



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 12:45 AM JST

PDB ID : 5XNN / pdb_00005xnn
EMDB ID : EMD-6743
Title : Structure of M-LHCII and CP24 complexes in the stacked C2S2M2-type PSII-LHCII supercomplex from *Pisum sativum*
Authors : Su, X.D.; Ma, J.; Wei, X.P.; Cao, P.; Zhu, D.J.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on : 2017-05-23
Resolution : 3.60 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 Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

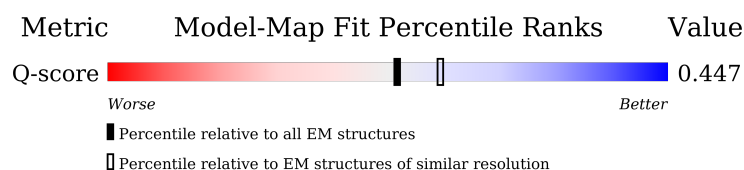
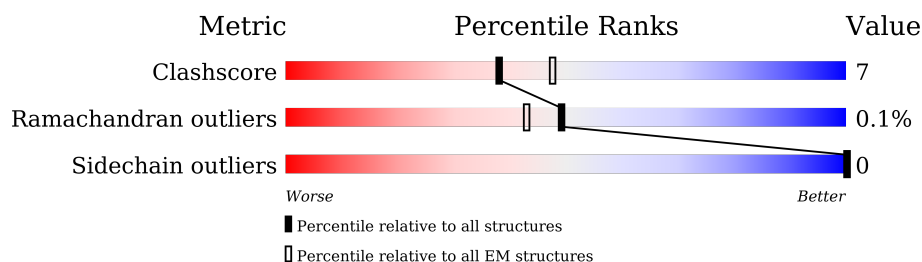
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	1	232	
1	2	232	
2	3	243	
3	4	210	

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
4	CHL	1	607	X	-	-	-
4	CHL	1	609	X	-	-	-
4	CHL	2	607	X	-	-	-
4	CHL	2	609	X	-	-	-
4	CHL	3	601	X	-	-	-
4	CHL	3	609	X	-	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10020 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 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	2	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		

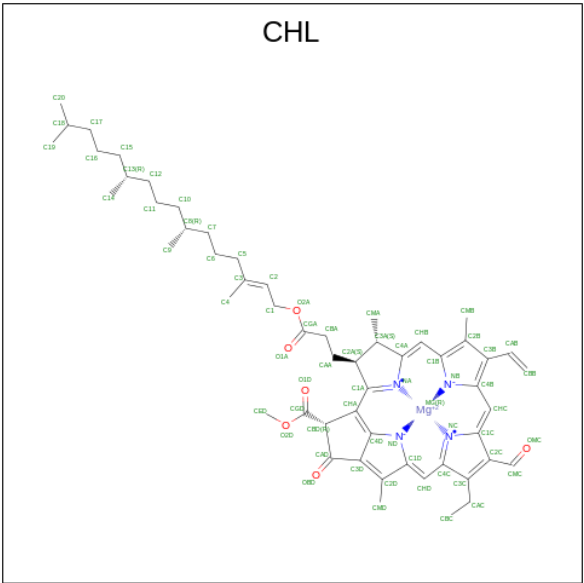
- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		

- Molecule 3 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

- Molecule 4 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



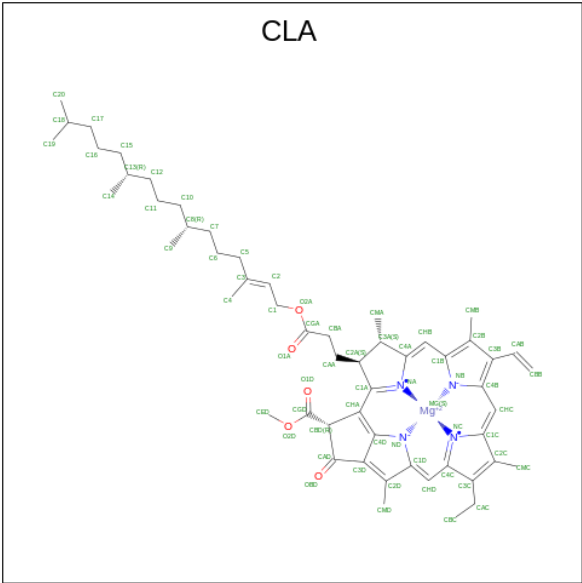
Mol	Chain	Residues	Atoms					AltConf
4	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	1	1	Total 63	C 52	Mg 1	N 4	O 6	0
4	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	1	1	Total 62	C 51	Mg 1	N 4	O 6	0
4	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	2	1	Total 61	C 50	Mg 1	N 4	O 6	0
4	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	2	1	Total 61	C 50	Mg 1	N 4	O 6	0
4	3	1	Total 64	C 53	Mg 1	N 4	O 6	0
4	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	3	1	Total 53	C 42	Mg 1	N 4	O 6	0
4	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	3	1	Total 61	C 50	Mg 1	N 4	O 6	0
4	4	1	Total 45	C 34	Mg 1	N 4	O 6	0
4	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
4	4	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
4	4	1	46	35	1	4	6	0

- Molecule 5 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



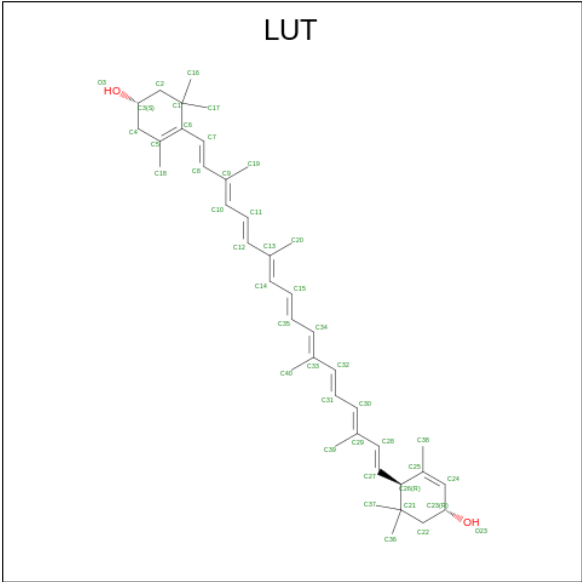
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
5	1	1	Total 61	51	1	4	5	0
5	1	1	Total 55	45	1	4	5	0
5	1	1	Total 50	40	1	4	5	0
5	1	1	Total 56	46	1	4	5	0
5	1	1	Total 45	35	1	4	5	0
5	1	1	Total 45	35	1	4	5	0
5	1	1	Total 55	45	1	4	5	0
5	1	1	Total 45	35	1	4	5	0
5	2	1	Total 61	51	1	4	5	0
5	2	1	Total 55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
5	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
5	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 6 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3, 3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).

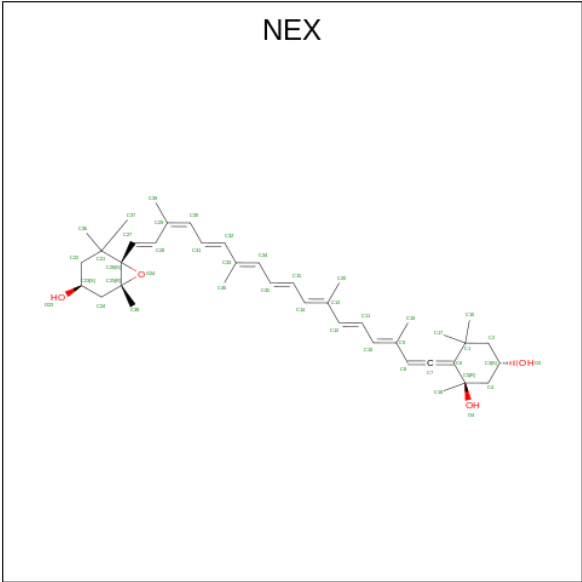


Mol	Chain	Residues	Atoms			AltConf
6	1	1	Total	C	O	0
			42	40	2	
6	1	1	Total	C	O	0
			42	40	2	
6	2	1	Total	C	O	0
			42	40	2	
6	2	1	Total	C	O	0
			42	40	2	
6	3	1	Total	C	O	0
			42	40	2	
6	3	1	Total	C	O	0
			42	40	2	
6	4	1	Total	C	O	0
			42	40	2	

- Molecule 7 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).

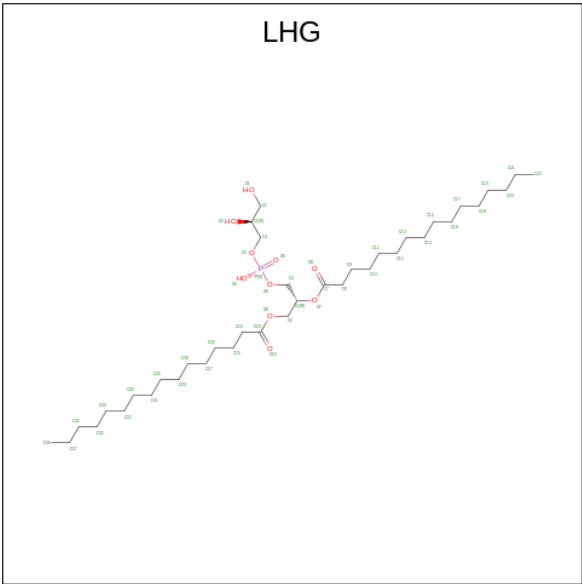


- Molecule 8 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



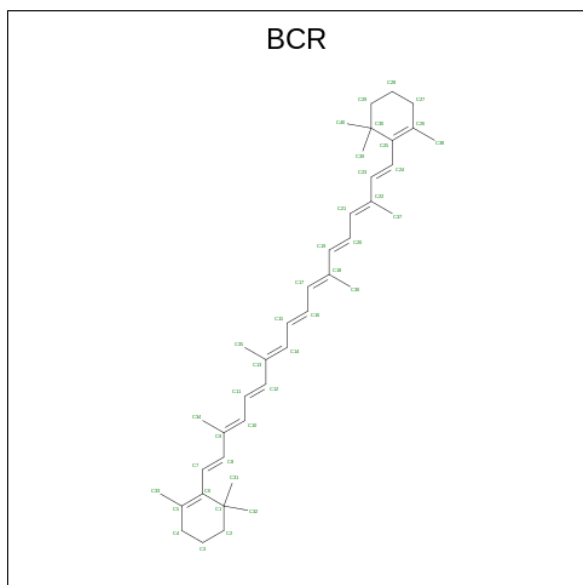
Mol	Chain	Residues	Atoms			AltConf
8	1	1	Total	C	O	0
			44	40	4	
8	2	1	Total	C	O	0
			44	40	4	
8	3	1	Total	C	O	0
			44	40	4	

- Molecule 9 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
9	1	1	Total	C	O	P	0
			41	30	10	1	
9	2	1	Total	C	O	P	0
			37	26	10	1	
9	3	1	Total	C	O	P	0
			47	36	10	1	
9	4	1	Total	C	O	P	0
			21	10	10	1	

- Molecule 10 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).

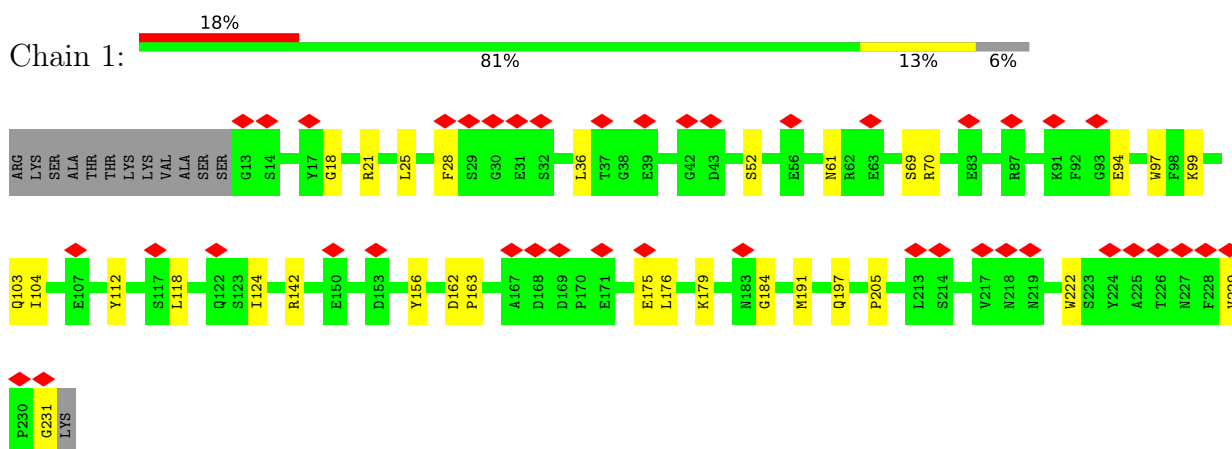


Mol	Chain	Residues	Atoms		AltConf
10	4	1	Total	C	0
			40	40	

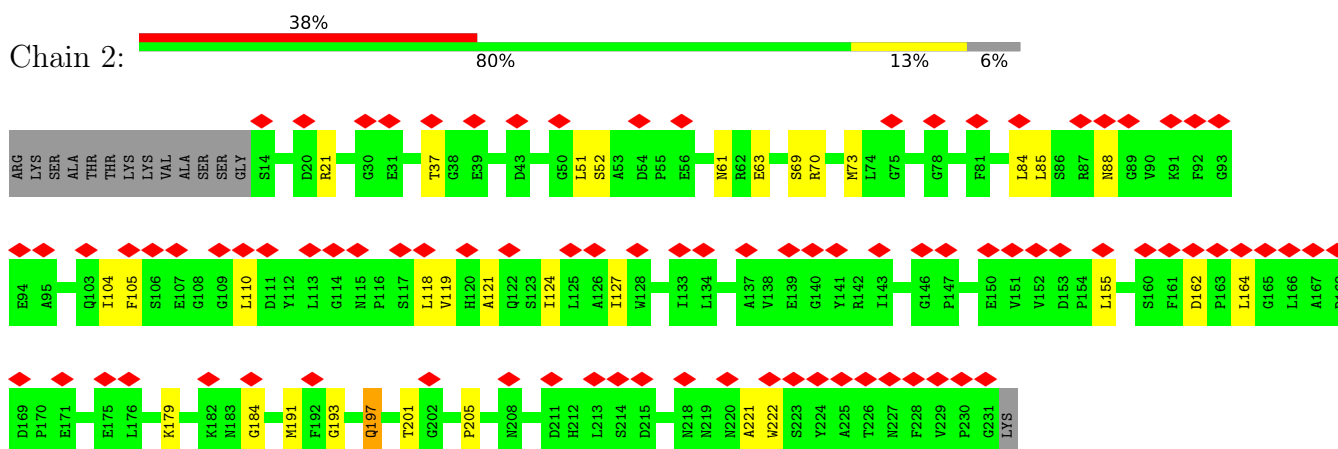
3 Residue-property plots

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.

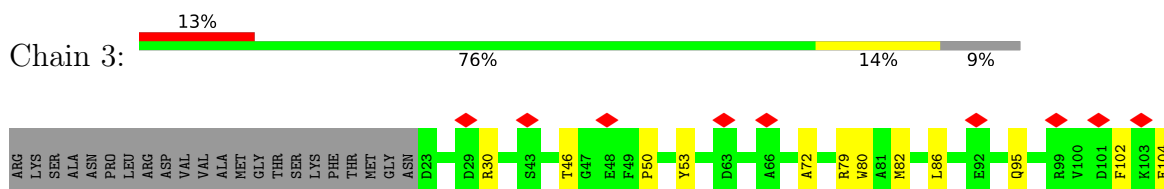
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

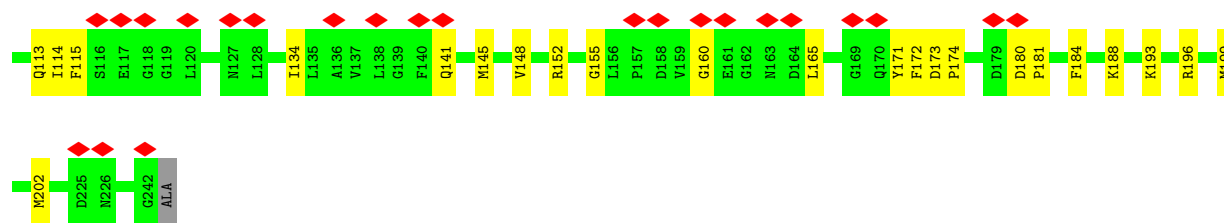


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



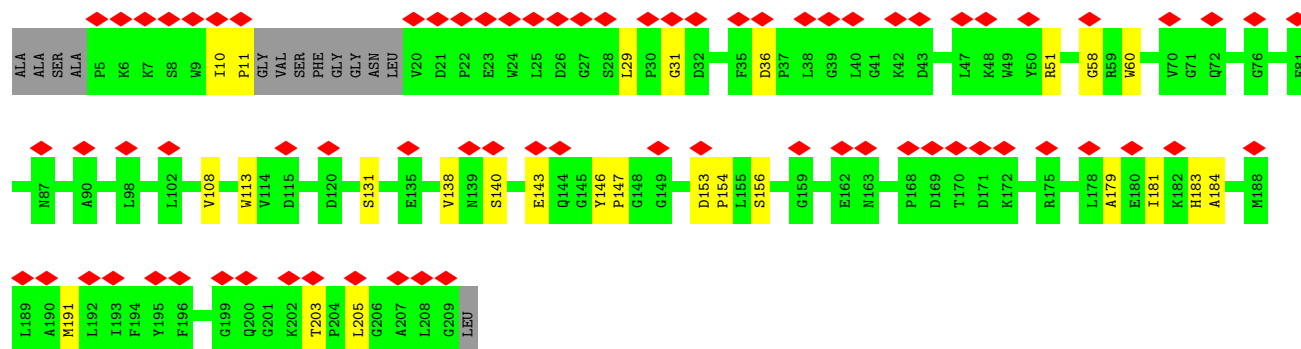
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic





- Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

Chain 4: 35% 81% 12% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	136521	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.112	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	156.0, 156.0, 156.0	wwPDB
Map dimensions	150, 150, 150	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: XAT, CLA, NEX, BCR, CHL, LHG, 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	1	0.27	0/1720	0.46	0/2342
1	2	0.25	0/1716	0.49	1/2337 (0.0%)
2	3	0.31	0/1759	0.50	0/2396
3	4	0.27	0/1586	0.59	0/2158
All	All	0.28	0/6781	0.51	1/9233 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	197	GLN	CA-CB-CG	5.92	125.95	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1668	0	1596	23	0
1	2	1664	0	1593	24	0
2	3	1707	0	1659	26	0
3	4	1534	0	1486	18	0
4	1	309	0	244	8	0
4	2	306	0	238	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	316	0	254	18	0
4	4	229	0	152	7	0
5	1	412	0	348	7	0
5	2	391	0	314	7	0
5	3	426	0	373	10	0
5	4	270	0	198	2	0
6	1	84	0	112	11	0
6	2	84	0	112	7	0
6	3	84	0	112	7	0
6	4	42	0	56	3	0
7	1	44	0	56	2	0
7	2	44	0	56	4	0
7	3	44	0	56	2	0
7	4	44	0	56	4	0
8	1	44	0	56	2	0
8	2	44	0	56	0	0
8	3	44	0	56	3	0
9	1	41	0	55	2	0
9	2	37	0	44	1	0
9	3	47	0	67	1	0
9	4	21	0	12	1	0
10	4	40	0	56	5	0
All	All	10020	0	9473	144	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 7.

The worst 5 of 144 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)
1:2:191:MET:HE2	6:2:1621:LUT:H10	1.65	0.79
5:3:602:CLA:HAB	6:3:1621:LUT:H32	1.67	0.75
2:3:202:MET:HE2	6:3:1621:LUT:H10	1.71	0.73
5:1:602:CLA:HAB	6:1:1621:LUT:H32	1.72	0.72
1:1:191:MET:HE2	6:1:1621:LUT:H10	1.75	0.68

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	217/232 (94%)	209 (96%)	8 (4%)	0	100	100
1	2	216/232 (93%)	210 (97%)	5 (2%)	1 (0%)	24	57
2	3	218/243 (90%)	209 (96%)	9 (4%)	0	100	100
3	4	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
All	All	844/917 (92%)	807 (96%)	36 (4%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	119	VAL

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	171/182 (94%)	171 (100%)	0	100	100
1	2	171/182 (94%)	171 (100%)	0	100	100
2	3	175/193 (91%)	175 (100%)	0	100	100
3	4	154/162 (95%)	154 (100%)	0	100	100
All	All	671/719 (93%)	671 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	3	95	GLN
2	3	113	GLN
2	3	219	ASN
1	2	61	ASN
1	1	61	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

72 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	$\# Z > 2$
6	LUT	2	1621	-	42,43,43	0.84	1 (2%)	51,60,60	1.68	15 (29%)
4	CHL	2	607	-	65,69,74	1.96	18 (27%)	74,108,114	2.95	24 (32%)
4	CHL	2	601	1	50,54,74	2.27	18 (36%)	56,90,114	3.47	26 (46%)
4	CHL	2	608	-	50,54,74	2.21	18 (36%)	56,90,114	3.36	21 (37%)
4	CHL	4	608	-	50,54,74	2.16	17 (34%)	56,90,114	3.42	21 (37%)
5	CLA	1	612	1	49,53,73	1.48	9 (18%)	59,89,113	1.45	10 (16%)
5	CLA	1	614	1	49,53,73	1.47	7 (14%)	59,89,113	1.29	6 (10%)
9	LHG	3	2630	5	46,46,48	0.70	1 (2%)	49,52,54	1.24	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CHL	2	606	-	50,54,74	2.26	18 (36%)	56,90,114	3.22	22 (39%)
7	XAT	3	1622	-	39,47,47	1.03	3 (7%)	54,74,74	2.85	24 (44%)
4	CHL	1	608	-	50,54,74	2.18	17 (34%)	56,90,114	3.36	19 (33%)
4	CHL	1	607	-	67,71,74	1.92	19 (28%)	76,110,114	3.11	24 (31%)
4	CHL	2	609	1	65,69,74	1.99	18 (27%)	74,108,114	2.87	24 (32%)
5	CLA	1	603	1	59,63,73	1.32	10 (16%)	71,101,113	1.44	7 (9%)
5	CLA	2	611	9	49,53,73	1.46	7 (14%)	59,89,113	1.38	7 (11%)
4	CHL	4	609	3	50,54,74	2.31	19 (38%)	56,90,114	3.26	20 (35%)
5	CLA	4	612	3	49,53,73	1.47	7 (14%)	59,89,113	1.35	6 (10%)
6	LUT	2	1620	-	42,43,43	0.80	0	51,60,60	1.80	15 (29%)
4	CHL	1	609	1	66,70,74	1.95	18 (27%)	75,109,114	2.86	22 (29%)
8	NEX	3	1623	-	38,46,46	0.87	1 (2%)	50,70,70	2.40	16 (32%)
5	CLA	2	602	1	65,69,73	1.30	10 (15%)	78,108,113	1.19	8 (10%)
5	CLA	3	613	2	62,66,73	1.32	9 (14%)	74,104,113	1.28	7 (9%)
9	LHG	2	2630	5	36,36,48	0.74	0	39,42,54	1.27	4 (10%)
9	LHG	4	2630	5	20,20,48	0.91	0	23,26,54	1.30	2 (8%)
5	CLA	4	602	3	49,53,73	1.45	9 (18%)	59,89,113	1.41	6 (10%)
4	CHL	3	606	-	50,54,74	2.19	18 (36%)	56,90,114	3.24	23 (41%)
5	CLA	2	603	1	59,63,73	1.34	9 (15%)	71,101,113	1.40	8 (11%)
5	CLA	4	603	3	49,53,73	1.49	10 (20%)	59,89,113	1.44	6 (10%)
5	CLA	1	604	-	54,58,73	1.43	10 (18%)	65,95,113	1.37	10 (15%)
4	CHL	3	605	2	50,54,74	2.27	18 (36%)	56,90,114	3.31	24 (42%)
5	CLA	3	611	9	59,63,73	1.38	9 (15%)	71,101,113	1.45	10 (14%)
6	LUT	1	1620	-	42,43,43	0.80	0	51,60,60	1.66	15 (29%)
7	XAT	2	1622	-	39,47,47	0.91	1 (2%)	54,74,74	2.81	21 (38%)
5	CLA	3	604	-	49,53,73	1.48	9 (18%)	59,89,113	1.32	6 (10%)
5	CLA	3	614	2	52,56,73	1.42	8 (15%)	62,92,113	1.16	5 (8%)
5	CLA	3	610	2	64,68,73	1.28	7 (10%)	77,107,113	1.18	7 (9%)
8	NEX	2	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.39	16 (32%)
7	XAT	4	622	-	39,47,47	0.92	1 (2%)	54,74,74	2.62	22 (40%)
5	CLA	1	611	9	49,53,73	1.47	9 (18%)	59,89,113	1.28	6 (10%)
4	CHL	4	607	-	50,54,74	2.30	18 (36%)	56,90,114	3.17	21 (37%)
9	LHG	1	2630	5	40,40,48	0.72	1 (2%)	43,46,54	1.33	6 (13%)
5	CLA	2	613	1	49,53,73	1.47	9 (18%)	59,89,113	1.29	6 (10%)
8	NEX	1	1623	-	38,46,46	0.98	2 (5%)	50,70,70	2.42	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BCR	4	623	-	41,41,41	0.74	0	56,56,56	2.31	17 (30%)
5	CLA	3	603	2	59,63,73	1.31	10 (16%)	71,101,113	1.46	8 (11%)
4	CHL	4	606	-	50,54,74	2.29	18 (36%)	56,90,114	3.30	25 (44%)
4	CHL	3	608	-	50,54,74	2.19	18 (36%)	56,90,114	3.42	21 (37%)
5	CLA	3	612	2	49,53,73	1.47	10 (20%)	59,89,113	1.39	9 (15%)
4	CHL	2	605	1	50,54,74	2.28	18 (36%)	56,90,114	3.31	22 (39%)
7	XAT	1	1622	-	39,47,47	0.90	0	54,74,74	2.77	22 (40%)
4	CHL	1	601	1	50,54,74	2.32	18 (36%)	56,90,114	3.26	24 (42%)
6	LUT	4	620	-	42,43,43	0.81	0	51,60,60	1.87	17 (33%)
5	CLA	4	611	9	49,53,73	1.49	7 (14%)	59,89,113	1.31	4 (6%)
5	CLA	1	613	1	59,63,73	1.36	9 (15%)	71,101,113	1.23	5 (7%)
5	CLA	2	604	-	49,53,73	1.47	9 (18%)	59,89,113	1.36	6 (10%)
6	LUT	3	1621	-	42,43,43	0.84	1 (2%)	51,60,60	1.60	11 (21%)
5	CLA	2	610	1	54,58,73	1.36	8 (14%)	65,95,113	1.22	8 (12%)
4	CHL	3	601	2	68,72,74	1.95	16 (23%)	77,111,114	3.10	27 (35%)
5	CLA	4	610	3	49,53,73	1.48	9 (18%)	59,89,113	1.18	6 (10%)
4	CHL	1	606	-	50,54,74	2.24	17 (34%)	56,90,114	3.15	22 (39%)
4	CHL	3	607	-	57,61,74	2.25	19 (33%)	64,98,114	3.11	26 (40%)
4	CHL	3	609	2	65,69,74	2.04	17 (26%)	74,108,114	2.72	24 (32%)
4	CHL	1	605	1	50,54,74	2.23	18 (36%)	56,90,114	3.37	24 (42%)
5	CLA	1	602	1	65,69,73	1.28	10 (15%)	78,108,113	1.19	8 (10%)
6	LUT	1	1621	-	42,43,43	0.90	2 (4%)	51,60,60	1.74	15 (29%)
4	CHL	4	601	3	48,53,74	2.38	19 (39%)	53,89,114	3.18	19 (35%)
5	CLA	2	614	1	49,53,73	1.48	7 (14%)	59,89,113	1.27	4 (6%)
5	CLA	3	602	2	64,68,73	1.30	8 (12%)	77,107,113	1.21	8 (10%)
5	CLA	2	612	1	49,53,73	1.51	8 (16%)	59,89,113	1.37	6 (10%)
5	CLA	4	604	-	49,53,73	1.50	8 (16%)	59,89,113	1.28	5 (8%)
5	CLA	1	610	1	60,64,73	1.30	8 (13%)	72,102,113	1.16	6 (8%)
6	LUT	3	1620	-	42,43,43	0.85	0	51,60,60	1.72	12 (23%)

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
6	LUT	2	1621	-	-	3/29/67/67	0/2/2/2
4	CHL	2	607	-	1/1/14/21	16/35/111/117	-
4	CHL	2	601	1	-	6/17/93/117	-
4	CHL	2	608	-	-	7/17/93/117	-
4	CHL	4	608	-	-	7/17/93/117	-
5	CLA	1	612	1	-	5/15/91/115	-
5	CLA	1	614	1	-	4/15/91/115	-
9	LHG	3	2630	5	-	24/51/51/53	-
4	CHL	2	606	-	-	6/17/93/117	-
7	XAT	3	1622	-	-	2/31/93/93	0/4/4/4
4	CHL	1	608	-	-	7/17/93/117	-
4	CHL	1	607	-	1/1/14/21	22/38/114/117	-
4	CHL	2	609	1	1/1/14/21	13/35/111/117	-
5	CLA	1	603	1	-	14/27/103/115	-
5	CLA	2	611	9	-	5/15/91/115	-
4	CHL	4	609	3	-	6/17/93/117	-
5	CLA	4	612	3	-	7/15/91/115	-
6	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
4	CHL	1	609	1	1/1/14/21	18/37/113/117	-
8	NEX	3	1623	-	-	4/27/83/83	0/3/3/3
5	CLA	2	602	1	-	12/35/111/115	-
5	CLA	3	613	2	-	11/31/107/115	-
9	LHG	2	2630	5	-	16/41/41/53	-
9	LHG	4	2630	5	-	8/23/23/53	-
5	CLA	4	602	3	-	9/15/91/115	-
4	CHL	3	606	-	-	9/17/93/117	-
5	CLA	2	603	1	-	13/27/103/115	-
5	CLA	4	603	3	-	6/15/91/115	-
5	CLA	1	604	-	-	12/21/97/115	-
4	CHL	3	605	2	-	11/17/93/117	-
5	CLA	3	611	9	-	9/27/103/115	-
6	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
7	XAT	2	1622	-	-	3/31/93/93	0/4/4/4
5	CLA	3	604	-	-	11/15/91/115	-
5	CLA	3	614	2	-	11/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	3	610	2	-	9/33/109/115	-
8	NEX	2	1623	-	-	7/27/83/83	0/3/3/3
7	XAT	4	622	-	-	2/31/93/93	0/4/4/4
5	CLA	1	611	9	-	8/15/91/115	-
4	CHL	4	607	-	-	10/17/93/117	-
9	LHG	1	2630	5	-	15/45/45/53	-
5	CLA	2	613	1	-	7/15/91/115	-
8	NEX	1	1623	-	-	6/27/83/83	0/3/3/3
10	BCR	4	623	-	-	9/29/63/63	0/2/2/2
5	CLA	3	603	2	-	15/27/103/115	-
4	CHL	4	606	-	-	8/17/93/117	-
4	CHL	3	608	-	-	5/17/93/117	-
5	CLA	3	612	2	-	10/15/91/115	-
4	CHL	2	605	1	-	11/17/93/117	-
7	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
4	CHL	1	601	1	-	6/17/93/117	-
6	LUT	4	620	-	-	4/29/67/67	0/2/2/2
5	CLA	4	611	9	-	6/15/91/115	-
5	CLA	1	613	1	-	10/27/103/115	-
5	CLA	2	604	-	-	10/15/91/115	-
6	LUT	3	1621	-	-	3/29/67/67	0/2/2/2
5	CLA	2	610	1	-	6/21/97/115	-
4	CHL	3	601	2	1/1/14/21	18/39/115/117	-
5	CLA	4	610	3	-	6/15/91/115	-
4	CHL	1	606	-	-	10/17/93/117	-
4	CHL	3	607	-	-	8/26/102/117	-
4	CHL	3	609	2	1/1/14/21	15/35/111/117	-
4	CHL	1	605	1	-	10/17/93/117	-
5	CLA	1	602	1	-	14/35/111/115	-
6	LUT	1	1621	-	-	3/29/67/67	0/2/2/2
4	CHL	4	601	3	-	9/15/91/117	-
5	CLA	2	614	1	-	7/15/91/115	-
5	CLA	3	602	2	-	16/33/109/115	-
5	CLA	2	612	1	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	4	604	-	-	10/15/91/115	-
5	CLA	1	610	1	-	7/29/105/115	-
6	LUT	3	1620	-	-	2/29/67/67	0/2/2/2

The worst 5 of 686 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	601	CHL	C3D-C4D	-5.50	1.31	1.44
4	1	601	CHL	C3D-C4D	-5.38	1.32	1.44
4	2	601	CHL	C3D-C4D	-5.34	1.32	1.44
4	3	606	CHL	C3D-C4D	-5.17	1.32	1.44
4	3	605	CHL	O2D-CGD	5.16	1.45	1.33

The worst 5 of 999 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	601	CHL	CMD-C2D-C1D	10.43	143.09	124.71
7	2	1622	XAT	O24-C25-C24	10.30	121.12	113.38
4	1	607	CHL	C2B-C1B-NB	10.15	117.04	110.23
4	2	601	CHL	CMD-C2D-C1D	9.97	142.28	124.71
4	3	601	CHL	C2B-C1B-NB	9.95	116.90	110.23

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	1	607	CHL	C8
4	1	609	CHL	C8
4	2	607	CHL	C8
4	2	609	CHL	C8
4	3	601	CHL	C8

5 of 630 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	1	601	CHL	C1C-C2C-CMC-OMC
4	1	601	CHL	C3C-C2C-CMC-OMC
4	1	601	CHL	CHA-CBD-CGD-O1D
4	1	601	CHL	CHA-CBD-CGD-O2D
4	1	605	CHL	C1C-C2C-CMC-OMC

There are no ring outliers.

53 monomers are involved in 97 short contacts:

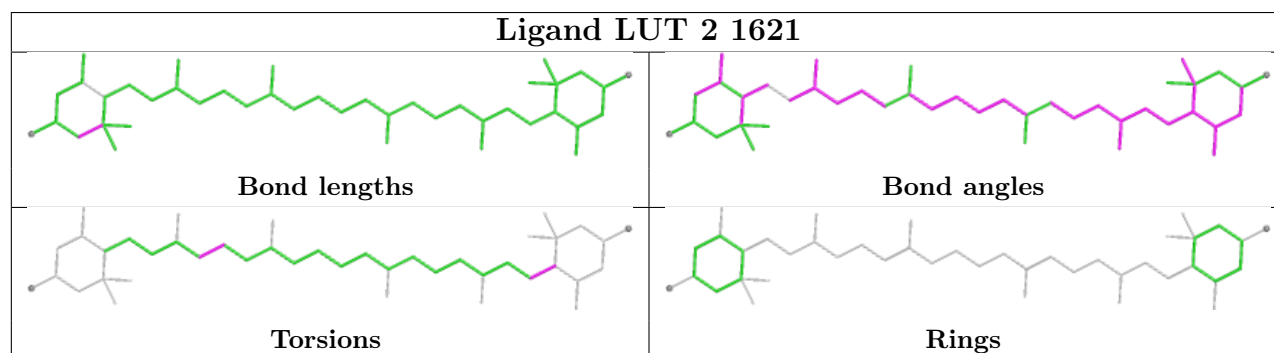
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	2	1621	LUT	3	0
4	2	607	CHL	2	0
4	4	608	CHL	2	0
9	3	2630	LHG	1	0
4	2	606	CHL	1	0
7	3	1622	XAT	2	0
4	1	608	CHL	1	0
4	1	607	CHL	4	0
4	2	609	CHL	2	0
5	1	603	CLA	2	0
5	2	611	CLA	1	0
4	4	609	CHL	1	0
5	4	612	CLA	1	0
6	2	1620	LUT	4	0
4	1	609	CHL	3	0
8	3	1623	NEX	3	0
5	2	602	CLA	2	0
9	2	2630	LHG	1	0
9	4	2630	LHG	1	0
4	3	606	CHL	3	0
5	2	603	CLA	1	0
5	1	604	CLA	1	0
5	3	611	CLA	2	0
6	1	1620	LUT	5	0
7	2	1622	XAT	4	0
5	3	604	CLA	1	0
7	4	622	XAT	4	0
9	1	2630	LHG	2	0
5	2	613	CLA	1	0
8	1	1623	NEX	2	0
10	4	623	BCR	5	0
5	3	603	CLA	4	0
4	4	606	CHL	2	0
4	3	608	CHL	4	0
5	3	612	CLA	1	0
4	2	605	CHL	1	0
7	1	1622	XAT	2	0
4	1	601	CHL	1	0
6	4	620	LUT	3	0
5	1	613	CLA	1	0
5	2	604	CLA	1	0
6	3	1621	LUT	4	0

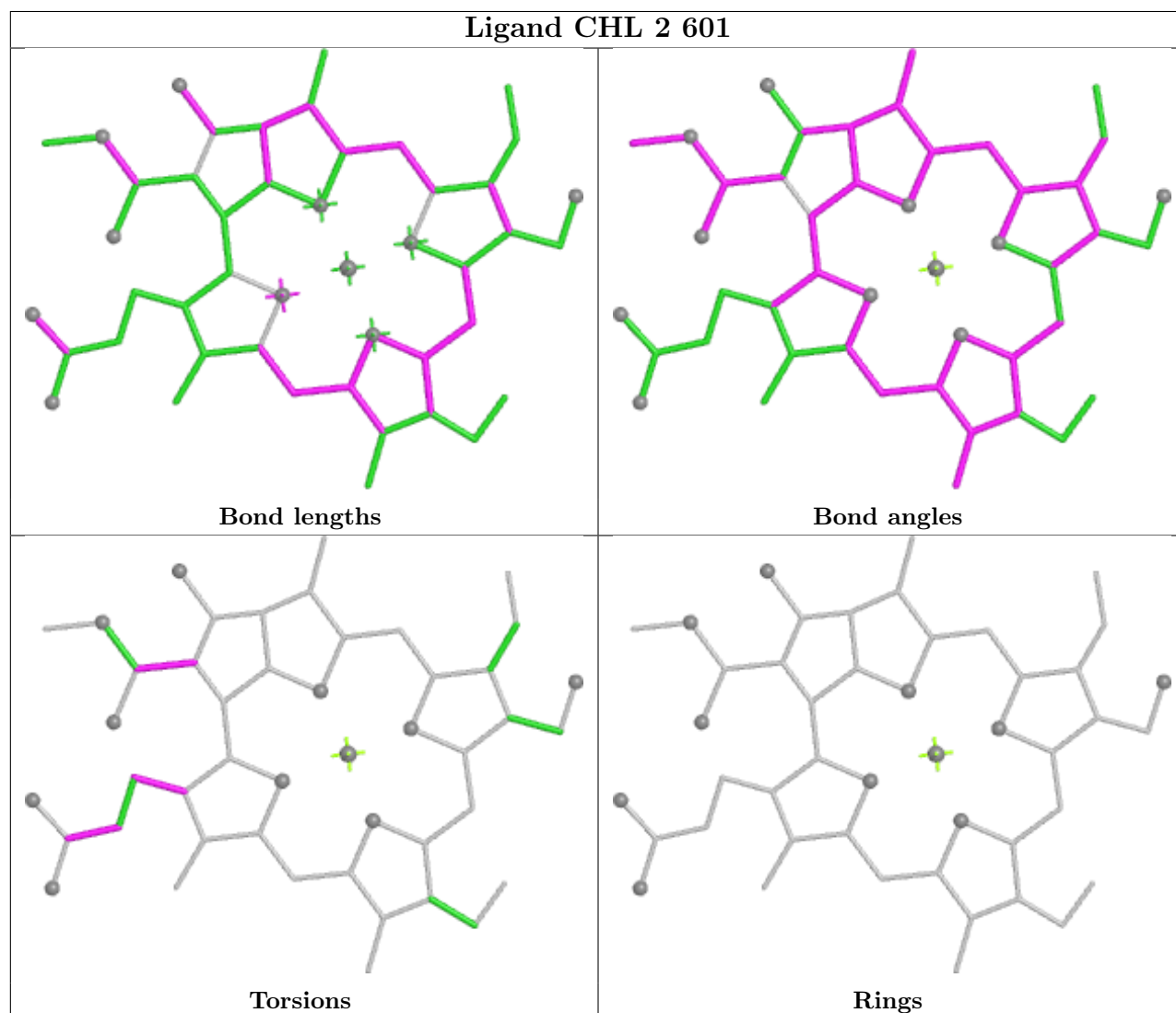
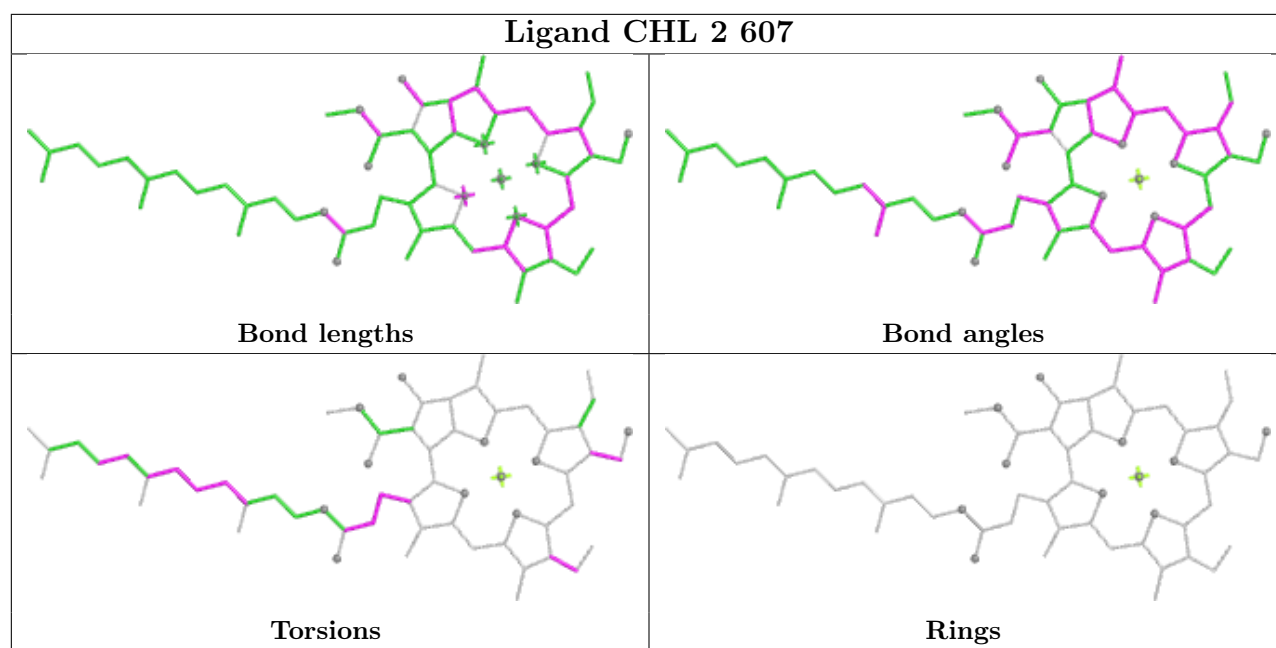
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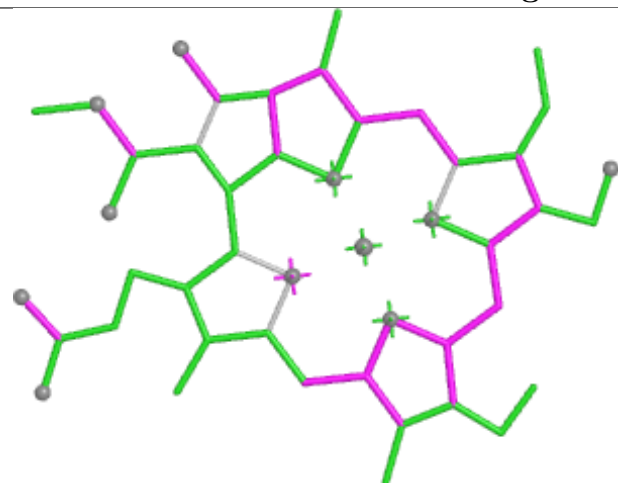
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3	601	CHL	2	0
5	4	610	CLA	1	0
4	3	607	CHL	4	0
4	3	609	CHL	7	0
5	1	602	CLA	2	0
6	1	1621	LUT	6	0
4	4	601	CHL	2	0
5	3	602	CLA	3	0
5	2	612	CLA	2	0
5	1	610	CLA	1	0
6	3	1620	LUT	3	0

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.

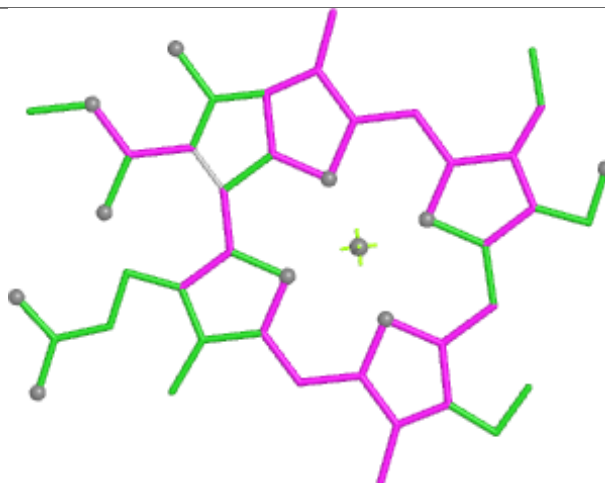




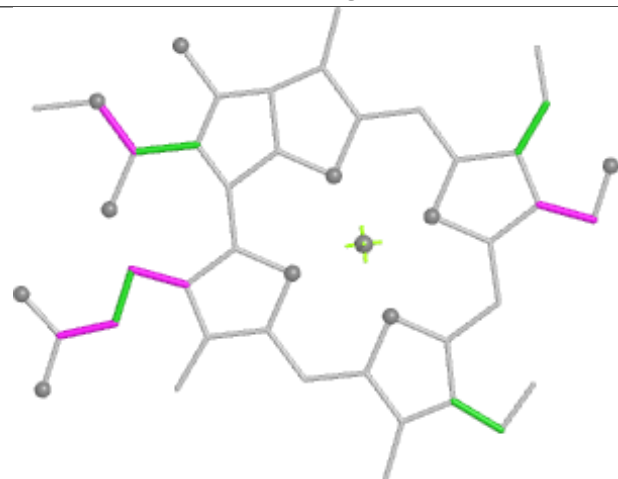
Ligand CHL 2 608



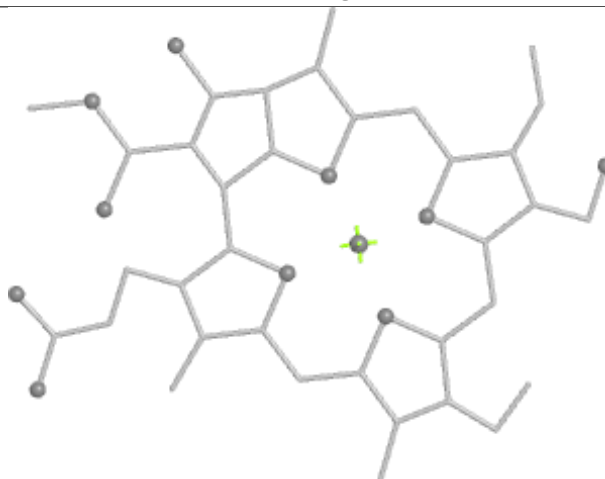
Bond lengths



Bond angles

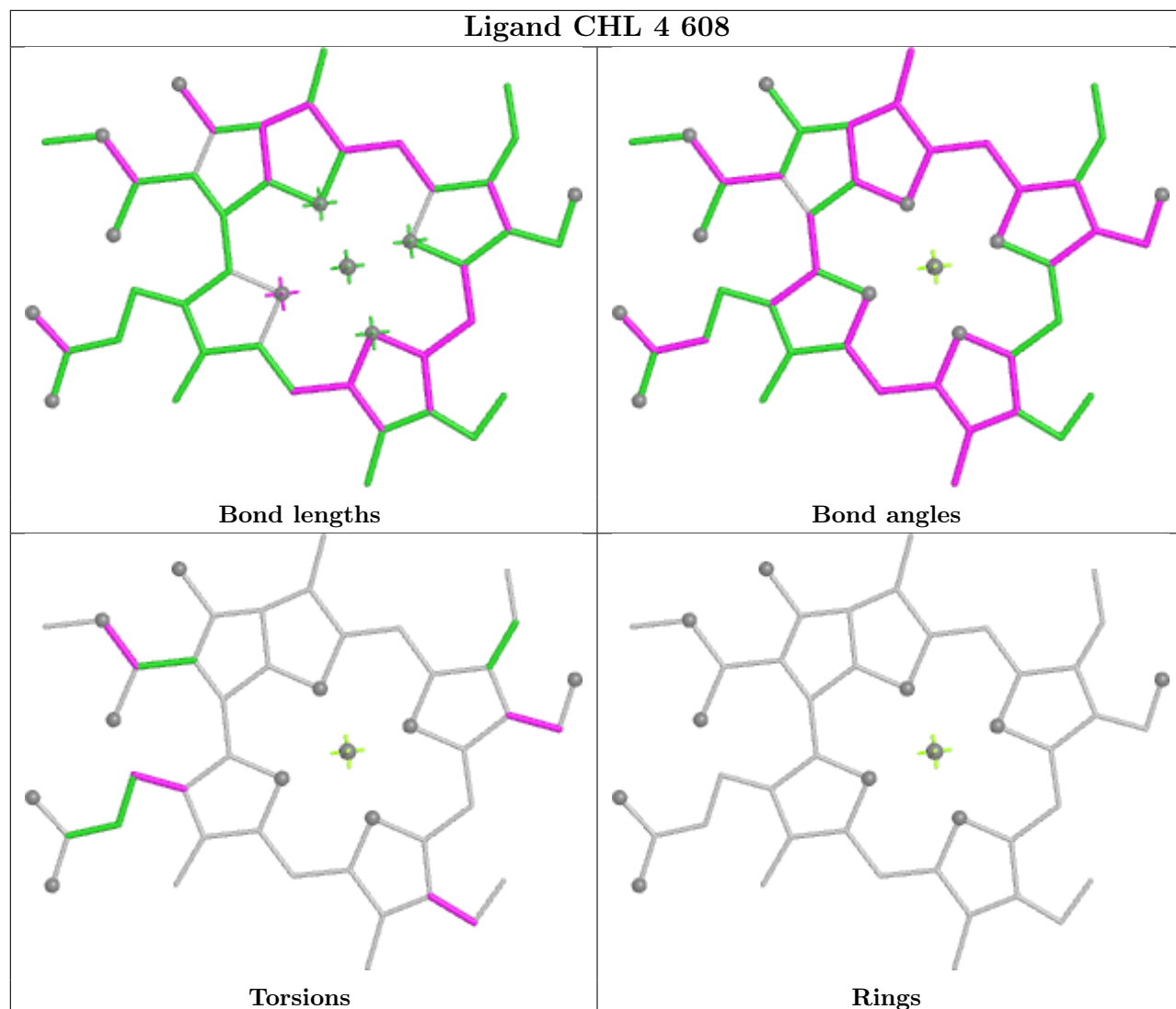


Torsions

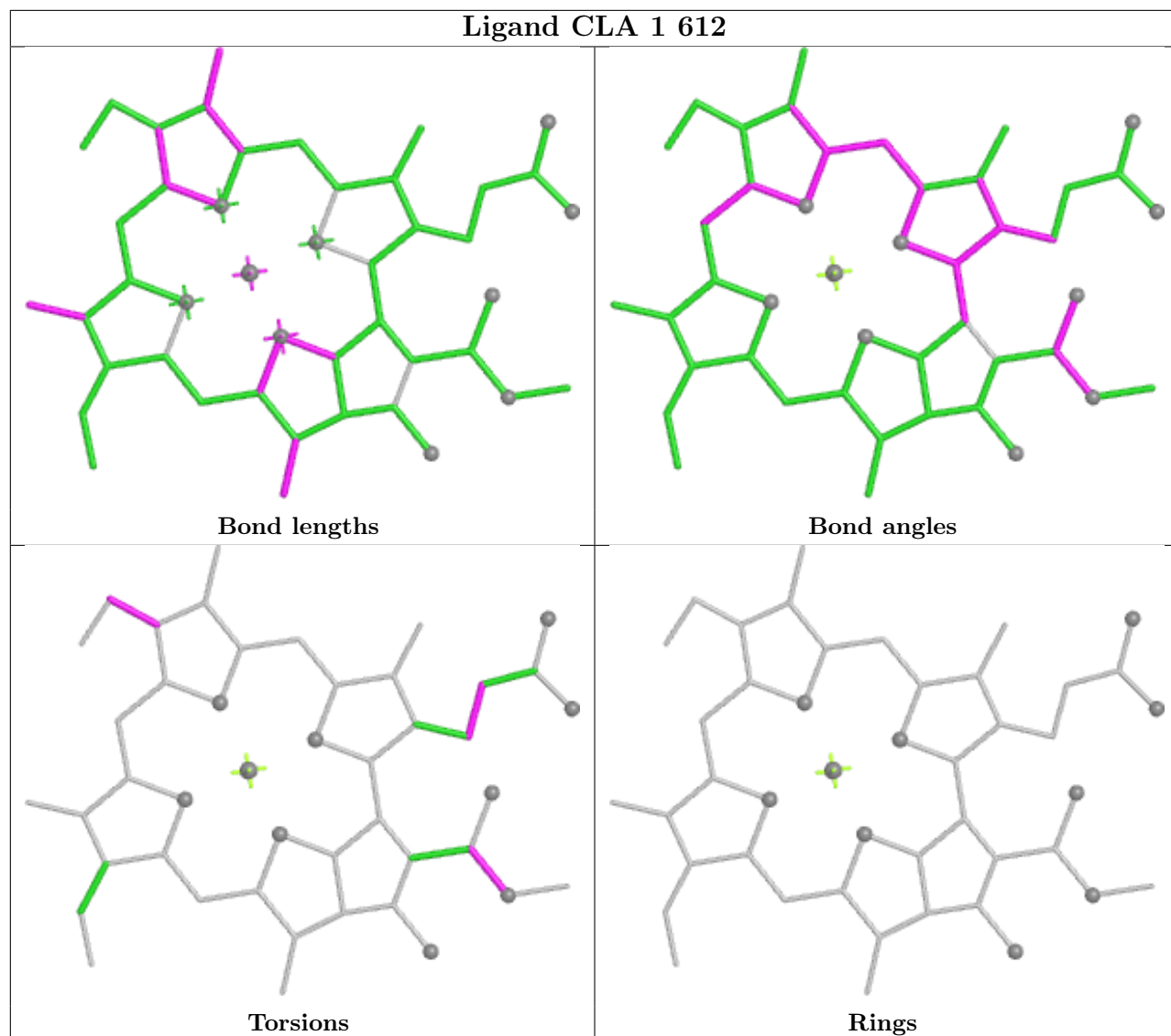


Rings

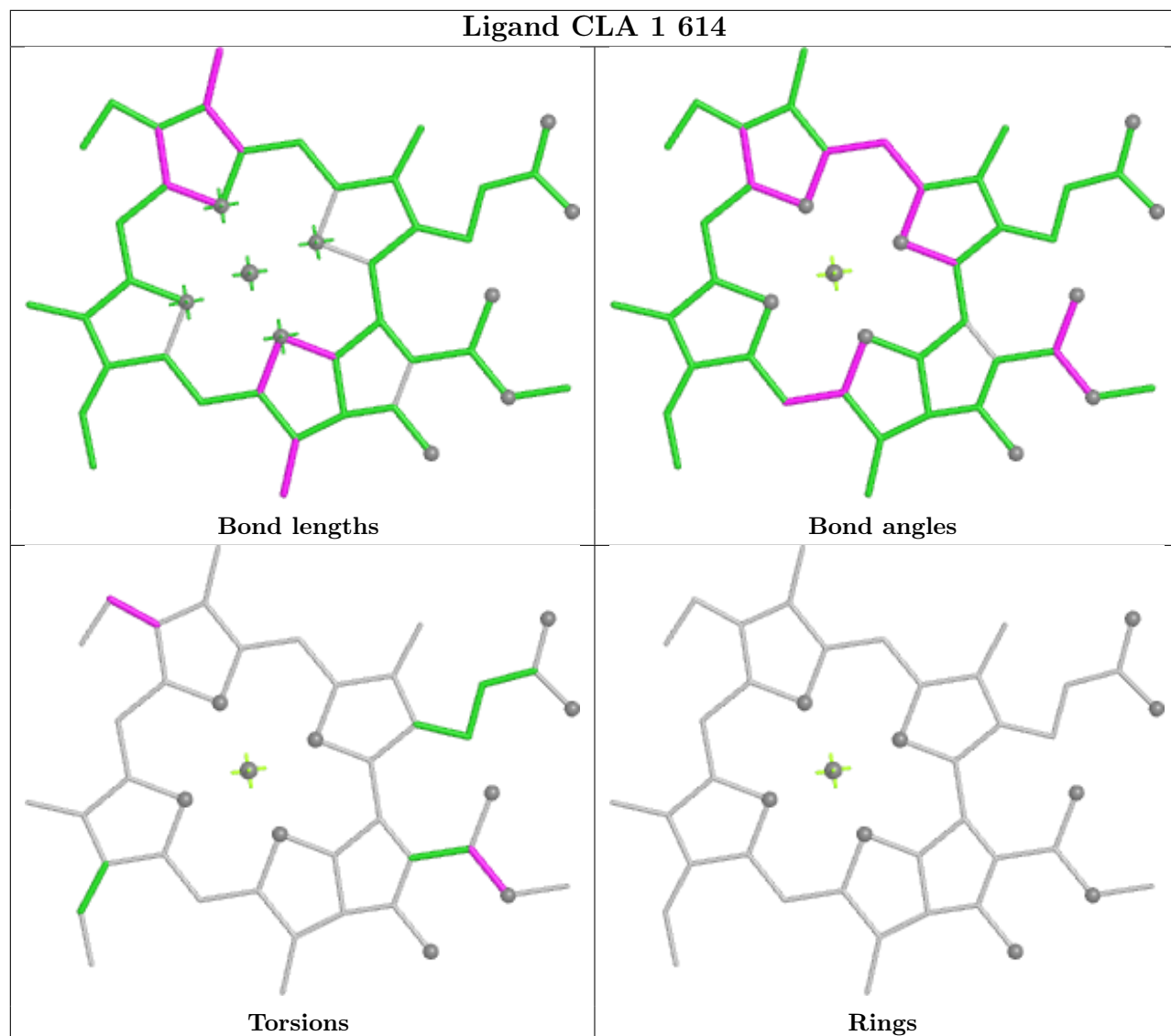
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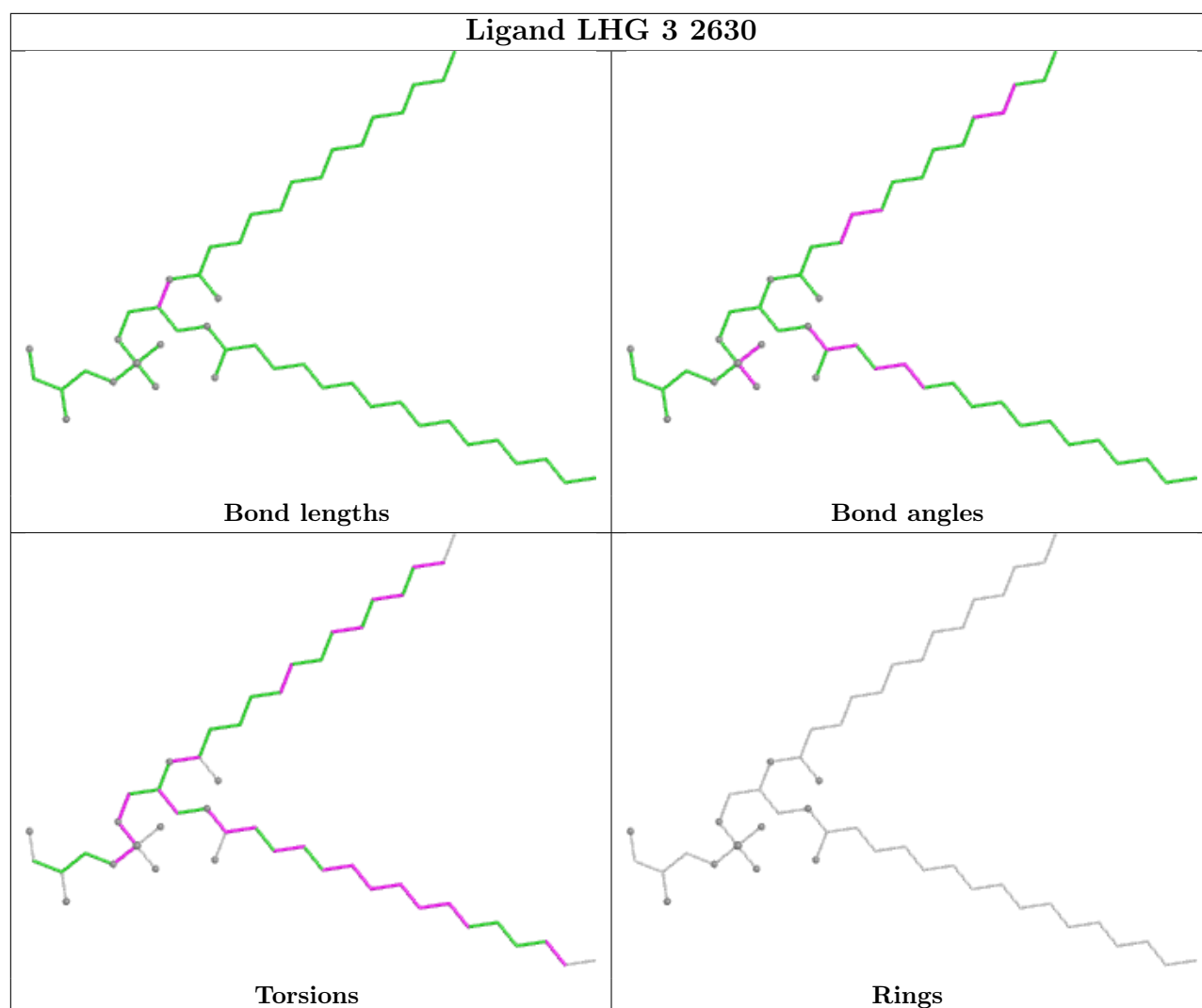


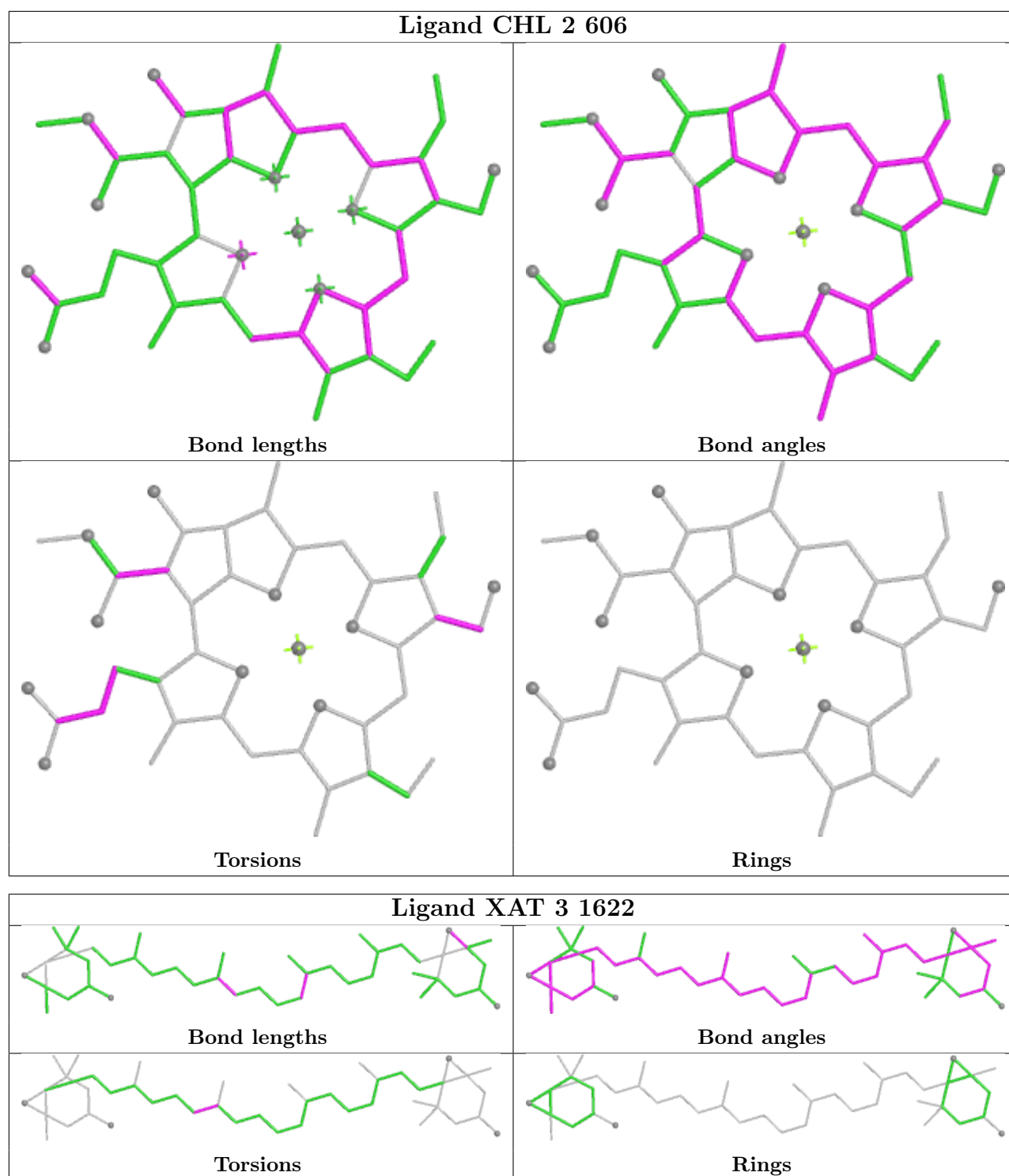
Ligand CLA 1 612

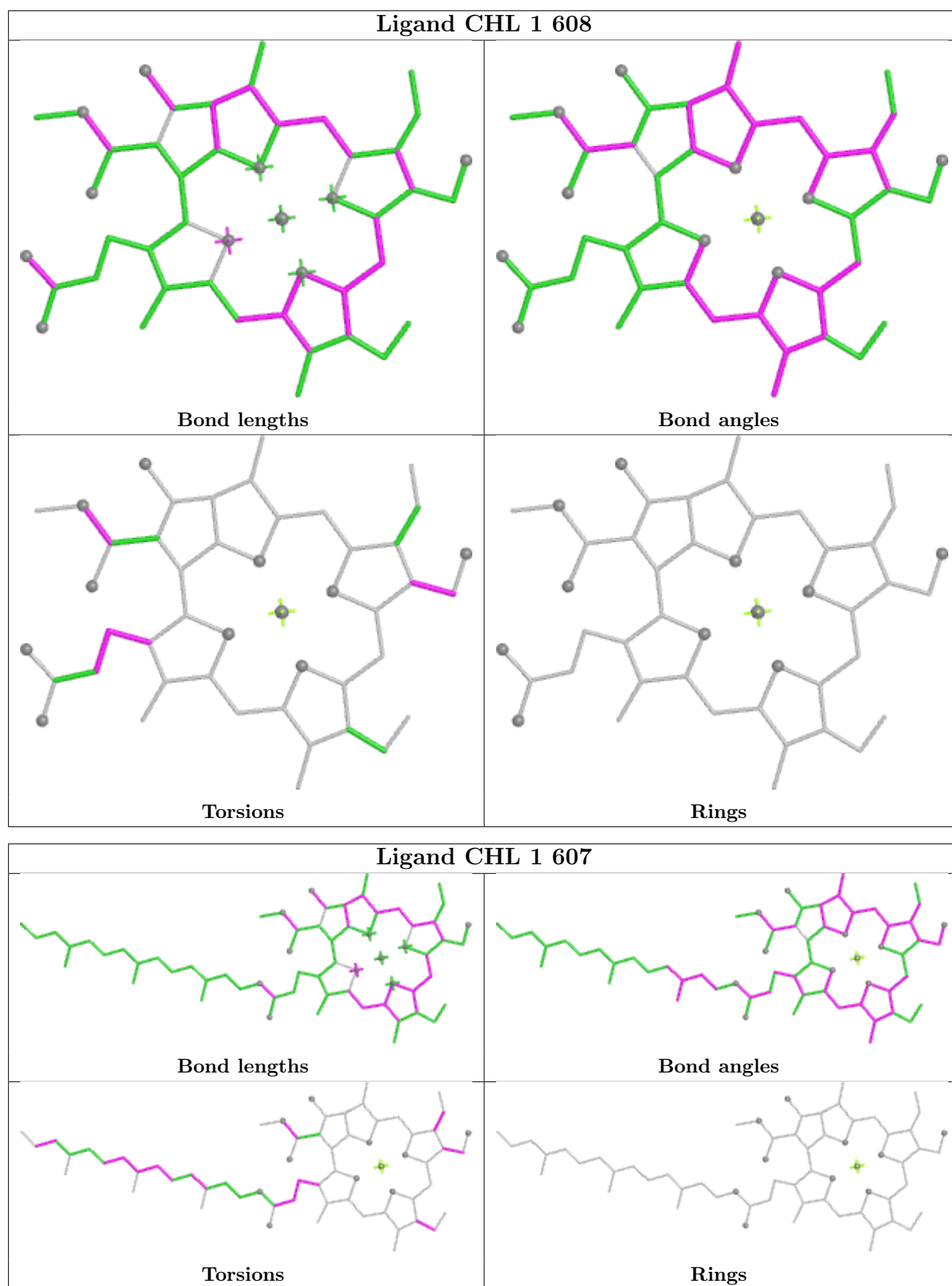


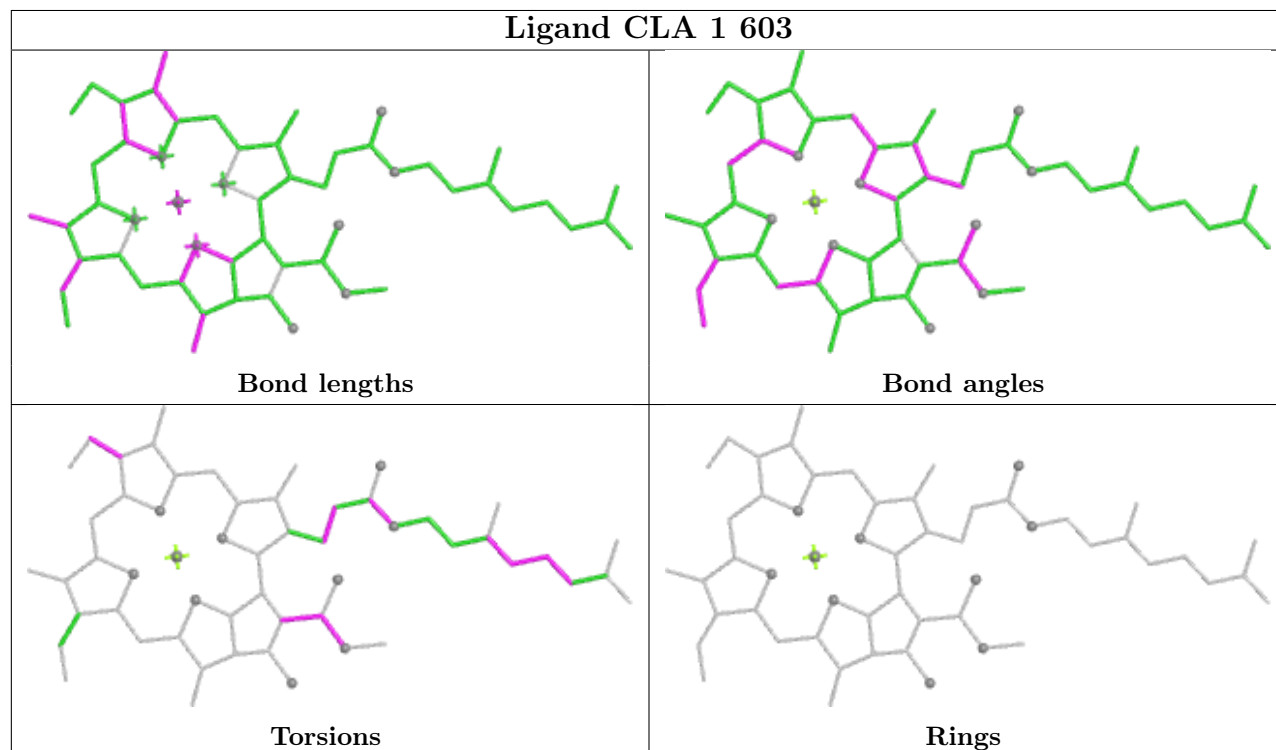
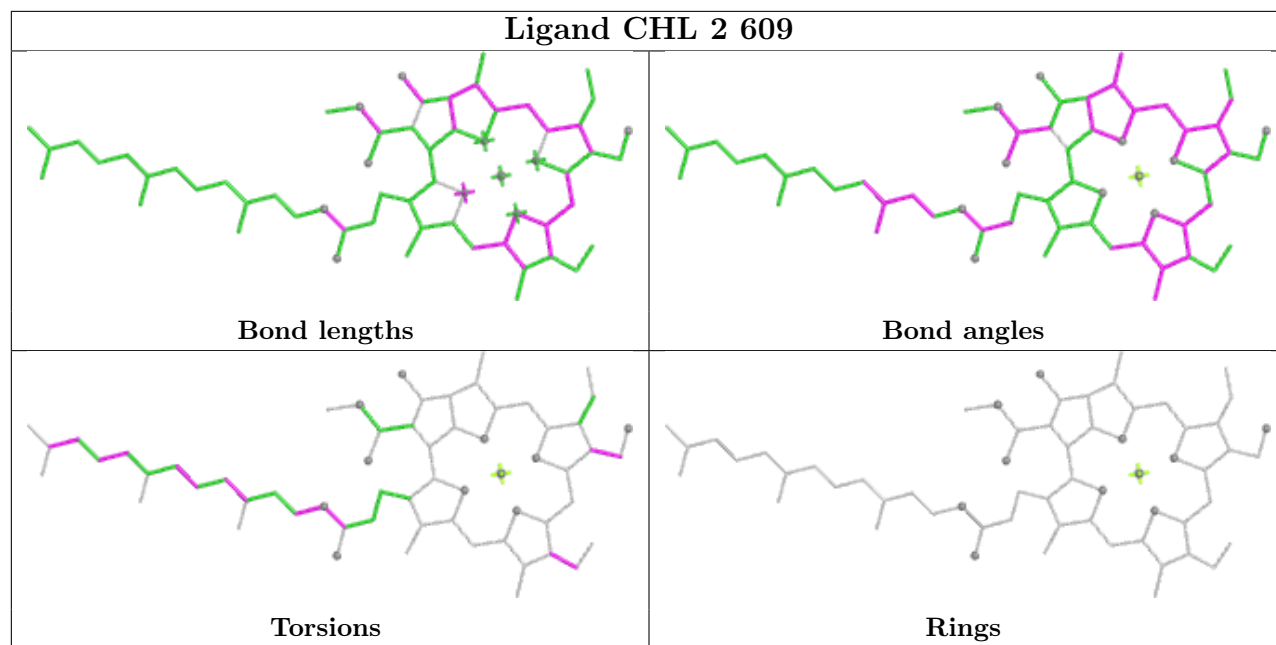
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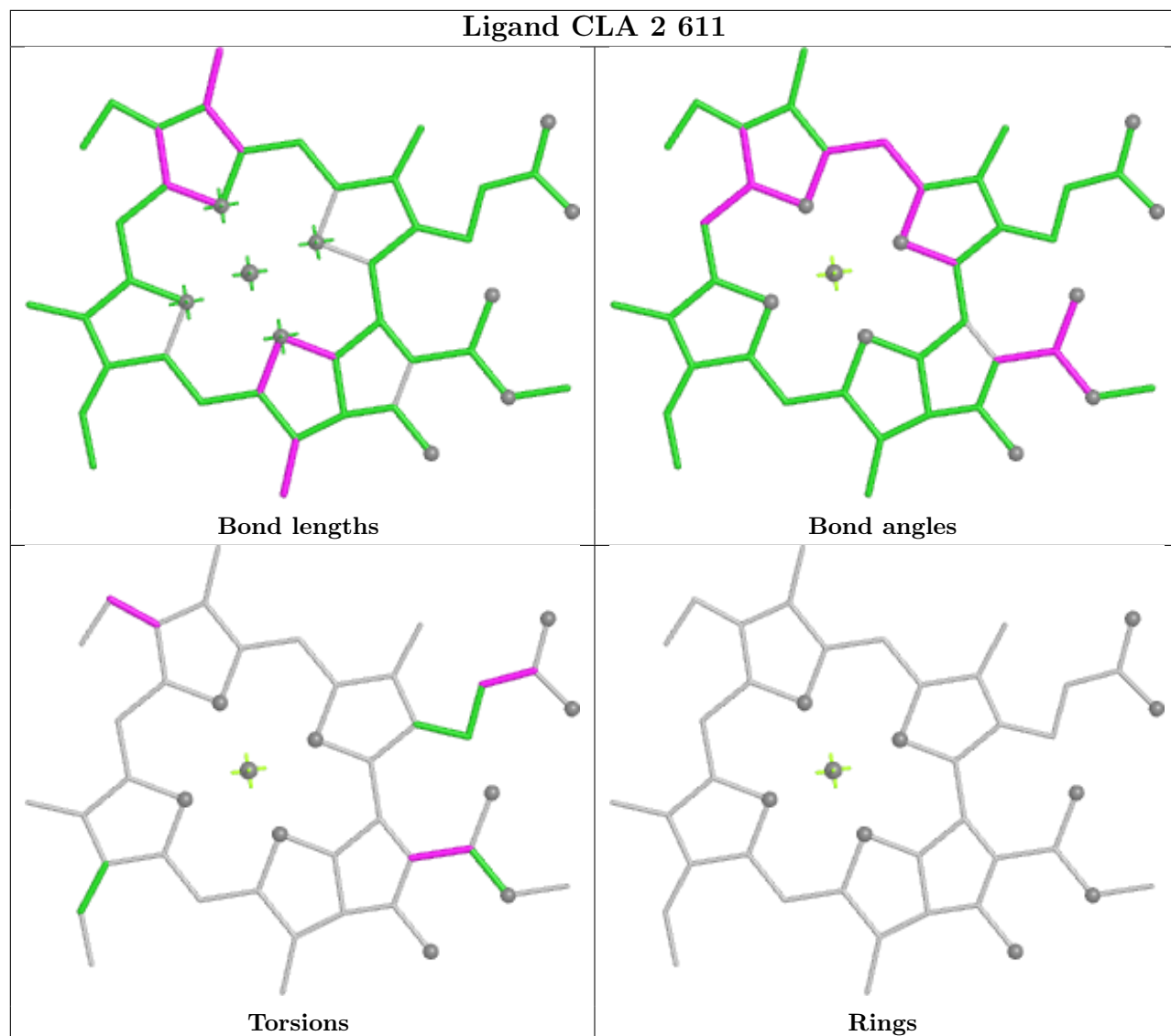




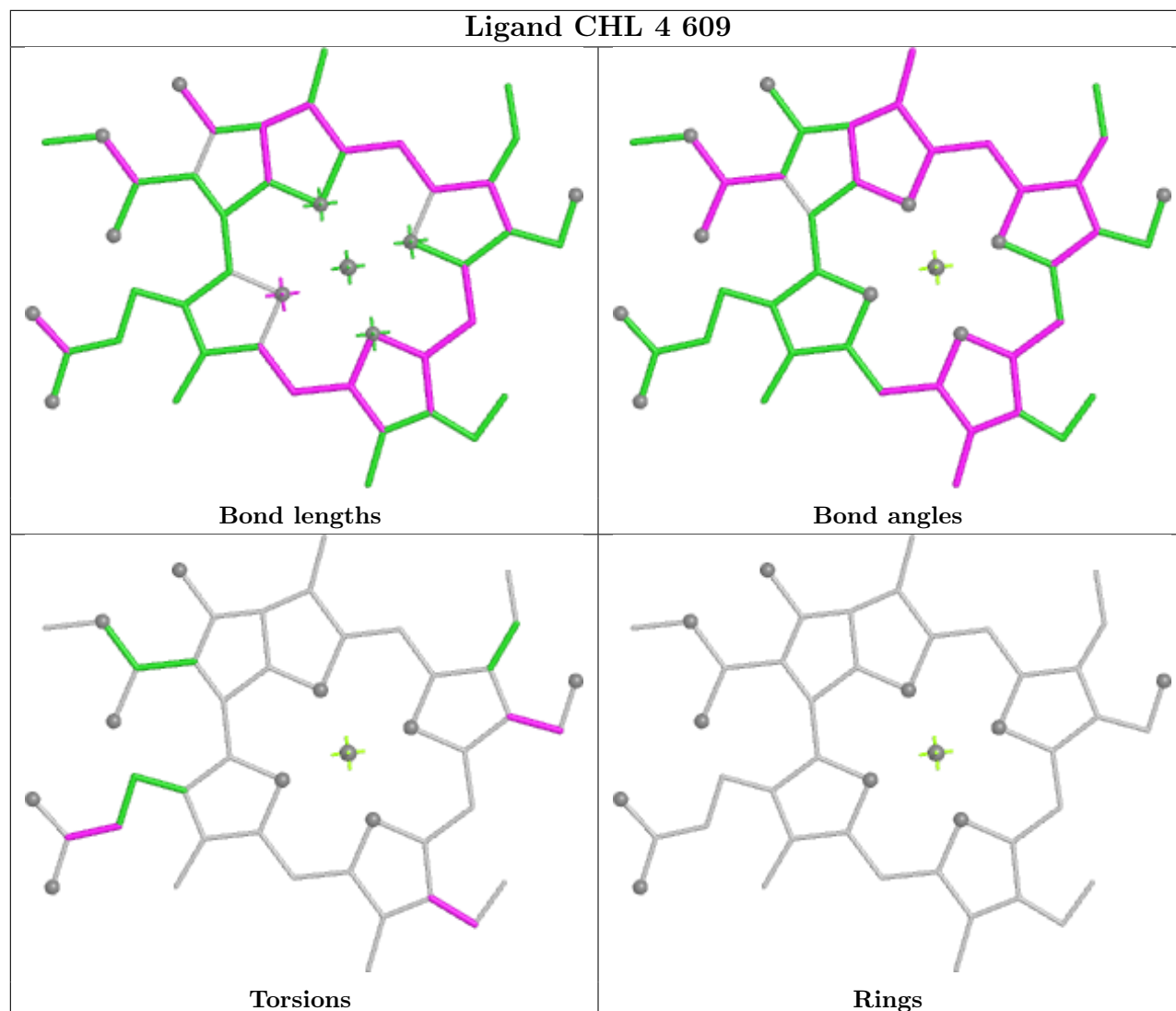




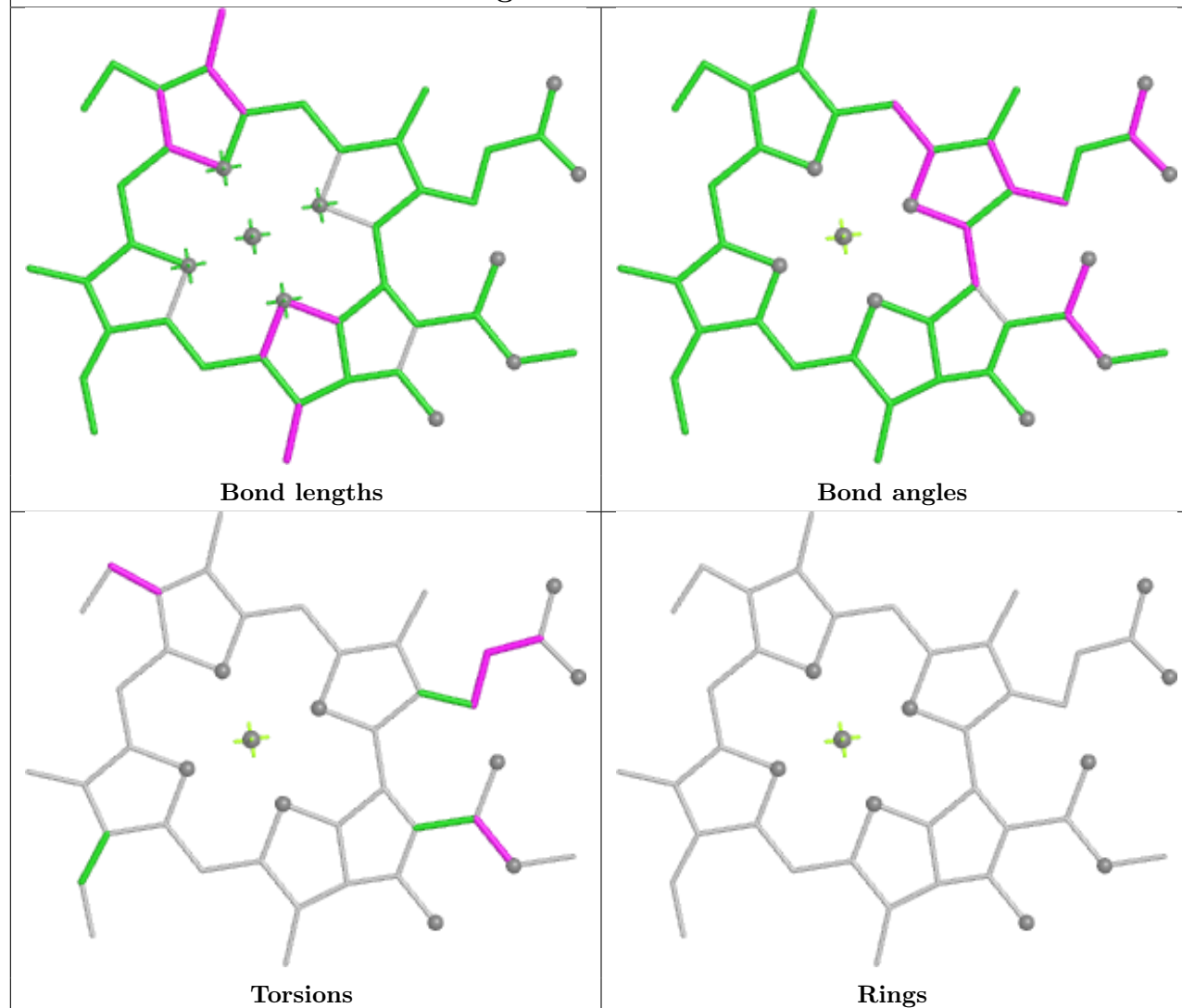
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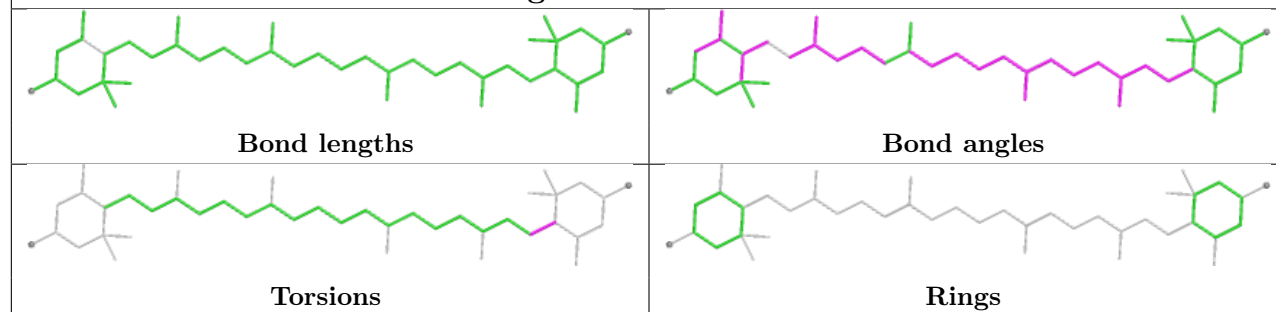
Ligand CHL 4 609

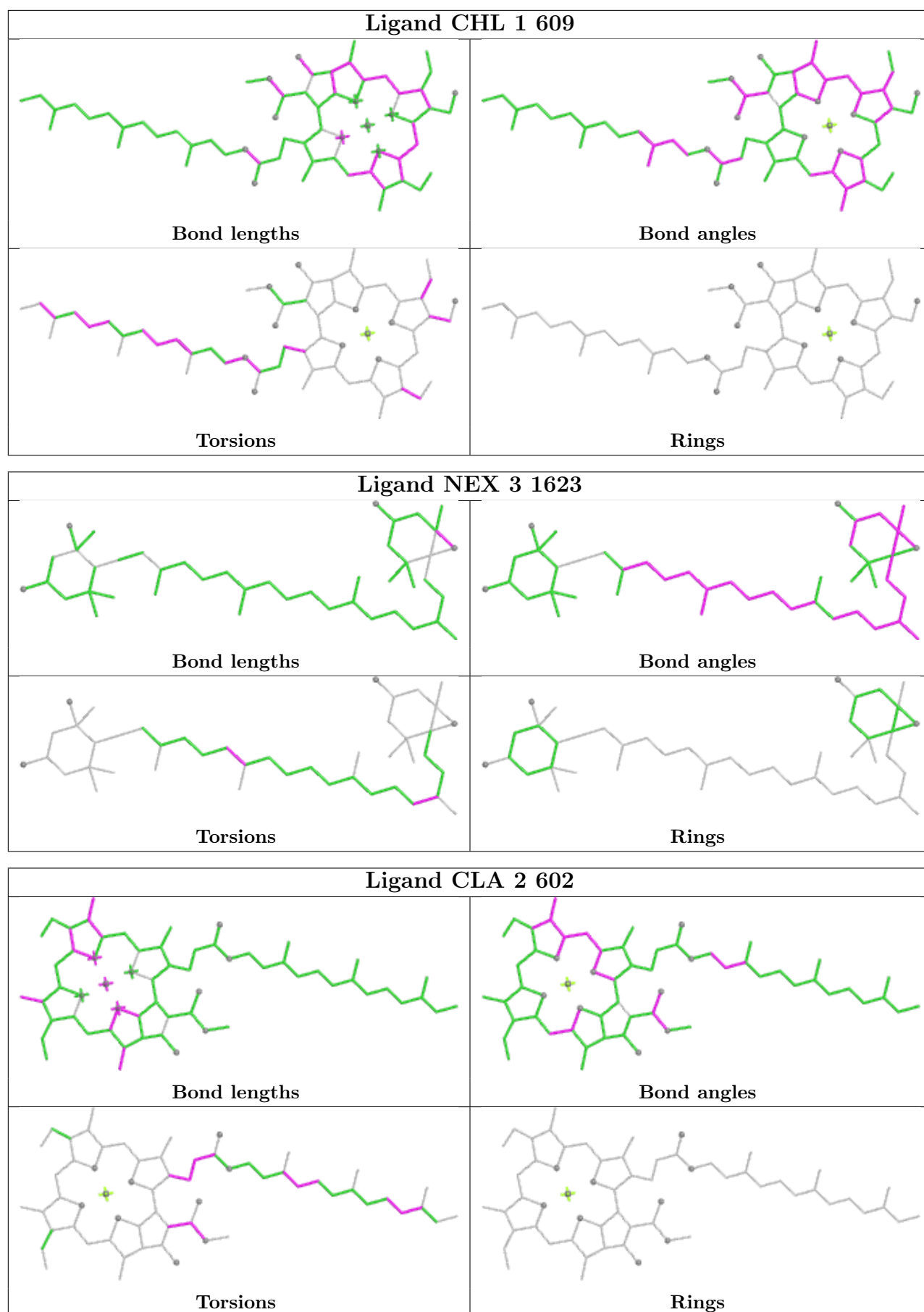


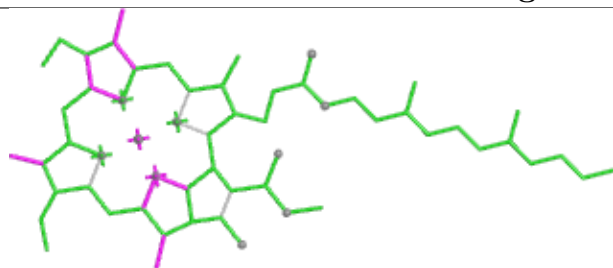
Ligand CLA 4 612



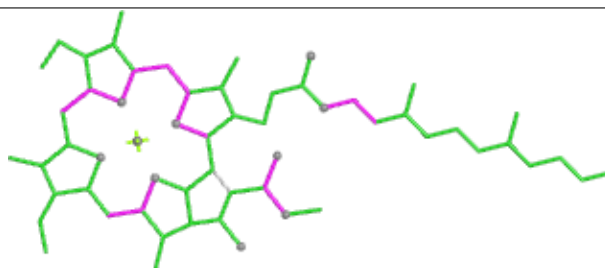
Ligand LUT 2 1620



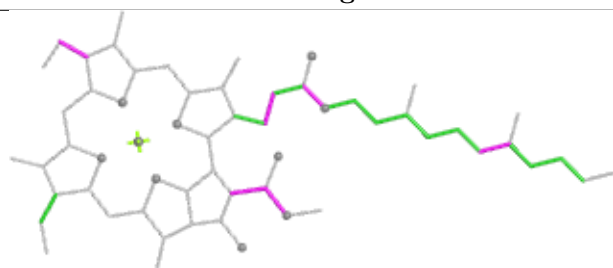


Ligand CLA 3 613

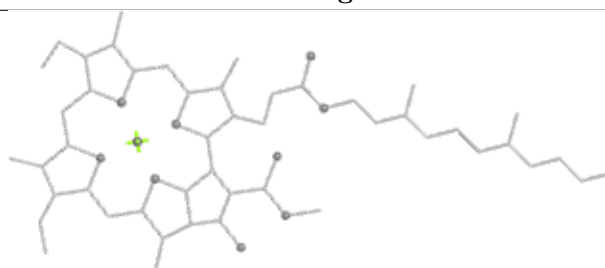
Bond lengths



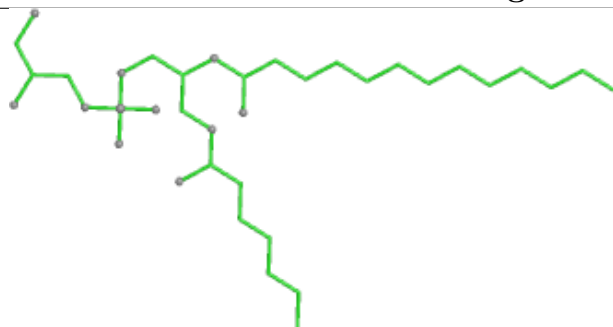
Bond angles



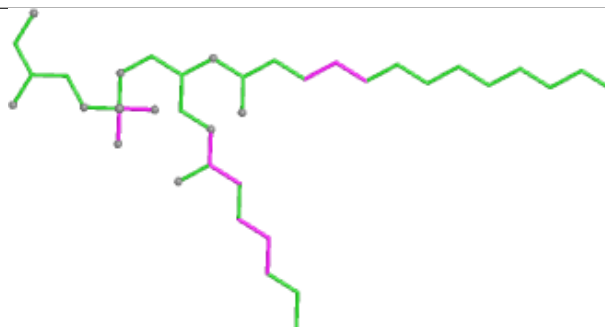
Torsions



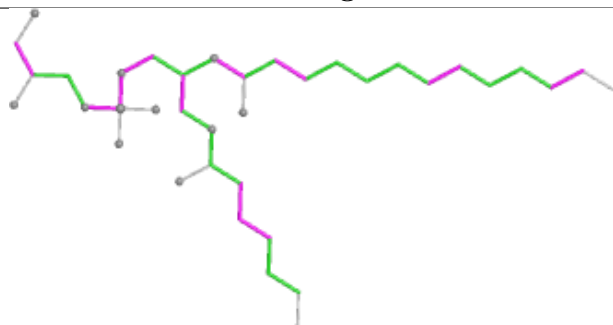
Rings

Ligand LHG 2 2630

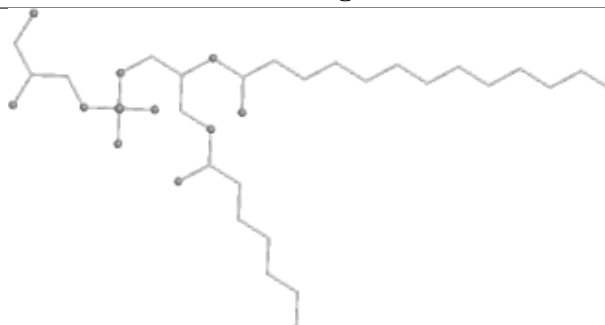
Bond lengths



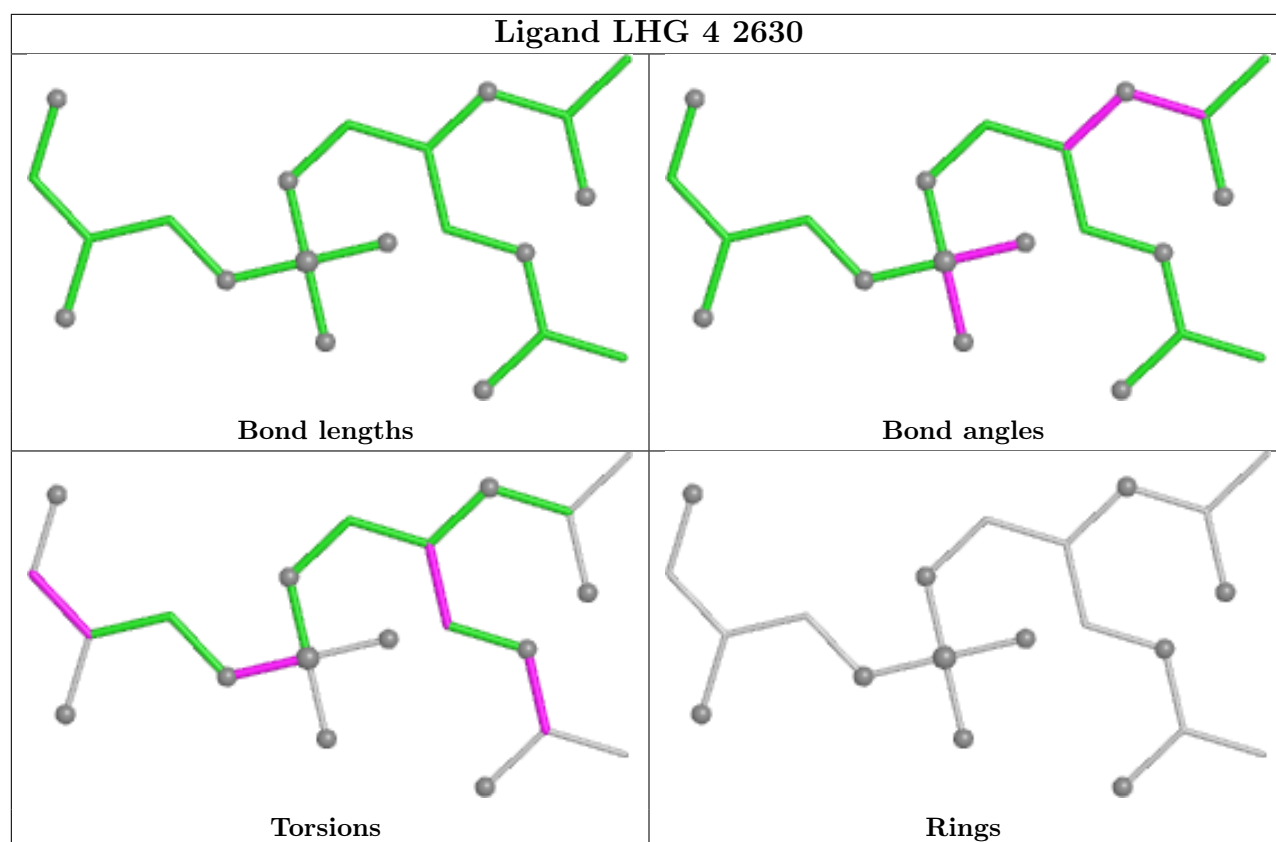
Bond angles



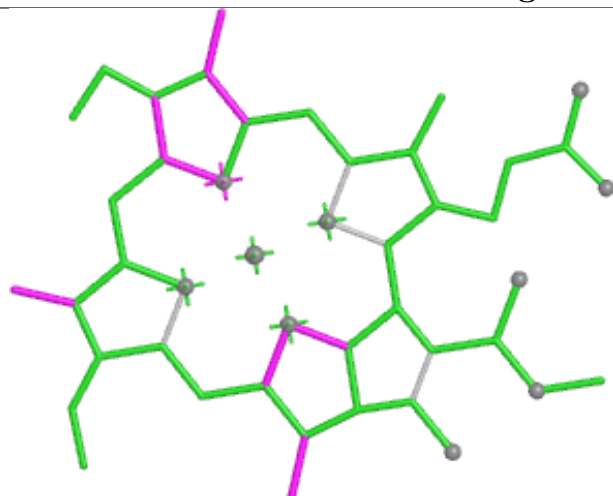
Torsions



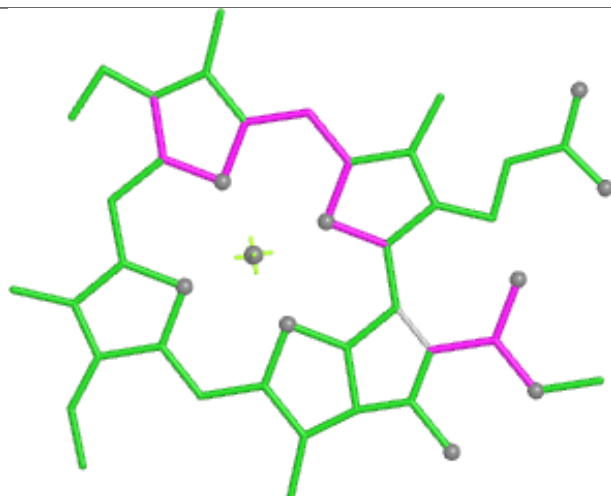
Rings



Ligand CLA 4 602



Bond lengths



Bond angles

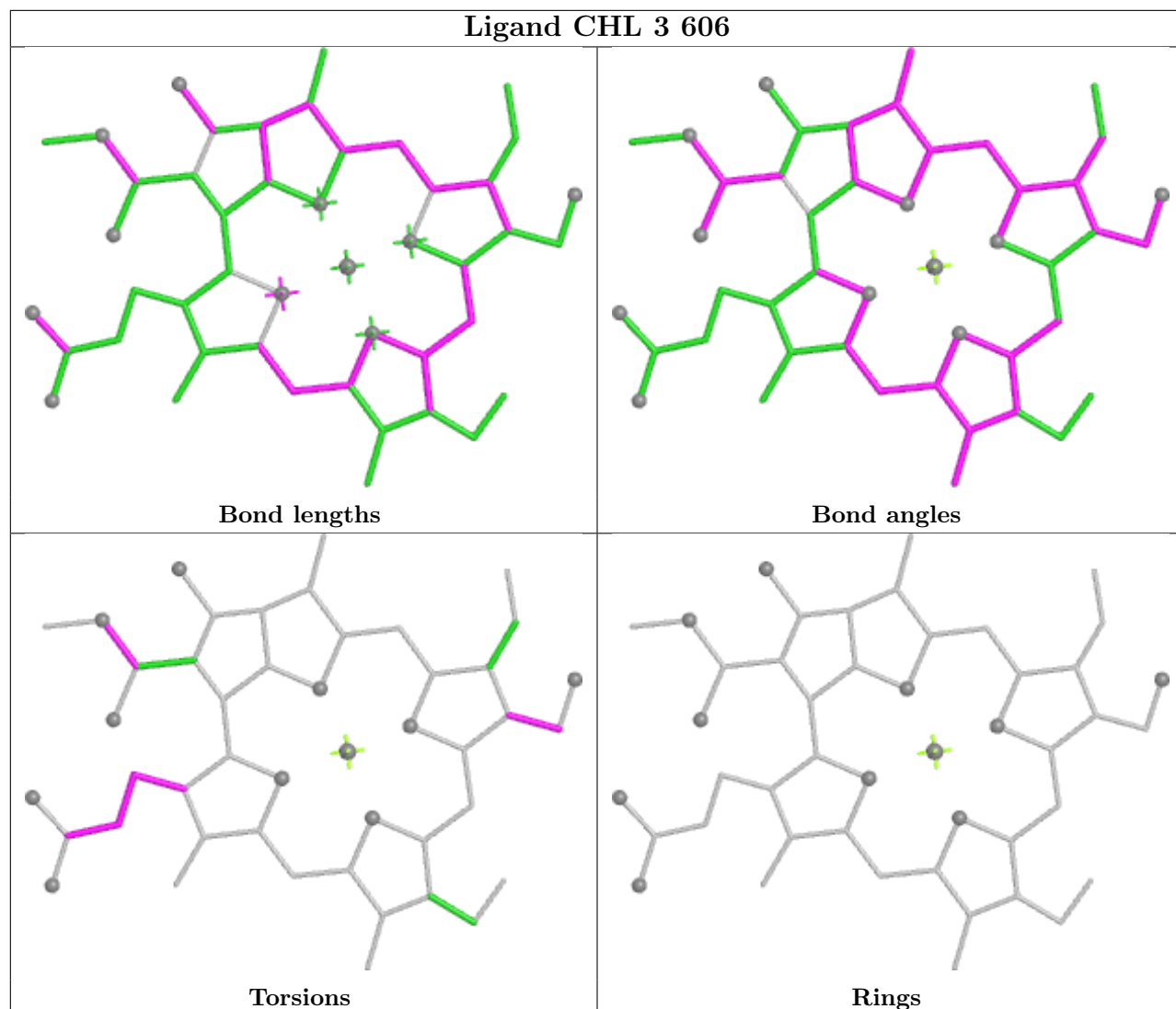


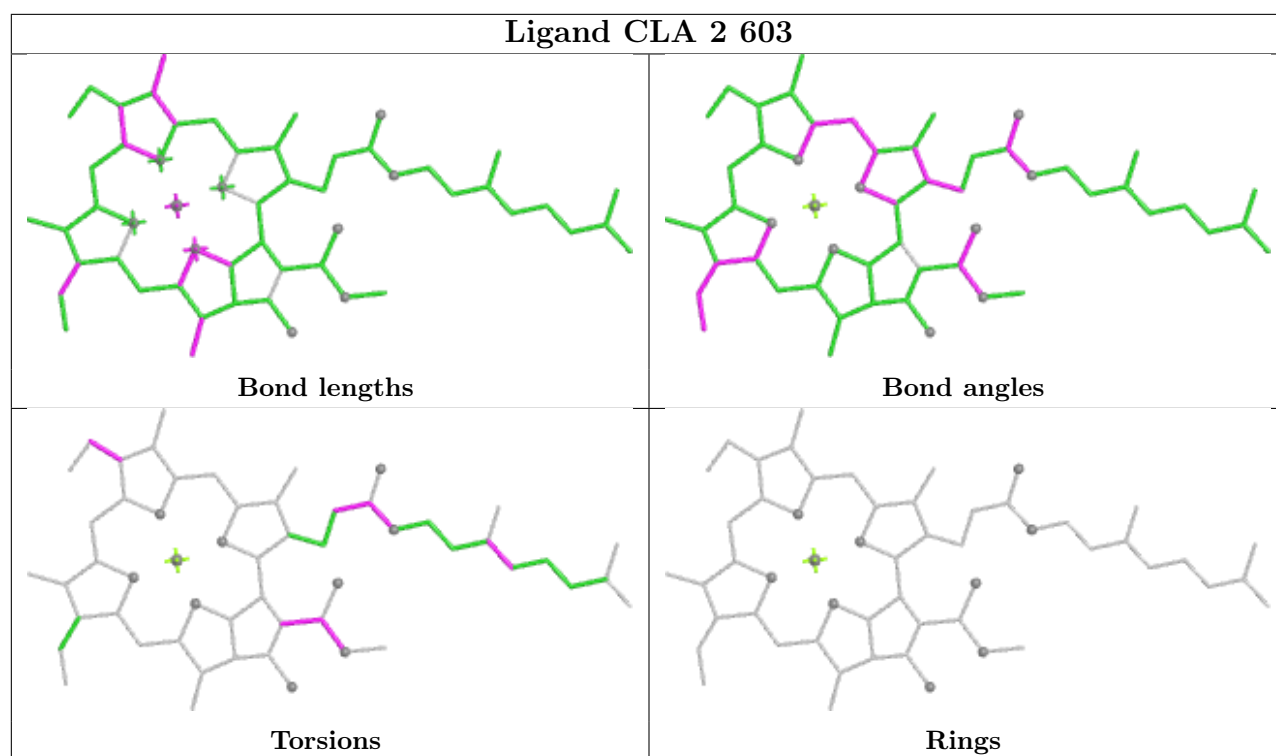
Torsions



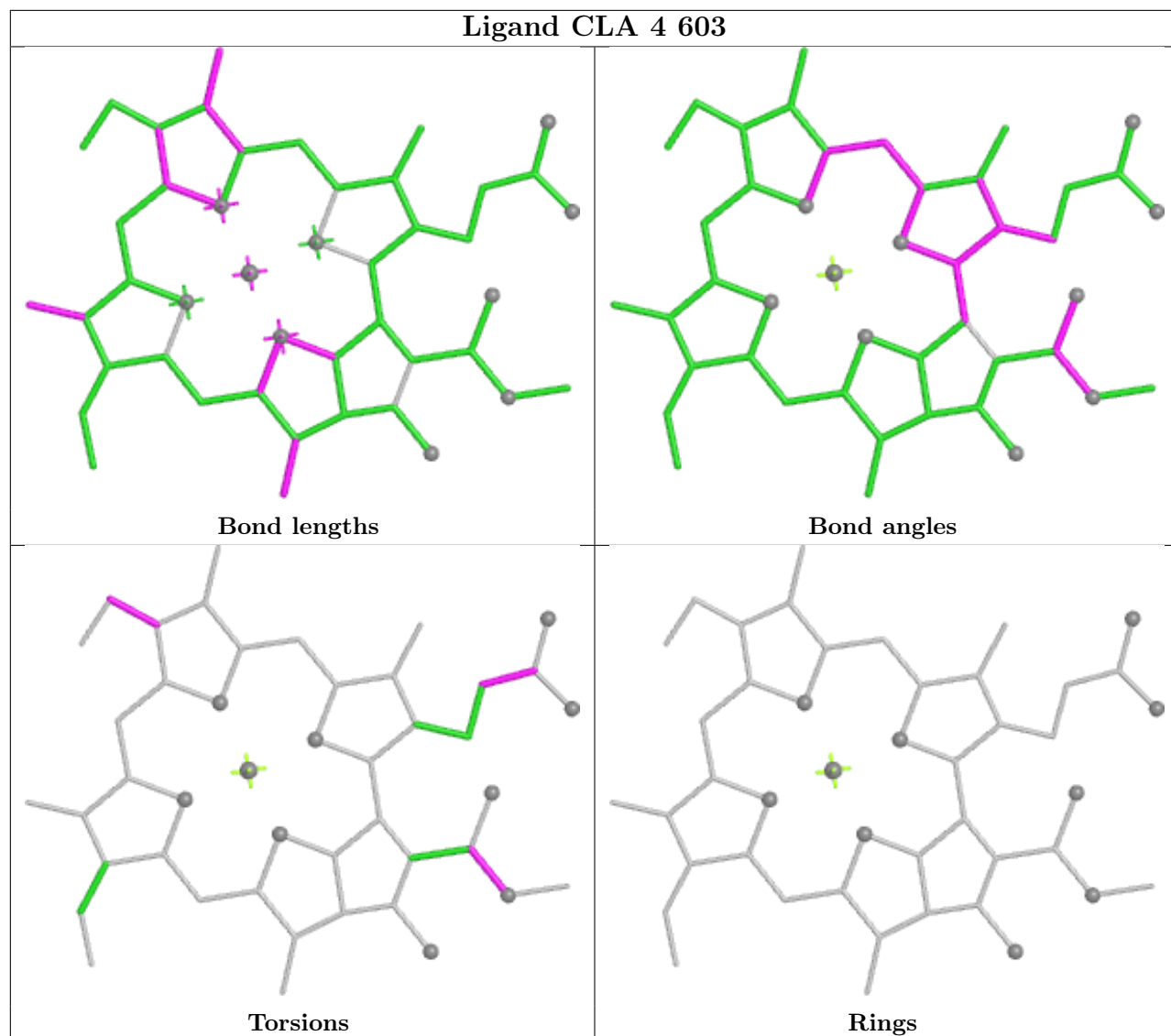
Rings

Ligand CHL 3 606

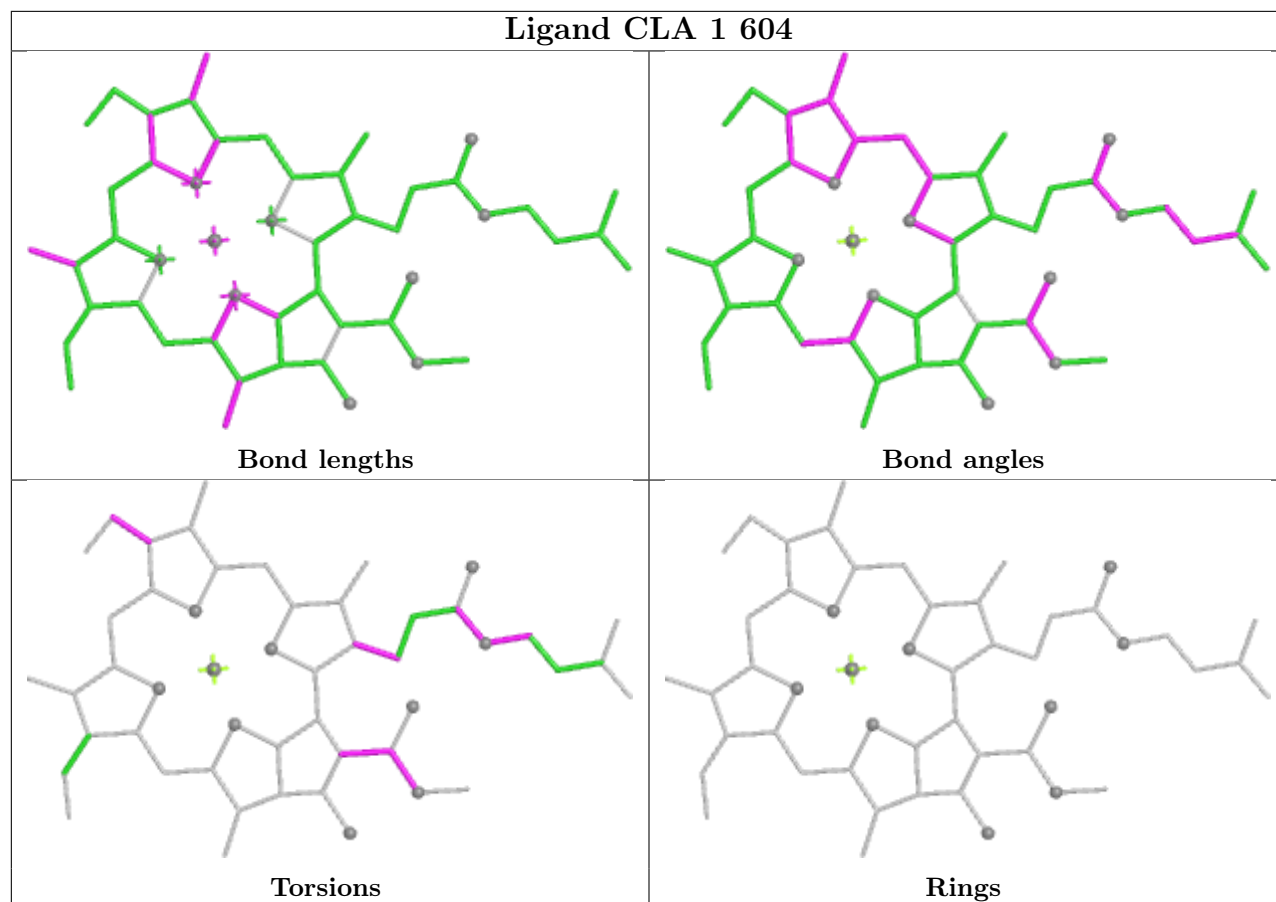




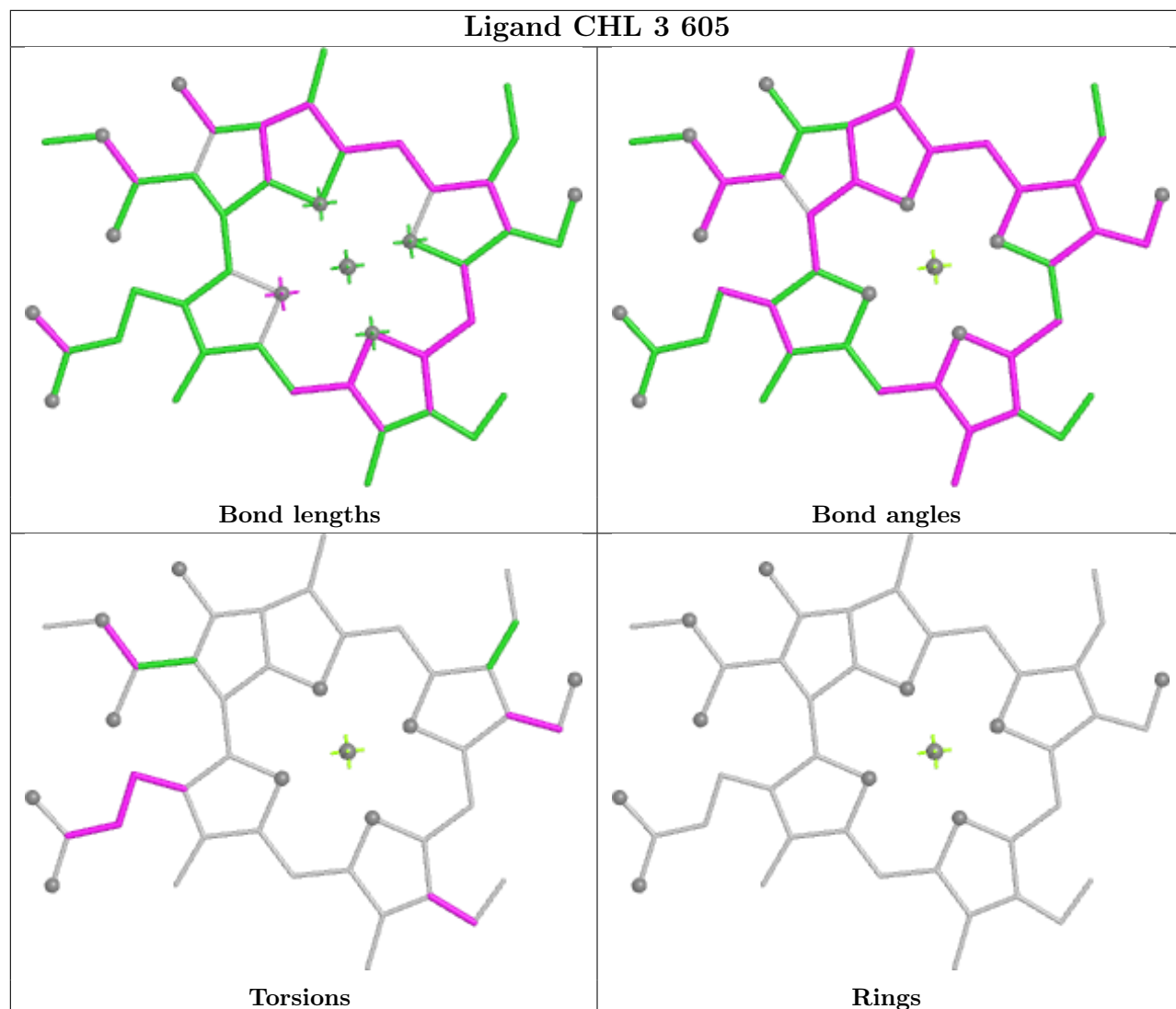
Ligand CLA 4 603

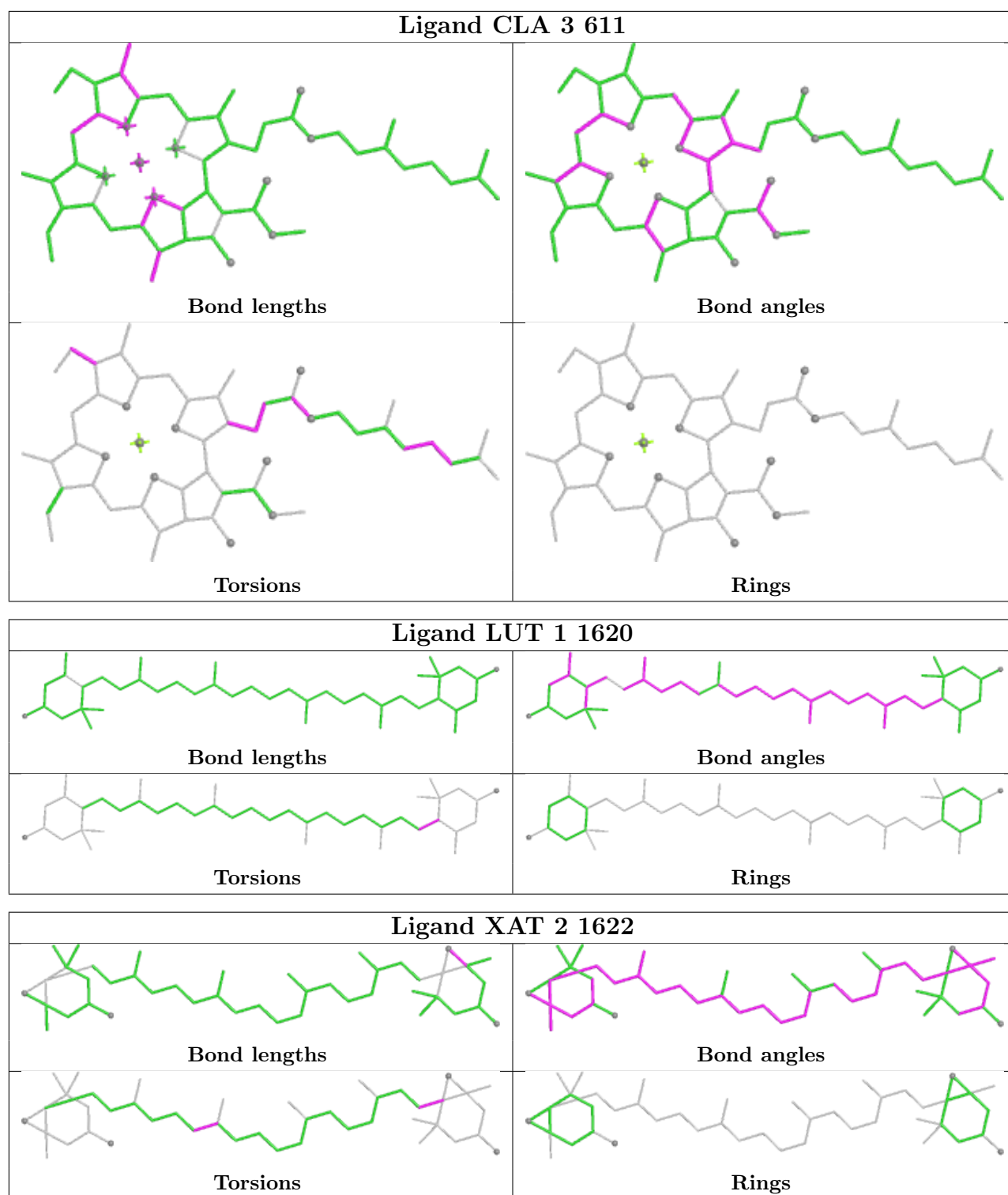


Ligand CLA 1 604

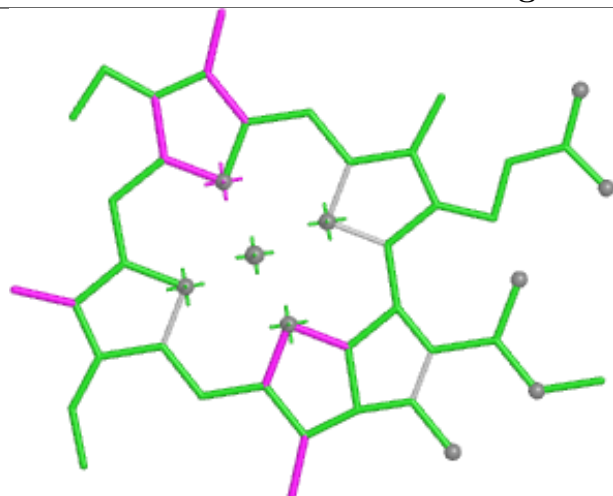


Ligand CHL 3 605

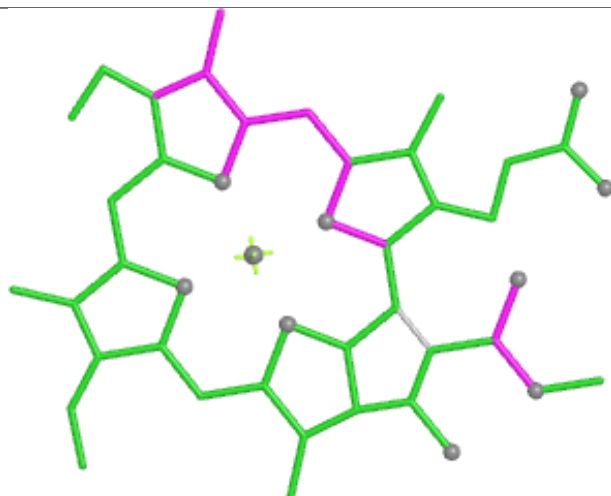




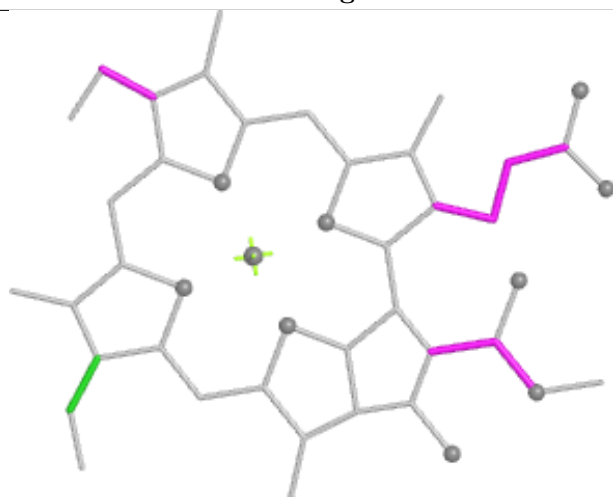
Ligand CLA 3 604



Bond lengths



Bond angles

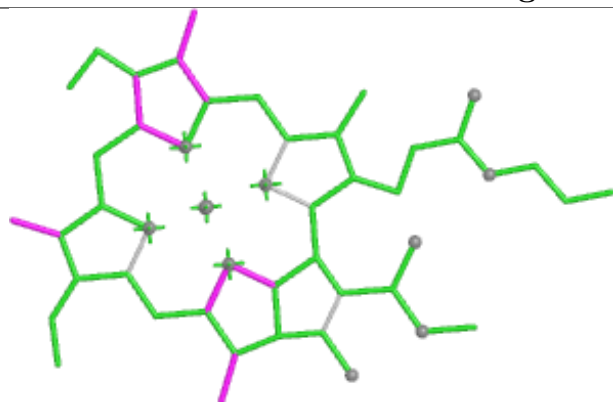


Torsions

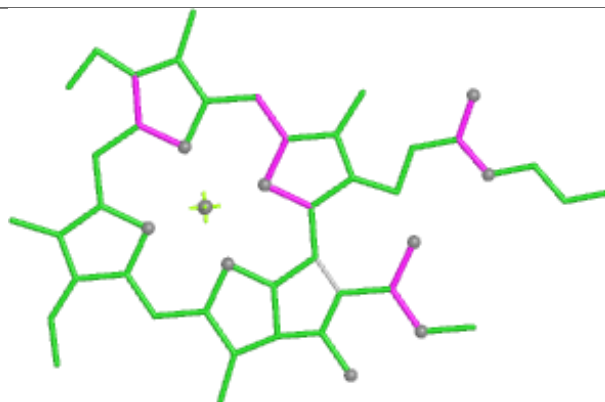


Rings

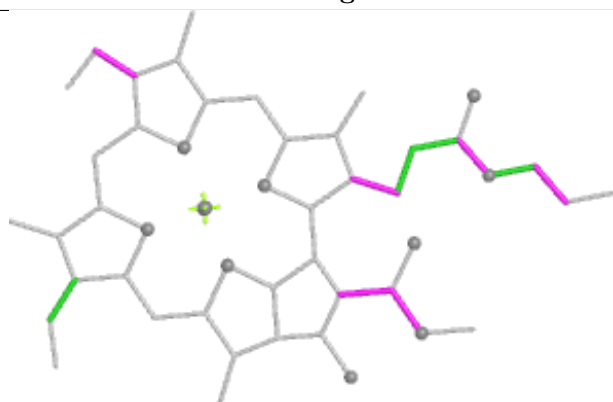
Ligand CLA 3 614



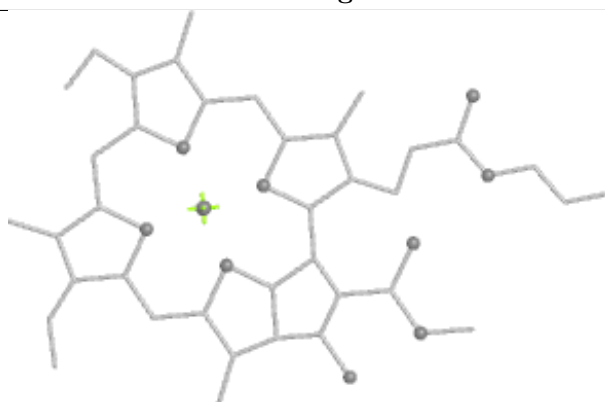
Bond lengths



Bond angles

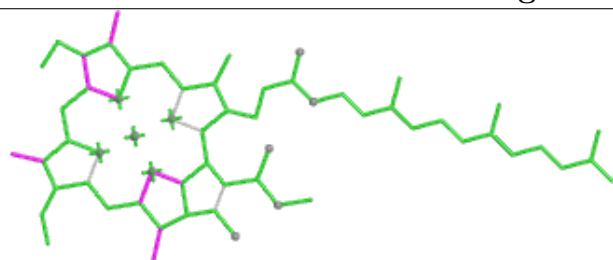


Torsions

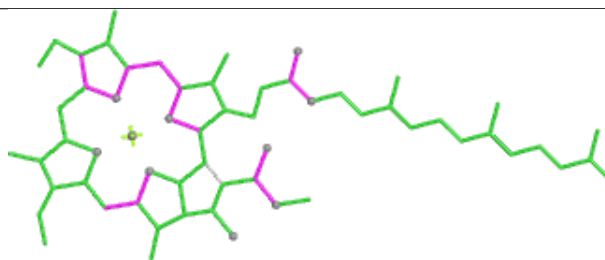


Rings

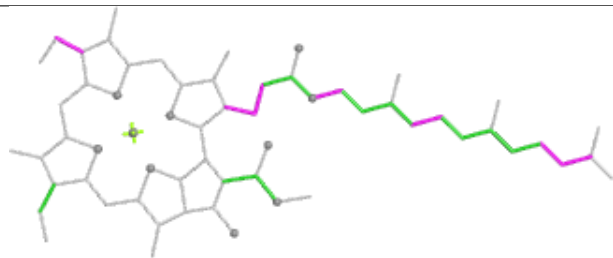
Ligand CLA 3 610



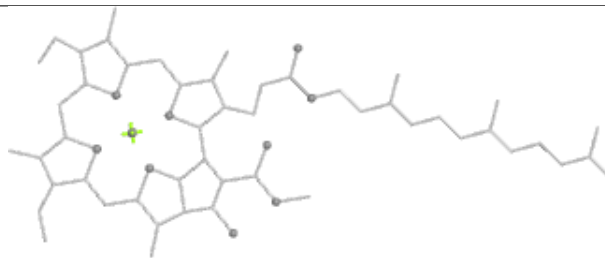
Bond lengths



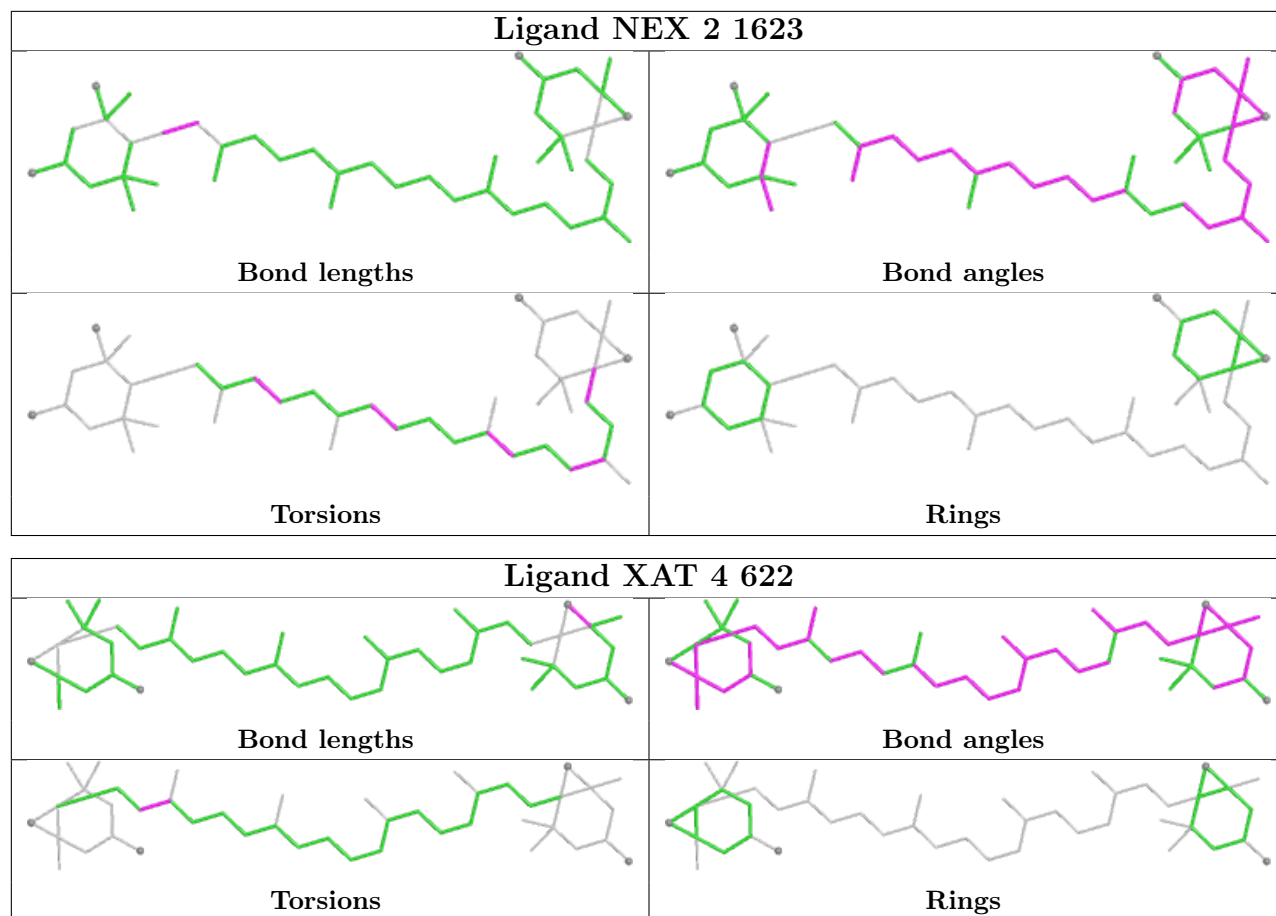
Bond angles



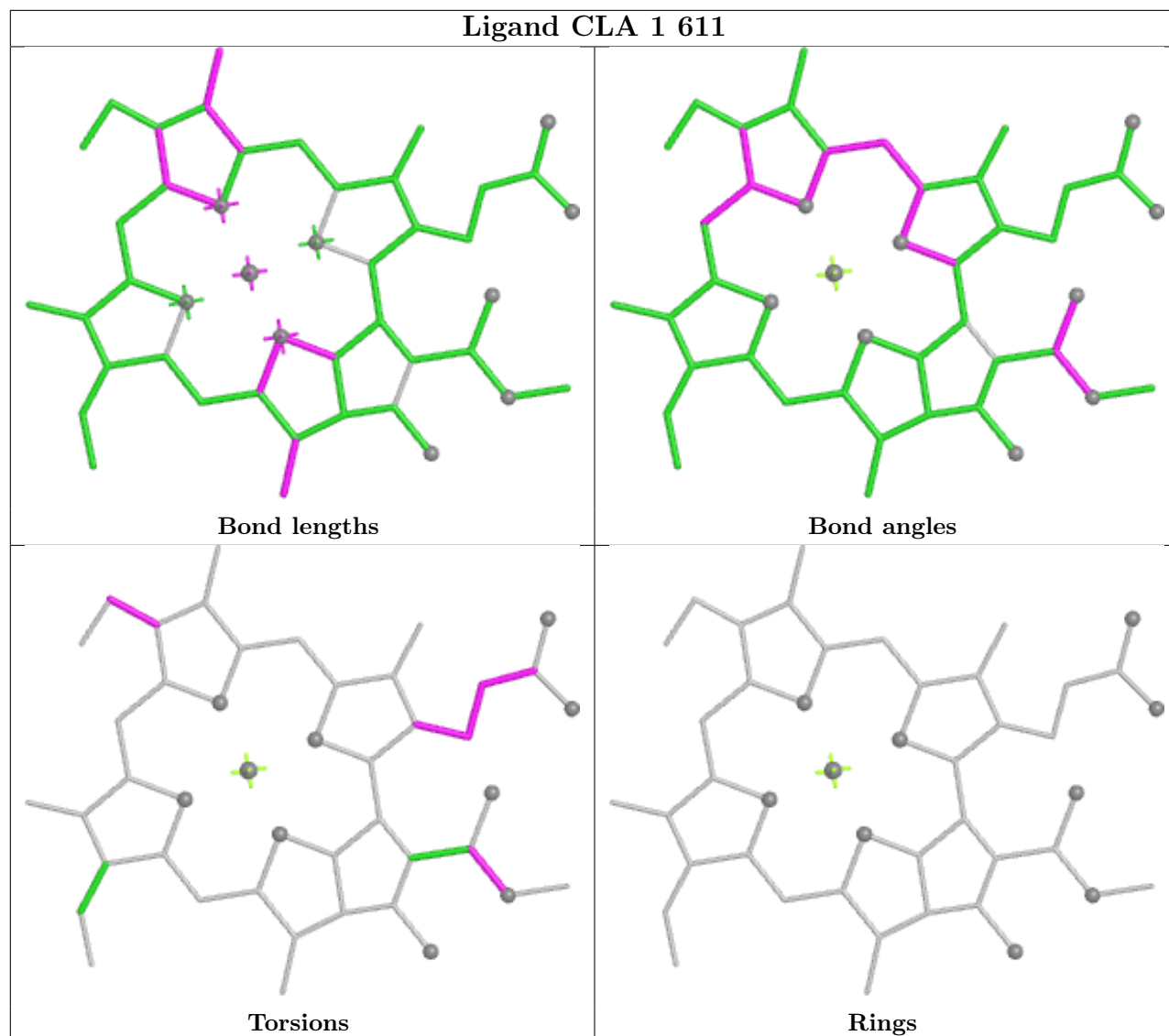
Torsions



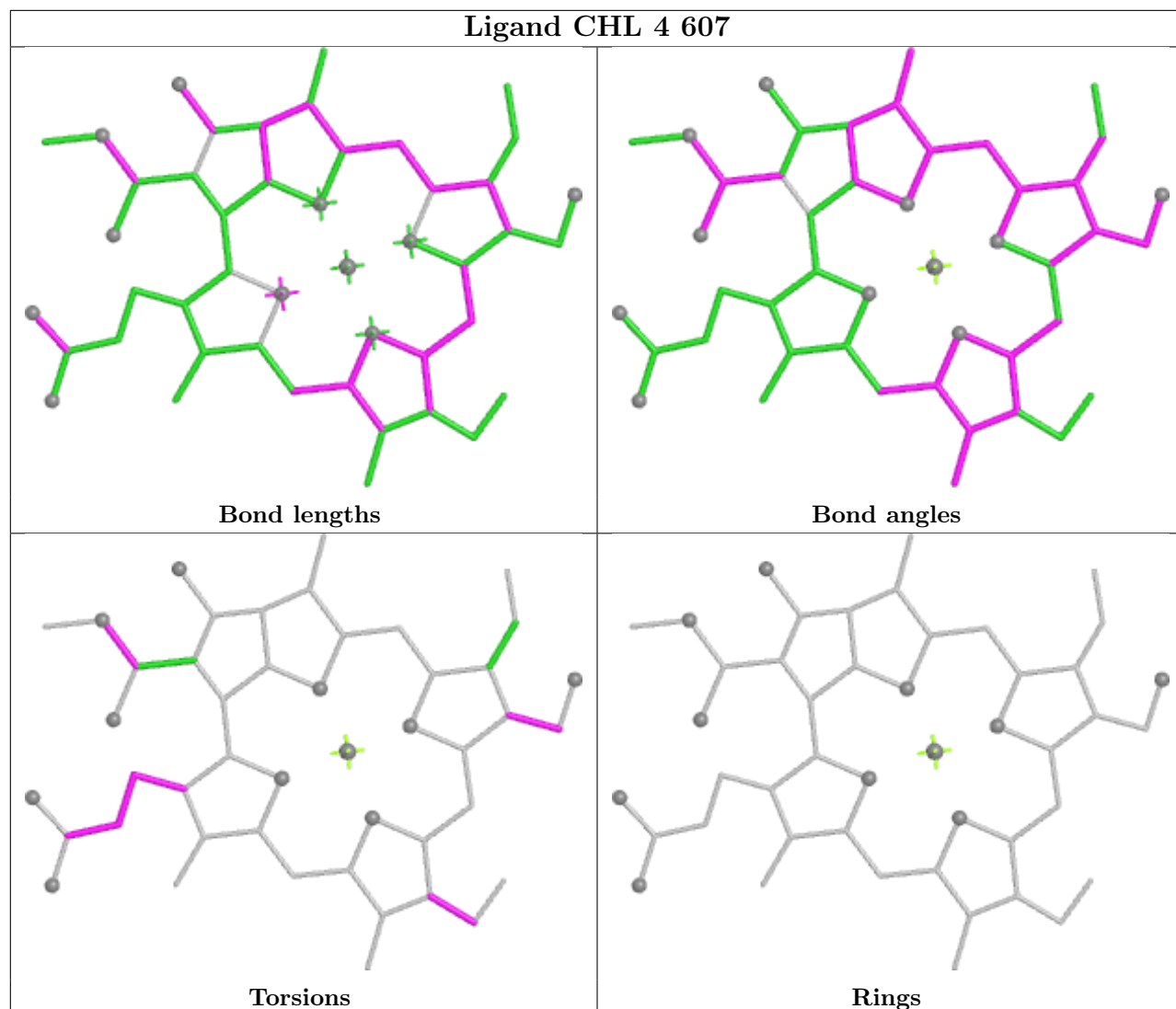
Rings

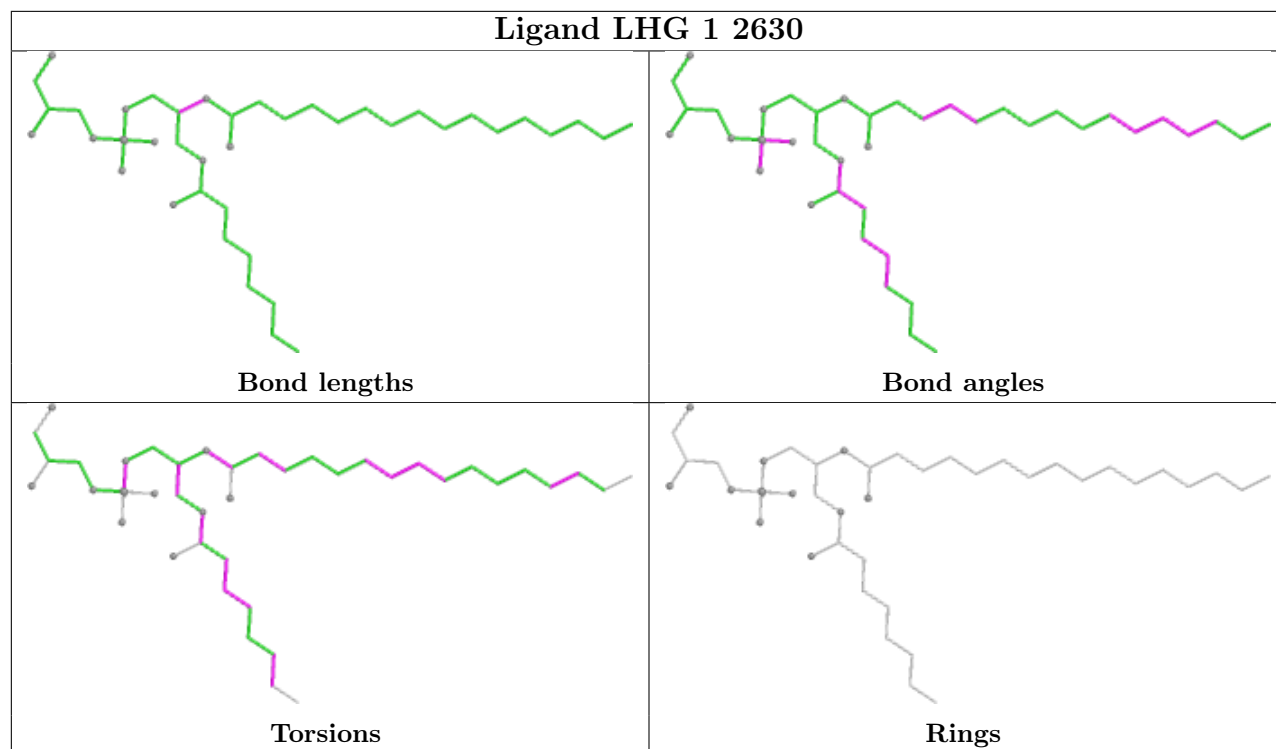


Ligand CLA 1 611

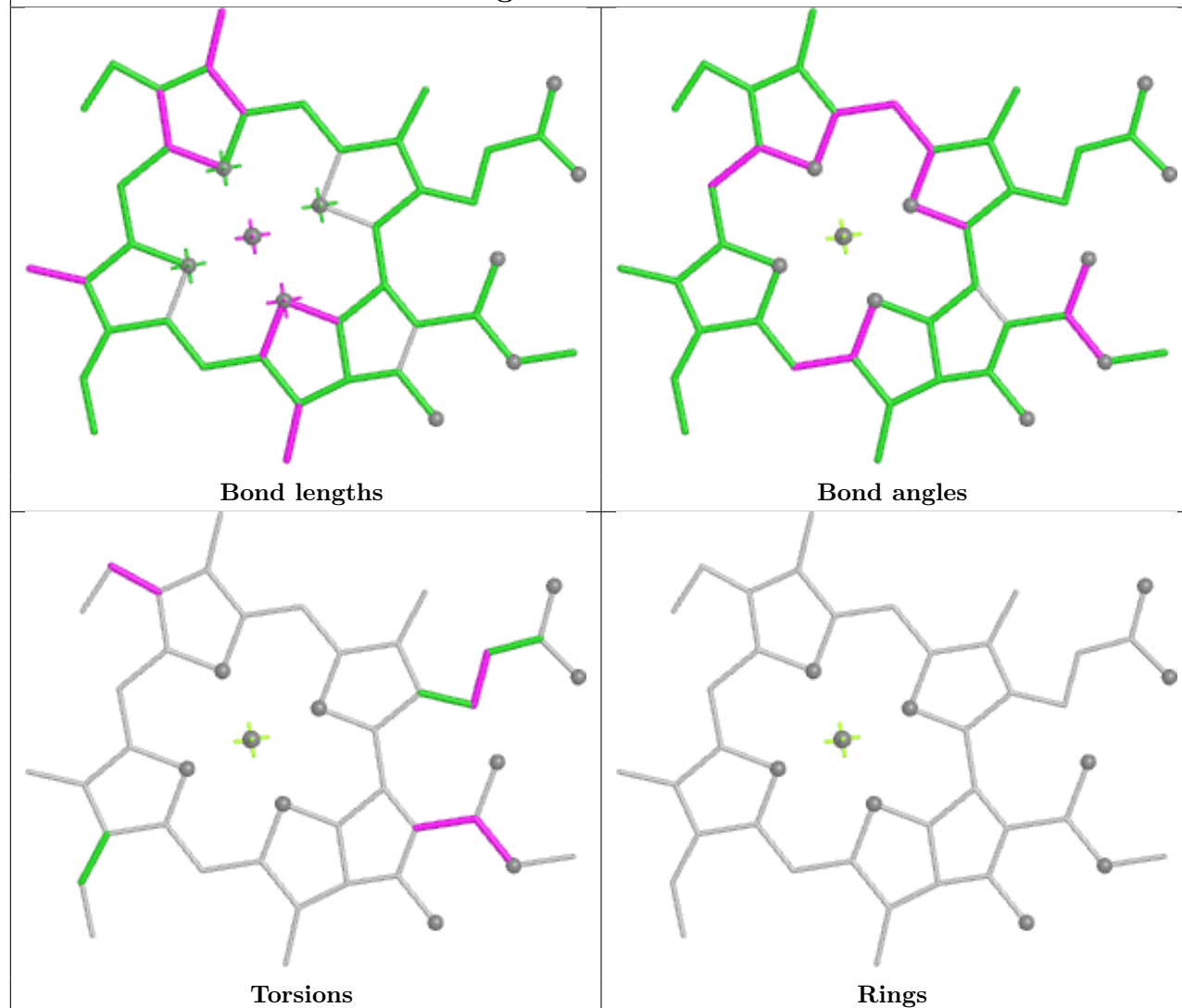


Ligand CHL 4 607

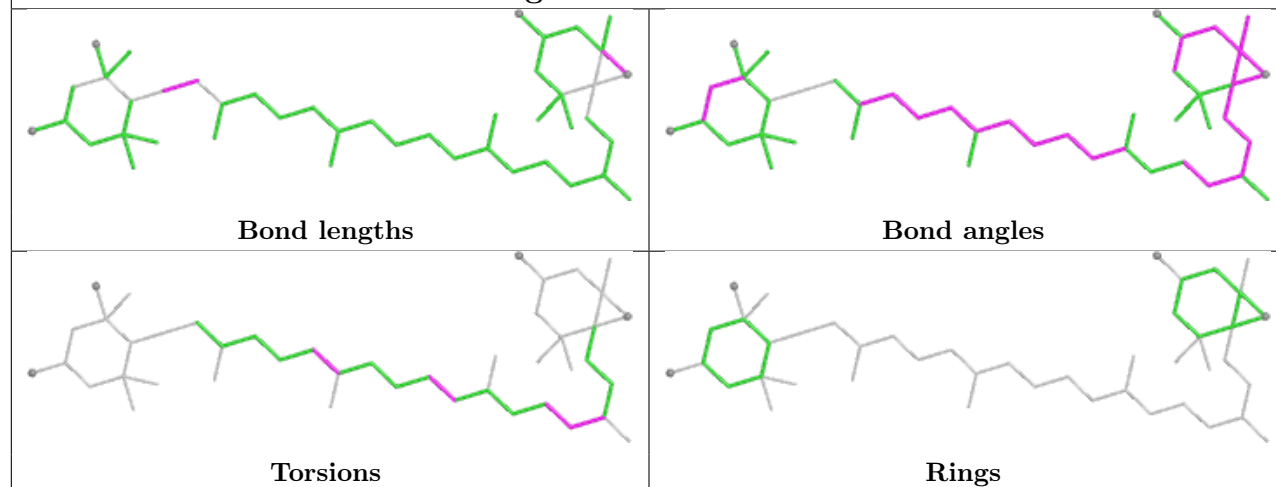


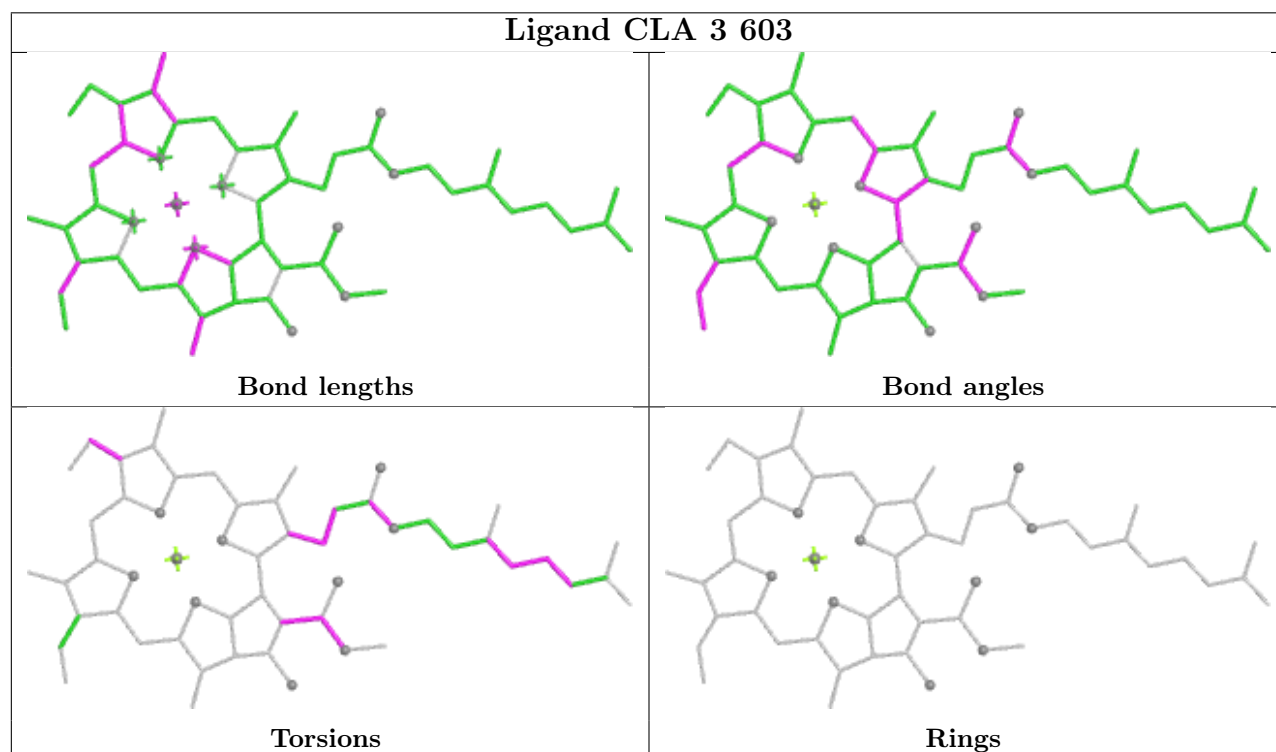
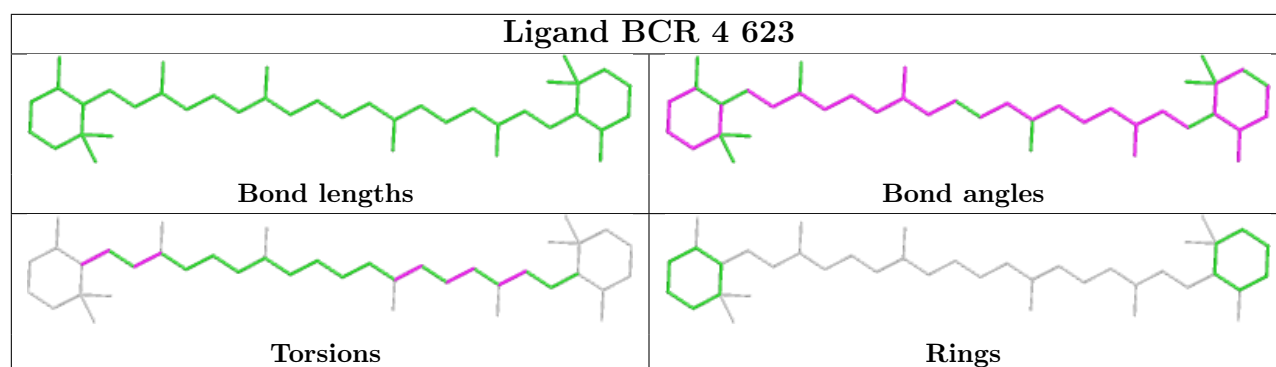


Ligand CLA 2 613

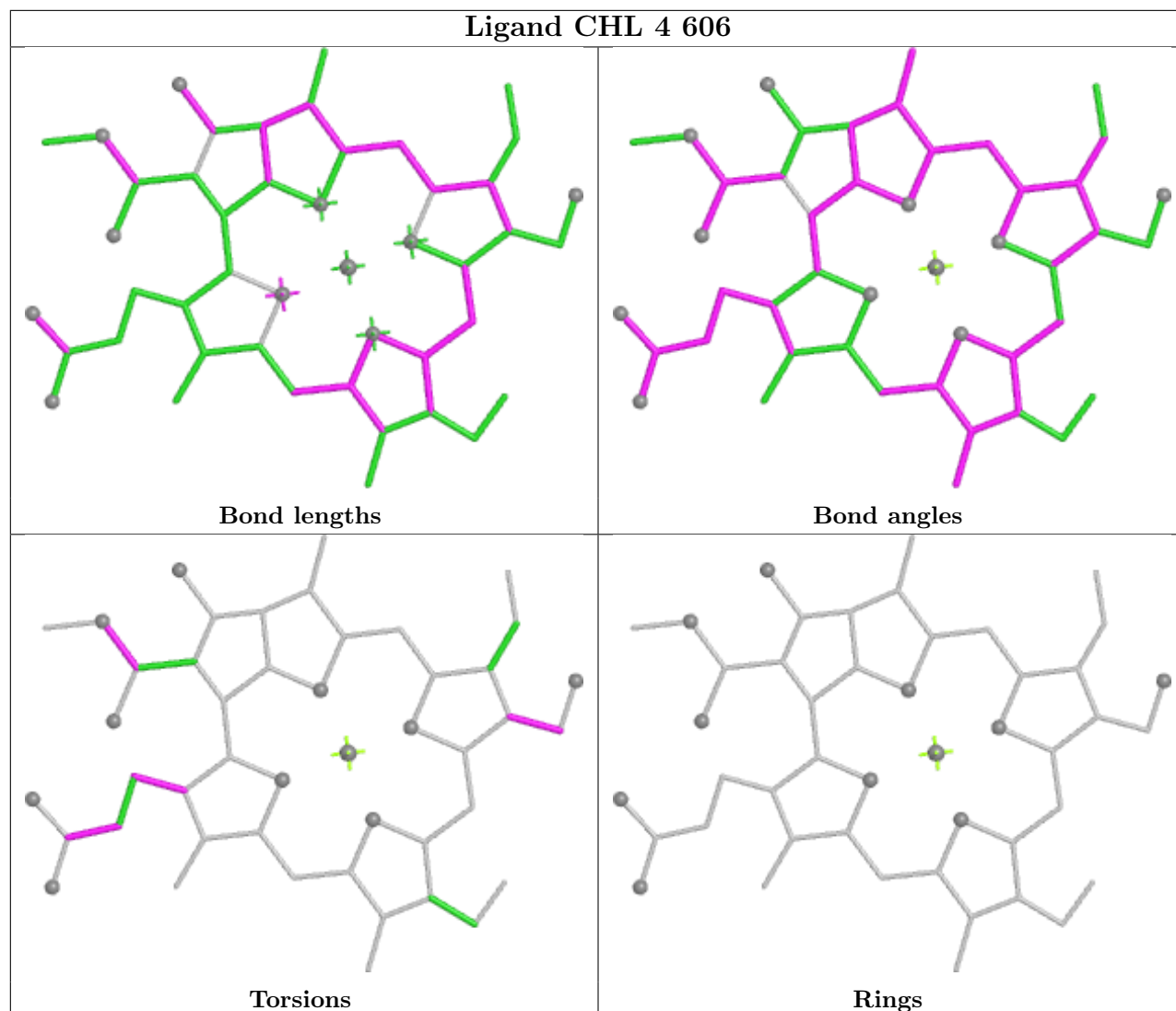


Ligand NEX 1 1623

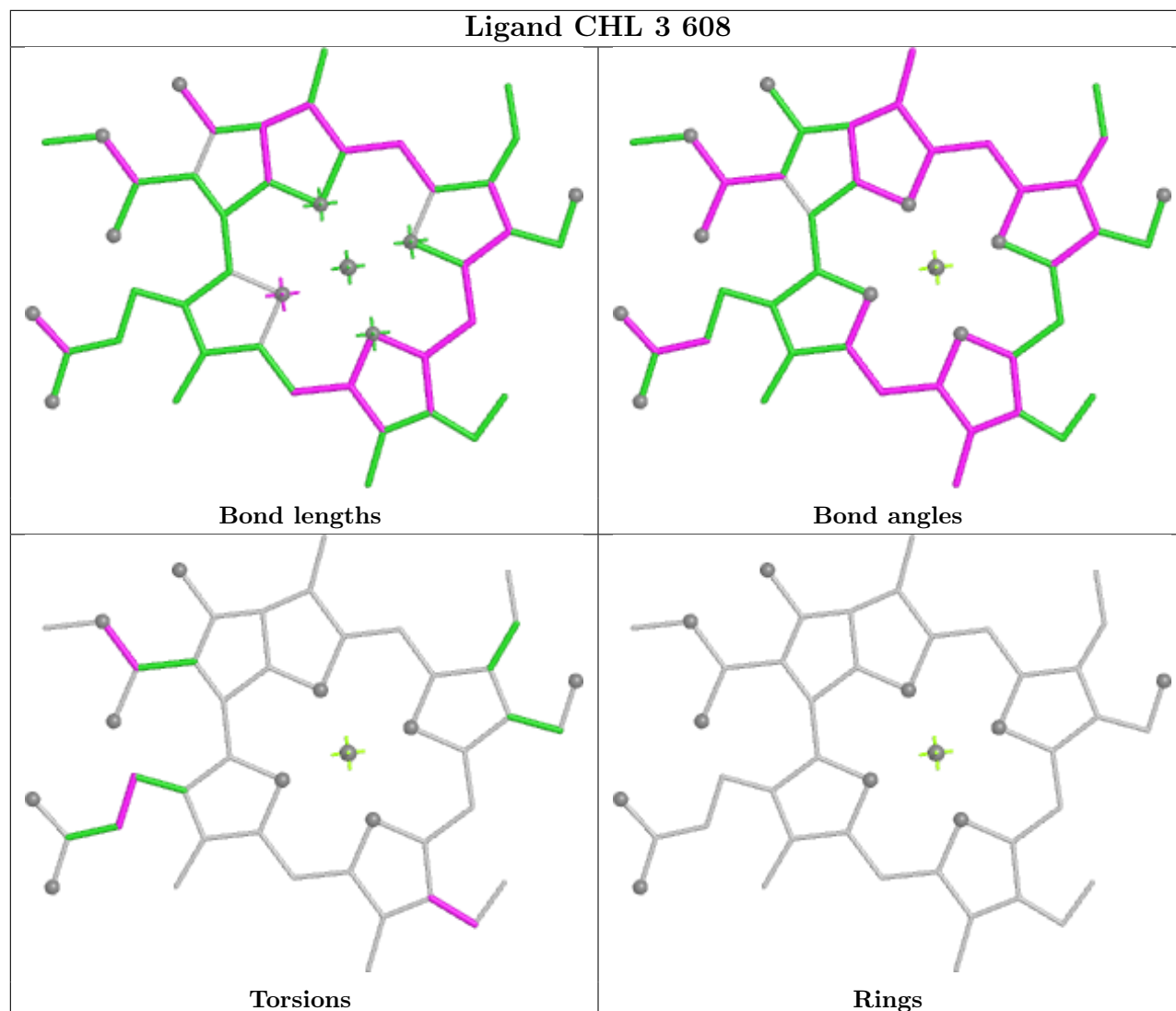




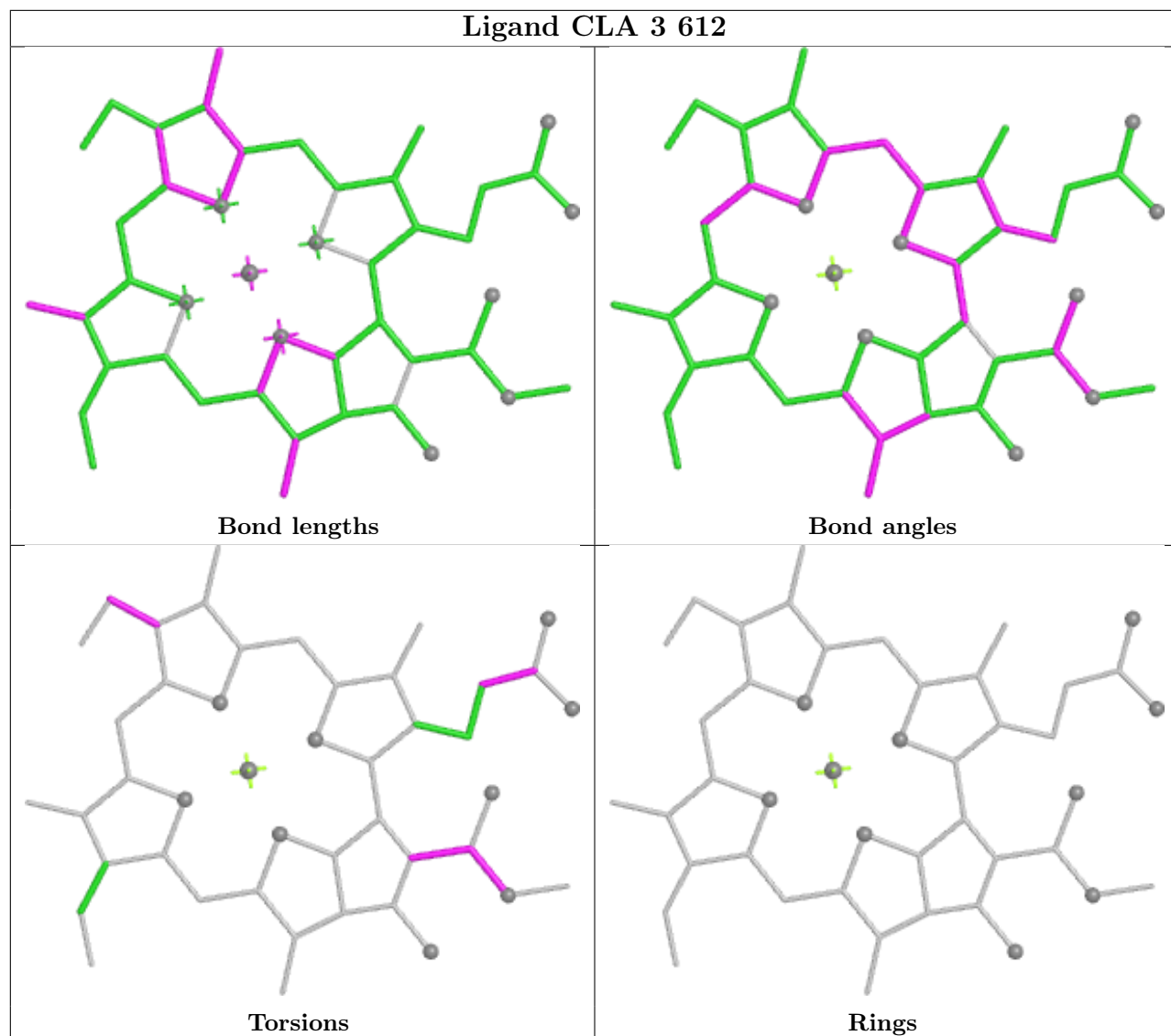
Ligand CHL 4 606

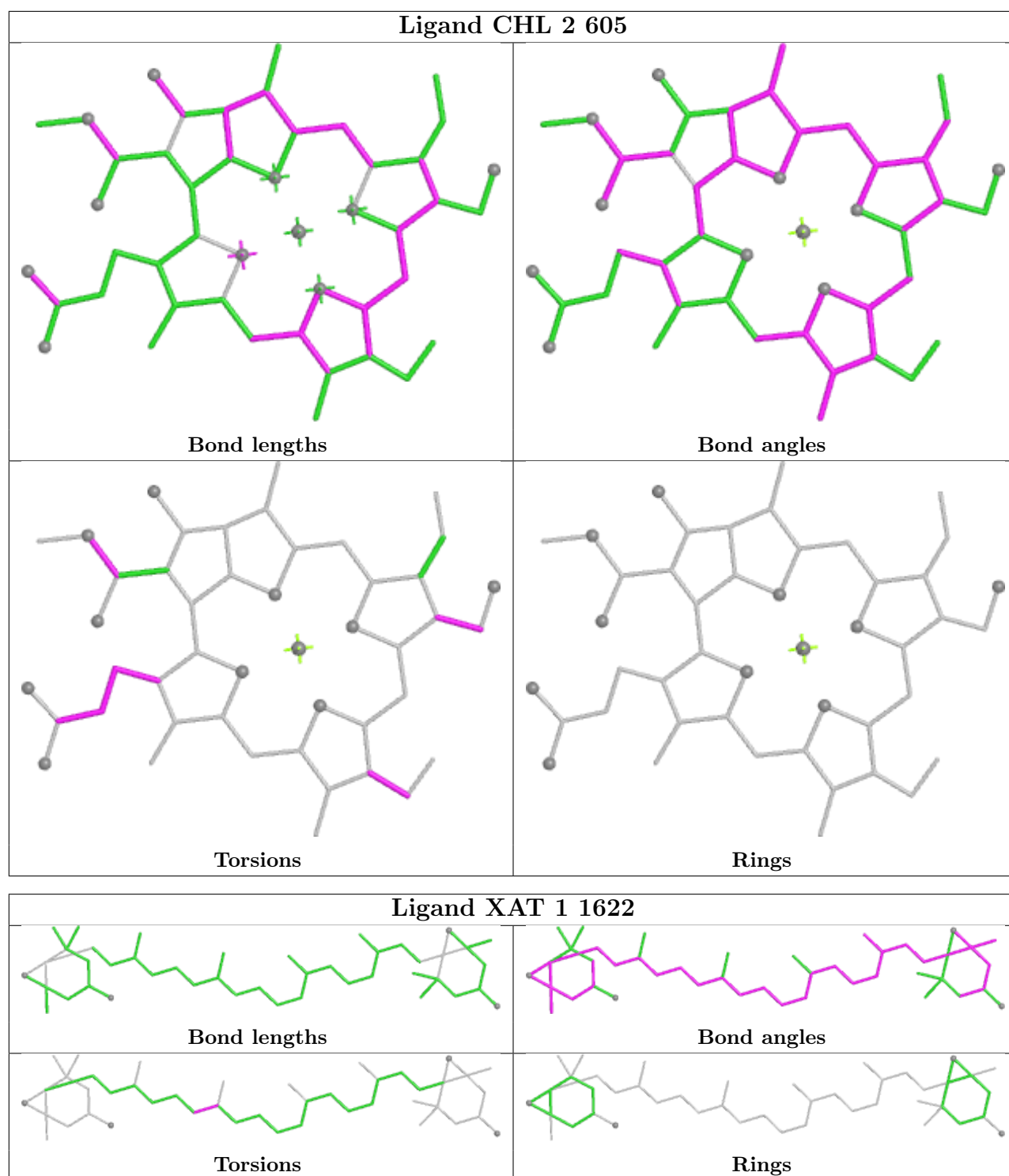


Ligand CHL 3 608

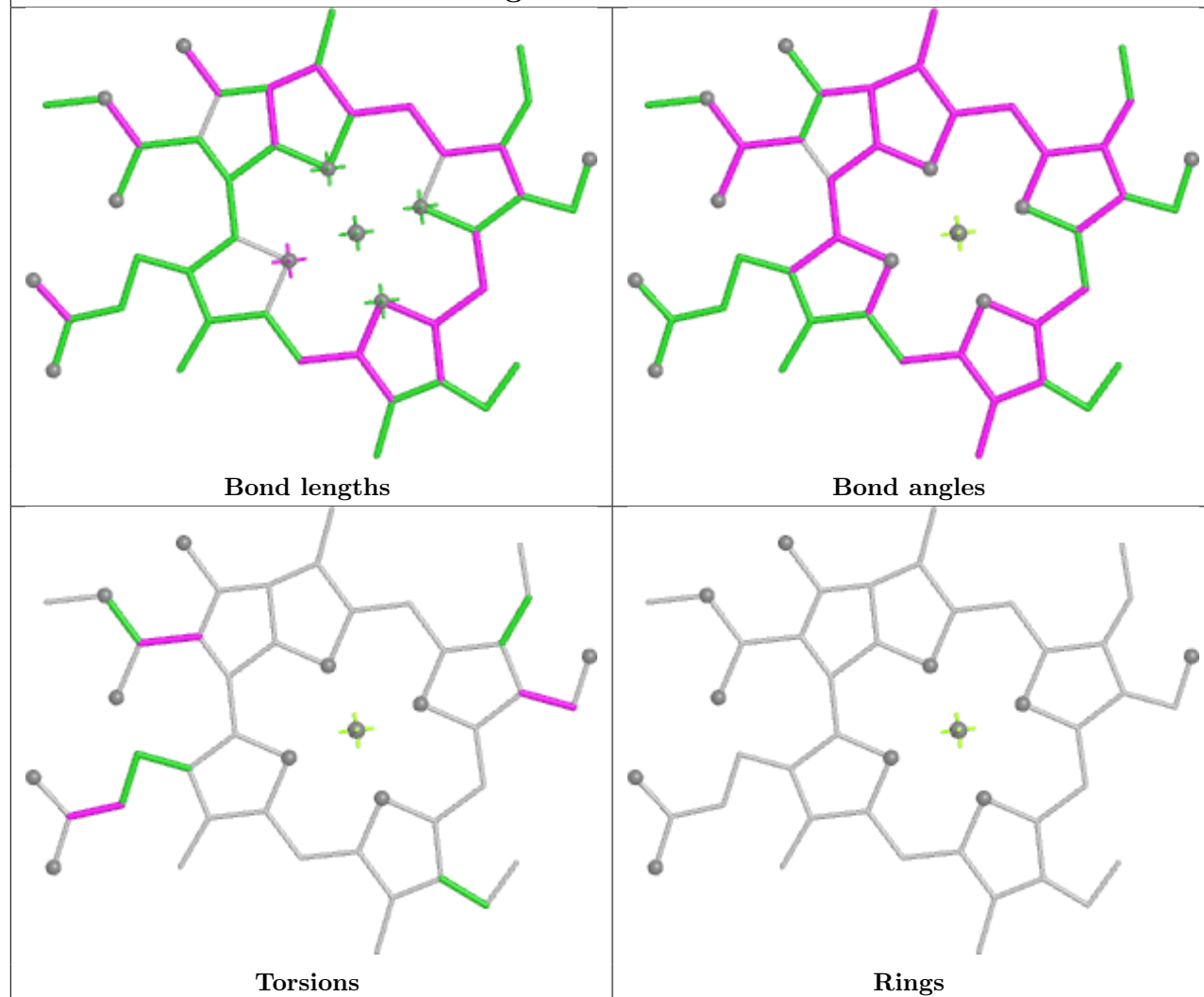


Ligand CLA 3 612

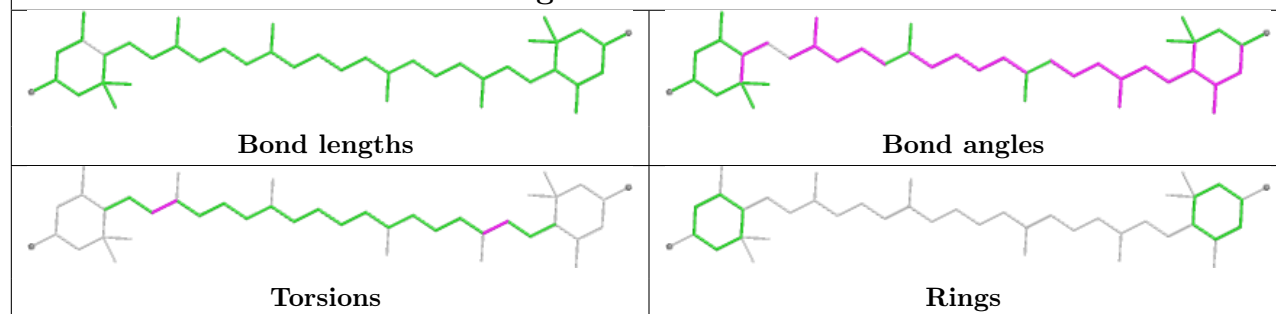




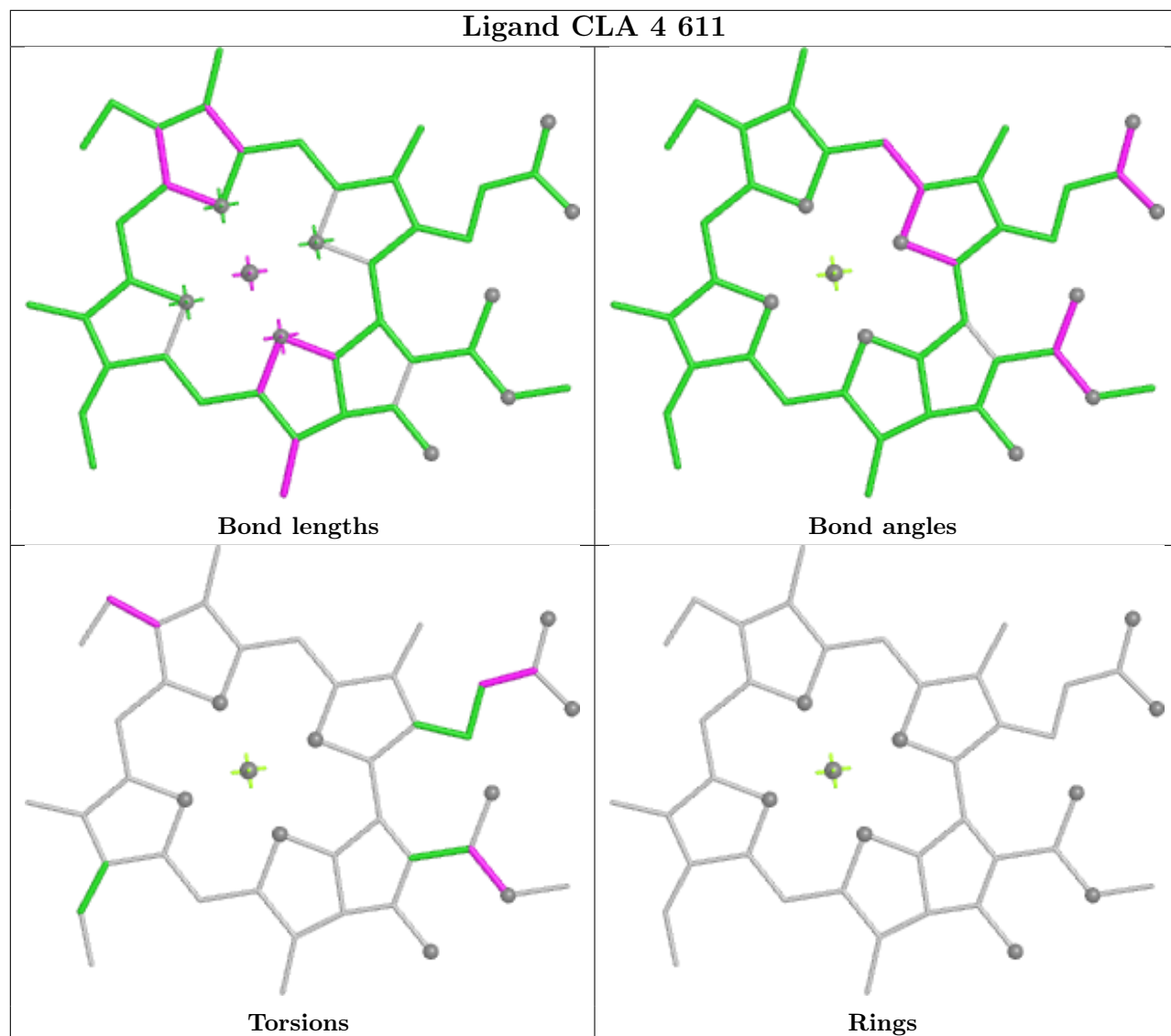
Ligand CHL 1 601

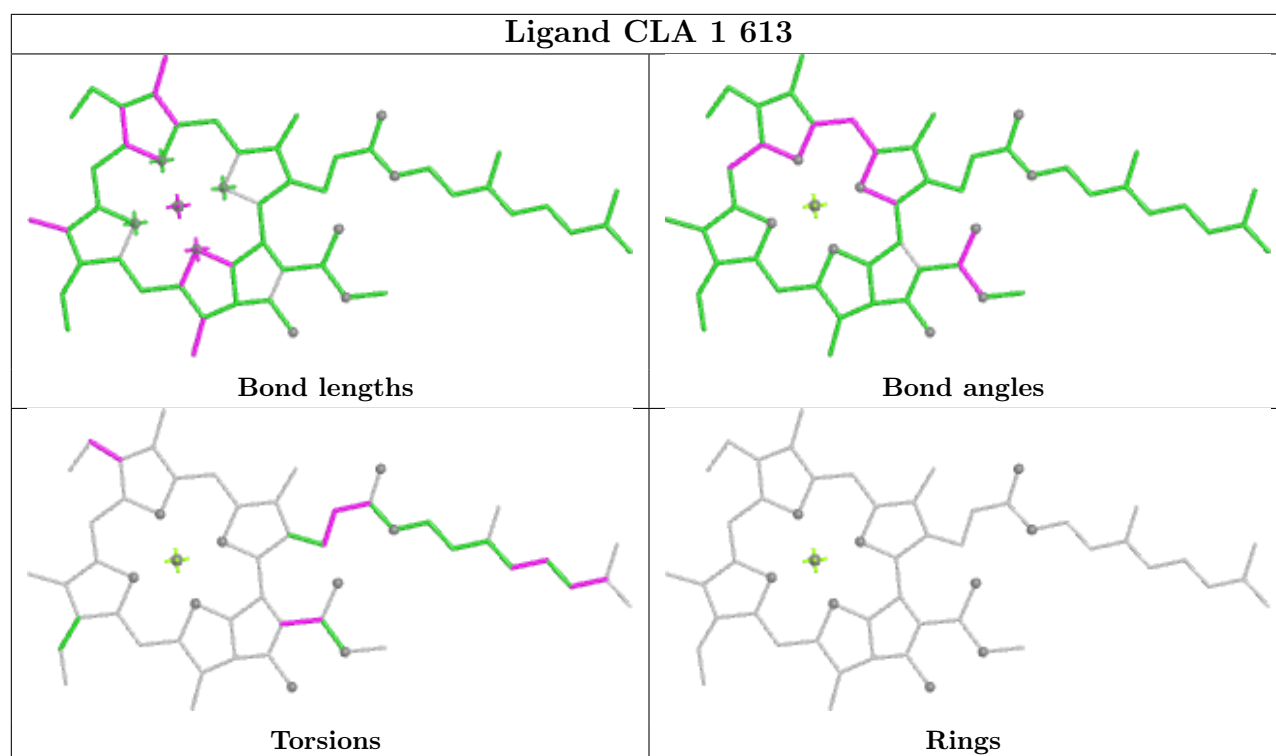


Ligand LUT 4 620

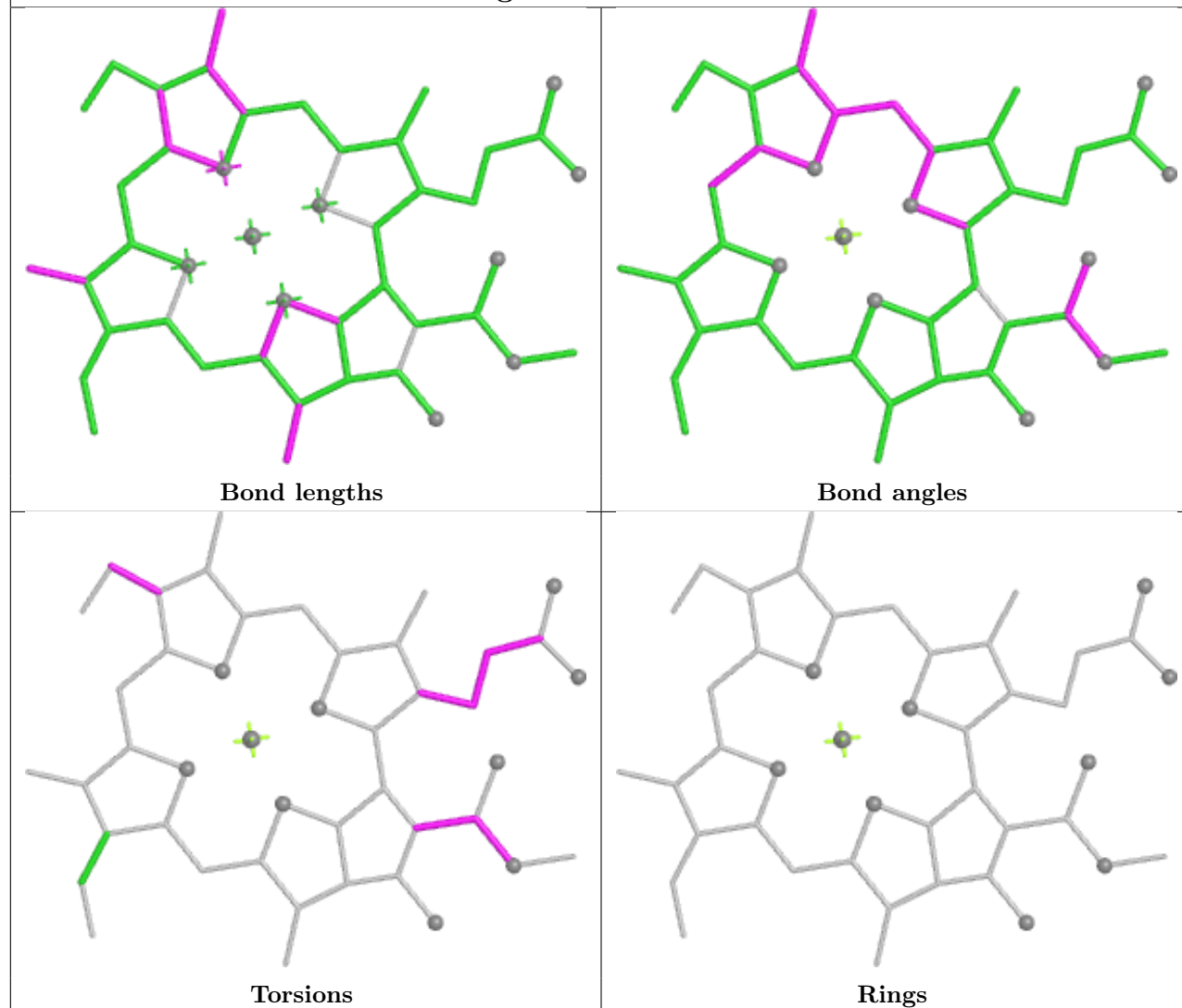


Ligand CLA 4 611

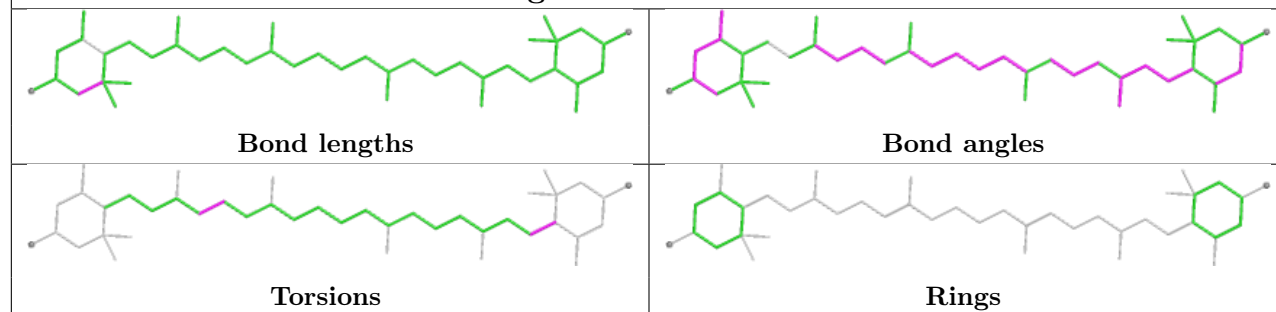




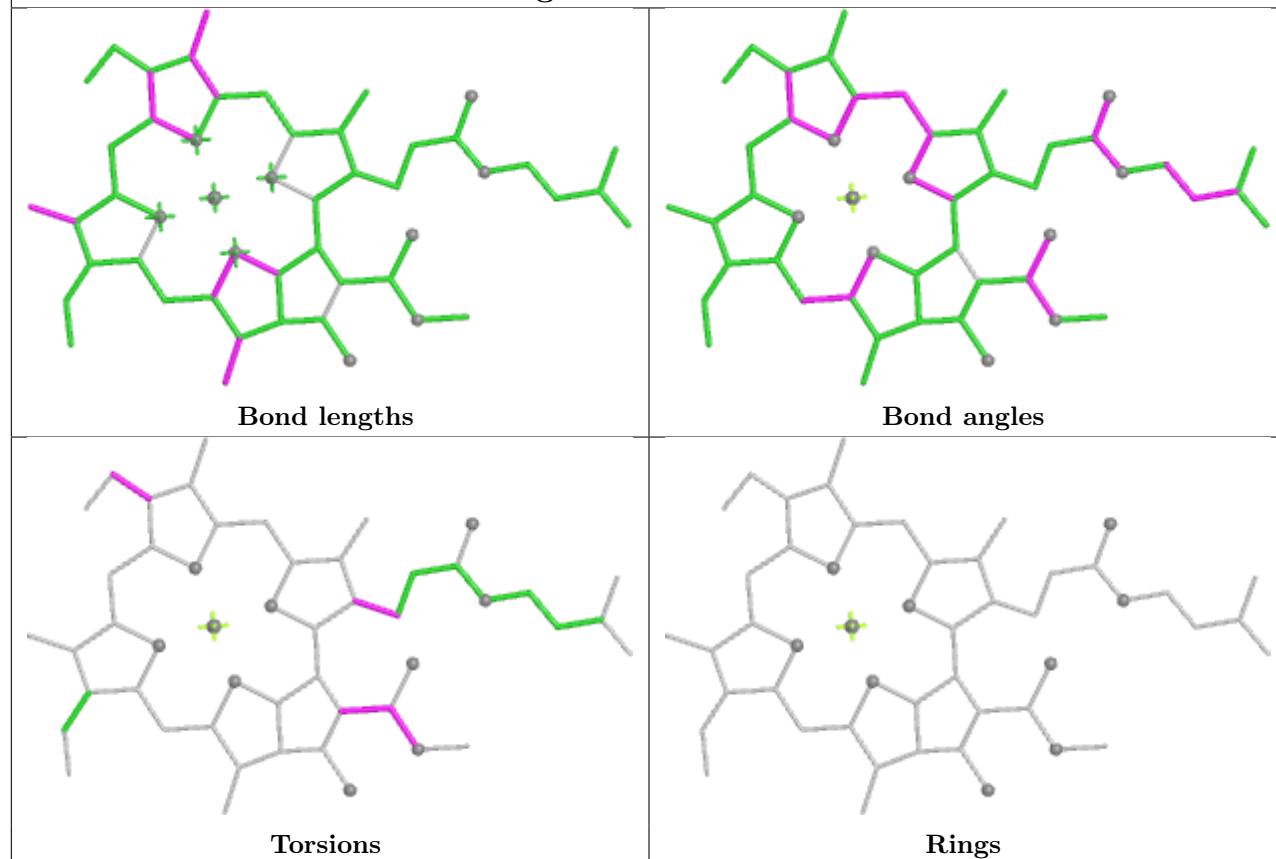
Ligand CLA 2 604



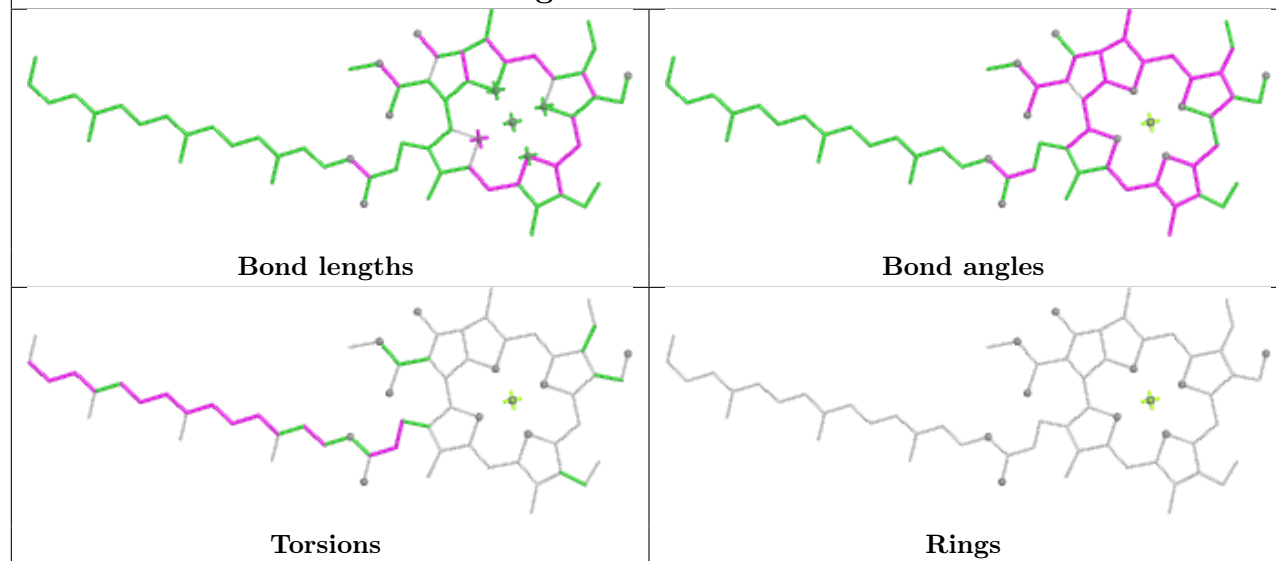
Ligand LUT 3 1621



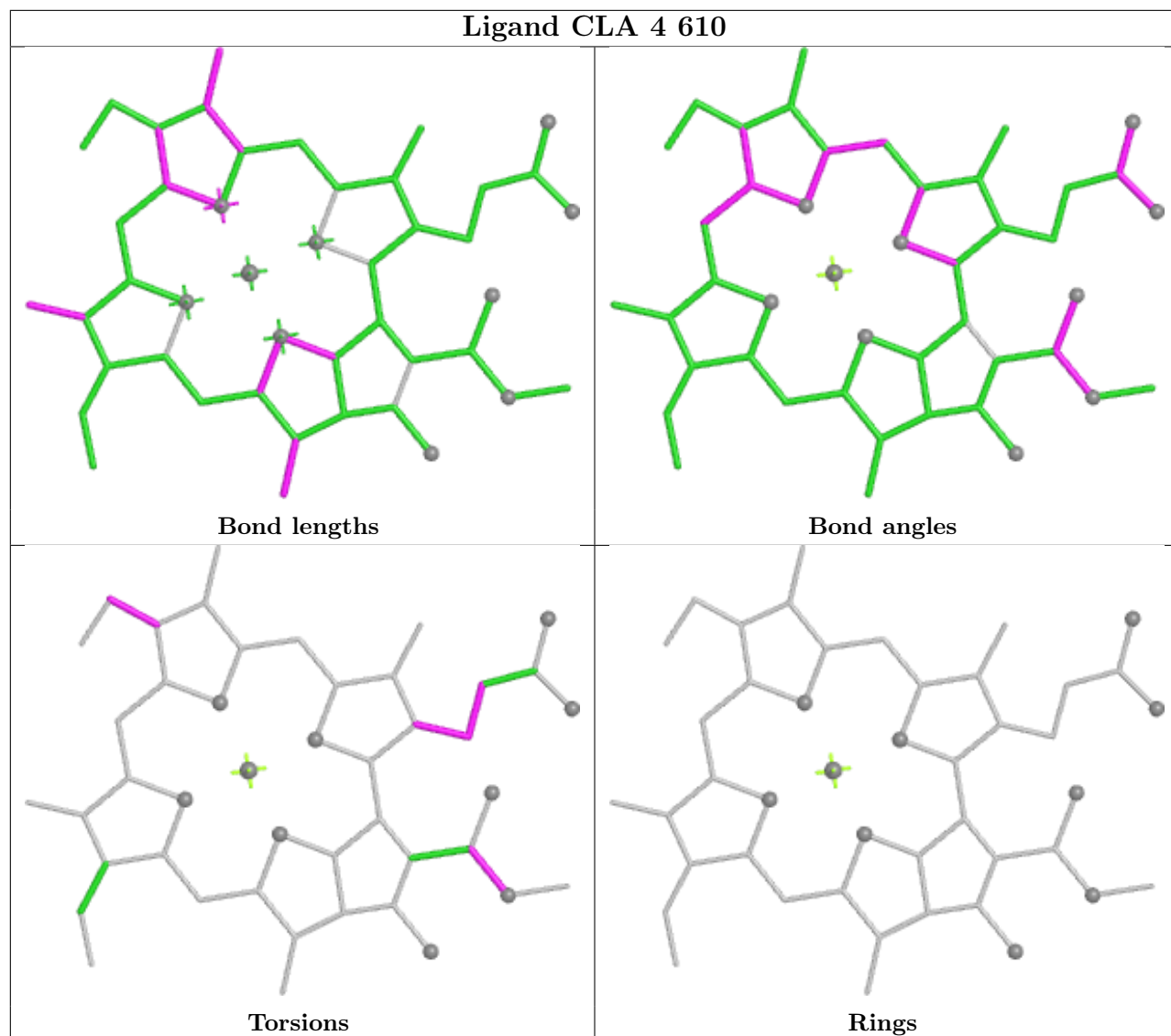
Ligand CLA 2 610



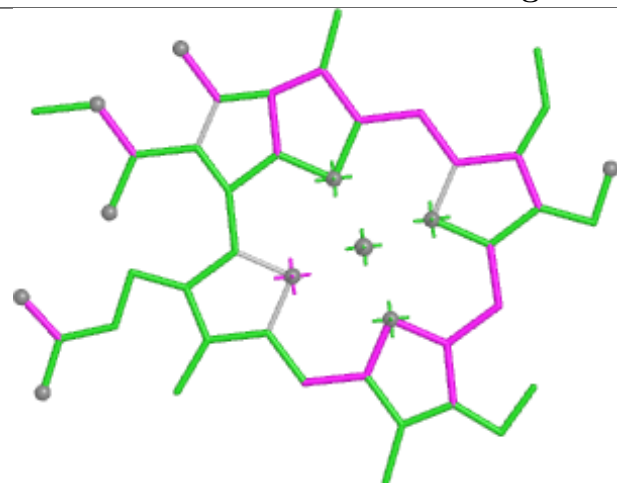
Ligand CHL 3 601



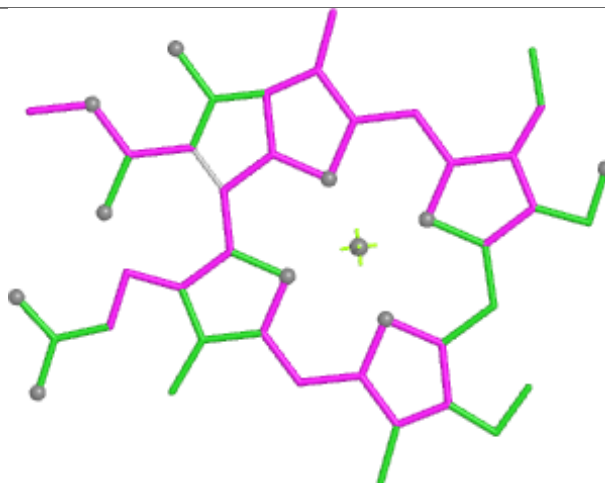
Ligand CLA 4 610



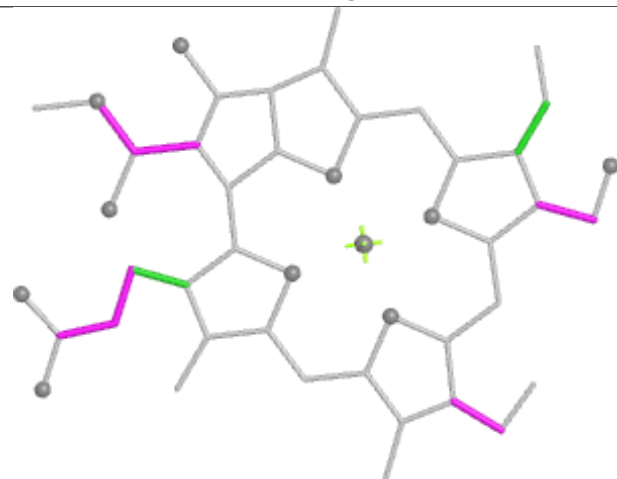
Ligand CHL 1 606



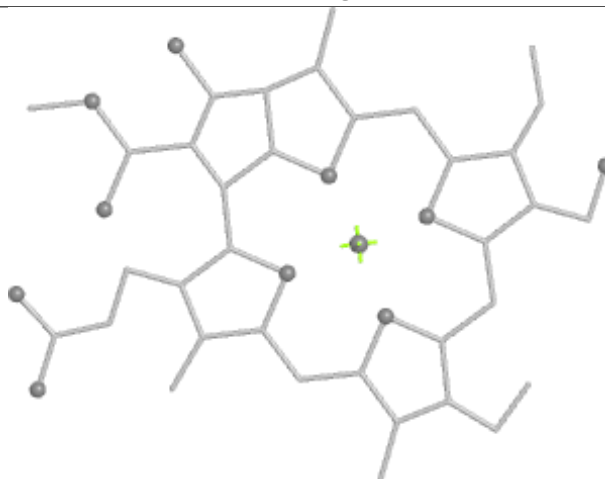
Bond lengths



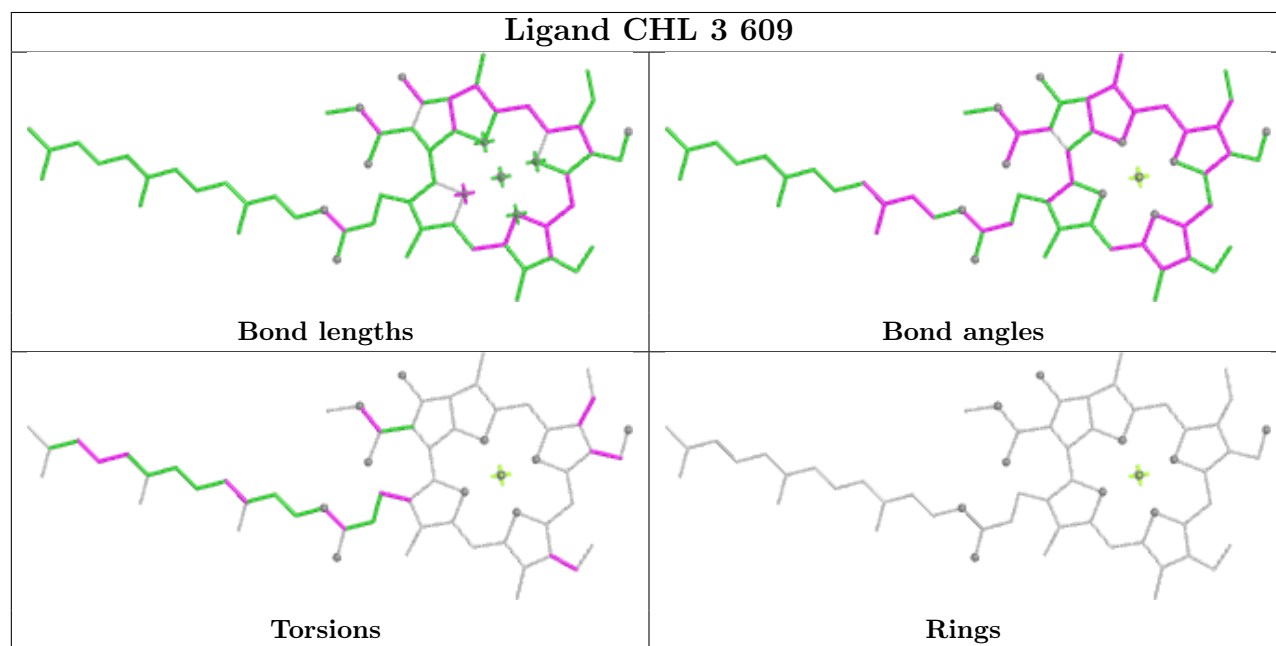
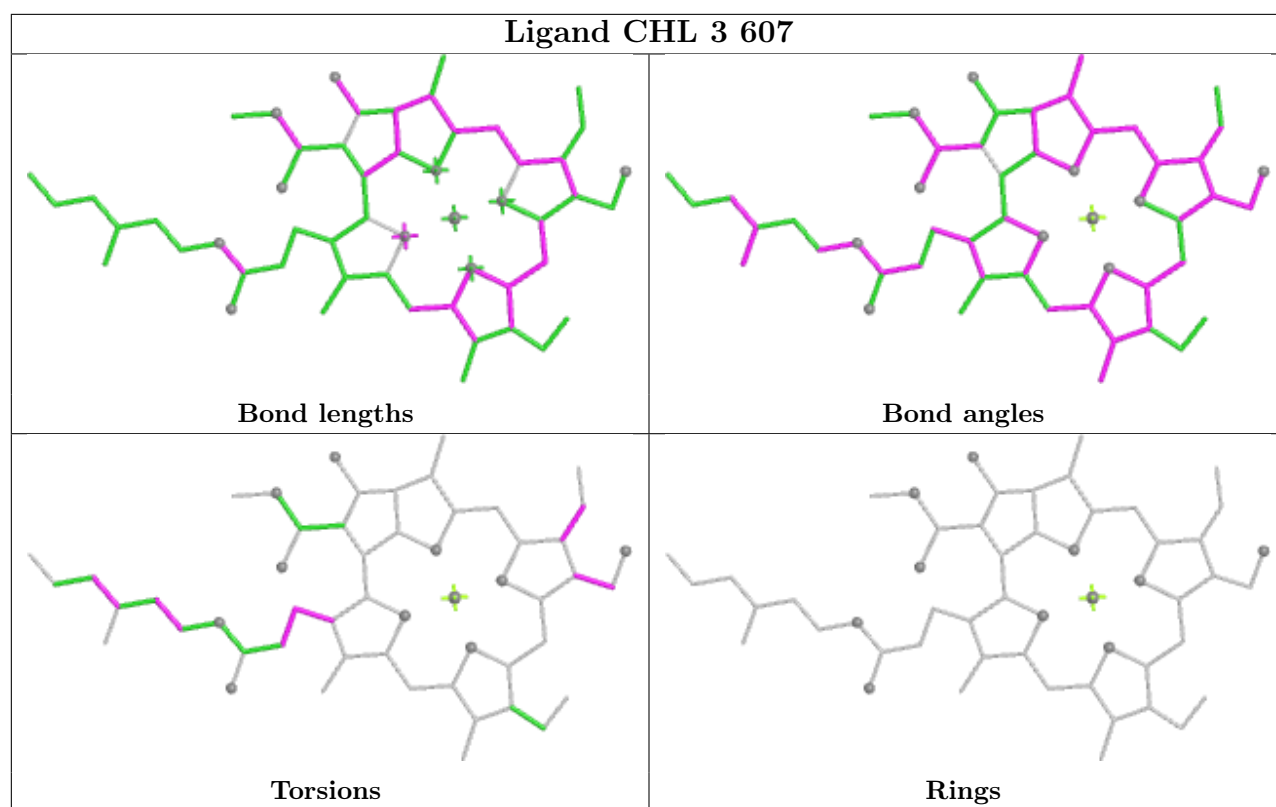
Bond angles



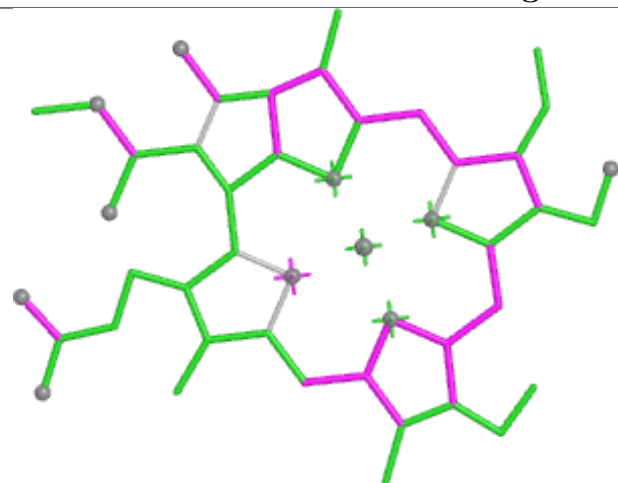
Torsions



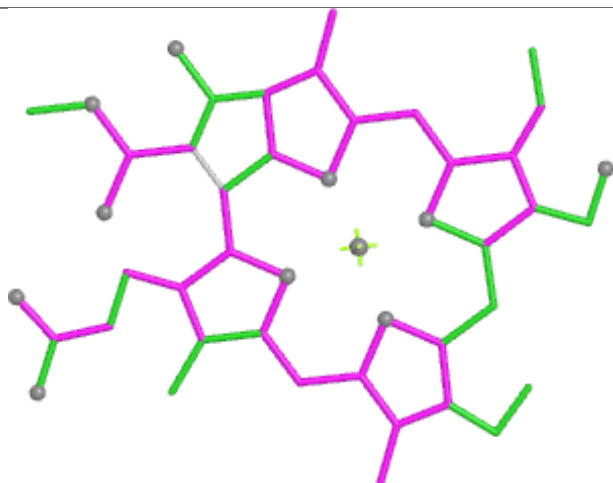
Rings



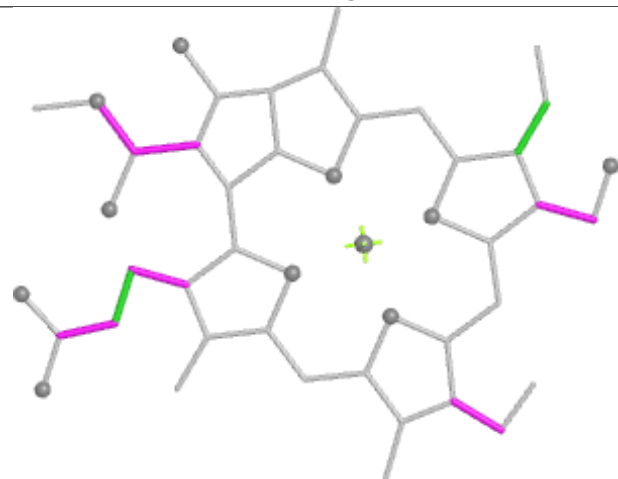
Ligand CHL 1 605



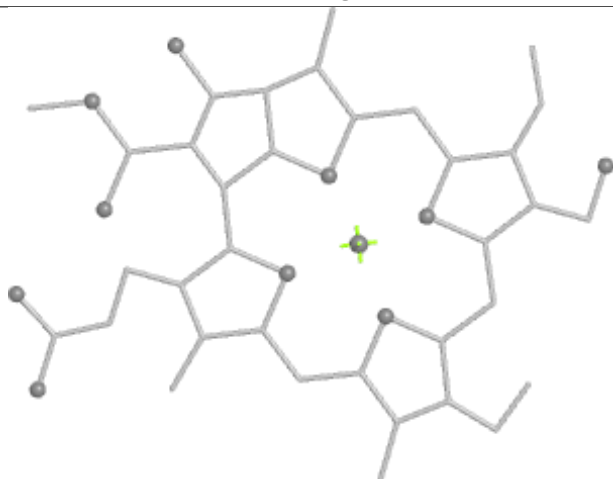
Bond lengths



Bond angles

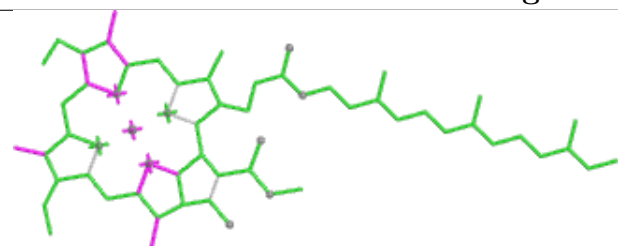


Torsions

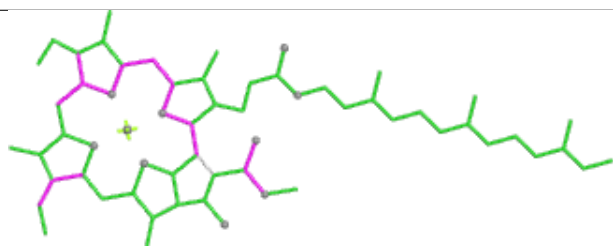


Rings

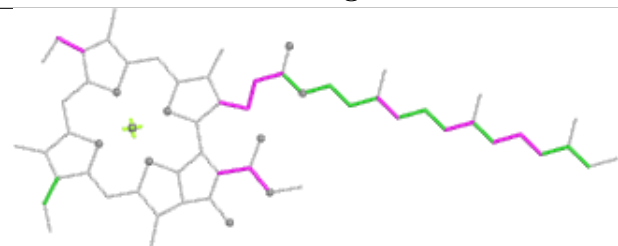
Ligand CLA 1 602



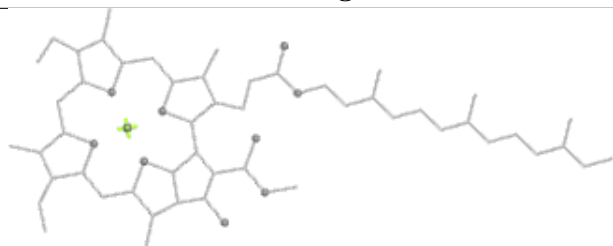
Bond lengths



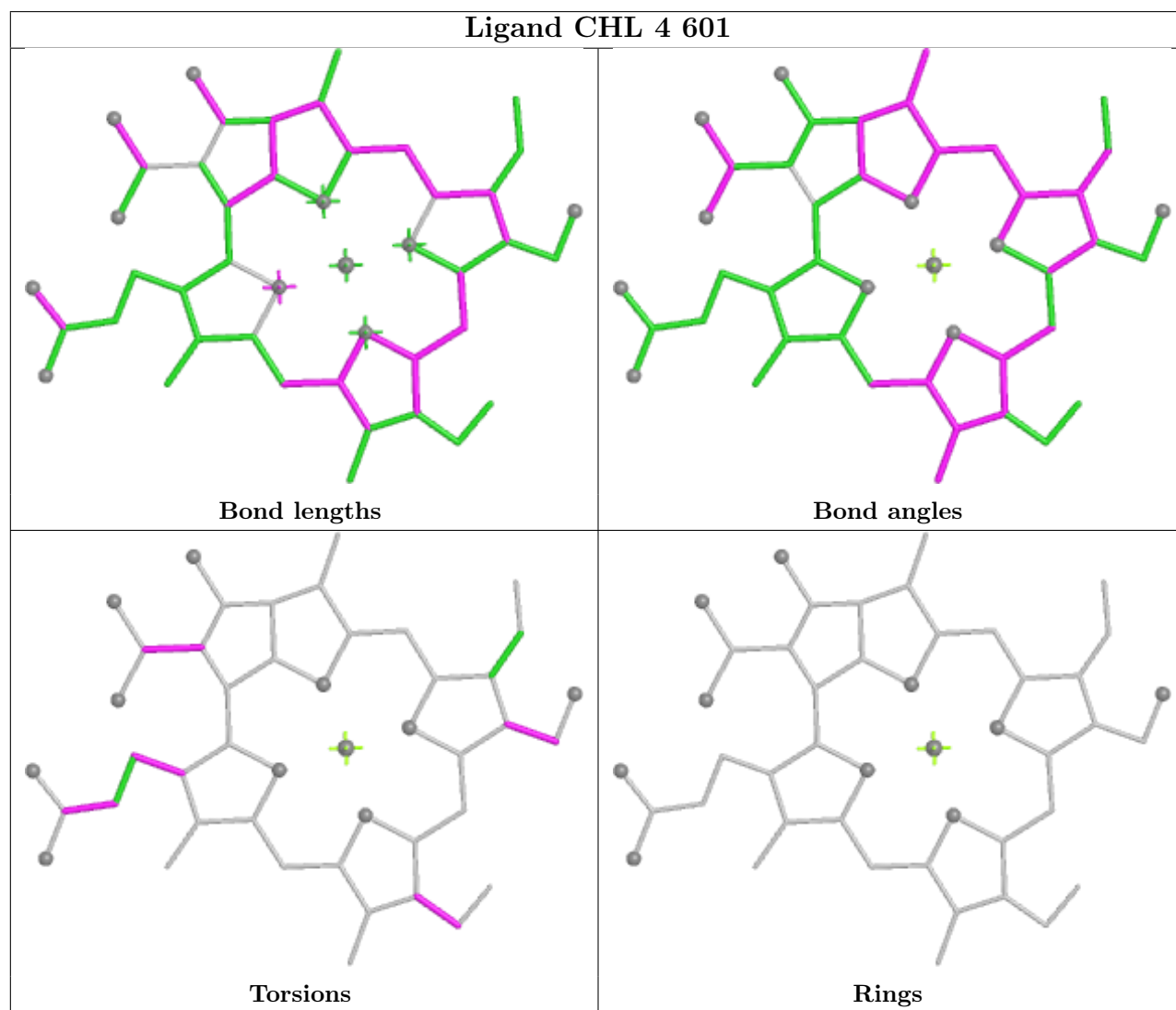
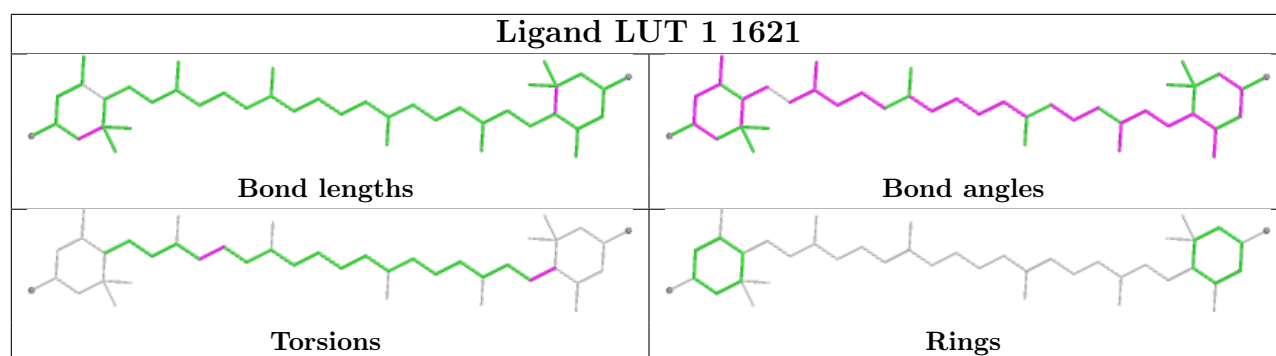
Bond angles



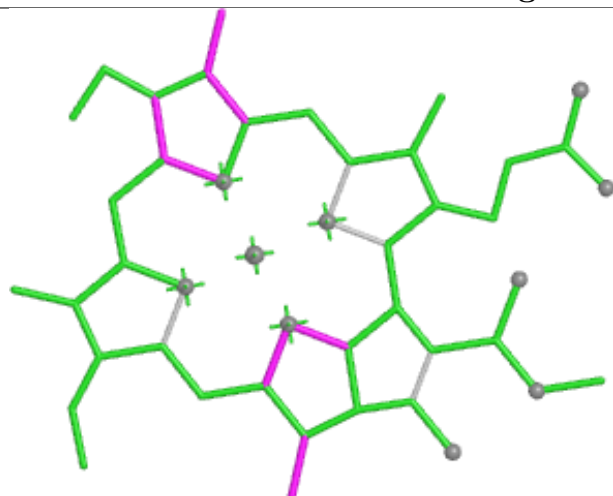
Torsions



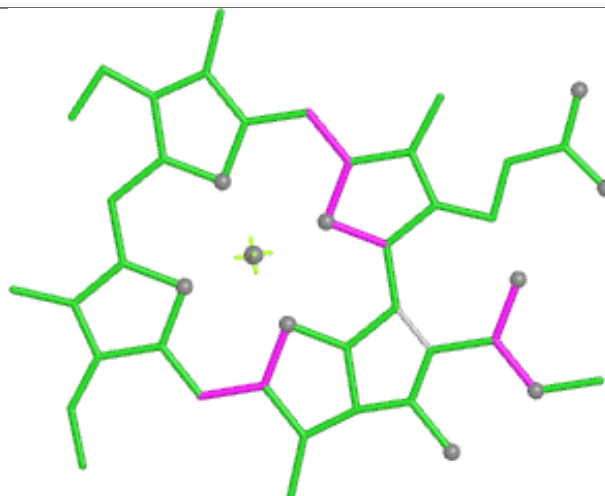
Rings



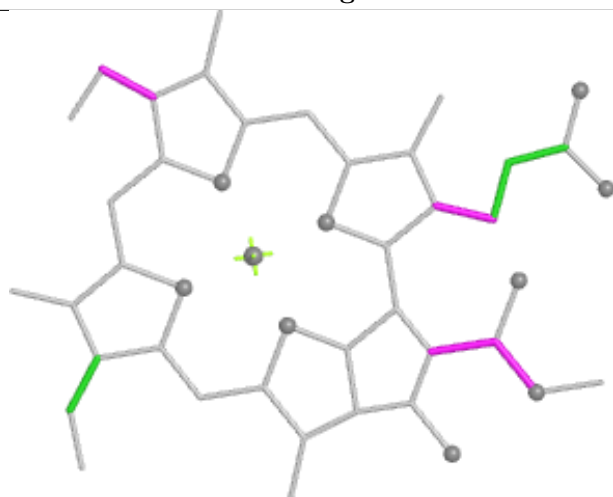
Ligand CLA 2 614



Bond lengths



Bond angles

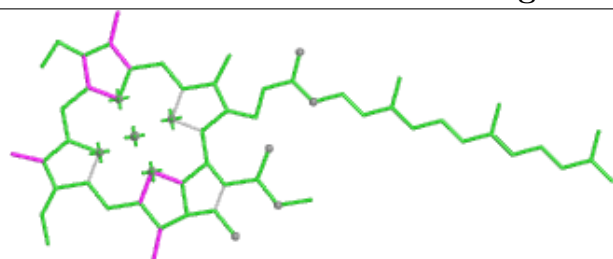


Torsions

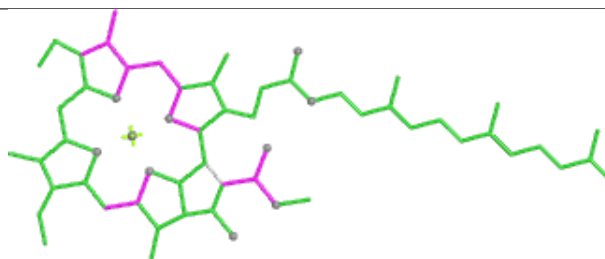


Rings

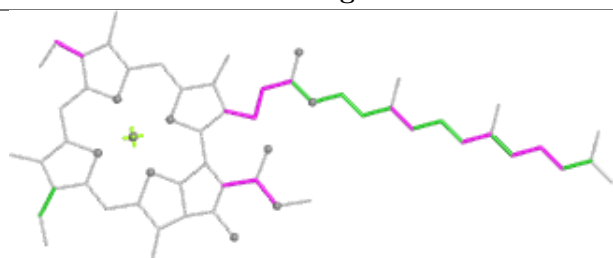
Ligand CLA 3 602



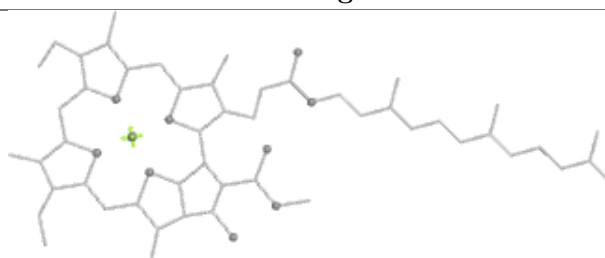
Bond lengths



Bond angles

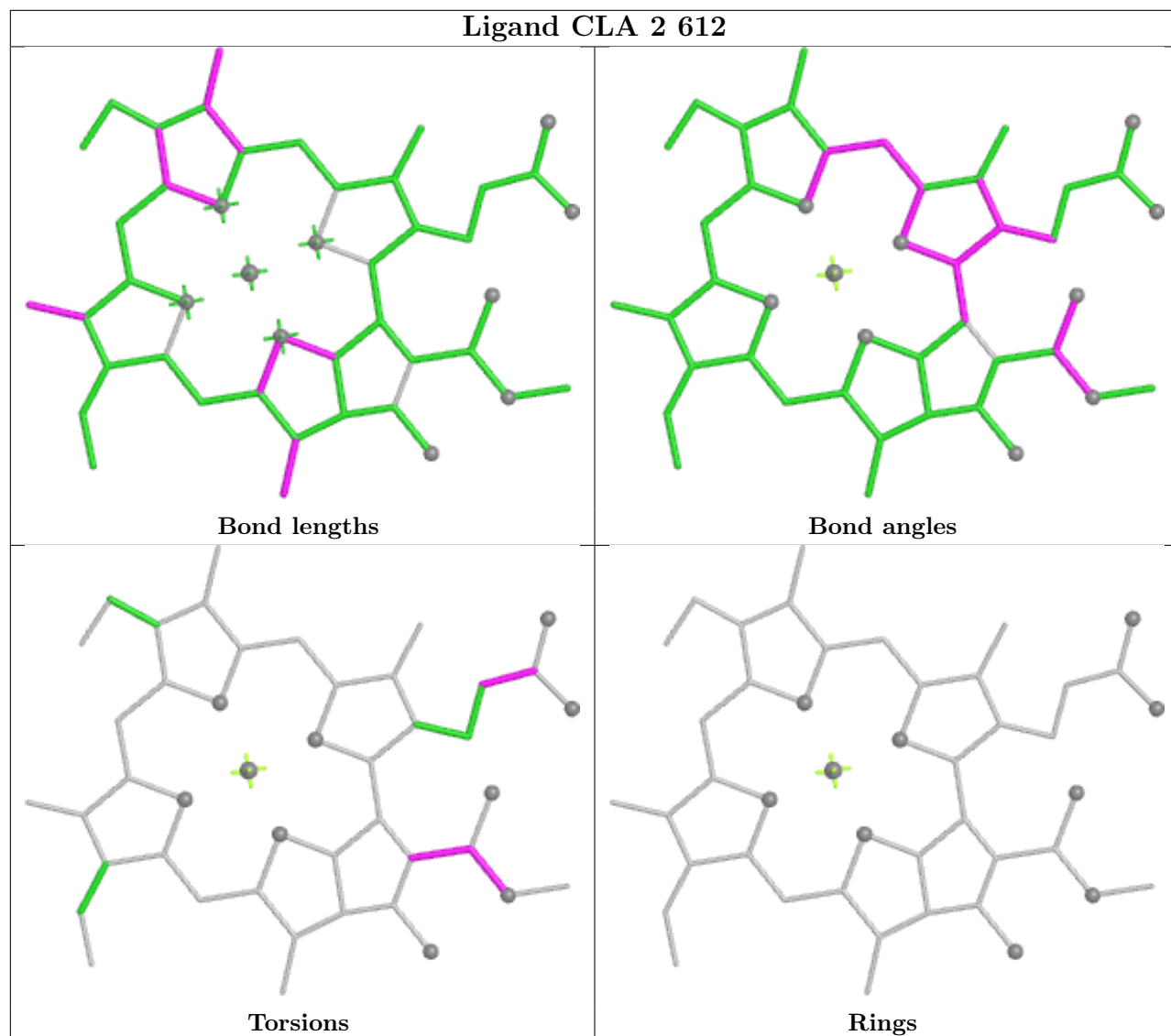


Torsions

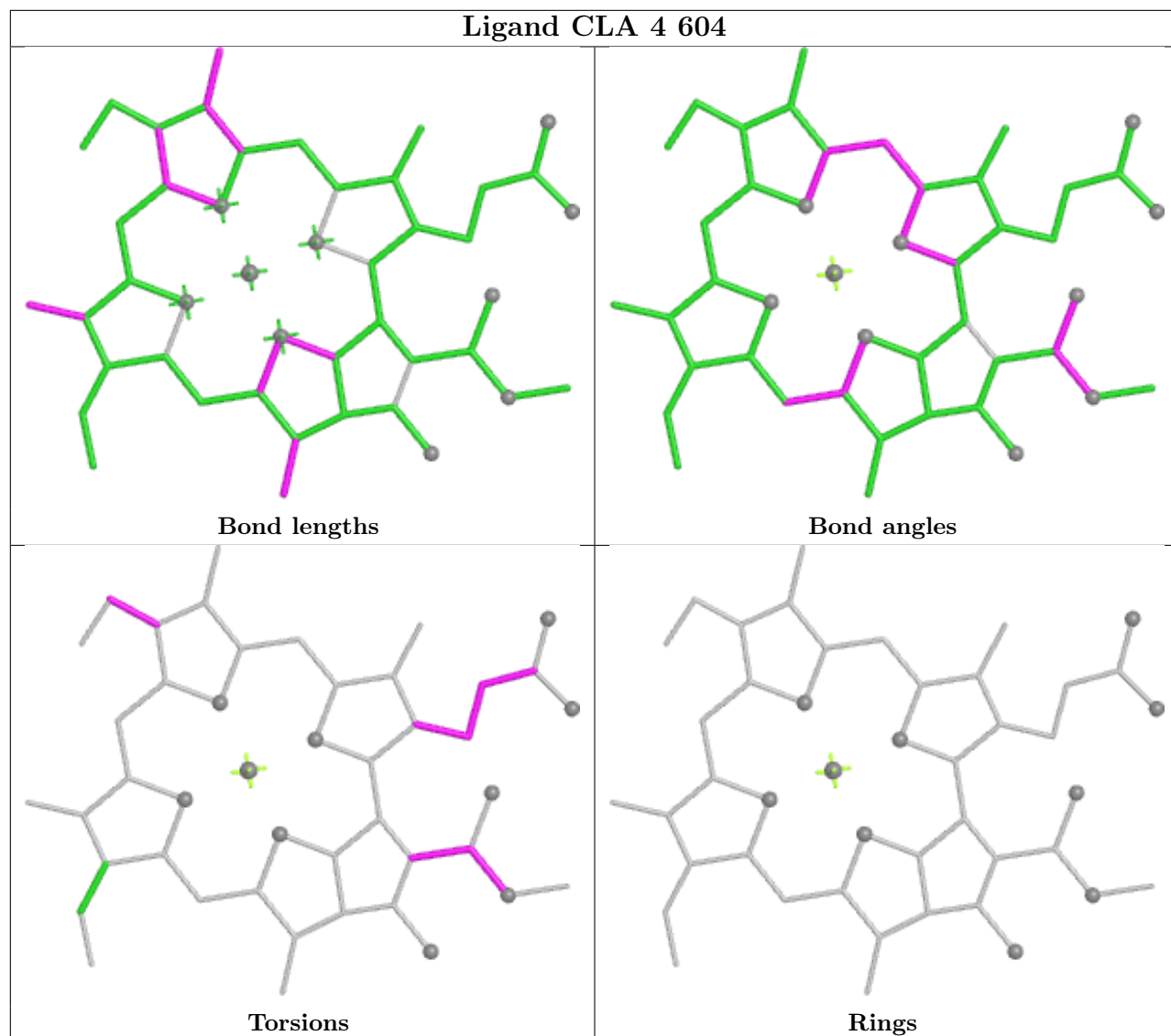


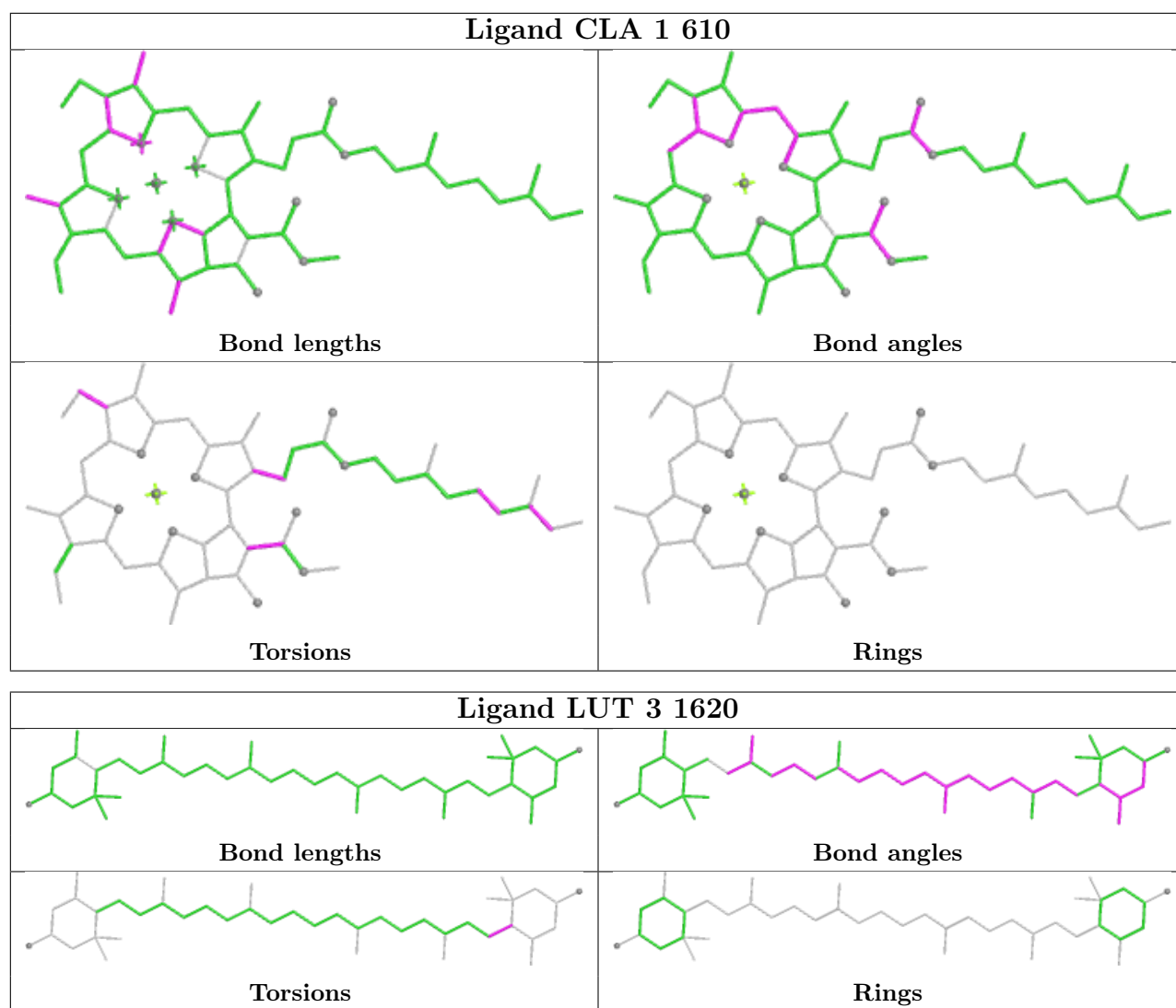
Rings

Ligand CLA 2 612



Ligand CLA 4 604





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.

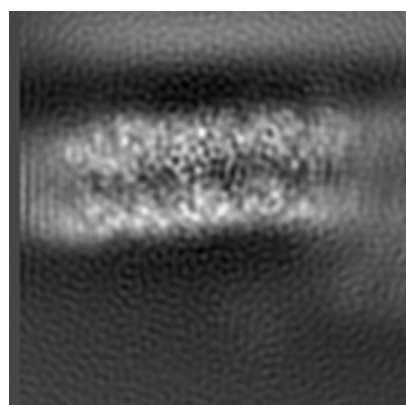
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6743. These allow visual inspection of the internal detail of the map and identification of artifacts.

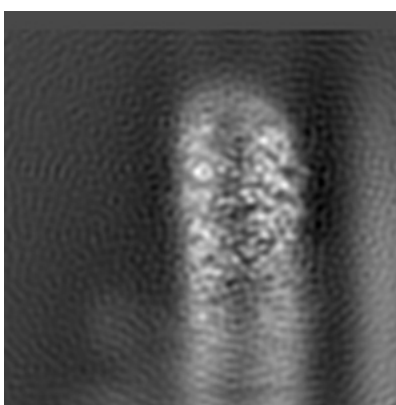
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

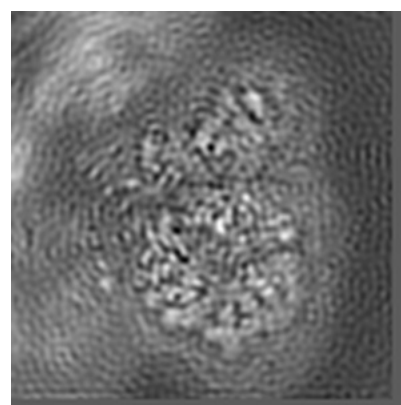
6.1.1 Primary map



X



Y

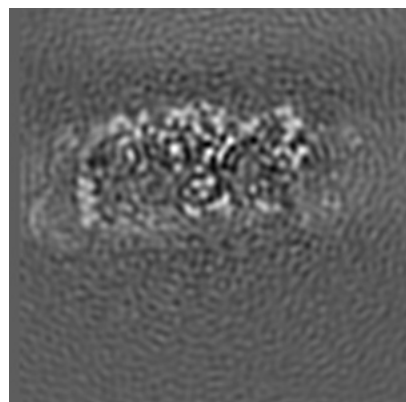


Z

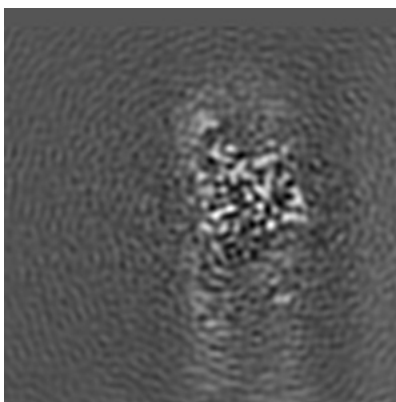
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

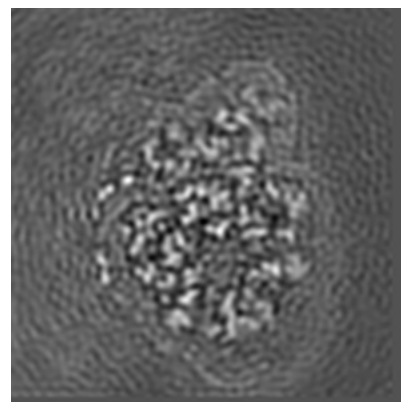
6.2.1 Primary map



X Index: 75



Y Index: 75

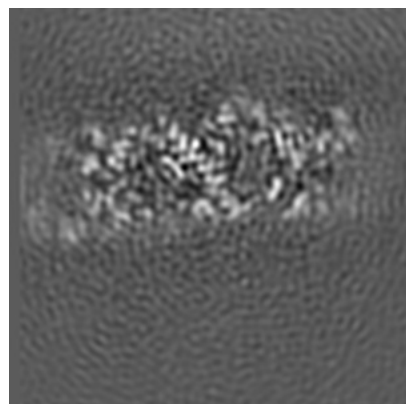


Z Index: 75

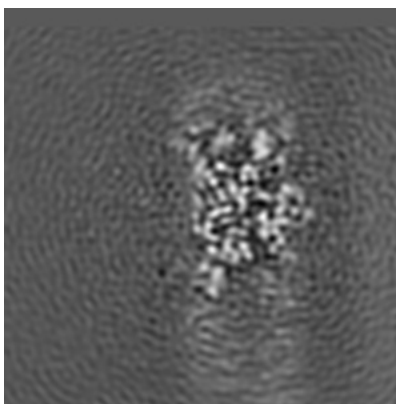
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

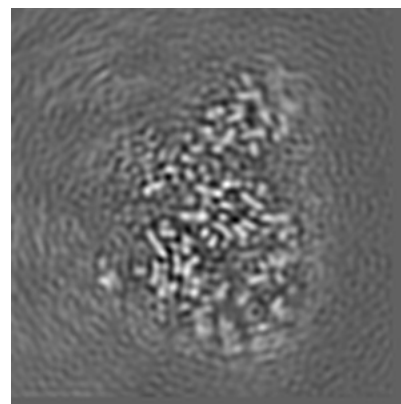
6.3.1 Primary map



X Index: 87



Y Index: 71

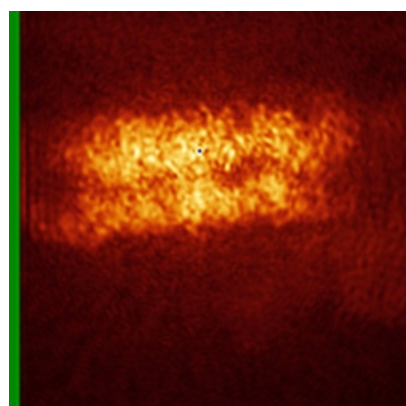


Z Index: 97

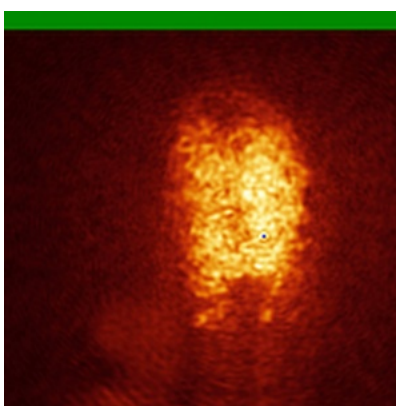
The images above show the largest variance slices of the map in three orthogonal directions.

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

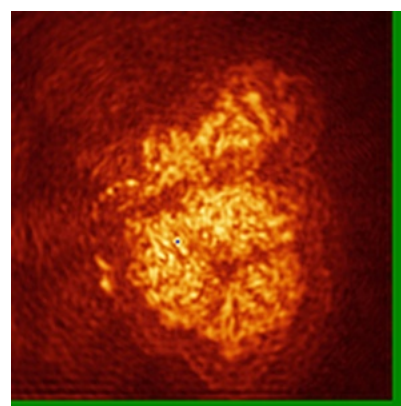
6.4.1 Primary map



X



Y

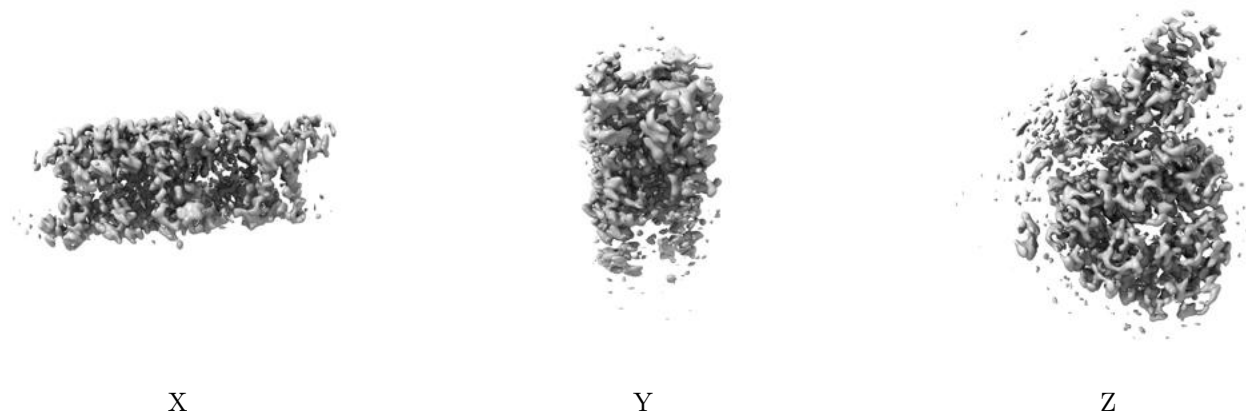


Z

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 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

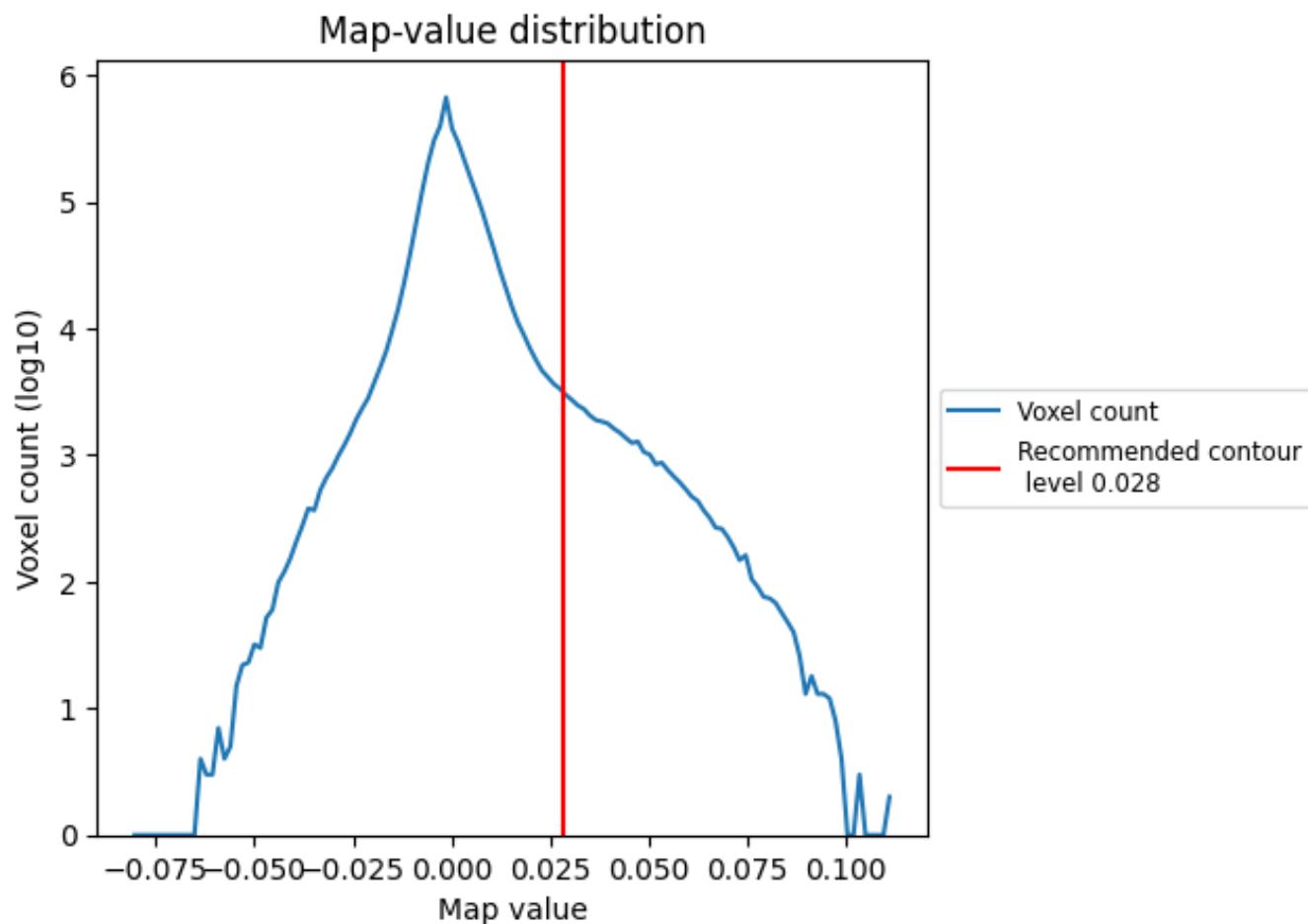
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

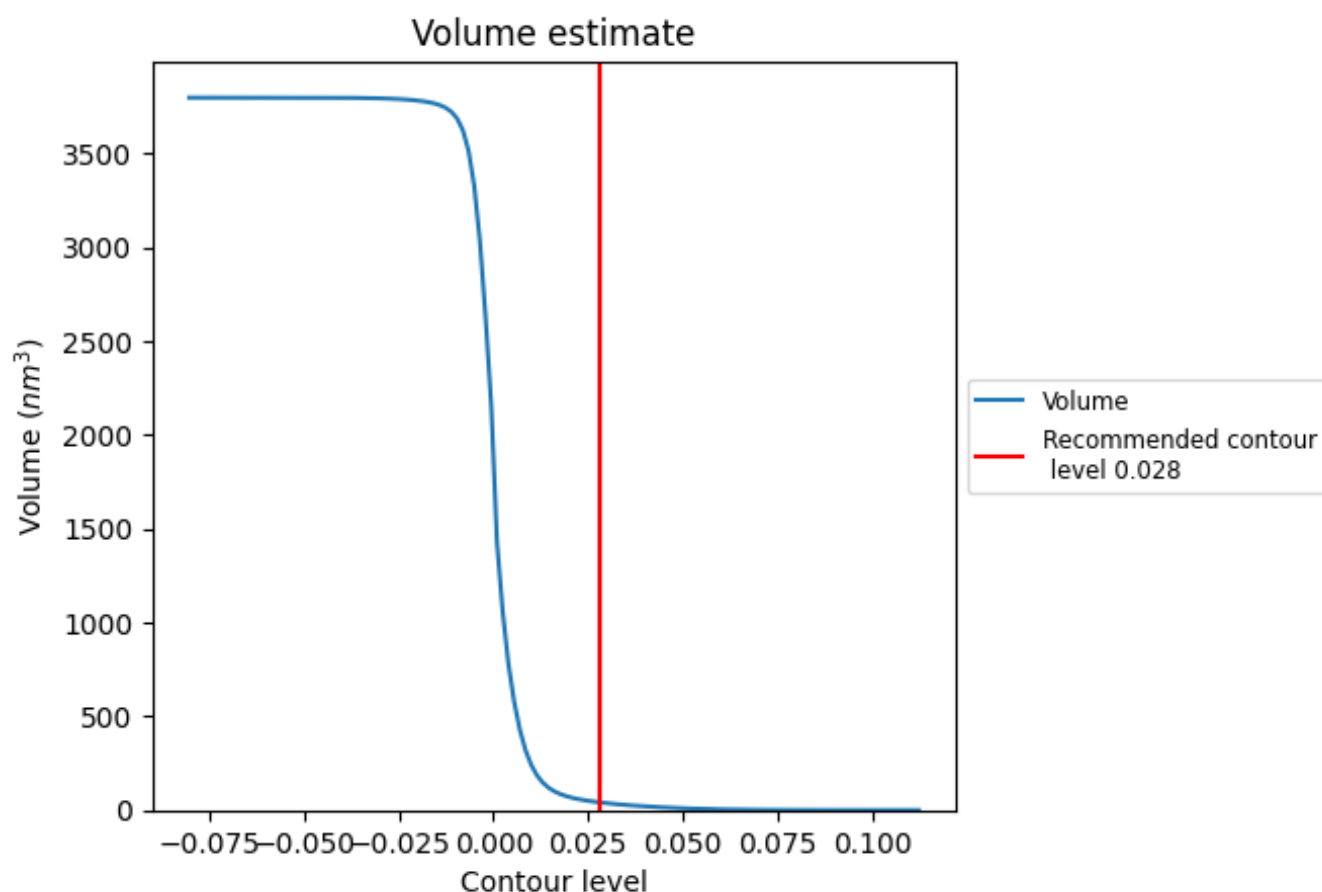
This section contains the results of statistical analysis of the map.

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.

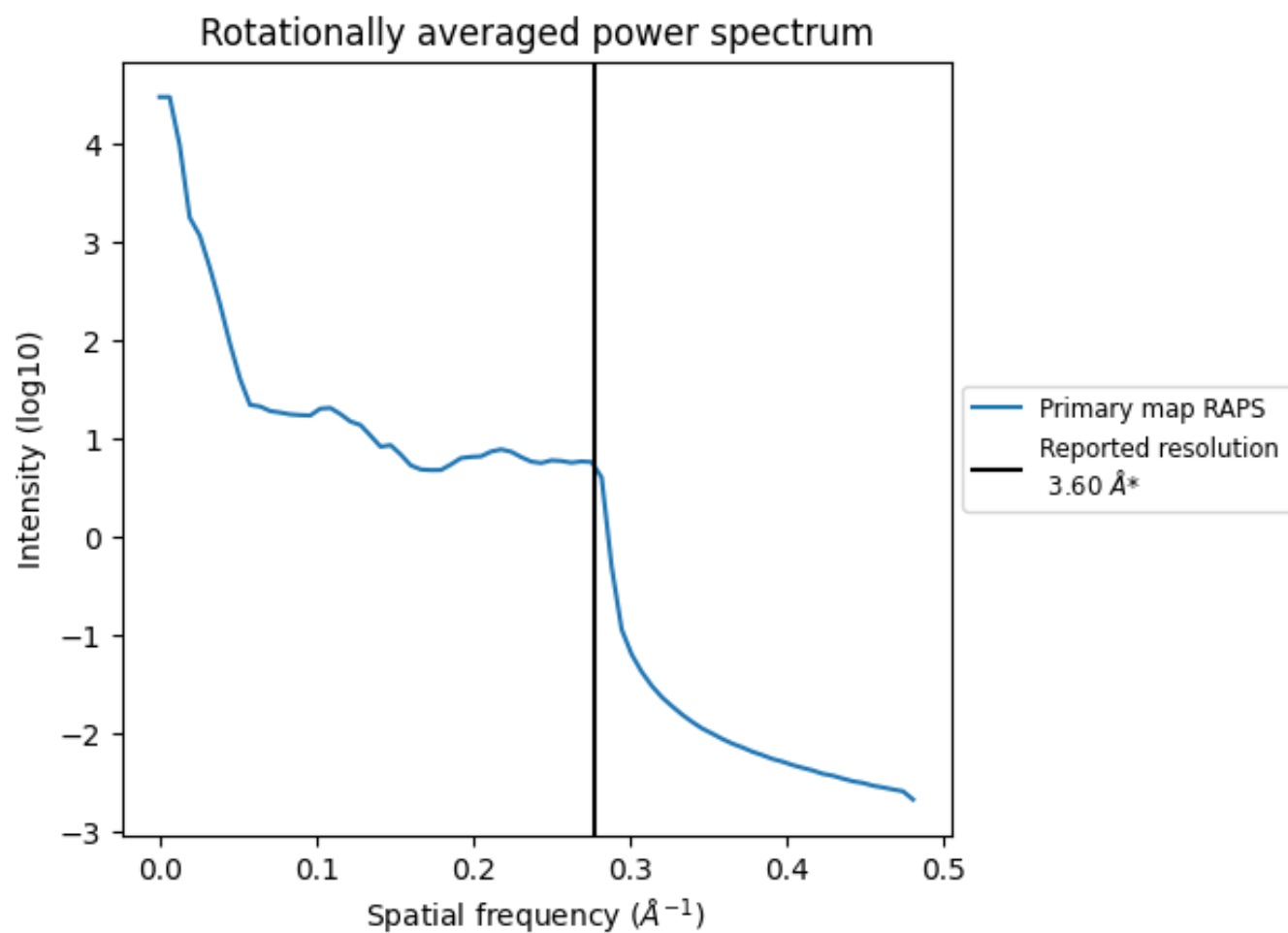
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 42 nm^3 ; this corresponds to an approximate mass of 38 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 0.278 Å⁻¹

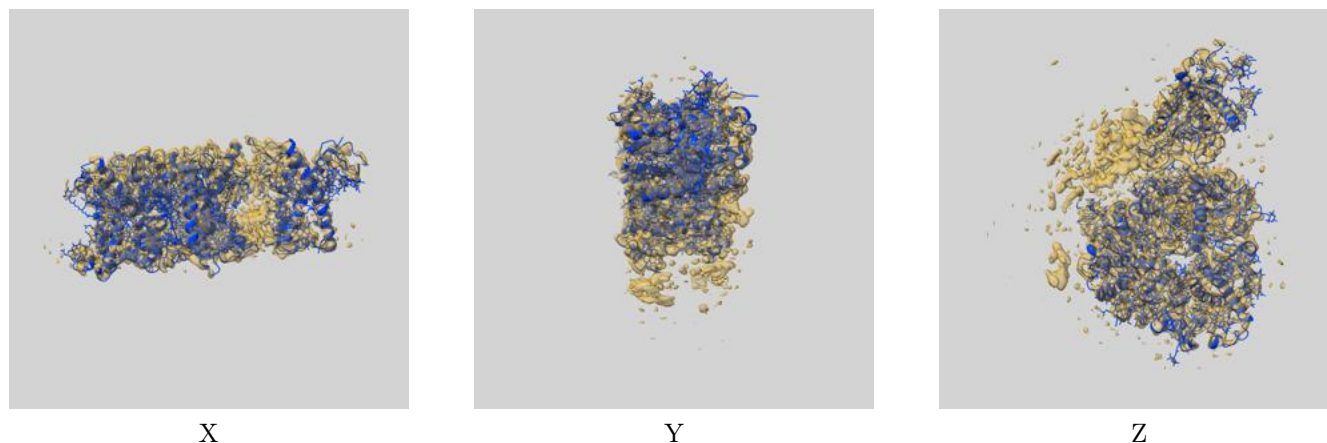
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

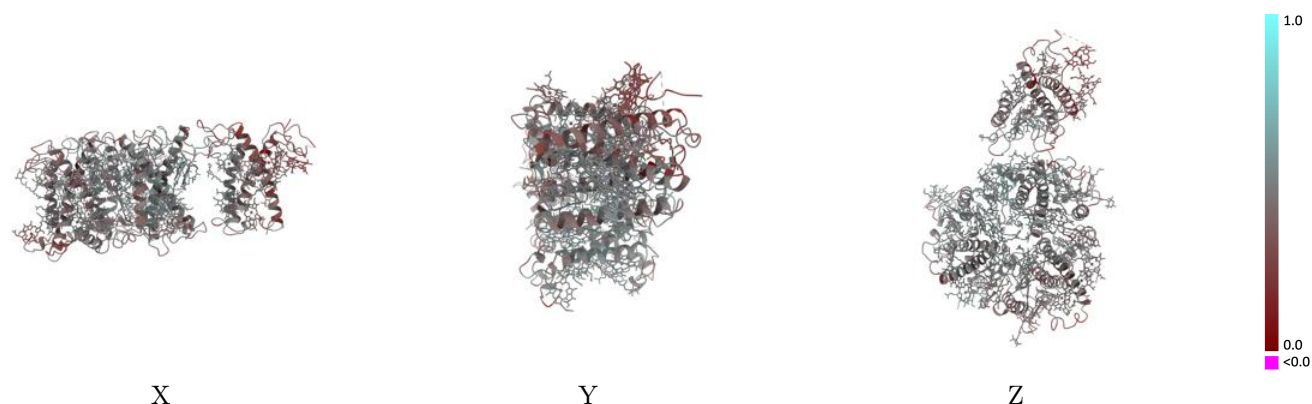
This section contains information regarding the fit between EMDB map EMD-6743 and PDB model 5XNN. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



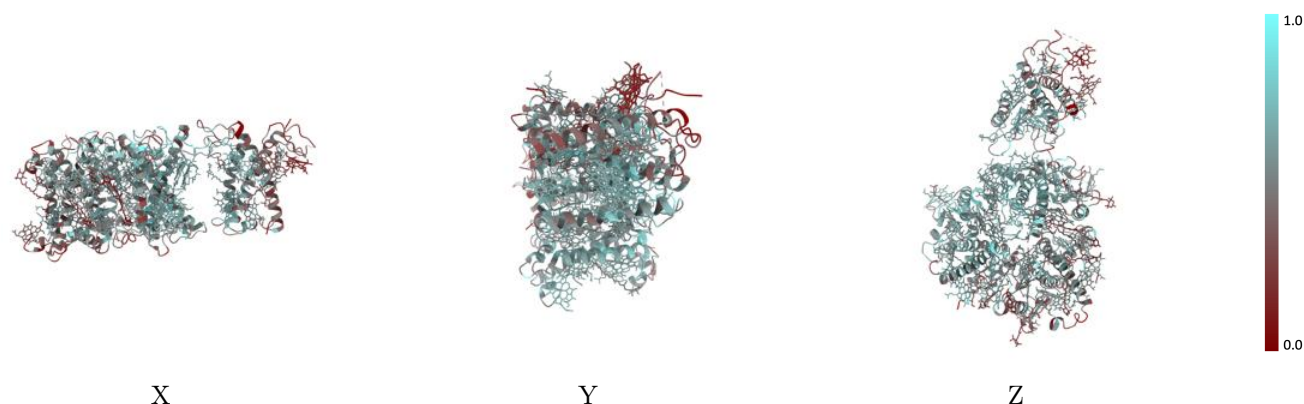
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



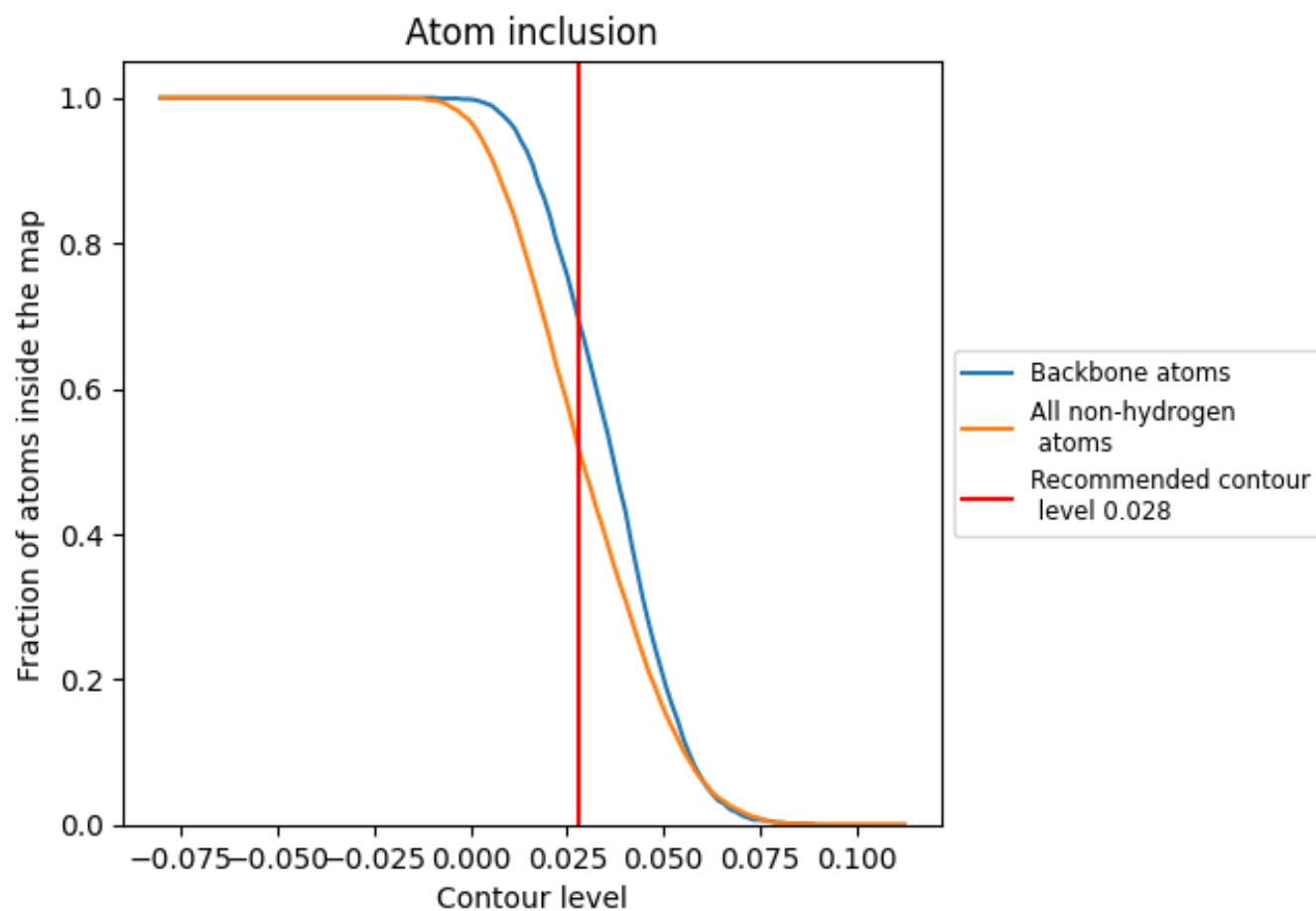
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.028).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 52% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5160	0.4470
1	0.5560	0.4700
2	0.4450	0.4310
3	0.5820	0.4800
4	0.4720	0.4010

