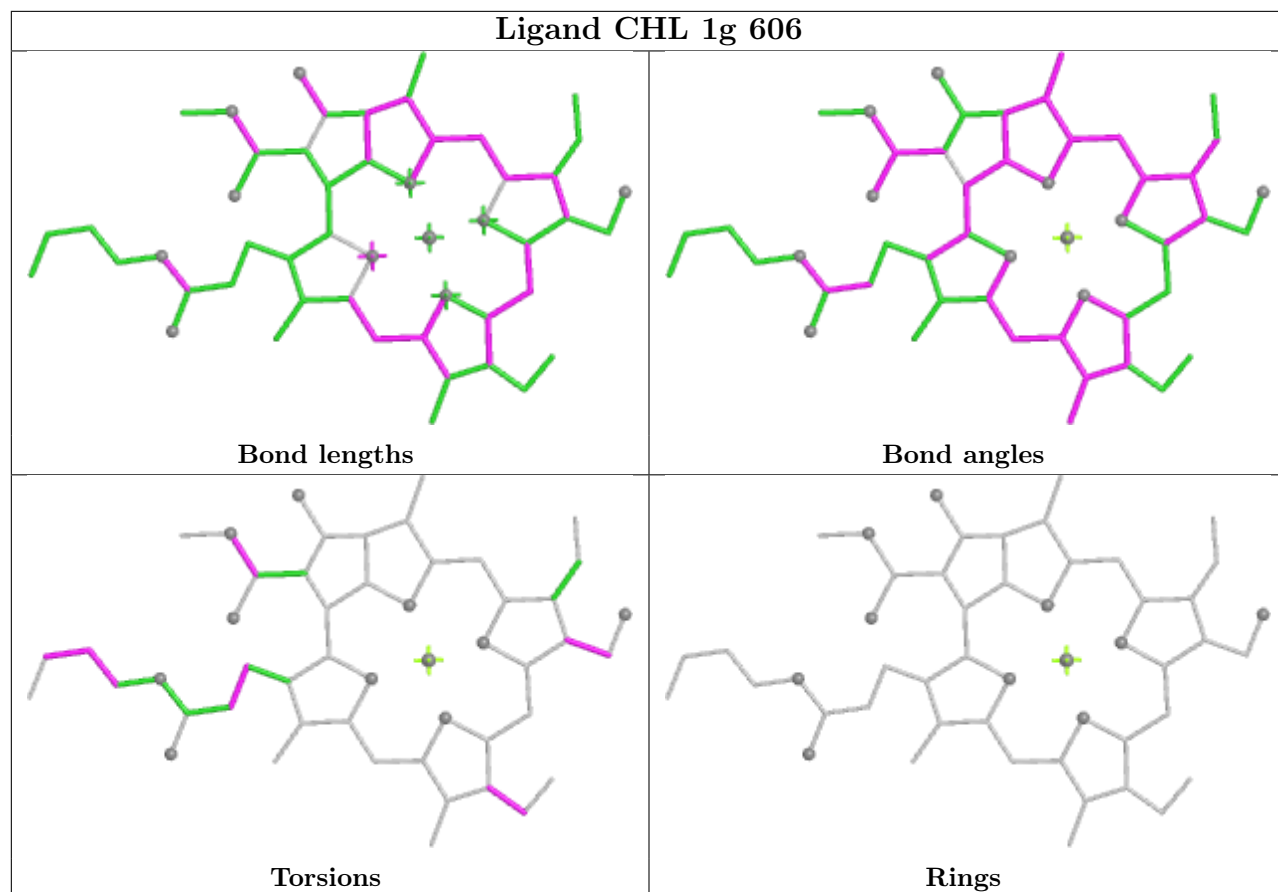


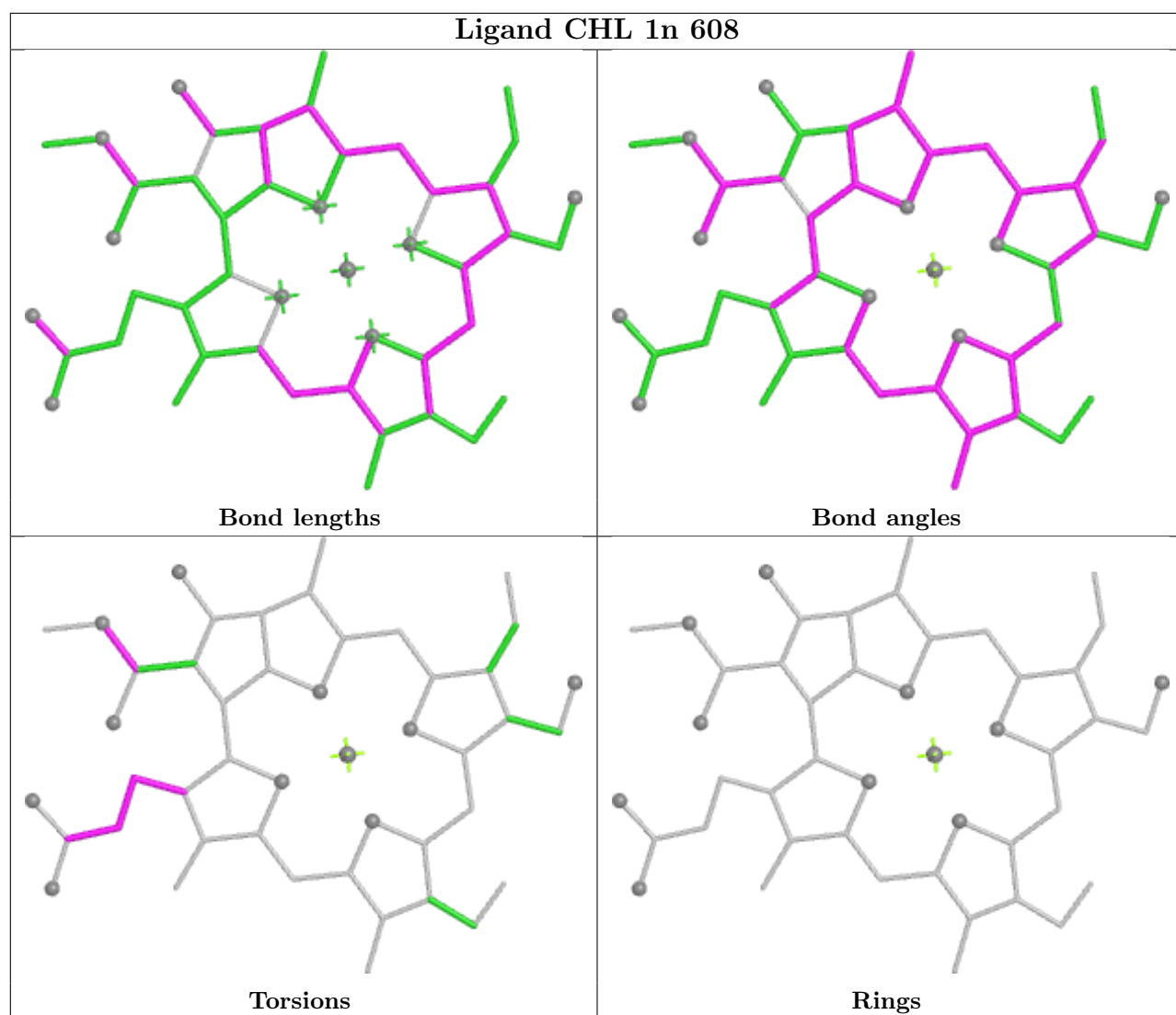


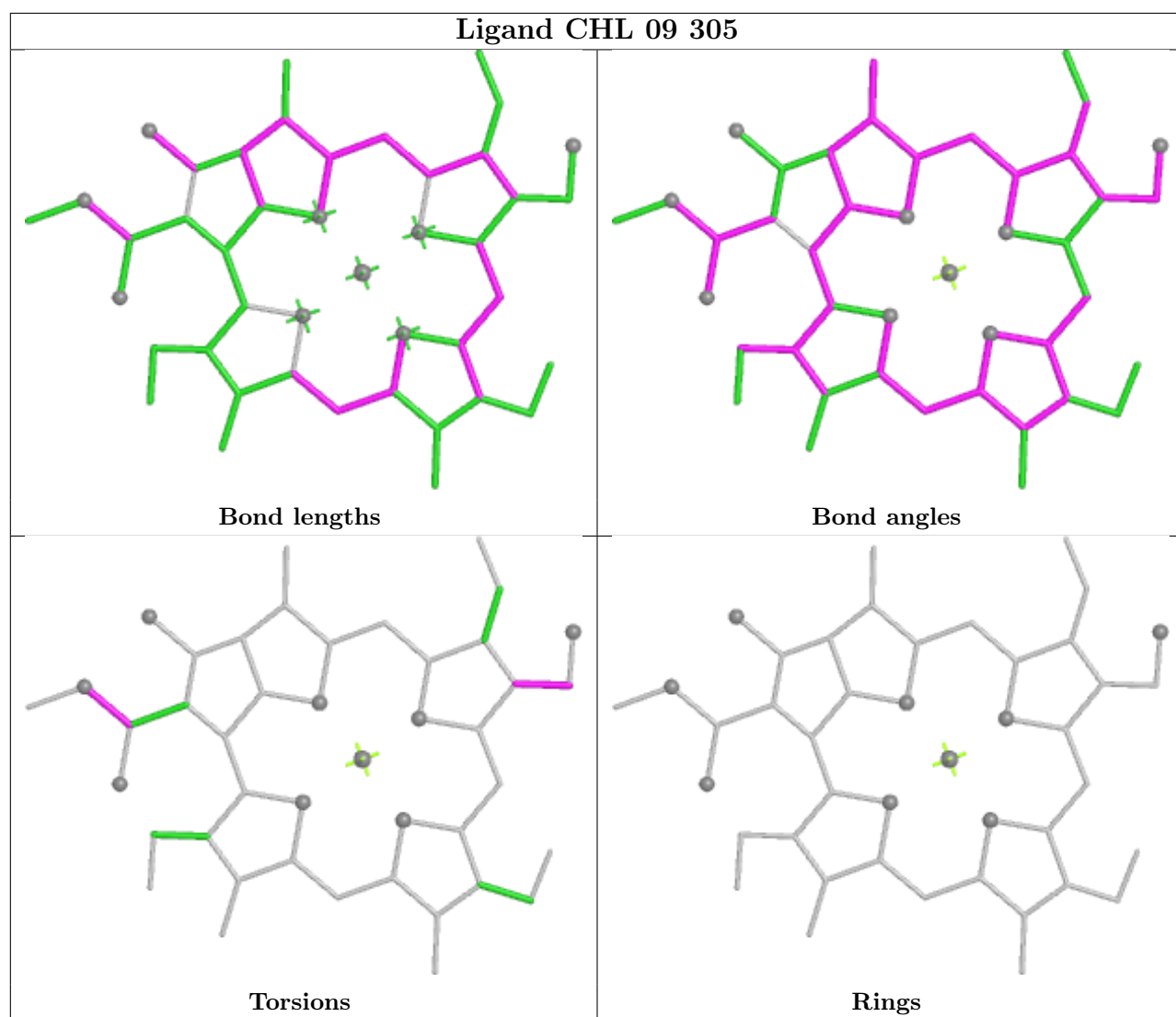


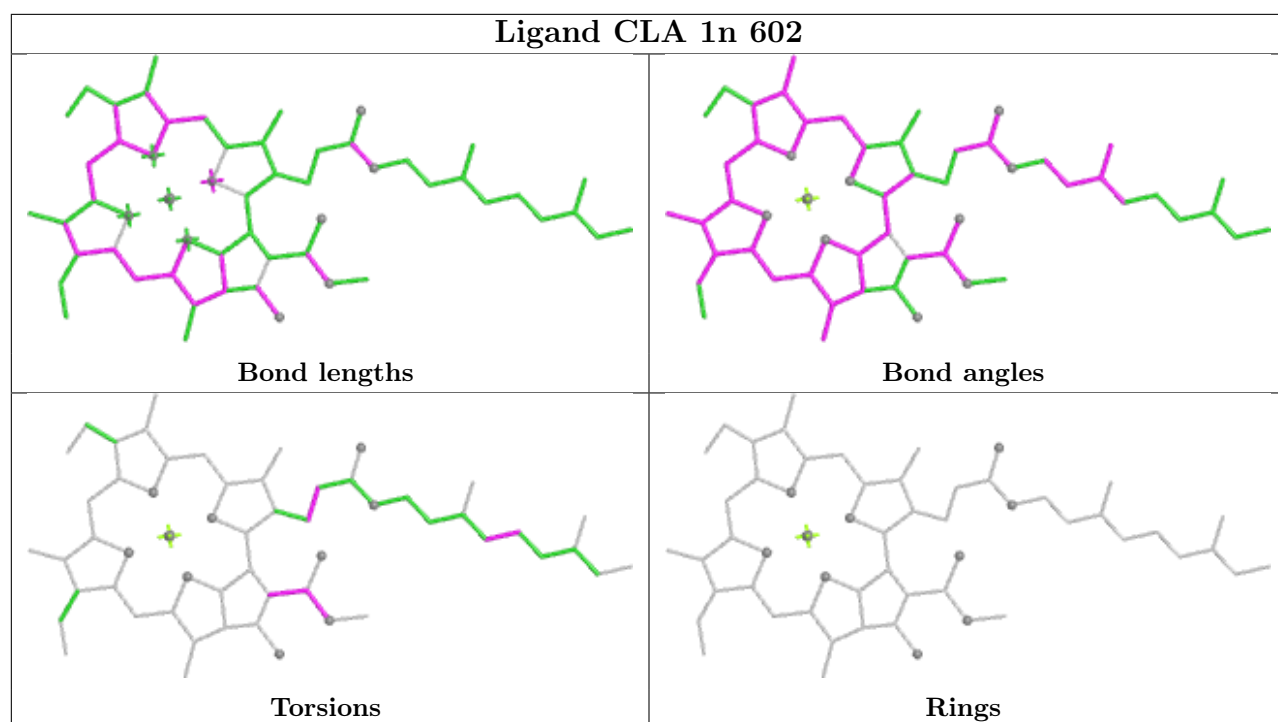


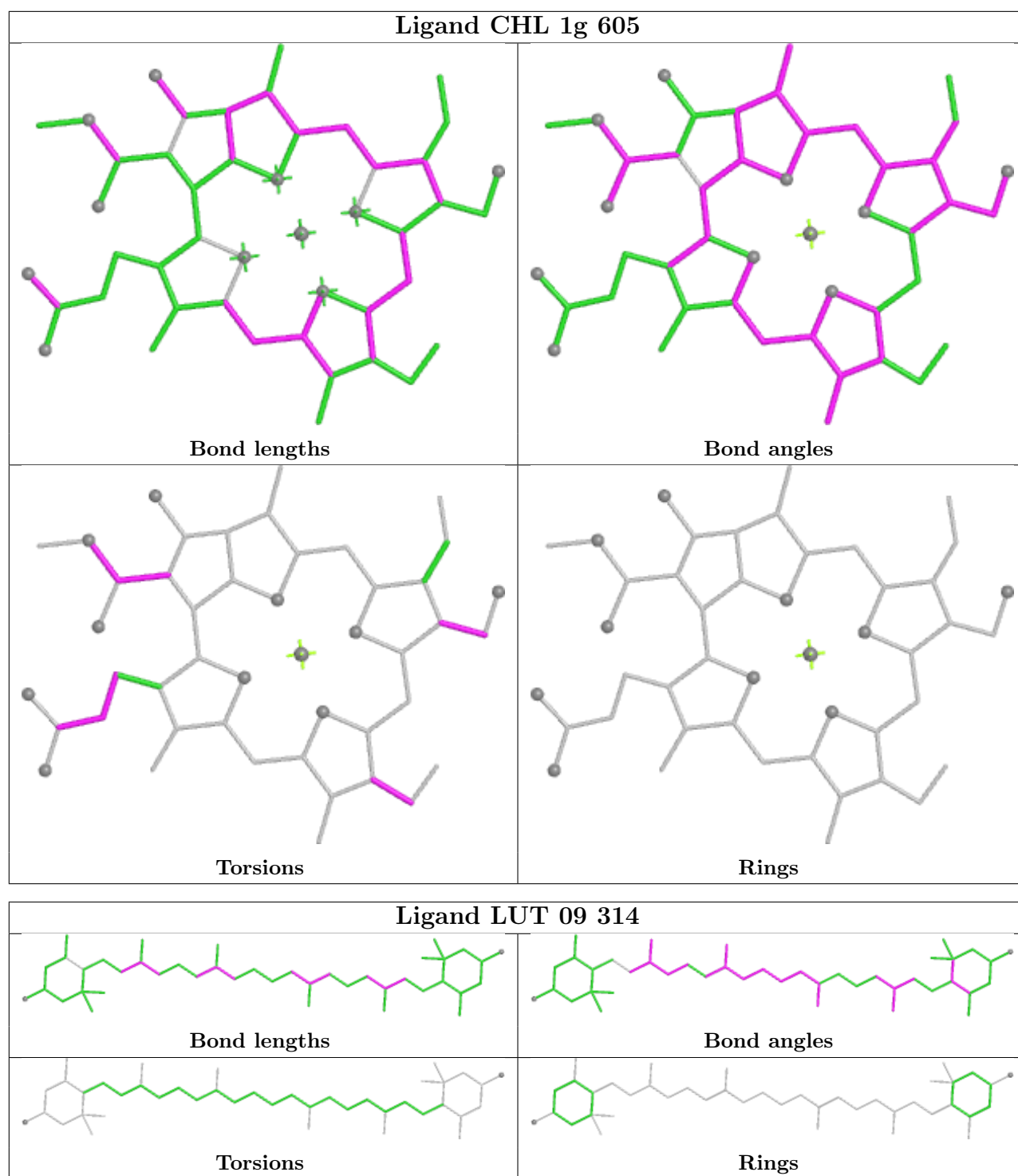


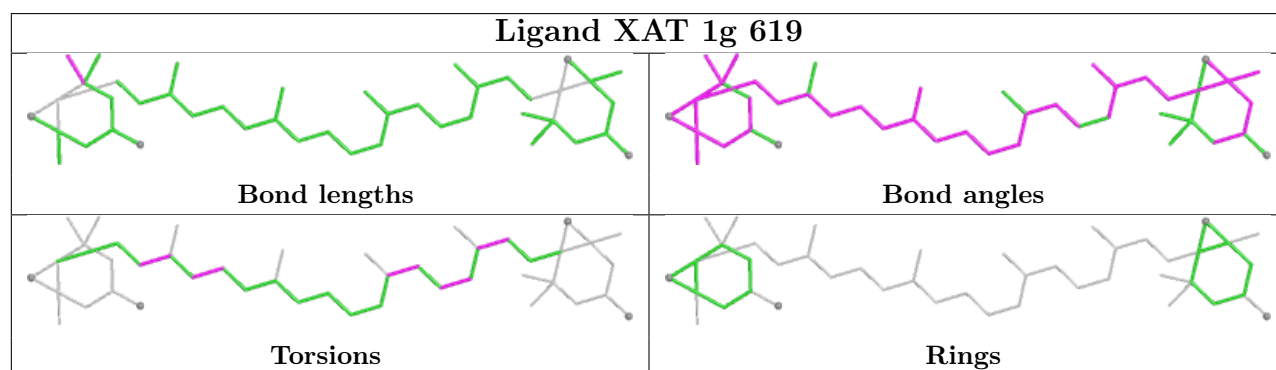
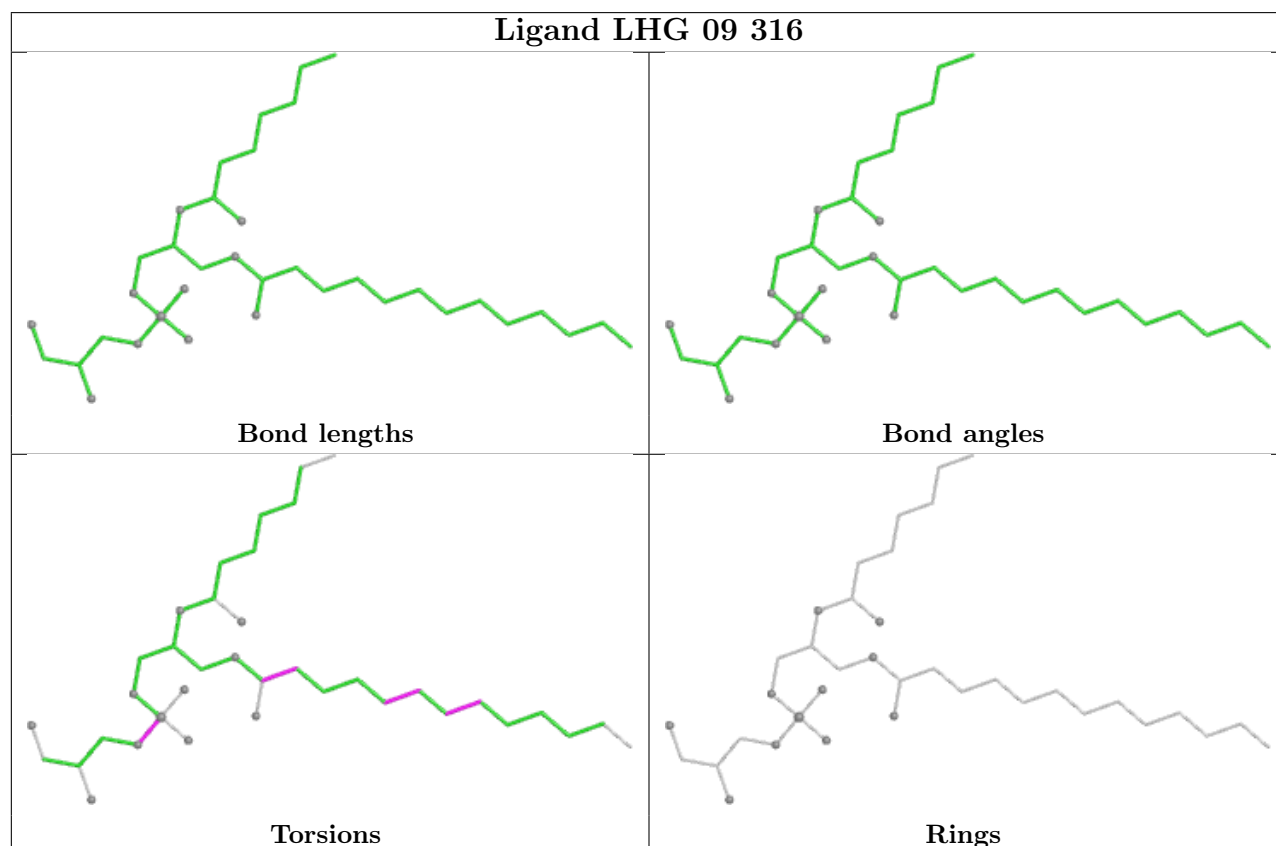
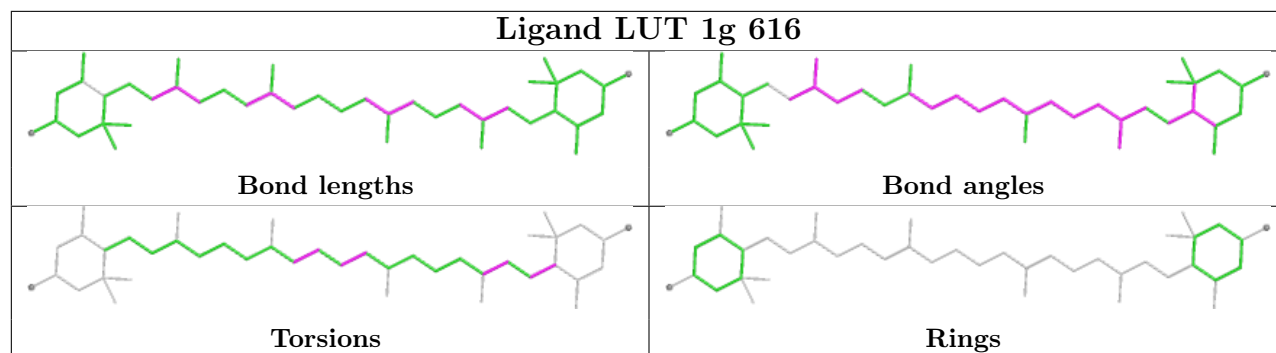


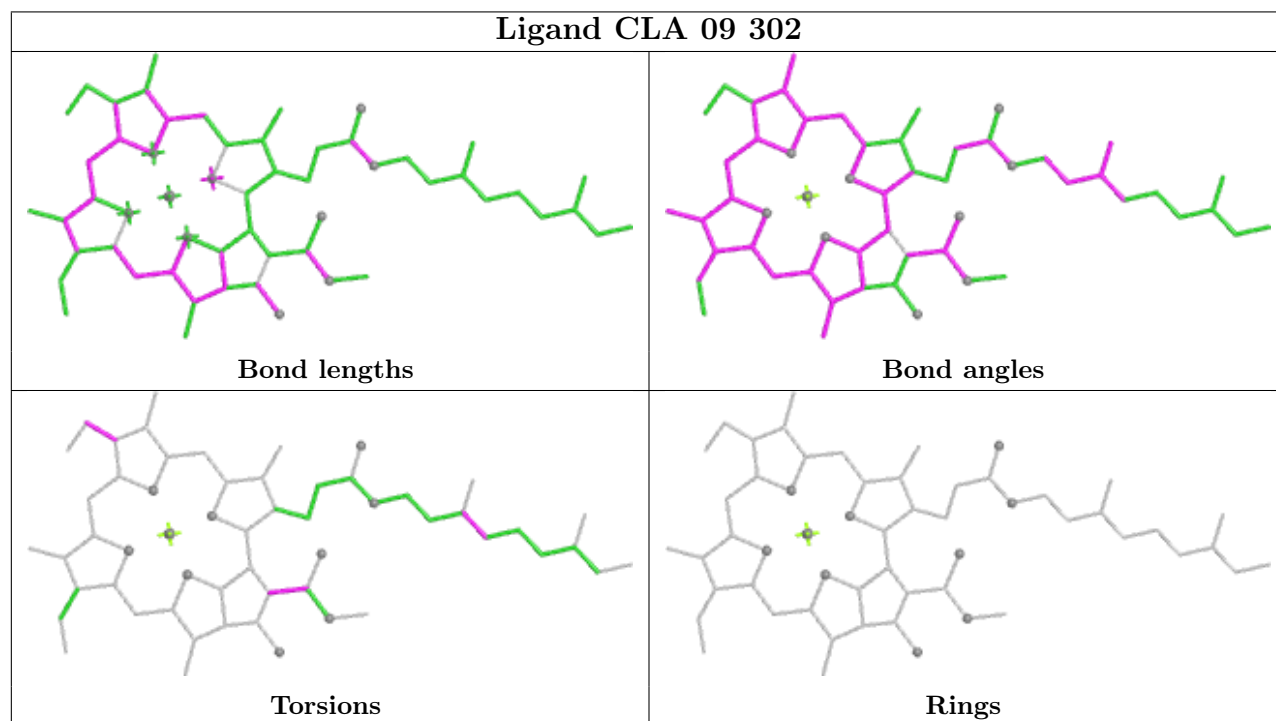
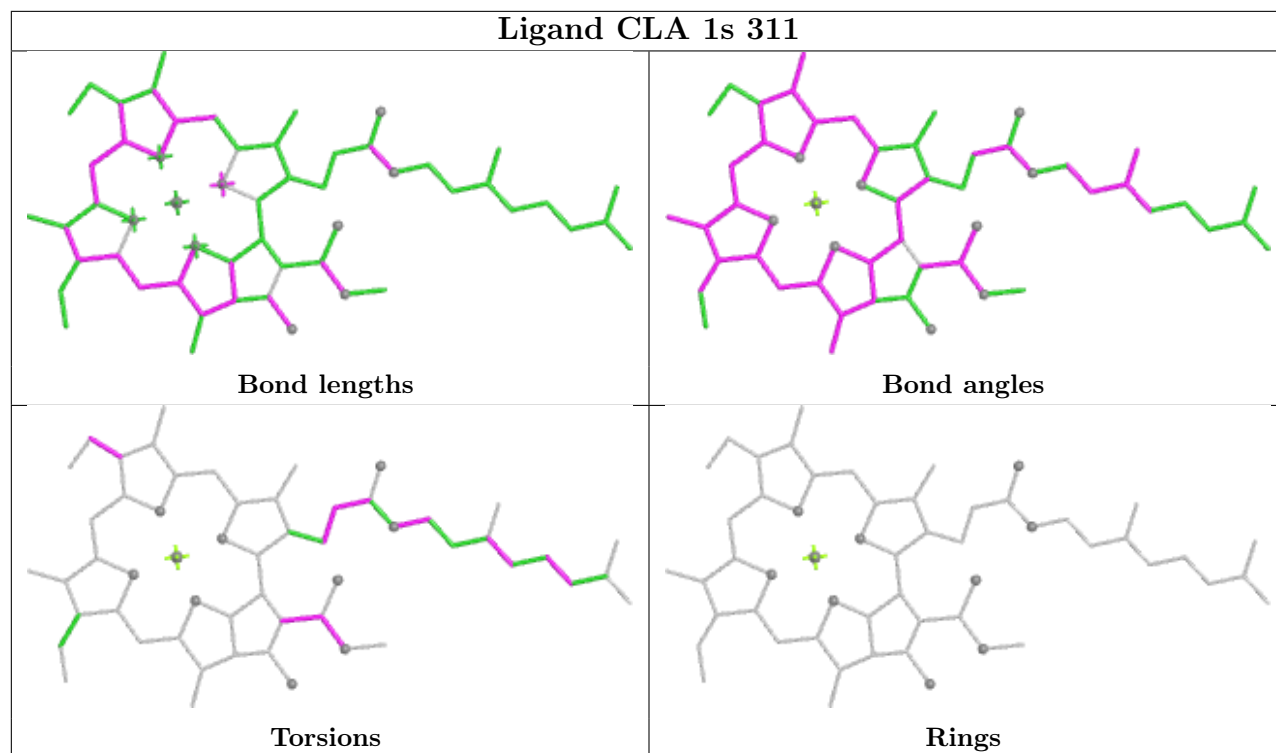


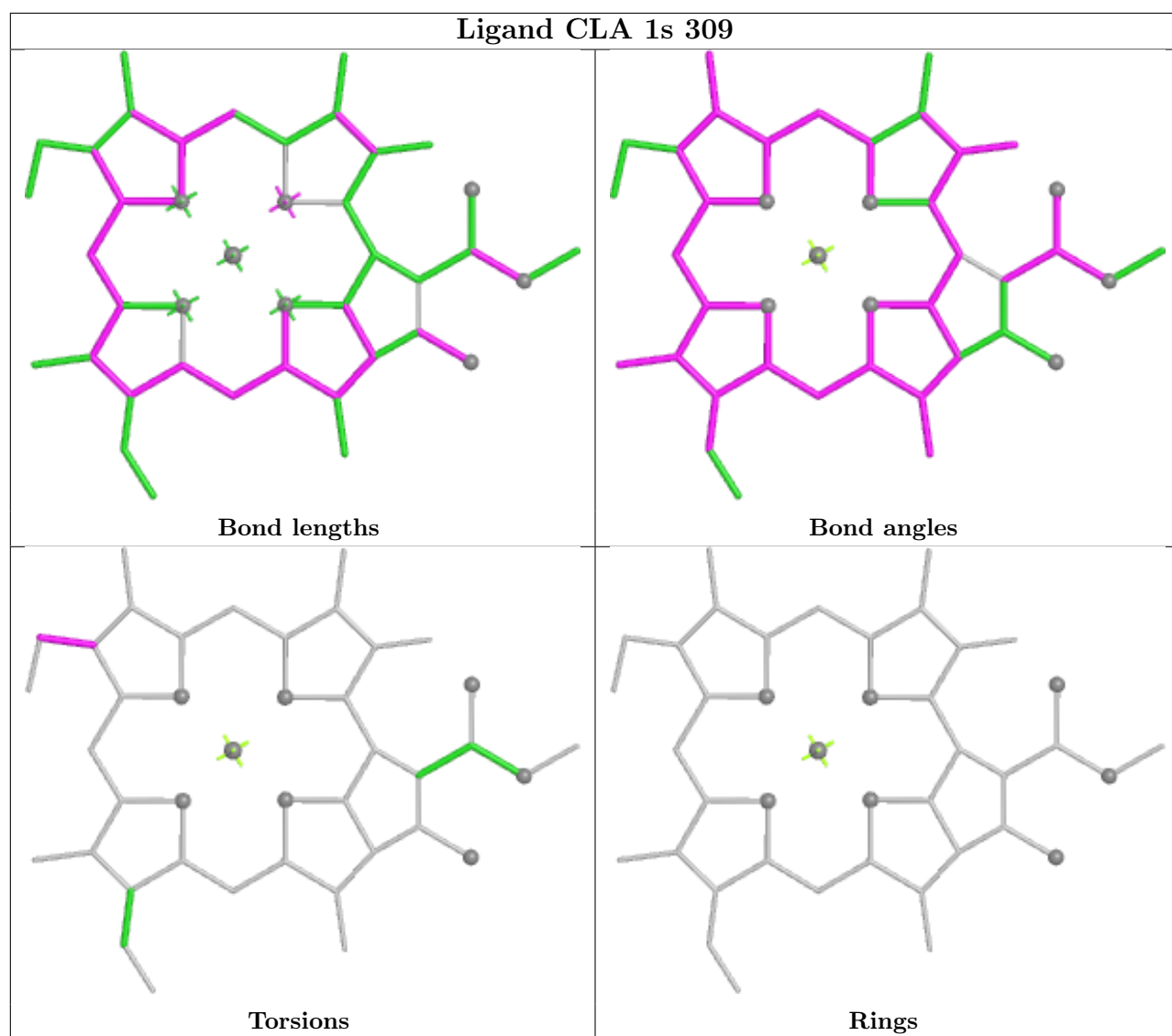


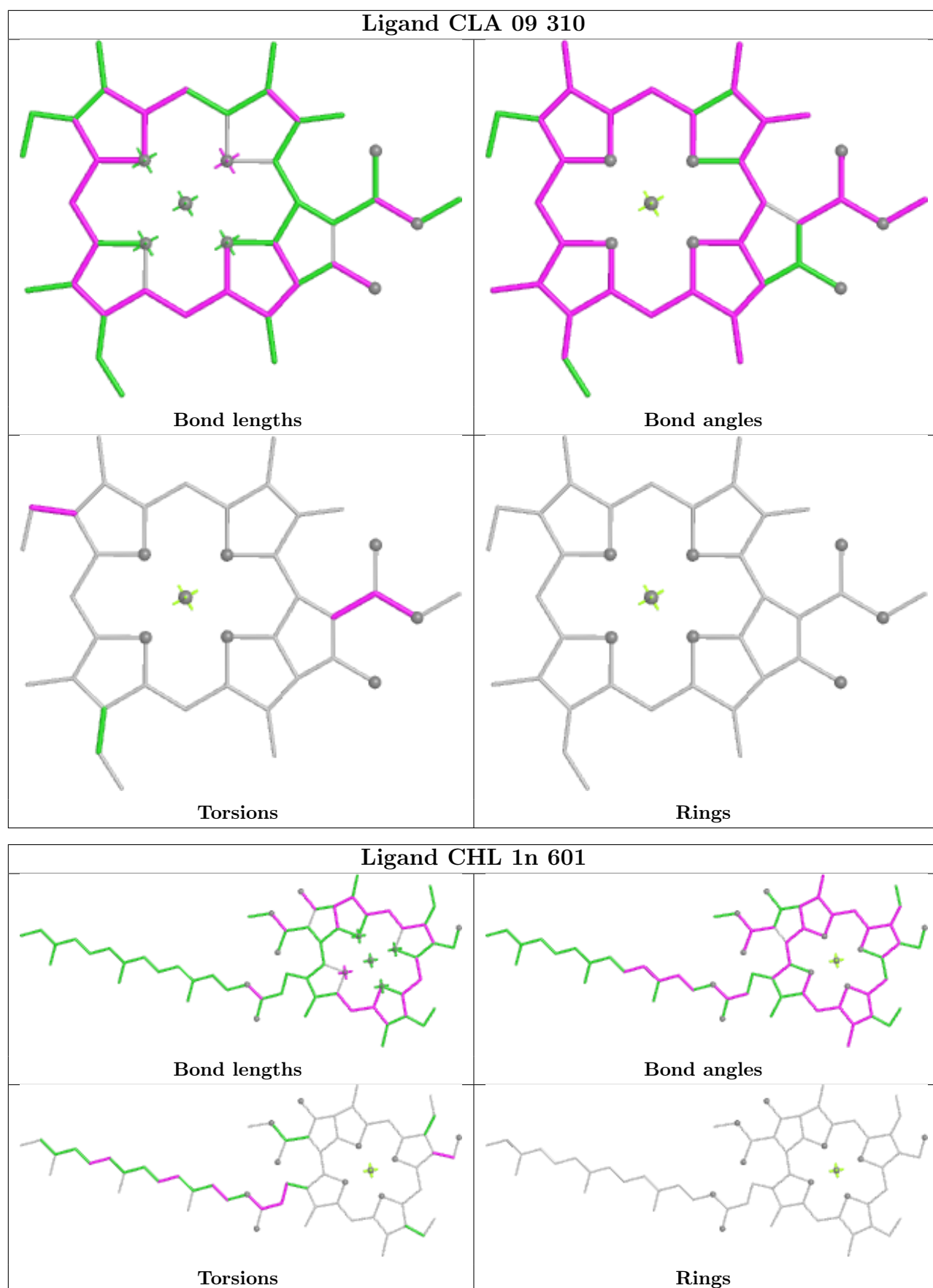


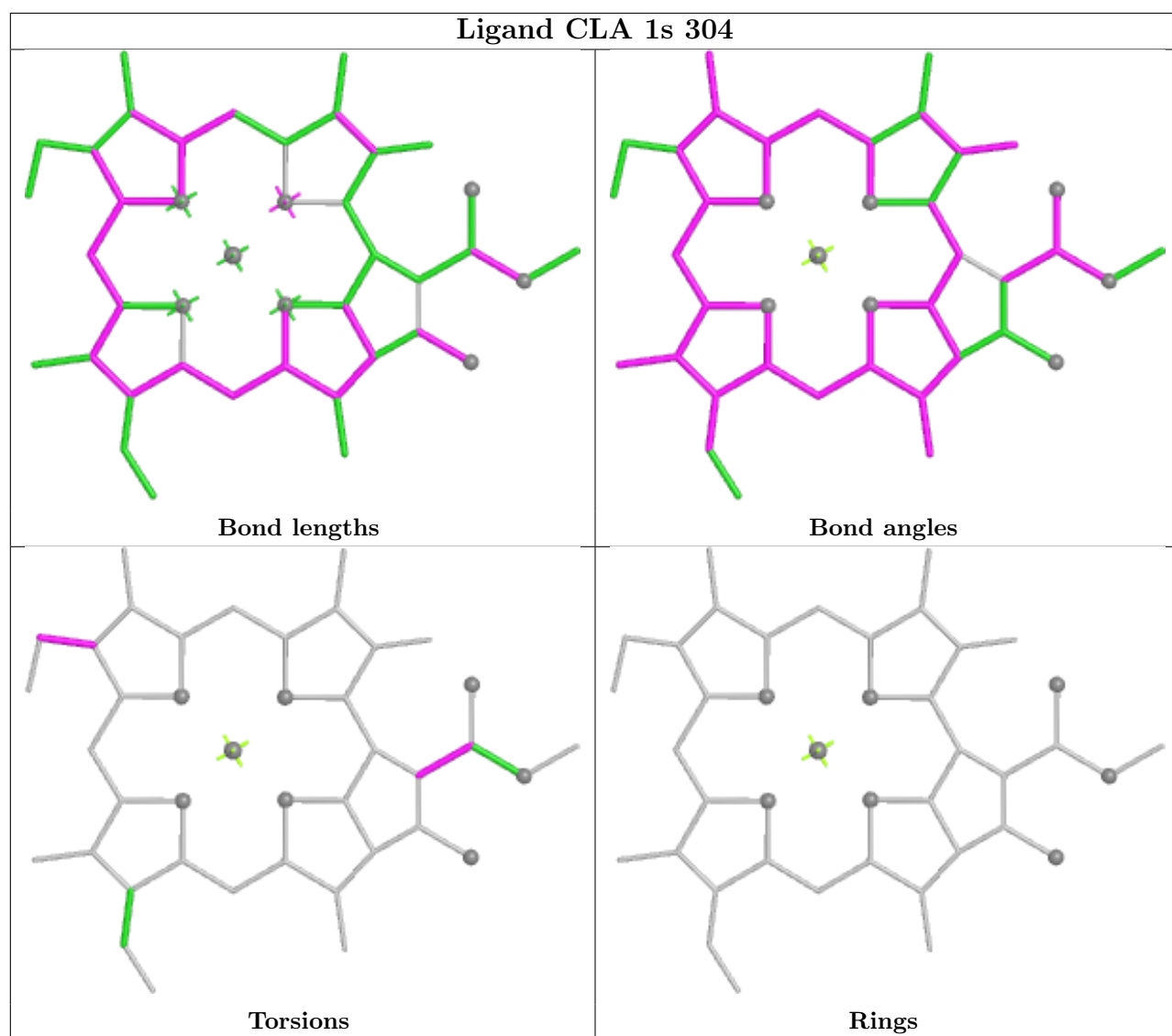


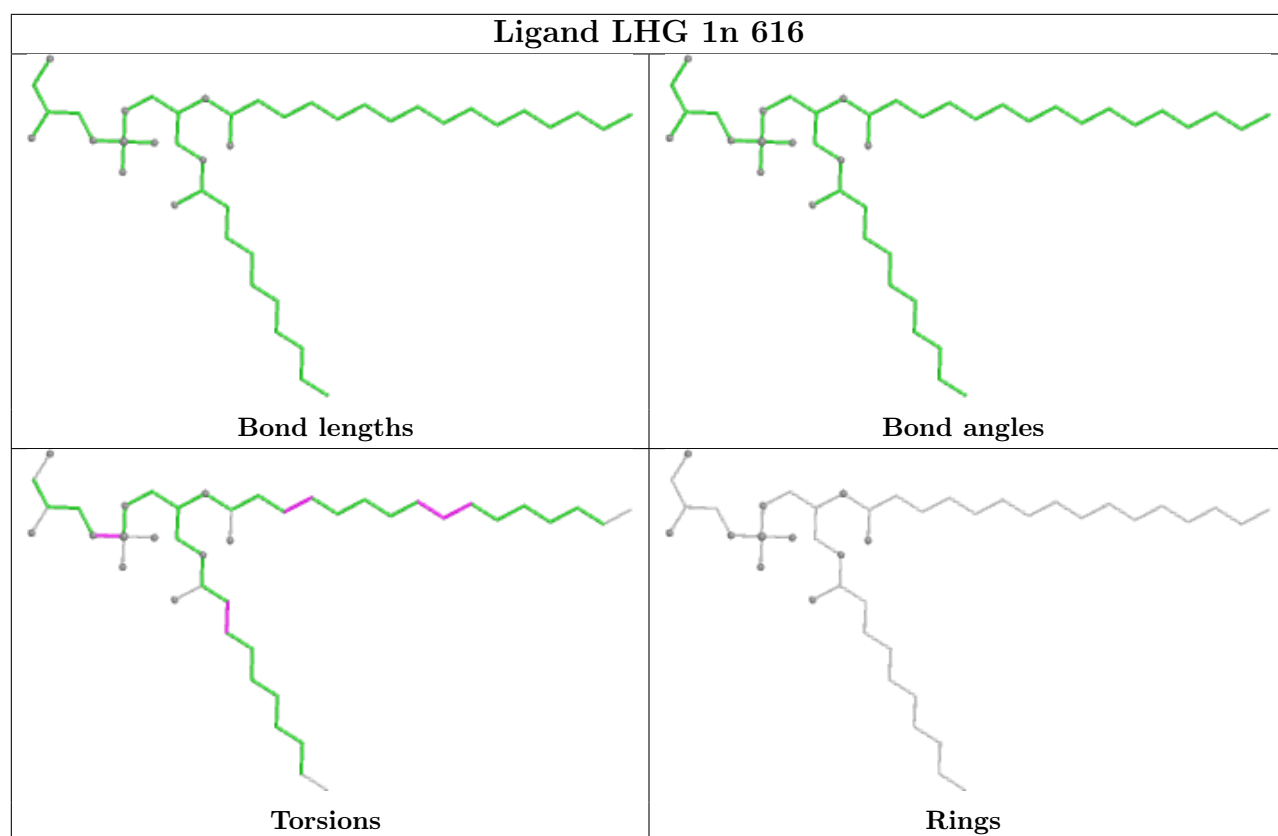


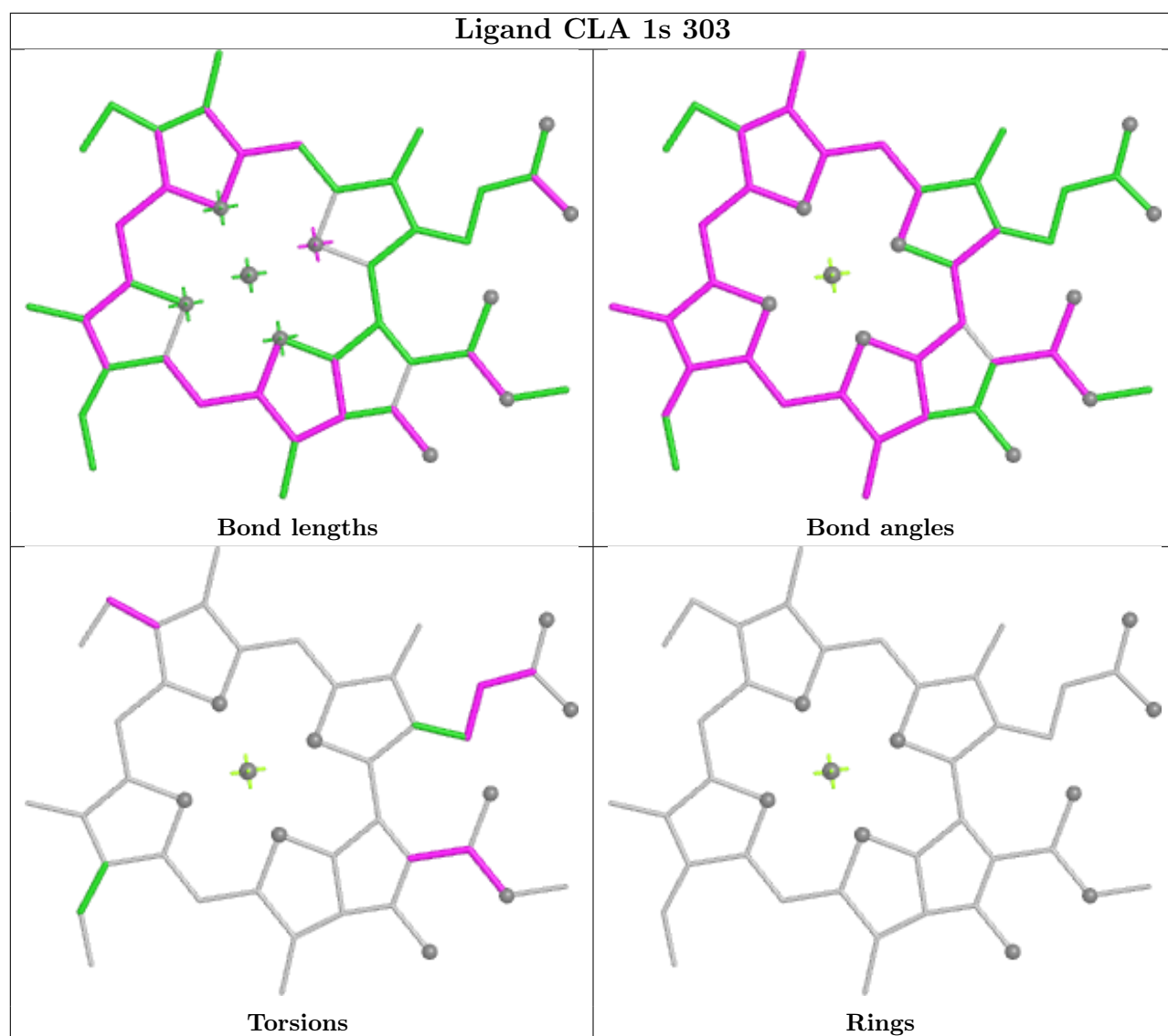


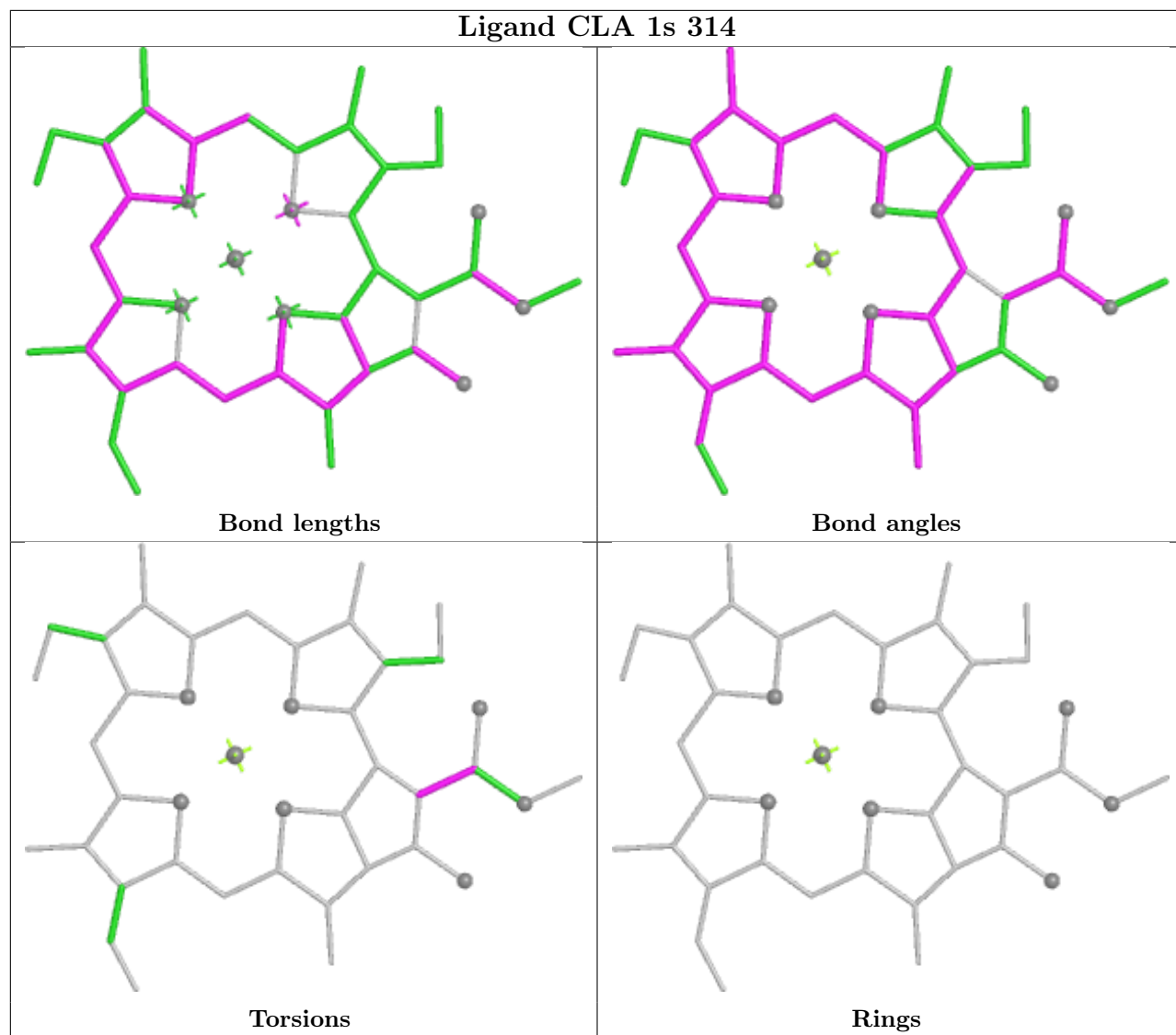


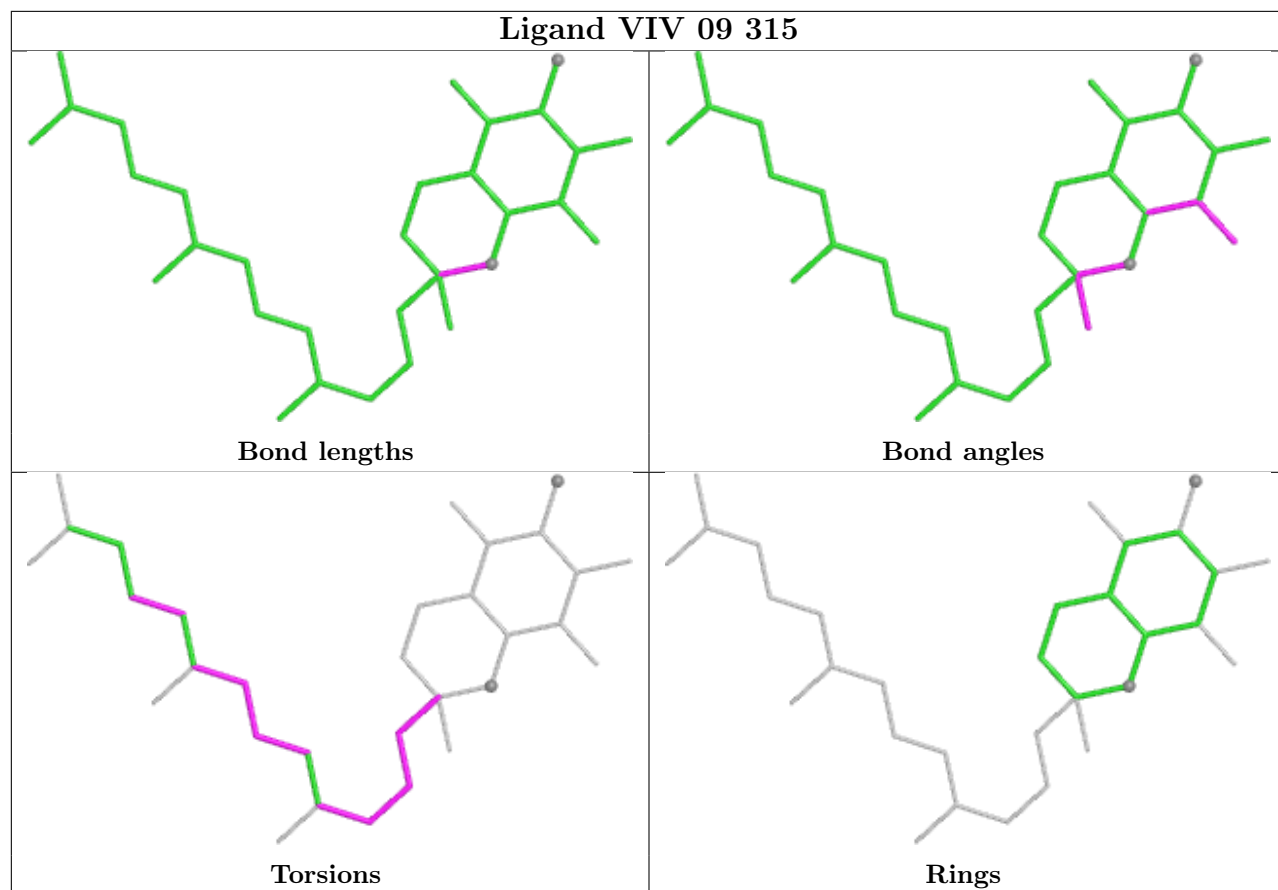


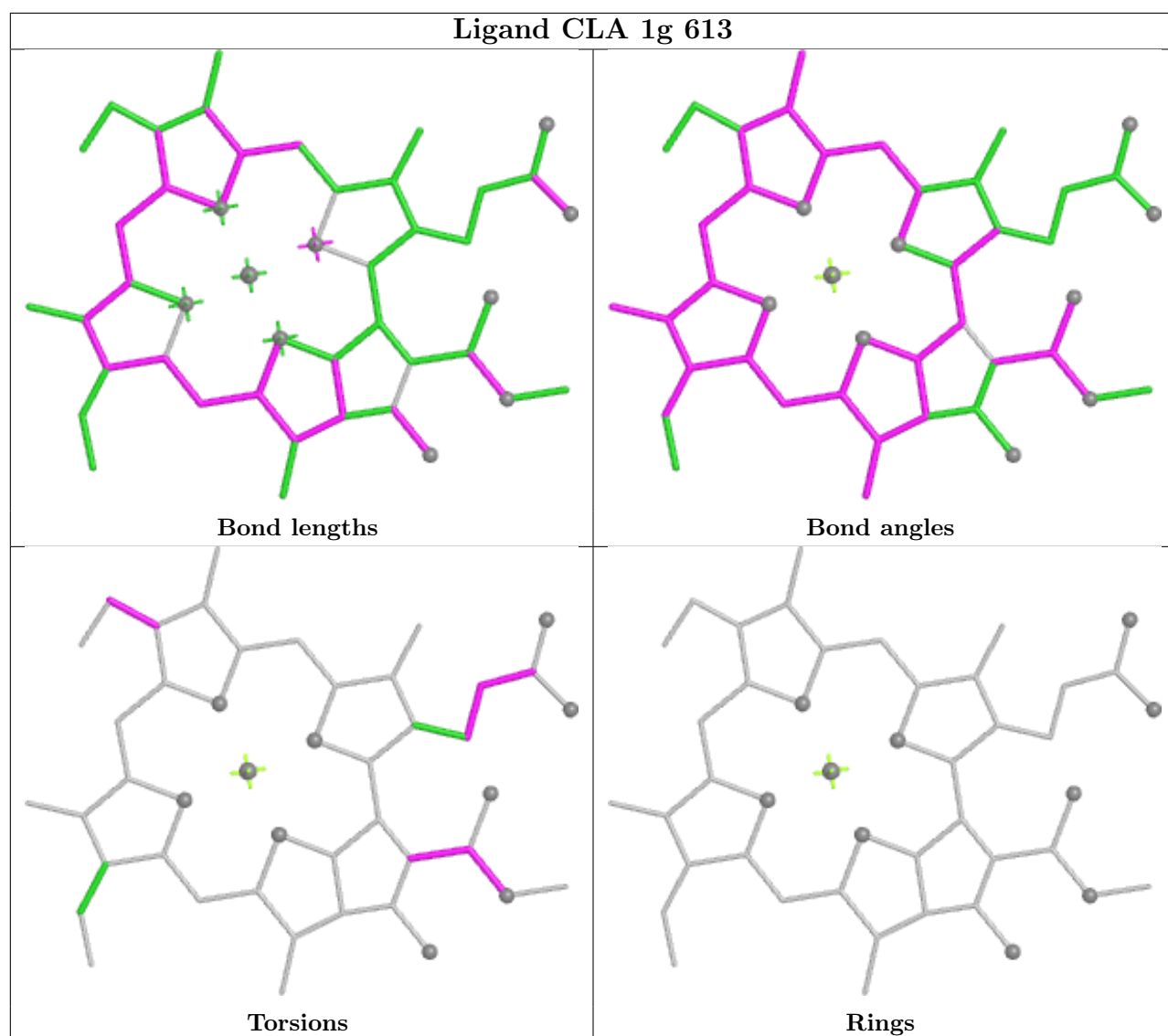


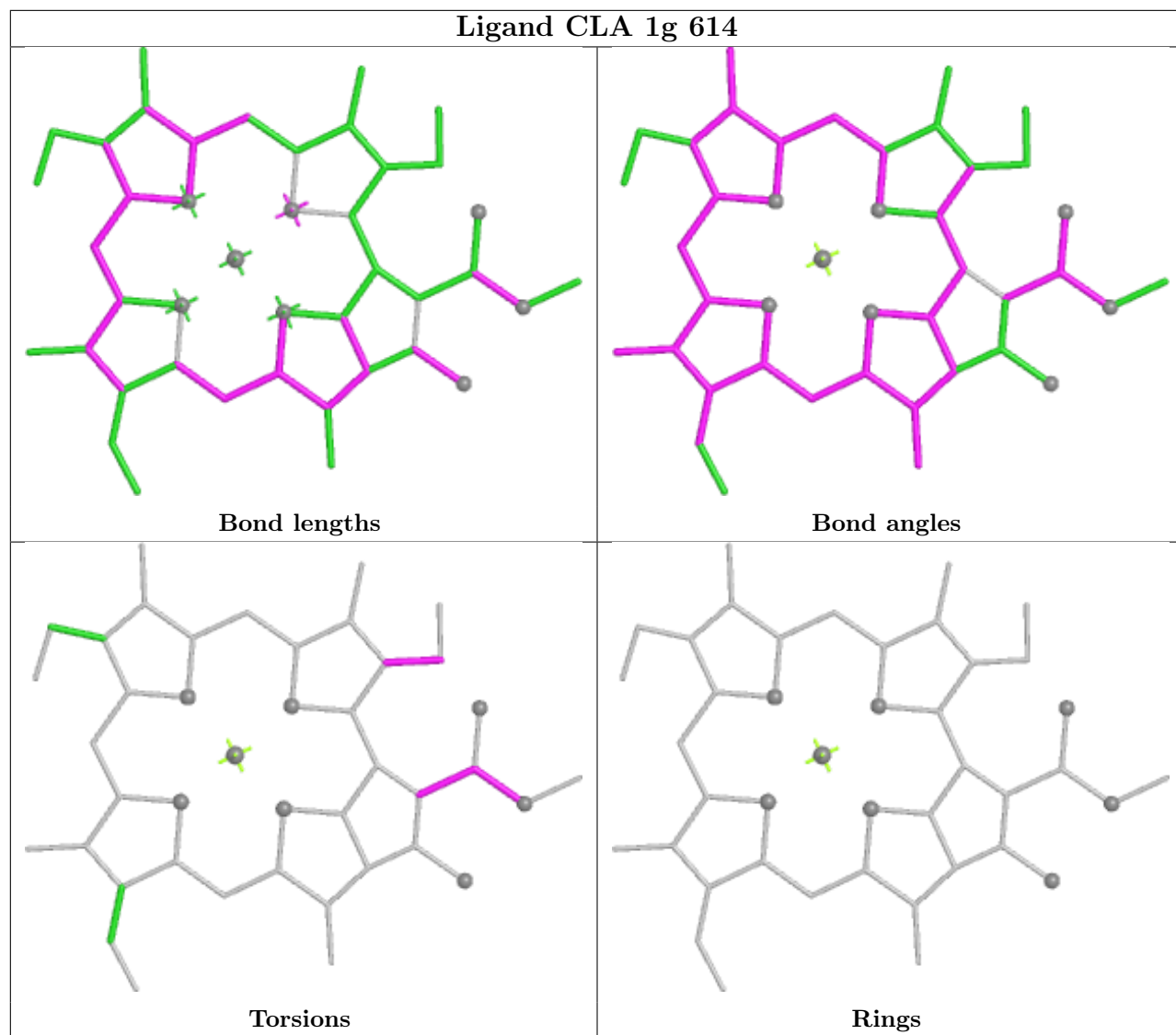


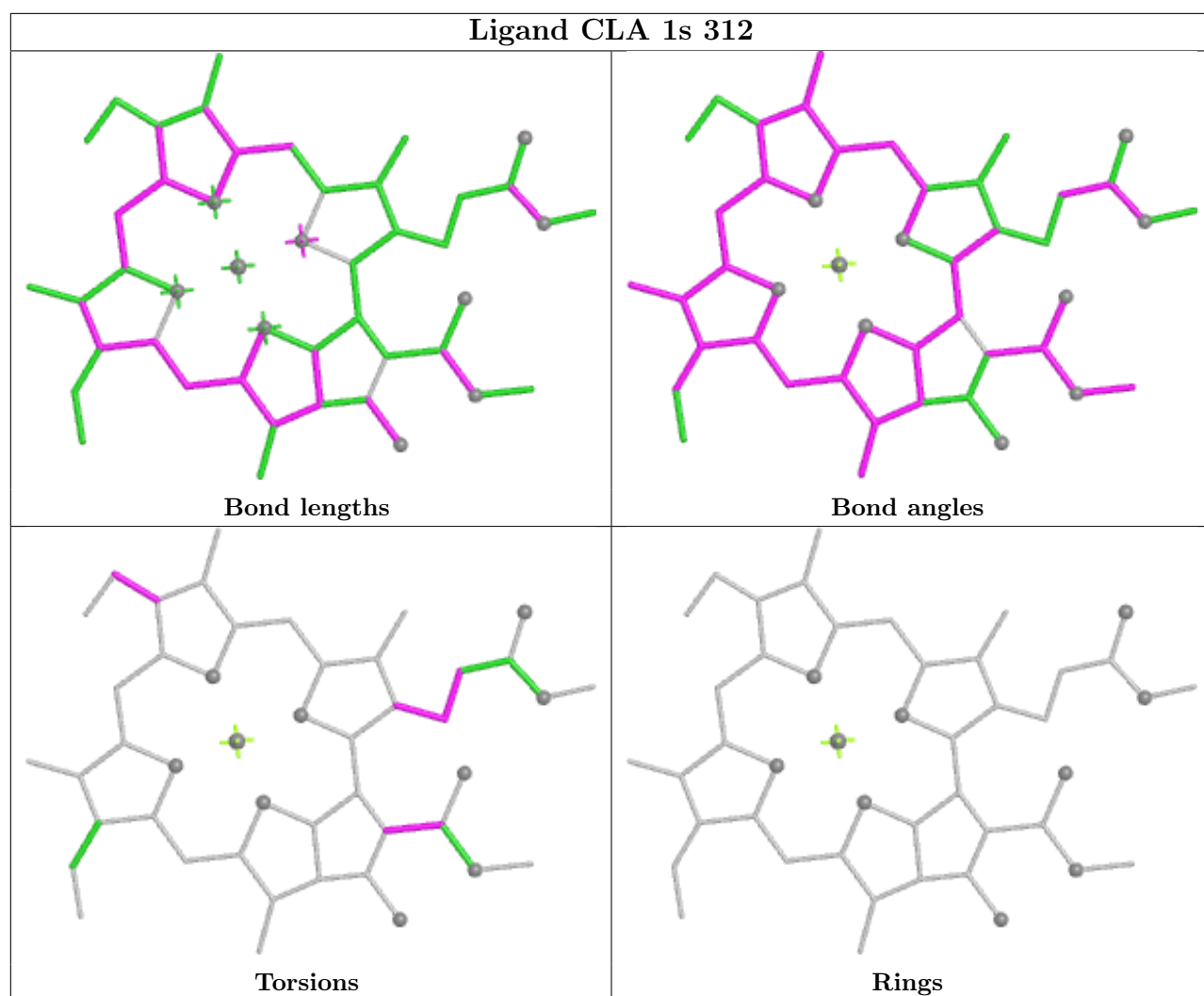


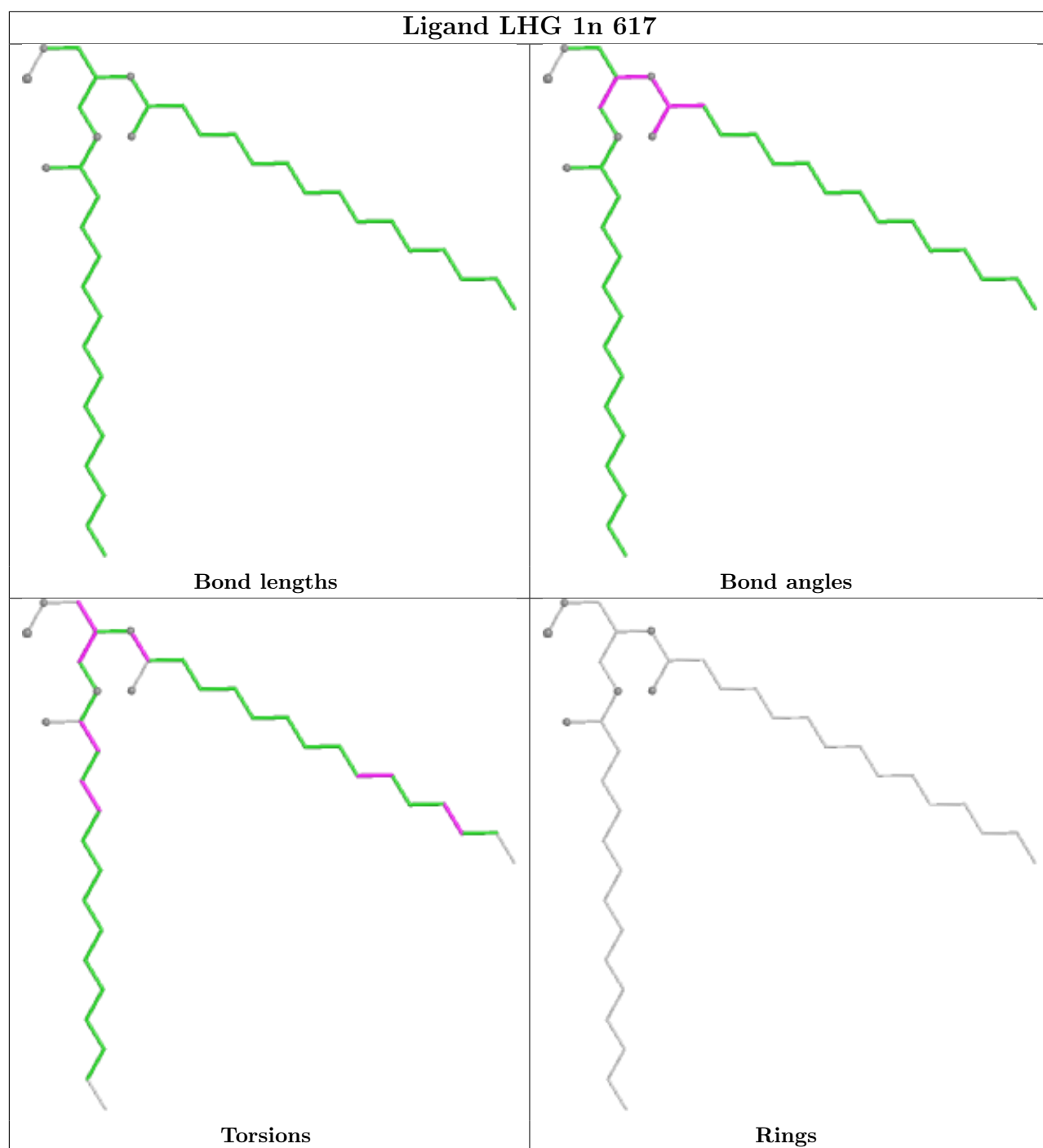


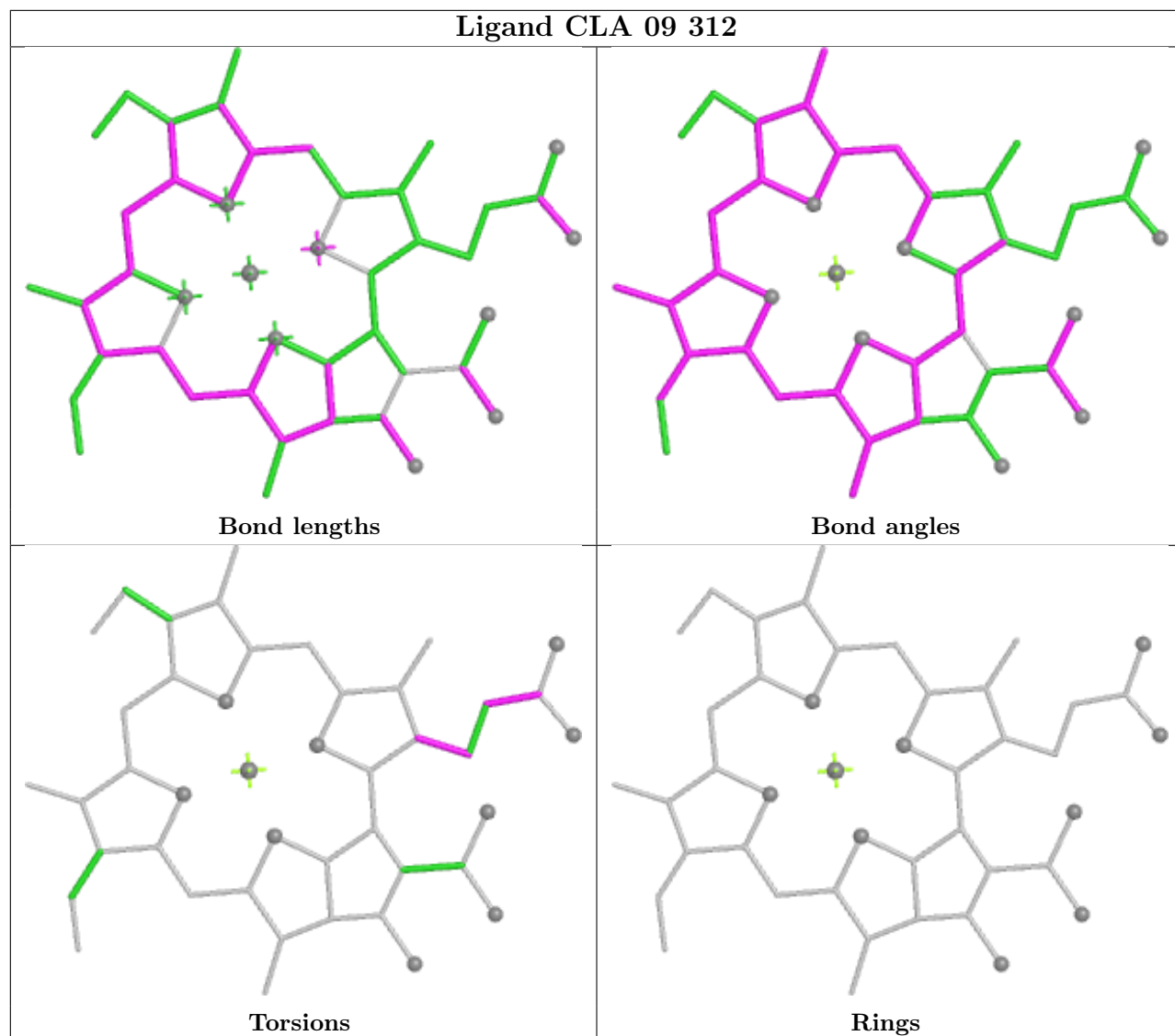


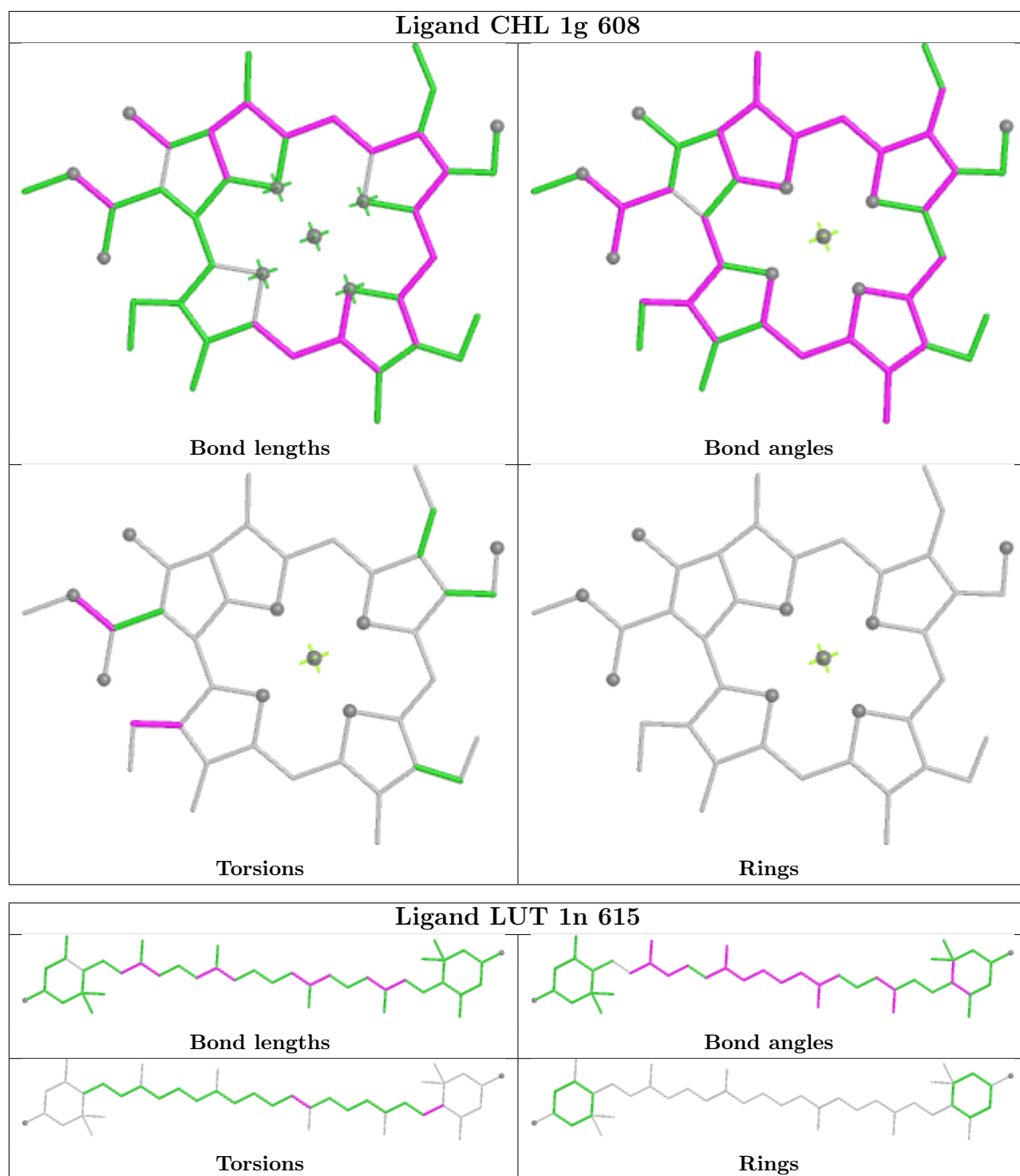


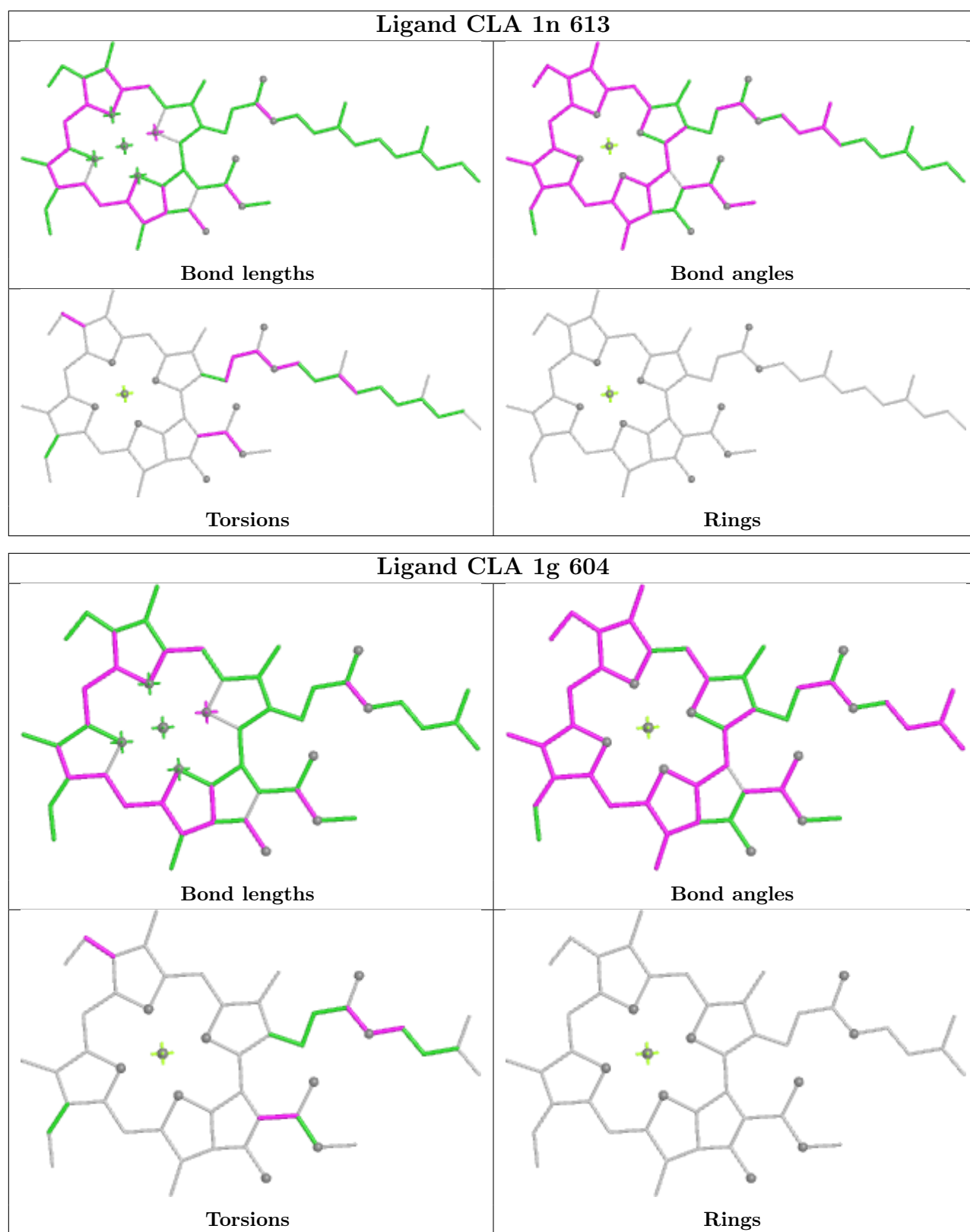


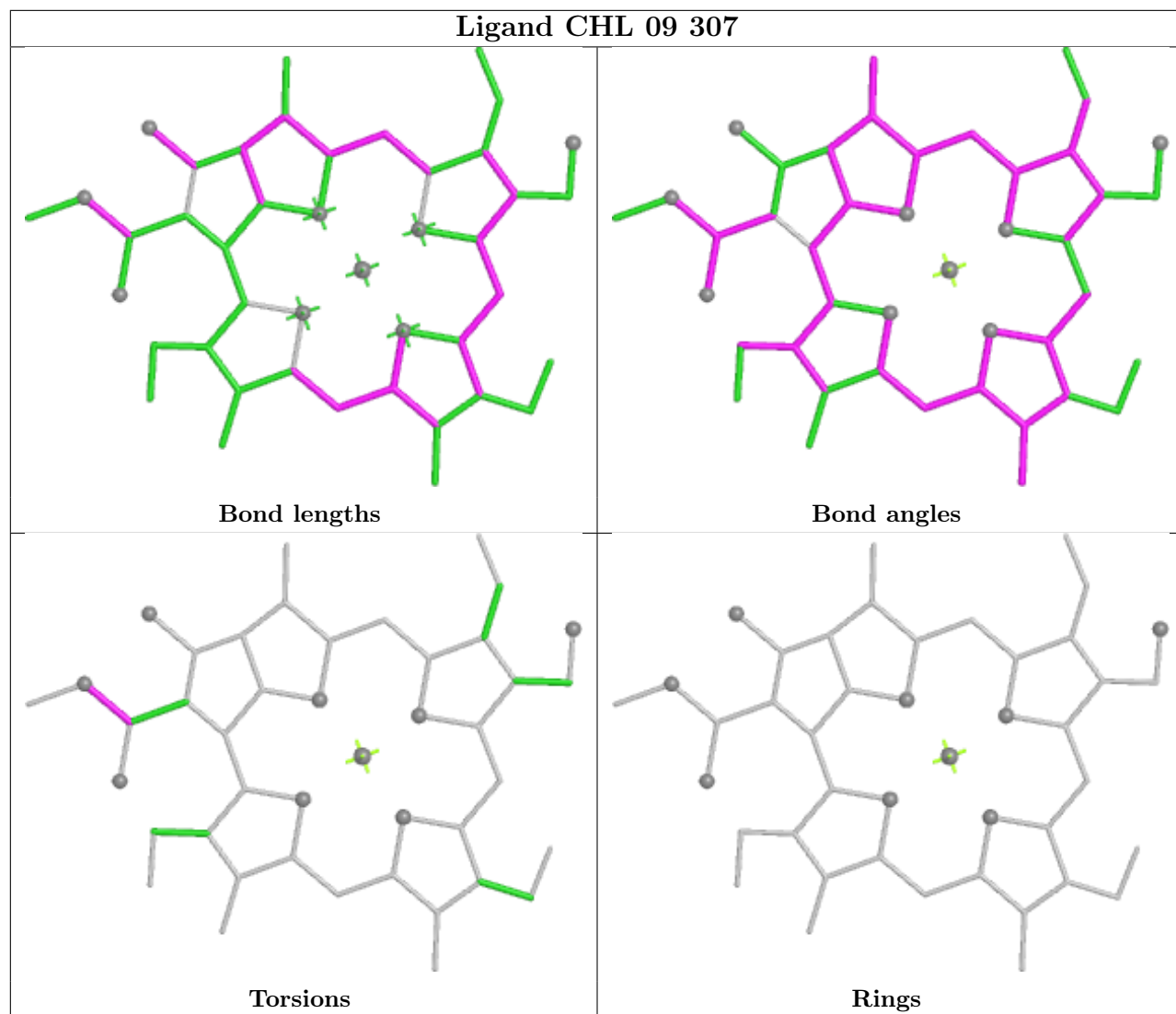


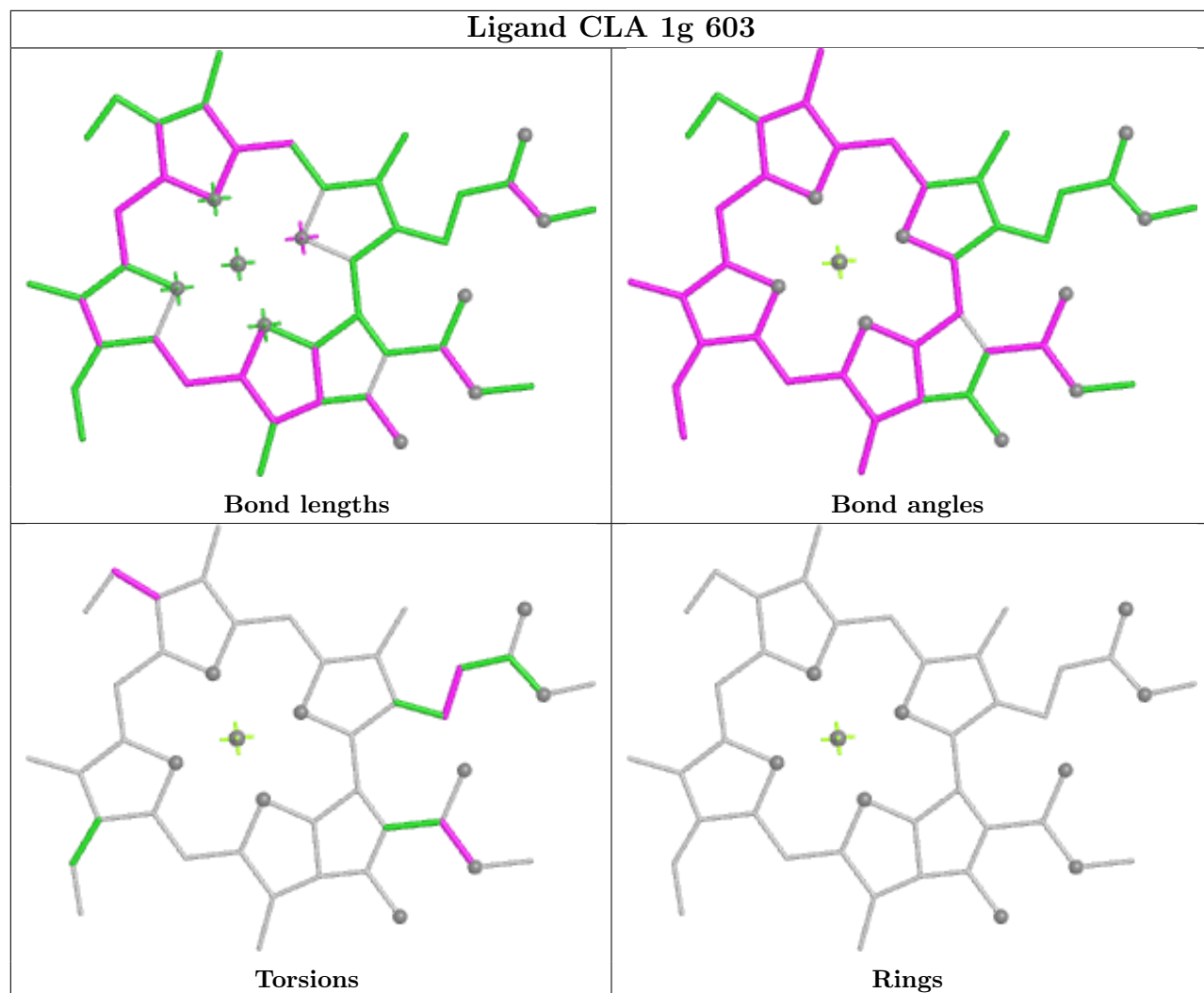


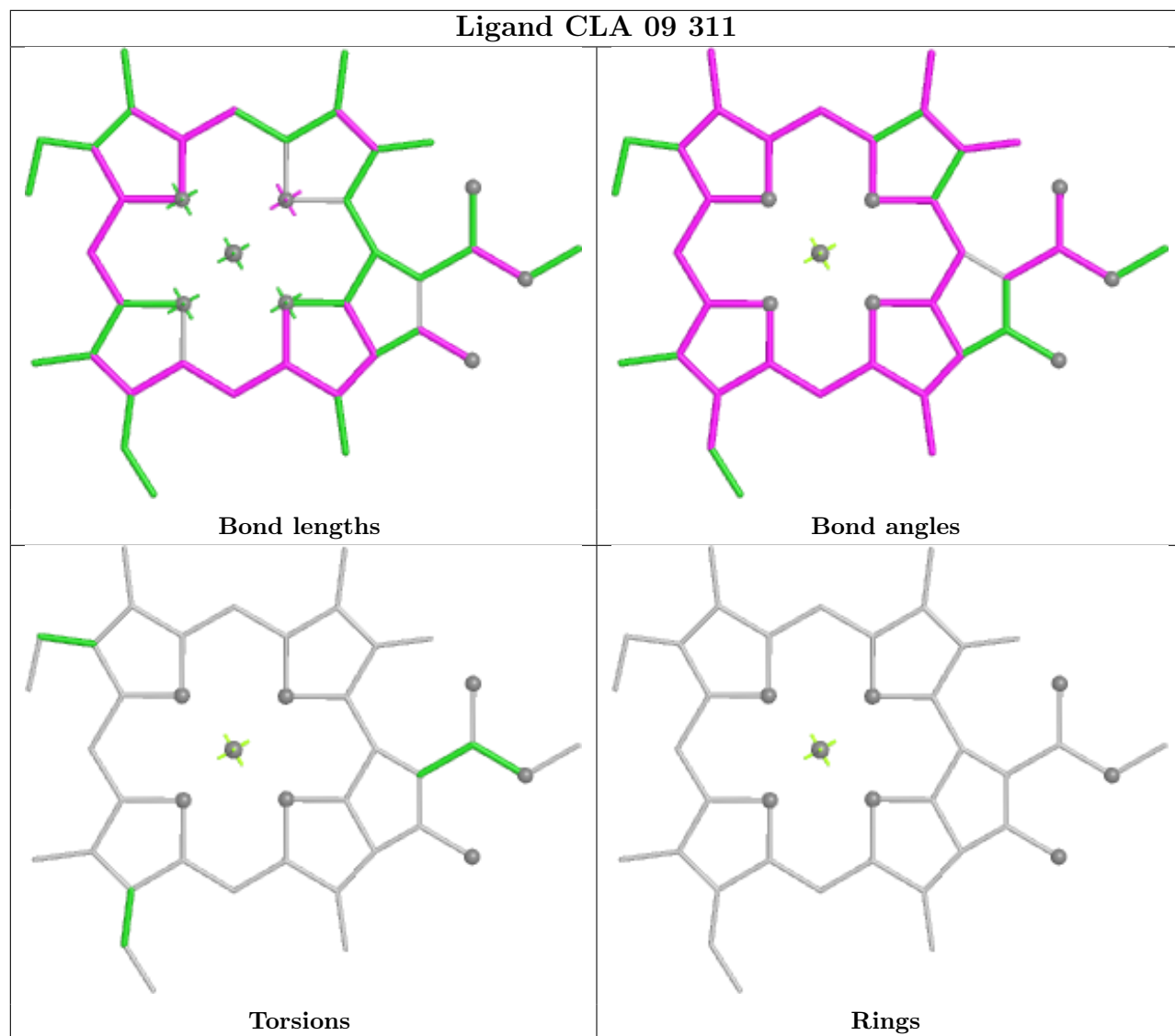


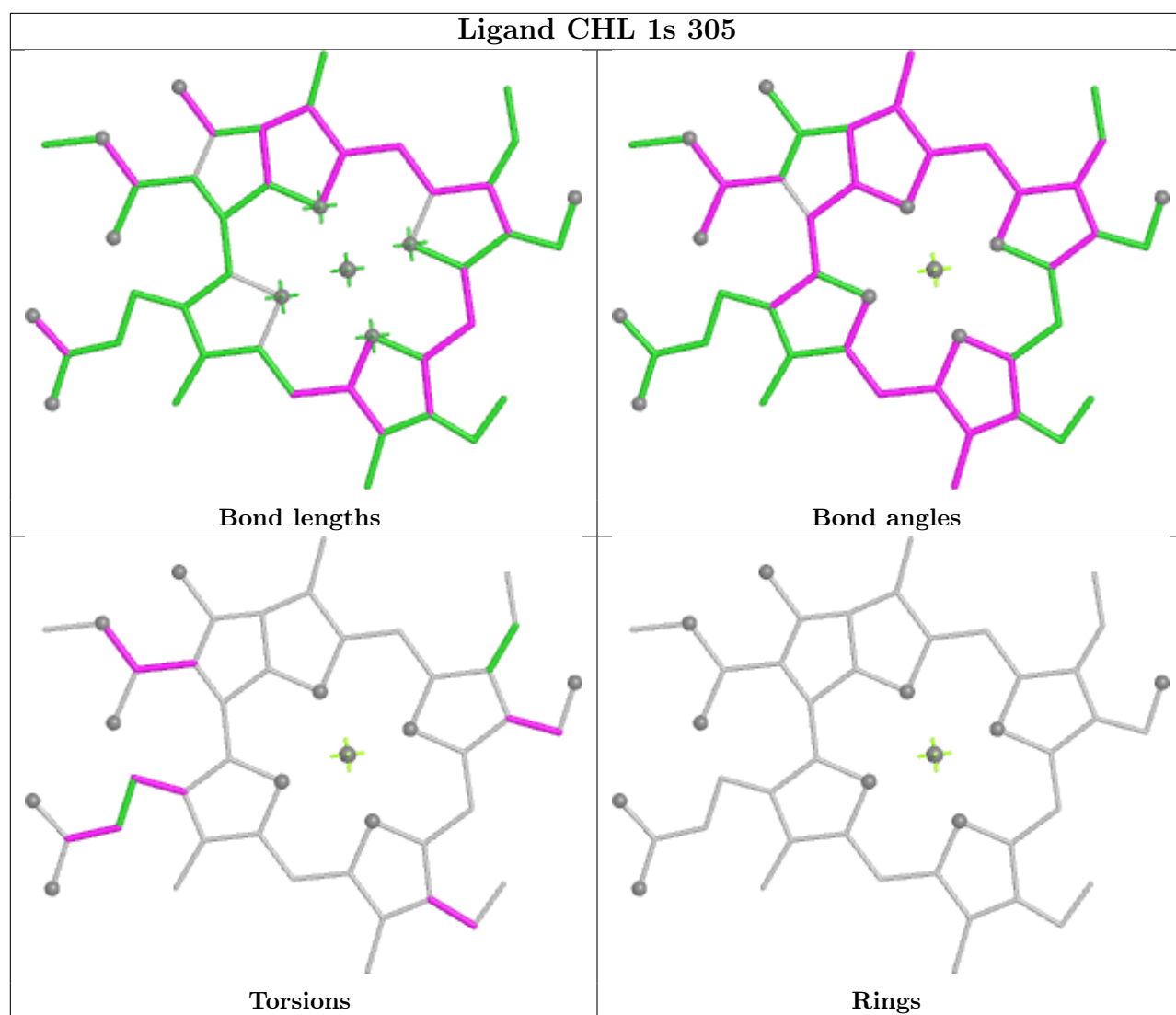


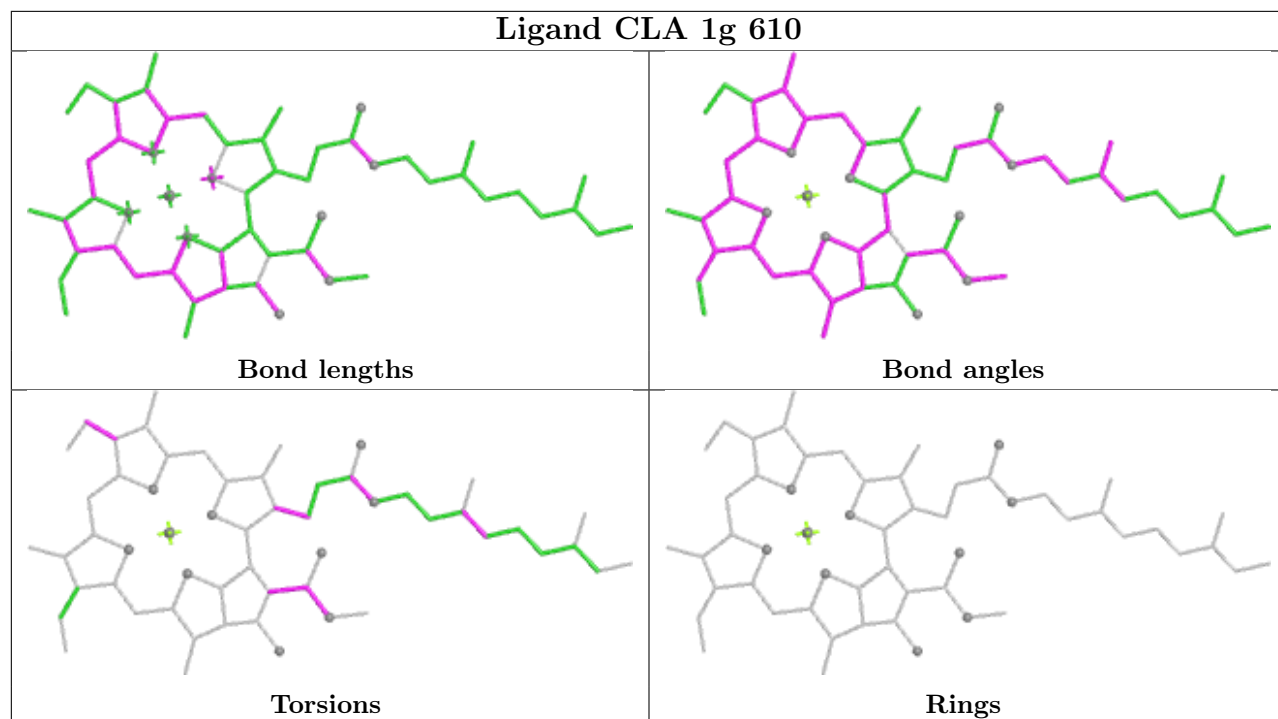


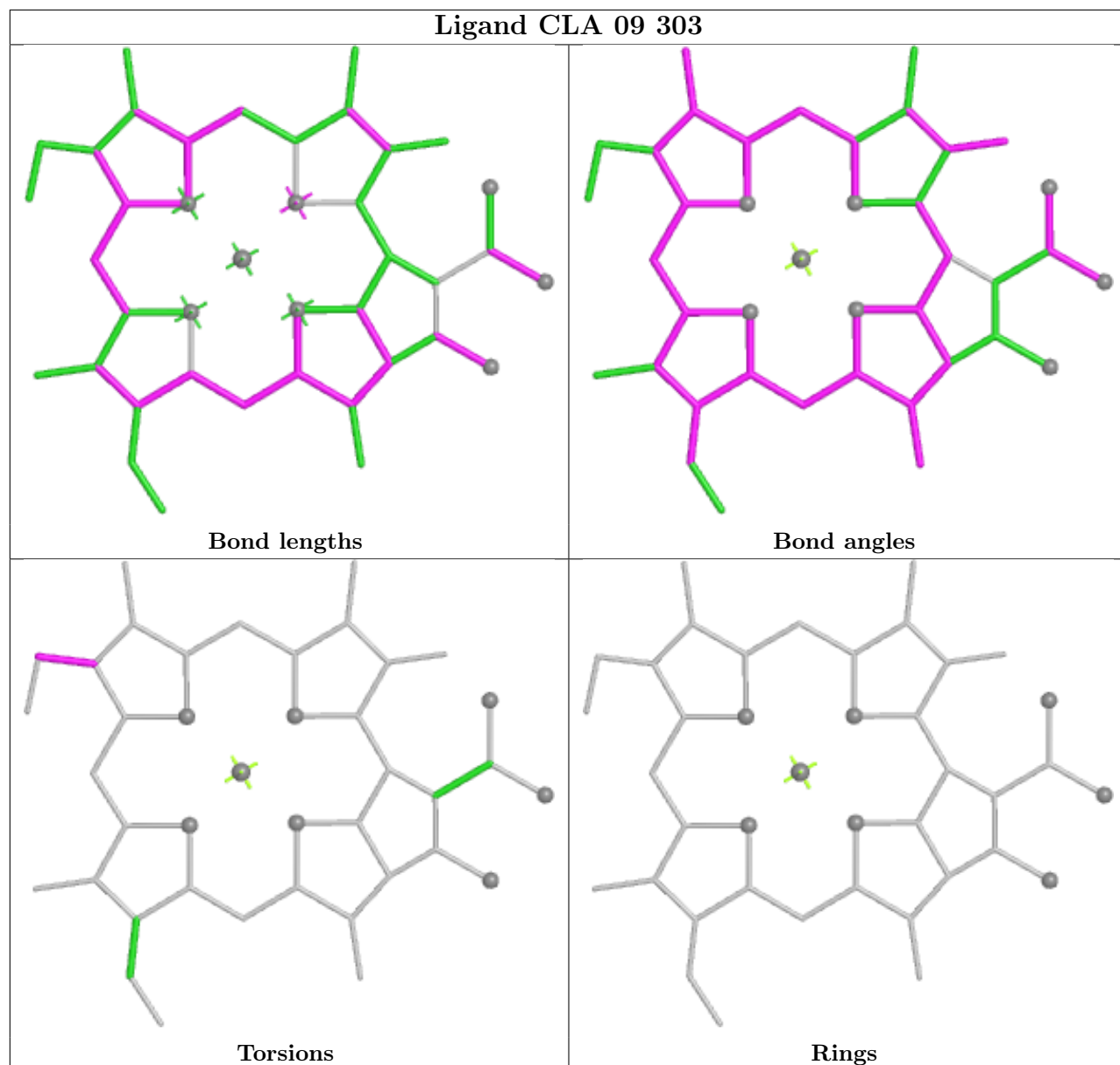


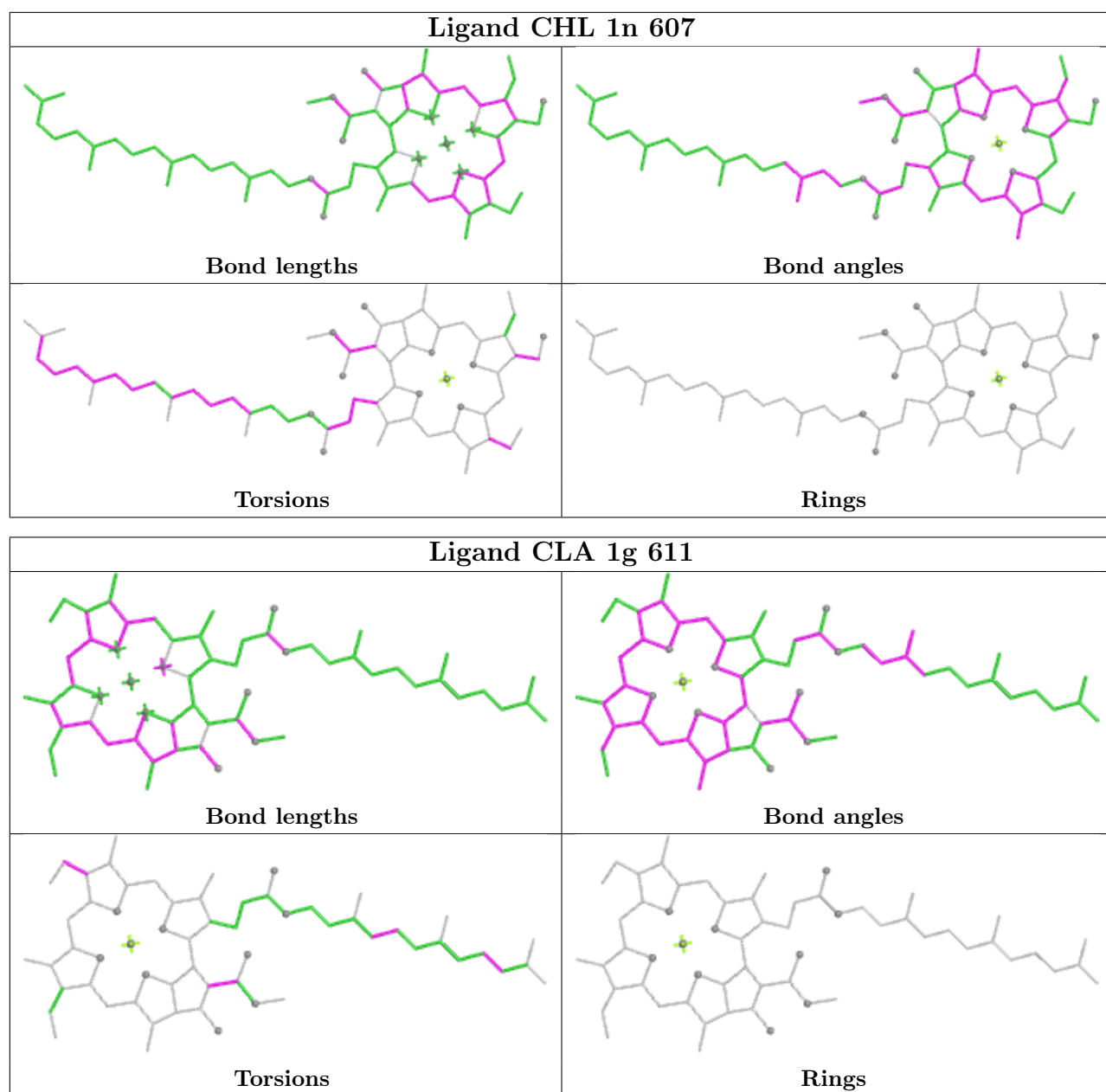


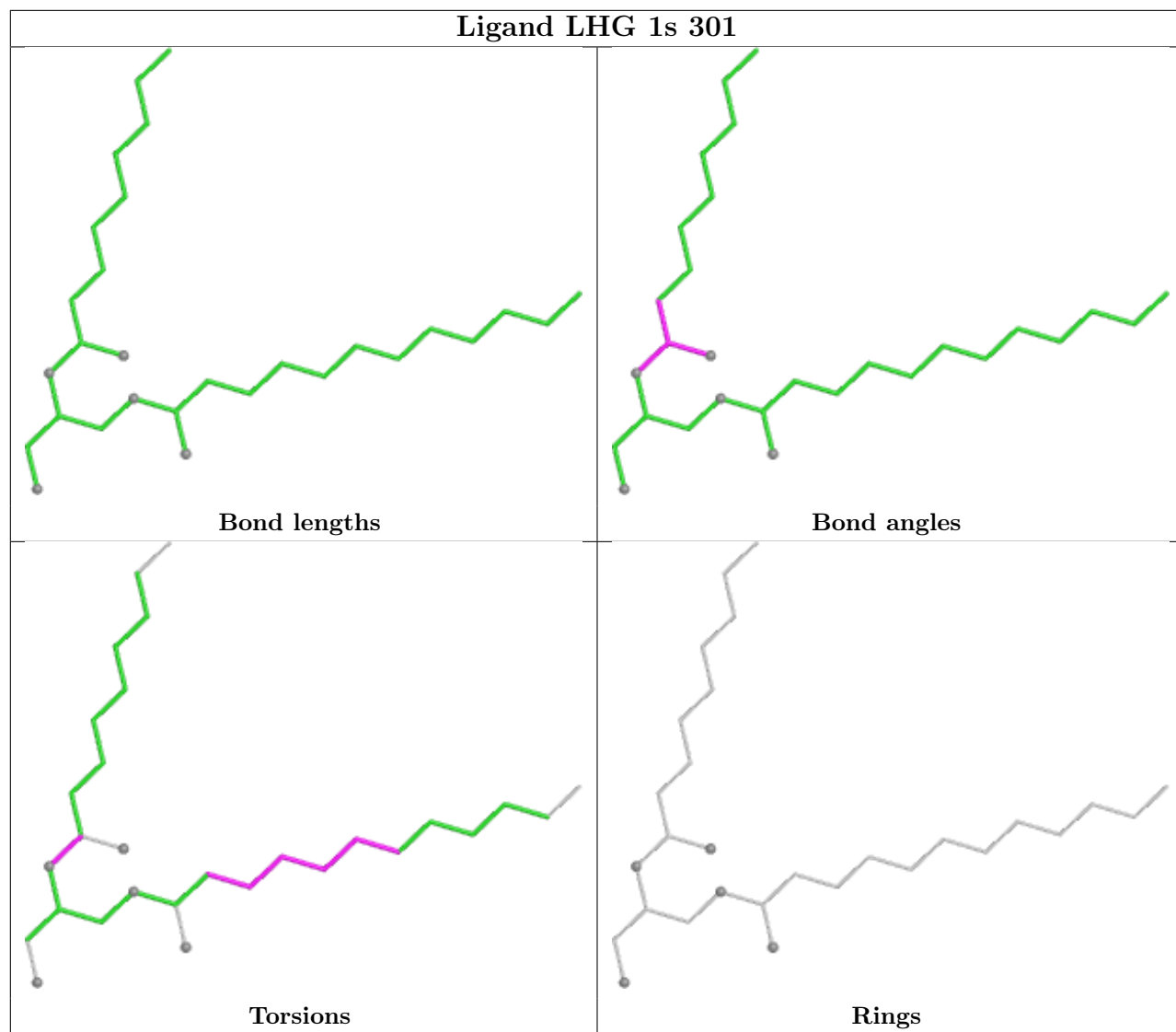


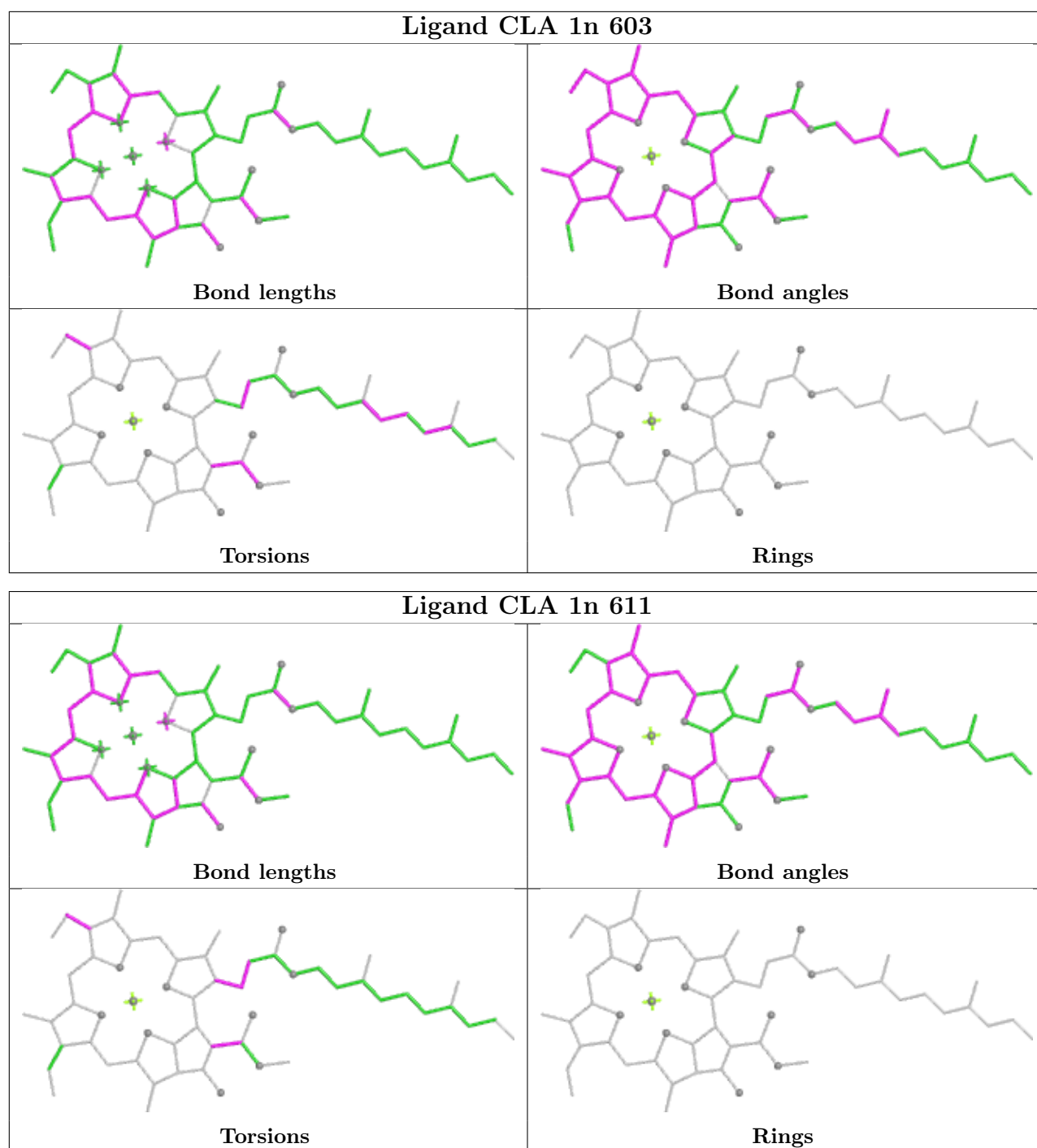


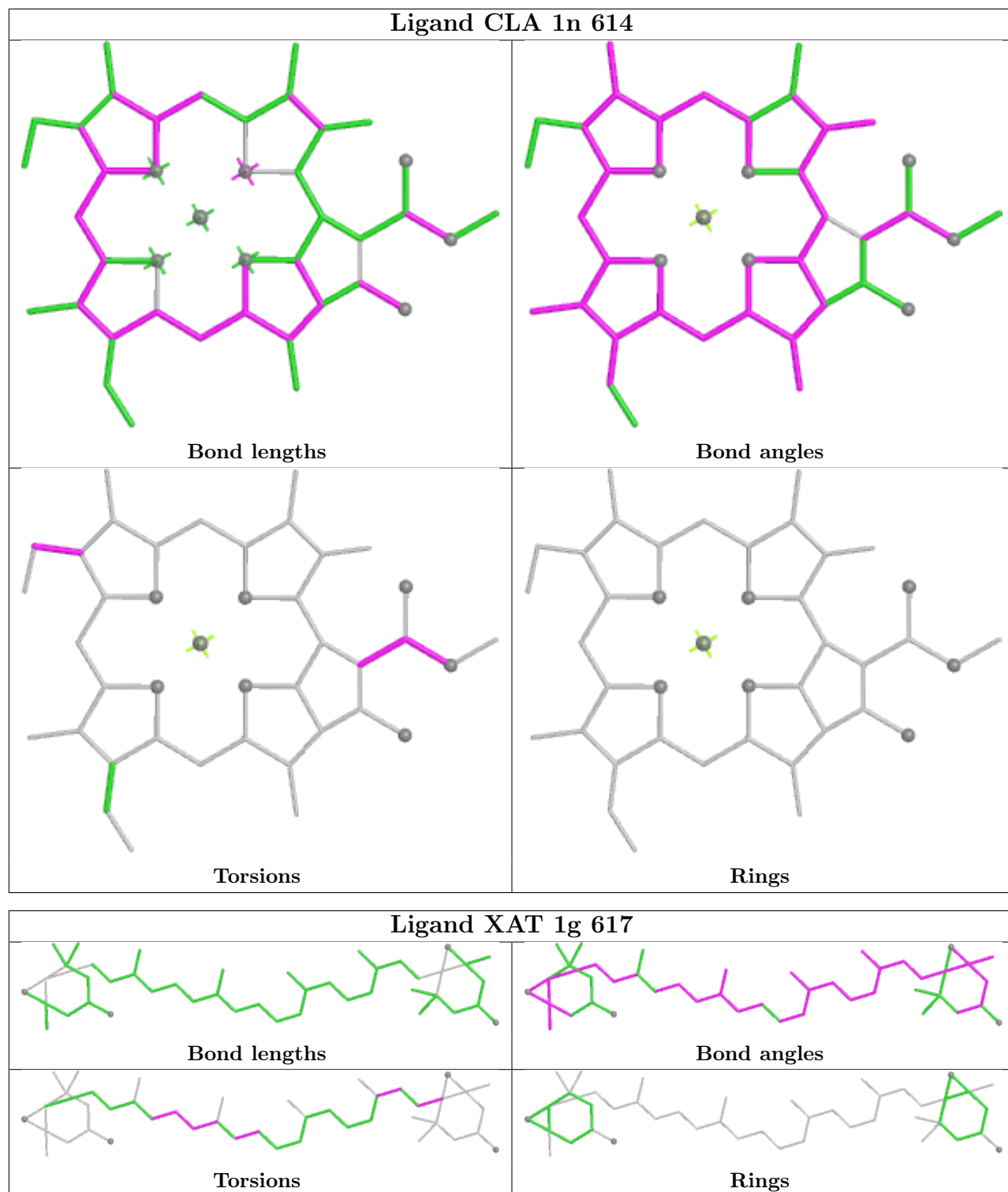


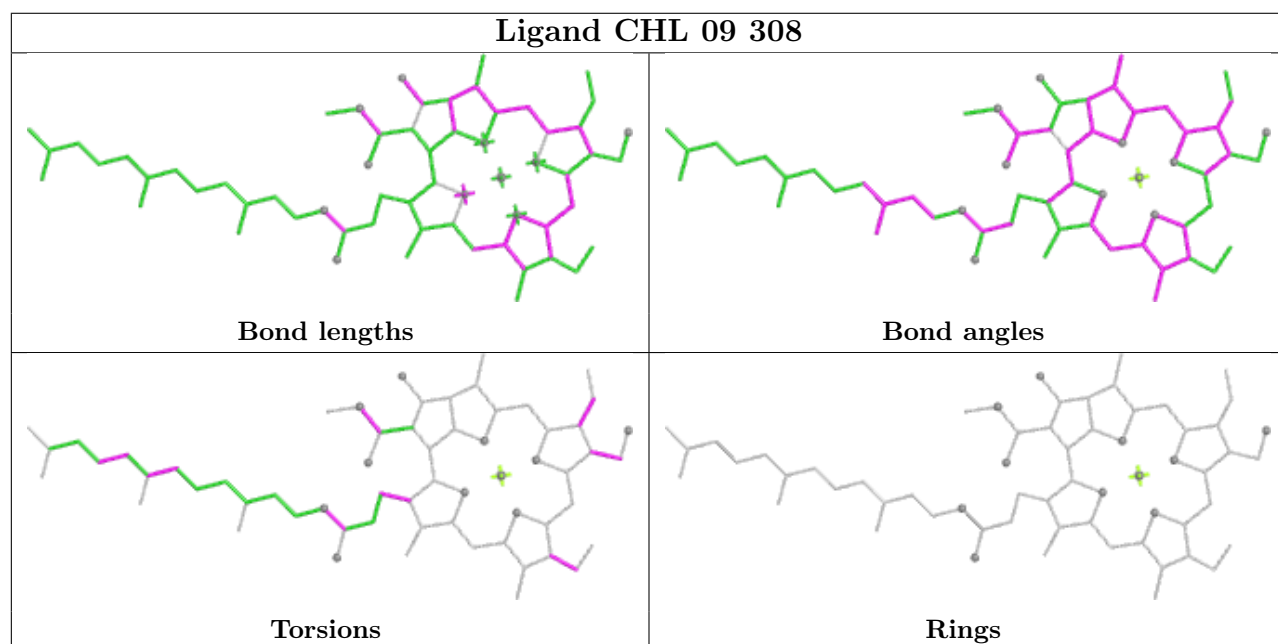
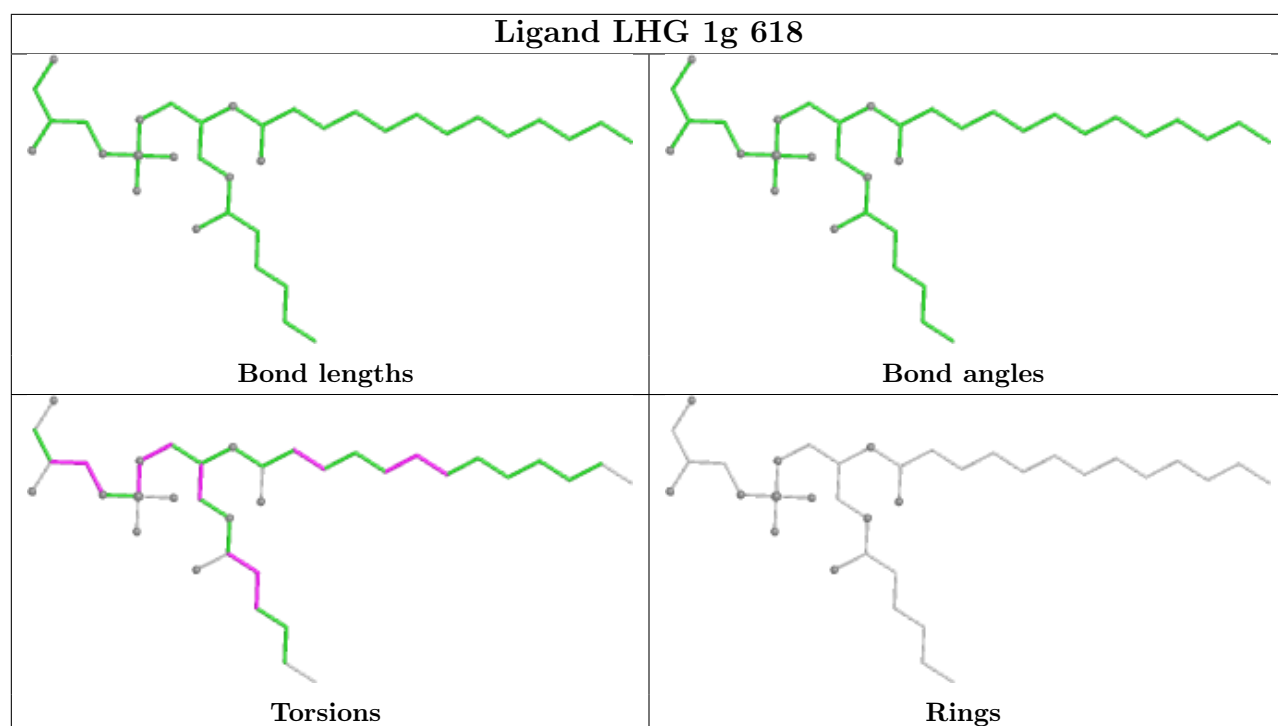


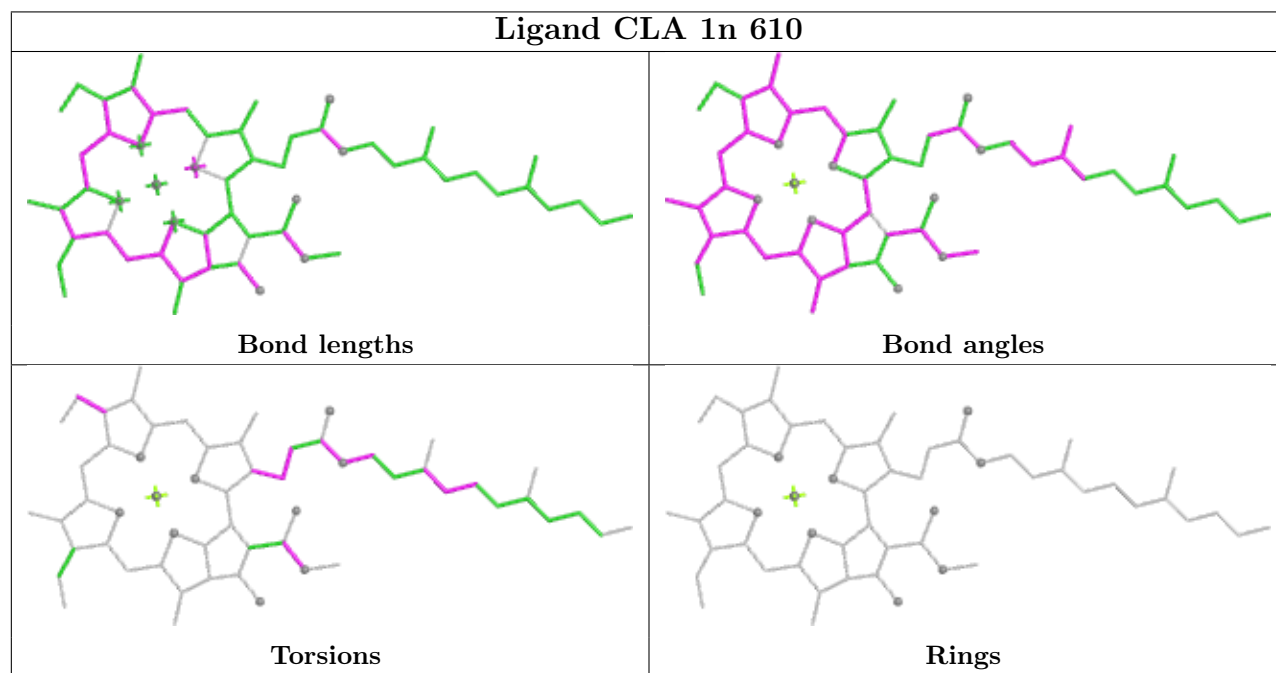
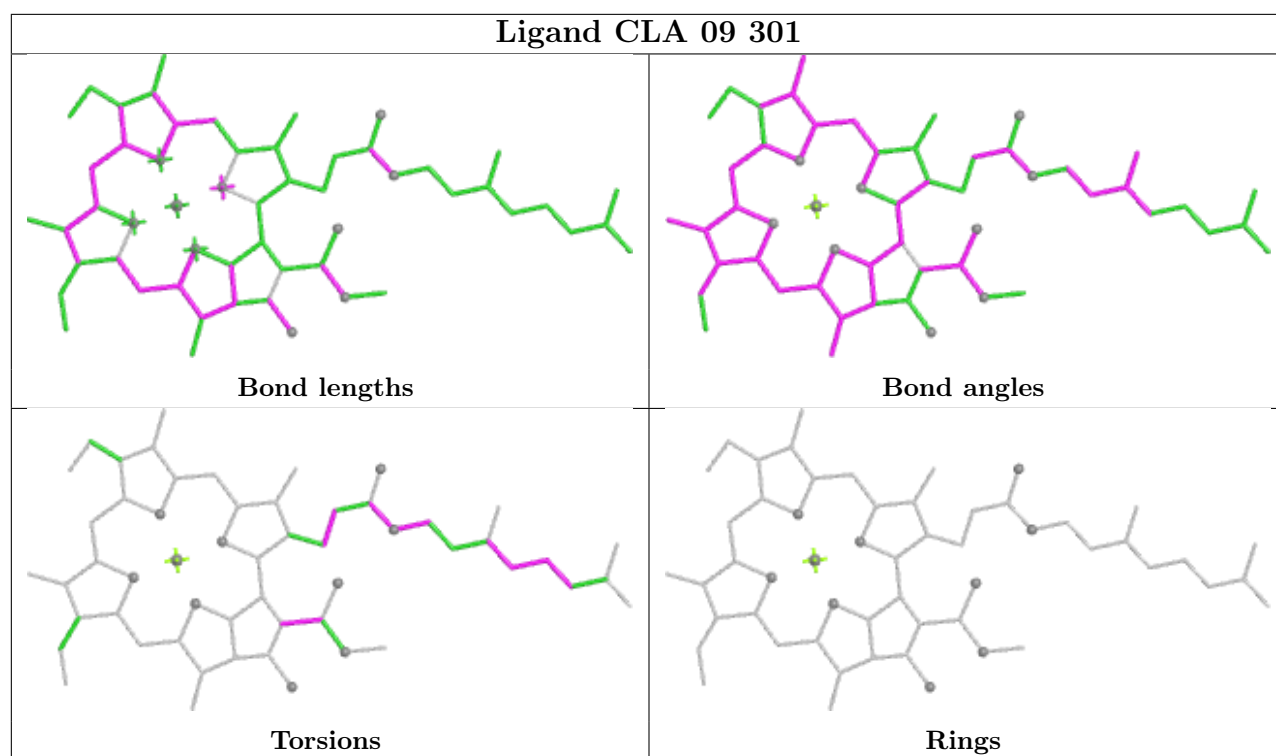


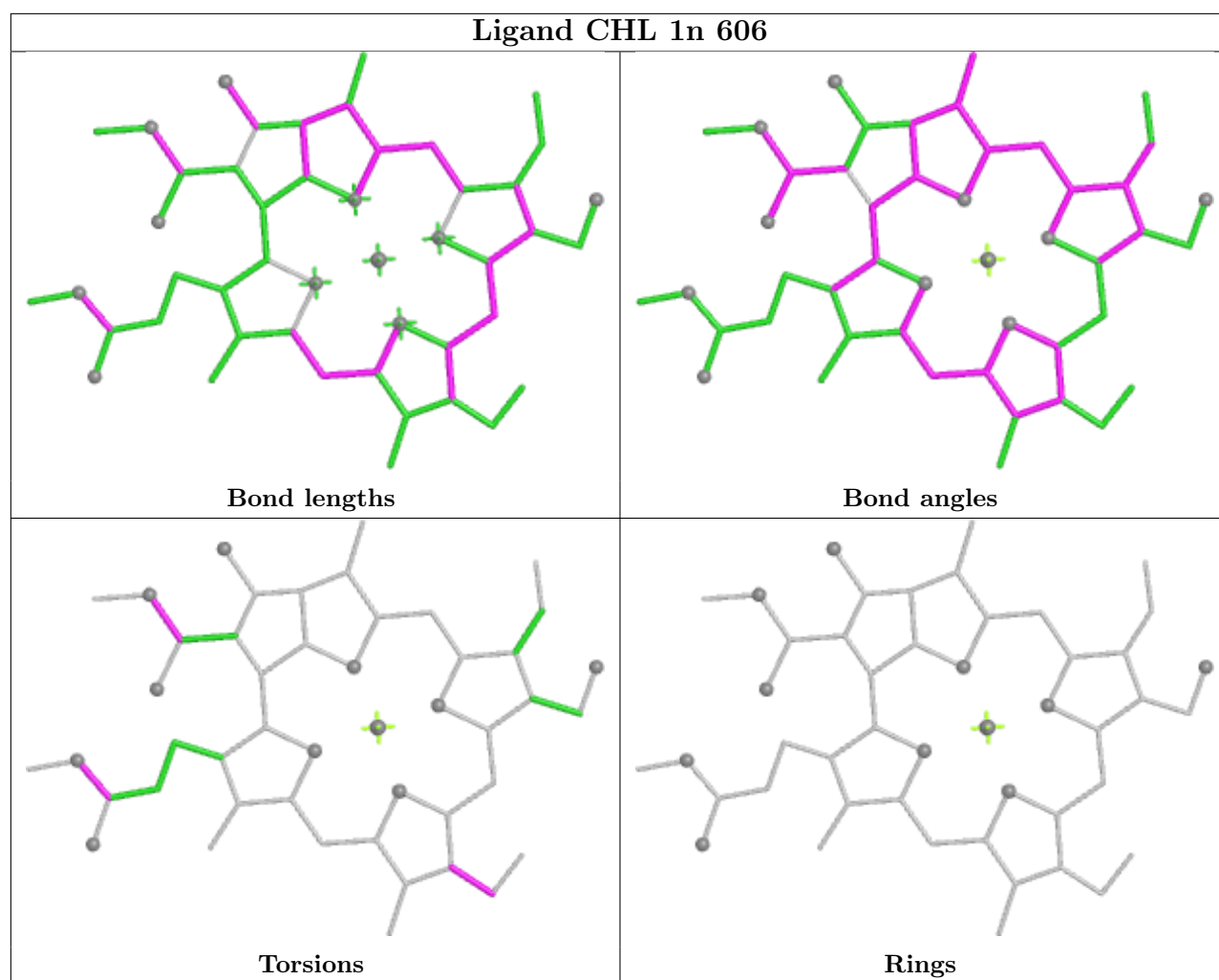


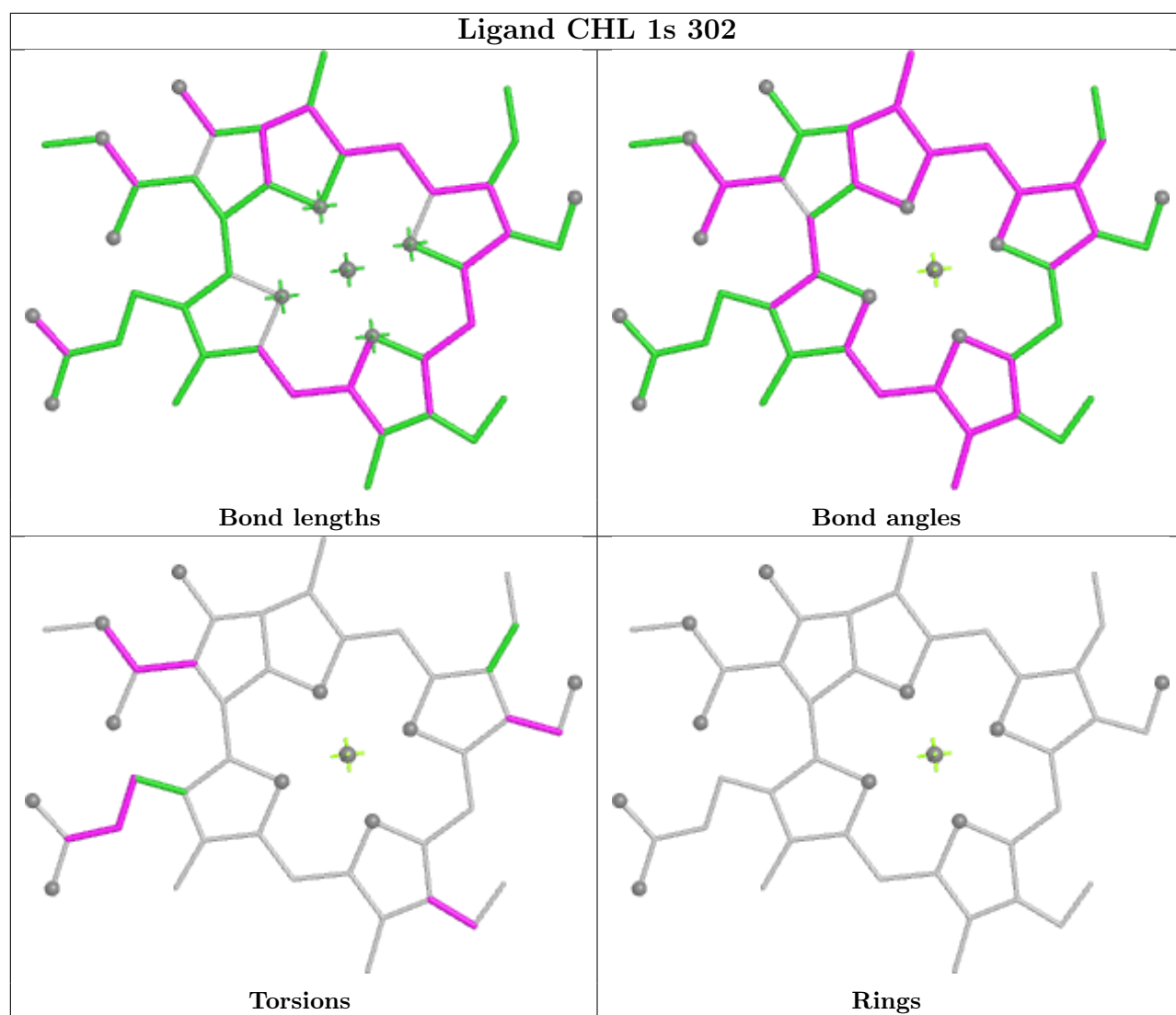


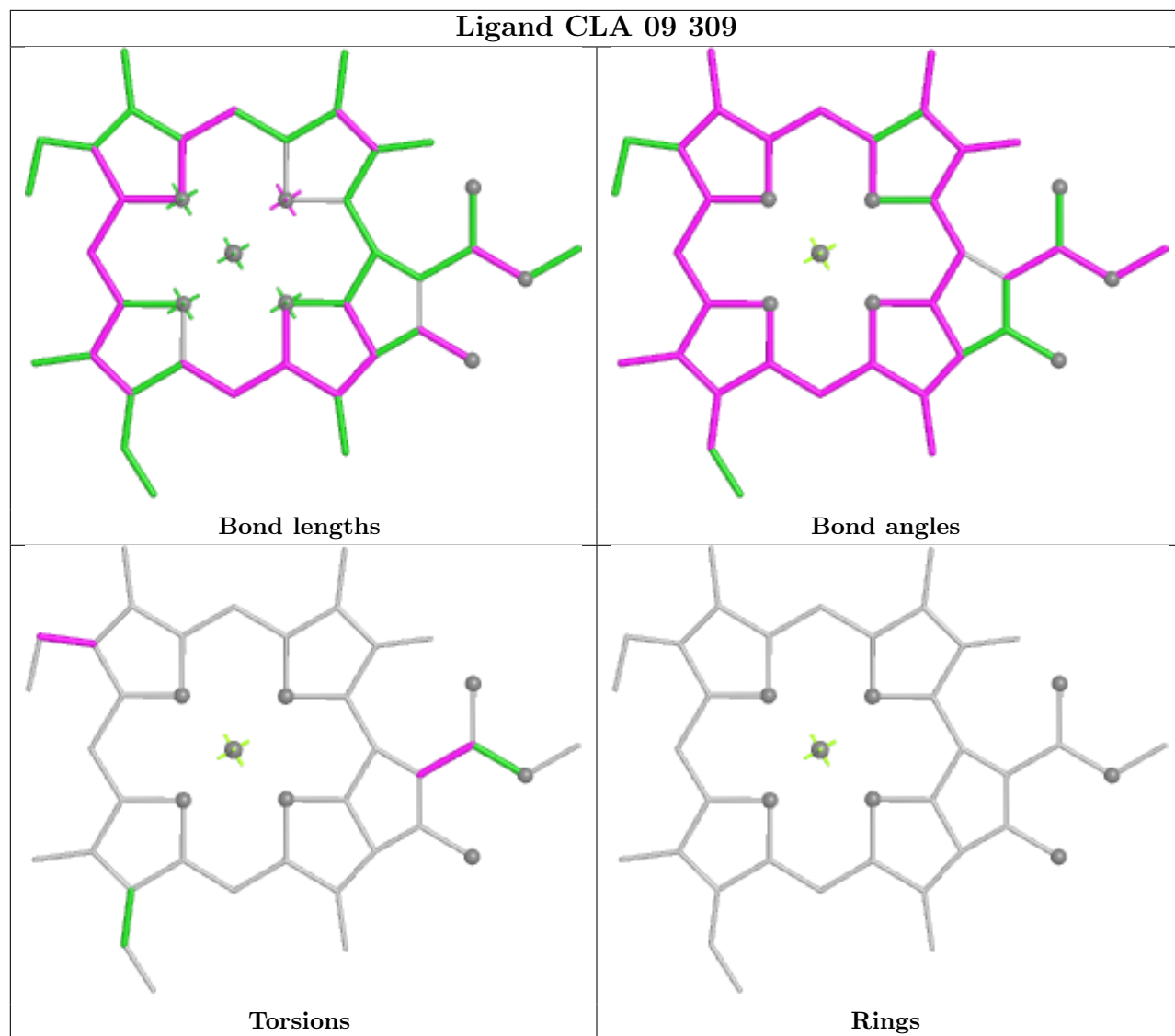


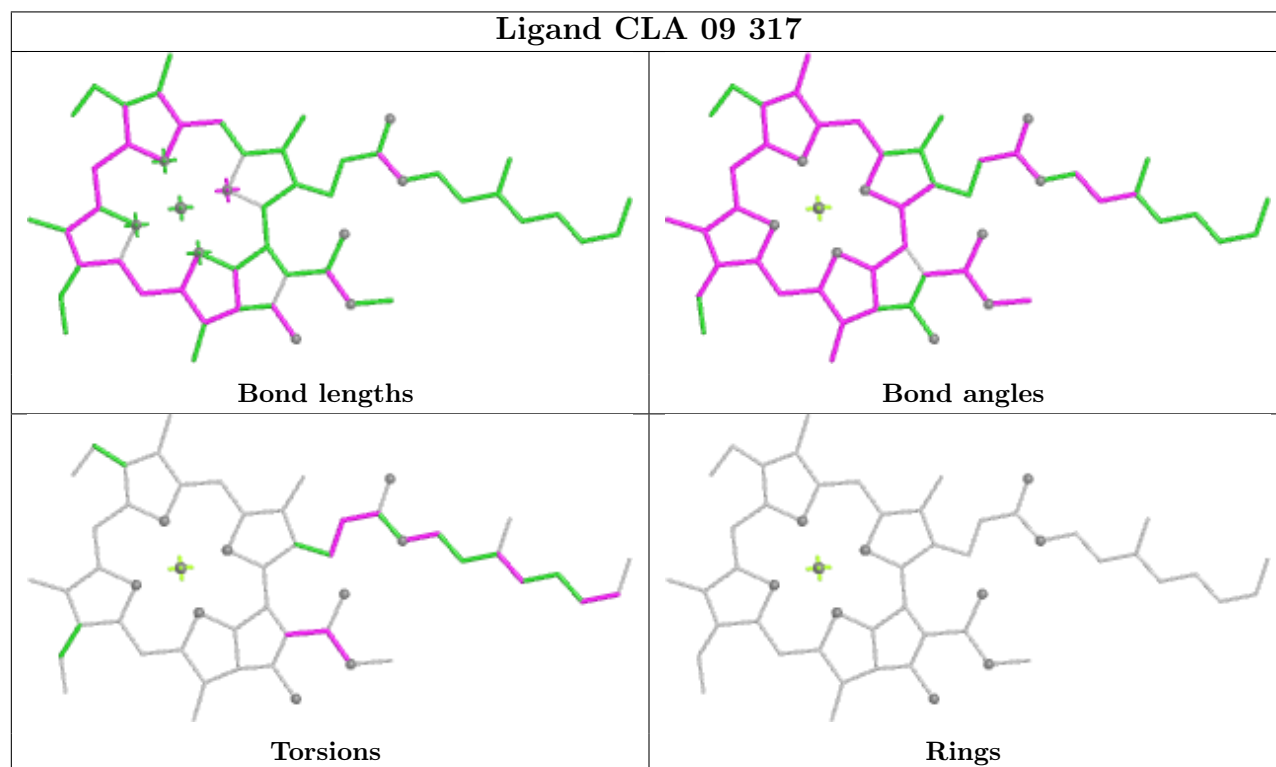
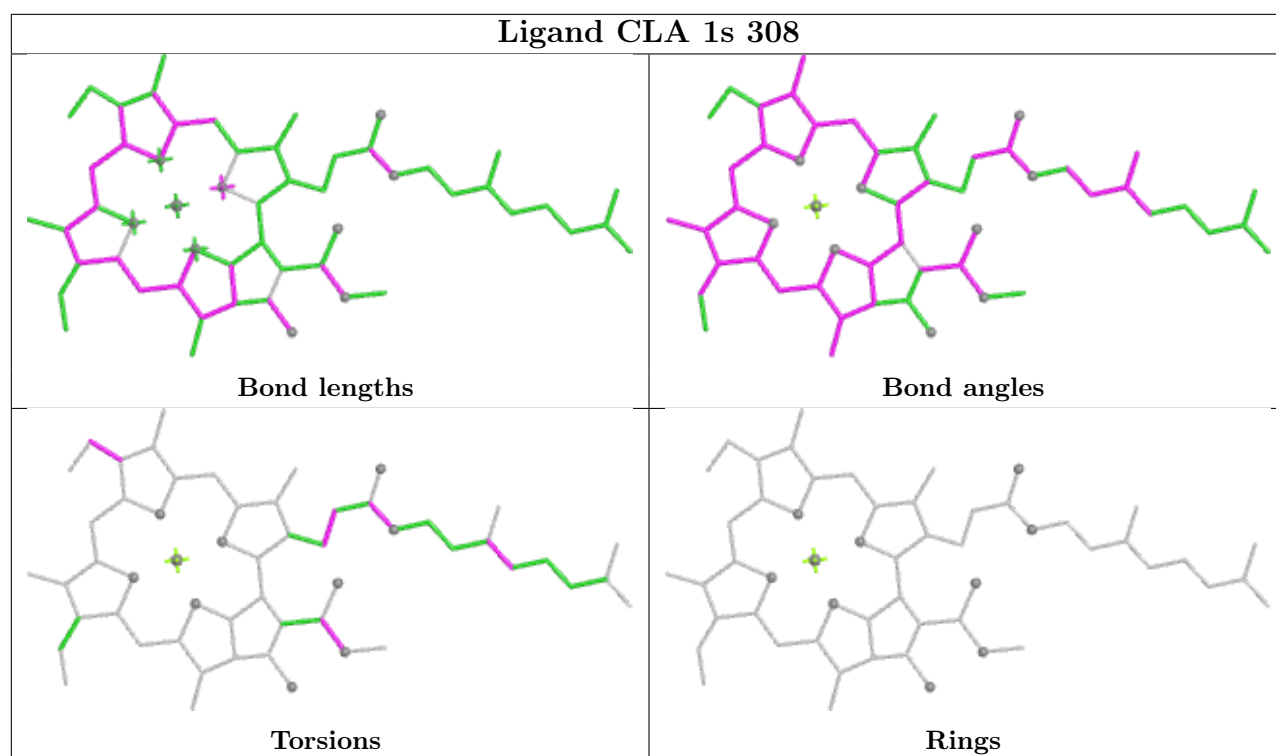


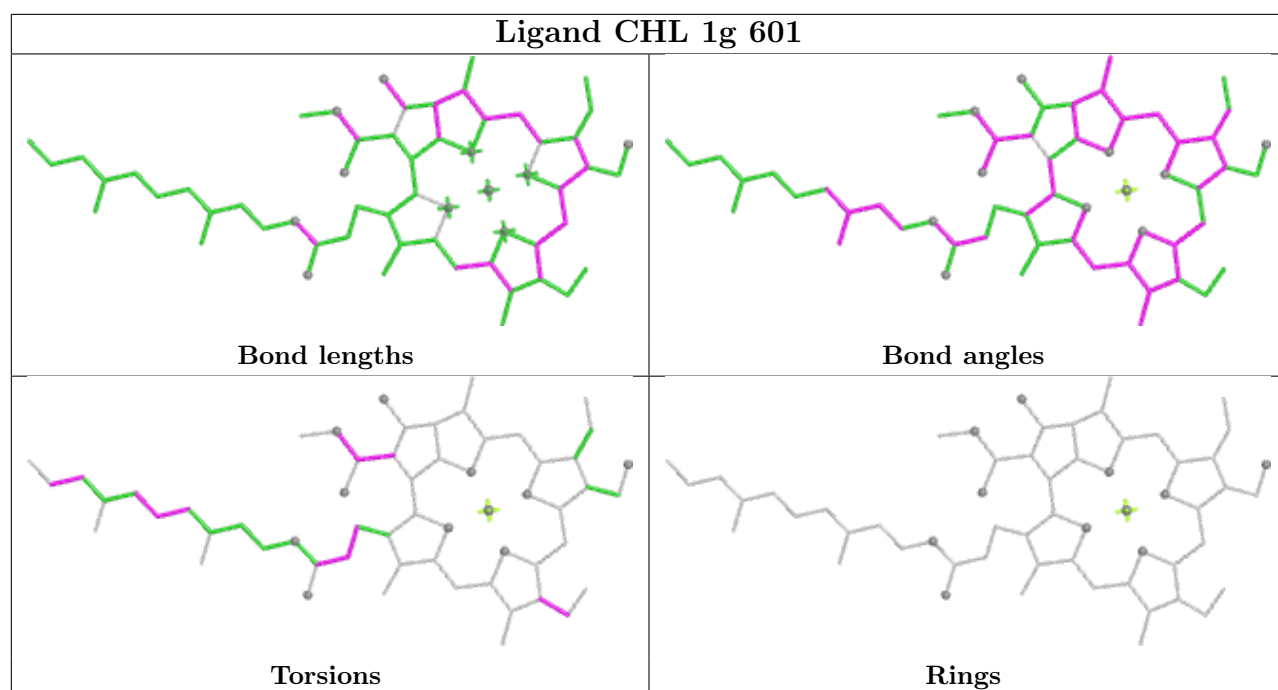


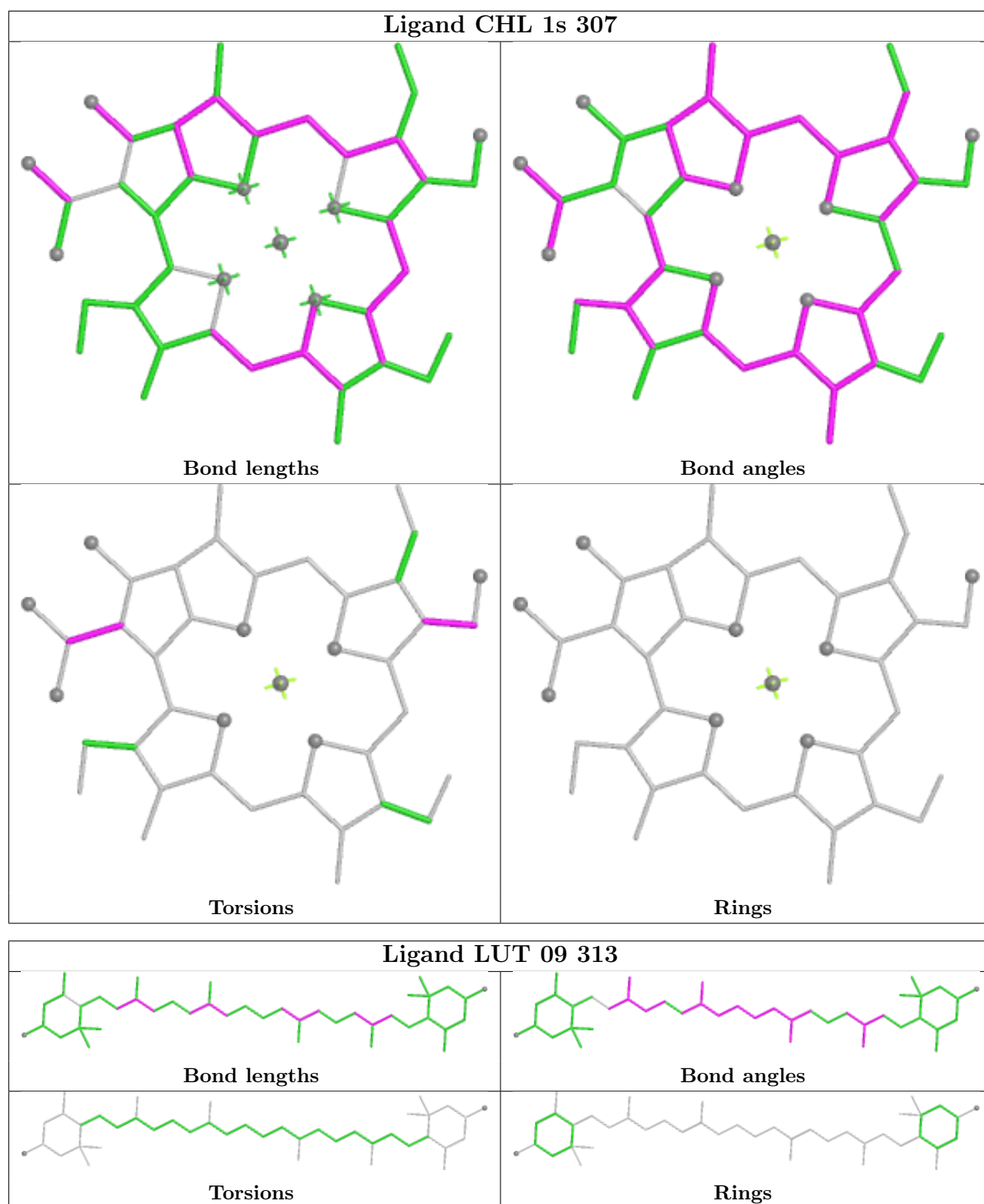


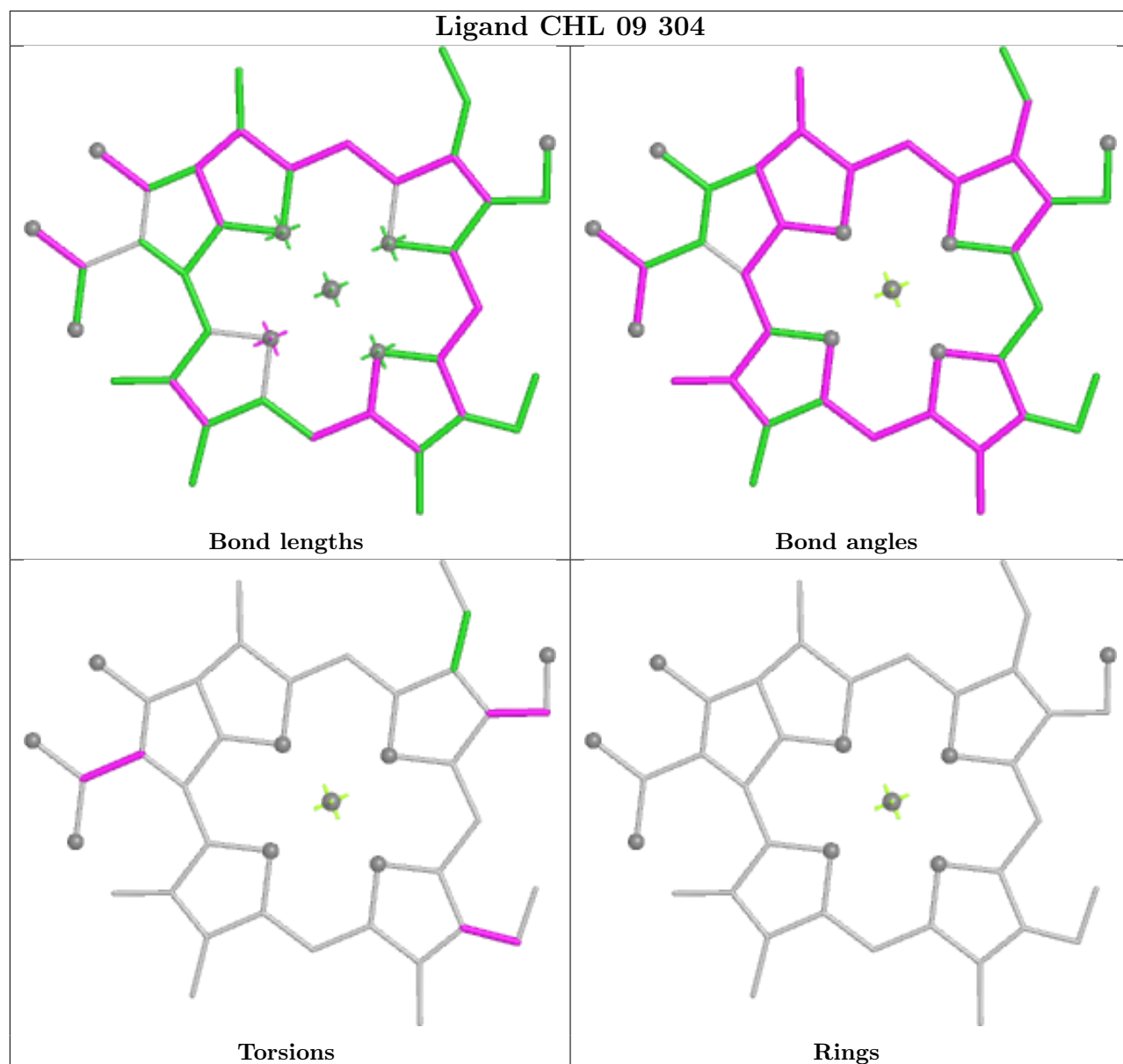
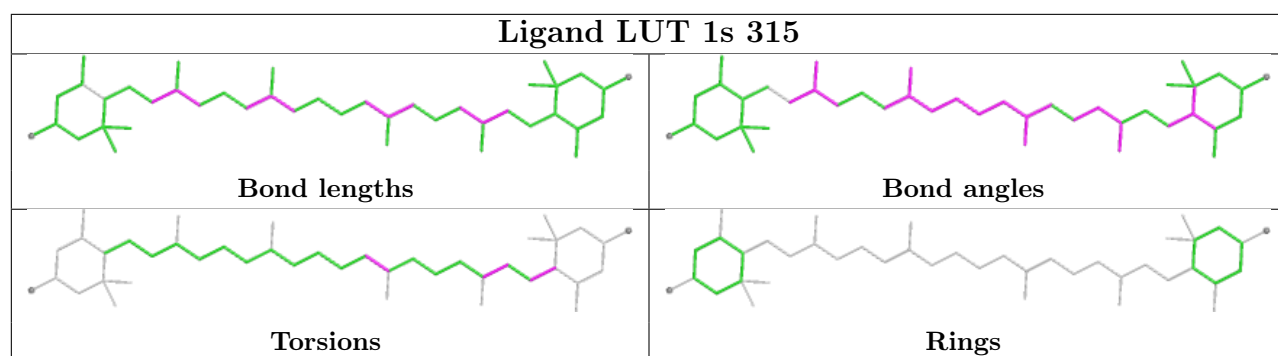


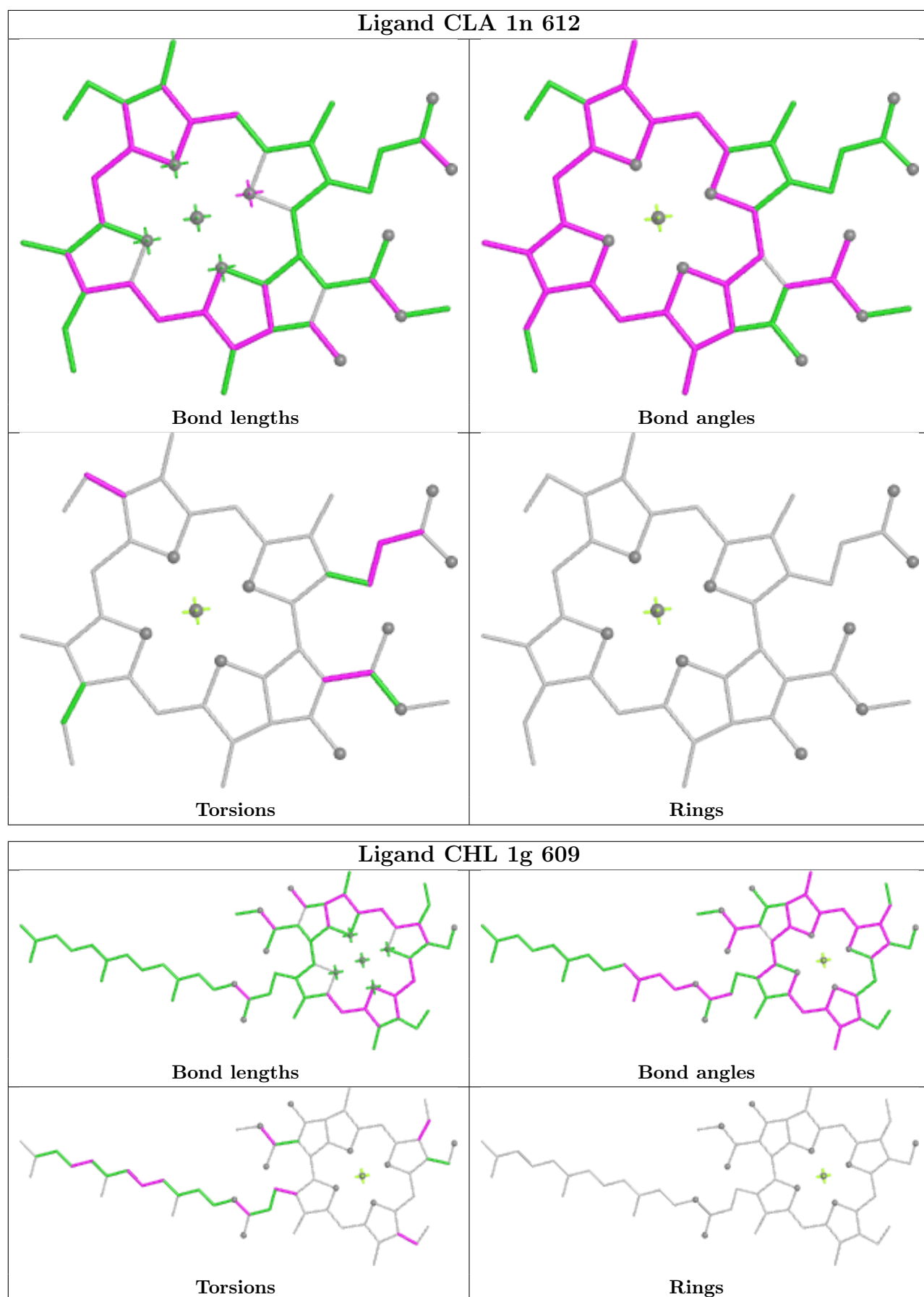


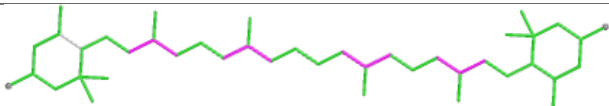
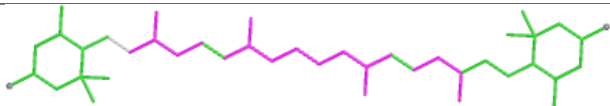
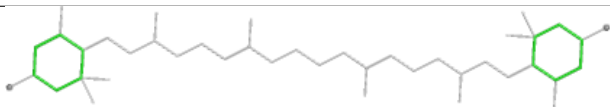


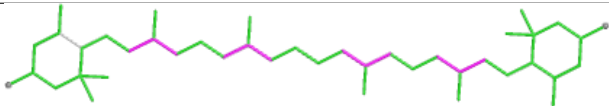
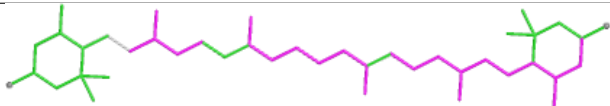
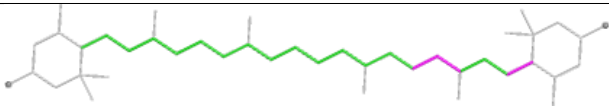
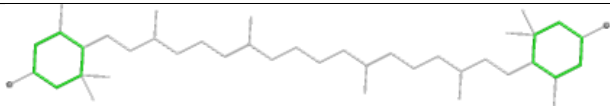


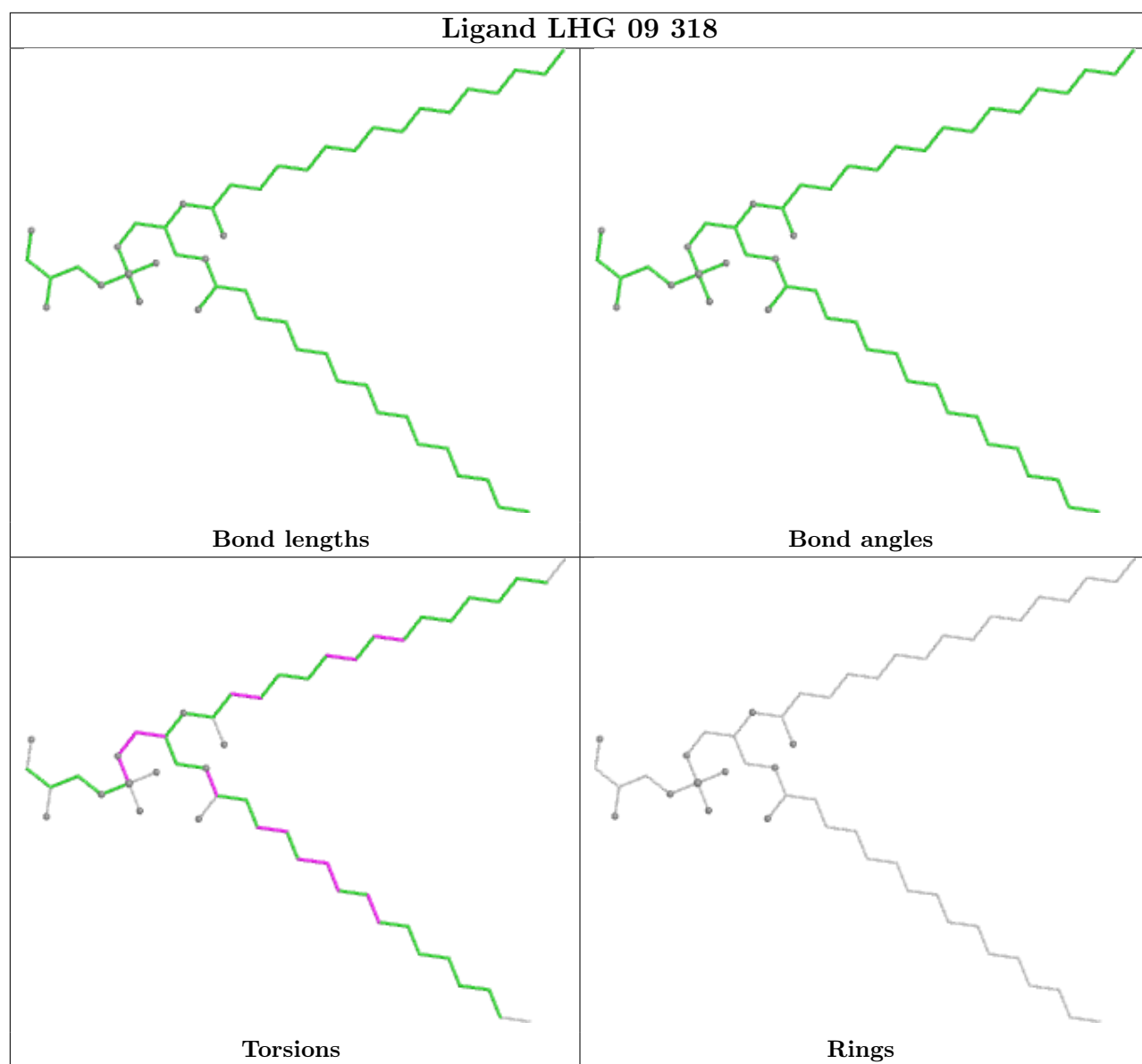


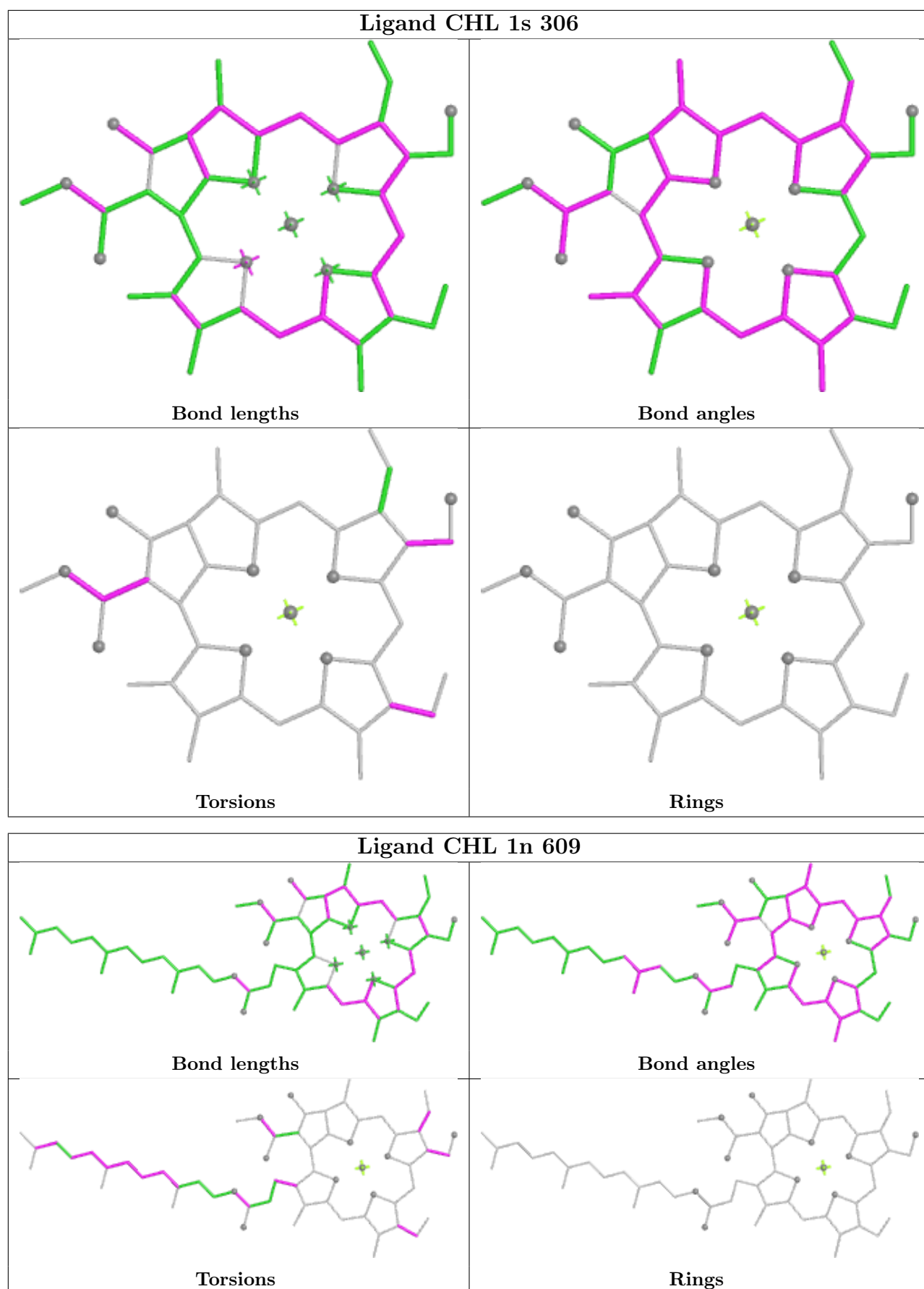


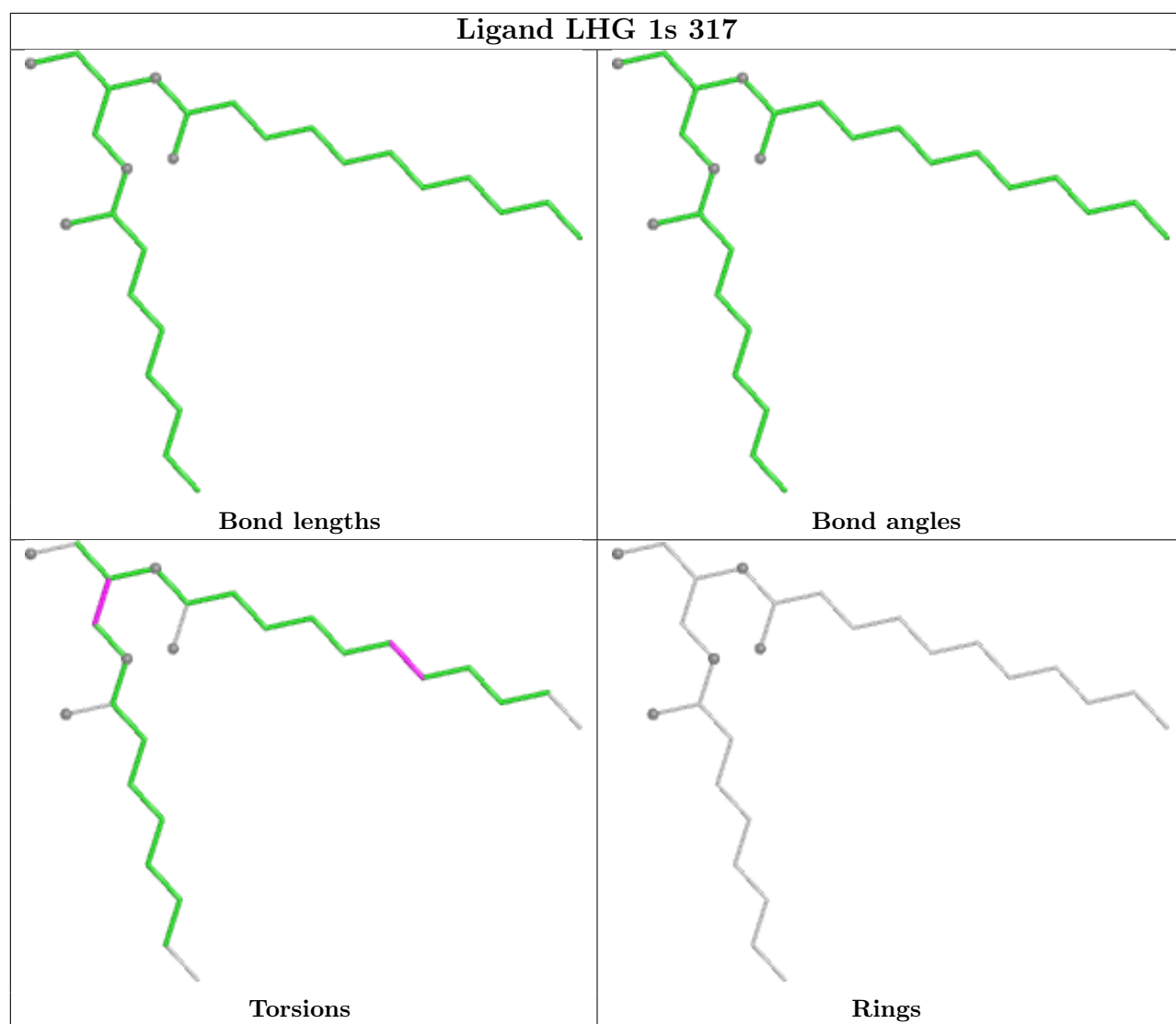


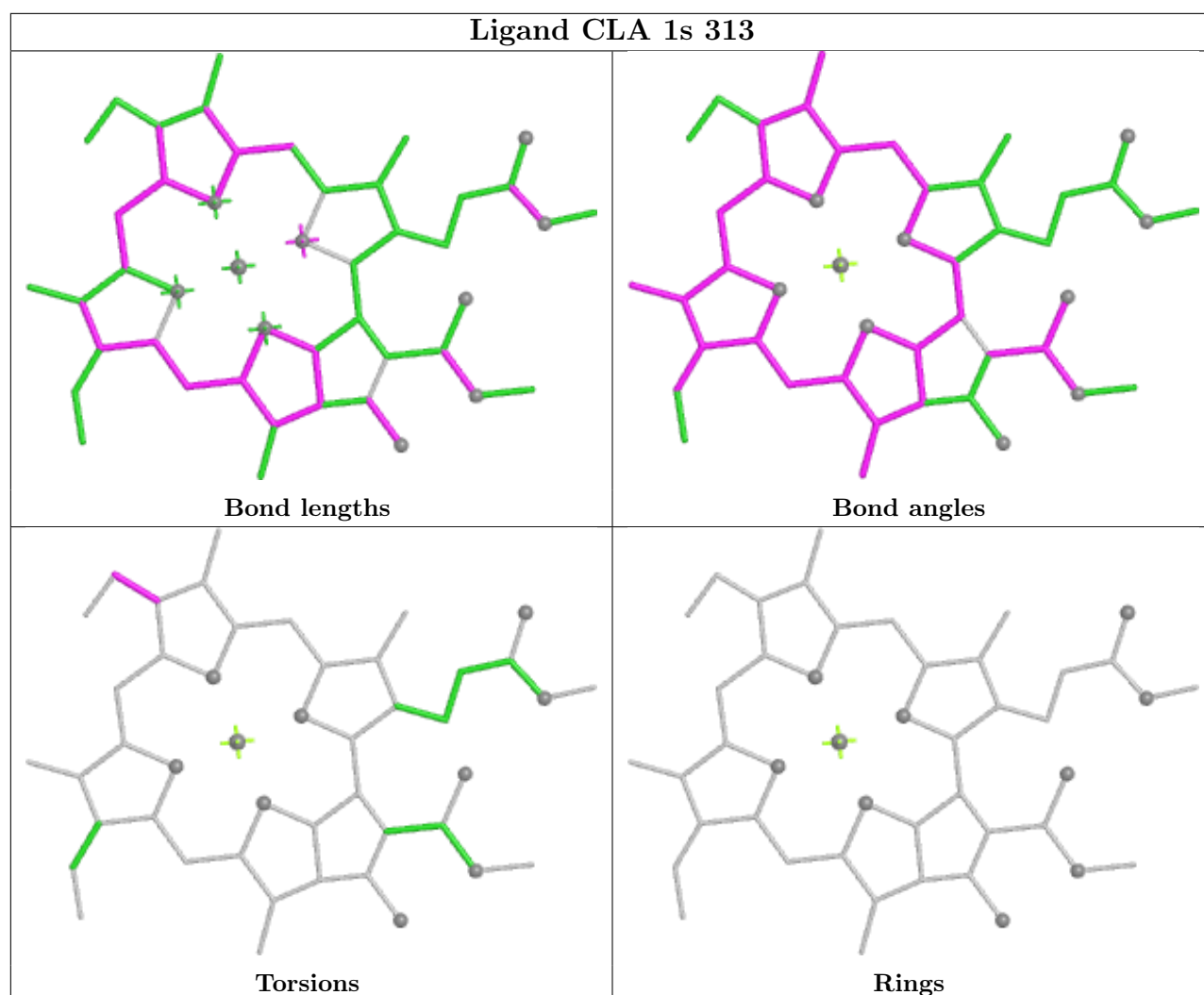
Ligand LUT 1g 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 1s 316	
	
Bond lengths	Bond angles
	
Torsions	Rings









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.

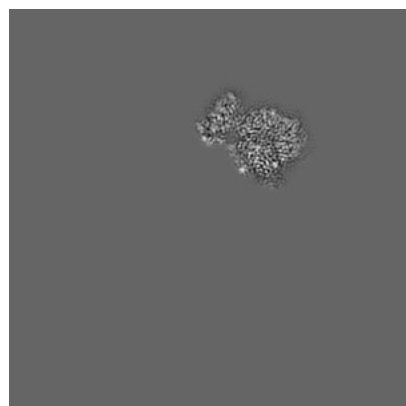
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66950. These allow visual inspection of the internal detail of the map and identification of artifacts.

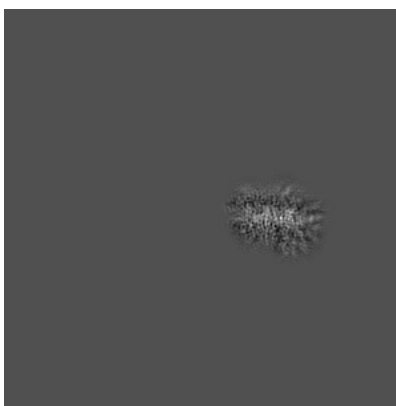
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

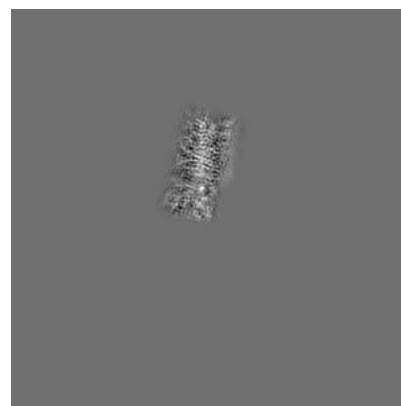
6.1.1 Primary map



X

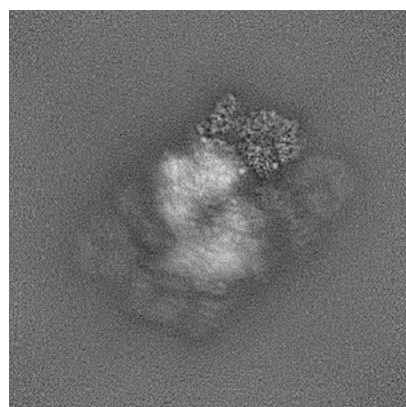


Y

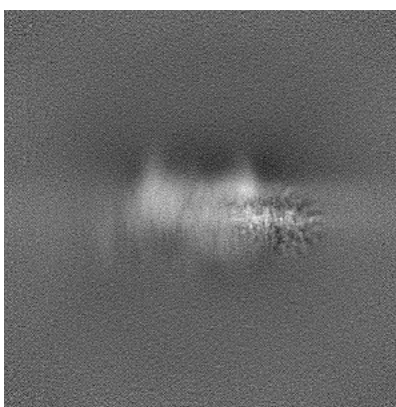


Z

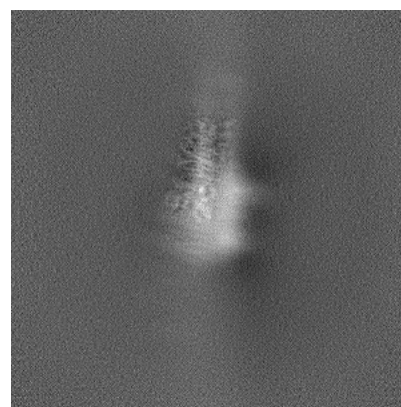
6.1.2 Raw map



X



Y

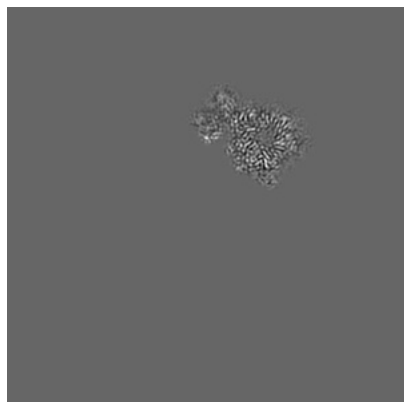


Z

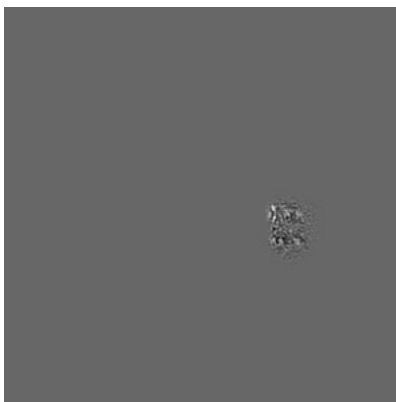
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

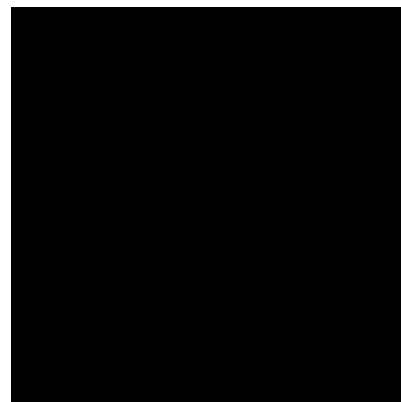
6.2.1 Primary map



X Index: 256

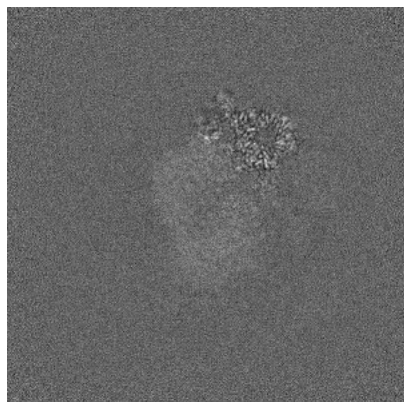


Y Index: 256



Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

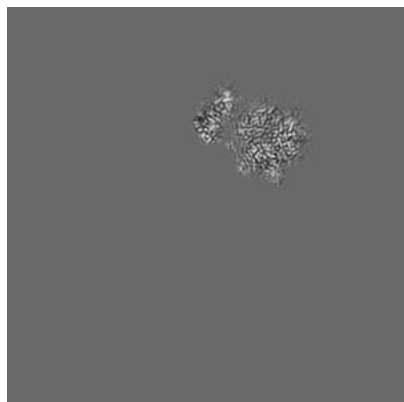


Z Index: 256

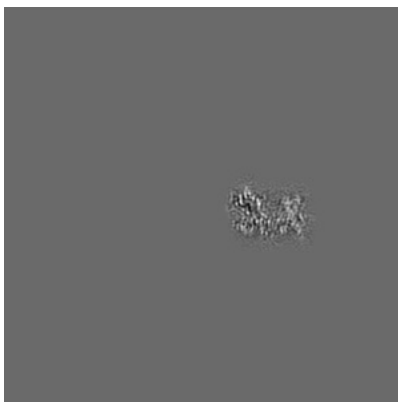
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

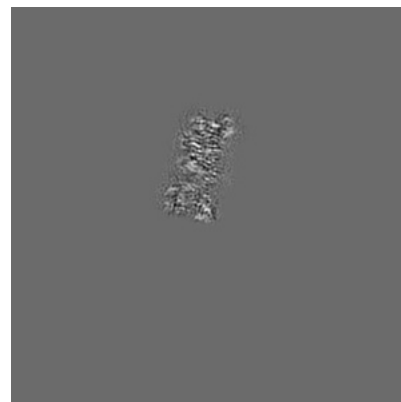
6.3.1 Primary map



X Index: 243

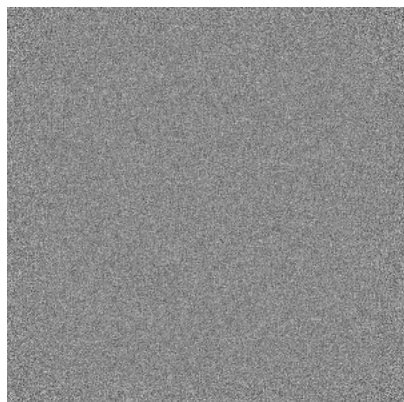


Y Index: 328

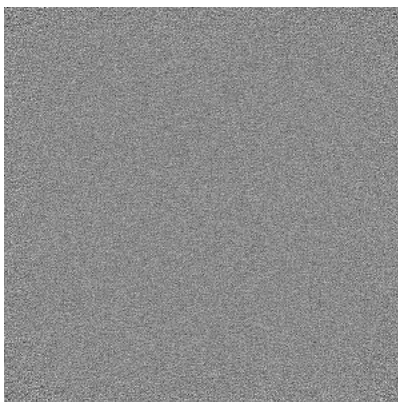


Z Index: 363

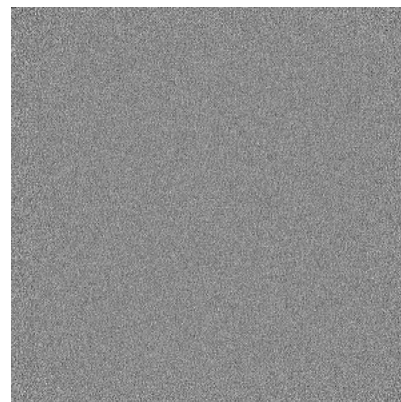
6.3.2 Raw map



X Index: 0



Y Index: 0

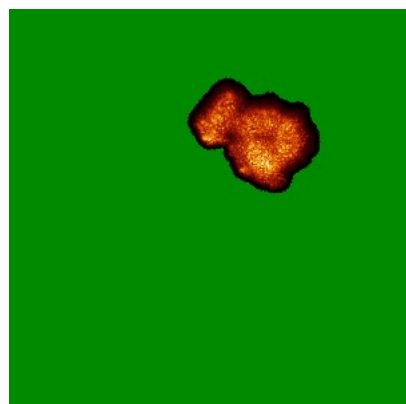


Z Index: 0

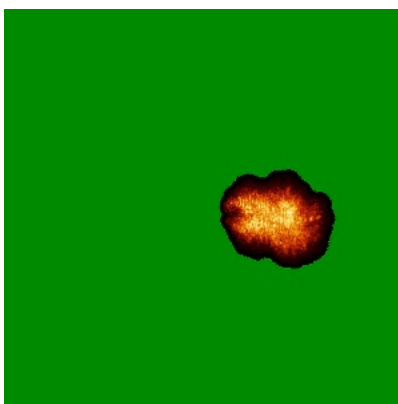
The images above show the largest variance slices of the map in three orthogonal directions.

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

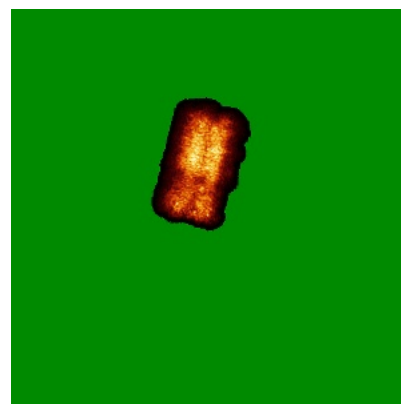
6.4.1 Primary map



X

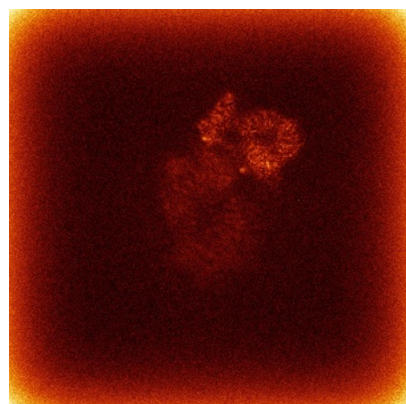


Y

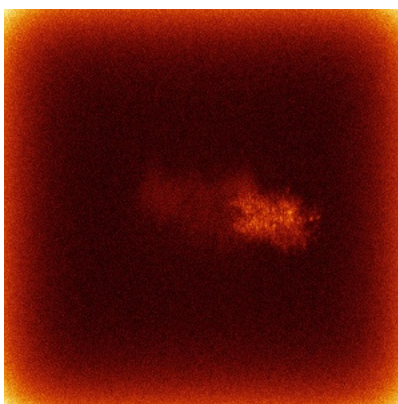


Z

6.4.2 Raw map



X



Y

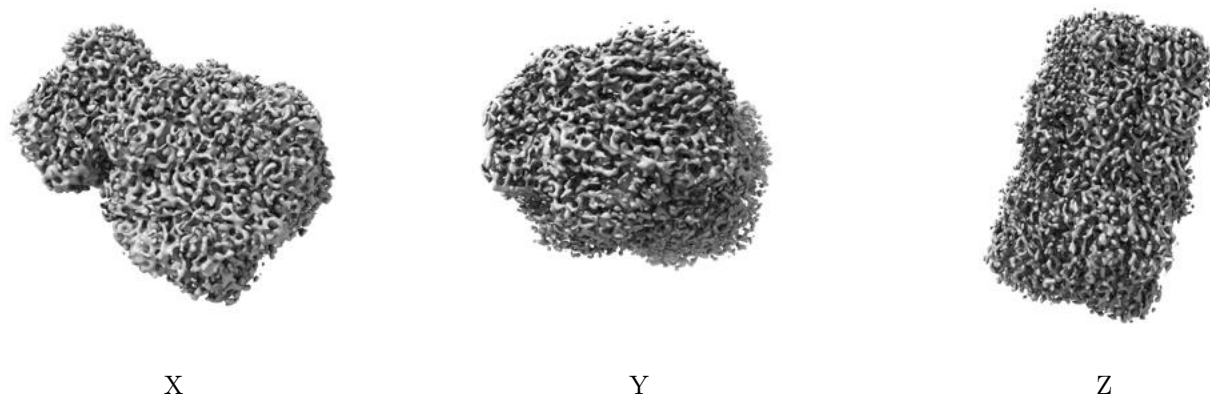


Z

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.

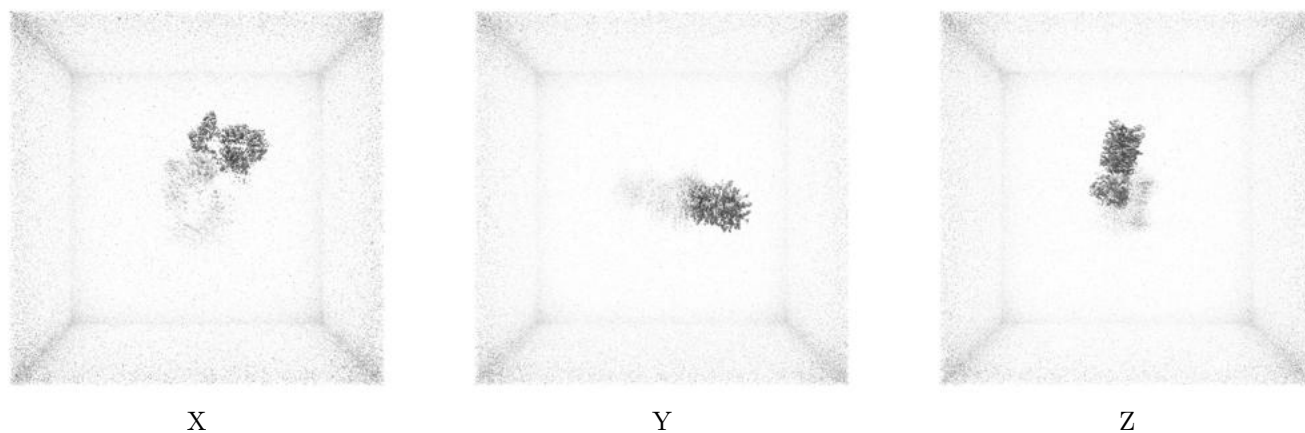
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

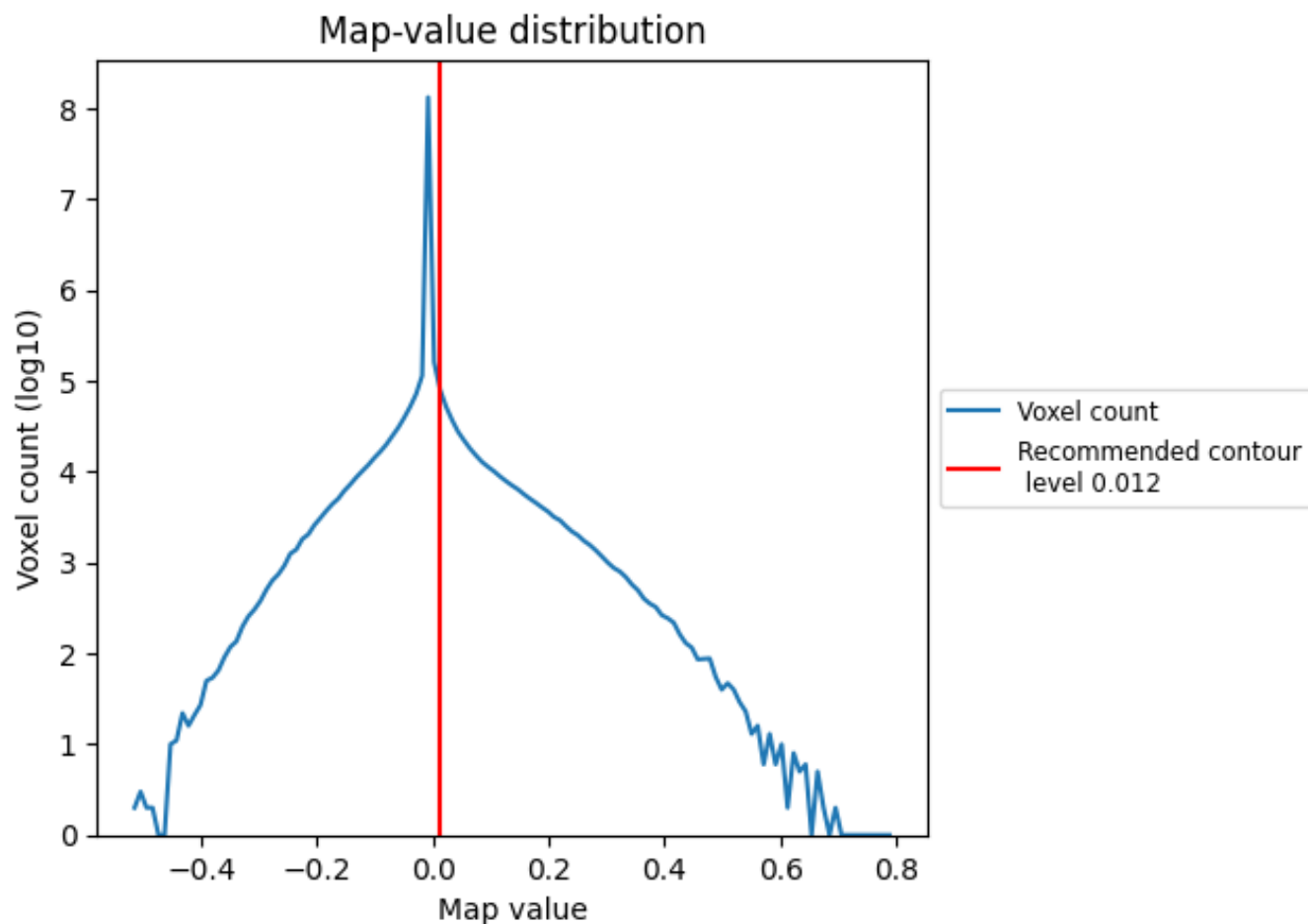
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

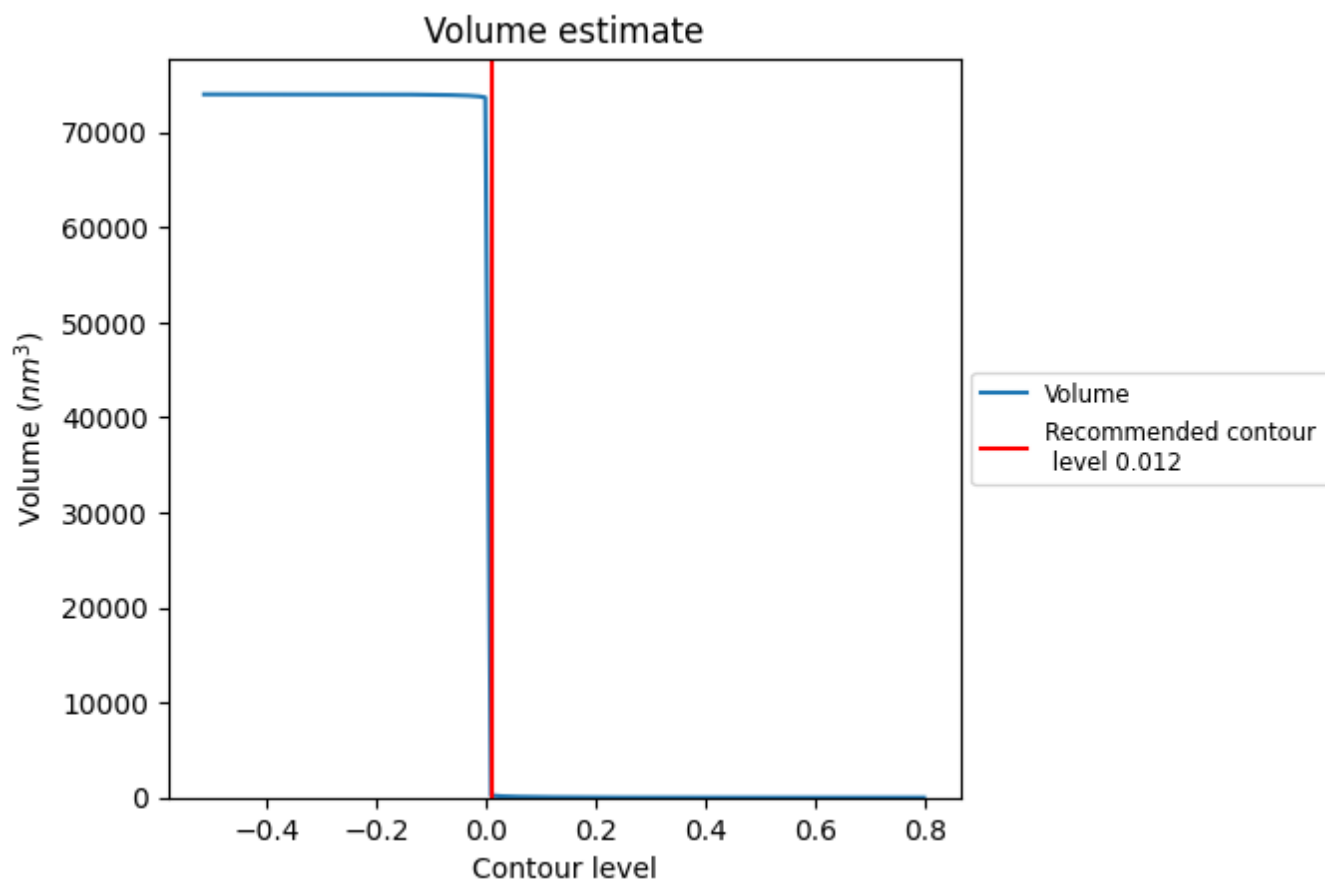
This section contains the results of statistical analysis of the map.

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.

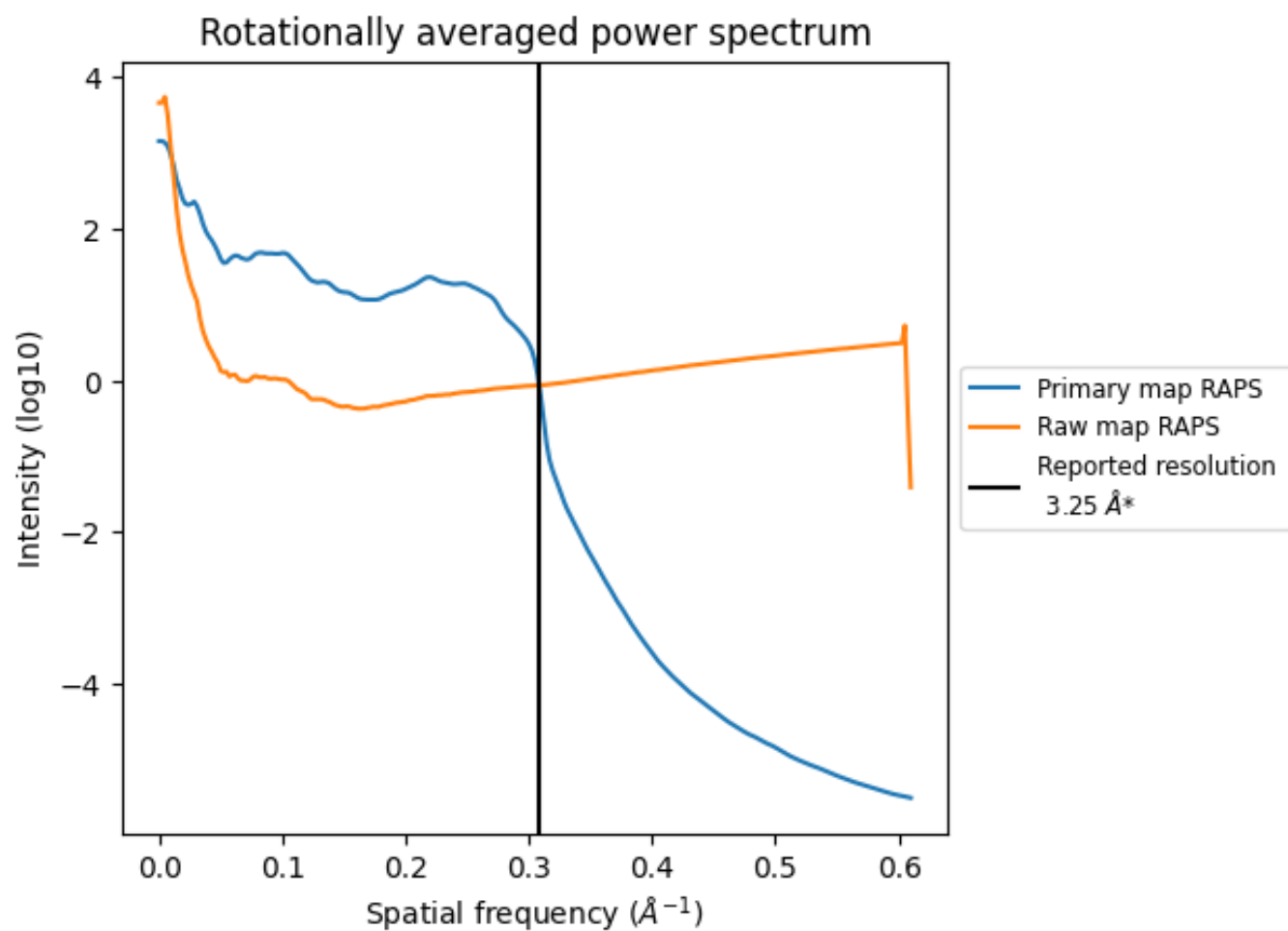
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 209 nm^3 ; this corresponds to an approximate mass of 189 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 ⓘ

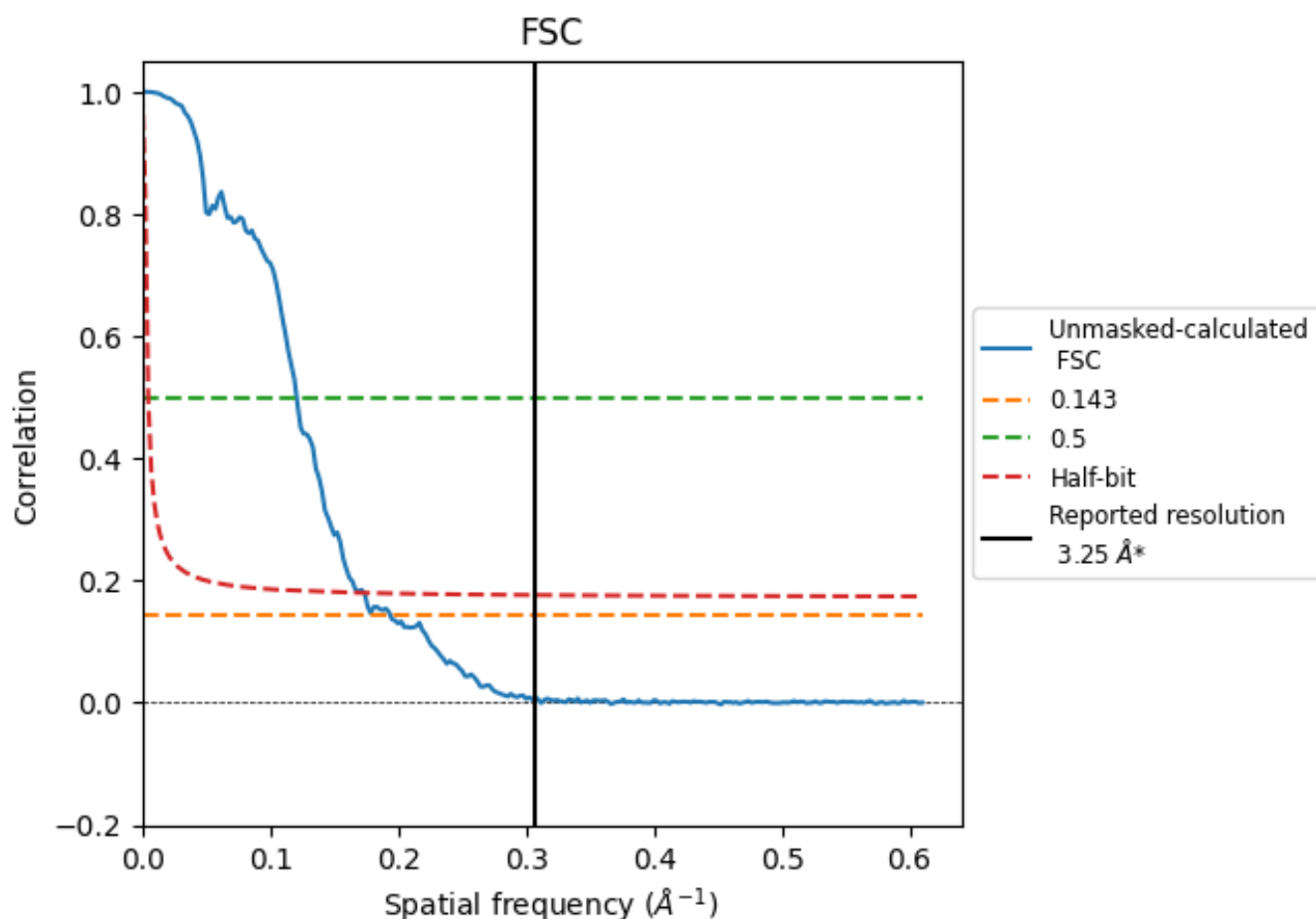


*Reported resolution corresponds to spatial frequency of $0.308 \text{ \AA}^{-1}$

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 0.308 Å⁻¹

8.2 Resolution estimates [i](#)

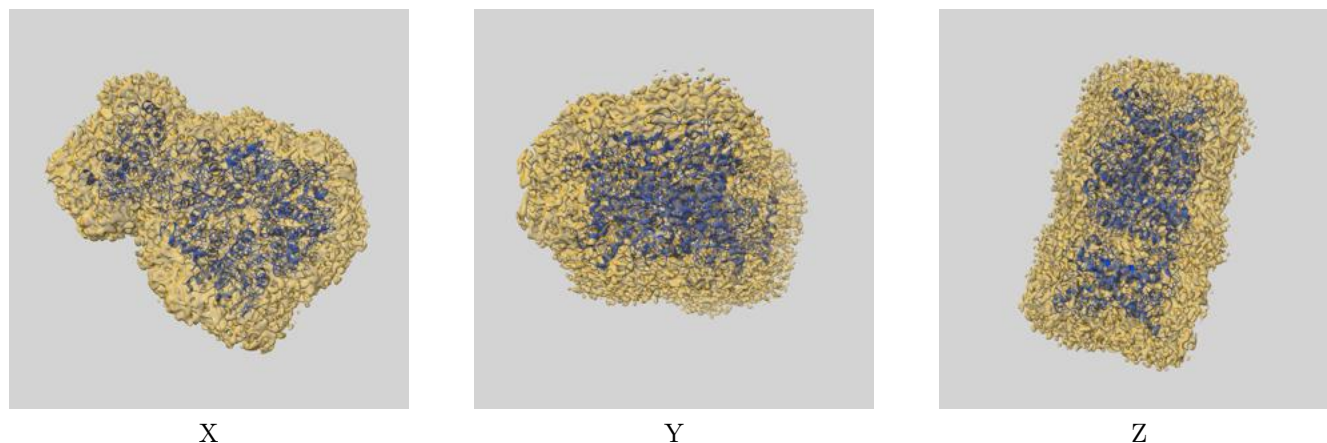
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.15	8.29	5.76

*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 5.15 differs from the reported value 3.25 by more than 10 %

9 Map-model fit [i](#)

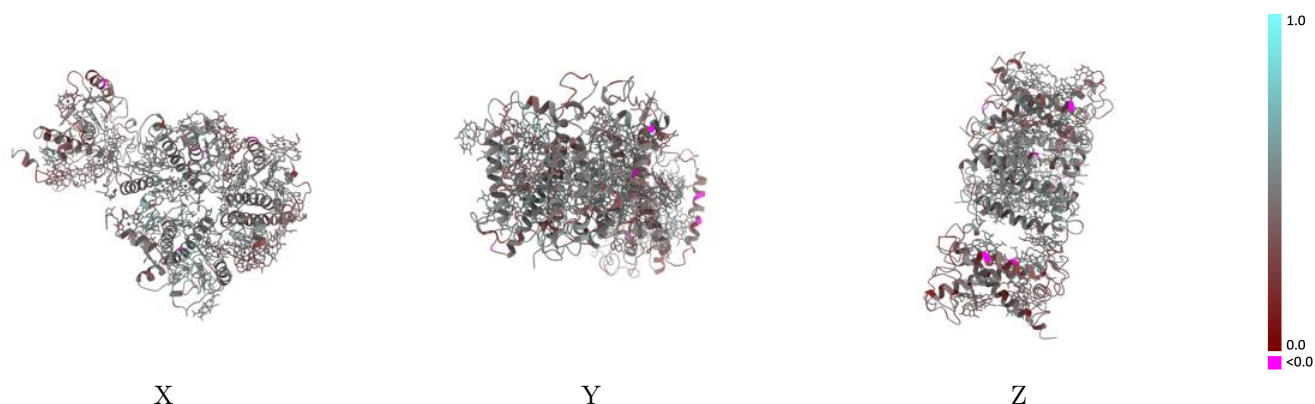
This section contains information regarding the fit between EMDB map EMD-66950 and PDB model 9XK7. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



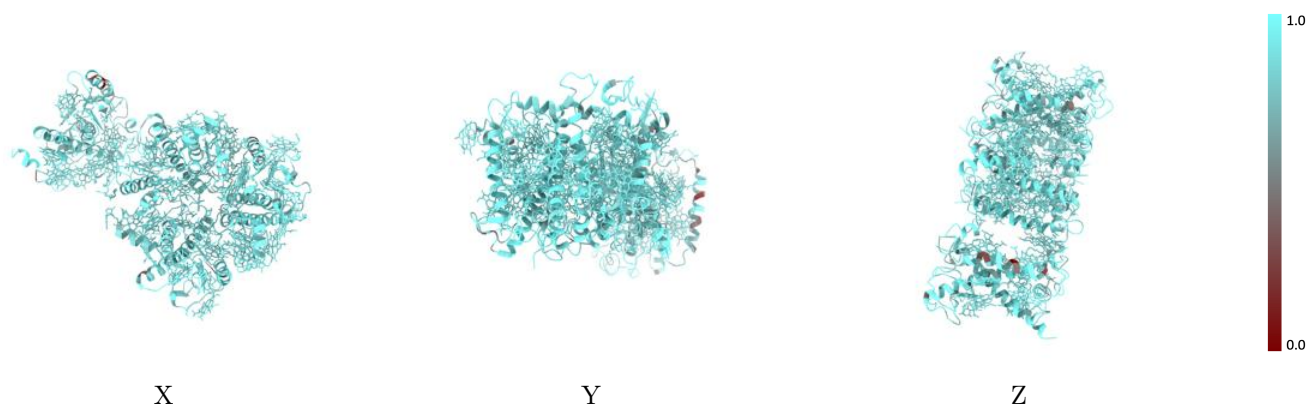
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



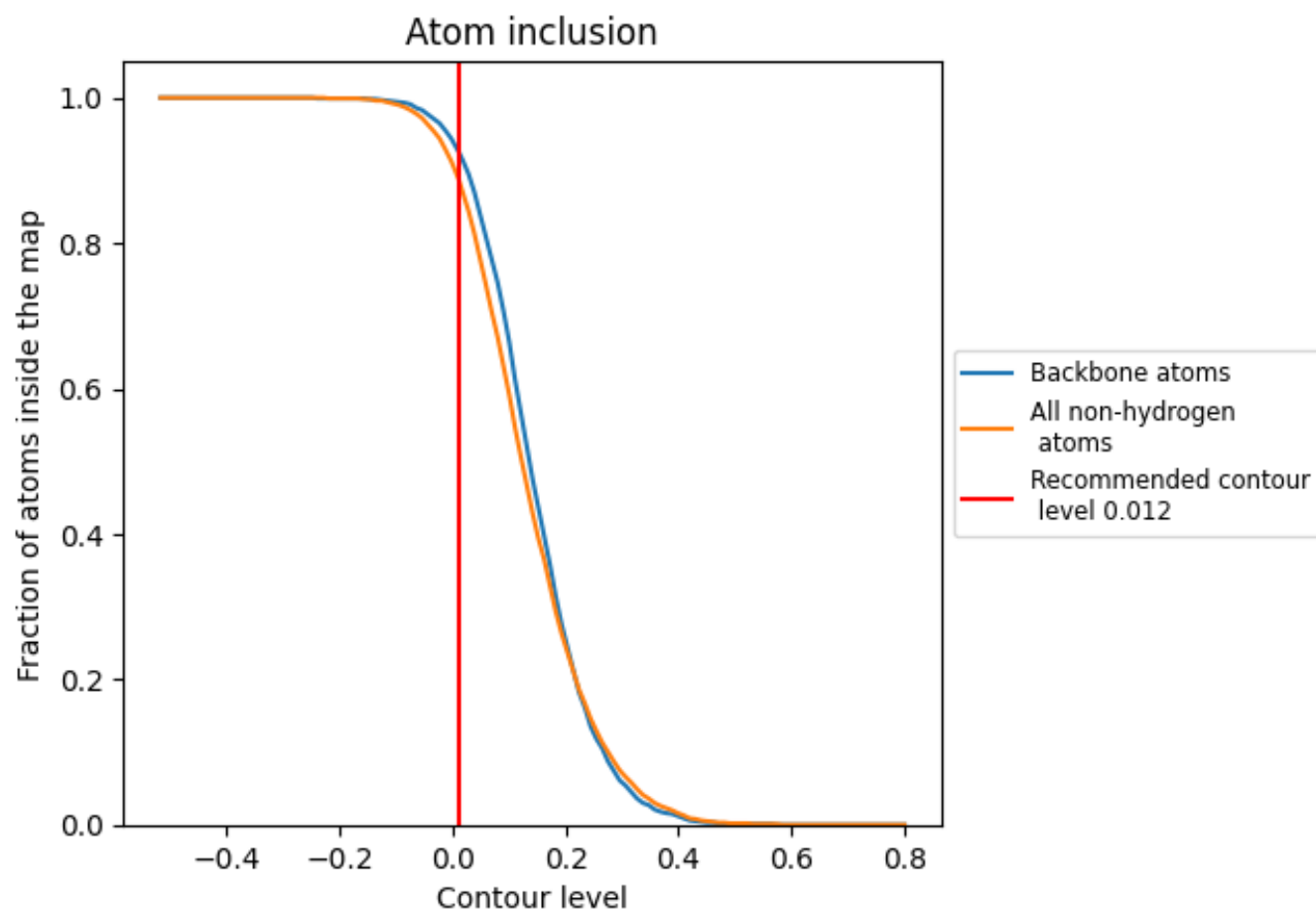
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% 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	0.8870	0.4330
09	0.9050	0.4690
1g	0.8910	0.4310
1n	0.8920	0.4410
1s	0.8570	0.3890

