



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2026 – 12:35 PM JST

PDB ID : 9XK4 / pdb_00009xk4
EMDB ID : EMD-66947
Title : In situ C2S2M2L4-type PSII-LHCII supercomplex, core, protomer 2
Authors : Li, J.; Elias, E.; Zhang, K.; Croce, R.; Zhu, J.
Deposited on : 2025-11-05
Resolution : 2.78 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

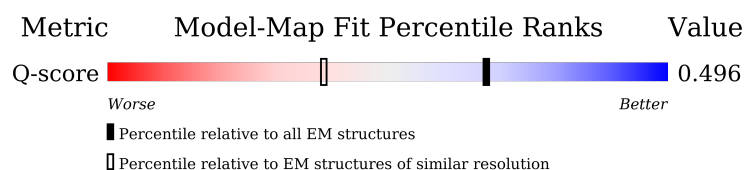
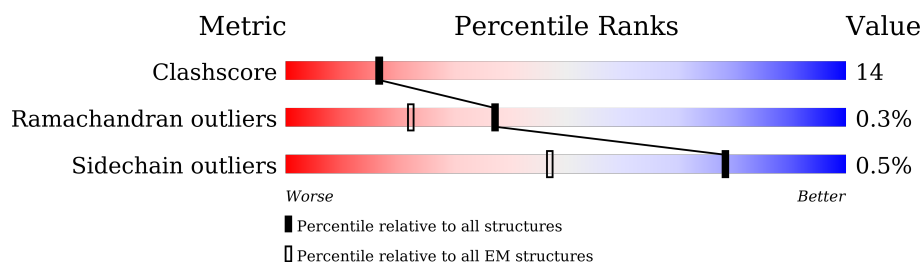
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 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.



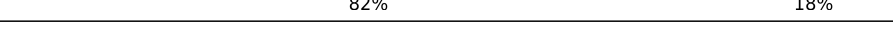
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10754 (2.28 - 3.28)

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	1a	333	64% 35% .
2	1b	503	71% 28%
3	1c	450	74% 26%
4	1d	341	66% 34% .

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Mol	Chain	Length	Quality of chain
5	1e	75	
6	1f	31	
7	1h	60	
8	1i	34	
9	1j	35	
10	1k	37	
11	1l	37	
12	1m	34	
13	1o	248	
14	1p	186	
15	1t	32	
16	1u	27	
17	1v	105	
18	1w	44	
19	1x	39	
20	1y	36	
21	1z	62	

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
26	CLA	1a	408	X	-	-	-
26	CLA	1b	601	X	-	-	-
26	CLA	1b	602	X	-	-	-
26	CLA	1b	603	X	-	-	-
26	CLA	1b	605	X	-	-	-
26	CLA	1b	607	X	-	-	-
26	CLA	1b	608	X	-	-	-
26	CLA	1b	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	1b	610	X	-	-	-
26	CLA	1b	611	X	-	-	-
26	CLA	1b	612	X	-	-	-
26	CLA	1b	613	X	-	-	-
26	CLA	1b	614	X	-	-	-
26	CLA	1b	615	X	-	-	-
26	CLA	1c	502	X	-	-	-
26	CLA	1c	503	X	-	-	-
26	CLA	1c	504	X	-	-	-
26	CLA	1c	505	X	-	-	-
26	CLA	1c	507	X	-	-	-
26	CLA	1c	508	X	-	-	-
26	CLA	1c	509	X	-	-	-
26	CLA	1c	511	X	-	-	-
26	CLA	1c	513	X	-	-	-
26	CLA	1c	514	X	-	-	-
26	CLA	1d	403	X	-	-	-
26	CLA	1d	406	X	-	-	-
26	CLA	1d	407	X	-	-	-
30	PL9	1a	413	-	-	X	-

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 25527 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 Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1a	333	Total	C	N	O	S	0	0
			2606	1703	429	461	13		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1b	503	Total	C	N	O	S	0	0
			3945	2577	663	693	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1c	450	Total	C	N	O	S	0	0
			3498	2304	583	601	10		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1d	341	Total	C	N	O	S	0	0
			2716	1794	444	466	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	1e	75	Total	C	N	O	0	0
			614	400	100	114		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1f	30	Total	C	N	O	S	0	0
			241	162	41	37	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1h	60	Total	C	N	O	S	0	0
			454	299	73	79	3		

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1i	34	Total	C	N	O	S	0	0
			277	190	43	43	1		

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1j	35	Total	C	N	O	S	0	0
			255	172	39	44			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1k	37	Total	C	N	O	S	0	0
			305	214	44	46	1		

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1l	35	Total	C	N	O	S	0	0
			295	196	46	53			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1m	33	Total	C	N	O	S	0	0
			251	173	37	41			

- Molecule 13 is a protein called 33 kDa subunit of oxygen evolving system of photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1o	237	Total	C	N	O	S	0	0
			1795	1136	294	360	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1o	248	SER	-	insertion	UNP Q943W1

- Molecule 14 is a protein called 23 kDa subunit of oxygen evolving system of photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1p	186	Total	C	N	O	S	0	0
			1422	901	236	284	1		

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1t	31	Total	C	N	O	S	0	0
			252	176	35	40	1		

- Molecule 16 is a protein called Os02g0581100 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1u	27	Total	C	N	O	S	0	0
			208	130	39	36	3		

- Molecule 17 is a protein called Photosystem II 10 kDa polypeptide, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	1v	99	Total	C	N	O	0	0
			683	437	113	133		

- Molecule 18 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1w	44	Total	C	N	O	S	0	0
			333	219	51	62	1		

- Molecule 19 is a protein called Os07g0673550 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	1x	38	Total	C	N	O	0	0
			272	179	45	48		

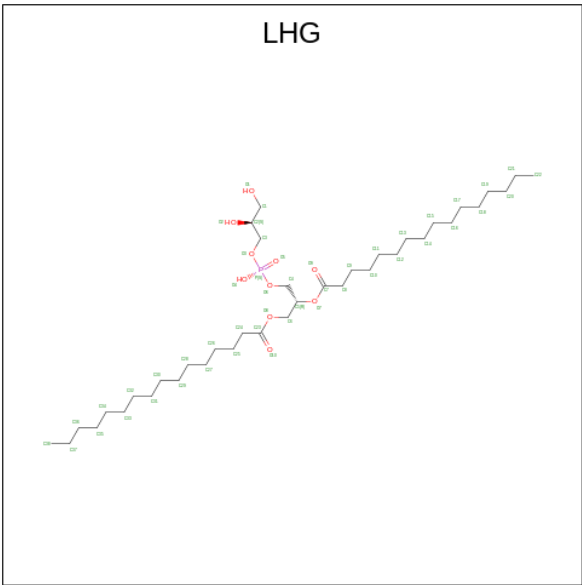
- Molecule 20 is a protein called Os08g0119800 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1y	34	Total	C	N	O	S	0	0
			268	175	50	42	1		

- Molecule 21 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1z	62	Total	C	N	O	S	0	0
			466	313	70	82	1		

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



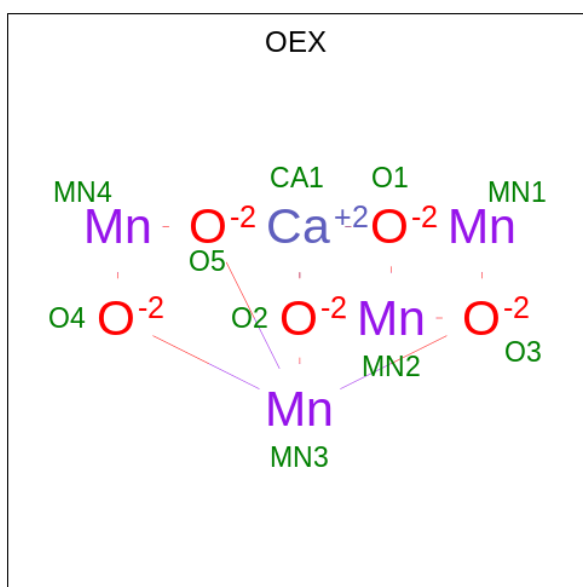
Mol	Chain	Residues	Atoms				AltConf
22	1a	1	Total	C	O	P	0
			32	21	10	1	
22	1a	1	Total	C	O	P	0
			41	30	10	1	
22	1b	1	Total	C	O	P	0
			27	18	8	1	
22	1b	1	Total	C	O	P	0
			36	25	10	1	
22	1b	1	Total	C	O	P	0
			45	34	10	1	
22	1b	1	Total	C	O	P	0
			49	38	10	1	
22	1c	1	Total	C	O	P	0
			29	20	8	1	

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Mol	Chain	Residues	Atoms				AltConf
22	1c	1	Total	C	O	P	0
			42	31	10	1	
22	1d	1	Total	C	O	P	0
			39	28	10	1	
22	1d	1	Total	C	O	P	0
			38	27	10	1	
22	1e	1	Total	C	O	P	0
			42	31	10	1	
22	1j	1	Total	C	O	P	0
			41	30	10	1	
22	1v	1	Total	C	O	P	0
			41	30	10	1	
22	1w	1	Total	C	O	P	0
			35	26	8	1	
22	1w	1	Total	C	O	P	0
			42	31	10	1	
22	1w	1	Total	C	O	P	0
			37	27	9	1	

- Molecule 23 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
23	1a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 24 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest")

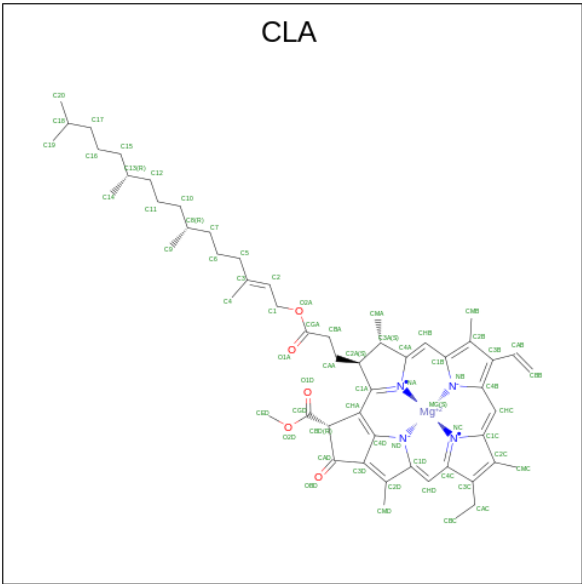
by depositor).

Mol	Chain	Residues	Atoms		AltConf
24	1a	1	Total	Fe	0
			1	1	

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
25	1a	1	Total	Cl	0
			1	1	
25	1c	1	Total	Cl	0
			1	1	

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	1a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
26	1a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	1a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	1b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	1b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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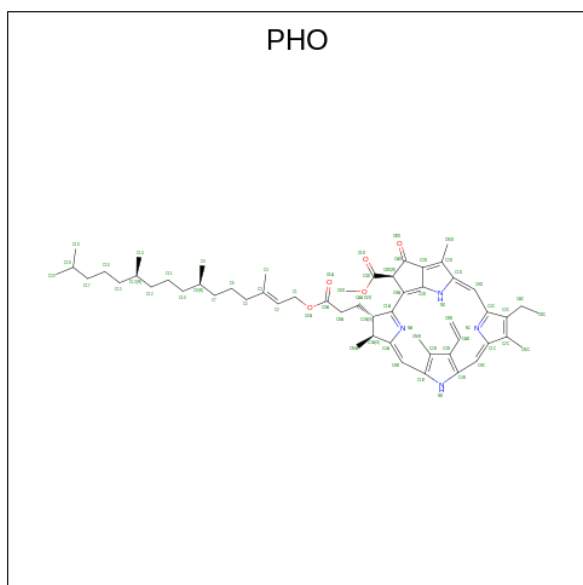
Mol	Chain	Residues	Atoms					AltConf
26	1b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	1b	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	1b	1	Total 58	C 48	Mg 1	N 4	O 5	0
26	1b	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	1b	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	1b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	1b	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	1b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	1b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	1b	1	Total 58	C 48	Mg 1	N 4	O 5	0
26	1b	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	1b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	1b	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	1b	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	1c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	1c	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	1c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	1c	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	1c	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	1c	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	1c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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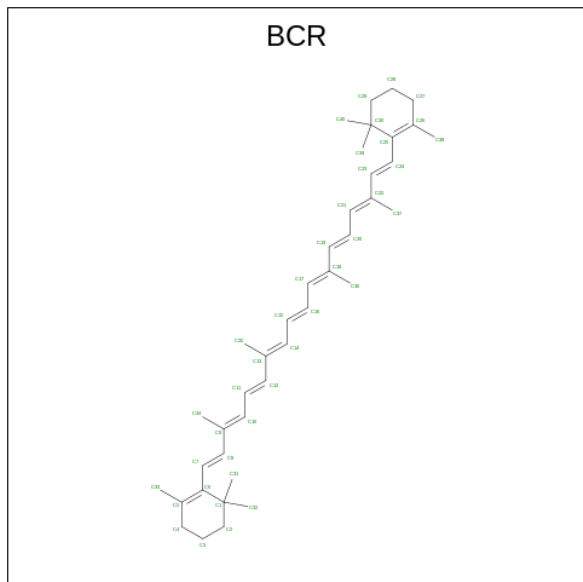
Mol	Chain	Residues	Atoms					AltConf
26	1c	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	1c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	1c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	1c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	1c	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	1c	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	1d	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	1d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	1d	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
27	1a	1	Total	C	N	O	0
			40	33	4	3	
27	1d	1	Total	C	N	O	0
			64	55	4	5	

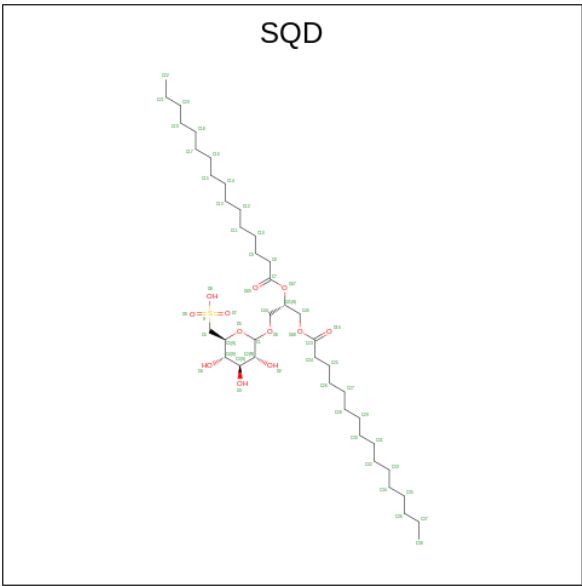
- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
28	1a	1	Total C 40 40	0
28	1b	1	Total C 40 40	0
28	1b	1	Total C 40 40	0
28	1b	1	Total C 40 40	0
28	1c	1	Total C 40 40	0
28	1d	1	Total C 40 40	0
28	1h	1	Total C 40 40	0
28	1i	1	Total C 40 40	0
28	1j	1	Total C 40 40	0
28	1k	1	Total C 40 40	0
28	1t	1	Total C 40 40	0

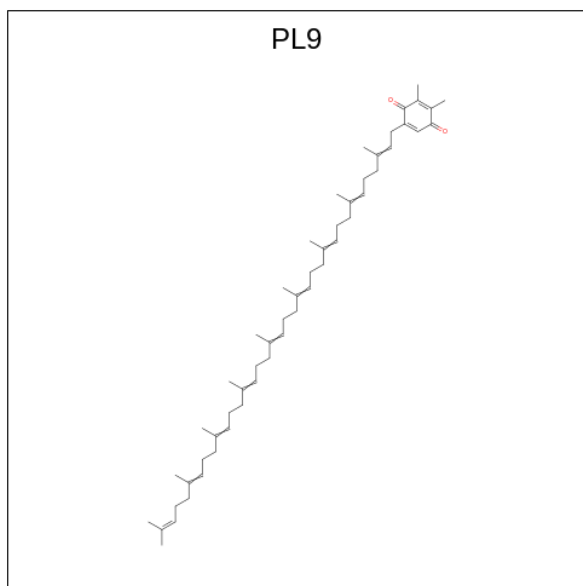
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest")

by depositor).



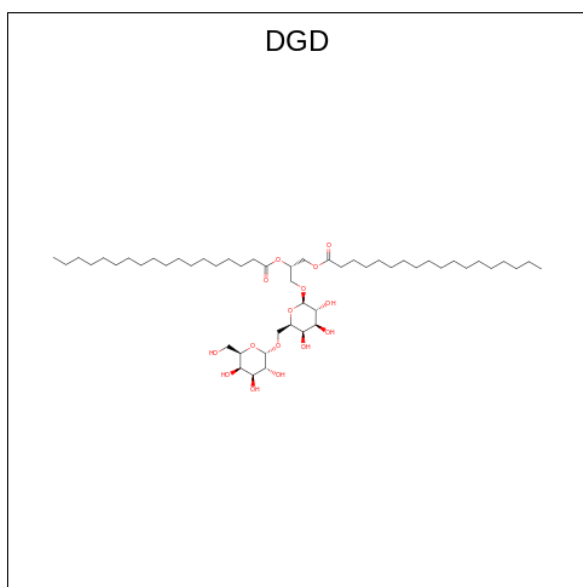
Mol	Chain	Residues	Atoms				AltConf
29	1a	1	Total	C	O	S	0
			50	37	12	1	
29	1a	1	Total	C	O	S	0
			54	41	12	1	
29	1a	1	Total	C	O	S	0
			46	33	12	1	
29	1b	1	Total	C	O	S	0
			53	40	12	1	
29	1b	1	Total	C	O	S	0
			54	41	12	1	
29	1b	1	Total	C	O	S	0
			48	35	12	1	
29	1c	1	Total	C	O	S	0
			54	41	12	1	
29	1c	1	Total	C	O	S	0
			44	31	12	1	
29	1d	1	Total	C	O	S	0
			48	35	12	1	
29	1d	1	Total	C	O	S	0
			39	26	12	1	
29	1i	1	Total	C	O	S	0
			40	27	12	1	
29	1l	1	Total	C	O	S	0
			42	29	12	1	
29	1w	1	Total	C	O	S	0
			40	27	12	1	

- Molecule 30 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



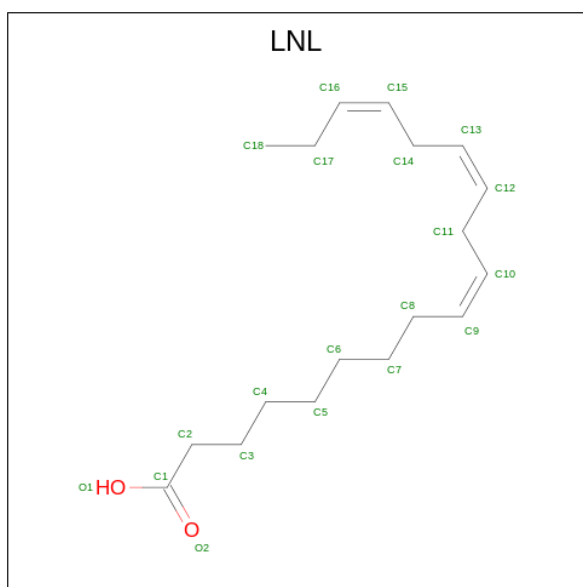
Mol	Chain	Residues	Atoms			AltConf
30	1a	1	Total	C	O	0
			55	53	2	
30	1d	1	Total	C	O	0
			55	53	2	
30	1e	1	Total	C	O	0
			21	19	2	
30	1h	1	Total	C	O	0
			55	53	2	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



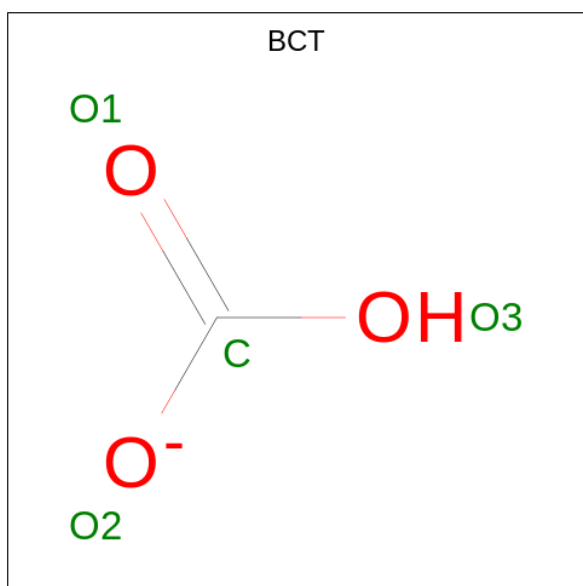
Mol	Chain	Residues	Atoms			AltConf
31	1b	1	Total	C	O	0
			55	40	15	
31	1b	1	Total	C	O	0
			62	47	15	
31	1c	1	Total	C	O	0
			47	32	15	
31	1c	1	Total	C	O	0
			52	37	15	
31	1c	1	Total	C	O	0
			57	42	15	

- Molecule 32 is ALPHA-LINOLENIC ACID (CCD ID: LNL) (formula: C₁₈H₃₀O₂) (labeled as "Ligand of Interest" by depositor).



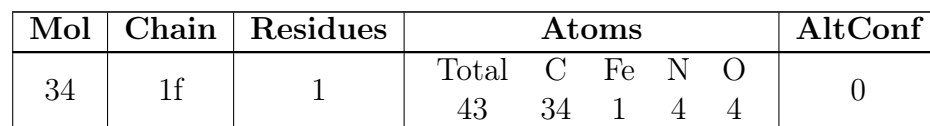
Mol	Chain	Residues	Atoms			AltConf
32	1c	1	Total	C	O	0
			17	15	2	

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).

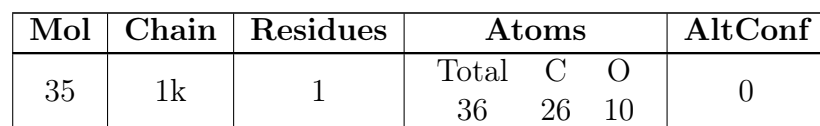


Mol	Chain	Residues	Atoms			AltConf
33	1d	1	Total	C	O	0
			4	1	3	

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



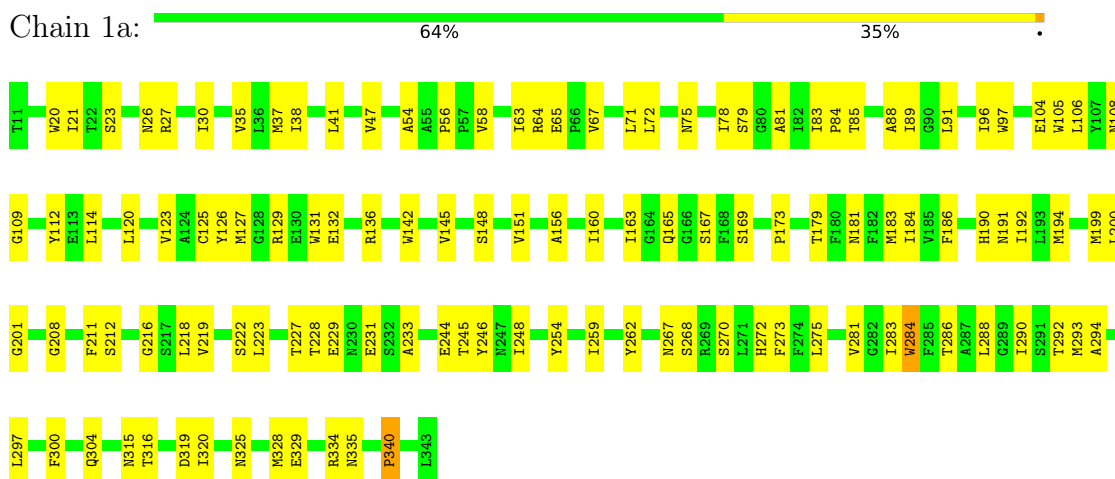
- Molecule 35 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: C₃₈H₇₂O₁₀) (labeled as "Ligand of Interest" by depositor).



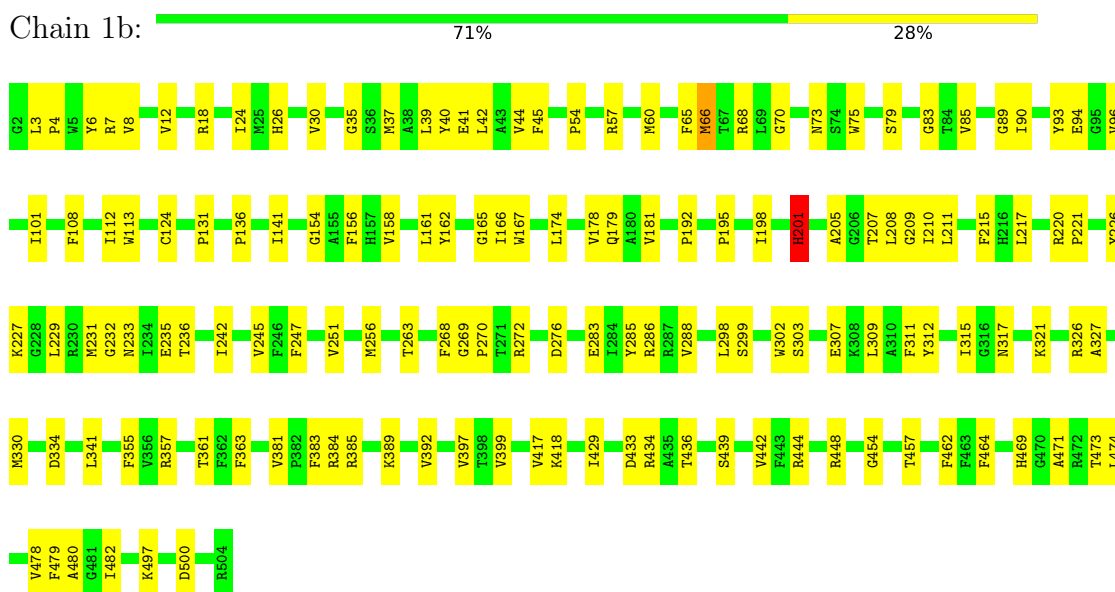
3 Residue-property plots

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.

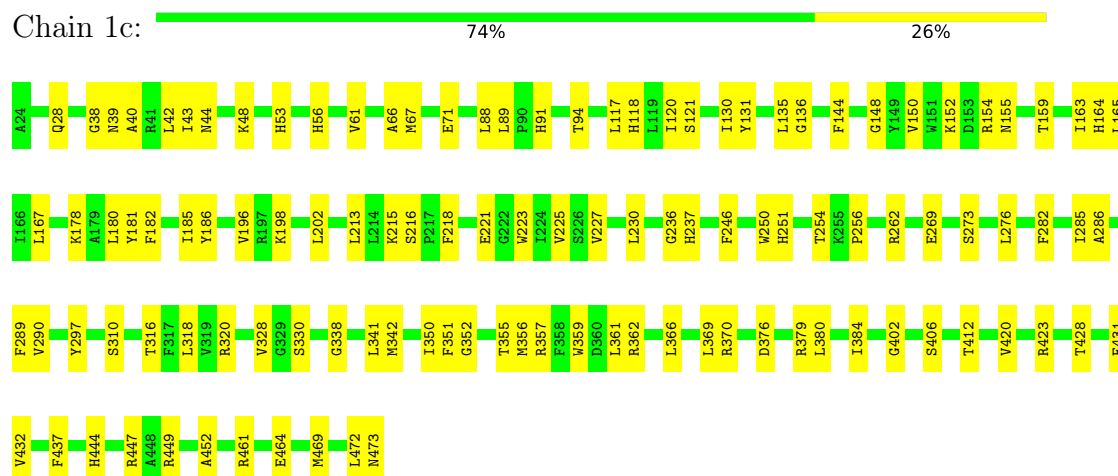
• Molecule 1: Photosystem II protein D1



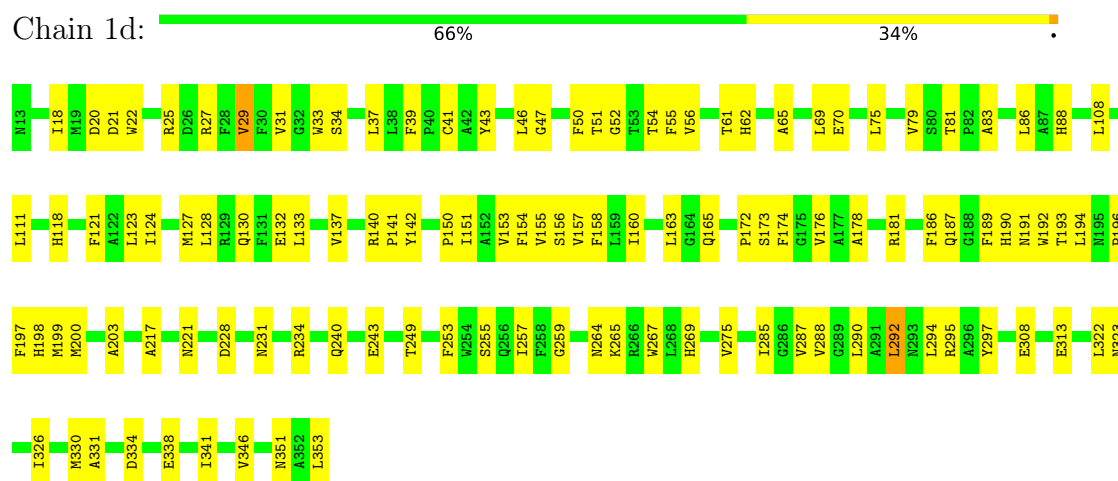
• Molecule 2: Photosystem II CP47 reaction center protein



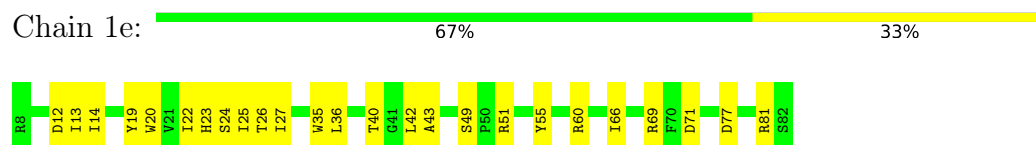
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 4: Photosystem II D2 protein



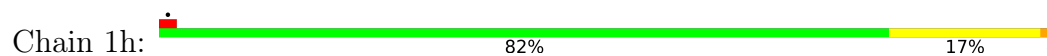
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 6: Cytochrome b559 subunit beta



• Molecule 7: Photosystem II reaction center protein H





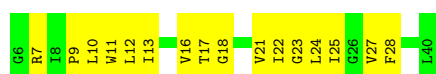
- Molecule 8: Photosystem II reaction center protein I

Chain 1i: 56% 44%



- Molecule 9: Photosystem II reaction center protein J

Chain 1j: 54% 46%



- Molecule 10: Photosystem II reaction center protein K

Chain 1k: 62% 35%



- Molecule 11: Photosystem II reaction center protein L

Chain 1l: 62% 32% 5%



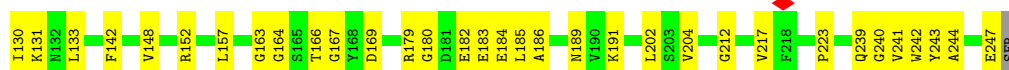
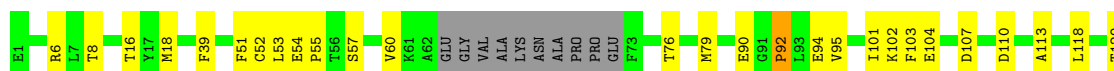
- Molecule 12: Photosystem II reaction center protein M

Chain 1m: 68% 29%

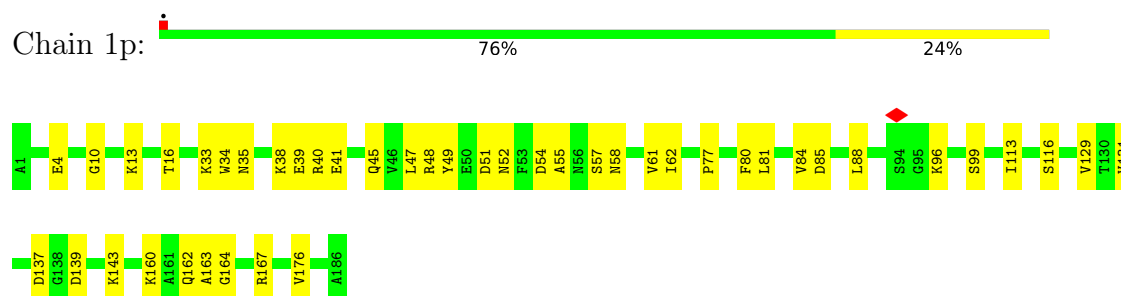


- Molecule 13: 33 kDa subunit of oxygen evolving system of photosystem II

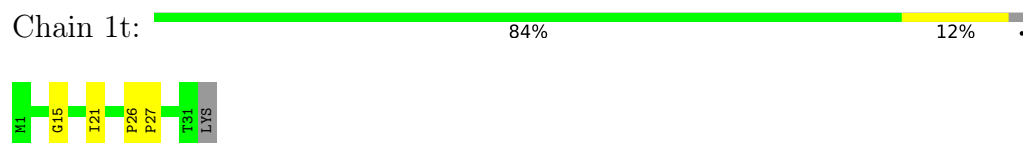
Chain 1o: 71% 24%



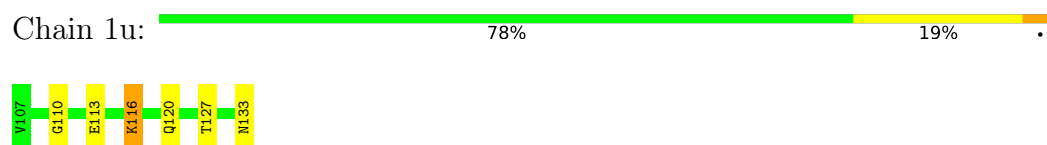
- Molecule 14: 23 kDa subunit of oxygen evolving system of photosystem II



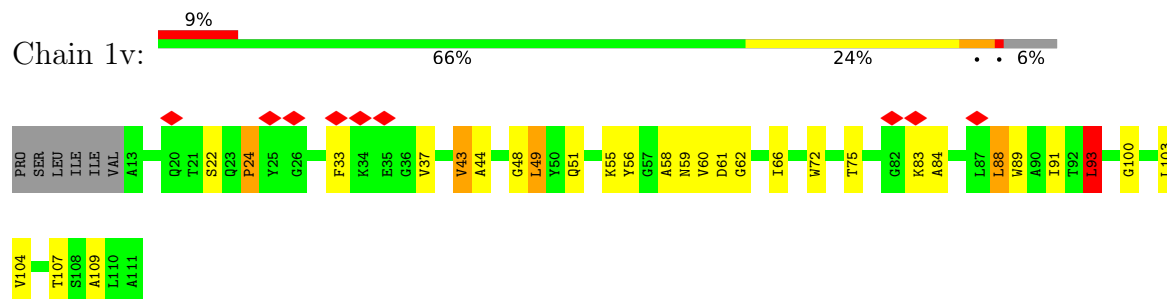
- Molecule 15: Photosystem II reaction center protein T



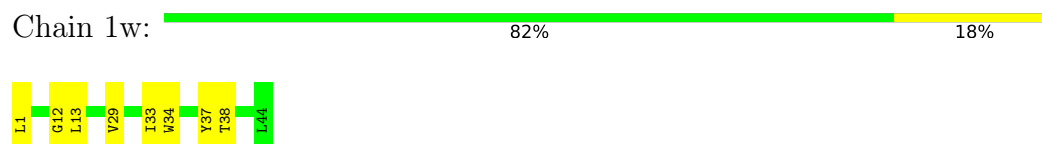
- Molecule 16: Os02g0581100 protein



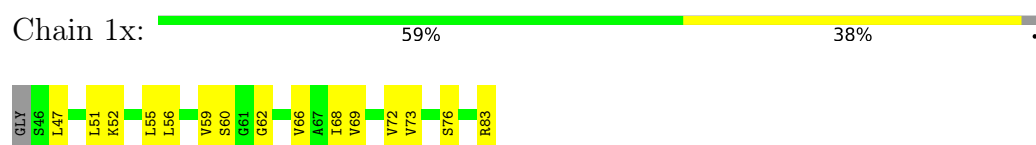
- Molecule 17: Photosystem II 10 kDa polypeptide, chloroplastic



- Molecule 18: Photosystem II reaction center W protein, chloroplastic

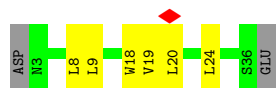


- Molecule 19: Os07g0673550 protein



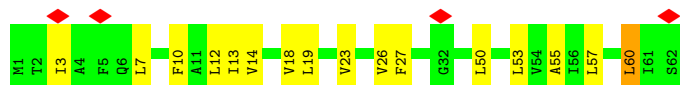
• Molecule 20: Os08g0119800 protein

Chain 1y:  78% 17% 6%



• Molecule 21: Photosystem II reaction center protein Z

Chain 1z:  6% 74% 24%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	173752	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	0.451	Depositor
Minimum map value	-0.243	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	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: PHO, OEX, SQD, HEM, PL9, DGD, BCT, LNL, LHG, MGE, BCR, FE2, CLA, CL

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	1a	0.31	0/2687	0.58	2/3665 (0.1%)
2	1b	0.26	0/4077	0.52	3/5551 (0.1%)
3	1c	0.25	0/3615	0.50	0/4922
4	1d	0.29	0/2809	0.58	2/3829 (0.1%)
5	1e	0.24	0/632	0.52	0/860
6	1f	0.22	0/248	0.46	0/335
7	1h	0.26	0/464	0.62	0/630
8	1i	0.26	0/285	0.60	0/385
9	1j	0.30	0/261	0.71	1/353 (0.3%)
10	1k	0.25	0/317	0.51	0/433
11	1l	0.29	0/303	0.61	0/412
12	1m	0.32	0/255	0.64	0/350
13	1o	0.24	0/1829	0.52	0/2470
14	1p	0.19	0/1452	0.43	0/1961
15	1t	0.17	0/260	0.37	0/354
16	1u	0.21	0/211	0.63	1/281 (0.4%)
17	1v	0.28	0/697	0.68	2/952 (0.2%)
18	1w	0.23	0/339	0.57	0/462
19	1x	0.23	0/275	0.48	0/375
20	1y	0.25	0/273	0.56	0/373
21	1z	0.23	0/476	0.51	0/652
All	All	0.26	0/21765	0.54	11/29605 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1a	0	1
2	1b	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	1o	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1b	201	HIS	CB-CA-C	7.84	122.24	109.07
2	1b	201	HIS	CA-CB-CG	7.61	121.41	113.80
2	1b	192	PRO	CA-N-CD	-7.53	101.46	112.00
1	1a	320	ILE	N-CA-C	-6.73	107.32	113.71
1	1a	284	TRP	CA-CB-CG	5.79	124.59	113.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1a	340	PRO	Peptide
2	1b	201	HIS	Sidechain
13	1o	92	PRO	Peptide

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	1a	2606	0	2517	114	0
2	1b	3945	0	3810	112	0
3	1c	3498	0	3421	94	0
4	1d	2716	0	2604	109	0
5	1e	614	0	592	28	0
6	1f	241	0	246	13	0
7	1h	454	0	473	10	0
8	1i	277	0	289	14	0
9	1j	255	0	265	12	0
10	1k	305	0	311	13	0
11	1l	295	0	284	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	1m	251	0	274	8	0
13	1o	1795	0	1783	39	0
14	1p	1422	0	1384	31	0
15	1t	252	0	267	4	0
16	1u	208	0	221	6	0
17	1v	683	0	648	27	0
18	1w	333	0	332	9	0
19	1x	272	0	300	10	0
20	1y	268	0	290	4	0
21	1z	466	0	494	13	0
22	1a	73	0	86	13	0
22	1b	157	0	204	14	0
22	1c	71	0	86	5	0
22	1d	77	0	97	4	0
22	1e	42	0	57	4	0
22	1j	41	0	52	2	0
22	1v	41	0	52	3	0
22	1w	114	0	147	8	0
23	1a	10	0	0	0	0
24	1a	1	0	0	0	0
25	1a	1	0	0	1	0
25	1c	1	0	0	0	0
26	1a	162	0	141	6	0
26	1b	940	0	935	45	0
26	1c	751	0	731	44	0
26	1d	174	0	166	11	0
27	1a	40	0	31	1	0
27	1d	64	0	74	6	0
28	1a	40	0	56	5	0
28	1b	120	0	168	16	0
28	1c	40	0	56	6	0
28	1d	40	0	56	1	0
28	1h	40	0	56	3	0
28	1i	40	0	56	7	0
28	1j	40	0	56	5	0
28	1k	40	0	56	4	0
28	1t	40	0	56	5	0
29	1a	150	0	201	9	0
29	1b	155	0	211	18	0
29	1c	98	0	130	8	0
29	1d	87	0	105	6	0
29	1i	40	0	44	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	1l	42	0	48	4	0
29	1w	40	0	44	3	0
30	1a	55	0	80	21	0
30	1d	55	0	80	7	0
30	1e	21	0	23	9	0
30	1h	55	0	80	4	0
31	1b	117	0	150	8	0
31	1c	156	0	186	8	0
32	1c	17	0	22	4	0
33	1d	4	0	0	0	0
34	1f	43	0	30	6	0
35	1k	36	0	42	5	0
All	All	25527	0	25756	719	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 14.

The worst 5 of 719 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)
30:1a:413:PL9:H312	27:1d:404:PHO:H2	1.55	0.88
30:1a:413:PL9:H503	4:1d:39:PHE:HB2	1.67	0.76
2:1b:141:ILE:HG13	2:1b:217:LEU:HD21	1.70	0.72
13:1o:130:ILE:HD11	13:1o:133:LEU:HD22	1.71	0.71
1:1a:186:PHE:HB3	1:1a:192:ILE:HD11	1.71	0.71

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	1a	331/333 (99%)	313 (95%)	18 (5%)	0	100	100
2	1b	501/503 (100%)	486 (97%)	15 (3%)	0	100	100
3	1c	448/450 (100%)	428 (96%)	17 (4%)	3 (1%)	18	44
4	1d	339/341 (99%)	316 (93%)	23 (7%)	0	100	100
5	1e	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
6	1f	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
7	1h	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
8	1i	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
9	1j	33/35 (94%)	33 (100%)	0	0	100	100
10	1k	35/37 (95%)	34 (97%)	0	1 (3%)	3	11
11	1l	33/37 (89%)	33 (100%)	0	0	100	100
12	1m	31/34 (91%)	31 (100%)	0	0	100	100
13	1o	233/248 (94%)	208 (89%)	25 (11%)	0	100	100
14	1p	184/186 (99%)	170 (92%)	14 (8%)	0	100	100
15	1t	29/32 (91%)	29 (100%)	0	0	100	100
16	1u	25/27 (93%)	22 (88%)	3 (12%)	0	100	100
17	1v	97/105 (92%)	81 (84%)	12 (12%)	4 (4%)	2	6
18	1w	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
19	1x	36/39 (92%)	34 (94%)	2 (6%)	0	100	100
20	1y	32/36 (89%)	32 (100%)	0	0	100	100
21	1z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	2680/2749 (98%)	2530 (94%)	142 (5%)	8 (0%)	37	63

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1c	43	ILE
3	1c	384	ILE
10	1k	40	MET
17	1v	43	VAL
17	1v	51	GLN

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	1a	270/270 (100%)	269 (100%)	1 (0%)	84	93
2	1b	402/402 (100%)	400 (100%)	2 (0%)	81	92
3	1c	349/350 (100%)	348 (100%)	1 (0%)	86	94
4	1d	275/275 (100%)	274 (100%)	1 (0%)	84	93
5	1e	68/68 (100%)	68 (100%)	0	100	100
6	1f	25/26 (96%)	25 (100%)	0	100	100
7	1h	49/49 (100%)	48 (98%)	1 (2%)	48	77
8	1i	31/31 (100%)	31 (100%)	0	100	100
9	1j	26/26 (100%)	26 (100%)	0	100	100
10	1k	32/32 (100%)	32 (100%)	0	100	100
11	1l	33/35 (94%)	33 (100%)	0	100	100
12	1m	27/30 (90%)	27 (100%)	0	100	100
13	1o	196/204 (96%)	195 (100%)	1 (0%)	81	92
14	1p	149/149 (100%)	149 (100%)	0	100	100
15	1t	28/29 (97%)	28 (100%)	0	100	100
16	1u	23/23 (100%)	23 (100%)	0	100	100
17	1v	62/77 (80%)	60 (97%)	2 (3%)	34	67
18	1w	35/38 (92%)	35 (100%)	0	100	100
19	1x	32/32 (100%)	32 (100%)	0	100	100
20	1y	28/30 (93%)	27 (96%)	1 (4%)	31	63
21	1z	54/54 (100%)	53 (98%)	1 (2%)	50	78
All	All	2194/2230 (98%)	2183 (100%)	11 (0%)	78	92

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	1v	49	LEU
17	1v	93	LEU

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Mol	Chain	Res	Type
21	1z	60	LEU
20	1y	9	LEU
4	1d	292	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
4	1d	302	GLN
6	1f	38	GLN
16	1u	132	HIS
5	1e	61	GLN
11	1l	7	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 94 ligands modelled in this entry, 3 are monoatomic - leaving 91 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
26	CLA	1b	606	2	54,58,73	2.41	19 (35%)	65,95,113	3.24	31 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	1b	619	-	41,41,41	1.65	8 (19%)	56,56,56	1.81	16 (28%)
26	CLA	1b	608	2	69,73,73	2.04	16 (23%)	83,113,113	2.67	28 (33%)
31	DGD	1c	518	-	48,48,67	0.99	2 (4%)	62,62,81	1.20	7 (11%)
28	BCR	1b	618	-	41,41,41	1.69	8 (19%)	56,56,56	1.73	15 (26%)
22	LHG	1d	402	-	37,37,48	0.33	0	40,43,54	0.38	0
22	LHG	1c	521	-	28,28,48	0.37	0	31,33,54	0.44	0
28	BCR	1j	101	-	41,41,41	1.79	8 (19%)	56,56,56	2.11	15 (26%)
26	CLA	1b	614	2	69,73,73	2.13	20 (28%)	83,113,113	2.83	30 (36%)
26	CLA	1b	612	-	62,66,73	2.16	19 (30%)	74,104,113	2.98	33 (44%)
27	PHO	1d	404	-	58,69,69	0.82	2 (3%)	56,99,99	1.06	5 (8%)
31	DGD	1b	627	-	63,63,67	0.85	2 (3%)	77,77,81	0.91	2 (2%)
33	BCT	1d	408	24	2,3,3	0.98	0	2,3,3	0.37	0
28	BCR	1b	617	-	41,41,41	1.67	12 (29%)	56,56,56	1.58	12 (21%)
22	LHG	1w	102	-	34,34,48	0.33	0	37,39,54	0.40	0
29	SQD	1l	101	-	41,42,54	0.44	1 (2%)	50,53,65	0.76	2 (4%)
26	CLA	1a	406	-	54,58,73	2.42	19 (35%)	65,95,113	3.26	31 (47%)
30	PL9	1a	413	-	55,55,55	0.58	1 (1%)	68,69,69	1.85	20 (29%)
29	SQD	1a	412	-	45,46,54	0.41	1 (2%)	54,57,65	0.52	1 (1%)
26	CLA	1b	613	2	64,68,73	2.28	21 (32%)	77,107,113	3.29	31 (40%)
26	CLA	1c	509	3	63,67,73	2.11	17 (26%)	75,105,113	2.95	31 (41%)
31	DGD	1c	519	-	53,53,67	0.92	2 (3%)	67,67,81	1.05	5 (7%)
22	LHG	1e	102	-	41,41,48	0.29	0	44,47,54	0.39	0
26	CLA	1b	610	-	69,73,73	2.13	20 (28%)	83,113,113	2.93	29 (34%)
26	CLA	1c	511	3	69,73,73	2.12	19 (27%)	83,113,113	2.87	27 (32%)
31	DGD	1c	520	-	58,58,67	0.90	2 (3%)	72,72,81	0.91	3 (4%)
28	BCR	1d	409	-	41,41,41	1.80	10 (24%)	56,56,56	1.89	17 (30%)
22	LHG	1a	401	-	31,31,48	0.34	0	34,37,54	0.48	0
30	PL9	1h	101	-	55,55,55	0.66	1 (1%)	68,69,69	0.86	4 (5%)
28	BCR	1a	409	-	41,41,41	1.73	8 (19%)	56,56,56	1.65	13 (23%)
22	LHG	1w	104	-	36,36,48	0.46	0	38,41,54	0.37	0
26	CLA	1c	510	3	49,53,73	2.55	20 (40%)	59,89,113	3.32	27 (45%)
26	CLA	1a	405	1	56,60,73	2.29	18 (32%)	67,97,113	3.14	31 (46%)
30	PL9	1d	410	-	55,55,55	0.78	1 (1%)	68,69,69	0.53	1 (1%)
22	LHG	1j	102	-	40,40,48	0.29	0	43,46,54	0.78	1 (2%)
26	CLA	1c	513	-	65,69,73	2.11	18 (27%)	78,108,113	3.02	30 (38%)
22	LHG	1d	401	-	38,38,48	0.30	0	41,44,54	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HEM	1f	101	6	50,50,50	1.57	7 (14%)	66,82,82	1.64	11 (16%)
26	CLA	1c	503	-	64,68,73	2.12	19 (29%)	77,107,113	2.97	30 (38%)
26	CLA	1c	502	3	69,73,73	2.13	19 (27%)	83,113,113	2.87	29 (34%)
23	OEX	1a	402	3,1	0,14,14	-	-	-	-	-
26	CLA	1c	504	3	69,73,73	2.07	20 (28%)	83,113,113	2.91	31 (37%)
26	CLA	1b	611	2	69,73,73	2.01	17 (24%)	83,113,113	2.70	29 (34%)
26	CLA	1b	604	2	46,50,73	2.48	18 (39%)	55,85,113	3.42	29 (52%)
29	SQD	1d	405	-	47,48,54	0.42	1 (2%)	56,59,65	0.65	2 (3%)
31	DGD	1b	623	-	56,56,67	0.90	2 (3%)	70,70,81	0.95	3 (4%)
26	CLA	1c	506	3	56,60,73	2.32	20 (35%)	67,97,113	3.14	31 (46%)
22	LHG	1c	522	-	41,41,48	0.29	0	44,47,54	0.39	0
26	CLA	1a	408	1	64,68,73	2.16	19 (29%)	77,107,113	2.93	30 (38%)
22	LHG	1b	628	-	48,48,48	0.27	0	51,54,54	0.32	0
29	SQD	1i	102	-	39,40,54	0.44	1 (2%)	48,51,65	0.39	0
29	SQD	1d	411	-	38,39,54	0.48	1 (2%)	47,50,65	0.65	2 (4%)
32	LNL	1c	523	-	16,16,19	0.61	0	15,16,19	0.63	0
22	LHG	1w	103	-	41,41,48	0.30	0	44,47,54	0.33	0
35	MGE	1k	101	-	36,36,48	0.29	0	44,44,56	0.59	0
27	PHO	1a	407	-	34,45,69	1.05	2 (5%)	28,70,99	1.48	5 (17%)
22	LHG	1v	201	-	40,40,48	0.29	0	43,46,54	0.39	0
30	PL9	1e	101	-	21,21,55	0.87	1 (4%)	27,28,69	1.82	7 (25%)
26	CLA	1d	403	-	63,67,73	2.23	19 (30%)	75,105,113	3.13	30 (40%)
29	SQD	1a	411	-	53,54,54	0.39	1 (1%)	62,65,65	0.47	1 (1%)
28	BCR	1c	515	-	41,41,41	1.72	8 (19%)	56,56,56	1.68	17 (30%)
26	CLA	1d	406	4	64,68,73	2.15	18 (28%)	77,107,113	2.94	32 (41%)
26	CLA	1b	602	2	60,64,73	2.19	16 (26%)	72,102,113	3.07	30 (41%)
26	CLA	1b	601	-	69,73,73	2.16	19 (27%)	83,113,113	2.81	27 (32%)
26	CLA	1b	605	2	62,66,73	2.21	18 (29%)	74,104,113	3.21	32 (43%)
29	SQD	1b	620	-	52,53,54	0.39	1 (1%)	61,64,65	0.64	1 (1%)
28	BCR	1h	102	-	41,41,41	1.79	10 (24%)	56,56,56	2.06	17 (30%)
26	CLA	1b	603	-	69,73,73	2.07	18 (26%)	83,113,113	2.63	25 (30%)
26	CLA	1c	505	-	59,63,73	2.25	20 (33%)	71,101,113	2.99	29 (40%)
29	SQD	1b	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.88	3 (4%)
26	CLA	1c	508	-	69,73,73	2.14	20 (28%)	83,113,113	2.90	30 (36%)
29	SQD	1a	410	-	49,50,54	0.40	1 (2%)	58,61,65	0.93	3 (5%)
29	SQD	1b	622	-	47,48,54	0.42	1 (2%)	56,59,65	0.58	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SQD	1w	101	-	39,40,54	0.43	1 (2%)	48,51,65	0.71	1 (2%)
22	LHG	1b	624	-	26,26,48	0.38	0	29,31,54	0.92	2 (6%)
28	BCR	1k	102	-	41,41,41	1.81	8 (19%)	56,56,56	1.83	13 (23%)
26	CLA	1b	607	-	63,67,73	2.16	19 (30%)	75,105,113	2.92	32 (42%)
26	CLA	1c	507	3	59,63,73	2.27	18 (30%)	71,101,113	2.92	27 (38%)
22	LHG	1b	625	-	35,35,48	0.31	0	38,41,54	0.53	0
26	CLA	1b	609	2	65,69,73	2.12	18 (27%)	78,108,113	2.99	30 (38%)
29	SQD	1c	517	-	43,44,54	0.44	1 (2%)	52,55,65	0.48	0
26	CLA	1c	512	3	49,53,73	2.49	20 (40%)	59,89,113	3.40	28 (47%)
28	BCR	1i	101	-	41,41,41	1.70	8 (19%)	56,56,56	1.61	11 (19%)
26	CLA	1b	615	-	65,69,73	2.16	18 (27%)	78,108,113	3.03	29 (37%)
22	LHG	1a	414	-	40,40,48	1.01	2 (5%)	43,46,54	1.10	3 (6%)
29	SQD	1c	516	-	53,54,54	0.39	1 (1%)	62,65,65	0.88	4 (6%)
22	LHG	1b	626	-	44,44,48	0.29	0	47,50,54	0.34	0
26	CLA	1d	407	4	59,63,73	2.28	20 (33%)	71,101,113	3.11	30 (42%)
26	CLA	1c	514	3	63,67,73	2.23	20 (31%)	75,105,113	3.04	30 (40%)
28	BCR	1t	101	-	41,41,41	1.68	9 (21%)	56,56,56	1.83	15 (26%)
26	CLA	1b	616	-	49,53,73	2.49	19 (38%)	59,89,113	3.29	26 (44%)

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
26	CLA	1b	606	2	-	4/21/97/115	-
28	BCR	1b	619	-	-	2/29/63/63	0/2/2/2
26	CLA	1b	608	2	1/1/15/20	4/39/115/115	-
31	DGD	1c	518	-	-	8/36/76/95	0/2/2/2
28	BCR	1b	618	-	-	4/29/63/63	0/2/2/2
22	LHG	1d	402	-	-	3/42/42/53	-
22	LHG	1c	521	-	-	4/32/32/53	-
28	BCR	1j	101	-	-	5/29/63/63	0/2/2/2
26	CLA	1b	614	2	1/1/15/20	14/39/115/115	-
26	CLA	1b	612	-	1/1/13/20	18/31/107/115	-
27	PHO	1d	404	-	-	3/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	1b	627	-	-	9/51/91/95	0/2/2/2
28	BCR	1b	617	-	-	2/29/63/63	0/2/2/2
22	LHG	1w	102	-	-	10/38/38/53	-
29	SQD	1l	101	-	-	4/37/57/69	0/1/1/1
26	CLA	1a	406	-	-	3/21/97/115	-
30	PL9	1a	413	-	-	16/53/73/73	0/1/1/1
29	SQD	1a	412	-	-	3/41/61/69	0/1/1/1
26	CLA	1b	613	2	1/1/14/20	7/33/109/115	-
26	CLA	1c	509	3	1/1/13/20	6/32/108/115	-
31	DGD	1c	519	-	-	14/41/81/95	0/2/2/2
22	LHG	1e	102	-	-	10/46/46/53	-
26	CLA	1b	610	-	1/1/15/20	13/39/115/115	-
26	CLA	1c	511	3	1/1/15/20	12/39/115/115	-
31	DGD	1c	520	-	-	8/46/86/95	0/2/2/2
28	BCR	1d	409	-	-	4/29/63/63	0/2/2/2
22	LHG	1a	401	-	-	4/36/36/53	-
30	PL9	1h	101	-	-	13/53/73/73	0/1/1/1
28	BCR	1a	409	-	-	1/29/63/63	0/2/2/2
22	LHG	1w	104	-	-	10/40/40/53	-
26	CLA	1c	510	3	-	7/15/91/115	-
26	CLA	1a	405	1	-	6/24/100/115	-
30	PL9	1d	410	-	-	3/53/73/73	0/1/1/1
22	LHG	1j	102	-	-	14/45/45/53	-
26	CLA	1c	513	-	1/1/14/20	11/35/111/115	-
22	LHG	1d	401	-	-	10/43/43/53	-
34	HEM	1f	101	6	-	8/14/54/54	-
26	CLA	1c	503	-	1/1/14/20	11/33/109/115	-
26	CLA	1c	502	3	1/1/15/20	8/39/115/115	-
26	CLA	1c	504	3	1/1/15/20	15/39/115/115	-
26	CLA	1b	611	2	1/1/15/20	11/39/115/115	-
26	CLA	1b	604	2	-	1/12/88/115	-
29	SQD	1d	405	-	-	3/43/63/69	0/1/1/1
31	DGD	1b	623	-	-	10/44/84/95	0/2/2/2
26	CLA	1c	506	3	-	10/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	1a	408	1	1/1/14/20	5/33/109/115	-
22	LHG	1c	522	-	-	9/46/46/53	-
22	LHG	1b	628	-	-	3/53/53/53	-
29	SQD	1i	102	-	-	3/35/55/69	0/1/1/1
29	SQD	1d	411	-	-	0/34/54/69	0/1/1/1
32	LNL	1c	523	-	-	2/14/14/17	-
22	LHG	1w	103	-	-	7/46/46/53	-
35	MGE	1k	101	-	-	11/31/51/63	0/1/1/1
27	PHO	1a	407	-	-	1/8/74/103	0/5/6/6
22	LHG	1v	201	-	-	8/45/45/53	-
30	PL9	1e	101	-	-	4/13/33/73	0/1/1/1
26	CLA	1d	403	-	1/1/13/20	10/32/108/115	-
29	SQD	1a	411	-	-	8/49/69/69	0/1/1/1
28	BCR	1c	515	-	-	1/29/63/63	0/2/2/2
26	CLA	1d	406	4	1/1/14/20	7/33/109/115	-
26	CLA	1b	602	2	1/1/13/20	8/29/105/115	-
26	CLA	1b	601	-	1/1/15/20	6/39/115/115	-
26	CLA	1b	605	2	1/1/13/20	9/31/107/115	-
29	SQD	1b	620	-	-	10/48/68/69	0/1/1/1
28	BCR	1h	102	-	-	3/29/63/63	0/2/2/2
26	CLA	1b	603	-	1/1/15/20	9/39/115/115	-
26	CLA	1c	505	-	1/1/13/20	8/27/103/115	-
29	SQD	1b	621	-	-	7/49/69/69	0/1/1/1
26	CLA	1c	508	-	1/1/15/20	9/39/115/115	-
29	SQD	1a	410	-	-	9/45/65/69	0/1/1/1
29	SQD	1b	622	-	-	13/43/63/69	0/1/1/1
29	SQD	1w	101	-	-	5/35/55/69	0/1/1/1
22	LHG	1b	624	-	-	4/30/30/53	-
28	BCR	1k	102	-	-	5/29/63/63	0/2/2/2
26	CLA	1b	607	-	1/1/13/20	10/32/108/115	-
26	CLA	1c	507	3	1/1/13/20	14/27/103/115	-
22	LHG	1b	625	-	-	7/40/40/53	-
26	CLA	1b	609	2	1/1/14/20	10/35/111/115	-
29	SQD	1c	517	-	-	2/39/59/69	0/1/1/1
26	CLA	1c	512	3	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	1i	101	-	-	1/29/63/63	0/2/2/2
26	CLA	1b	615	-	1/1/14/20	10/35/111/115	-
22	LHG	1a	414	-	-	29/45/45/53	-
29	SQD	1c	516	-	-	3/49/69/69	0/1/1/1
26	CLA	1d	407	4	1/1/13/20	9/27/103/115	-
22	LHG	1b	626	-	-	7/49/49/53	-
26	CLA	1c	514	3	1/1/13/20	7/32/108/115	-
28	BCR	1t	101	-	-	2/29/63/63	0/2/2/2
26	CLA	1b	616	-	-	8/15/91/115	-

The worst 5 of 795 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1b	601	CLA	C1D-ND	8.88	1.48	1.37
26	1c	510	CLA	C1D-ND	8.86	1.48	1.37
26	1b	602	CLA	C1D-ND	8.77	1.48	1.37
26	1b	606	CLA	C1D-ND	8.66	1.48	1.37
26	1a	406	CLA	C1D-ND	8.63	1.48	1.37

The worst 5 of 1297 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1d	403	CLA	C1D-ND-C4D	-10.31	99.01	106.33
26	1b	613	CLA	C1D-ND-C4D	-10.30	99.02	106.33
26	1b	605	CLA	C1D-ND-C4D	-10.01	99.23	106.33
26	1c	514	CLA	C1D-ND-C4D	-9.83	99.36	106.33
26	1c	510	CLA	C2C-C1C-NC	9.68	119.04	109.97

5 of 27 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	1a	408	CLA	C8
26	1b	601	CLA	C8
26	1b	602	CLA	C8
26	1b	603	CLA	C8
26	1b	605	CLA	C8

5 of 652 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1a	414	LHG	C1-C2-C3-O3
22	1a	414	LHG	C4-O6-P-O3
22	1a	414	LHG	C4-O6-P-O4
22	1a	414	LHG	C4-O6-P-O5
22	1a	414	LHG	O9-C7-O7-C5

There are no ring outliers.

85 monomers are involved in 279 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	1b	619	BCR	3	0
26	1b	608	CLA	7	0
31	1c	518	DGD	1	0
28	1b	618	BCR	5	0
22	1d	402	LHG	2	0
22	1c	521	LHG	1	0
28	1j	101	BCR	5	0
26	1b	614	CLA	2	0
26	1b	612	CLA	3	0
27	1d	404	PHO	6	0
31	1b	627	DGD	4	0
28	1b	617	BCR	8	0
29	1l	101	SQD	4	0
26	1a	406	CLA	1	0
30	1a	413	PL9	21	0
29	1a	412	SQD	1	0
26	1b	613	CLA	5	0
26	1c	509	CLA	5	0
31	1c	519	DGD	5	0
22	1e	102	LHG	4	0
26	1b	610	CLA	2	0
26	1c	511	CLA	9	0
31	1c	520	DGD	3	0
28	1d	409	BCR	1	0
22	1a	401	LHG	2	0
30	1h	101	PL9	4	0
28	1a	409	BCR	5	0
22	1w	104	LHG	6	0
26	1c	510	CLA	3	0
26	1a	405	CLA	4	0
30	1d	410	PL9	7	0
22	1j	102	LHG	2	0
26	1c	513	CLA	2	0

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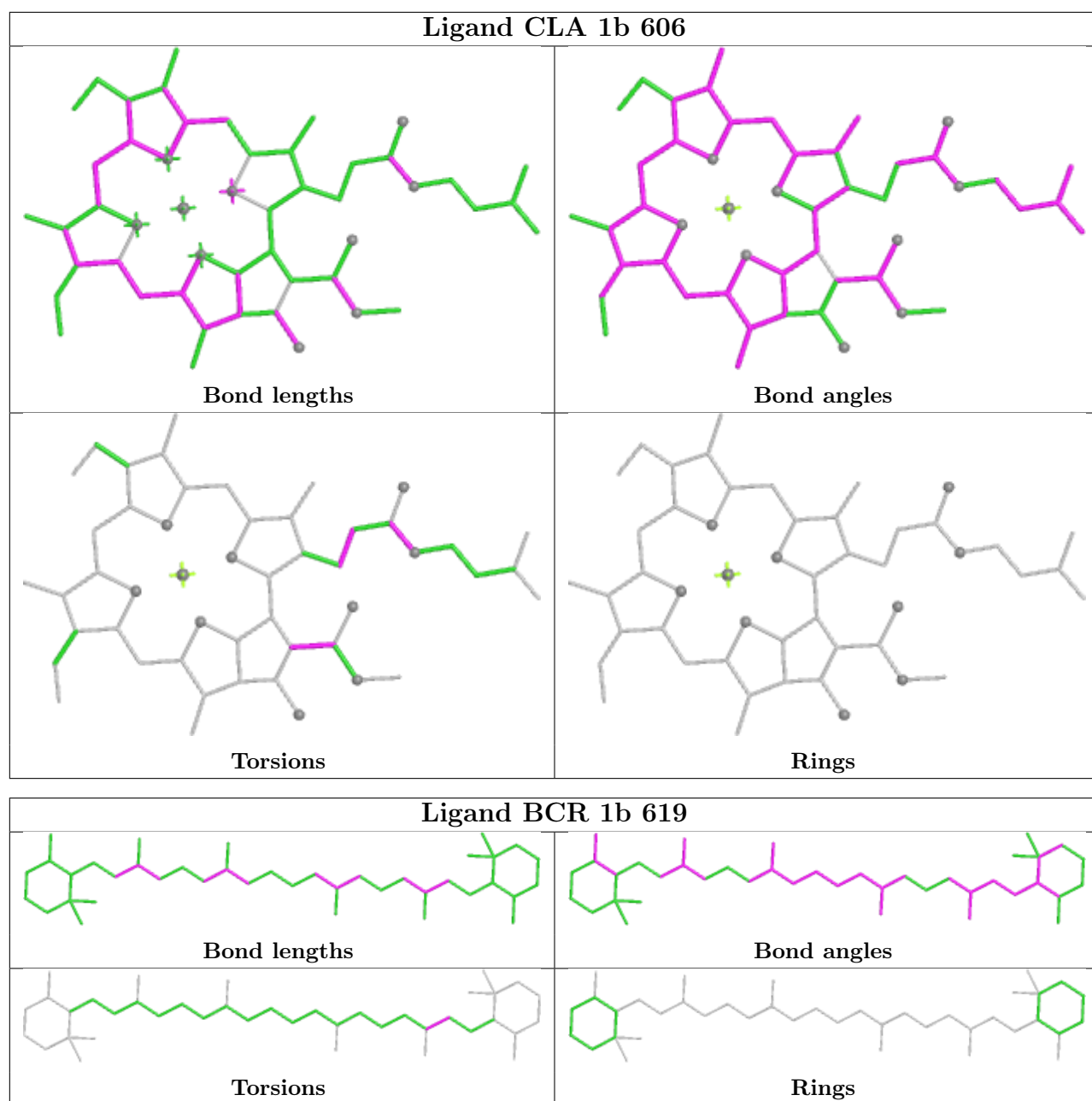
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1d	401	LHG	2	0
34	1f	101	HEM	6	0
26	1c	503	CLA	1	0
26	1c	502	CLA	4	0
26	1c	504	CLA	3	0
26	1b	611	CLA	8	0
26	1b	604	CLA	1	0
29	1d	405	SQD	4	0
31	1b	623	DGD	4	0
26	1c	506	CLA	2	0
22	1c	522	LHG	4	0
26	1a	408	CLA	1	0
22	1b	628	LHG	7	0
29	1i	102	SQD	3	0
29	1d	411	SQD	2	0
32	1c	523	LNL	4	0
22	1w	103	LHG	3	0
35	1k	101	MGE	5	0
27	1a	407	PHO	1	0
22	1v	201	LHG	3	0
30	1e	101	PL9	9	0
26	1d	403	CLA	2	0
29	1a	411	SQD	2	0
28	1c	515	BCR	6	0
26	1d	406	CLA	8	0
26	1b	602	CLA	4	0
26	1b	601	CLA	5	0
26	1b	605	CLA	3	0
29	1b	620	SQD	5	0
28	1h	102	BCR	3	0
26	1b	603	CLA	2	0
26	1c	505	CLA	2	0
29	1b	621	SQD	9	0
26	1c	508	CLA	9	0
29	1a	410	SQD	6	0
29	1b	622	SQD	4	0
29	1w	101	SQD	3	0
22	1b	624	LHG	1	0
28	1k	102	BCR	4	0
26	1b	607	CLA	5	0
26	1c	507	CLA	10	0
22	1b	625	LHG	3	0

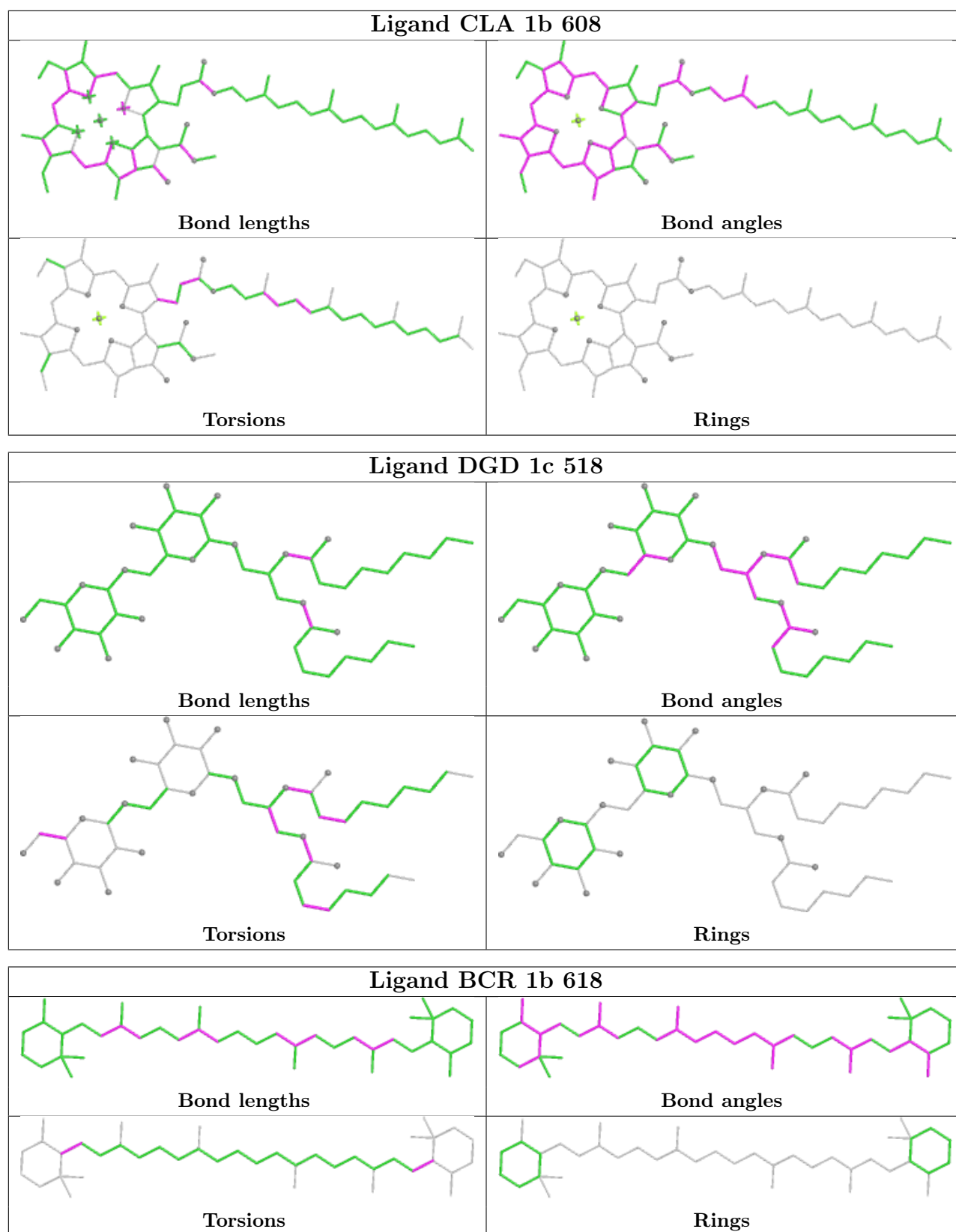
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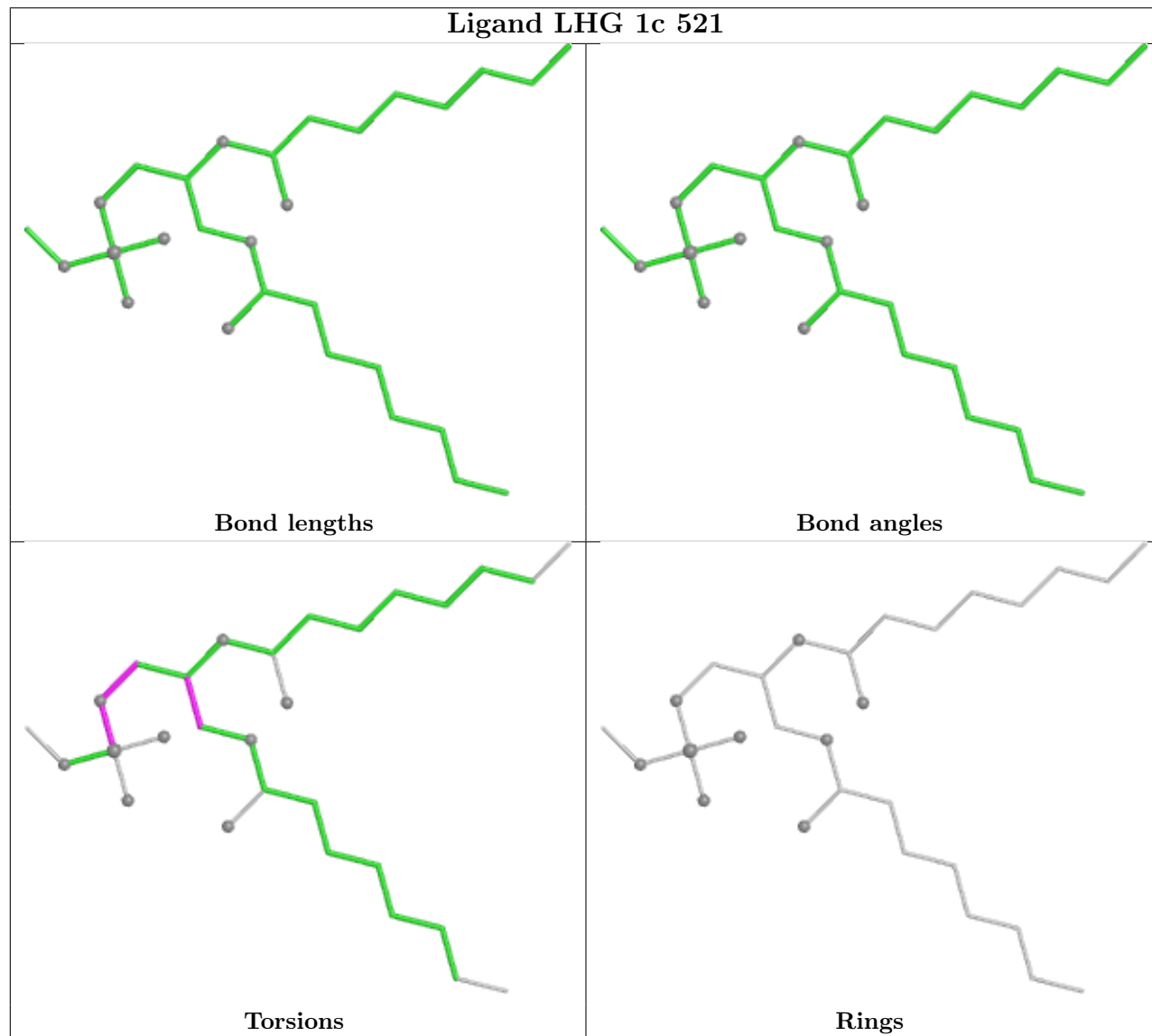
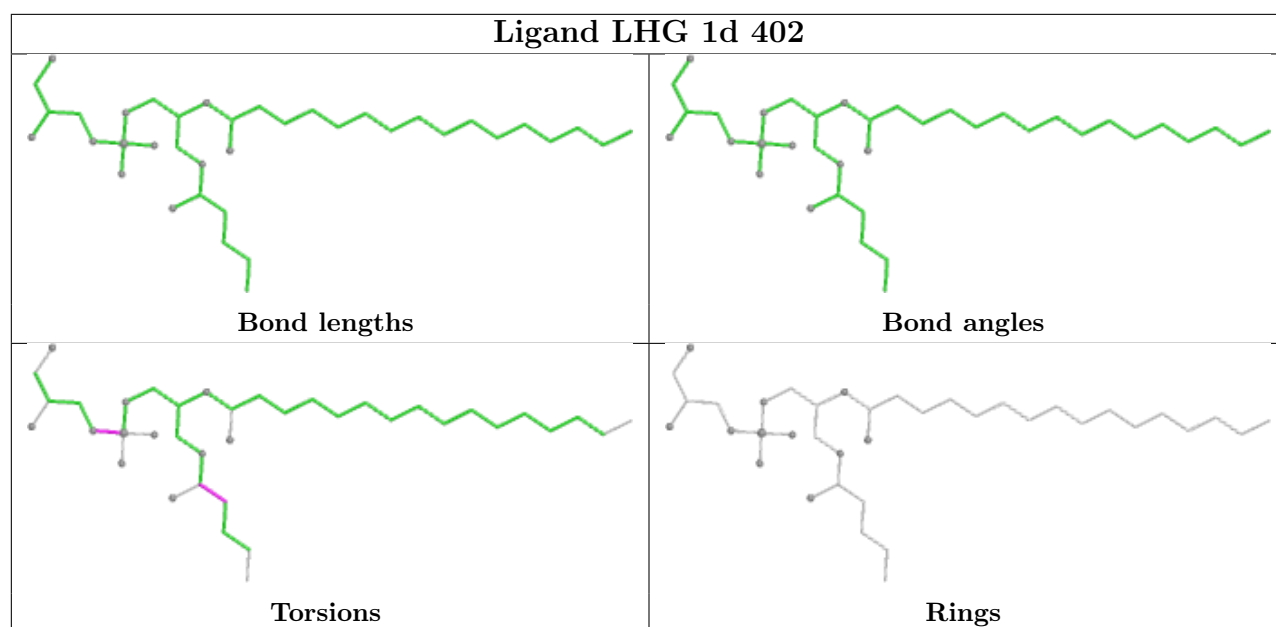
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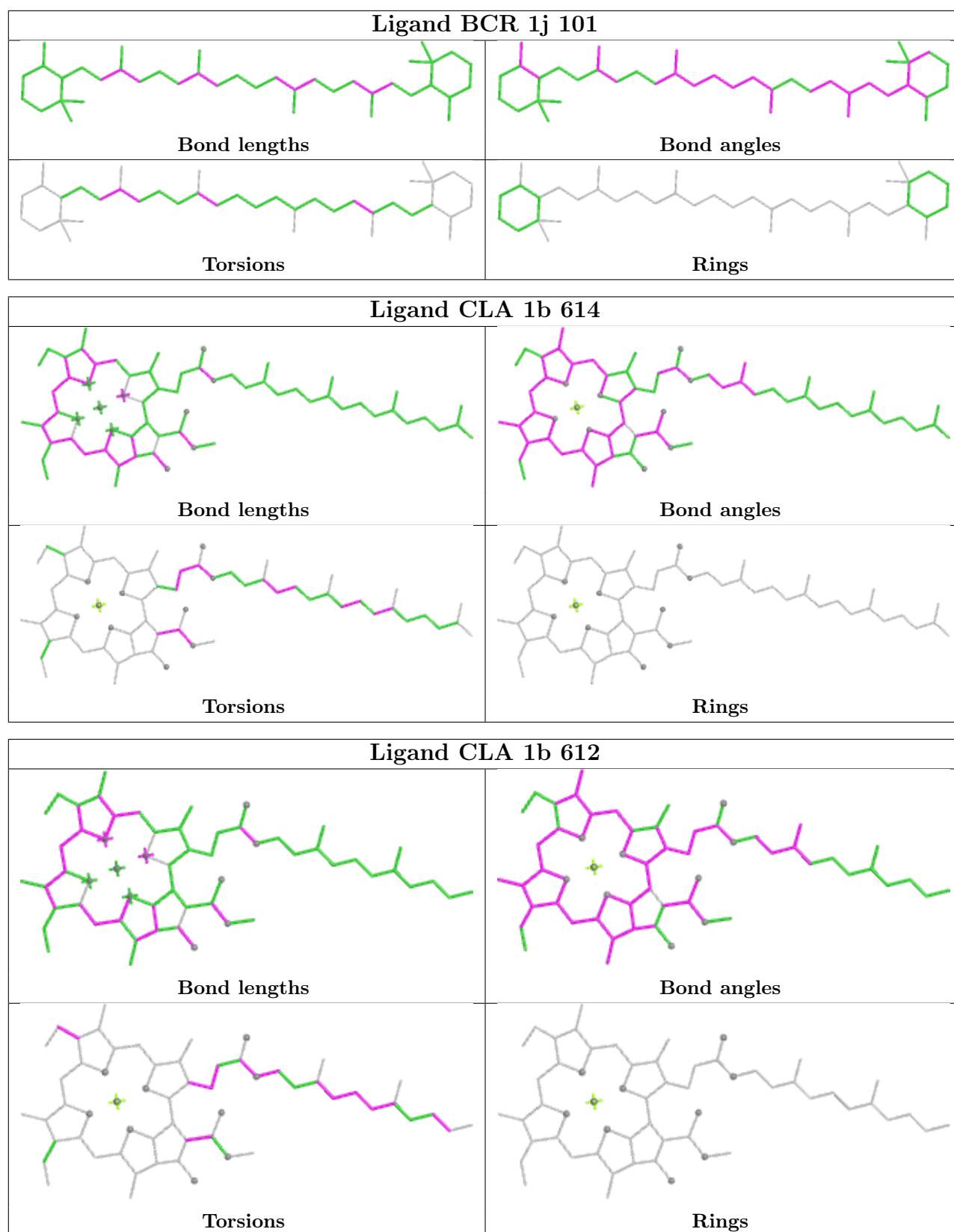
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1b	609	CLA	2	0
26	1c	512	CLA	2	0
28	1i	101	BCR	7	0
26	1b	615	CLA	3	0
22	1a	414	LHG	11	0
29	1c	516	SQD	8	0
22	1b	626	LHG	3	0
26	1d	407	CLA	1	0
28	1t	101	BCR	5	0
26	1b	616	CLA	1	0

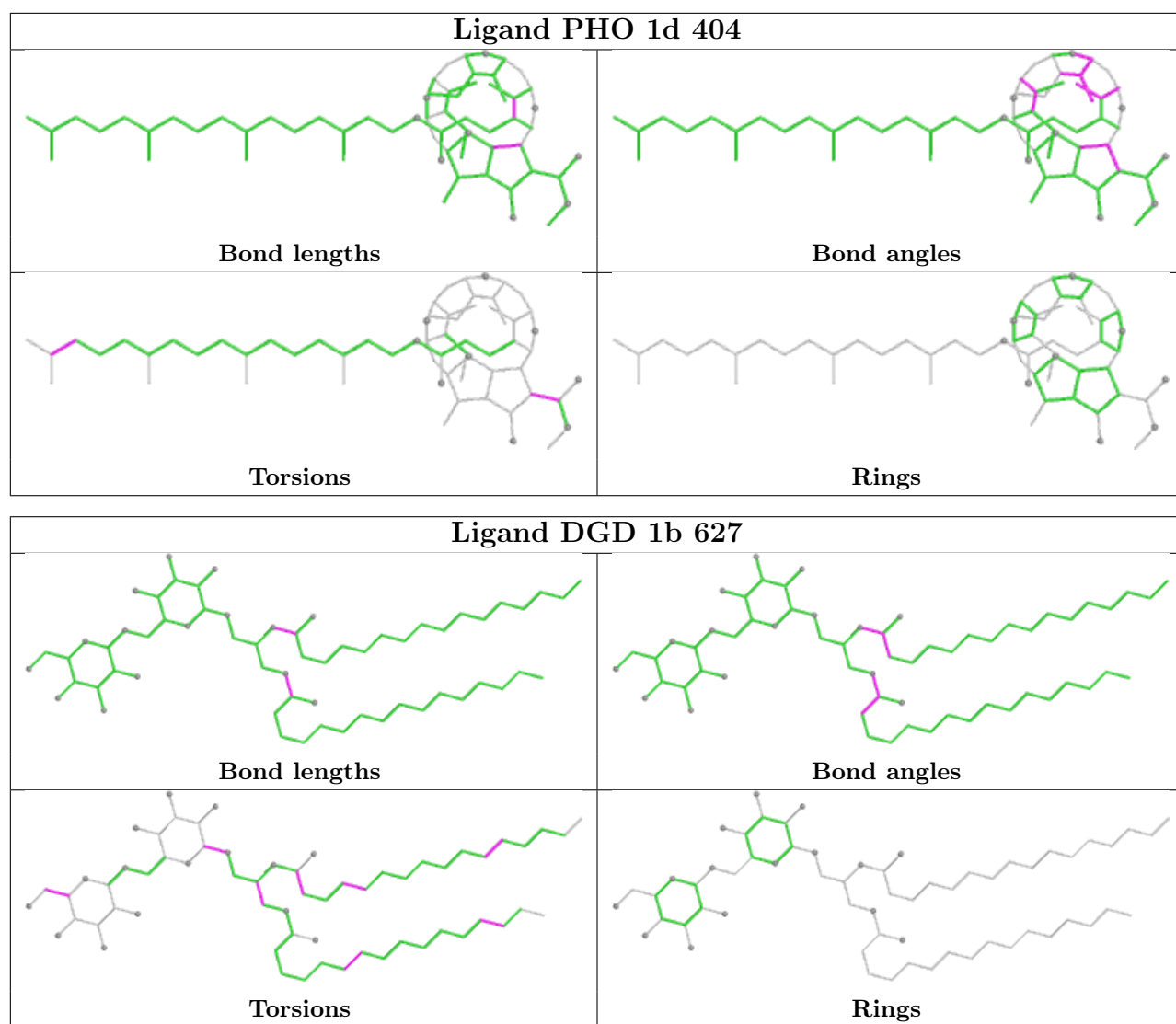
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

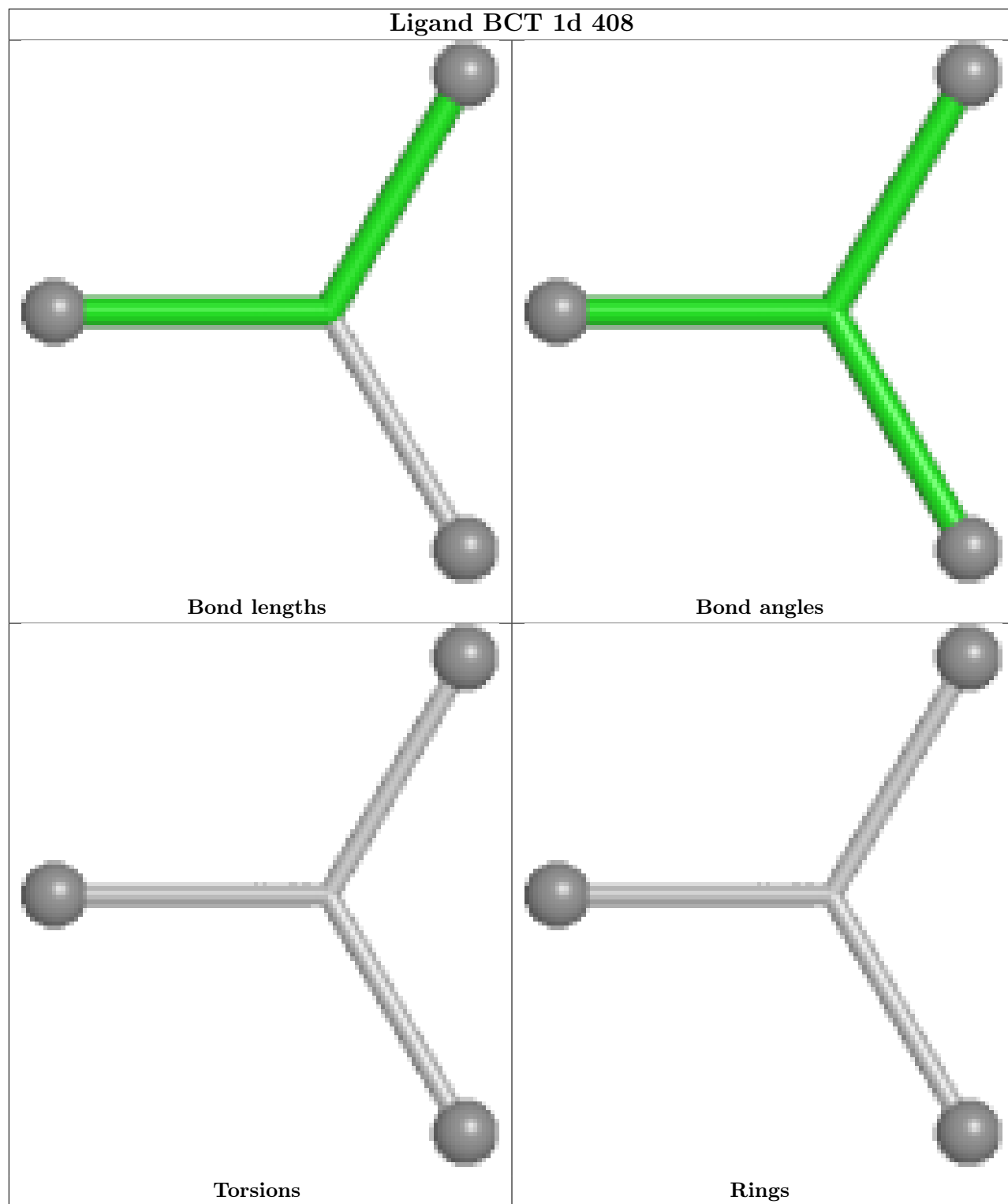


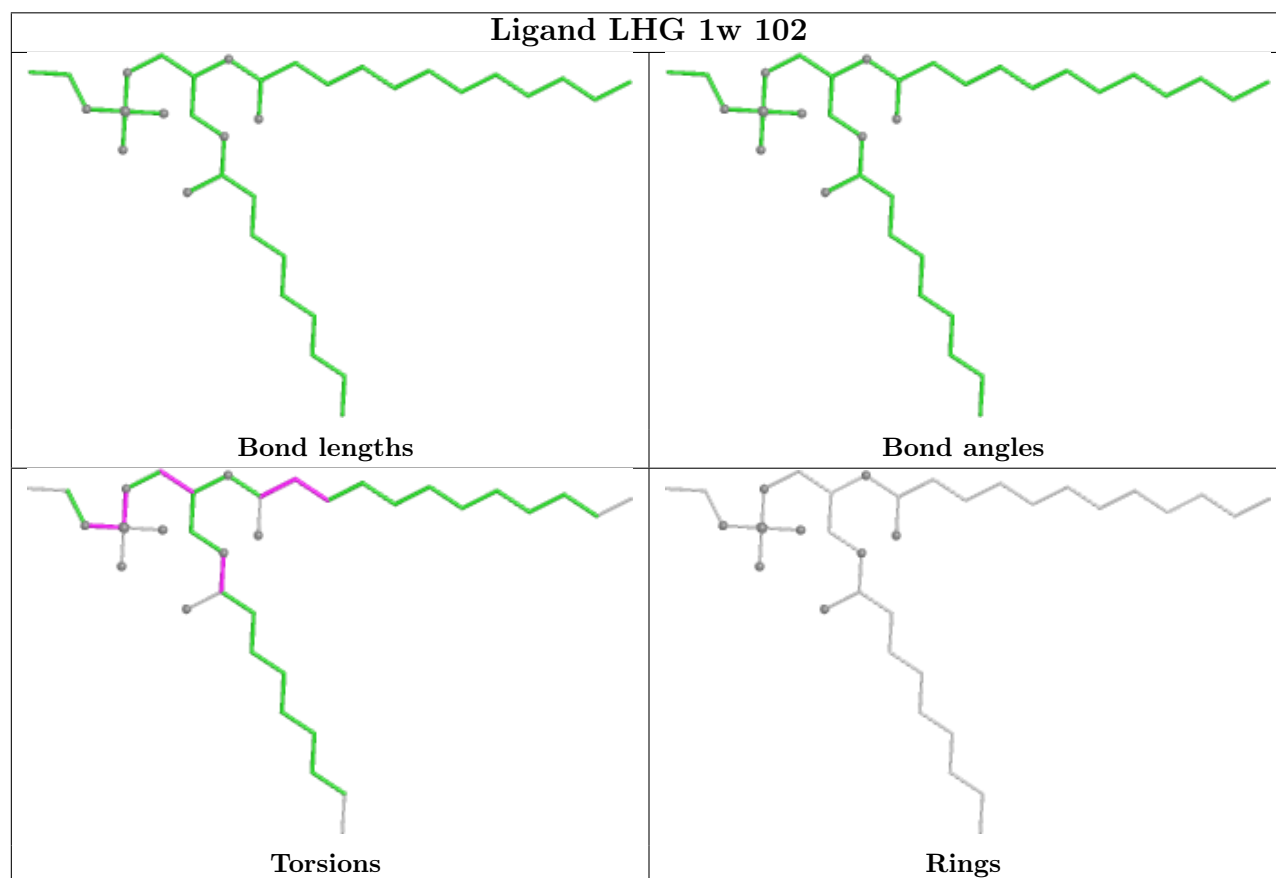
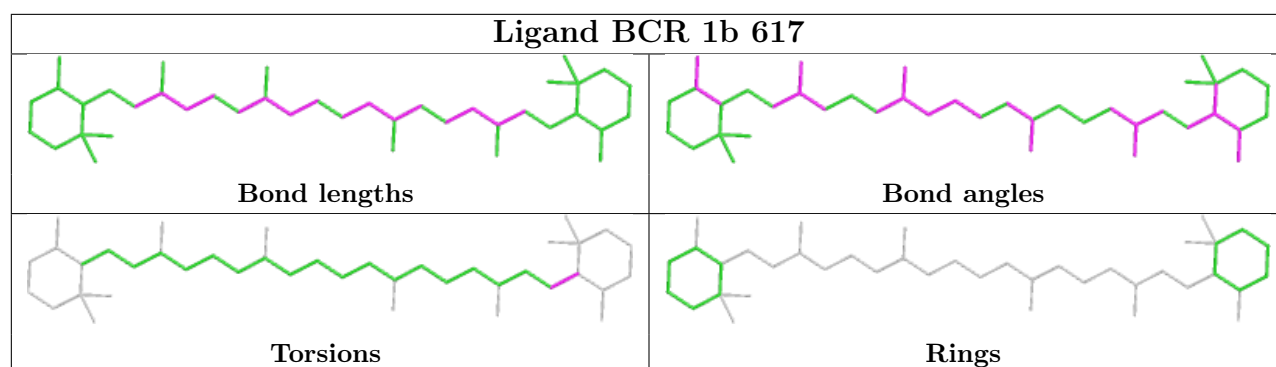


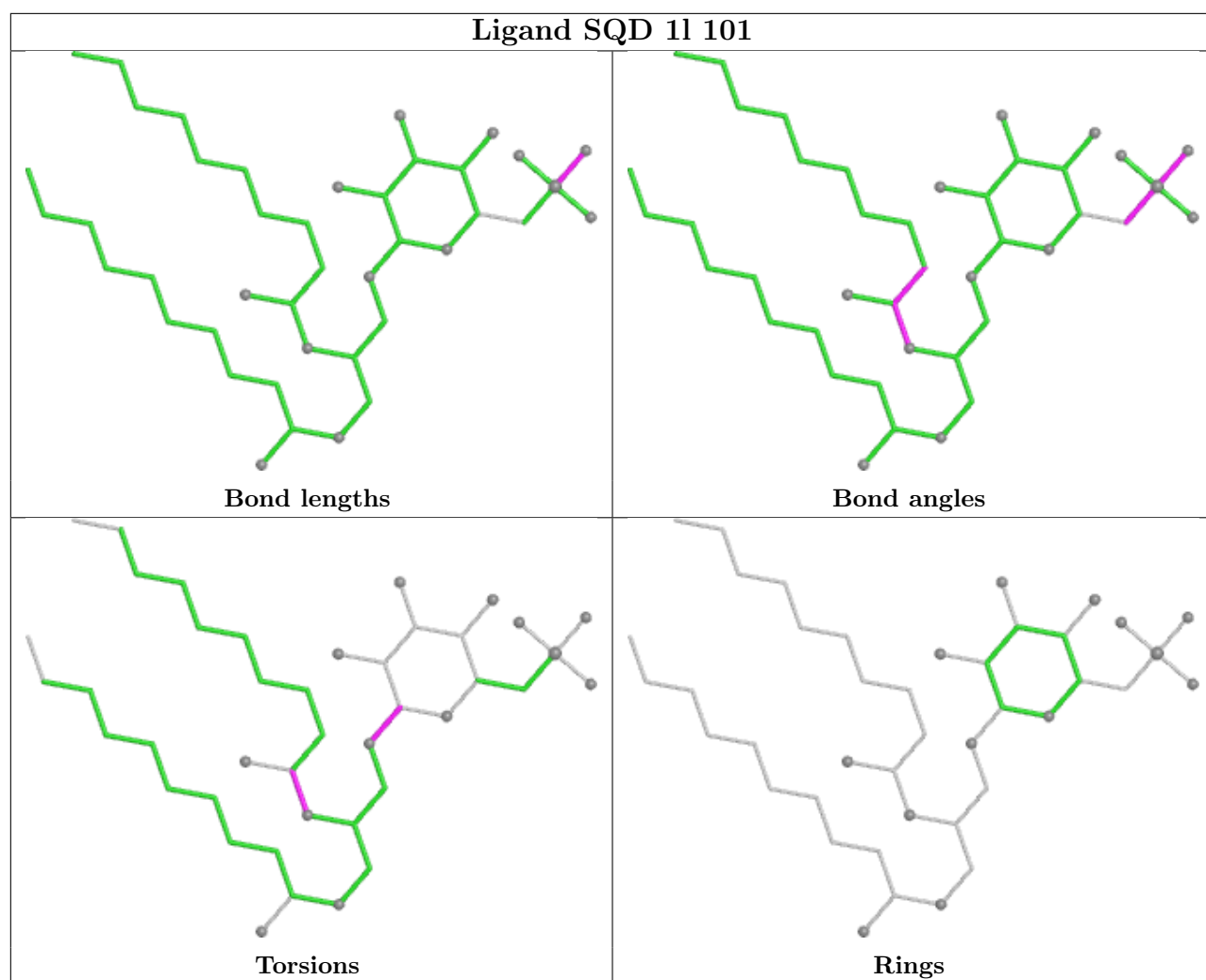


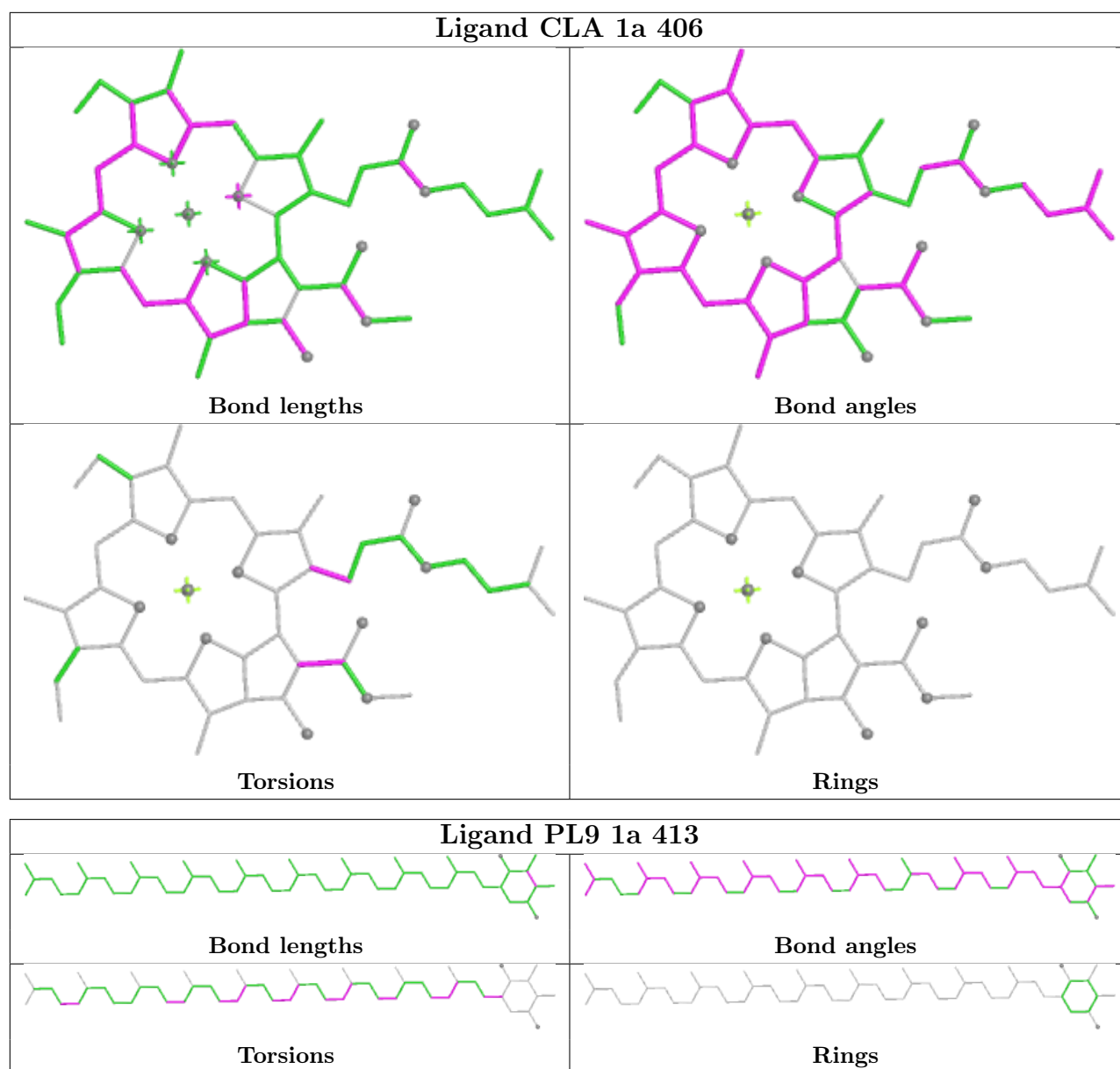


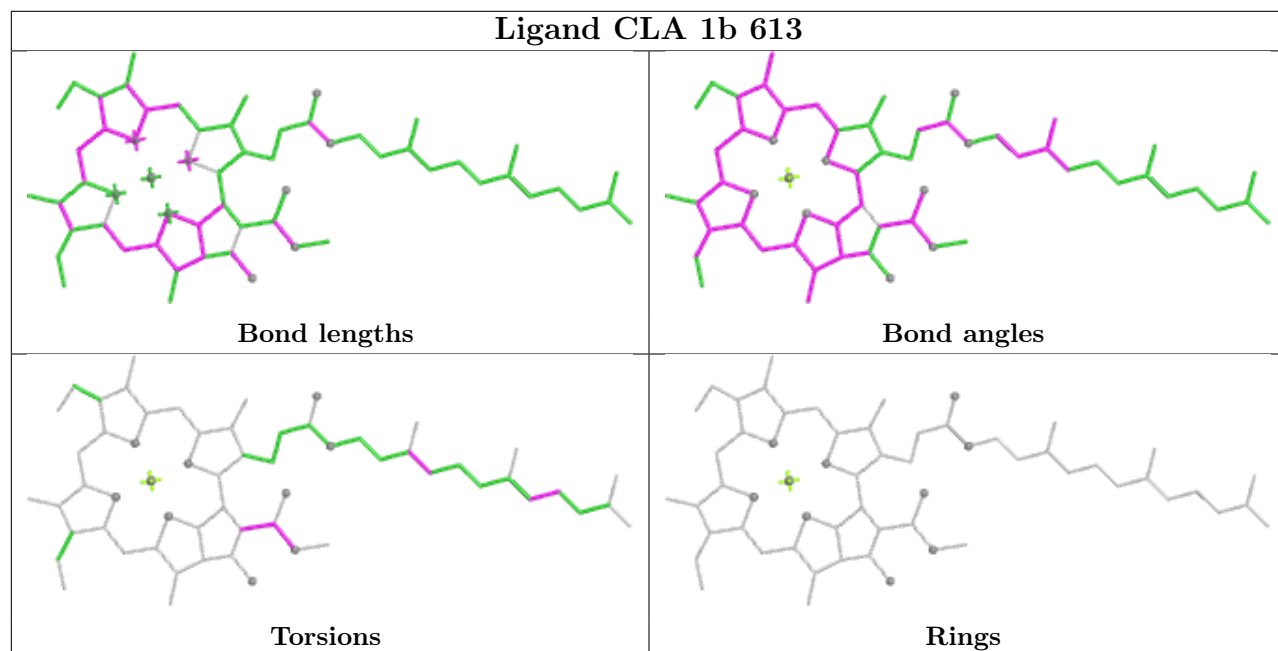
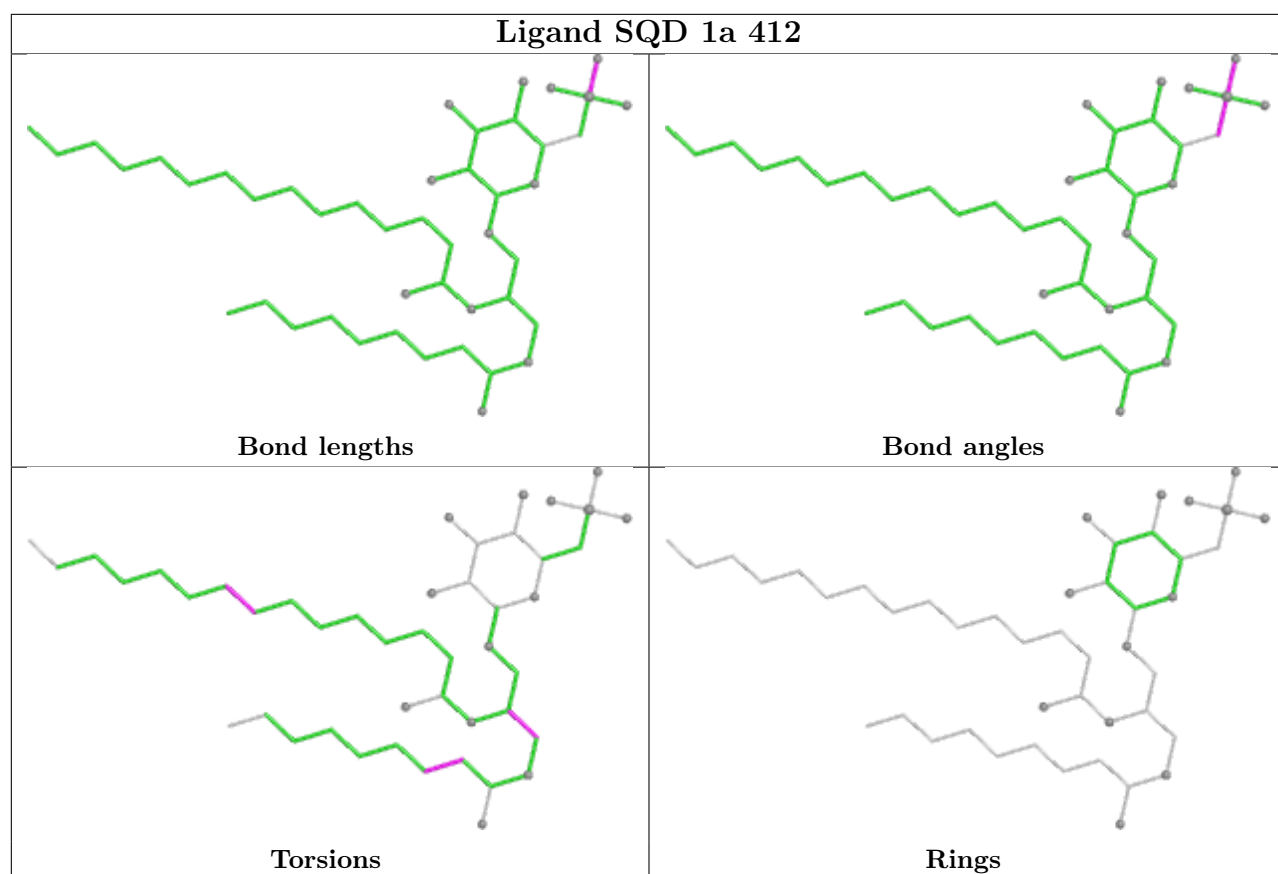


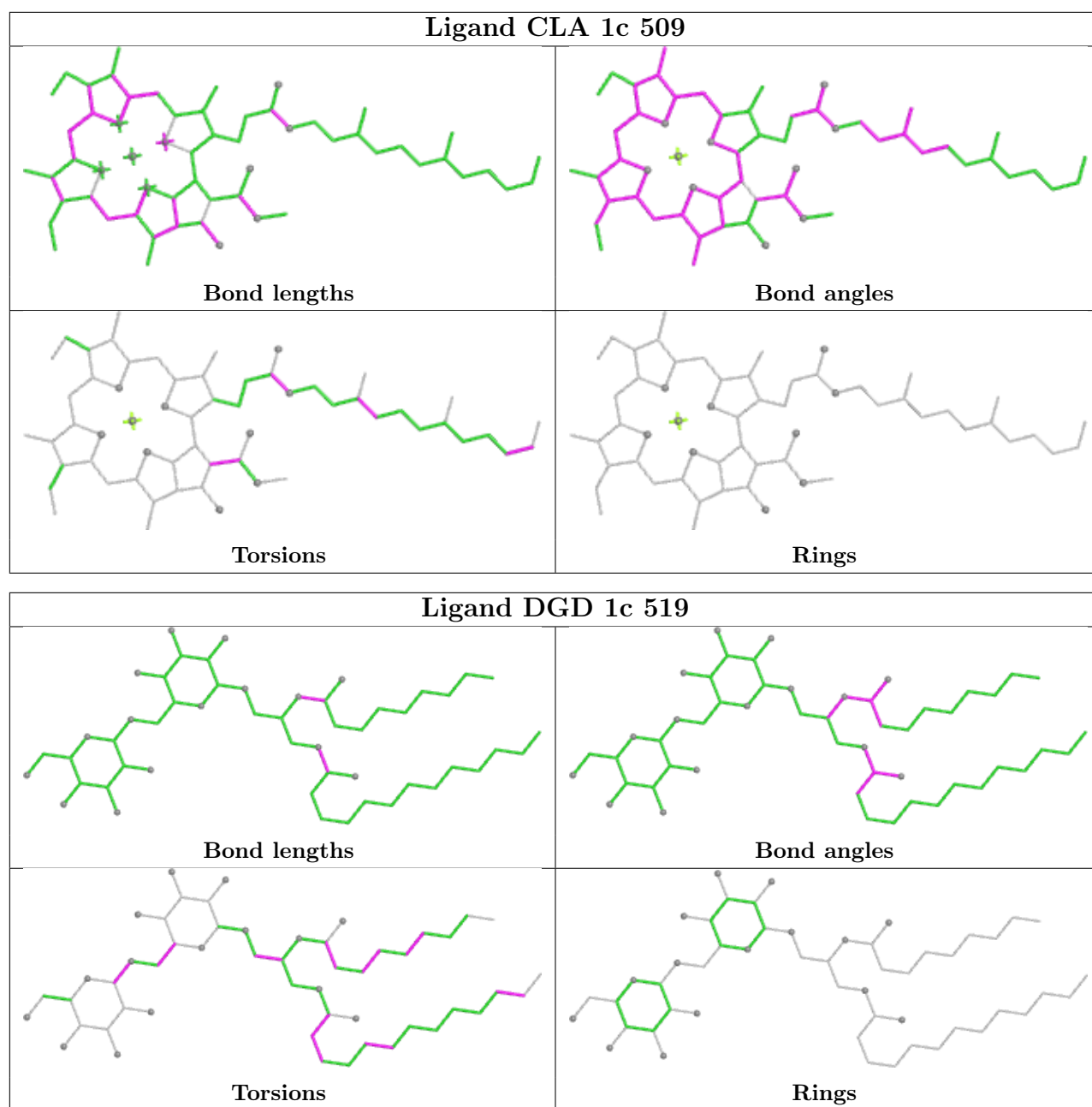


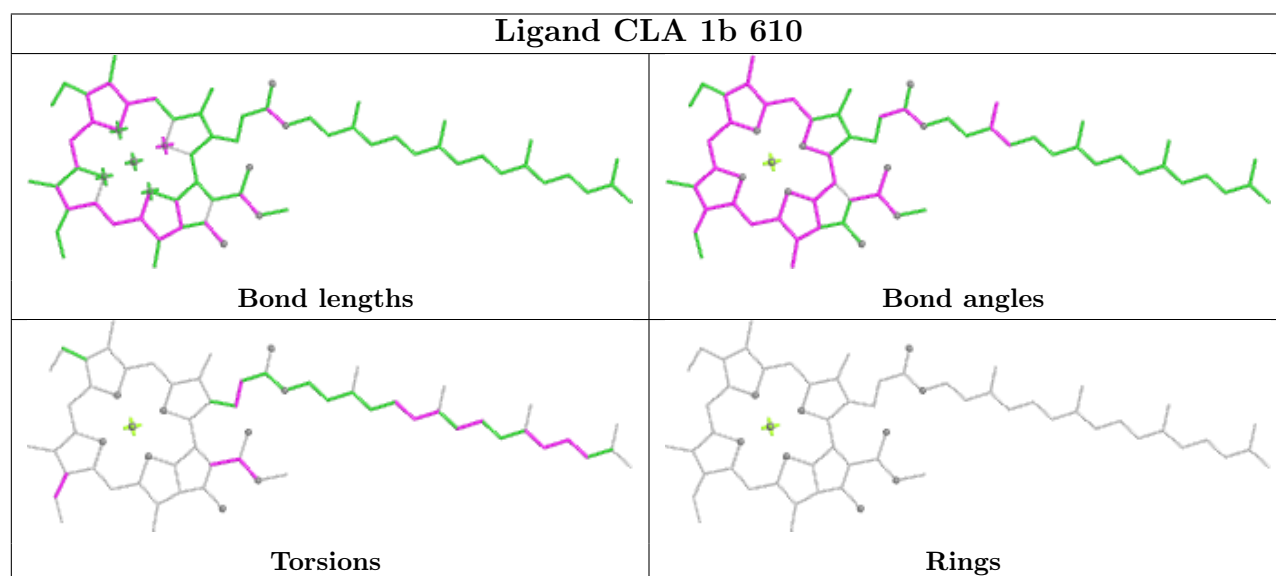
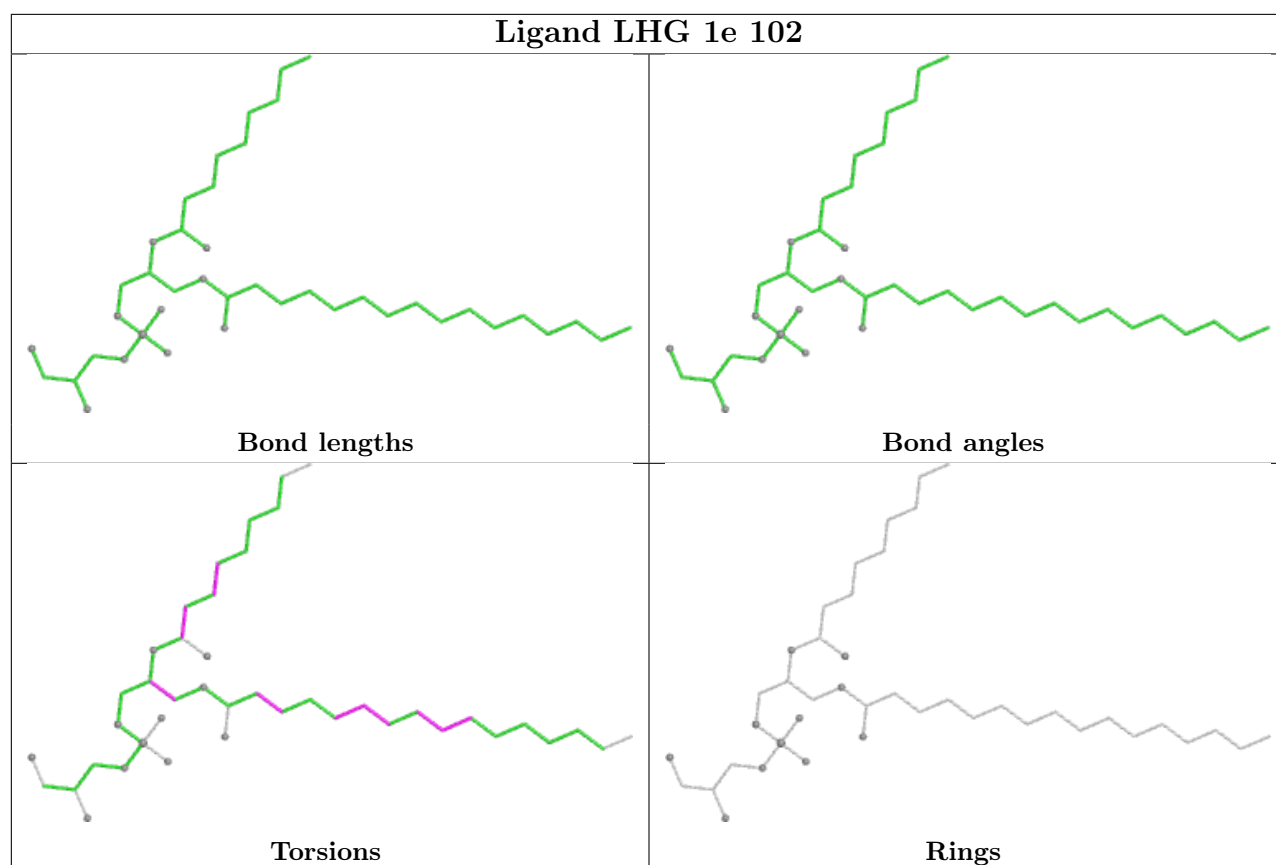


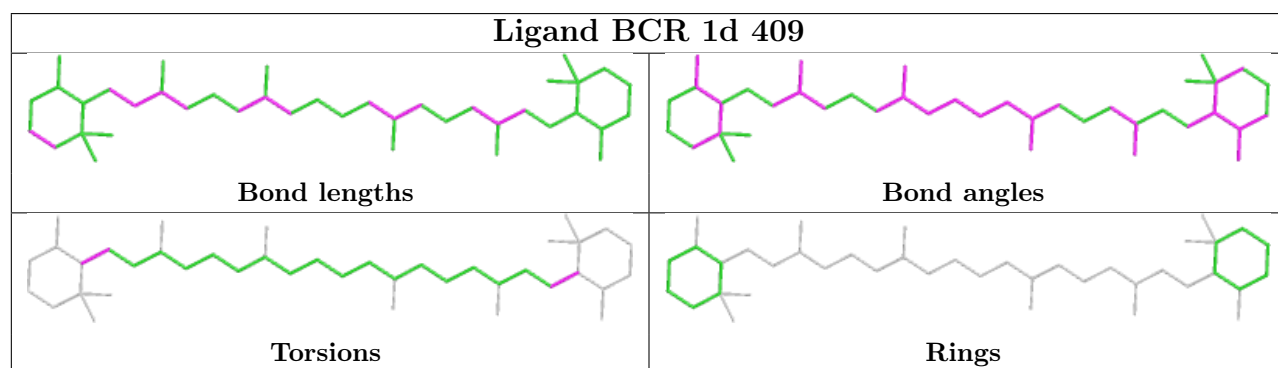
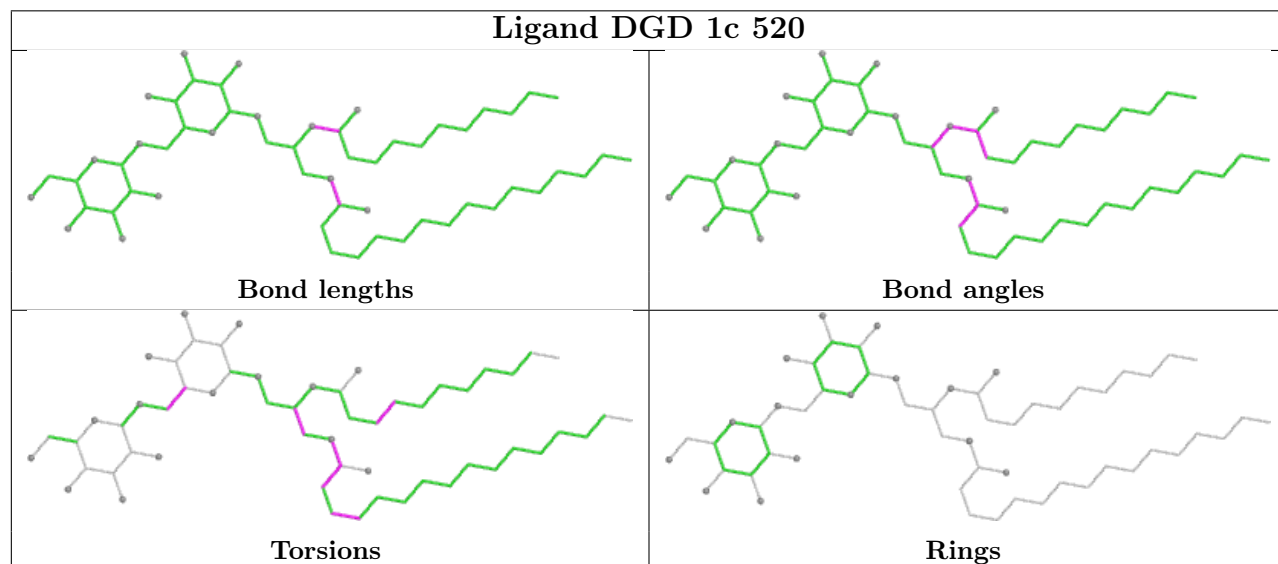
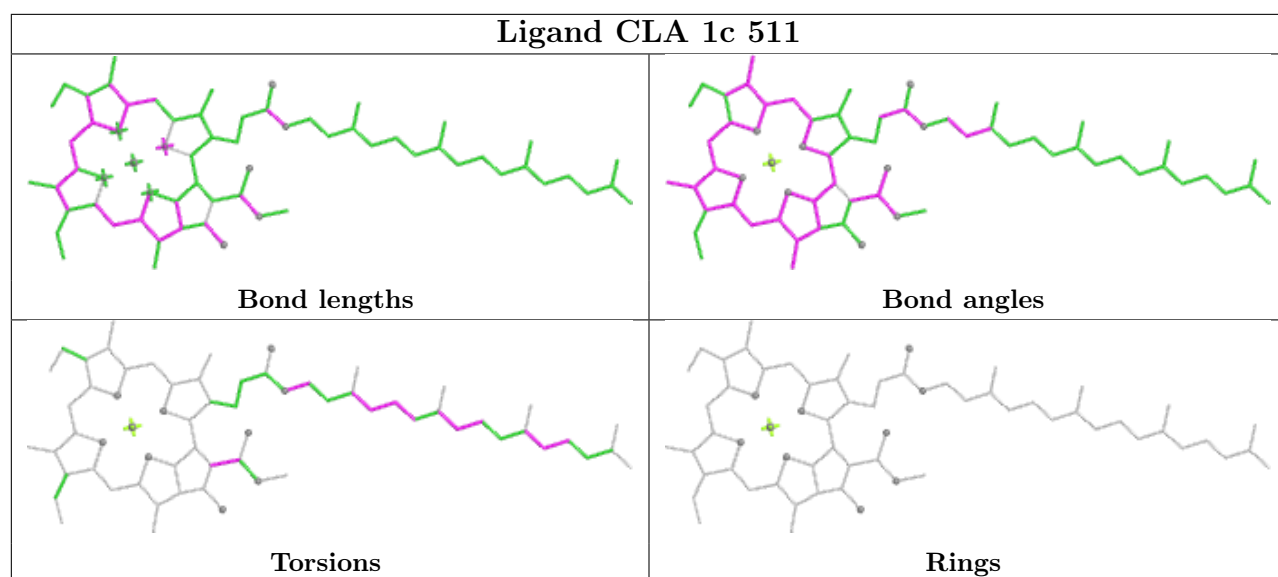


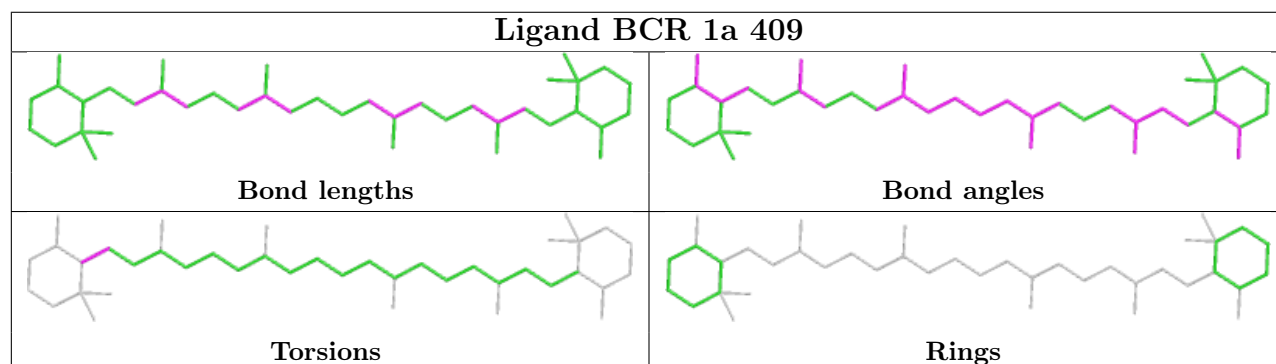
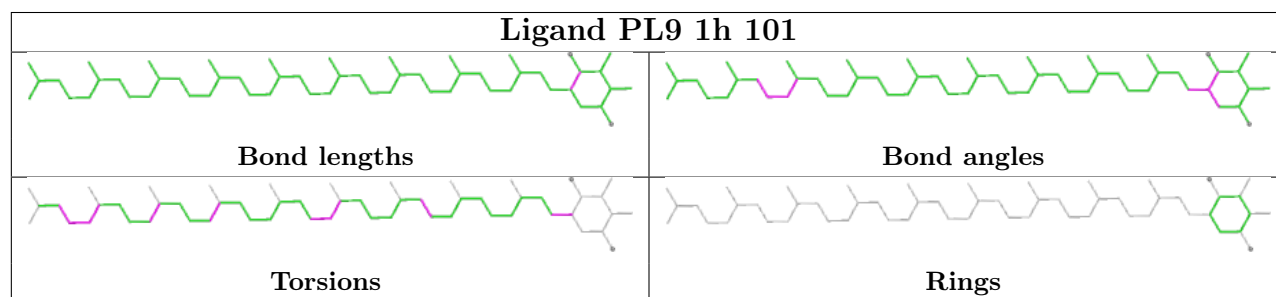
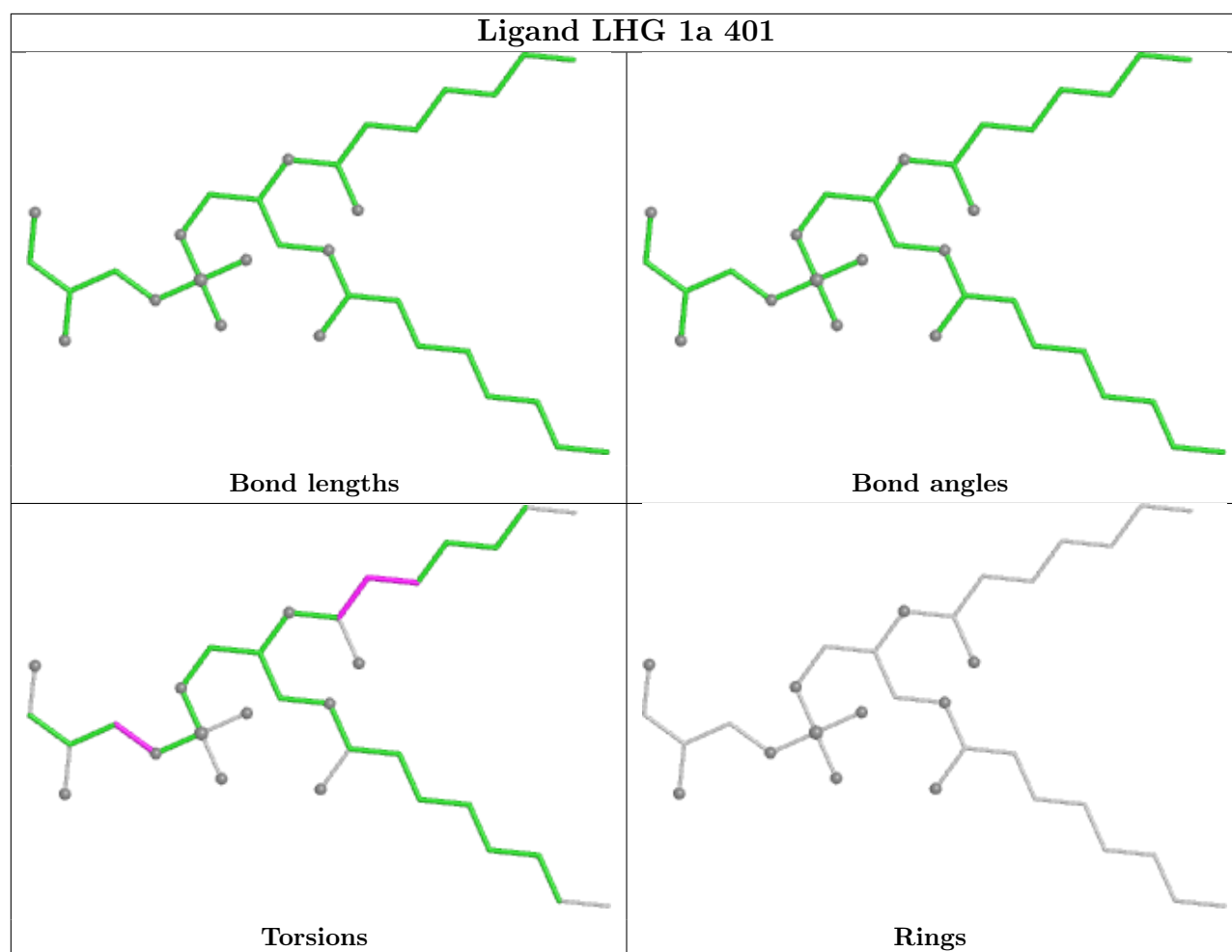


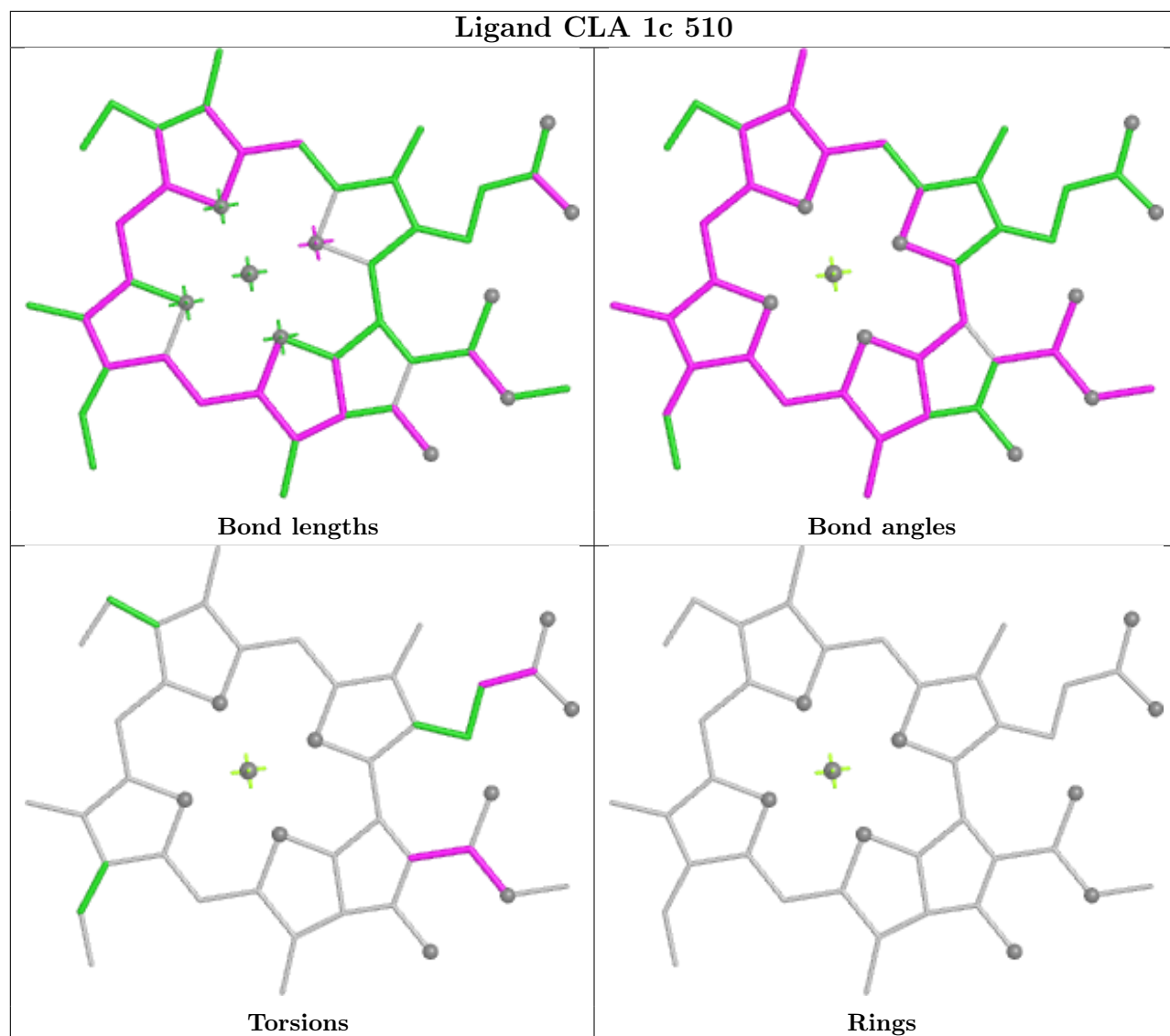
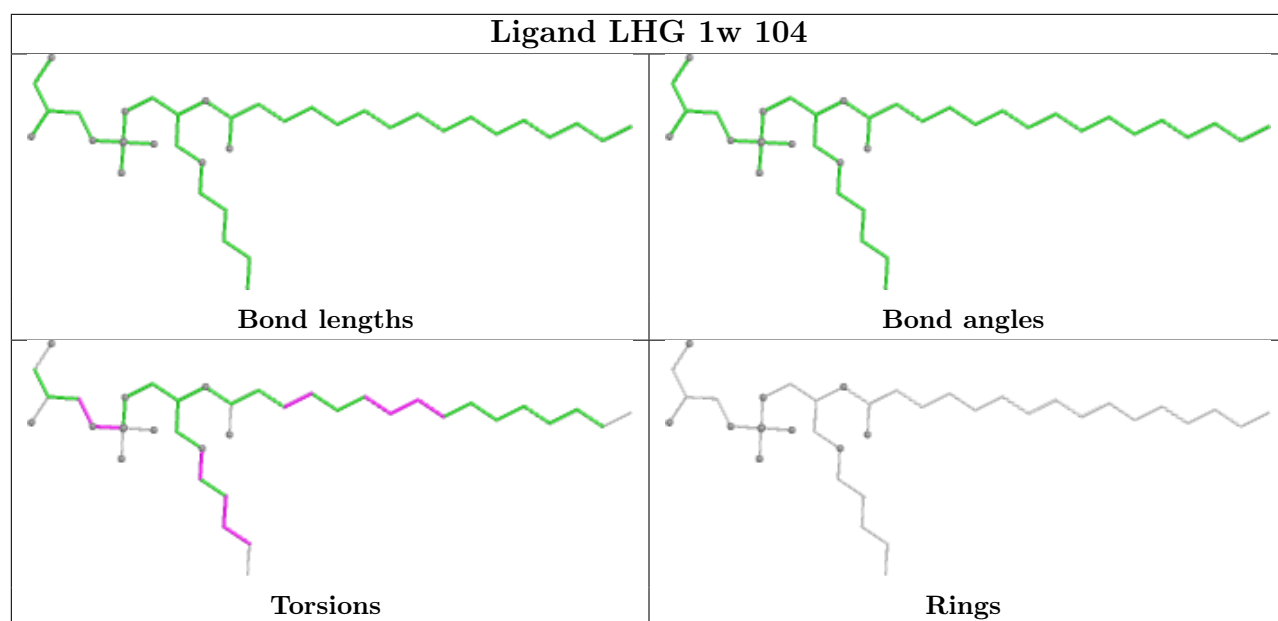


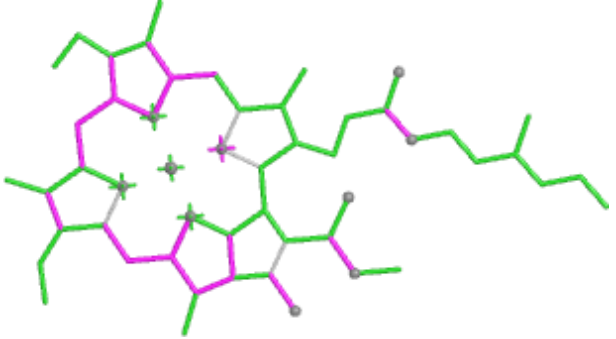
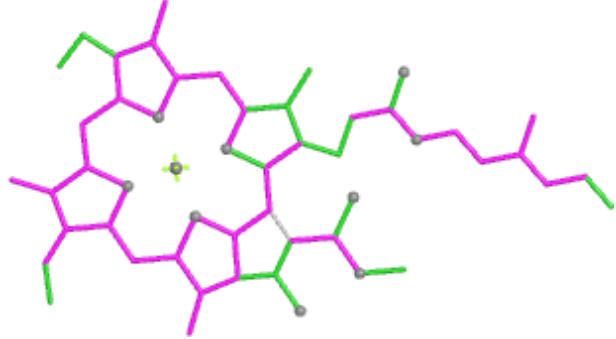
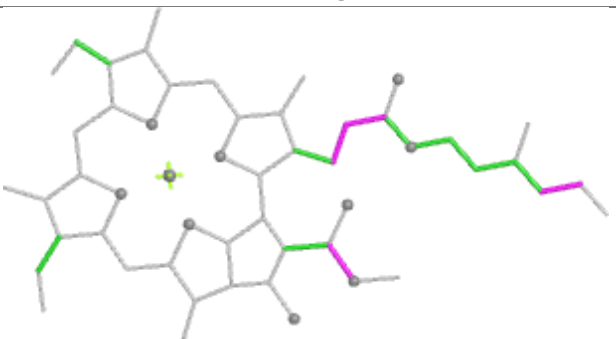
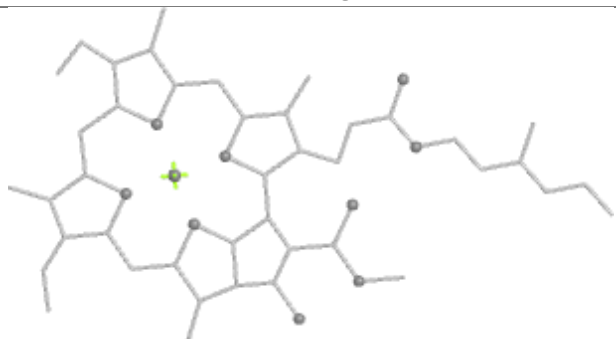
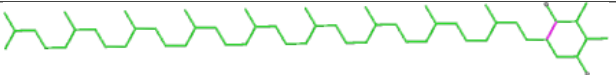
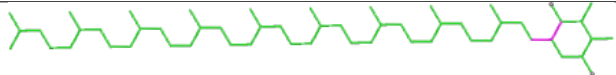
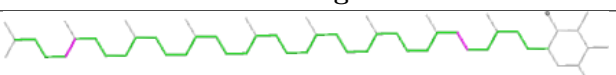
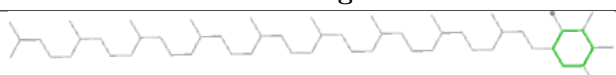


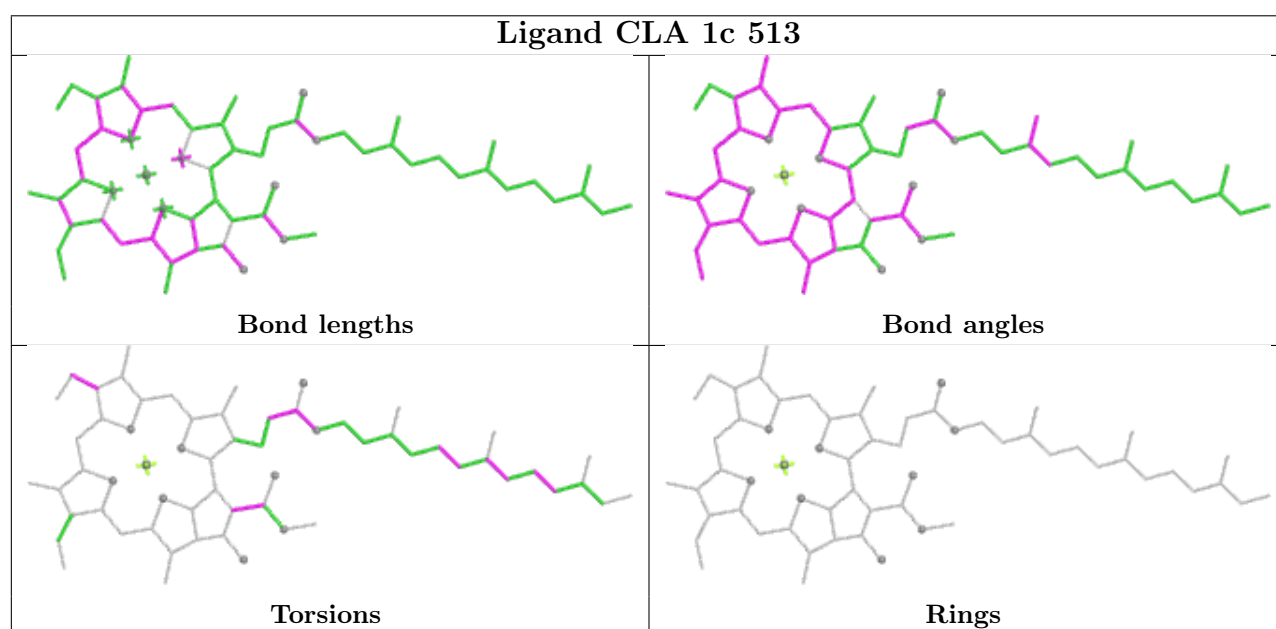
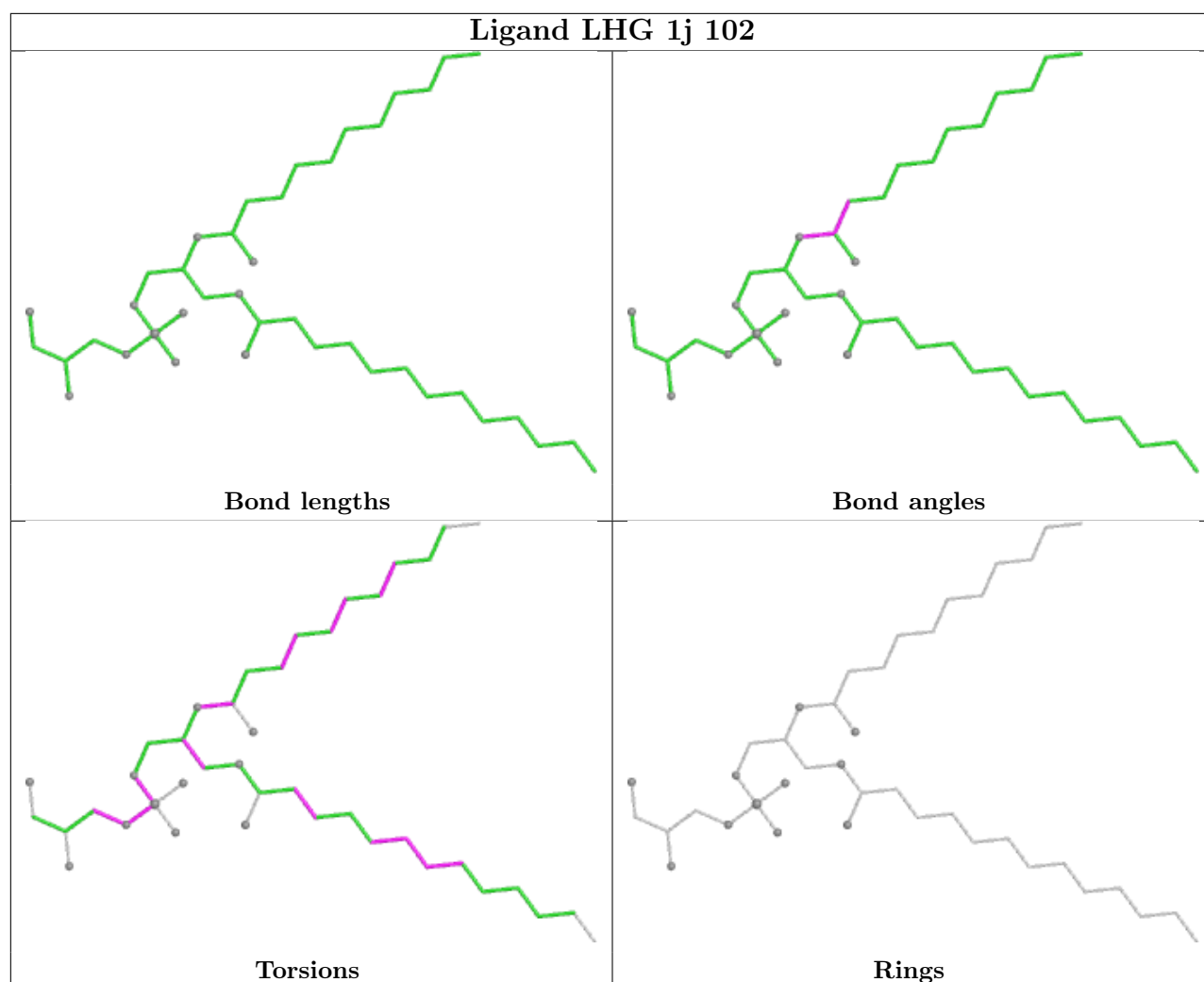


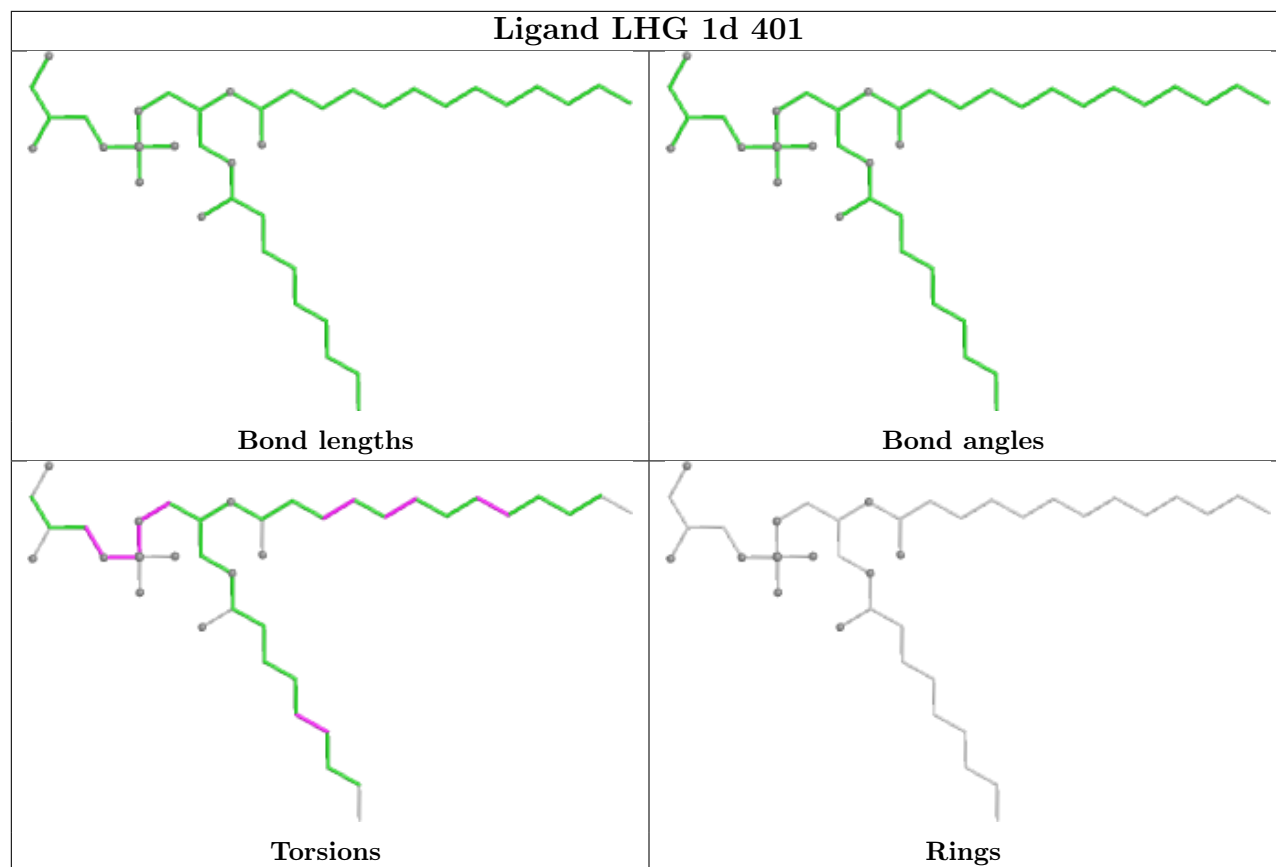


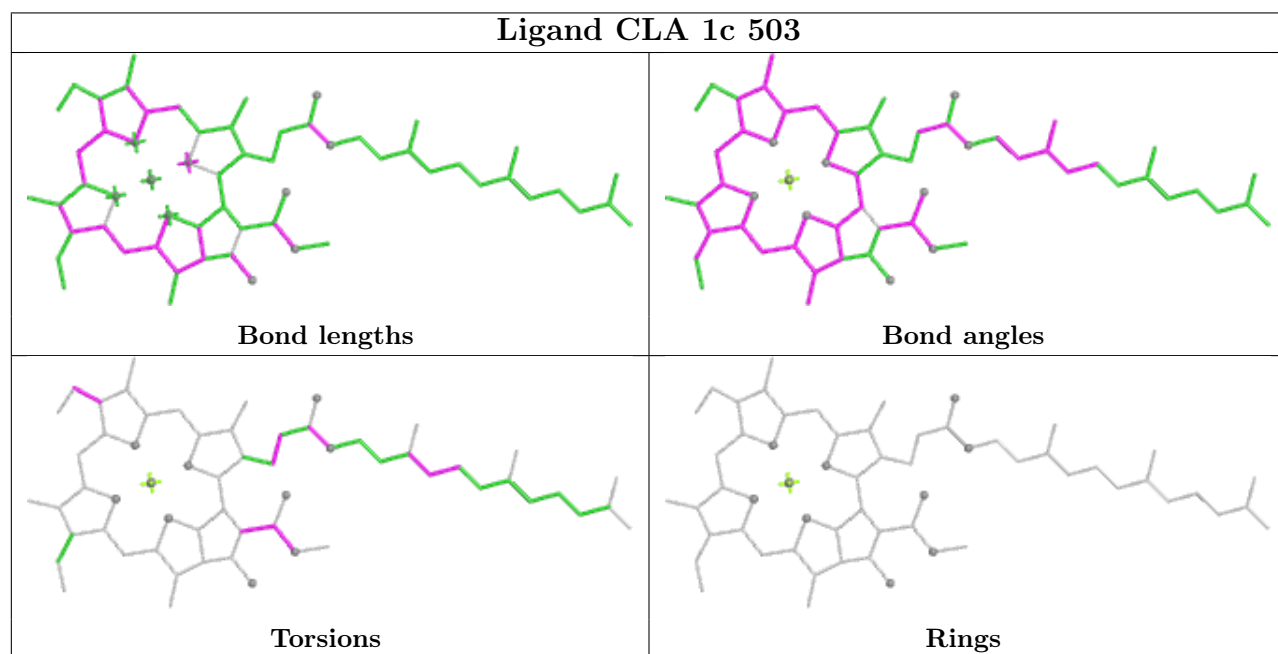
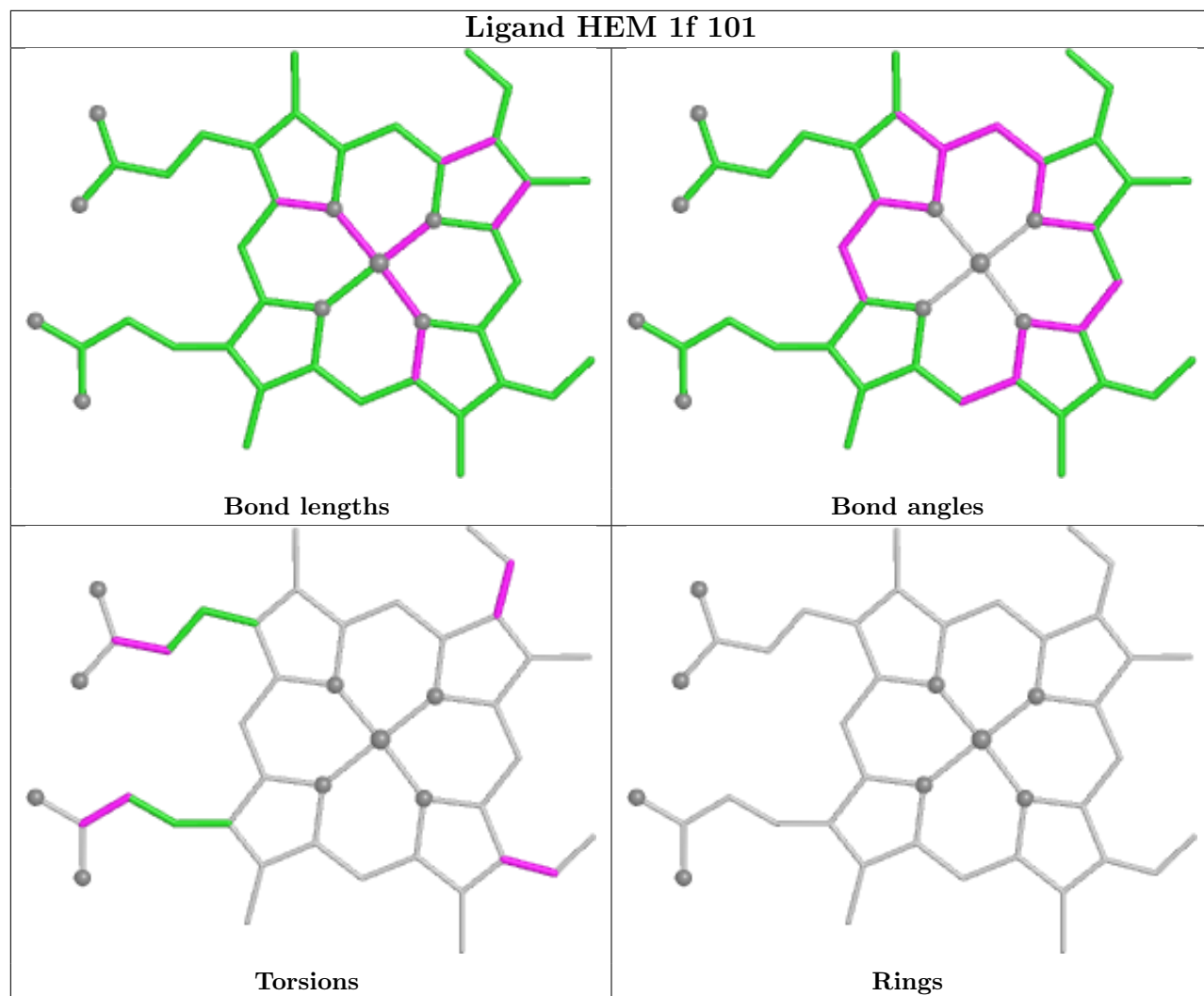


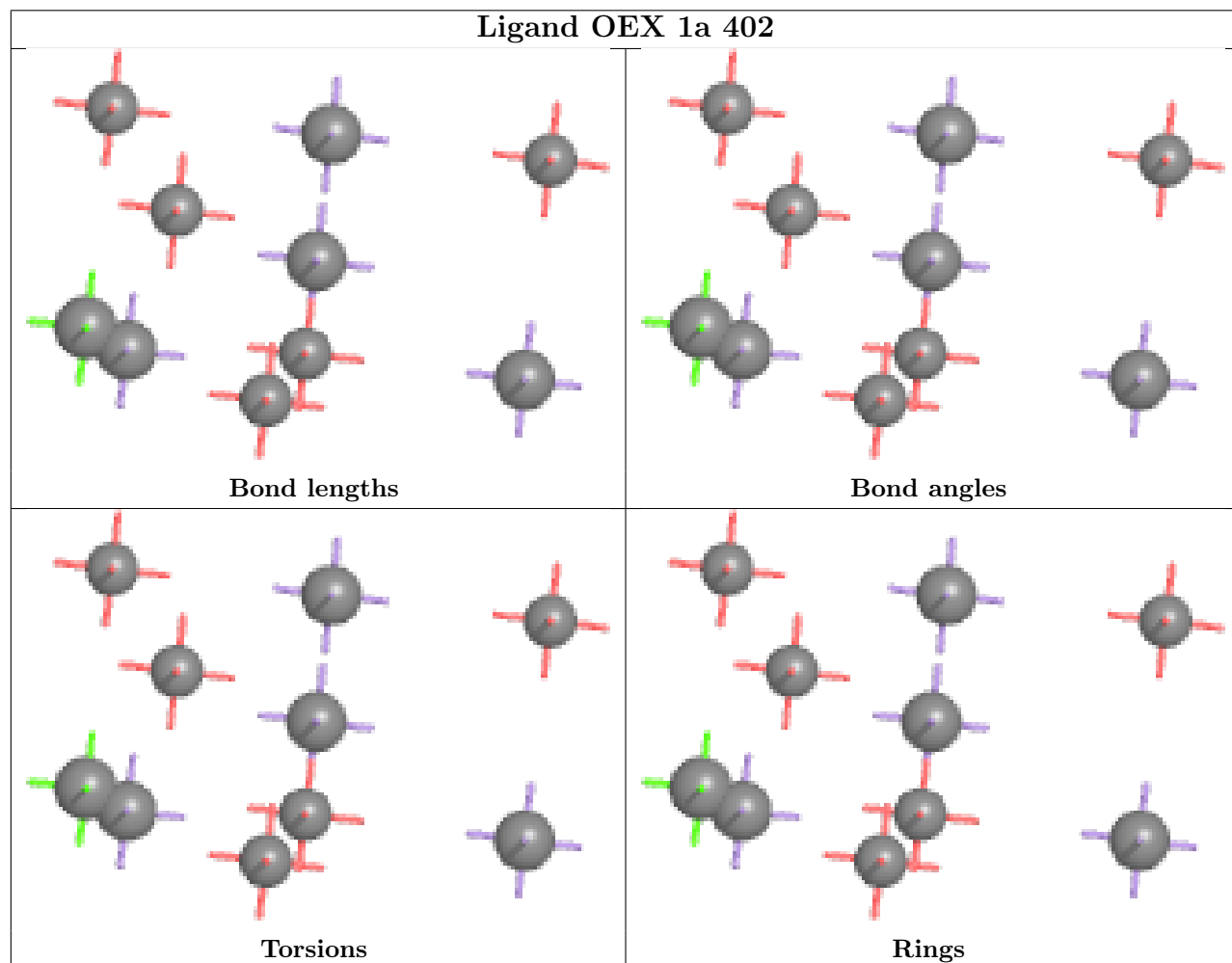
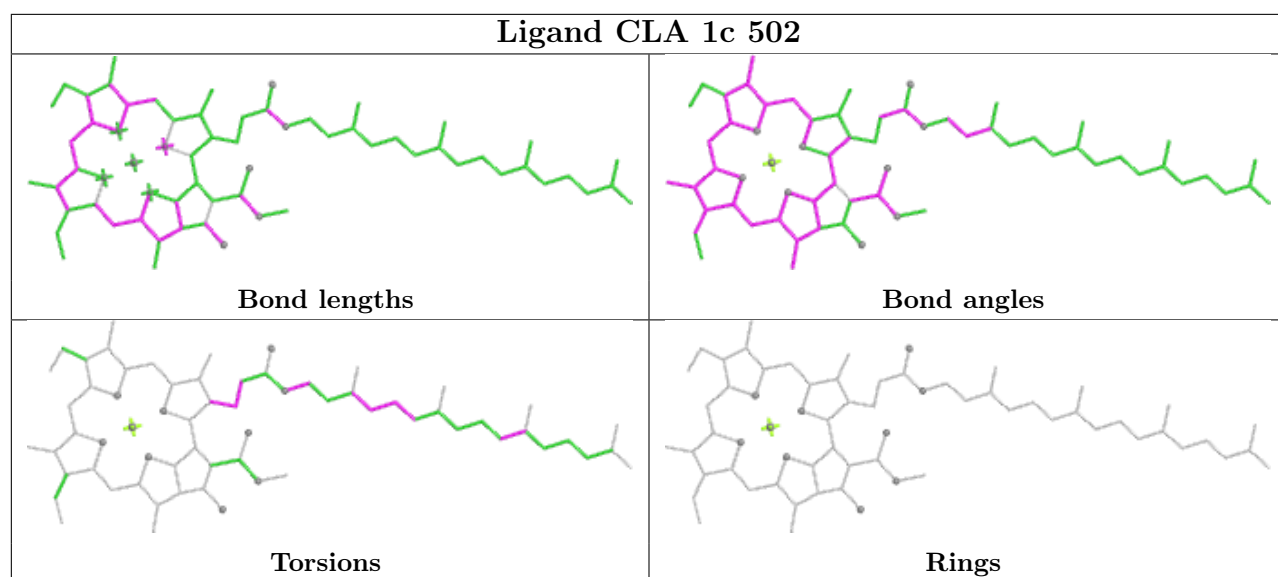


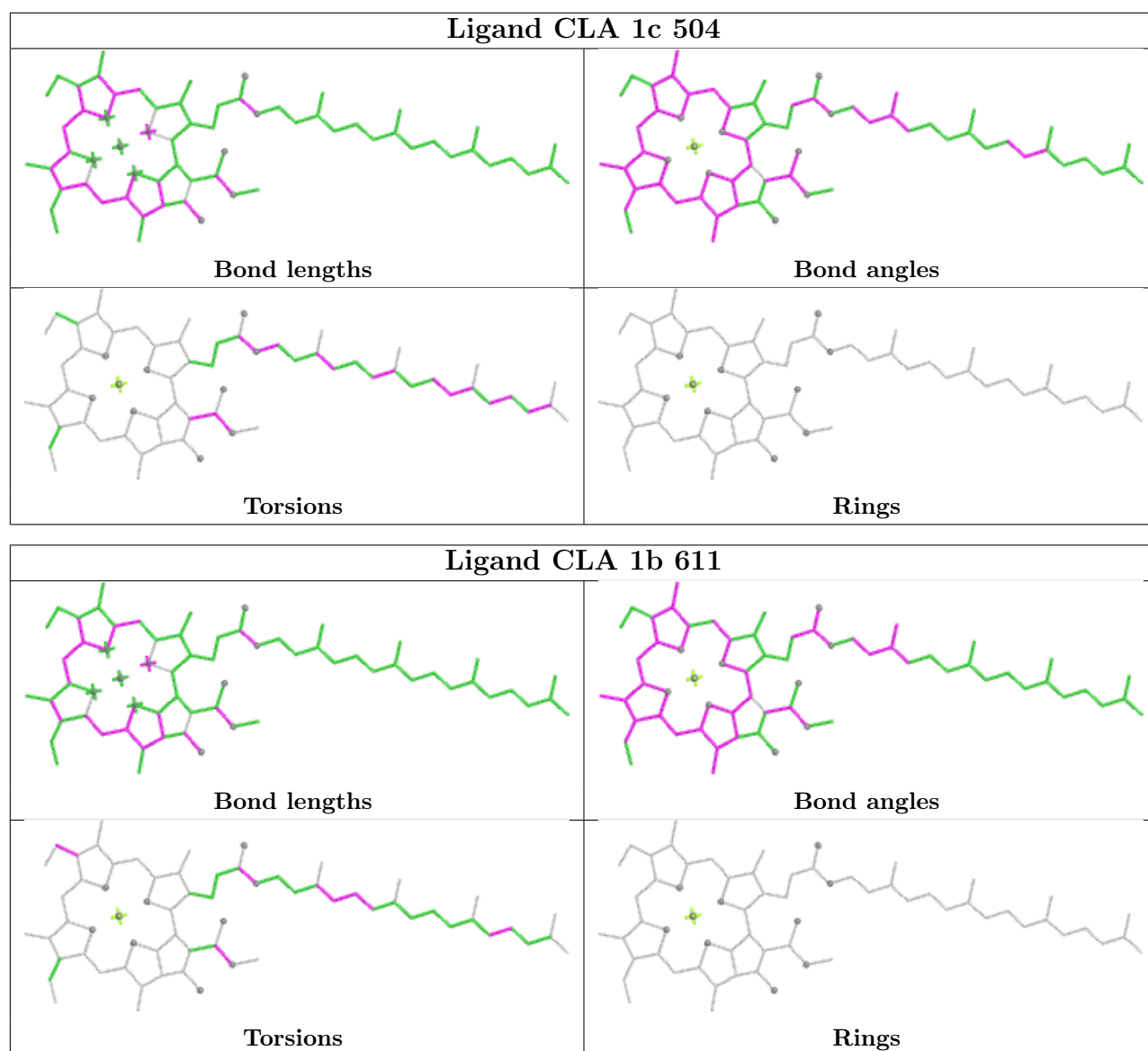
Ligand CLA 1a 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 1d 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

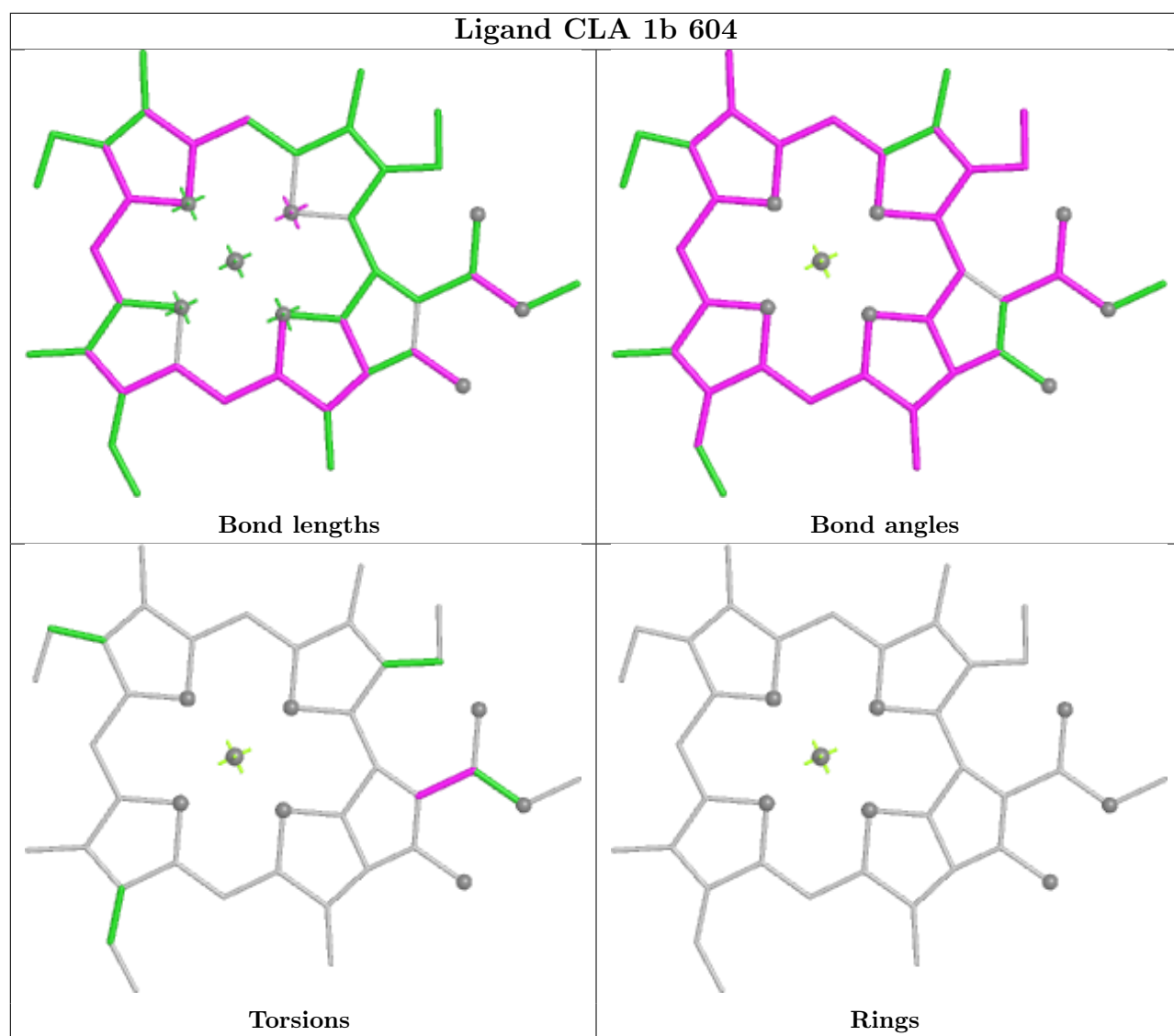


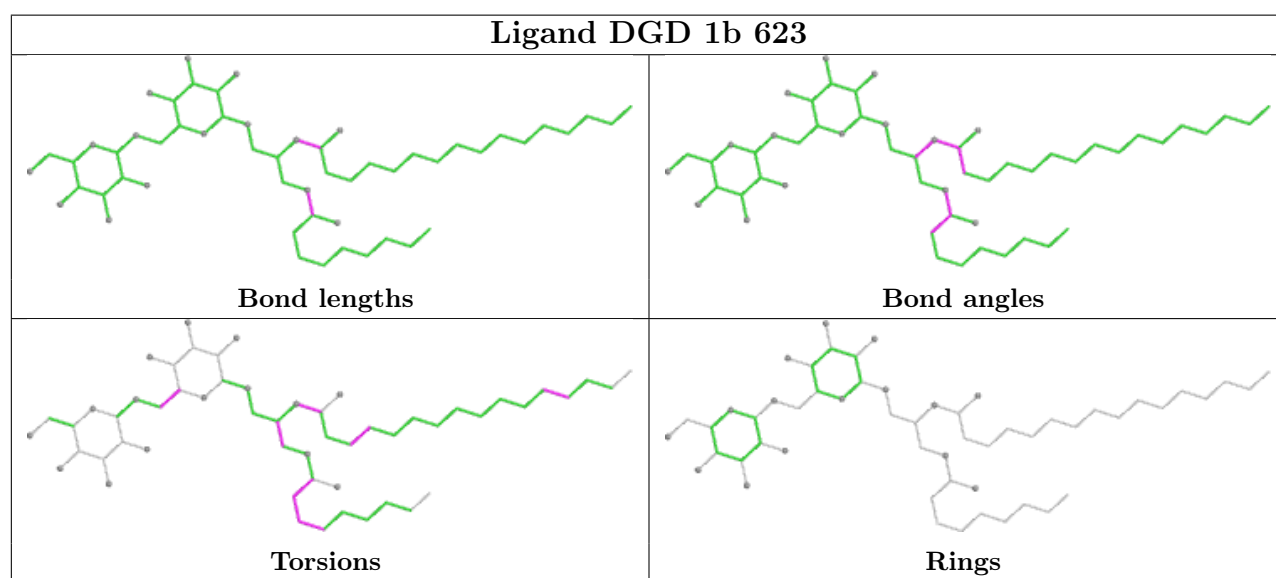
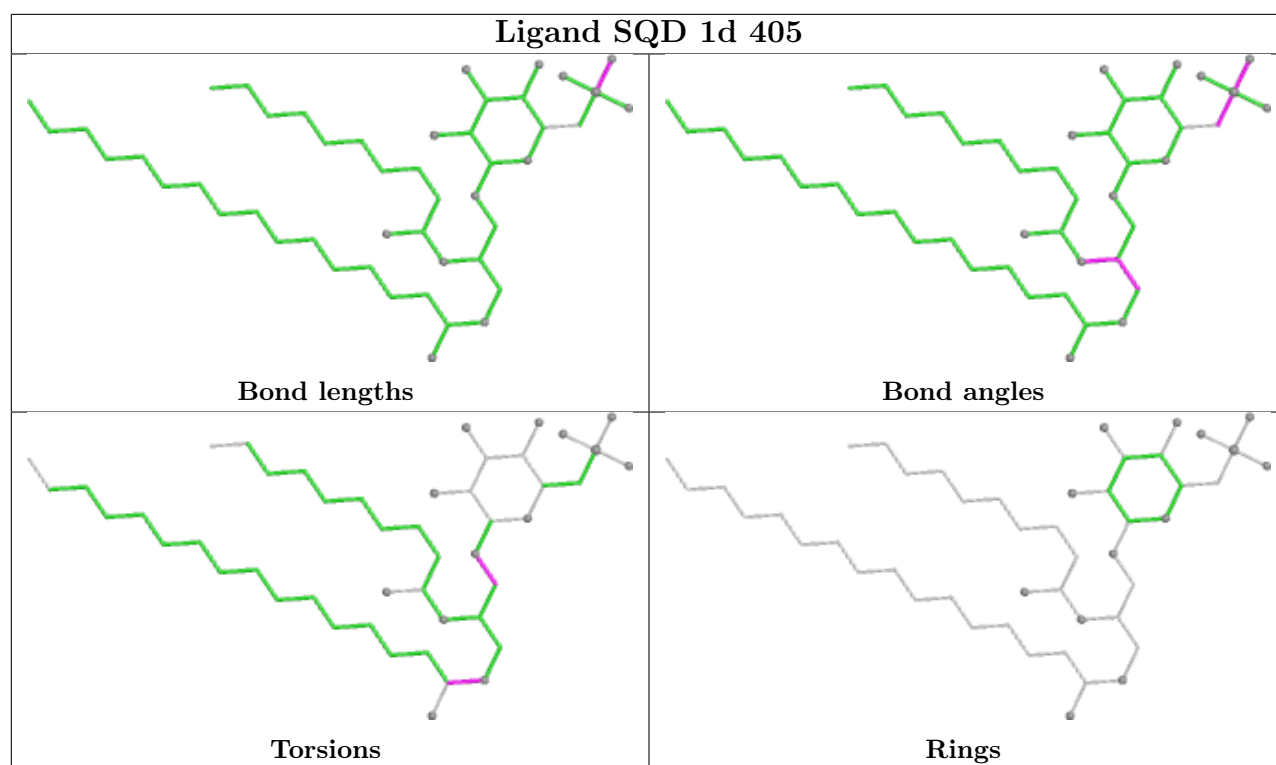


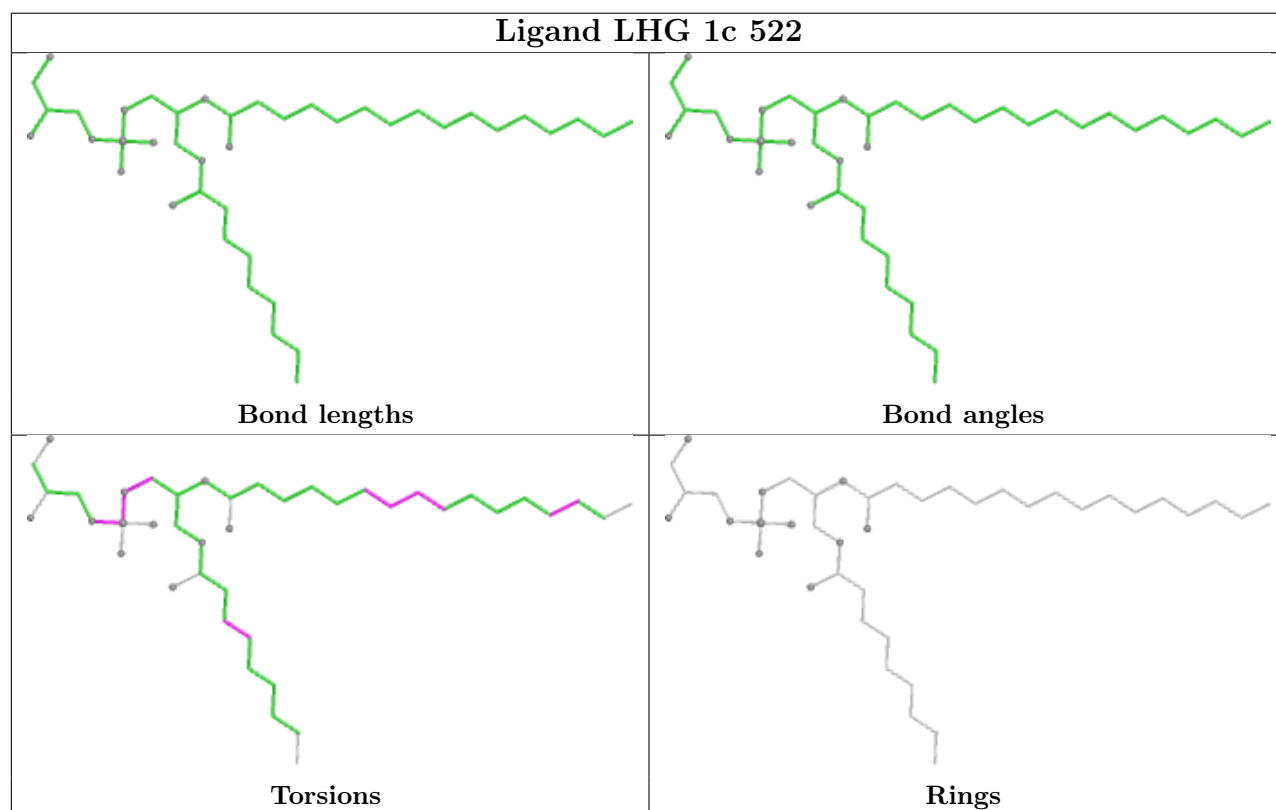
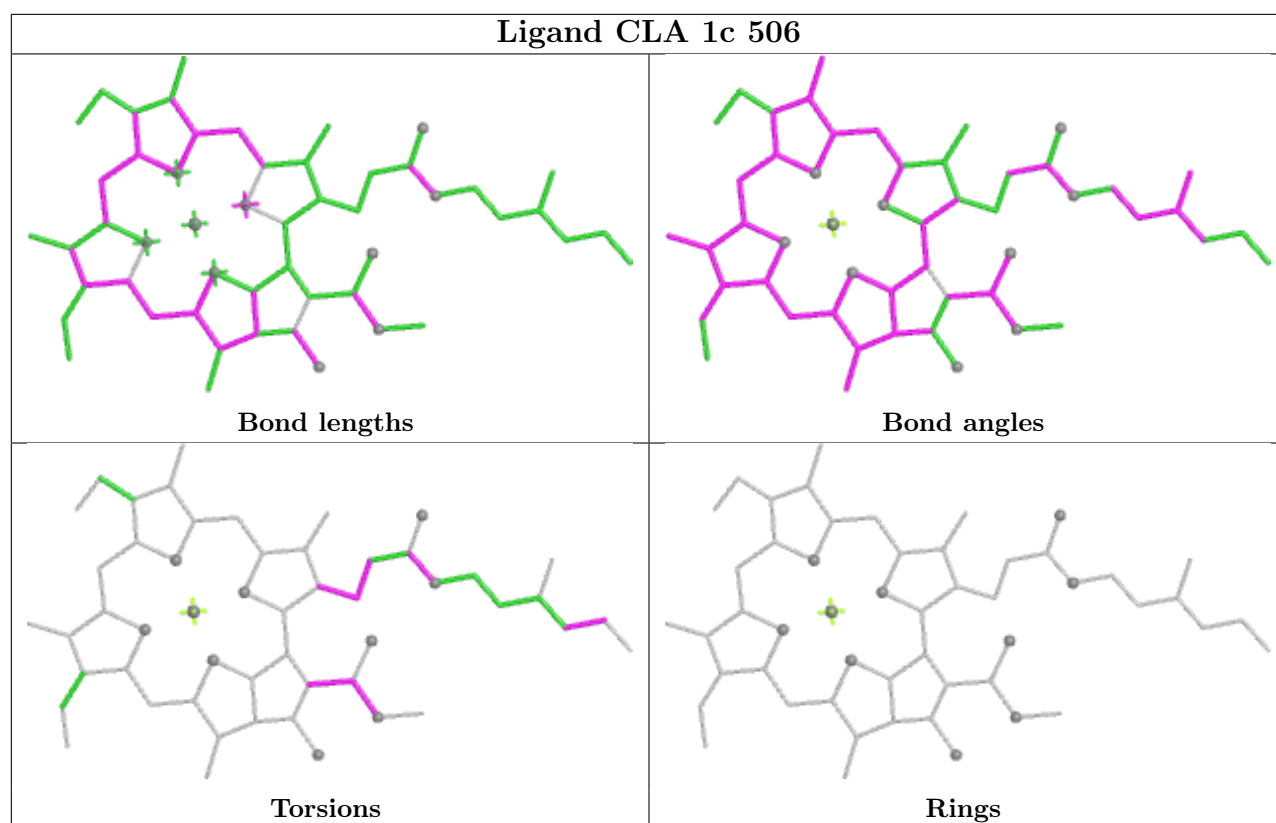


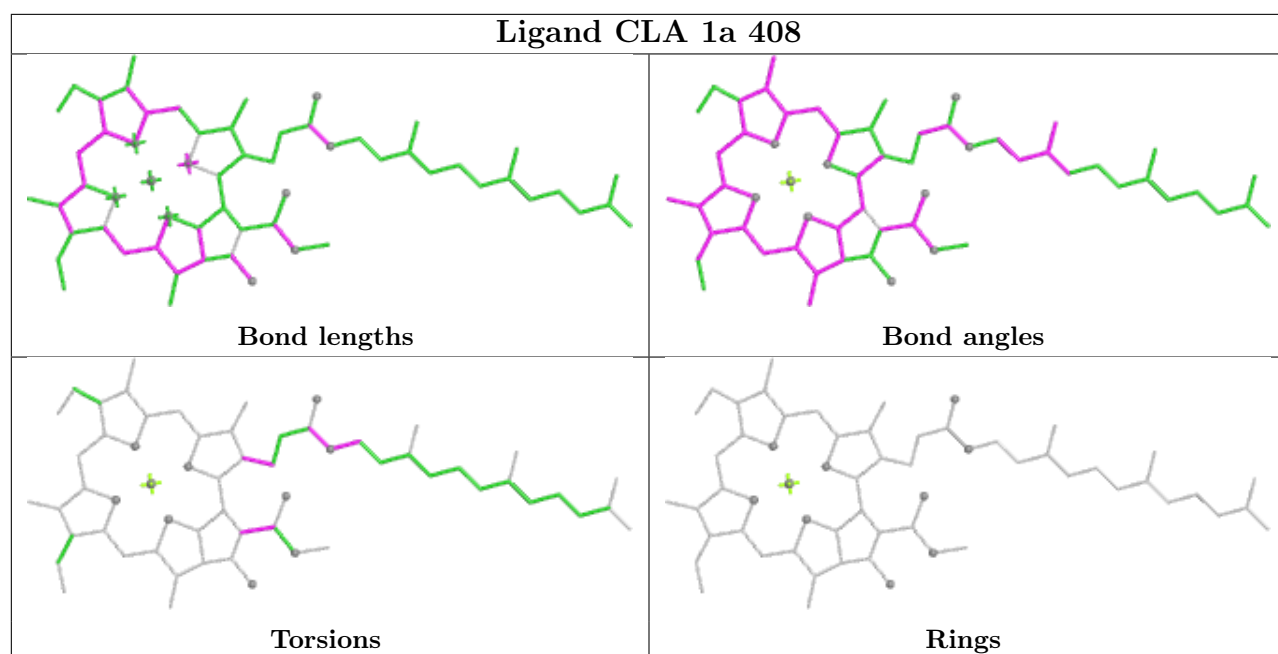


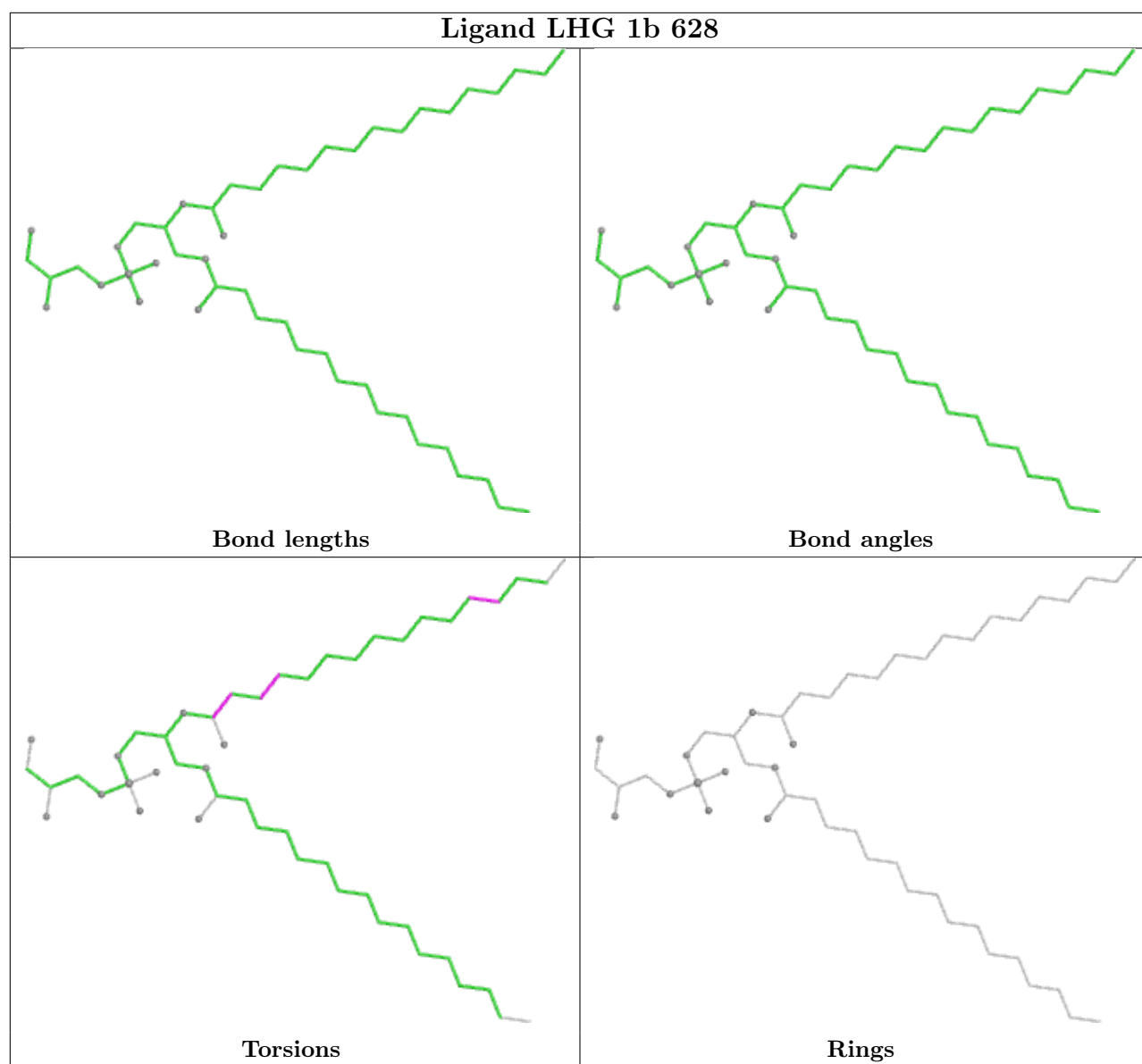


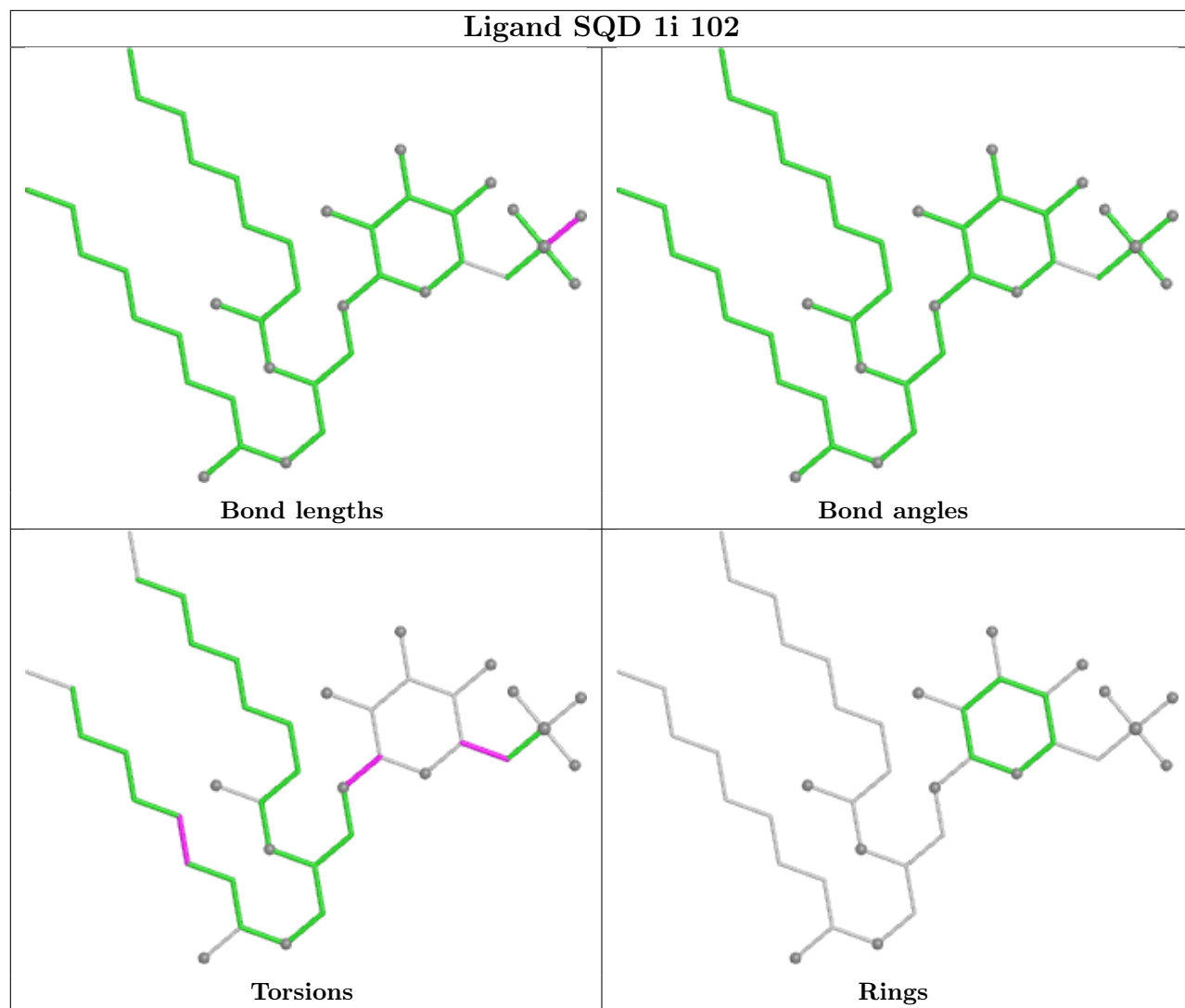


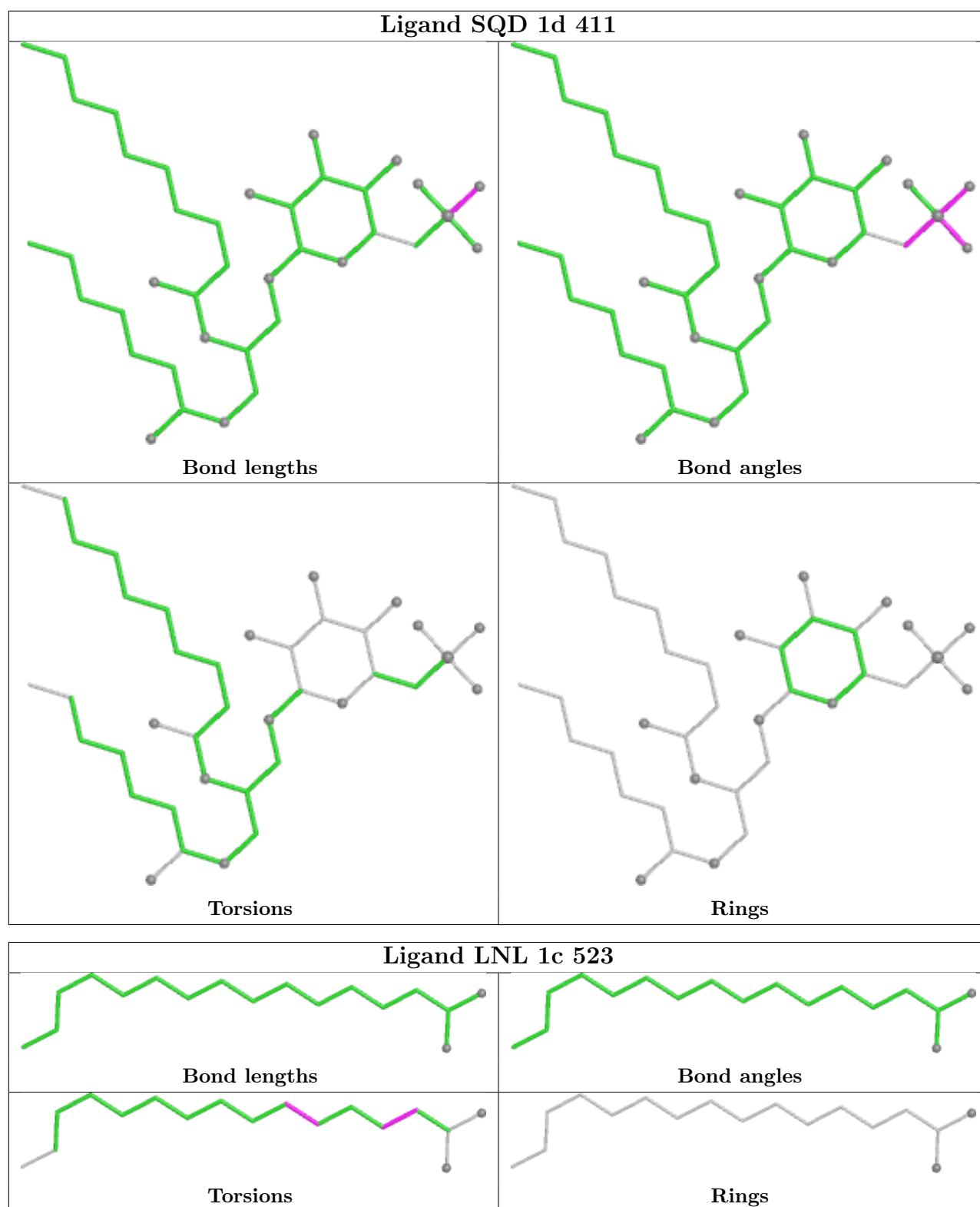


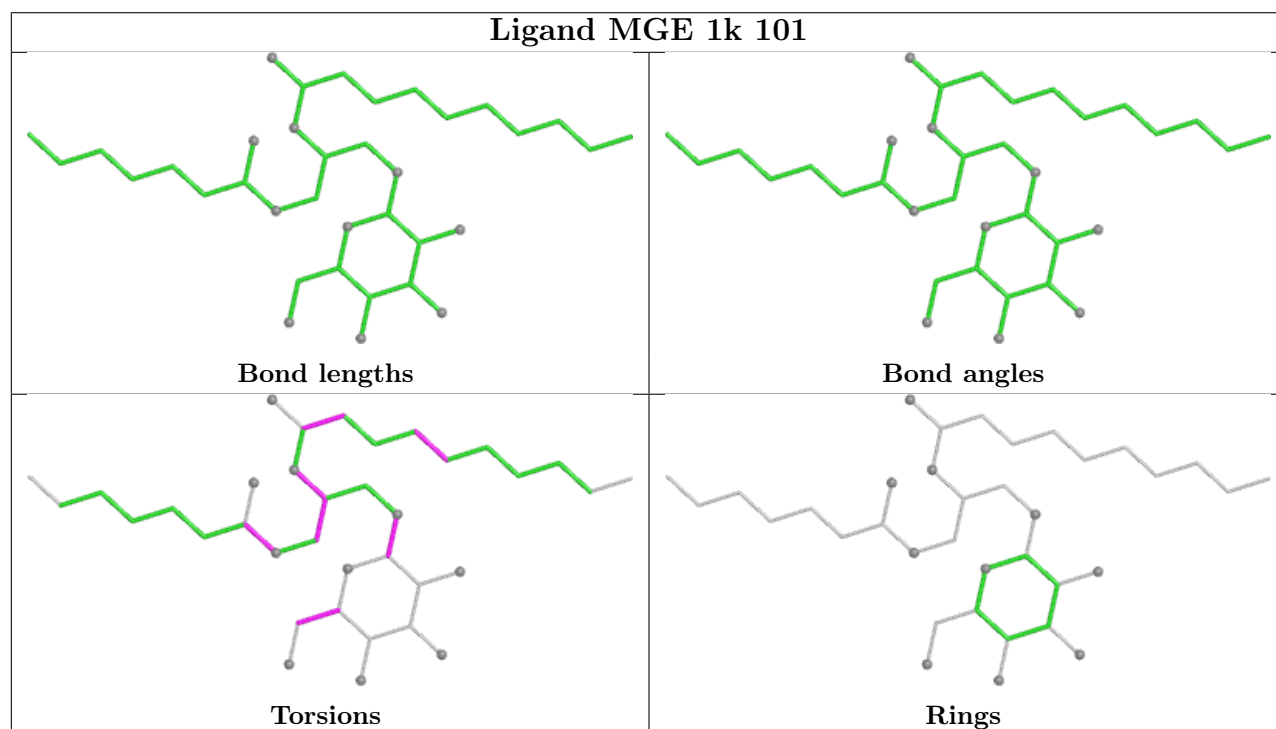
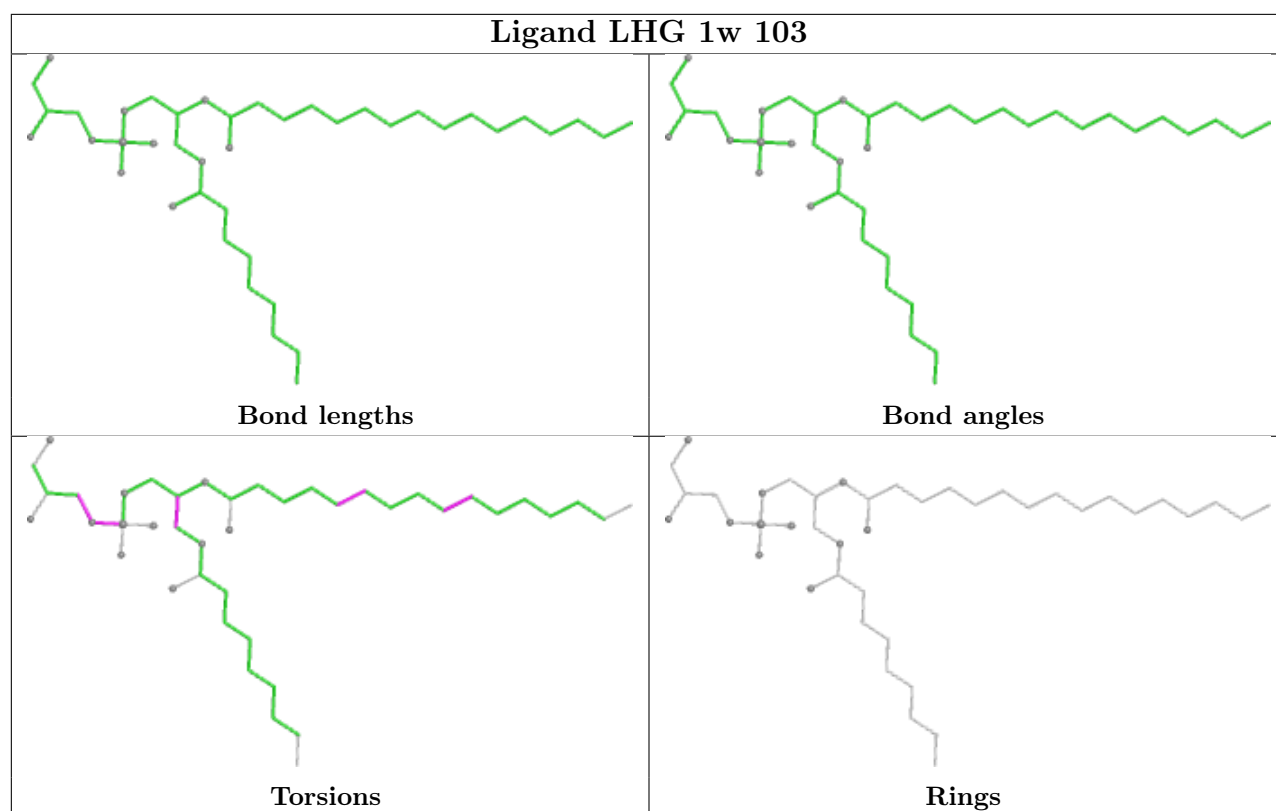


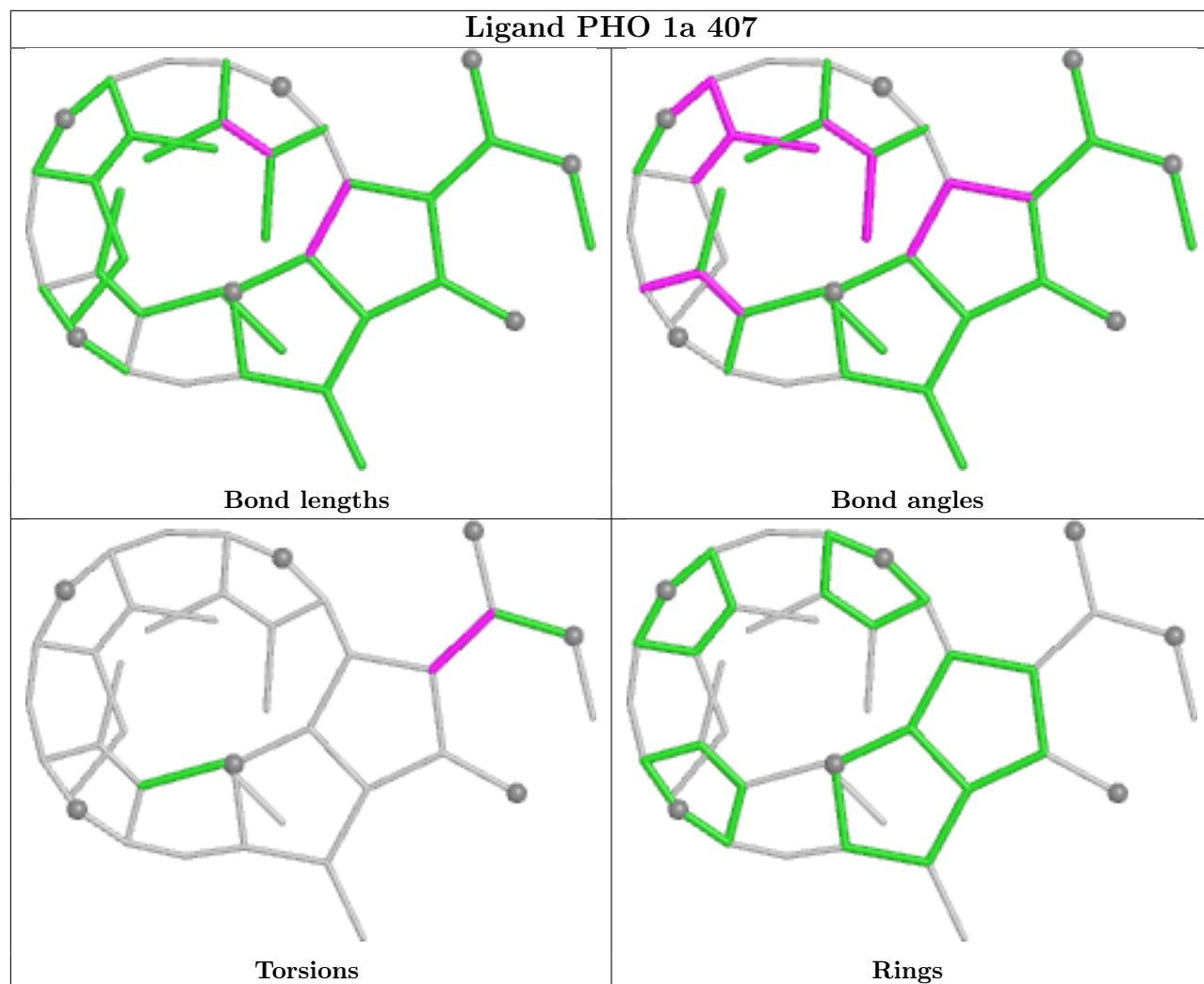


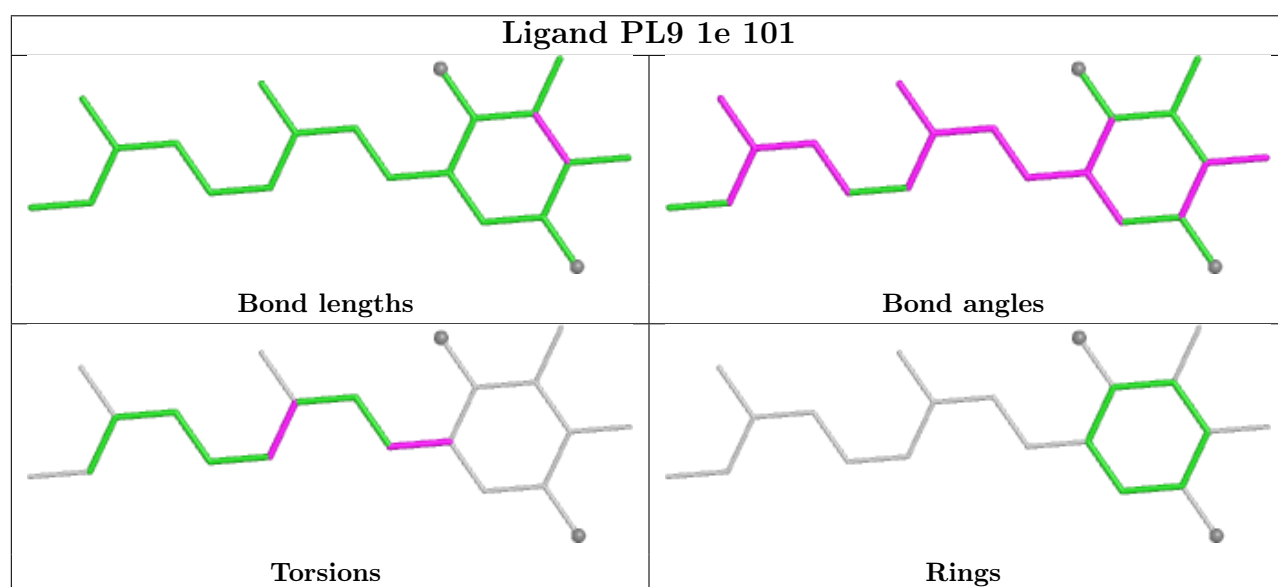
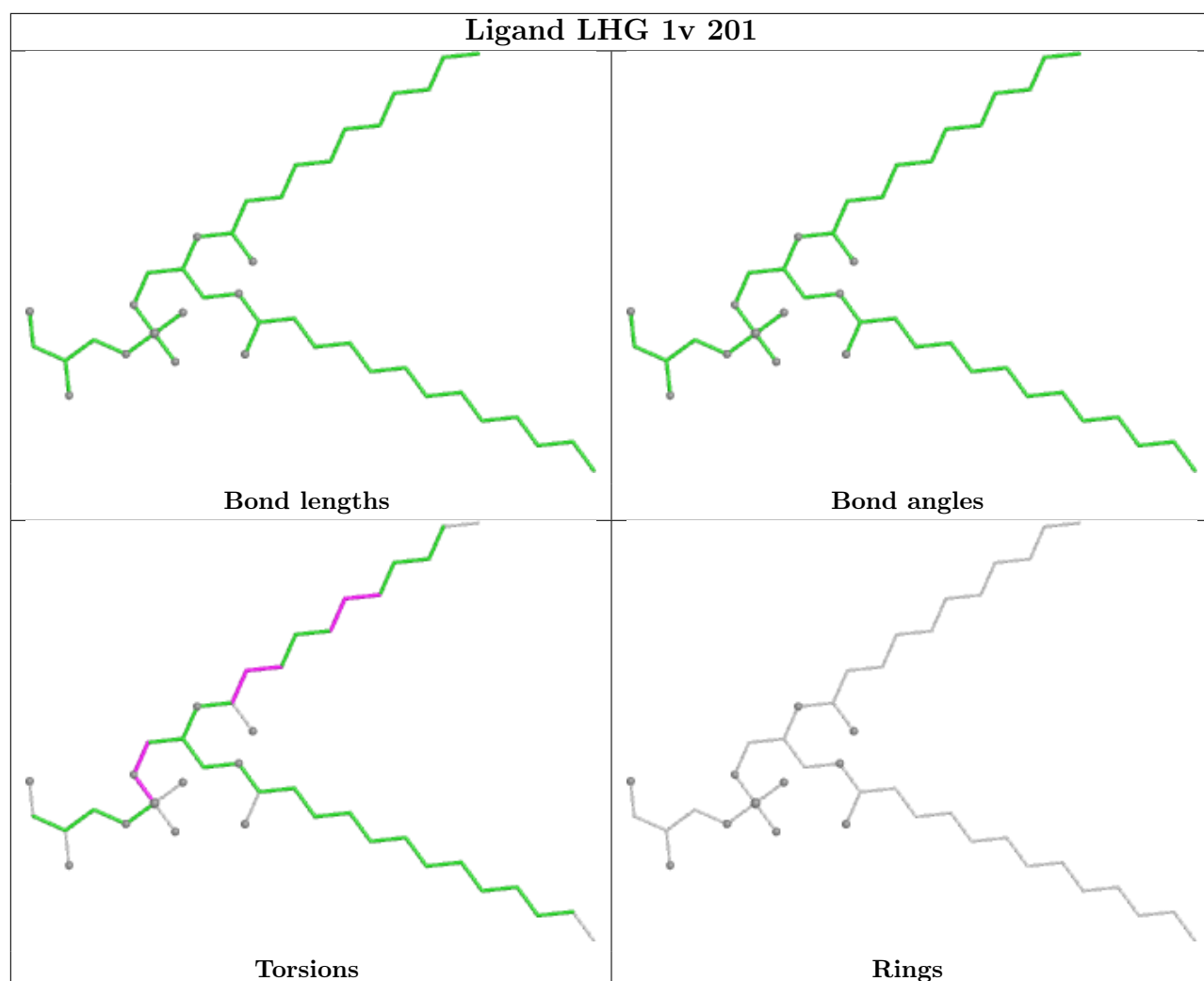


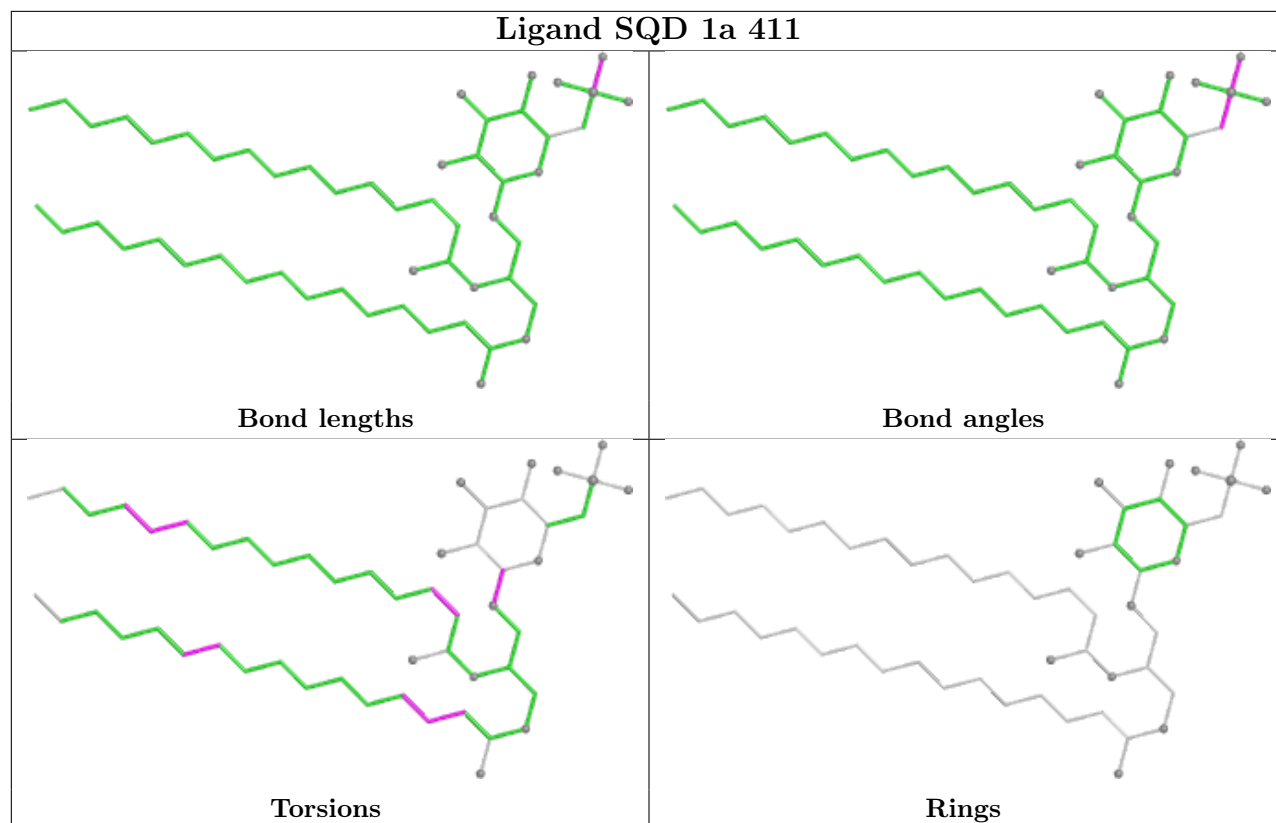
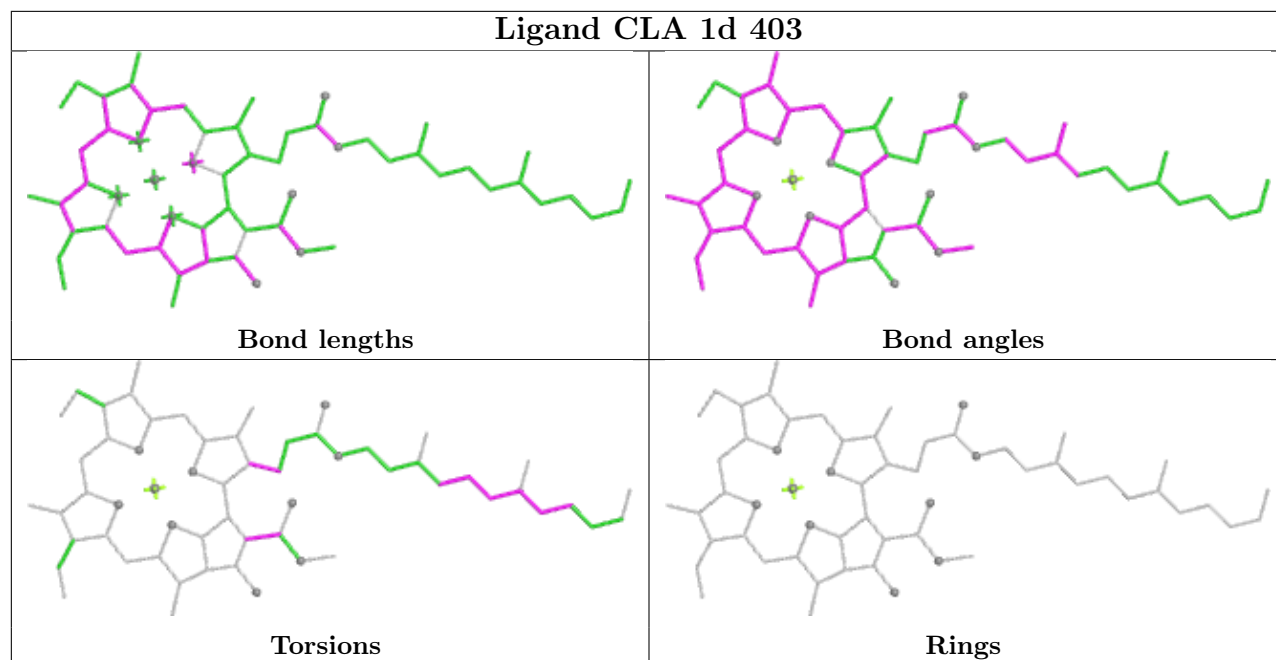


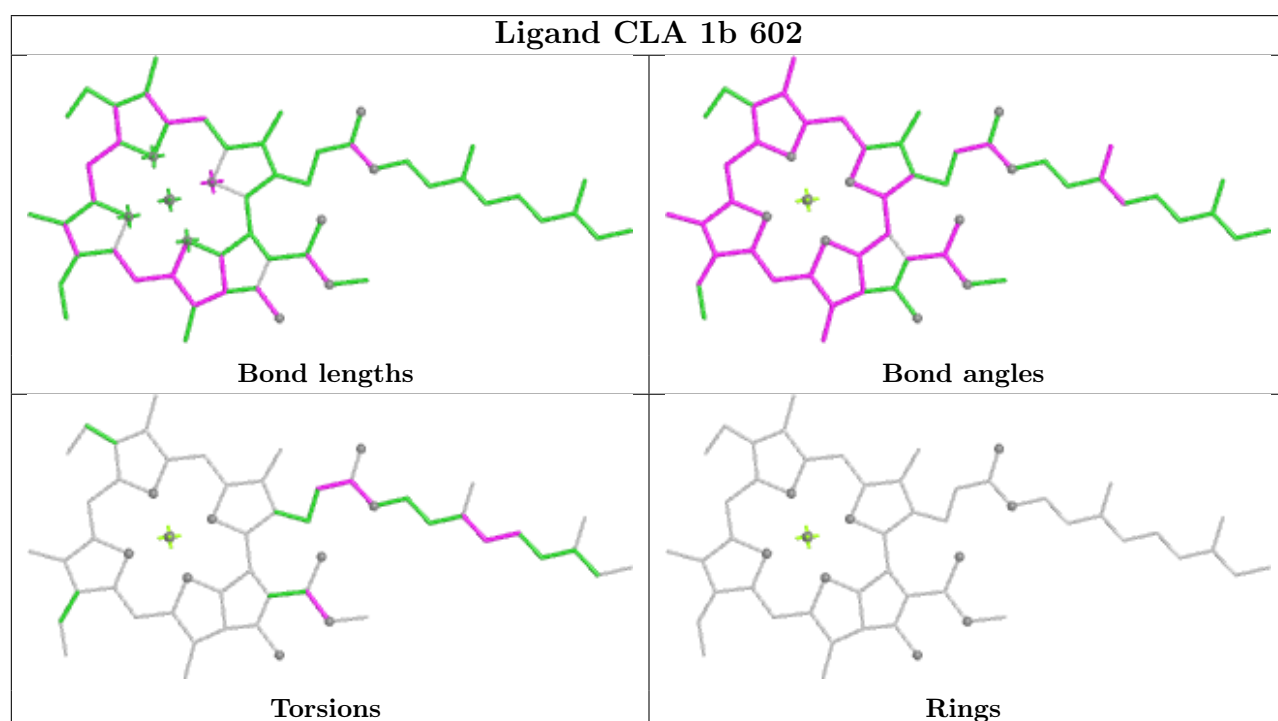
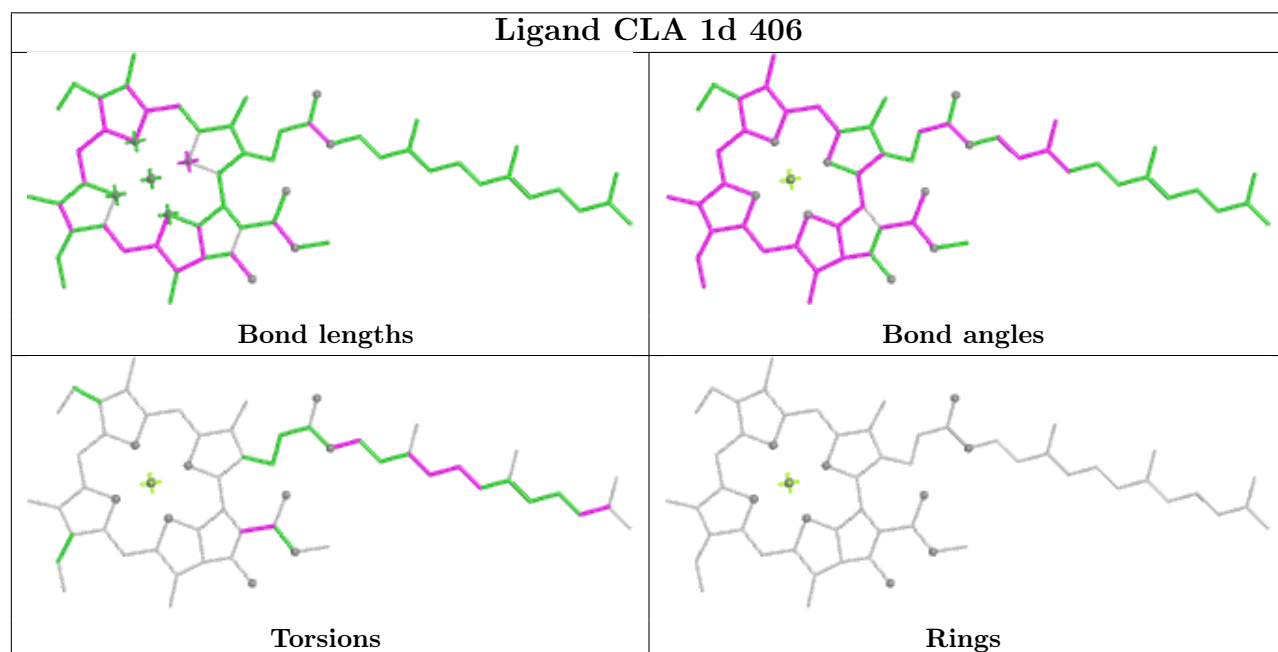
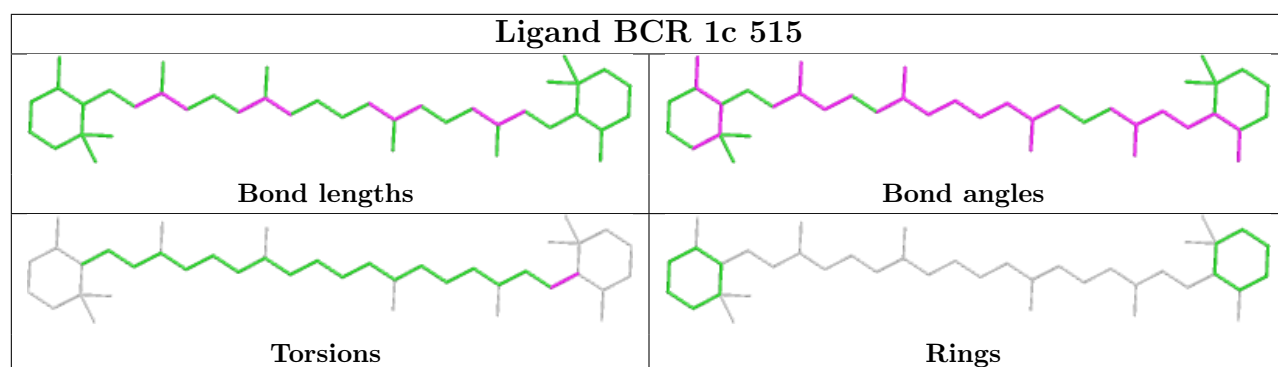


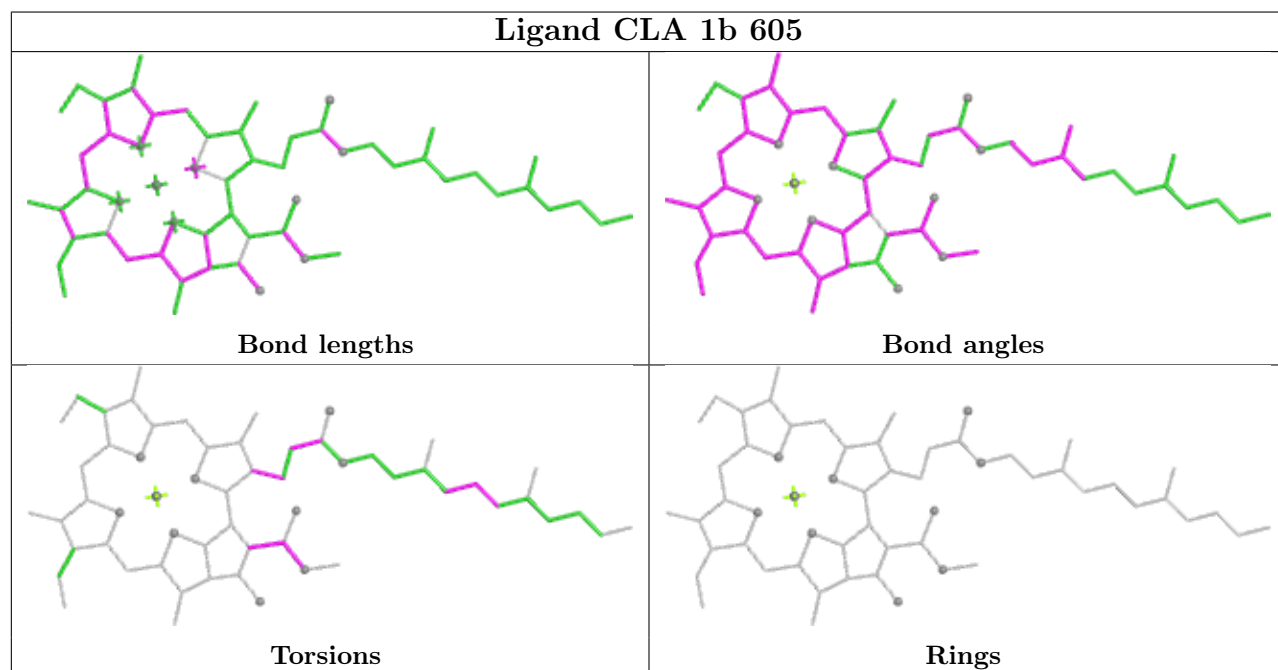
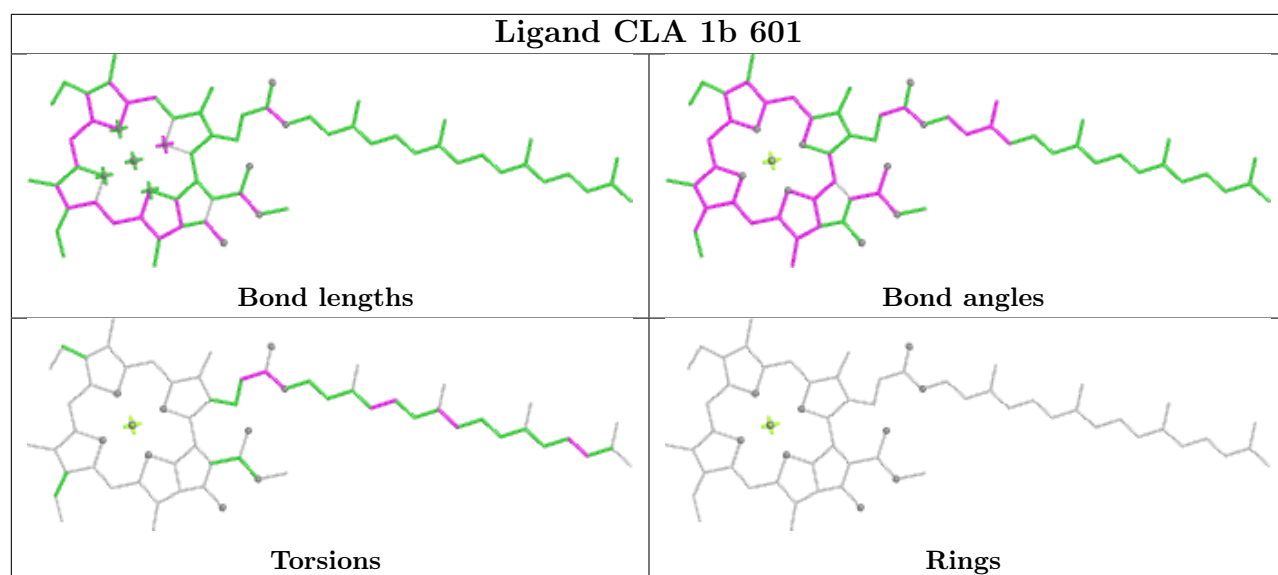


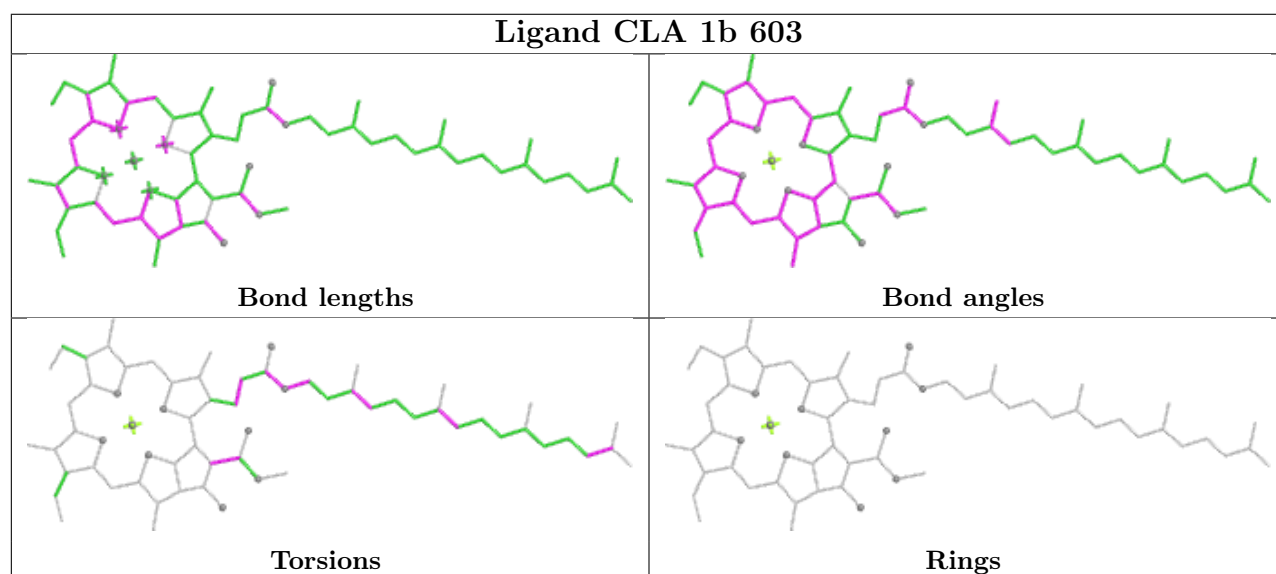
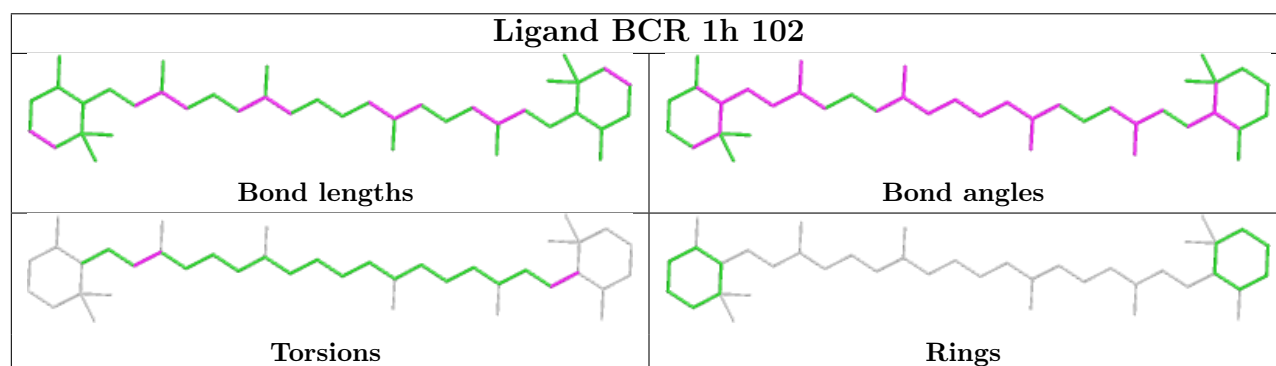
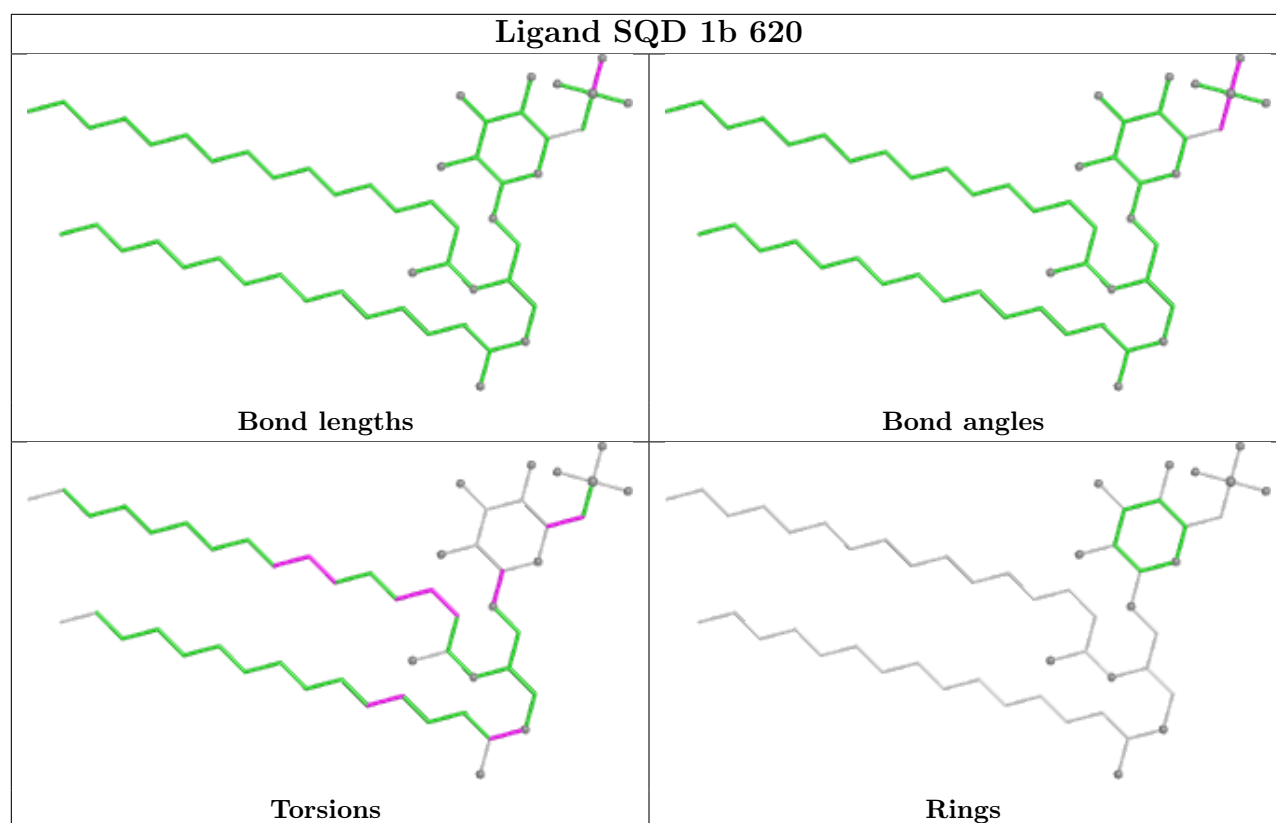


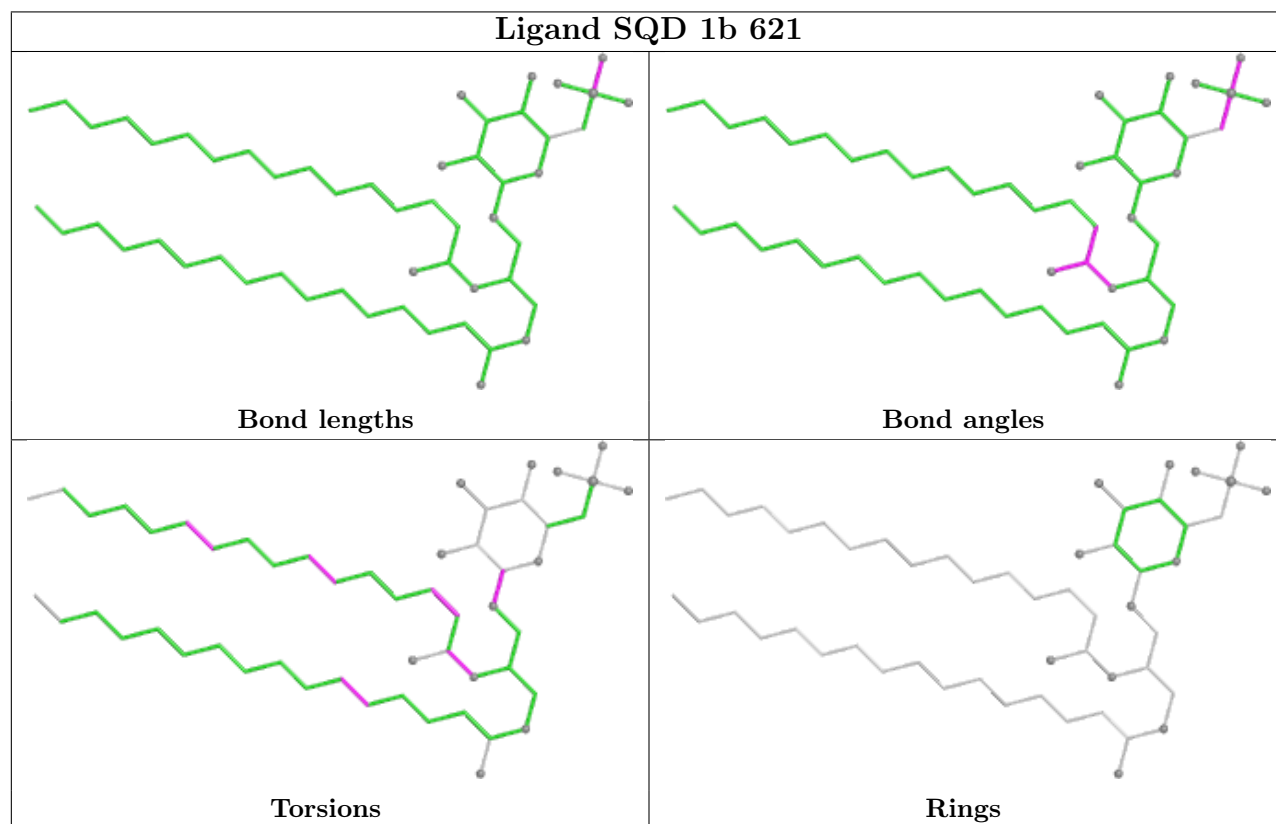
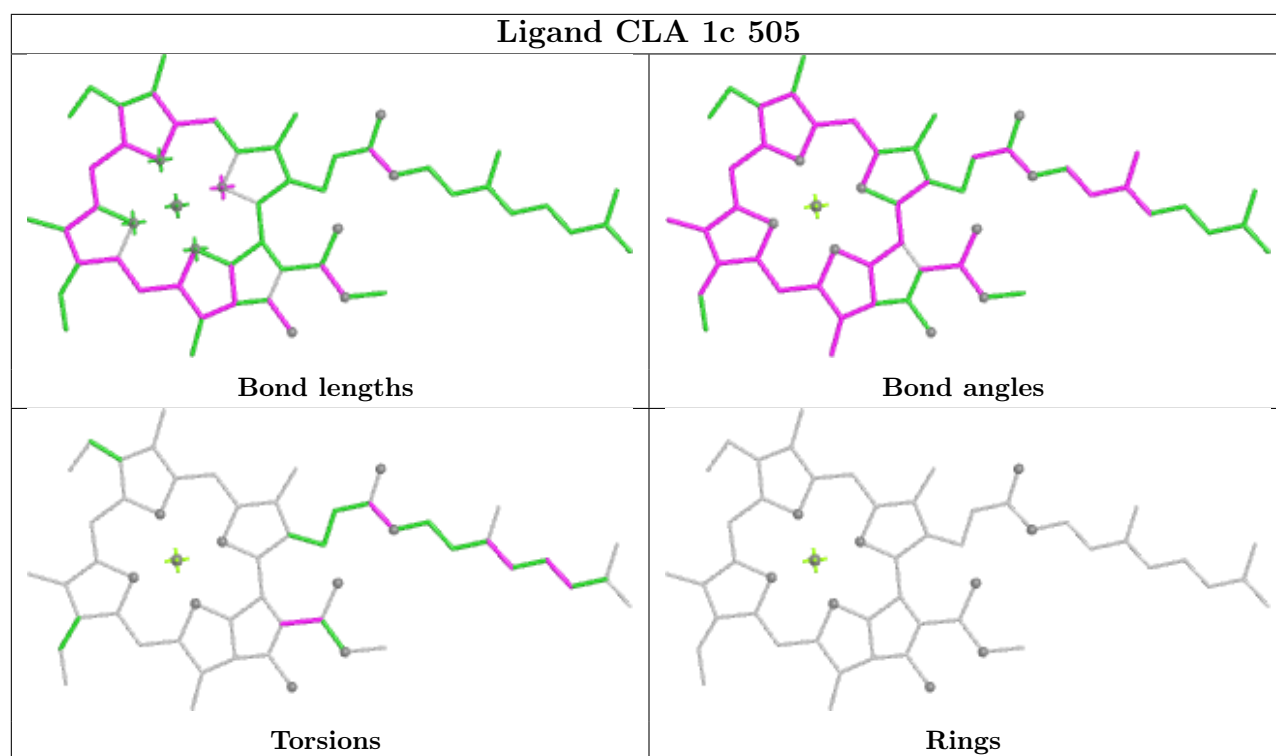


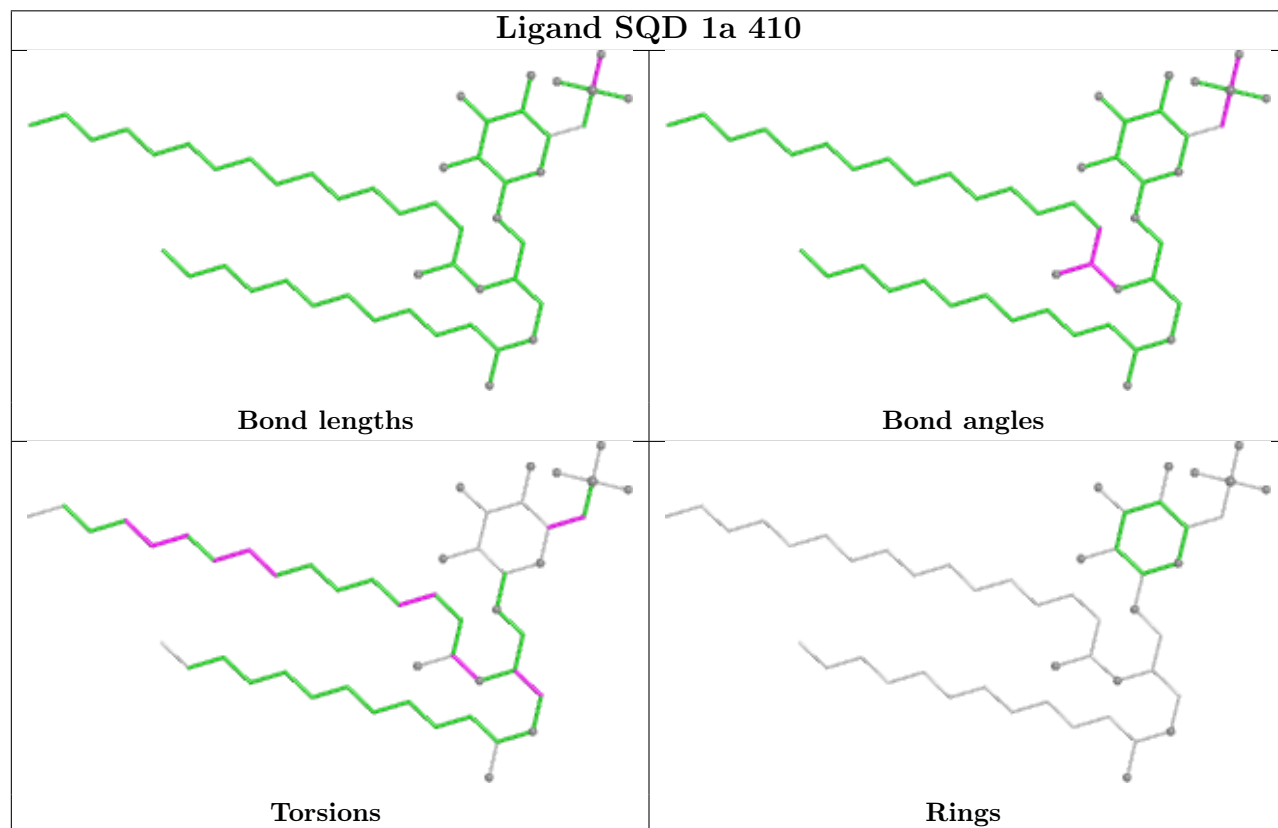
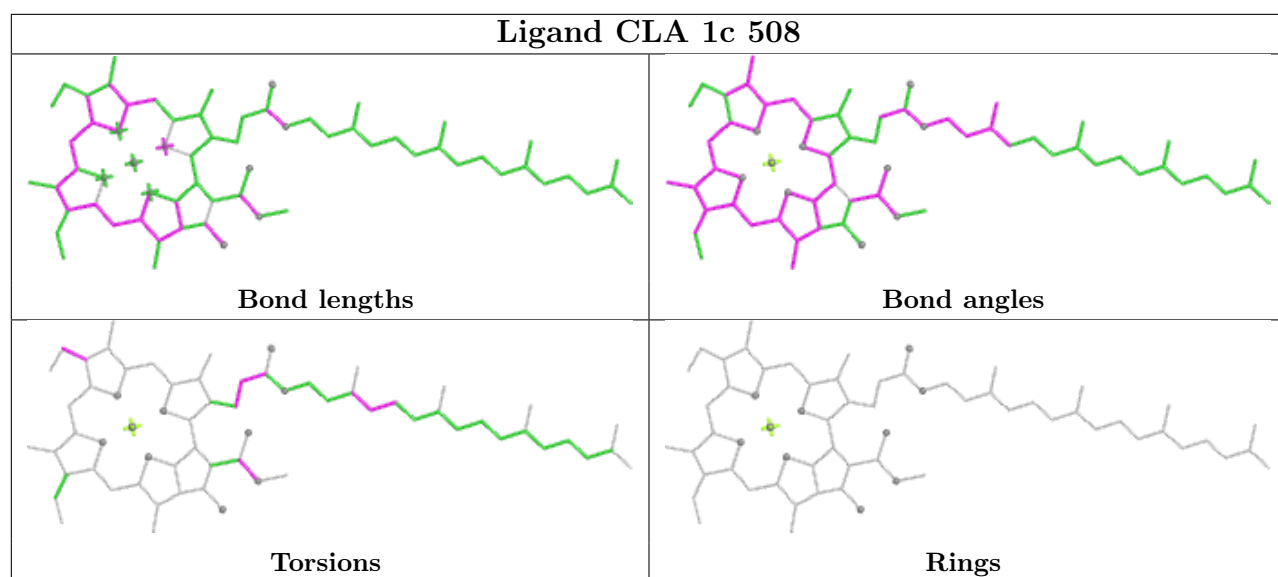


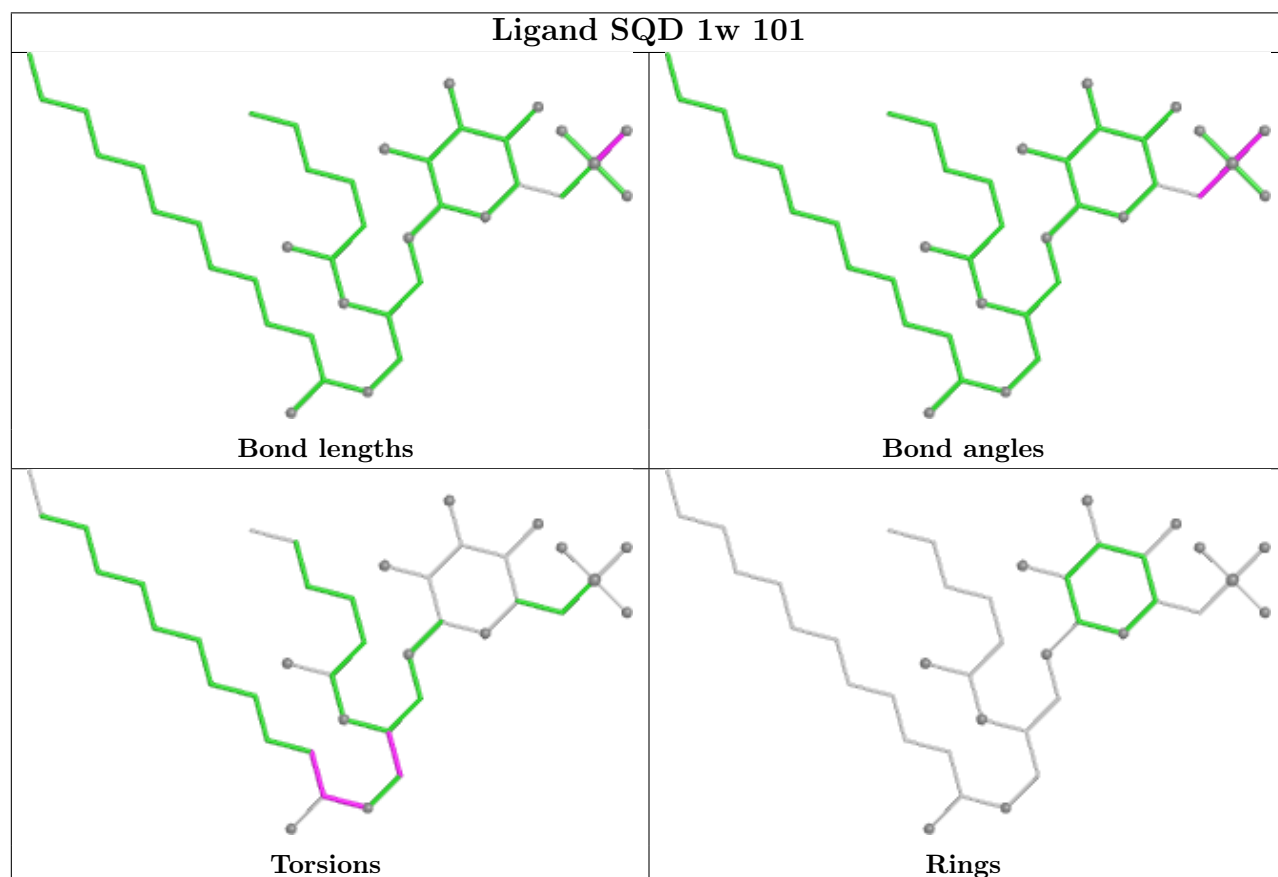
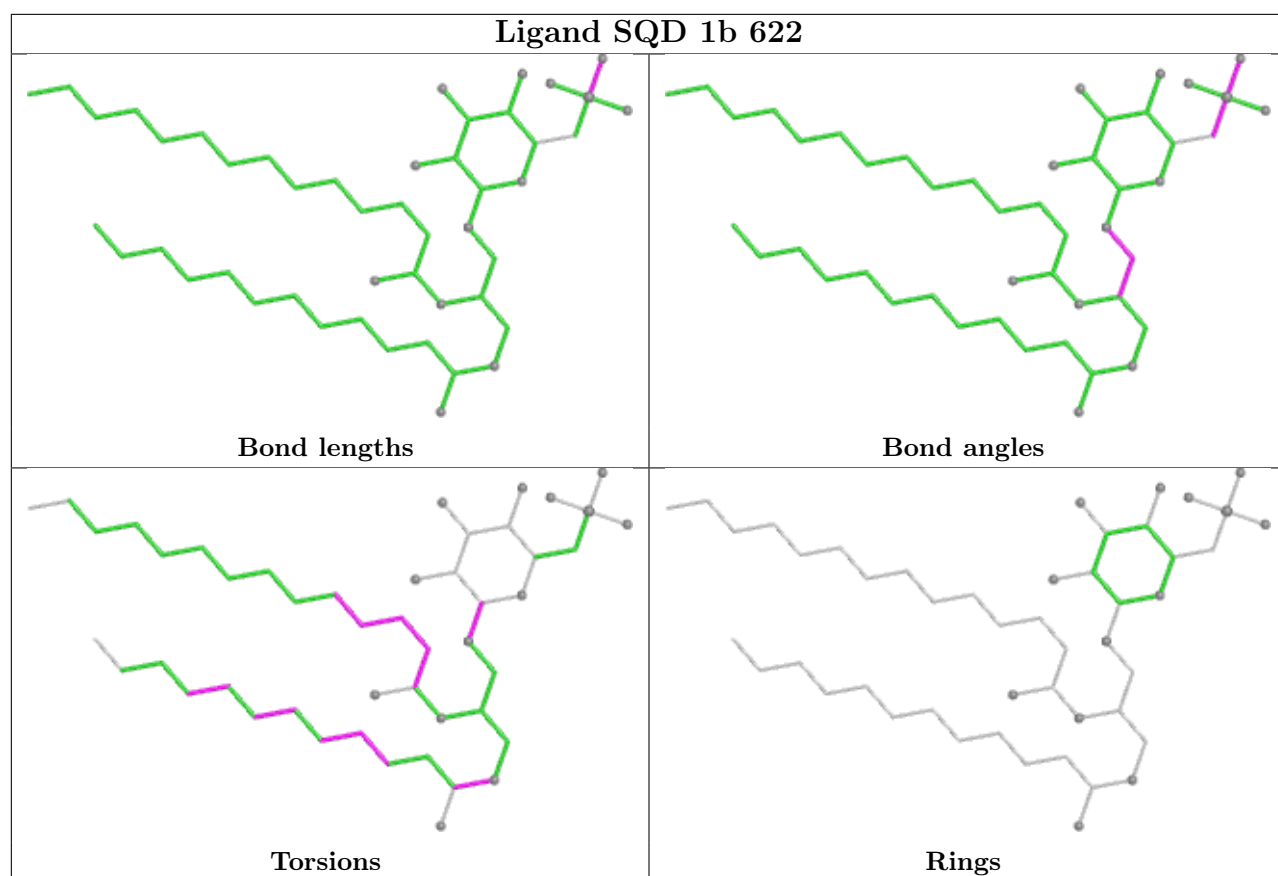


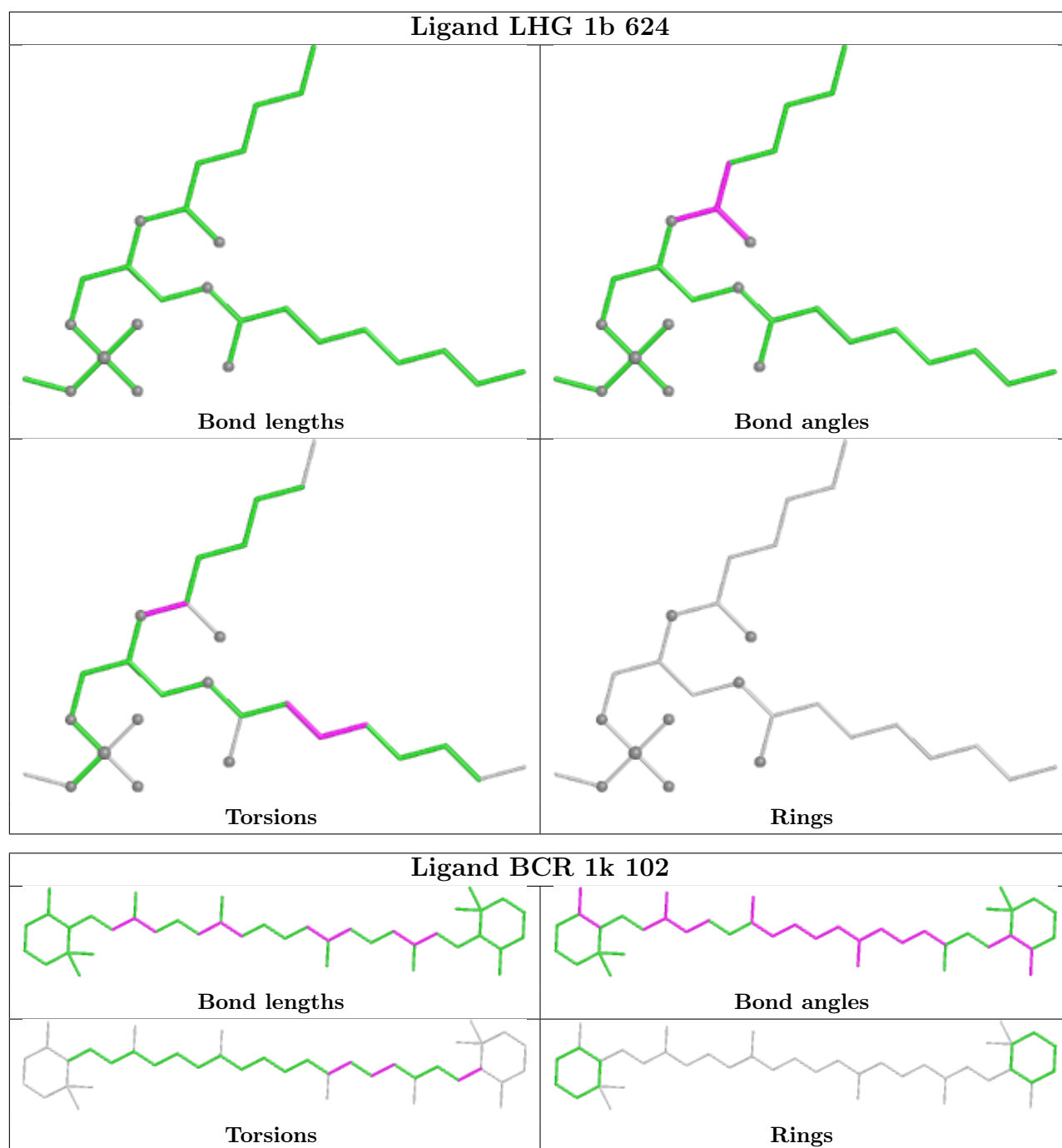


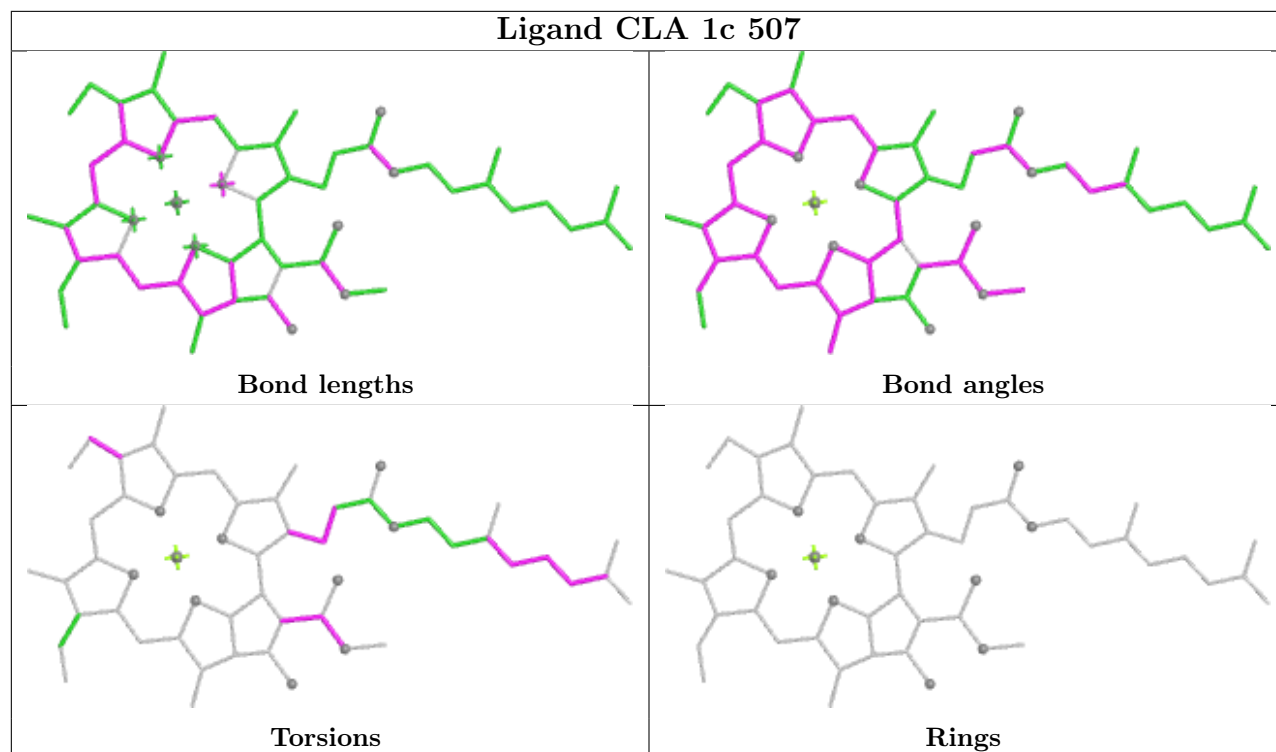
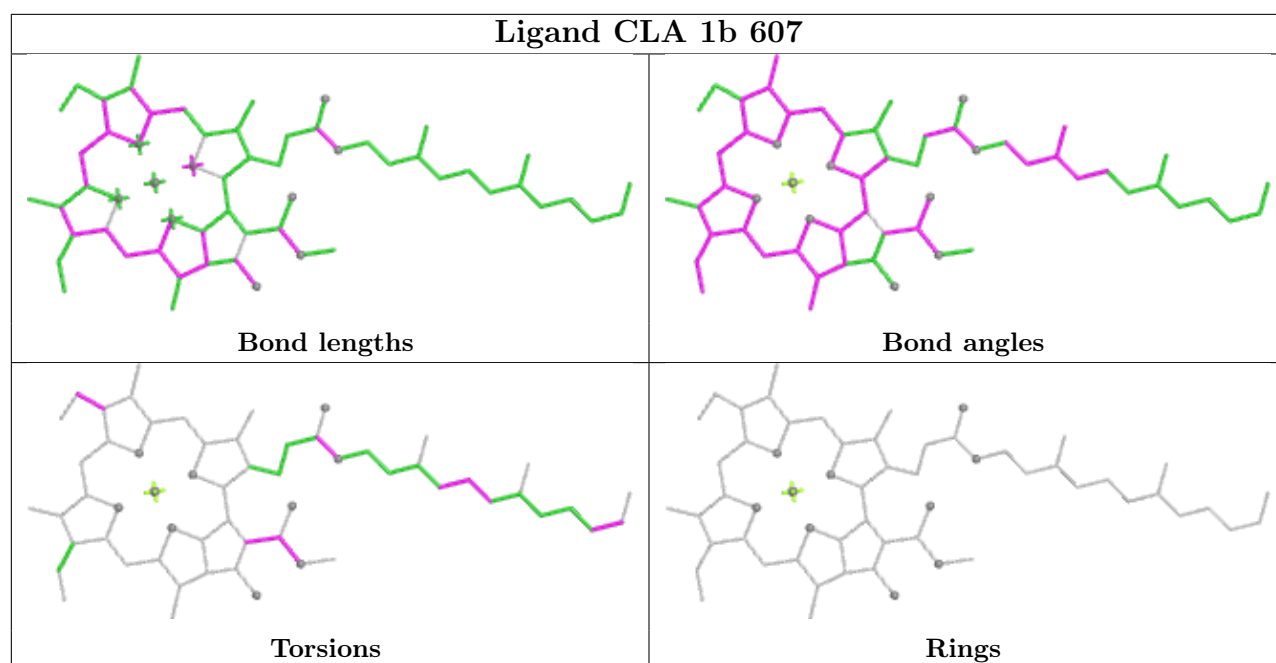


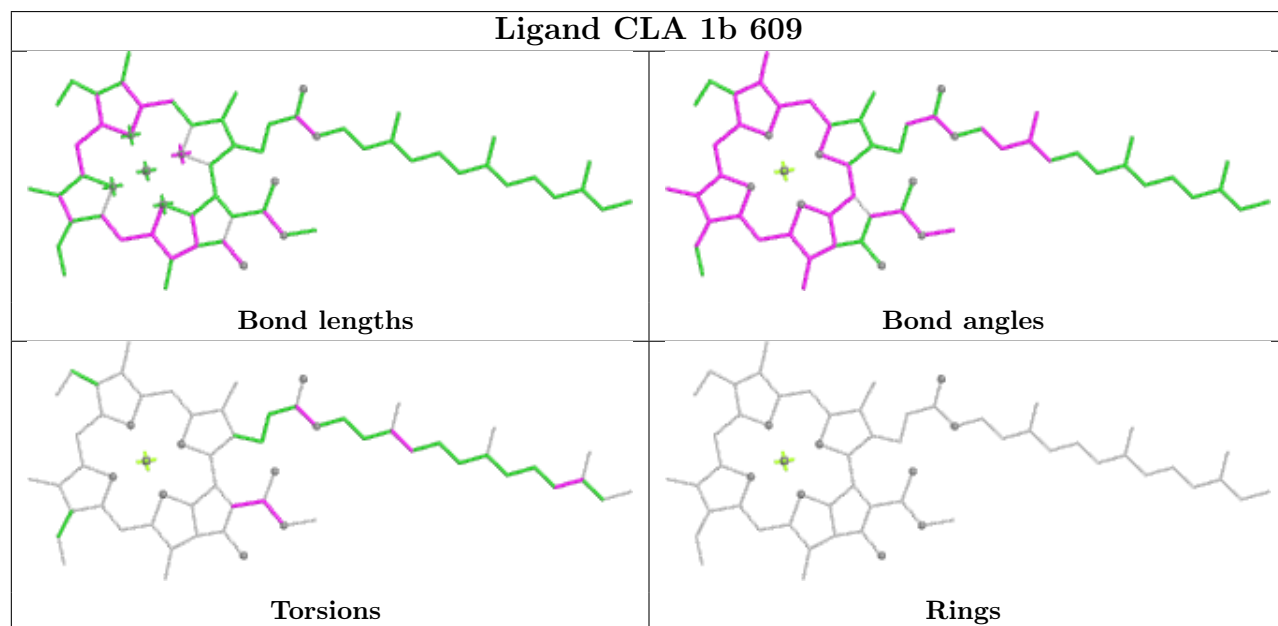
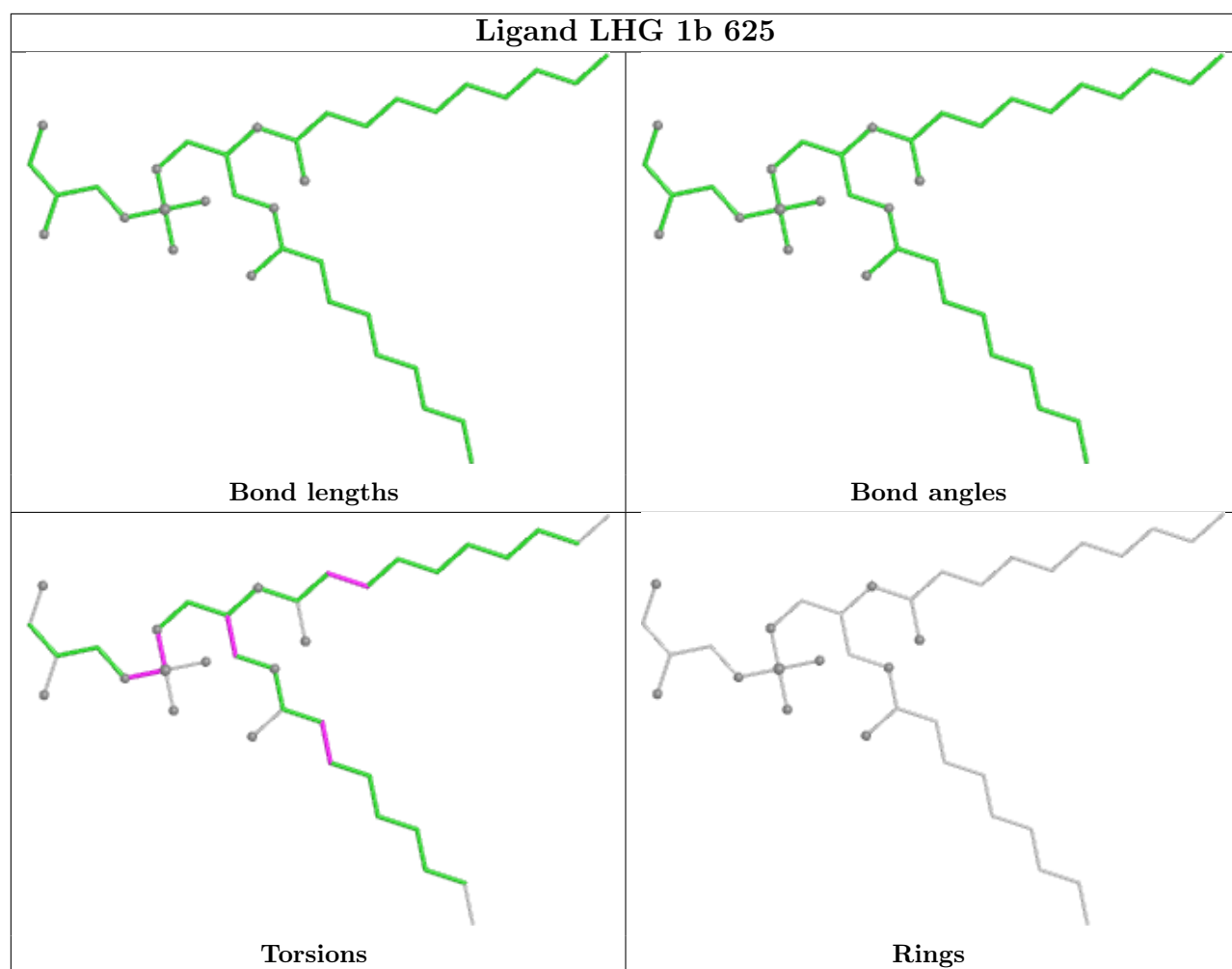


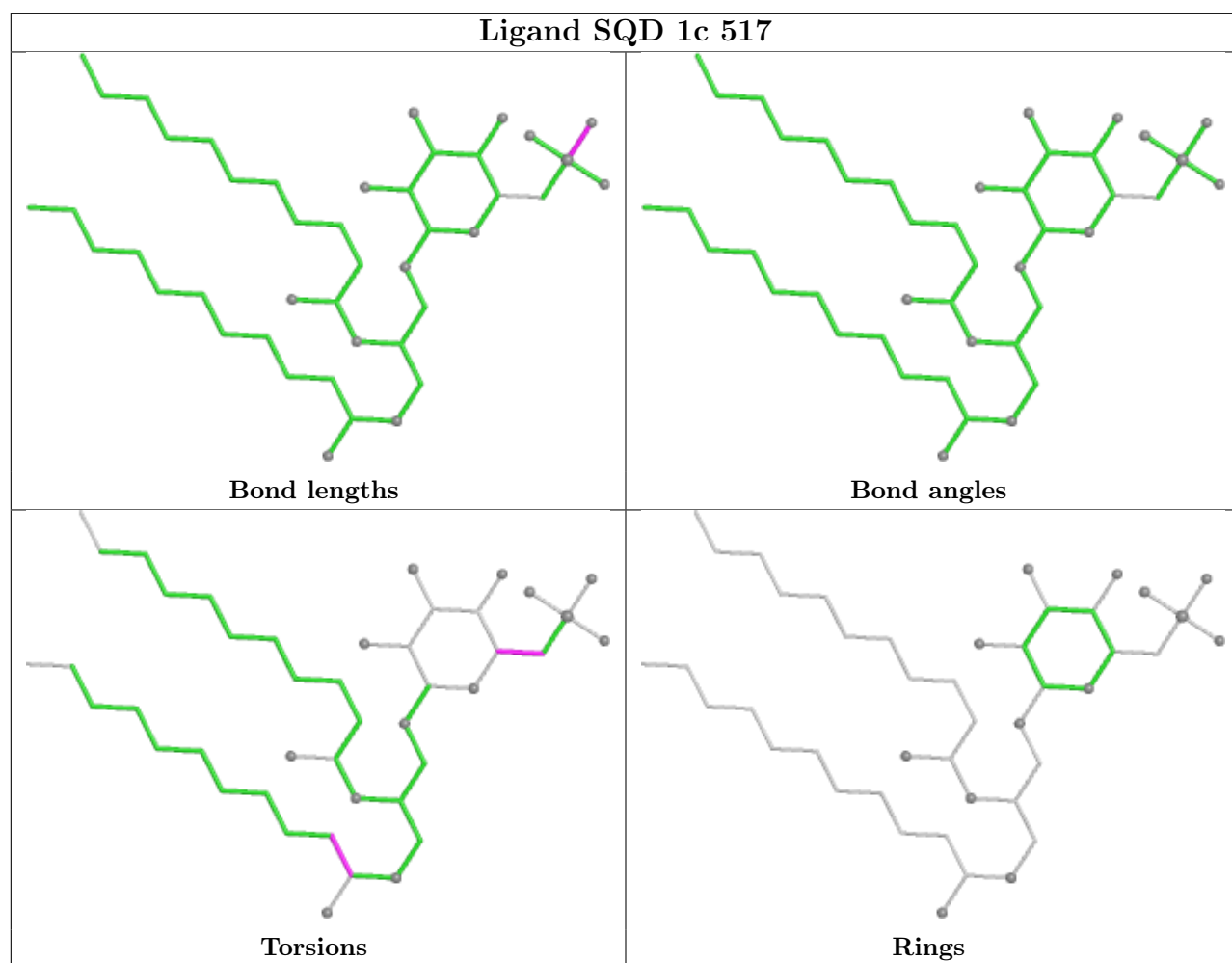


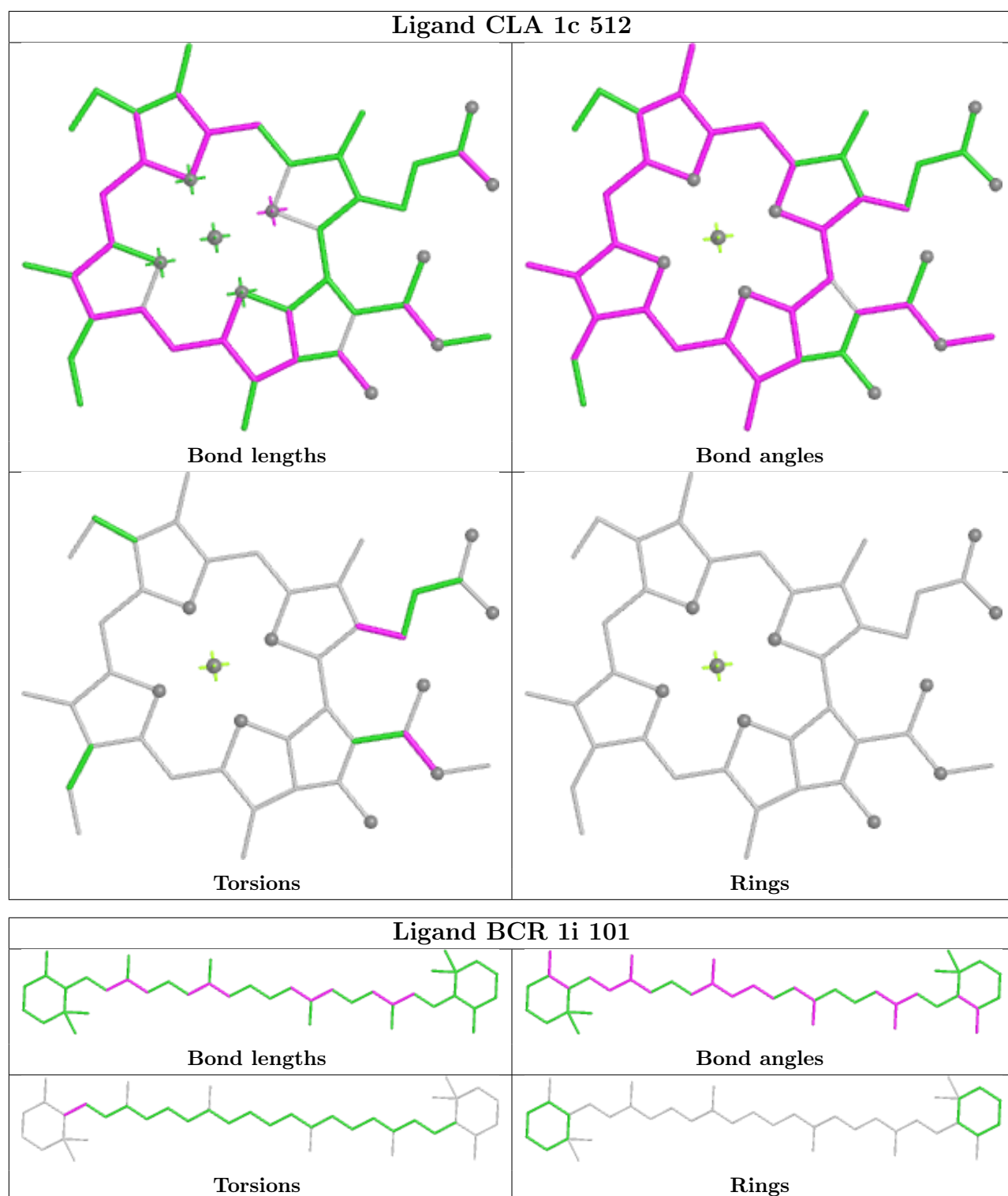


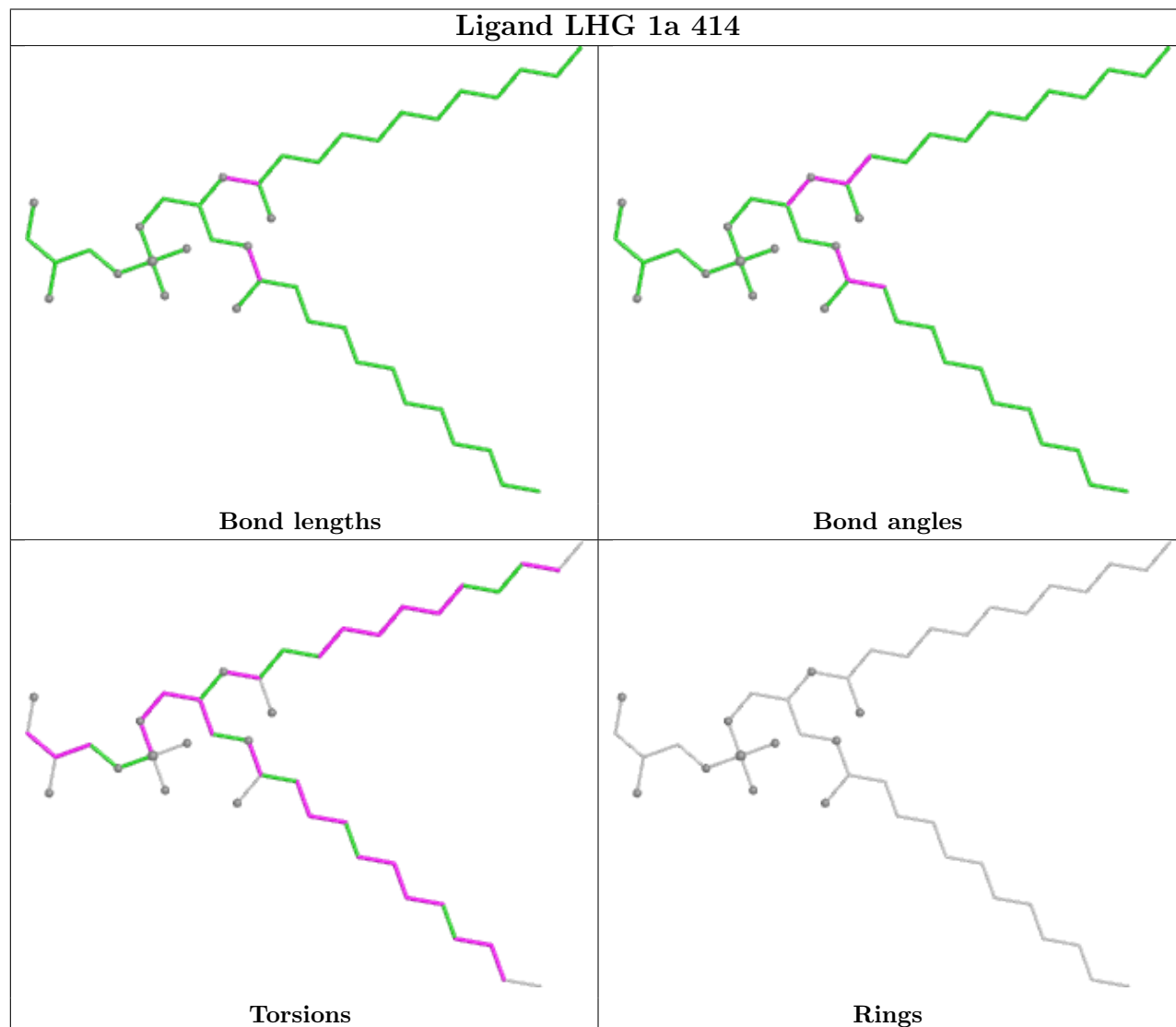
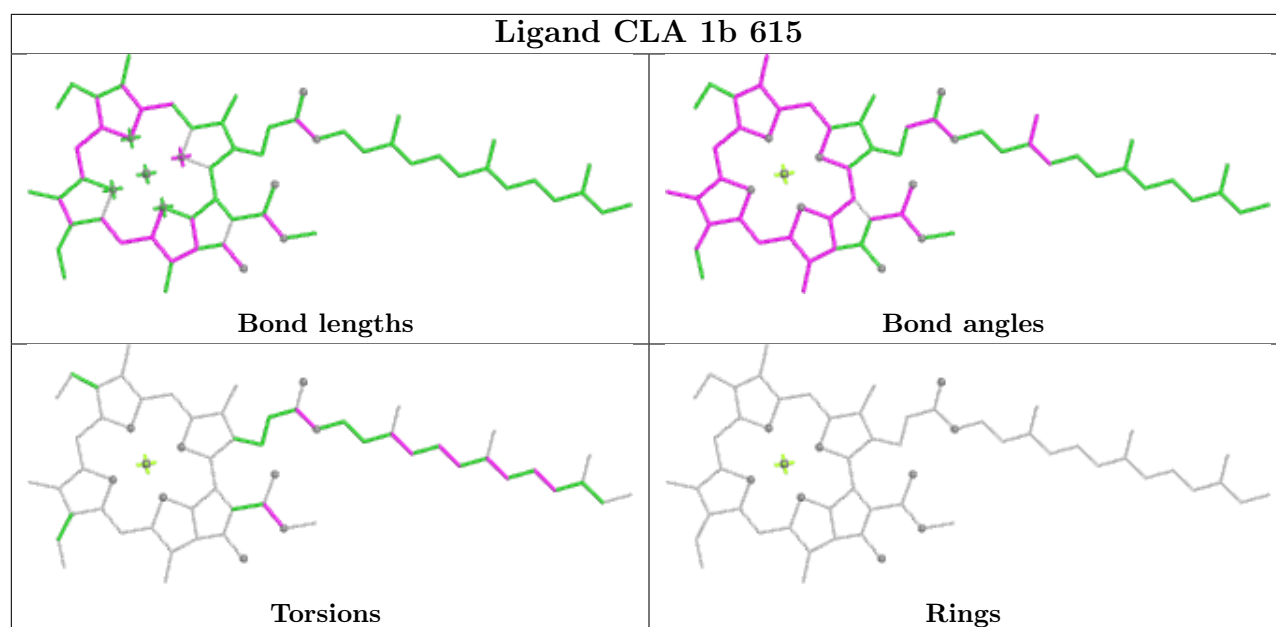


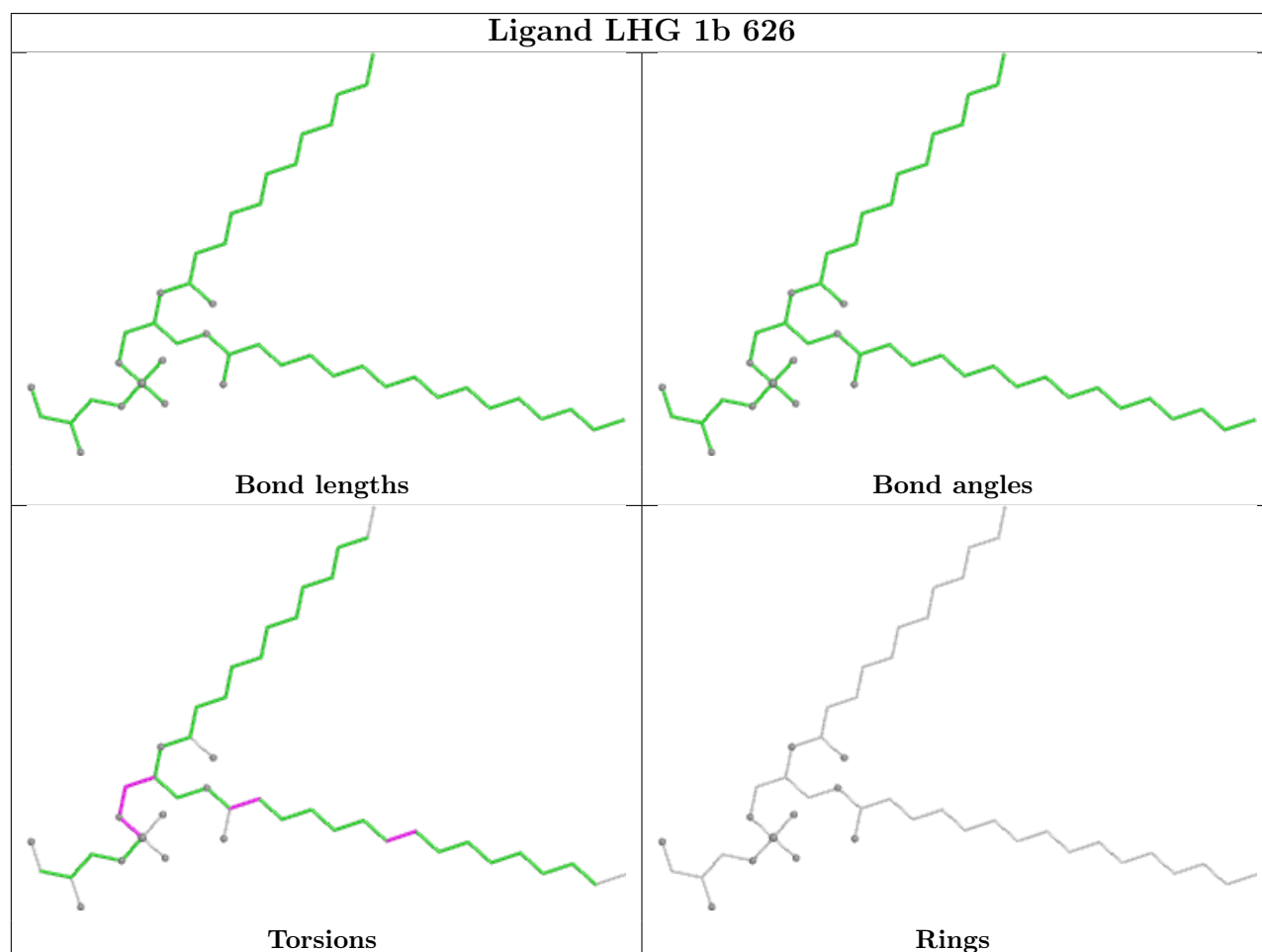
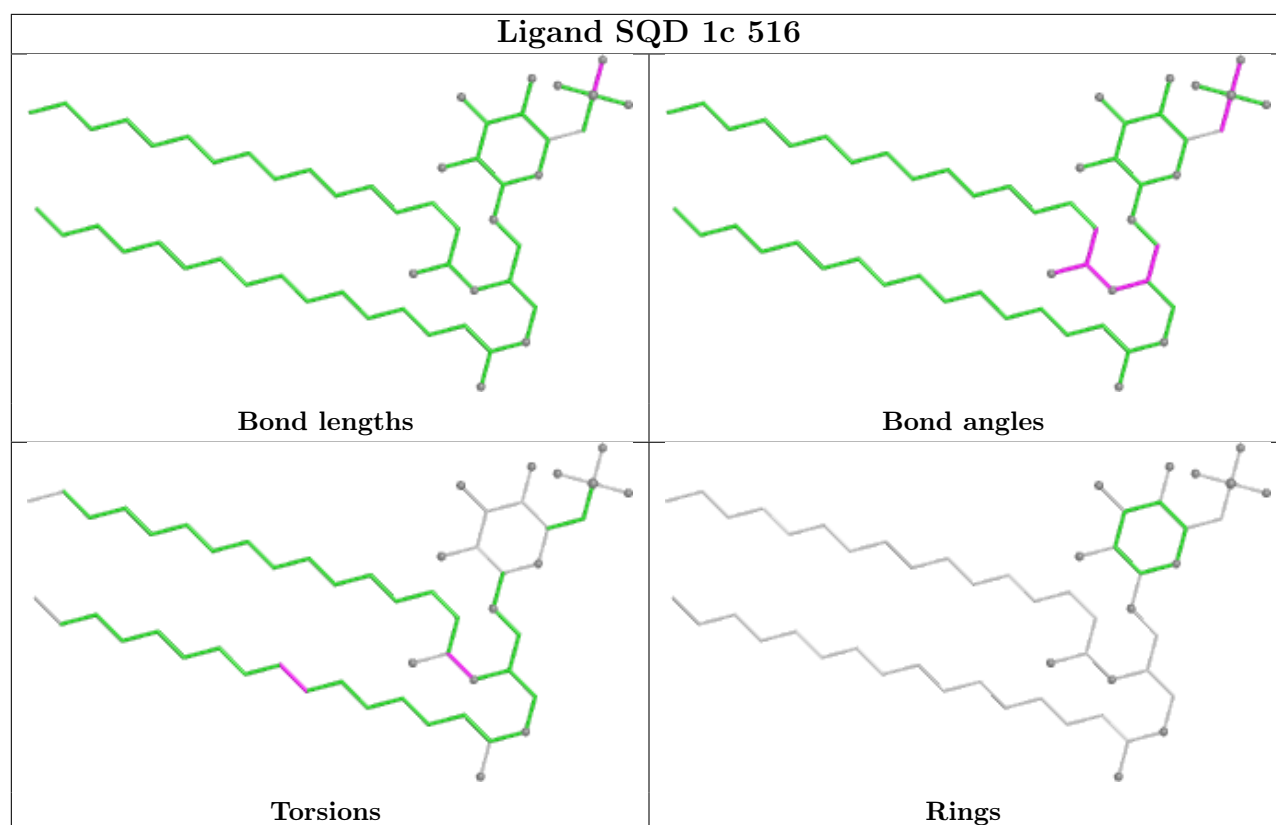


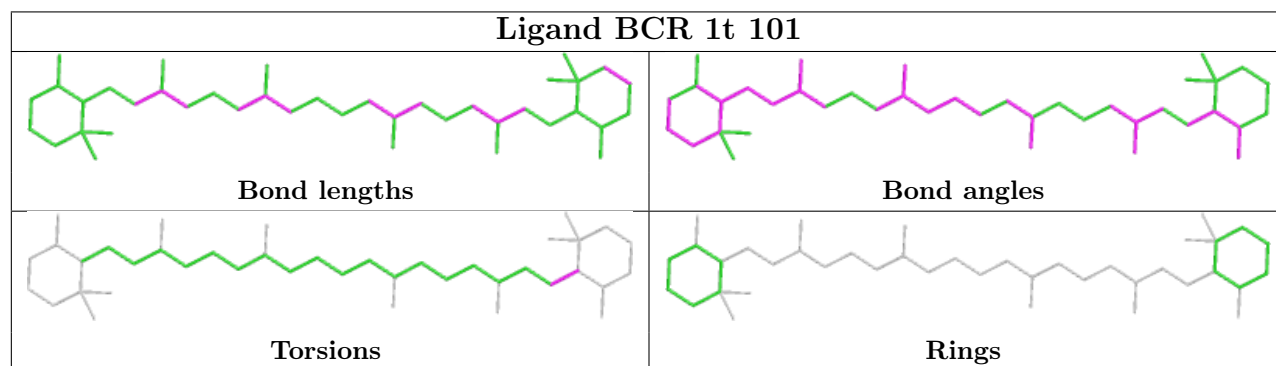
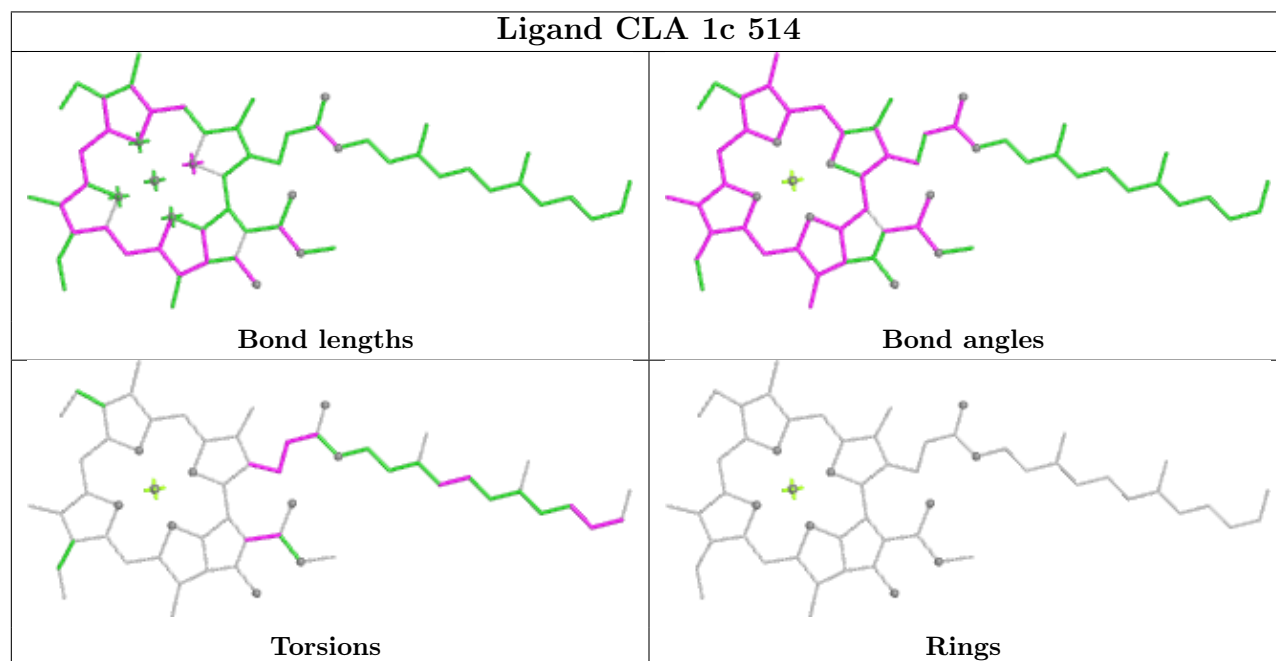
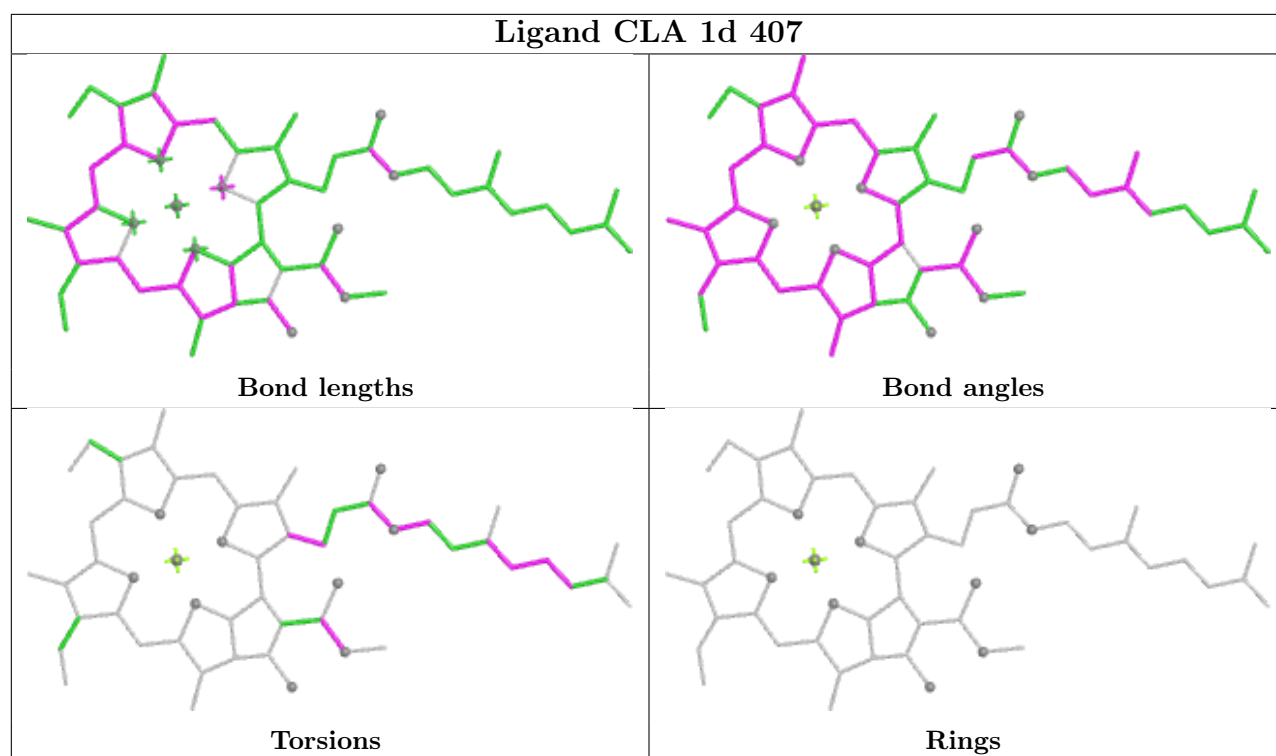


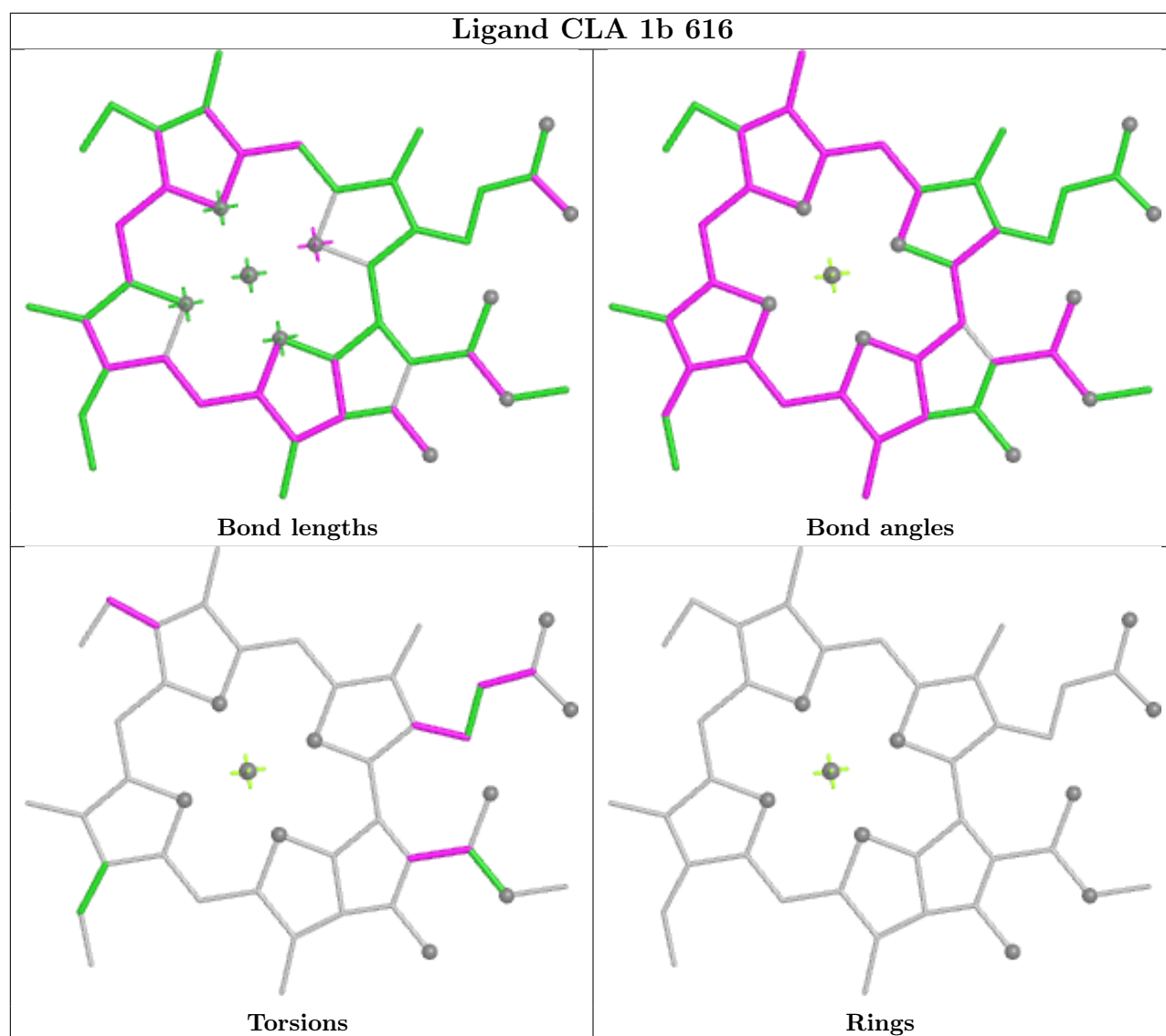












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

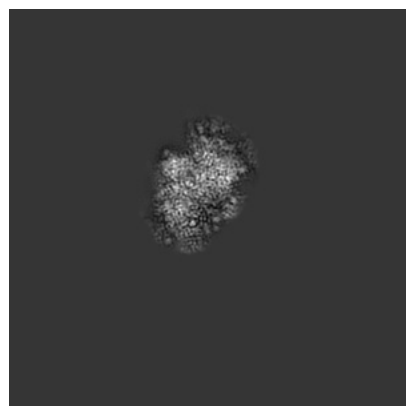
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66947. These allow visual inspection of the internal detail of the map and identification of artifacts.

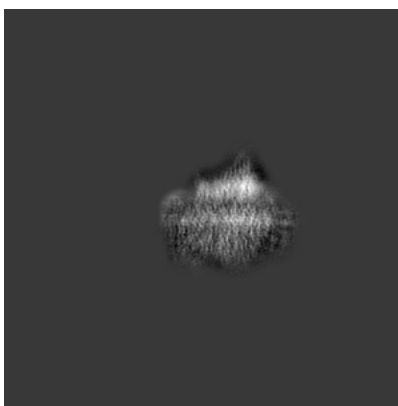
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

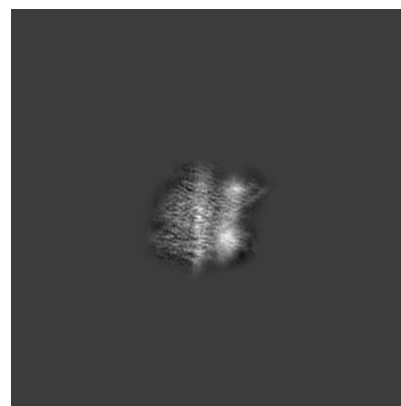
6.1.1 Primary map



X

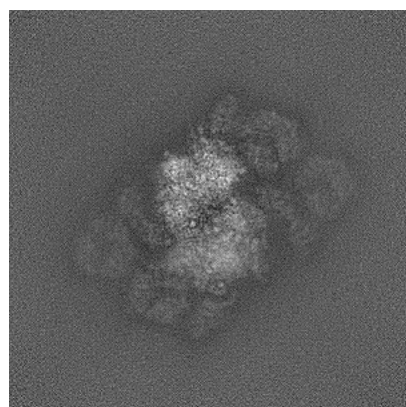


Y

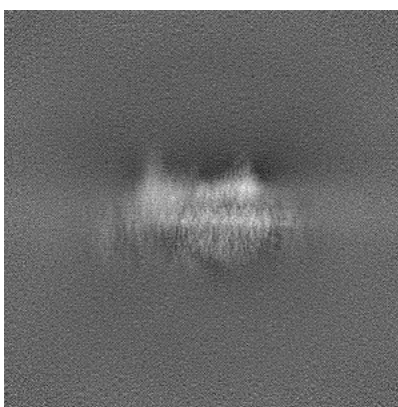


Z

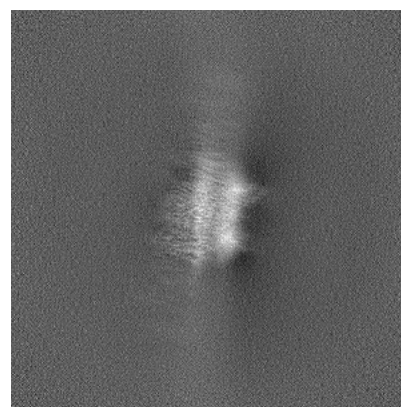
6.1.2 Raw map



X



Y

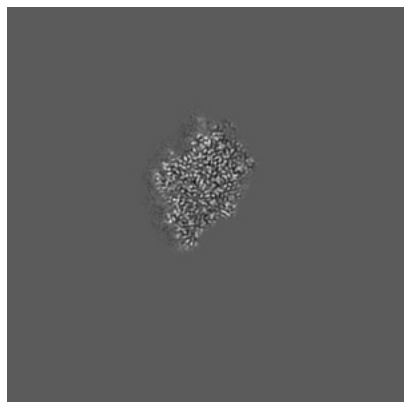


Z

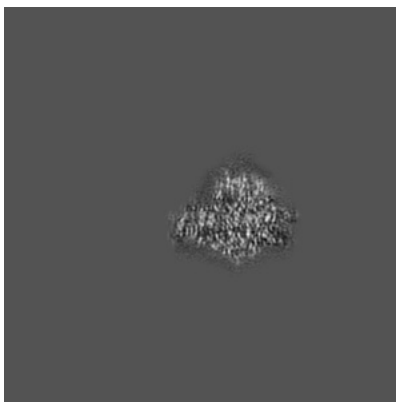
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

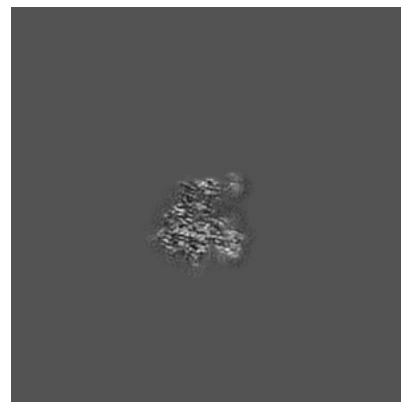
6.2.1 Primary map



X Index: 256

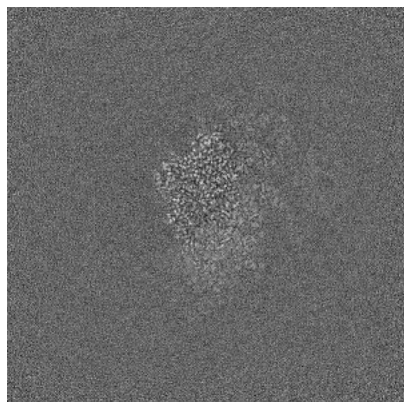


Y Index: 256

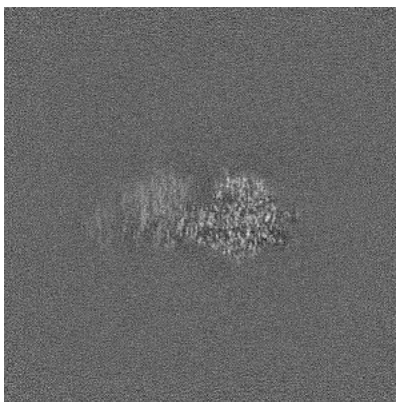


Z Index: 256

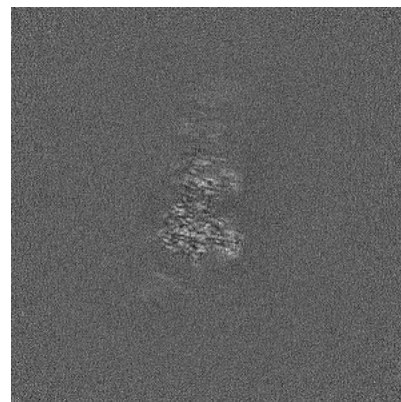
6.2.2 Raw map



X Index: 256



Y Index: 256

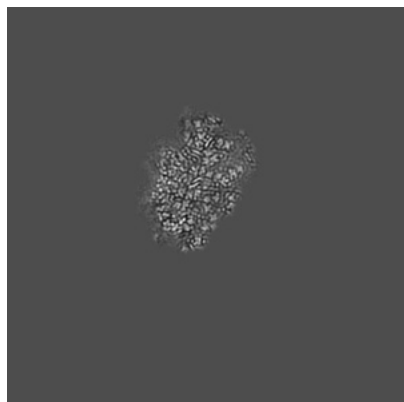


Z Index: 256

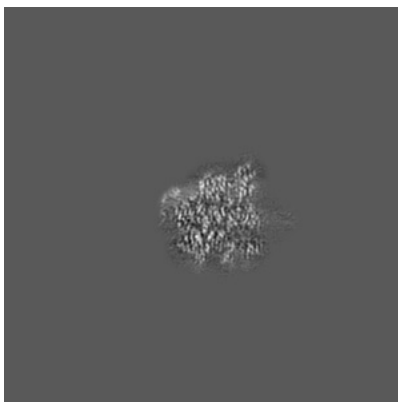
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

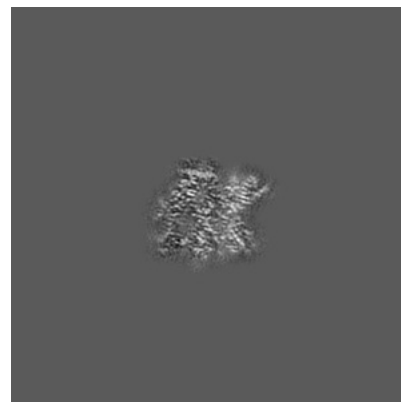
6.3.1 Primary map



X Index: 241

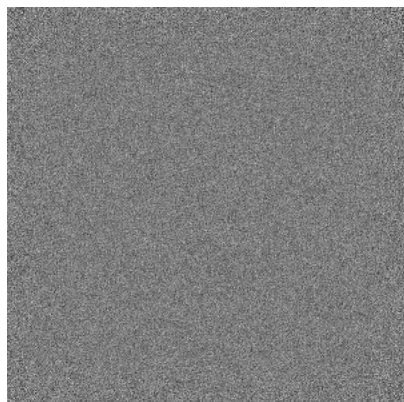


Y Index: 220

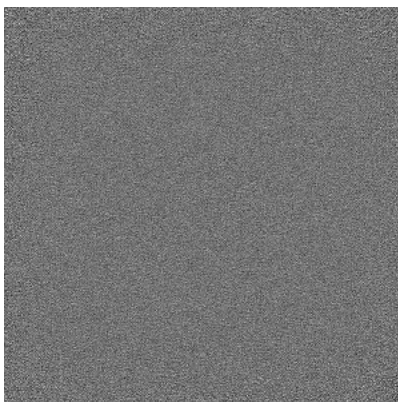


Z Index: 306

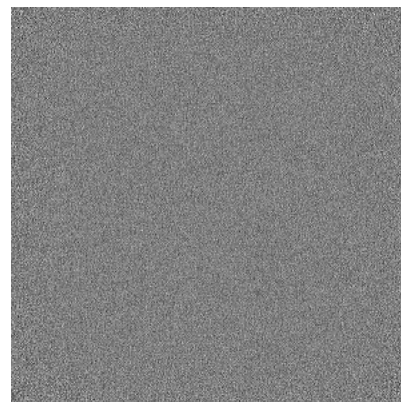
6.3.2 Raw map



X Index: 0



Y Index: 0

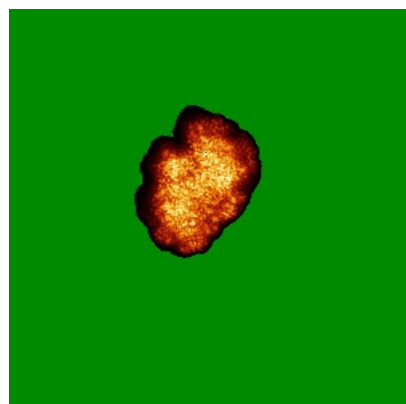


Z Index: 0

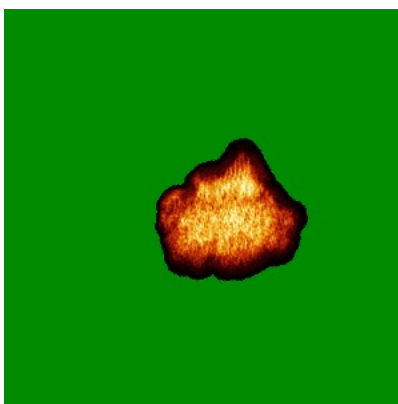
The images above show the largest variance slices of the map in three orthogonal directions.

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

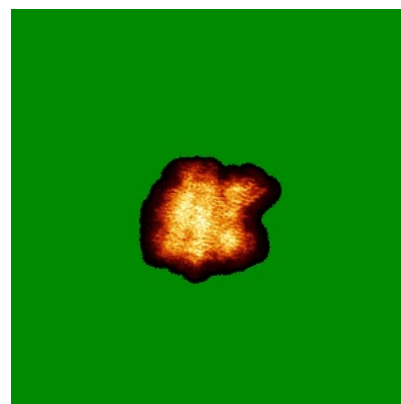
6.4.1 Primary map



X

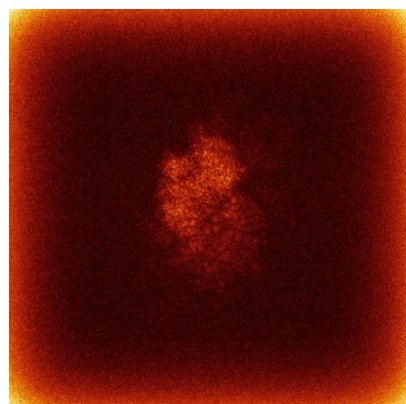


Y

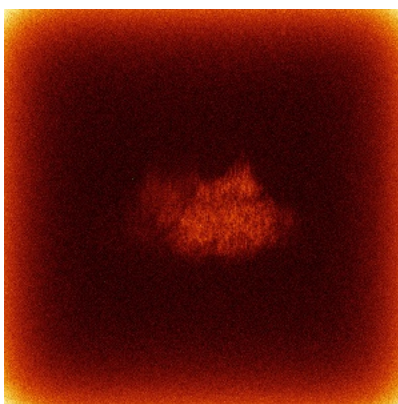


Z

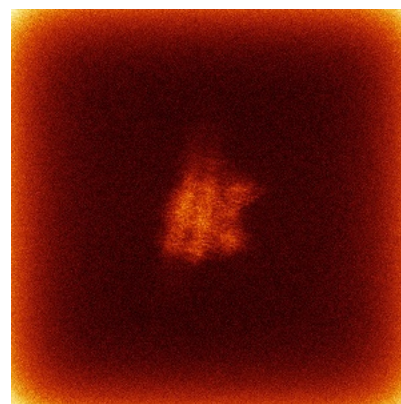
6.4.2 Raw map



X



Y

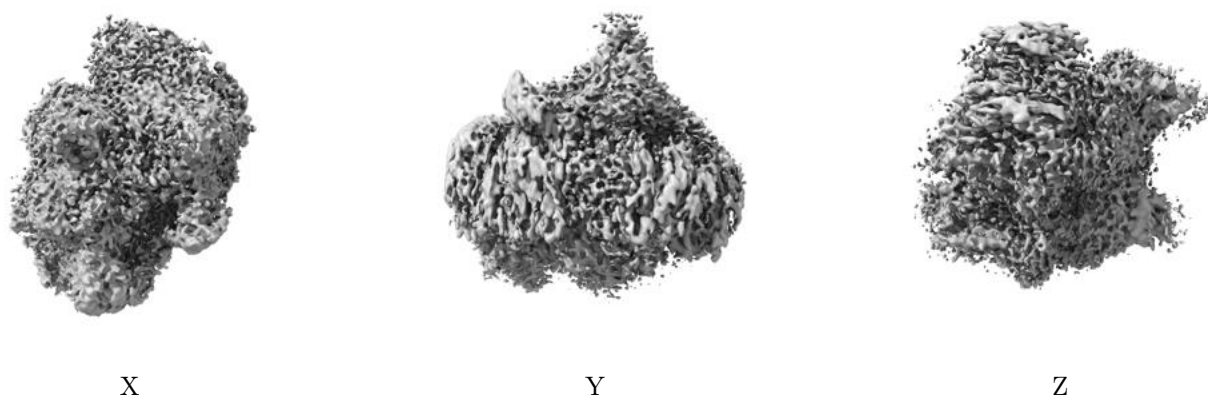


Z

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.

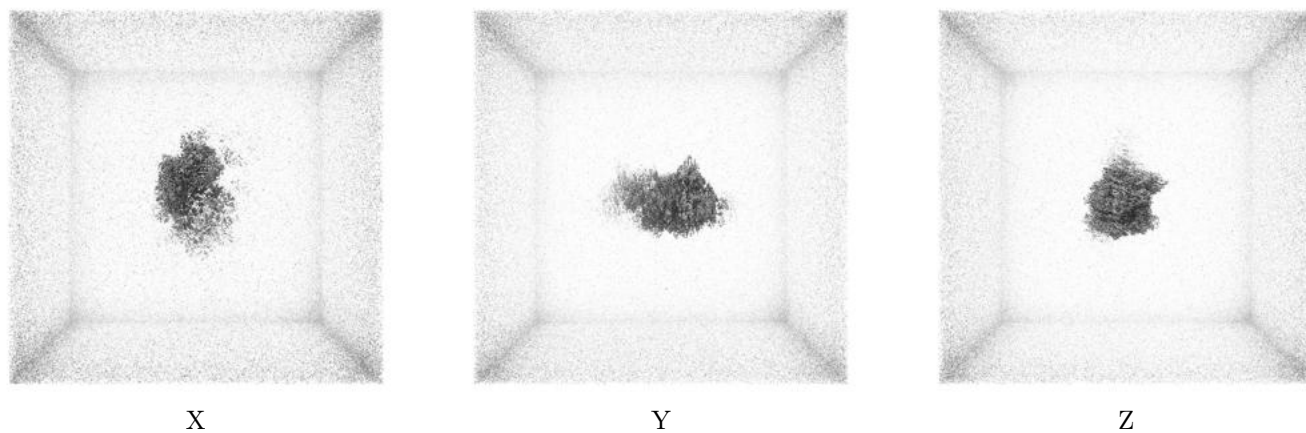
6.5 Orthogonal surface views [i](#)

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.

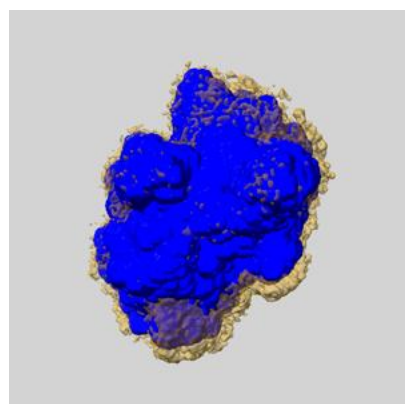
6.6 Mask visualisation [i](#)

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

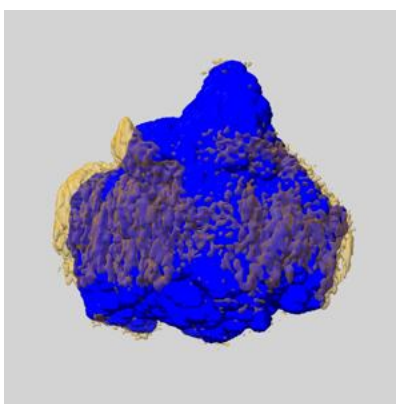
A mask typically either:

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

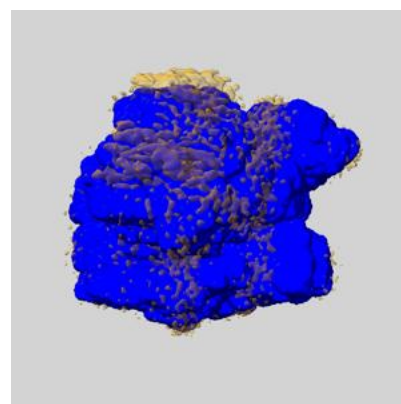
6.6.1 emd_66947_msk_1.map [i](#)



X



Y

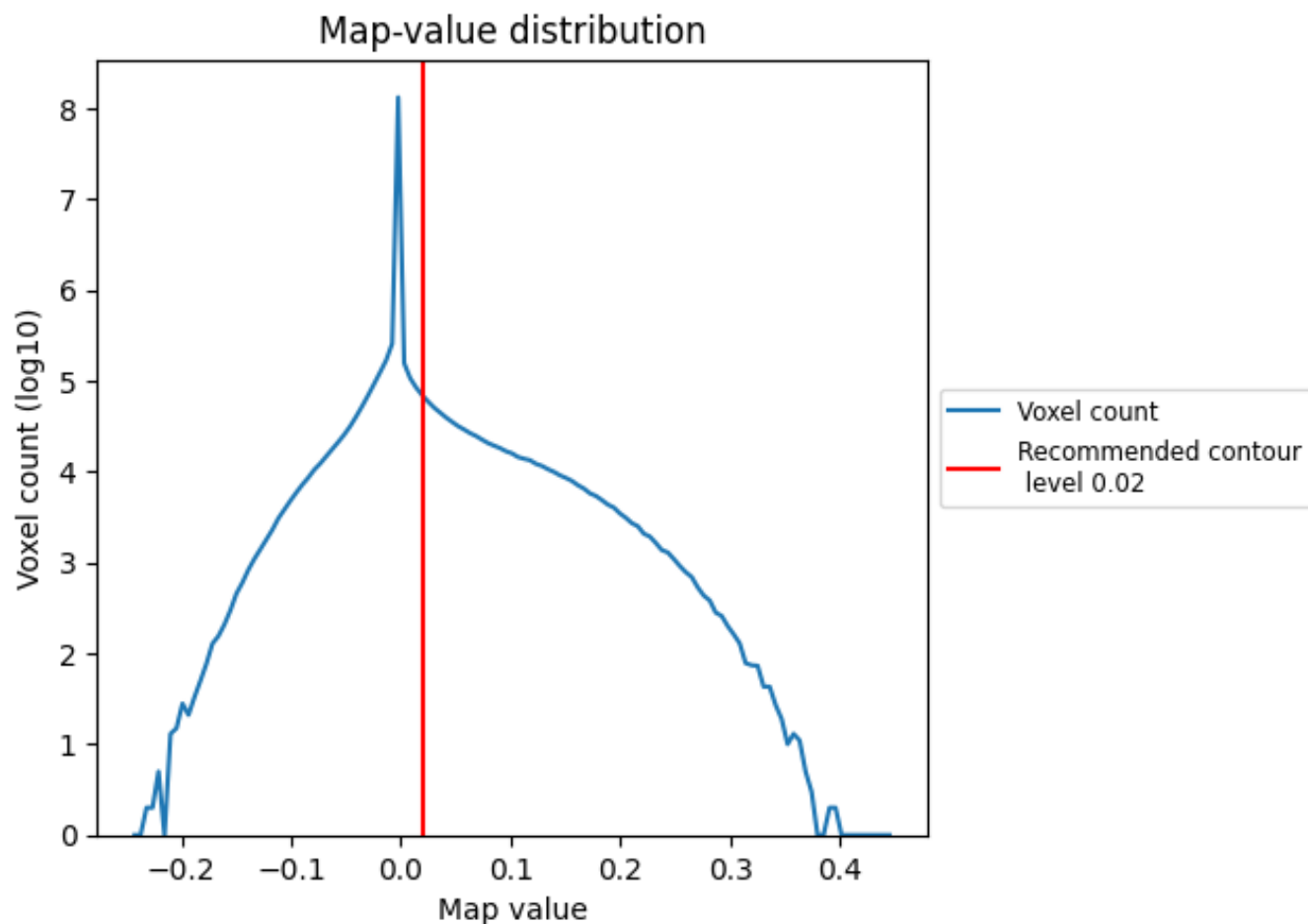


Z

7 Map analysis [i](#)

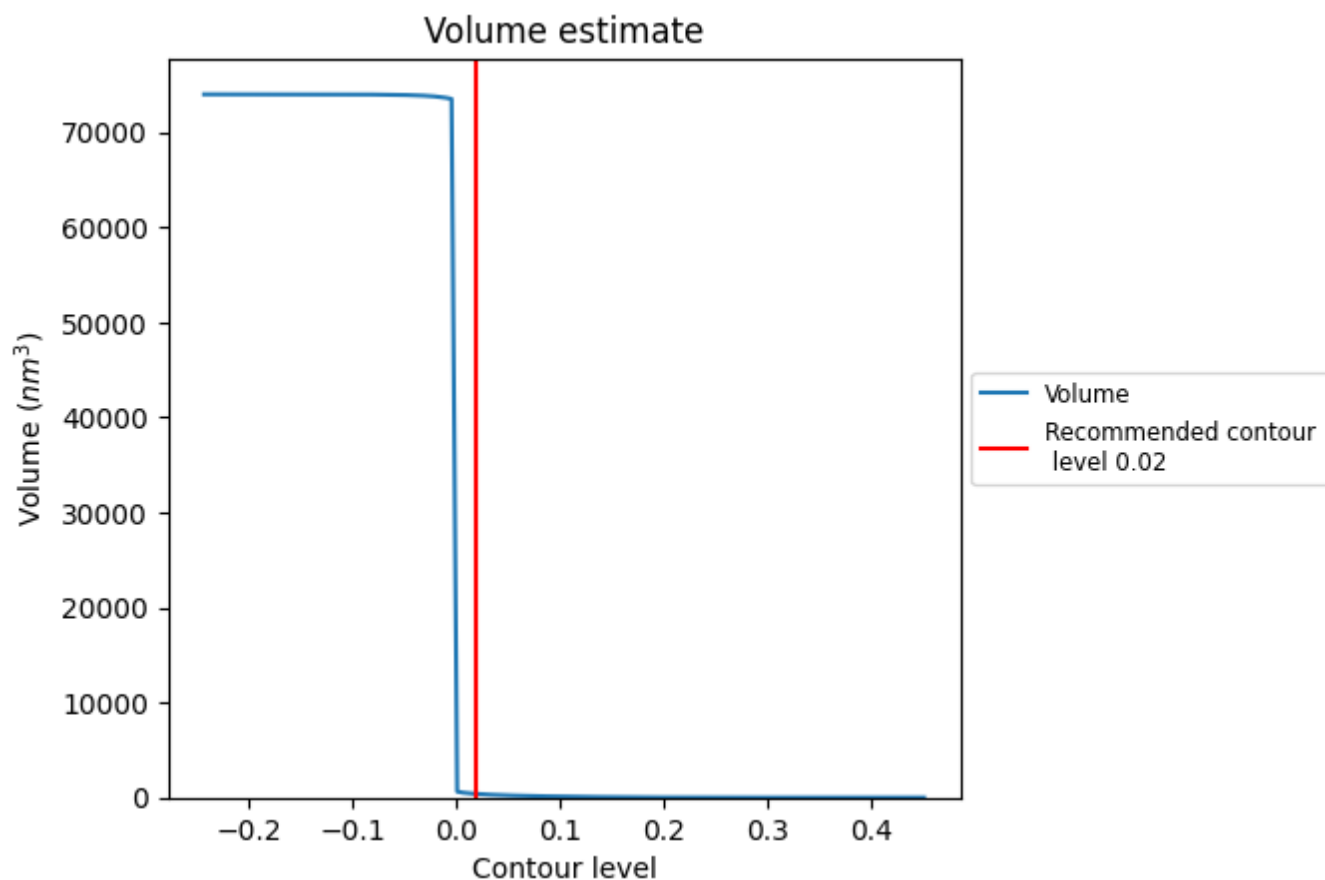
This section contains the results of statistical analysis of the map.

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.

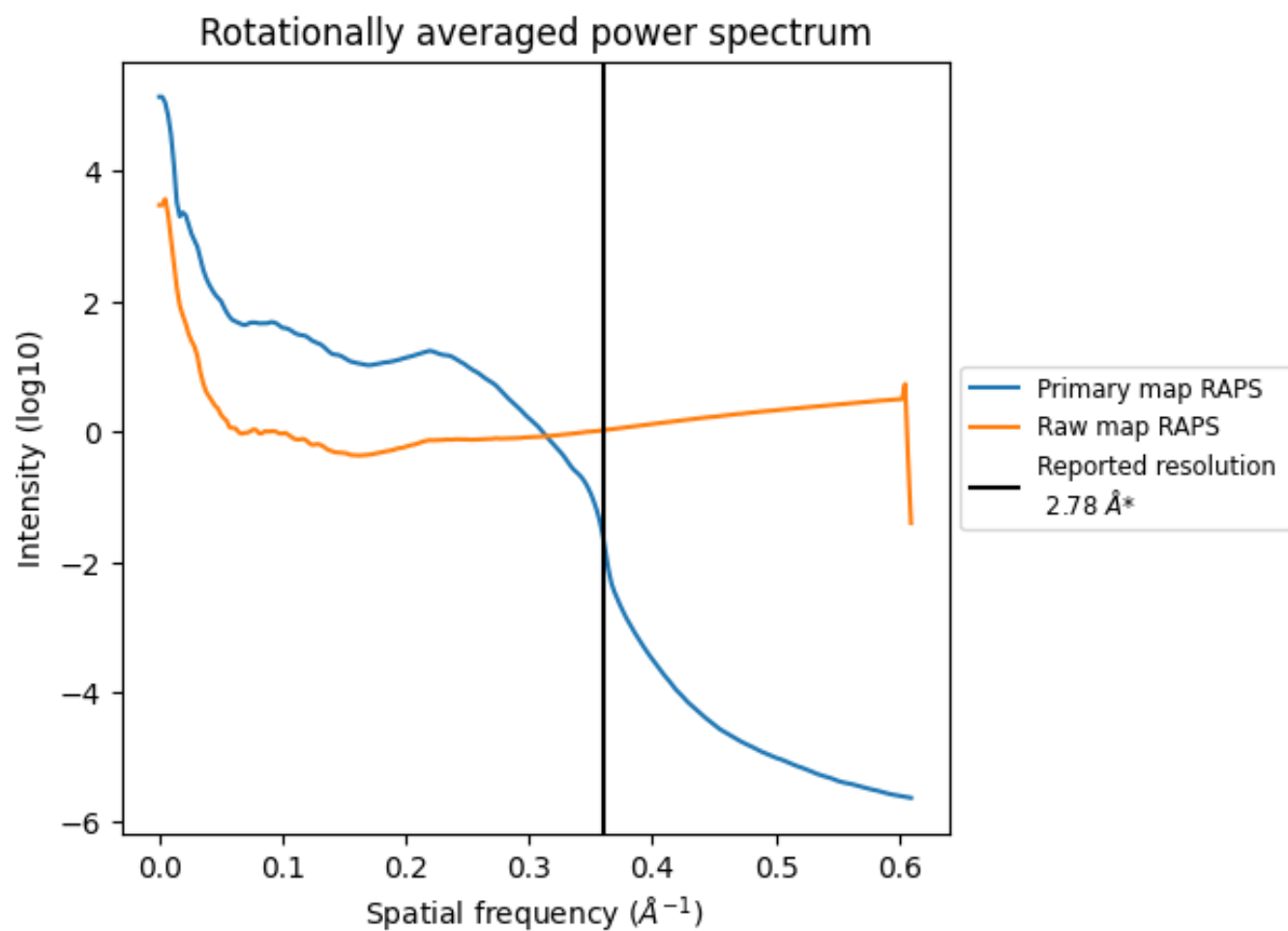
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 382 nm^3 ; this corresponds to an approximate mass of 345 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 ⓘ

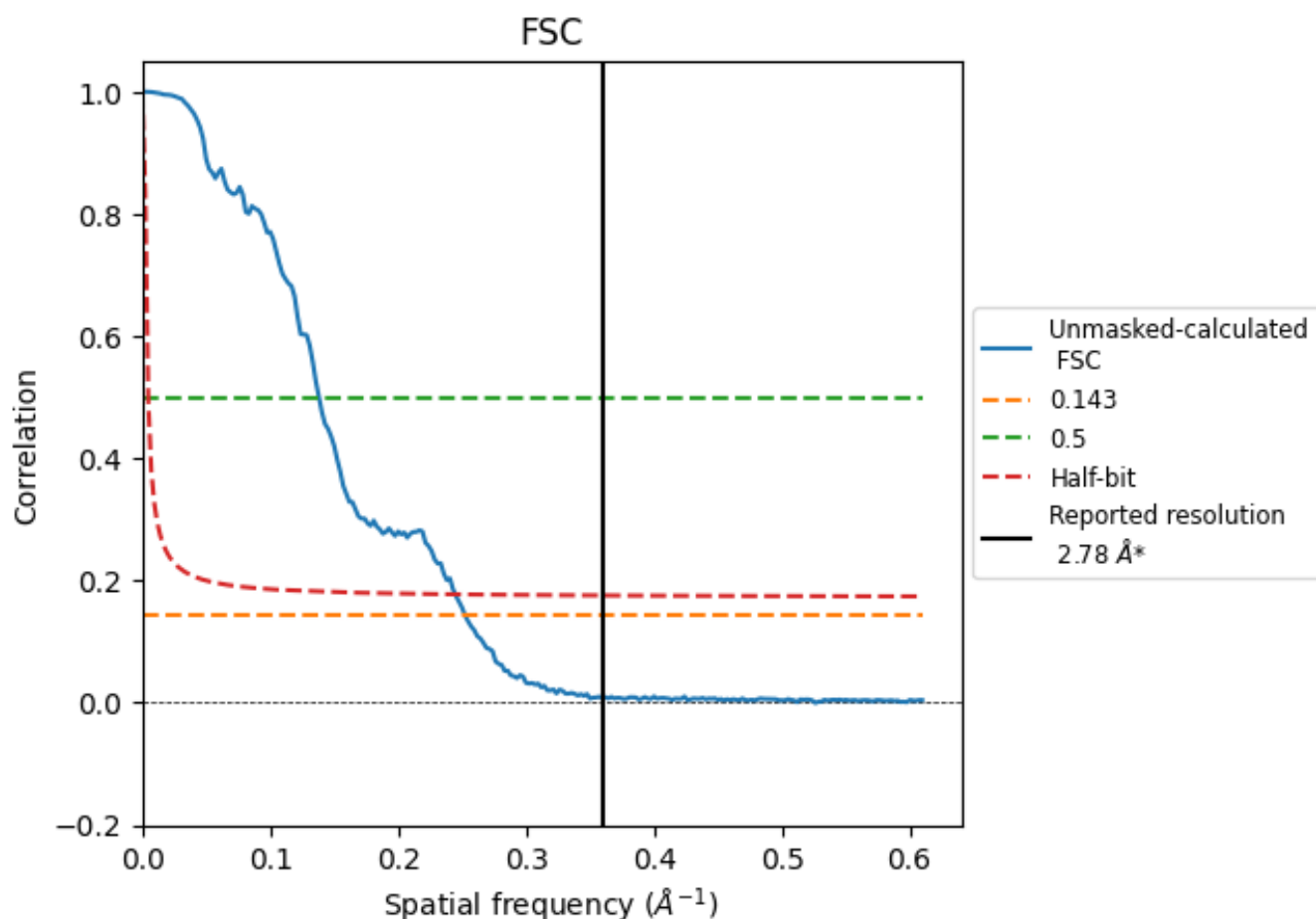


*Reported resolution corresponds to spatial frequency of 0.360 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.360 Å⁻¹

8.2 Resolution estimates [i](#)

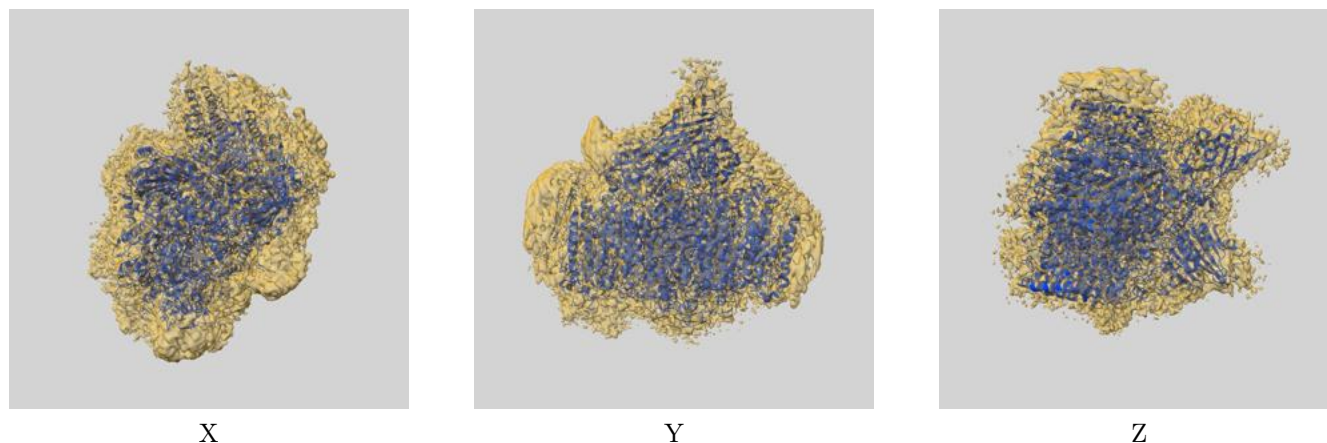
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	7.24	4.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 2.78 by more than 10 %

9 Map-model fit [i](#)

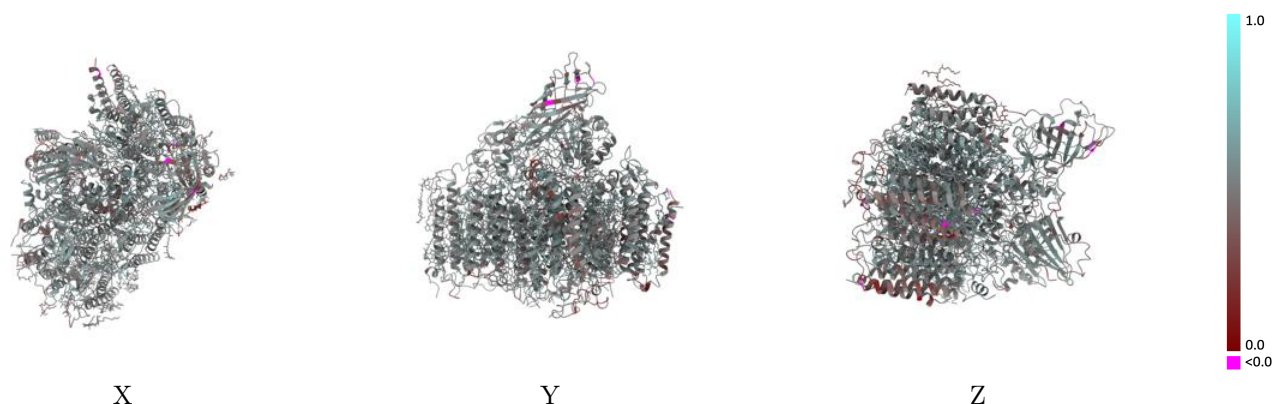
This section contains information regarding the fit between EMDB map EMD-66947 and PDB model 9XK4. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

9.1 Map-model overlay [i](#)



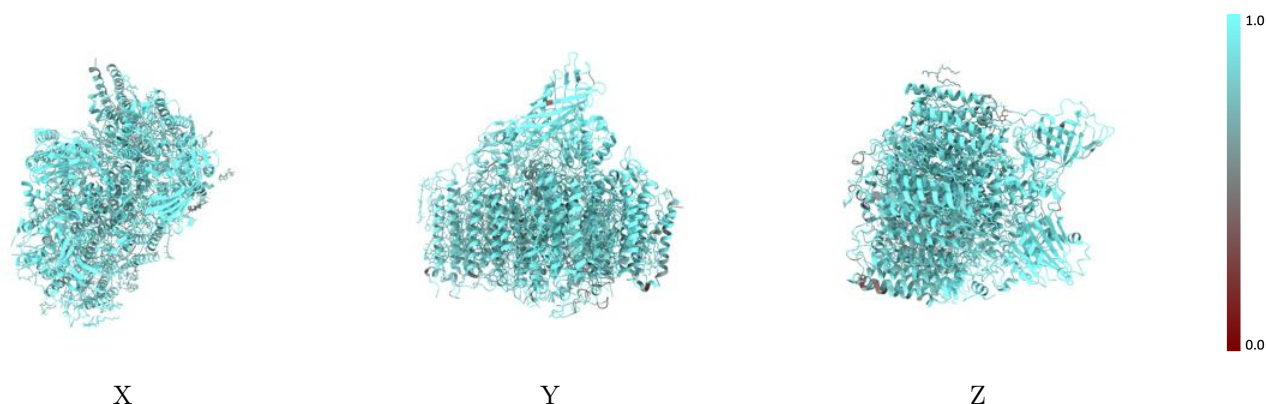
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



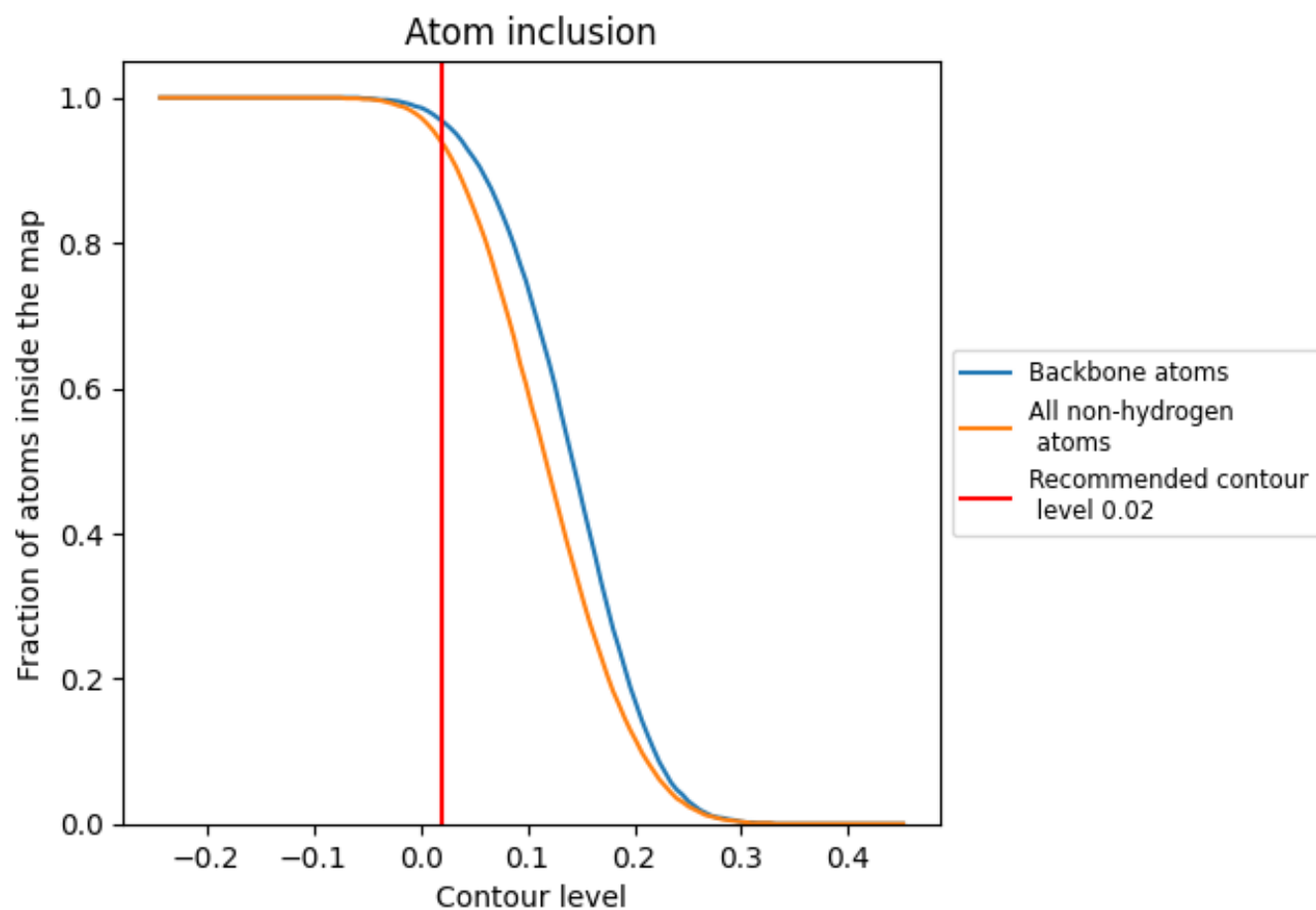
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 97% of all backbone atoms, 94% 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	 0.9380	 0.4960
1a	 0.9510	 0.5120
1b	 0.9450	 0.5050
1c	 0.9540	 0.5160
1d	 0.9640	 0.5190
1e	 0.9520	 0.5040
1f	 0.9640	 0.5070
1h	 0.8980	 0.4920
1i	 0.8670	 0.4550
1j	 0.9330	 0.4780
1k	 0.9180	 0.5030
1l	 0.9250	 0.5080
1m	 0.8680	 0.4740
1o	 0.9650	 0.4740
1p	 0.9730	 0.4840
1t	 0.9130	 0.4920
1u	 0.9850	 0.4730
1v	 0.7690	 0.3820
1w	 0.8960	 0.4540
1x	 0.9070	 0.4700
1y	 0.7770	 0.4080
1z	 0.7970	 0.3920

