



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2026 – 12:31 PM JST

PDB ID : 9XK9 / pdb_00009xk9
EMDB ID : EMD-66952
Title : In situ C2S2M2L4-type PSII-LHCII supercomplex, moderately bound (M-) LHCII trimer with CP29 and CP24, protomer 2
Authors : Li, J.; Elias, E.; Zhang, K.; Croce, R.; Zhu, J.
Deposited on : 2025-11-05
Resolution : 3.64 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

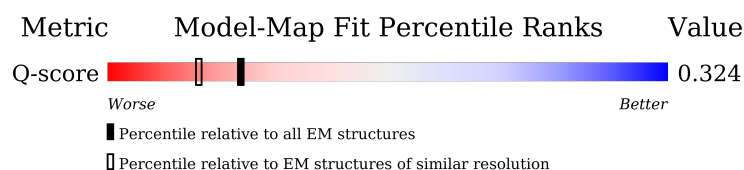
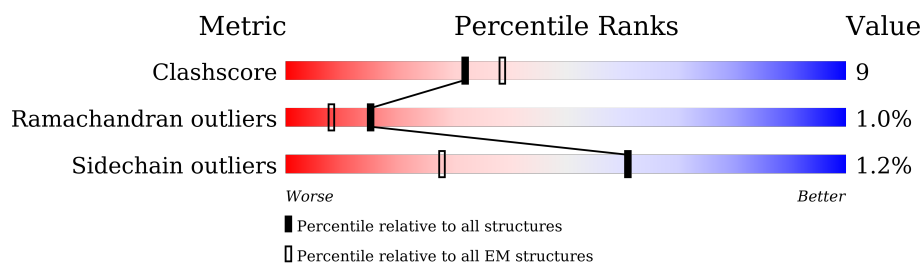
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.64 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	11633 (3.14 - 4.14)

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	05	219	11% 77% 18% 5%
1	06	219	7% 78% 16% 5%
2	07	220	6% 81% 18% 5%
3	08	205	6% 78% 21% 5%

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Mol	Chain	Length	Quality of chain
4	1r	234	 80%19%

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
5	CLA	06	602	X	-	-	-
5	CLA	1r	306	X	-	-	-
6	CHL	05	305	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10982 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	05	210	Total	C	N	O	S	0	0
			1555	1003	258	289	5		
1	06	207	Total	C	N	O	S	0	0
			1450	927	242	276	5		

- Molecule 2 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	07	220	Total	C	N	O	S	0	0
			1648	1070	273	300	5		

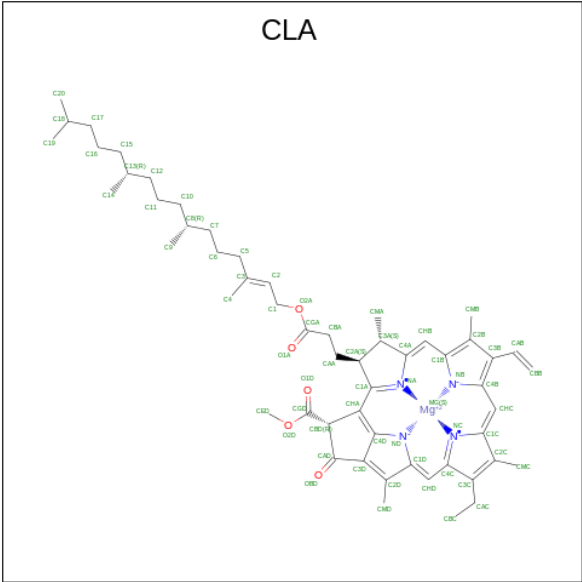
- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	08	205	Total	C	N	O	S	0	0
			1570	1029	255	282	4		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1r	234	Total	C	N	O	S	0	0
			1837	1193	299	342	3		

- Molecule 5 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	05	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
5	05	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
5	05	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
5	05	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
5	05	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
5	05	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
5	05	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
5	06	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	06	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
5	06	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
5	06	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
5	06	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
5	06	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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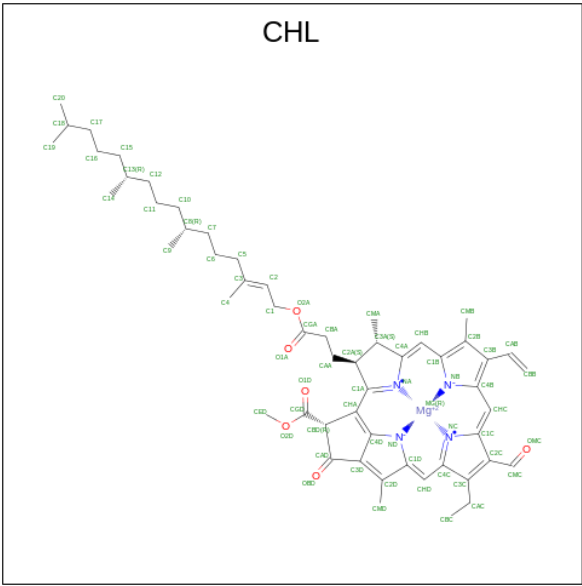
Mol	Chain	Residues	Atoms					AltConf
5	07	1	Total 40	C 32	Mg 1	N 4	O 3	0
5	07	1	Total 40	C 32	Mg 1	N 4	O 3	0
5	07	1	Total 40	C 32	Mg 1	N 4	O 3	0
5	07	1	Total 41	C 33	Mg 1	N 4	O 3	0
5	07	1	Total 48	C 38	Mg 1	N 4	O 5	0
5	07	1	Total 39	C 31	Mg 1	N 4	O 3	0
5	07	1	Total 44	C 34	Mg 1	N 4	O 5	0
5	08	1	Total 41	C 33	Mg 1	N 4	O 3	0
5	08	1	Total 40	C 32	Mg 1	N 4	O 3	0
5	08	1	Total 41	C 33	Mg 1	N 4	O 3	0
5	08	1	Total 40	C 32	Mg 1	N 4	O 3	0
5	08	1	Total 38	C 32	Mg 1	N 4	O 1	0
5	08	1	Total 40	C 32	Mg 1	N 4	O 3	0
5	08	1	Total 42	C 34	Mg 1	N 4	O 3	0
5	1r	1	Total 41	C 33	Mg 1	N 4	O 3	0
5	1r	1	Total 52	C 42	Mg 1	N 4	O 5	0
5	1r	1	Total 56	C 46	Mg 1	N 4	O 5	0
5	1r	1	Total 42	C 34	Mg 1	N 4	O 3	0
5	1r	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	1r	1	Total 52	C 42	Mg 1	N 4	O 5	0
5	1r	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
5	1r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
5	1r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

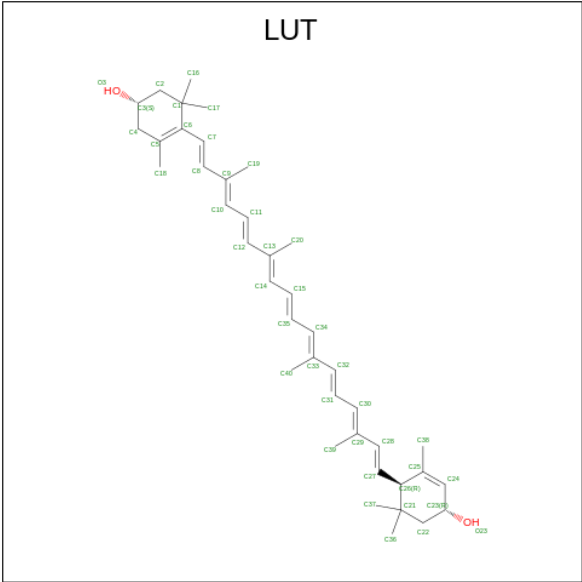
- Molecule 6 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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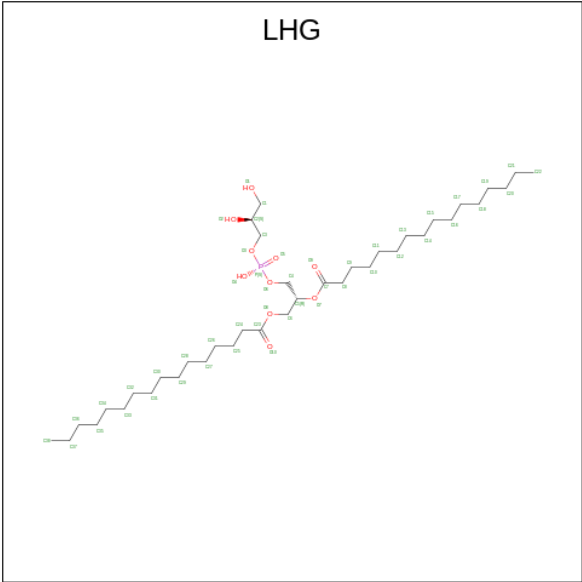
Mol	Chain	Residues	Atoms					AltConf
6	06	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
6	06	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	07	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
6	07	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
6	07	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
6	07	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
6	07	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
6	08	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
6	08	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
6	08	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
6	08	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
6	08	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
6	1r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	1r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	1r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
6	1r	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

- Molecule 7 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



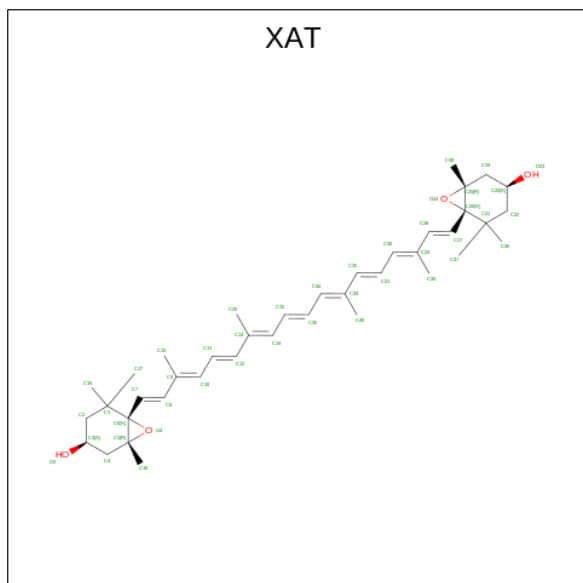
Mol	Chain	Residues	Atoms			AltConf
7	05	1	Total	C	O	0
			42	40	2	
7	07	1	Total	C	O	0
			42	40	2	
7	1r	1	Total	C	O	0
			42	40	2	

- Molecule 8 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
8	07	1	Total	C	O	P	0
			49	38	10	1	
8	1r	1	Total	C	O	P	0
			29	20	8	1	

- Molecule 9 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).

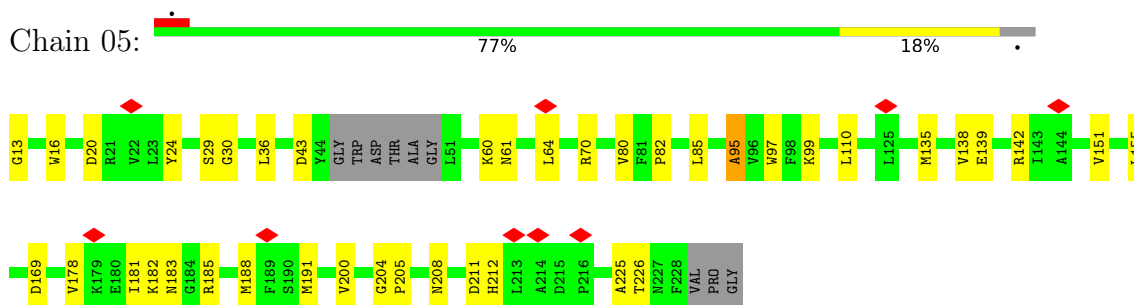


Mol	Chain	Residues	Atoms			AltConf
9	1r	1	Total	C	O	0
			44	40	4	

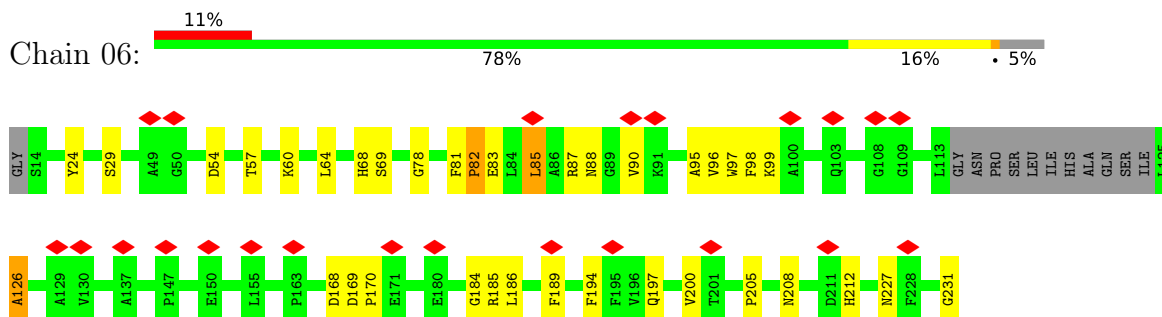
3 Residue-property plots

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.

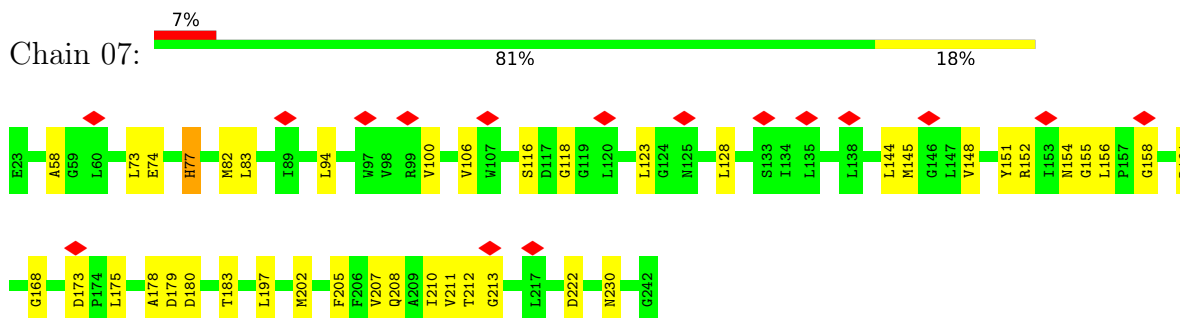
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic



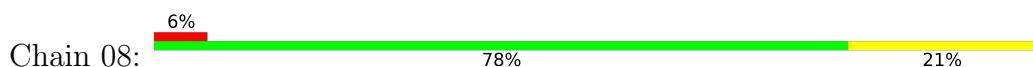
- Molecule 1: Chlorophyll a-b binding protein 2, chloroplastic

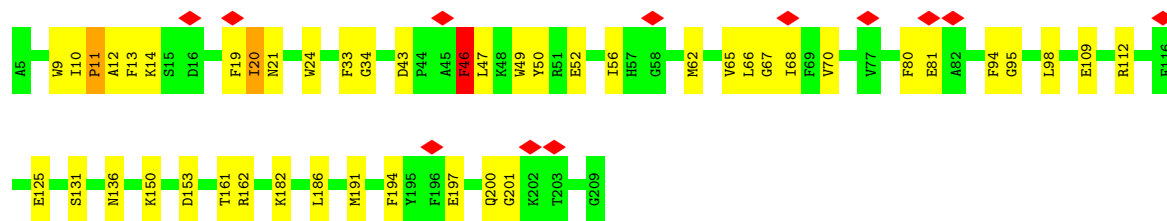


- Molecule 2: Chlorophyll a/b-binding protein

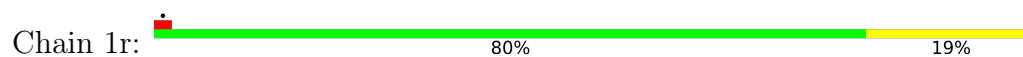


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic





- Molecule 4: 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	0.671	Depositor
Minimum map value	-0.420	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	419.84, 419.84, 419.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: CLA, LHG, XAT, CHL, 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	05	0.26	0/1597	0.67	0/2176
1	06	0.35	1/1485 (0.1%)	0.71	5/2030 (0.2%)
2	07	0.28	0/1696	0.69	1/2312 (0.0%)
3	08	0.32	0/1626	0.69	1/2217 (0.0%)
4	1r	0.22	0/1890	0.54	0/2574
All	All	0.29	1/8294 (0.0%)	0.66	7/11309 (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	05	0	1
1	06	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	06	170	PRO	CG-CD	-9.05	1.20	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	06	170	PRO	N-CD-CG	-10.77	87.04	103.20
1	06	170	PRO	CA-N-CD	-10.40	97.44	112.00
1	06	170	PRO	CA-CB-CG	-6.97	91.26	104.50
3	08	46	PHE	N-CA-C	-6.64	105.31	113.41
2	07	77	HIS	N-CA-CB	5.57	118.41	110.06

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	05	95	ALA	Peptide
1	06	189	PHE	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	05	1555	0	1473	31	0
1	06	1450	0	1320	28	0
2	07	1648	0	1561	31	0
3	08	1570	0	1469	31	0
4	1r	1837	0	1785	36	0
5	05	331	0	224	7	0
5	06	257	0	183	8	0
5	07	292	0	198	4	0
5	08	282	0	191	8	0
5	1r	425	0	329	16	0
6	05	274	0	191	10	0
6	06	218	0	137	1	0
6	07	203	0	120	3	0
6	08	207	0	125	1	0
6	1r	185	0	124	4	0
7	05	42	0	56	5	0
7	07	42	0	56	7	0
7	1r	42	0	56	6	0
8	07	49	0	74	1	0
8	1r	29	0	29	1	0
9	1r	44	0	56	2	0
All	All	10982	0	9757	179	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 9.

The worst 5 of 179 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)
1:06:68:HIS:HE1	5:06:602:CLA:NC	1.81	0.78
1:06:97:TRP:H	1:06:205:PRO:HG3	1.51	0.75
4:1r:108:LEU:HD21	5:1r:308:CLA:HAB	1.72	0.72
4:1r:97:LEU:HD21	4:1r:172:LEU:HD12	1.72	0.71
1:05:70:ARG:NH2	1:05:155:LEU:O	2.27	0.68

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	05	206/219 (94%)	175 (85%)	29 (14%)	2 (1%)	12	41
1	06	203/219 (93%)	167 (82%)	33 (16%)	3 (2%)	8	33
2	07	218/220 (99%)	188 (86%)	29 (13%)	1 (0%)	24	55
3	08	203/205 (99%)	170 (84%)	28 (14%)	5 (2%)	4	24
4	1r	232/234 (99%)	216 (93%)	16 (7%)	0	100	100
All	All	1062/1097 (97%)	916 (86%)	135 (13%)	11 (1%)	15	41

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	08	13	PHE
1	05	95	ALA
1	06	126	ALA
2	07	179	ASP
3	08	20	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	05	150/166 (90%)	149 (99%)	1 (1%)	76	75
1	06	129/166 (78%)	128 (99%)	1 (1%)	73	74
2	07	159/172 (92%)	157 (99%)	2 (1%)	61	69
3	08	149/157 (95%)	146 (98%)	3 (2%)	48	63
4	1r	191/191 (100%)	189 (99%)	2 (1%)	68	72
All	All	778/852 (91%)	769 (99%)	9 (1%)	61	70

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	1r	29	VAL
4	1r	138	GLN
2	07	106	VAL
3	08	46	PHE
3	08	66	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
4	1r	163	ASN
4	1r	225	ASN
2	07	40	GLN
2	07	141	GLN
2	07	208	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

68 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
5	CLA	1r	308	-	49,53,73	2.53	19 (38%)	59,89,113	3.33	26 (44%)
6	CHL	07	303	2	44,49,74	2.33	17 (38%)	48,84,114	3.33	21 (43%)
6	CHL	05	313	1	44,49,74	2.34	15 (34%)	48,84,114	3.31	21 (43%)
5	CLA	08	307	-	43,48,73	2.64	20 (46%)	51,83,113	3.46	27 (52%)
6	CHL	06	605	-	48,53,74	2.29	15 (31%)	53,89,114	3.16	21 (39%)
6	CHL	05	315	-	46,50,74	2.35	16 (34%)	51,85,114	3.30	24 (47%)
6	CHL	1r	303	-	50,54,74	2.23	18 (36%)	56,90,114	3.18	24 (42%)
9	XAT	1r	315	-	39,47,47	0.88	0	54,74,74	3.46	24 (44%)
5	CLA	05	302	1	47,52,73	2.57	19 (40%)	56,88,113	3.40	27 (48%)
5	CLA	05	301	1	45,49,73	2.64	20 (44%)	54,84,113	3.41	28 (51%)
5	CLA	1r	313	4	50,54,73	2.47	20 (40%)	60,90,113	3.36	28 (46%)
7	LUT	05	314	-	42,43,43	1.70	9 (21%)	51,60,60	1.97	14 (27%)
5	CLA	07	302	2	43,48,73	2.75	21 (48%)	51,83,113	4.04	29 (56%)
8	LHG	07	314	-	48,48,48	0.29	0	51,54,54	0.67	1 (1%)
5	CLA	06	609	-	44,49,73	2.56	19 (43%)	52,84,113	3.47	26 (50%)
6	CHL	1r	302	-	50,54,74	2.24	18 (36%)	56,90,114	3.11	23 (41%)
5	CLA	06	611	-	43,48,73	2.66	20 (46%)	51,83,113	3.52	26 (50%)
5	CLA	08	310	3	41,46,73	2.65	19 (46%)	51,80,113	3.55	27 (52%)
5	CLA	1r	310	-	49,53,73	2.51	18 (36%)	59,89,113	3.34	27 (45%)
6	CHL	06	601	-	50,54,74	2.27	15 (30%)	56,90,114	3.15	21 (37%)
5	CLA	07	310	-	41,47,73	2.64	19 (46%)	49,81,113	3.57	27 (55%)
5	CLA	1r	311	-	50,54,73	2.46	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
5	CLA	1r	306	4	60,64,73	2.30	19 (31%)	72,102,113	3.03	33 (45%)
8	LHG	1r	316	5	28,28,48	0.36	0	31,33,54	0.77	2 (6%)
6	CHL	08	303	-	48,53,74	2.23	17 (35%)	53,89,114	3.14	20 (37%)
6	CHL	1r	304	-	50,54,74	2.23	18 (36%)	56,90,114	3.17	20 (35%)
6	CHL	05	307	1	46,50,74	2.32	14 (30%)	51,85,114	3.26	24 (47%)
5	CLA	06	602	1	59,63,73	2.35	22 (37%)	71,101,113	3.15	31 (43%)
5	CLA	07	308	-	45,49,73	2.59	20 (44%)	54,84,113	3.46	28 (51%)
6	CHL	07	311	-	44,49,74	2.31	17 (38%)	48,84,114	3.23	21 (43%)
5	CLA	08	312	-	46,50,73	2.53	18 (39%)	55,85,113	3.41	29 (52%)
5	CLA	05	308	1	45,49,73	2.67	19 (42%)	54,84,113	3.46	31 (57%)
5	CLA	1r	305	4	56,60,73	2.32	20 (35%)	67,97,113	3.14	31 (46%)
5	CLA	05	309	-	43,48,73	2.62	20 (46%)	51,83,113	3.53	26 (50%)
6	CHL	1r	312	4	51,55,74	2.21	17 (33%)	57,91,114	3.13	23 (40%)
5	CLA	08	309	3	43,48,73	2.74	19 (44%)	51,83,113	3.50	27 (52%)
5	CLA	1r	301	4	45,49,73	2.62	19 (42%)	54,84,113	3.42	29 (53%)
5	CLA	07	307	-	43,48,73	2.64	19 (44%)	51,83,113	3.53	27 (52%)
5	CLA	07	309	2	52,56,73	2.48	19 (36%)	62,92,113	3.29	27 (43%)
5	CLA	05	303	-	47,52,73	2.55	19 (40%)	56,88,113	3.27	27 (48%)
5	CLA	07	301	-	43,48,73	2.61	20 (46%)	51,83,113	3.45	28 (54%)
5	CLA	08	311	-	43,48,73	2.69	19 (44%)	51,83,113	3.51	28 (54%)
5	CLA	07	312	-	47,52,73	2.56	20 (42%)	56,88,113	3.34	26 (46%)
5	CLA	05	311	-	43,48,73	2.62	19 (44%)	51,83,113	3.60	30 (58%)
5	CLA	06	608	-	43,48,73	2.66	20 (46%)	51,83,113	3.48	27 (52%)
5	CLA	08	306	-	44,49,73	2.55	17 (38%)	52,84,113	3.49	26 (50%)
6	CHL	05	305	-	67,71,74	1.93	18 (26%)	76,110,114	2.79	27 (35%)
5	CLA	08	308	3	44,49,73	2.57	18 (40%)	52,84,113	3.38	26 (50%)
6	CHL	07	306	-	44,49,74	2.35	16 (36%)	48,84,114	3.32	22 (45%)
5	CLA	05	310	1	44,49,73	2.56	19 (43%)	52,84,113	3.46	26 (50%)
6	CHL	08	305	-	44,47,74	2.11	14 (31%)	48,80,114	3.29	21 (43%)
5	CLA	1r	309	4	56,60,73	2.36	20 (35%)	67,97,113	3.20	31 (46%)
6	CHL	05	306	-	44,49,74	2.37	19 (43%)	48,84,114	3.35	21 (43%)
6	CHL	06	603	-	42,48,74	2.32	15 (35%)	46,82,114	3.38	23 (50%)
5	CLA	06	607	1	43,48,73	2.68	20 (46%)	51,83,113	3.47	28 (54%)
6	CHL	07	305	-	42,47,74	2.30	16 (38%)	48,81,114	3.33	21 (43%)
5	CLA	06	610	-	44,49,73	2.58	19 (43%)	52,84,113	3.44	26 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CHL	05	304	-	48,53,74	2.21	15 (31%)	53,89,114	2.77	19 (35%)
6	CHL	06	606	-	50,54,74	2.25	16 (32%)	56,90,114	3.13	22 (39%)
6	CHL	08	302	-	44,49,74	2.36	18 (40%)	48,84,114	3.36	22 (45%)
5	CLA	05	312	1	43,48,73	2.74	21 (48%)	51,83,113	3.62	28 (54%)
5	CLA	1r	307	8	46,50,73	2.52	19 (41%)	55,85,113	3.41	26 (47%)
6	CHL	08	301	-	44,49,74	2.38	16 (36%)	48,84,114	3.23	22 (45%)
6	CHL	08	304	3	44,49,74	2.36	17 (38%)	48,84,114	3.35	22 (45%)
7	LUT	07	313	-	42,43,43	1.59	7 (16%)	51,60,60	1.91	13 (25%)
6	CHL	06	604	-	44,49,74	2.36	16 (36%)	48,84,114	3.32	22 (45%)
6	CHL	07	304	2	44,49,74	2.36	16 (36%)	48,84,114	3.31	22 (45%)
7	LUT	1r	314	-	42,43,43	1.68	8 (19%)	51,60,60	1.72	11 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	1r	308	-	-	4/15/91/115	-
6	CHL	07	303	2	-	6/10/86/117	-
6	CHL	05	313	1	-	6/10/86/117	-
5	CLA	08	307	-	-	1/8/84/115	-
6	CHL	06	605	-	-	7/15/91/117	-
6	CHL	05	315	-	-	7/12/88/117	-
6	CHL	1r	303	-	-	9/17/93/117	-
9	XAT	1r	315	-	-	5/31/93/93	0/4/4/4
5	CLA	05	302	1	-	4/13/89/115	-
5	CLA	05	301	1	-	5/10/86/115	-
5	CLA	1r	313	4	-	8/17/93/115	-
7	LUT	05	314	-	-	2/29/67/67	0/2/2/2
5	CLA	07	302	2	-	1/8/84/115	-
8	LHG	07	314	-	-	13/53/53/53	-
5	CLA	06	609	-	-	0/10/86/115	-
6	CHL	1r	302	-	-	9/17/93/117	-
5	CLA	06	611	-	-	0/8/84/115	-
5	CLA	08	310	3	-	0/4/80/115	-
5	CLA	1r	310	-	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CHL	06	601	-	-	11/17/93/117	-
5	CLA	07	310	-	-	2/8/80/115	-
5	CLA	1r	311	-	-	4/17/93/115	-
5	CLA	1r	306	4	1/1/13/20	5/29/105/115	-
8	LHG	1r	316	5	-	4/32/32/53	-
6	CHL	08	303	-	-	8/15/91/117	-
6	CHL	1r	304	-	-	7/17/93/117	-
6	CHL	05	307	1	-	6/12/88/117	-
5	CLA	06	602	1	1/1/13/20	6/27/103/115	-
5	CLA	07	308	-	-	4/10/86/115	-
6	CHL	07	311	-	-	8/10/86/117	-
5	CLA	08	312	-	-	9/12/88/115	-
5	CLA	05	308	1	-	2/10/86/115	-
5	CLA	1r	305	4	-	9/24/100/115	-
5	CLA	05	309	-	-	2/8/84/115	-
6	CHL	1r	312	4	-	8/19/95/117	-
5	CLA	08	309	3	-	3/8/84/115	-
5	CLA	1r	301	4	-	2/10/86/115	-
5	CLA	07	307	-	-	1/8/84/115	-
5	CLA	07	309	2	-	7/19/95/115	-
5	CLA	05	303	-	-	6/13/89/115	-
5	CLA	07	301	-	-	2/8/84/115	-
5	CLA	08	311	-	-	1/8/84/115	-
5	CLA	07	312	-	-	2/13/89/115	-
5	CLA	05	311	-	-	0/8/84/115	-
5	CLA	06	608	-	-	1/8/84/115	-
6	CHL	05	305	-	1/1/14/21	18/38/114/117	-
5	CLA	08	306	-	-	2/10/86/115	-
5	CLA	08	308	3	-	4/10/86/115	-
6	CHL	07	306	-	-	4/10/86/117	-
5	CLA	05	310	1	-	2/10/86/115	-
6	CHL	08	305	-	-	5/8/80/117	-
5	CLA	1r	309	4	-	7/24/100/115	-
6	CHL	05	306	-	-	2/10/86/117	-
6	CHL	06	603	-	-	6/10/82/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	06	607	1	-	0/8/84/115	-
6	CHL	07	305	-	-	4/6/82/117	-
5	CLA	06	610	-	-	0/10/86/115	-
6	CHL	05	304	-	-	9/15/91/117	-
6	CHL	06	606	-	-	10/17/93/117	-
6	CHL	08	302	-	-	2/10/86/117	-
5	CLA	05	312	1	-	0/8/84/115	-
5	CLA	1r	307	8	-	3/12/88/115	-
6	CHL	08	301	-	-	4/10/86/117	-
6	CHL	08	304	3	-	6/10/86/117	-
7	LUT	07	313	-	-	0/29/67/67	0/2/2/2
6	CHL	06	604	-	-	3/10/86/117	-
6	CHL	07	304	2	-	4/10/86/117	-
7	LUT	1r	314	-	-	0/29/67/67	0/2/2/2

The worst 5 of 1150 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	08	309	CLA	C1D-ND	8.80	1.48	1.37
5	08	306	CLA	C1D-ND	8.77	1.48	1.37
5	07	309	CLA	C1D-ND	8.68	1.48	1.37
5	06	610	CLA	C1D-ND	8.68	1.48	1.37
5	07	312	CLA	C1D-ND	8.67	1.48	1.37

The worst 5 of 1643 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	05	311	CLA	C1D-ND-C4D	-10.88	98.61	106.33
5	07	302	CLA	C2C-C1C-NC	10.78	120.07	109.97
6	1r	304	CHL	C2B-C1B-NB	10.60	117.34	110.23
5	07	302	CLA	C4A-NA-C1A	10.58	111.46	106.71
6	08	302	CHL	C2B-C1B-NB	10.52	117.28	110.23

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	06	602	CLA	C8
5	1r	306	CLA	C8
6	05	305	CHL	C8

5 of 305 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	05	301	CLA	C2B-C3B-CAB-CBB
5	05	301	CLA	C4B-C3B-CAB-CBB
5	05	303	CLA	C4B-C3B-CAB-CBB
5	06	602	CLA	C4-C3-C5-C6
5	07	309	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

42 monomers are involved in 76 short contacts:

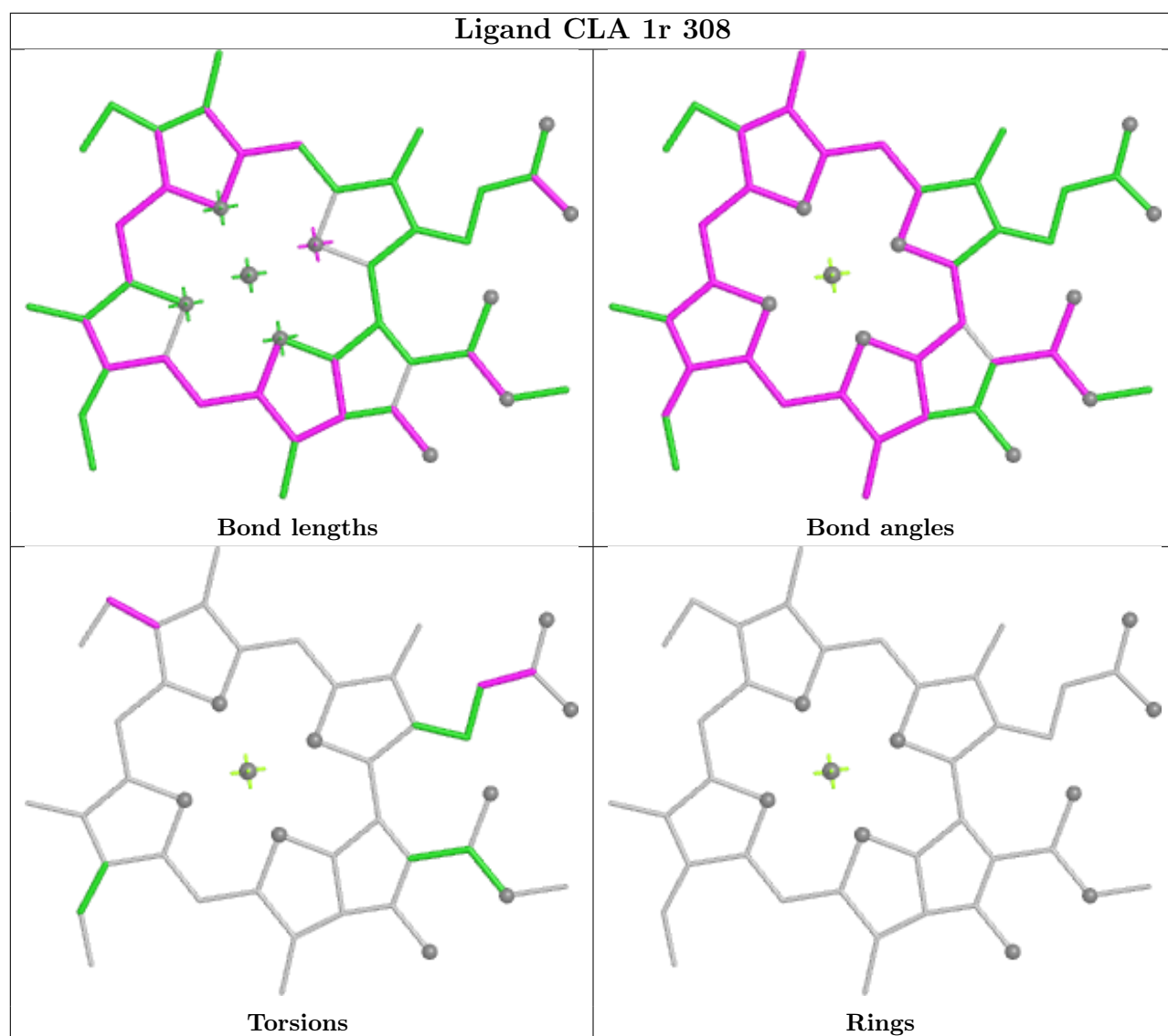
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1r	308	CLA	1	0
5	08	307	CLA	1	0
6	05	315	CHL	1	0
6	1r	303	CHL	2	0
9	1r	315	XAT	2	0
5	05	301	CLA	3	0
5	1r	313	CLA	1	0
7	05	314	LUT	5	0
8	07	314	LHG	1	0
5	06	609	CLA	1	0
6	1r	302	CHL	2	0
5	06	611	CLA	1	0
5	08	310	CLA	2	0
5	1r	310	CLA	1	0
5	07	310	CLA	1	0
5	1r	311	CLA	1	0
5	1r	306	CLA	3	0
8	1r	316	LHG	1	0
6	05	307	CHL	2	0
5	06	602	CLA	4	0
5	07	308	CLA	1	0
6	07	311	CHL	3	0
5	08	312	CLA	1	0
5	1r	305	CLA	2	0
5	05	309	CLA	1	0
6	1r	312	CHL	1	0
5	08	309	CLA	1	0
5	1r	301	CLA	4	0
5	07	307	CLA	2	0
5	08	311	CLA	3	0
5	05	311	CLA	1	0

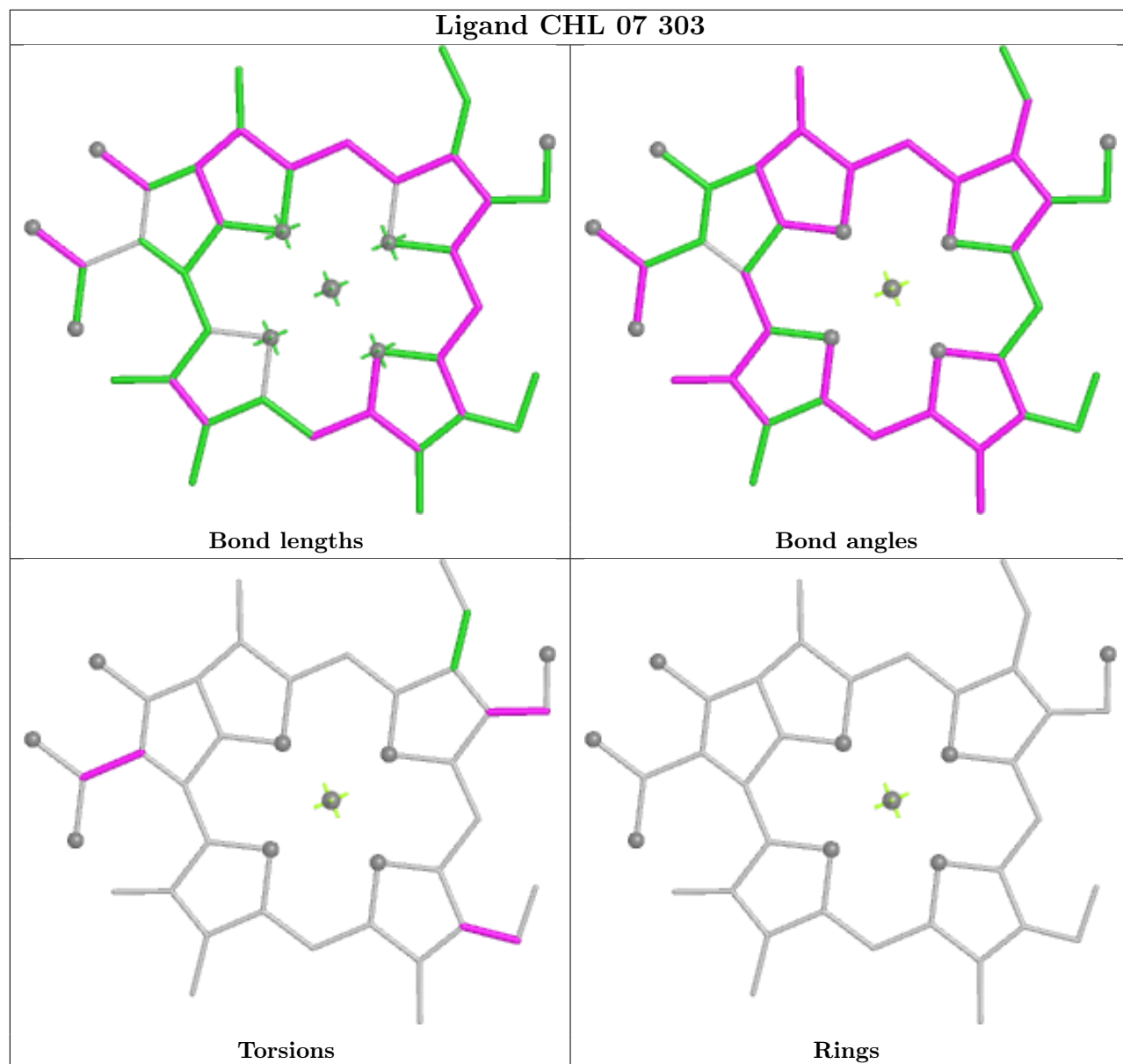
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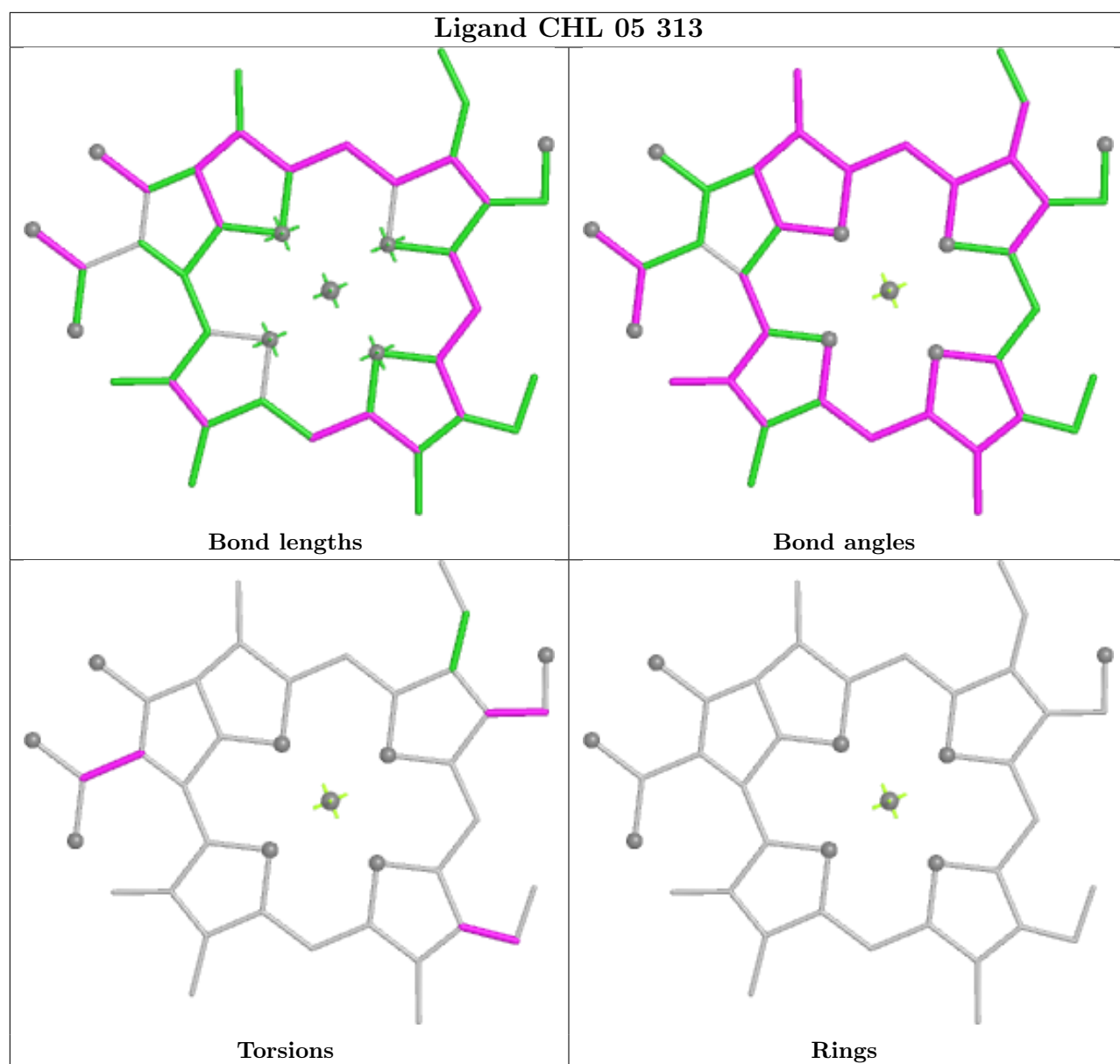
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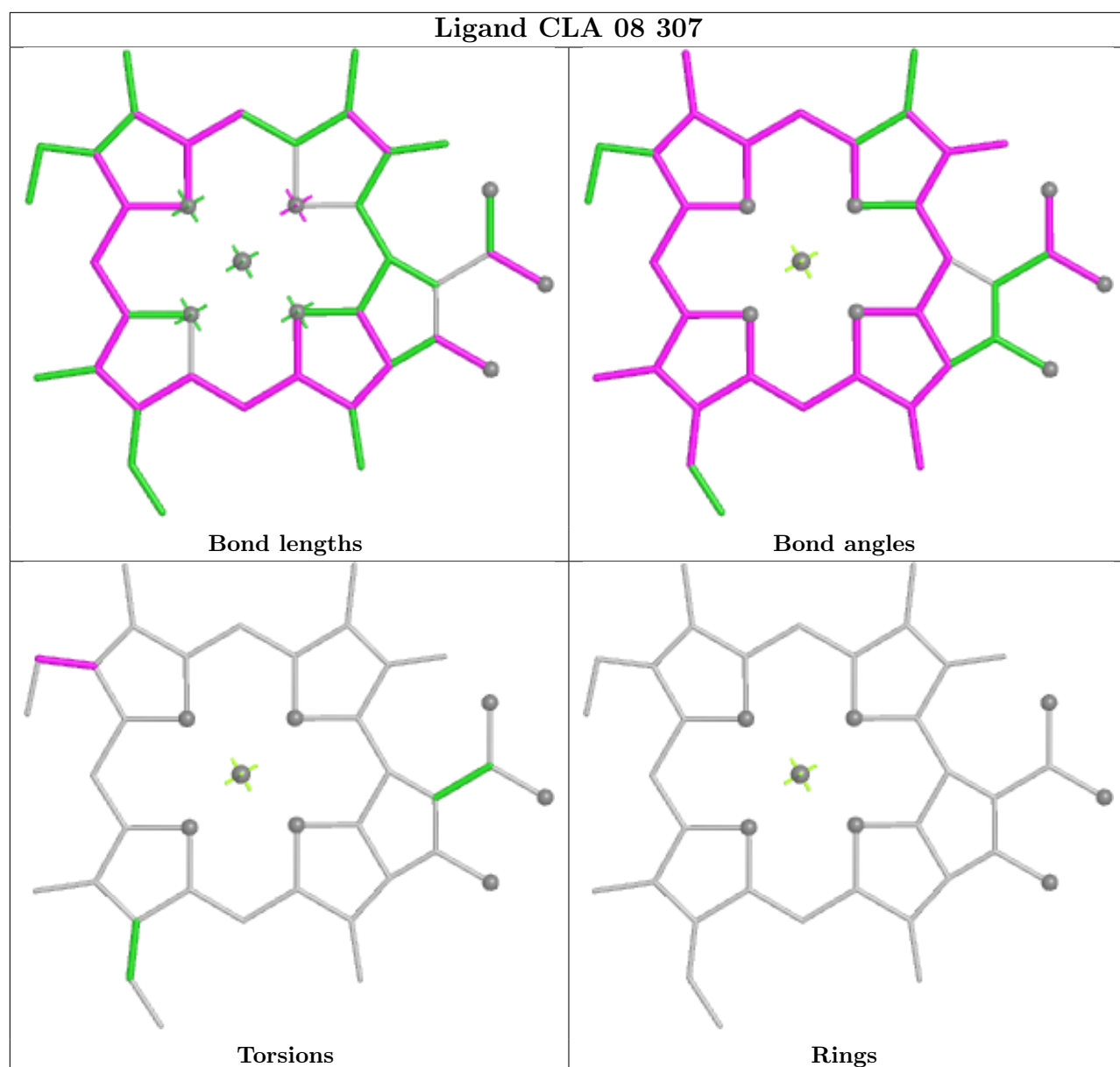
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	05	305	CHL	4	0
5	05	310	CLA	1	0
5	1r	309	CLA	3	0
6	06	603	CHL	1	0
5	06	607	CLA	2	0
6	05	304	CHL	5	0
5	05	312	CLA	1	0
6	08	304	CHL	1	0
7	07	313	LUT	7	0
6	07	304	CHL	1	0
7	1r	314	LUT	6	0

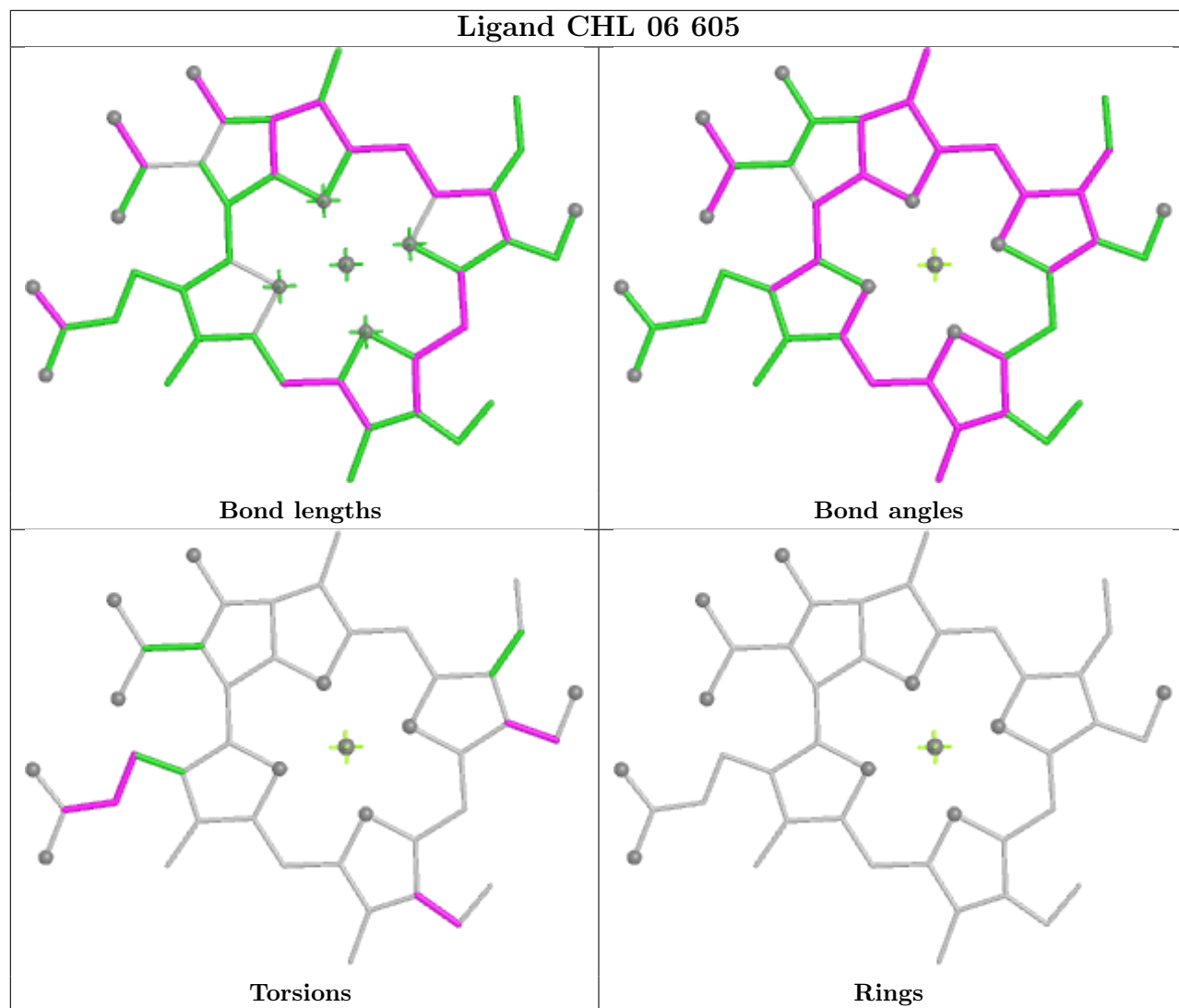
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

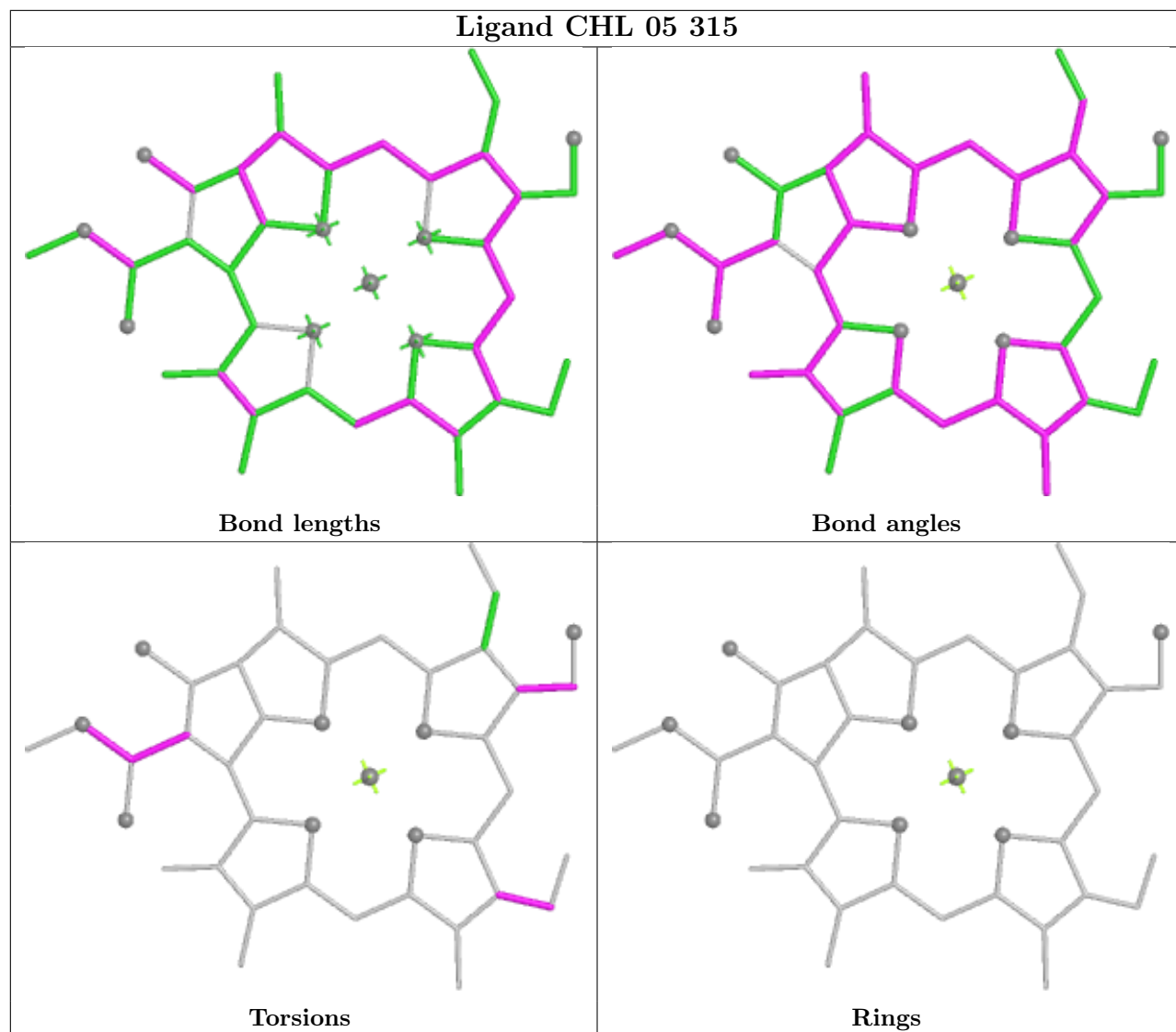


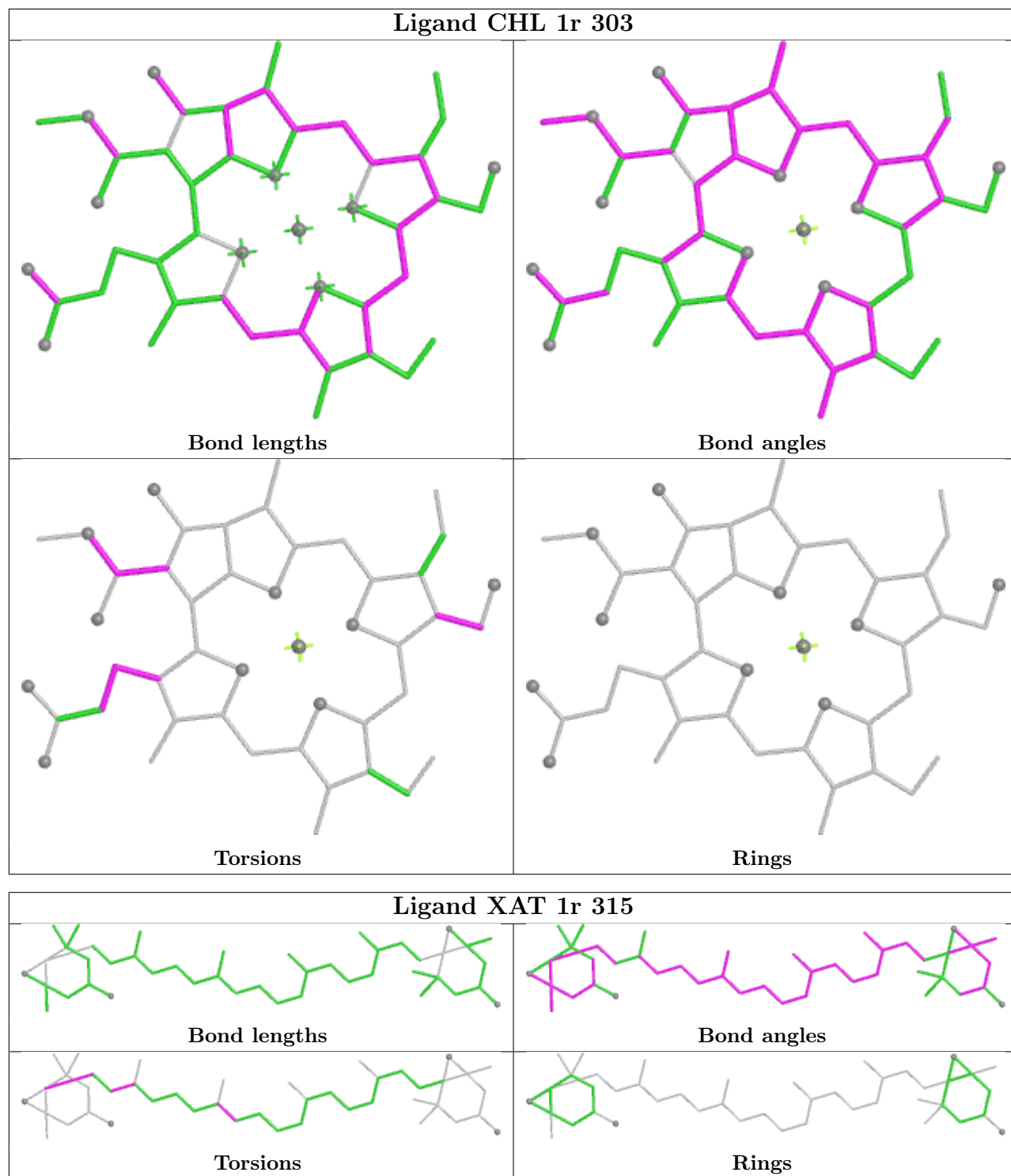


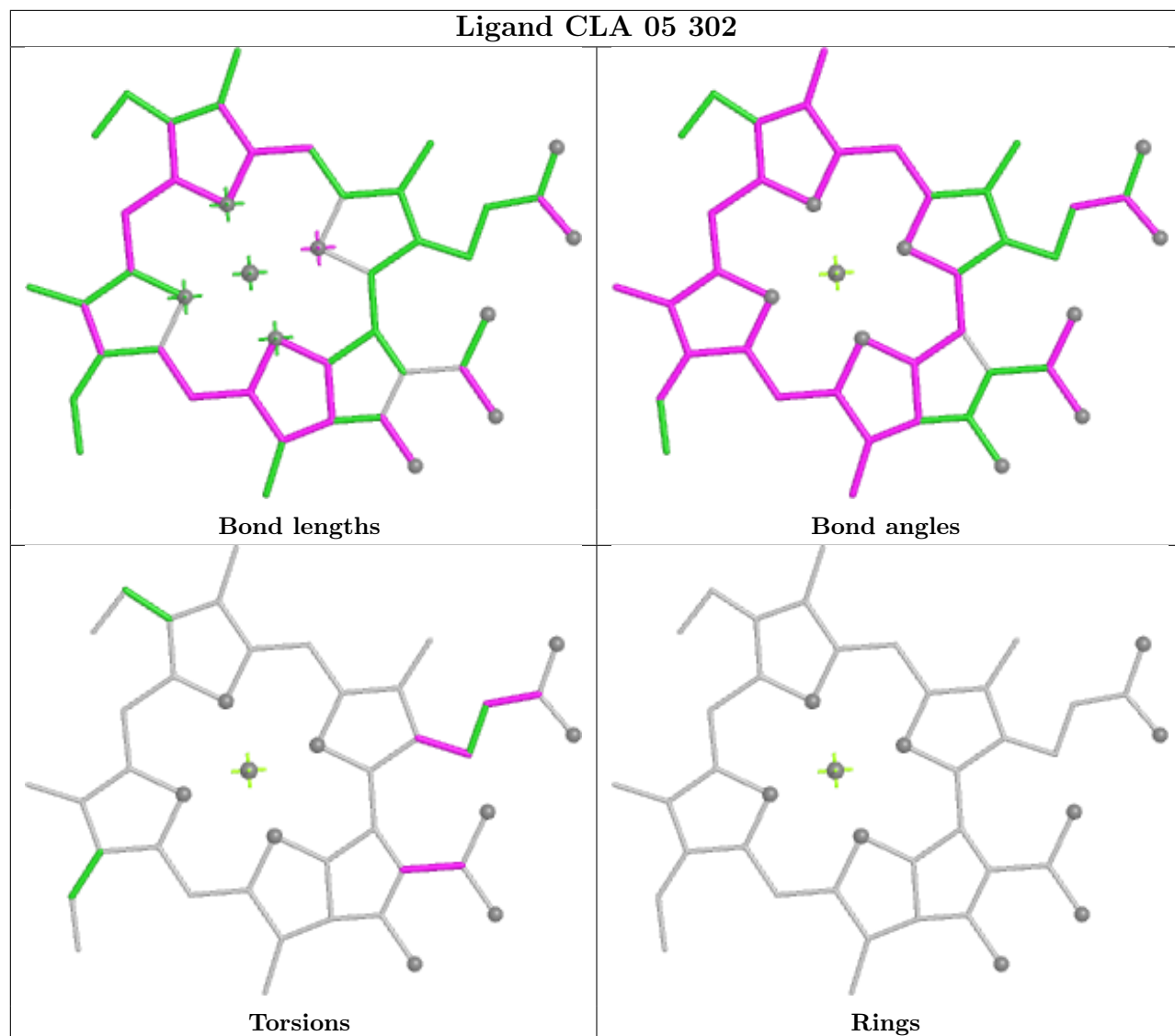


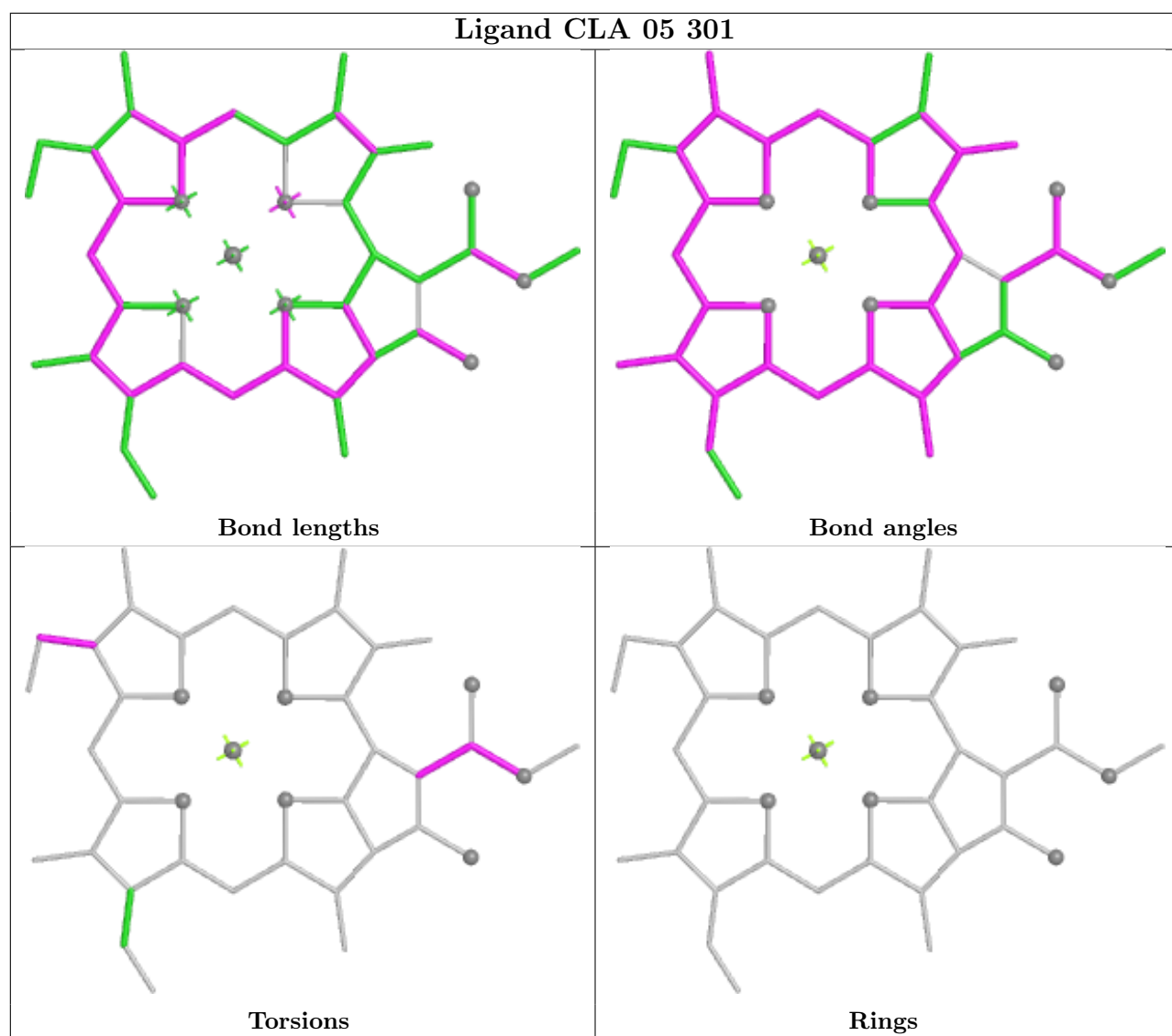


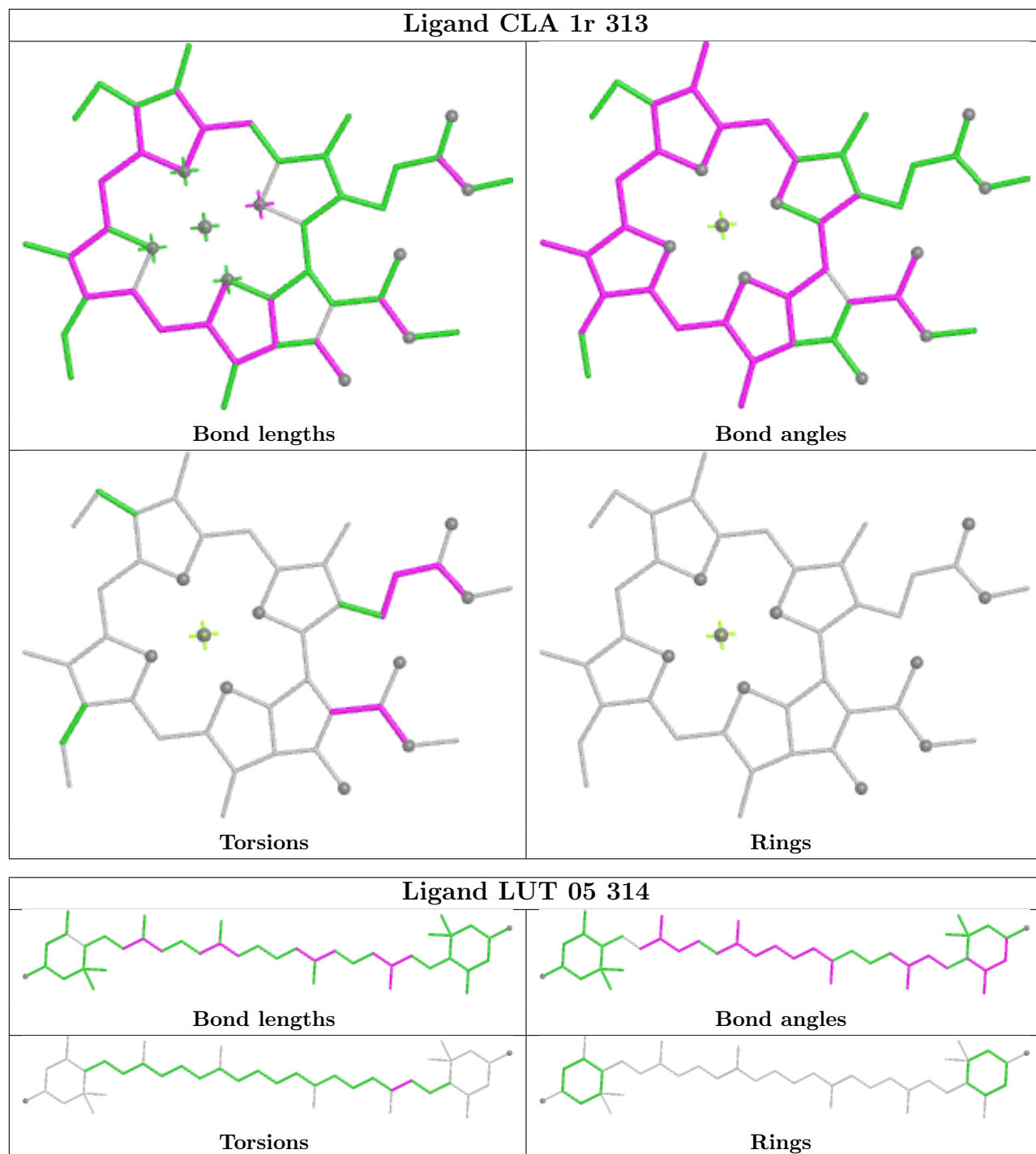


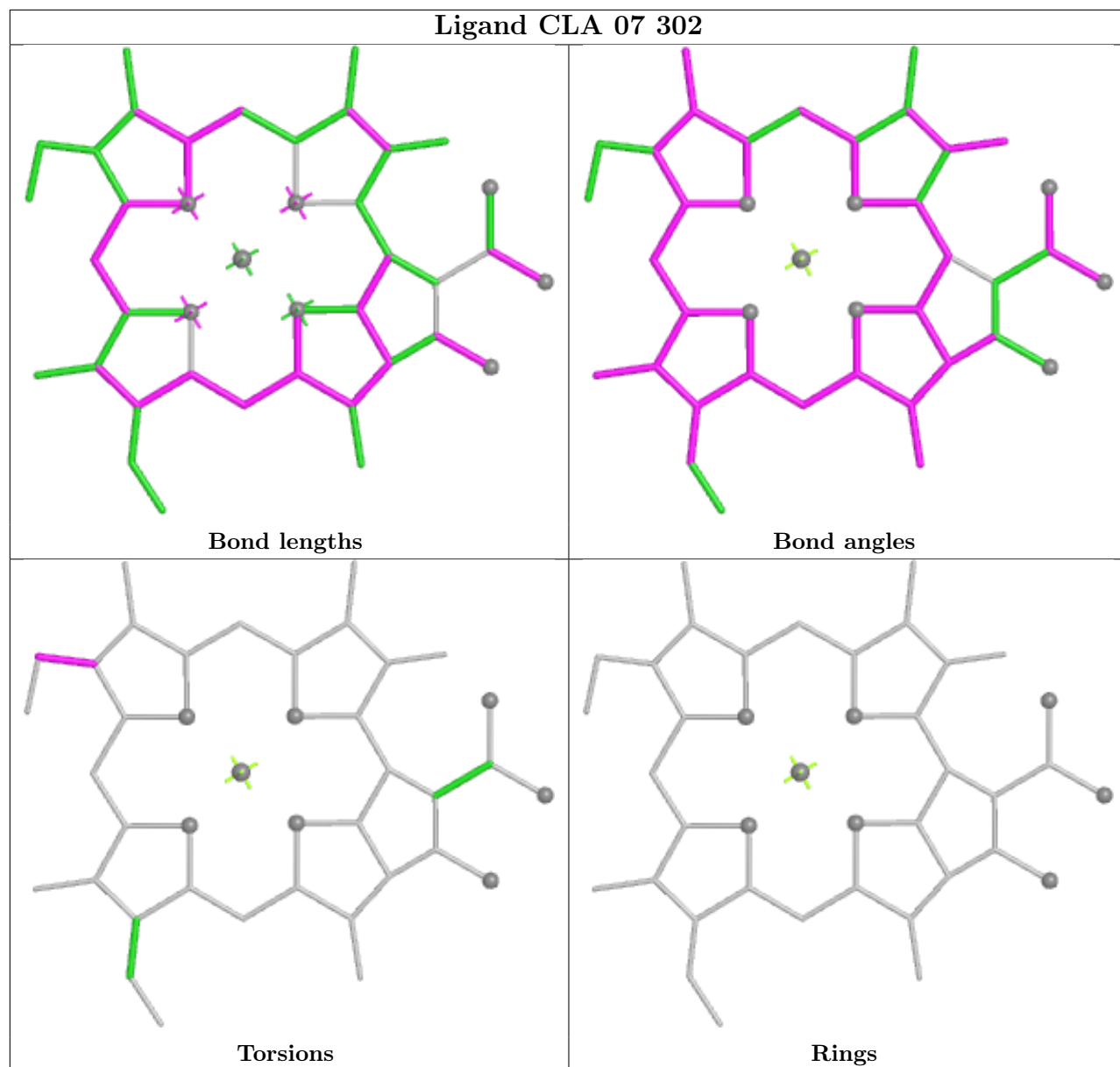


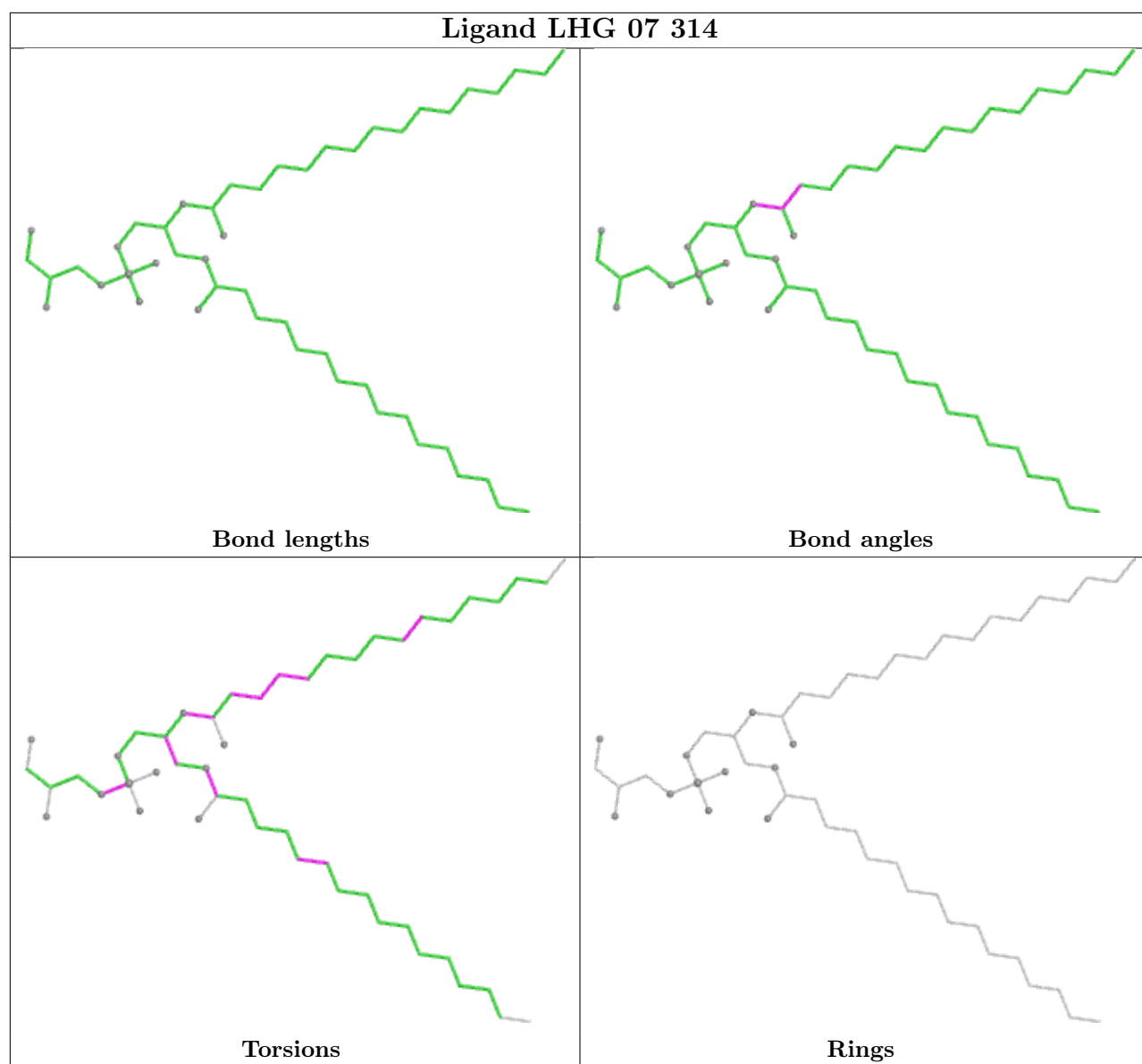


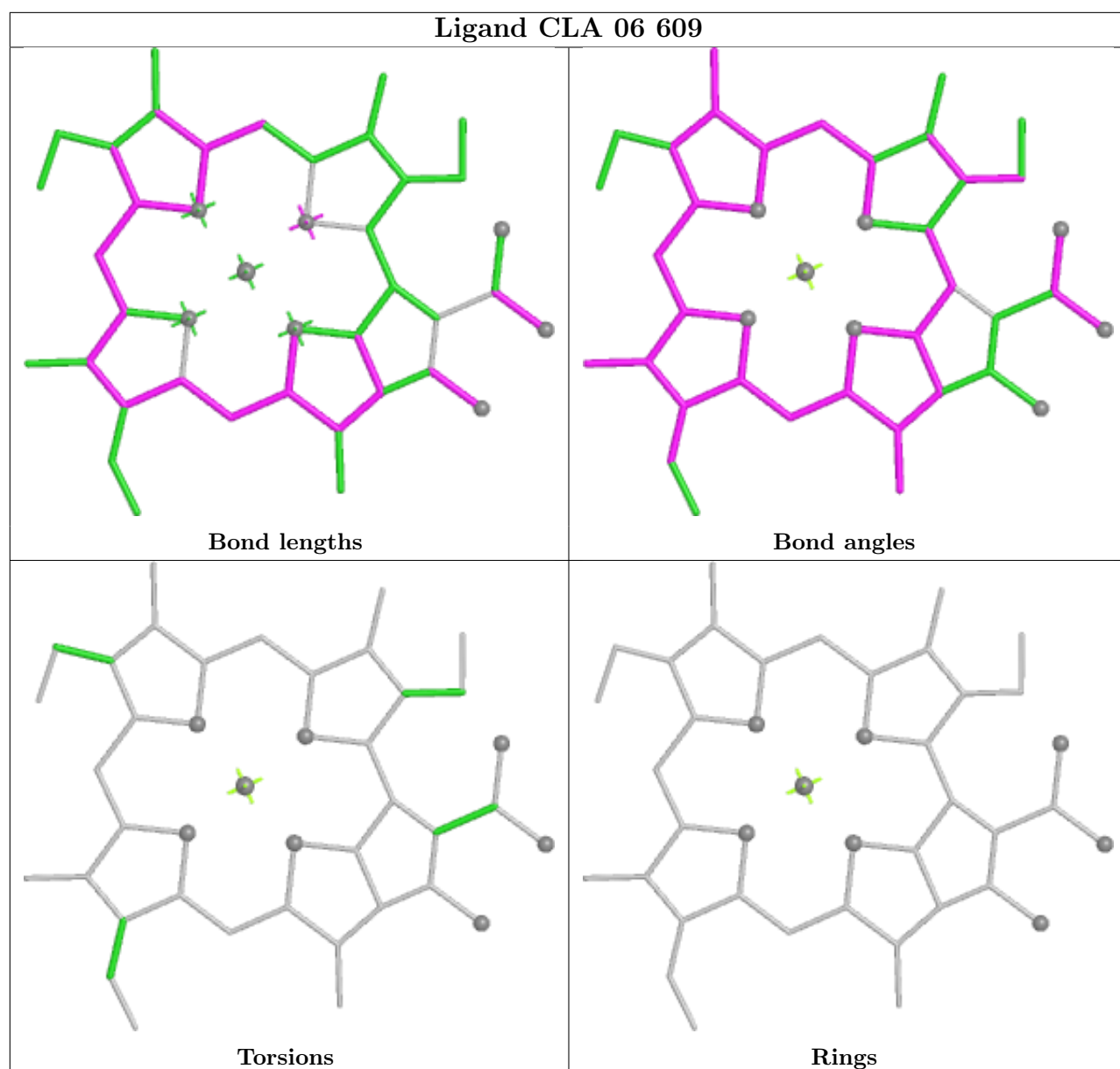


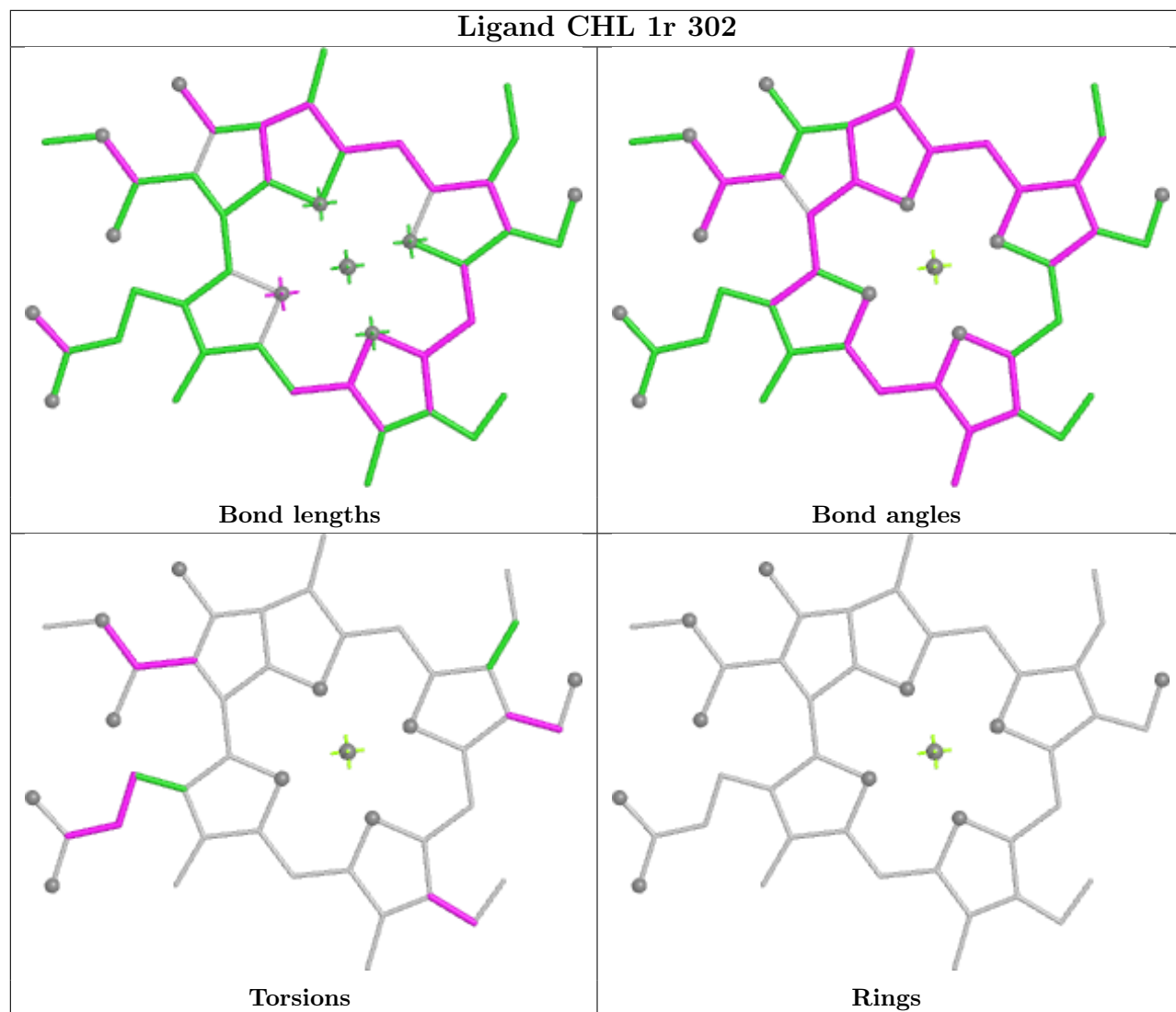


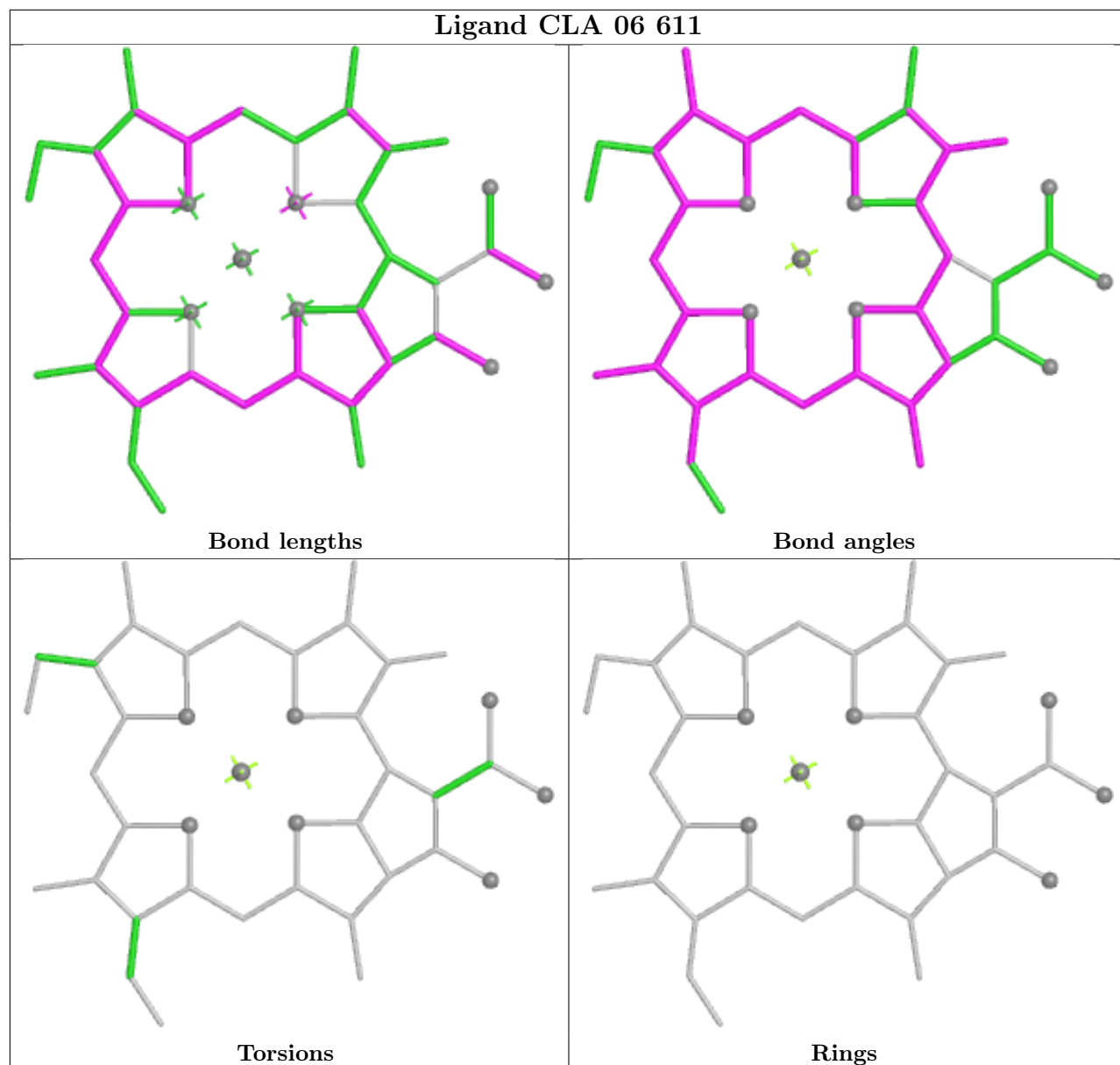


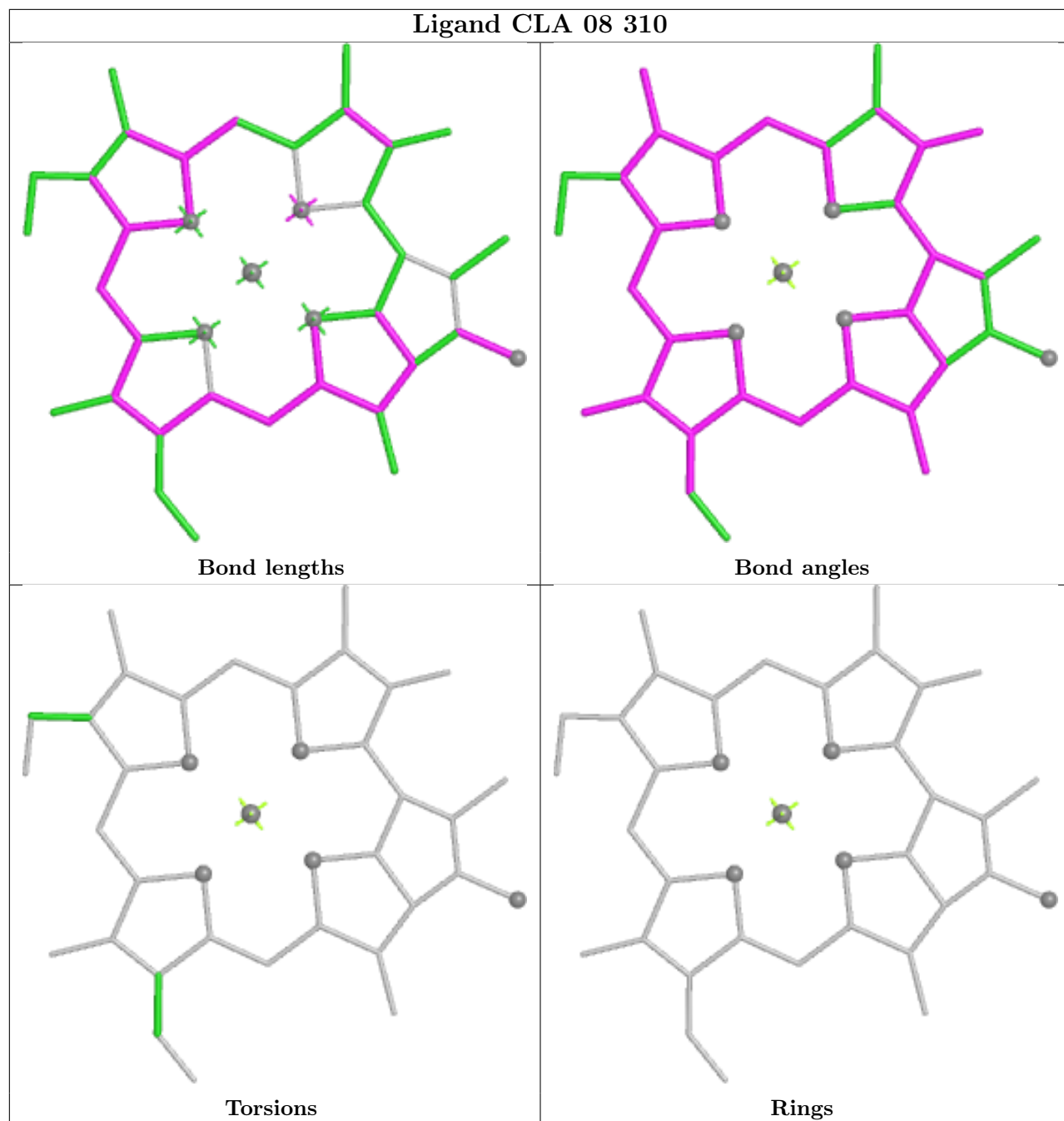


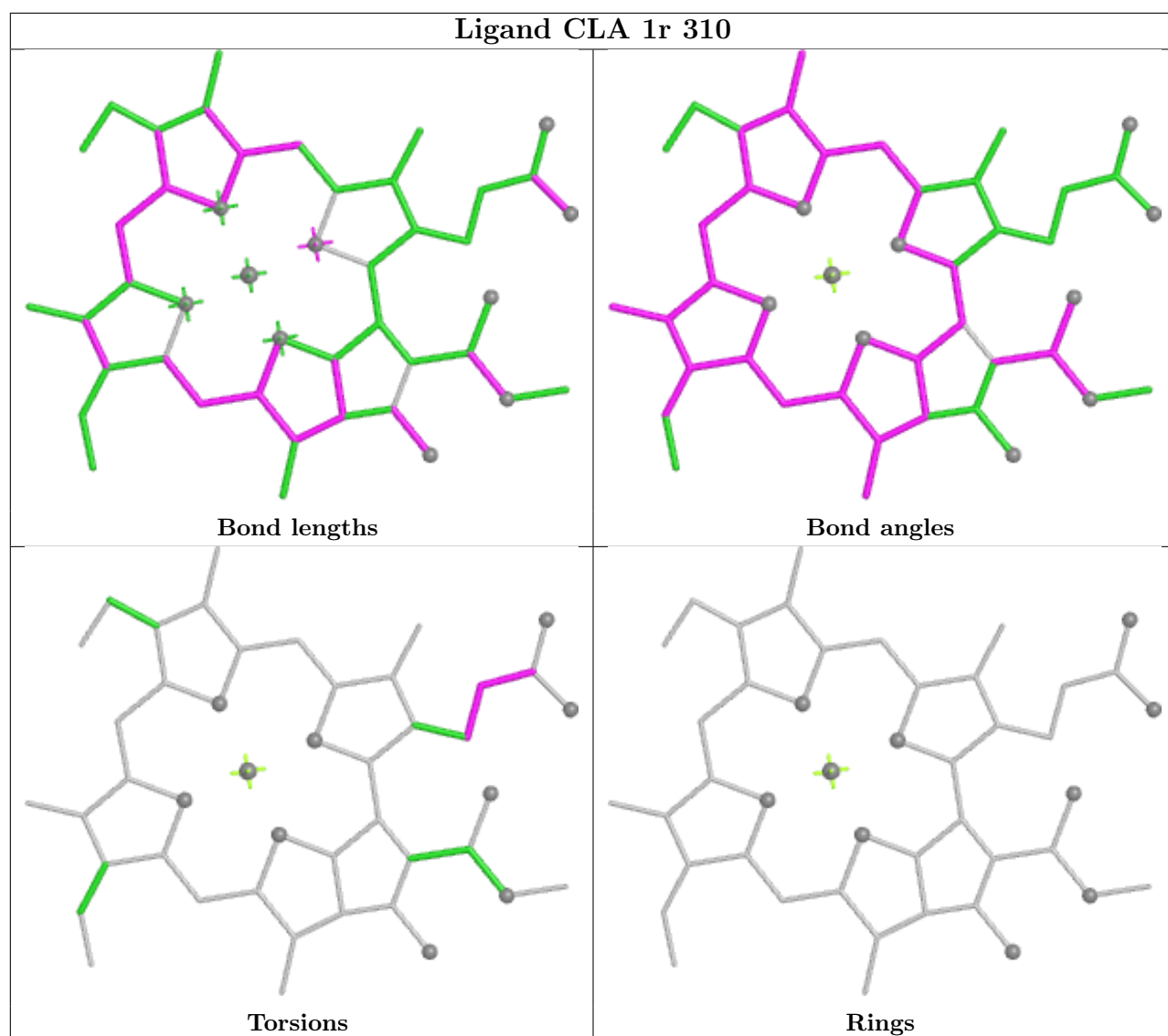


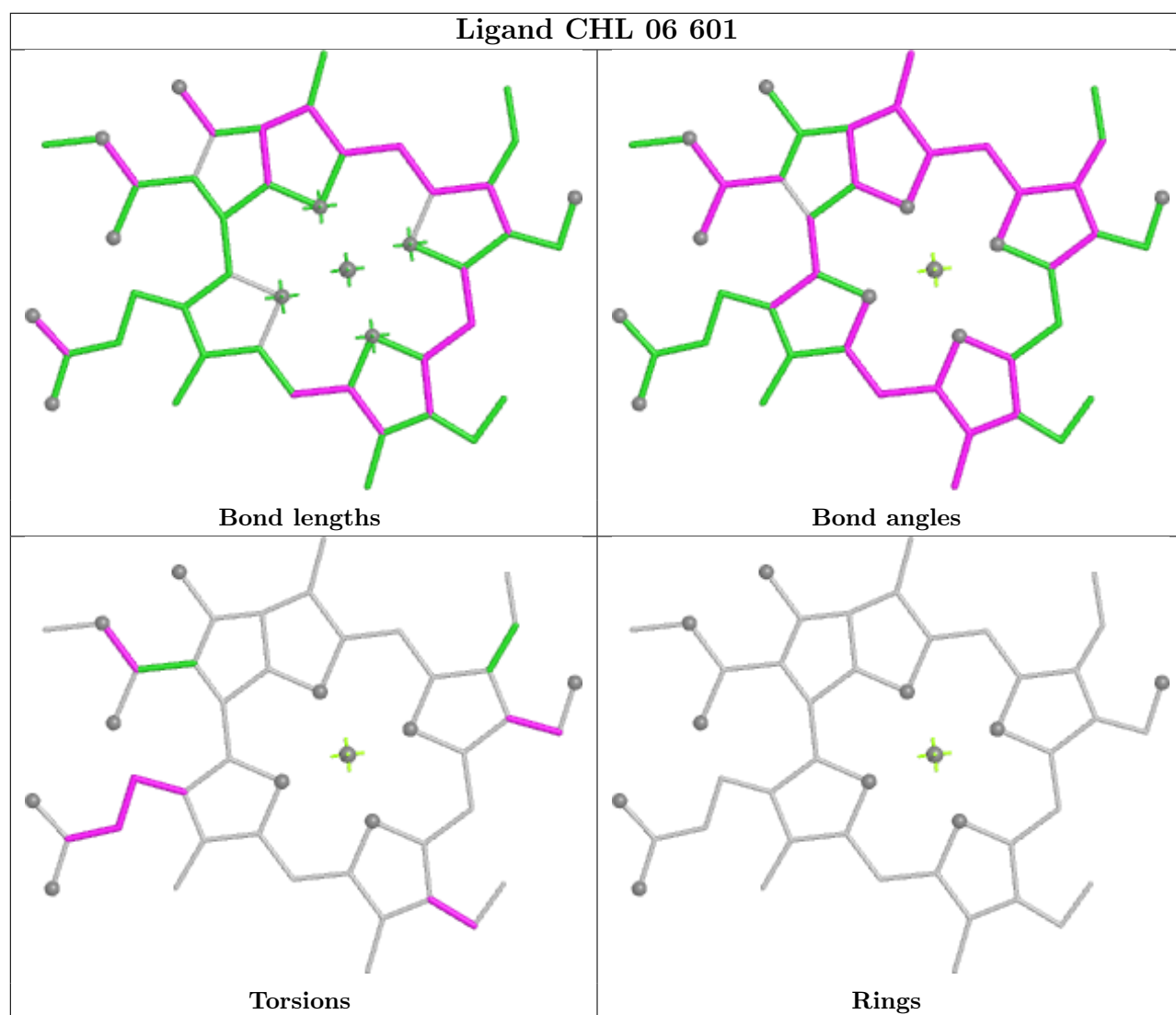


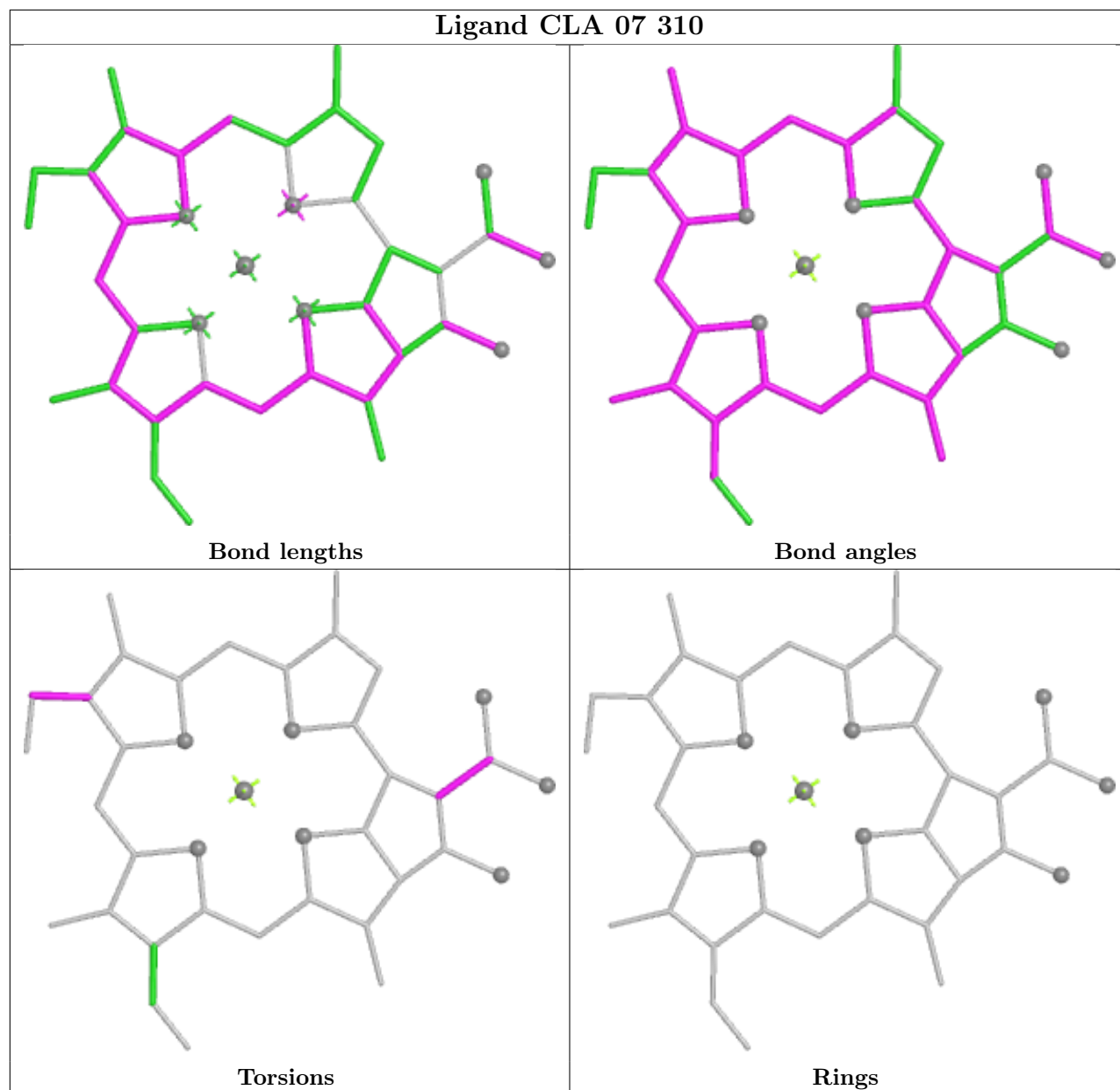


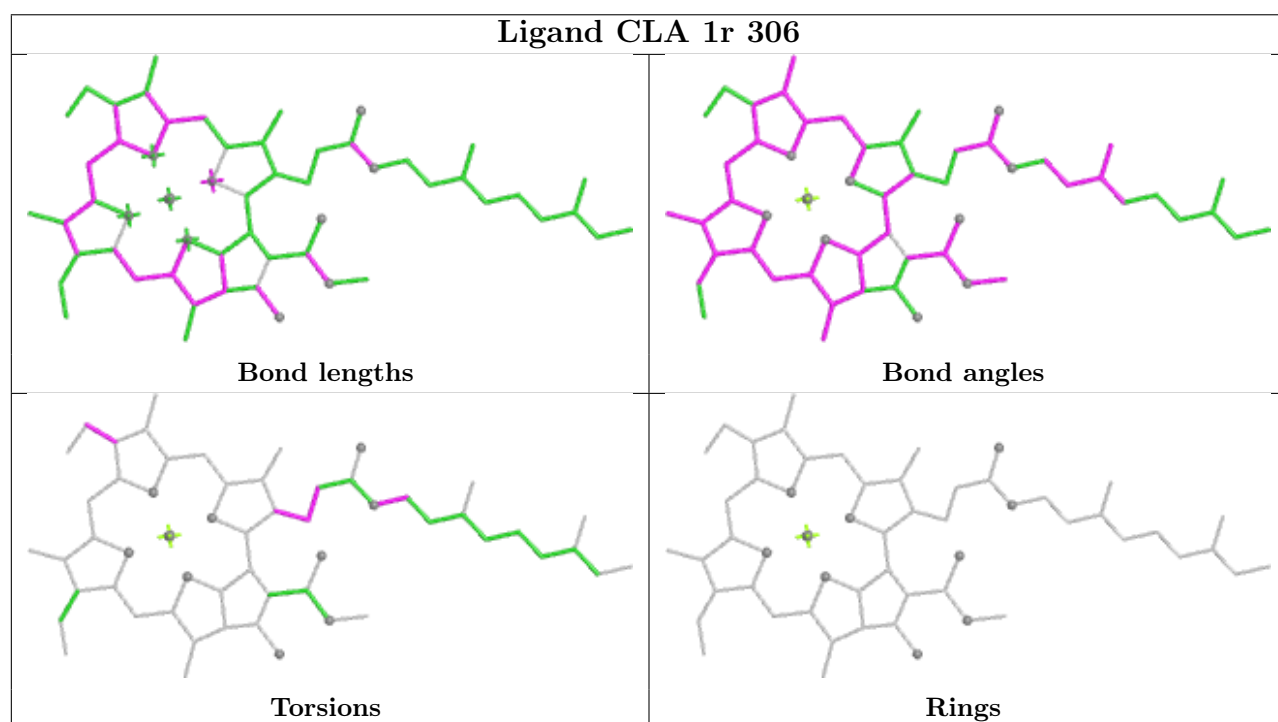
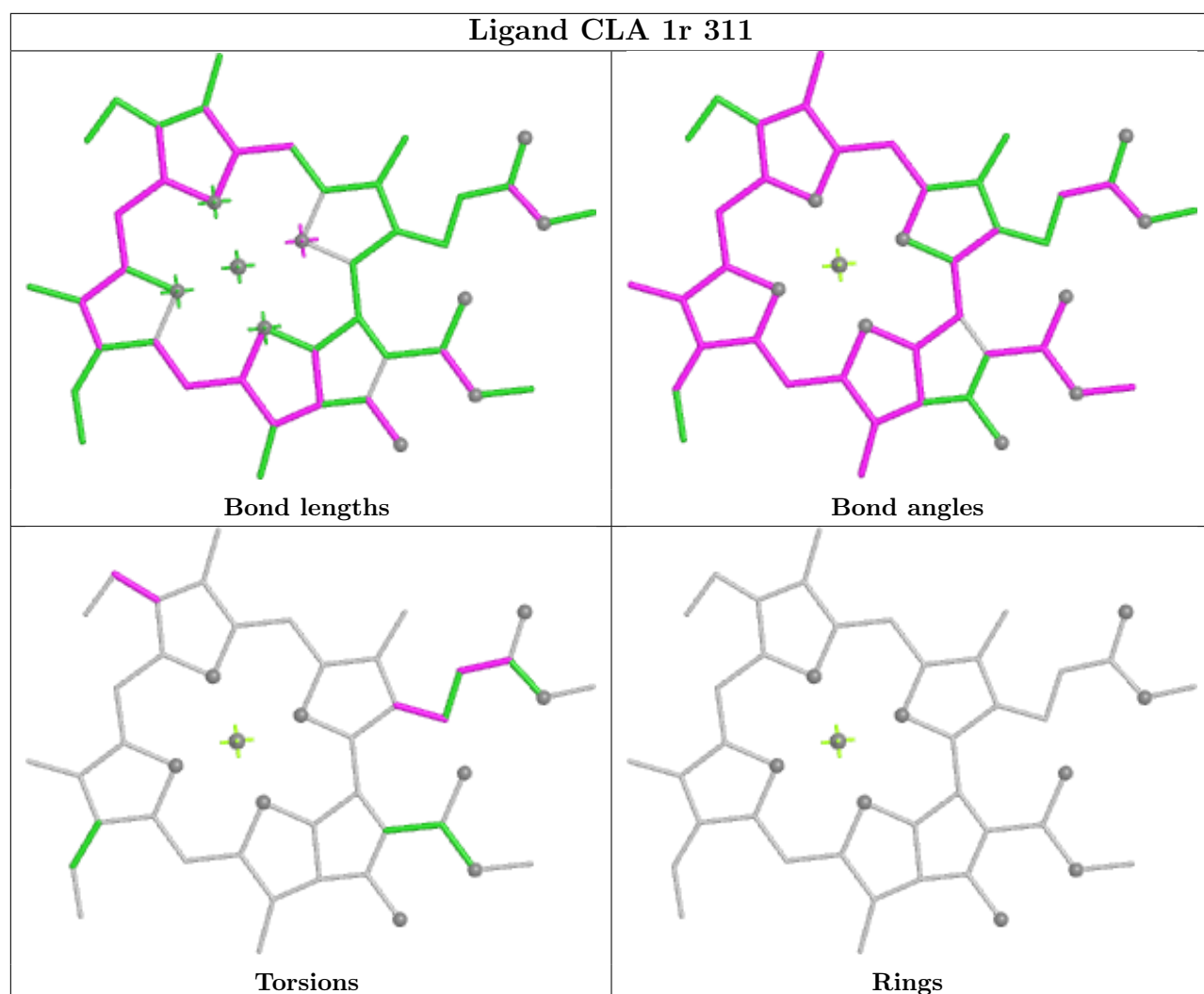


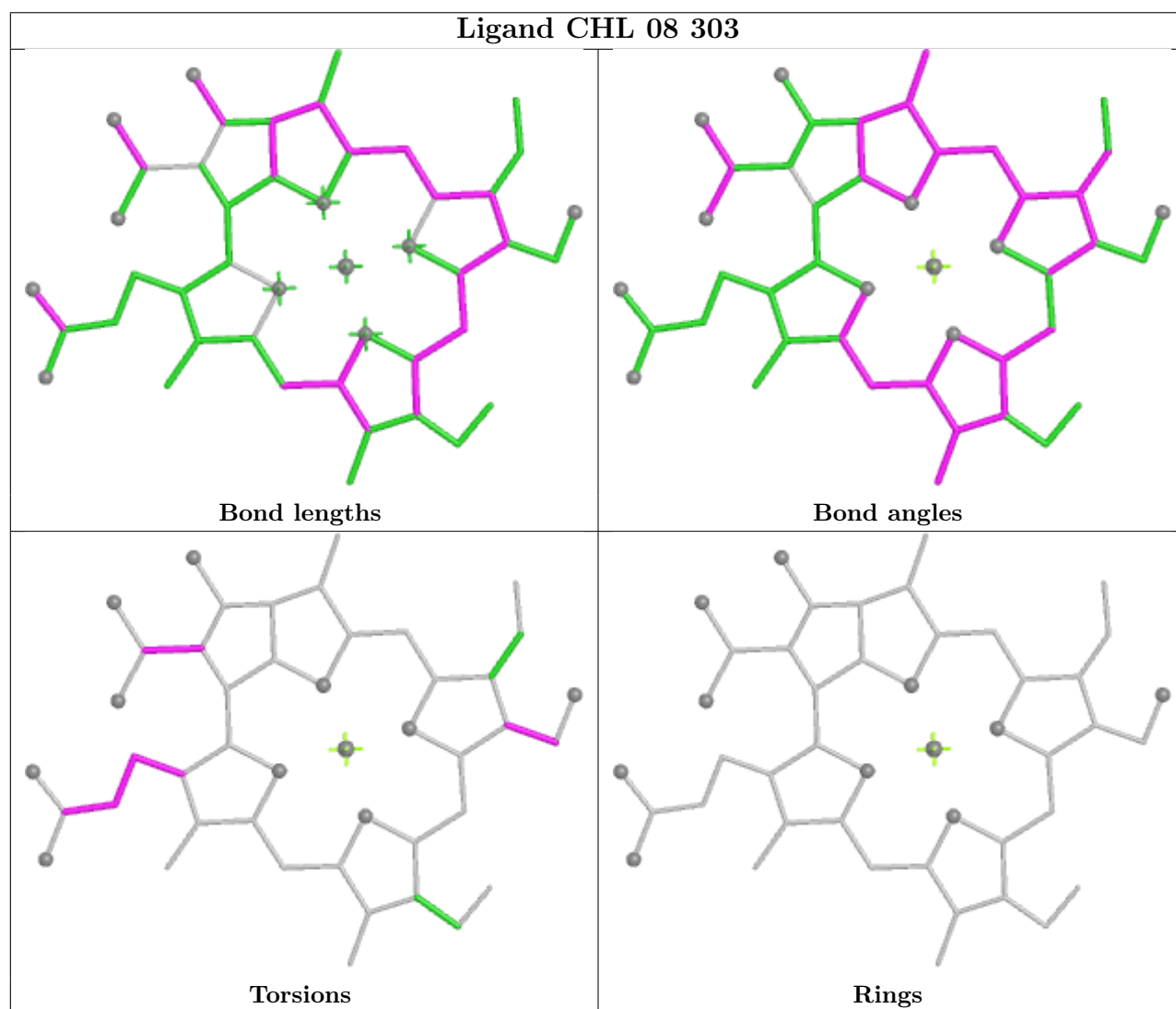
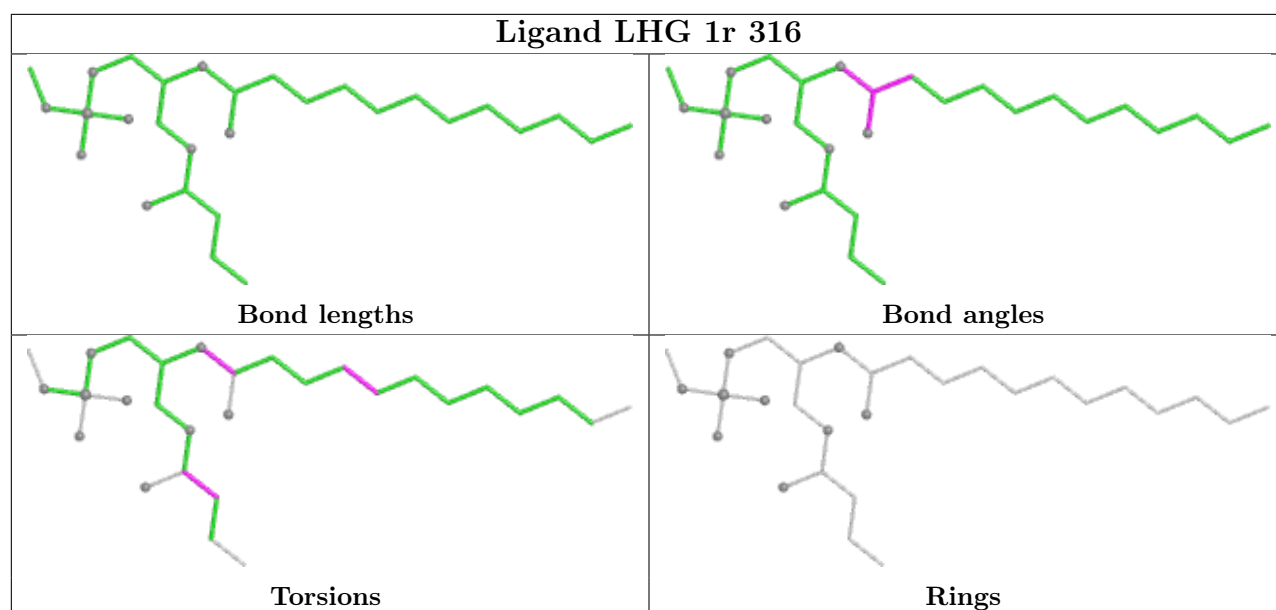


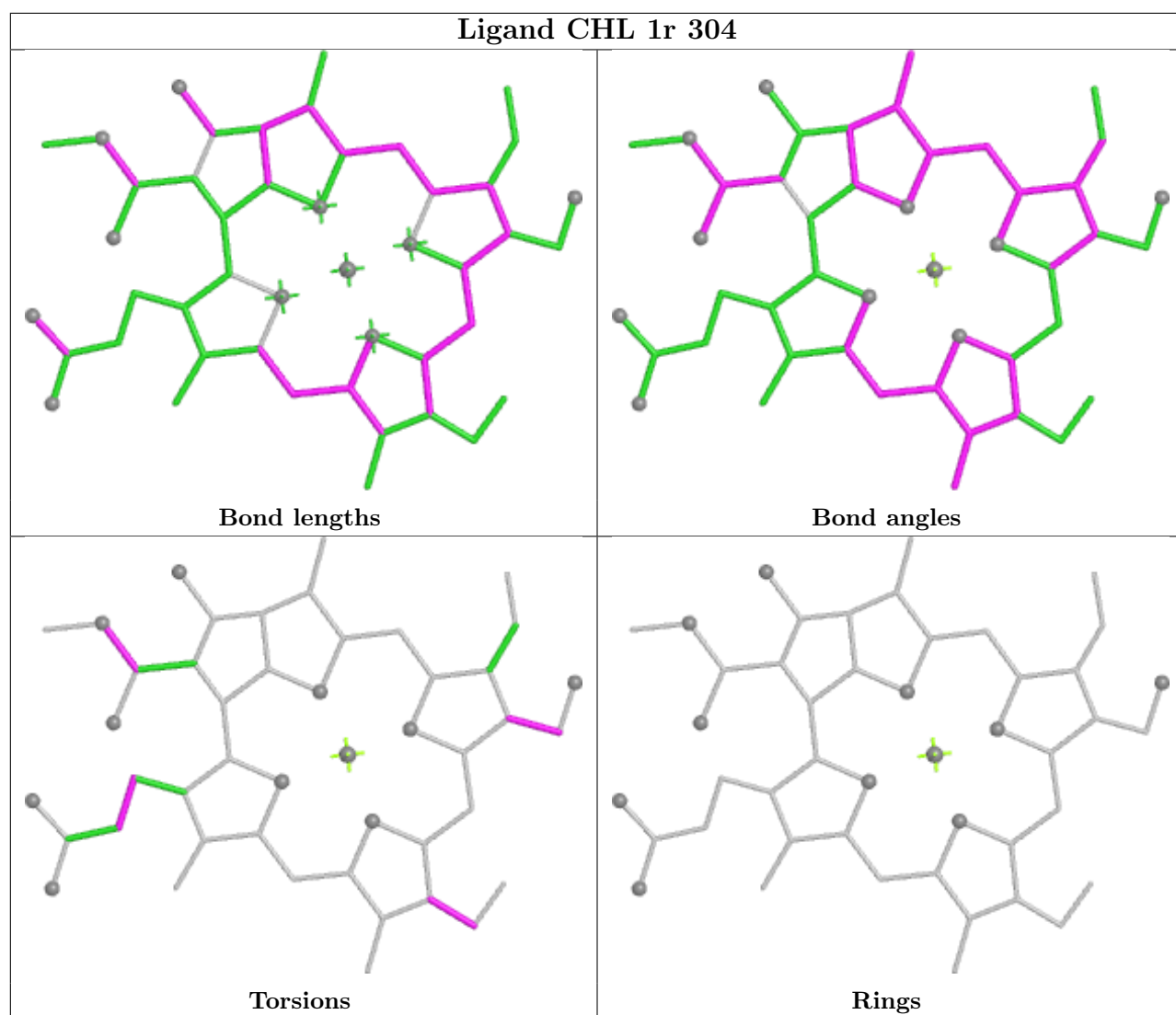


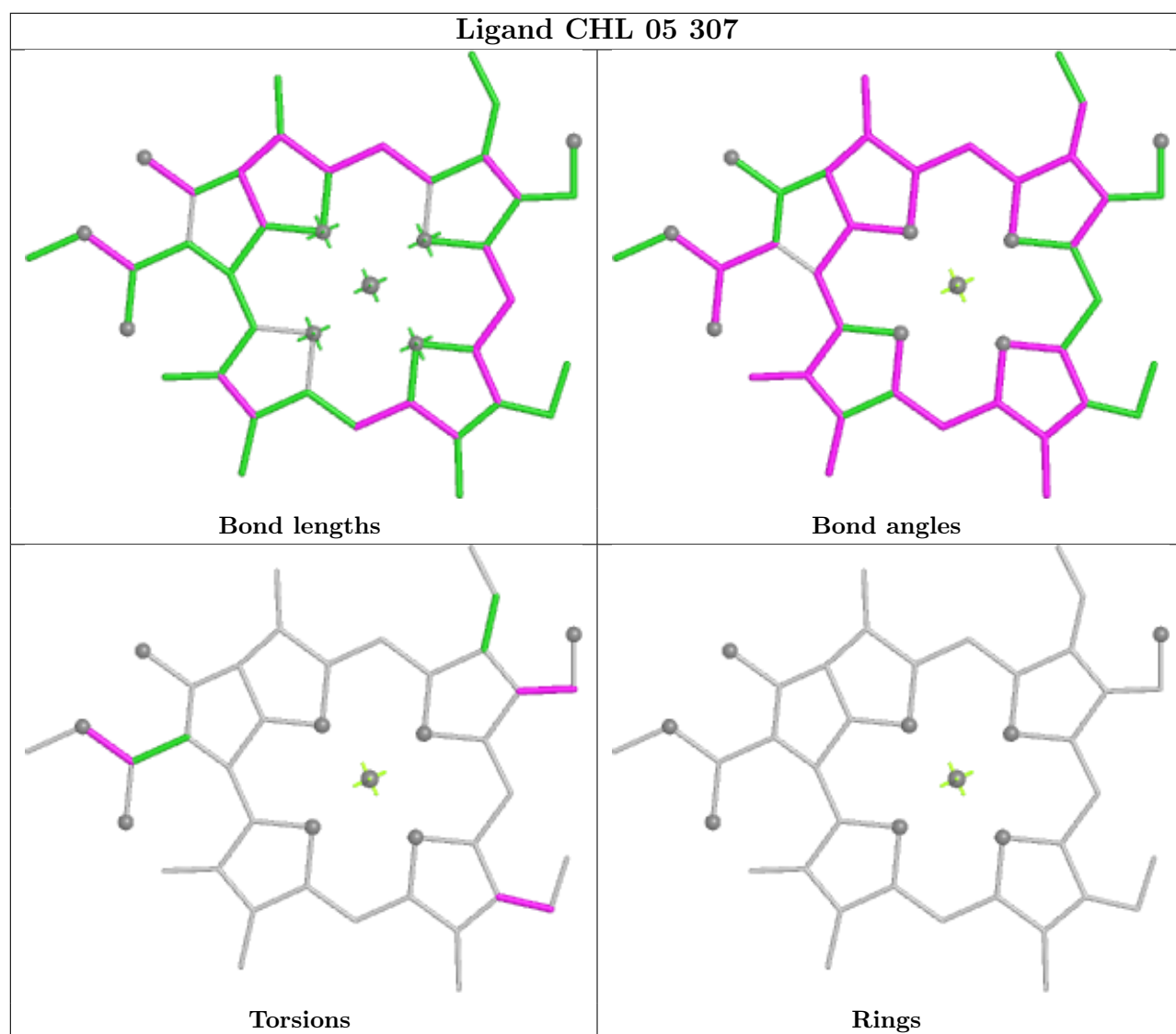


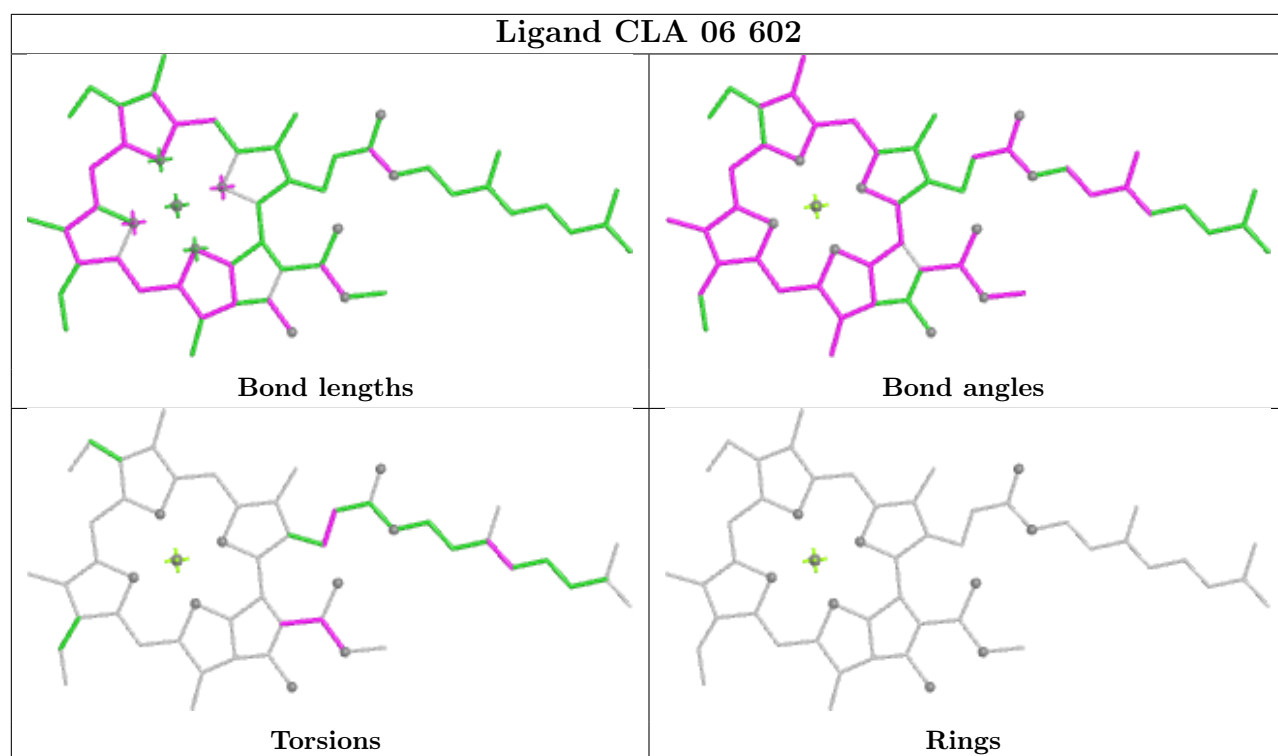


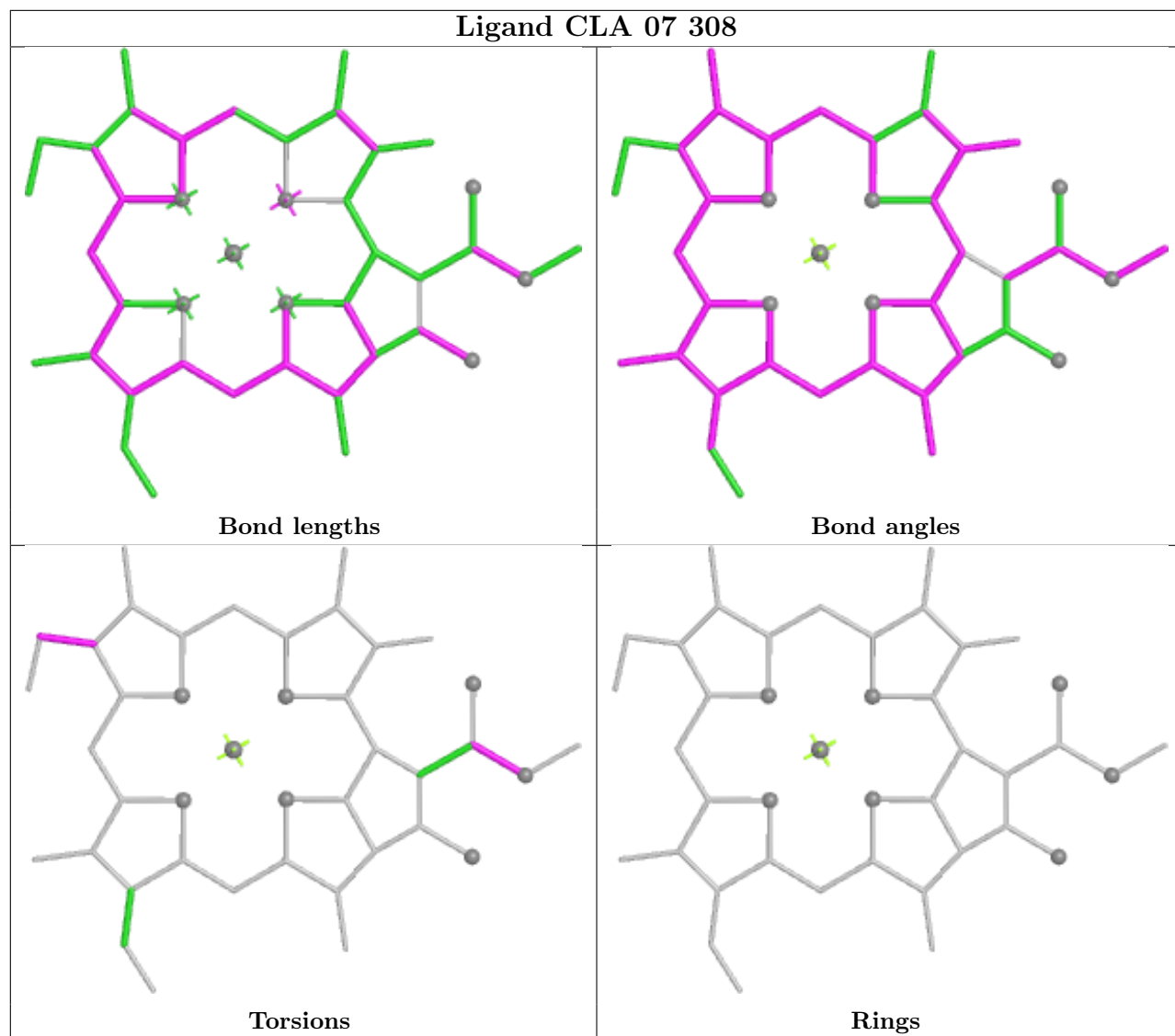


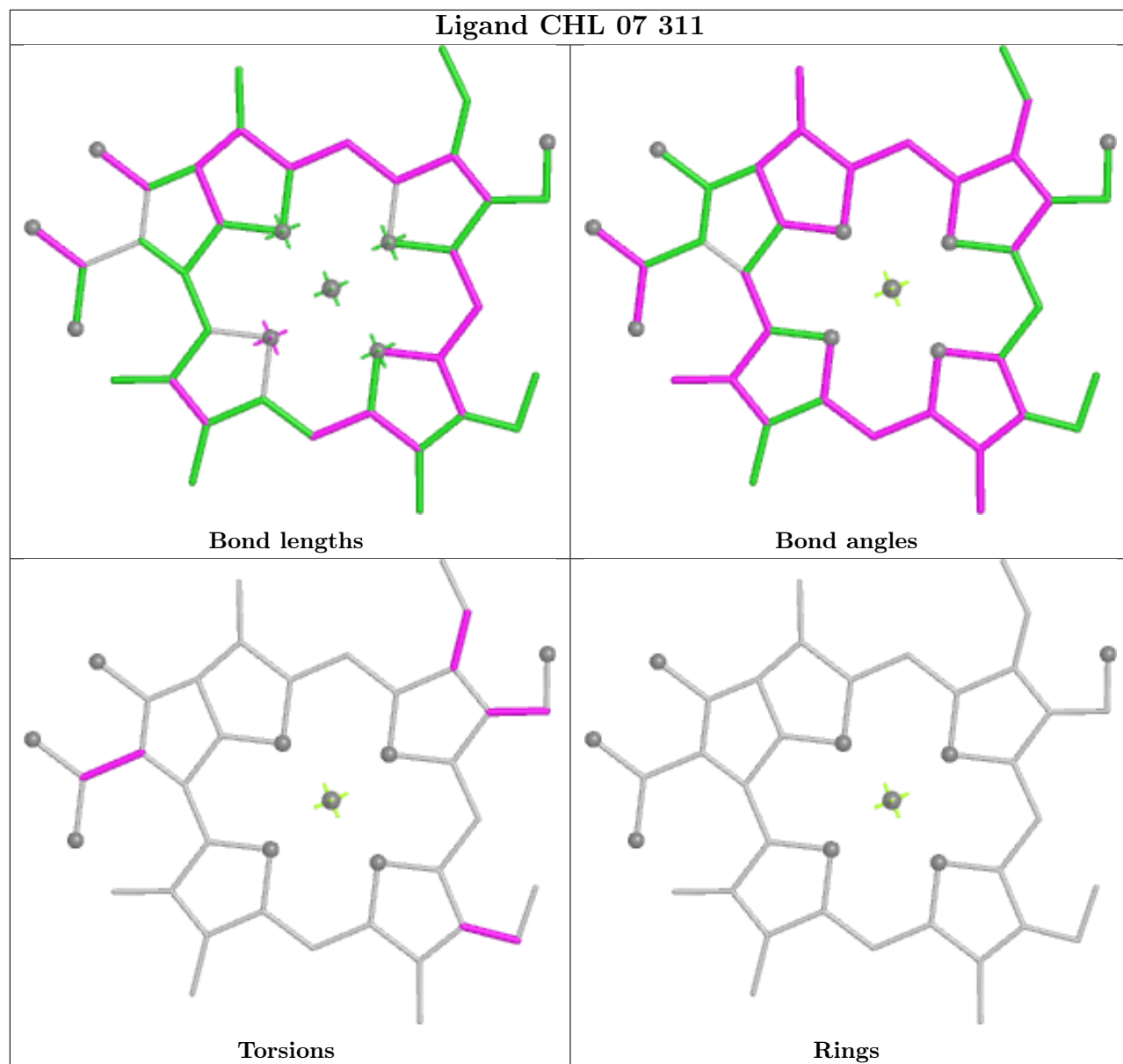


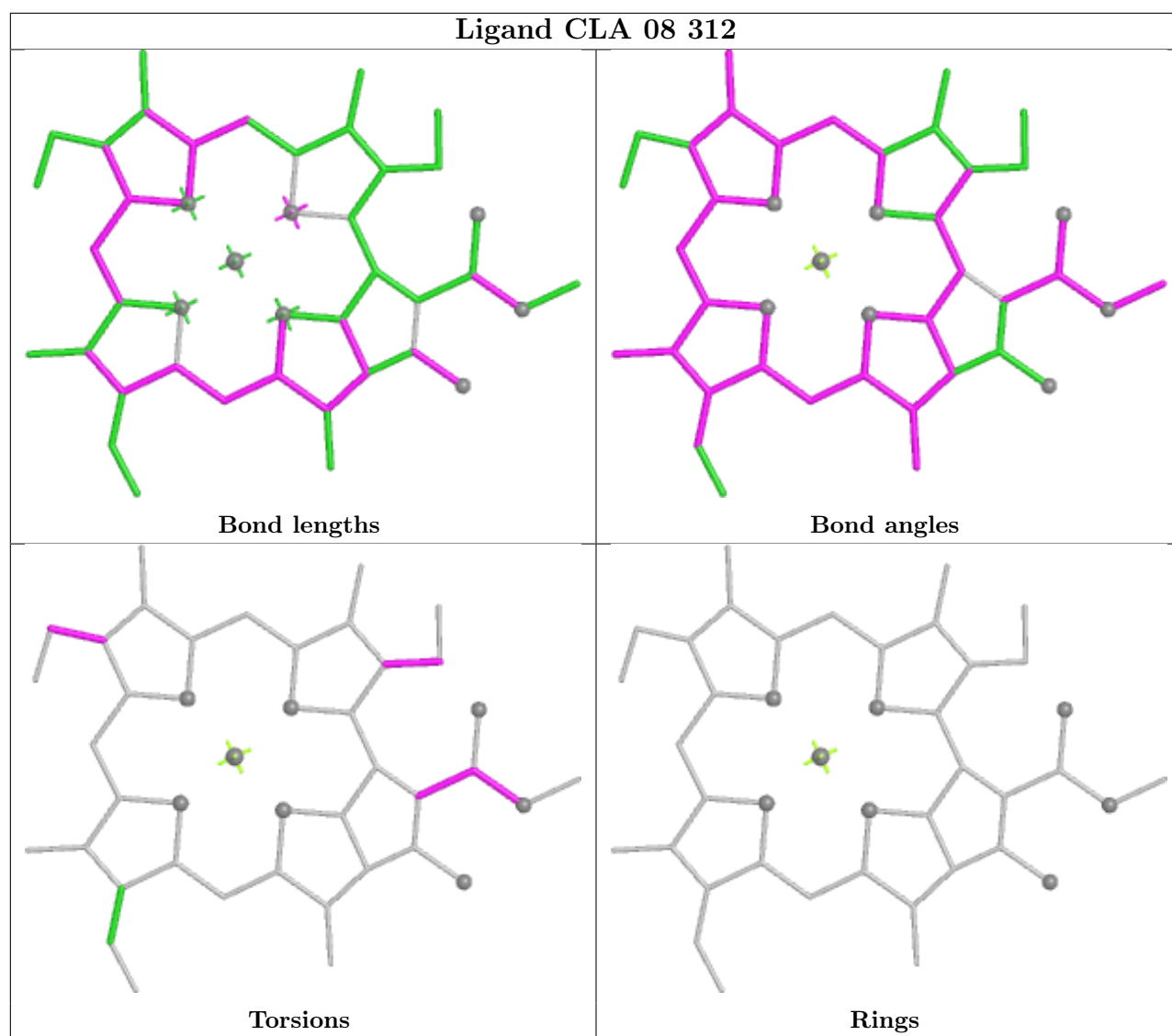


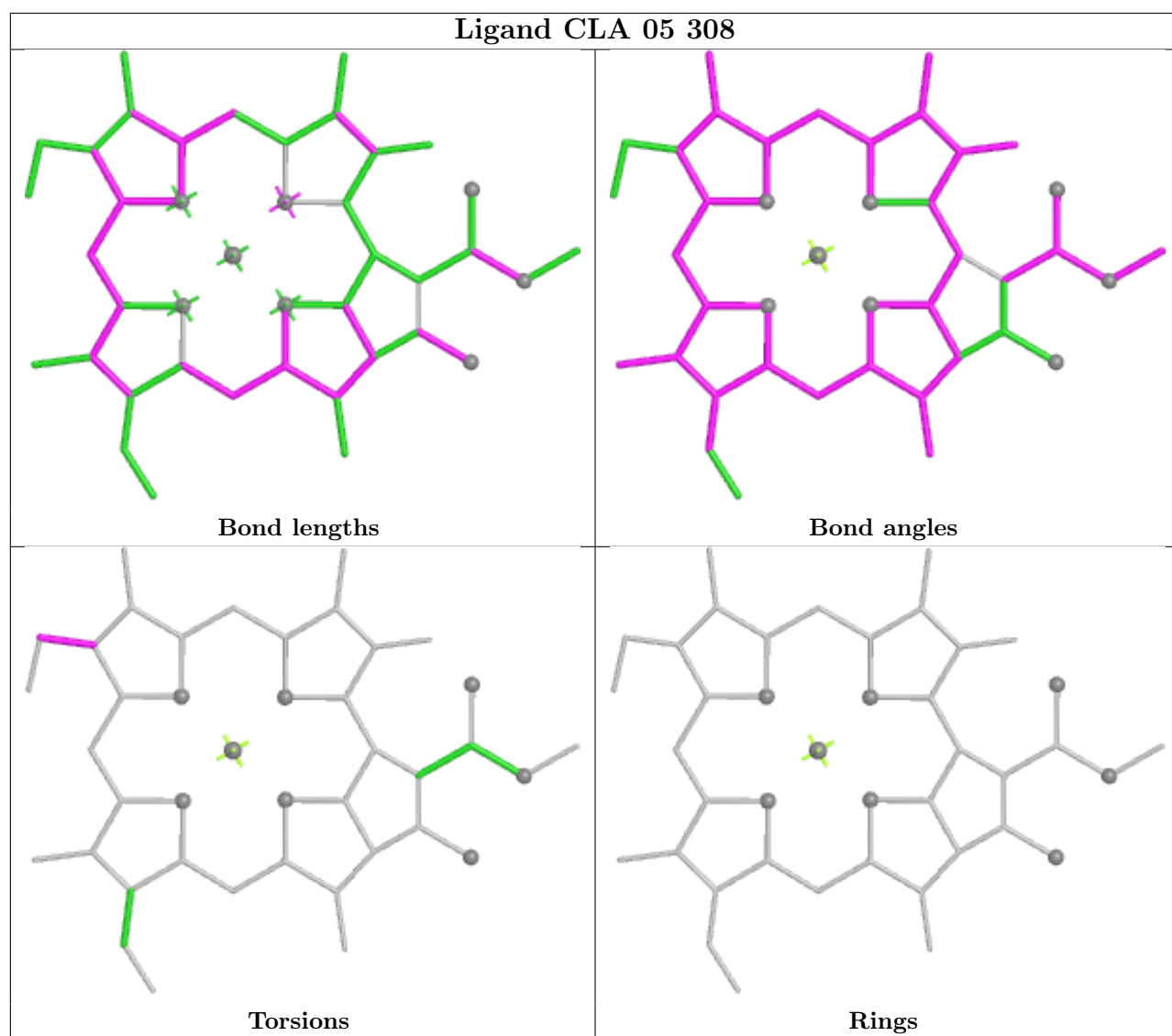


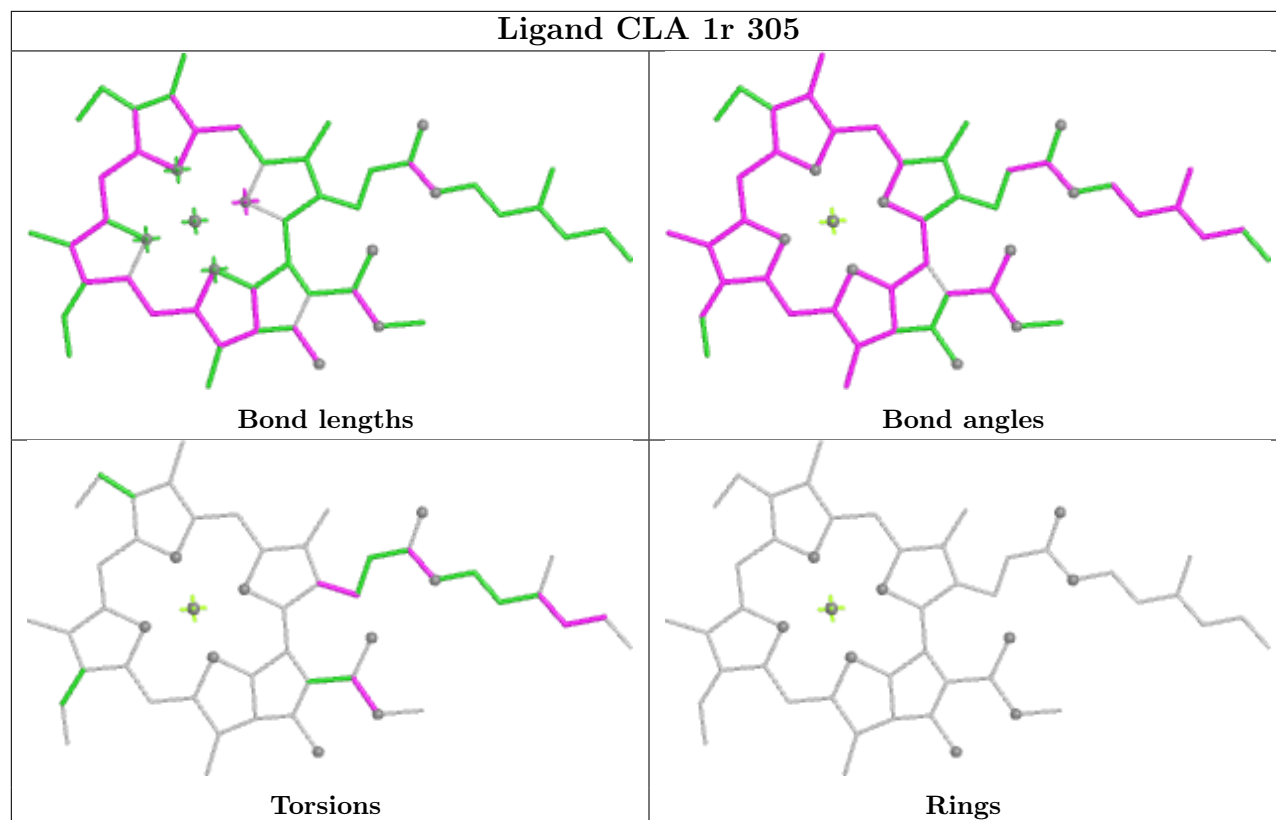


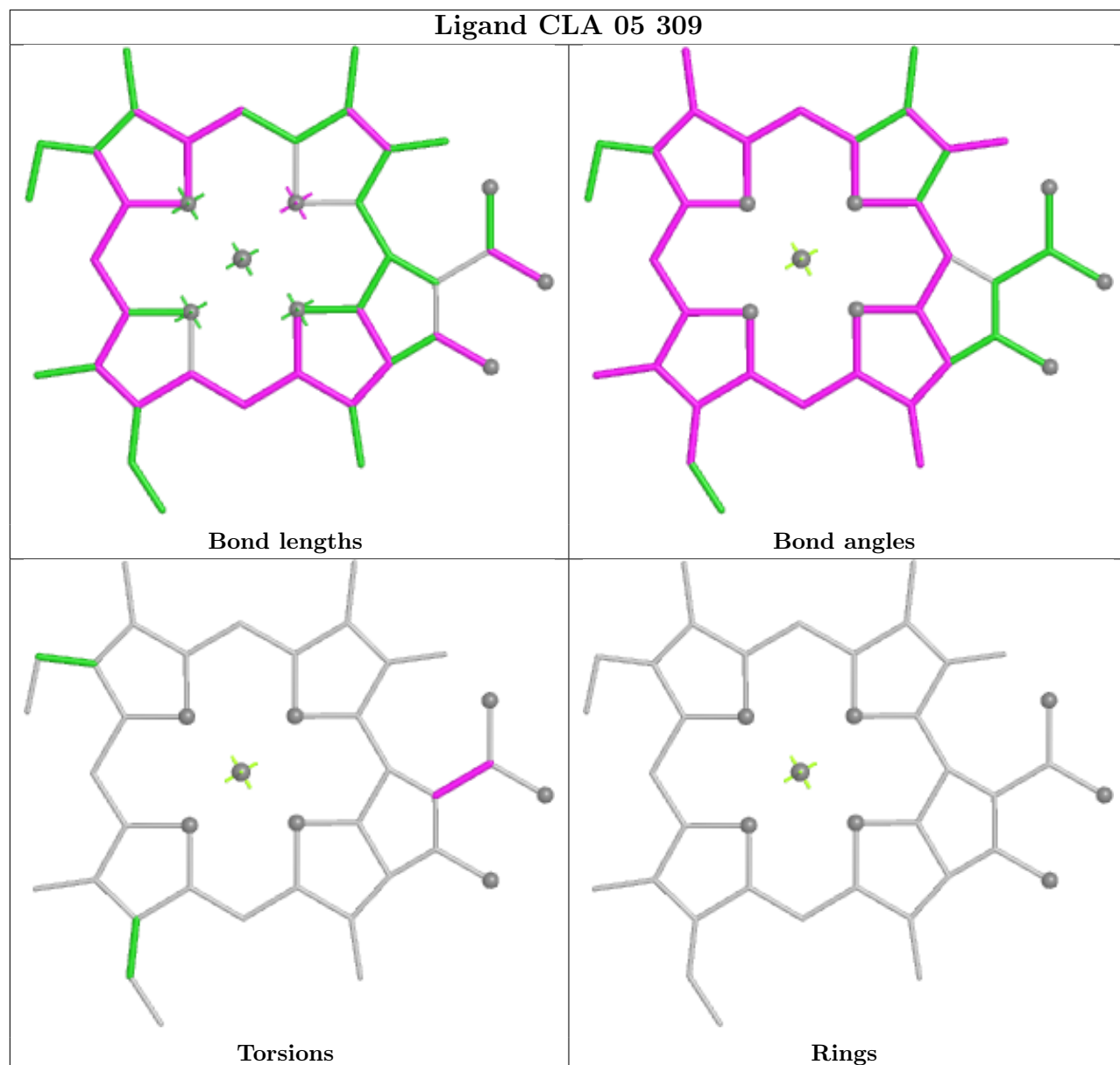


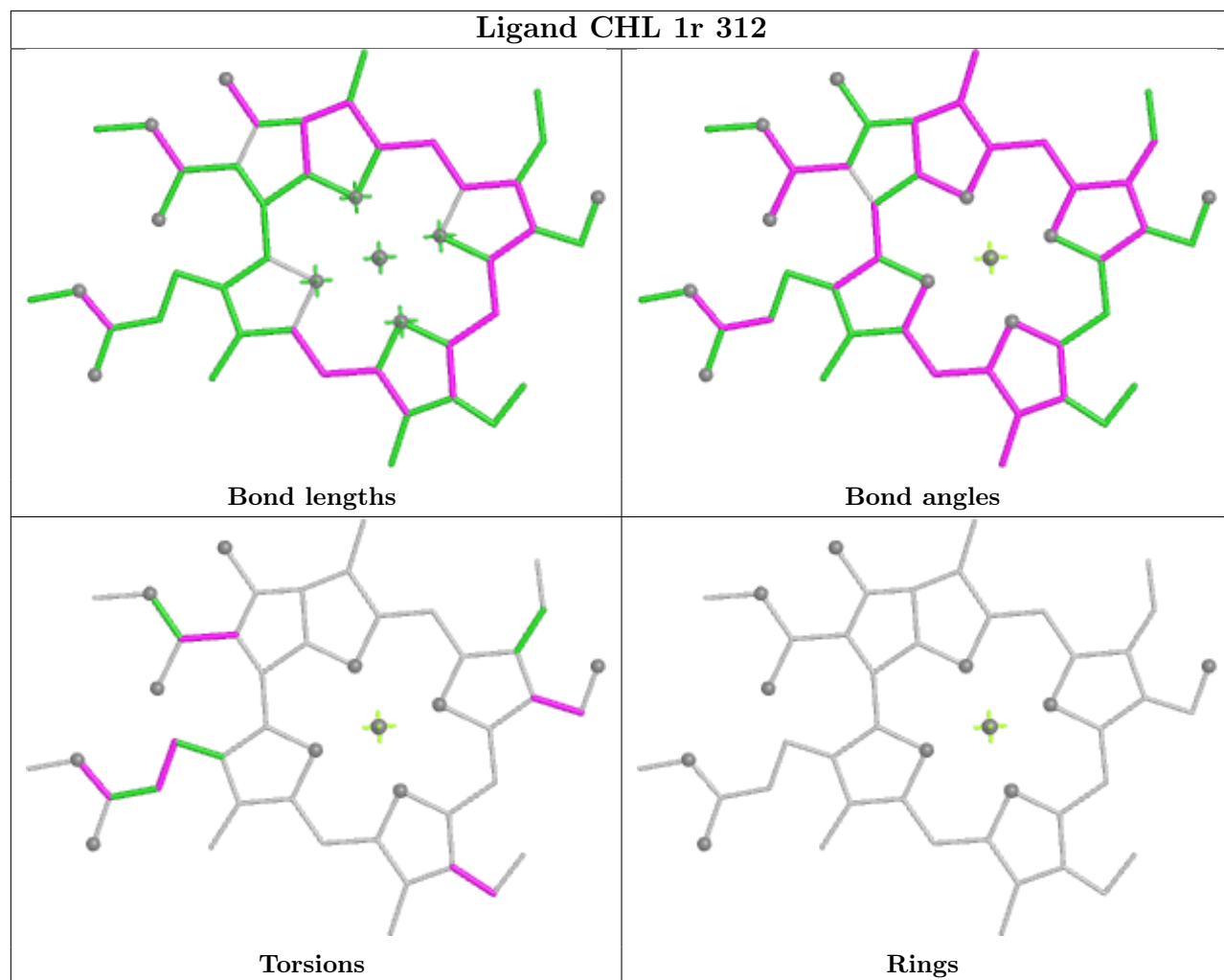


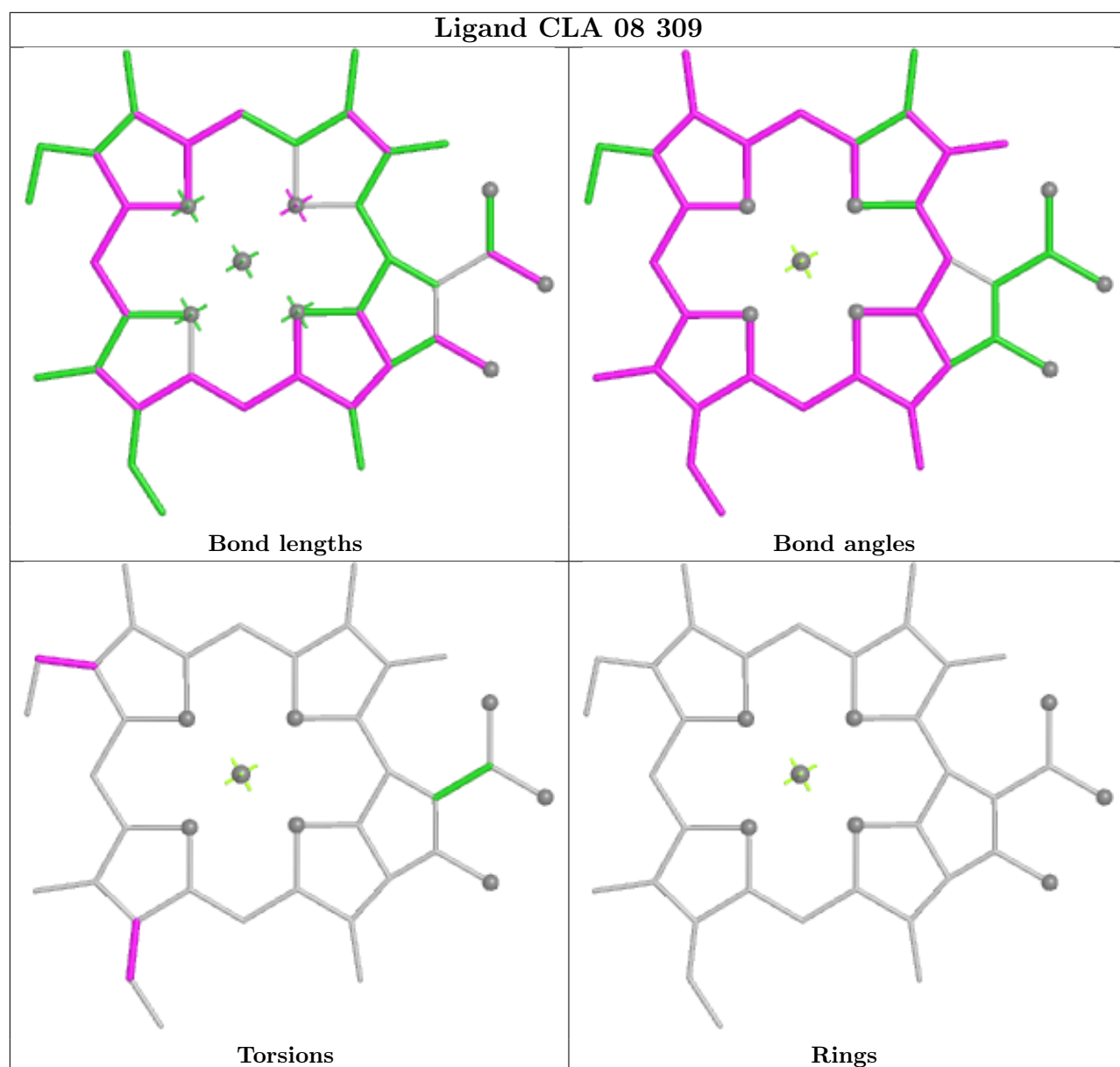


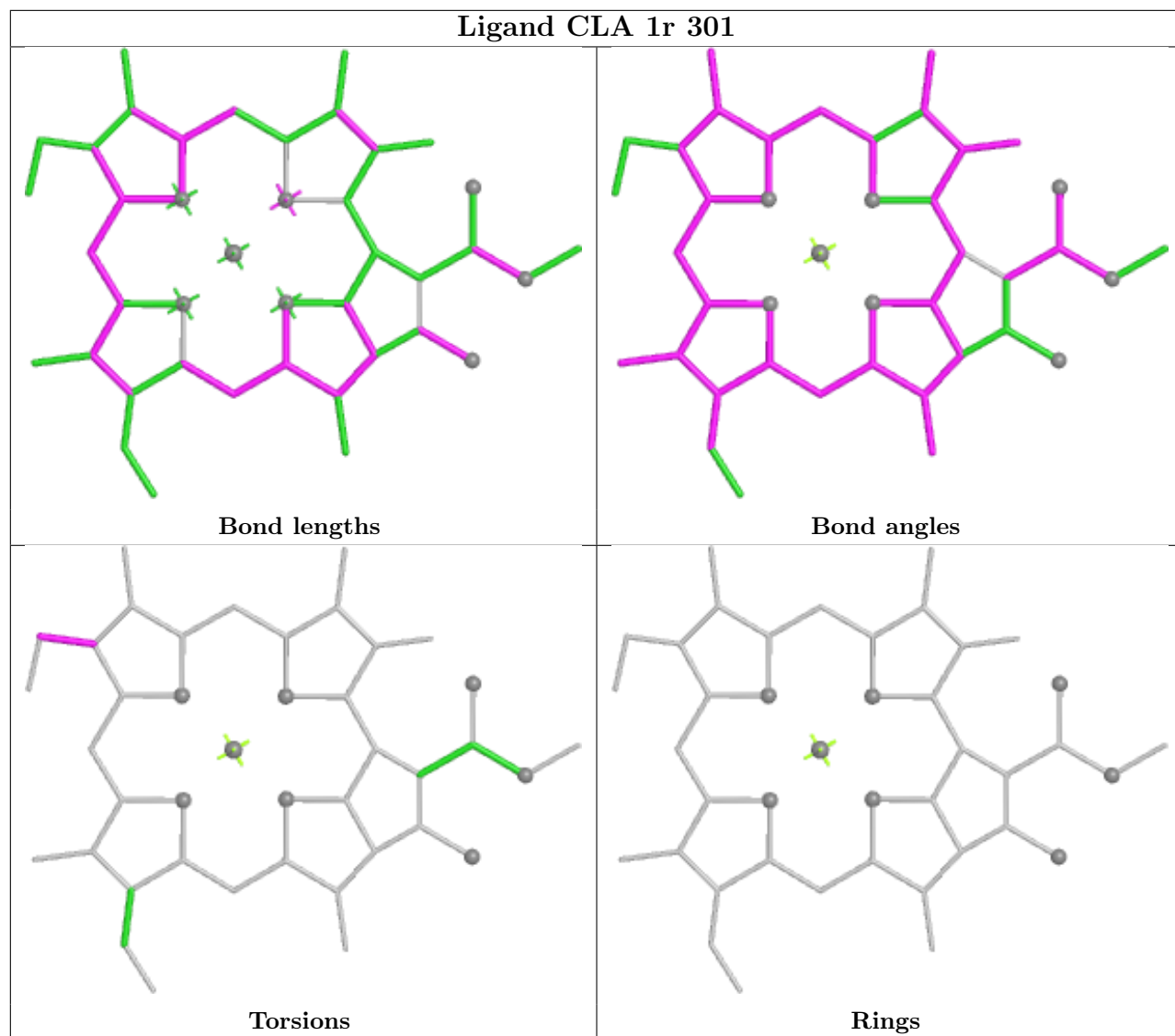


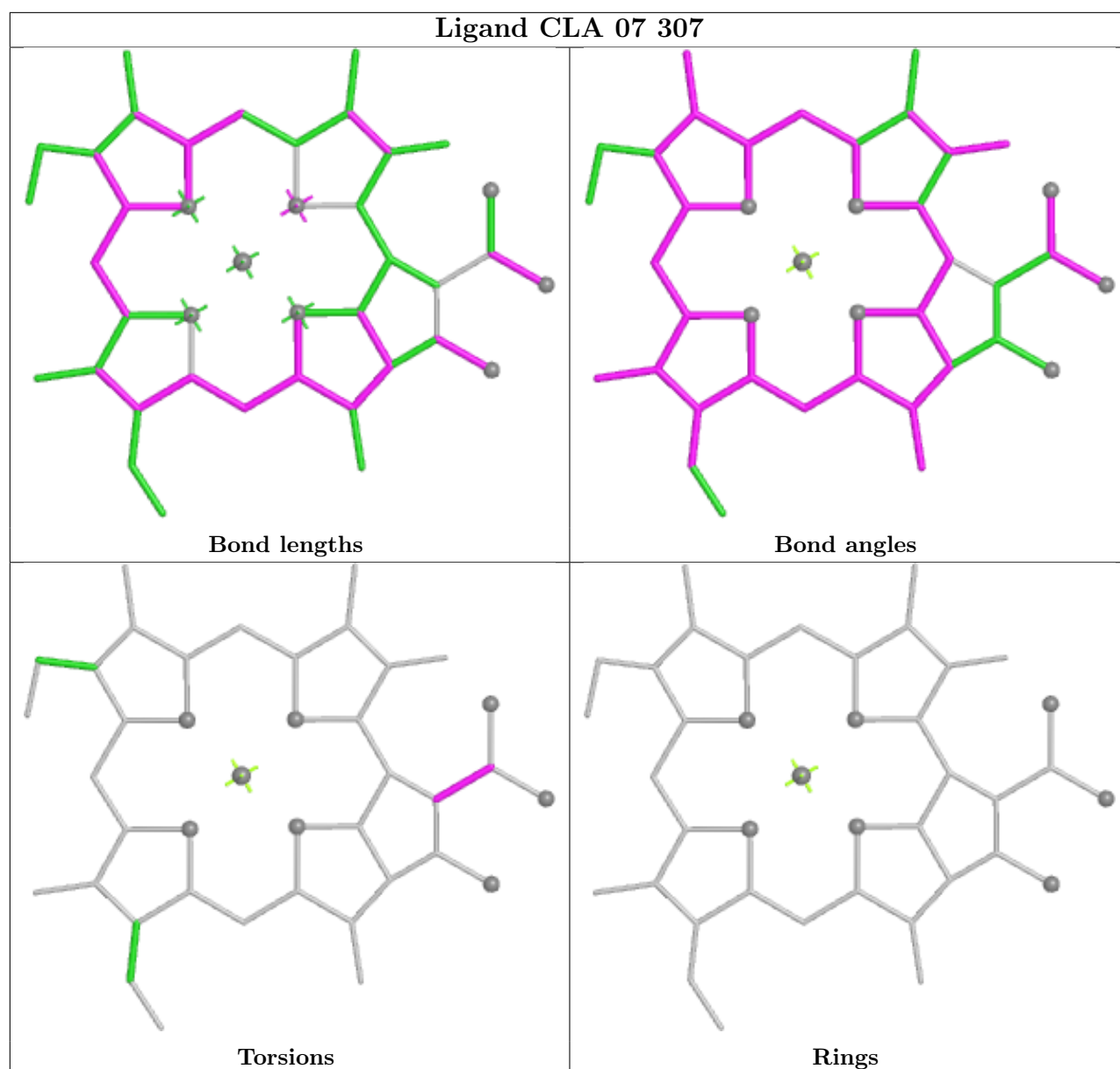


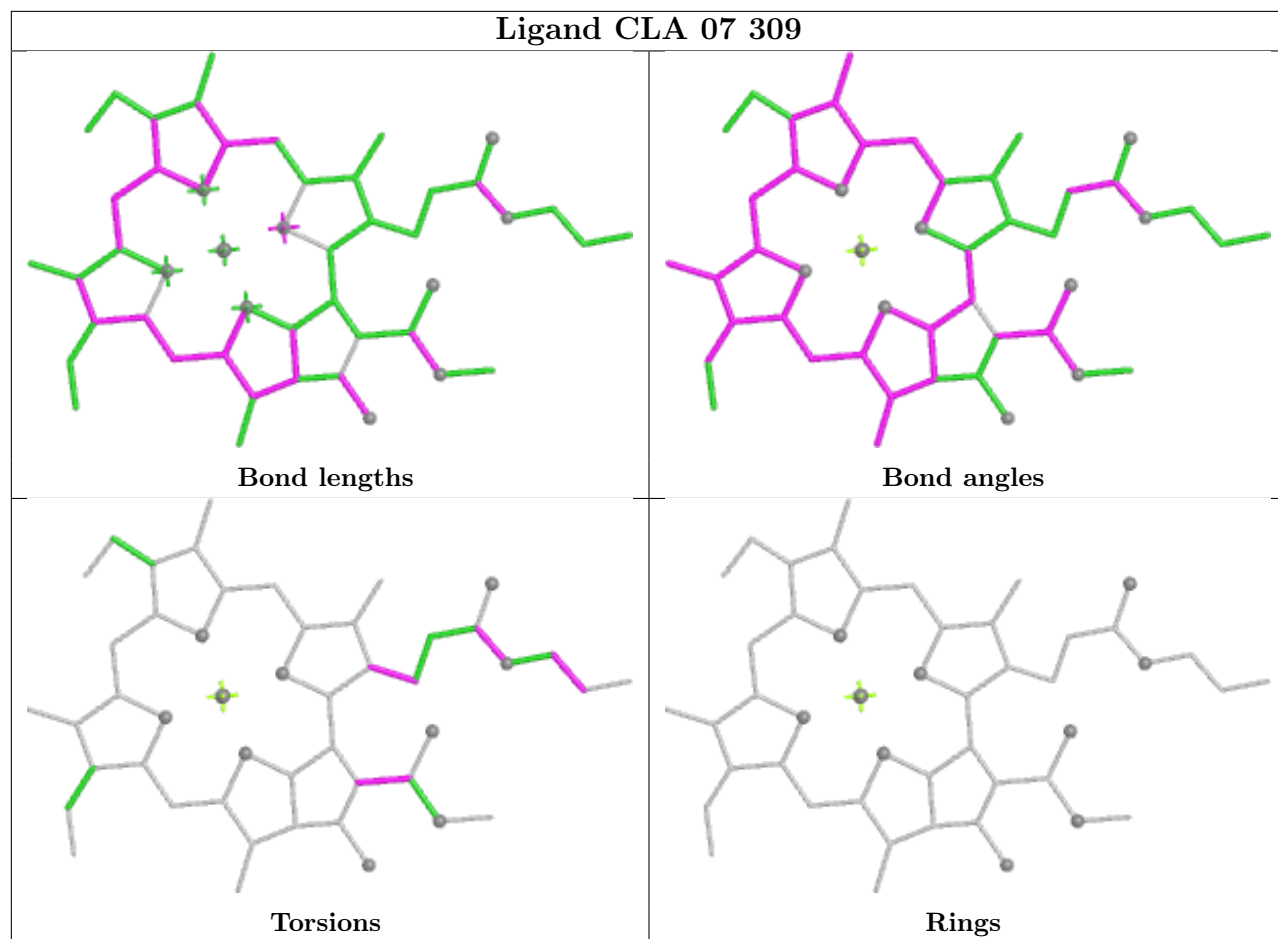


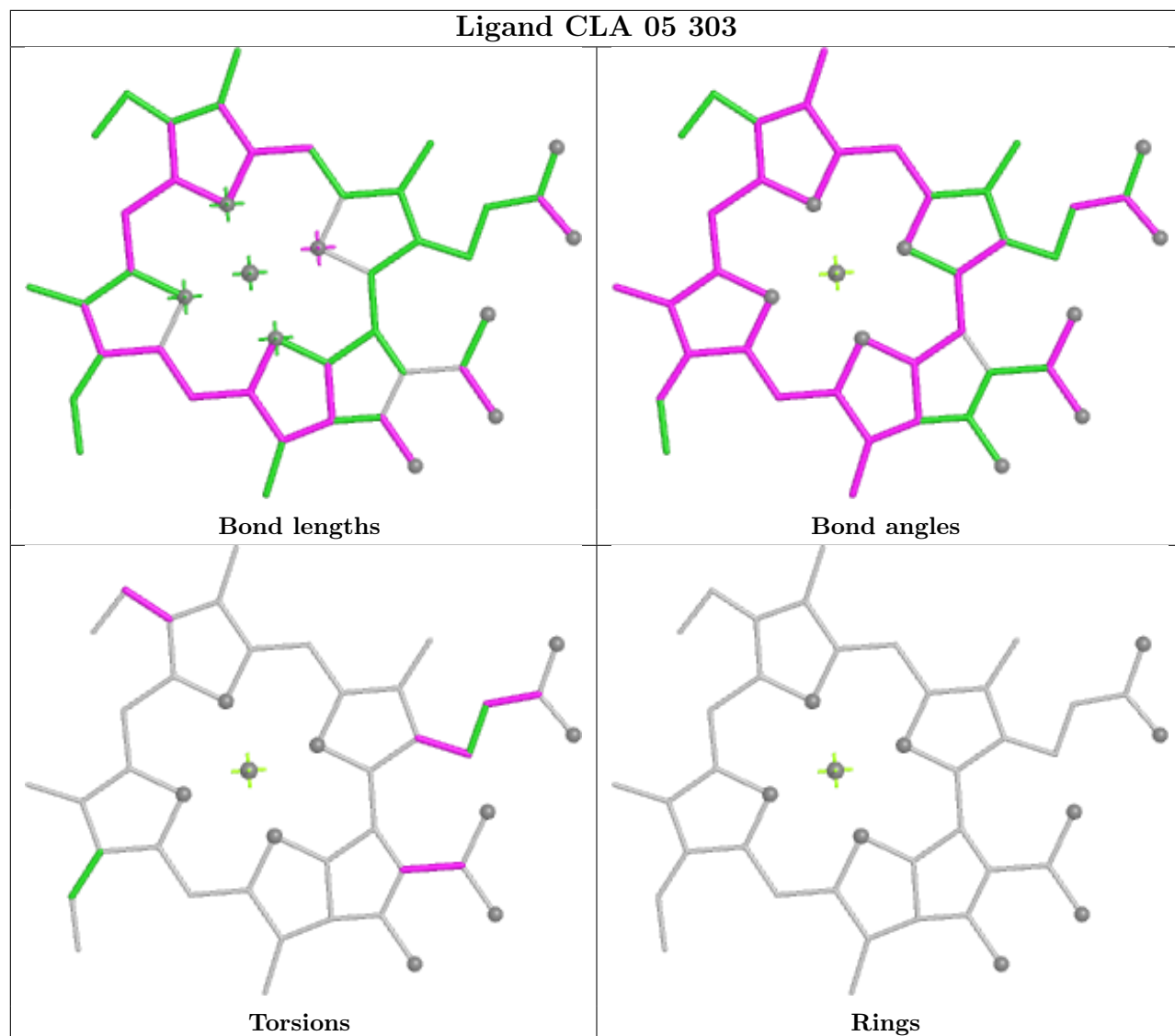


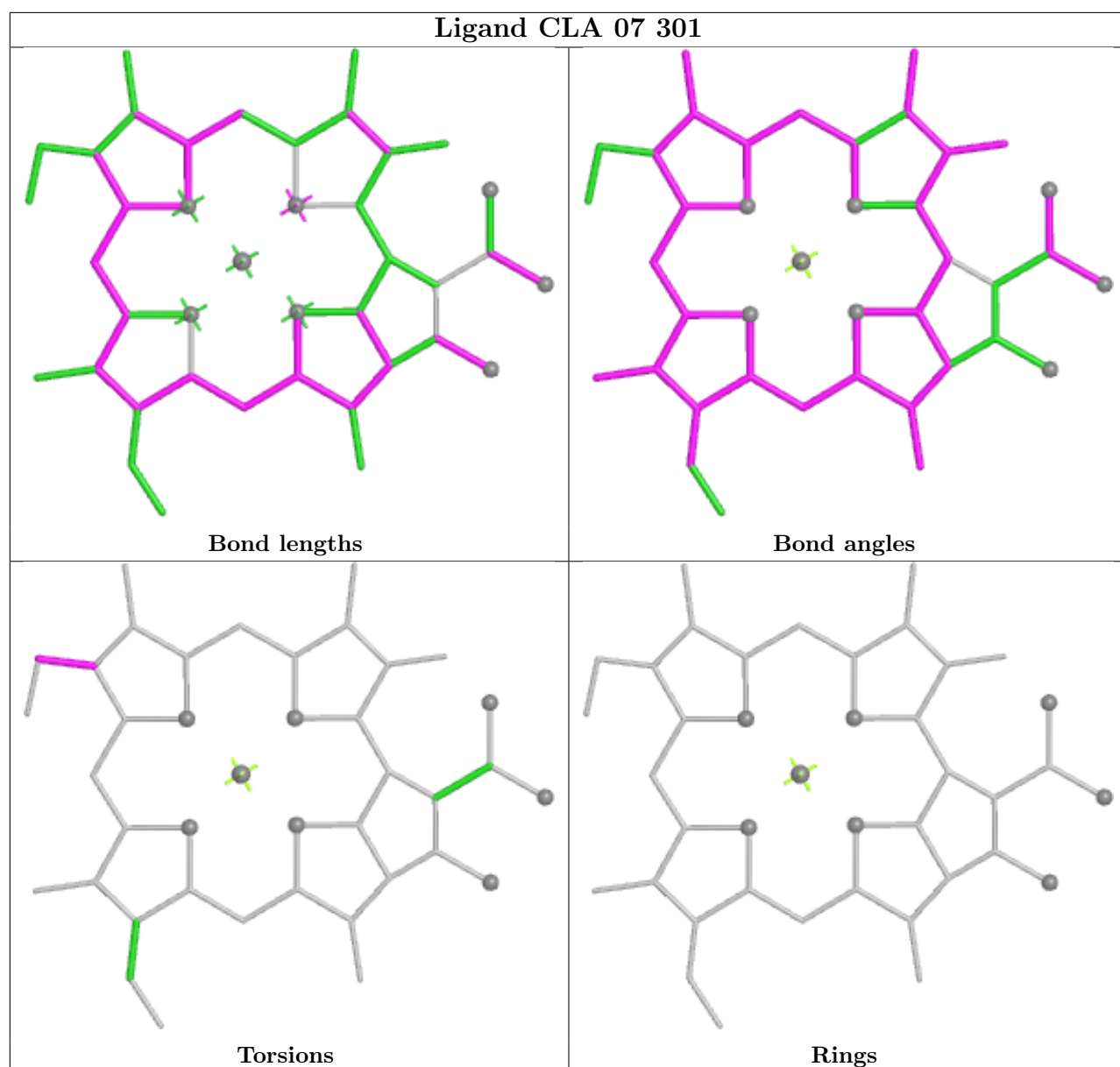


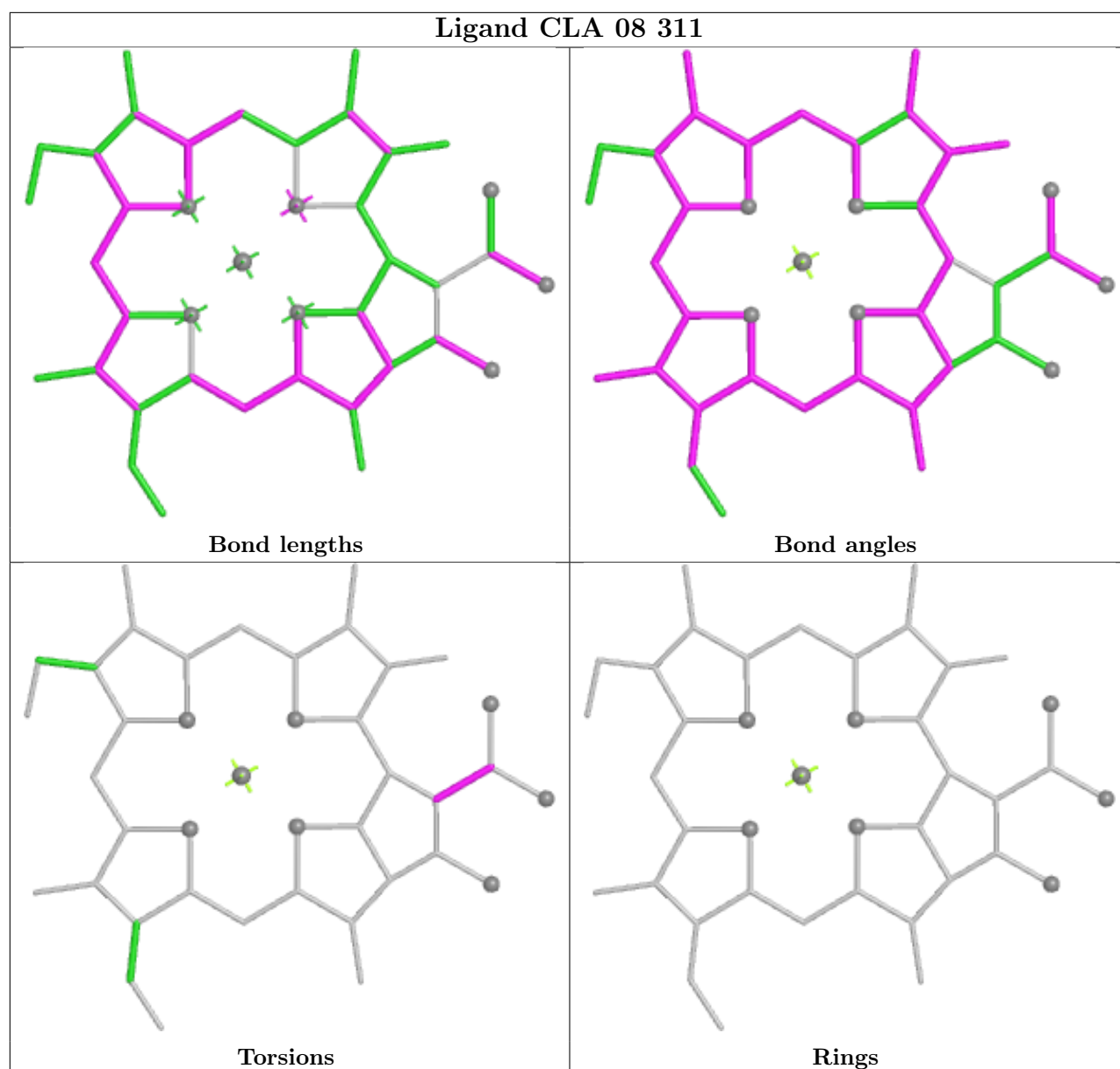


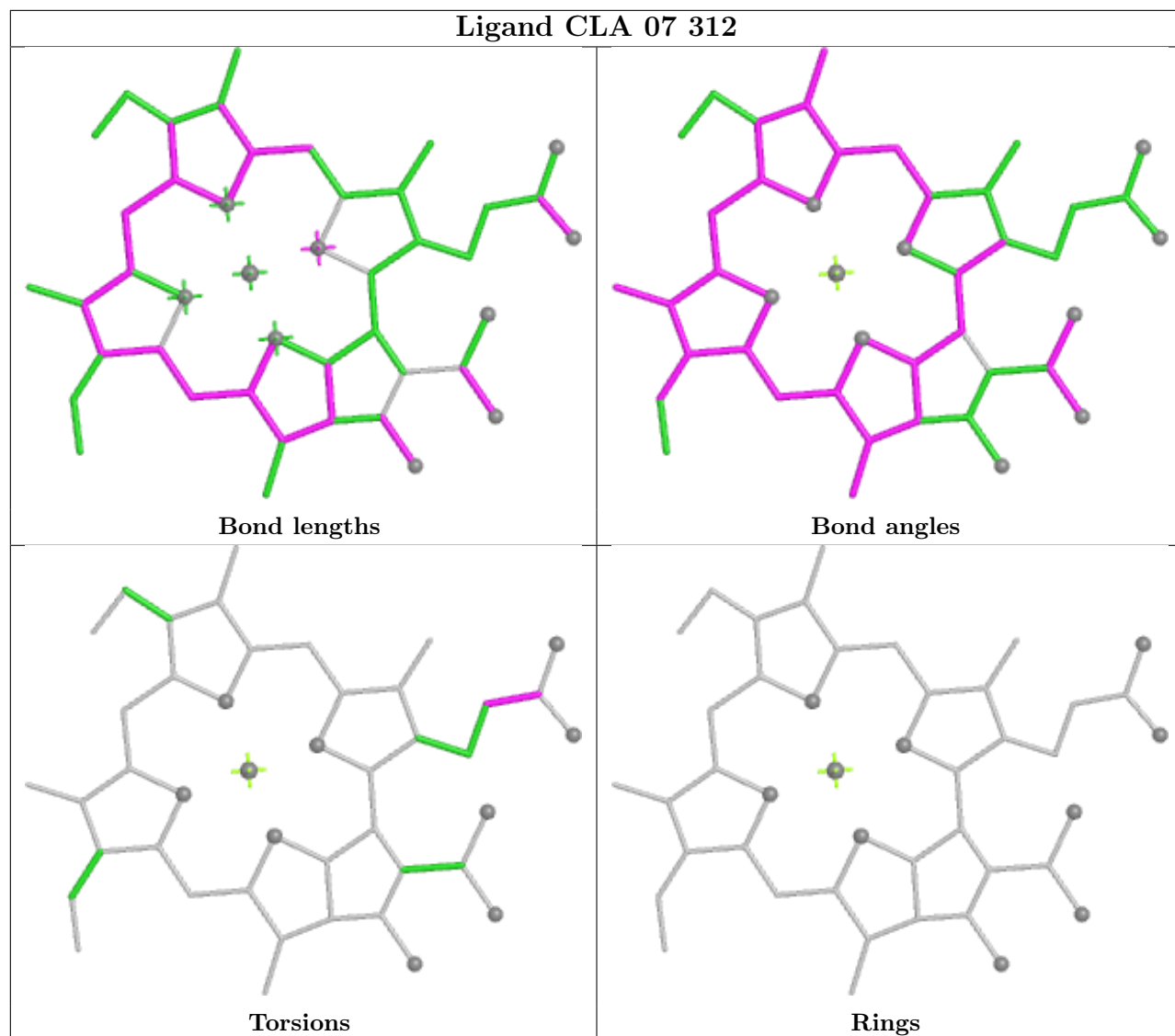


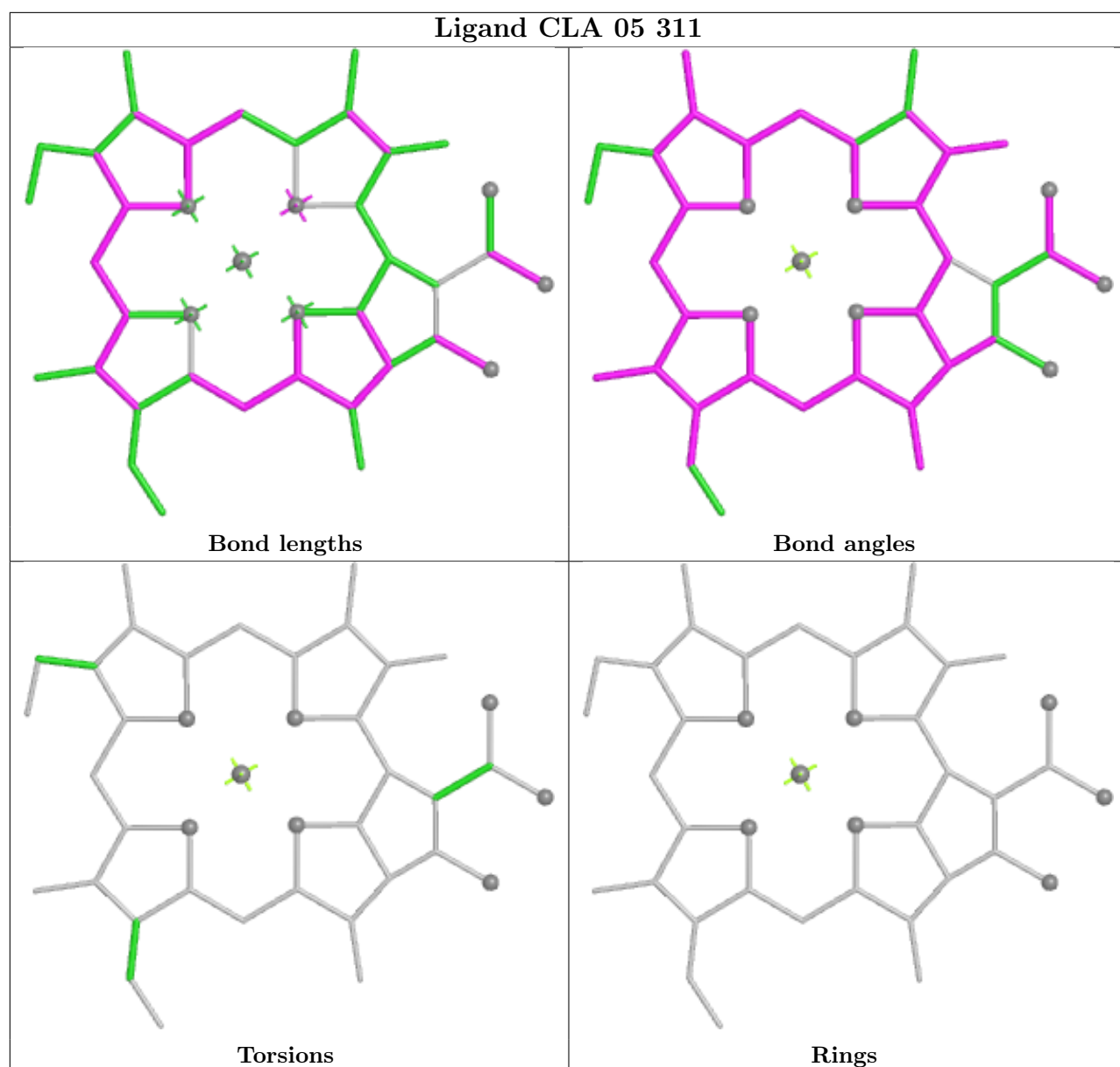


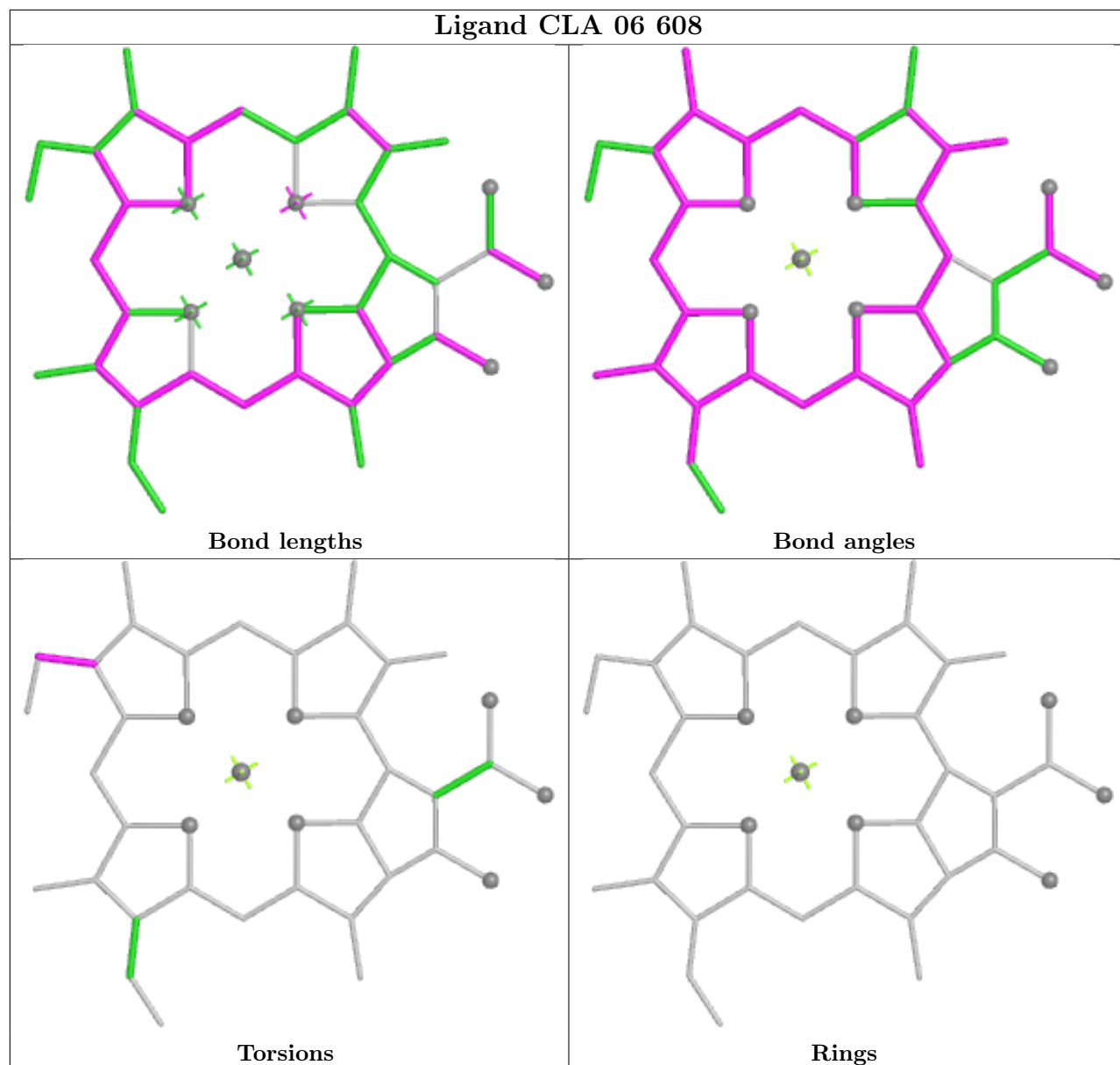


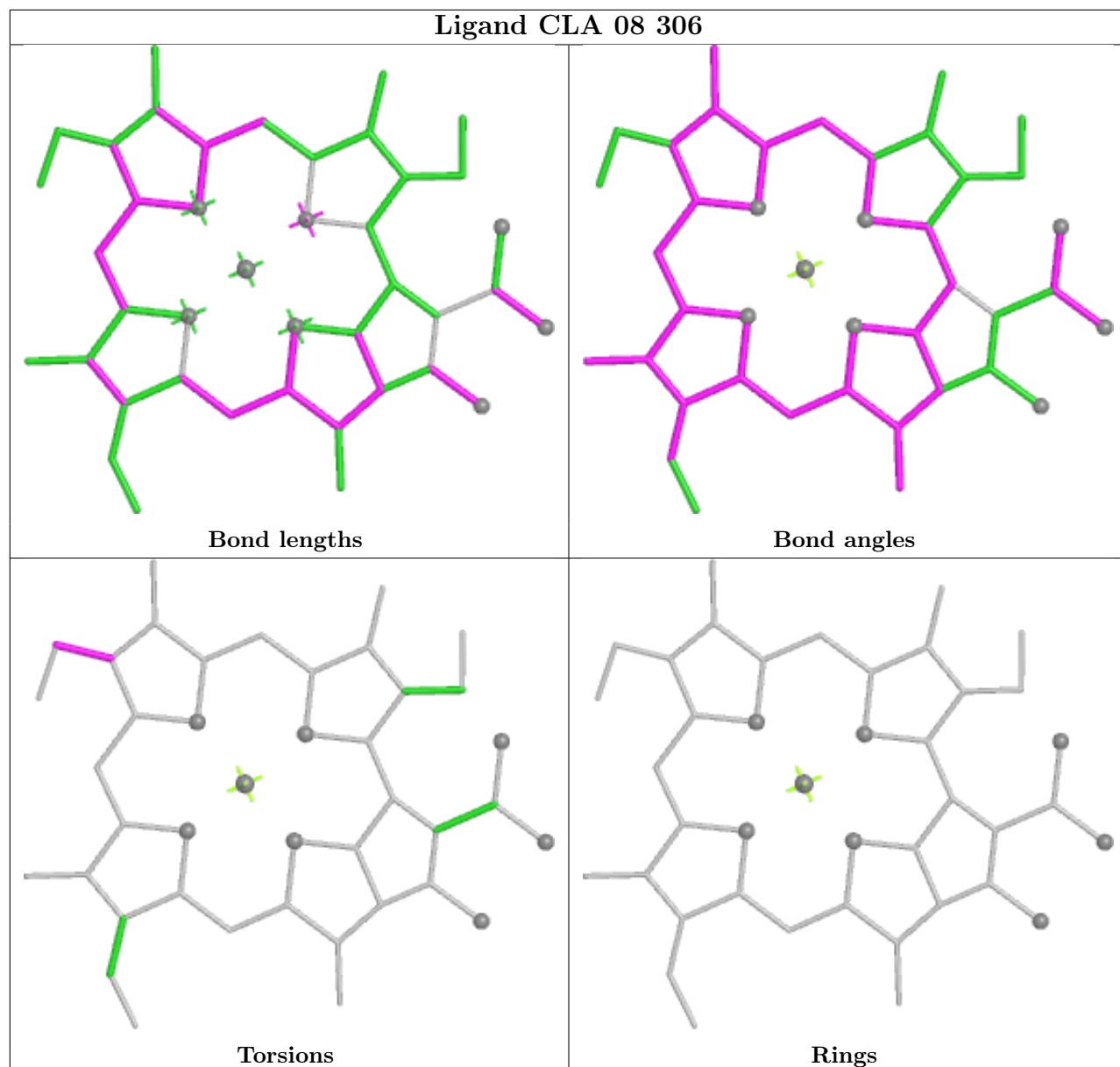


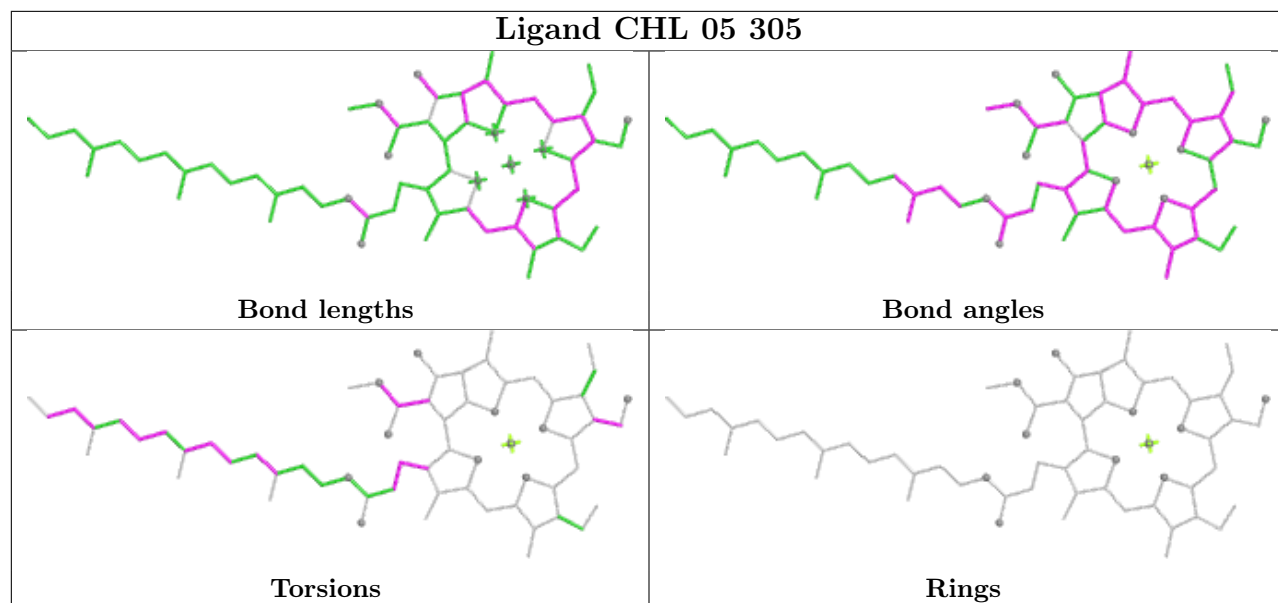


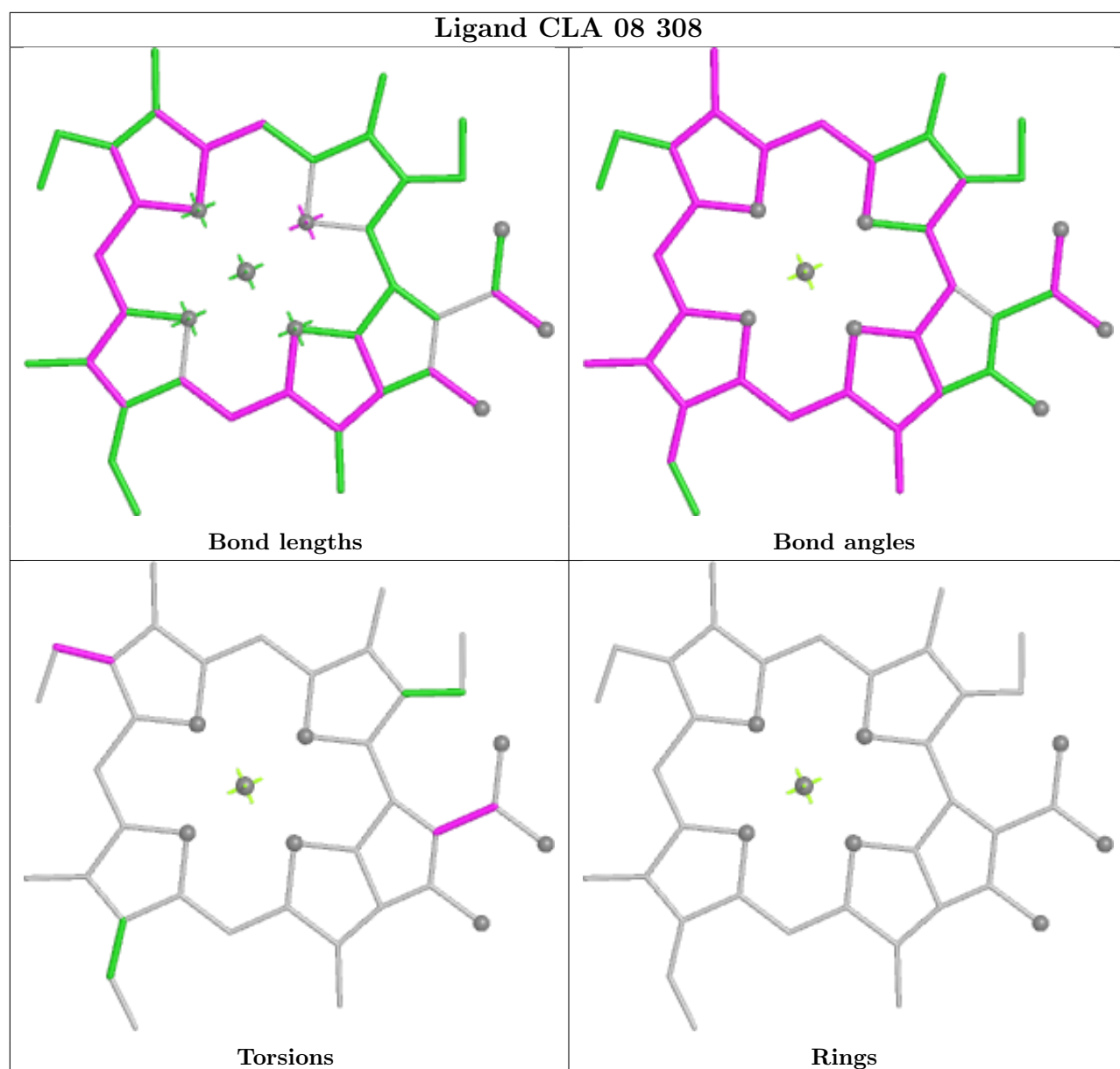


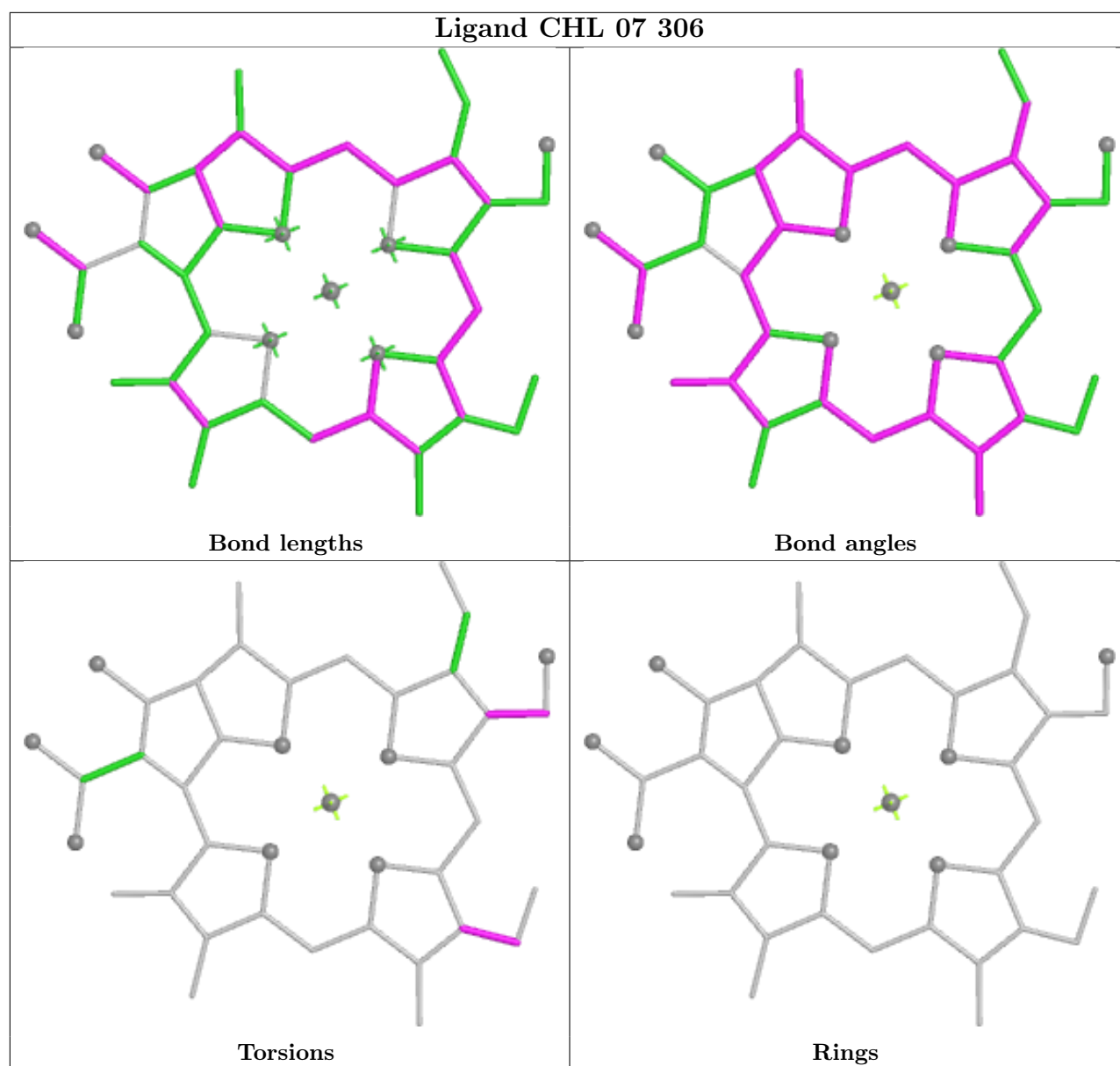


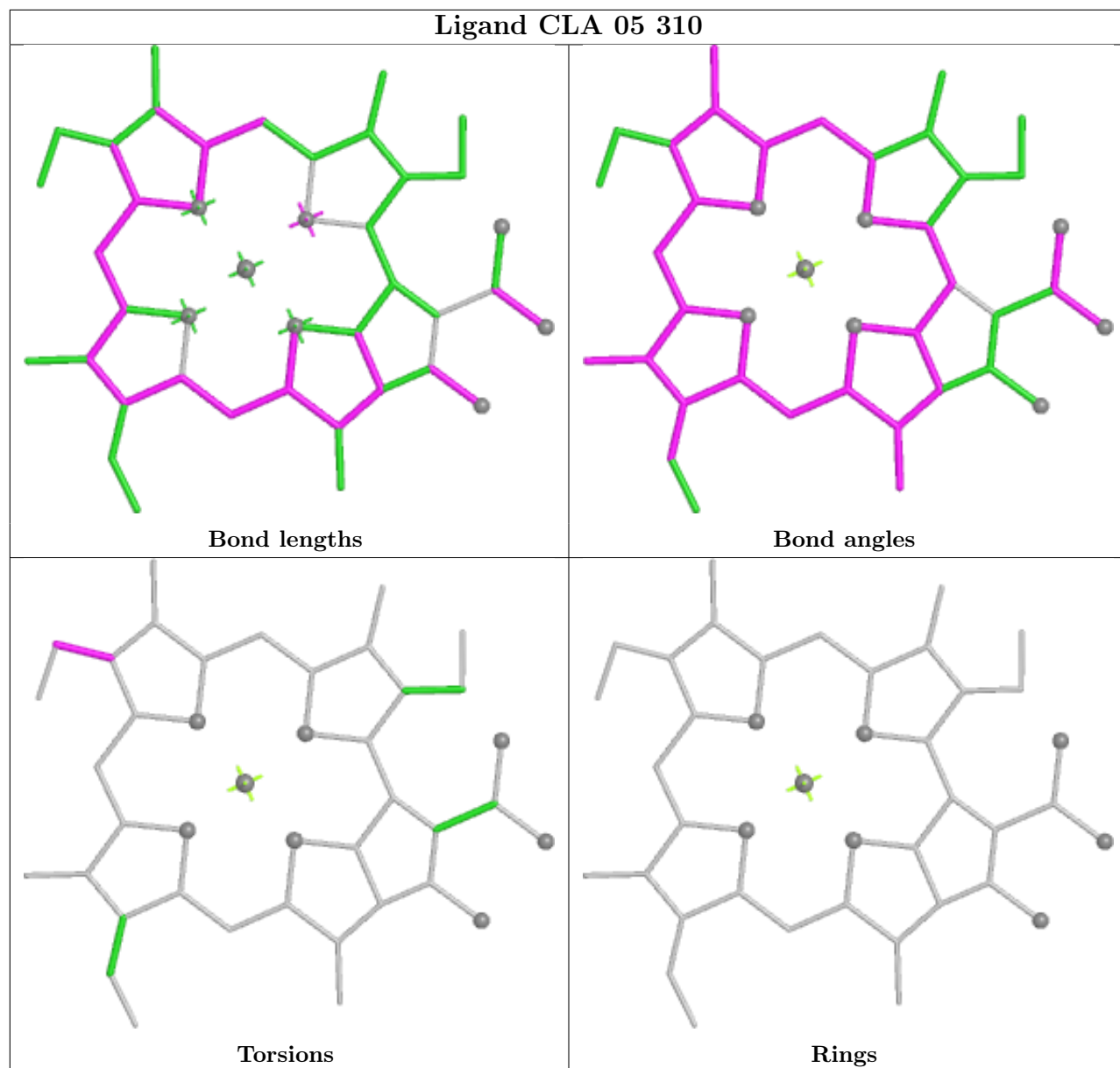


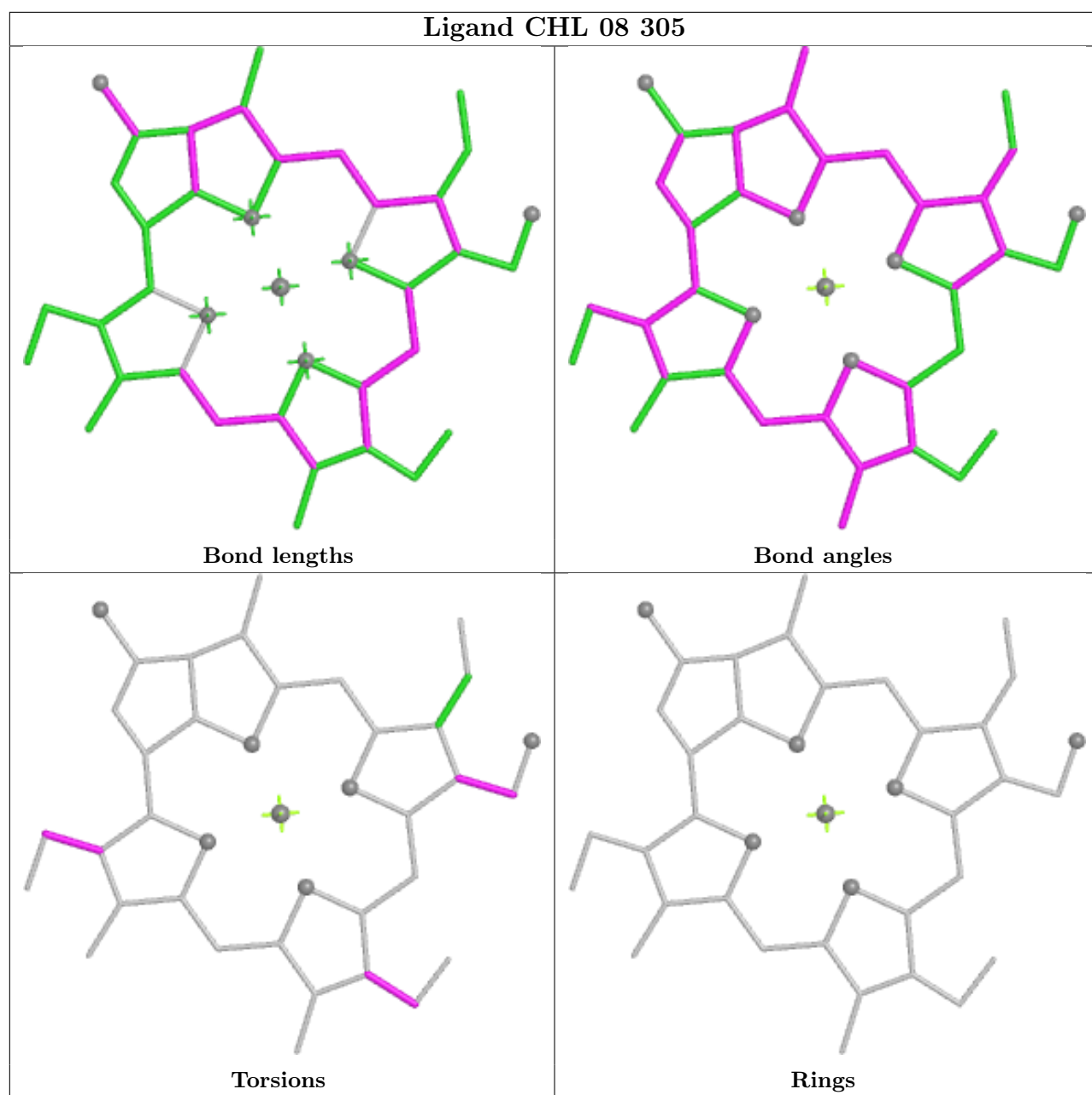


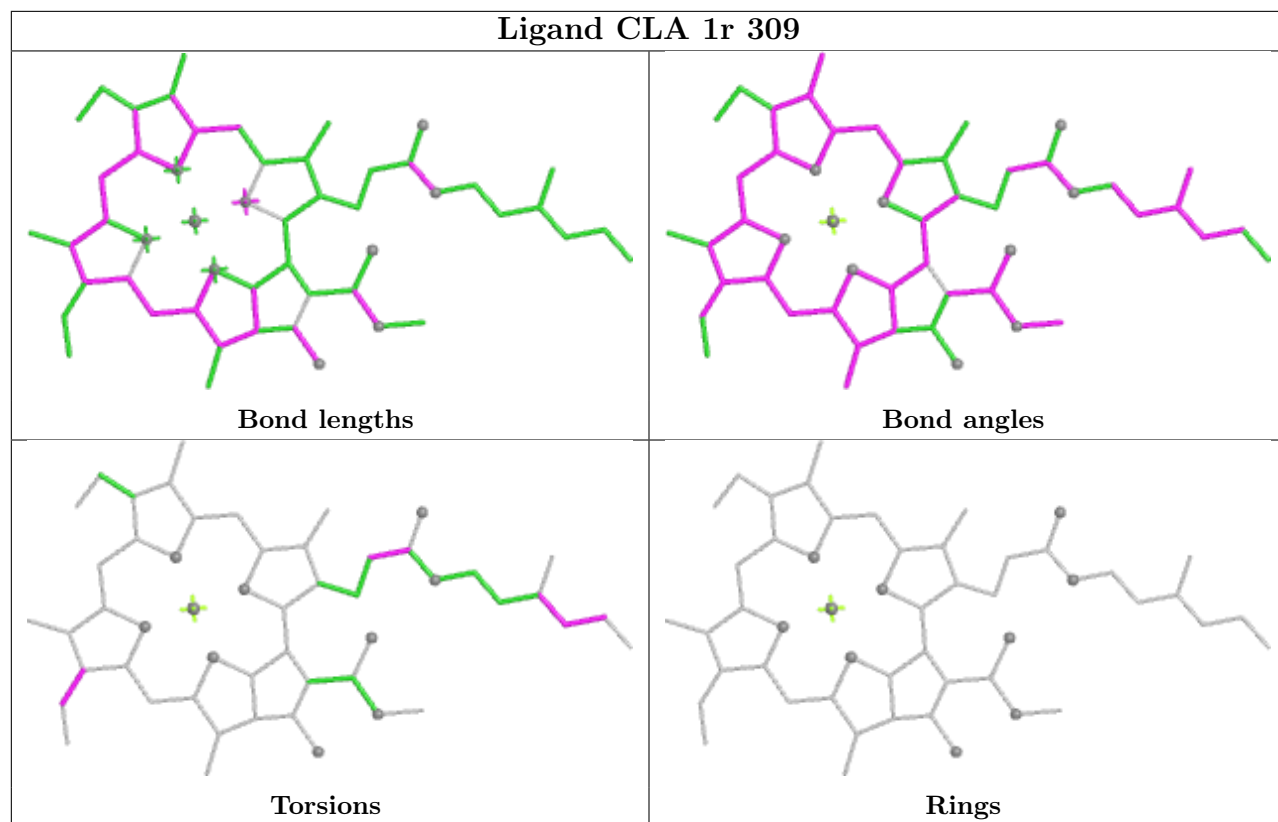


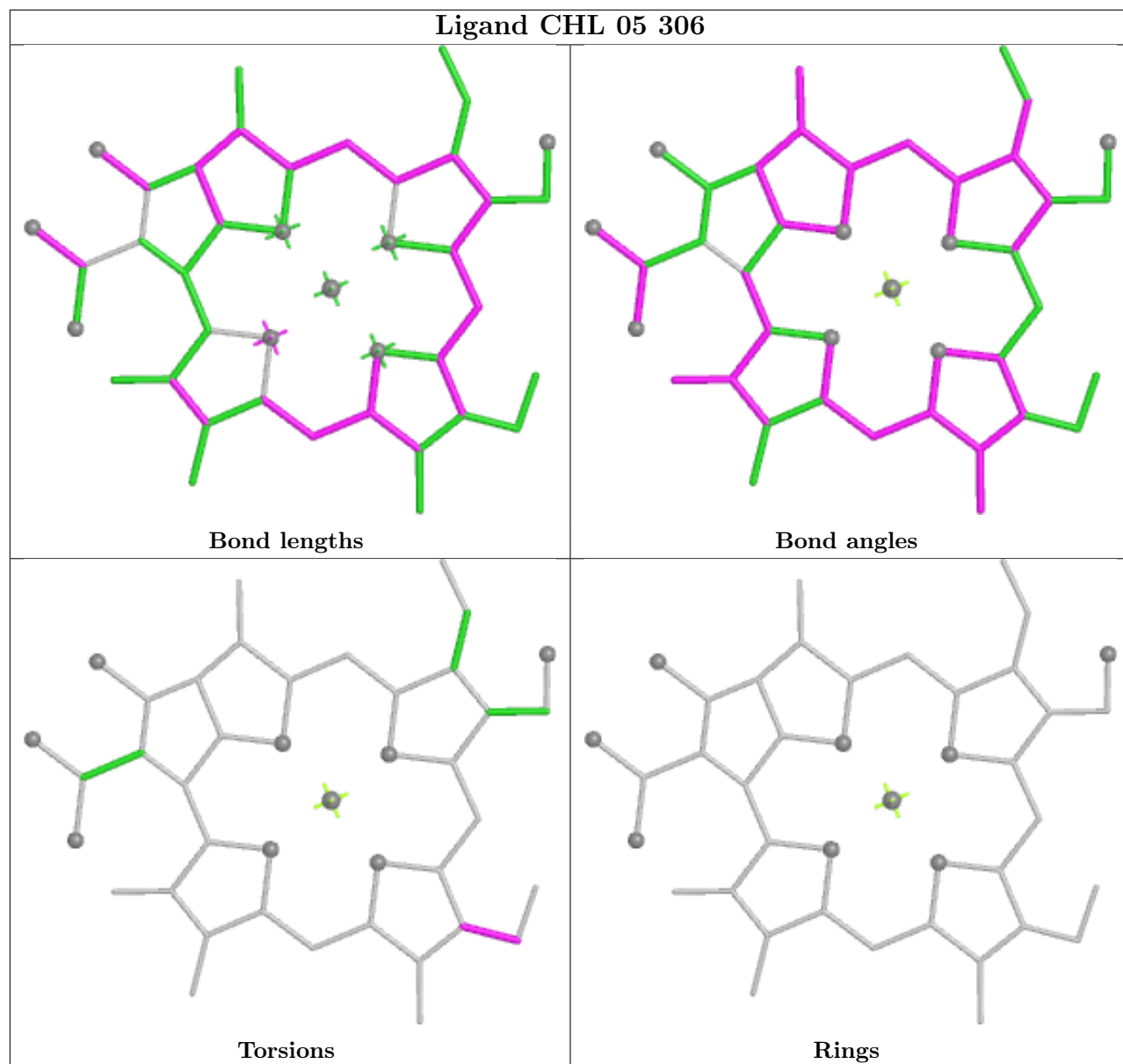


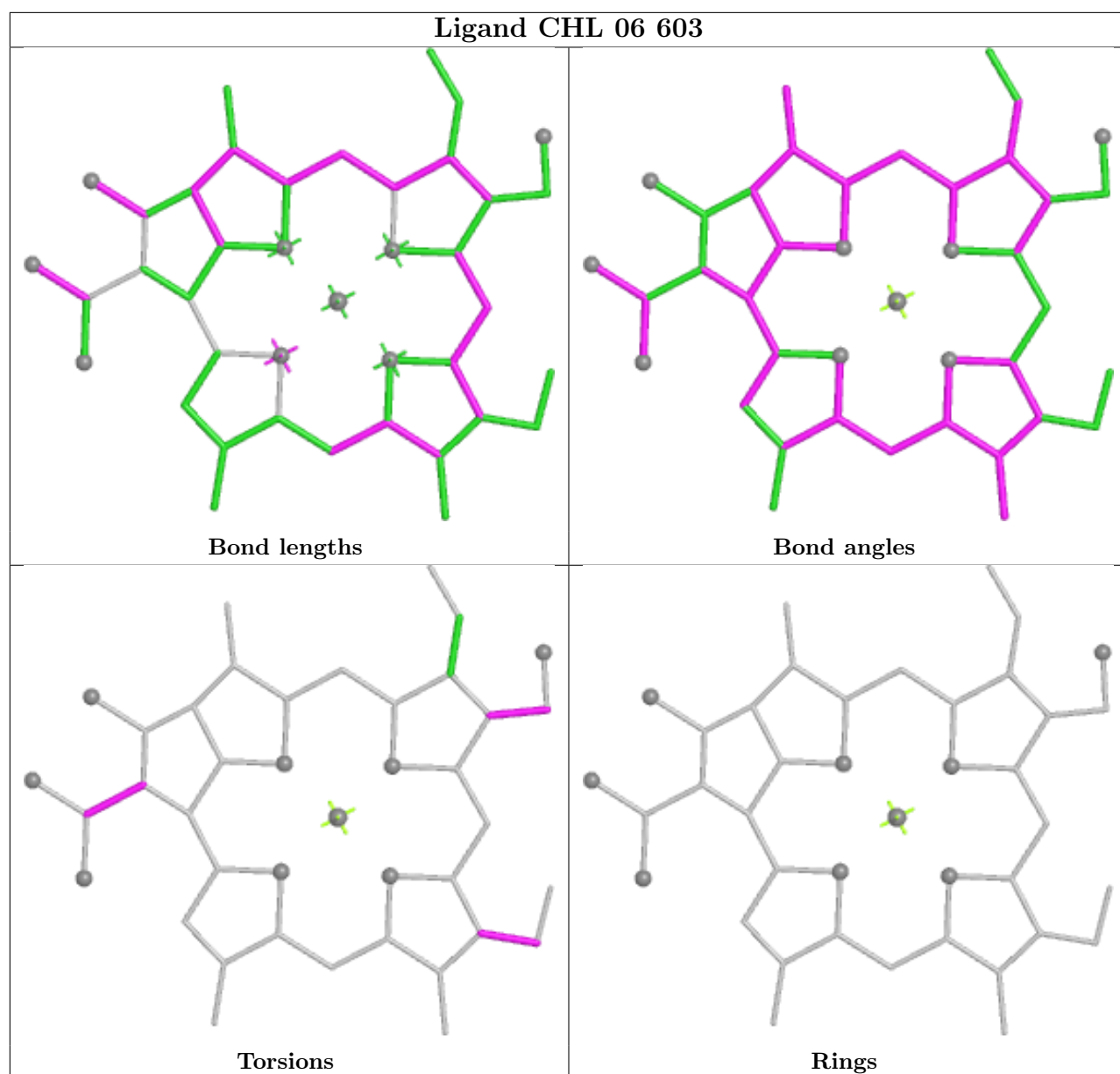


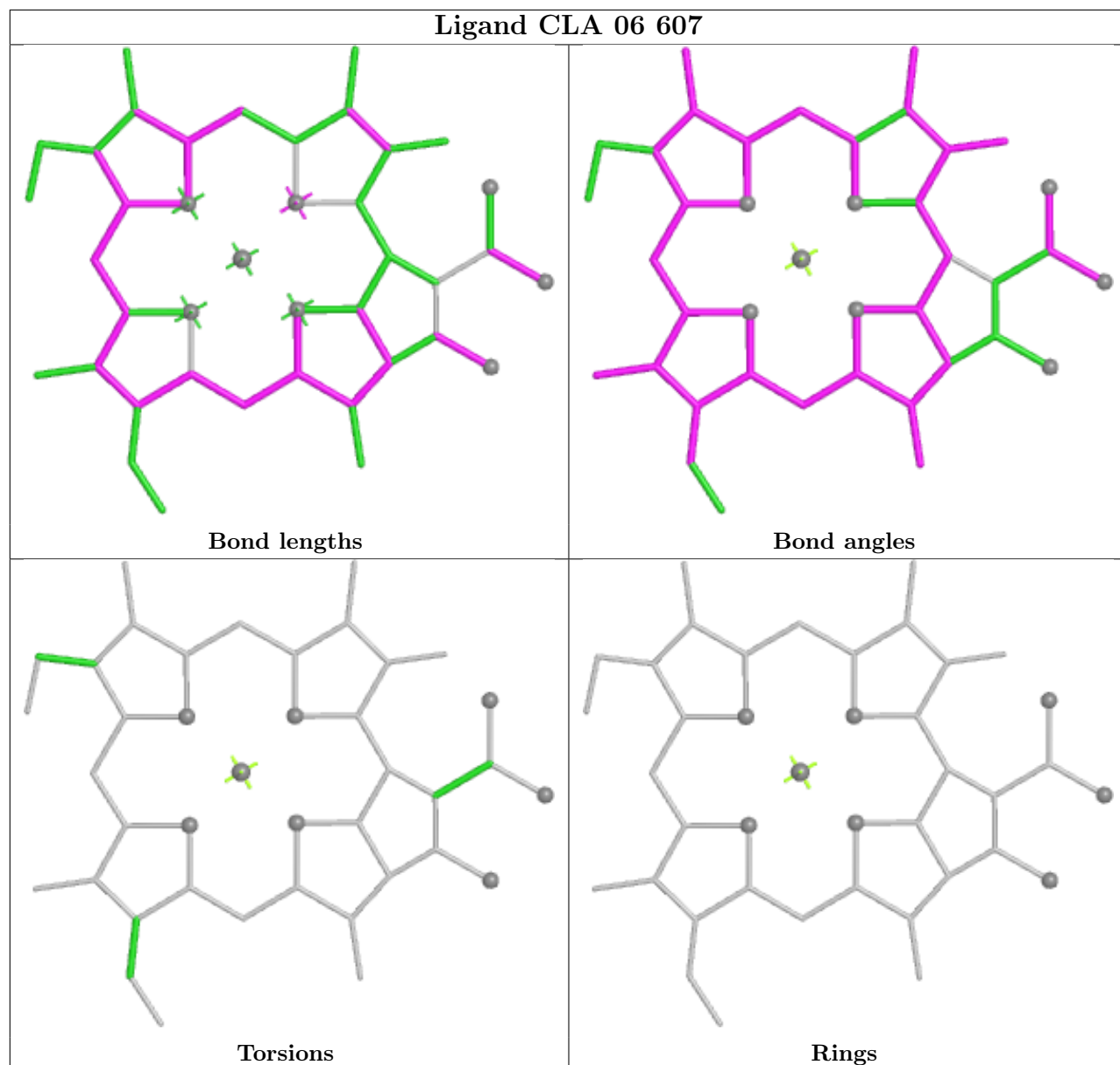


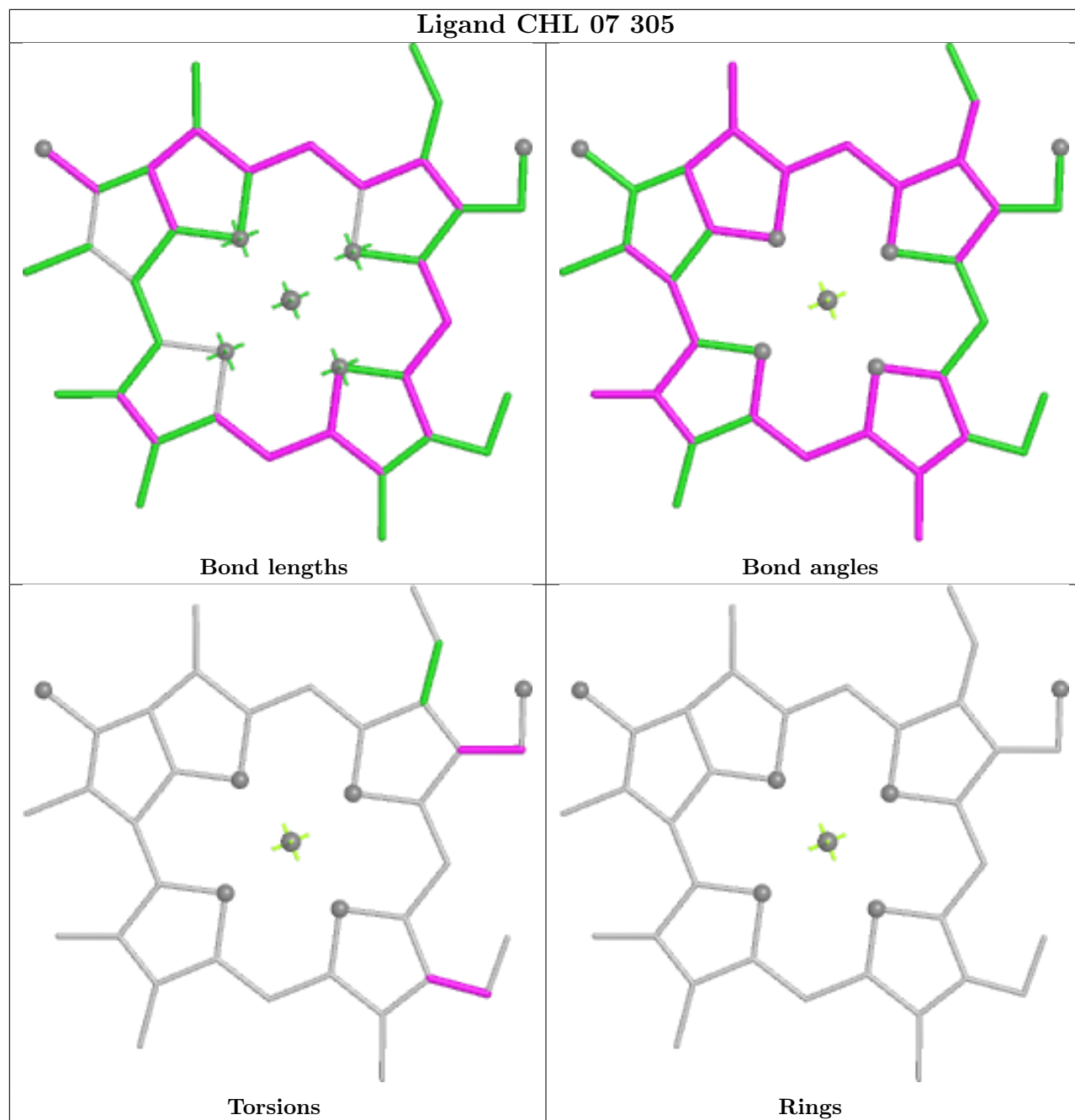


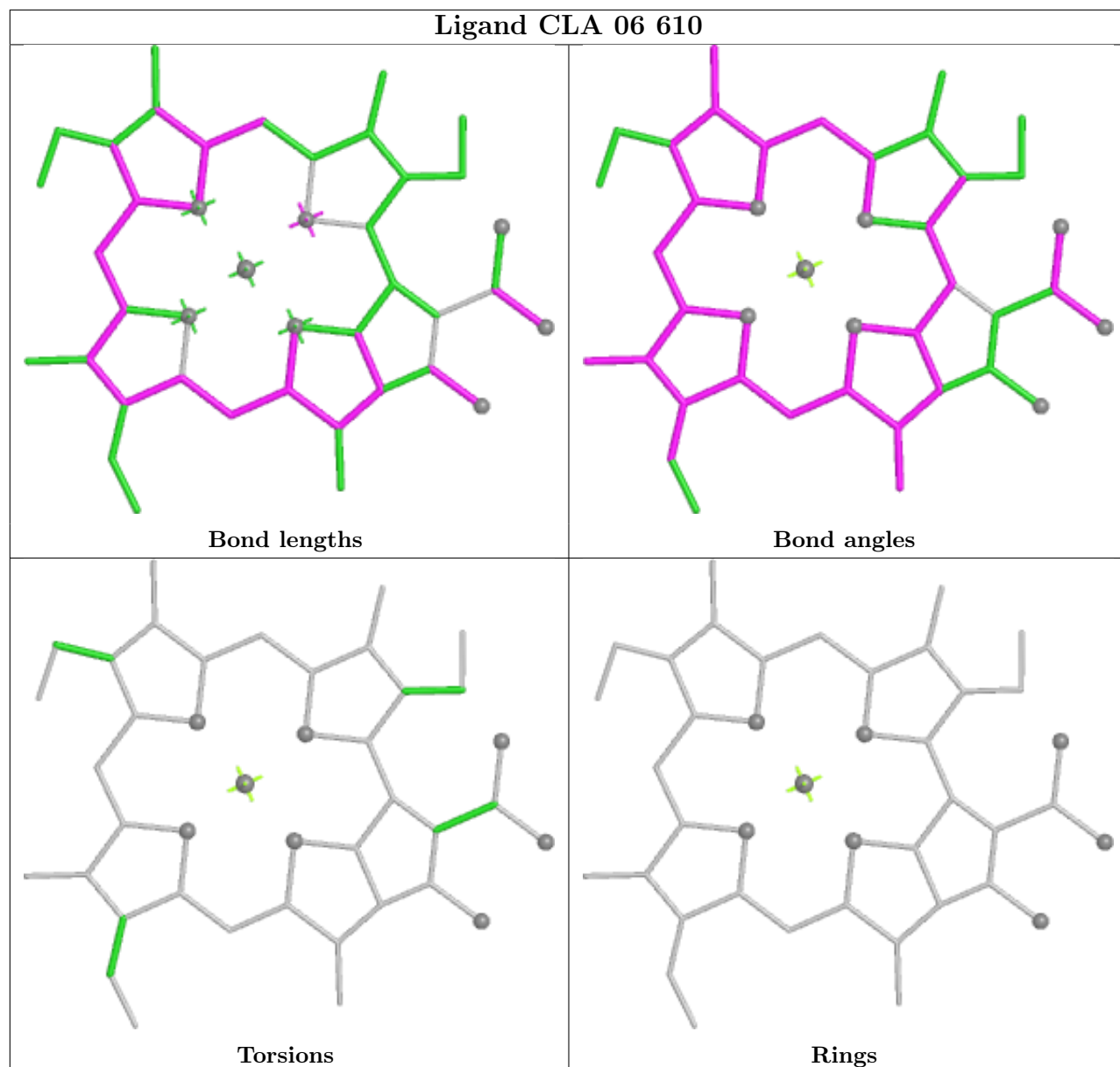


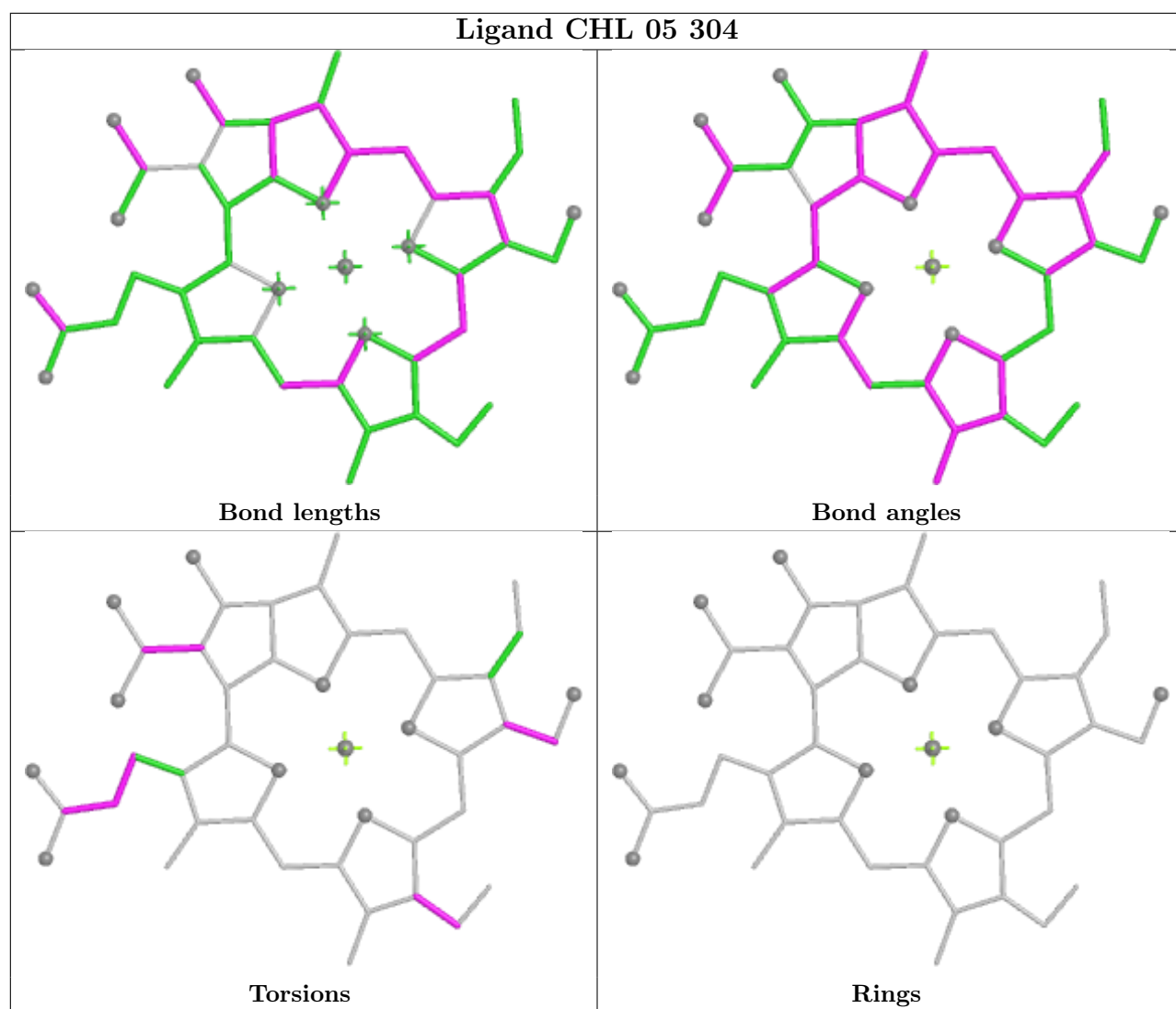


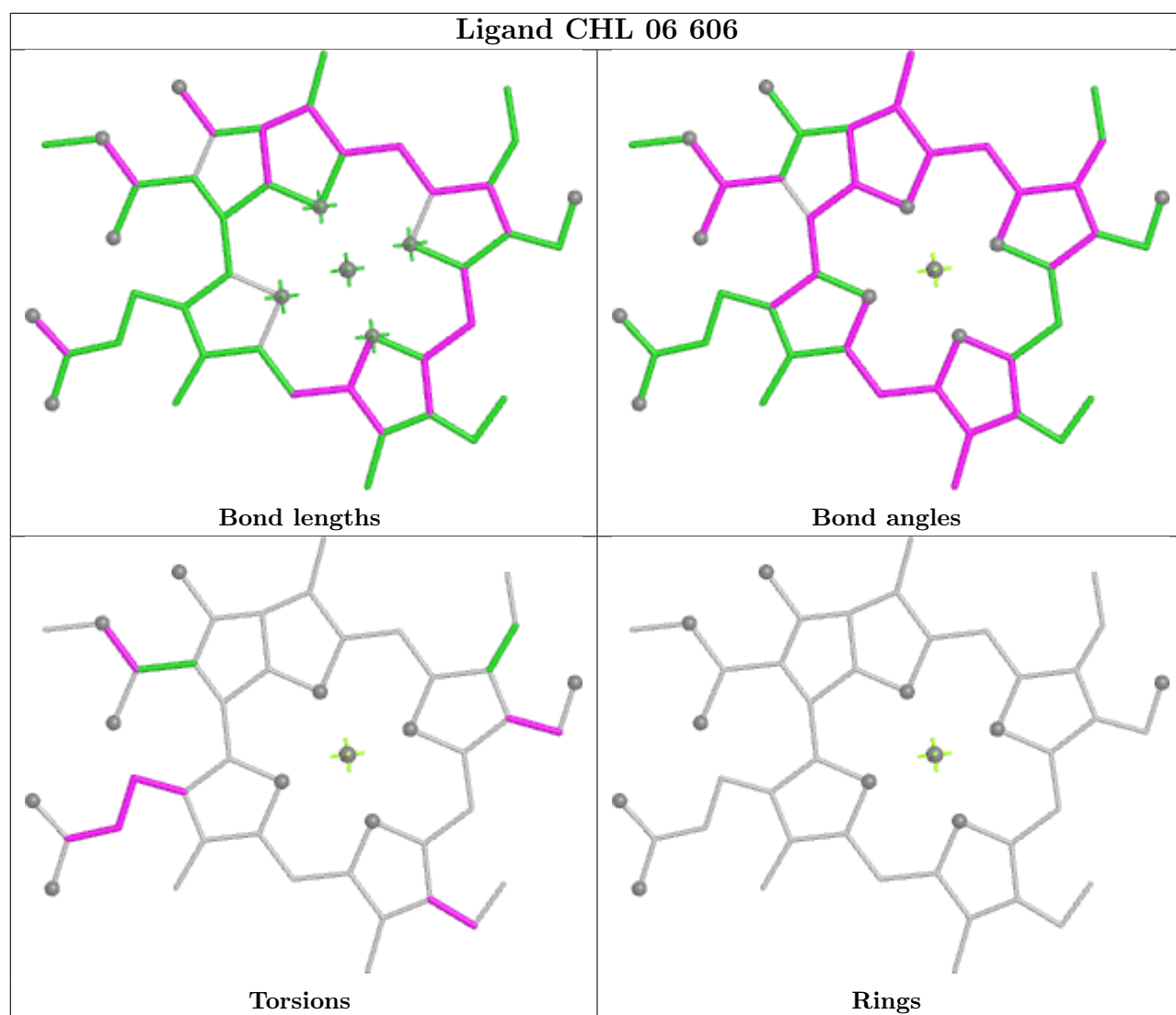


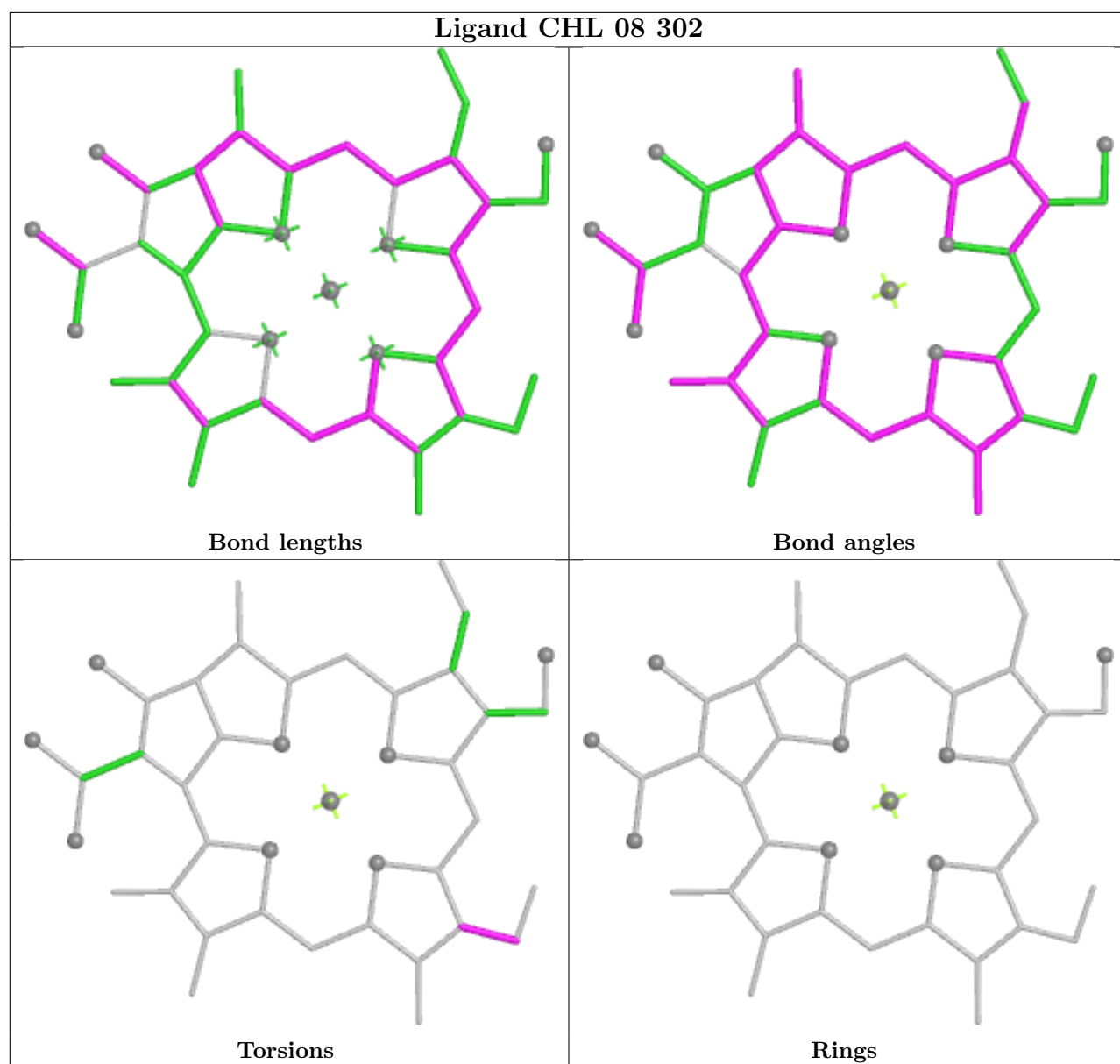


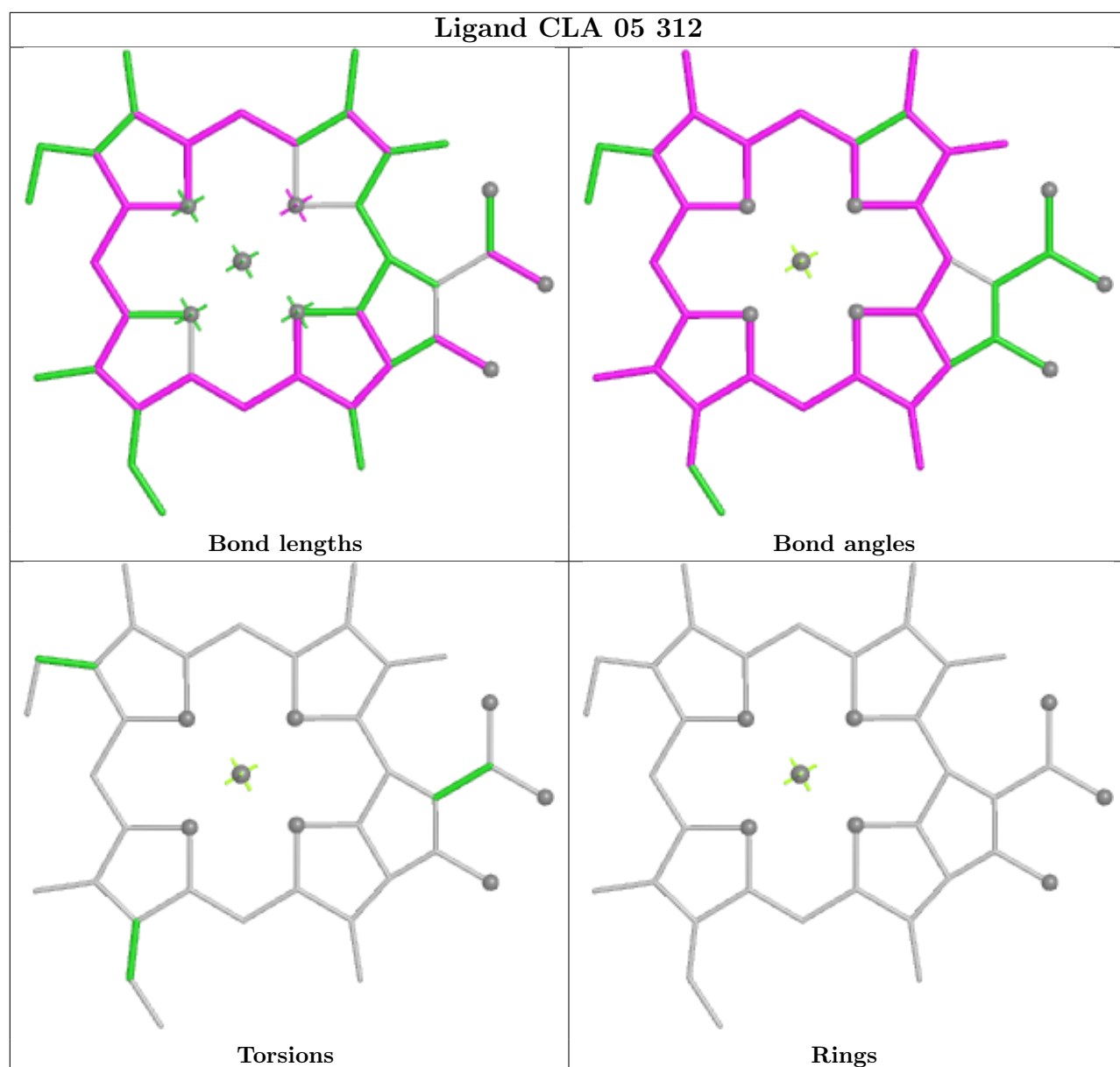


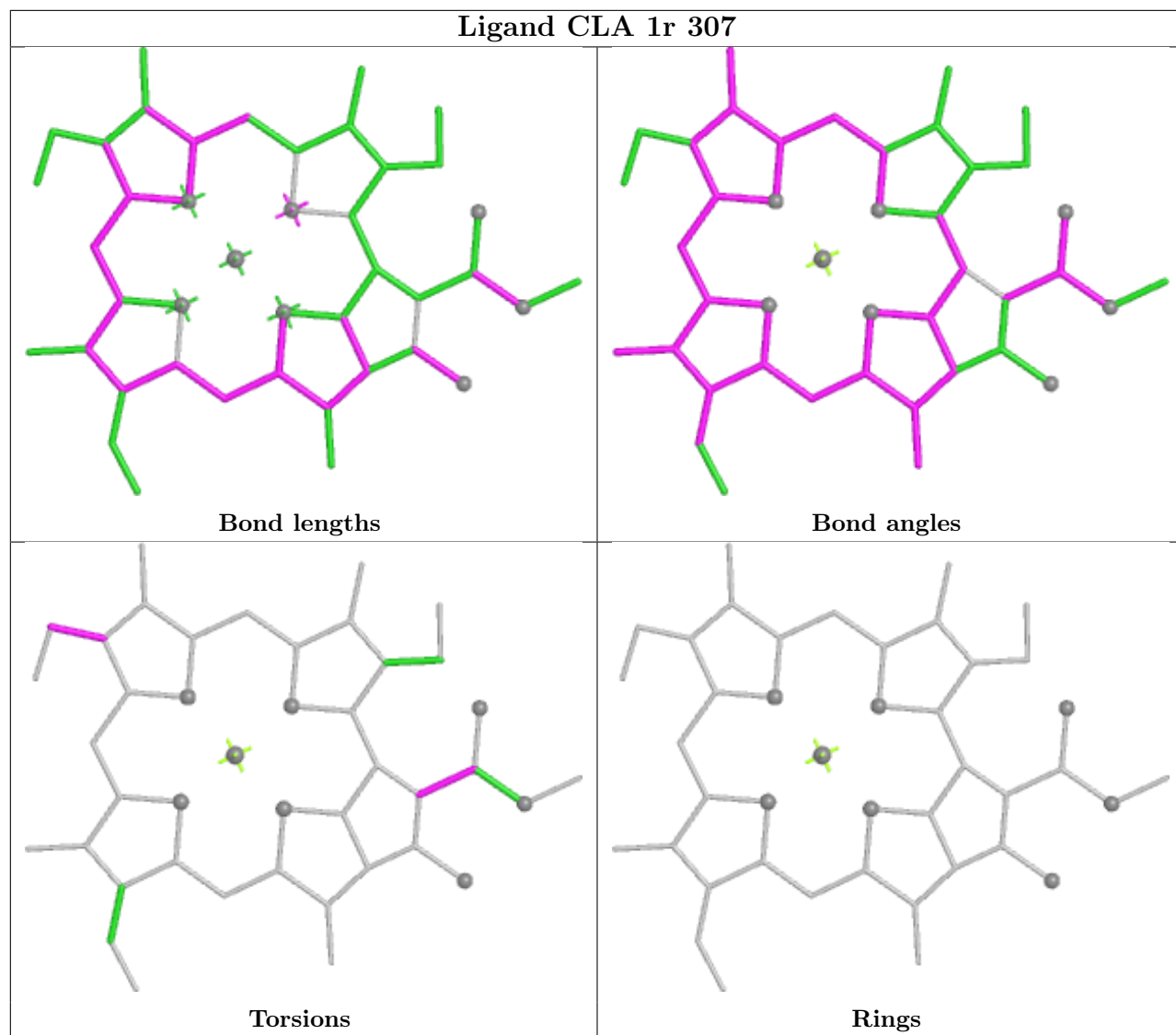


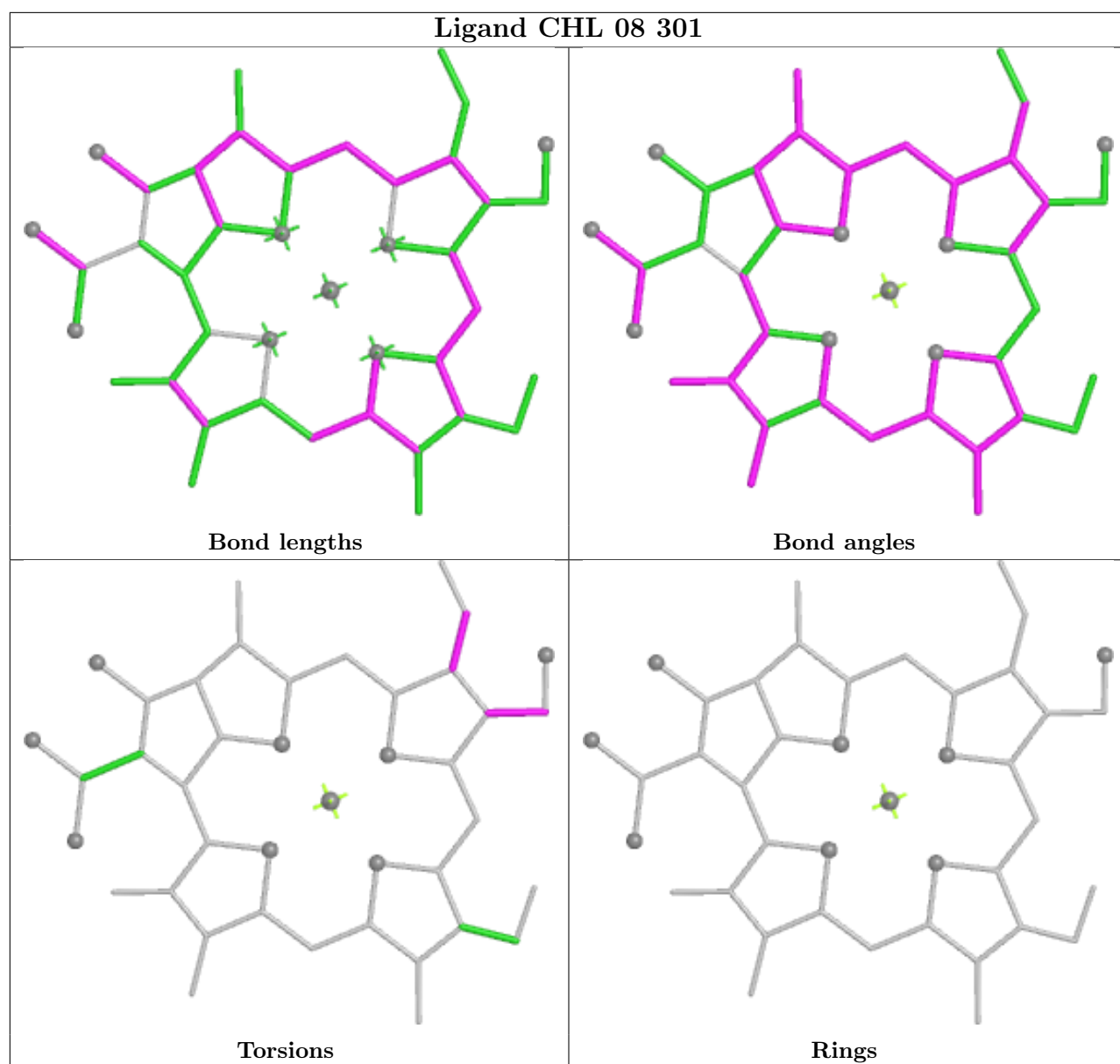


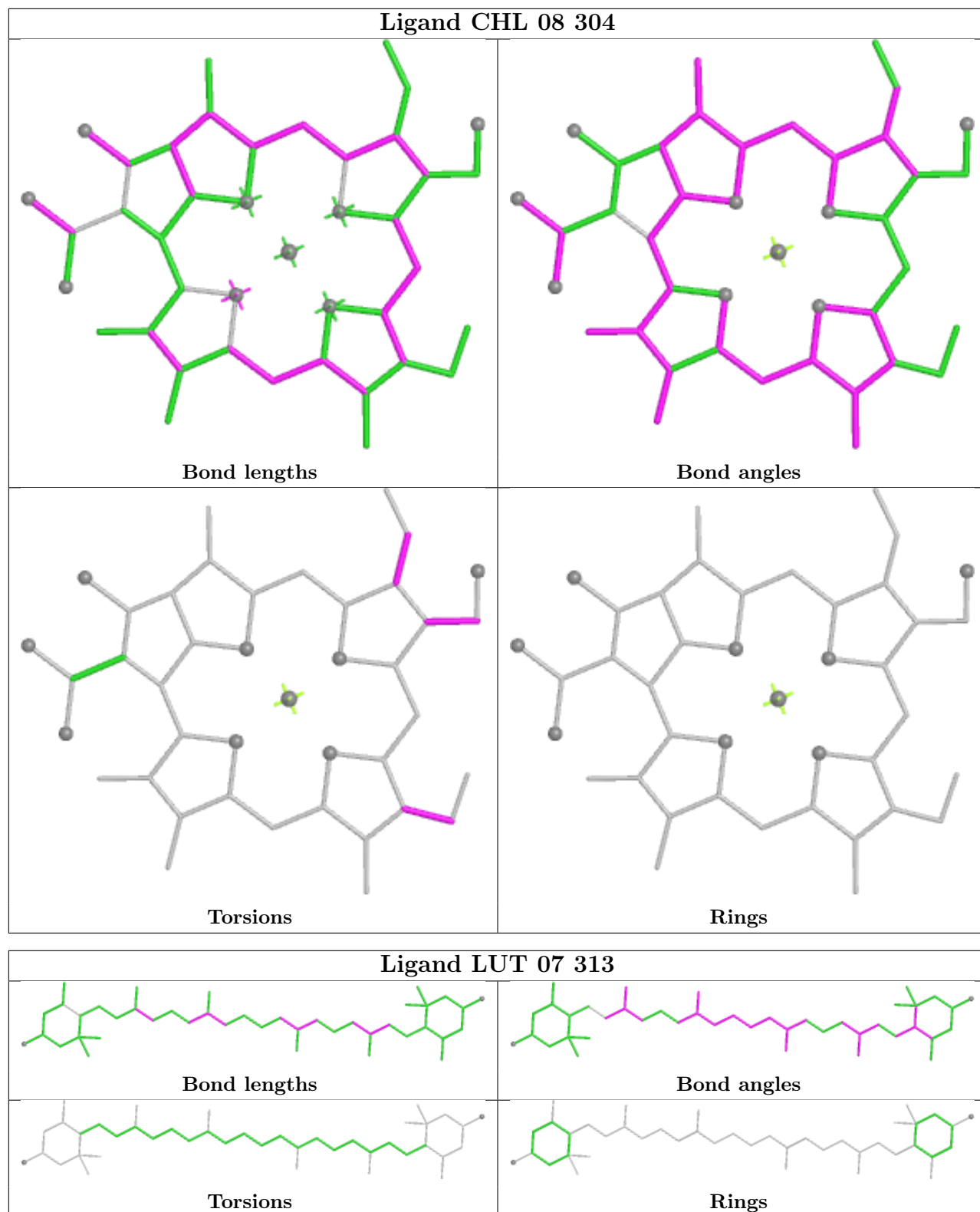


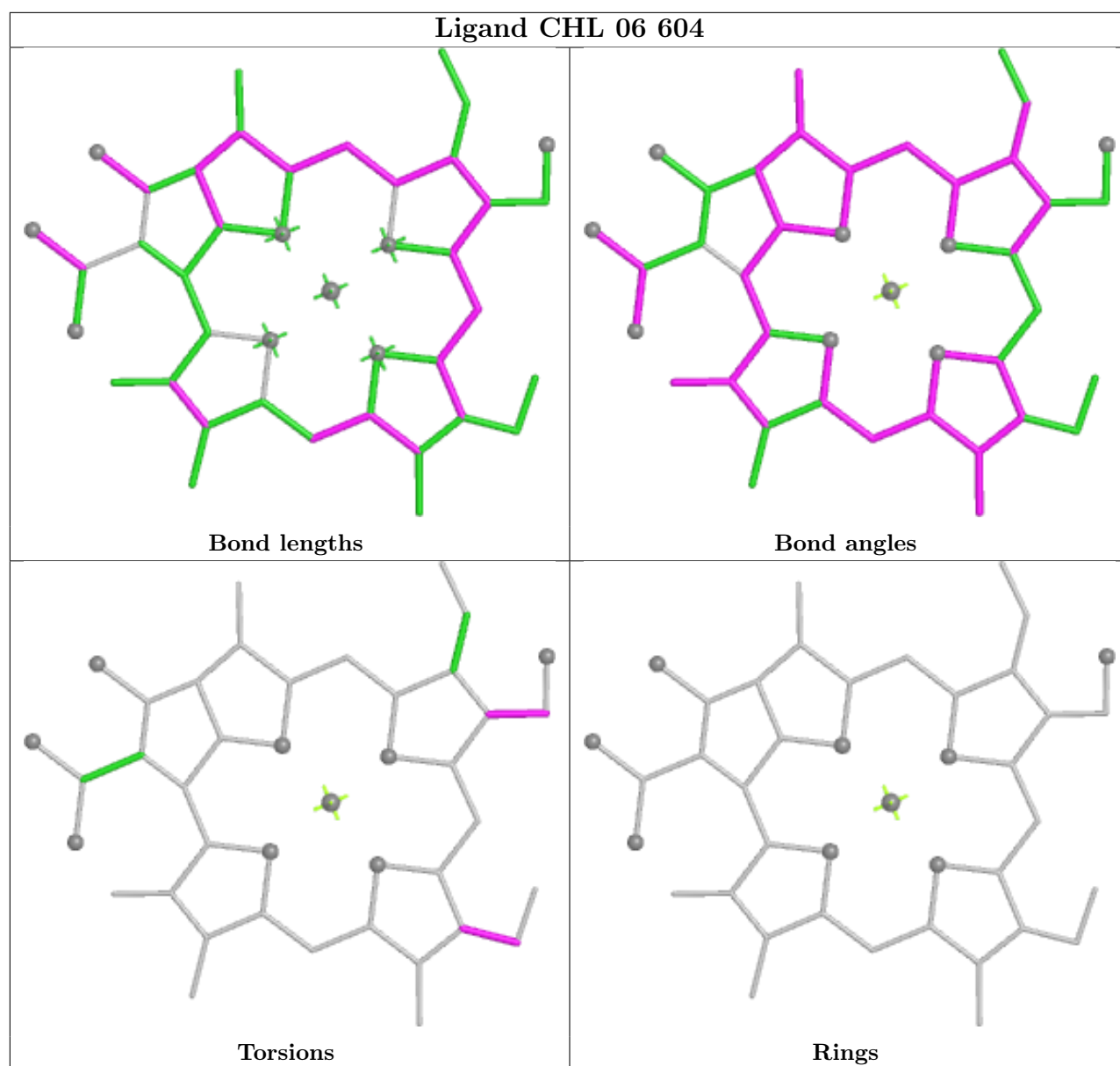


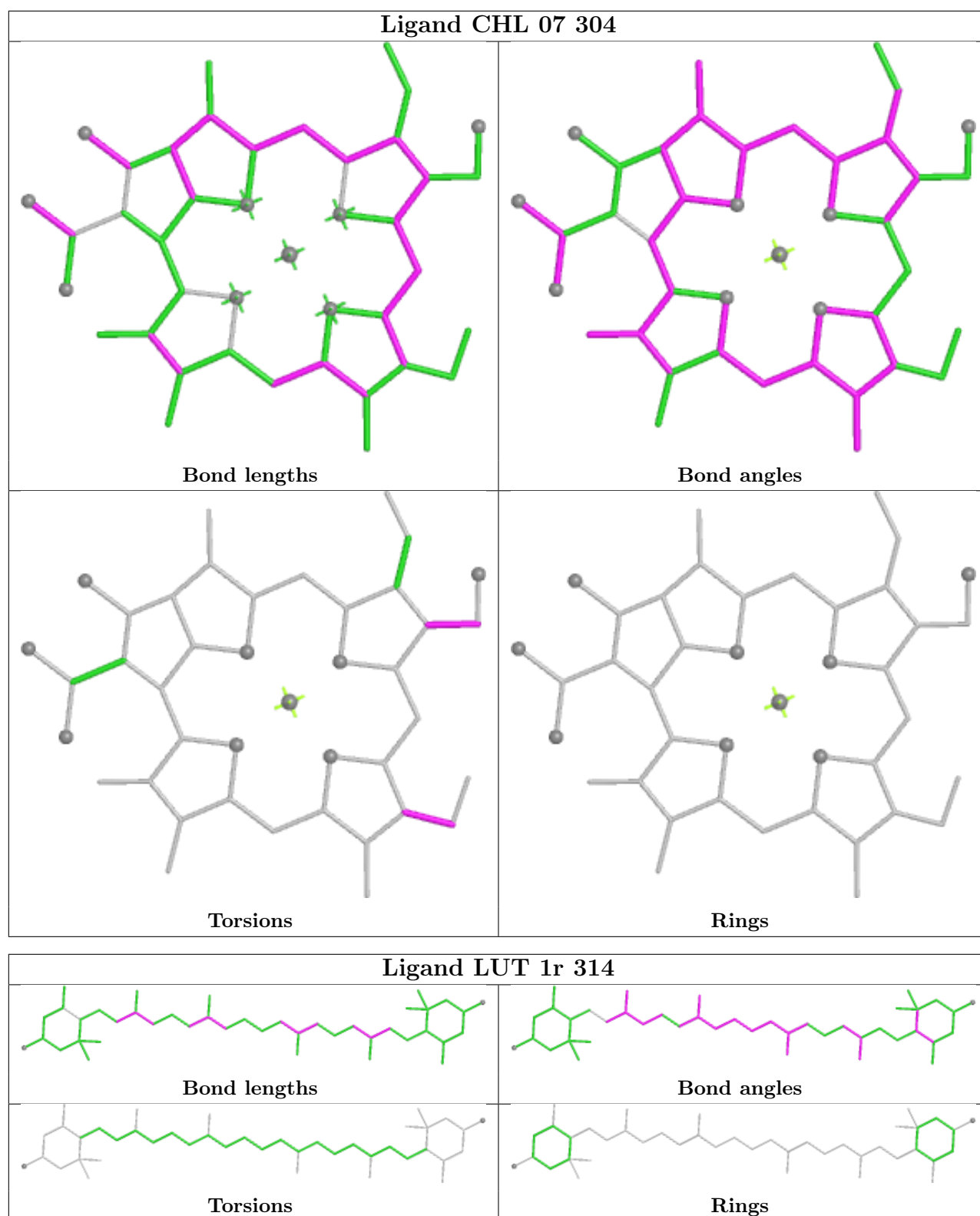












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

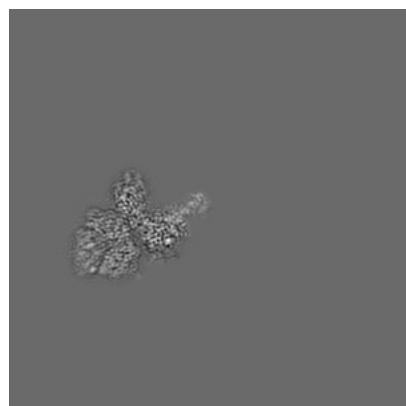
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66952. These allow visual inspection of the internal detail of the map and identification of artifacts.

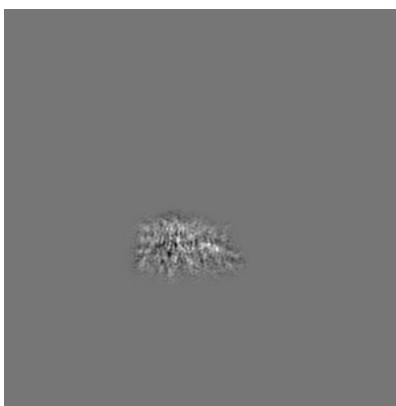
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

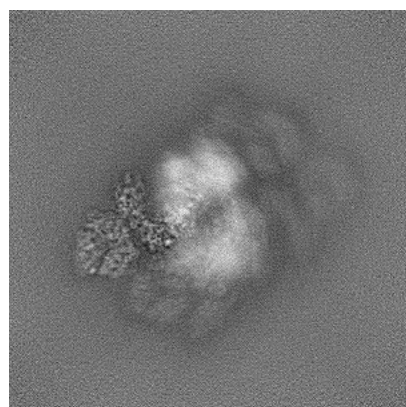


Y

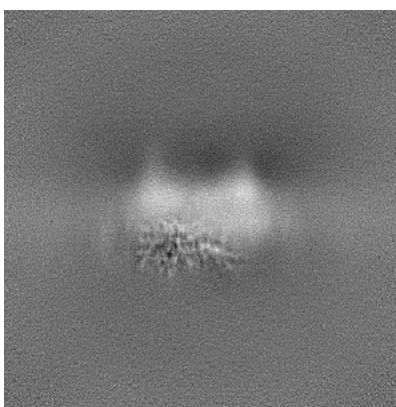


Z

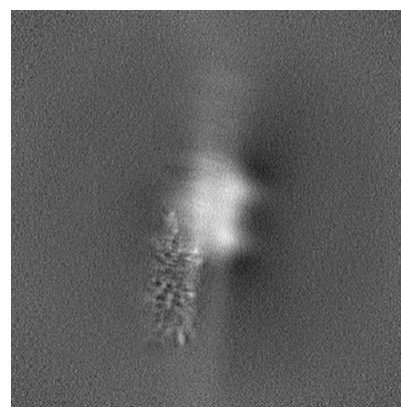
6.1.2 Raw map



X



Y

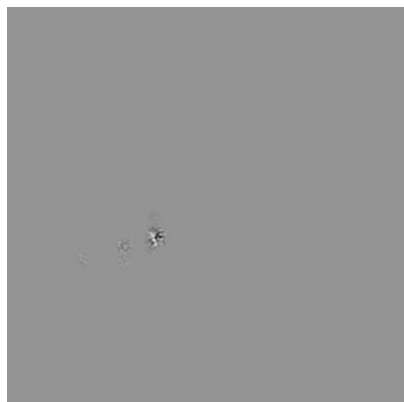


Z

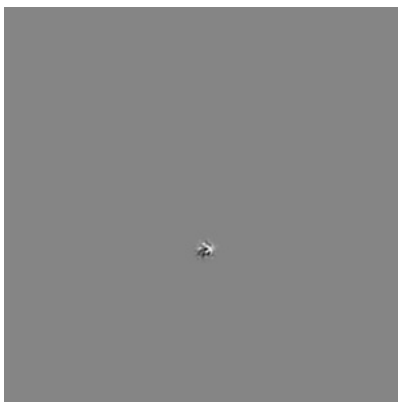
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

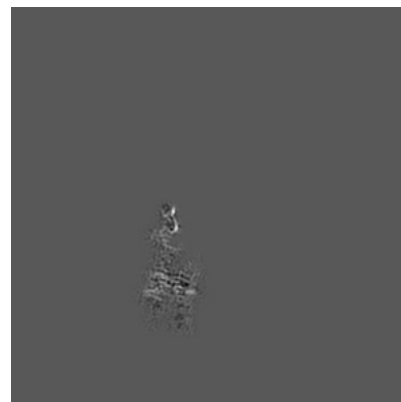
6.2.1 Primary map



X Index: 256

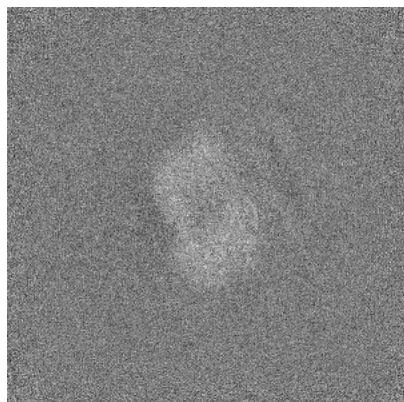


Y Index: 256



Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

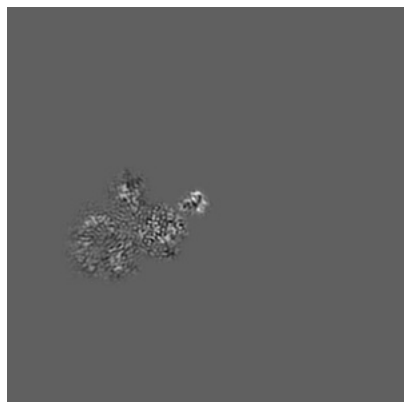


Z Index: 256

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

6.3 Largest variance slices [i](#)

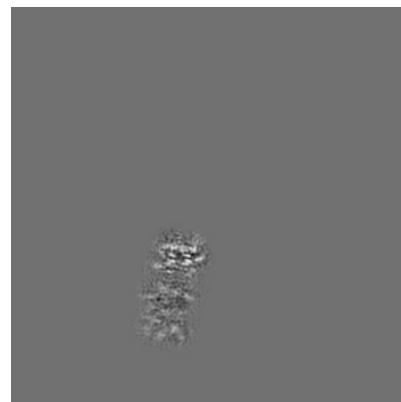
6.3.1 Primary map



X Index: 205

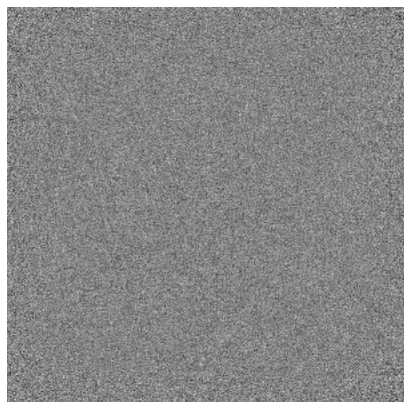


Y Index: 149

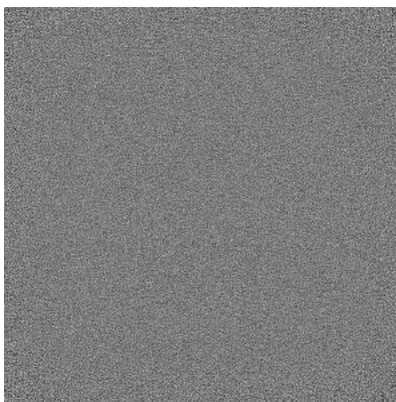


Z Index: 216

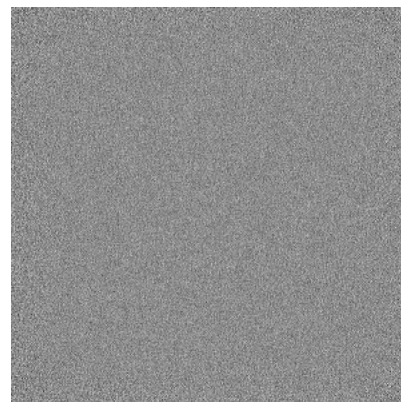
6.3.2 Raw map



X Index: 0



Y Index: 0

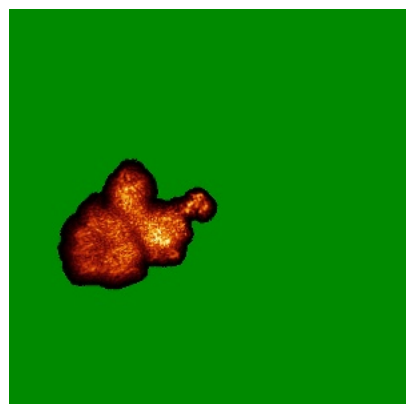


Z Index: 0

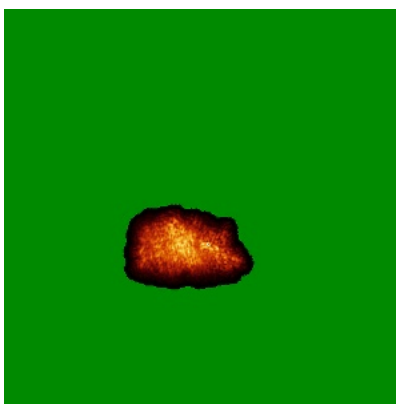
The images above show the largest variance slices of the map in three orthogonal directions.

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

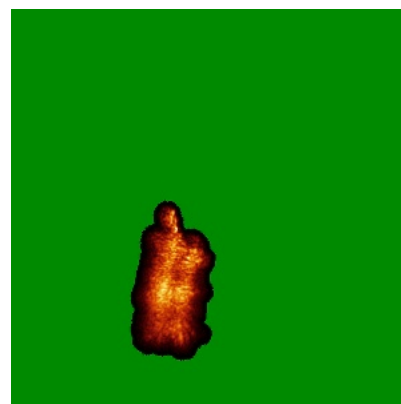
6.4.1 Primary map



X

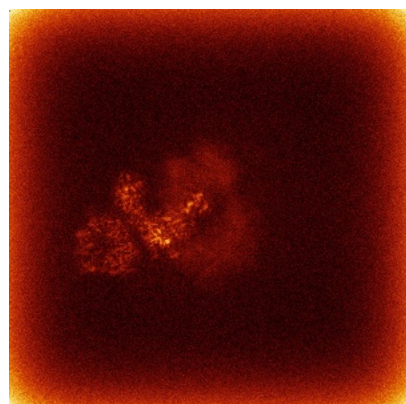


Y

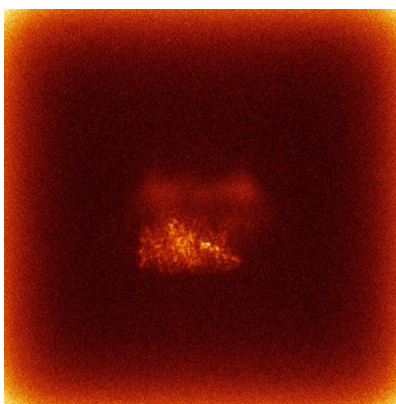


Z

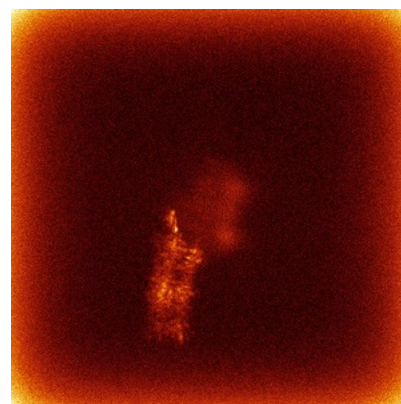
6.4.2 Raw map



X



Y

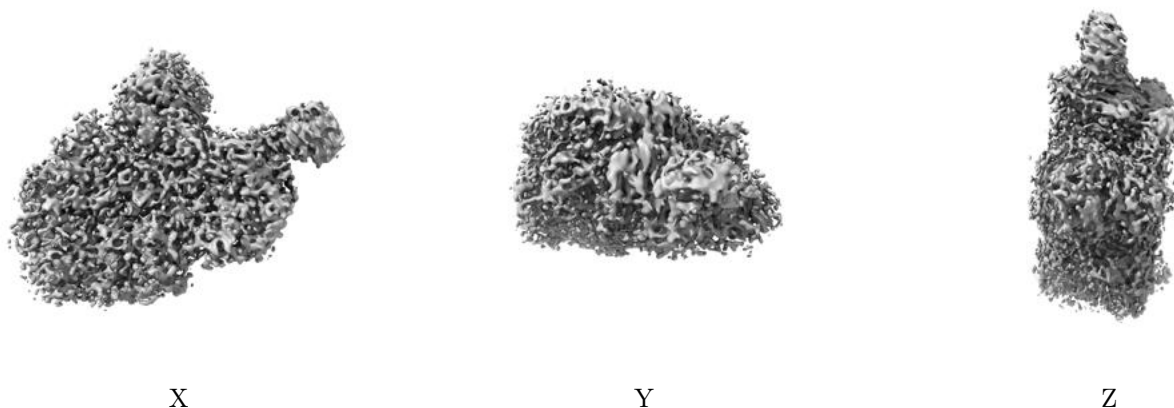


Z

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.

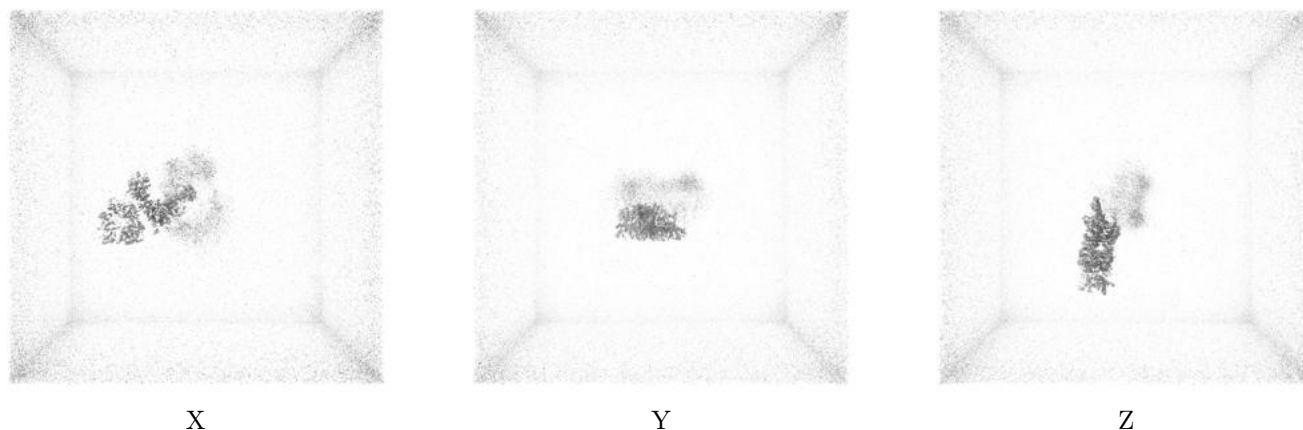
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

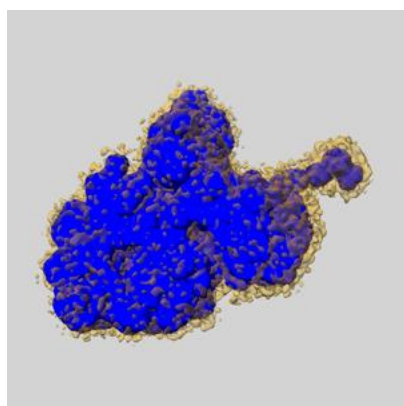
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

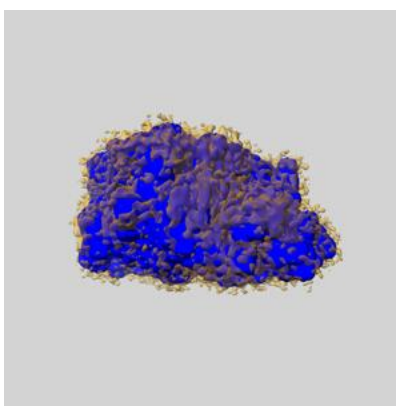
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

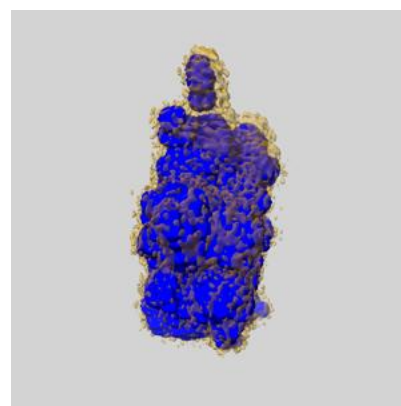
6.6.1 emd_66952_msk_1.map [i](#)



X



Y

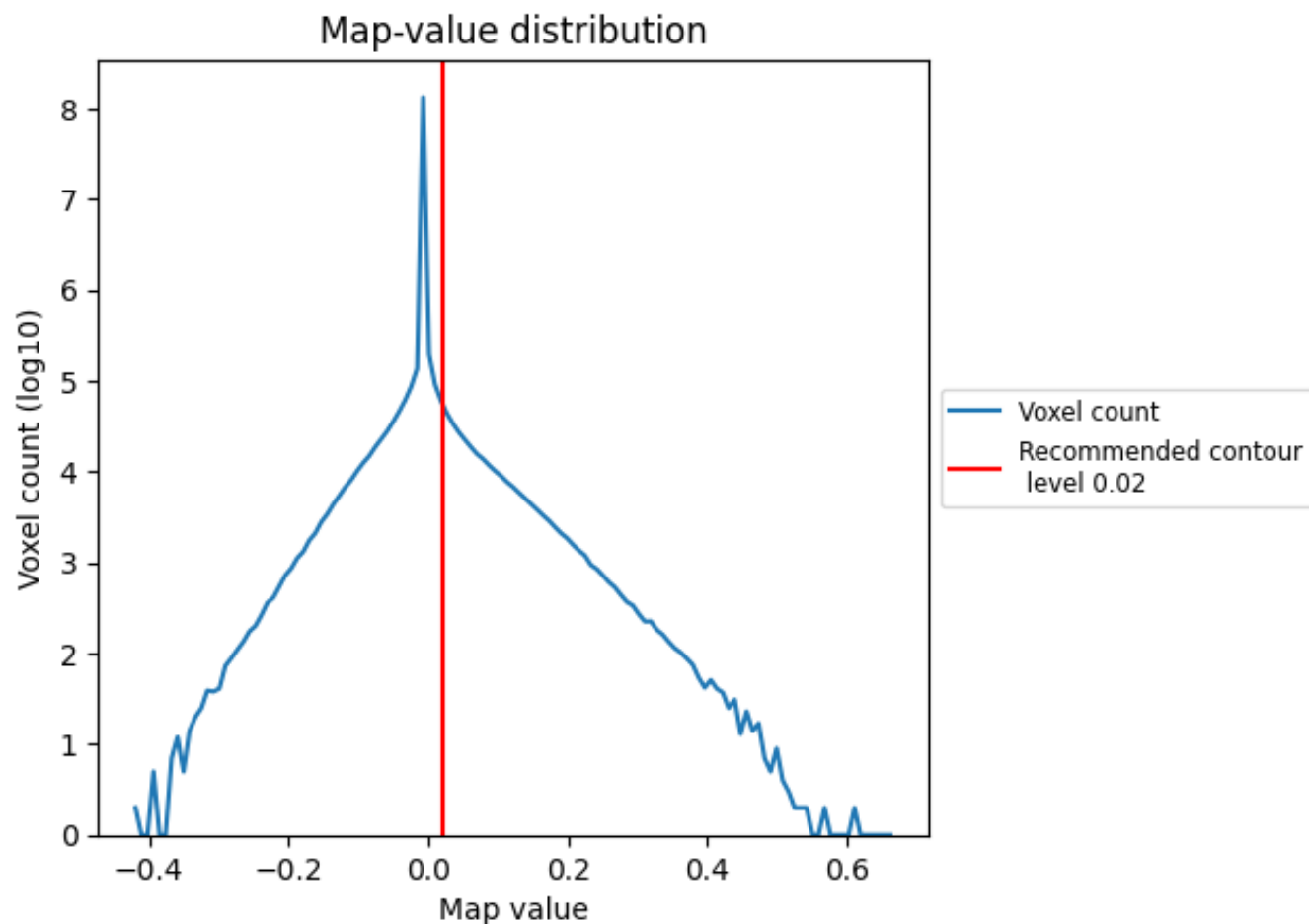


Z

7 Map analysis [i](#)

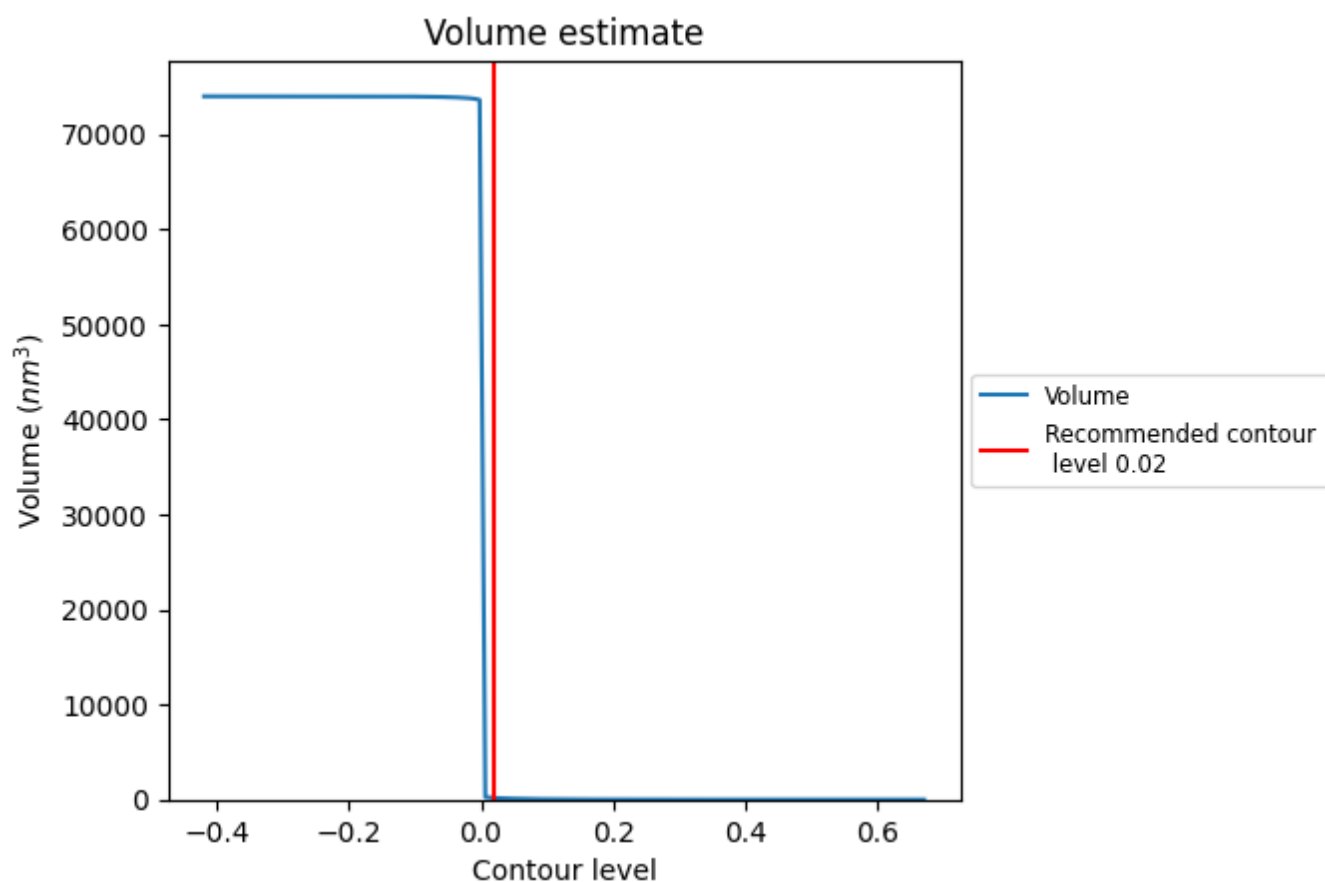
This section contains the results of statistical analysis of the map.

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.

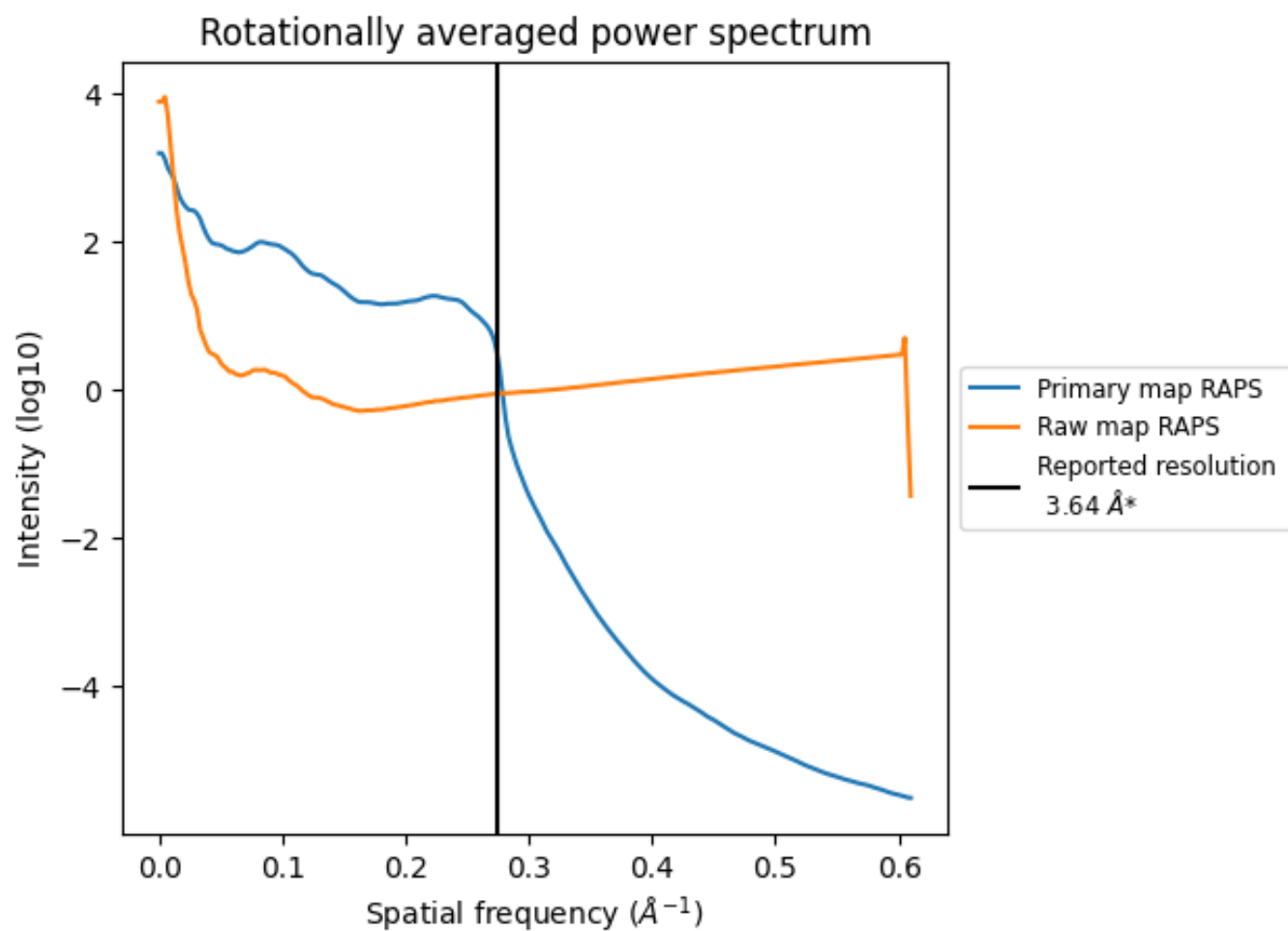
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm³; this corresponds to an approximate mass of 157 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 ⓘ

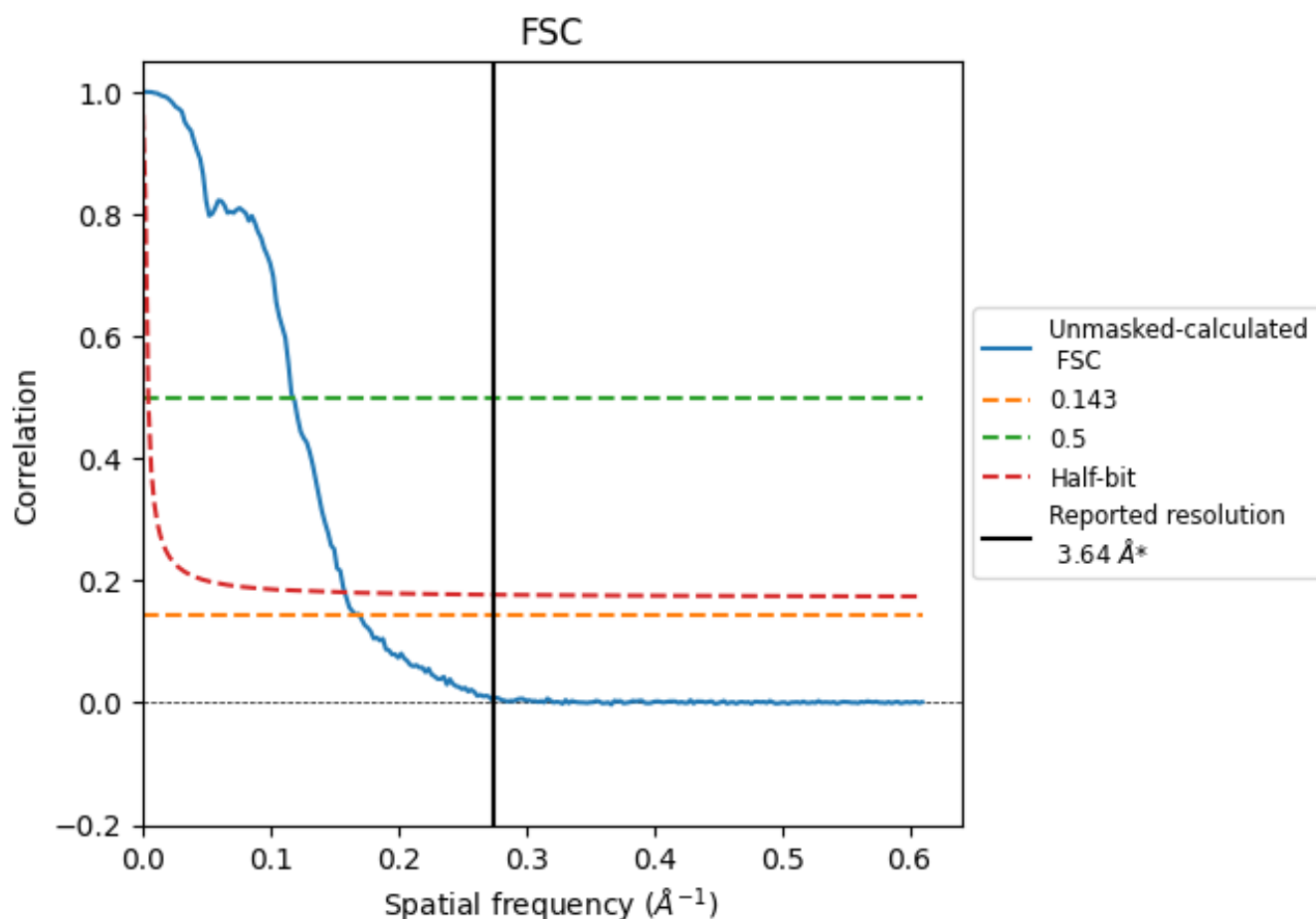


*Reported resolution corresponds to spatial frequency of $0.275 \text{ \AA}^{-1}$

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 0.275 Å⁻¹

8.2 Resolution estimates [i](#)

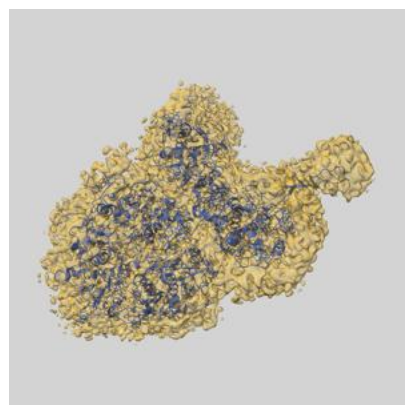
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.89	8.49	6.31

*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 5.89 differs from the reported value 3.64 by more than 10 %

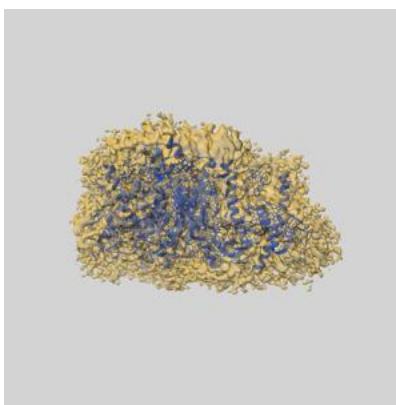
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66952 and PDB model 9XK9. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

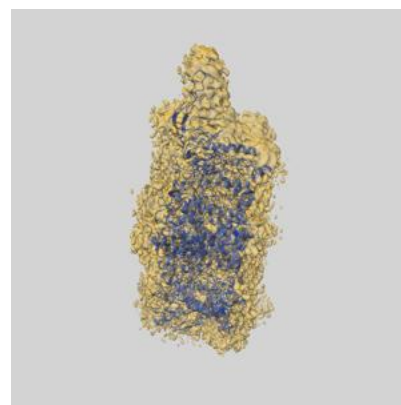
9.1 Map-model overlay [i](#)



X



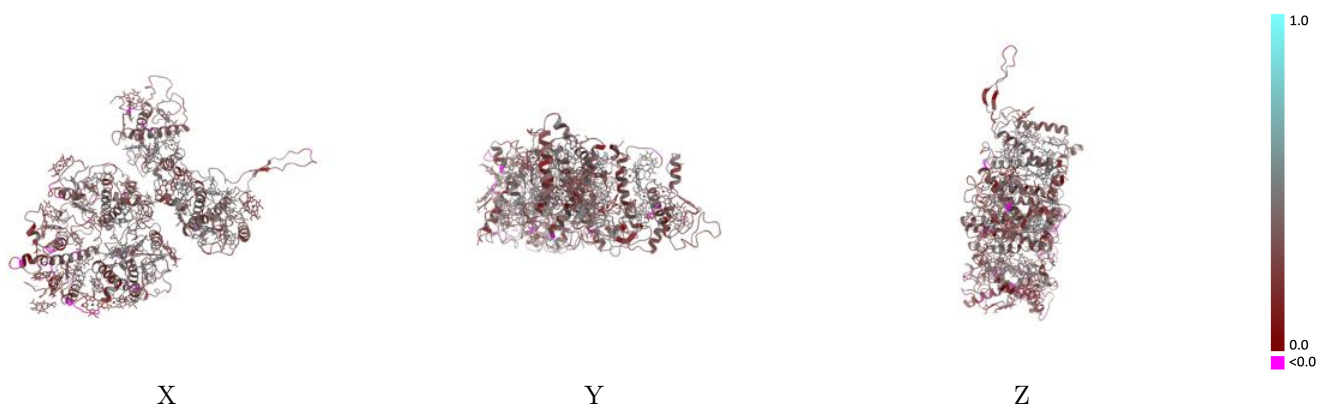
Y



Z

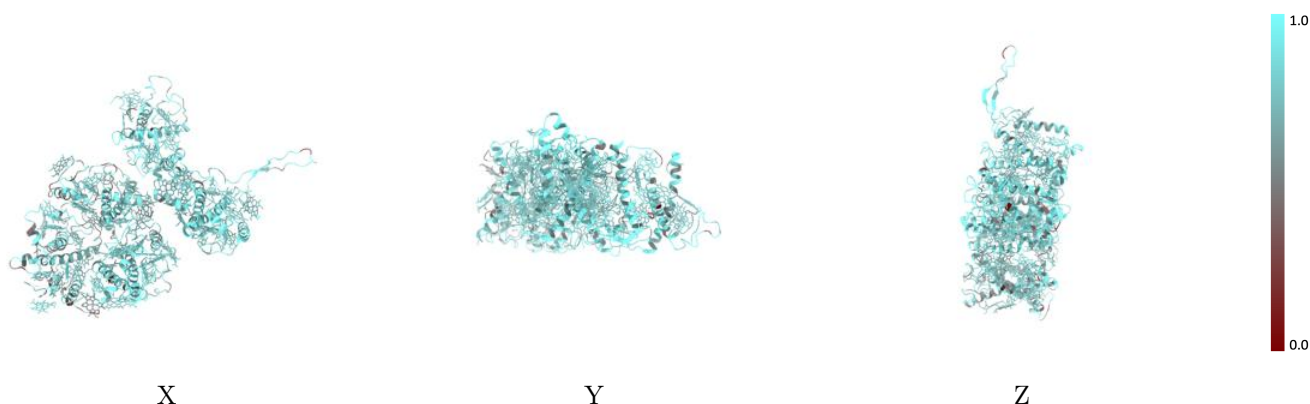
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



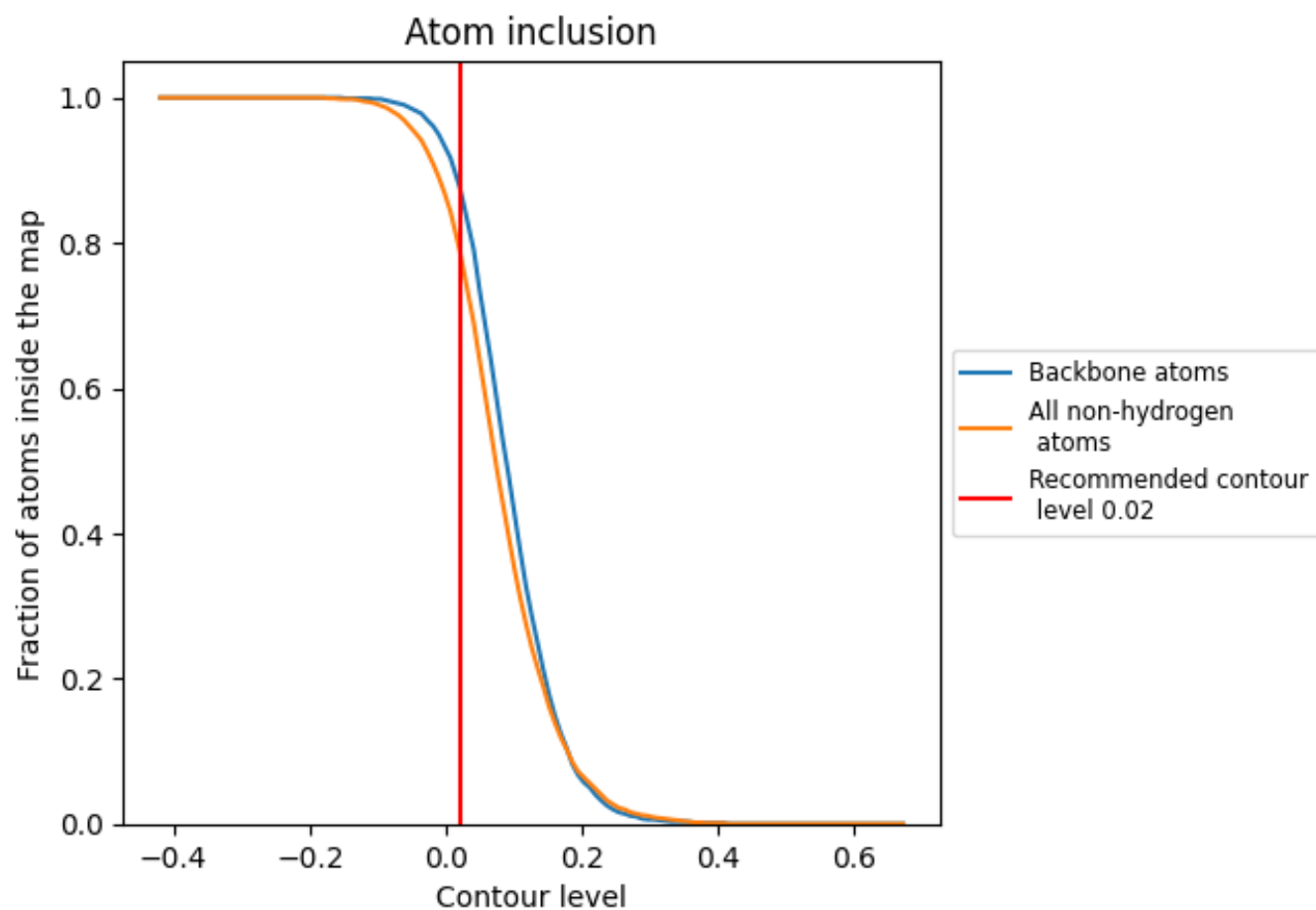
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 79% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7900	0.3240
05	0.7960	0.3290
06	0.7470	0.2650
07	0.7610	0.3240
08	0.8140	0.3370
1r	0.8220	0.3540

