



wwPDB EM Validation Summary Report ⓘ

Oct 15, 2026 – 05:51 pm BST

PDB ID : 31FD / pdb_000031fd
EMDB ID : EMD-58358
Title : Photosystem II from Arabidopsis thaliana following high light and high temperature treatment
Authors : Forsman, J.A.; Graca, A.T.; Hall, M.; Messinger, J.; Schroder, W.P.
Deposited on : 2026-06-01
Resolution : 2.74 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:

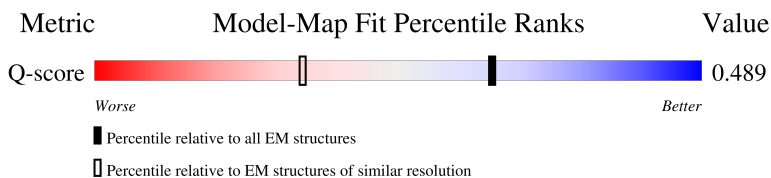
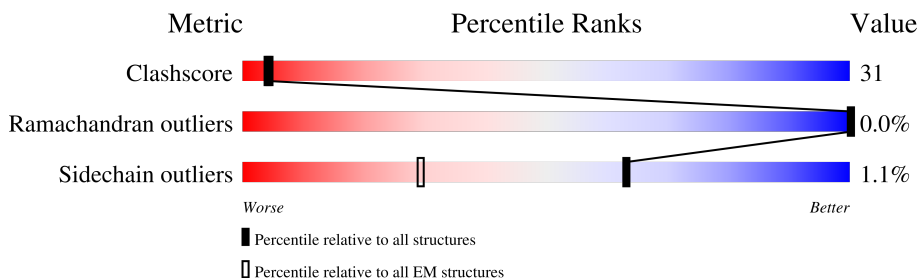
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.74 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	10492 (2.24 - 3.24)

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	A	353	9% 39% 49% 10%
1	a	353	8% 38% 50% 10%
2	B	508	12% 50% 42% 7%
2	b	508	13% 54% 38% 7%

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Mol	Chain	Length	Quality of chain
3	C	473	
3	c	473	
4	D	353	
4	d	353	
5	E	83	
5	e	83	
6	F	39	
6	f	39	
7	H	73	
7	h	73	
8	I	36	
8	i	36	
9	K	61	
9	k	61	
10	L	38	
10	l	38	
11	M	34	
11	m	34	
12	O	332	
12	o	332	
13	T	33	
13	t	33	
14	U	103	
14	u	103	
15	X	116	

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Mol	Chain	Length	Quality of chain
15	x	116	

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
18	CLA	c	505	-	-	X	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 39296 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	A	316	Total	C	N	O	S	0	0
			2466	1621	410	422	13		
1	a	316	Total	C	N	O	S	0	0
			2466	1621	410	422	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	473	Total	C	N	O	S	0	0
			3710	2436	625	637	12		
2	b	473	Total	C	N	O	S	0	0
			3710	2436	625	637	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	385	Total	C	N	O	S	0	0
			3022	1996	508	507	11		
3	c	385	Total	C	N	O	S	0	0
			3022	1996	508	507	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	326	Total	C	N	O	S	0	0
			2604	1729	422	441	12		
4	d	326	Total	C	N	O	S	0	0
			2604	1729	422	441	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	62	Total	C	N	O	0	0
			495	322	80	93		
5	e	62	Total	C	N	O	0	0
			495	322	80	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	28	Total	C	N	O	S	0	0
			220	151	35	33	1		
6	f	28	Total	C	N	O	S	0	0
			220	151	35	33	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	32	PHE	SER	variant	UNP P62095
f	32	PHE	SER	variant	UNP P62095

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	57	Total	C	N	O	S	0	0
			425	281	66	76	2		
7	h	57	Total	C	N	O	S	0	0
			425	281	66	76	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	33	Total	C	N	O	S	0	0
			266	184	39	42	1		
8	i	33	Total	C	N	O	S	0	0
			266	184	39	42	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	27	Total	C	N	O	S	0	0
			216	153	30	32	1		
9	k	27	Total	C	N	O	S	0	0
			216	153	30	32	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	35	Total	C	N	O	0	0
			293	195	45	53		
10	l	35	Total	C	N	O	0	0
			293	195	45	53		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	31	Total	C	N	O	0	0
			242	168	34	40		
11	m	31	Total	C	N	O	0	0
			242	168	34	40		

- Molecule 12 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	227	Total	C	N	O	S	0	0
			1742	1109	281	348	4		
12	o	227	Total	C	N	O	S	0	0
			1742	1109	281	348	4		

- Molecule 13 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	29	Total	C	N	O	S	0	0
			239	168	33	37	1		
13	t	29	Total	C	N	O	S	0	0
			239	168	33	37	1		

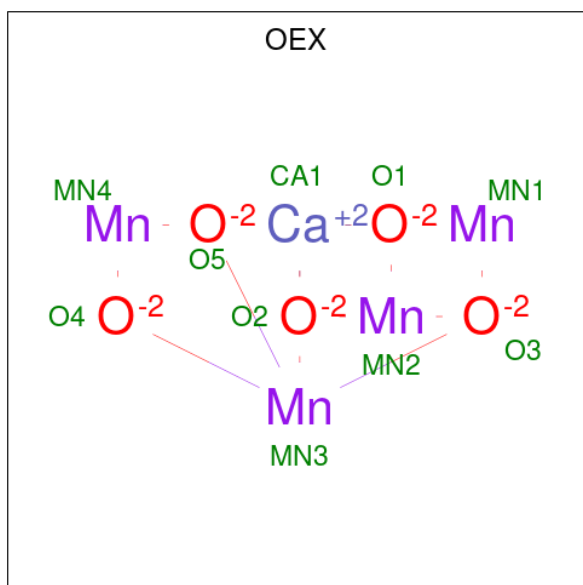
- Molecule 14 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	25	Total	C	N	O	S	0	0
			194	122	36	33	3		
14	u	25	Total	C	N	O	S	0	0
			194	122	36	33	3		

- Molecule 15 is a protein called Expressed protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	X	33	Total	C	N	O	0	0
			233	154	36	43		
15	x	33	Total	C	N	O	0	0
			233	154	36	43		

- Molecule 16 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Cl	0
			1	1	
17	C	1	Total	Cl	0
			1	1	
17	a	1	Total	Cl	0
			1	1	
17	c	1	Total	Cl	0
			1	1	

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 49	C 39	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	H	1	Total 65	C 55	Mg 1	N 4	O 5	0

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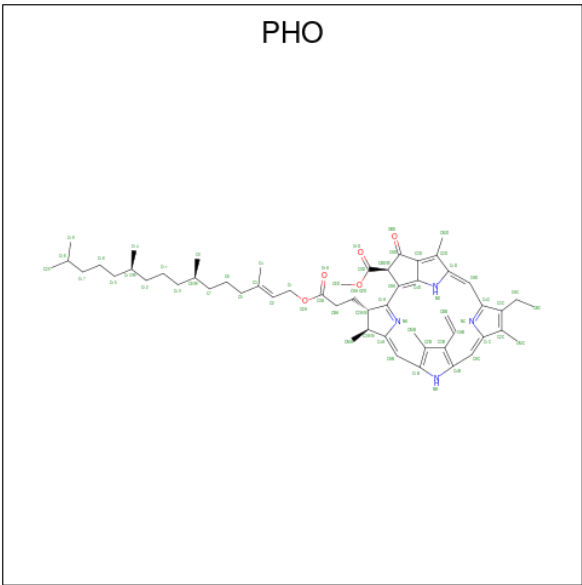
Mol	Chain	Residues	Atoms					AltConf
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
18	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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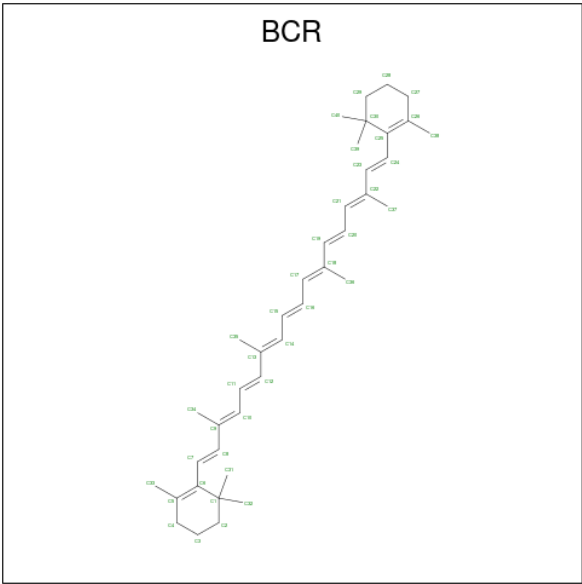
Mol	Chain	Residues	Atoms					AltConf
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 49	C 39	Mg 1	N 4	O 5	0
18	c	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	d	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 19 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



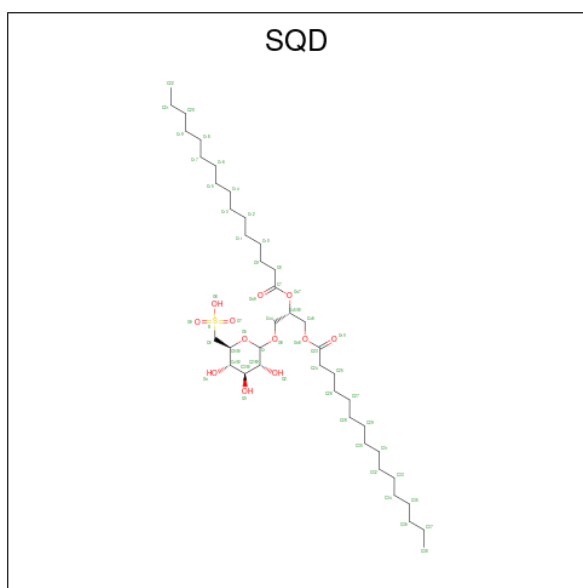
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	N	O	0
			64	55	4	5	
19	D	1	Total	C	N	O	0
			64	55	4	5	
19	a	1	Total	C	N	O	0
			64	55	4	5	
19	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



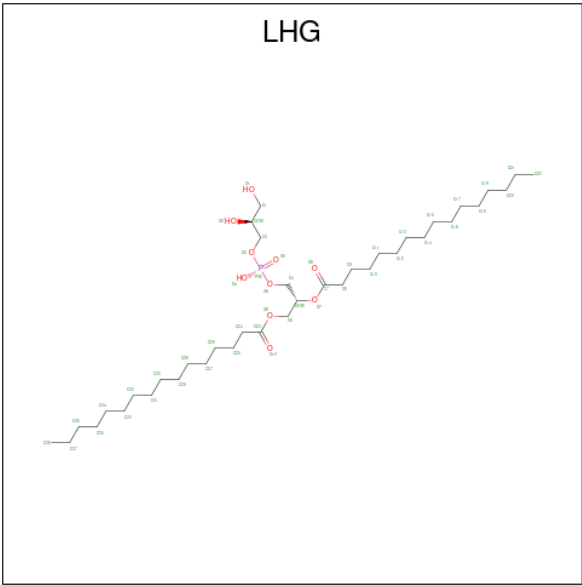
Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	D	1	Total C 40 40	0
20	H	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	d	1	Total C 40 40	0
20	h	1	Total C 40 40	0

- Molecule 21 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



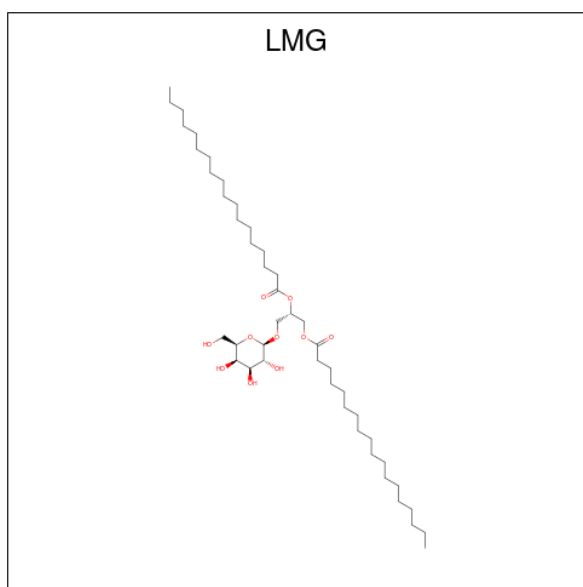
Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	C	O	S	0
			54	41	12	1	
21	a	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



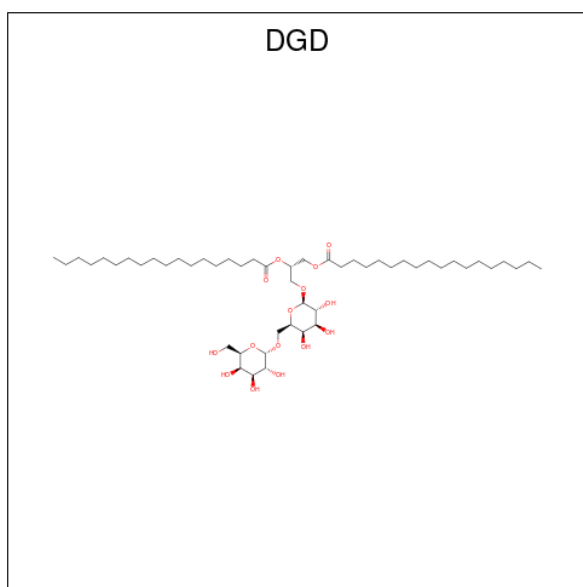
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			37	26	10	1	
22	D	1	Total	C	O	P	0
			49	38	10	1	
22	D	1	Total	C	O	P	0
			43	32	10	1	
22	L	1	Total	C	O	P	0
			49	38	10	1	
22	a	1	Total	C	O	P	0
			37	26	10	1	
22	d	1	Total	C	O	P	0
			43	32	10	1	
22	d	1	Total	C	O	P	0
			49	38	10	1	
22	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			51	41	10	
23	C	1	Total	C	O	0
			48	38	10	
23	D	1	Total	C	O	0
			46	36	10	
23	b	1	Total	C	O	0
			51	41	10	
23	c	1	Total	C	O	0
			48	38	10	
23	d	1	Total	C	O	0
			46	36	10	

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

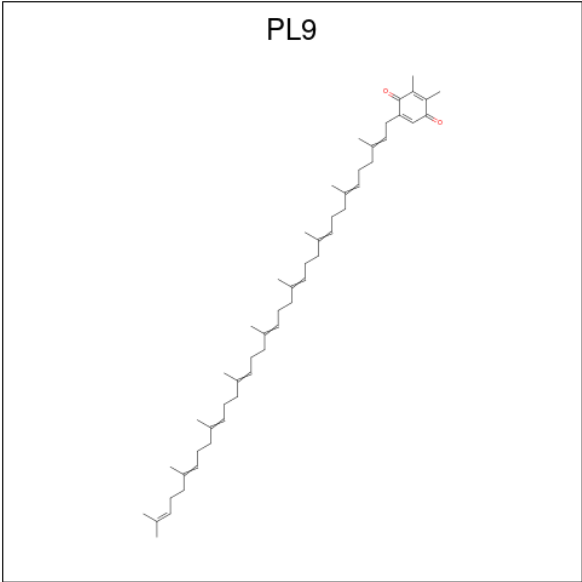


Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	C	O	0
			62	47	15	
24	C	1	Total	C	O	0
			50	35	15	
24	C	1	Total	C	O	0
			62	47	15	
24	b	1	Total	C	O	0
			62	47	15	
24	c	1	Total	C	O	0
			50	35	15	
24	c	1	Total	C	O	0
			62	47	15	

- Molecule 25 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

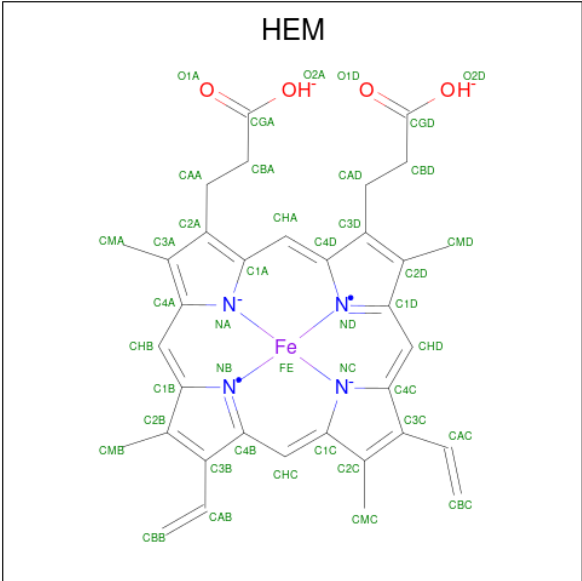
Mol	Chain	Residues	Atoms		AltConf
25	D	1	Total	Fe	0
			1	1	
25	d	1	Total	Fe	0
			1	1	

- Molecule 26 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: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms			AltConf
26	D	1	Total	C	O	0
			55	53	2	
26	d	1	Total	C	O	0
			55	53	2	

- Molecule 27 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
27	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
27	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

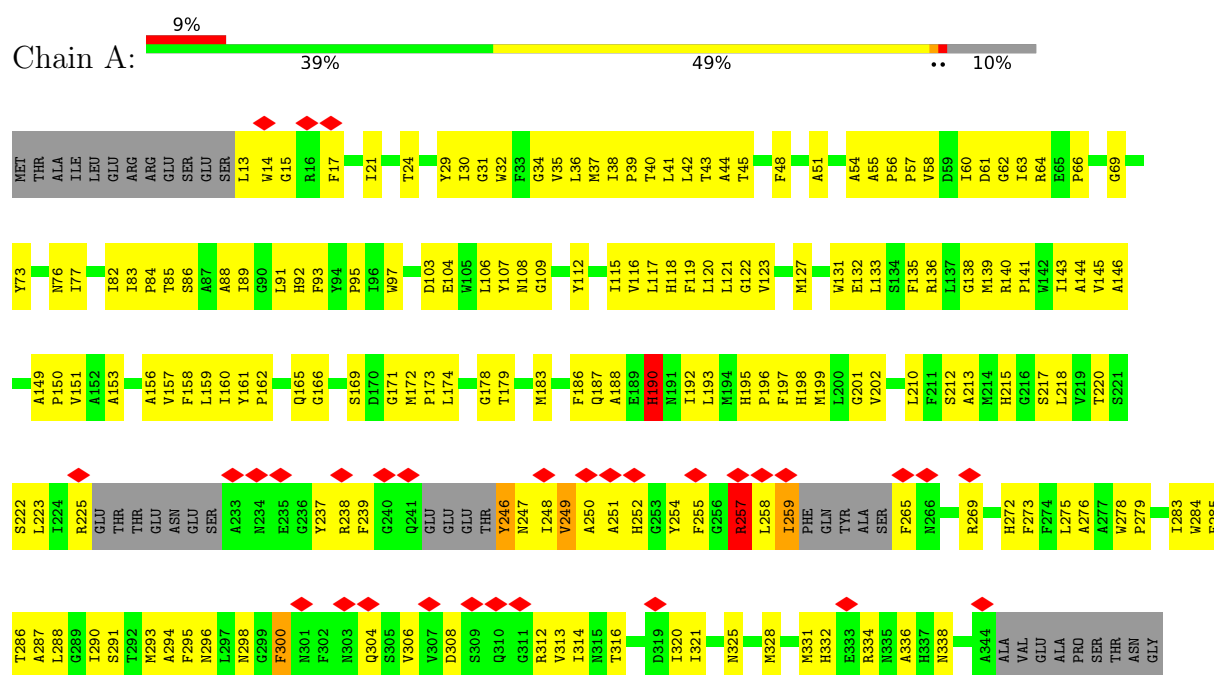
- Molecule 28 is water.

Mol	Chain	Residues	Atoms		AltConf
28	A	14	Total	O	0
			14	14	
28	B	5	Total	O	0
			5	5	
28	C	2	Total	O	0
			2	2	
28	D	5	Total	O	0
			5	5	
28	a	14	Total	O	0
			14	14	
28	b	5	Total	O	0
			5	5	
28	c	2	Total	O	0
			2	2	
28	d	5	Total	O	0
			5	5	

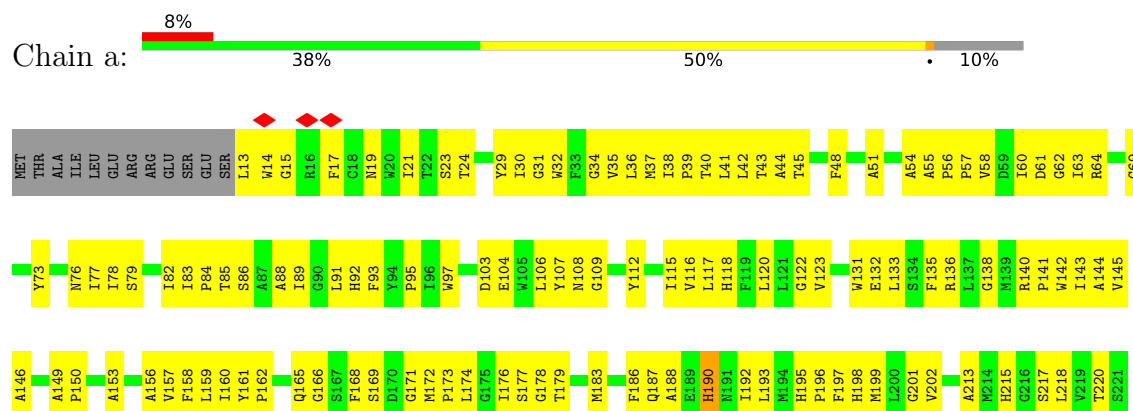
3 Residue-property plots

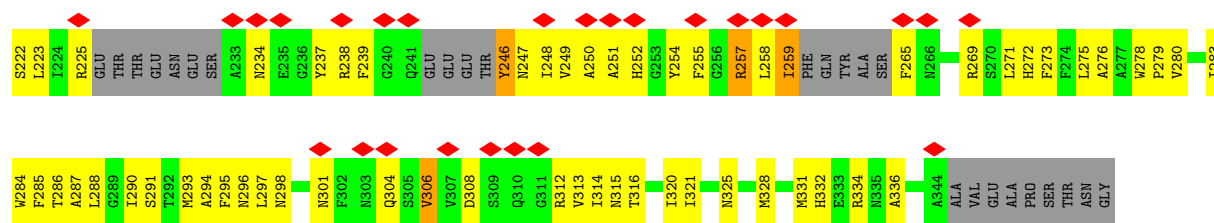
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

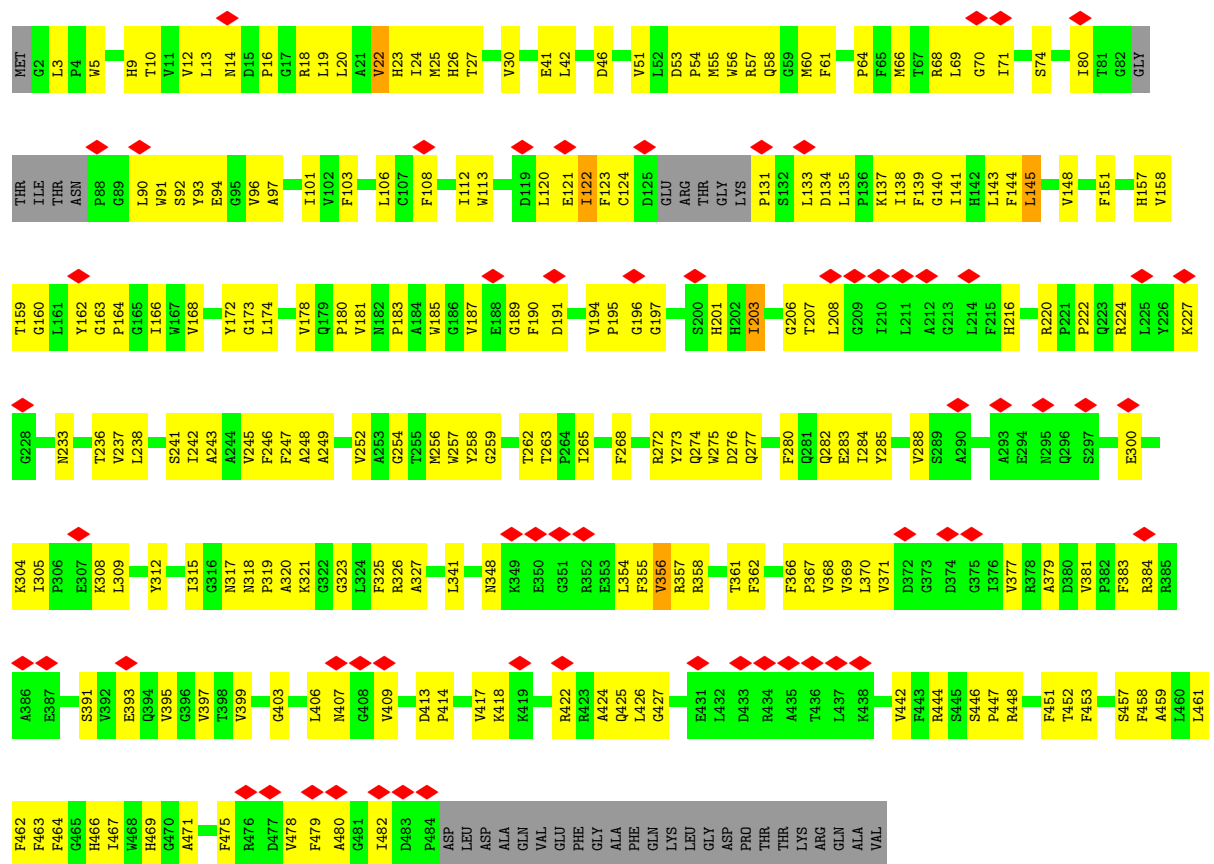


• Molecule 1: Photosystem II protein D1

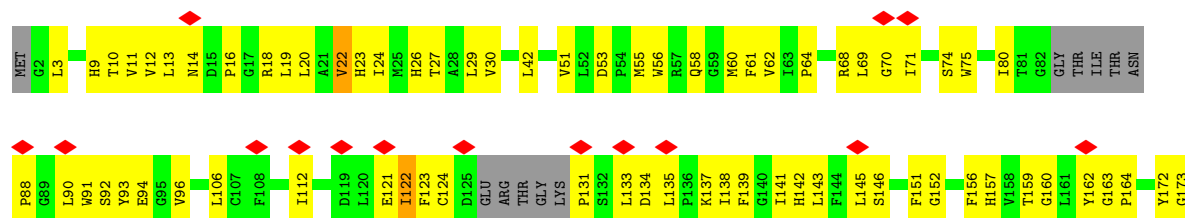


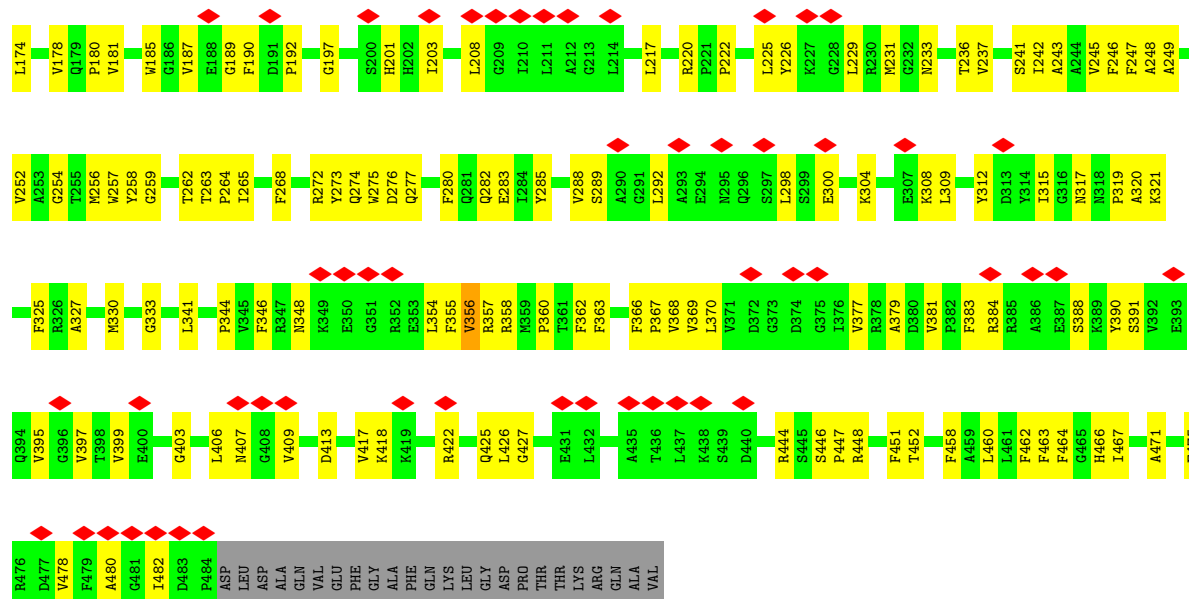


• Molecule 2: Photosystem II CP47 reaction center protein

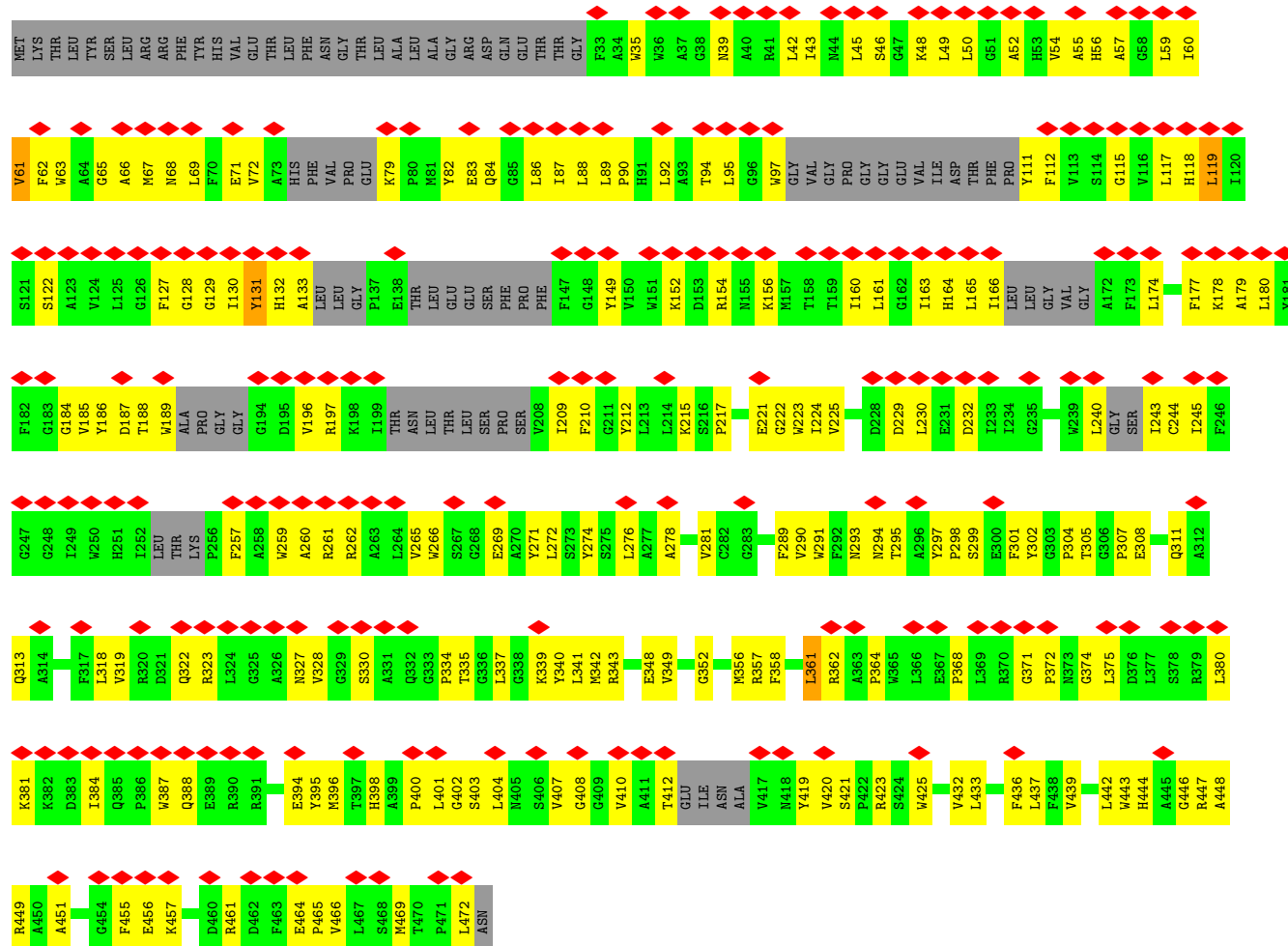


• Molecule 2: Photosystem II CP47 reaction center protein

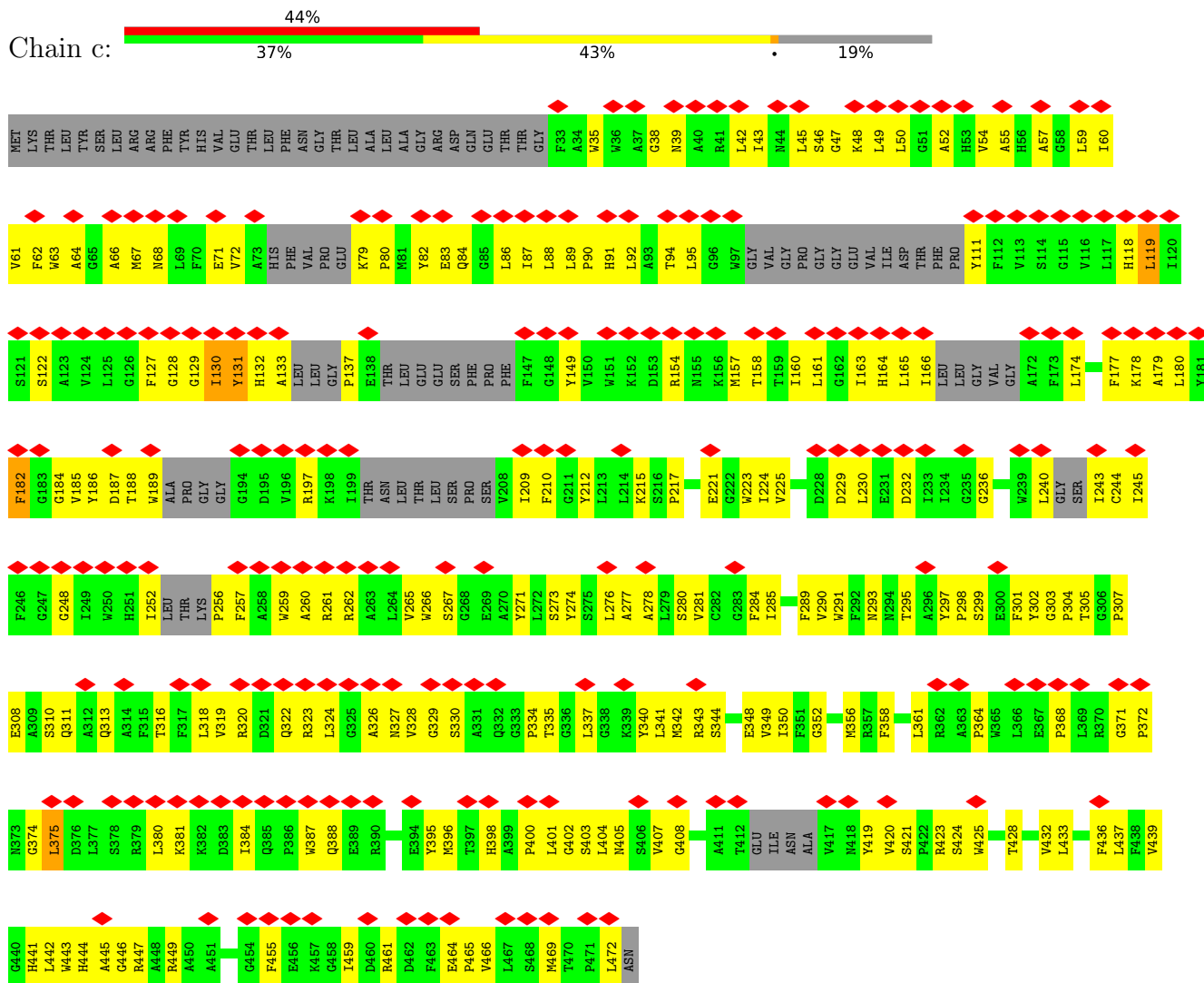




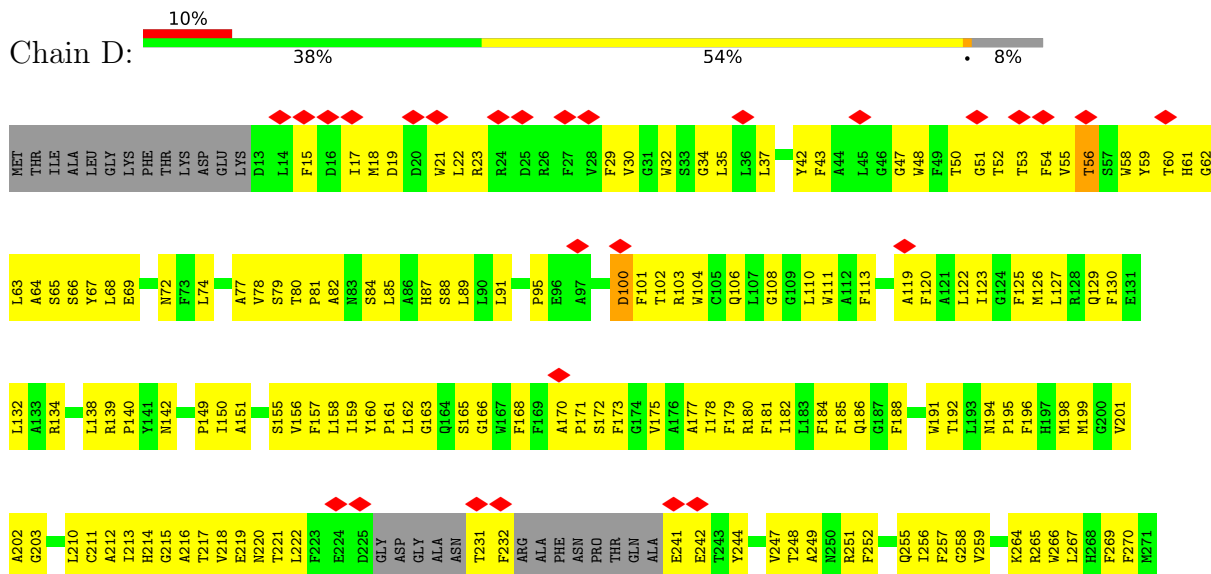
• Molecule 3: Photosystem II CP43 reaction center protein

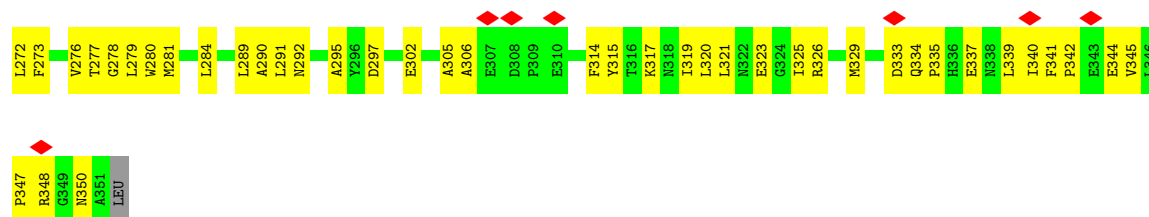


Chain c:

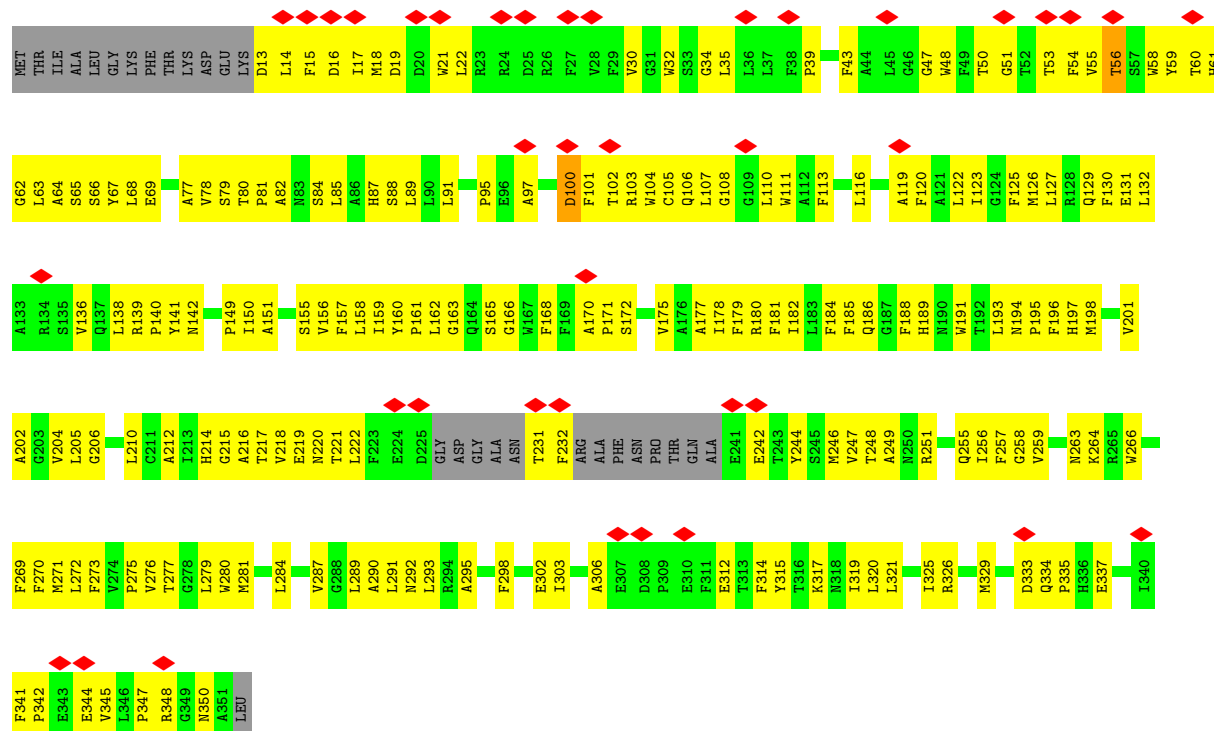


Chain D:

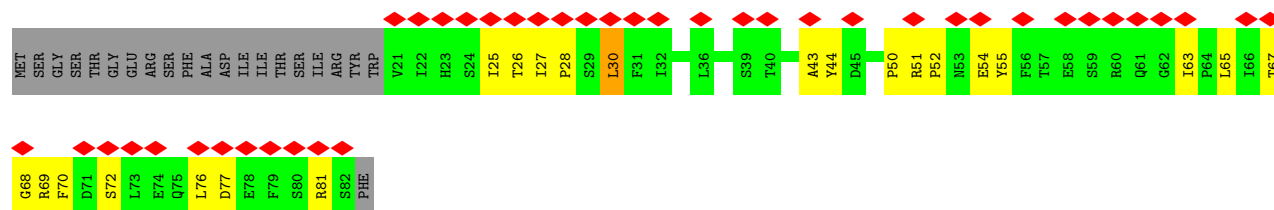




• Molecule 4: Photosystem II D2 protein

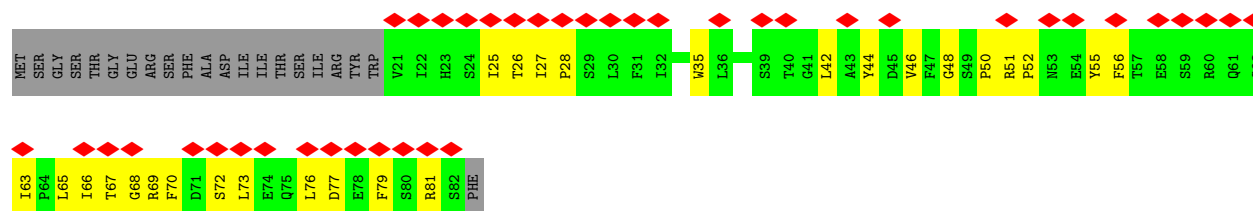


• Molecule 5: Cytochrome b559 subunit alpha

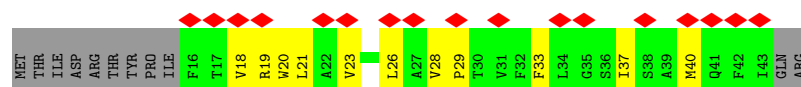


• Molecule 5: Cytochrome b559 subunit alpha

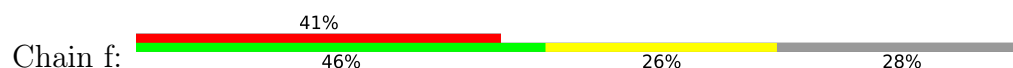




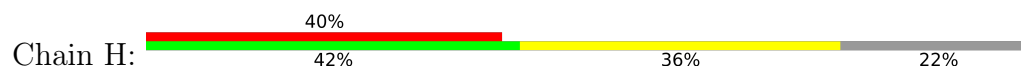
• Molecule 6: Cytochrome b559 subunit beta



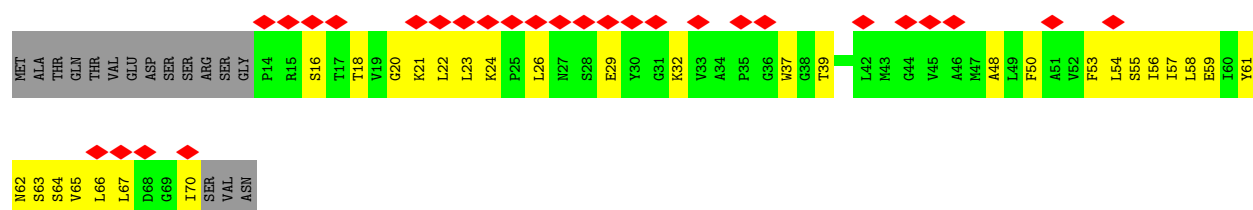
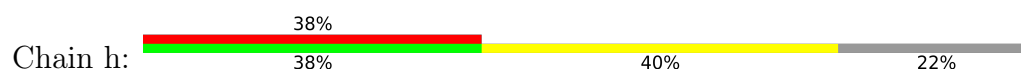
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 7: Photosystem II reaction center protein H

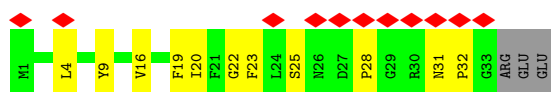


• Molecule 7: Photosystem II reaction center protein H

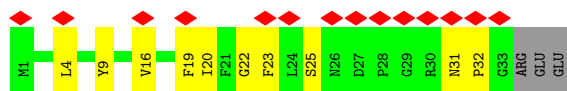
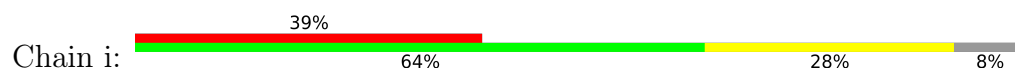


• Molecule 8: Photosystem II reaction center protein I

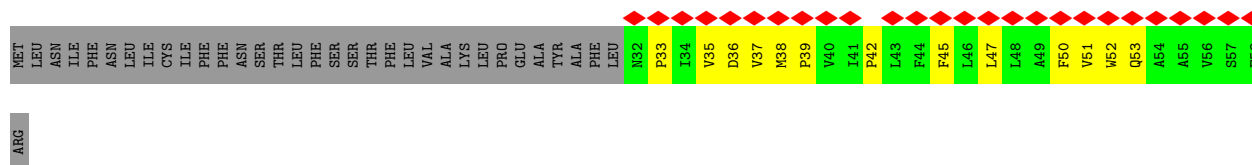




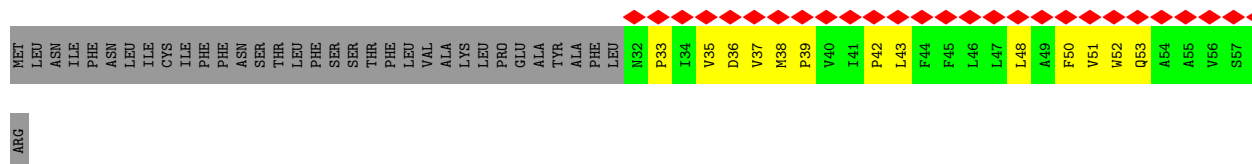
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein K



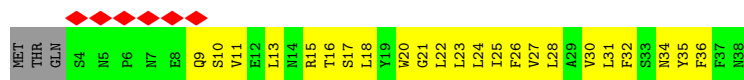
- Molecule 9: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein L

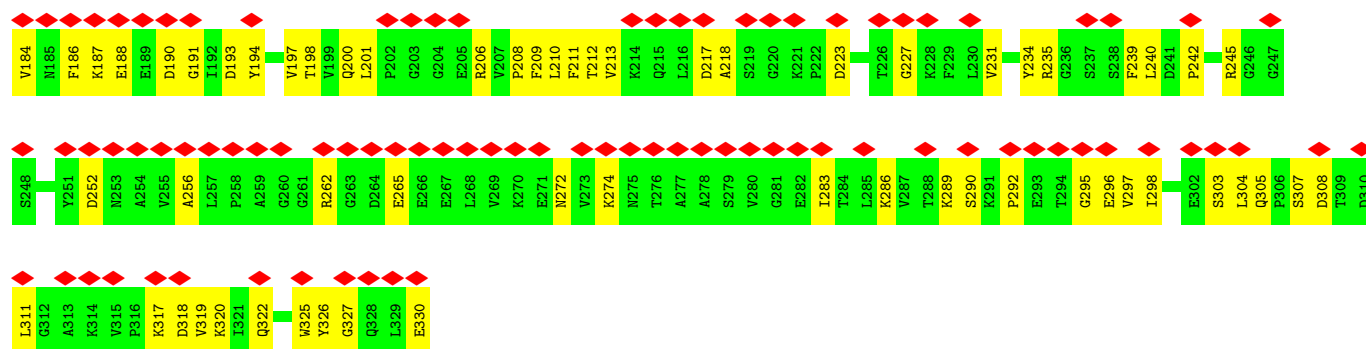


- Molecule 10: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein M





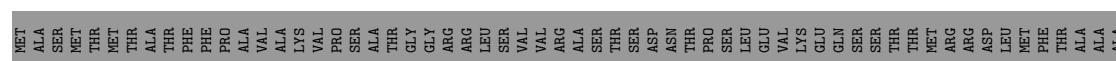
- Molecule 13: Photosystem II reaction center protein T



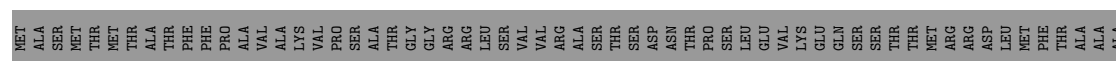
- Molecule 13: Photosystem II reaction center protein T



- Molecule 14: Photosystem II 5 kDa protein, chloroplastic



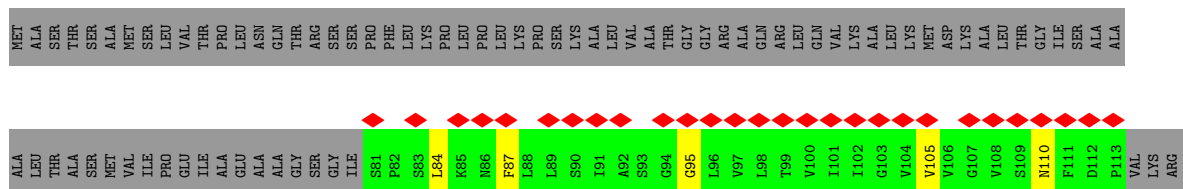
- Molecule 14: Photosystem II 5 kDa protein, chloroplastic



- Molecule 15: Expressed protein



- Molecule 15: Expressed protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57560	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	10.181	Depositor
Minimum map value	-6.342	Depositor
Average map value	0.040	Depositor
Map value standard deviation	1.021	Depositor
Recommended contour level	2.216	Depositor
Map size (Å)	151.4675, 165.55751, 109.902	wwPDB
Map dimensions	156, 235, 215	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7045, 0.7045, 0.7045	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, LHG, OEX, FE2, PHO, PL9, LMG, HEM, CL, BCR, DGD, SQD

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	A	0.35	0/2542	0.55	2/3463 (0.1%)
1	a	0.34	0/2542	0.51	0/3463
2	B	0.26	0/3838	0.36	0/5225
2	b	0.26	0/3838	0.39	0/5225
3	C	0.25	0/3116	0.45	2/4226 (0.0%)
3	c	0.26	0/3116	0.47	3/4226 (0.1%)
4	D	0.28	0/2693	0.41	0/3669
4	d	0.32	0/2693	0.45	0/3669
5	E	0.24	0/509	0.46	0/692
5	e	0.22	0/509	0.43	0/692
6	F	0.18	0/227	0.32	0/309
6	f	0.20	0/227	0.42	0/309
7	H	0.25	0/434	0.39	0/590
7	h	0.25	0/434	0.43	0/590
8	I	0.17	0/274	0.37	0/371
8	i	0.18	0/274	0.38	0/371
9	K	0.21	0/224	0.42	0/309
9	k	0.24	0/224	0.49	0/309
10	L	0.25	0/301	0.32	0/409
10	l	0.27	0/301	0.33	0/409
11	M	0.18	0/246	0.31	0/337
11	m	0.23	0/246	0.37	0/337
12	O	0.24	0/1776	0.45	0/2396
12	o	0.24	0/1776	0.47	0/2396
13	T	0.23	0/246	0.31	0/333
13	t	0.23	0/246	0.32	0/333
14	U	0.17	0/196	0.39	0/261
14	u	0.18	0/196	0.39	0/261
15	X	0.16	0/236	0.29	0/322
15	x	0.21	0/236	0.33	0/322
All	All	0.27	0/33716	0.44	7/45824 (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	A	0	1
1	a	0	1
3	c	0	1
All	All	0	3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	131	TYR	CB-CA-C	-6.87	96.75	110.42
1	A	300	PHE	CA-CB-CG	6.32	120.11	113.80
3	C	61	VAL	CG1-CB-CG2	-5.64	98.38	110.80
3	c	131	TYR	N-CA-CB	5.60	118.10	109.98
3	c	130	ILE	CA-C-N	-5.27	113.46	120.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	ARG	Sidechain
1	a	257	ARG	Sidechain
3	c	182	PHE	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	A	2466	0	2403	221	0
1	a	2466	0	2403	222	0
2	B	3710	0	3590	251	0
2	b	3710	0	3590	220	0
3	C	3022	0	2959	244	0
3	c	3022	0	2959	258	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2604	0	2502	227	0
4	d	2604	0	2502	251	0
5	E	495	0	478	30	0
5	e	495	0	478	32	0
6	F	220	0	225	11	0
6	f	220	0	225	9	0
7	H	425	0	451	33	0
7	h	425	0	451	38	0
8	I	266	0	276	19	0
8	i	266	0	276	14	0
9	K	216	0	224	15	0
9	k	216	0	224	15	0
10	L	293	0	283	26	0
10	l	293	0	283	30	0
11	M	242	0	267	17	0
11	m	242	0	267	25	0
12	O	1742	0	1715	97	0
12	o	1742	0	1715	101	0
13	T	239	0	255	10	0
13	t	239	0	255	9	0
14	U	194	0	208	17	0
14	u	194	0	208	17	0
15	X	233	0	251	9	0
15	x	233	0	251	8	0
16	A	10	0	0	1	0
16	a	10	0	0	1	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	a	1	0	0	0	0
17	c	1	0	0	0	0
18	A	239	0	242	40	0
18	B	975	0	1080	136	0
18	C	816	0	874	125	0
18	D	130	0	144	19	0
18	H	65	0	72	17	0
18	a	239	0	242	40	0
18	b	1040	0	1152	153	0
18	c	816	0	874	125	0
18	d	130	0	144	22	0
19	A	64	0	74	9	0
19	D	64	0	74	8	0
19	a	64	0	74	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	d	64	0	74	11	0
20	A	40	0	56	7	0
20	B	120	0	168	18	0
20	D	40	0	56	6	0
20	H	40	0	56	9	0
20	a	40	0	56	7	0
20	b	120	0	168	19	0
20	d	40	0	56	4	0
20	h	40	0	56	7	0
21	A	54	0	78	4	0
21	a	54	0	78	5	0
22	A	37	0	44	4	0
22	D	92	0	133	21	0
22	L	49	0	74	9	0
22	a	37	0	44	4	0
22	d	92	0	133	20	0
22	l	49	0	74	9	0
23	B	51	0	72	9	0
23	C	48	0	66	12	0
23	D	46	0	62	4	0
23	b	51	0	72	10	0
23	c	48	0	66	14	0
23	d	46	0	62	3	0
24	B	62	0	82	14	0
24	C	112	0	140	18	0
24	b	62	0	82	11	0
24	c	112	0	140	15	0
25	D	1	0	0	0	0
25	d	1	0	0	0	0
26	D	55	0	80	7	0
26	d	55	0	80	11	0
27	F	43	0	30	3	0
27	f	43	0	30	2	0
28	A	14	0	0	3	0
28	B	5	0	0	1	0
28	C	2	0	0	0	0
28	D	5	0	0	0	0
28	a	14	0	0	2	0
28	b	5	0	0	1	0
28	c	2	0	0	0	0
28	d	5	0	0	1	0
All	All	39296	0	39688	2479	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 31.

The worst 5 of 2479 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)
3:c:131:TYR:HB3	18:c:507:CLA:HAC1	1.49	0.94
3:c:82:TYR:HD2	3:c:419:TYR:HH	1.01	0.94
3:c:119:LEU:HD11	9:k:38:MET:HE1	1.48	0.93
18:B:609:CLA:H122	18:D:405:CLA:HMB2	1.51	0.92
18:b:604:CLA:H122	18:d:408:CLA:HMB2	1.52	0.91

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	A	308/353 (87%)	303 (98%)	5 (2%)	0	100	100
1	a	308/353 (87%)	300 (97%)	8 (3%)	0	100	100
2	B	467/508 (92%)	462 (99%)	5 (1%)	0	100	100
2	b	467/508 (92%)	461 (99%)	6 (1%)	0	100	100
3	C	363/473 (77%)	353 (97%)	10 (3%)	0	100	100
3	c	363/473 (77%)	352 (97%)	11 (3%)	0	100	100
4	D	320/353 (91%)	311 (97%)	8 (2%)	1 (0%)	36	54
4	d	320/353 (91%)	310 (97%)	9 (3%)	1 (0%)	36	54
5	E	60/83 (72%)	58 (97%)	2 (3%)	0	100	100
5	e	60/83 (72%)	58 (97%)	2 (3%)	0	100	100
6	F	26/39 (67%)	26 (100%)	0	0	100	100
6	f	26/39 (67%)	24 (92%)	2 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	55/73 (75%)	52 (94%)	3 (6%)	0	100	100
7	h	55/73 (75%)	53 (96%)	2 (4%)	0	100	100
8	I	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
8	i	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
9	K	25/61 (41%)	25 (100%)	0	0	100	100
9	k	25/61 (41%)	24 (96%)	1 (4%)	0	100	100
10	L	33/38 (87%)	33 (100%)	0	0	100	100
10	l	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
11	M	29/34 (85%)	28 (97%)	1 (3%)	0	100	100
11	m	29/34 (85%)	28 (97%)	1 (3%)	0	100	100
12	O	219/332 (66%)	206 (94%)	13 (6%)	0	100	100
12	o	219/332 (66%)	204 (93%)	15 (7%)	0	100	100
13	T	27/33 (82%)	27 (100%)	0	0	100	100
13	t	27/33 (82%)	27 (100%)	0	0	100	100
14	U	23/103 (22%)	21 (91%)	2 (9%)	0	100	100
14	u	23/103 (22%)	20 (87%)	3 (13%)	0	100	100
15	X	31/116 (27%)	31 (100%)	0	0	100	100
15	x	31/116 (27%)	30 (97%)	1 (3%)	0	100	100
All	All	4034/5270 (76%)	3919 (97%)	113 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	100	ASP
4	d	100	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/285 (89%)	246 (97%)	7 (3%)	38	60
1	a	253/285 (89%)	245 (97%)	8 (3%)	34	56
2	B	374/402 (93%)	369 (99%)	5 (1%)	61	75
2	b	374/402 (93%)	371 (99%)	3 (1%)	73	83
3	C	302/373 (81%)	298 (99%)	4 (1%)	61	75
3	c	302/373 (81%)	299 (99%)	3 (1%)	68	80
4	D	263/283 (93%)	262 (100%)	1 (0%)	84	90
4	d	263/283 (93%)	262 (100%)	1 (0%)	84	90
5	E	55/73 (75%)	54 (98%)	1 (2%)	51	69
5	e	55/73 (75%)	55 (100%)	0	100	100
6	F	23/34 (68%)	23 (100%)	0	100	100
6	f	23/34 (68%)	23 (100%)	0	100	100
7	H	47/61 (77%)	47 (100%)	0	100	100
7	h	47/61 (77%)	47 (100%)	0	100	100
8	I	30/33 (91%)	30 (100%)	0	100	100
8	i	30/33 (91%)	30 (100%)	0	100	100
9	K	24/55 (44%)	24 (100%)	0	100	100
9	k	24/55 (44%)	24 (100%)	0	100	100
10	L	33/36 (92%)	33 (100%)	0	100	100
10	l	33/36 (92%)	33 (100%)	0	100	100
11	M	27/30 (90%)	27 (100%)	0	100	100
11	m	27/30 (90%)	27 (100%)	0	100	100
12	O	190/268 (71%)	188 (99%)	2 (1%)	65	79
12	o	190/268 (71%)	189 (100%)	1 (0%)	81	88
13	T	26/30 (87%)	25 (96%)	1 (4%)	29	51
13	t	26/30 (87%)	26 (100%)	0	100	100
14	U	20/82 (24%)	20 (100%)	0	100	100
14	u	20/82 (24%)	20 (100%)	0	100	100
15	X	28/92 (30%)	28 (100%)	0	100	100
15	x	28/92 (30%)	28 (100%)	0	100	100
All	All	3390/4274 (79%)	3353 (99%)	37 (1%)	63	79

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	306	VAL
4	d	56	THR
2	b	22	VAL
3	c	119	LEU
3	C	119	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	350	ASN
10	l	34	ASN
10	L	7	ASN
4	D	292	ASN
12	o	305	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 120 ligands modelled in this entry, 6 are monoatomic - leaving 114 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	PL9	d	405	-	55,55,55	1.36	5 (9%)	68,69,69	1.54	12 (17%)
20	BCR	B	613	-	41,41,41	0.37	0	56,56,56	2.32	14 (25%)
27	HEM	F	101	-	50,50,50	1.39	7 (14%)	66,82,82	1.27	7 (10%)
18	CLA	B	609	2	69,73,73	1.36	11 (15%)	83,113,113	1.21	9 (10%)
24	DGD	C	513	-	63,63,67	0.54	0	77,77,81	0.80	1 (1%)
18	CLA	a	403	-	69,73,73	1.23	9 (13%)	83,113,113	1.25	8 (9%)
18	CLA	a	405	-	53,57,73	1.41	10 (18%)	62,93,113	1.29	7 (11%)
18	CLA	b	608	-	69,73,73	1.28	9 (13%)	83,113,113	1.27	12 (14%)
16	OEX	A	401	3,1	0,14,14	-	-	-	-	-
23	LMG	b	618	-	51,51,55	0.52	0	59,59,63	0.64	0
27	HEM	f	101	-	50,50,50	1.40	7 (14%)	66,82,82	1.27	7 (10%)
18	CLA	b	604	2	69,73,73	1.37	11 (15%)	83,113,113	1.21	9 (10%)
18	CLA	b	609	-	69,73,73	1.25	8 (11%)	83,113,113	1.16	9 (10%)
18	CLA	c	513	-	69,73,73	1.34	8 (11%)	83,113,113	1.22	9 (10%)
18	CLA	B	603	-	69,73,73	1.23	8 (11%)	83,113,113	1.17	6 (7%)
18	CLA	c	512	3	69,73,73	1.24	8 (11%)	83,113,113	1.15	6 (7%)
24	DGD	C	503	-	51,51,67	0.68	0	65,65,81	1.16	5 (7%)
18	CLA	b	612	2	69,73,73	1.25	9 (13%)	83,113,113	1.09	7 (8%)
18	CLA	H	101	2	69,73,73	1.36	10 (14%)	83,113,113	1.18	5 (6%)
22	LHG	l	101	-	48,48,48	0.51	0	51,54,54	0.51	0
18	CLA	c	511	3	69,73,73	1.25	8 (11%)	83,113,113	1.27	9 (10%)
18	CLA	b	606	2	69,73,73	1.27	9 (13%)	83,113,113	1.41	8 (9%)
18	CLA	b	603	2	69,73,73	1.22	8 (11%)	83,113,113	1.17	5 (6%)
18	CLA	C	514	3	69,73,73	1.23	8 (11%)	83,113,113	1.16	7 (8%)
18	CLA	C	506	-	69,73,73	1.23	7 (10%)	83,113,113	1.25	5 (6%)
18	CLA	B	616	2	69,73,73	1.21	8 (11%)	83,113,113	1.34	8 (9%)
23	LMG	D	408	-	46,46,55	0.52	0	54,54,63	0.64	0
26	PL9	D	407	-	55,55,55	1.43	5 (9%)	68,69,69	1.52	13 (19%)
18	CLA	c	503	-	69,73,73	1.22	8 (11%)	83,113,113	1.21	11 (13%)
18	CLA	b	613	2	69,73,73	1.22	9 (13%)	83,113,113	1.28	10 (12%)
23	LMG	C	502	-	48,48,55	0.52	0	56,56,63	0.71	0
18	CLA	B	618	2	69,73,73	1.35	12 (17%)	83,113,113	1.52	16 (19%)
18	CLA	c	505	-	69,73,73	1.34	10 (14%)	83,113,113	1.53	9 (10%)
24	DGD	c	517	-	63,63,67	0.55	0	77,77,81	0.79	1 (1%)
18	CLA	B	605	2	69,73,73	1.27	9 (13%)	83,113,113	1.44	10 (12%)
18	CLA	C	516	-	69,73,73	1.30	9 (13%)	83,113,113	1.27	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	B	612	-	41,41,41	0.32	0	56,56,56	0.77	1 (1%)
18	CLA	C	509	3	69,73,73	1.20	7 (10%)	83,113,113	1.24	8 (9%)
18	CLA	c	515	-	69,73,73	1.20	6 (8%)	83,113,113	1.24	7 (8%)
18	CLA	B	611	-	69,73,73	1.24	8 (11%)	83,113,113	1.16	8 (9%)
19	PHO	D	402	-	58,69,69	1.97	10 (17%)	56,99,99	1.66	10 (17%)
18	CLA	B	608	2	69,73,73	1.24	9 (13%)	83,113,113	1.08	7 (8%)
23	LMG	B	604	-	51,51,55	0.51	0	59,59,63	0.64	0
18	CLA	b	601	-	69,73,73	1.22	9 (13%)	83,113,113	1.27	8 (9%)
18	CLA	A	404	-	69,73,73	1.24	9 (13%)	83,113,113	1.23	8 (9%)
20	BCR	b	602	-	41,41,41	0.34	0	56,56,56	1.63	11 (19%)
24	DGD	c	514	-	51,51,67	0.67	0	65,65,81	1.17	6 (9%)
18	CLA	C	504	-	53,57,73	1.76	10 (18%)	62,93,113	2.30	16 (25%)
18	CLA	D	405	-	69,73,73	1.26	10 (14%)	83,113,113	1.22	7 (8%)
18	CLA	c	507	-	53,57,73	1.80	11 (20%)	62,93,113	2.53	16 (25%)
18	CLA	b	617	2	69,73,73	1.27	10 (14%)	83,113,113	1.23	4 (4%)
18	CLA	B	614	2	69,73,73	1.25	8 (11%)	83,113,113	1.22	5 (6%)
18	CLA	b	614	2	69,73,73	1.33	12 (17%)	83,113,113	1.52	16 (19%)
18	CLA	B	607	-	69,73,73	1.27	8 (11%)	83,113,113	1.25	11 (13%)
18	CLA	b	607	2	69,73,73	1.24	10 (14%)	83,113,113	1.23	6 (7%)
18	CLA	B	601	2	69,73,73	1.36	10 (14%)	83,113,113	1.25	7 (8%)
18	CLA	B	619	-	69,73,73	1.30	10 (14%)	83,113,113	1.16	8 (9%)
18	CLA	b	619	-	69,73,73	1.23	8 (11%)	83,113,113	1.17	6 (7%)
19	PHO	a	409	-	58,69,69	1.97	11 (18%)	56,99,99	1.56	7 (12%)
18	CLA	c	510	-	69,73,73	1.23	6 (8%)	83,113,113	1.27	5 (6%)
18	CLA	a	407	1	69,73,73	1.23	8 (11%)	83,113,113	1.19	6 (7%)
21	SQD	A	409	-	53,54,54	1.55	8 (15%)	62,65,65	1.34	6 (9%)
18	CLA	b	620	2	69,73,73	1.21	7 (10%)	83,113,113	1.36	7 (8%)
20	BCR	b	610	-	41,41,41	0.31	0	56,56,56	0.75	1 (1%)
18	CLA	B	606	-	69,73,73	1.26	10 (14%)	83,113,113	1.19	9 (10%)
22	LHG	D	409	-	42,42,48	0.55	0	45,48,54	0.55	0
22	LHG	A	410	-	36,36,48	0.57	0	39,42,54	0.59	0
18	CLA	B	615	-	69,73,73	1.22	8 (11%)	83,113,113	1.28	8 (9%)
18	CLA	C	507	-	56,60,73	1.37	7 (12%)	67,97,113	1.57	10 (14%)
19	PHO	d	401	-	58,69,69	1.97	10 (17%)	56,99,99	1.65	7 (12%)
18	CLA	C	508	3	69,73,73	1.20	7 (10%)	83,113,113	1.21	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	c	516	3	69,73,73	1.20	7 (10%)	83,113,113	1.21	7 (8%)
22	LHG	d	403	-	42,42,48	0.55	0	45,48,54	0.55	0
22	LHG	a	410	-	36,36,48	0.55	0	39,42,54	0.63	0
16	OEX	a	402	3,1	0,14,14	-	-	-	-	-
18	CLA	a	404	1	64,68,73	1.30	9 (14%)	77,107,113	1.25	11 (14%)
18	CLA	C	512	3	69,73,73	1.23	9 (13%)	83,113,113	1.36	11 (13%)
18	CLA	b	611	-	69,73,73	1.27	9 (13%)	83,113,113	1.21	9 (10%)
24	DGD	B	620	-	63,63,67	0.59	0	77,77,81	0.90	4 (5%)
18	CLA	b	615	2	69,73,73	1.30	10 (14%)	83,113,113	1.15	8 (9%)
19	PHO	A	407	-	58,69,69	1.96	11 (18%)	56,99,99	1.54	7 (12%)
23	LMG	d	409	-	46,46,55	0.52	0	54,54,63	0.65	0
20	BCR	a	401	-	41,41,41	0.38	0	56,56,56	0.79	2 (3%)
18	CLA	C	510	-	69,73,73	1.34	8 (11%)	83,113,113	1.23	10 (12%)
18	CLA	D	406	4	69,73,73	1.28	10 (14%)	83,113,113	1.33	12 (14%)
18	CLA	B	617	2	69,73,73	1.21	8 (11%)	83,113,113	1.27	10 (12%)
20	BCR	B	610	-	41,41,41	0.34	0	56,56,56	1.63	11 (19%)
20	BCR	D	403	-	41,41,41	0.32	0	56,56,56	0.91	1 (1%)
22	LHG	D	404	-	48,48,48	0.51	0	51,54,54	0.56	0
18	CLA	C	515	3	69,73,73	1.24	9 (13%)	83,113,113	1.36	9 (10%)
20	BCR	d	407	-	41,41,41	0.32	0	56,56,56	0.91	1 (1%)
18	CLA	b	605	2	69,73,73	1.35	9 (13%)	83,113,113	1.24	6 (7%)
18	CLA	c	508	-	56,60,73	1.37	8 (14%)	67,97,113	1.60	11 (16%)
20	BCR	H	102	-	41,41,41	0.44	0	56,56,56	1.77	8 (14%)
18	CLA	C	505	-	69,73,73	1.22	7 (10%)	83,113,113	1.19	9 (10%)
18	CLA	B	602	2	69,73,73	1.24	10 (14%)	83,113,113	1.23	6 (7%)
22	LHG	d	406	-	48,48,48	0.52	0	51,54,54	0.56	0
23	LMG	c	502	-	48,48,55	0.52	0	56,56,63	0.73	0
18	CLA	A	406	1	64,68,73	1.31	10 (15%)	77,107,113	1.25	8 (10%)
20	BCR	A	408	-	41,41,41	0.38	0	56,56,56	0.79	1 (1%)
24	DGD	b	621	-	63,63,67	0.58	0	77,77,81	0.94	4 (5%)
22	LHG	L	101	-	48,48,48	0.51	0	51,54,54	0.52	0
18	CLA	c	506	3	69,73,73	1.22	8 (11%)	83,113,113	1.40	10 (12%)
18	CLA	c	504	3	69,73,73	1.20	7 (10%)	83,113,113	1.26	9 (10%)
20	BCR	b	616	-	41,41,41	0.37	0	56,56,56	2.33	14 (25%)
21	SQD	a	406	-	53,54,54	1.55	8 (15%)	62,65,65	1.33	6 (9%)
18	CLA	c	509	3	69,73,73	1.25	9 (13%)	83,113,113	1.40	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	C	511	3	69,73,73	1.24	8 (11%)	83,113,113	1.26	8 (9%)
18	CLA	A	403	1	69,73,73	1.24	8 (11%)	83,113,113	1.18	5 (6%)
20	BCR	h	101	-	41,41,41	0.44	0	56,56,56	1.77	8 (14%)
18	CLA	C	517	-	69,73,73	1.20	6 (8%)	83,113,113	1.23	7 (8%)
18	CLA	A	405	-	53,57,73	1.41	10 (18%)	62,93,113	1.29	7 (11%)
18	CLA	d	408	-	69,73,73	1.23	8 (11%)	83,113,113	1.24	7 (8%)
18	CLA	d	404	4	69,73,73	1.27	11 (15%)	83,113,113	1.33	12 (14%)

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	PL9	d	405	-	-	12/53/73/73	0/1/1/1
20	BCR	B	613	-	-	10/29/63/63	0/2/2/2
27	HEM	F	101	-	-	9/14/54/54	-
18	CLA	B	609	2	-	13/39/115/115	-
24	DGD	C	513	-	-	25/51/91/95	0/2/2/2
18	CLA	a	403	-	-	16/39/115/115	-
18	CLA	a	405	-	-	9/20/96/115	-
18	CLA	b	608	-	-	18/39/115/115	-
23	LMG	b	618	-	-	17/46/66/70	0/1/1/1
27	HEM	f	101	-	-	9/14/54/54	-
18	CLA	b	604	2	-	13/39/115/115	-
18	CLA	b	609	-	-	17/39/115/115	-
18	CLA	c	513	-	-	14/39/115/115	-
18	CLA	B	603	-	-	9/39/115/115	-
18	CLA	c	512	3	-	18/39/115/115	-
24	DGD	C	503	-	-	17/39/79/95	0/2/2/2
18	CLA	b	612	2	-	16/39/115/115	-
18	CLA	H	101	2	-	14/39/115/115	-
22	LHG	l	101	-	-	16/53/53/53	-
18	CLA	c	511	3	-	20/39/115/115	-
18	CLA	b	606	2	-	16/39/115/115	-
18	CLA	b	603	2	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	C	514	3	-	18/39/115/115	-
18	CLA	C	506	-	-	17/39/115/115	-
18	CLA	B	616	2	-	14/39/115/115	-
23	LMG	D	408	-	-	18/41/61/70	0/1/1/1
26	PL9	D	407	-	-	13/53/73/73	0/1/1/1
18	CLA	c	503	-	-	18/39/115/115	-
18	CLA	b	613	2	-	17/39/115/115	-
23	LMG	C	502	-	-	20/43/63/70	0/1/1/1
18	CLA	B	618	2	-	20/39/115/115	-
18	CLA	c	505	-	-	21/39/115/115	-
24	DGD	c	517	-	-	26/51/91/95	0/2/2/2
18	CLA	B	605	2	-	16/39/115/115	-
18	CLA	C	516	-	-	24/39/115/115	-
20	BCR	B	612	-	-	9/29/63/63	0/2/2/2
18	CLA	C	509	3	-	15/39/115/115	-
18	CLA	c	515	-	-	15/39/115/115	-
18	CLA	B	611	-	-	17/39/115/115	-
19	PHO	D	402	-	-	7/37/103/103	0/5/6/6
18	CLA	B	608	2	-	16/39/115/115	-
23	LMG	B	604	-	-	17/46/66/70	0/1/1/1
18	CLA	b	601	-	-	9/39/115/115	-
18	CLA	A	404	-	-	15/39/115/115	-
20	BCR	b	602	-	-	6/29/63/63	0/2/2/2
24	DGD	c	514	-	-	20/39/79/95	0/2/2/2
18	CLA	C	504	-	-	5/20/96/115	-
18	CLA	D	405	-	-	18/39/115/115	-
18	CLA	c	507	-	-	5/20/96/115	-
18	CLA	b	617	2	-	16/39/115/115	-
18	CLA	B	614	2	-	16/39/115/115	-
18	CLA	b	614	2	-	20/39/115/115	-
18	CLA	B	607	-	-	14/39/115/115	-
18	CLA	b	607	2	-	18/39/115/115	-
18	CLA	B	601	2	-	14/39/115/115	-
18	CLA	B	619	-	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	b	619	-	-	8/39/115/115	-
19	PHO	a	409	-	-	15/37/103/103	0/5/6/6
18	CLA	c	510	-	-	17/39/115/115	-
18	CLA	a	407	1	-	10/39/115/115	-
21	SQD	A	409	-	-	26/49/69/69	0/1/1/1
18	CLA	b	620	2	-	11/39/115/115	-
20	BCR	b	610	-	-	9/29/63/63	0/2/2/2
18	CLA	B	606	-	-	20/39/115/115	-
22	LHG	D	409	-	-	15/47/47/53	-
22	LHG	A	410	-	-	17/41/41/53	-
18	CLA	B	615	-	-	9/39/115/115	-
18	CLA	C	507	-	-	11/24/100/115	-
19	PHO	d	401	-	-	8/37/103/103	0/5/6/6
18	CLA	C	508	3	-	21/39/115/115	-
18	CLA	c	516	3	-	20/39/115/115	-
22	LHG	d	403	-	-	18/47/47/53	-
22	LHG	a	410	-	-	12/41/41/53	-
18	CLA	a	404	1	-	15/33/109/115	-
18	CLA	C	512	3	-	15/39/115/115	-
18	CLA	b	611	-	-	20/39/115/115	-
24	DGD	B	620	-	-	20/51/91/95	0/2/2/2
18	CLA	b	615	2	-	15/39/115/115	-
19	PHO	A	407	-	-	16/37/103/103	0/5/6/6
23	LMG	d	409	-	-	17/41/61/70	0/1/1/1
20	BCR	a	401	-	-	7/29/63/63	0/2/2/2
18	CLA	C	510	-	-	14/39/115/115	-
18	CLA	D	406	4	-	18/39/115/115	-
18	CLA	B	617	2	-	19/39/115/115	-
20	BCR	B	610	-	-	6/29/63/63	0/2/2/2
20	BCR	D	403	-	-	7/29/63/63	0/2/2/2
22	LHG	D	404	-	-	21/53/53/53	-
18	CLA	C	515	3	-	18/39/115/115	-
20	BCR	d	407	-	-	4/29/63/63	0/2/2/2
18	CLA	b	605	2	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	c	508	-	-	10/24/100/115	-
20	BCR	H	102	-	-	10/29/63/63	0/2/2/2
18	CLA	C	505	-	-	18/39/115/115	-
18	CLA	B	602	2	-	18/39/115/115	-
22	LHG	d	406	-	-	20/53/53/53	-
23	LMG	c	502	-	-	19/43/63/70	0/1/1/1
18	CLA	A	406	1	-	15/33/109/115	-
20	BCR	A	408	-	-	6/29/63/63	0/2/2/2
24	DGD	b	621	-	-	19/51/91/95	0/2/2/2
22	LHG	L	101	-	-	16/53/53/53	-
18	CLA	c	506	3	-	16/39/115/115	-
18	CLA	c	504	3	-	17/39/115/115	-
20	BCR	b	616	-	-	10/29/63/63	0/2/2/2
21	SQD	a	406	-	-	26/49/69/69	0/1/1/1
18	CLA	c	509	3	-	16/39/115/115	-
18	CLA	C	511	3	-	20/39/115/115	-
18	CLA	A	403	1	-	10/39/115/115	-
20	BCR	h	101	-	-	10/29/63/63	0/2/2/2
18	CLA	C	517	-	-	15/39/115/115	-
18	CLA	A	405	-	-	9/20/96/115	-
18	CLA	d	408	-	-	19/39/115/115	-
18	CLA	d	404	4	-	17/39/115/115	-

The worst 5 of 694 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	407	PHO	C1B-C2B	8.83	1.49	1.39
19	a	409	PHO	C1B-C2B	8.82	1.49	1.39
19	d	401	PHO	C1B-C2B	8.69	1.49	1.39
19	D	402	PHO	C1B-C2B	8.63	1.49	1.39
19	d	401	PHO	C3B-C4B	7.45	1.50	1.41

The worst 5 of 773 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	504	CLA	CHC-C4B-NB	-8.08	115.71	124.26
18	c	507	CLA	C4A-NA-C1A	7.92	110.27	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	504	CLA	C4A-NA-C1A	7.86	110.24	106.71
18	c	507	CLA	CHC-C4B-NB	-7.76	116.04	124.26
18	c	505	CLA	C4A-NA-C1A	7.72	110.18	106.71

There are no chirality outliers.

5 of 1679 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	405	CLA	C2B-C3B-CAB-CBB
18	A	405	CLA	C4B-C3B-CAB-CBB
18	A	405	CLA	CBD-CGD-O2D-CED
18	B	601	CLA	C3A-C2A-CAA-CBA
18	B	602	CLA	C2-C3-C5-C6

There are no ring outliers.

114 monomers are involved in 895 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	d	405	PL9	11	0
20	B	613	BCR	9	0
27	F	101	HEM	3	0
18	B	609	CLA	18	0
24	C	513	DGD	6	0
18	a	403	CLA	8	0
18	a	405	CLA	6	0
18	b	608	CLA	14	0
16	A	401	OEX	1	0
23	b	618	LMG	10	0
27	f	101	HEM	2	0
18	b	604	CLA	17	0
18	b	609	CLA	6	0
18	c	513	CLA	10	0
18	B	603	CLA	10	0
18	c	512	CLA	13	0
24	C	503	DGD	12	0
18	b	612	CLA	10	0
18	H	101	CLA	17	0
22	l	101	LHG	9	0
18	c	511	CLA	16	0
18	b	606	CLA	12	0
18	b	603	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	514	CLA	14	0
18	C	506	CLA	7	0
18	B	616	CLA	8	0
23	D	408	LMG	4	0
26	D	407	PL9	7	0
18	c	503	CLA	12	0
18	b	613	CLA	14	0
23	C	502	LMG	12	0
18	B	618	CLA	15	0
18	c	505	CLA	25	0
24	c	517	DGD	5	0
18	B	605	CLA	13	0
18	C	516	CLA	20	0
20	B	612	BCR	3	0
18	C	509	CLA	15	0
18	c	515	CLA	15	0
18	B	611	CLA	5	0
19	D	402	PHO	8	0
18	B	608	CLA	9	0
23	B	604	LMG	9	0
18	b	601	CLA	6	0
18	A	404	CLA	10	0
20	b	602	BCR	6	0
24	c	514	DGD	10	0
18	C	504	CLA	7	0
18	D	405	CLA	9	0
18	c	507	CLA	6	0
18	b	617	CLA	7	0
18	B	614	CLA	8	0
18	b	614	CLA	16	0
18	B	607	CLA	12	0
18	b	607	CLA	11	0
18	B	601	CLA	18	0
18	B	619	CLA	13	0
18	b	619	CLA	12	0
19	a	409	PHO	9	0
18	c	510	CLA	4	0
18	a	407	CLA	14	0
21	A	409	SQD	4	0
18	b	620	CLA	12	0
20	b	610	BCR	4	0
18	B	606	CLA	8	0

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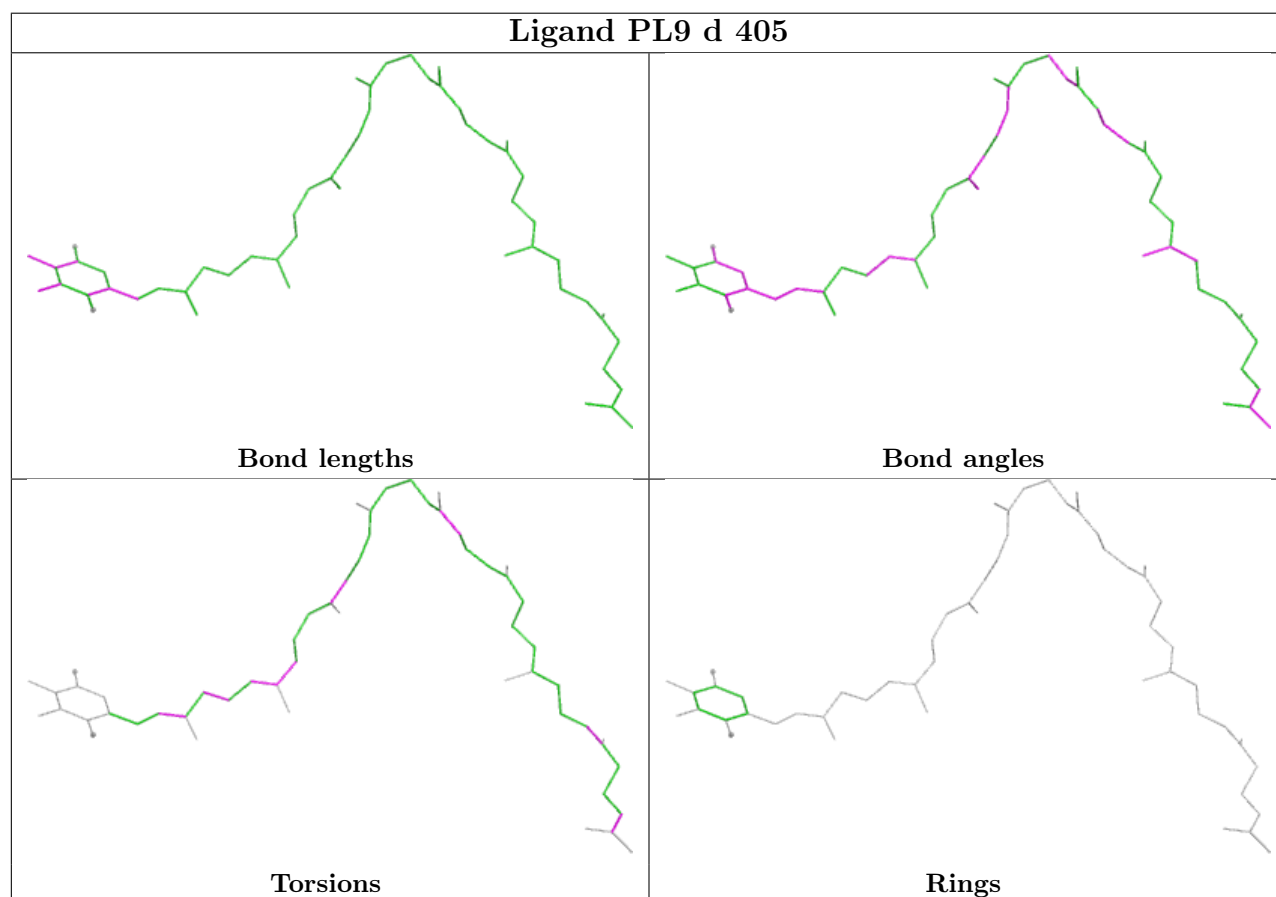
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	A	410	LHG	4	0
18	B	615	CLA	7	0
18	C	507	CLA	3	0
19	d	401	PHO	11	0
18	C	508	CLA	6	0
18	c	516	CLA	5	0
22	d	403	LHG	7	0
22	a	410	LHG	4	0
16	a	402	OEX	1	0
18	a	404	CLA	13	0
18	C	512	CLA	14	0
18	b	611	CLA	8	0
24	B	620	DGD	14	0
18	b	615	CLA	12	0
19	A	407	PHO	9	0
23	d	409	LMG	3	0
20	a	401	BCR	7	0
18	C	510	CLA	10	0
18	D	406	CLA	10	0
18	B	617	CLA	13	0
20	B	610	BCR	6	0
20	D	403	BCR	6	0
22	D	404	LHG	12	0
18	C	515	CLA	14	0
20	d	407	BCR	4	0
18	b	605	CLA	17	0
18	c	508	CLA	4	0
20	H	102	BCR	9	0
18	C	505	CLA	10	0
18	B	602	CLA	9	0
22	d	406	LHG	13	0
23	c	502	LMG	14	0
18	A	406	CLA	13	0
20	A	408	BCR	7	0
24	b	621	DGD	11	0
22	L	101	LHG	9	0
18	c	506	CLA	14	0
18	c	504	CLA	16	0
20	b	616	BCR	9	0
21	a	406	SQD	5	0
18	c	509	CLA	12	0

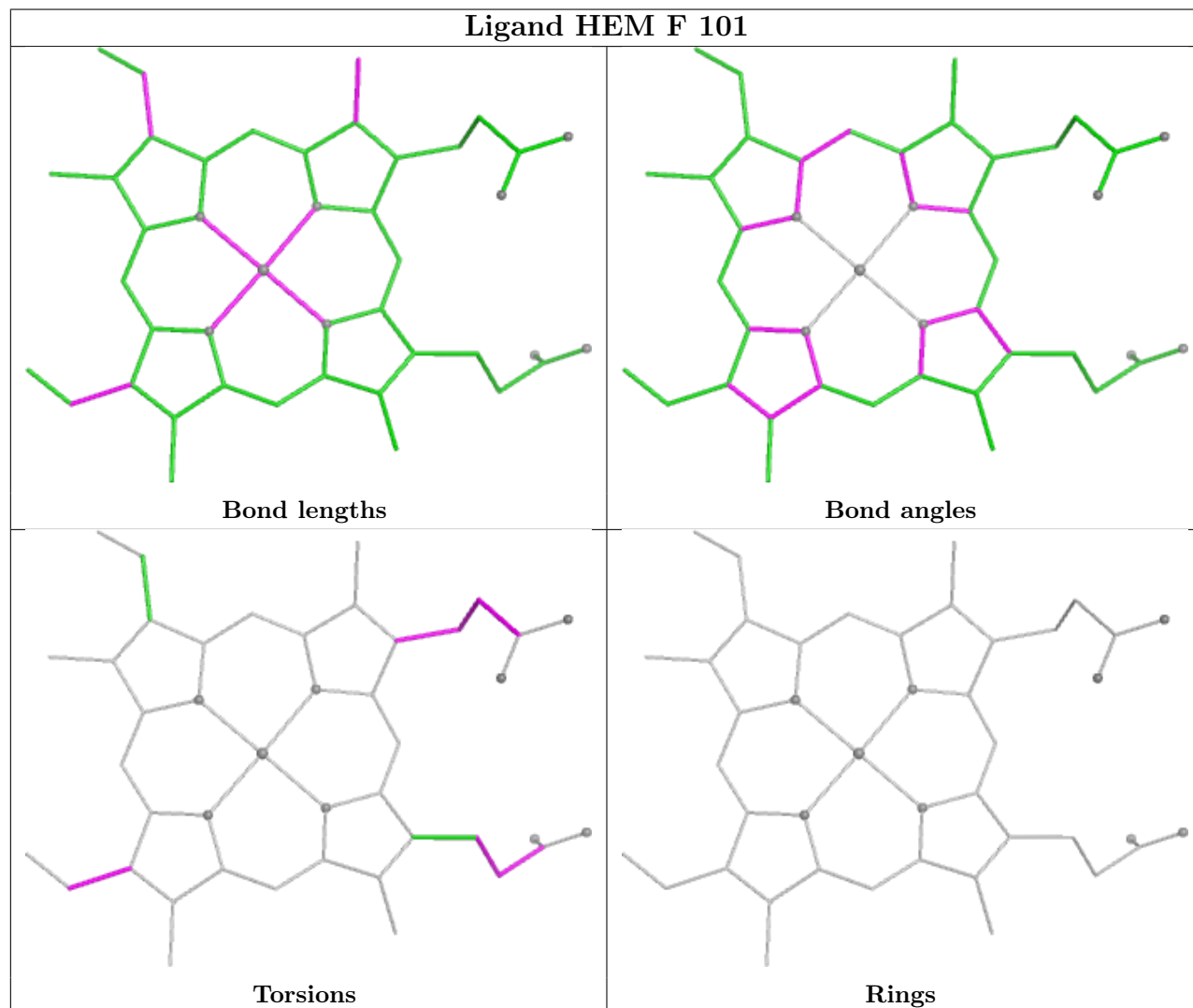
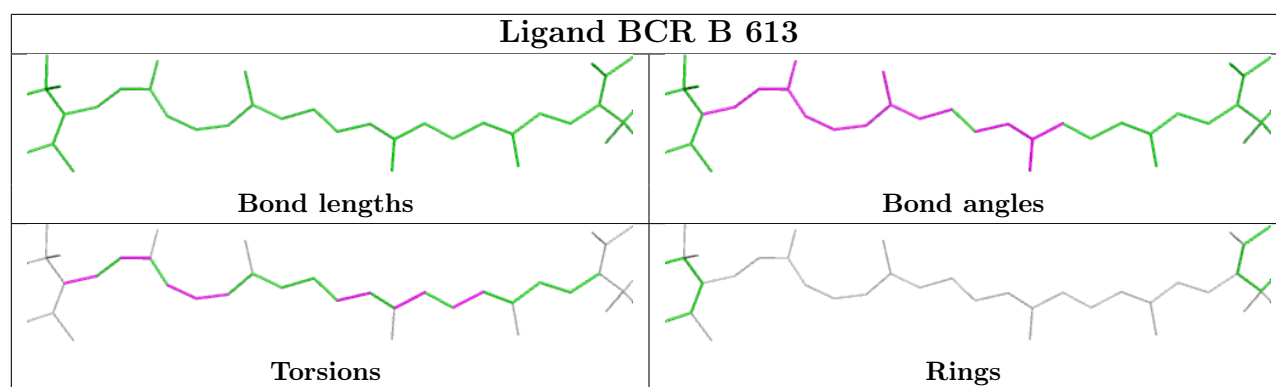
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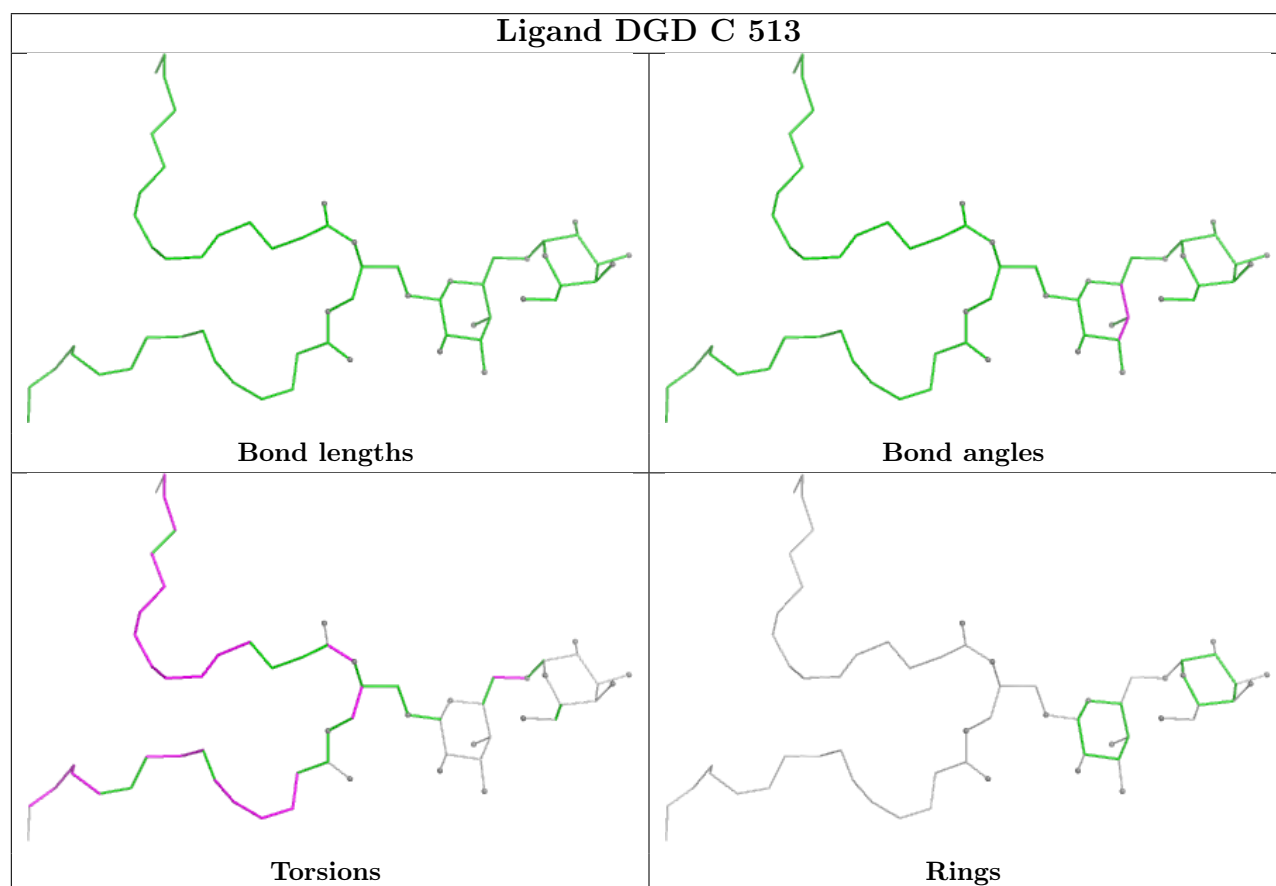
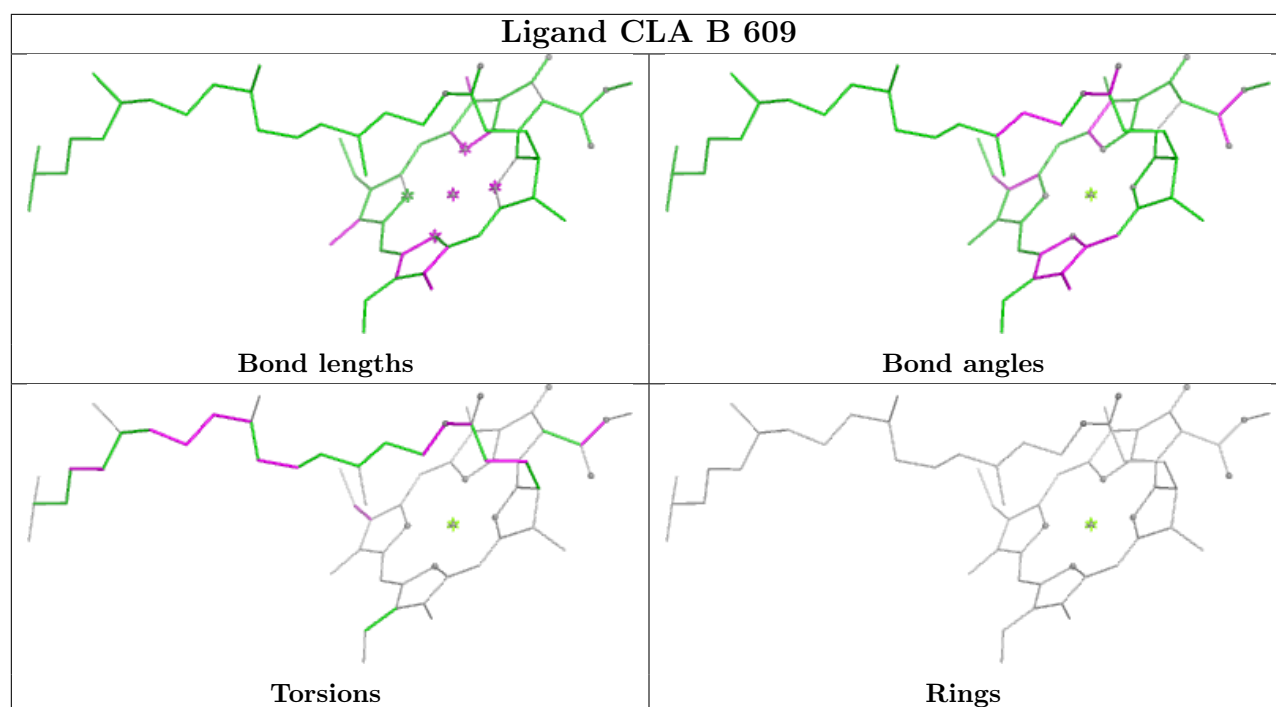
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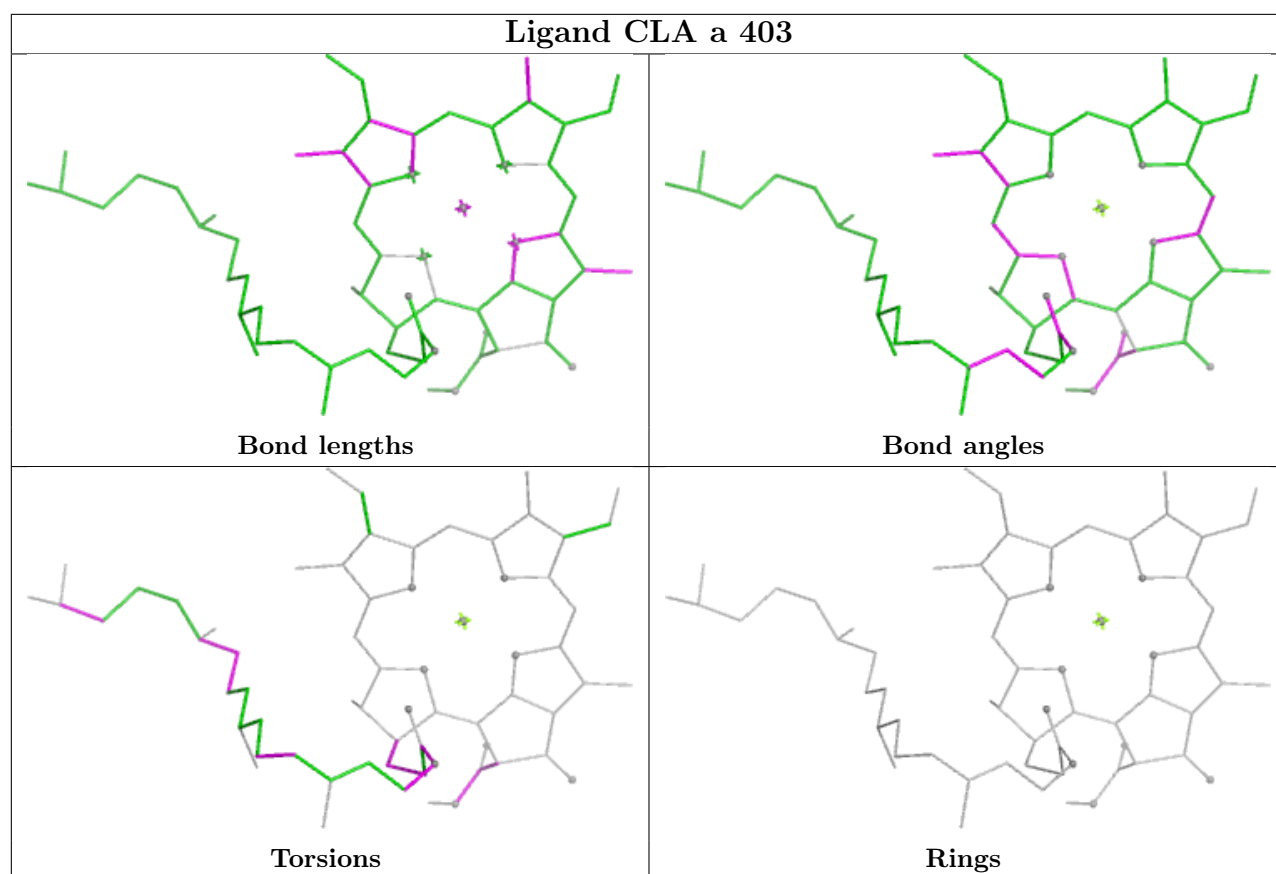
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	511	CLA	17	0
18	A	403	CLA	15	0
20	h	101	BCR	7	0
18	C	517	CLA	16	0
18	A	405	CLA	4	0
18	d	408	CLA	11	0
18	d	404	CLA	11	0

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.

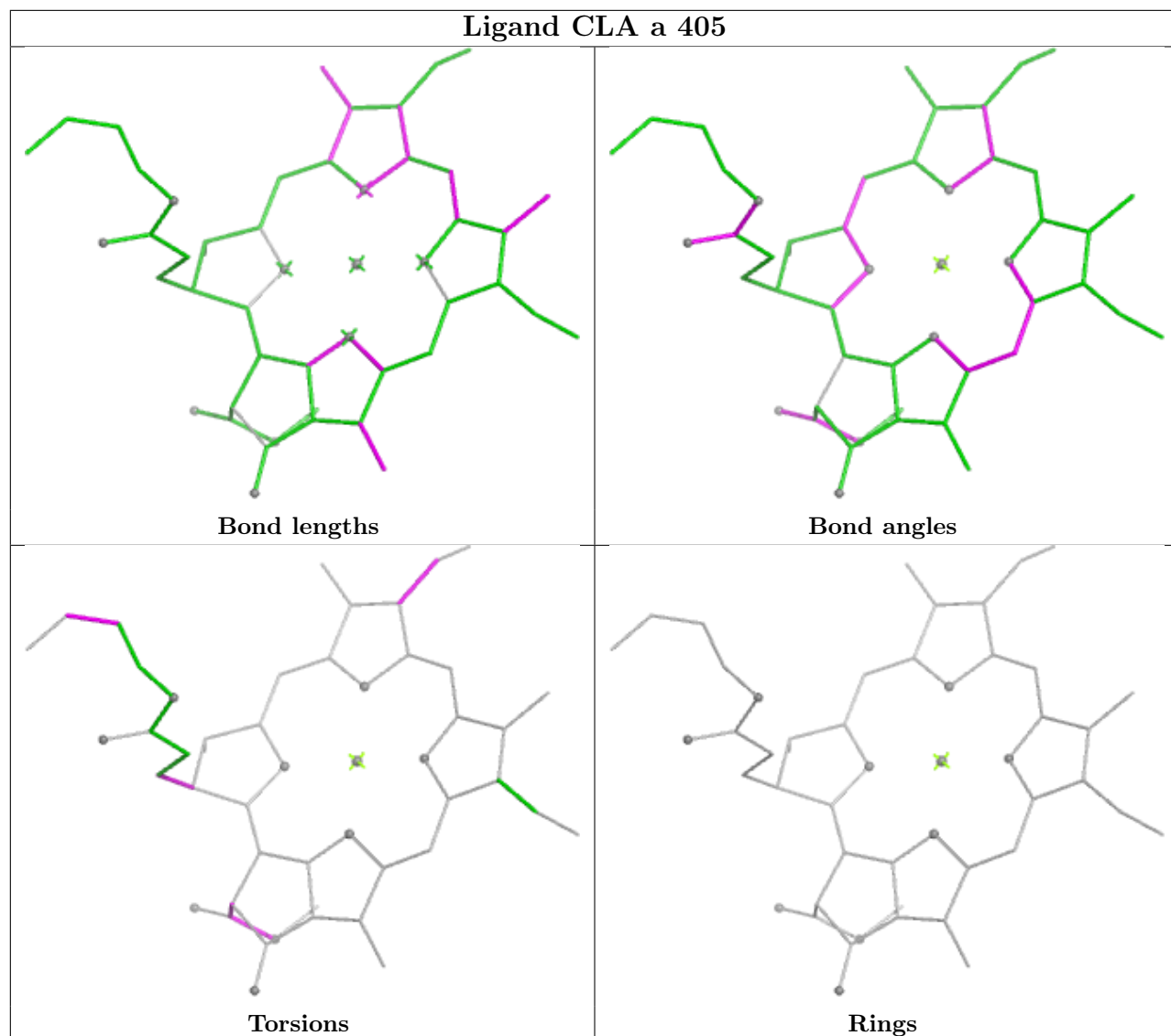


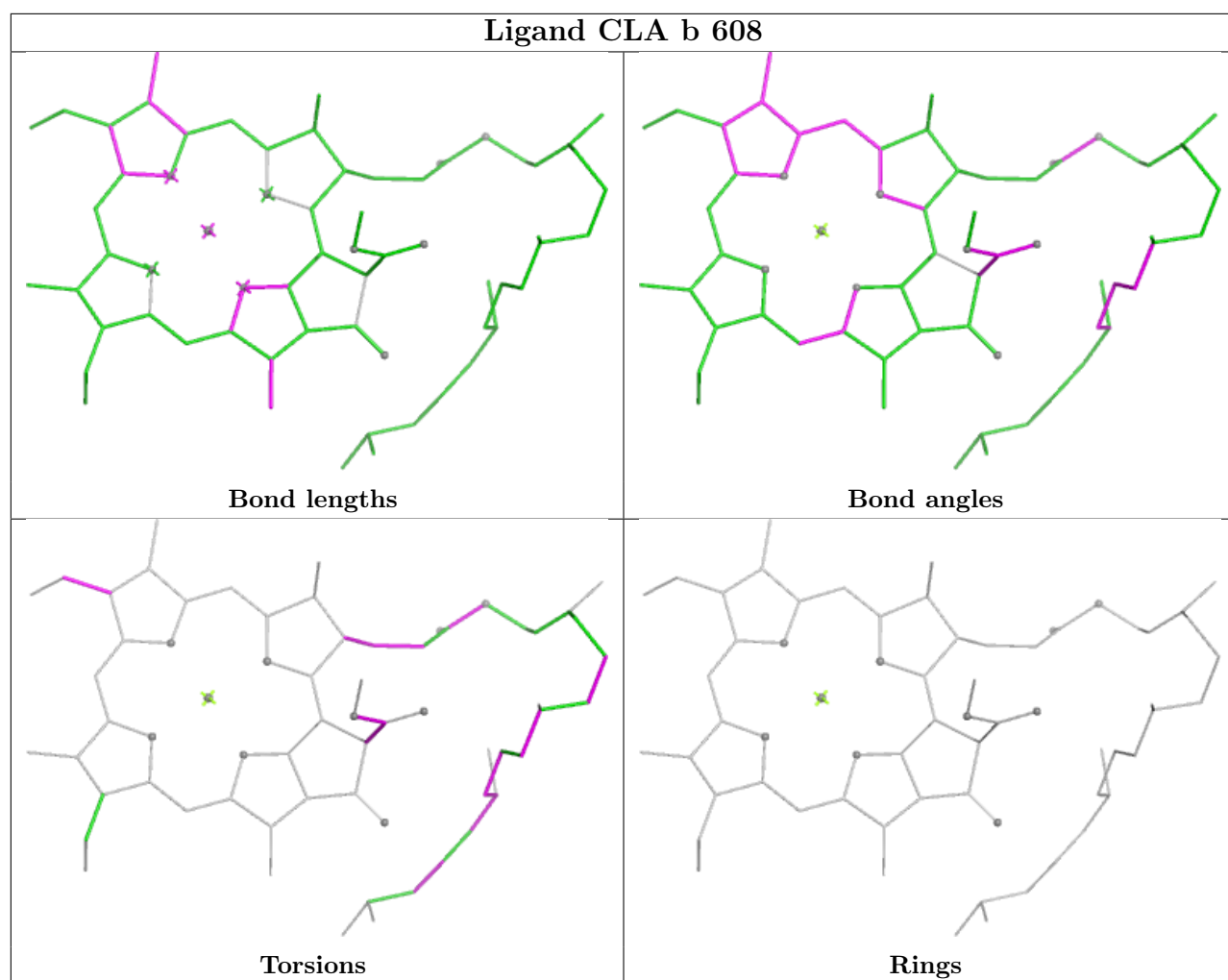


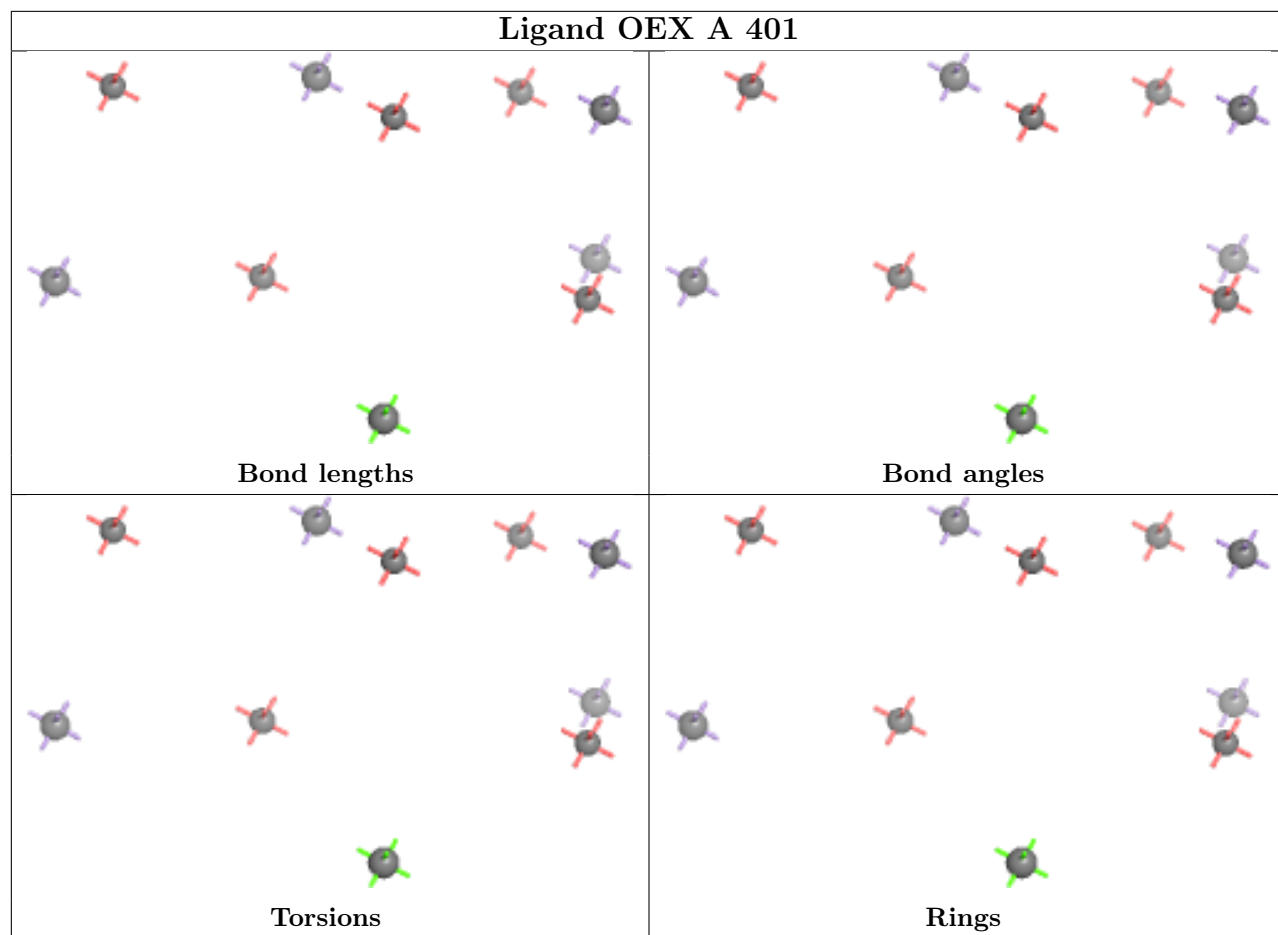


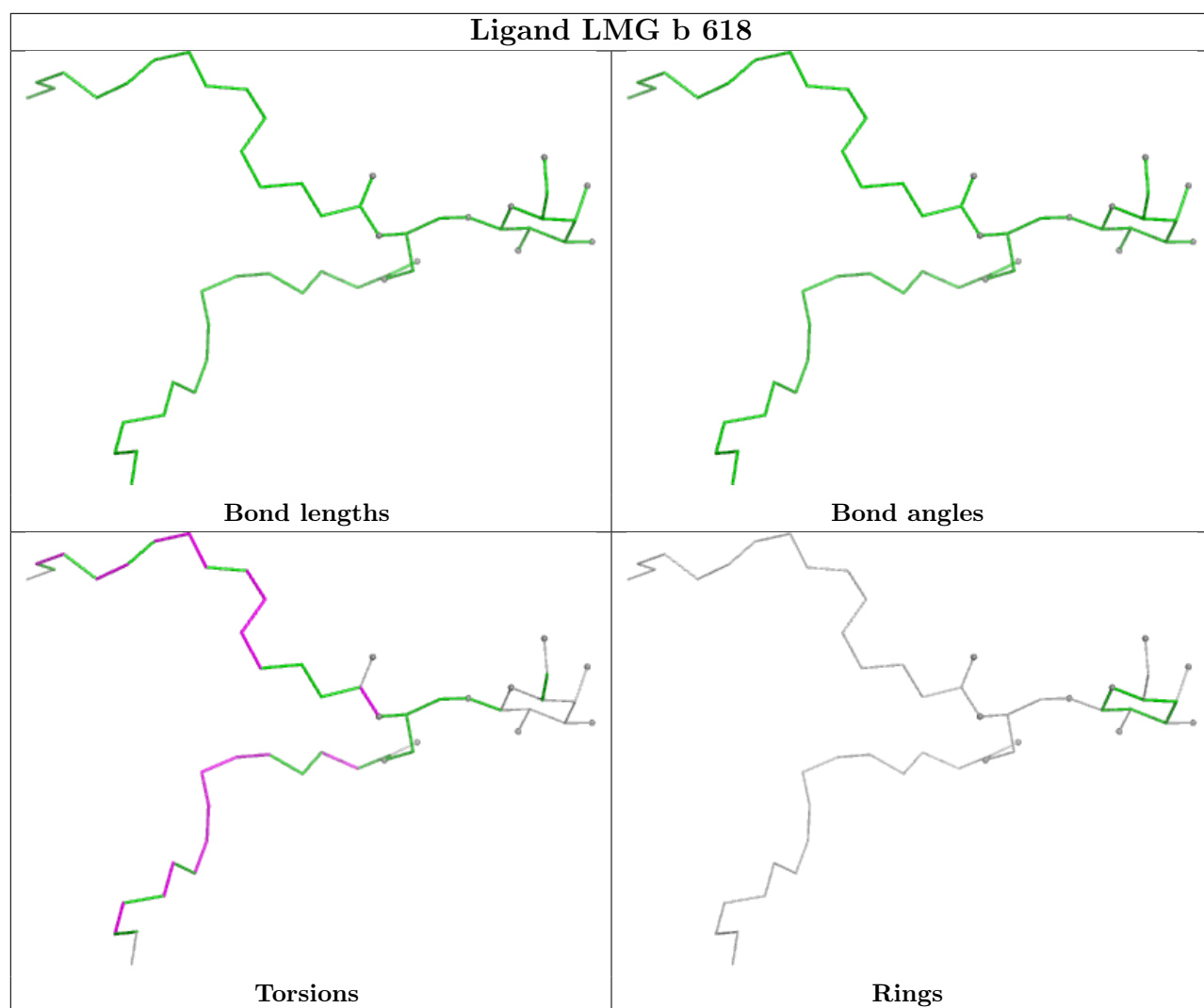


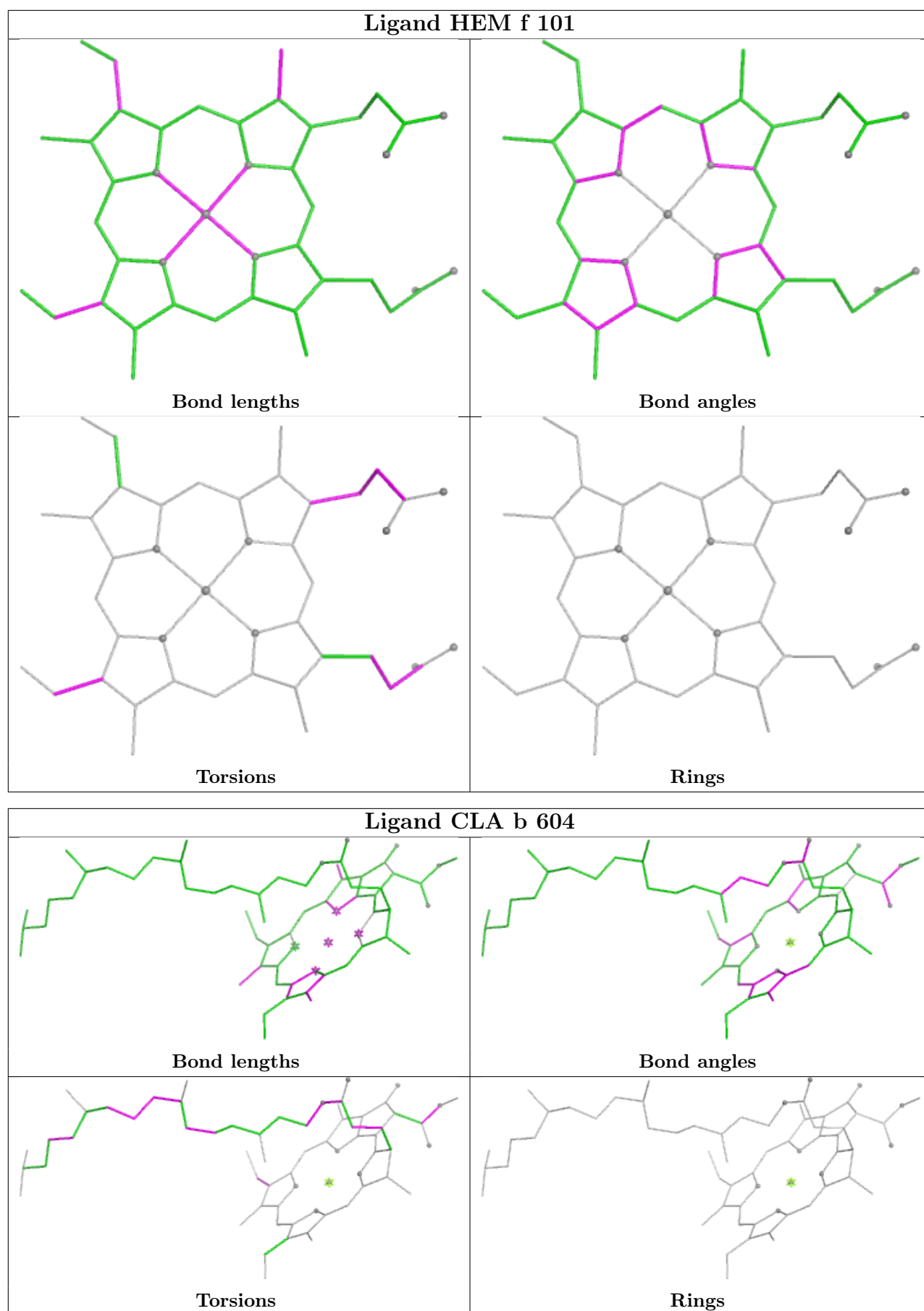
Ligand CLA a 405

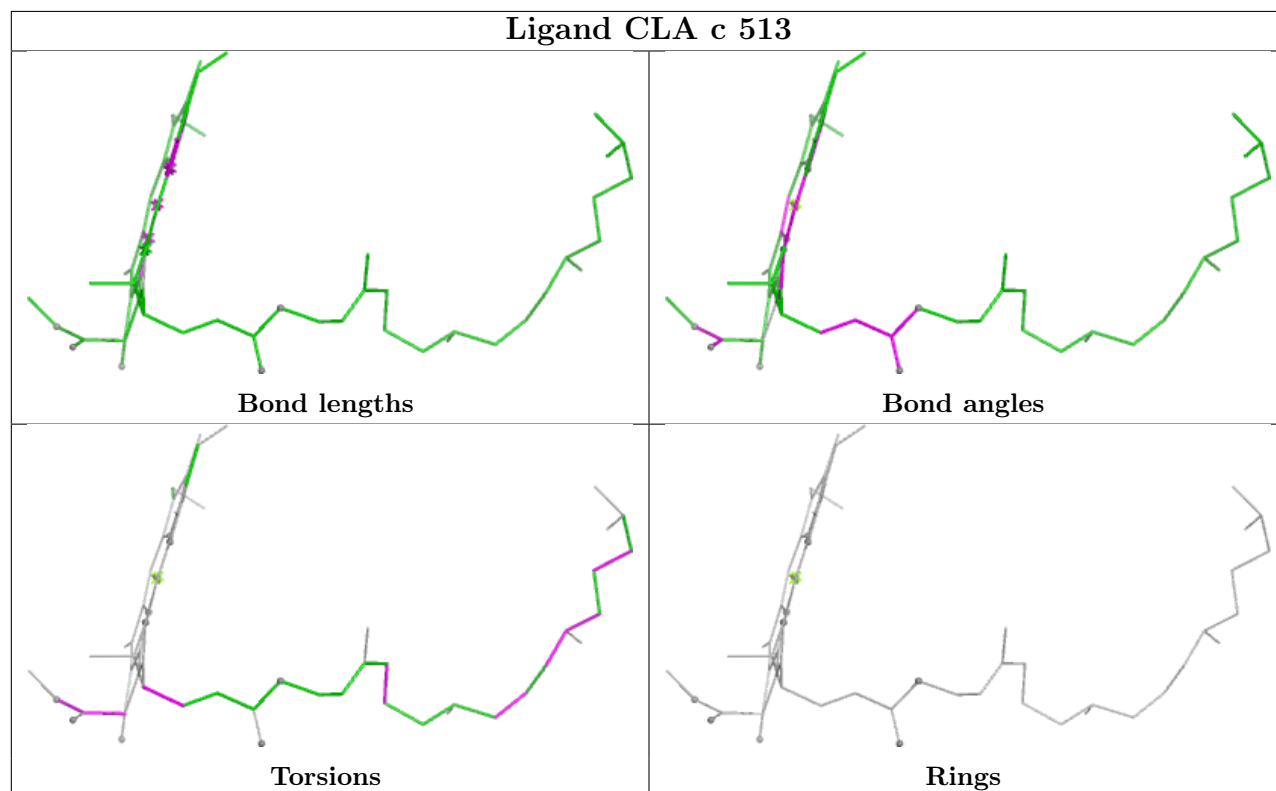
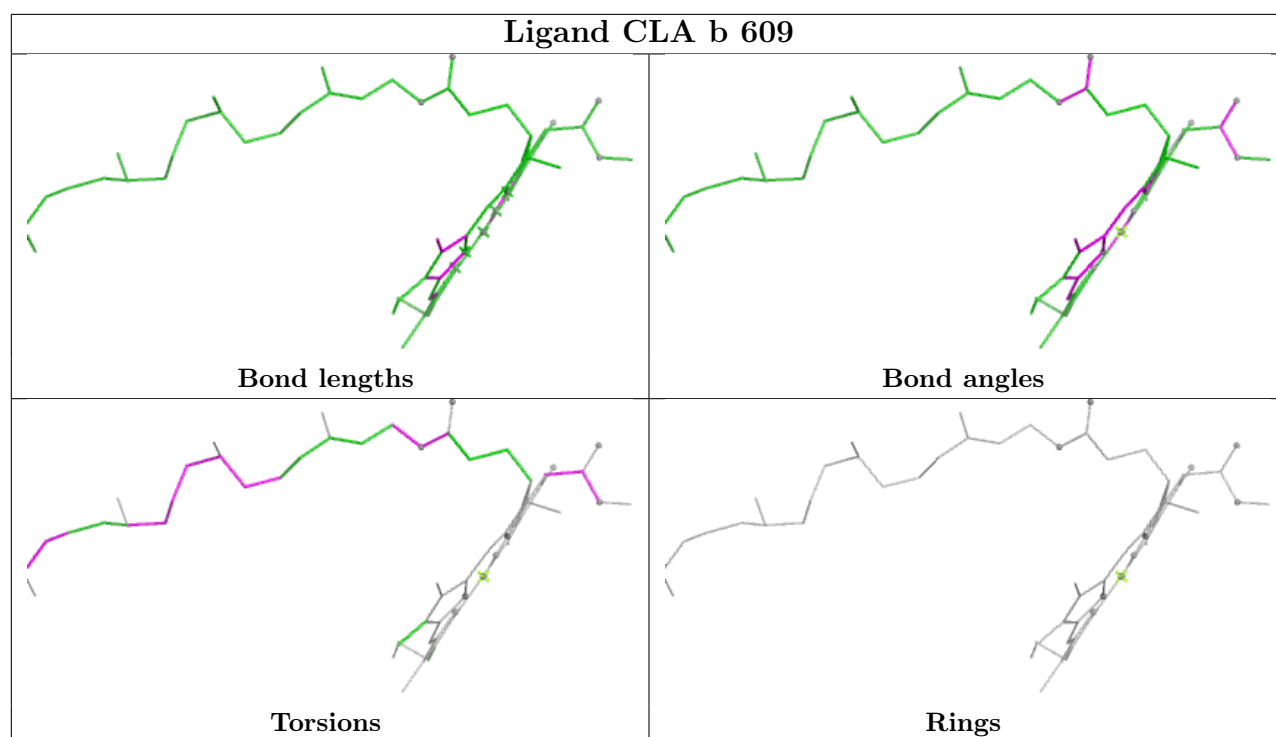


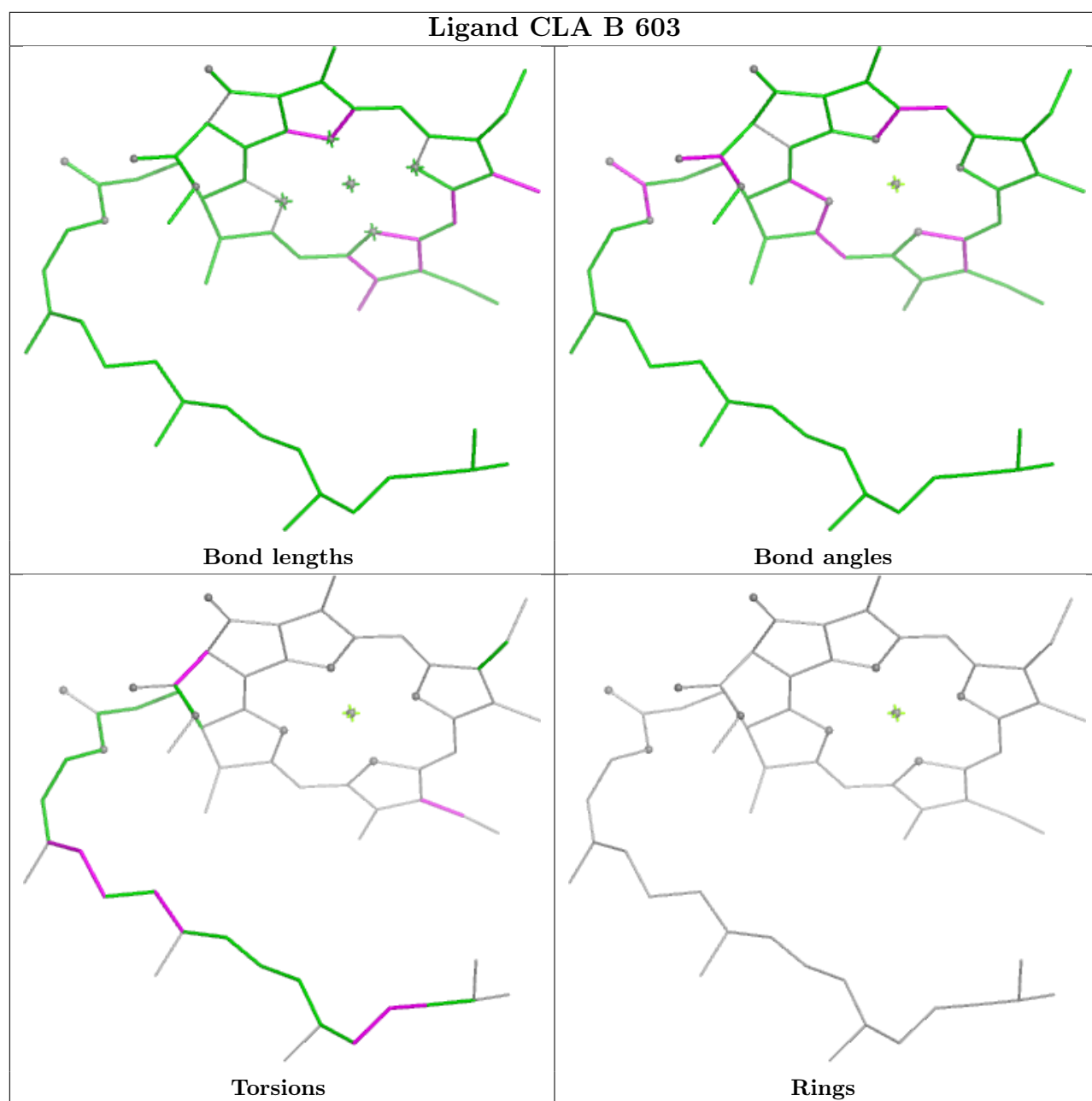


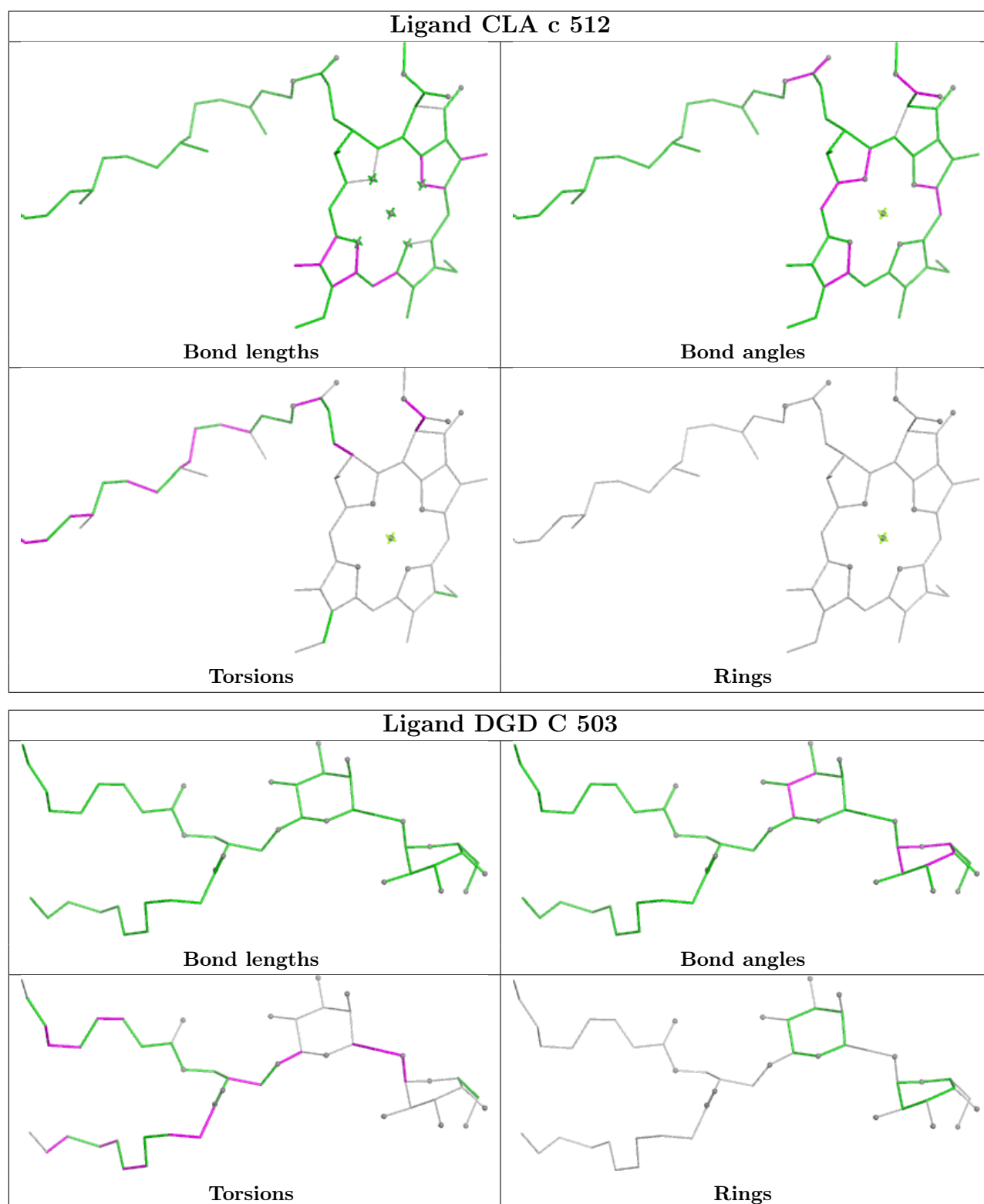


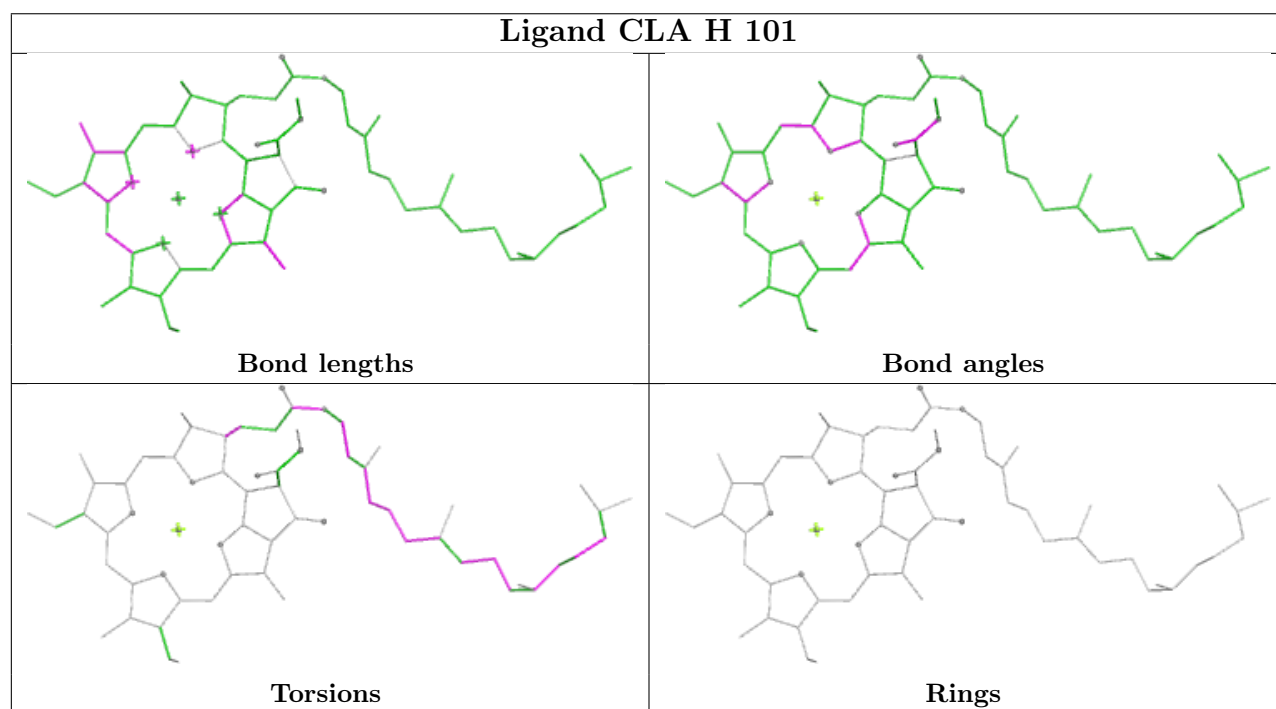
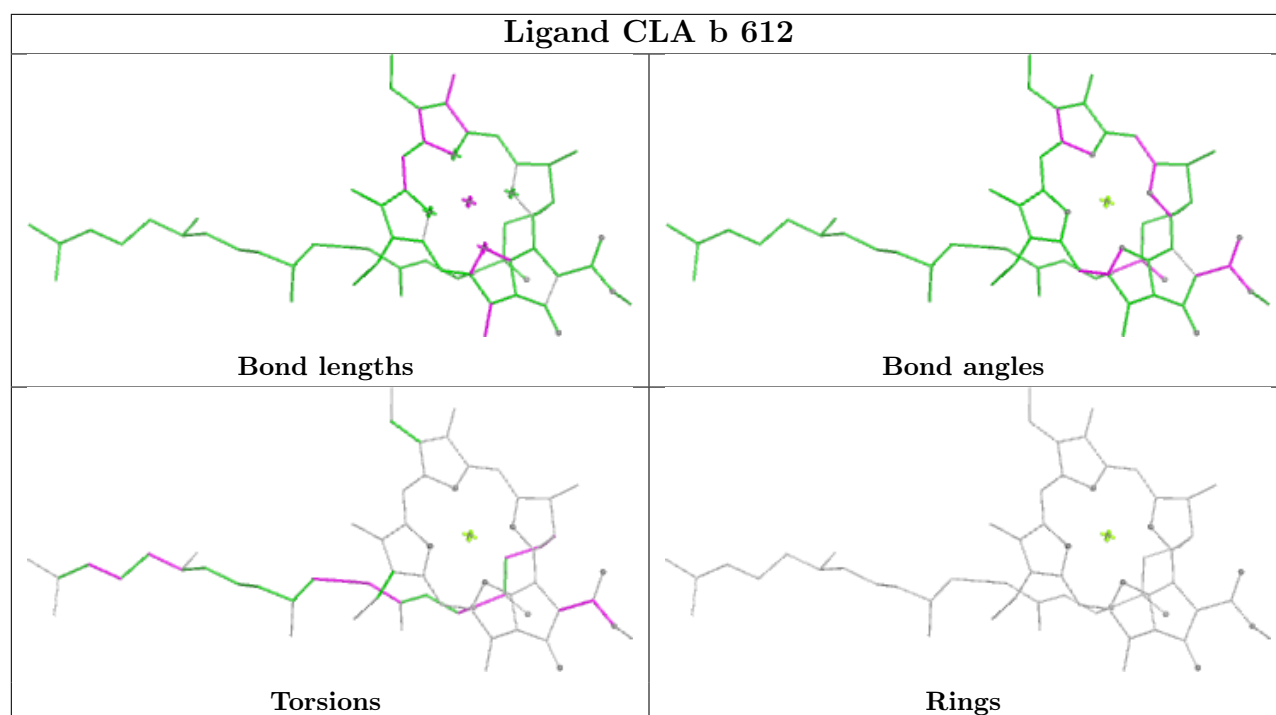


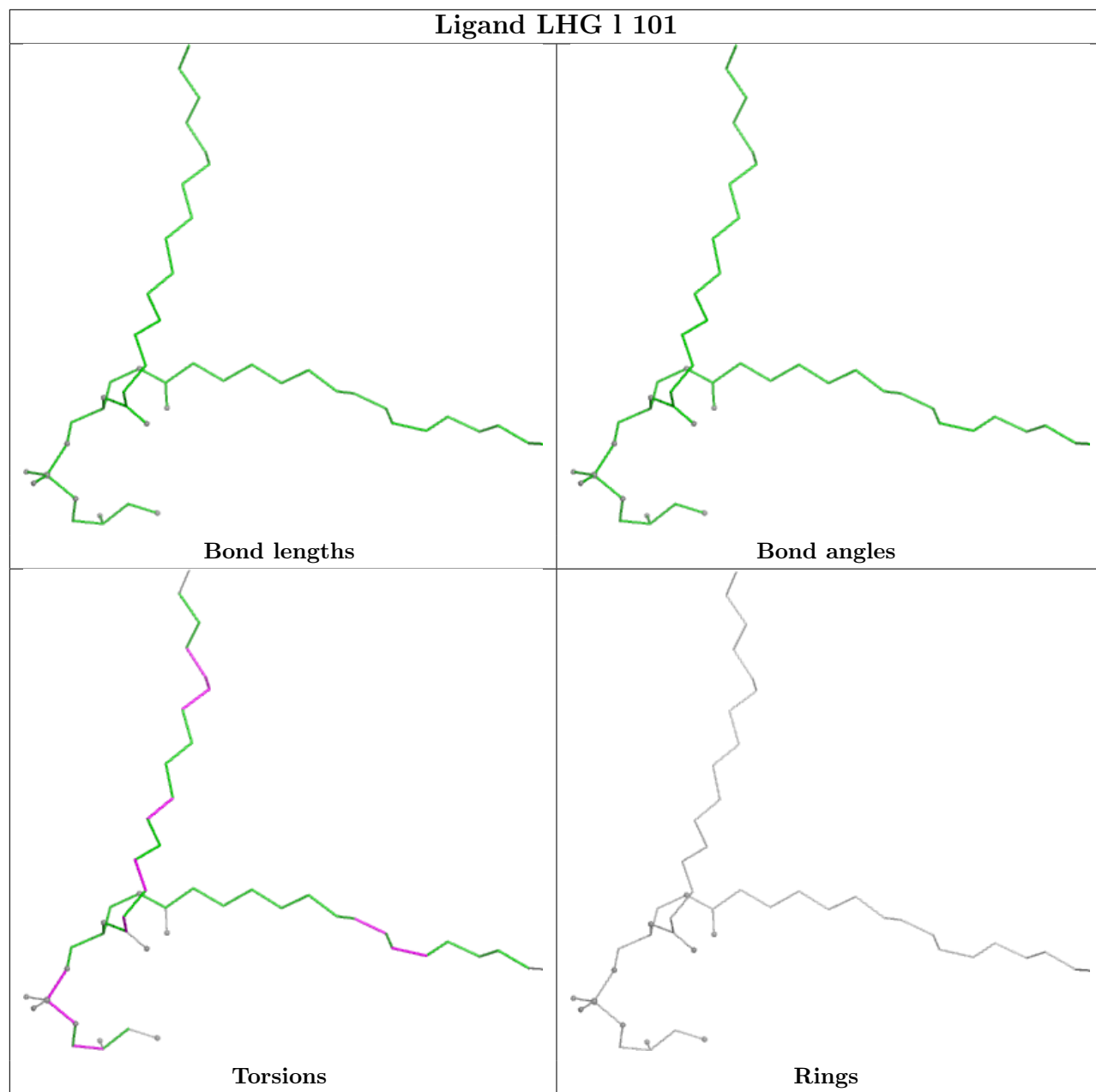


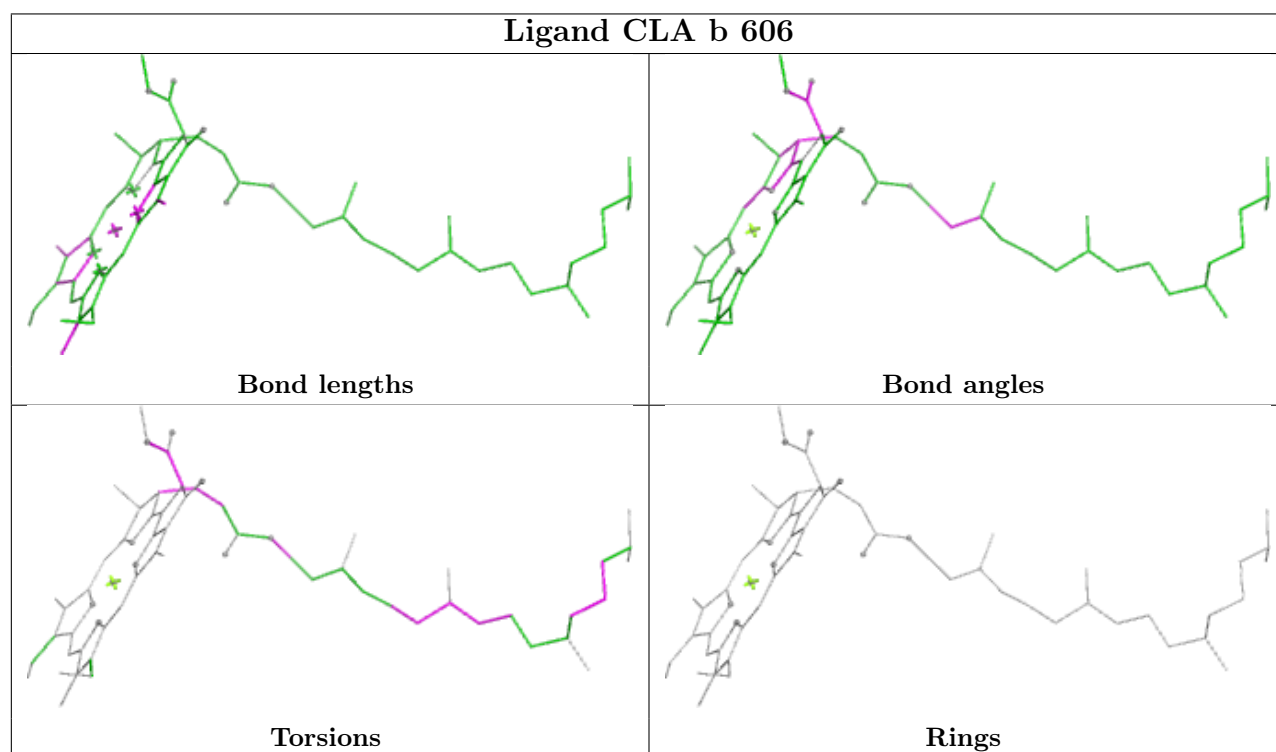
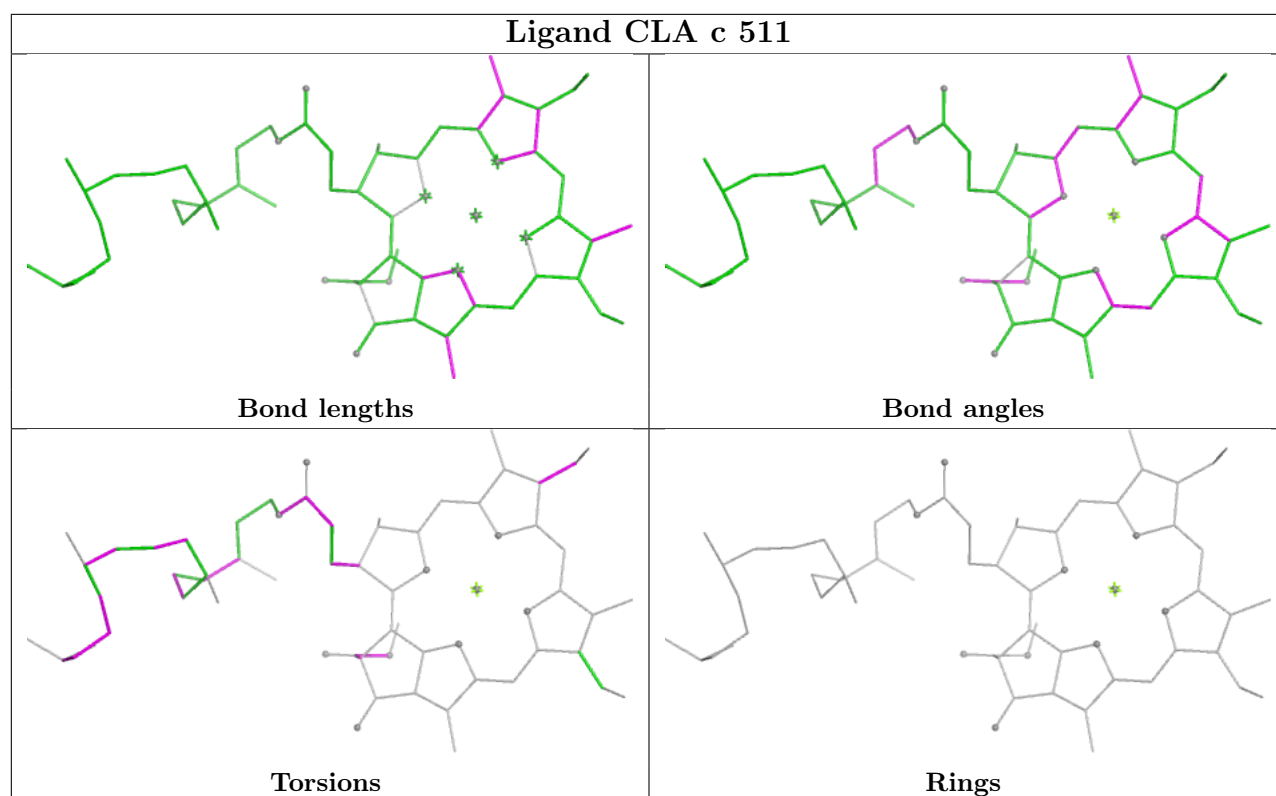


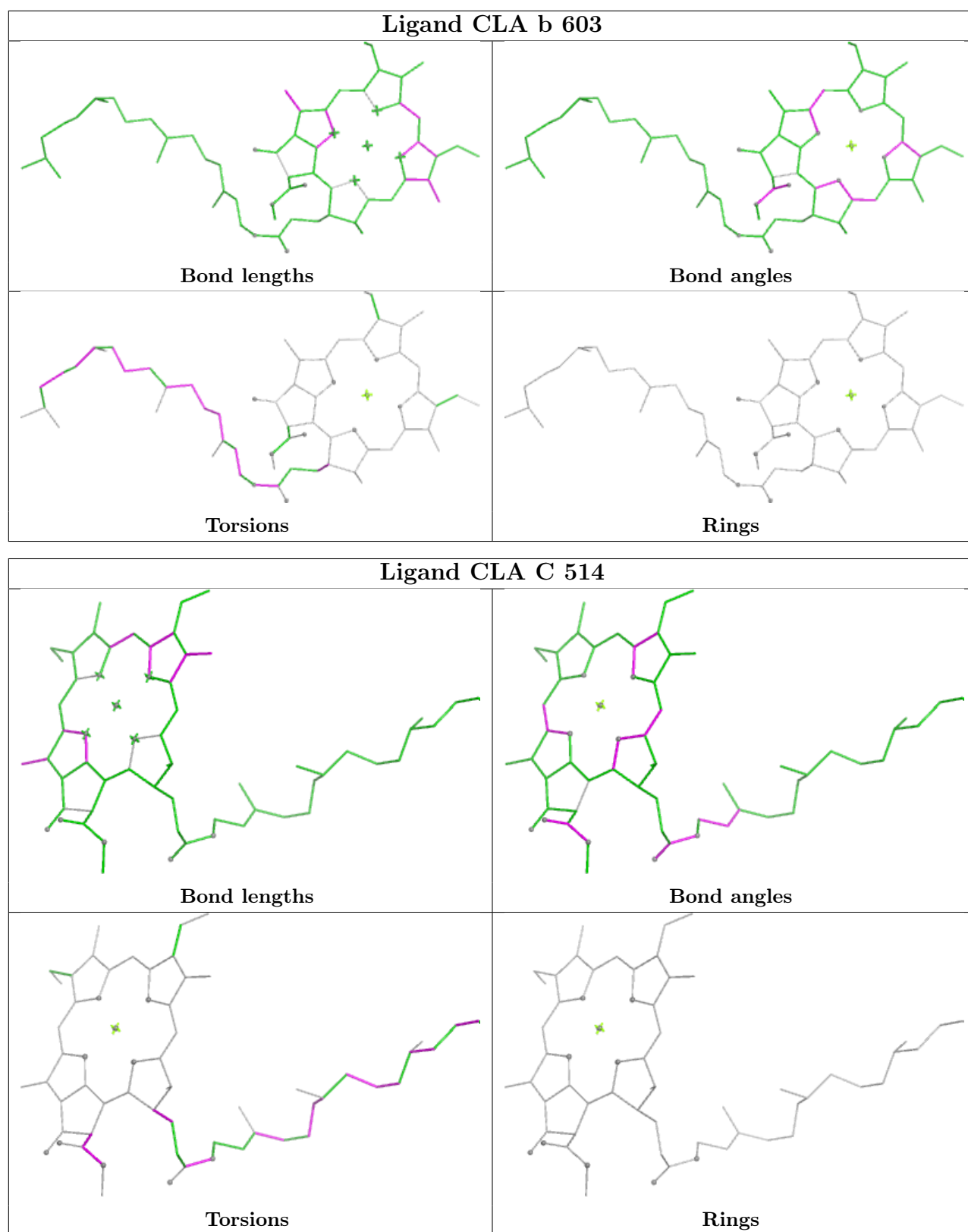


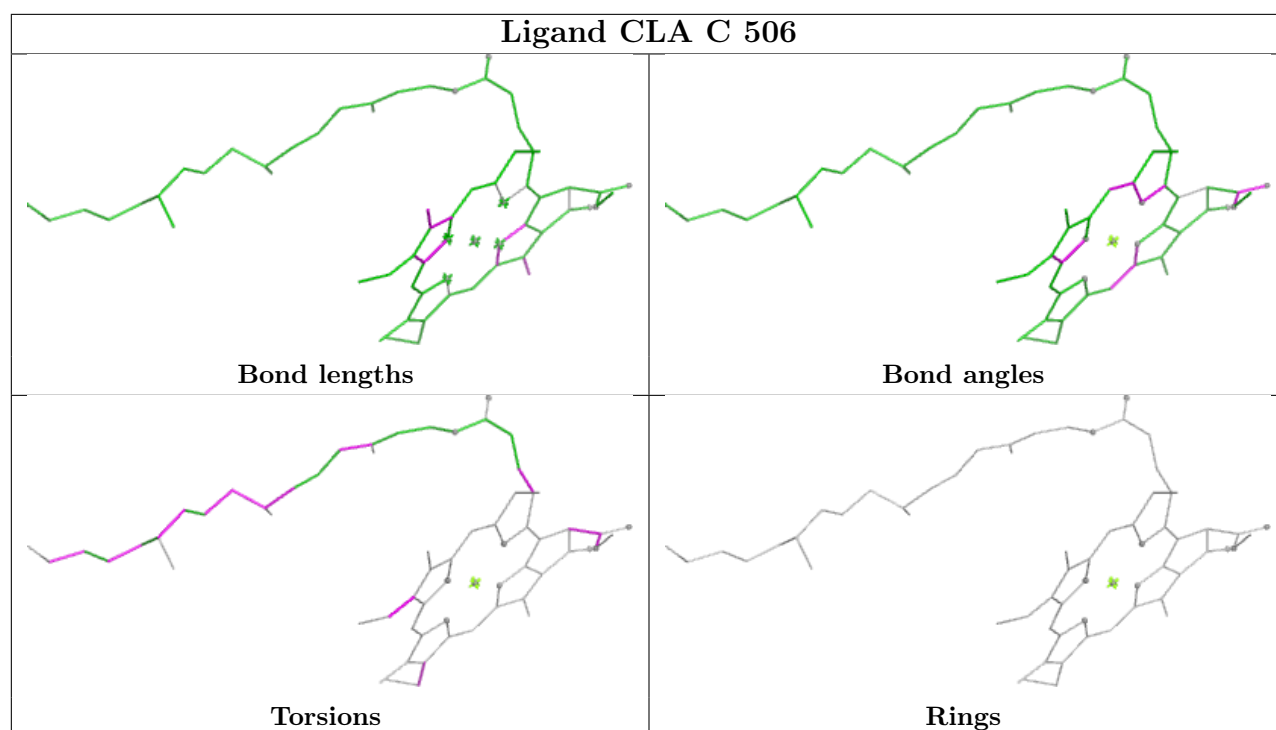




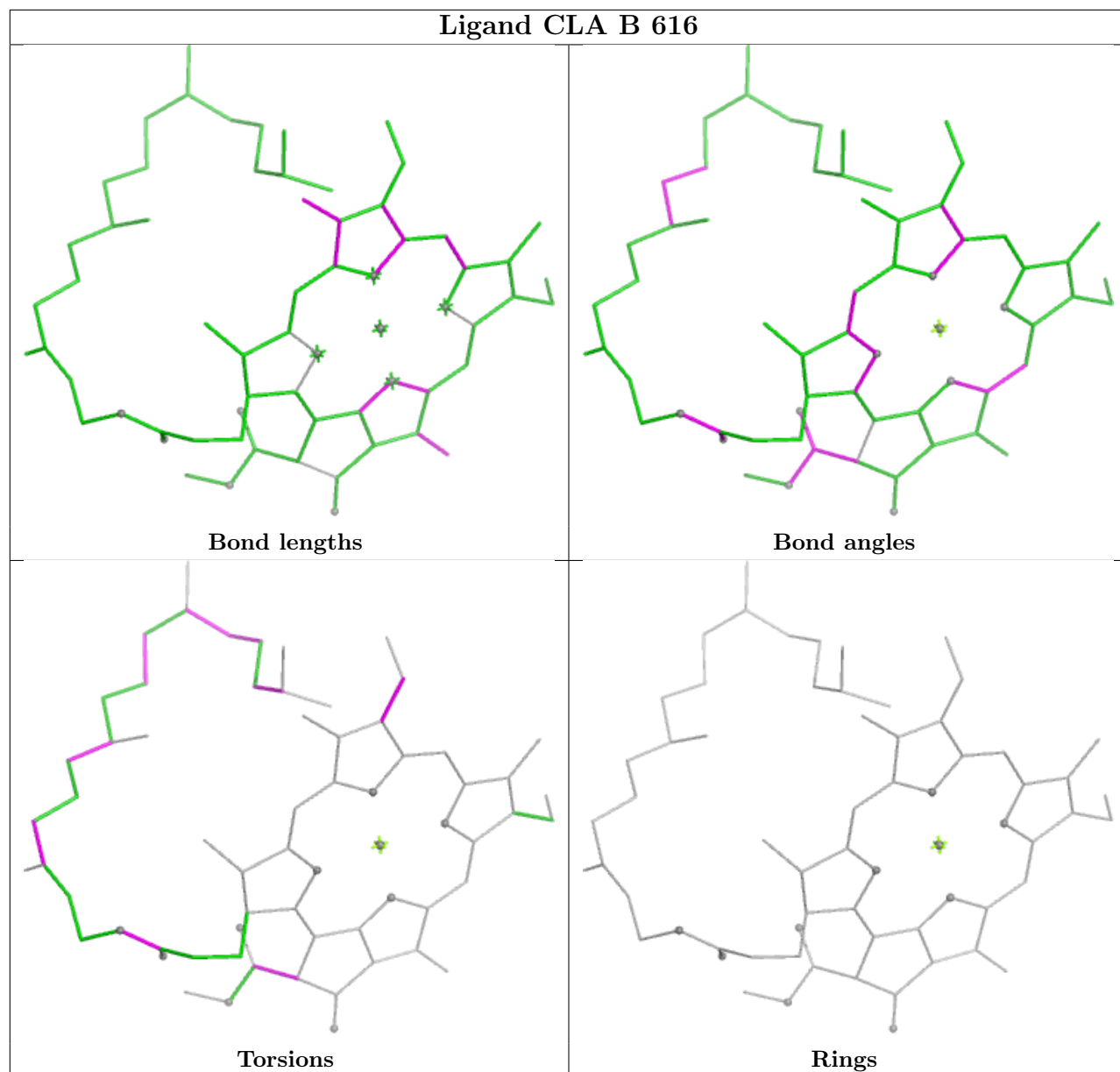


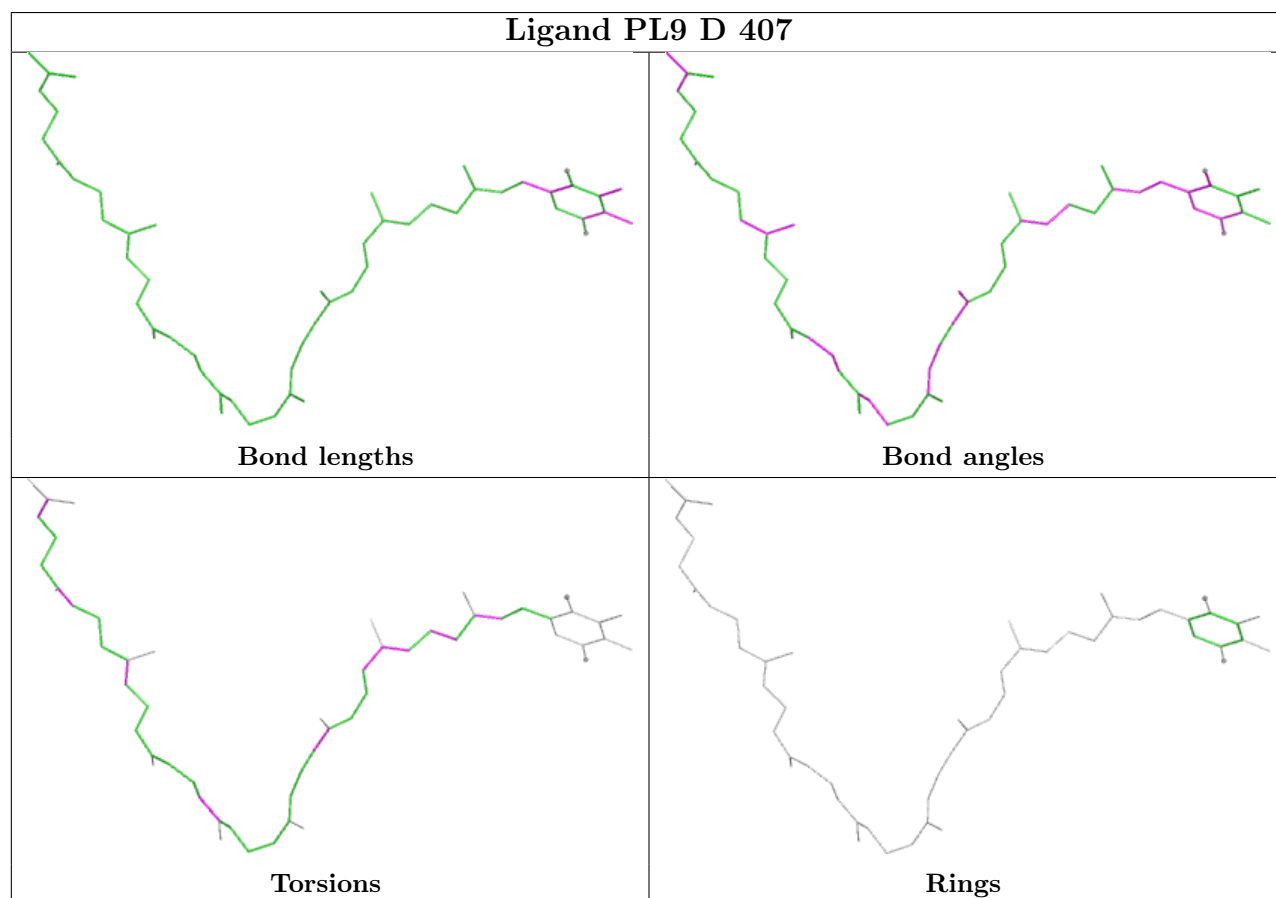
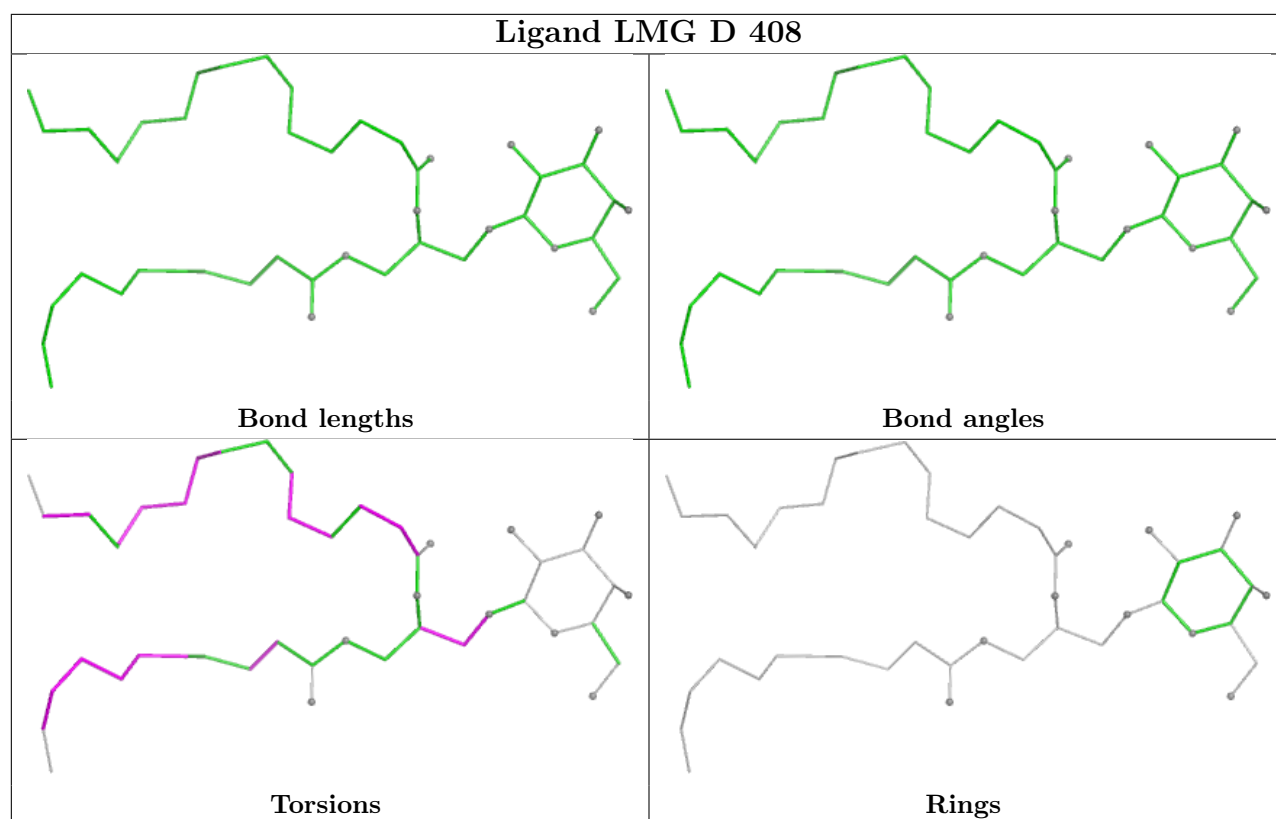


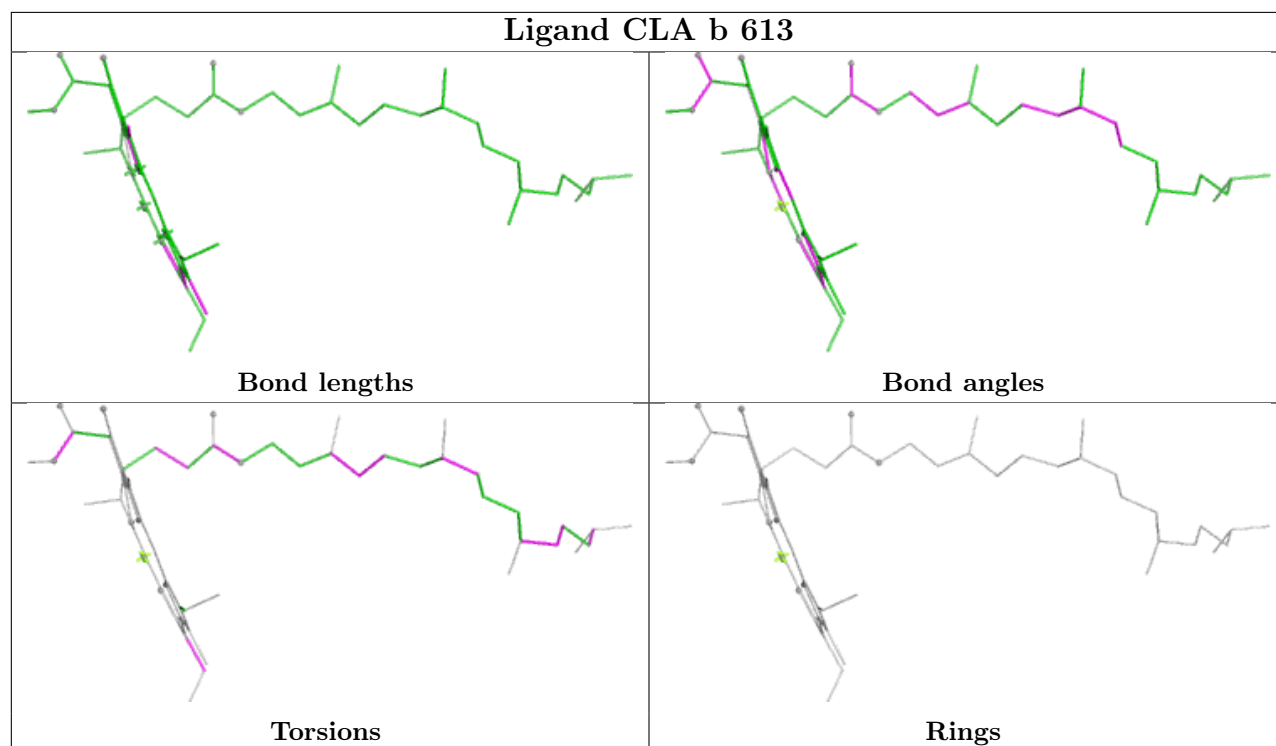
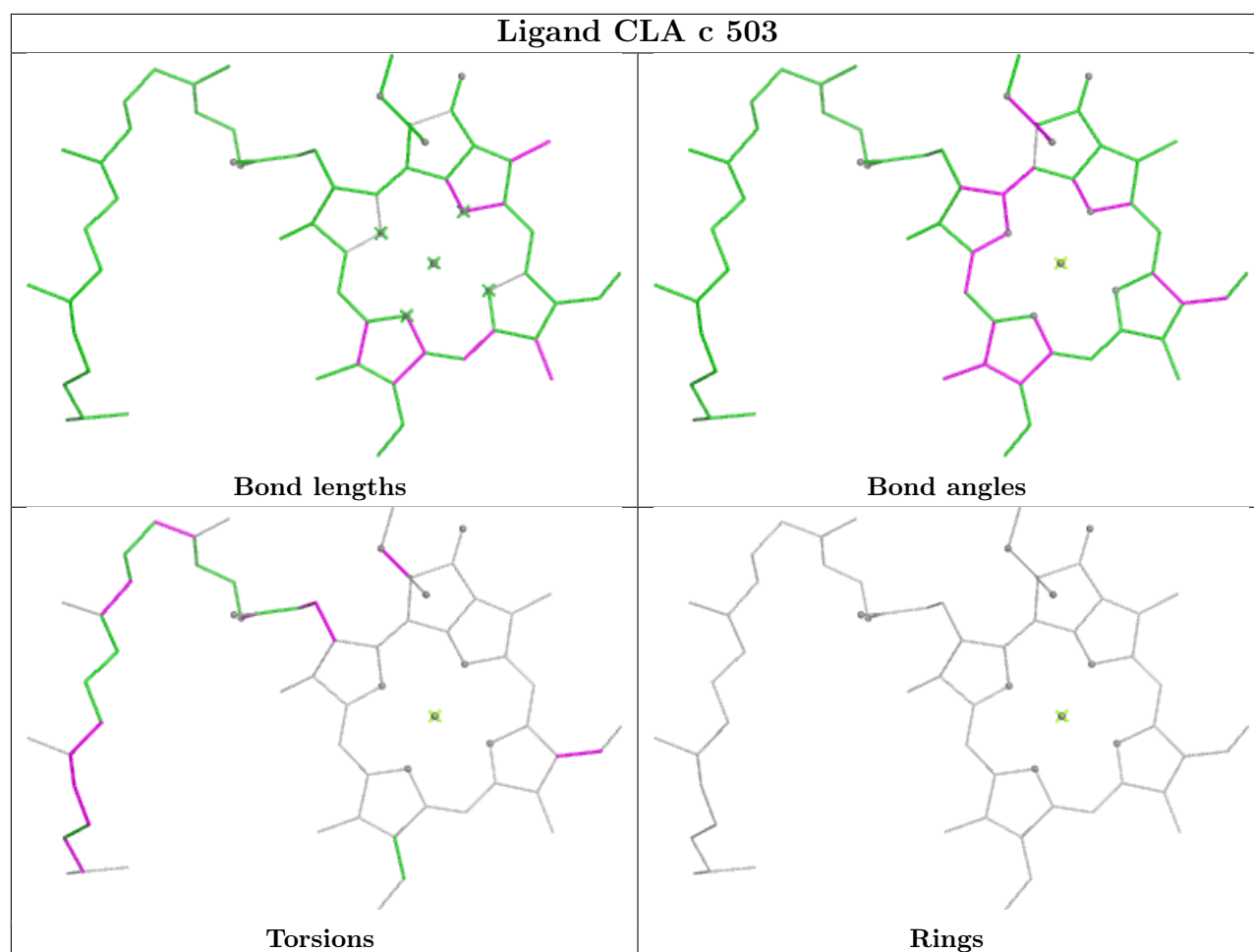


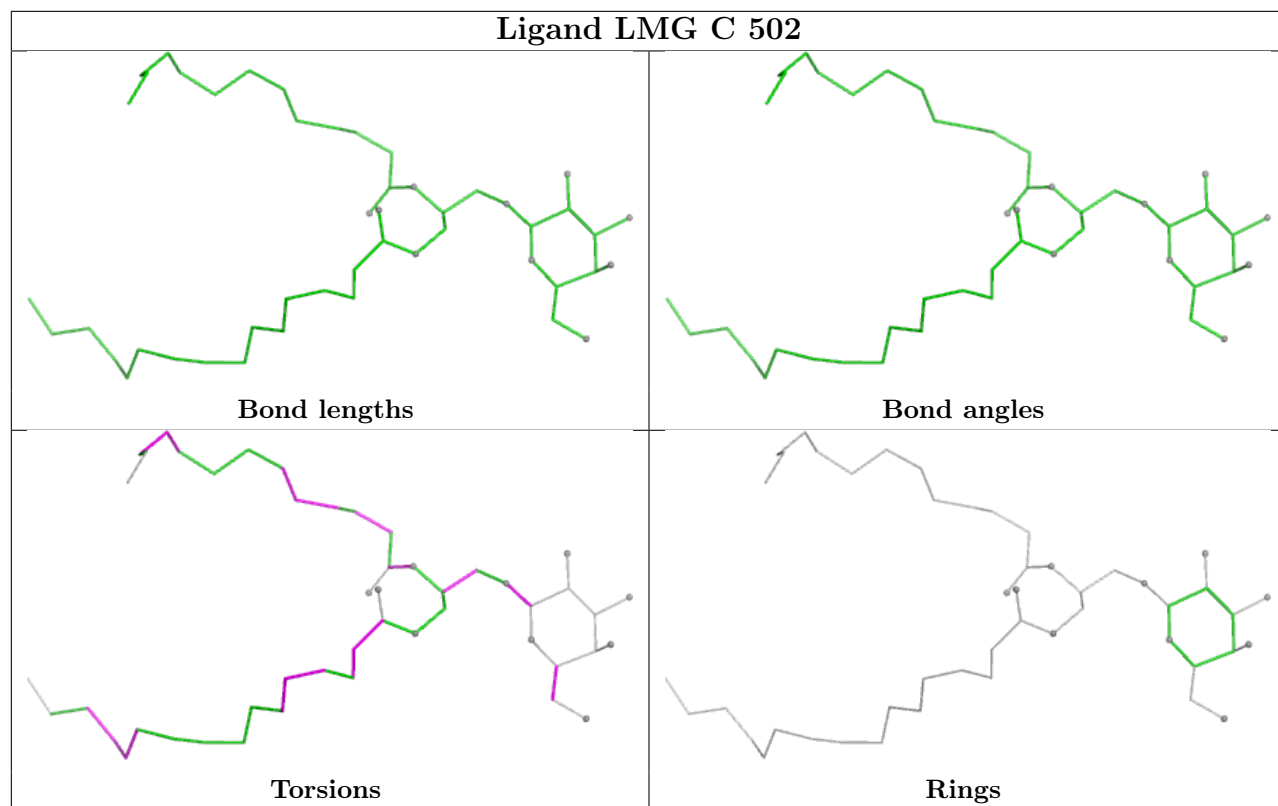


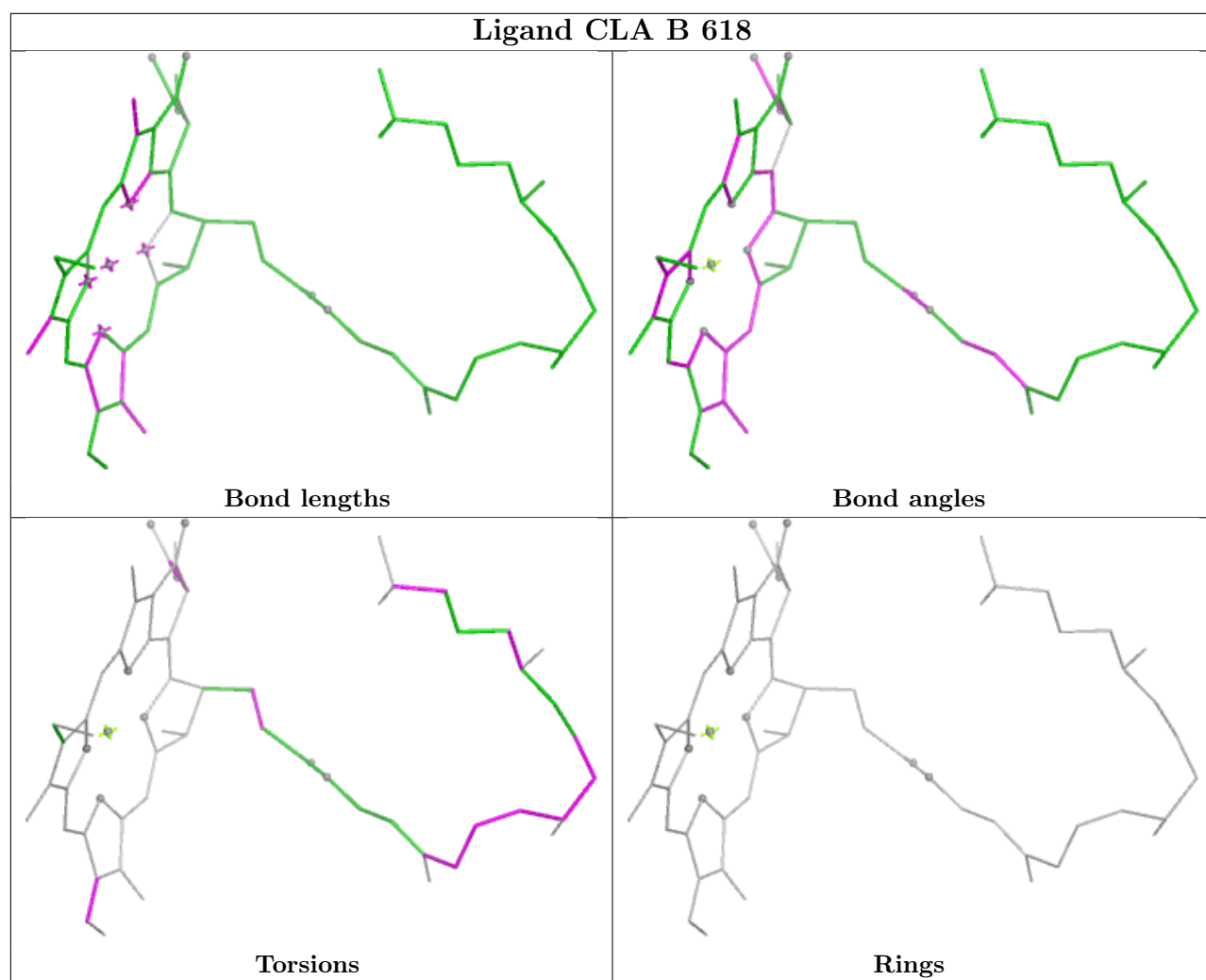
Ligand CLA B 616

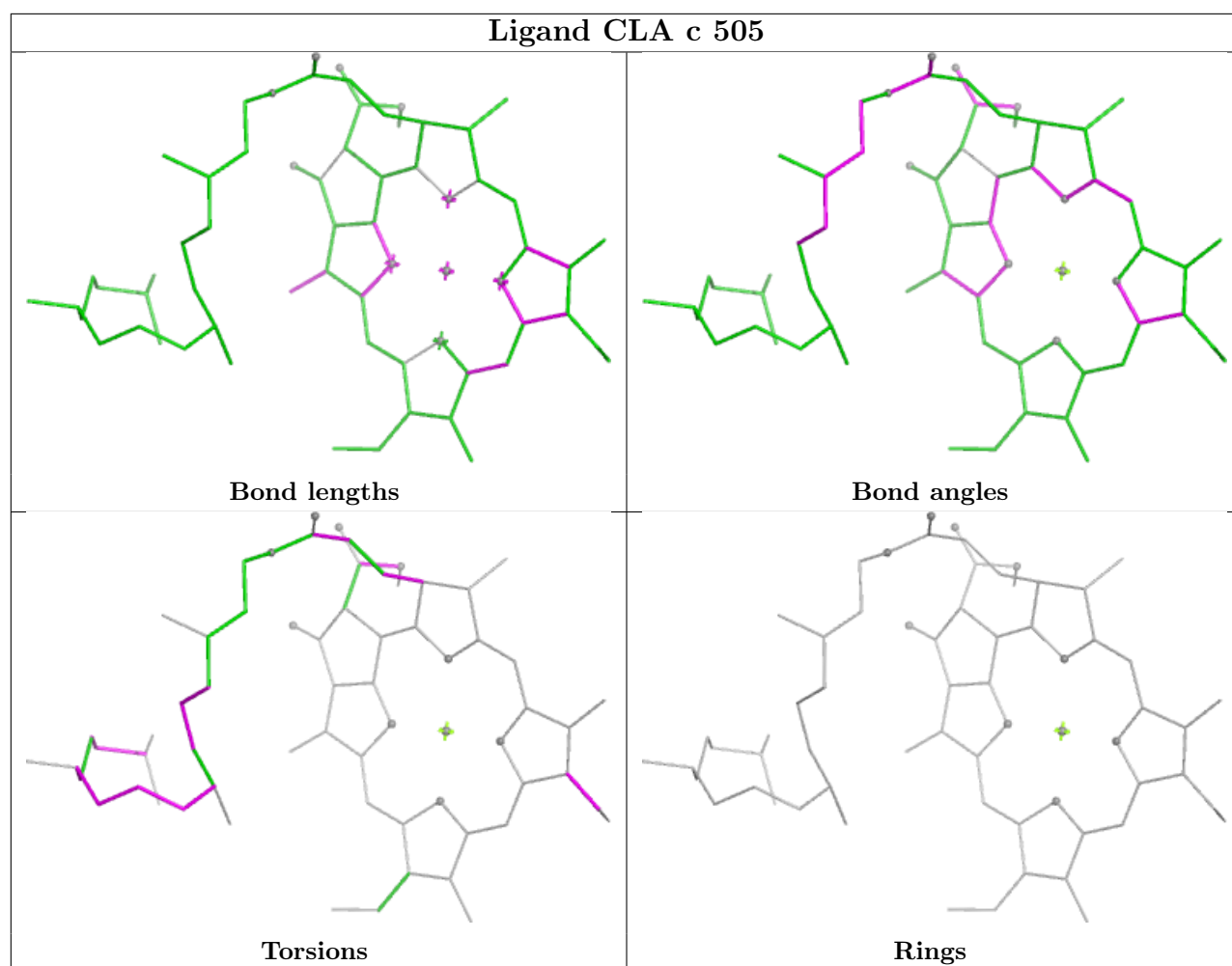


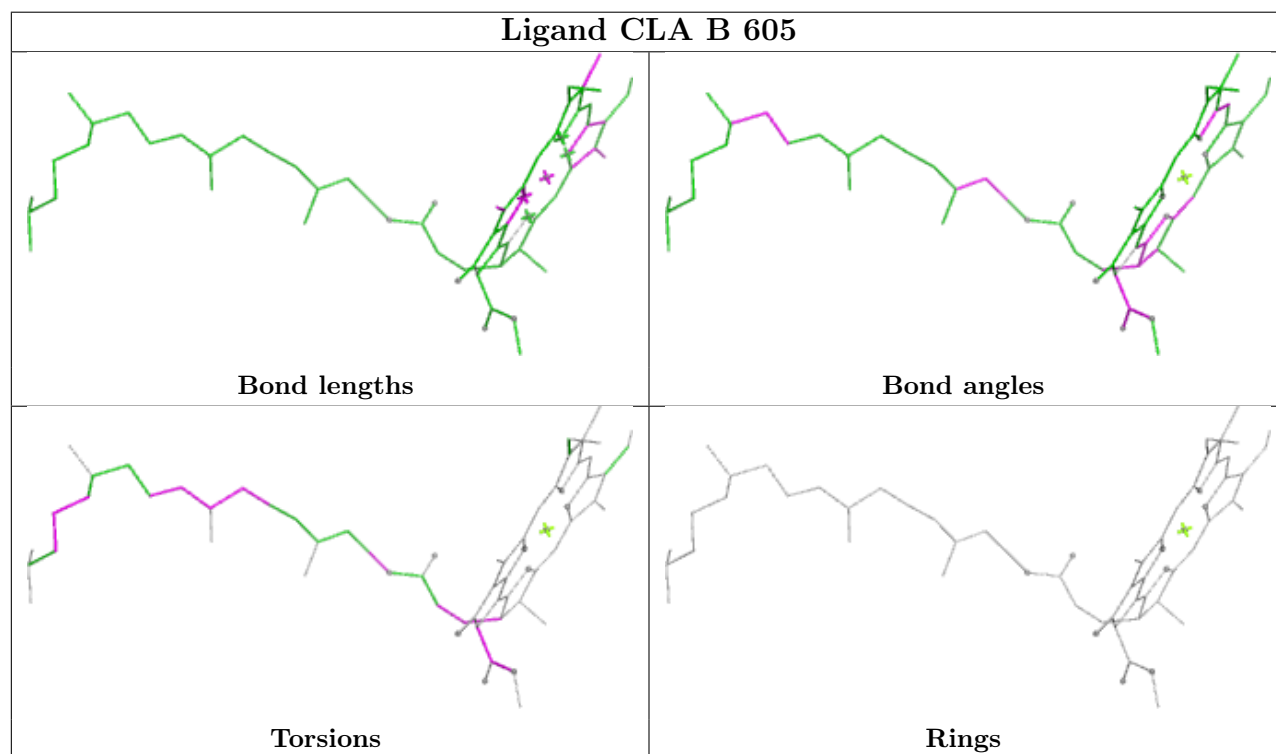
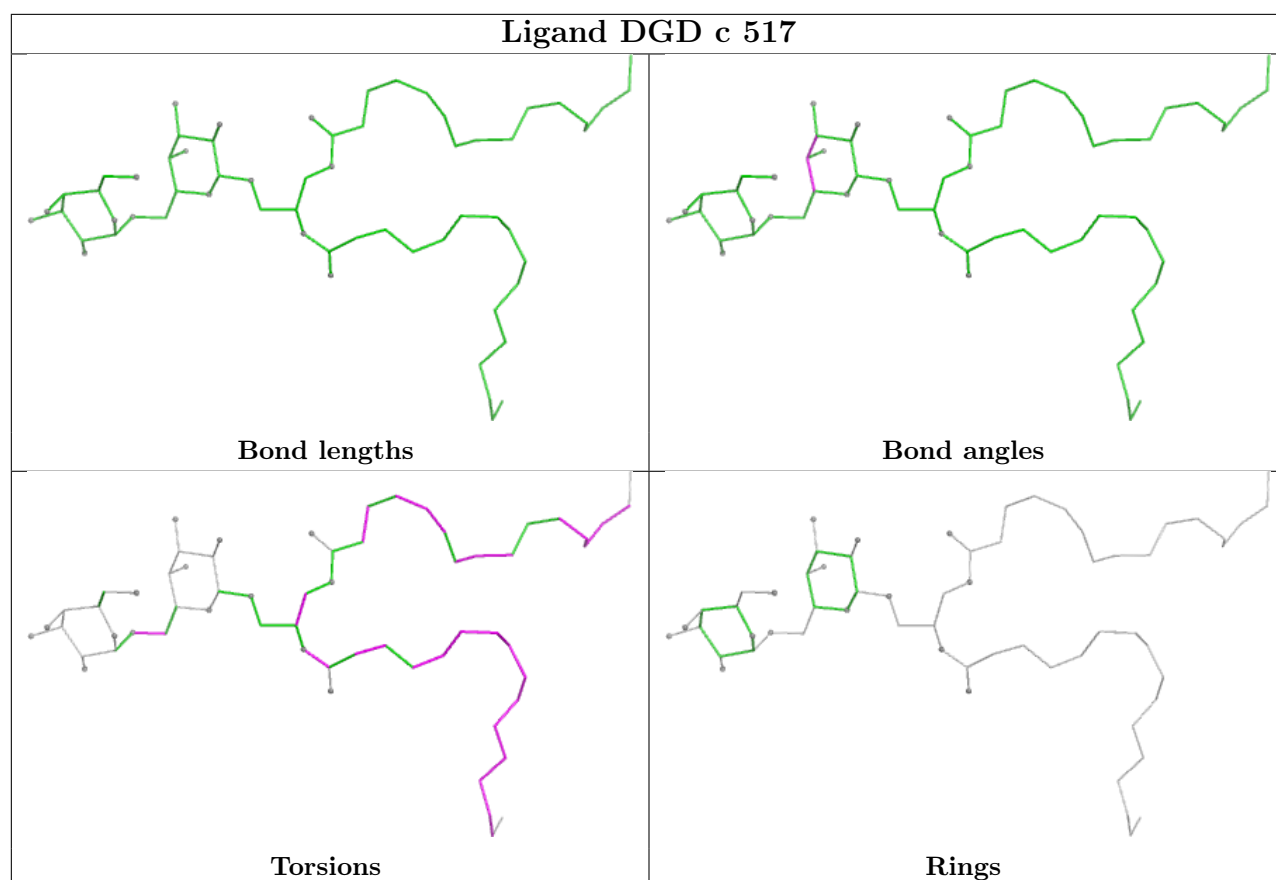


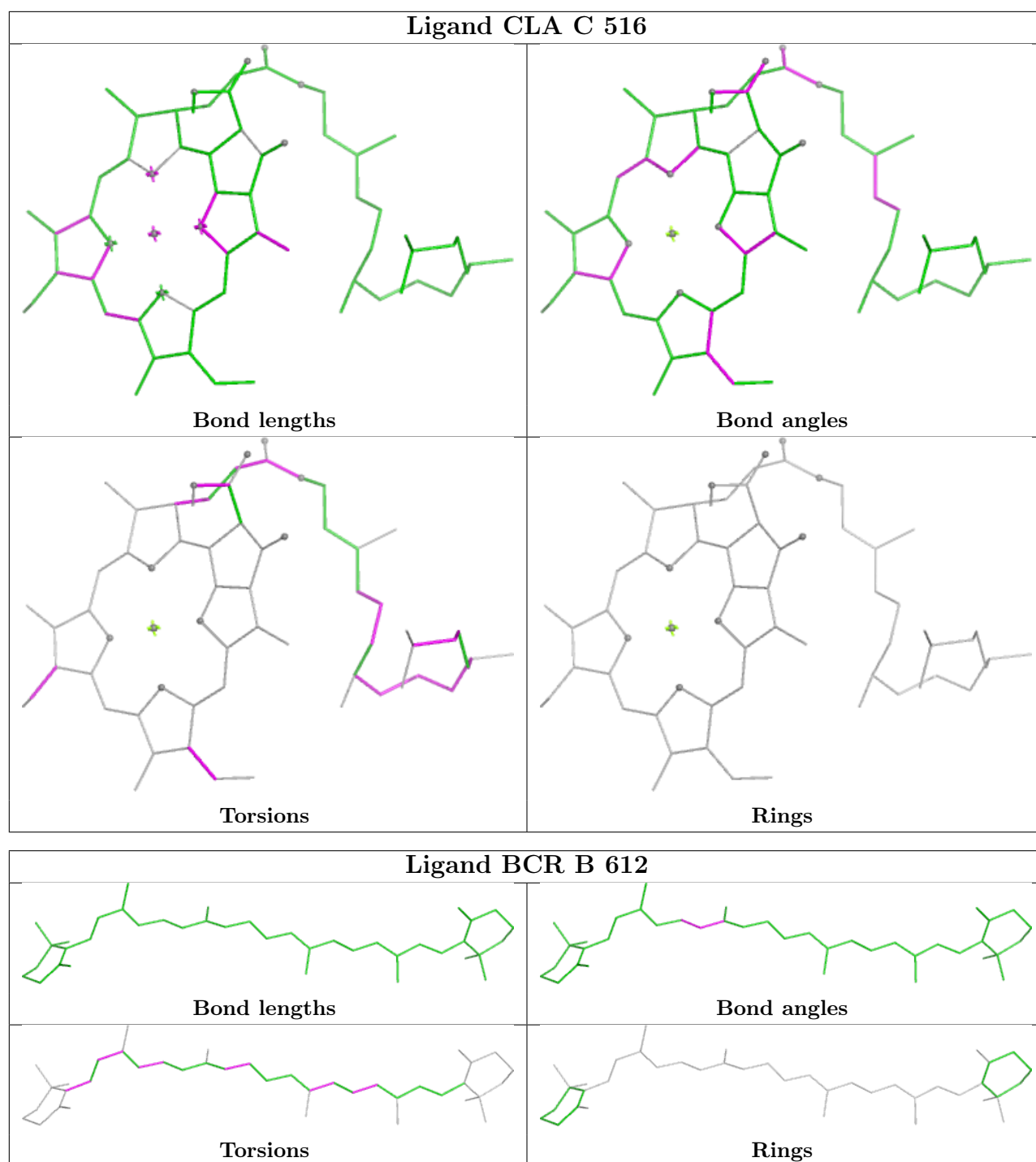




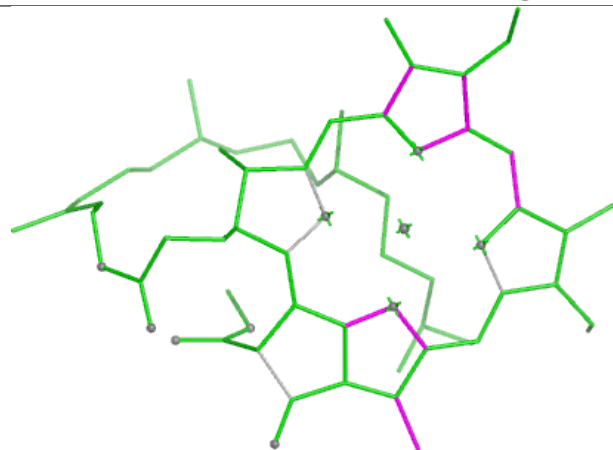




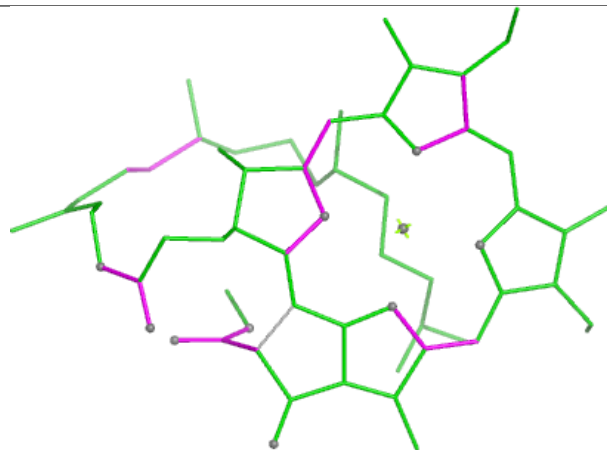




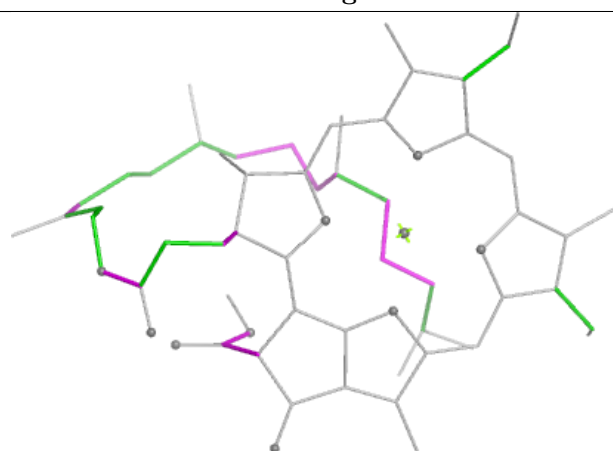
Ligand CLA C 509



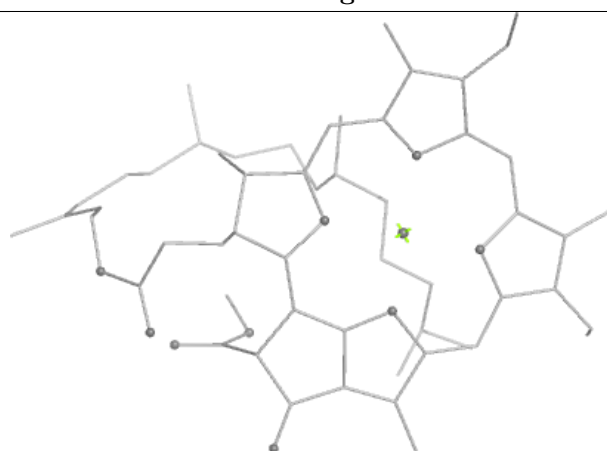
Bond lengths



Bond angles

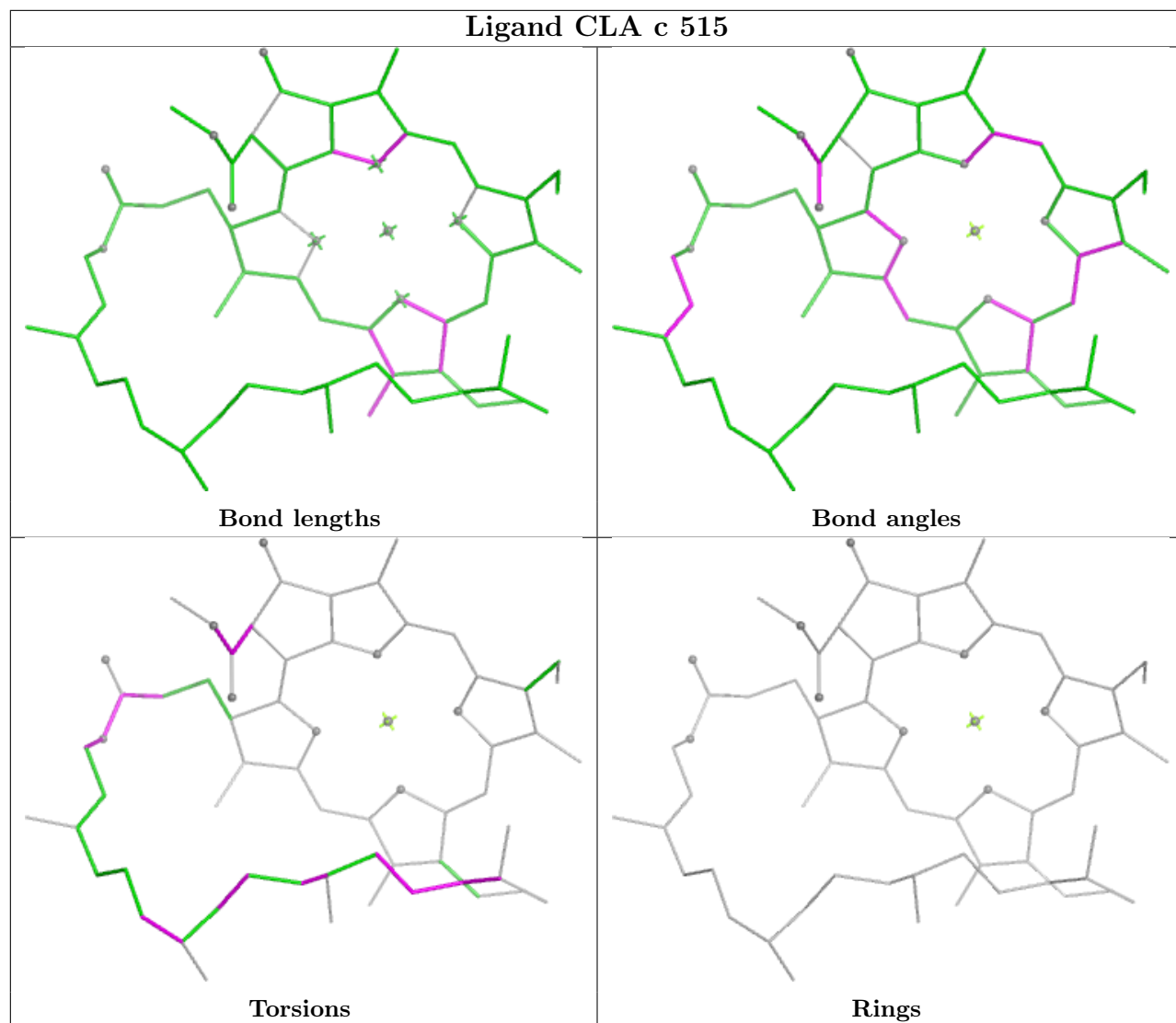


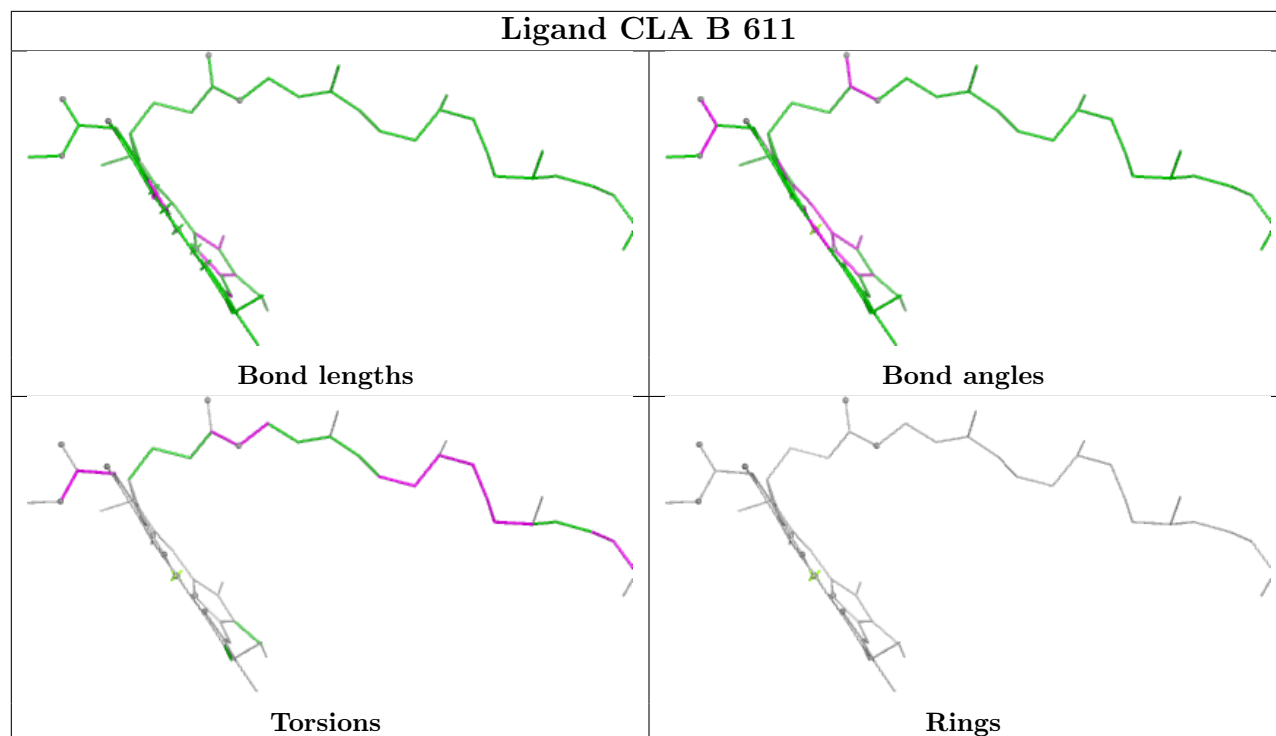
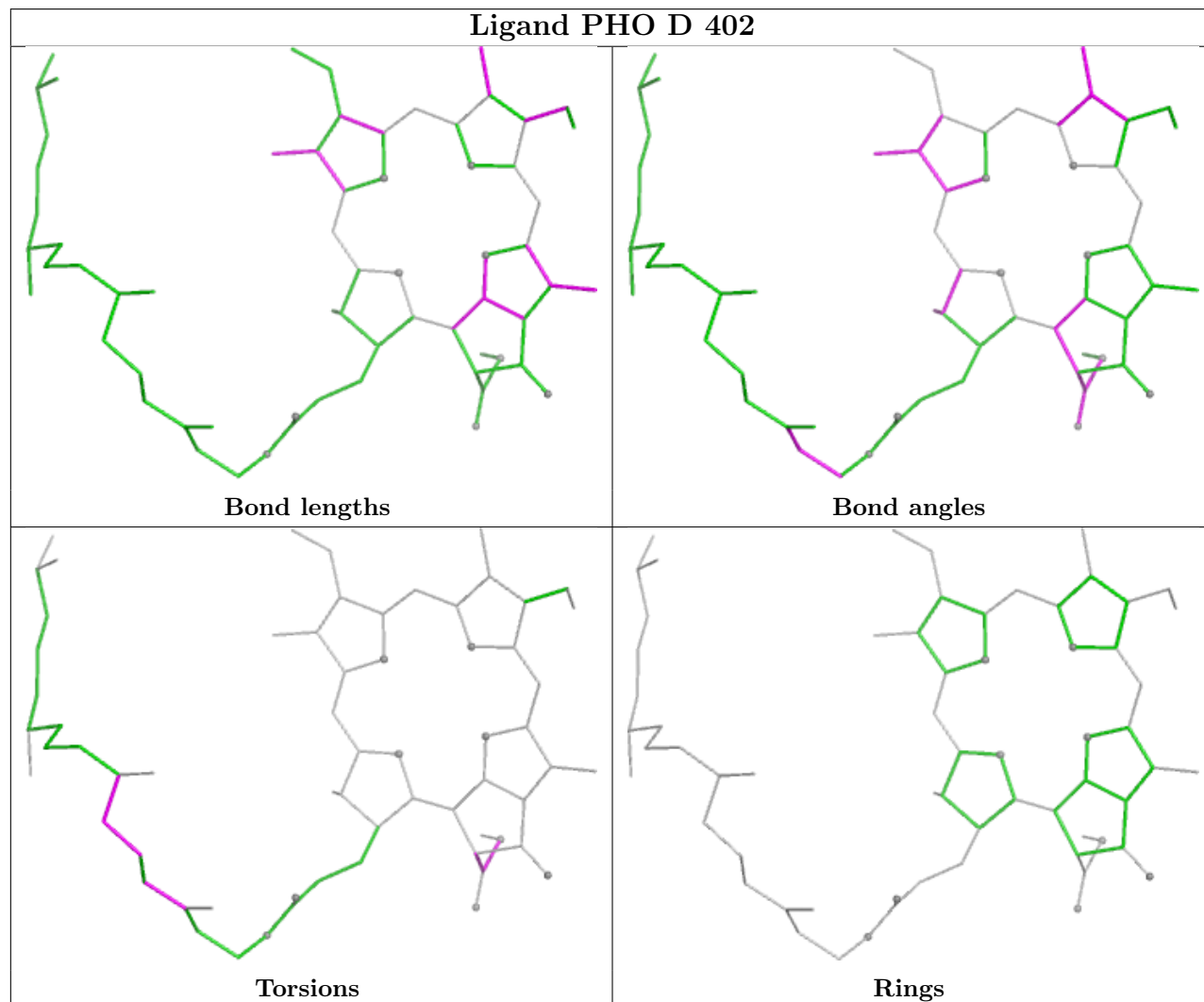
Torsions

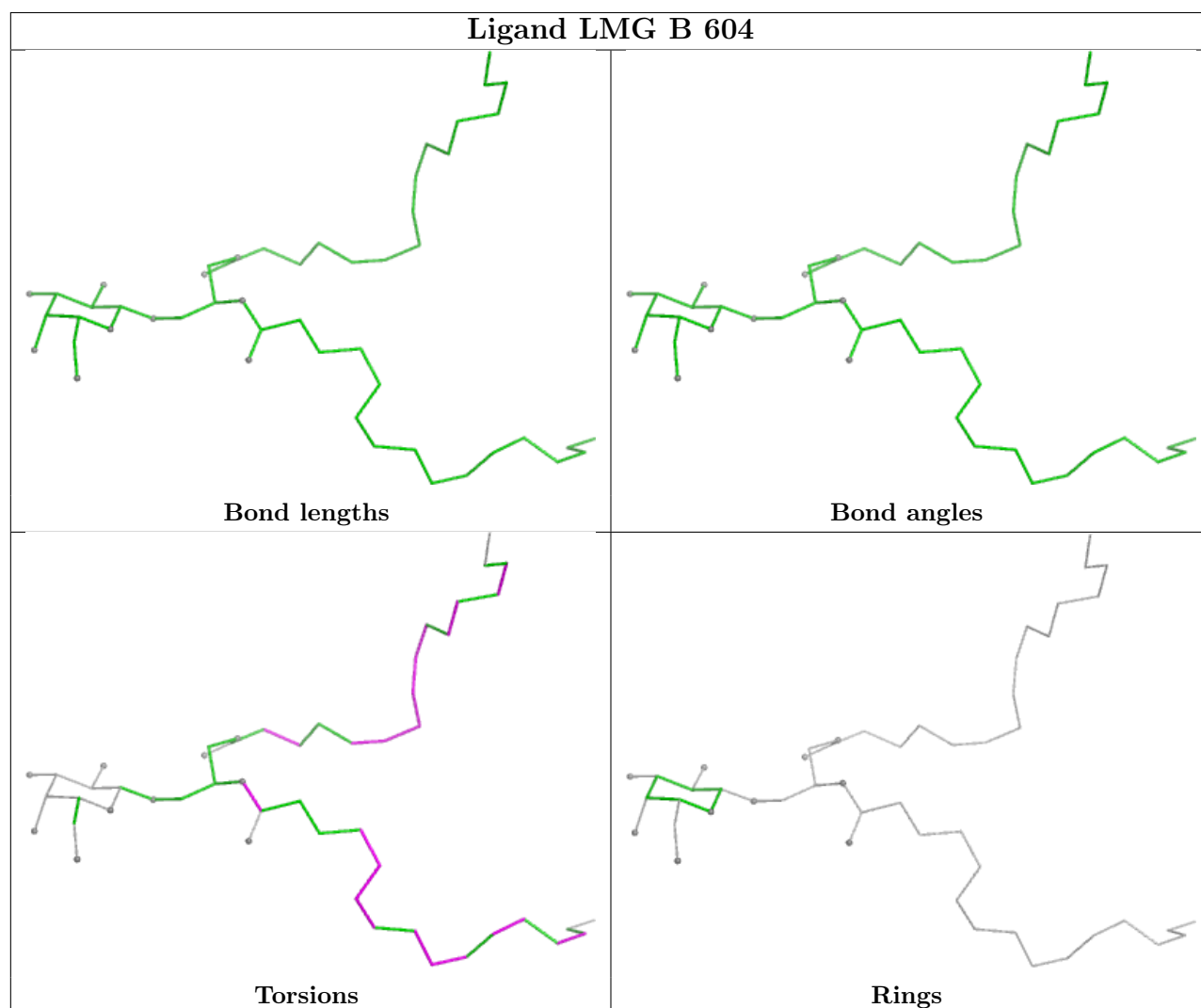
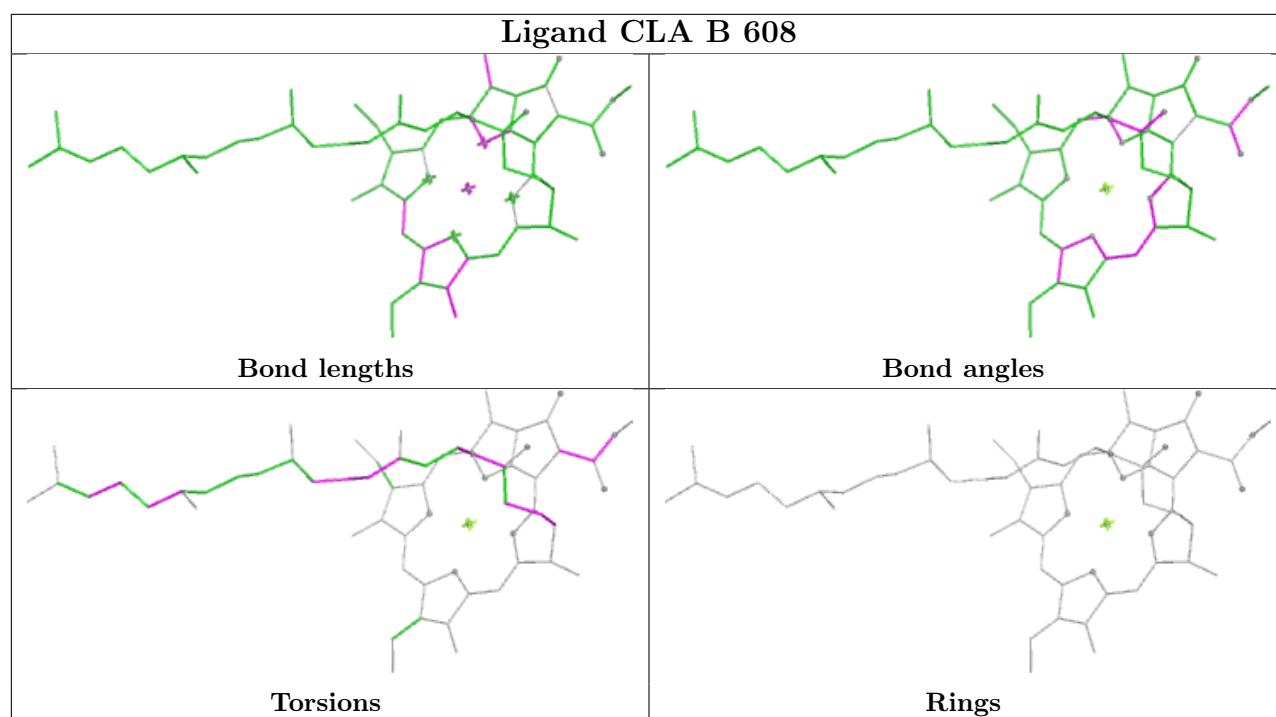


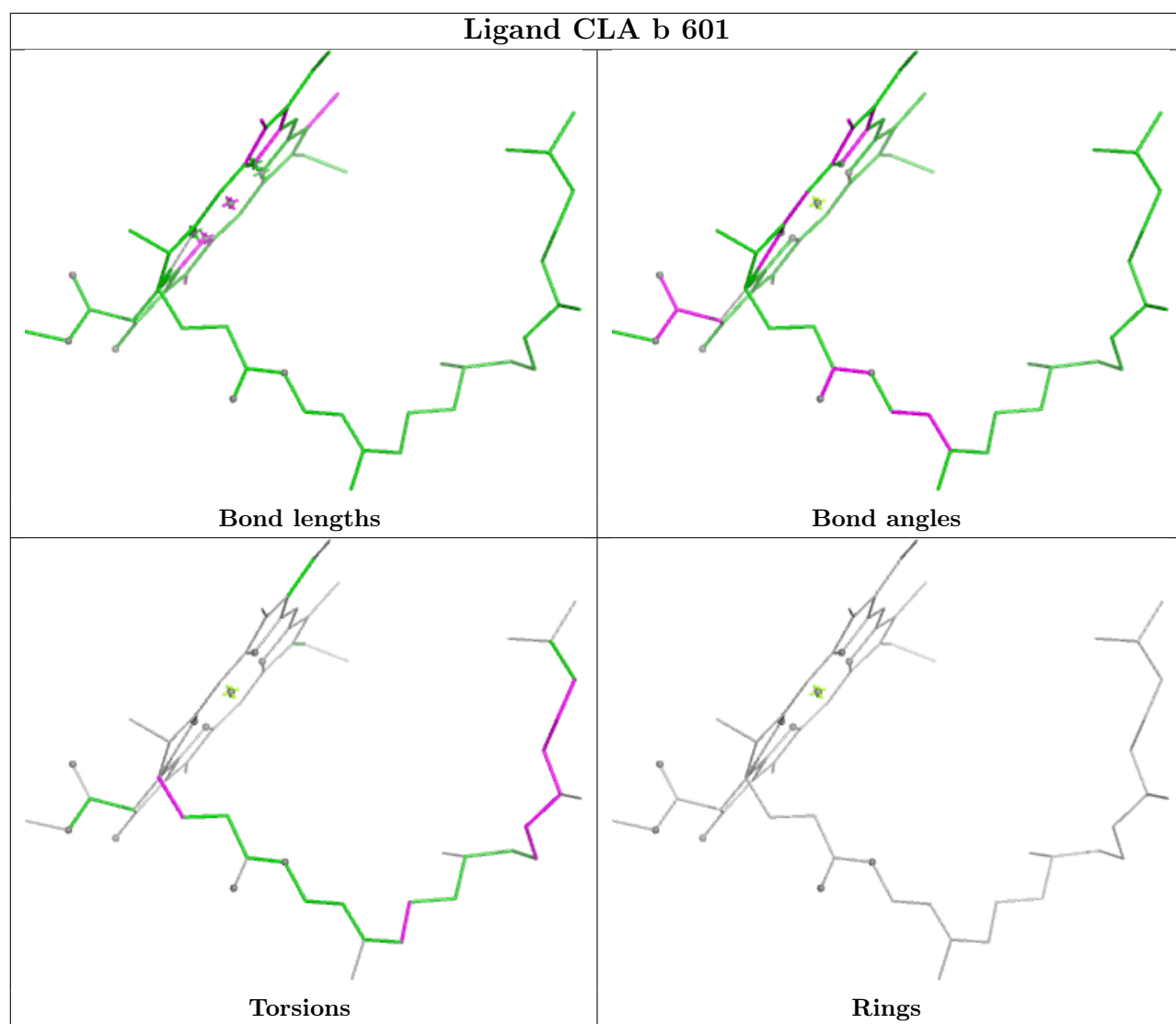
Rings

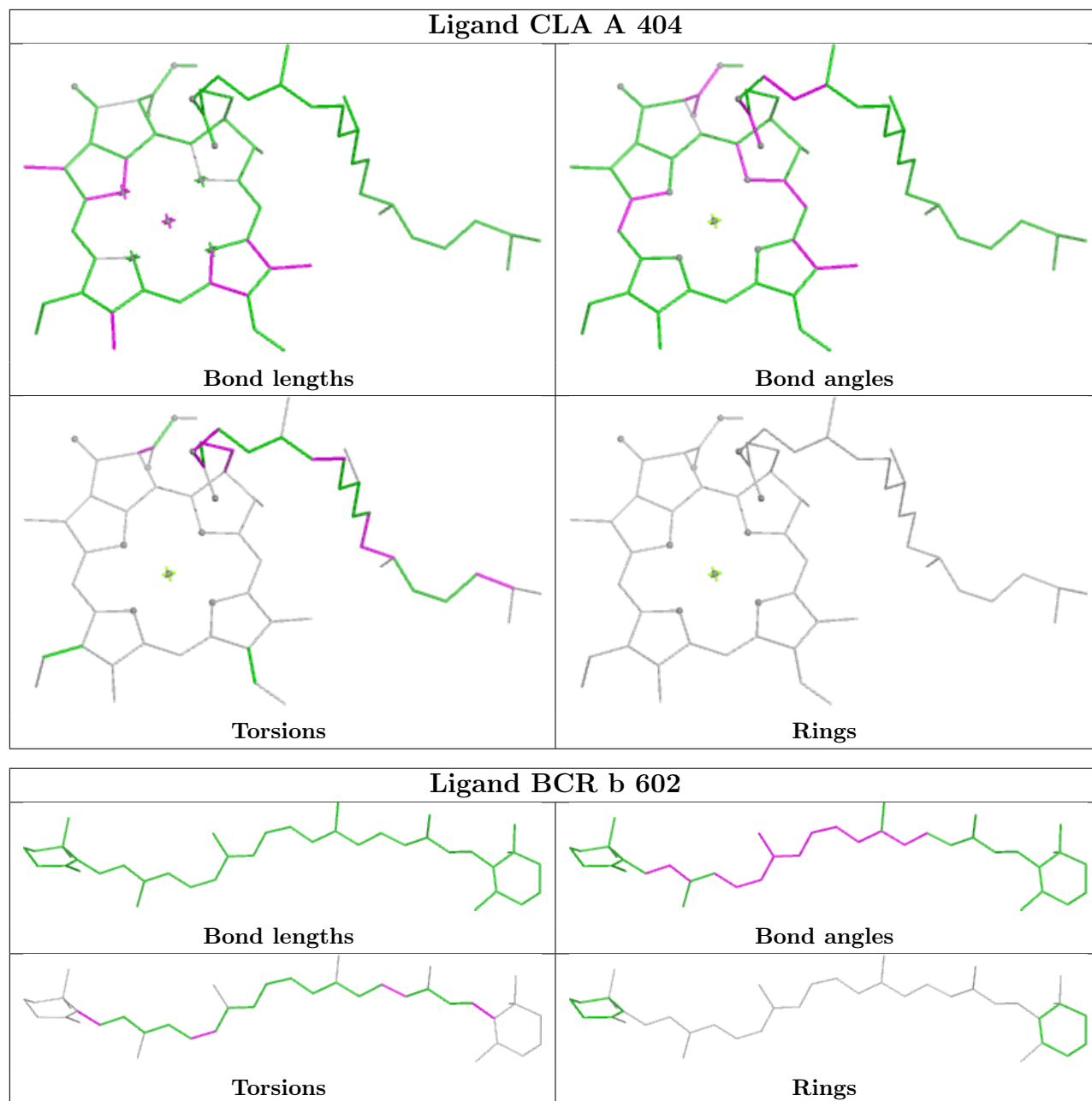
Ligand CLA c 515

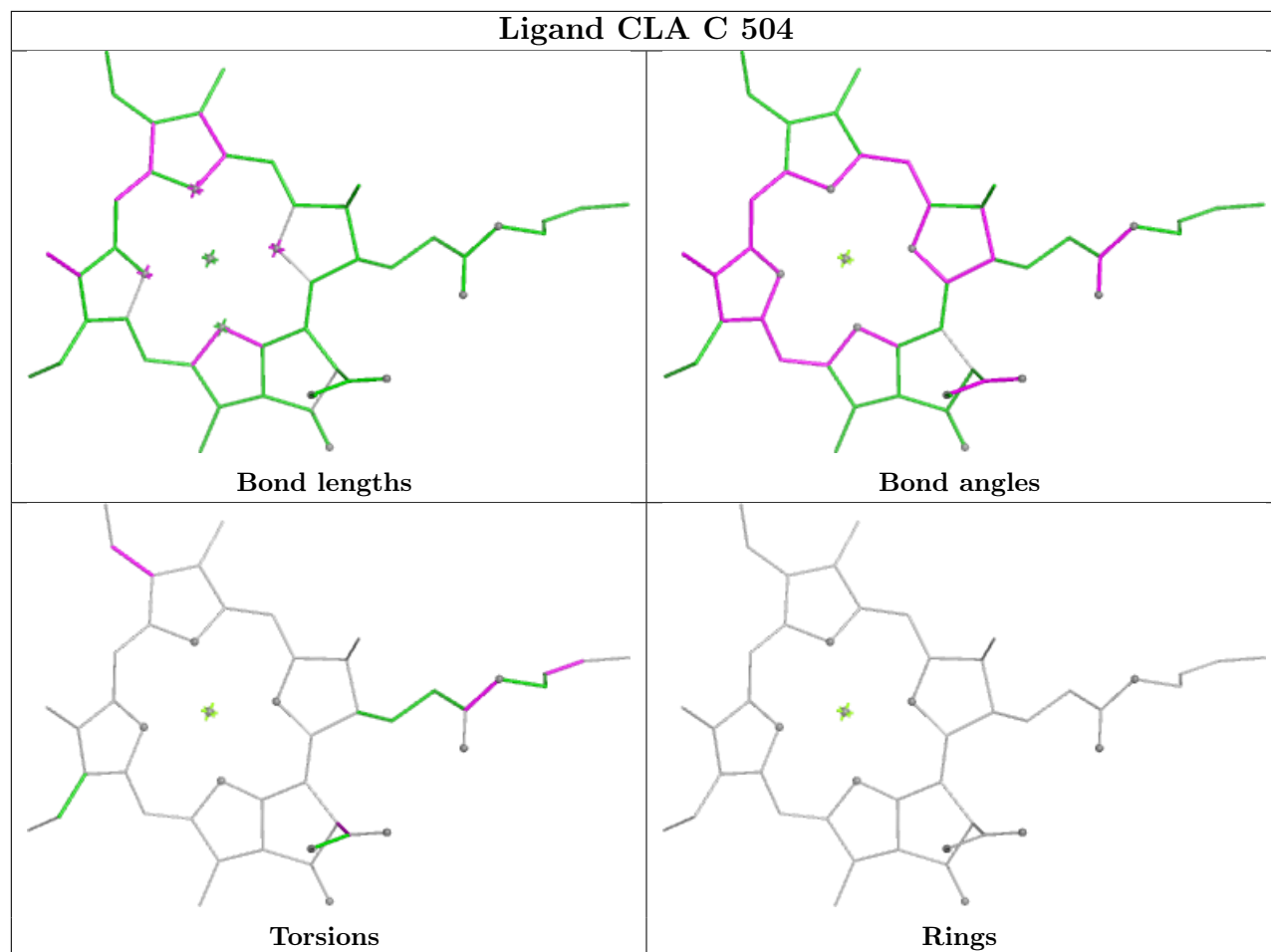
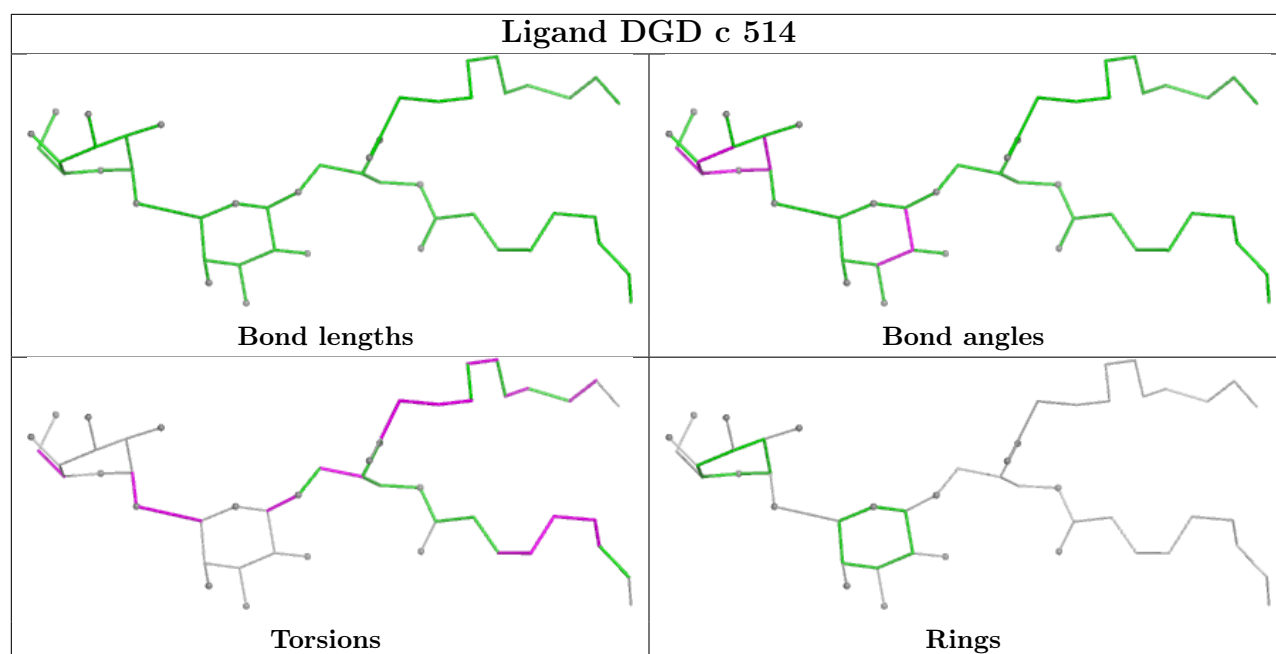


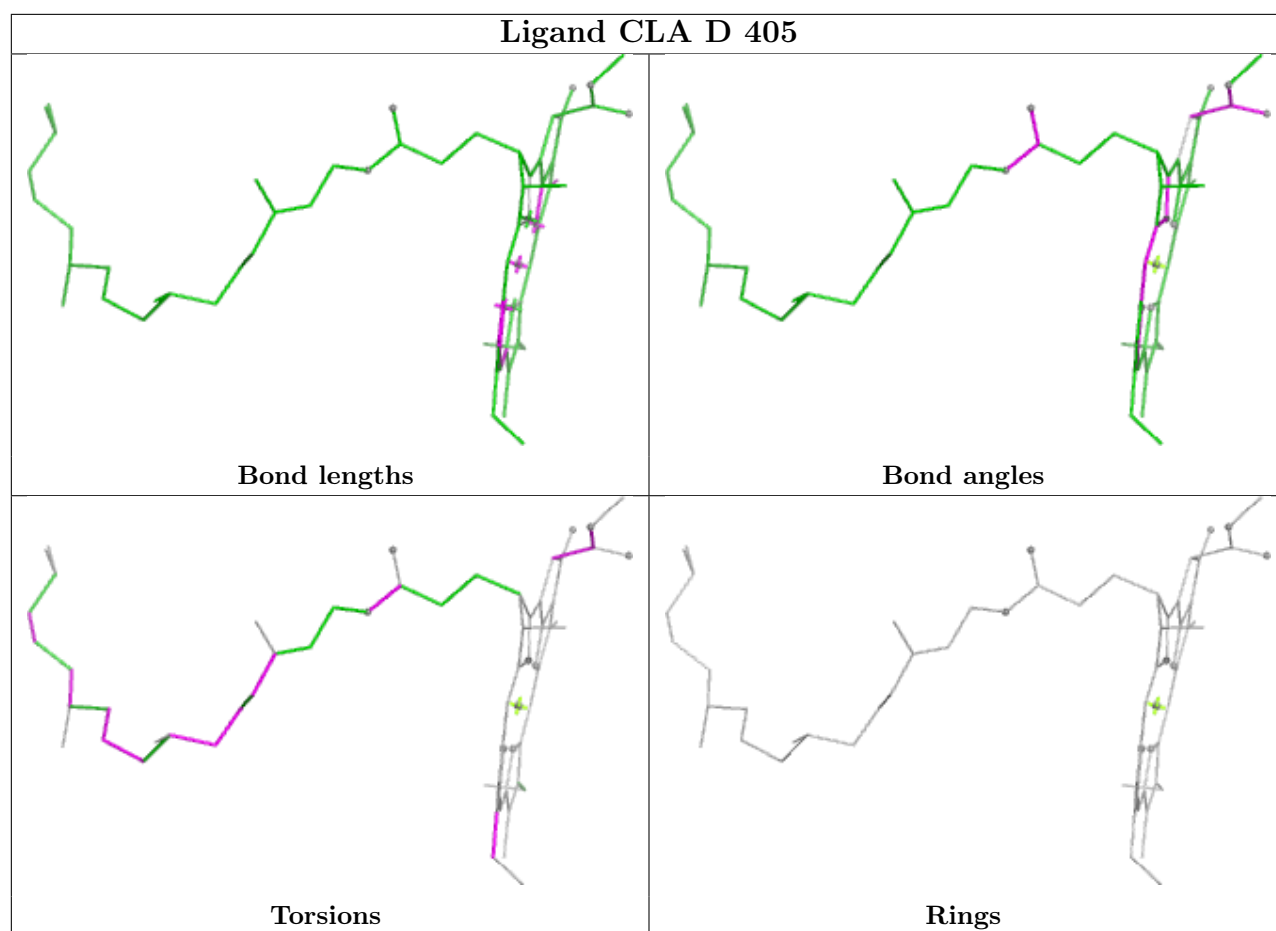
Ligand CLA B 611**Ligand PHO D 402**



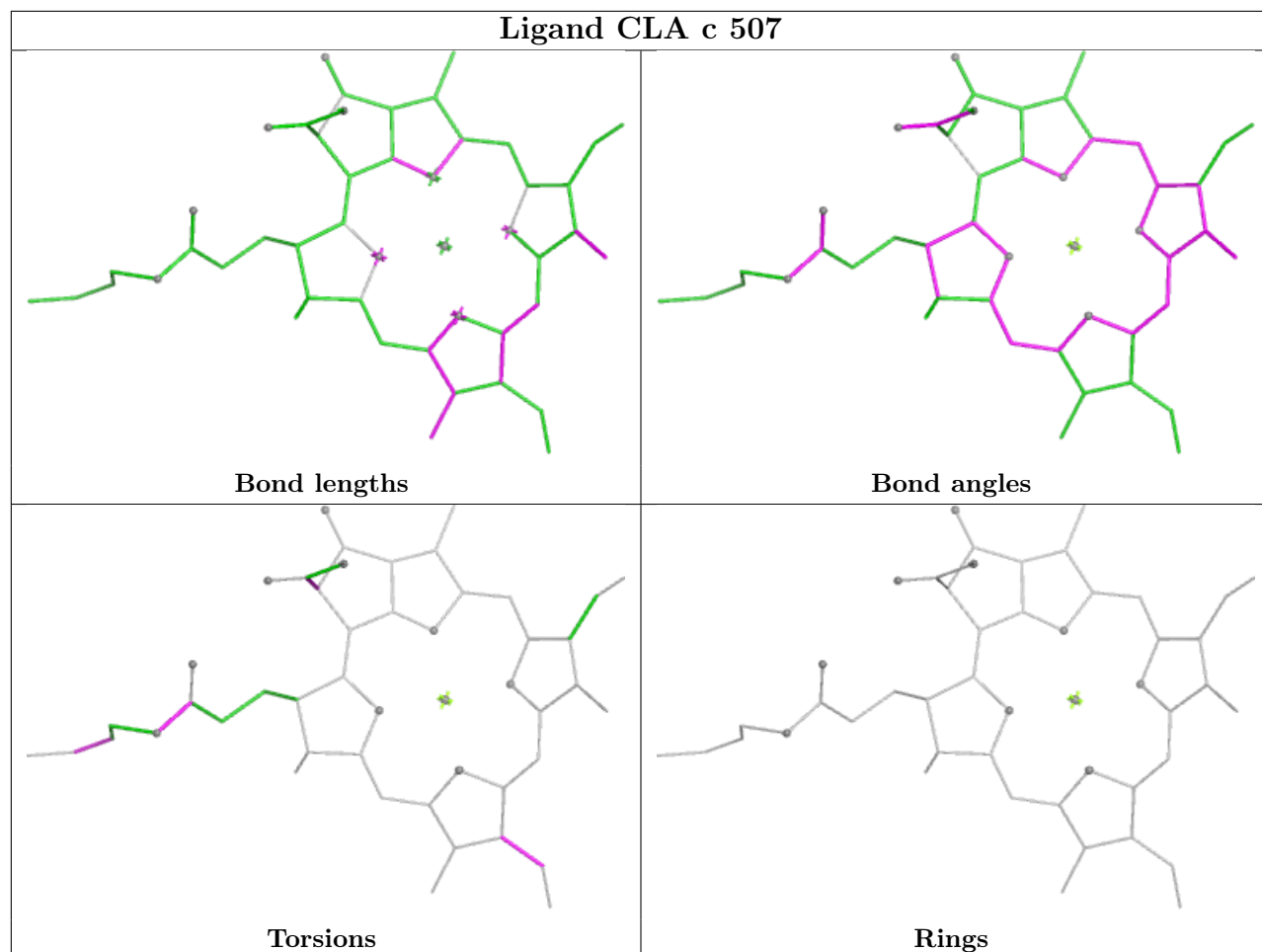


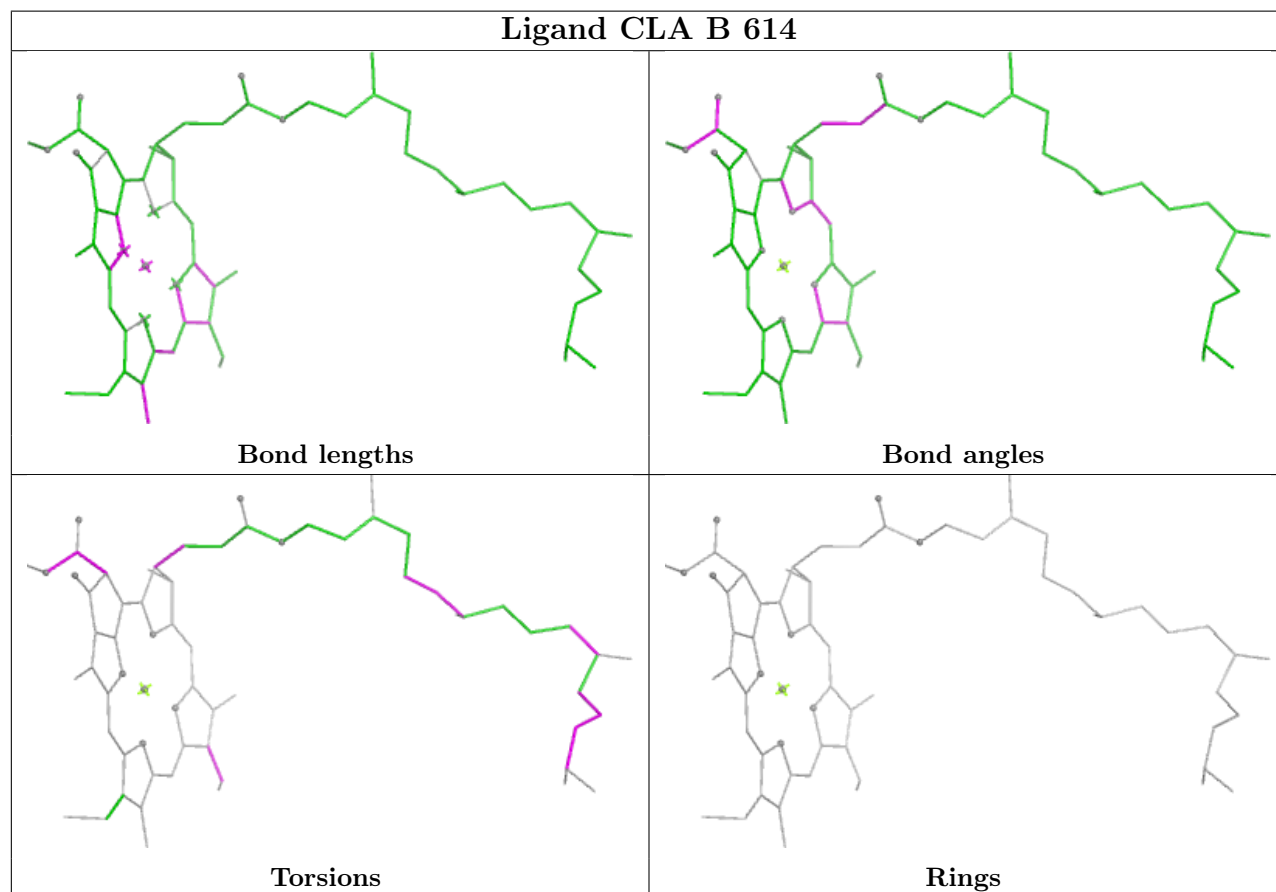
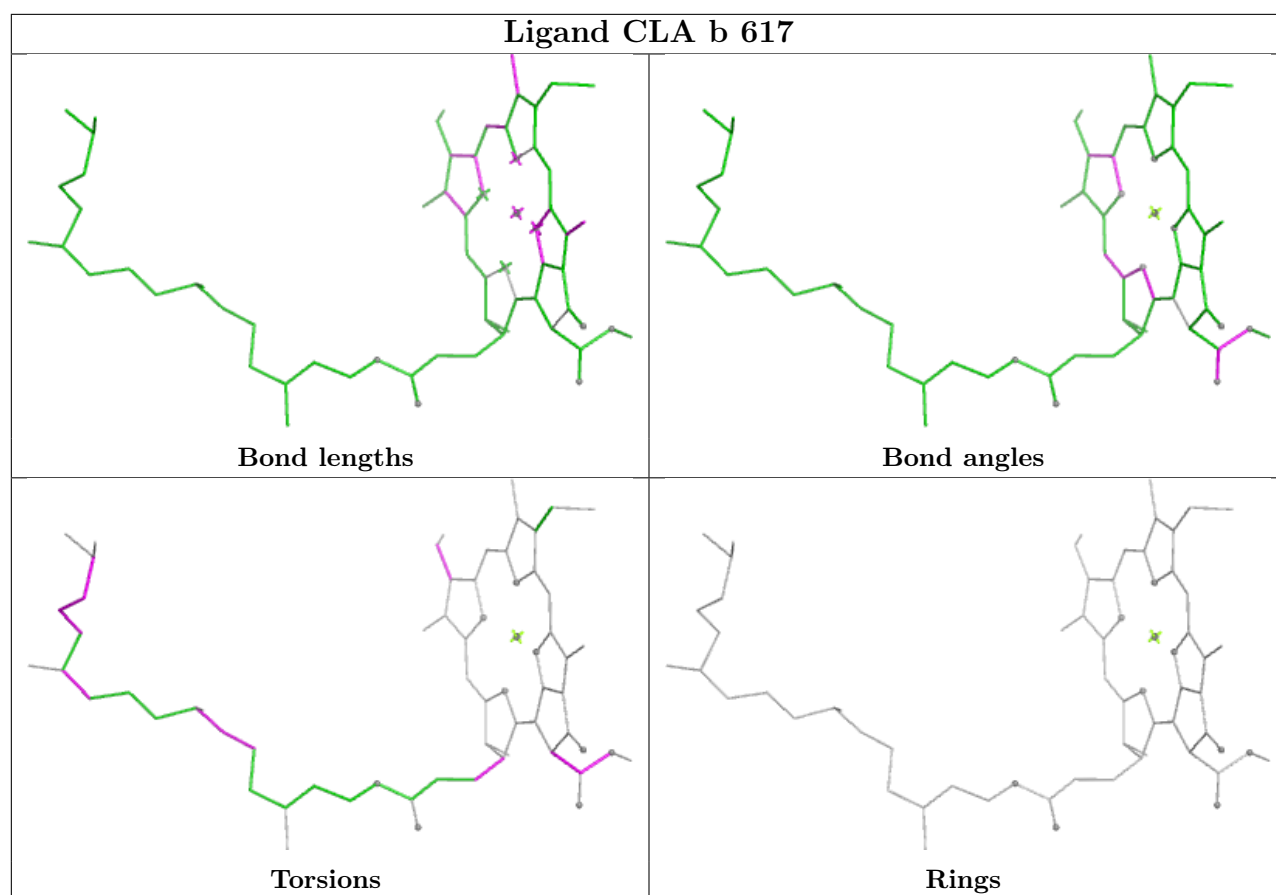


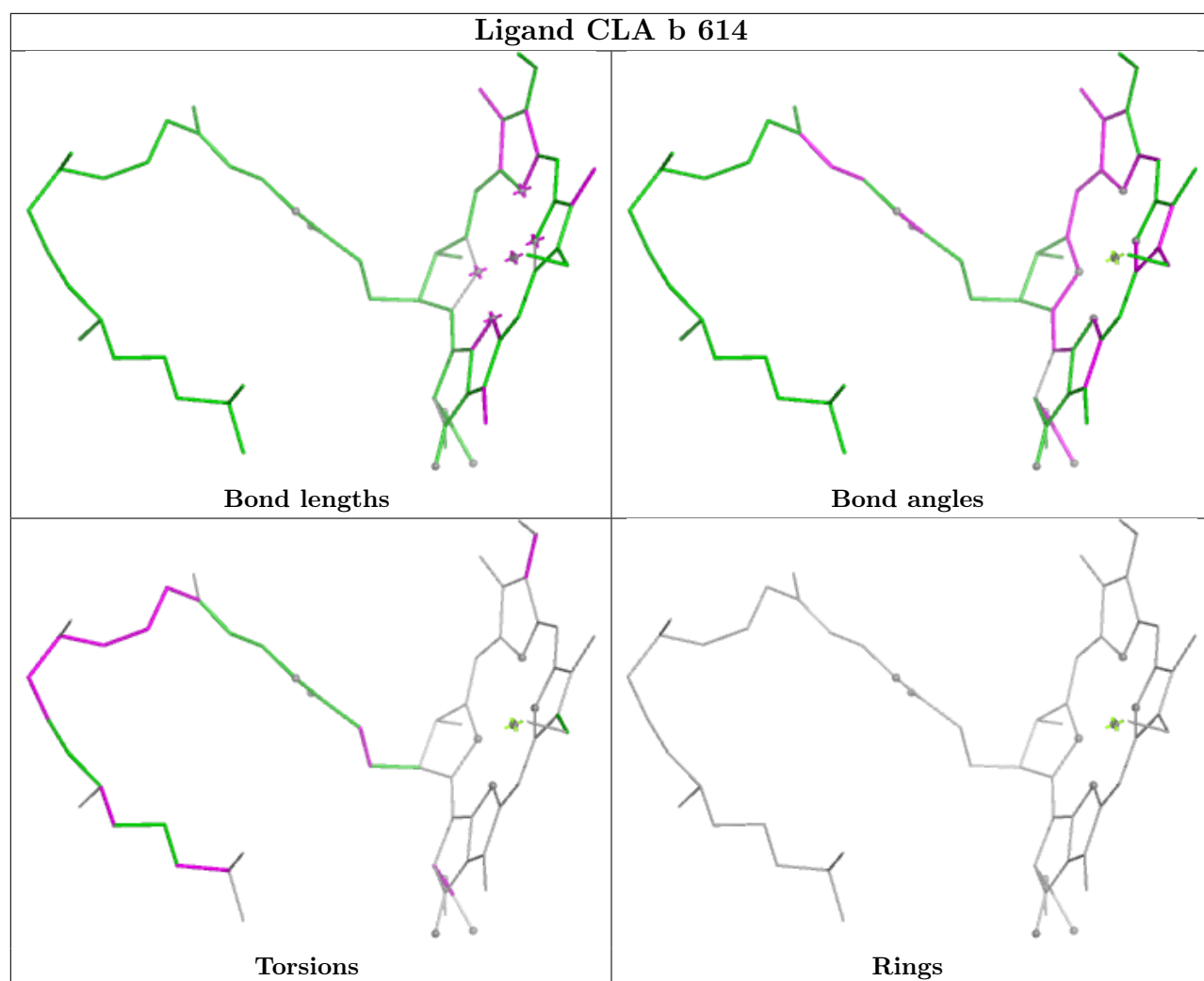


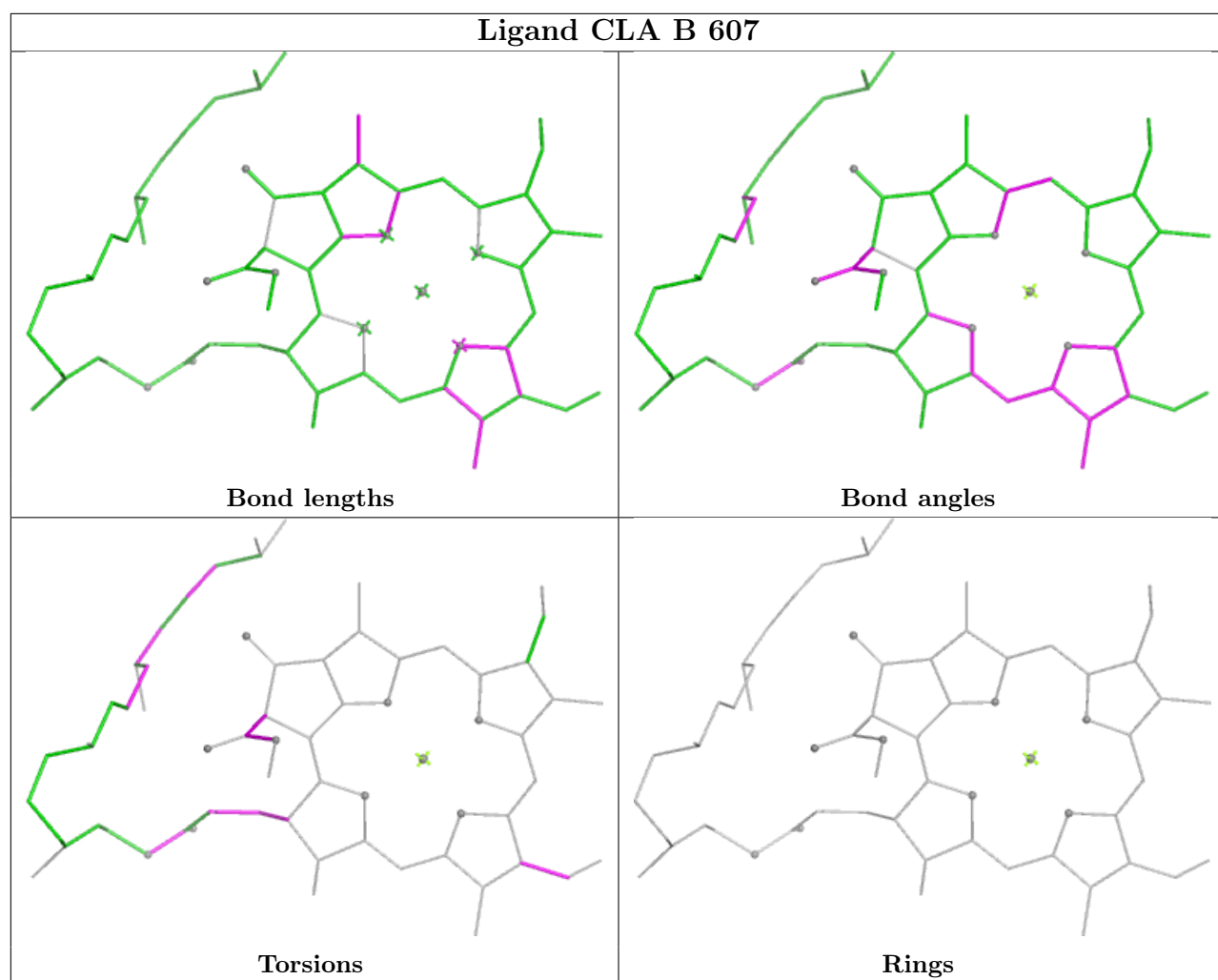


Ligand CLA c 507

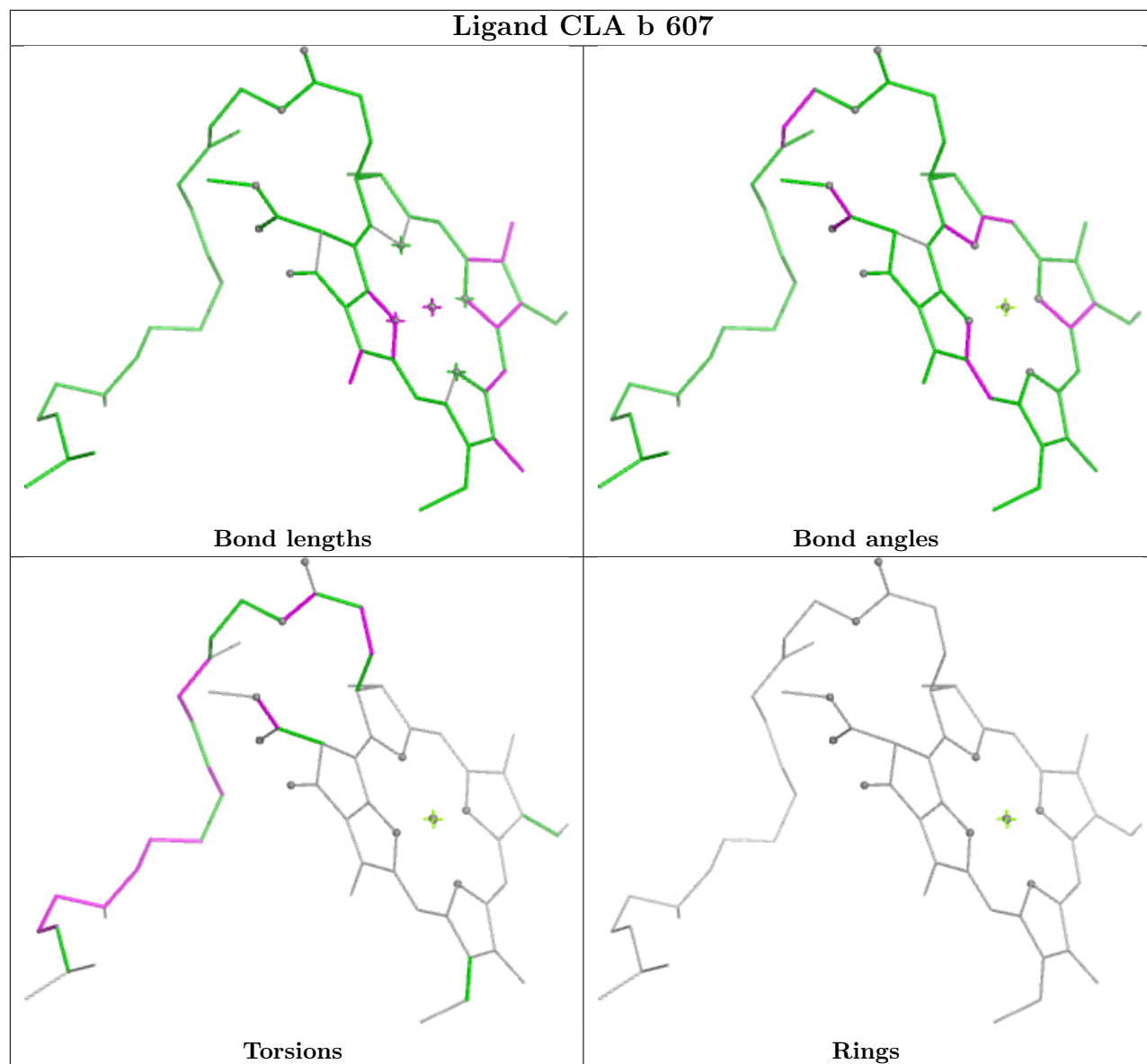


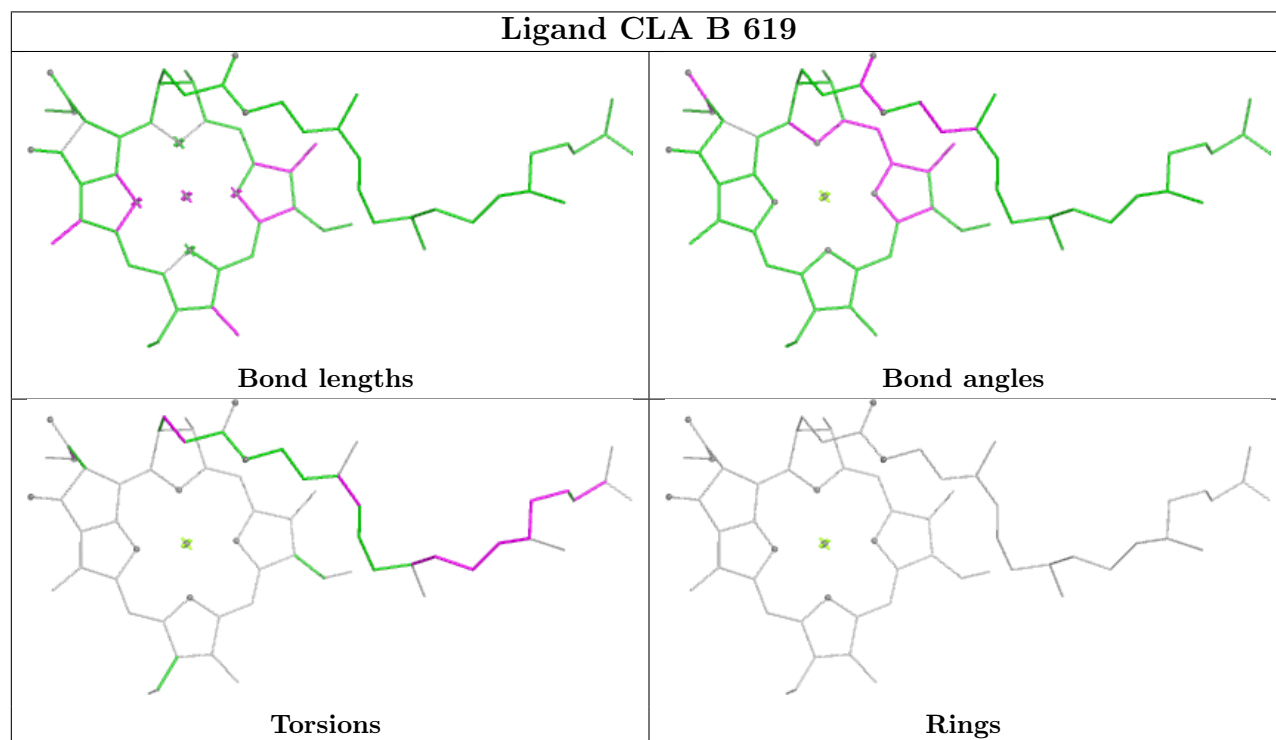
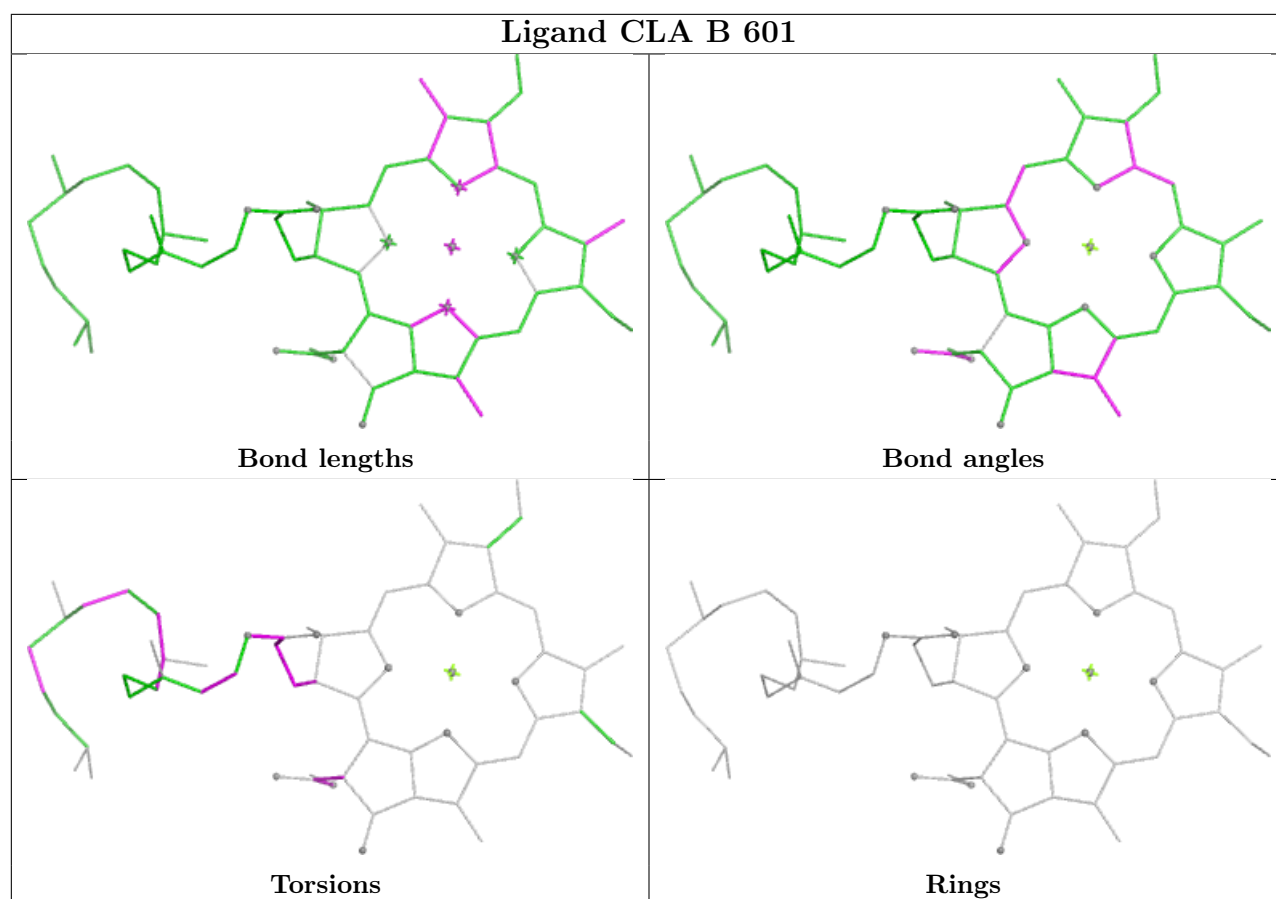


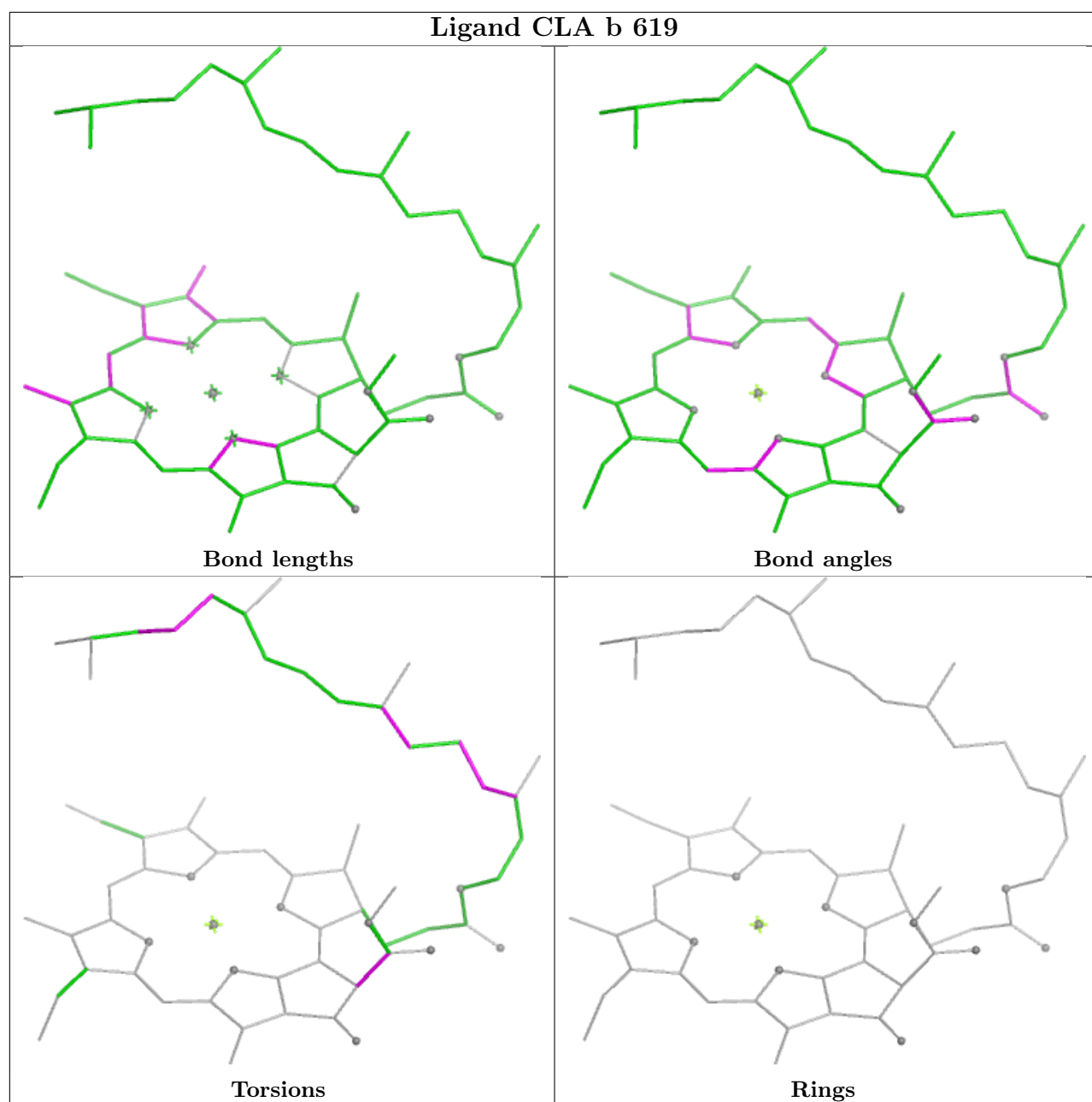


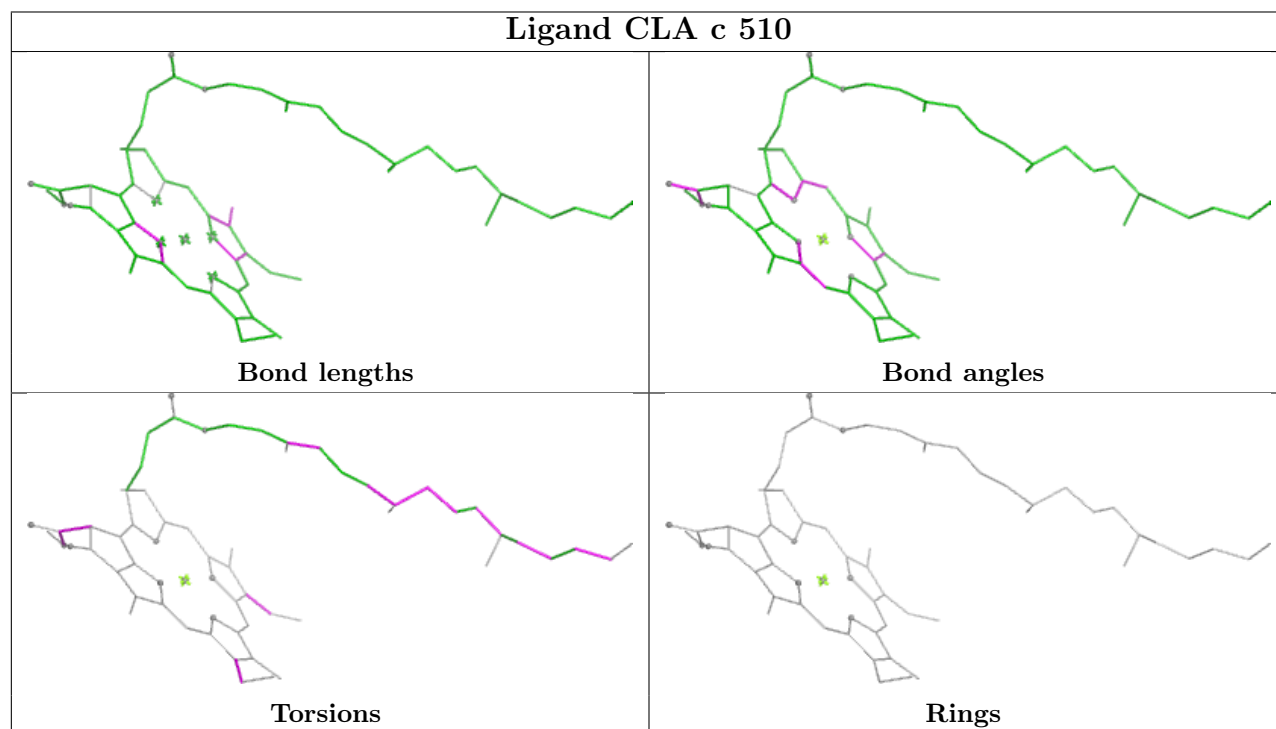
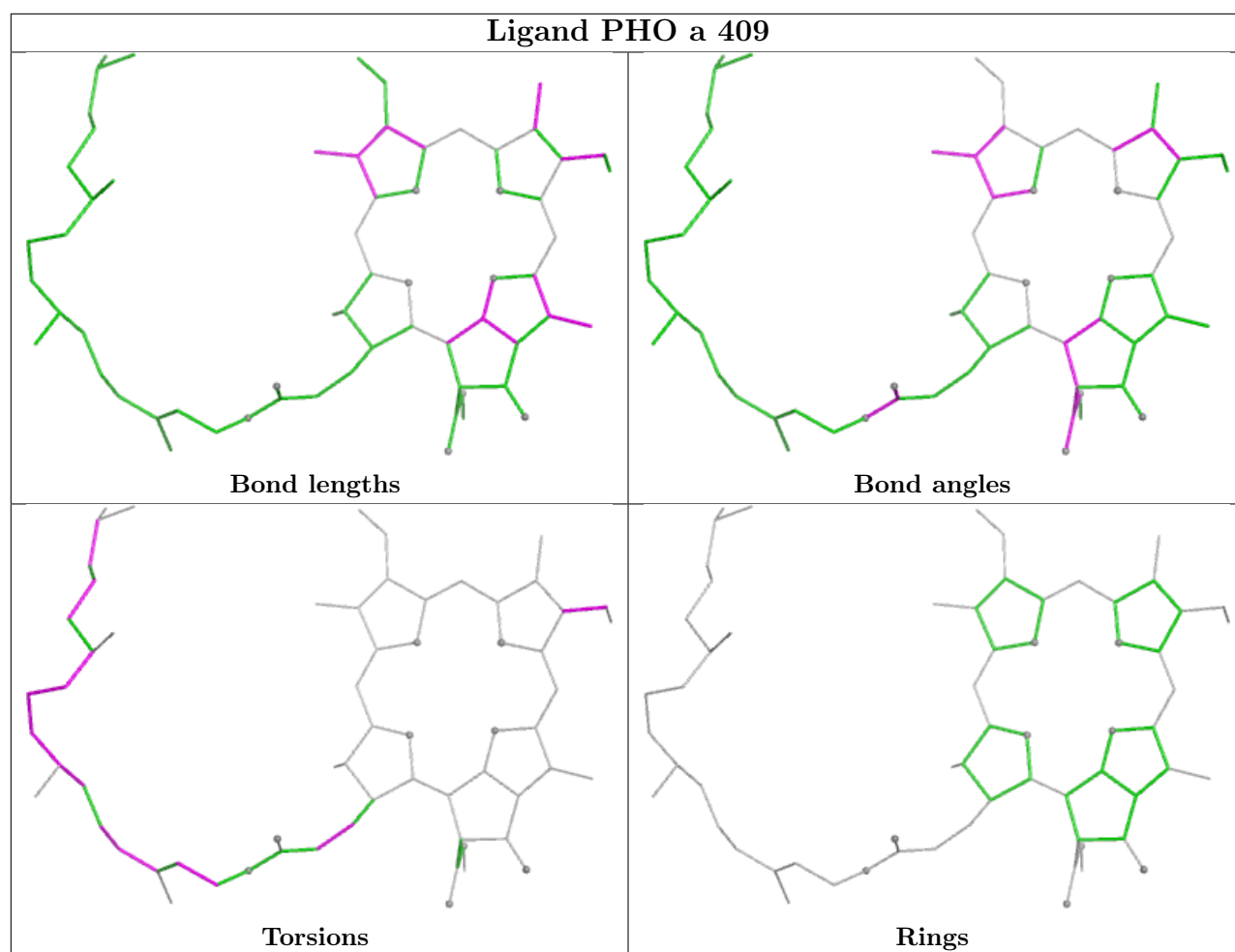


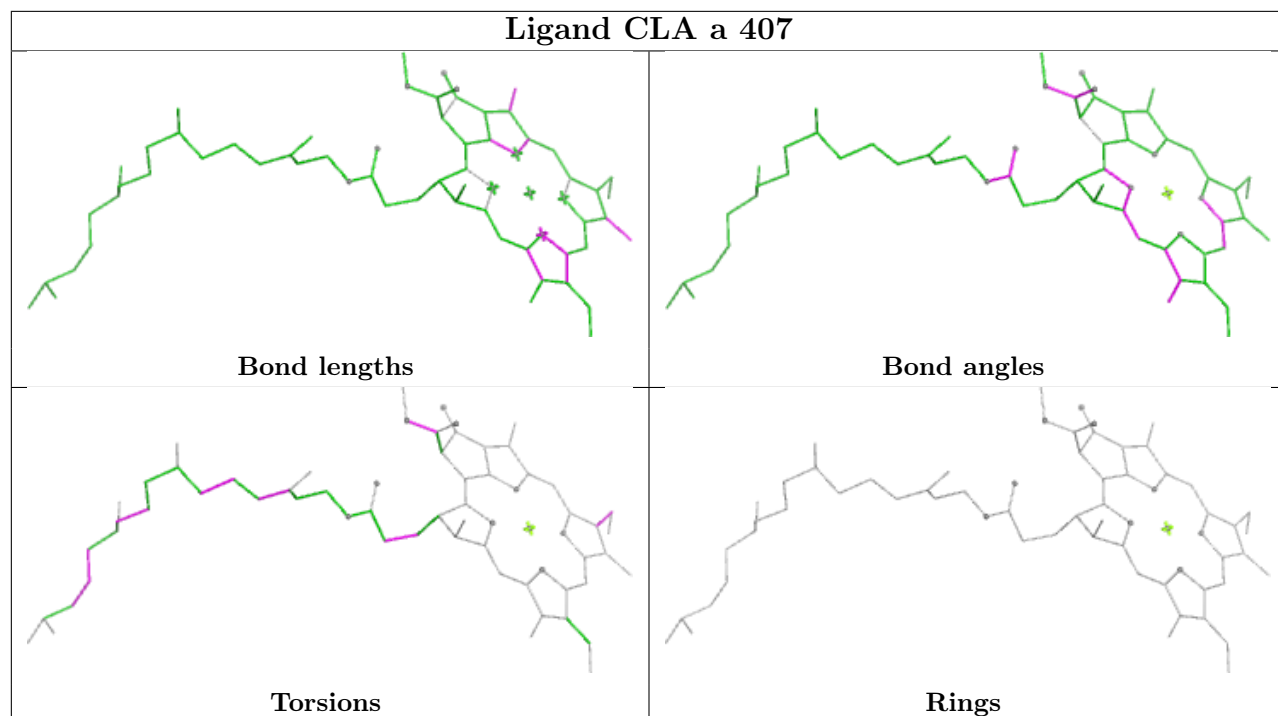
Ligand CLA b 607

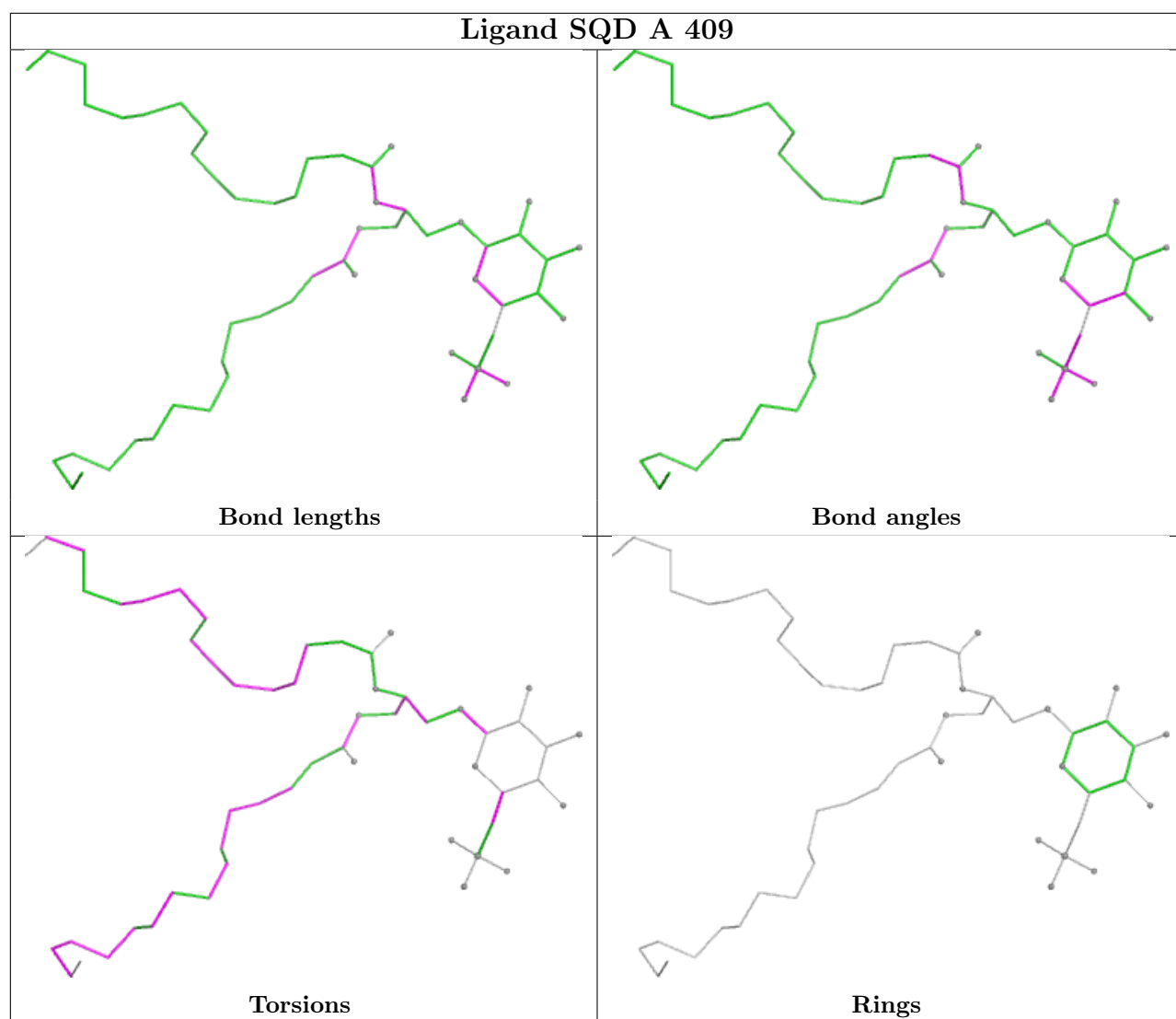


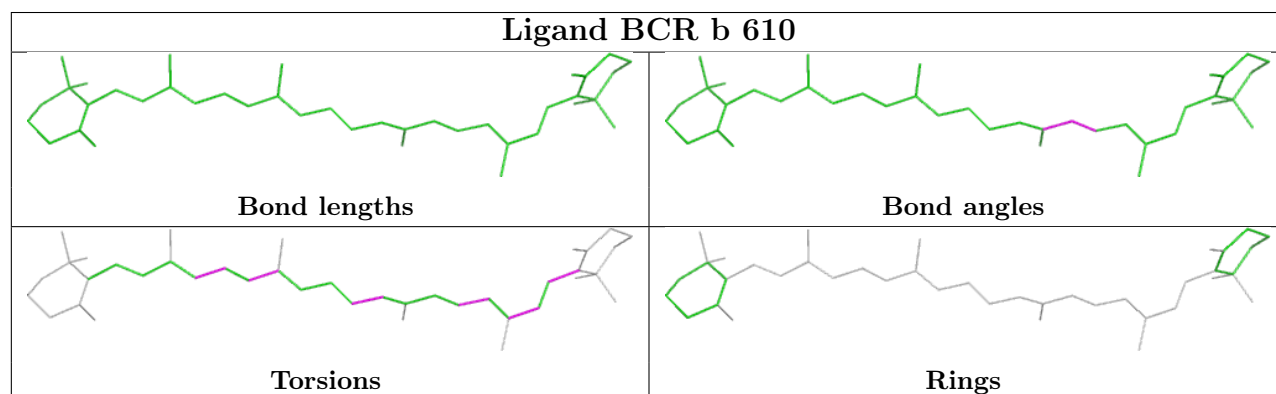
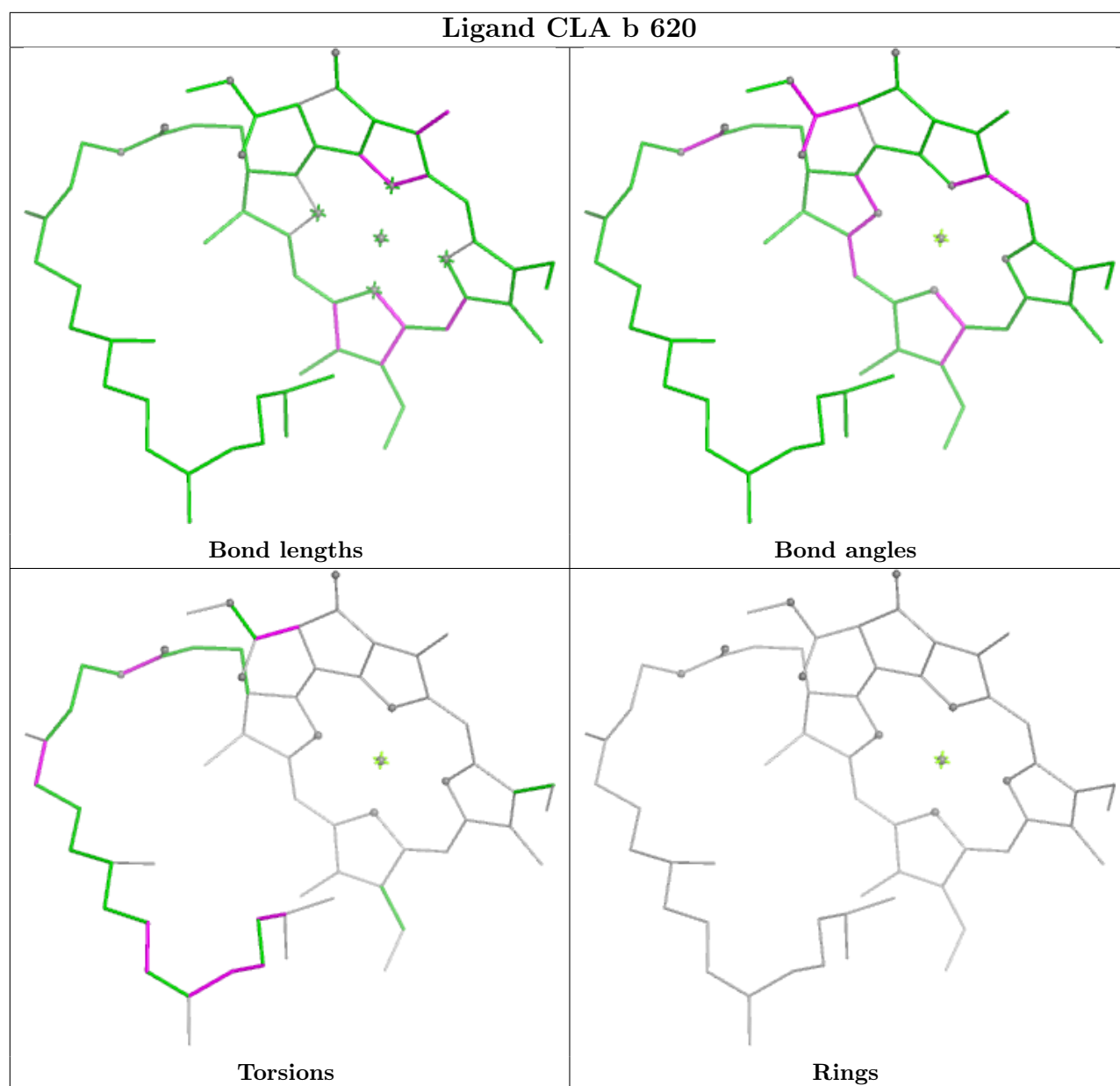


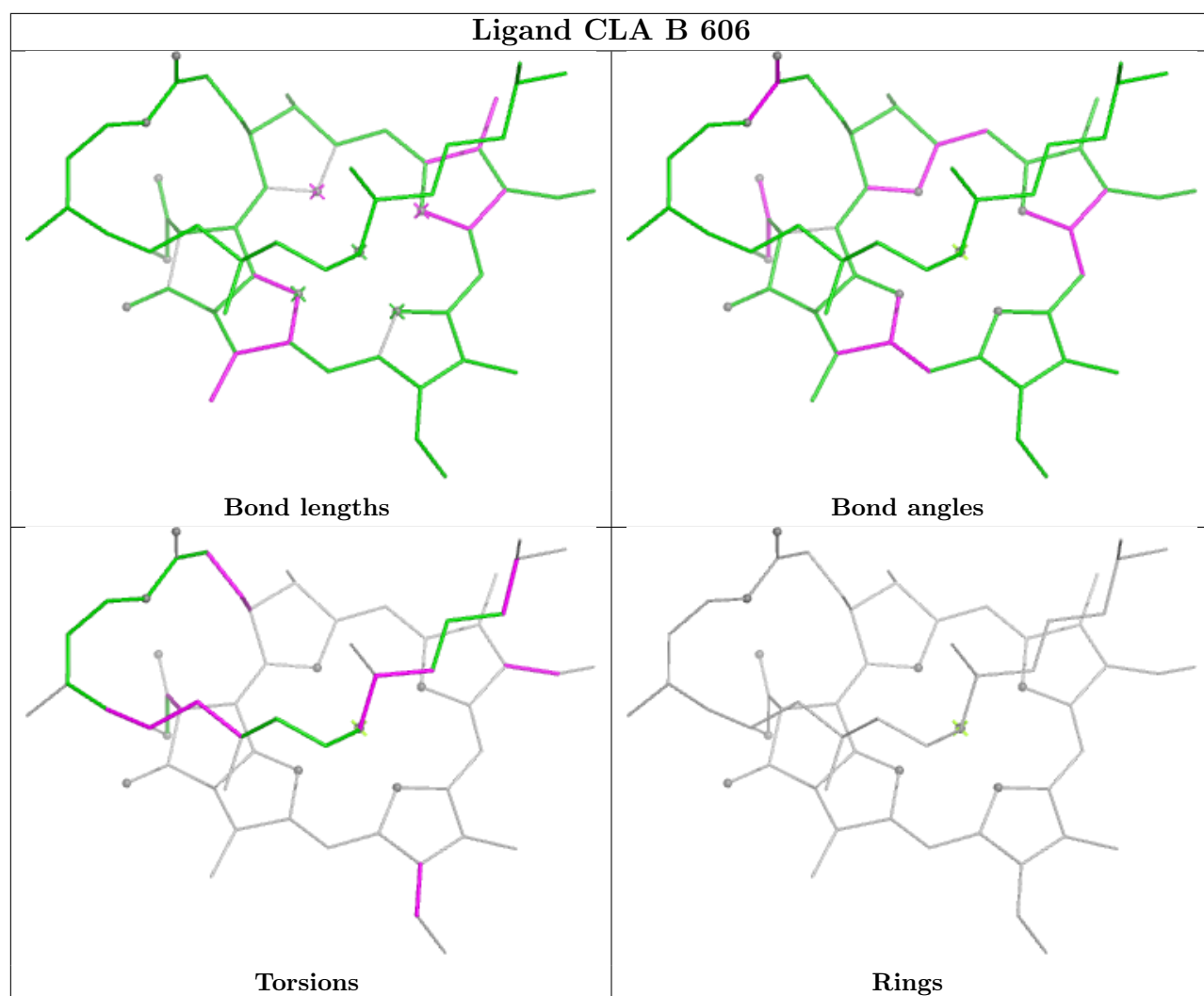


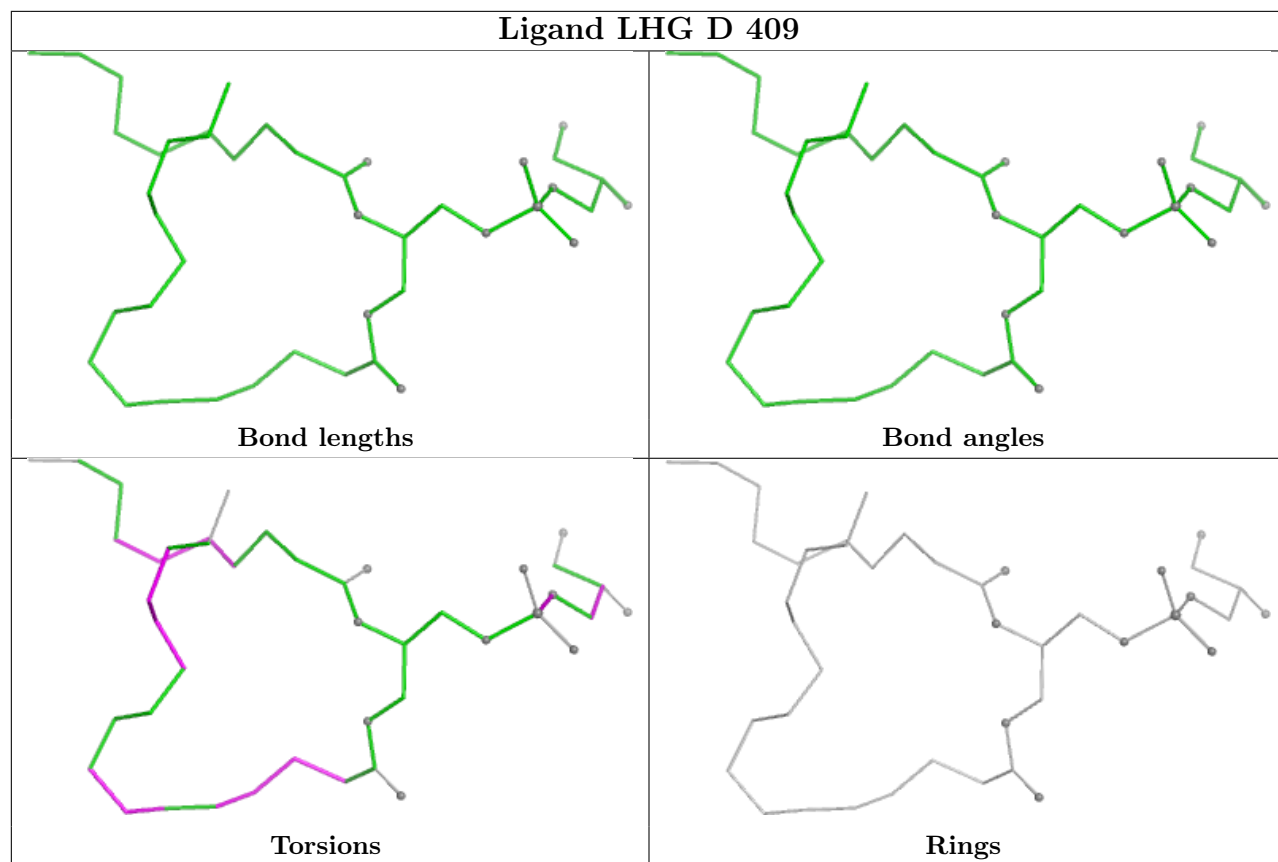


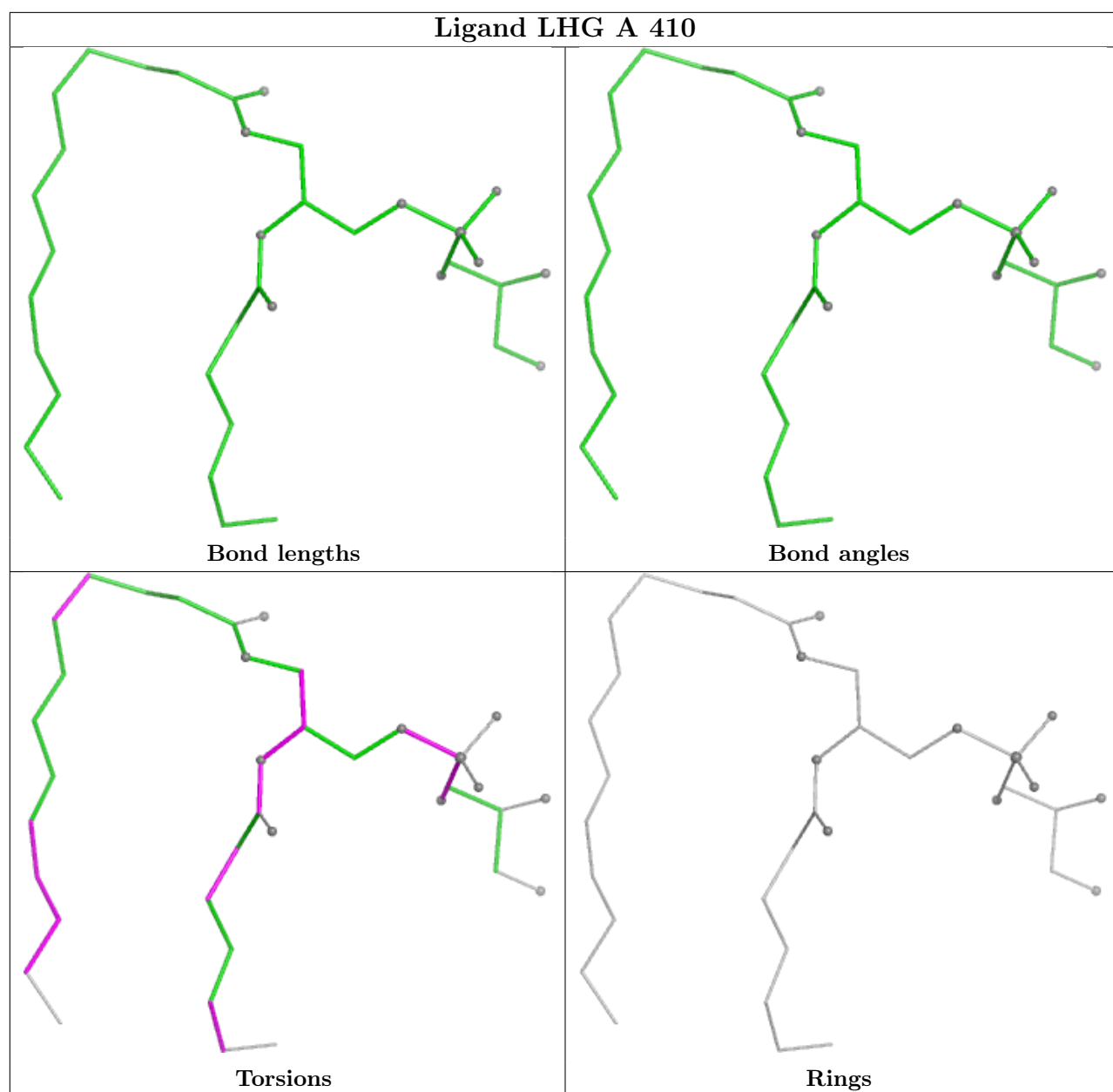


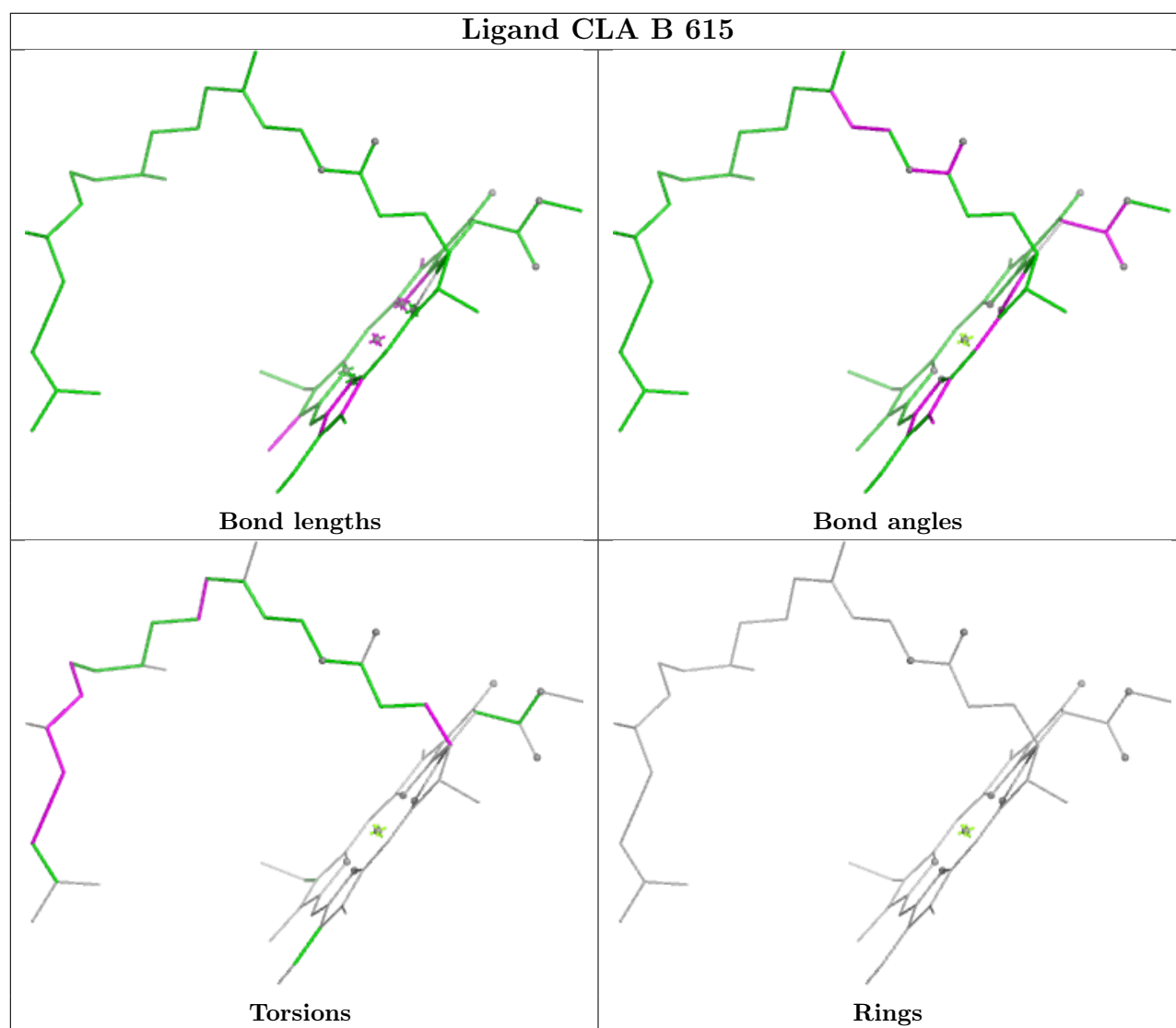


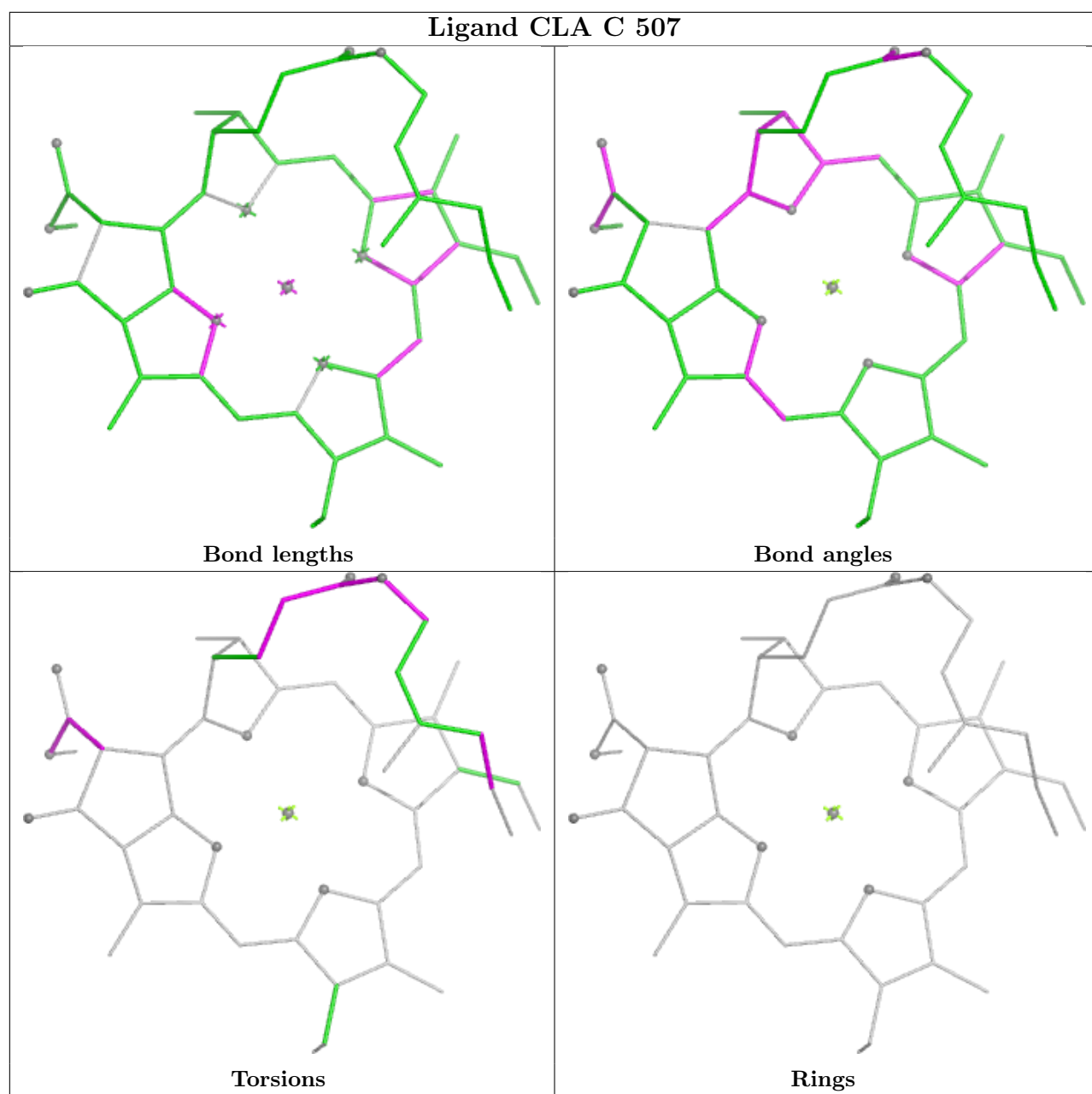


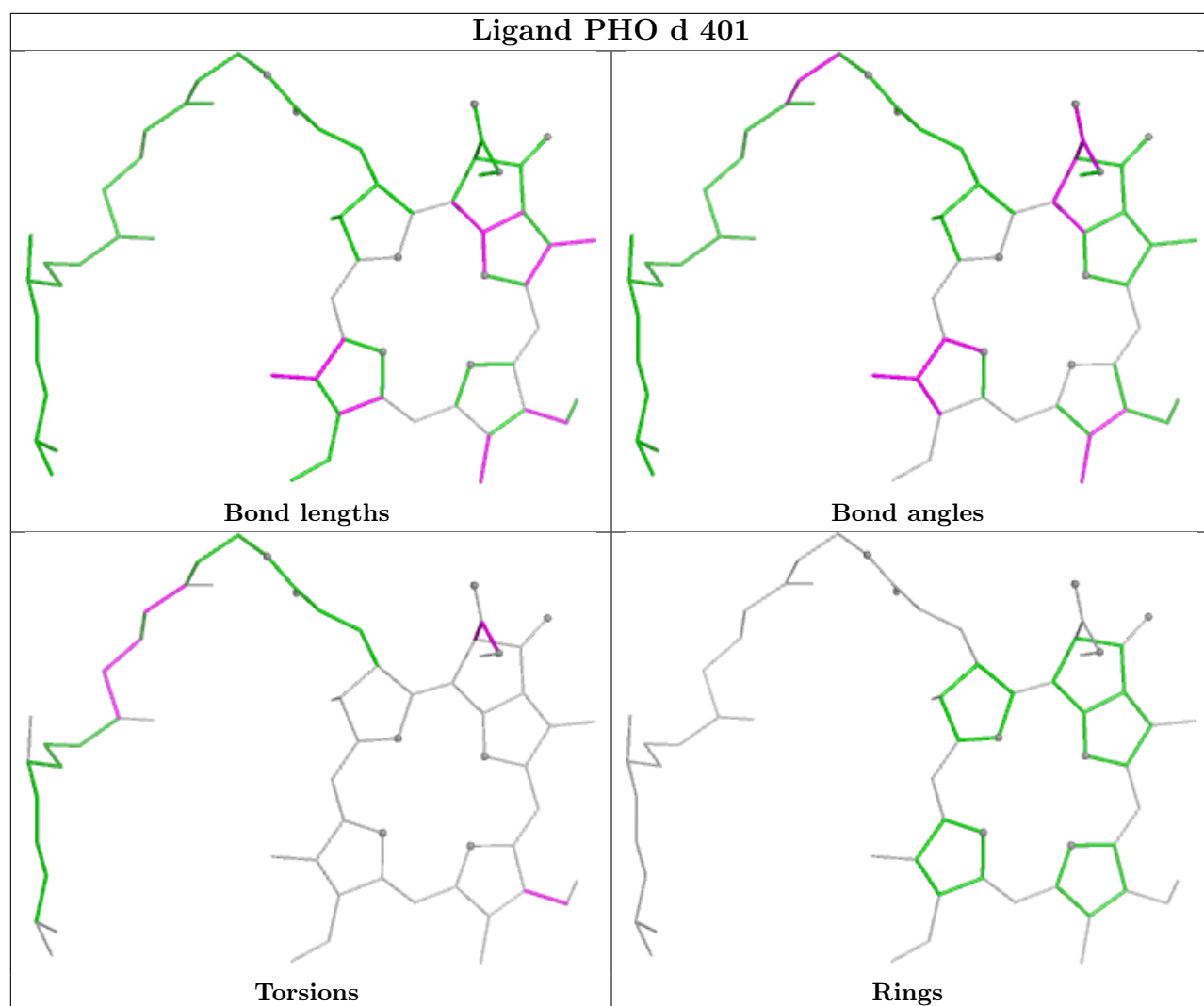




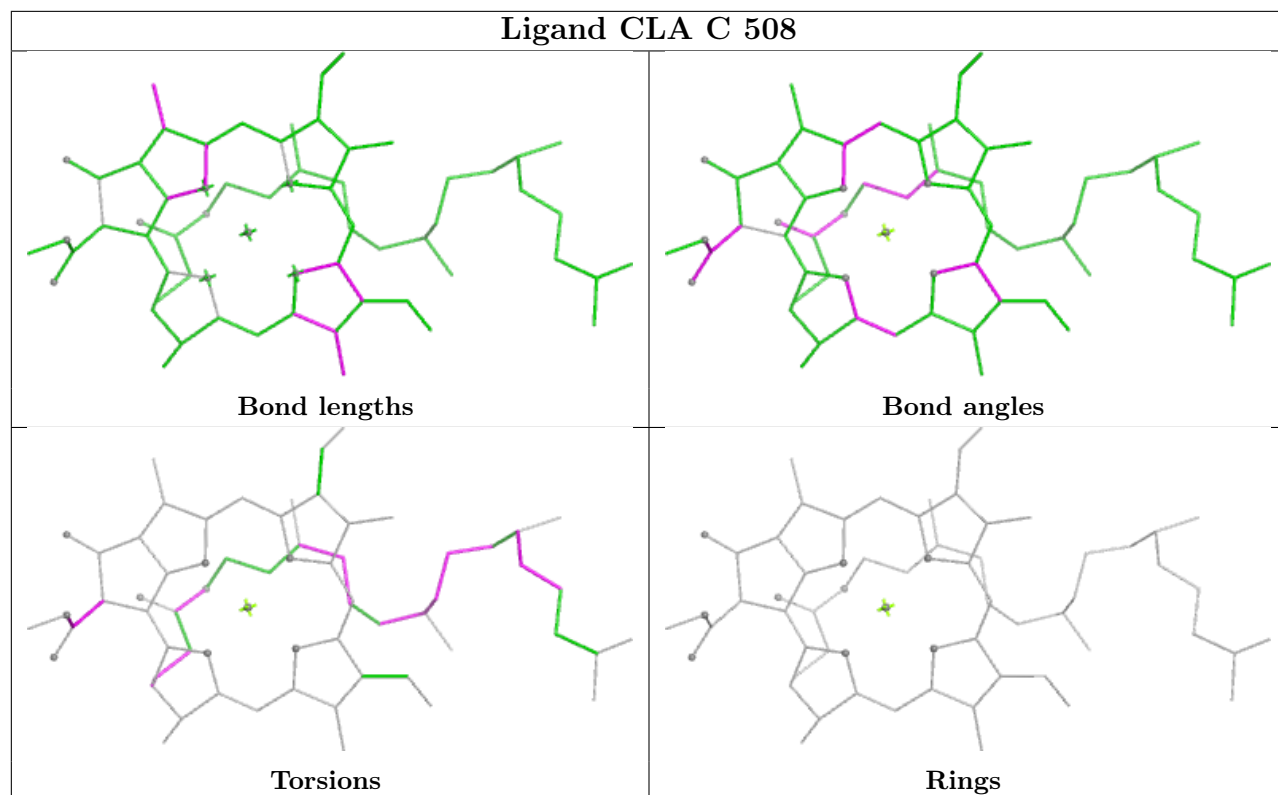




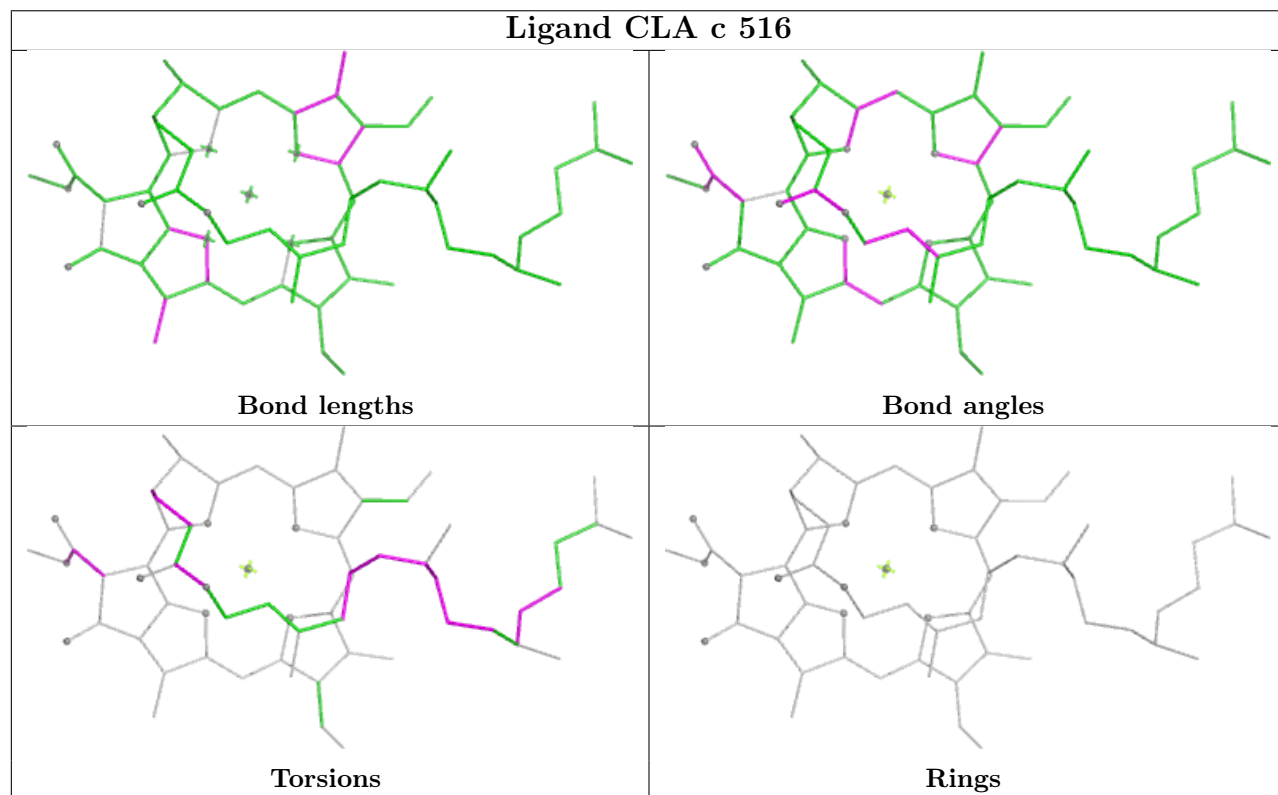


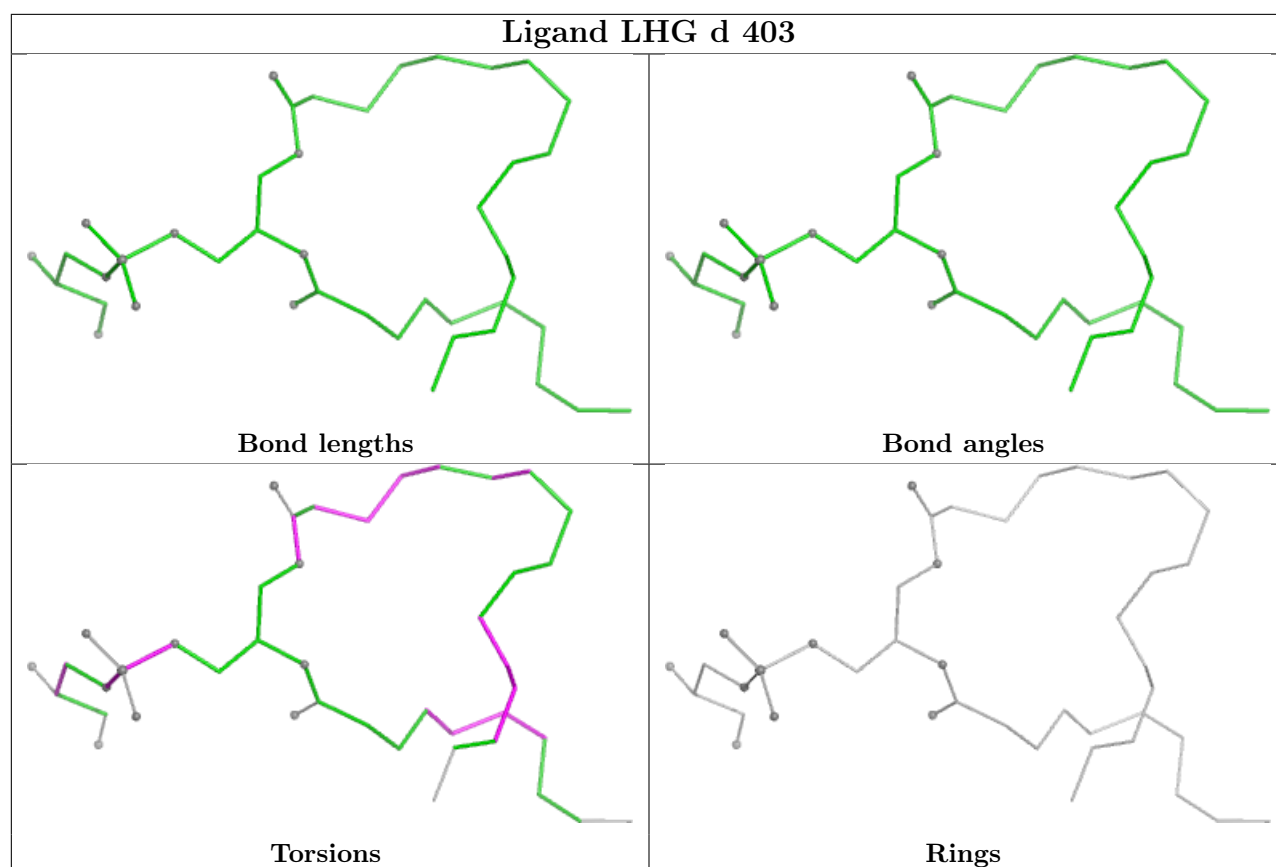


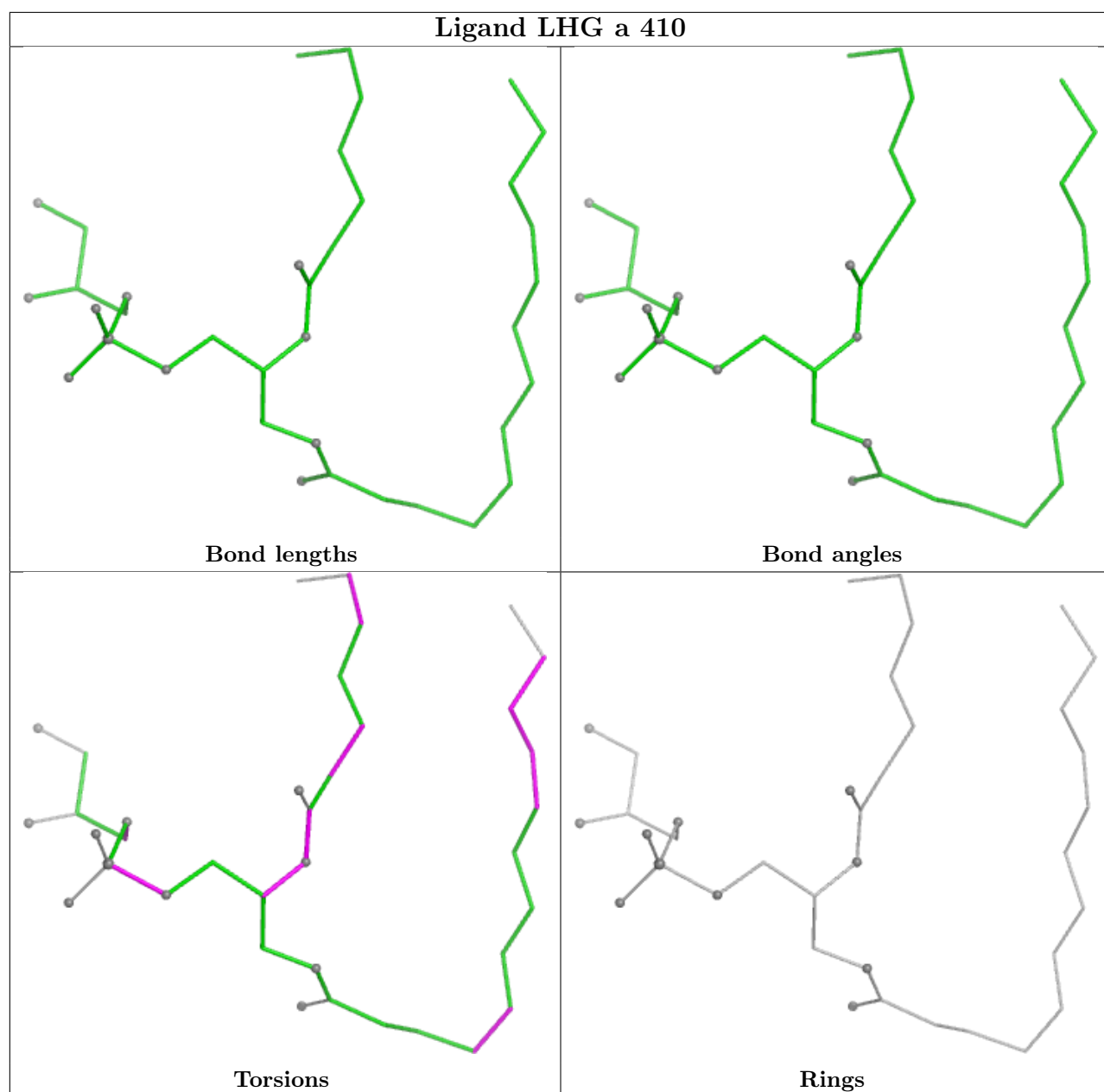
Ligand CLA C 508

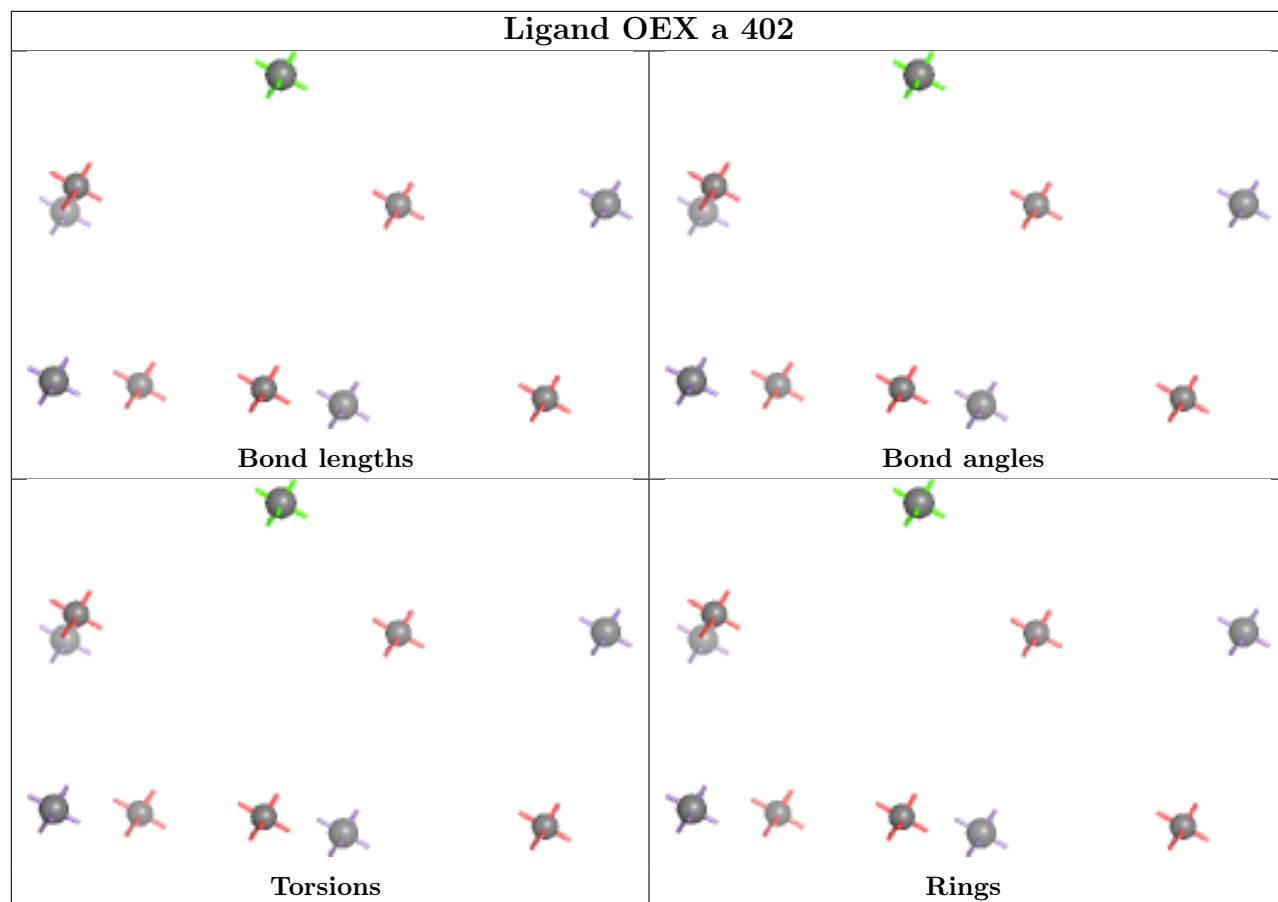


Ligand CLA c 516

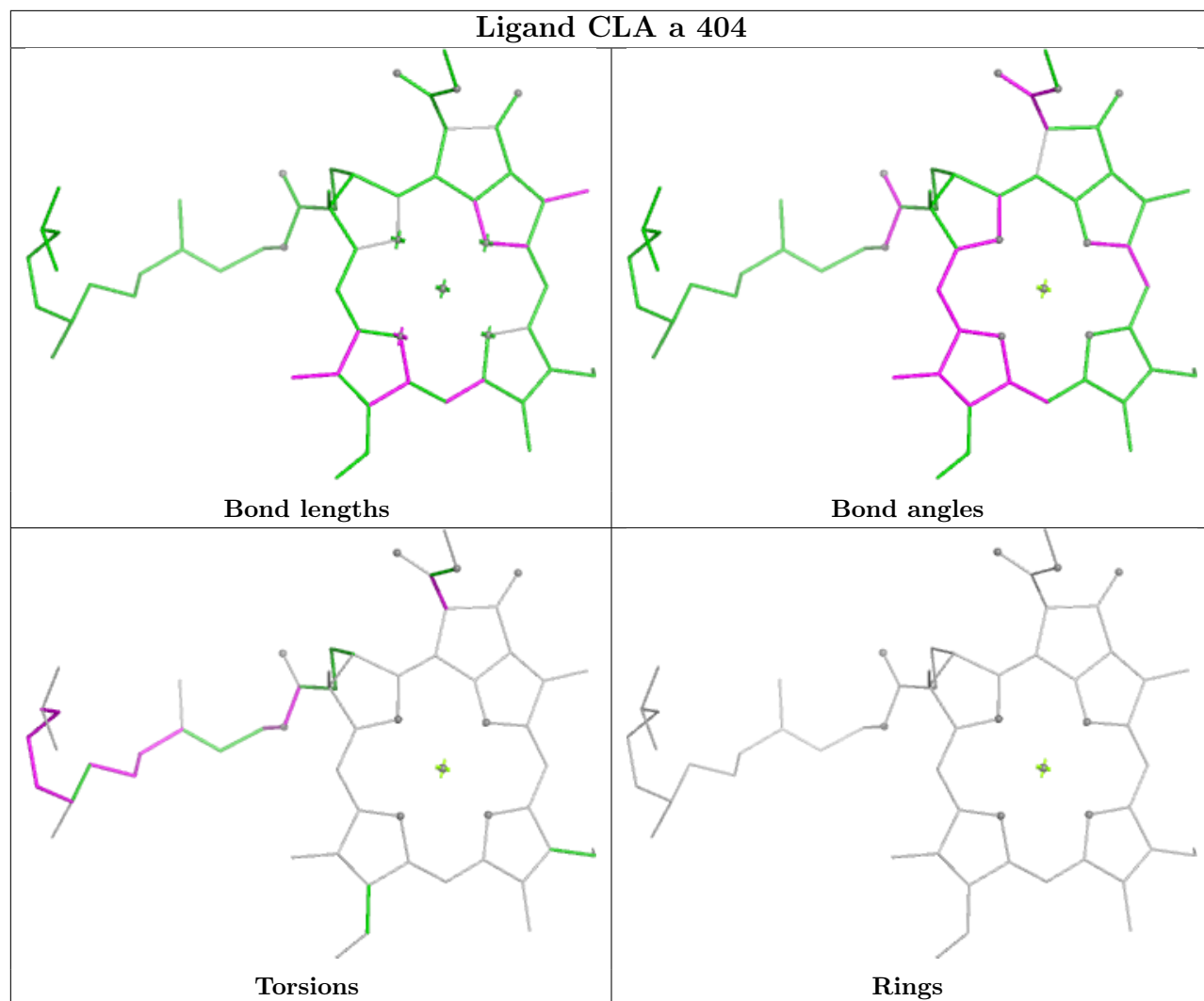


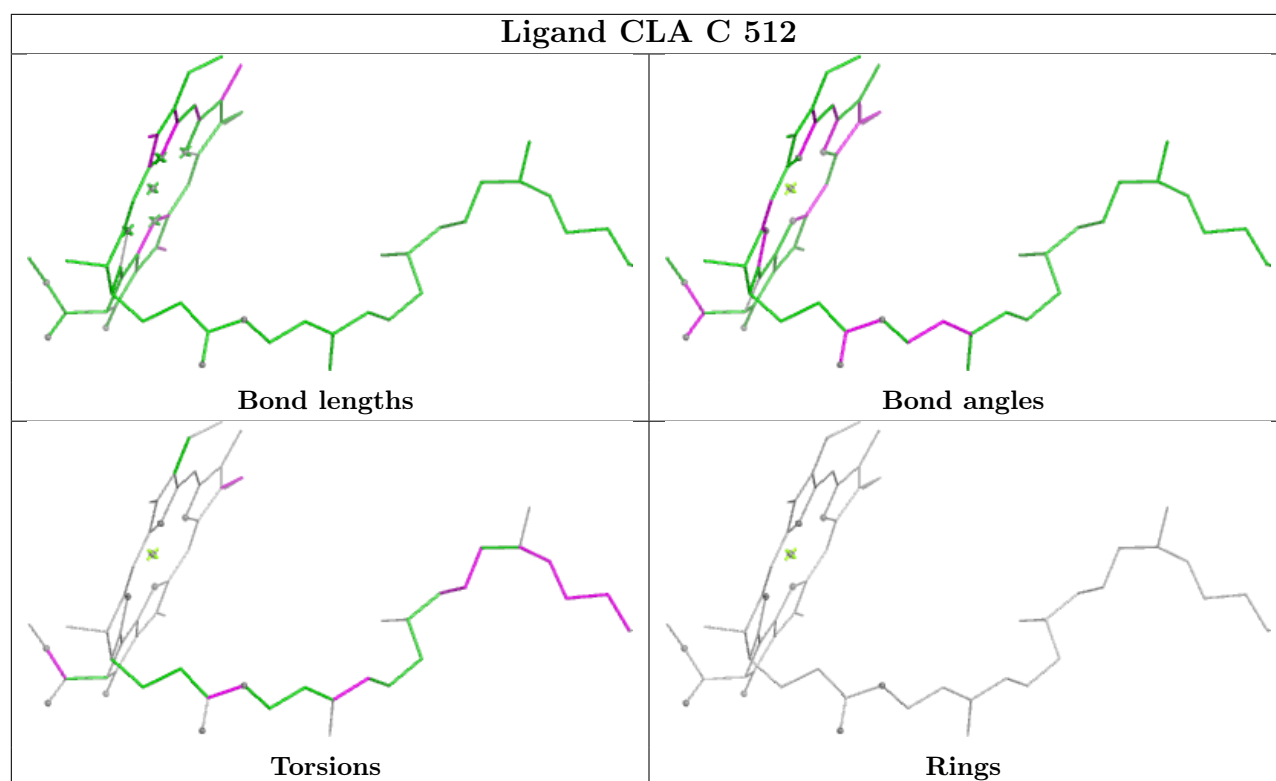




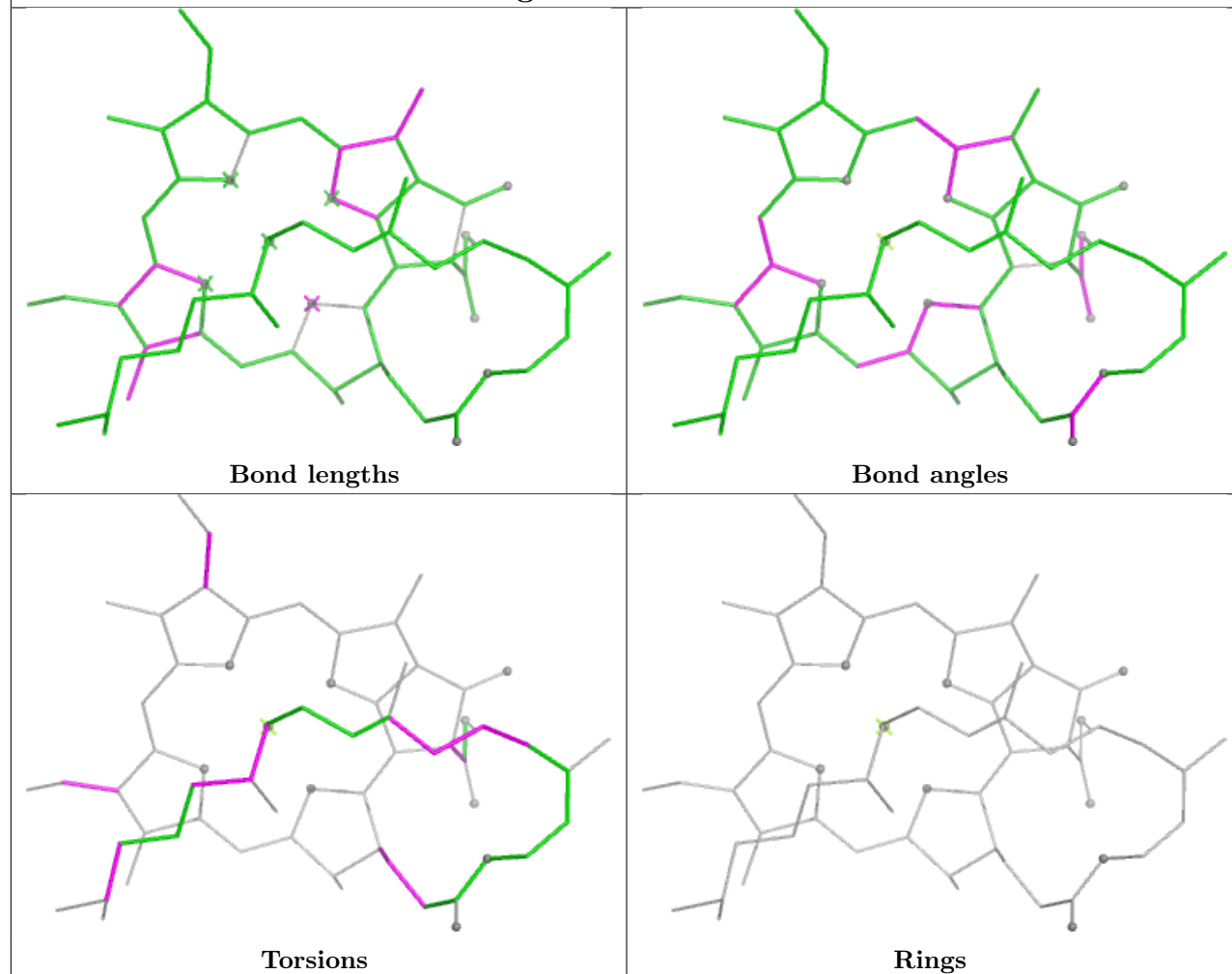


Ligand CLA a 404

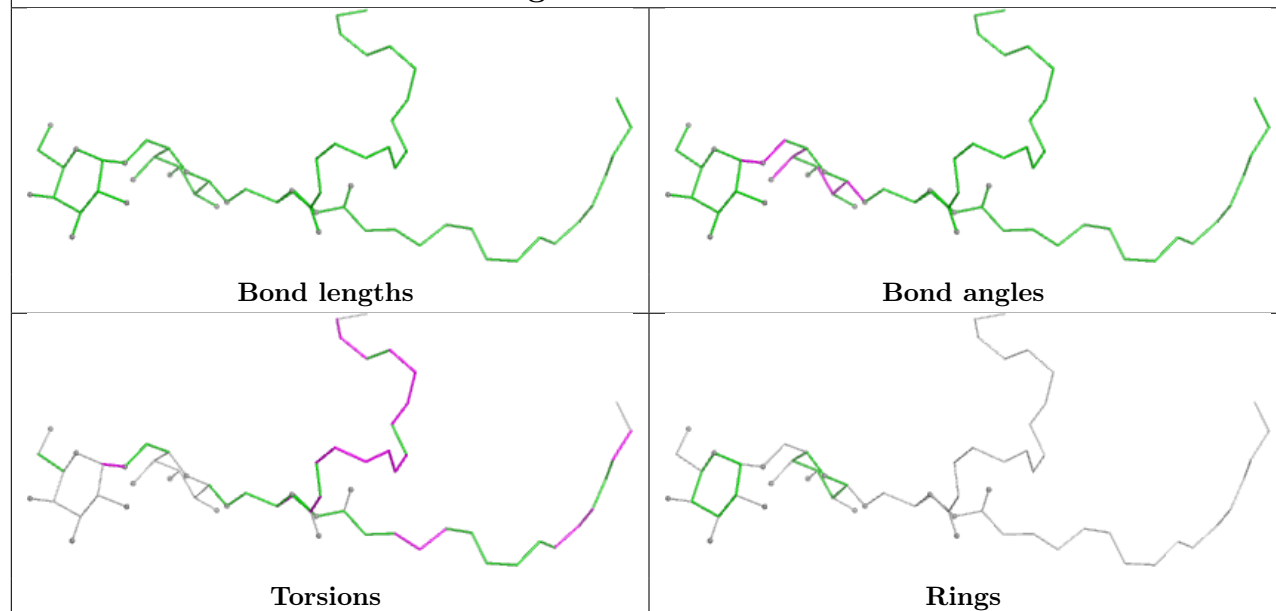


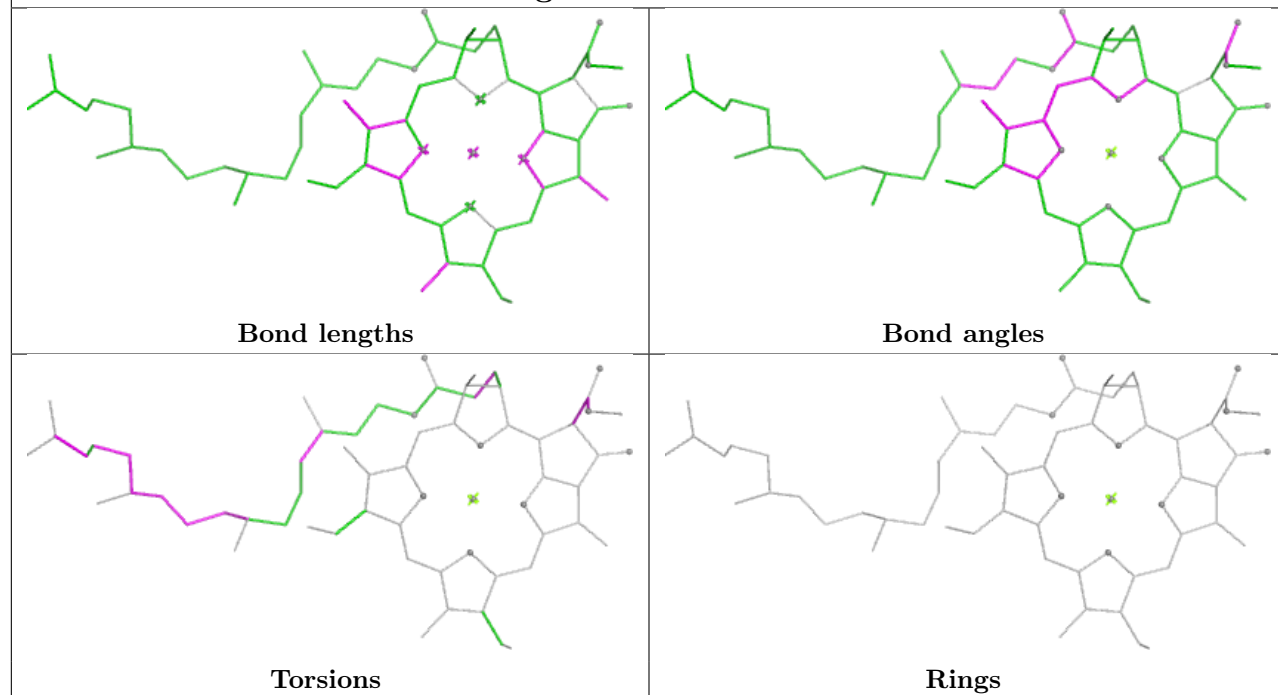
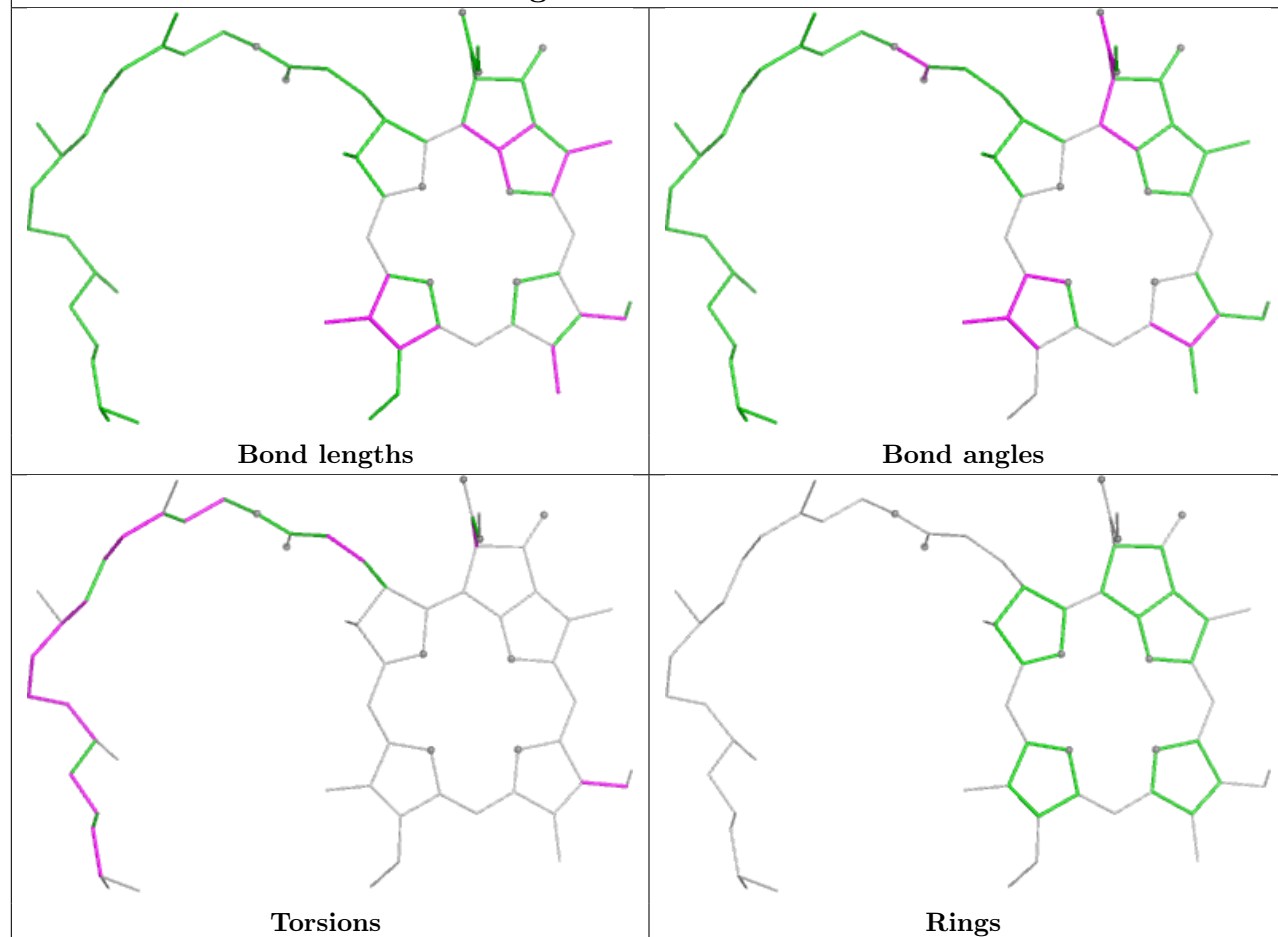


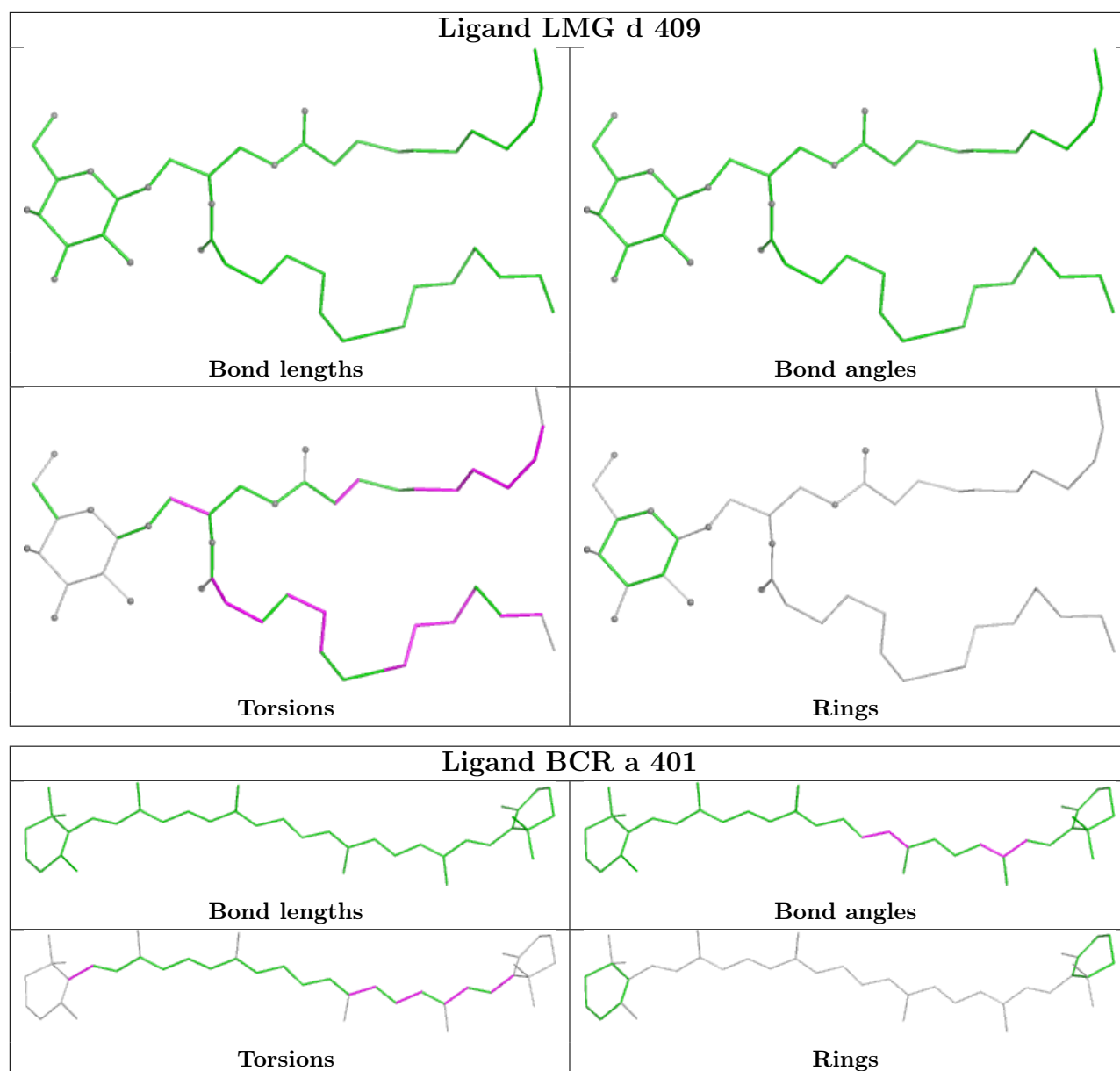
Ligand CLA b 611

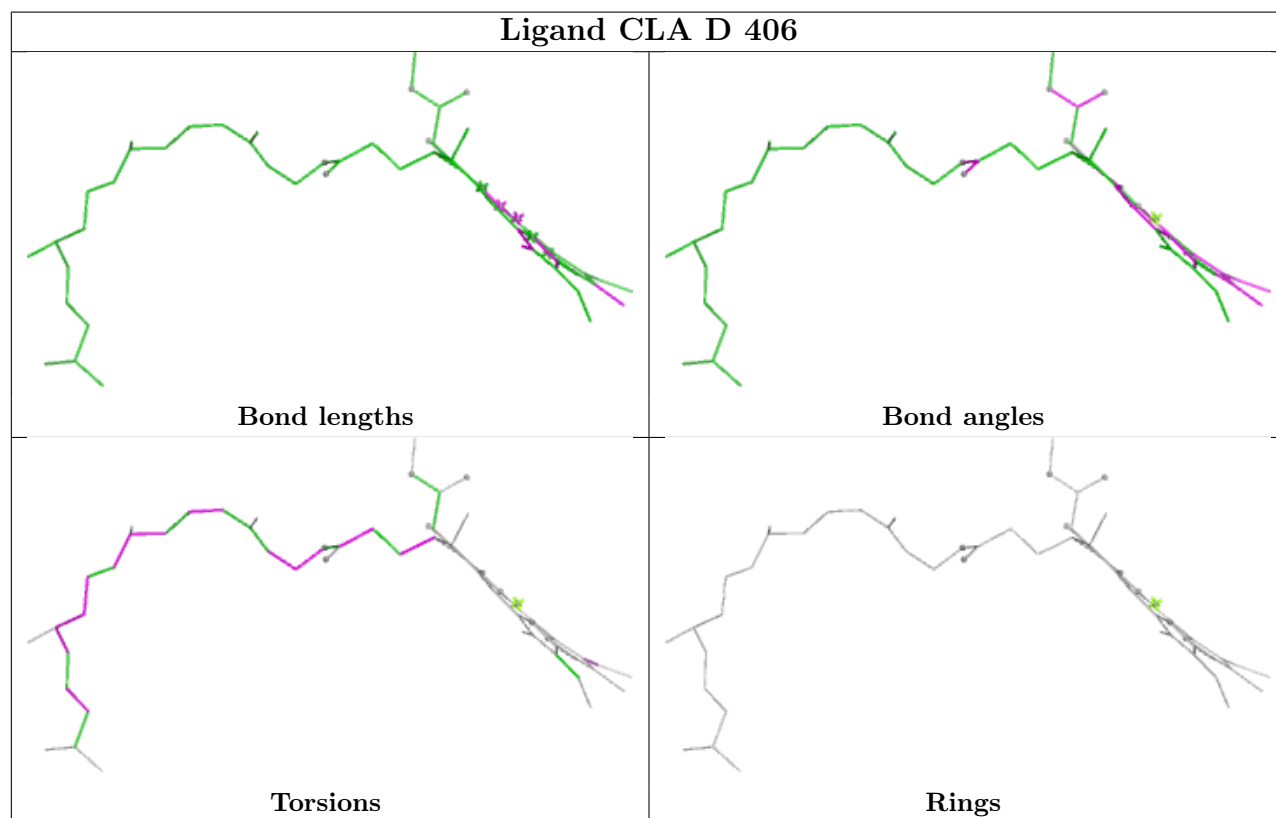
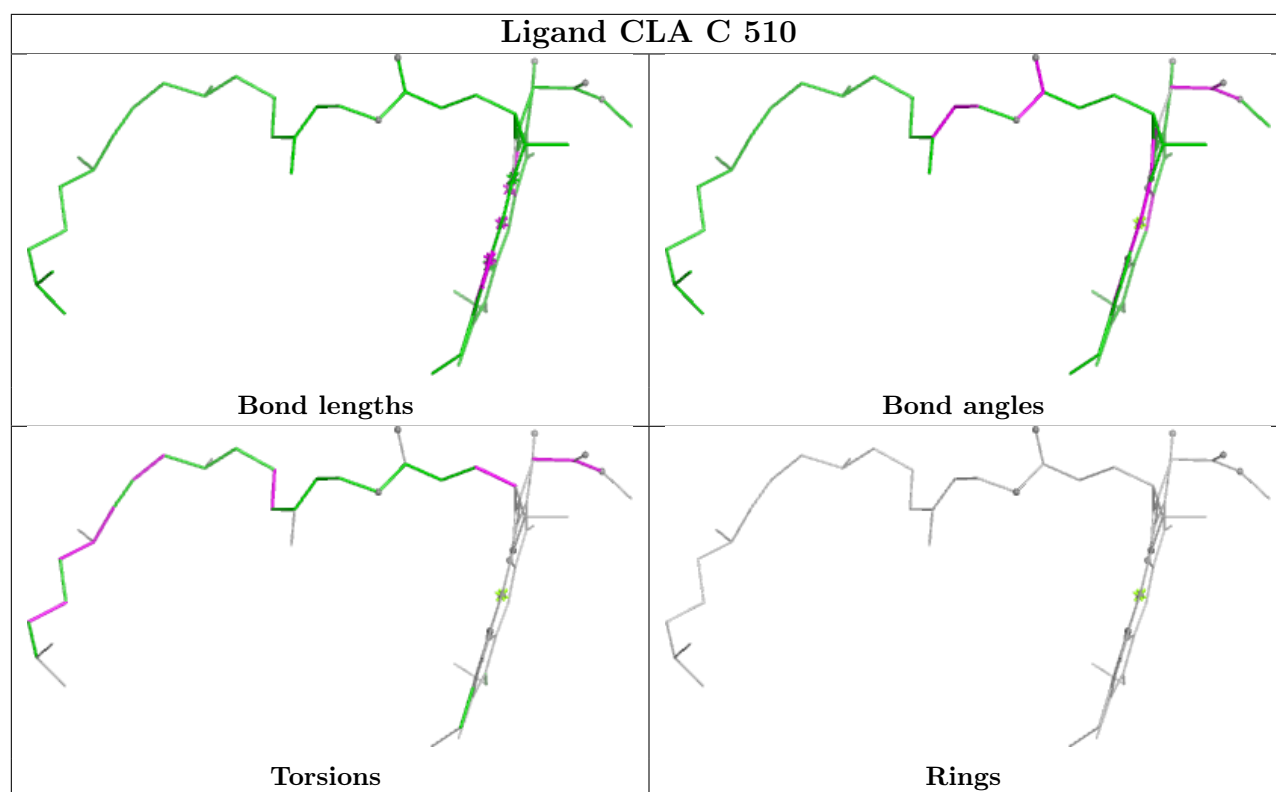


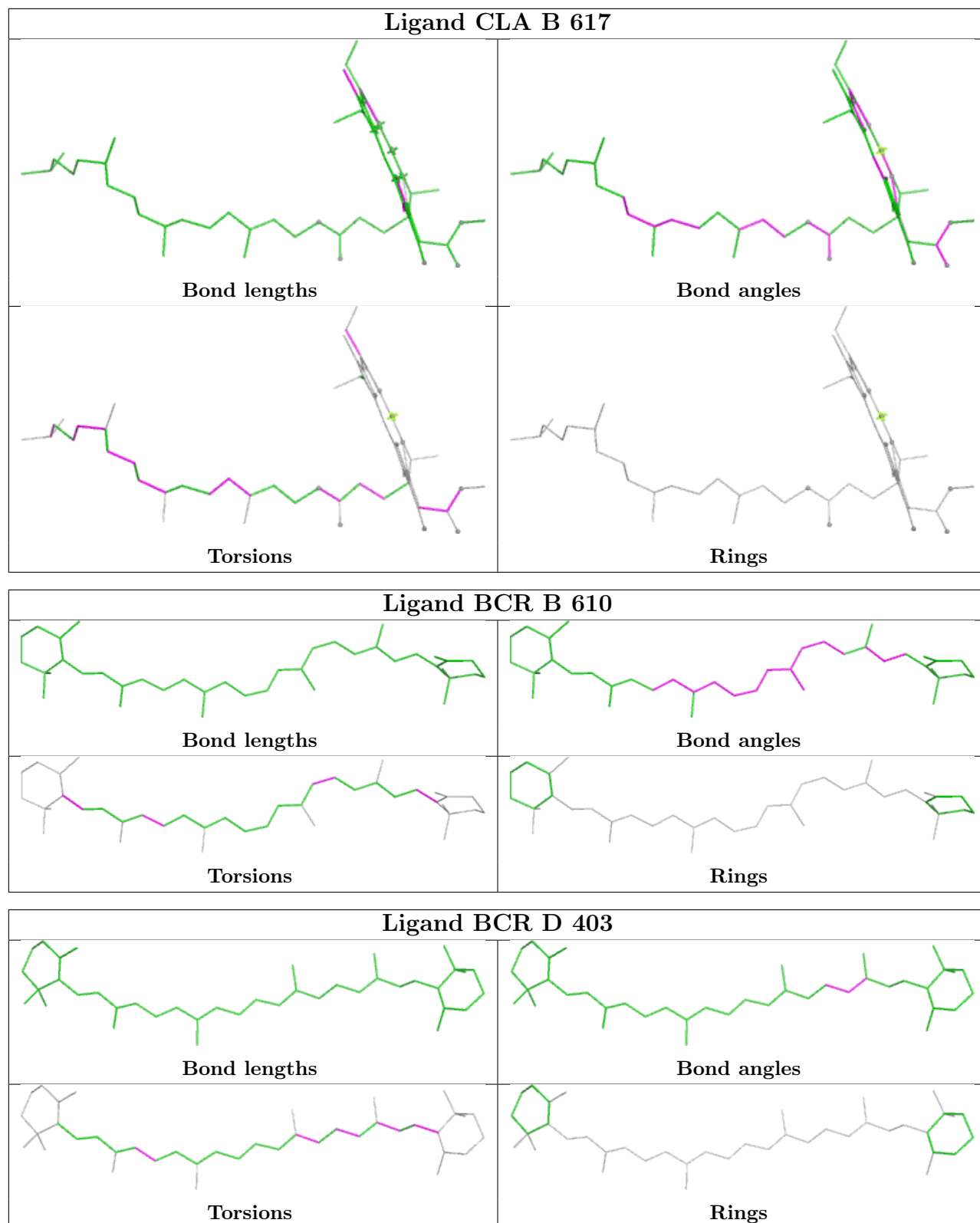
Ligand DGD B 620

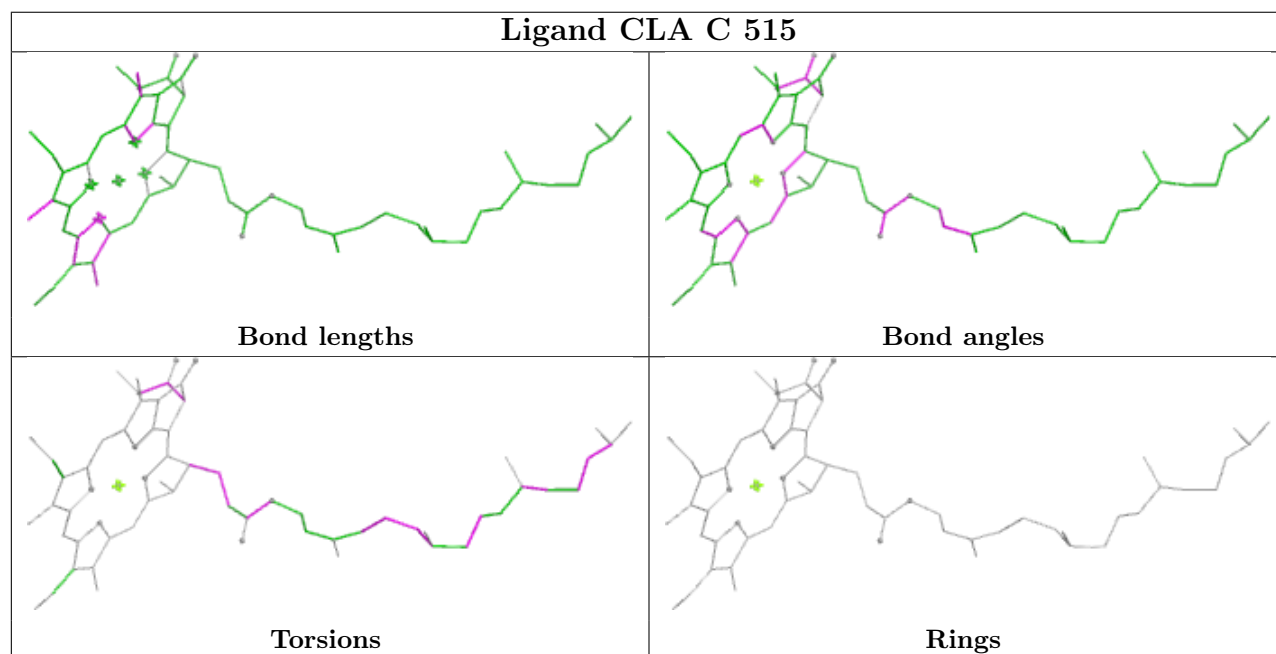
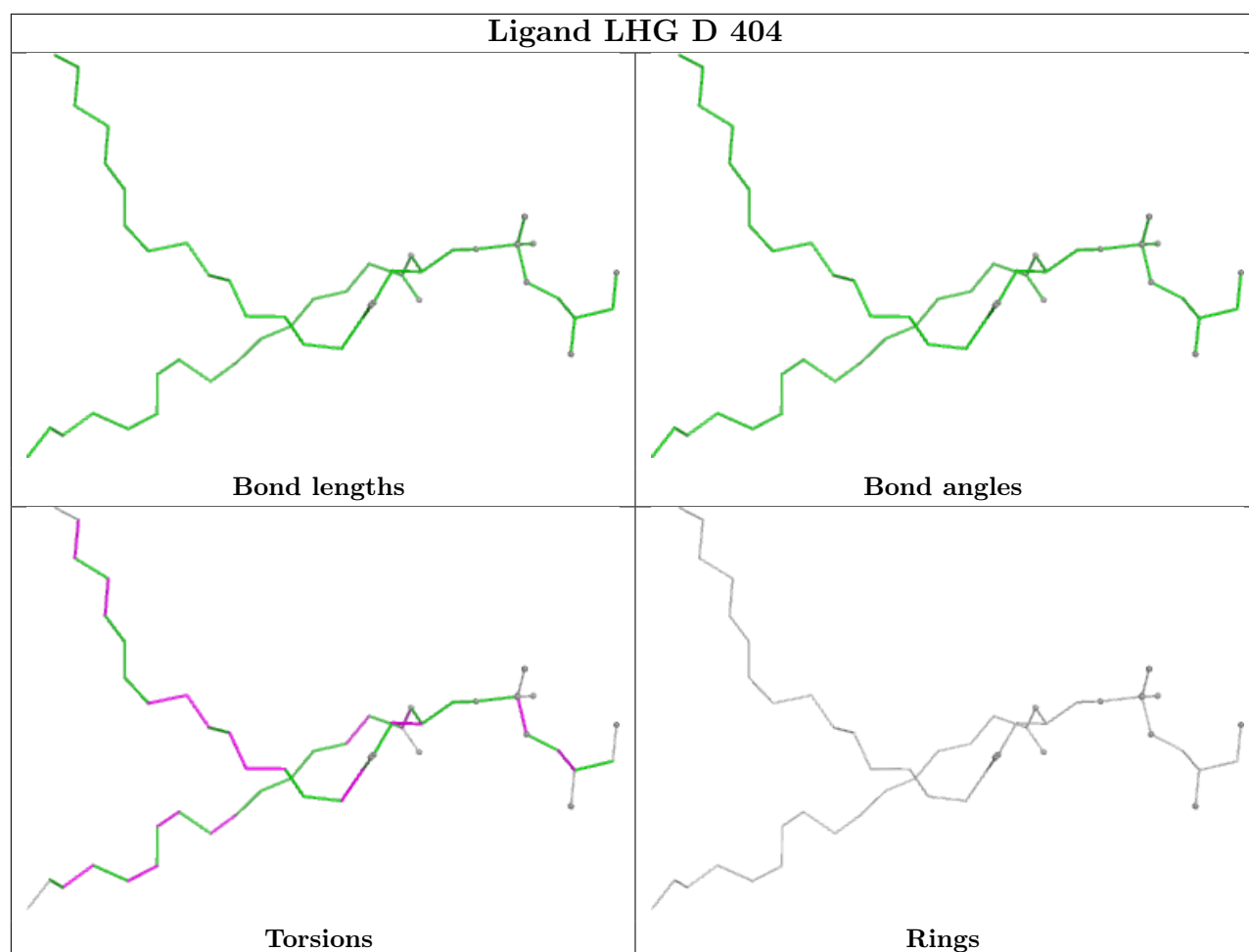


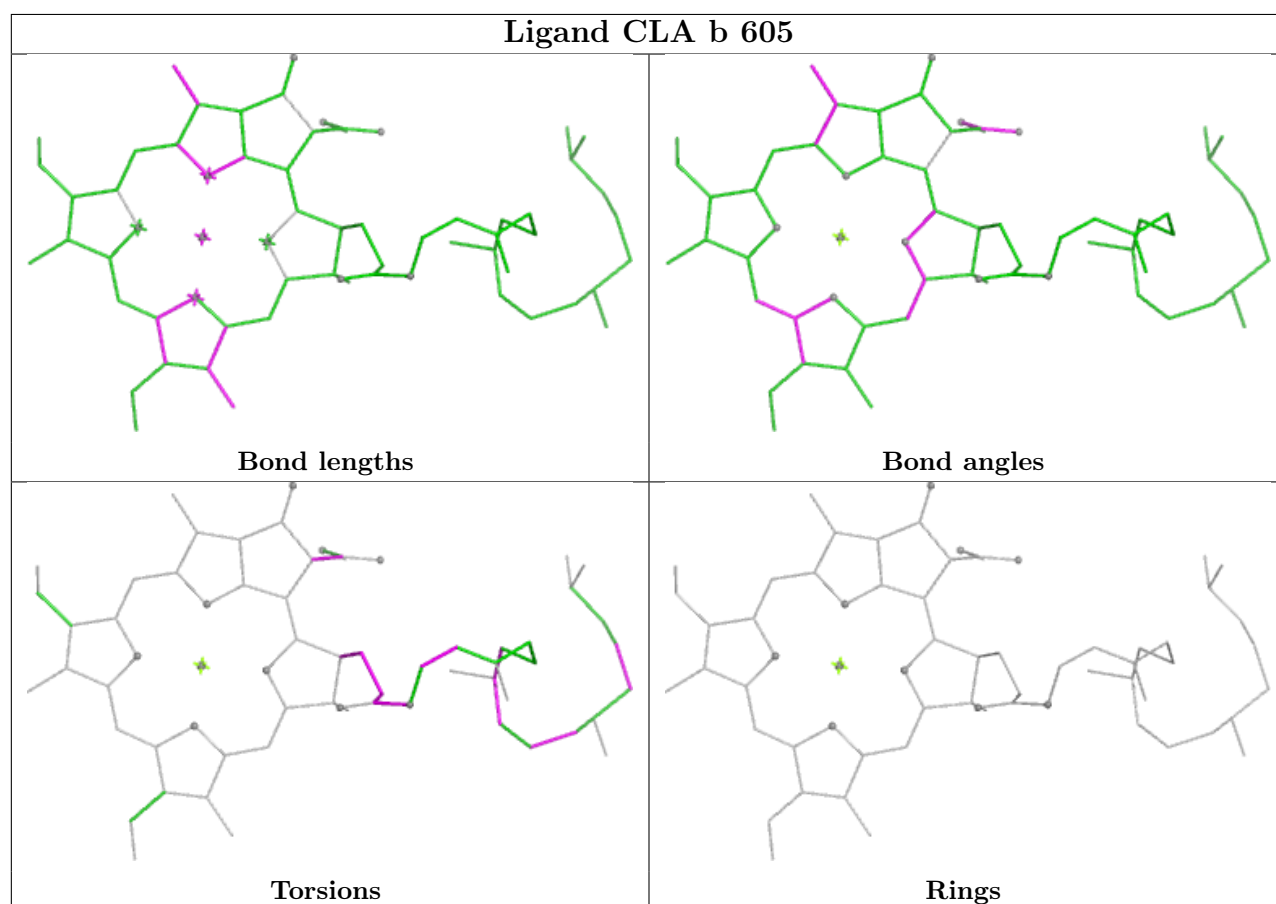
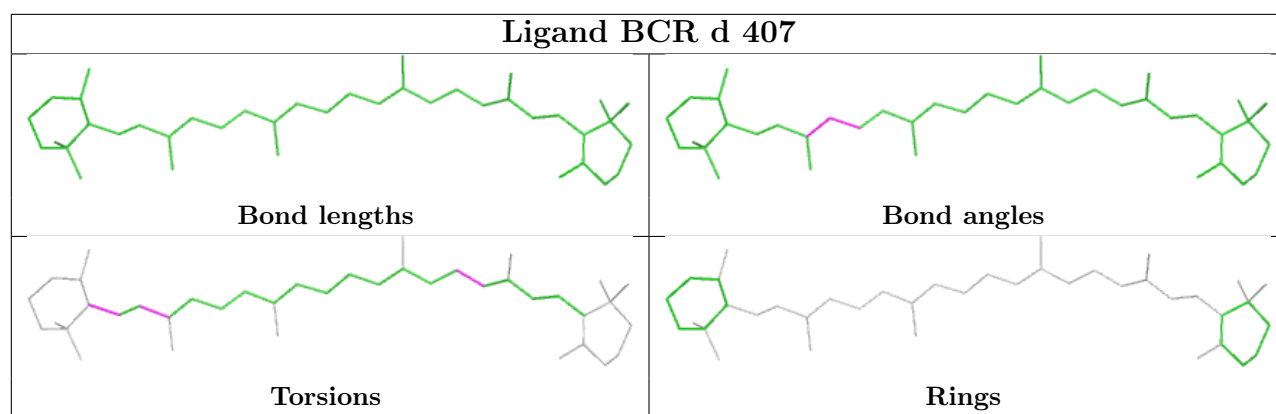
Ligand CLA b 615**Ligand PHO A 407**

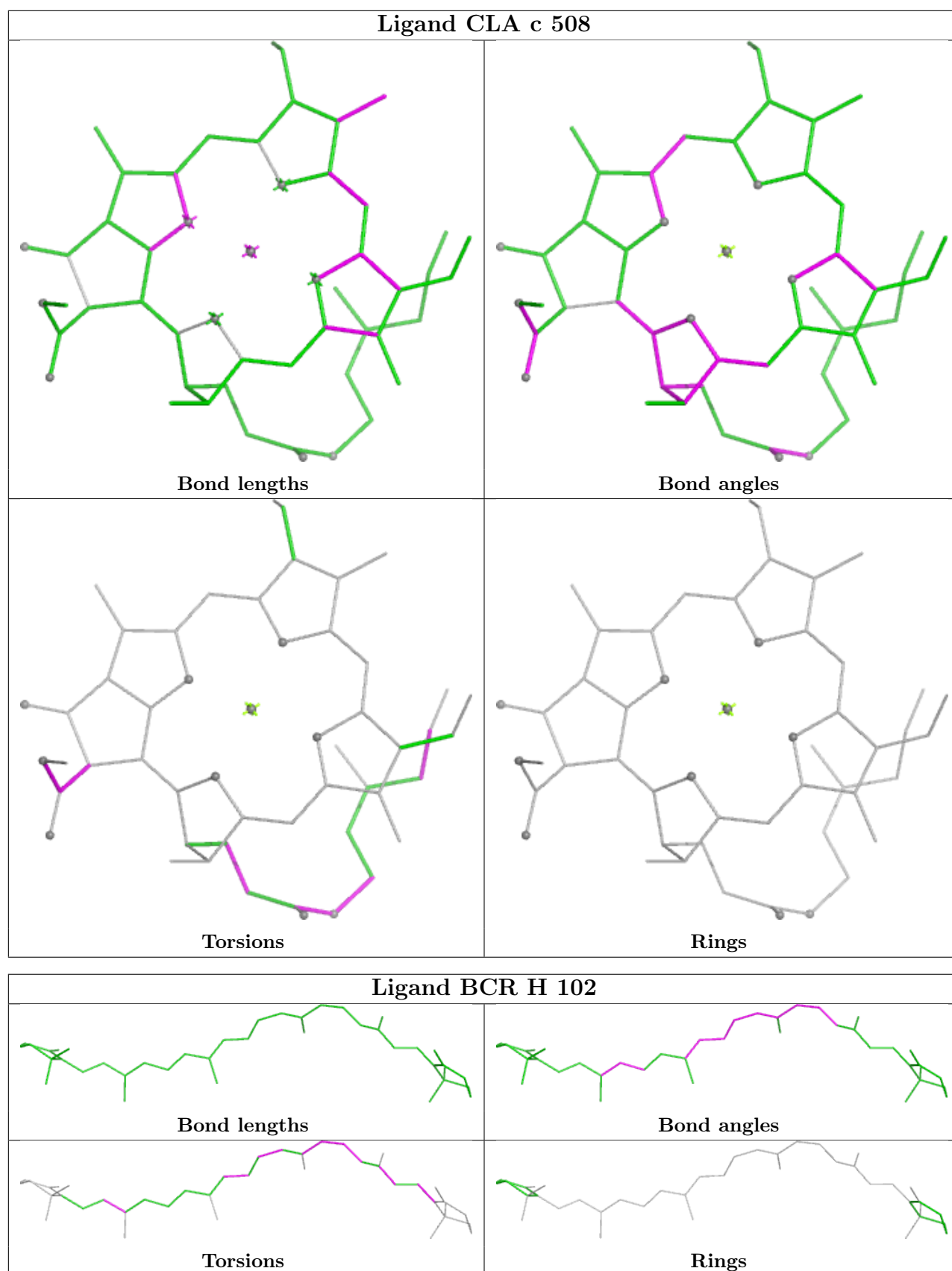


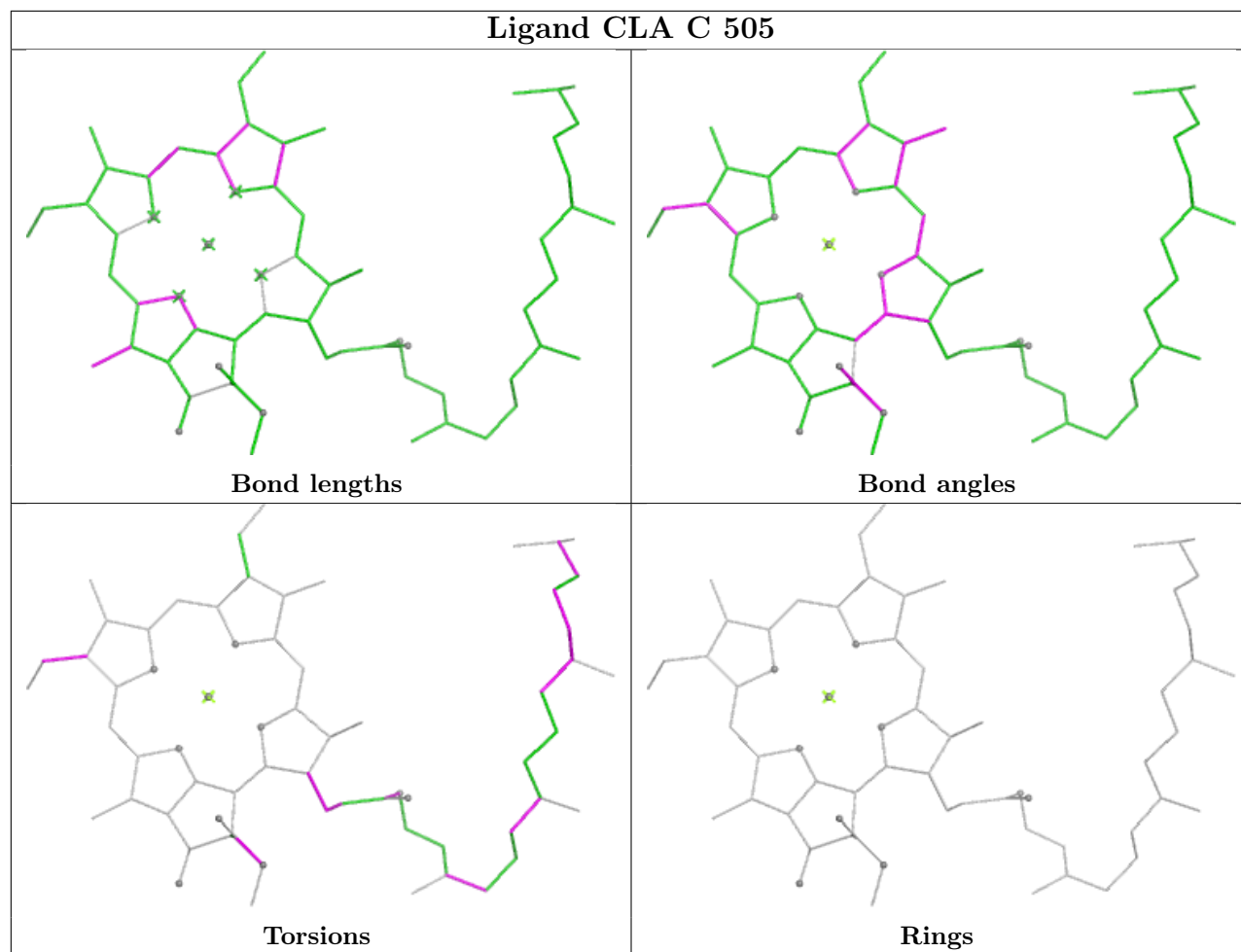


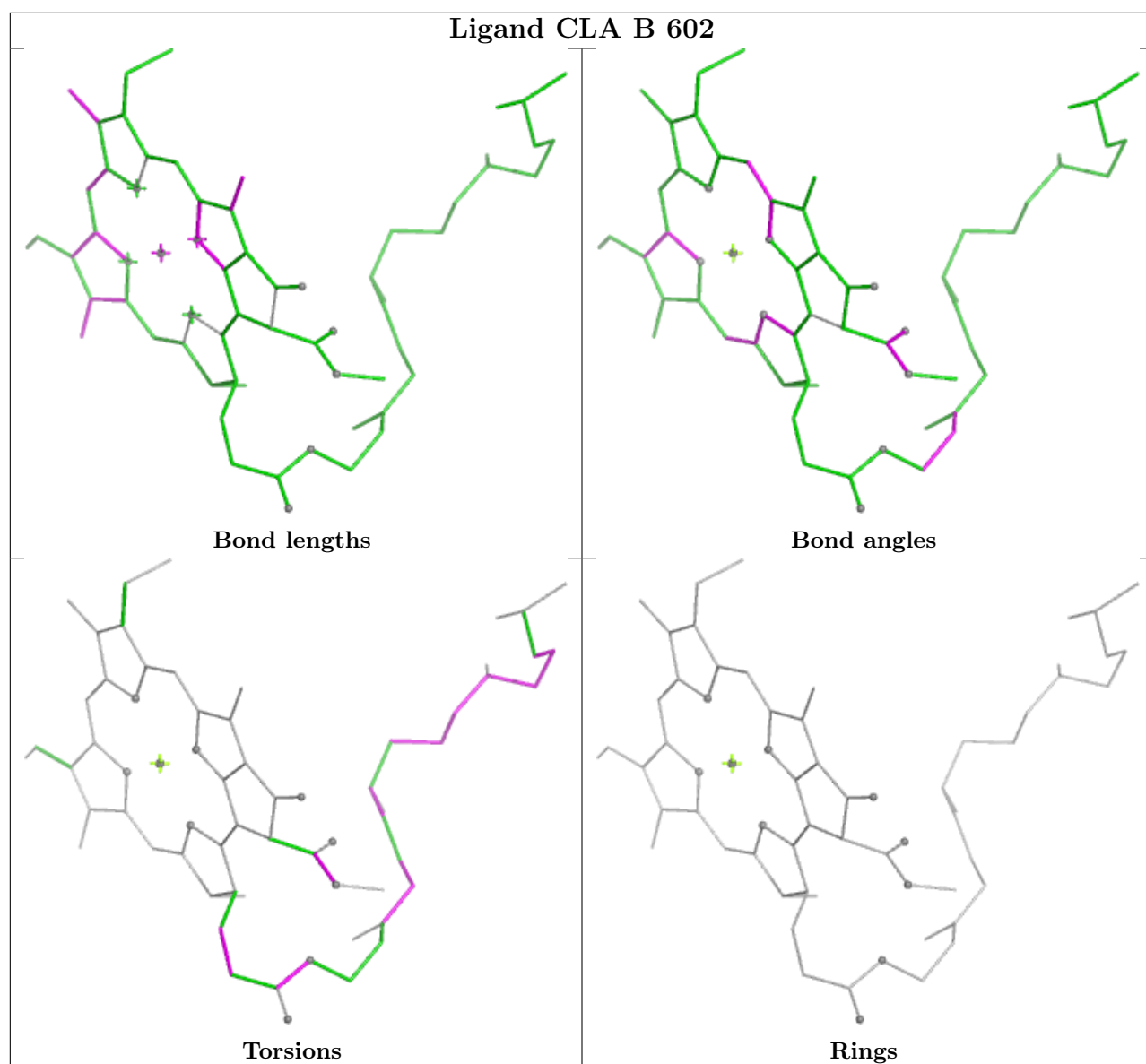


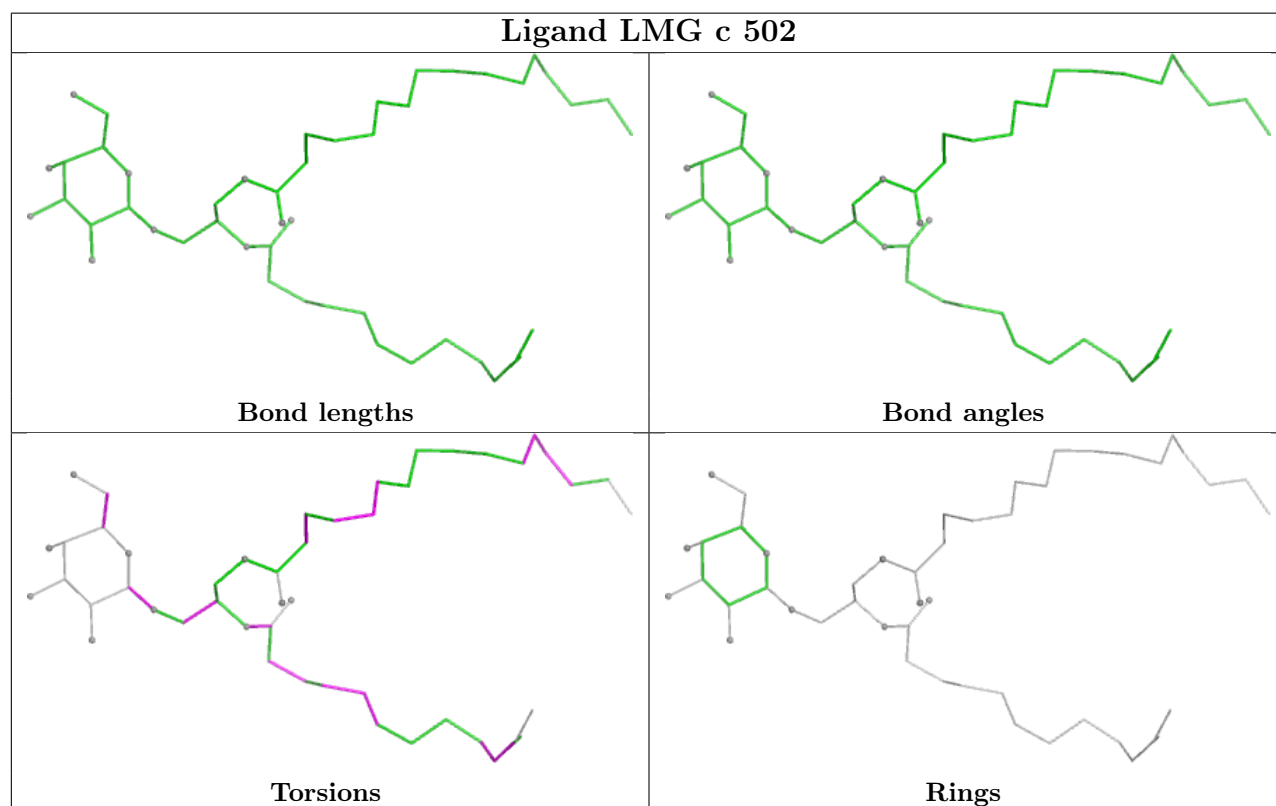
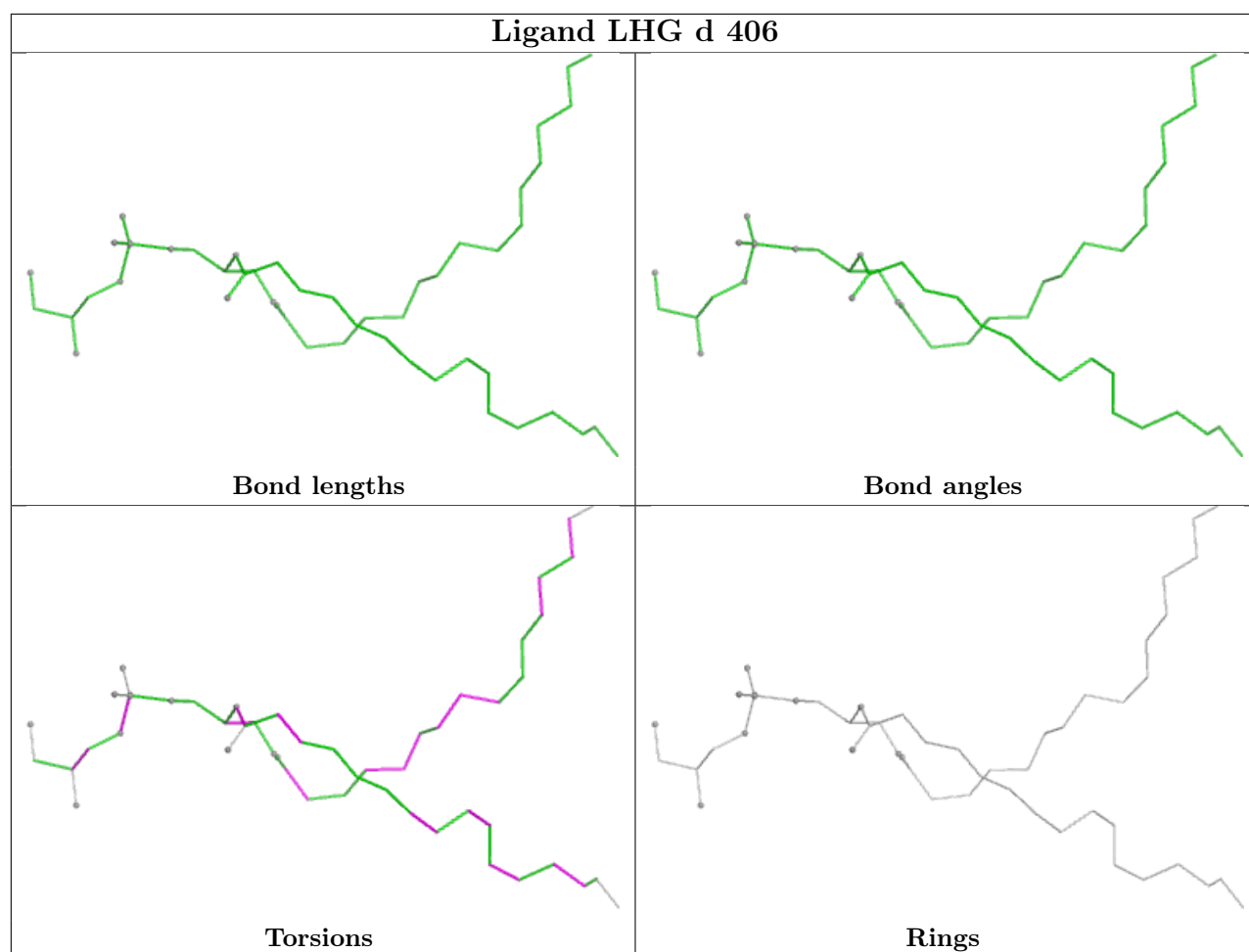




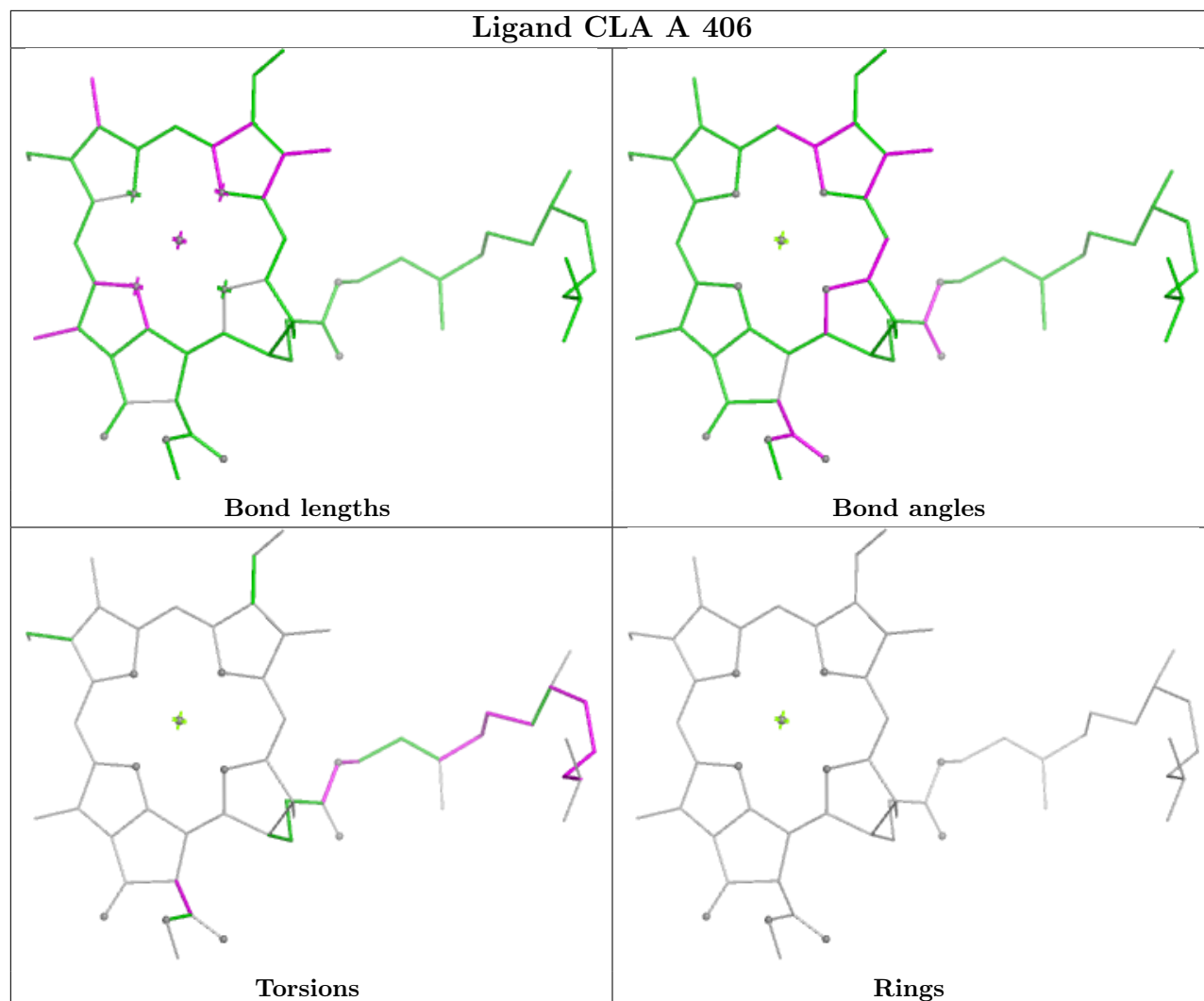




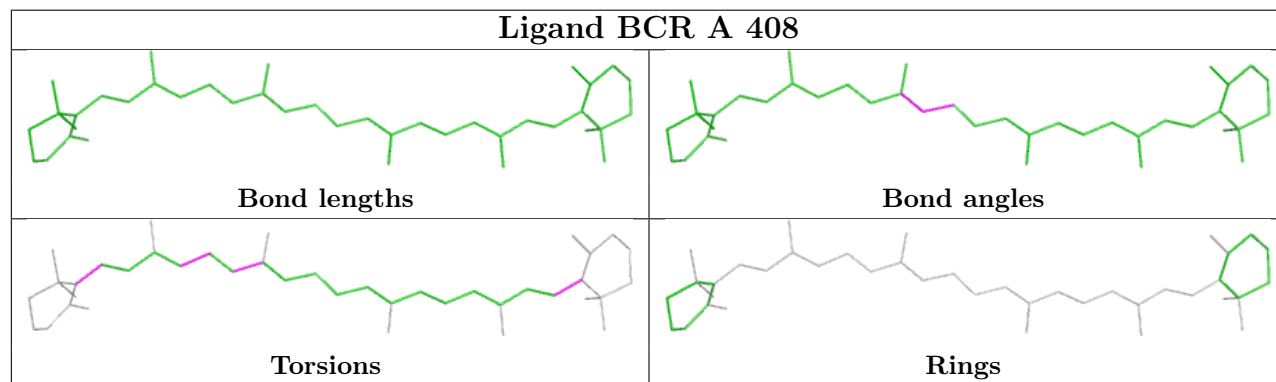


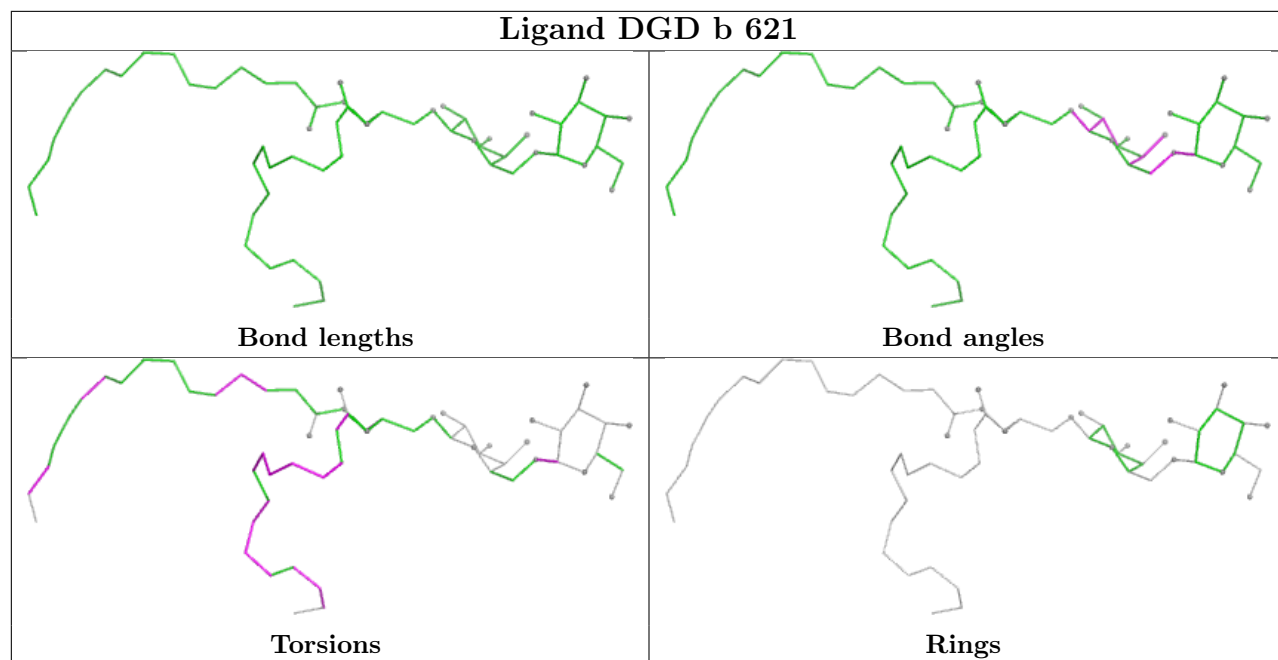


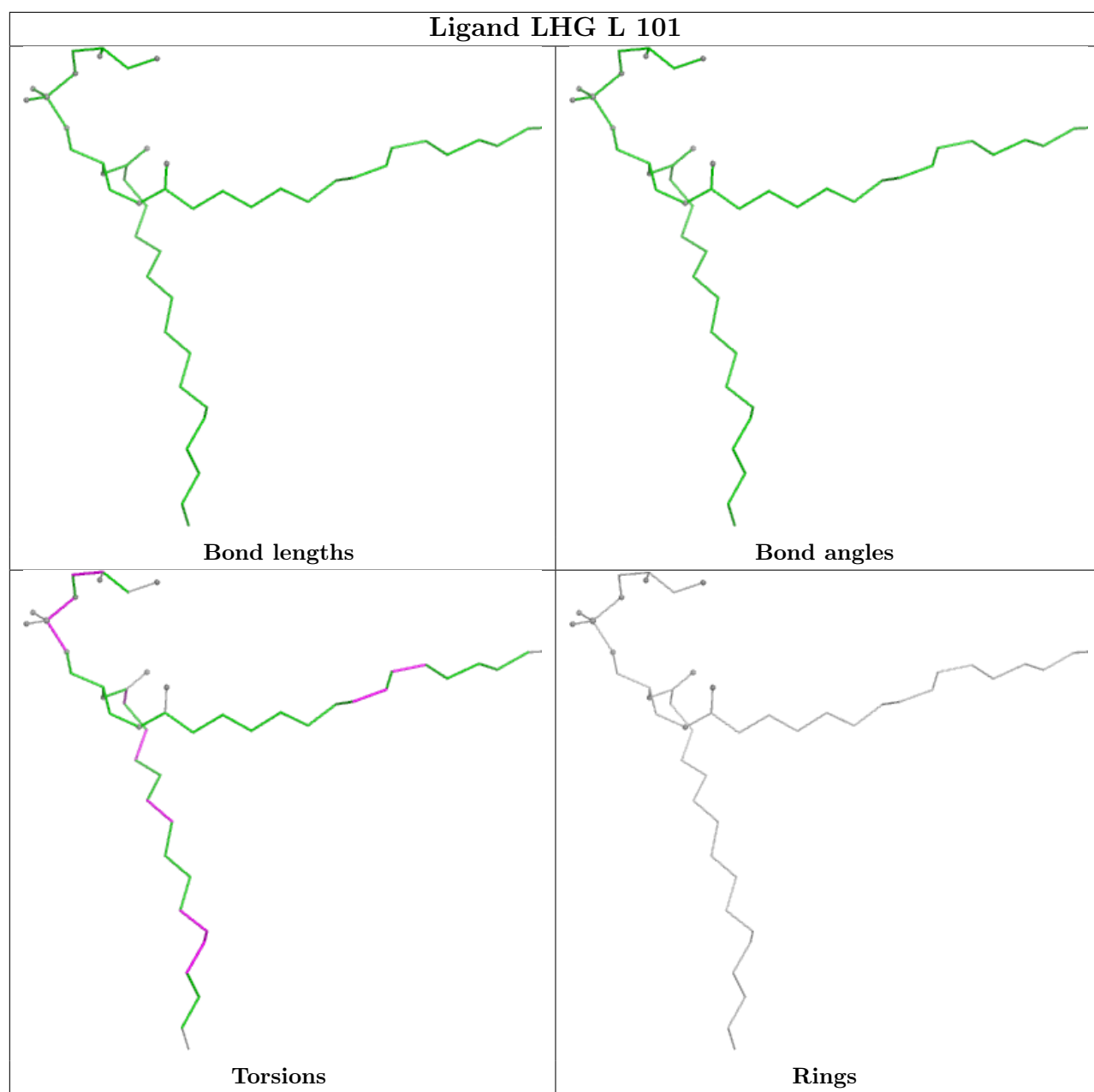
Ligand CLA A 406

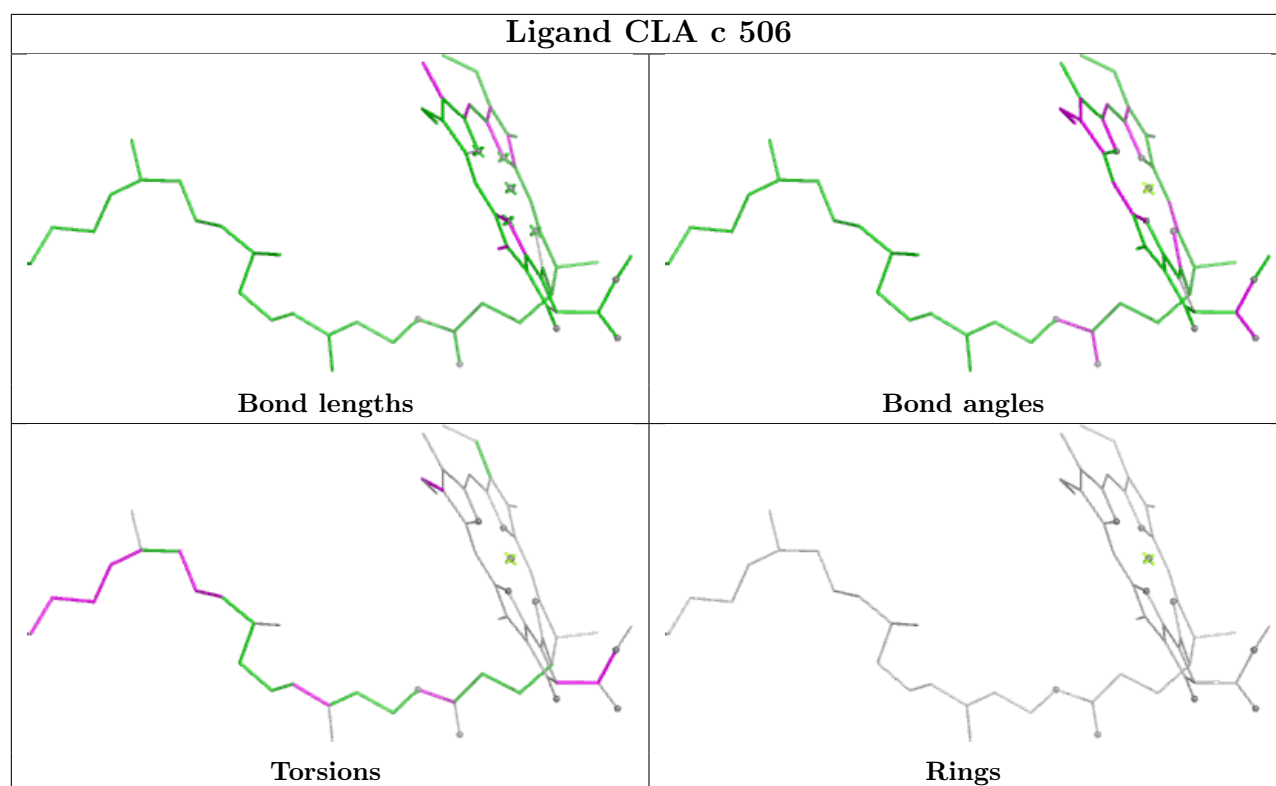


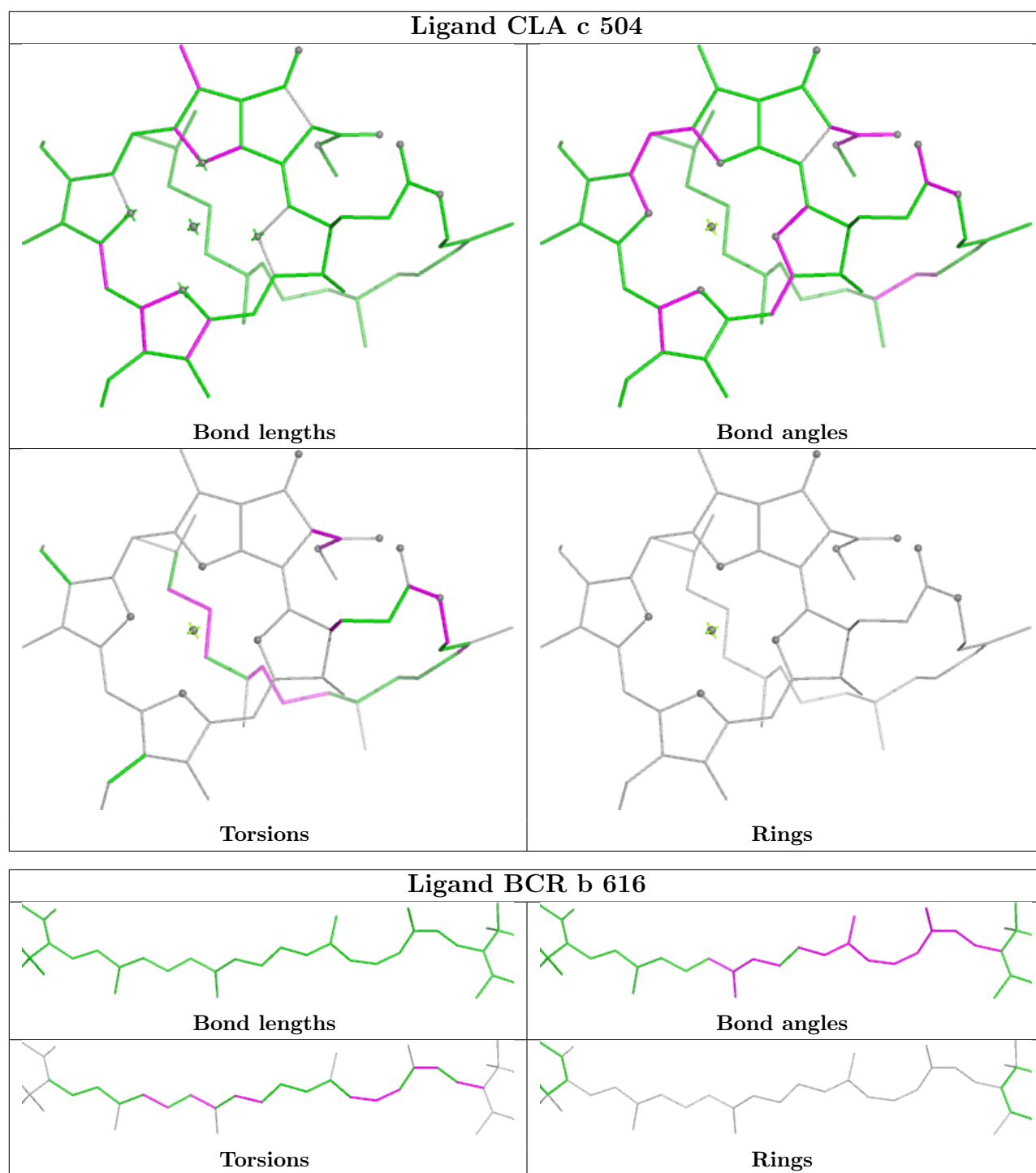
Ligand BCR A 408

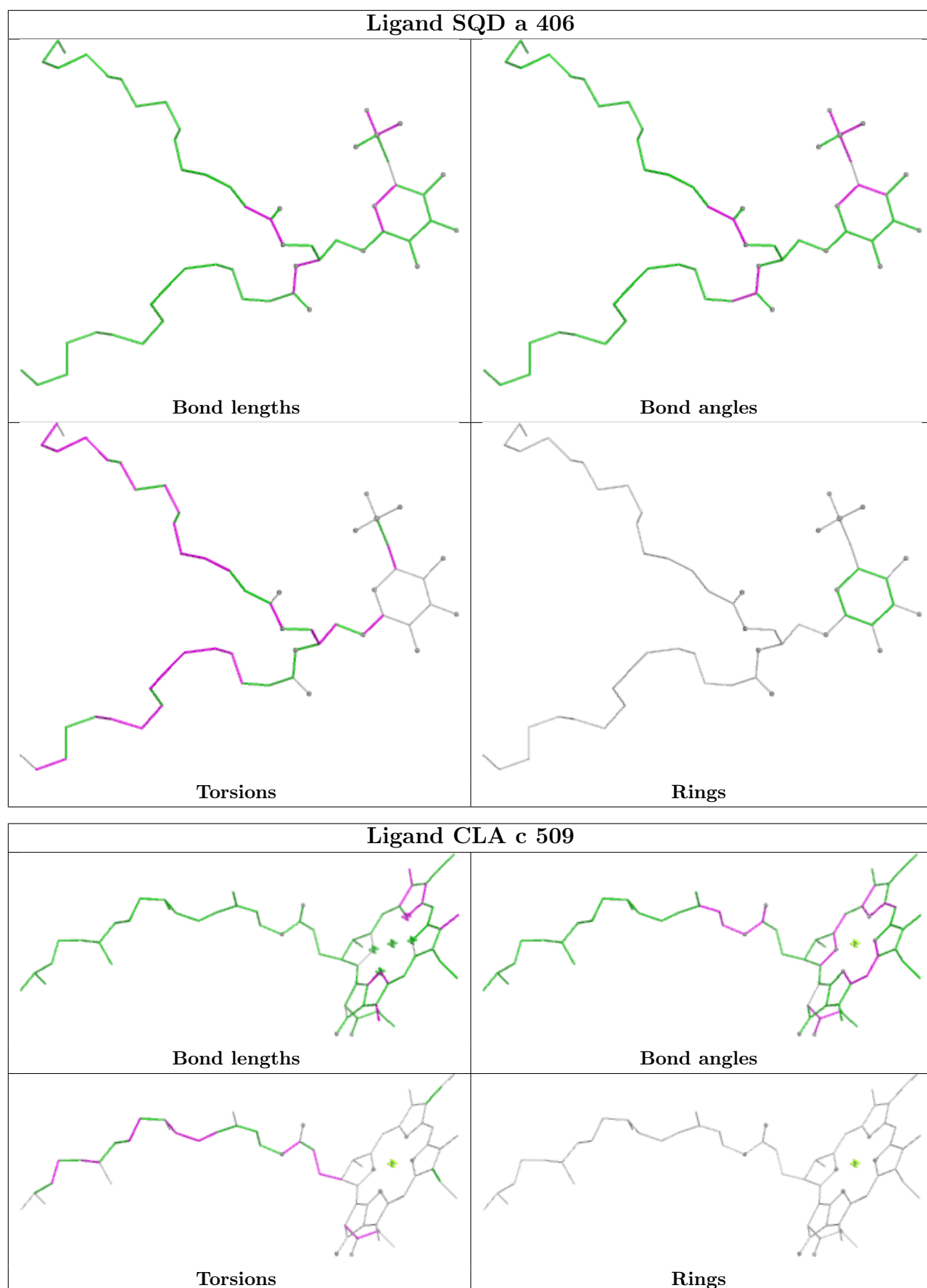


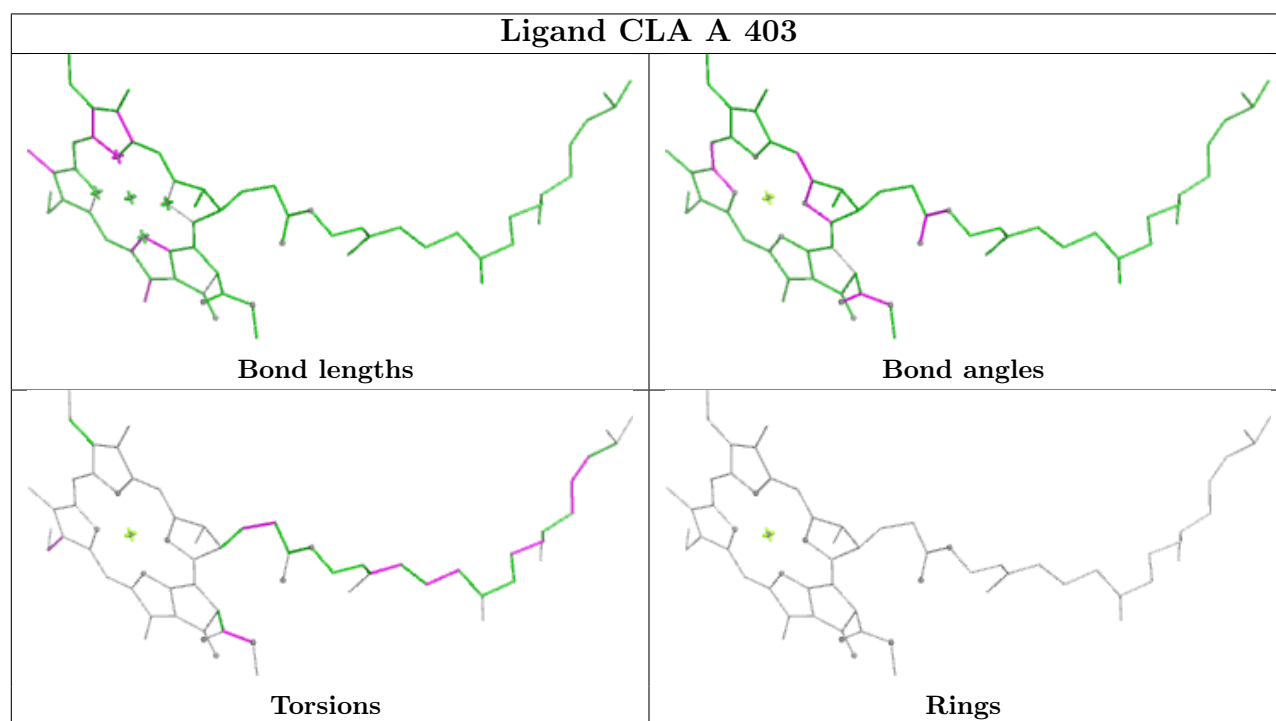
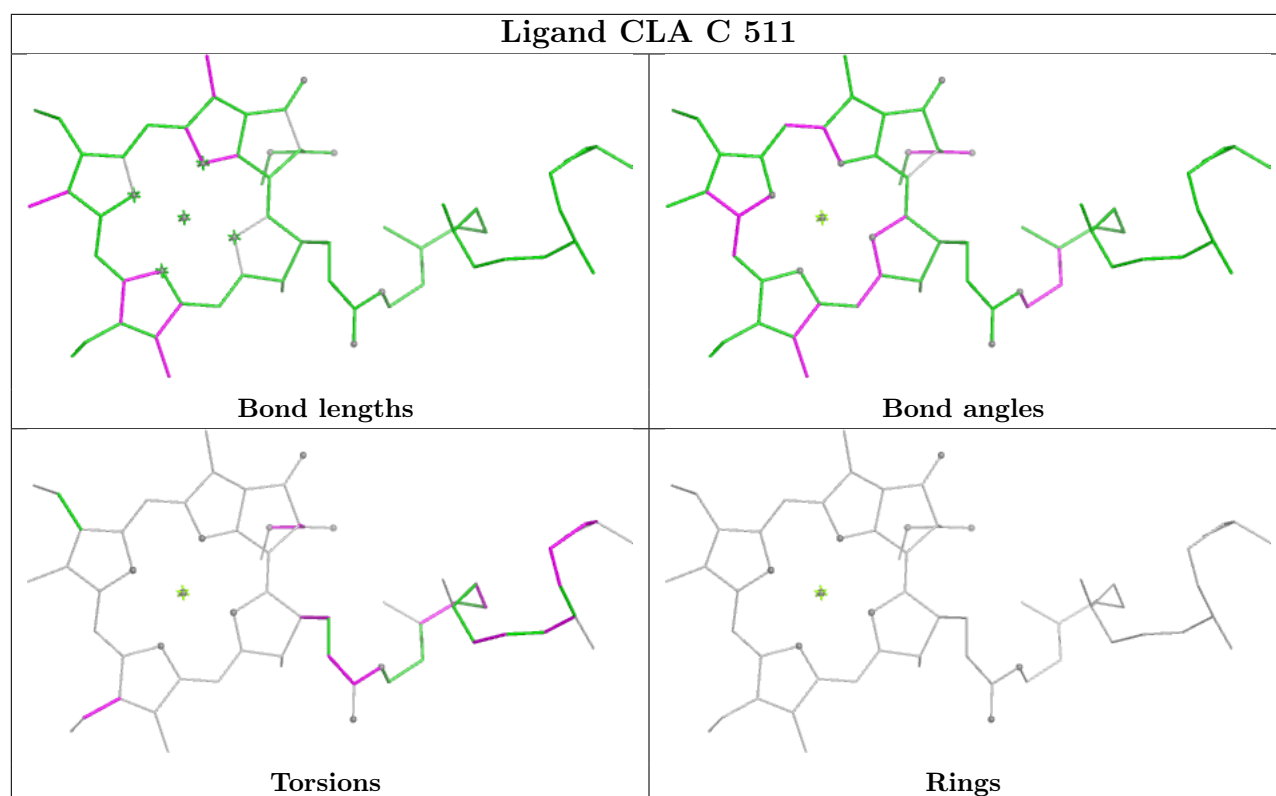


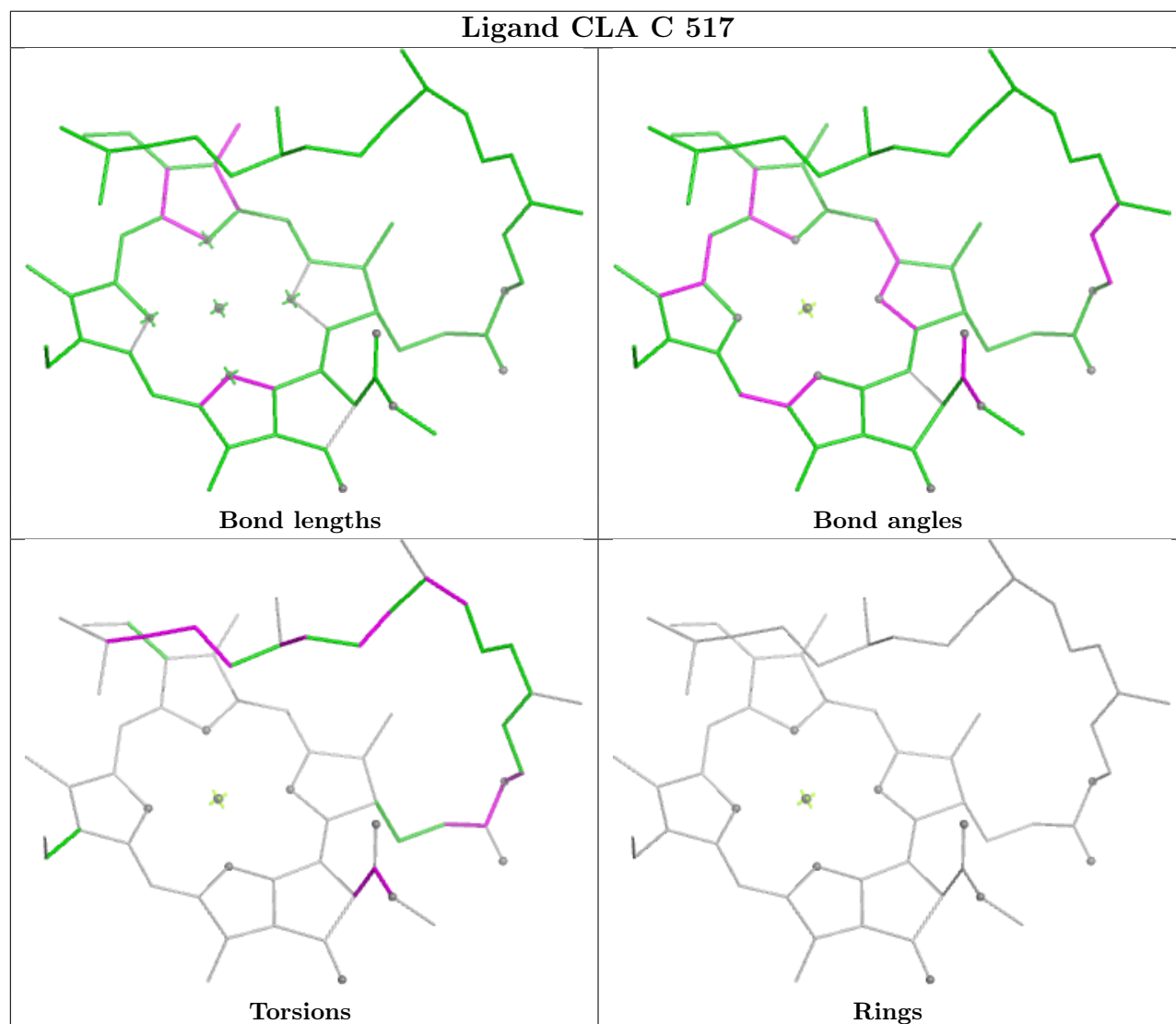
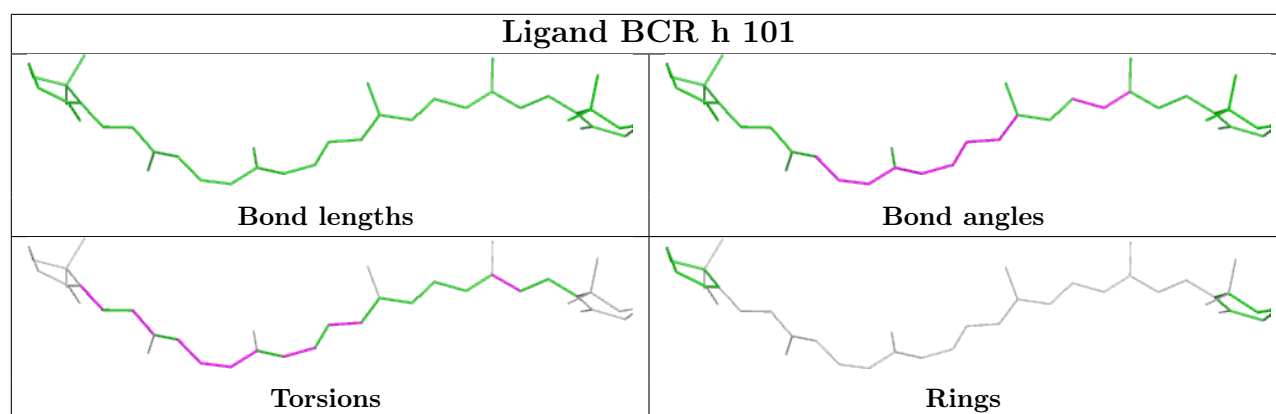


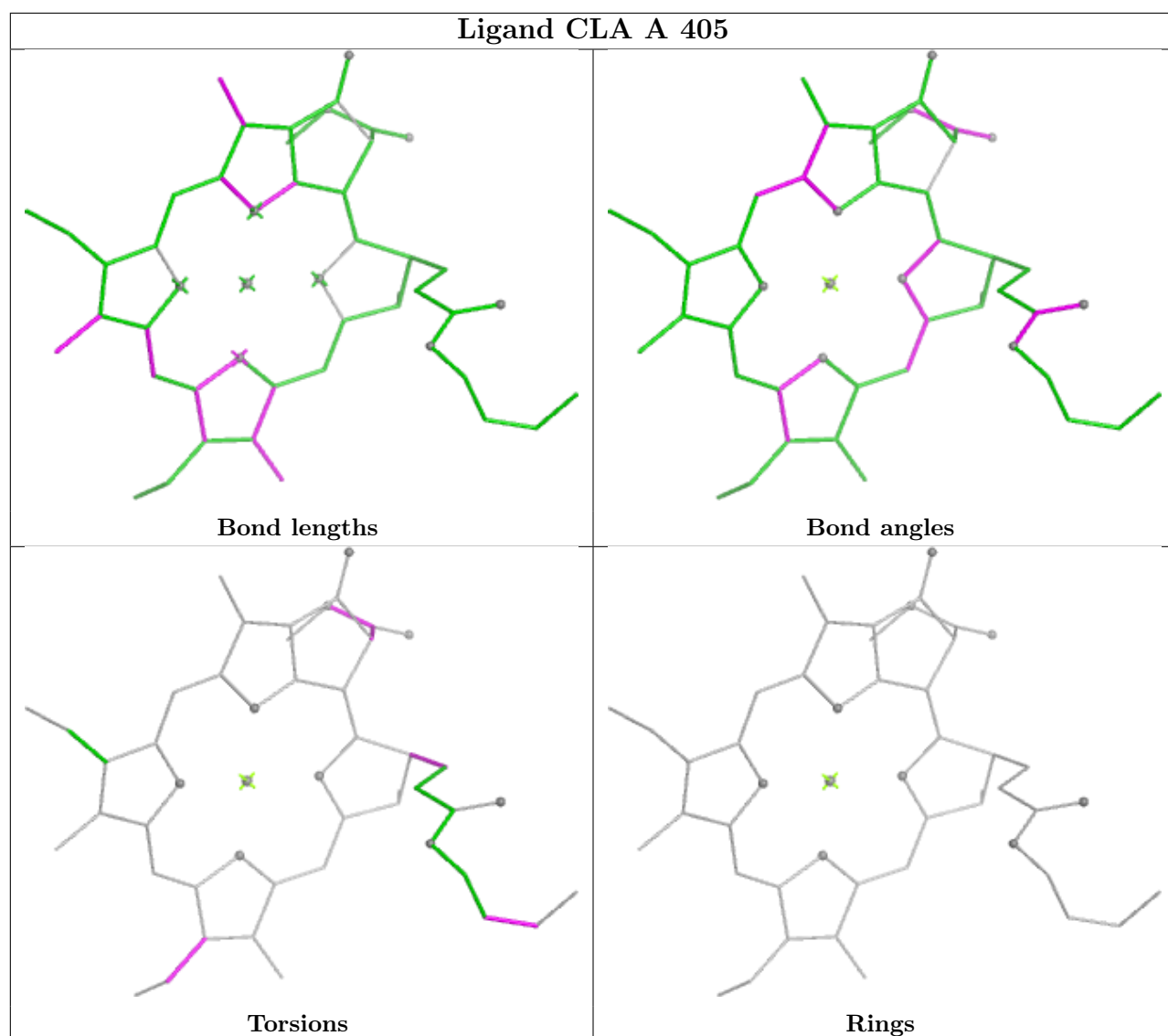


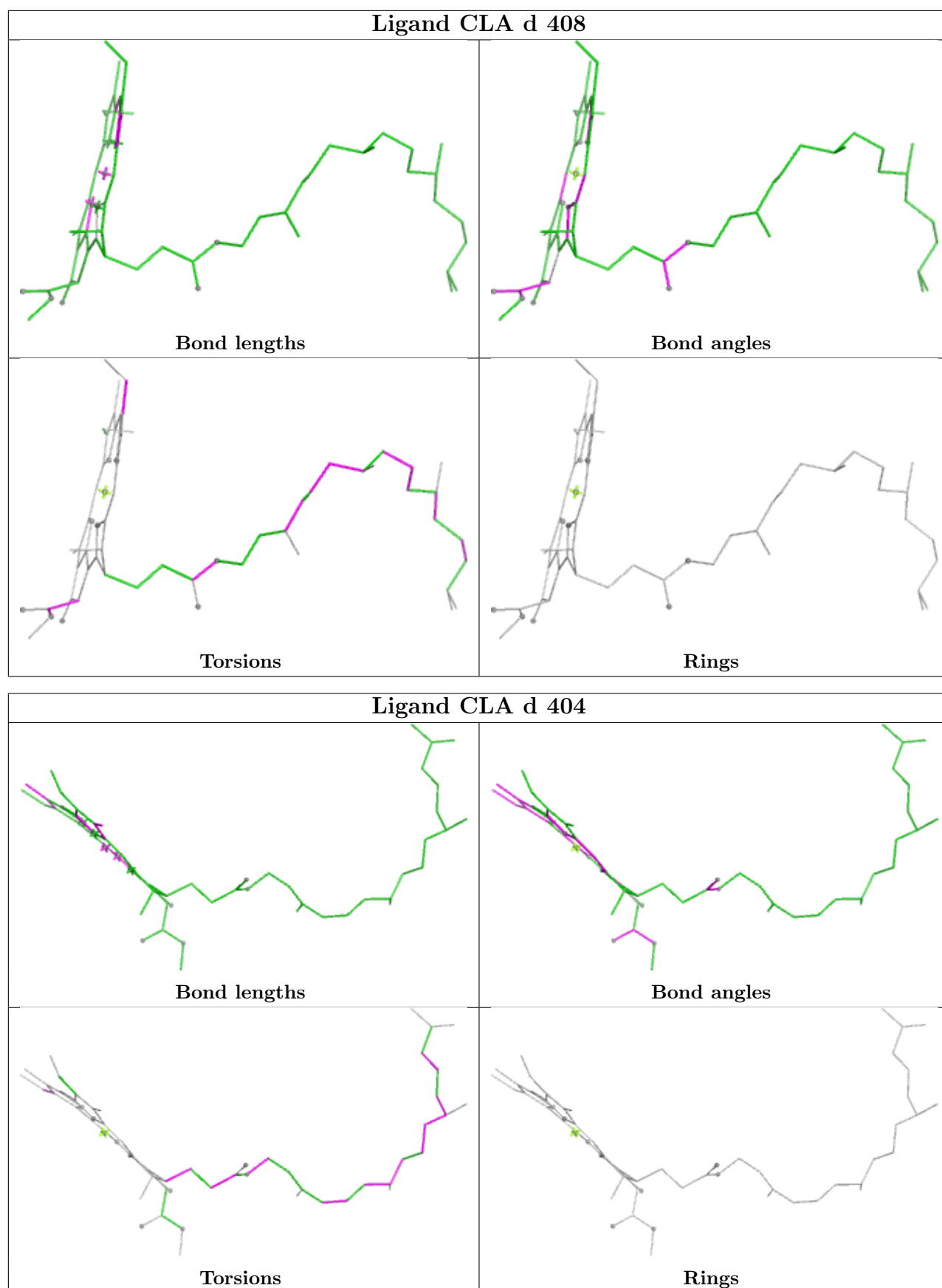












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

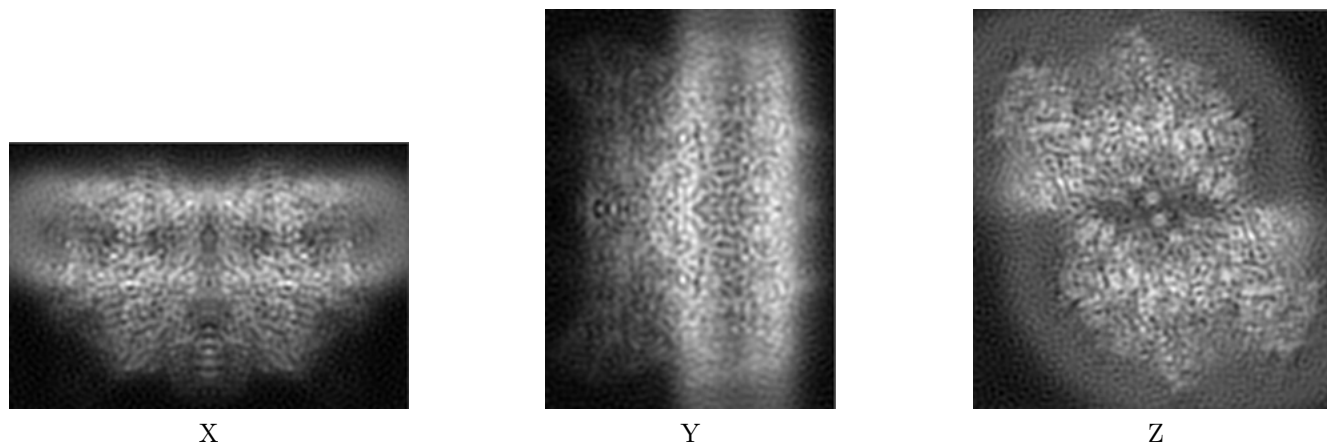
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-58358. These allow visual inspection of the internal detail of the map and identification of artifacts.

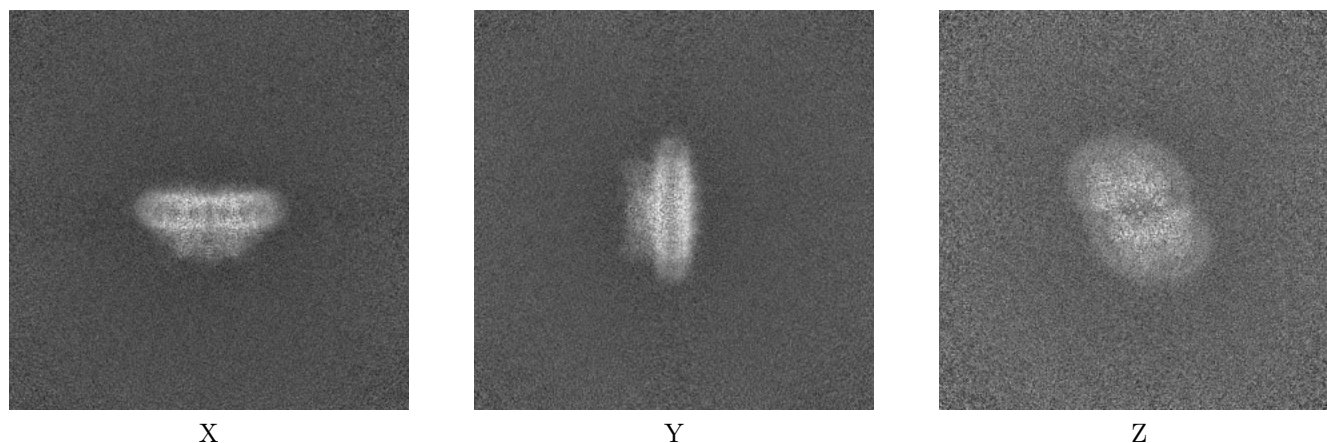
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



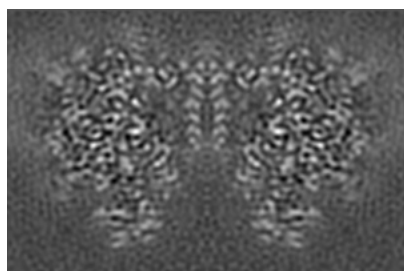
6.1.2 Raw map



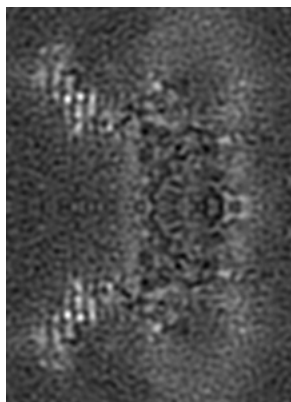
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

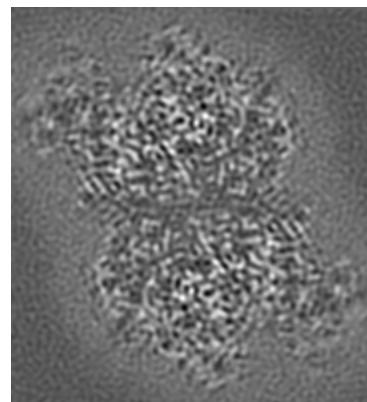
6.2.1 Primary map



X Index: 107

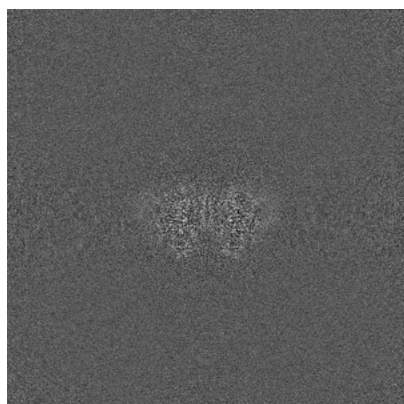


Y Index: 117

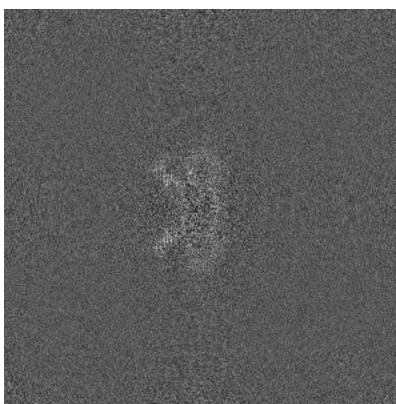


Z Index: 78

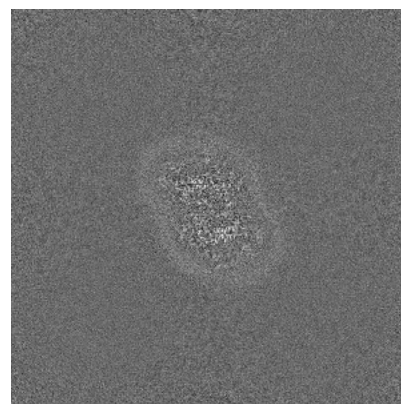
6.2.2 Raw map



X Index: 360



Y Index: 360

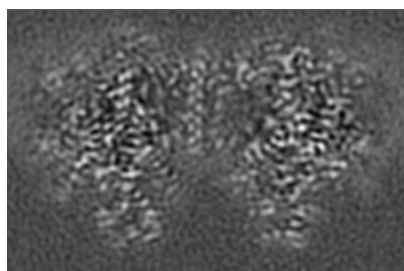


Z Index: 360

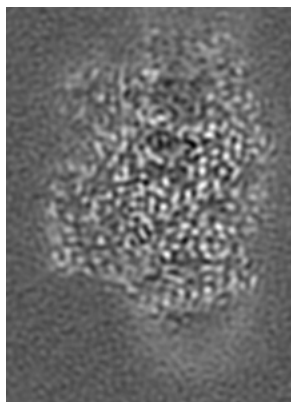
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

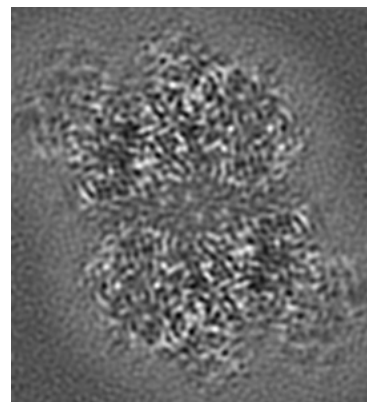
6.3.1 Primary map



X Index: 109

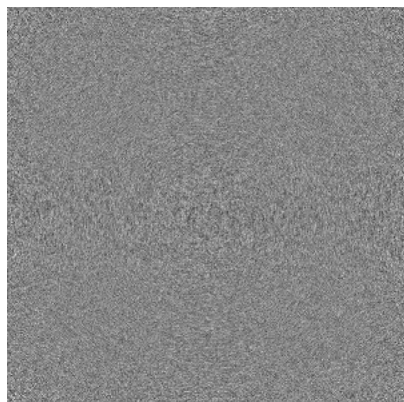


Y Index: 76

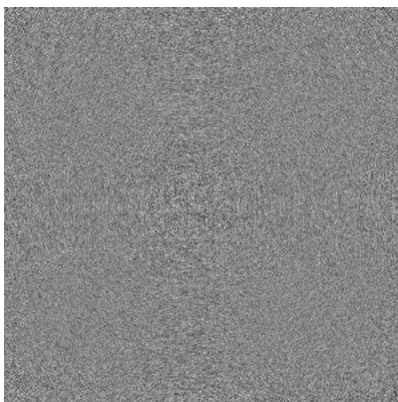


Z Index: 81

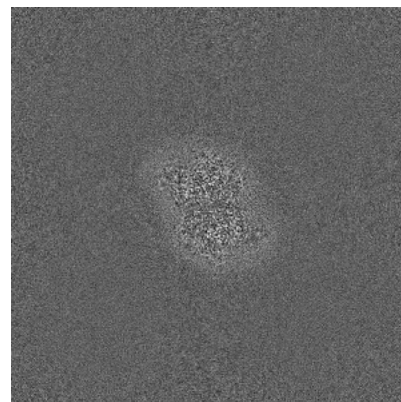
6.3.2 Raw map



X Index: 0



Y Index: 0

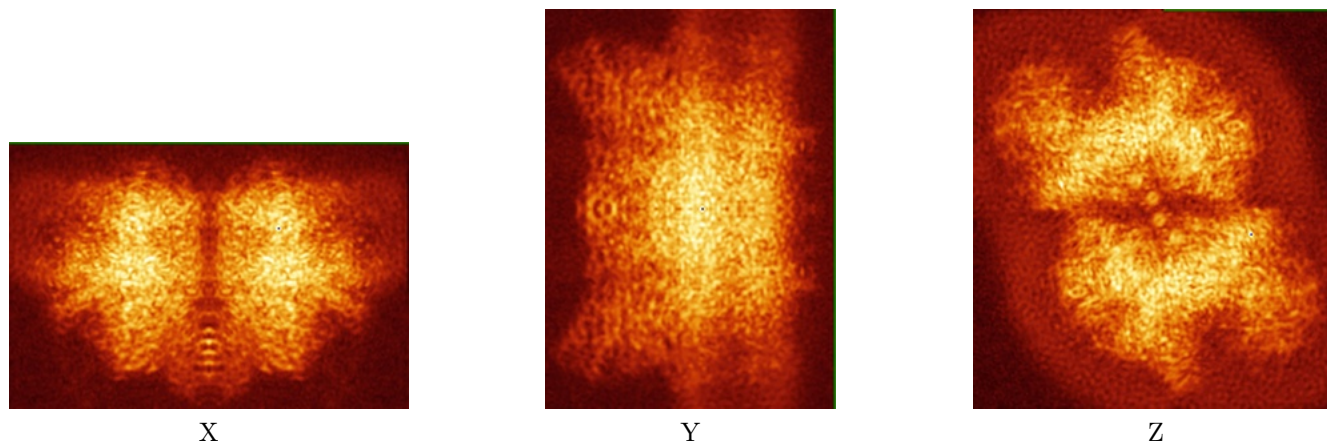


Z Index: 333

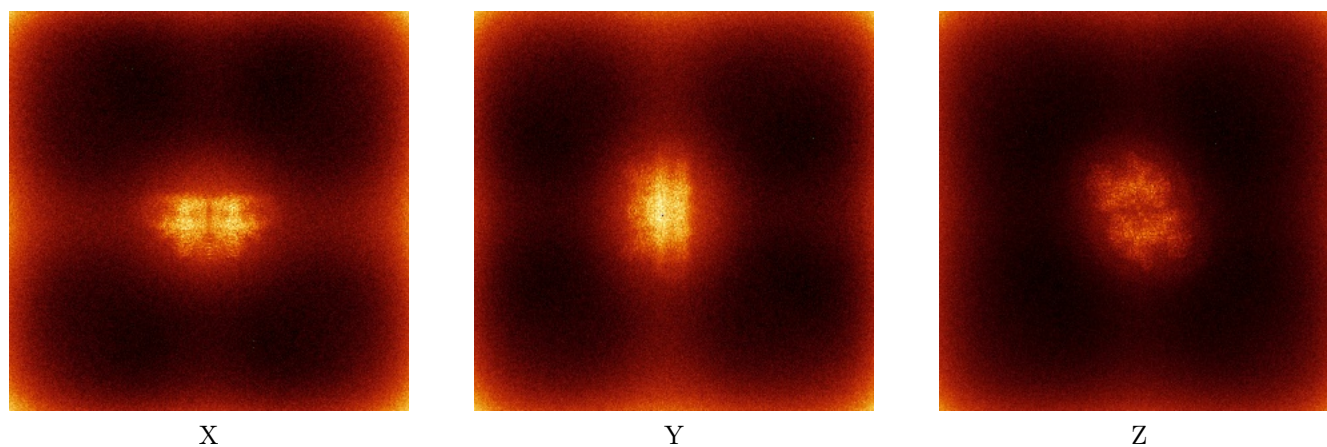
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



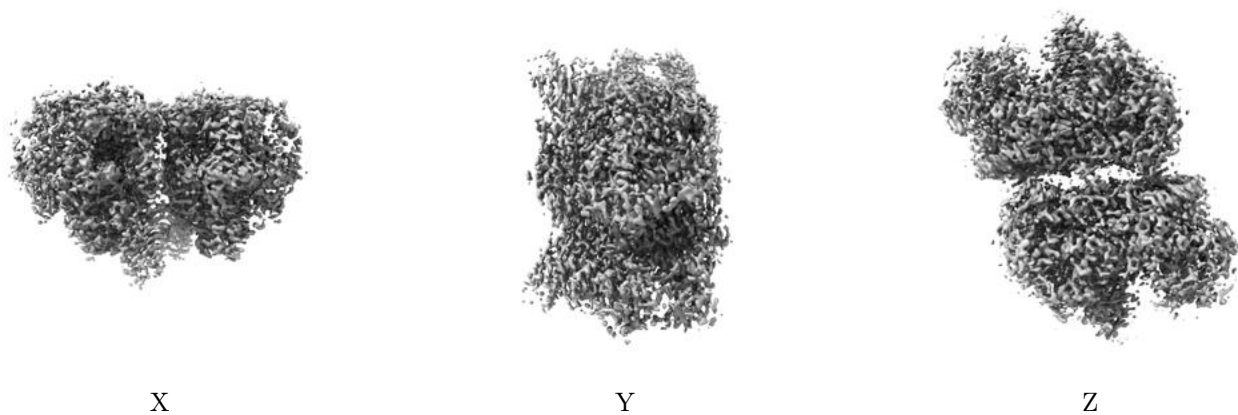
6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

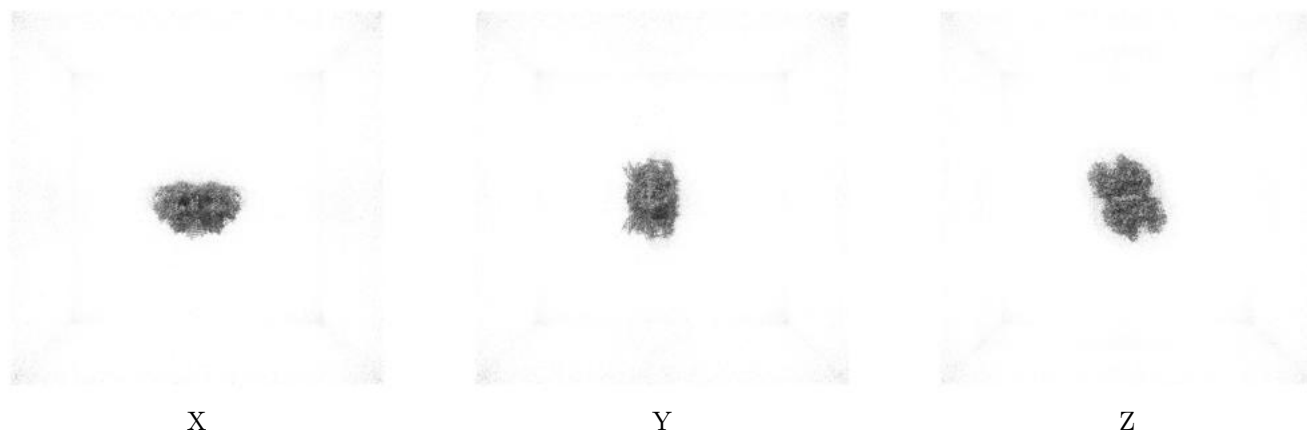
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.216. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

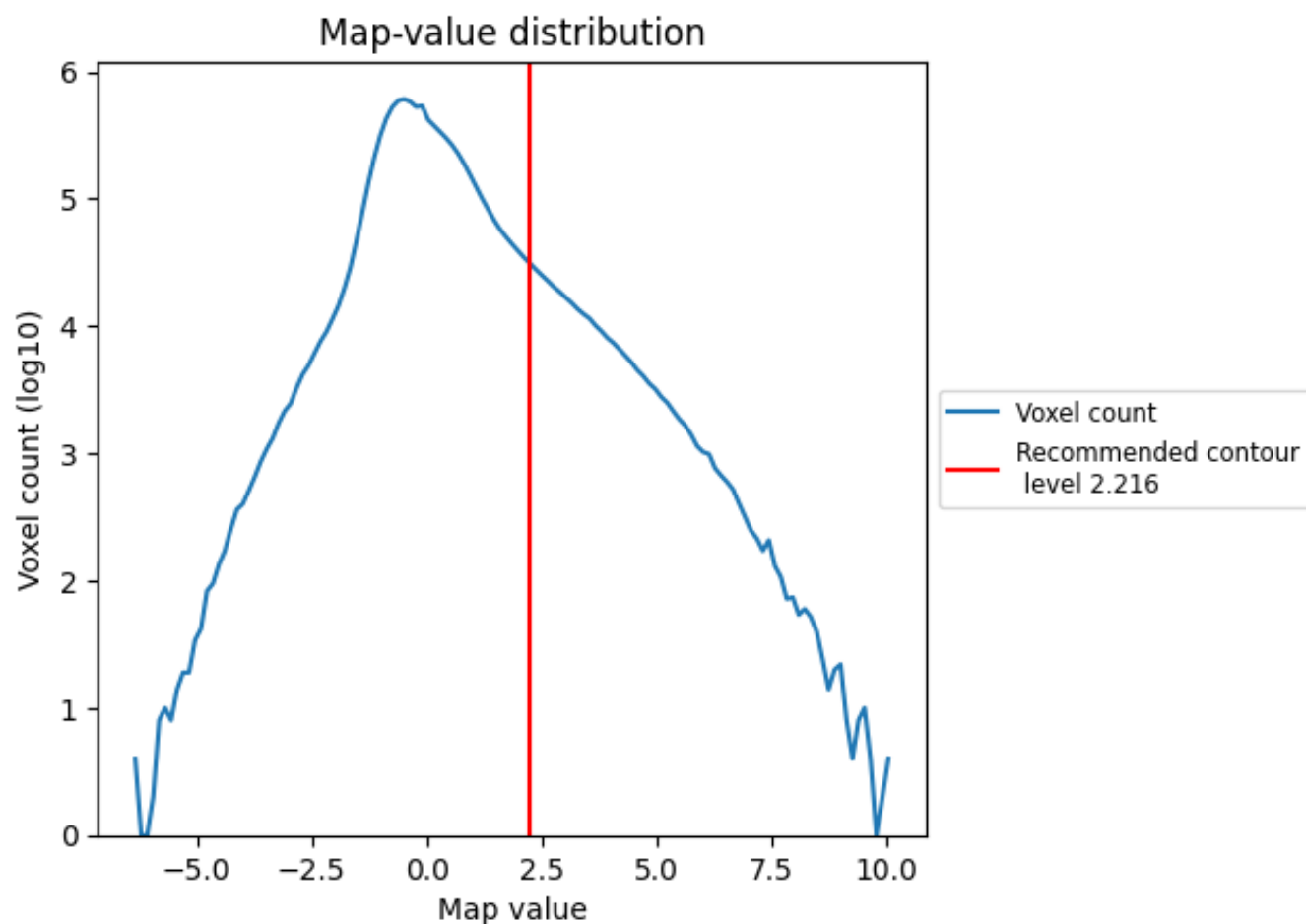
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

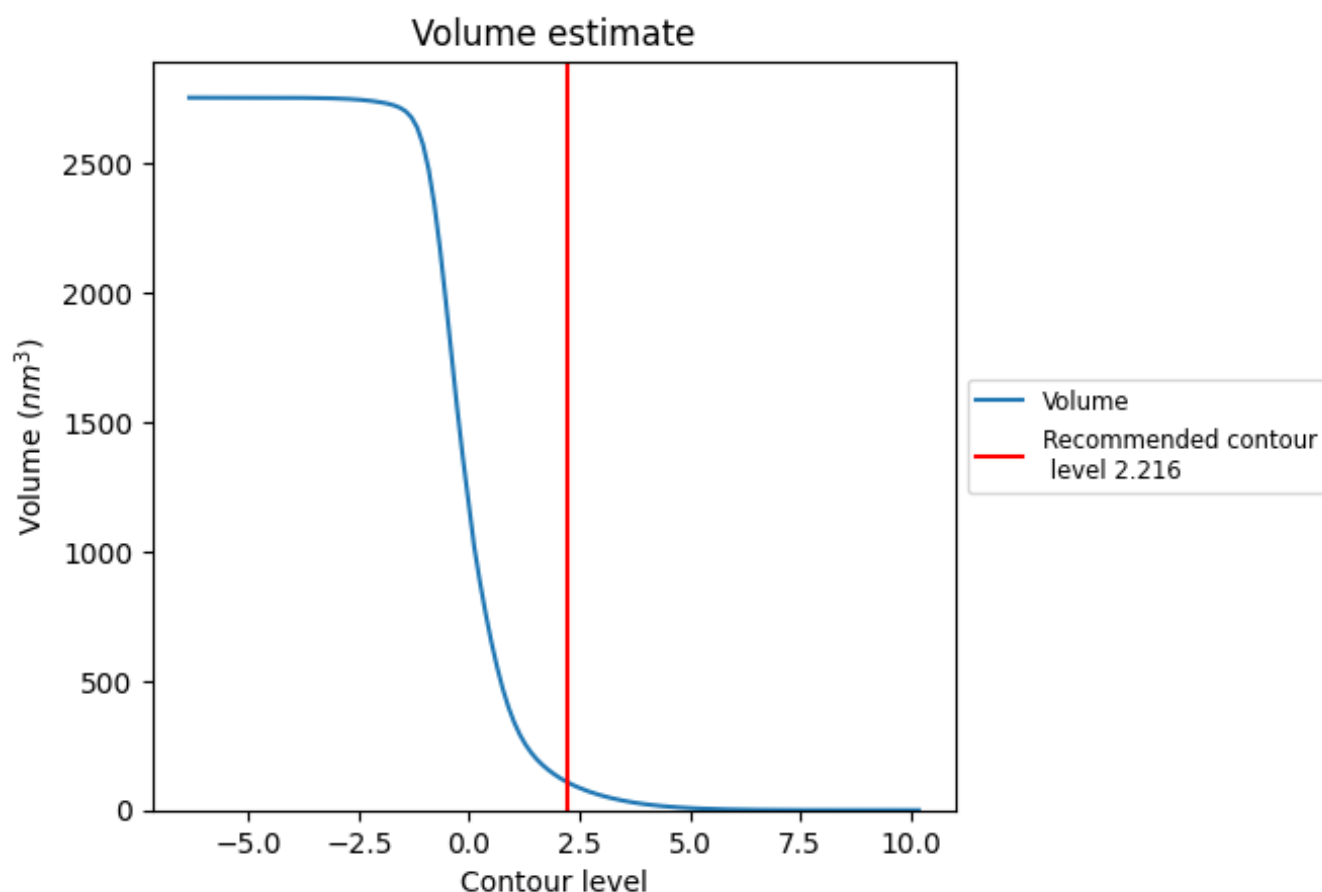
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm^3 ; this corresponds to an approximate mass of 98 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.

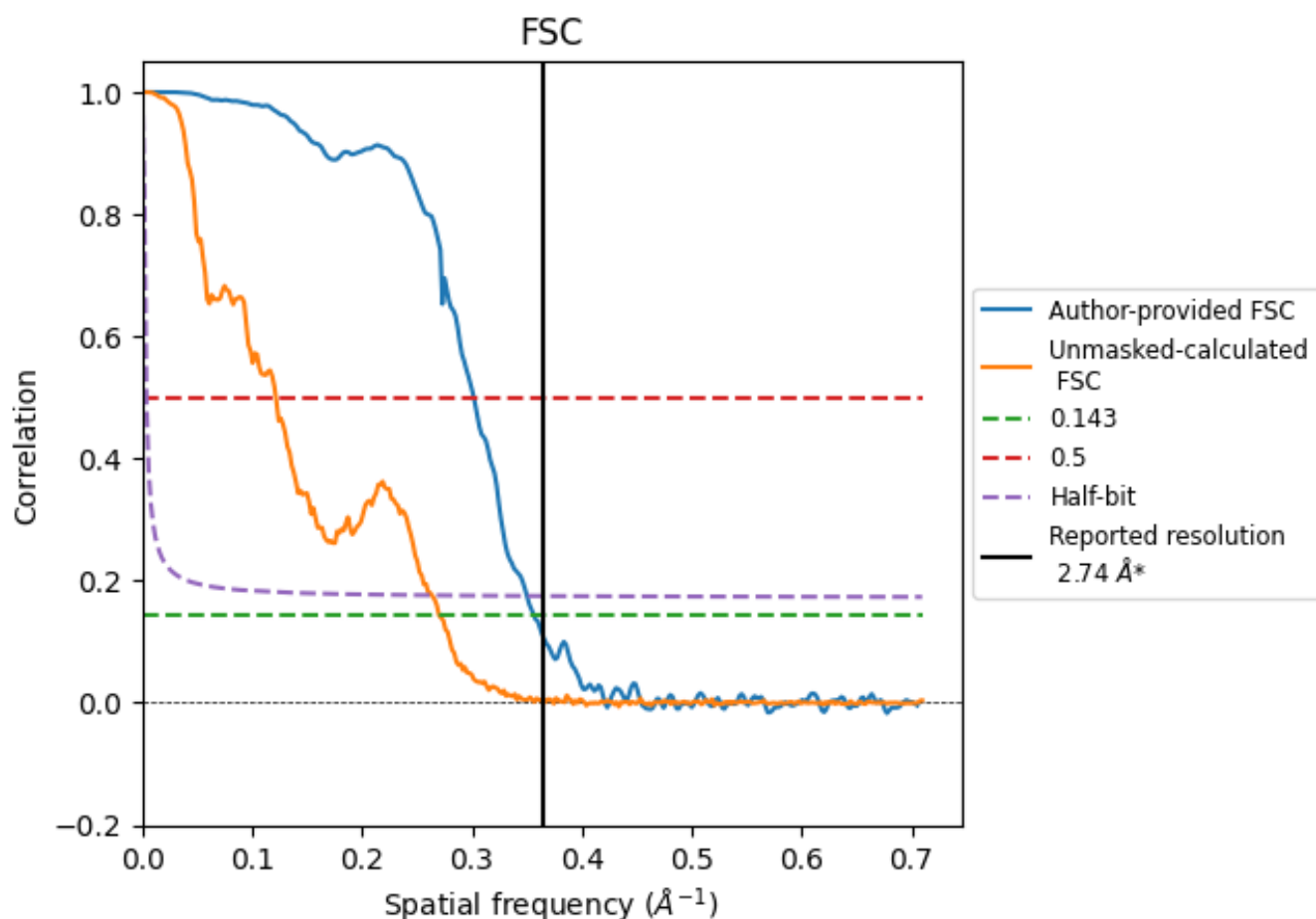
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.365 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.81	3.31	2.86
Unmasked-calculated*	3.70	8.22	3.79

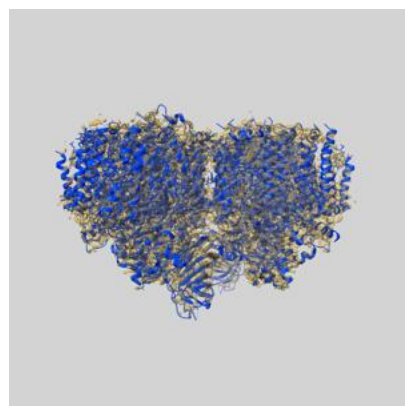
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 2.74 by more than 10 %

9 Map-model fit [i](#)

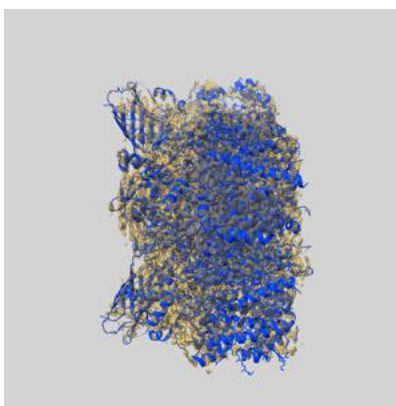
This section contains information regarding the fit between EMDB map EMD-58358 and PDB model 31FD. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlays

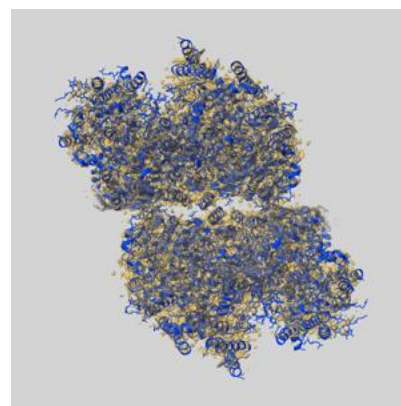
9.1.1 Map-model overlay [i](#)



X

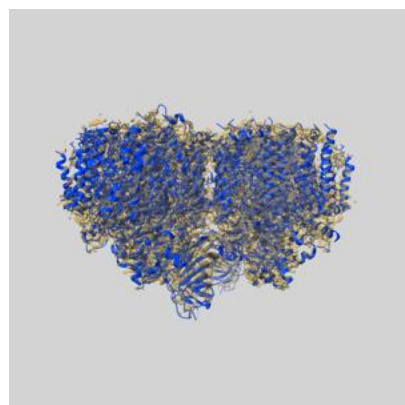


Y

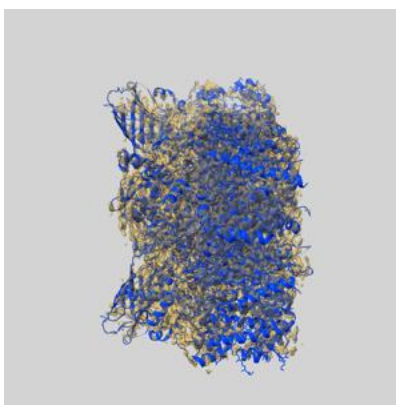


Z

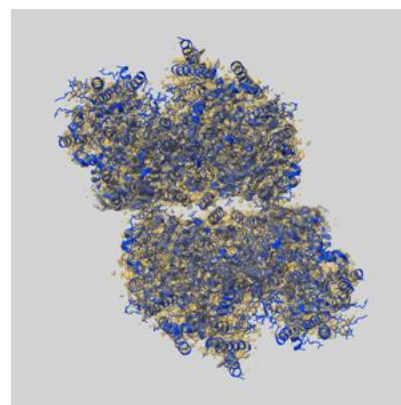
9.1.2 Map-model assembly overlay [i](#)



X



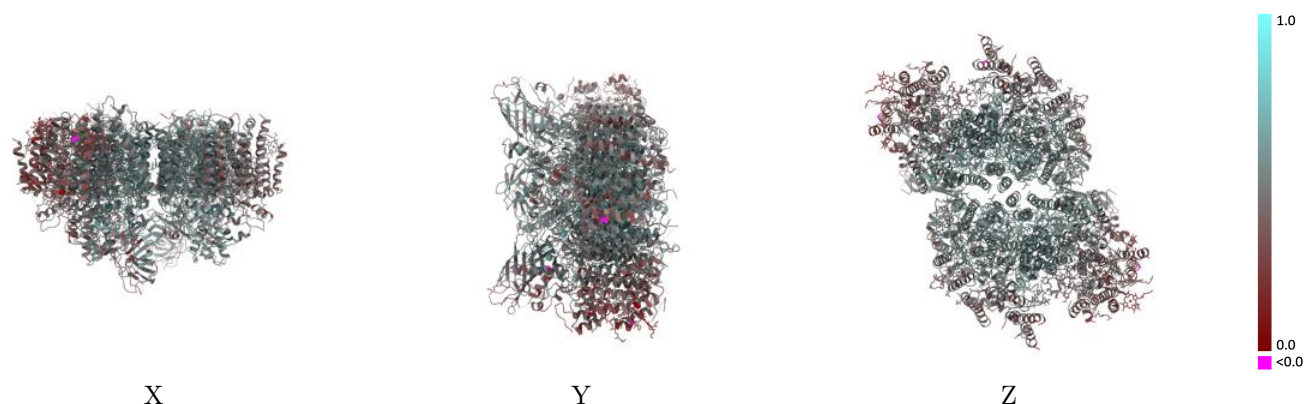
Y



Z

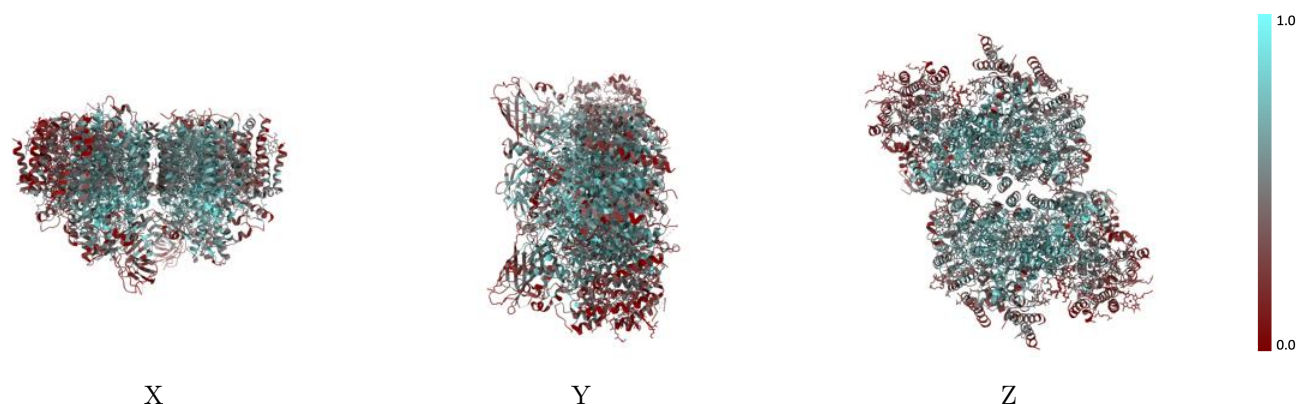
The images above show the 3D surface view of the map at the recommended contour level 2.216 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



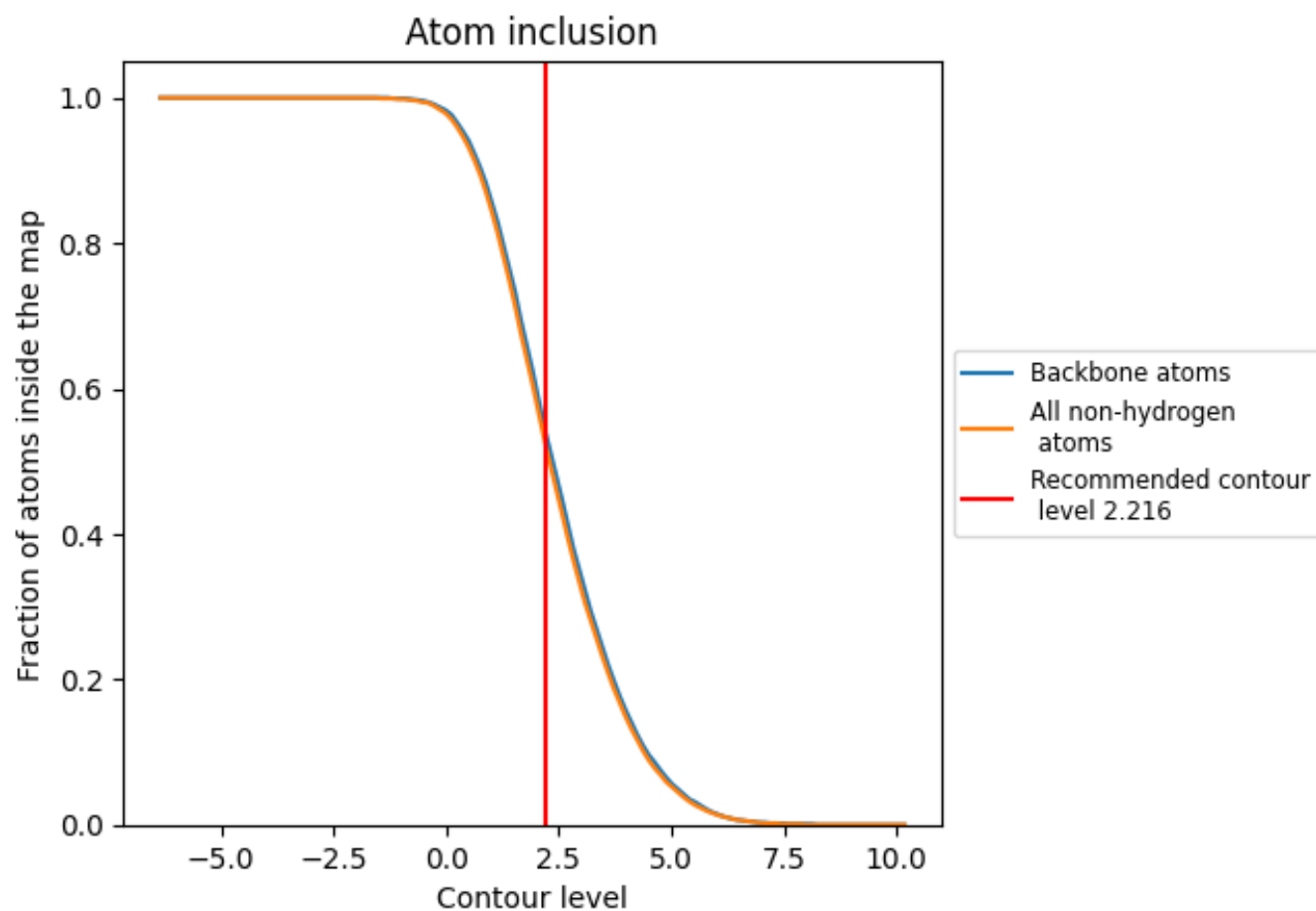
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.216).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% 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 (2.216) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5200	 0.4890
A	 0.6720	 0.5470
B	 0.6150	 0.5300
C	 0.3660	 0.3980
D	 0.6820	 0.5360
E	 0.3350	 0.4060
F	 0.3750	 0.3730
H	 0.3970	 0.4580
I	 0.4530	 0.4810
K	 0.1070	 0.3610
L	 0.5880	 0.5810
M	 0.4940	 0.5510
O	 0.3300	 0.4610
T	 0.5380	 0.5670
U	 0.3880	 0.4660
X	 0.2400	 0.3900
a	 0.6720	 0.5460
b	 0.6140	 0.5280
c	 0.3620	 0.3950
d	 0.6760	 0.5300
e	 0.3410	 0.4020
f	 0.3630	 0.3720
h	 0.3830	 0.4530
i	 0.4490	 0.4930
k	 0.1070	 0.3600
l	 0.5790	 0.5750
m	 0.4850	 0.5580
o	 0.3320	 0.4670
t	 0.5380	 0.5670
u	 0.3990	 0.4650
x	 0.2280	 0.3800

