



wwPDB EM Validation Summary Report ⓘ

Aug 27, 2026 – 08:48 am BST

PDB ID : 9GNW / pdb_00009gnw
EMDB ID : EMD-51482
Title : Universal PSII assembly intermediate
Authors : Fadeeva, M.; Klaiman, D.; Nelson, N.
Deposited on : 2024-09-04
Resolution : 2.93 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 Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

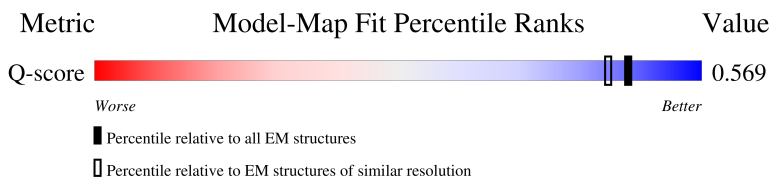
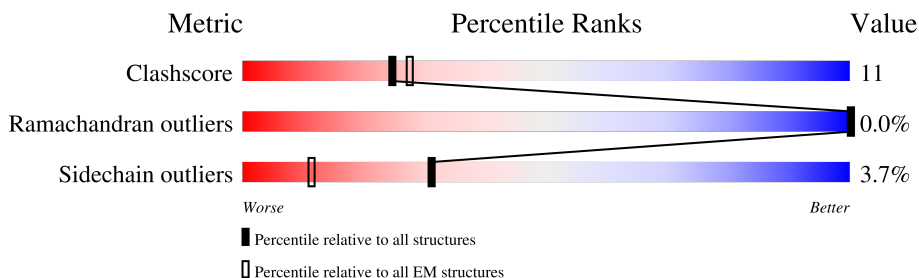
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.93 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.



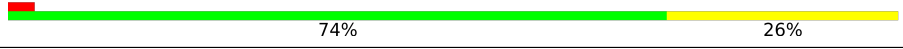
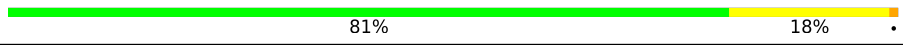
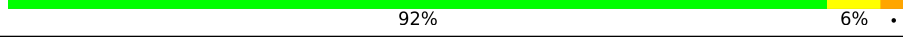
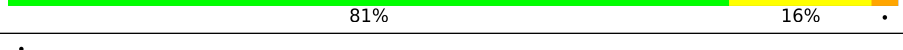
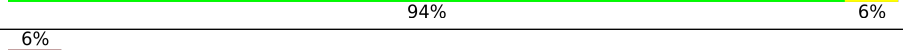
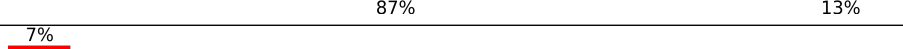
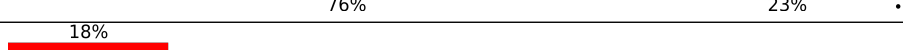
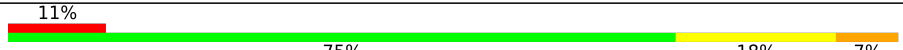
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13037 (2.43 - 3.43)

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	336	9% 74% 26%
2	B	484	79% 20%
3	V	33	82% 18%
4	C	449	79% 20%

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Mol	Chain	Length	Quality of chain
5	D	348	
6	E	76	
7	F	31	
8	H	67	
9	I	33	
10	J	36	
11	K	37	
12	L	36	
13	M	31	
14	O	238	
15	P	187	
16	T	30	
17	W	45	
18	X	33	
19	Z	61	
20	U	28	

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 24204 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	336	Total	C	N	O	S	0	0
			2635	1719	432	468	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		

- Molecule 3 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	33	Total	C	N	O	S	0	0
			235	157	38	39	1		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	76	Total	C	N	O	0	0
			621	404	102	115		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	33	Total	C	N	O	S	0	0
			265	182	39	43	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			265	181	40	44		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	42	LEU	GLN	conflict	UNP A0A1C8XRM8

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	207	43	47		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	36	Total	C	N	O	0	0
			300	201	49	50		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			235	161	33	41		

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1819	1148	295	370	6		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	101	ASP	ASN	conflict	UNP A0A7S3QTM3
O	103	LYS	ARG	conflict	UNP A0A7S3QTM3
O	150	ASN	GLY	conflict	UNP A0A7S3QTM3
O	151	ASN	GLY	conflict	UNP A0A7S3QTM3
O	156	GLU	GLN	conflict	UNP A0A7S3QTM3
O	160	ASP	GLU	conflict	UNP A0A7S3QTM3
O	219	ALA	SER	conflict	UNP A0A7S3QTM3
O	220	THR	SER	conflict	UNP A0A7S3QTM3
O	226	ILE	VAL	conflict	UNP A0A7S3QTM3
O	240	LEU	VAL	conflict	UNP A0A7S3QTM3
O	244	SER	THR	conflict	UNP A0A7S3QTM3
O	248	GLY	SER	conflict	UNP A0A7S3QTM3
O	261	THR	ALA	conflict	UNP A0A7S3QTM3
O	272	SER	THR	conflict	UNP A0A7S3QTM3
O	285	ALA	SER	conflict	UNP A0A7S3QTM3

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1453	923	243	286	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	96	GLN	GLU	conflict	UNP A0A9J4RF14
P	100	GLU	ASP	conflict	UNP A0A9J4RF14
P	107	GLU	ALA	conflict	UNP A0A9J4RF14
P	116	LEU	VAL	conflict	UNP A0A9J4RF14
P	119	VAL	ILE	conflict	UNP A0A9J4RF14
P	120	GLU	ALA	conflict	UNP A0A9J4RF14

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Chain	Residue	Modelled	Actual	Comment	Reference
P	121	ASP	GLN	conflict	UNP A0A9J4RF14
P	122	LYS	ASP	conflict	UNP A0A9J4RF14
P	123	SER	THR	conflict	UNP A0A9J4RF14
P	129	GLU	GLN	conflict	UNP A0A9J4RF14
P	130	ALA	ASP	conflict	UNP A0A9J4RF14
P	133	THR	SER	conflict	UNP A0A9J4RF14
P	147	LYS	ARG	conflict	UNP A0A9J4RF14
P	164	ARG	LYS	conflict	UNP A0A9J4RF14
P	167	ASN	SER	conflict	UNP A0A9J4RF14
P	191	THR	SER	conflict	UNP A0A9J4RF14

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PSII 6.1 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	45	Total	C	N	O	S	0	0
			335	217	54	63	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	104	GLY	-	expression tag	UNP A0A9J4RF15

- Molecule 18 is a protein called Photosystem II PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	33	Total	C	N	O	0	0
			225	148	36	41		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	81	VAL	THR	conflict	UNP A0A7S3VKF3

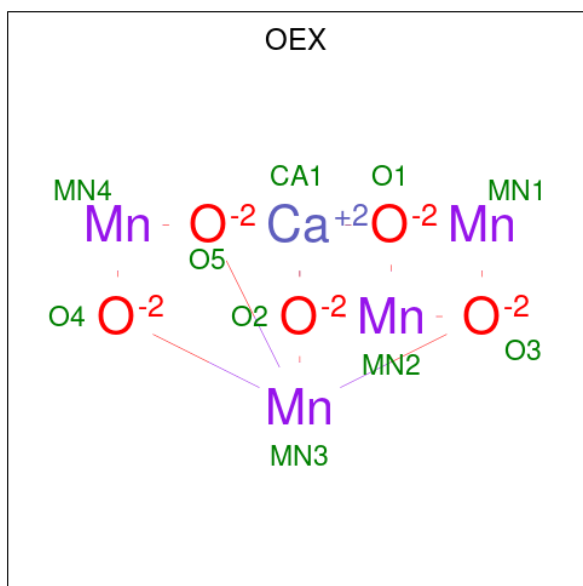
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called Photosystem II reaction center protein U, PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	28	Total	C	N	O	S	0	0
			235	141	46	47	1		

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

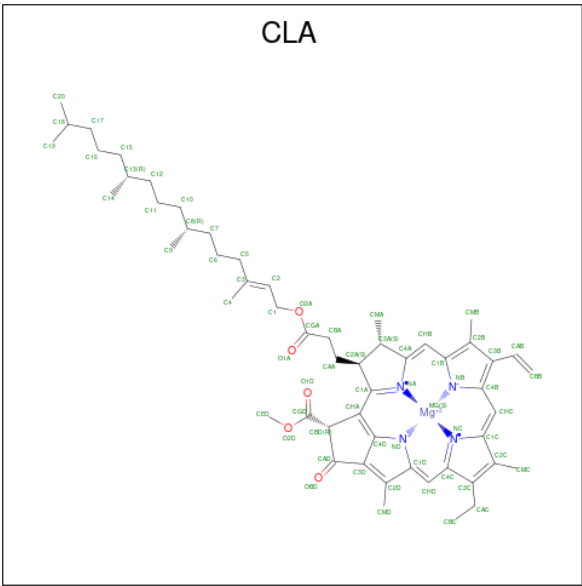
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	Fe	0
			1	1	

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Cl	0
			2	2	

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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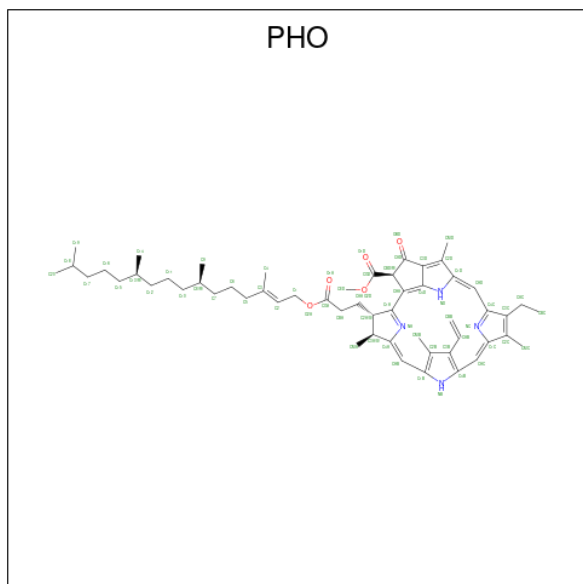
Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	C	1	Total 54	C 44	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

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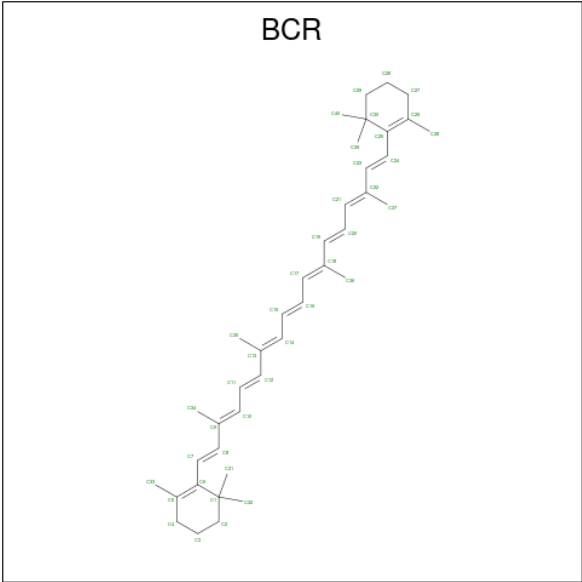
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	D	1	60	50	1	4	5	0

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



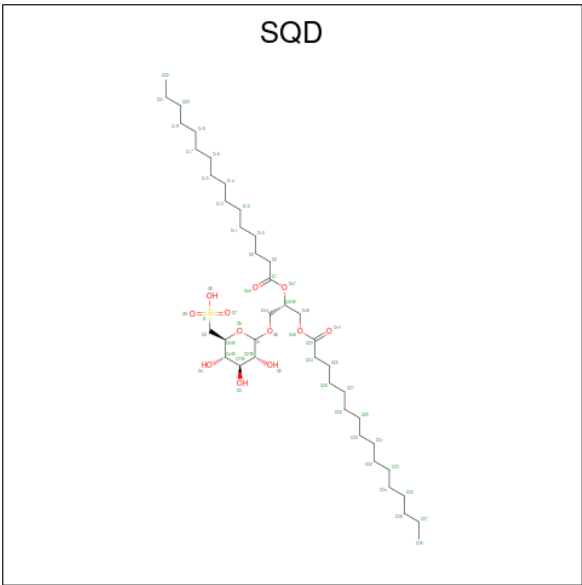
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
25	A	1	64	55	4	5	0
25	D	1	64	55	4	5	0

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



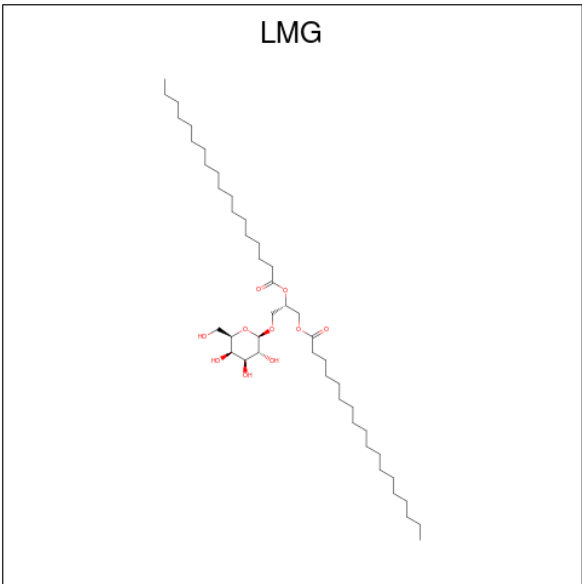
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	D	1	Total C 40 40	0
26	J	1	Total C 40 40	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	S	0
			42	29	12	1	
27	M	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			34	24	10	

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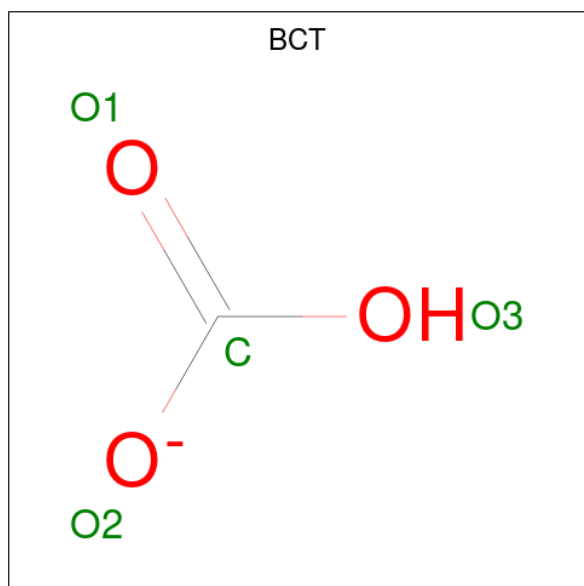
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Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			37	27	10	
28	B	1	Total	C	O	0
			44	34	10	
28	C	1	Total	C	O	0
			40	30	10	
28	C	1	Total	C	O	0
			47	37	10	
28	C	1	Total	C	O	0
			33	24	9	
28	D	1	Total	C	O	0
			42	32	10	
28	H	1	Total	C	O	0
			48	38	10	

- Molecule 29 is SODIUM ION (CCD ID: NA) (formula: Na).

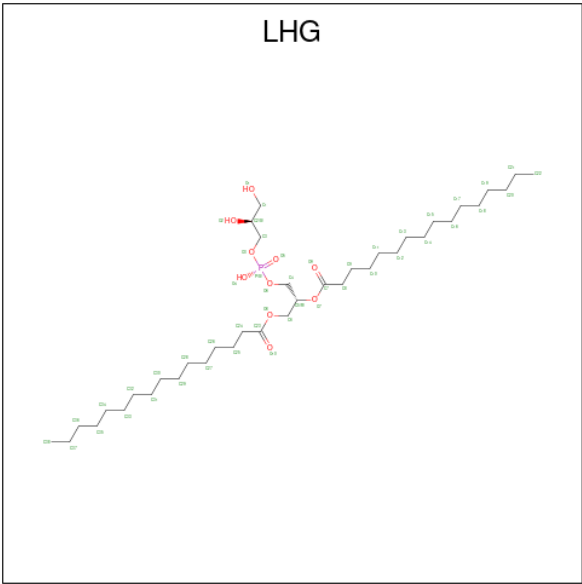
Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	Na	0
			1	1	

- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



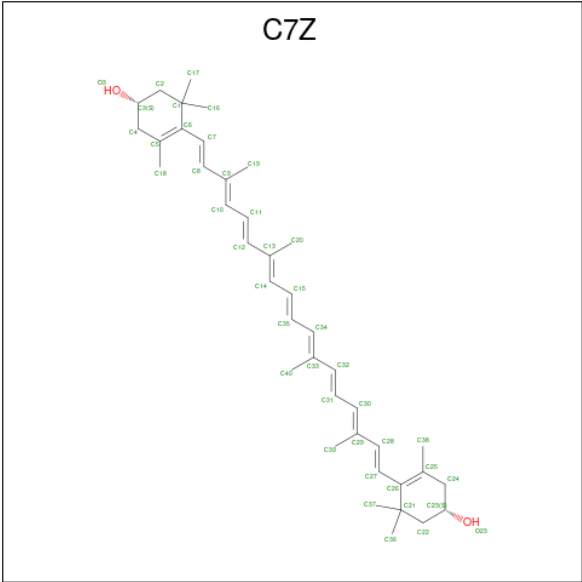
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			4	1	3	

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



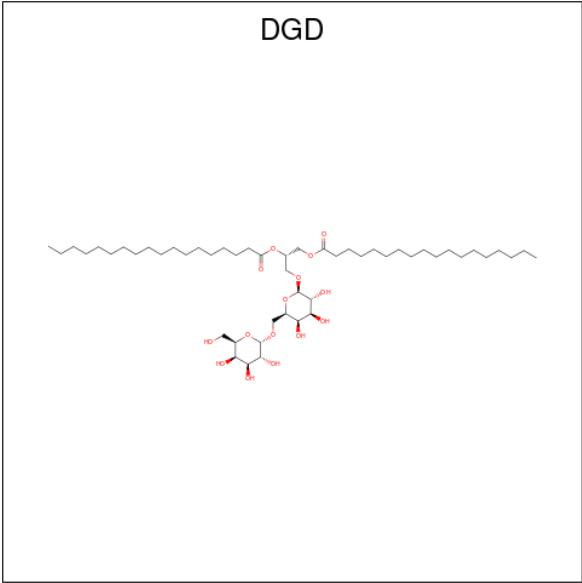
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	P	0
			39	28	10	1	
31	D	1	Total	C	O	P	0
			44	33	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	D	1	Total	C	O	P	0
			39	28	10	1	
31	L	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 32 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			42	40	2	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



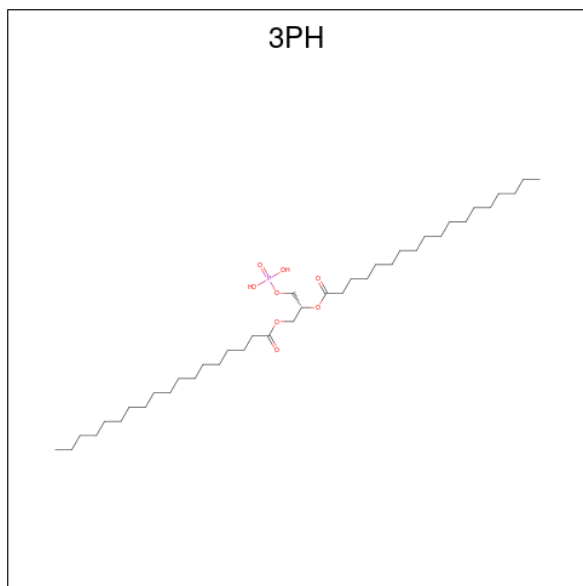
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			43	28	15	
33	C	1	Total	C	O	0
			44	29	15	

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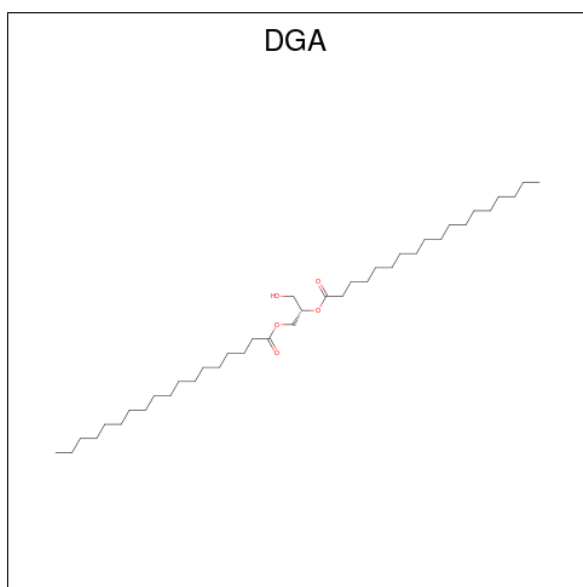
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			53	38	15	
33	C	1	Total	C	O	0
			53	38	15	

- Molecule 34 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



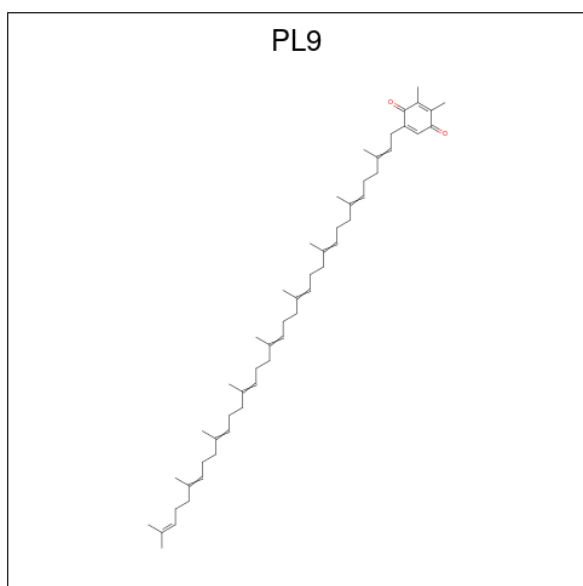
Mol	Chain	Residues	Atoms				AltConf
34	B	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 35 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			37	32	5	

- Molecule 36 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: $C_{53}H_{80}O_2$).

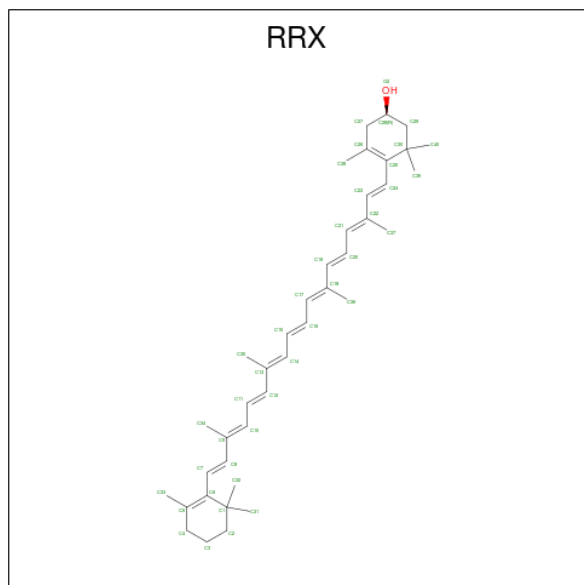


Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total	C	O	0
			55	53	2	

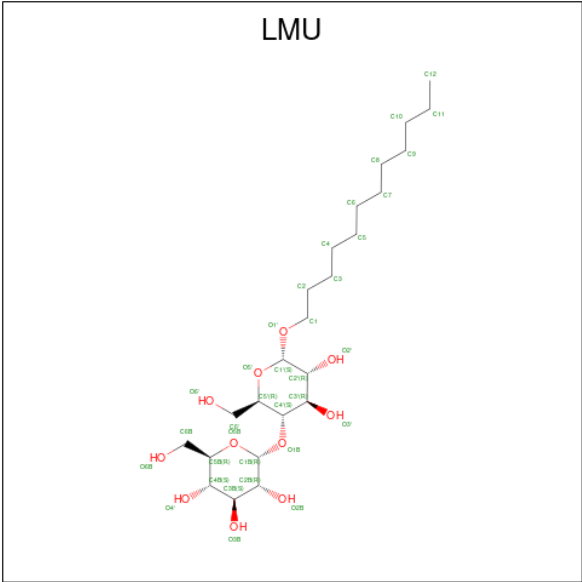
- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

HEM

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



- Molecule 39 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
39	J	1	Total	C	O	0
			35	24	11	

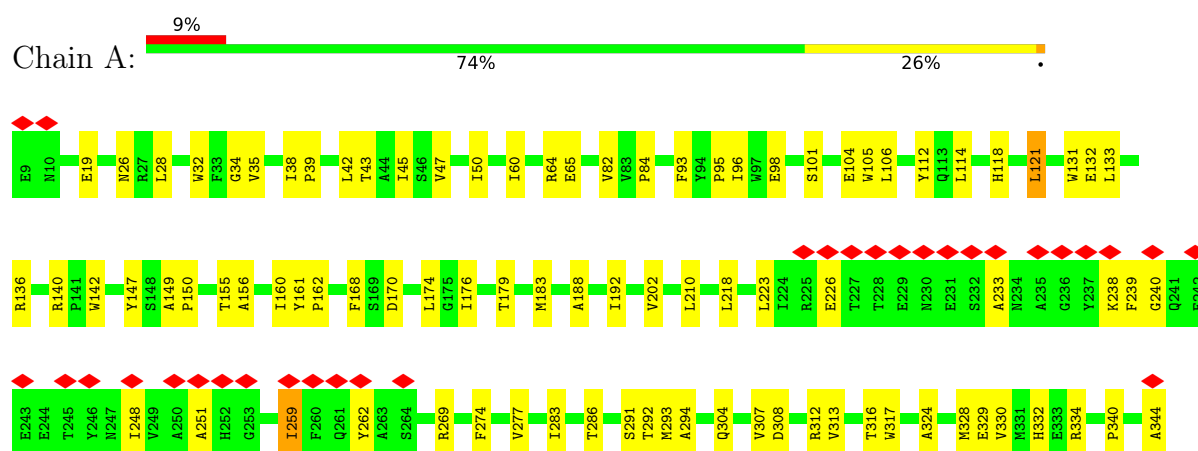
- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	A	6	Total	O	0
			6	6	
40	B	3	Total	O	0
			3	3	
40	C	1	Total	O	0
			1	1	
40	D	1	Total	O	0
			1	1	

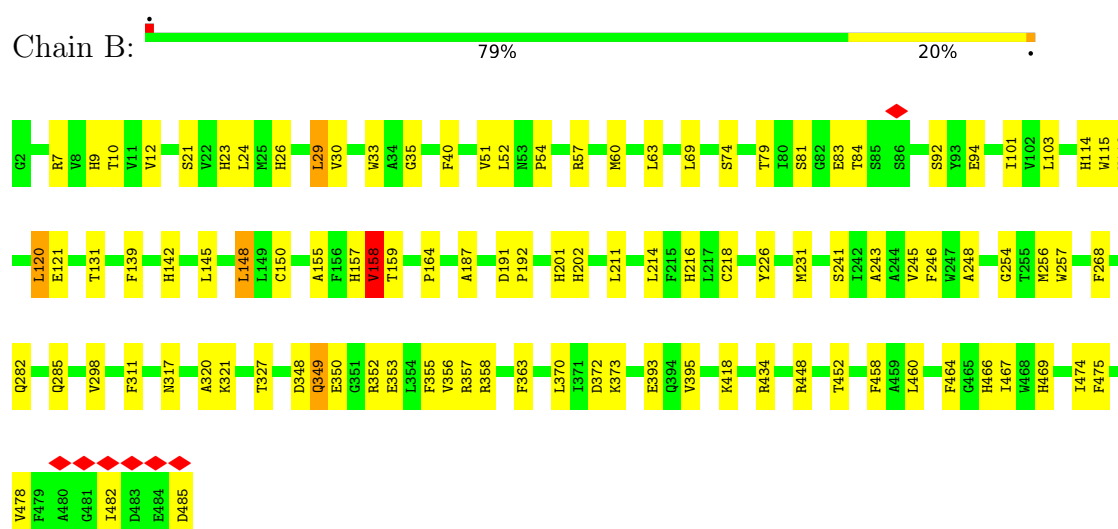
3 Residue-property plots

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.

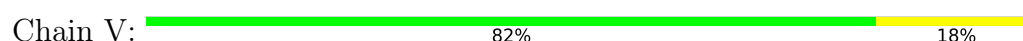
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein



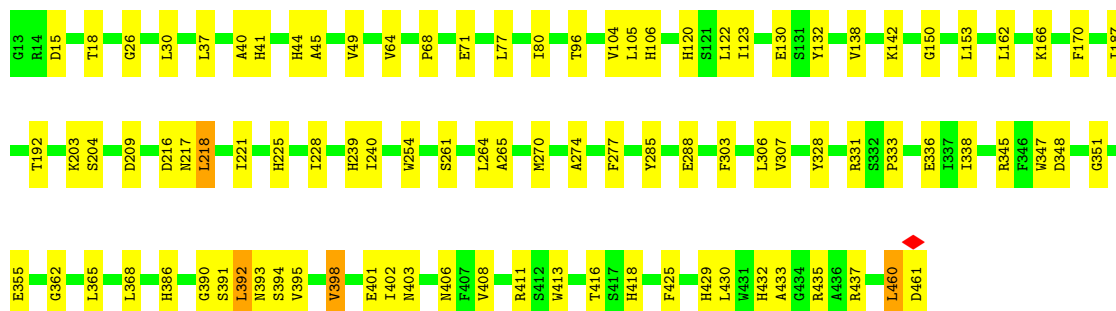
- Molecule 3: Photosystem II reaction center protein Psb30





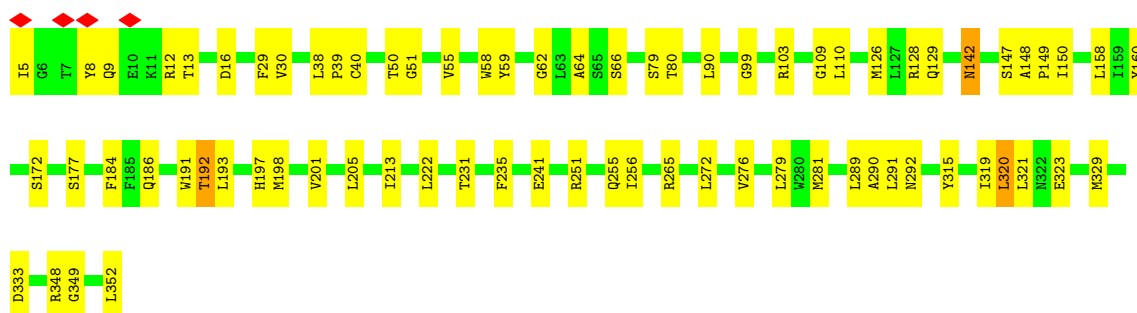
• Molecule 4: Photosystem II CP43 reaction center protein

Chain C: 79% 20%



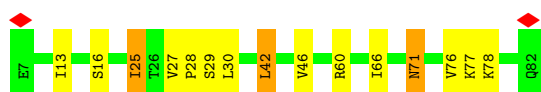
• Molecule 5: Photosystem II D2 protein

Chain D: 79% 20%



• Molecule 6: Cytochrome b559 subunit alpha

Chain E: 80% 16%



• Molecule 7: Cytochrome b559 subunit beta

Chain F: 74% 26%



• Molecule 8: Photosystem II reaction center protein H

Chain H: 81% 18%



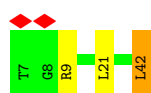
• Molecule 9: Photosystem II reaction center protein I

Chain I: 88% 12%



• Molecule 10: Photosystem II reaction center protein J

Chain J: 6% 92% 6%



• Molecule 11: Photosystem II reaction center protein K

Chain K: 81% 16%



• Molecule 12: Photosystem II reaction center protein L

Chain L: 94% 6%



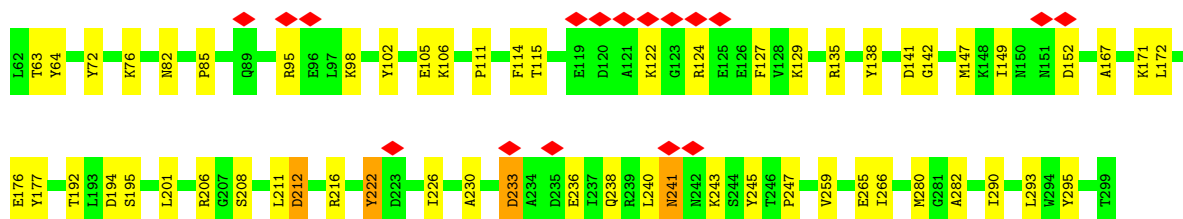
• Molecule 13: Photosystem II reaction center protein M

Chain M: 6% 87% 13%

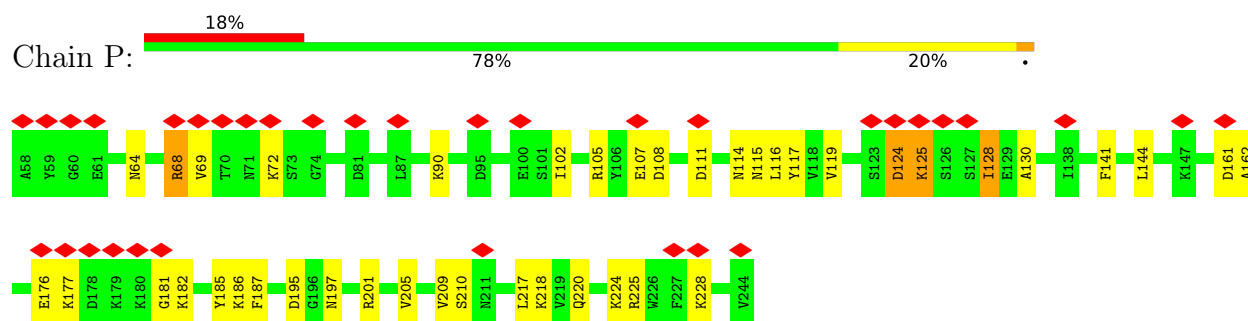


• Molecule 14: PsbO

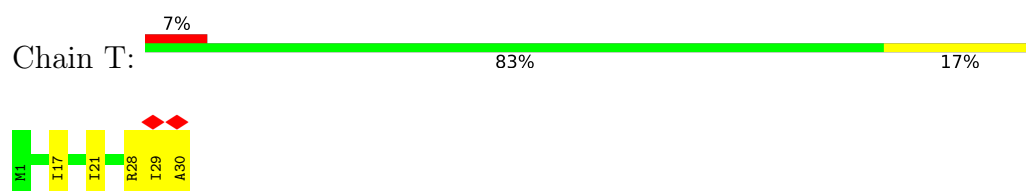
Chain O: 7% 76% 23%



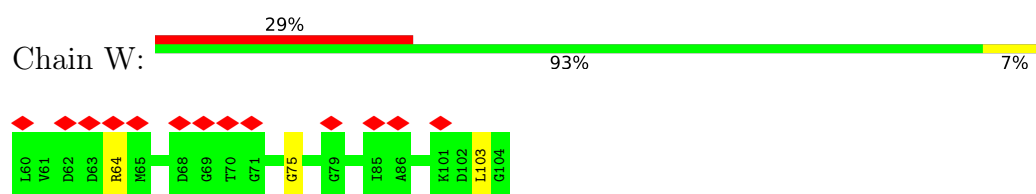
- Molecule 15: PsbP



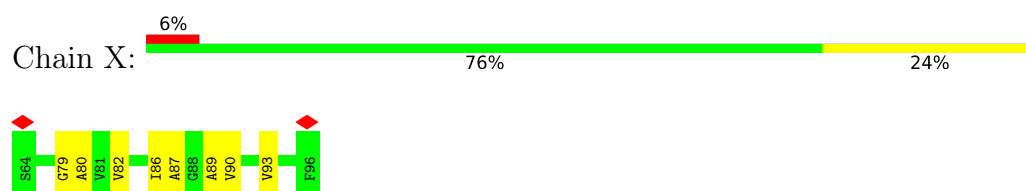
- Molecule 16: Photosystem II reaction center protein T



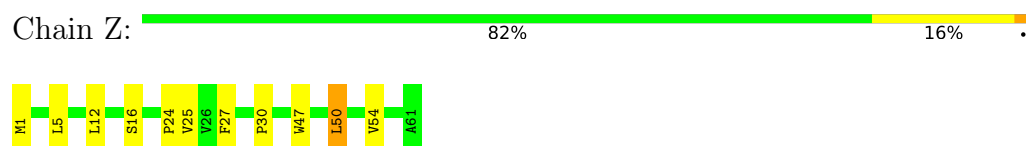
- Molecule 17: PSII 6.1 kDa protein



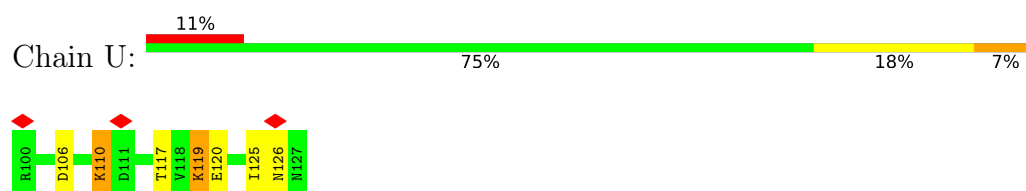
- Molecule 18: Photosystem II PsbX



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein U, PsbU



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	118340	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0047	Depositor
Map size ($\text{\AA}$)	193.5, 193.5, 193.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.645, 0.645, 0.645	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMG, CL, C7Z, FE2, LHG, CSD, CLA, PHO, OEX, NA, DGA, SQD, PL9, HEM, DGD, LMU, RRX, BCT, 3PH, BCR

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	0.26	0/2717	0.34	0/3707
2	B	0.22	0/3906	0.31	0/5319
3	V	0.16	0/236	0.24	0/321
4	C	0.30	0/3602	0.37	0/4913
5	D	0.31	0/2860	0.37	0/3899
6	E	0.18	0/639	0.31	0/870
7	F	0.19	0/259	0.29	0/351
8	H	0.19	0/513	0.24	0/703
9	I	0.21	0/273	0.29	0/370
10	J	0.25	0/271	0.29	0/368
11	K	0.23	0/308	0.36	0/423
12	L	0.21	0/308	0.26	0/418
13	M	0.17	0/238	0.24	0/324
14	O	0.21	0/1854	0.31	0/2503
15	P	0.13	0/1482	0.26	0/1999
16	T	0.18	0/254	0.23	0/342
17	W	0.14	0/342	0.26	0/465
18	X	0.18	0/227	0.27	0/311
19	Z	0.15	0/469	0.25	0/641
20	U	0.15	0/235	0.25	0/311
All	All	0.24	0/20993	0.32	0/28558

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2635	0	2536	84	0
2	B	3785	0	3662	85	0
3	V	235	0	273	8	0
4	C	3483	0	3376	76	0
5	D	2766	0	2655	58	0
6	E	621	0	605	8	0
7	F	252	0	265	6	0
8	H	503	0	532	11	0
9	I	265	0	272	2	0
10	J	265	0	282	4	0
11	K	297	0	312	6	0
12	L	300	0	308	2	0
13	M	235	0	262	3	0
14	O	1819	0	1772	39	0
15	P	1453	0	1416	27	0
16	T	247	0	260	7	0
17	W	335	0	326	3	0
18	X	225	0	244	5	0
19	Z	457	0	478	10	0
20	U	235	0	244	6	0
21	A	10	0	0	0	0
22	A	1	0	0	0	0
23	A	2	0	0	0	0
24	A	190	0	203	16	0
24	B	1017	0	1095	82	0
24	C	794	0	824	53	0
24	D	190	0	203	20	0
25	A	64	0	74	5	0
25	D	64	0	74	5	0
26	A	40	0	56	5	0
26	B	80	0	112	6	0
26	C	120	0	168	9	0
26	D	40	0	56	1	0
26	J	40	0	56	2	0
27	A	42	0	47	0	0
27	M	42	0	47	4	0
28	A	71	0	82	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	B	44	0	58	2	0
28	C	120	0	156	7	0
28	D	42	0	54	1	0
28	H	48	0	66	5	0
29	A	1	0	0	0	0
30	A	4	0	1	0	0
31	A	39	0	48	3	0
31	D	132	0	185	11	0
31	L	49	0	74	1	0
32	B	42	0	0	3	0
33	B	43	0	44	2	0
33	C	150	0	174	7	0
34	B	48	0	75	4	0
35	B	37	0	56	3	0
36	D	55	0	80	1	0
37	E	43	0	30	2	0
38	H	41	0	56	6	0
39	J	35	0	46	4	0
40	A	6	0	0	0	0
40	B	3	0	0	0	0
40	C	1	0	0	0	0
40	D	1	0	0	0	0
All	All	24204	0	24380	513	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 513 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)
2:B:24:LEU:HD21	24:B:516:CLA:HAB	1.56	0.88
5:D:192:THR:HG23	24:D:403:CLA:HBC2	1.67	0.77
24:B:514:CLA:H18	26:B:517:BCR:H11C	1.68	0.75
4:C:187:ILE:HD11	4:C:218:LEU:HD23	1.68	0.74
1:A:26:ASN:HA	28:A:415:LMG:HC71	1.68	0.73

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/336 (99%)	322 (96%)	12 (4%)	0	100	100
2	B	481/484 (99%)	466 (97%)	14 (3%)	1 (0%)	43	65
3	V	31/33 (94%)	31 (100%)	0	0	100	100
4	C	447/449 (100%)	431 (96%)	16 (4%)	0	100	100
5	D	346/348 (99%)	336 (97%)	10 (3%)	0	100	100
6	E	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	65 (100%)	0	0	100	100
9	I	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	L	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
13	M	29/31 (94%)	29 (100%)	0	0	100	100
14	O	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
15	P	185/187 (99%)	183 (99%)	2 (1%)	0	100	100
16	T	28/30 (93%)	28 (100%)	0	0	100	100
17	W	43/45 (96%)	42 (98%)	1 (2%)	0	100	100
18	X	31/33 (94%)	31 (100%)	0	0	100	100
19	Z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
20	U	26/28 (93%)	26 (100%)	0	0	100	100
All	All	2578/2619 (98%)	2498 (97%)	79 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	158	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/275 (100%)	270 (98%)	5 (2%)	51	72
2	B	387/387 (100%)	378 (98%)	9 (2%)	44	68
3	V	26/26 (100%)	26 (100%)	0	100	100
4	C	350/350 (100%)	332 (95%)	18 (5%)	21	45
5	D	279/279 (100%)	268 (96%)	11 (4%)	28	53
6	E	68/68 (100%)	62 (91%)	6 (9%)	9	23
7	F	25/25 (100%)	24 (96%)	1 (4%)	28	53
8	H	56/56 (100%)	52 (93%)	4 (7%)	13	31
9	I	30/30 (100%)	28 (93%)	2 (7%)	15	34
10	J	27/27 (100%)	26 (96%)	1 (4%)	30	55
11	K	33/33 (100%)	31 (94%)	2 (6%)	17	38
12	L	34/34 (100%)	34 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
14	O	195/195 (100%)	189 (97%)	6 (3%)	35	60
15	P	152/152 (100%)	145 (95%)	7 (5%)	24	49
16	T	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	33 (97%)	1 (3%)	37	62
18	X	24/24 (100%)	24 (100%)	0	100	100
19	Z	50/50 (100%)	49 (98%)	1 (2%)	48	70
20	U	27/27 (100%)	22 (82%)	5 (18%)	1	3
All	All	2124/2124 (100%)	2045 (96%)	79 (4%)	31	55

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	10	LYS
15	P	217	LEU
14	O	129	LYS

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Mol	Chain	Res	Type
15	P	68	ARG
20	U	119	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	336	HIS
8	H	79	ASN
15	P	197	ASN
15	P	71	ASN
15	P	115	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSD	B	218	2	3,7,8	0.87	0	1,8,10	0.10	0

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
2	CSD	B	218	2	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	218	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	218	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 77 ligands modelled in this entry, 4 are monoatomic - leaving 73 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	$\# Z > 2$
24	CLA	A	408	1	64,68,73	1.41	7 (10%)	77,107,113	2.13	20 (25%)
24	CLA	B	501	-	69,73,73	1.35	6 (8%)	83,113,113	1.98	20 (24%)
24	CLA	B	508	2	69,73,73	1.37	6 (8%)	83,113,113	1.88	17 (20%)
24	CLA	C	503	4	69,73,73	1.36	6 (8%)	83,113,113	1.97	19 (22%)
24	CLA	C	509	4	69,73,73	1.38	6 (8%)	83,113,113	1.92	18 (21%)
36	PL9	D	406	-	55,55,55	1.39	5 (9%)	68,69,69	1.52	13 (19%)
24	CLA	C	506	4	58,62,73	1.50	7 (12%)	69,99,113	2.08	17 (24%)
24	CLA	B	503	2	69,73,73	1.38	7 (10%)	83,113,113	1.88	17 (20%)
28	LMG	H	102	-	48,48,55	0.99	5 (10%)	56,56,63	1.13	2 (3%)
24	CLA	B	509	2	69,73,73	1.35	7 (10%)	83,113,113	1.94	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	D	408	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
24	CLA	C	505	-	59,63,73	1.46	7 (11%)	71,101,113	2.11	17 (23%)
28	LMG	C	521	-	47,47,55	0.96	4 (8%)	55,55,63	1.09	3 (5%)
24	CLA	C	513	4	59,63,73	1.47	7 (11%)	71,101,113	2.01	17 (23%)
25	PHO	D	402	-	58,69,69	1.98	10 (17%)	56,99,99	1.52	8 (14%)
30	BCT	A	413	22	2,3,3	1.28	0	2,3,3	4.11	1 (50%)
26	BCR	B	518	-	41,41,41	4.76	26 (63%)	56,56,56	2.24	19 (33%)
26	BCR	B	517	-	41,41,41	4.74	25 (60%)	56,56,56	2.47	20 (35%)
28	LMG	A	411	-	34,34,55	0.46	0	42,42,63	1.27	5 (11%)
24	CLA	B	515	2	69,73,73	1.34	7 (10%)	83,113,113	1.93	18 (21%)
37	HEM	E	101	7,6	50,50,50	1.36	6 (12%)	66,82,82	1.07	5 (7%)
24	CLA	C	511	4	69,73,73	1.35	6 (8%)	83,113,113	1.99	17 (20%)
24	CLA	D	404	-	64,68,73	1.42	7 (10%)	77,107,113	2.06	16 (20%)
24	CLA	C	512	4	69,73,73	1.37	6 (8%)	83,113,113	1.98	20 (24%)
24	CLA	A	406	40	69,73,73	1.37	7 (10%)	83,113,113	1.94	21 (25%)
28	LMG	B	520	-	44,44,55	0.87	3 (6%)	52,52,63	1.14	2 (3%)
28	LMG	C	522	-	33,33,55	0.93	2 (6%)	40,40,63	1.10	2 (5%)
24	CLA	B	512	2	69,73,73	1.36	6 (8%)	83,113,113	1.93	16 (19%)
21	OEX	A	401	4,1	0,14,14	-	-	-	-	-
24	CLA	C	504	4	69,73,73	1.37	7 (10%)	83,113,113	1.92	19 (22%)
28	LMG	C	501	-	40,40,55	0.76	2 (5%)	48,48,63	1.24	4 (8%)
33	DGD	C	520	-	54,54,67	0.94	4 (7%)	68,68,81	1.16	5 (7%)
26	BCR	J	101	-	41,41,41	4.79	26 (63%)	56,56,56	2.39	20 (35%)
28	LMG	D	409	-	42,42,55	0.77	2 (4%)	50,50,63	1.08	3 (6%)
24	CLA	B	511	2	69,73,73	1.37	6 (8%)	83,113,113	1.90	17 (20%)
24	CLA	D	403	5	69,73,73	1.36	7 (10%)	83,113,113	1.87	16 (19%)
24	CLA	B	506	-	61,65,73	1.45	6 (9%)	73,103,113	1.99	18 (24%)
24	CLA	B	510	40	69,73,73	1.36	6 (8%)	83,113,113	1.93	17 (20%)
26	BCR	D	405	-	41,41,41	4.77	26 (63%)	56,56,56	2.20	19 (33%)
31	LHG	L	101	-	48,48,48	0.39	0	51,54,54	1.12	4 (7%)
32	C7Z	B	519	-	43,43,43	5.30	27 (62%)	58,60,60	2.33	18 (31%)
33	DGD	C	519	-	54,54,67	1.01	4 (7%)	68,68,81	1.21	5 (7%)
39	LMU	J	102	-	36,36,36	0.39	0	47,47,47	0.77	2 (4%)
31	LHG	D	410	-	38,38,48	0.43	0	41,44,54	1.20	4 (9%)
24	CLA	B	516	2	59,63,73	1.47	6 (10%)	71,101,113	2.00	17 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PHO	A	407	-	58,69,69	1.97	10 (17%)	56,99,99	1.52	7 (12%)
27	SQD	M	101	-	41,42,54	0.87	0	50,53,65	0.93	2 (4%)
33	DGD	C	518	-	45,45,67	0.80	1 (2%)	59,59,81	1.11	4 (6%)
31	LHG	A	414	-	38,38,48	0.43	0	41,44,54	1.19	3 (7%)
24	CLA	B	505	2	69,73,73	1.36	6 (8%)	83,113,113	1.94	18 (21%)
26	BCR	C	516	-	41,41,41	4.73	25 (60%)	56,56,56	2.40	22 (39%)
24	CLA	D	401	40	69,73,73	1.36	6 (8%)	83,113,113	1.97	19 (22%)
26	BCR	C	517	-	41,41,41	4.78	26 (63%)	56,56,56	2.38	19 (33%)
34	3PH	B	522	-	47,47,47	0.85	4 (8%)	51,52,52	1.15	2 (3%)
24	CLA	A	405	1	69,73,73	1.36	6 (8%)	83,113,113	1.94	19 (22%)
35	DGA	B	523	-	36,36,43	1.17	3 (8%)	38,38,45	1.38	3 (7%)
24	CLA	C	514	4	49,53,73	1.61	6 (12%)	59,89,113	2.09	14 (23%)
24	CLA	B	513	2	69,73,73	1.36	6 (8%)	83,113,113	1.94	15 (18%)
38	RRX	H	101	-	42,42,42	5.02	26 (61%)	57,58,58	2.57	23 (40%)
24	CLA	B	504	2	64,68,73	1.44	7 (10%)	77,107,113	2.02	16 (20%)
24	CLA	B	514	2	69,73,73	1.37	6 (8%)	83,113,113	1.95	18 (21%)
33	DGD	B	521	-	44,44,67	0.86	1 (2%)	58,58,81	0.93	2 (3%)
24	CLA	B	507	40	69,73,73	1.36	7 (10%)	83,113,113	1.94	18 (21%)
24	CLA	C	502	4	69,73,73	1.35	6 (8%)	83,113,113	1.94	19 (22%)
28	LMG	A	415	-	37,37,55	0.59	1 (2%)	45,45,63	1.07	3 (6%)
24	CLA	C	508	40	69,73,73	1.36	6 (8%)	83,113,113	1.96	16 (19%)
26	BCR	C	515	-	41,41,41	4.77	26 (63%)	56,56,56	2.23	20 (35%)
24	CLA	C	507	4	69,73,73	1.37	6 (8%)	83,113,113	1.92	19 (22%)
27	SQD	A	410	-	41,42,54	0.87	0	50,53,65	1.01	2 (4%)
31	LHG	D	407	-	43,43,48	0.42	0	46,49,54	1.05	3 (6%)
24	CLA	B	502	2	69,73,73	1.35	6 (8%)	83,113,113	1.92	18 (21%)
24	CLA	C	510	4	69,73,73	1.37	6 (8%)	83,113,113	1.92	17 (20%)
26	BCR	A	409	-	41,41,41	4.79	26 (63%)	56,56,56	3.00	25 (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
24	CLA	A	408	1	-	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	501	-	-	16/39/115/115	-
24	CLA	B	508	2	-	15/39/115/115	-
24	CLA	C	503	4	-	15/39/115/115	-
24	CLA	C	509	4	-	15/39/115/115	-
36	PL9	D	406	-	-	8/53/73/73	0/1/1/1
24	CLA	C	506	4	-	13/26/102/115	-
24	CLA	B	503	2	-	21/39/115/115	-
28	LMG	H	102	-	-	13/43/63/70	0/1/1/1
24	CLA	B	509	2	-	15/39/115/115	-
31	LHG	D	408	-	-	26/53/53/53	-
24	CLA	C	505	-	-	9/27/103/115	-
28	LMG	C	521	-	-	9/42/62/70	0/1/1/1
24	CLA	C	513	4	-	11/27/103/115	-
25	PHO	D	402	-	-	7/37/103/103	0/5/6/6
26	BCR	B	518	-	-	13/29/63/63	0/2/2/2
26	BCR	B	517	-	-	10/29/63/63	0/2/2/2
28	LMG	A	411	-	-	8/29/49/70	0/1/1/1
24	CLA	B	515	2	-	20/39/115/115	-
37	HEM	E	101	7,6	-	2/14/54/54	-
24	CLA	C	511	4	-	16/39/115/115	-
24	CLA	D	404	-	-	16/33/109/115	-
24	CLA	C	512	4	-	13/39/115/115	-
24	CLA	A	406	40	-	13/39/115/115	-
28	LMG	B	520	-	-	9/39/59/70	0/1/1/1
28	LMG	C	522	-	-	8/27/47/70	0/1/1/1
24	CLA	B	512	2	-	15/39/115/115	-
24	CLA	C	504	4	-	15/39/115/115	-
28	LMG	C	501	-	-	8/35/55/70	0/1/1/1
33	DGD	C	520	-	-	9/42/82/95	0/2/2/2
26	BCR	J	101	-	-	11/29/63/63	0/2/2/2
28	LMG	D	409	-	-	9/37/57/70	0/1/1/1
24	CLA	B	511	2	-	16/39/115/115	-
24	CLA	D	403	5	-	14/39/115/115	-
24	CLA	B	506	-	-	7/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	510	40	-	19/39/115/115	-
26	BCR	D	405	-	-	8/29/63/63	0/2/2/2
31	LHG	L	101	-	-	30/53/53/53	-
32	C7Z	B	519	-	-	12/29/67/67	0/2/2/2
33	DGD	C	519	-	-	16/42/82/95	0/2/2/2
39	LMU	J	102	-	-	6/21/61/61	0/2/2/2
31	LHG	D	410	-	-	25/43/43/53	-
24	CLA	B	516	2	-	15/27/103/115	-
25	PHO	A	407	-	-	13/37/103/103	0/5/6/6
27	SQD	M	101	-	-	14/37/57/69	0/1/1/1
33	DGD	C	518	-	-	6/33/73/95	0/2/2/2
31	LHG	A	414	-	-	26/43/43/53	-
24	CLA	B	505	2	-	15/39/115/115	-
26	BCR	C	516	-	-	9/29/63/63	0/2/2/2
24	CLA	D	401	40	-	21/39/115/115	-
26	BCR	C	517	-	-	10/29/63/63	0/2/2/2
34	3PH	B	522	-	-	25/49/49/49	-
24	CLA	A	405	1	-	14/39/115/115	-
35	DGA	B	523	-	-	24/38/38/45	-
24	CLA	C	514	4	-	7/15/91/115	-
24	CLA	B	513	2	-	18/39/115/115	-
38	RRX	H	101	-	-	6/29/65/65	0/2/2/2
24	CLA	B	504	2	-	18/33/109/115	-
24	CLA	B	514	2	-	17/39/115/115	-
33	DGD	B	521	-	-	14/32/72/95	0/2/2/2
24	CLA	B	507	40	-	24/39/115/115	-
24	CLA	C	502	4	-	18/39/115/115	-
28	LMG	A	415	-	-	4/32/52/70	0/1/1/1
24	CLA	C	508	40	-	14/39/115/115	-
26	BCR	C	515	-	-	13/29/63/63	0/2/2/2
24	CLA	C	507	4	-	19/39/115/115	-
27	SQD	A	410	-	-	8/37/57/69	0/1/1/1
31	LHG	D	407	-	-	23/48/48/53	-
24	CLA	B	502	2	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	510	4	-	9/39/115/115	-
26	BCR	A	409	-	-	13/29/63/63	0/2/2/2

The worst 5 of 549 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	519	C7Z	C25-C26	15.87	1.61	1.34
26	A	409	BCR	C26-C25	15.47	1.61	1.34
26	D	405	BCR	C26-C25	15.44	1.61	1.34
26	J	101	BCR	C26-C25	15.43	1.61	1.34
26	B	518	BCR	C26-C25	15.41	1.61	1.34

The worst 5 of 926 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	408	CLA	C4A-NA-C1A	9.70	111.06	106.71
26	A	409	BCR	C7-C8-C9	-9.68	111.60	126.23
24	B	512	CLA	C4A-NA-C1A	9.65	111.05	106.71
24	D	404	CLA	C4A-NA-C1A	9.55	111.00	106.71
24	B	509	CLA	C4A-NA-C1A	9.44	110.95	106.71

There are no chirality outliers.

5 of 987 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	405	CLA	C1A-C2A-CAA-CBA
24	A	405	CLA	C3A-C2A-CAA-CBA
24	A	406	CLA	C1A-C2A-CAA-CBA
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

70 monomers are involved in 245 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	408	CLA	8	0
24	B	501	CLA	4	0
24	B	508	CLA	9	0
24	C	503	CLA	2	0
24	C	509	CLA	7	0

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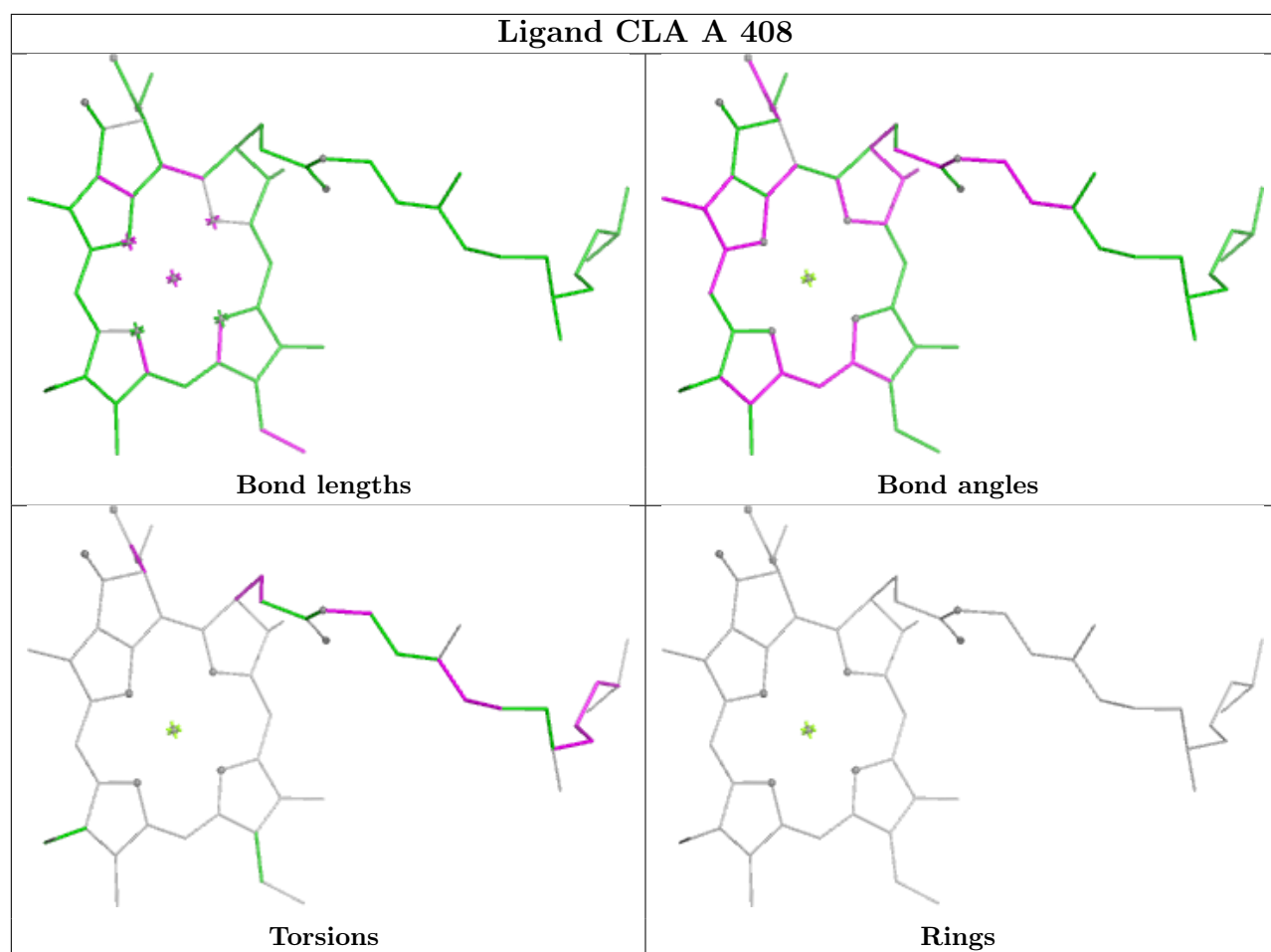
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	D	406	PL9	1	0
24	C	506	CLA	3	0
24	B	503	CLA	9	0
28	H	102	LMG	5	0
24	B	509	CLA	3	0
31	D	408	LHG	4	0
24	C	505	CLA	1	0
28	C	521	LMG	1	0
24	C	513	CLA	1	0
25	D	402	PHO	5	0
26	B	518	BCR	1	0
26	B	517	BCR	5	0
28	A	411	LMG	1	0
24	B	515	CLA	4	0
37	E	101	HEM	2	0
24	C	511	CLA	5	0
24	D	404	CLA	8	0
24	C	512	CLA	7	0
24	A	406	CLA	4	0
28	B	520	LMG	2	0
28	C	522	LMG	2	0
24	B	512	CLA	5	0
24	C	504	CLA	4	0
28	C	501	LMG	4	0
33	C	520	DGD	2	0
26	J	101	BCR	2	0
28	D	409	LMG	1	0
24	B	511	CLA	8	0
24	D	403	CLA	6	0
24	B	506	CLA	2	0
24	B	510	CLA	5	0
26	D	405	BCR	1	0
31	L	101	LHG	1	0
32	B	519	C7Z	3	0
33	C	519	DGD	4	0
39	J	102	LMU	4	0
31	D	410	LHG	5	0
24	B	516	CLA	4	0
25	A	407	PHO	5	0
27	M	101	SQD	4	0
33	C	518	DGD	1	0
31	A	414	LHG	3	0

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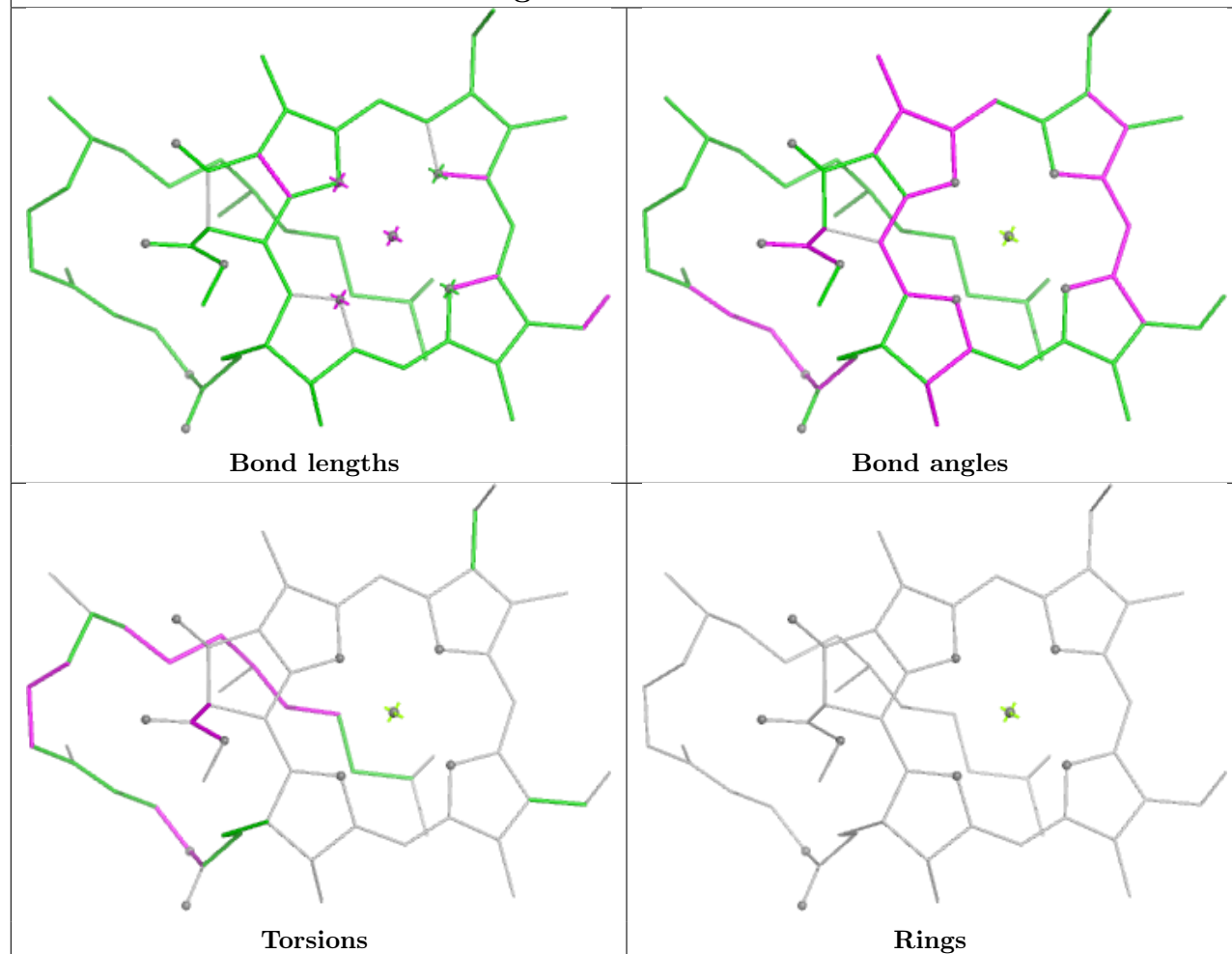
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	505	CLA	6	0
26	C	516	BCR	5	0
24	D	401	CLA	6	0
26	C	517	BCR	2	0
34	B	522	3PH	4	0
24	A	405	CLA	4	0
35	B	523	DGA	3	0
24	C	514	CLA	2	0
24	B	513	CLA	6	0
38	H	101	RRX	6	0
24	B	504	CLA	9	0
24	B	514	CLA	6	0
33	B	521	DGD	2	0
24	B	507	CLA	5	0
24	C	502	CLA	5	0
28	A	415	LMG	4	0
24	C	508	CLA	6	0
26	C	515	BCR	2	0
24	C	507	CLA	8	0
31	D	407	LHG	2	0
24	B	502	CLA	8	0
24	C	510	CLA	6	0
26	A	409	BCR	5	0

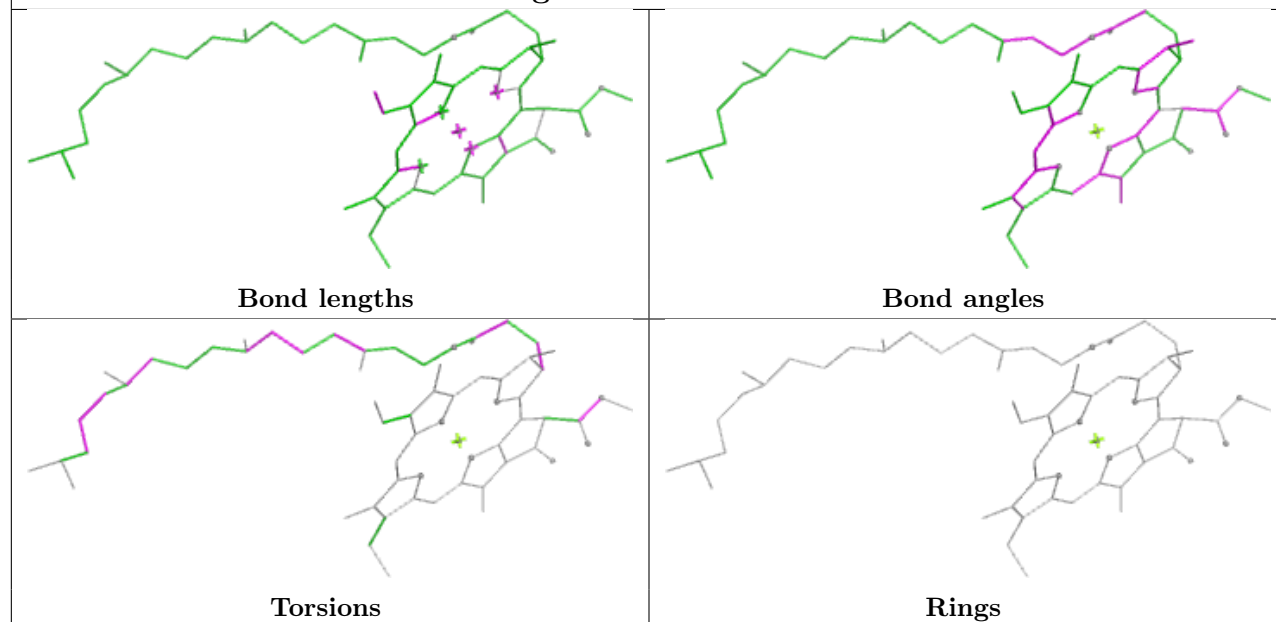
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

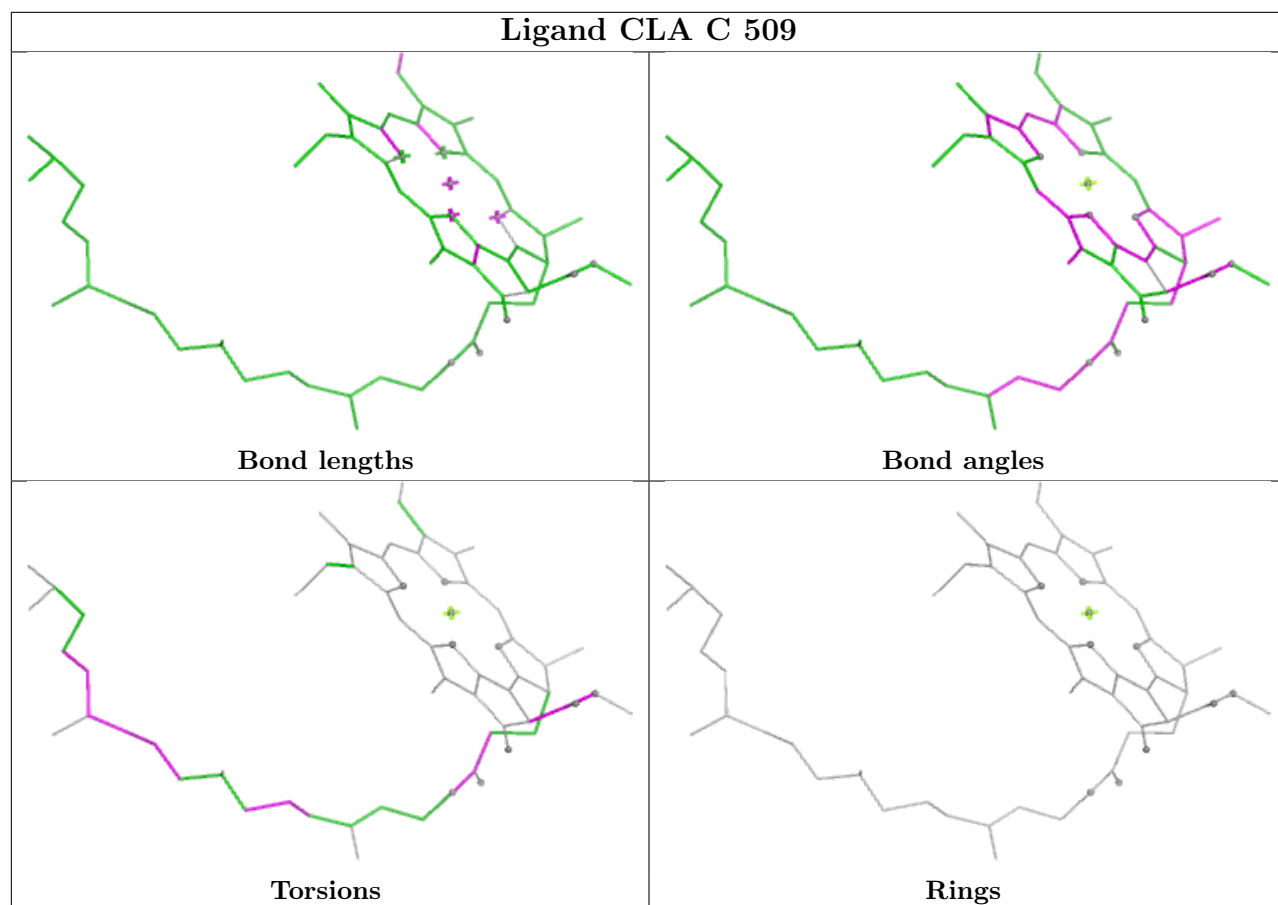
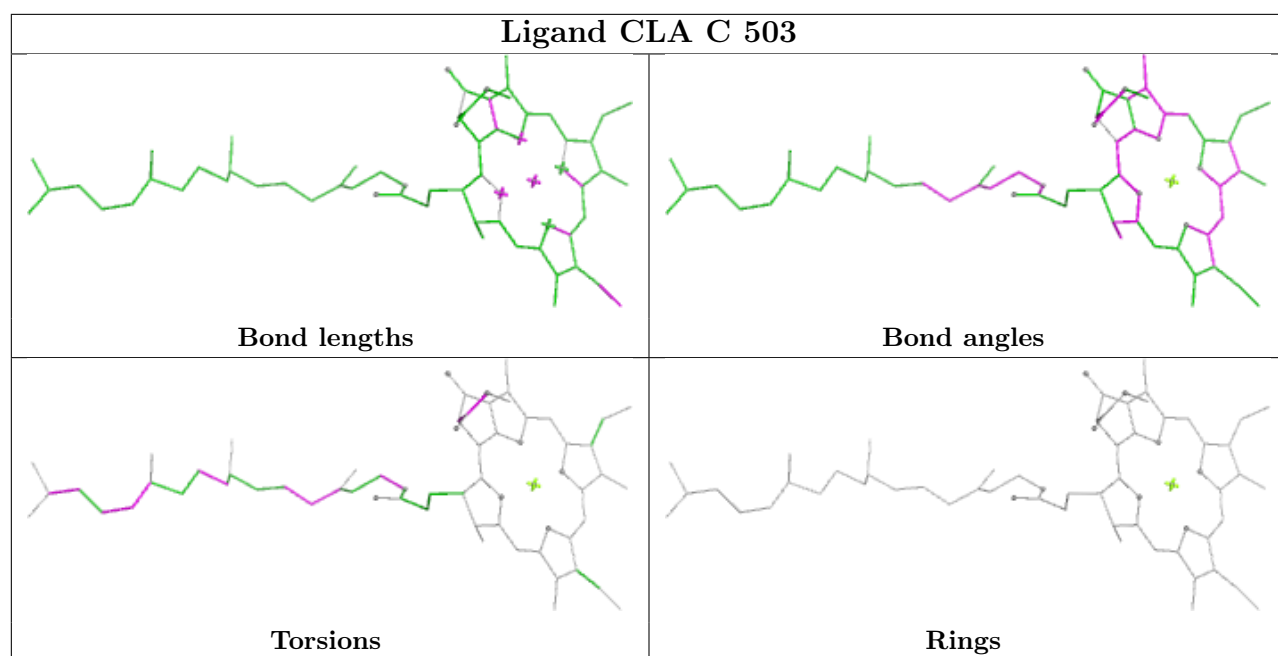


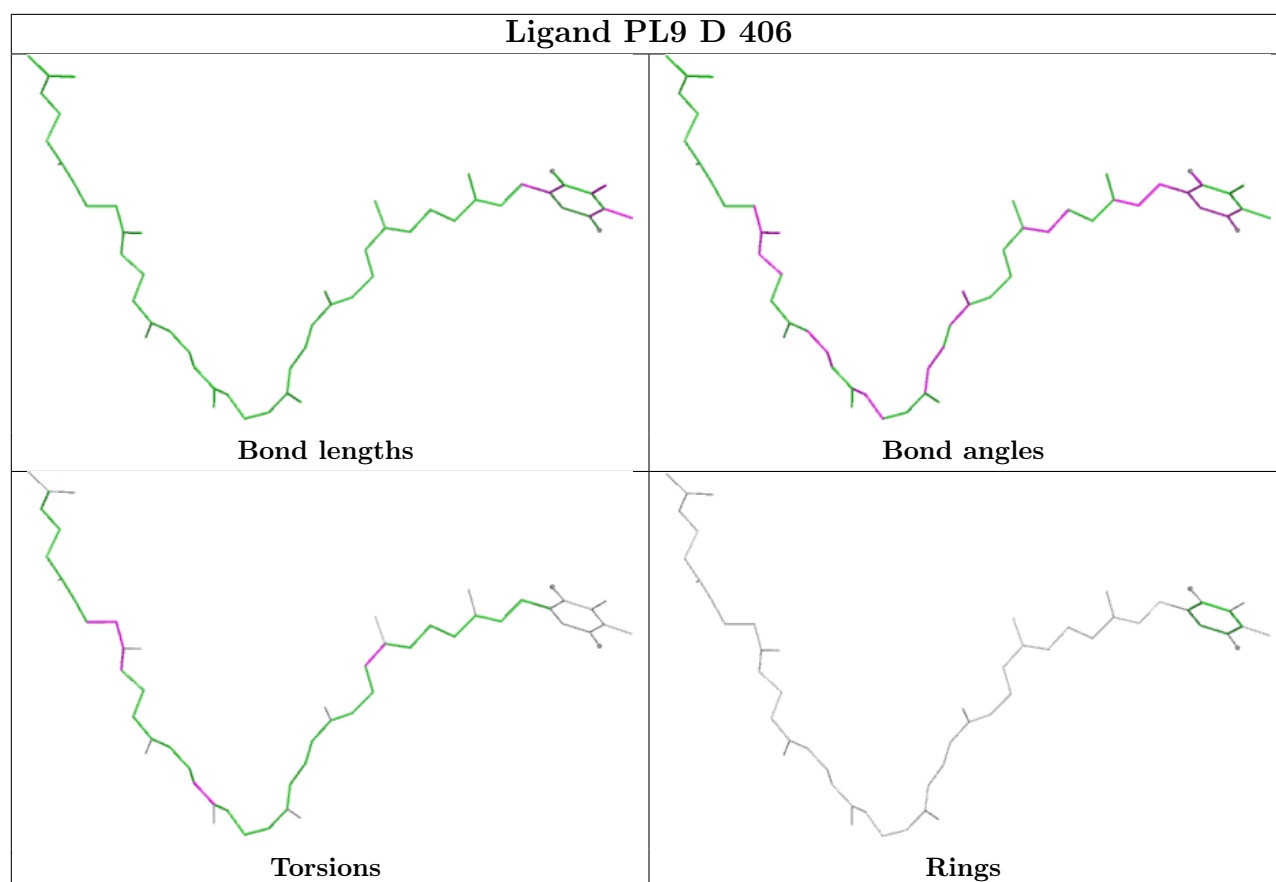
Ligand CLA B 501



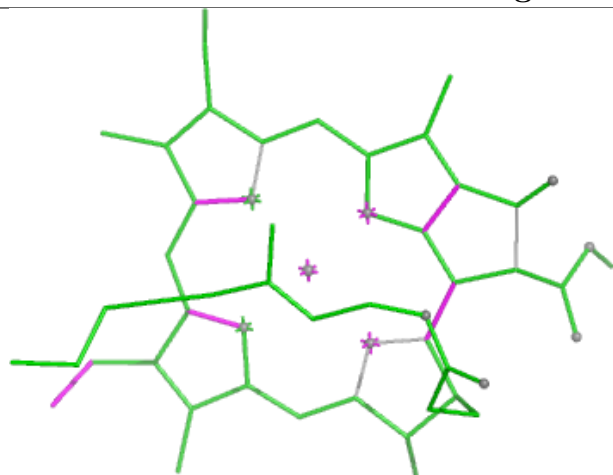
Ligand CLA B 508



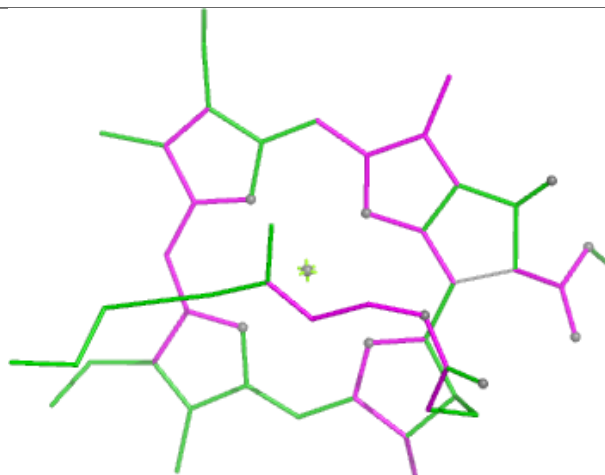




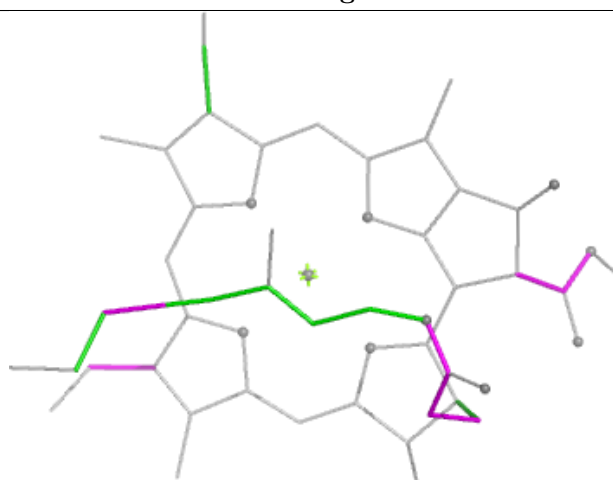
Ligand CLA C 506



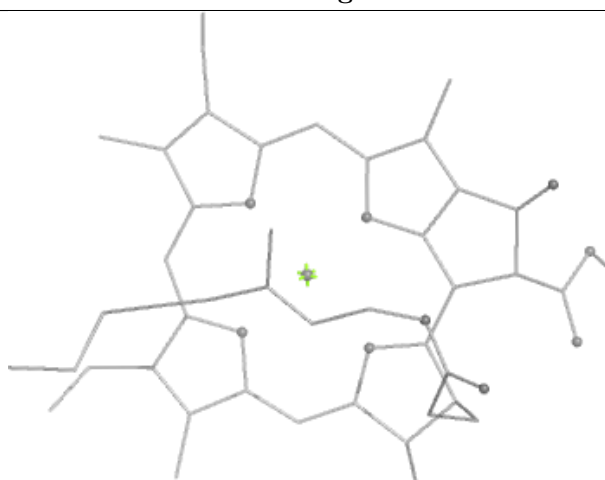
Bond lengths



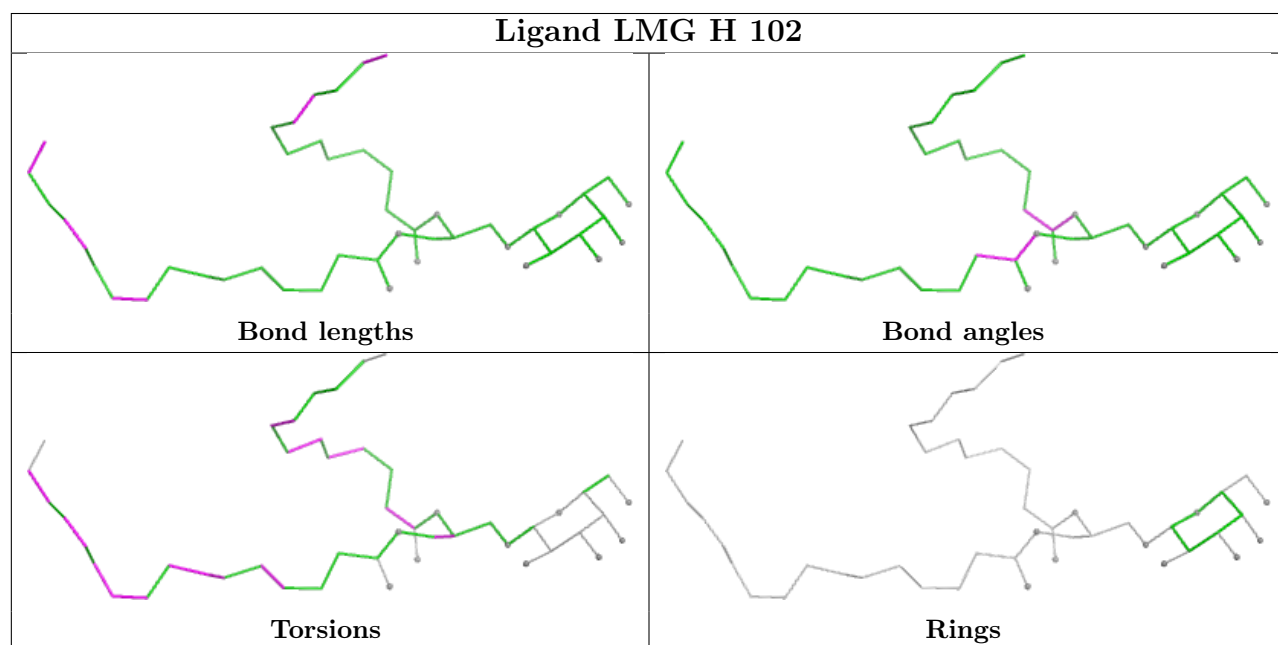
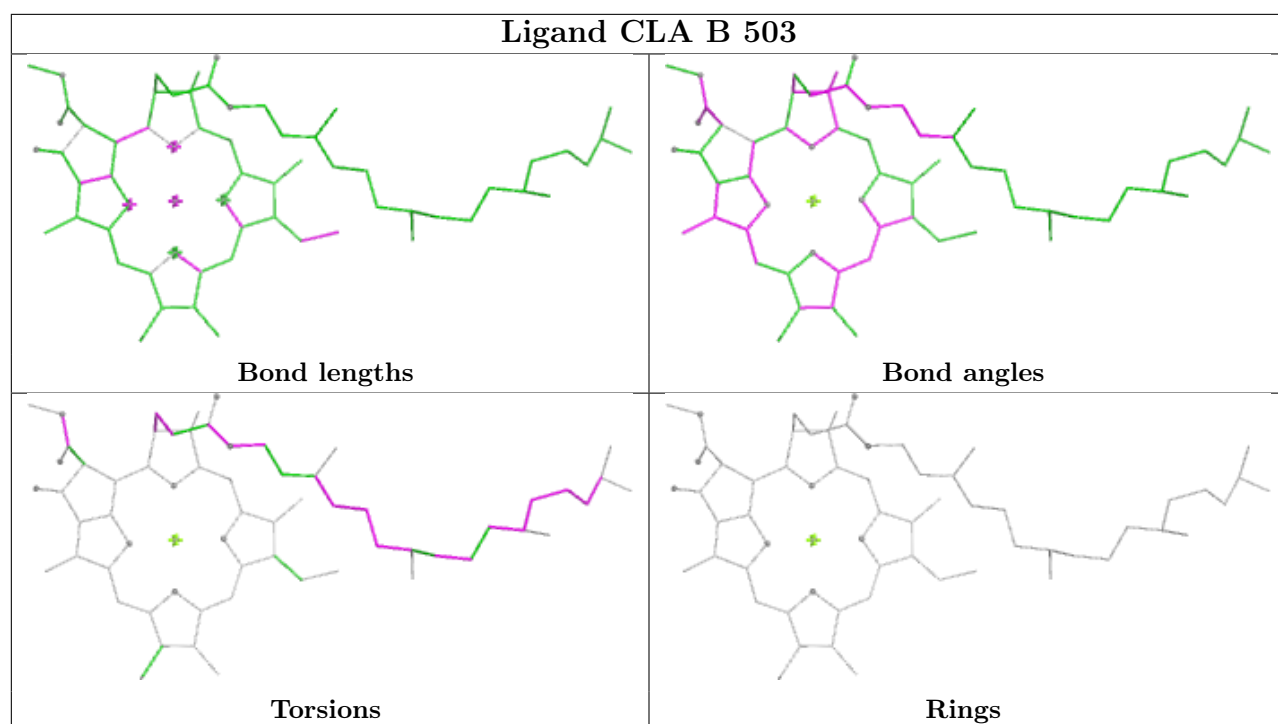
Bond angles

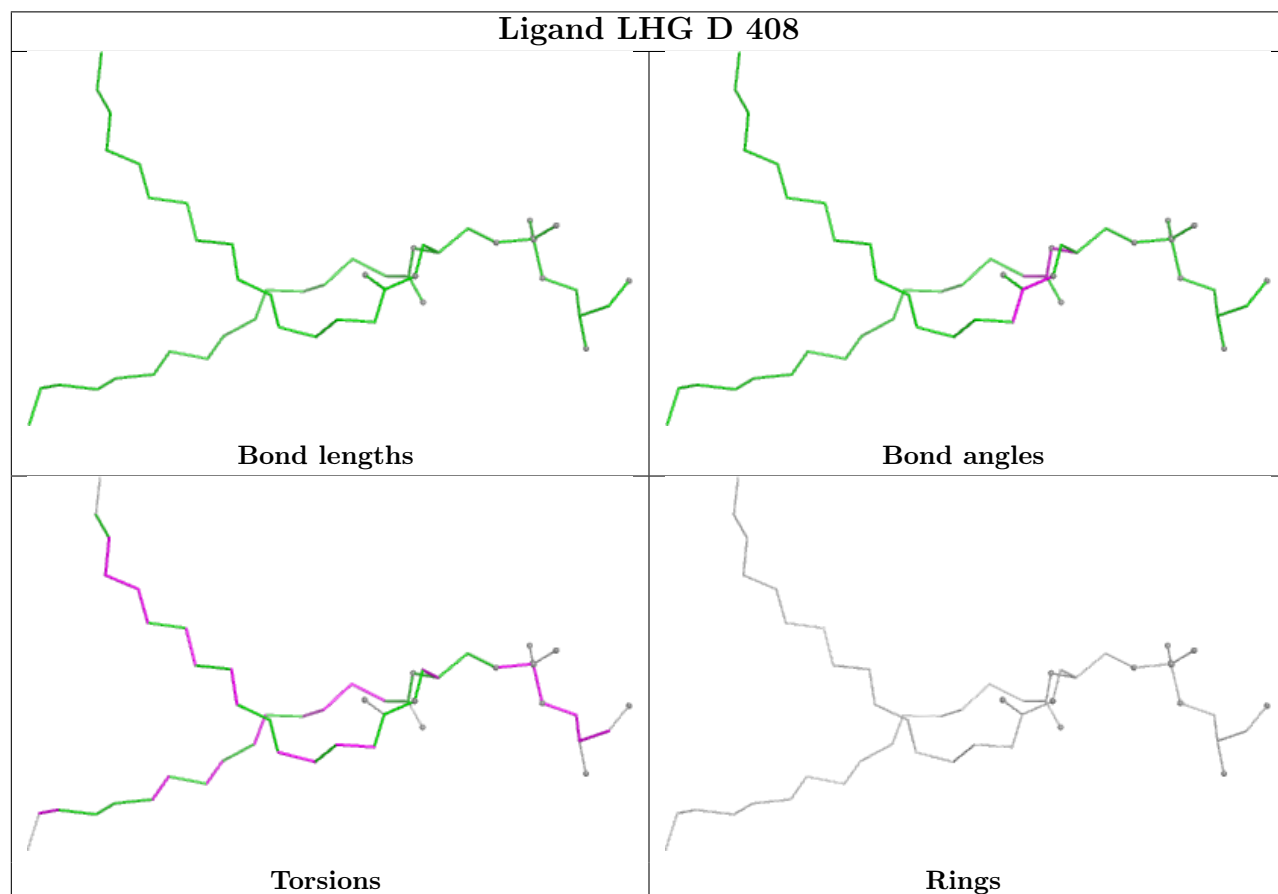
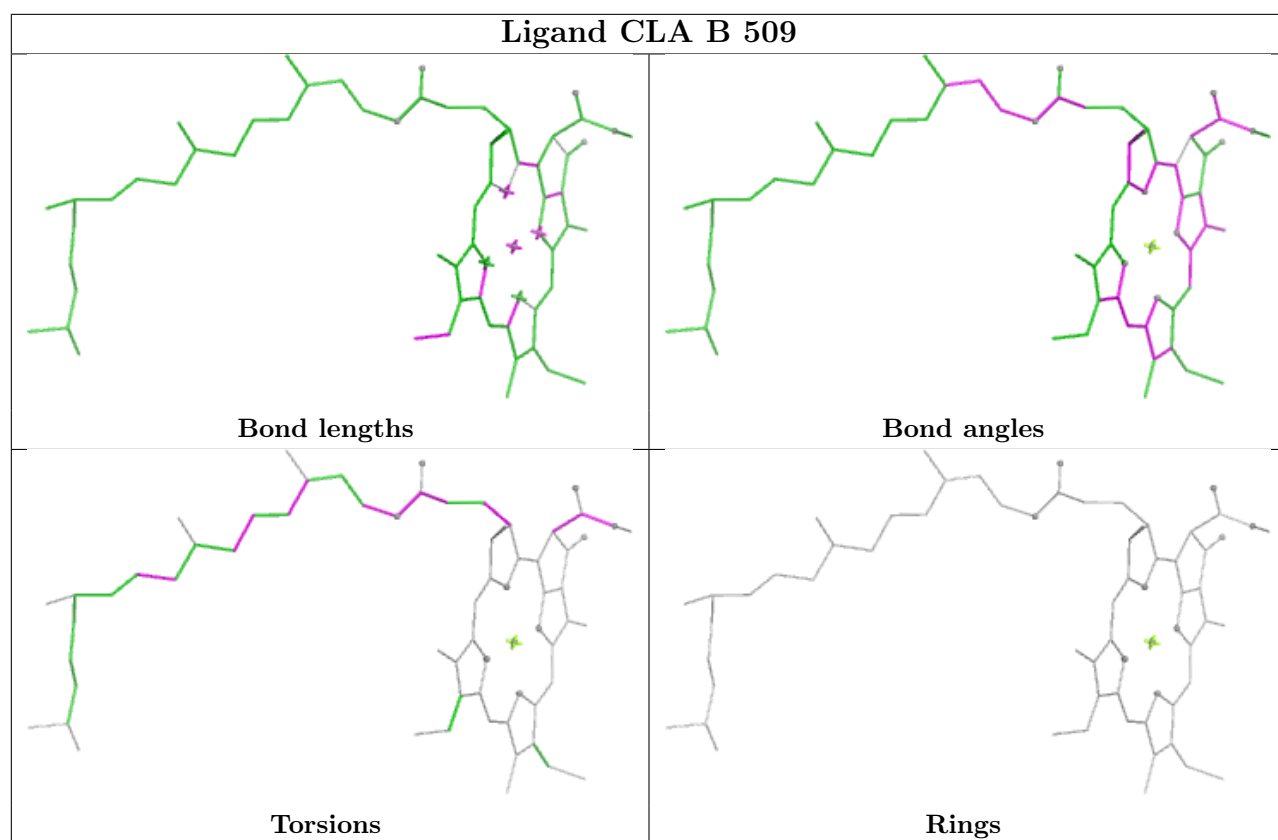


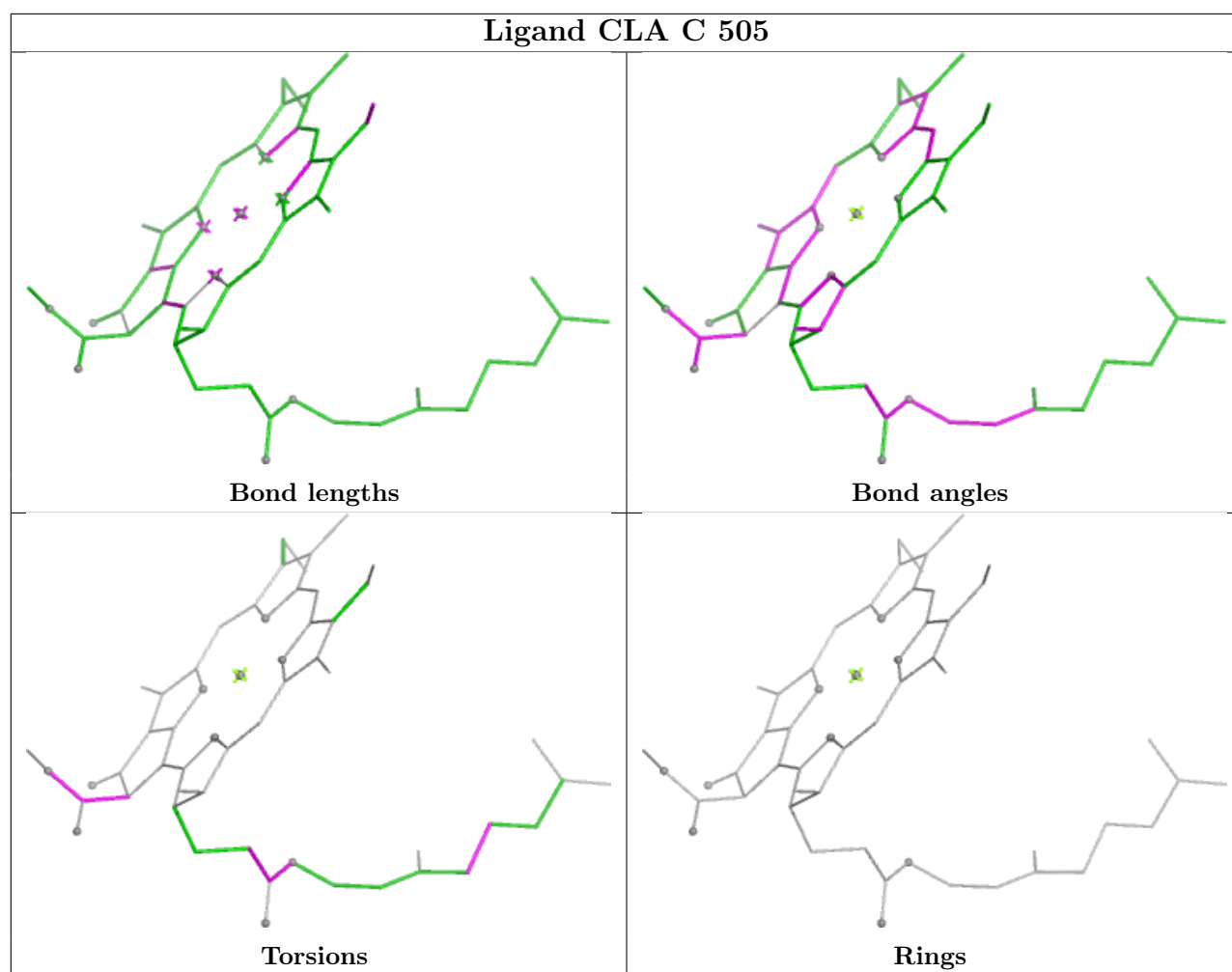
Torsions

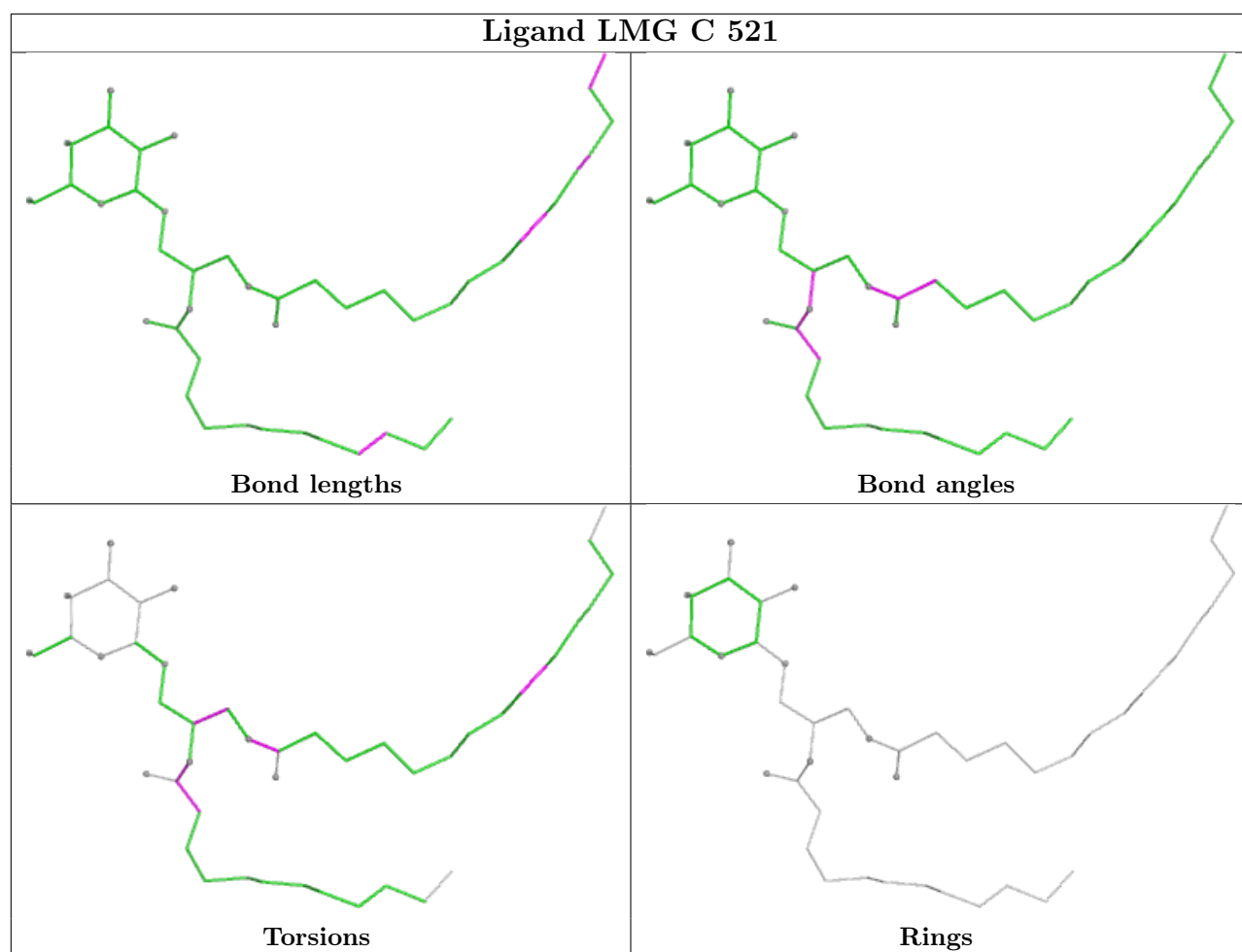


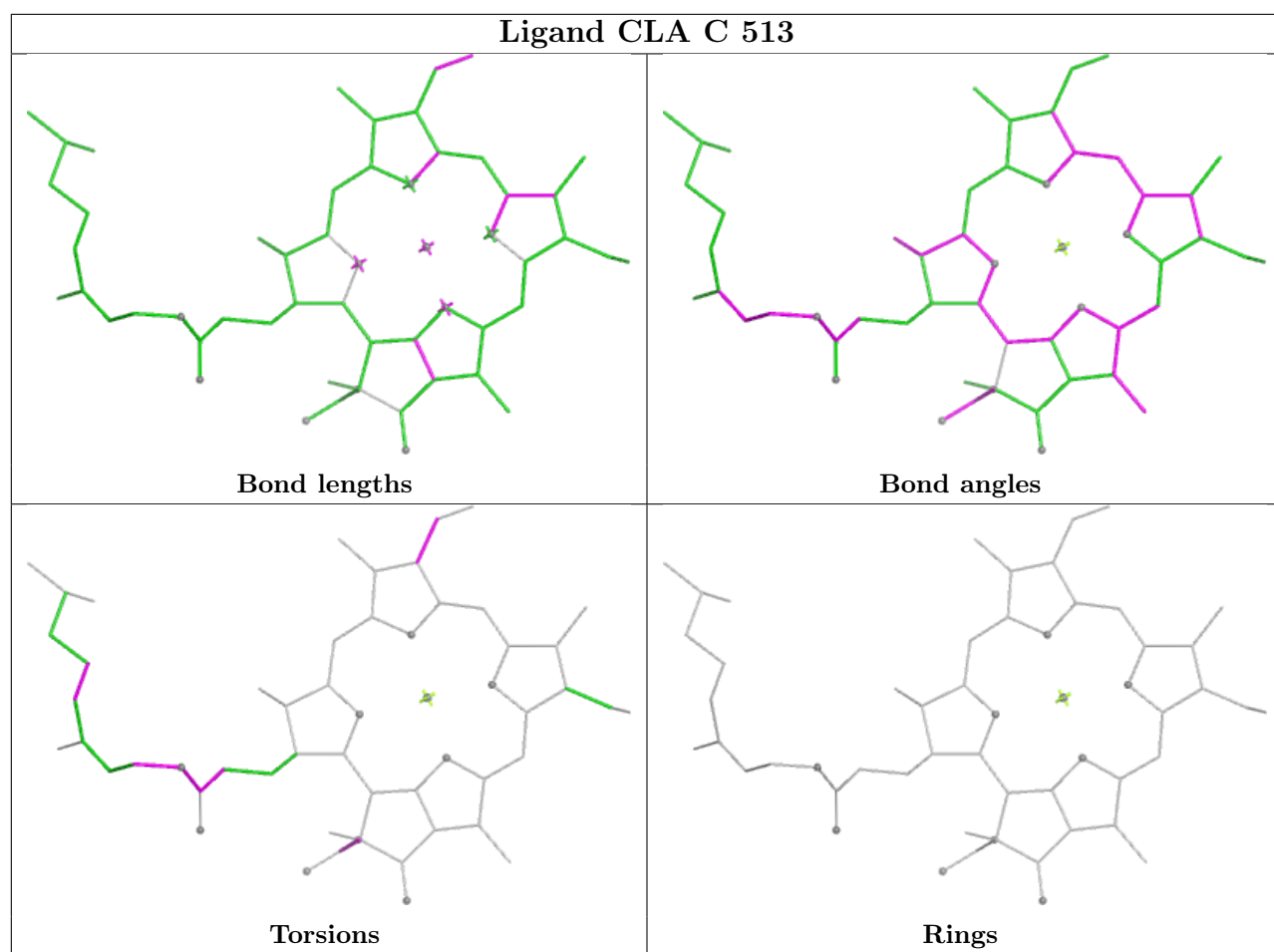
Rings

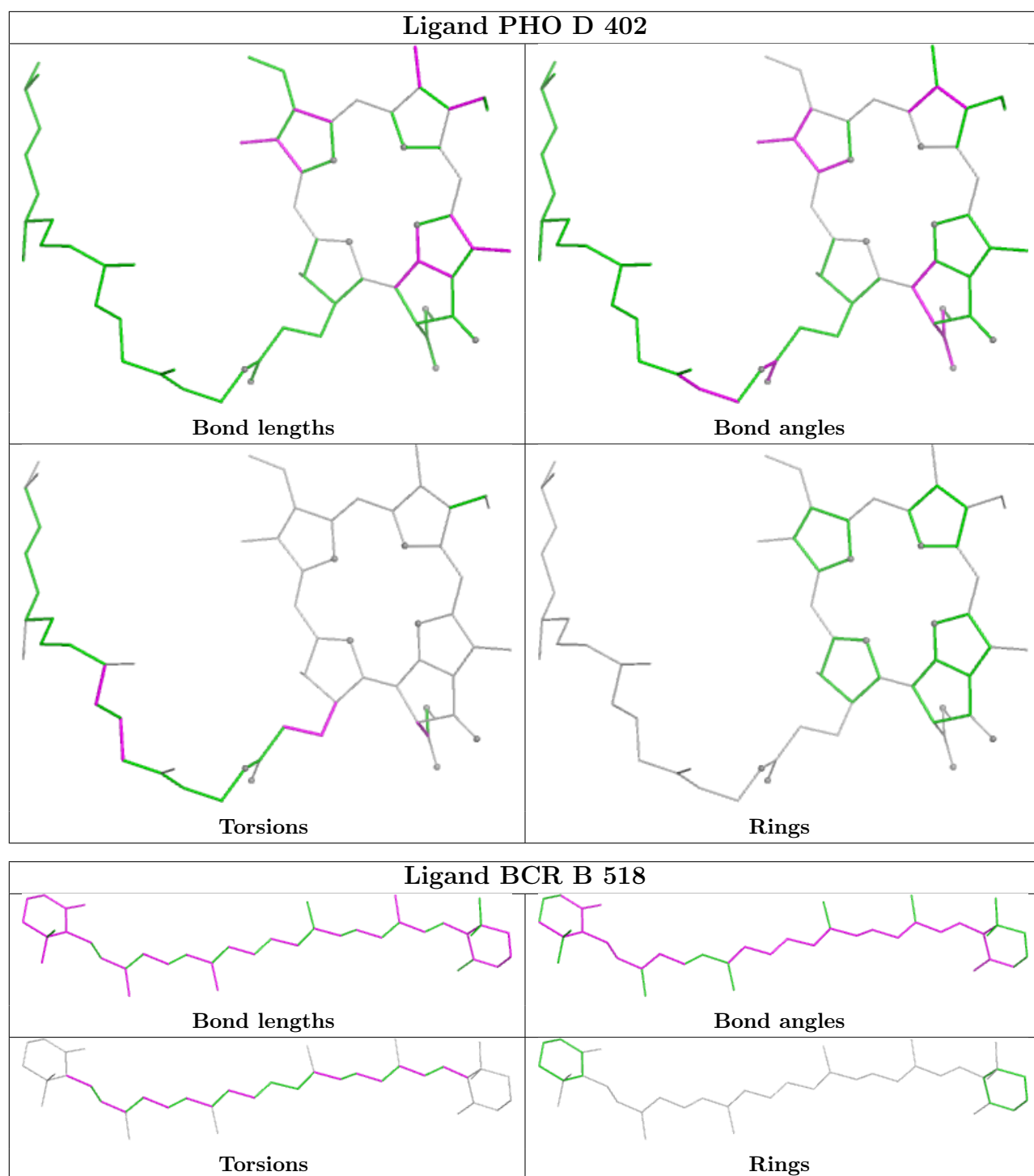


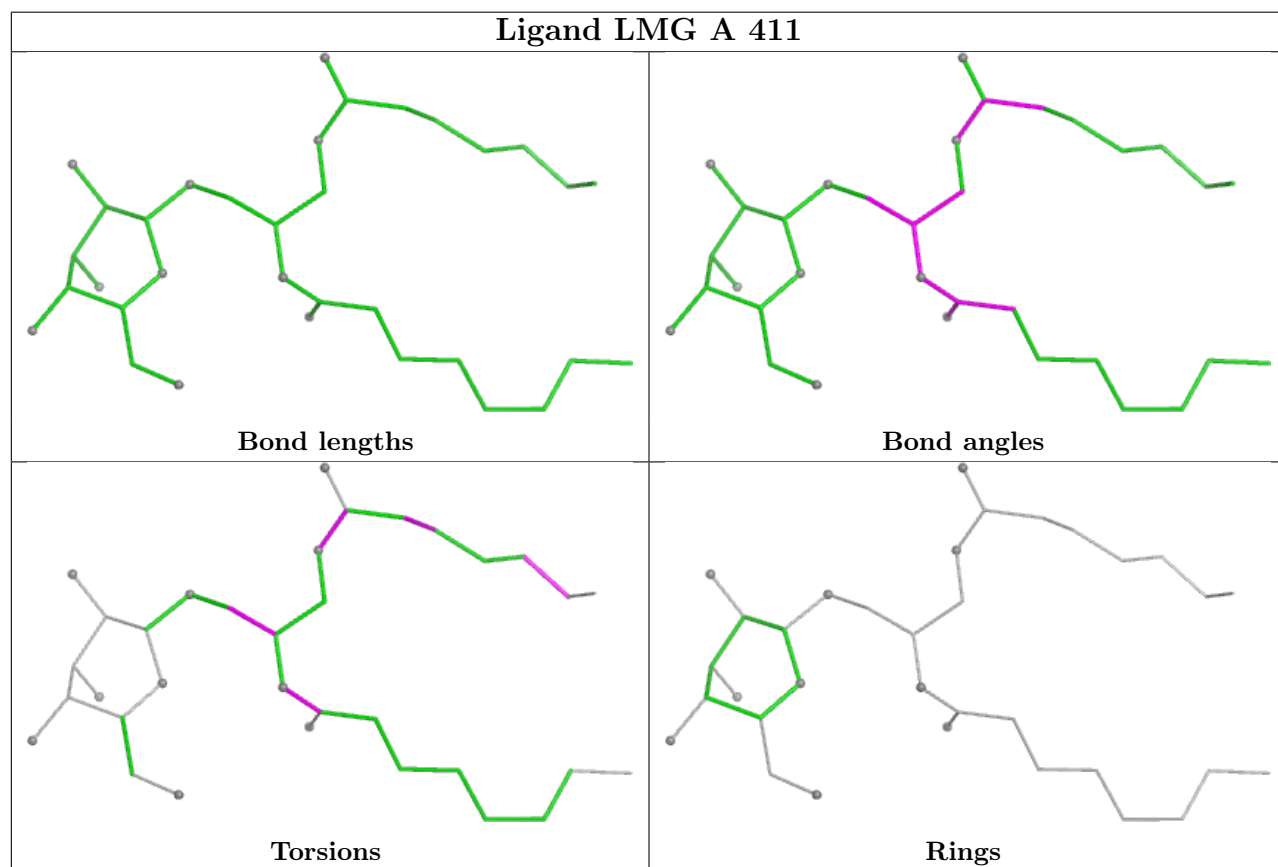
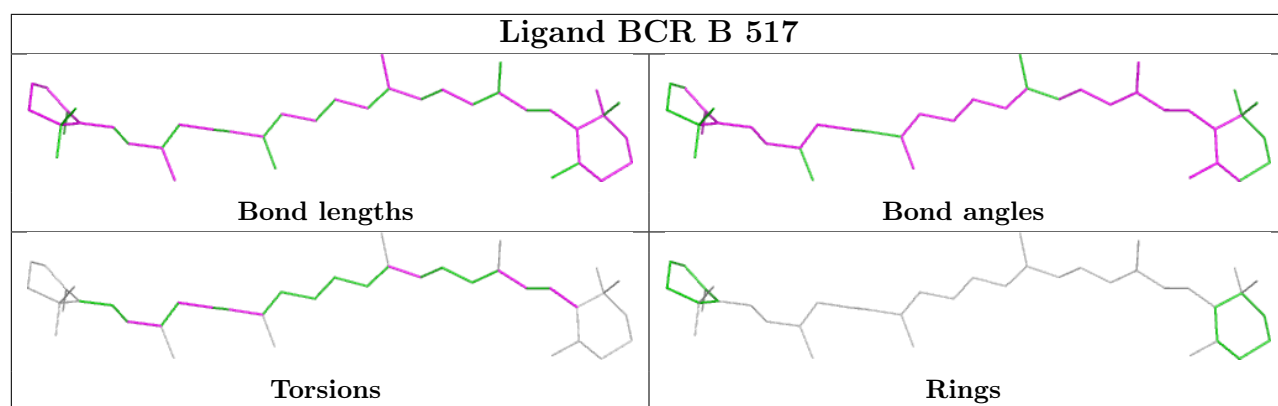


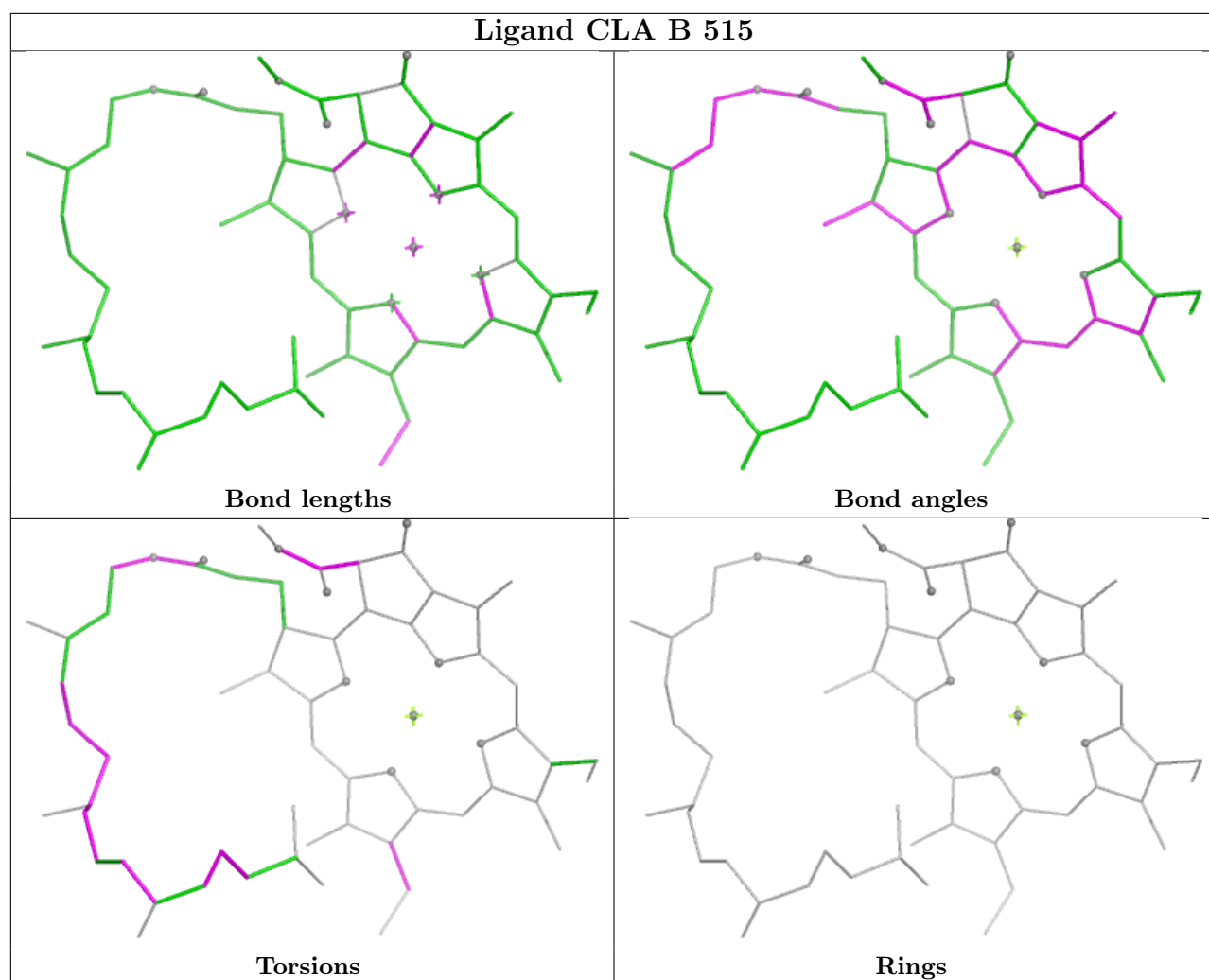


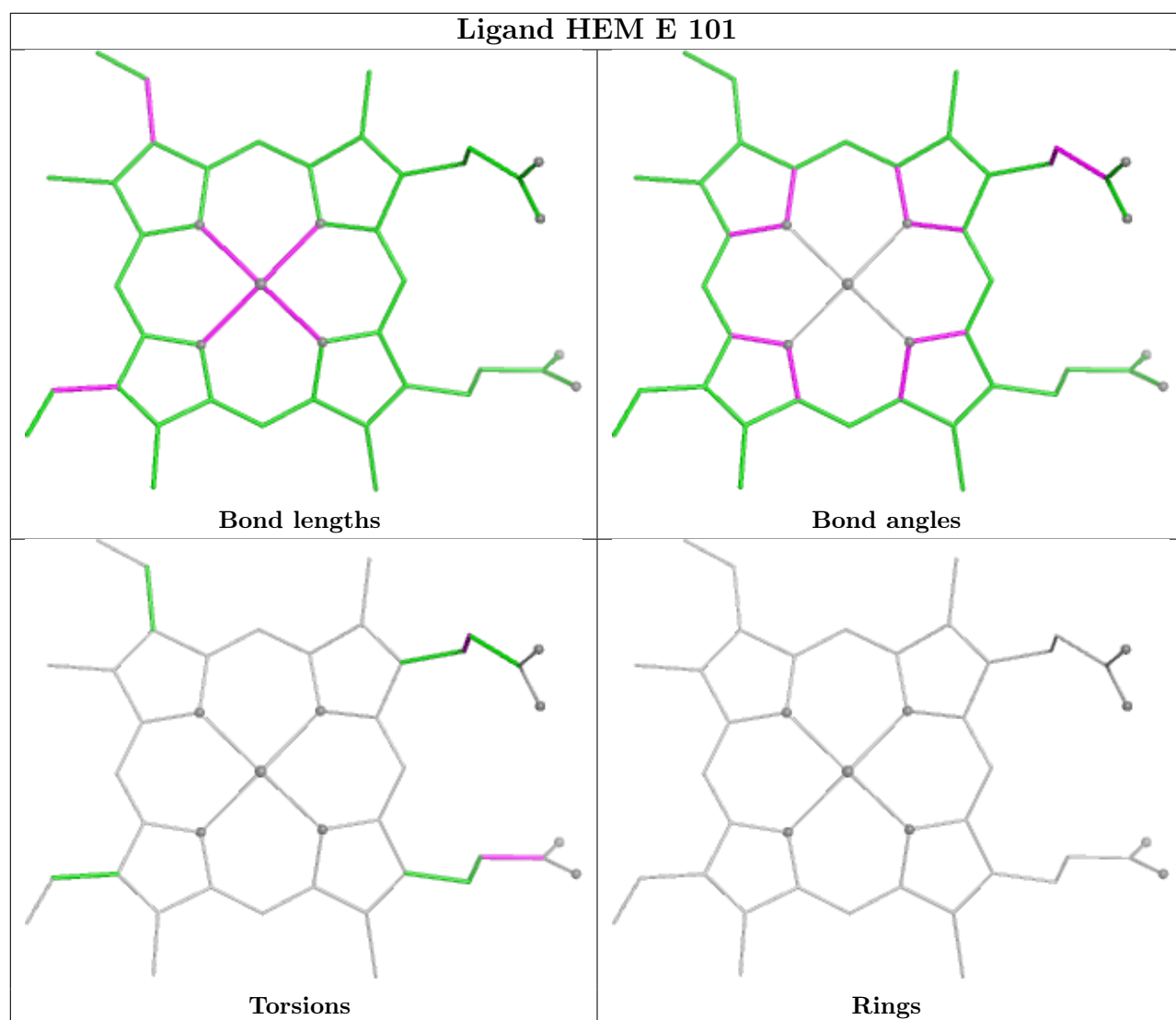




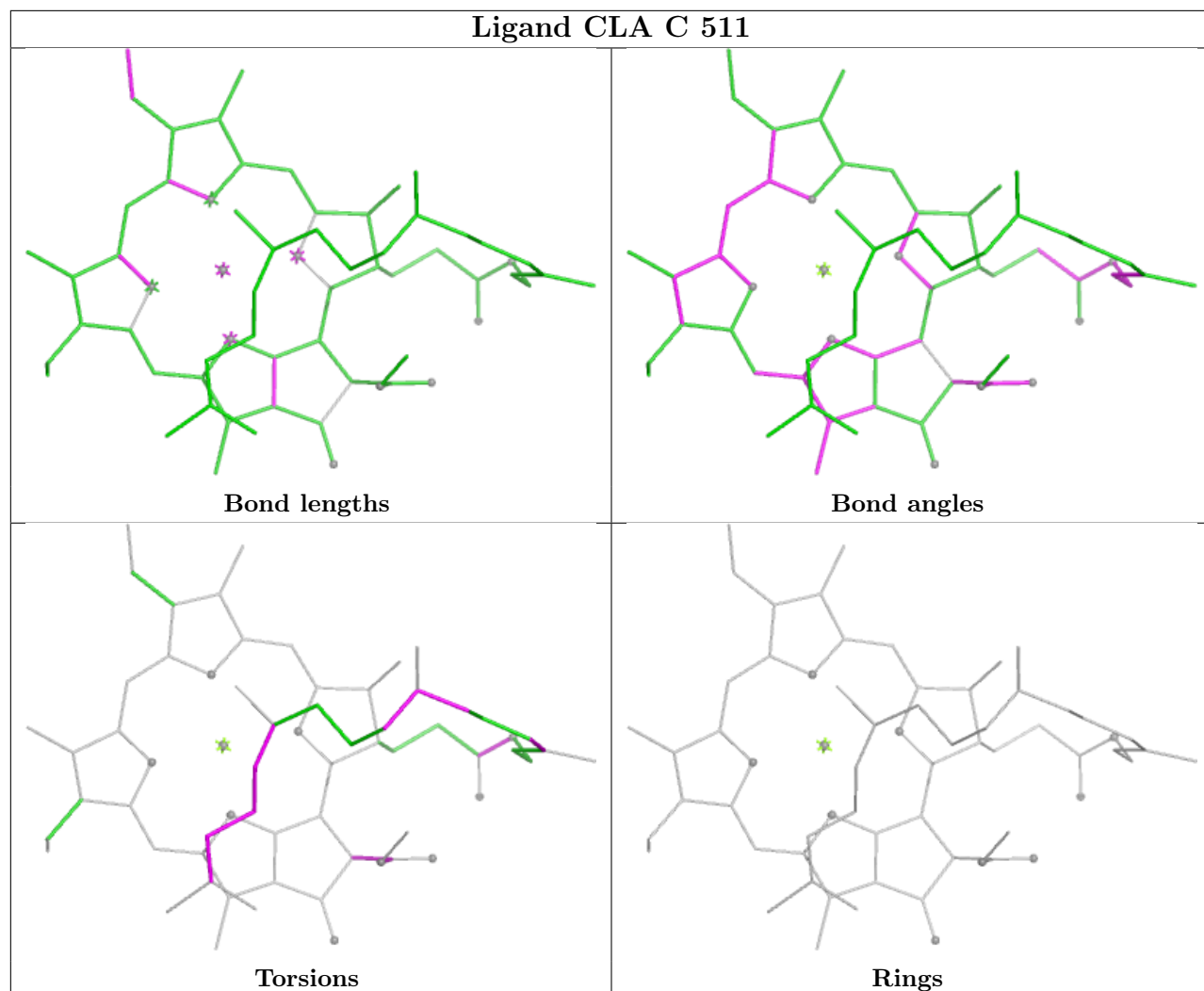


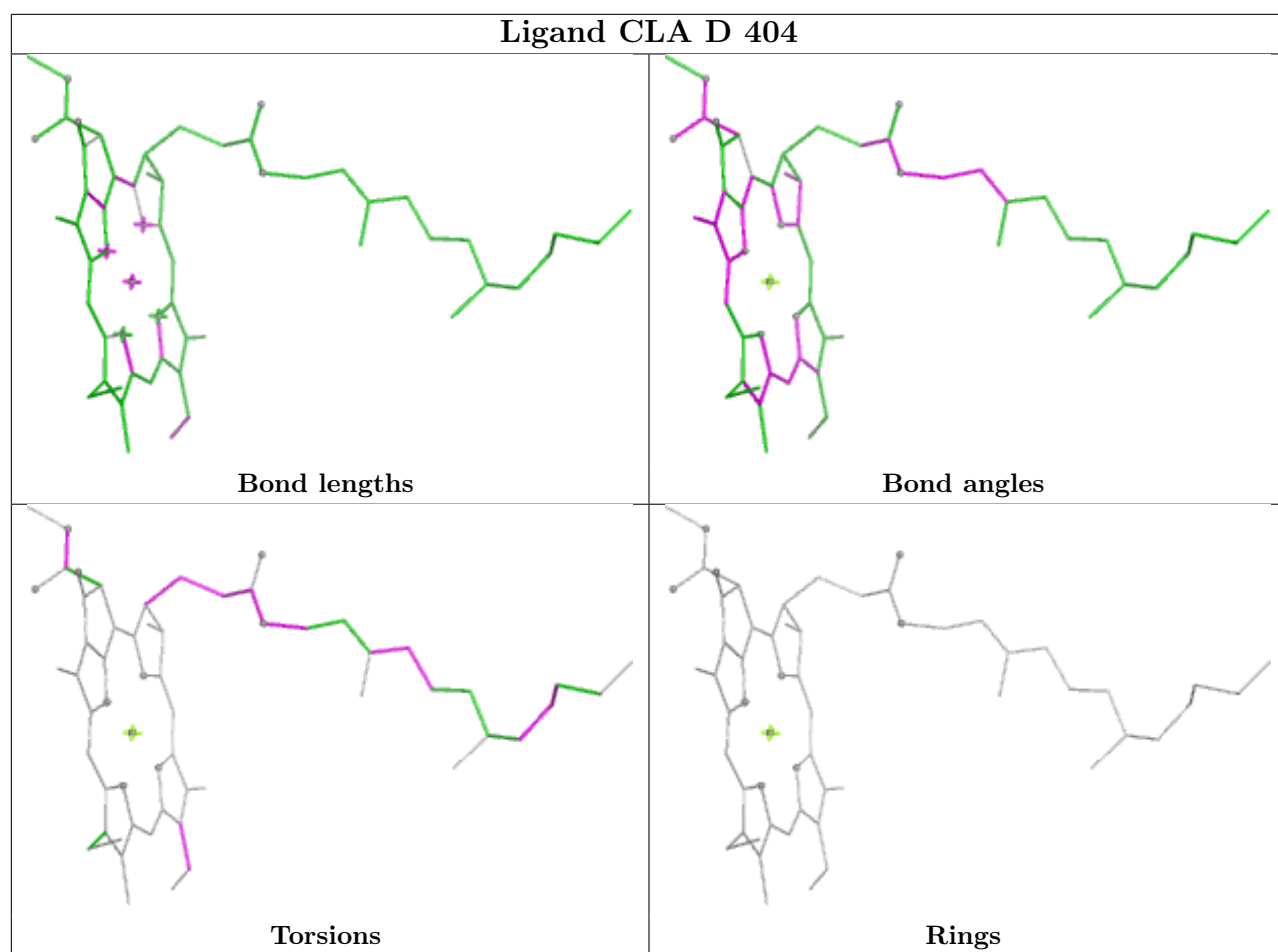


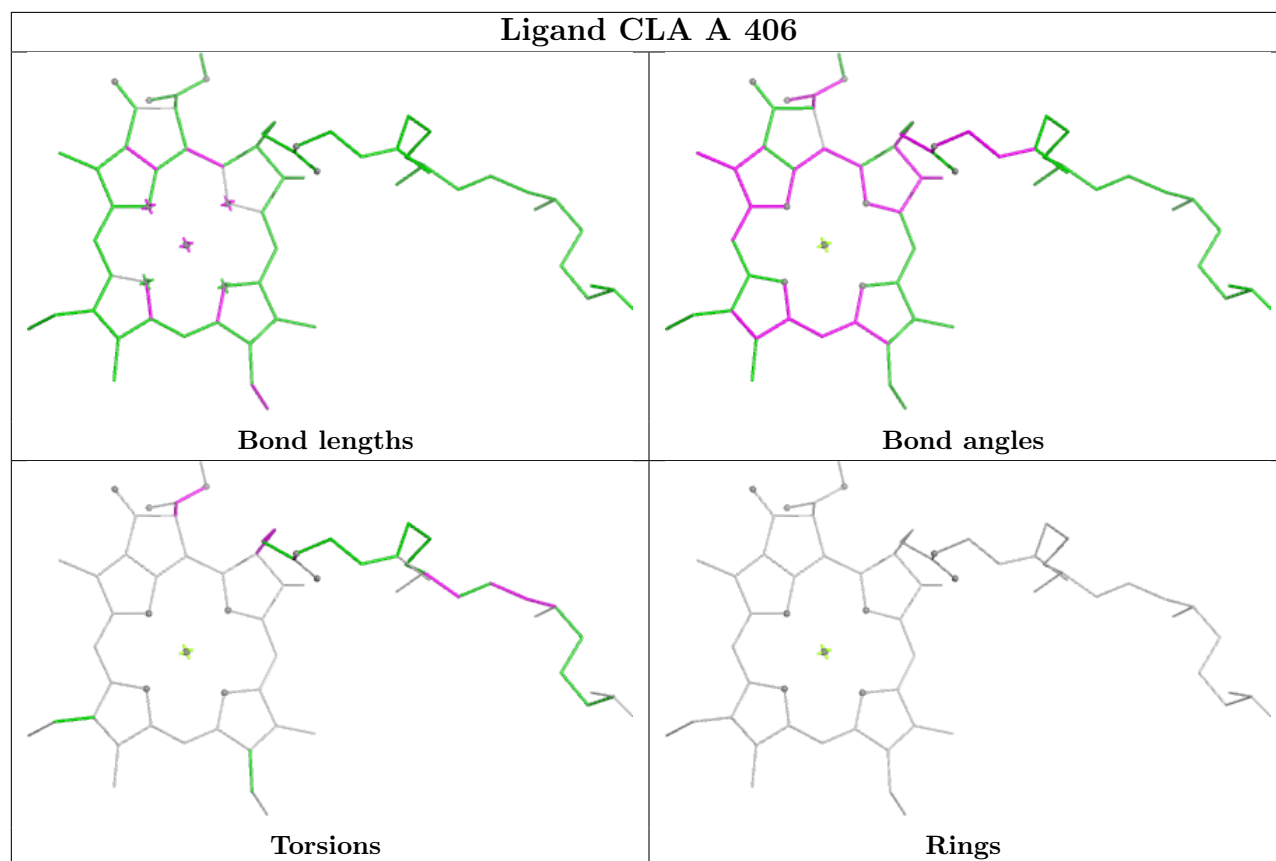
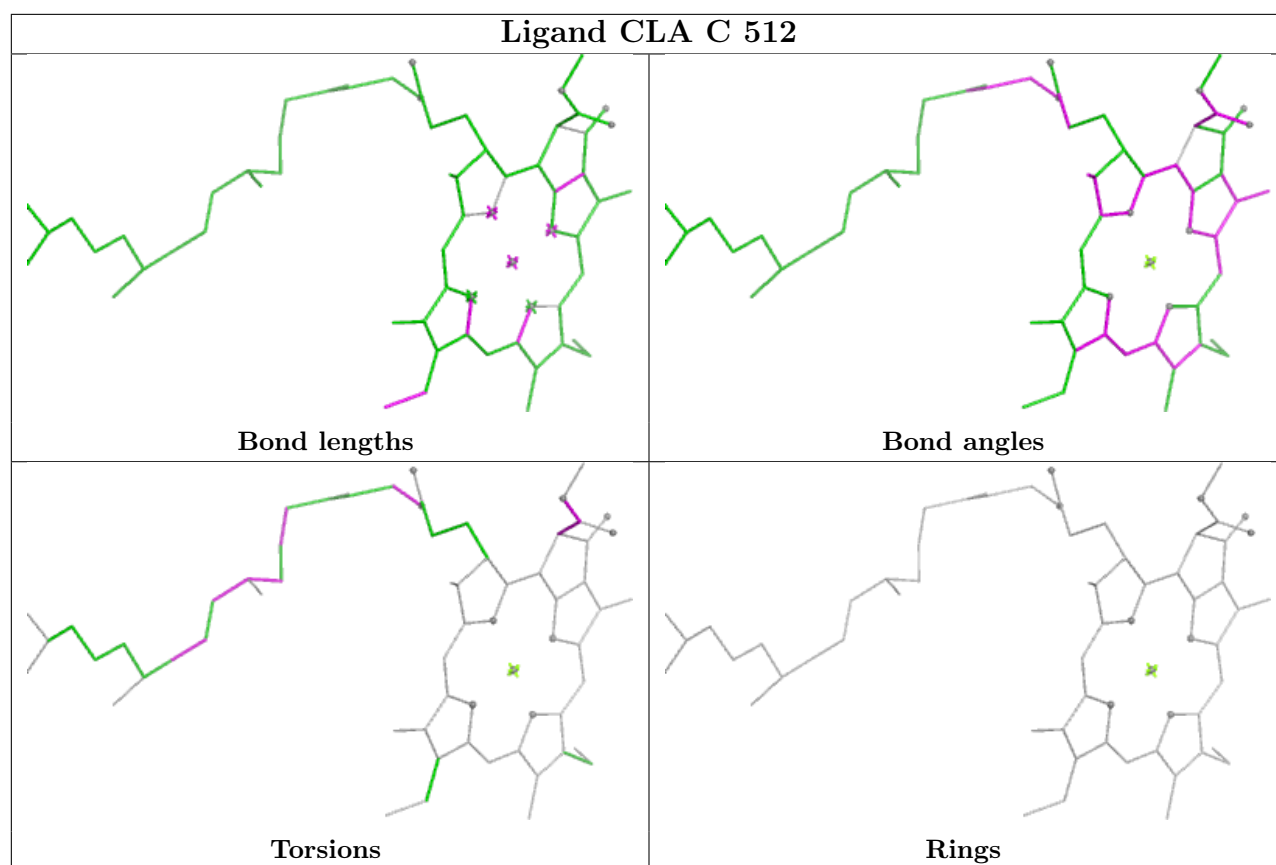


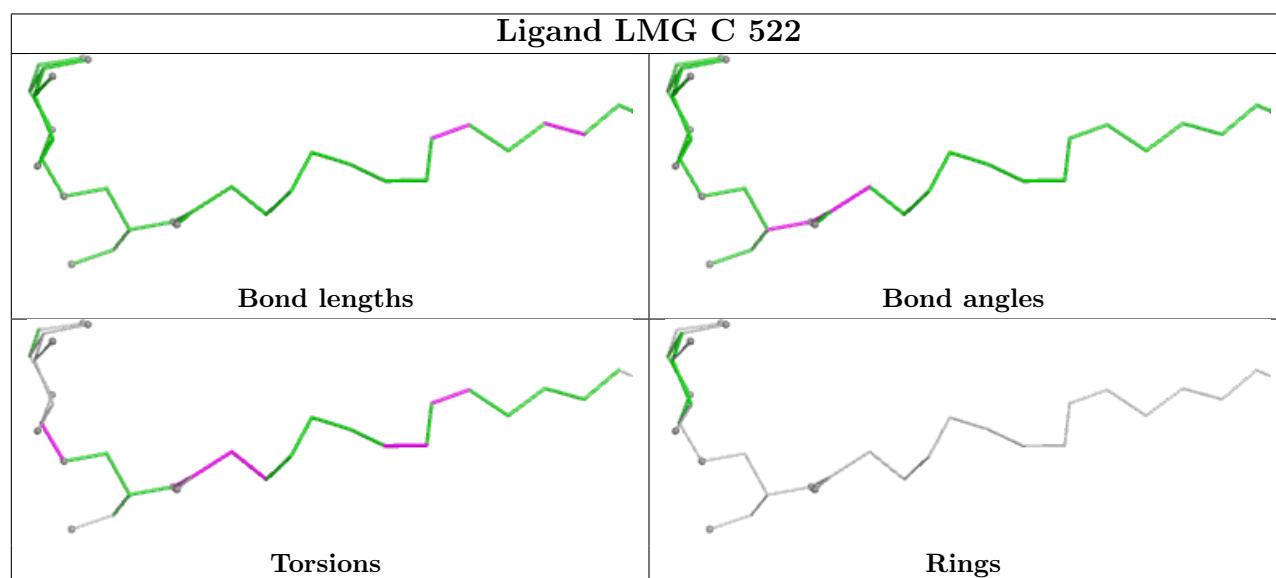
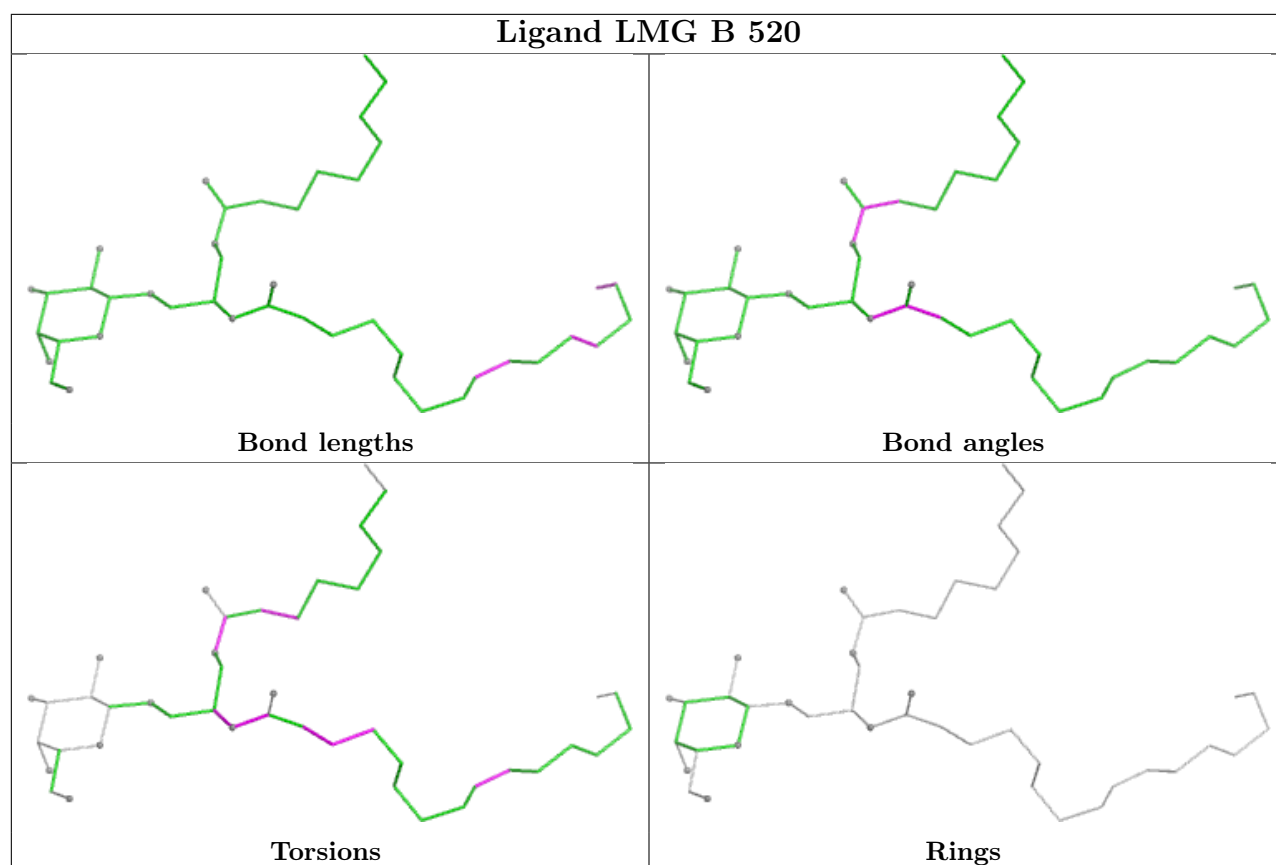


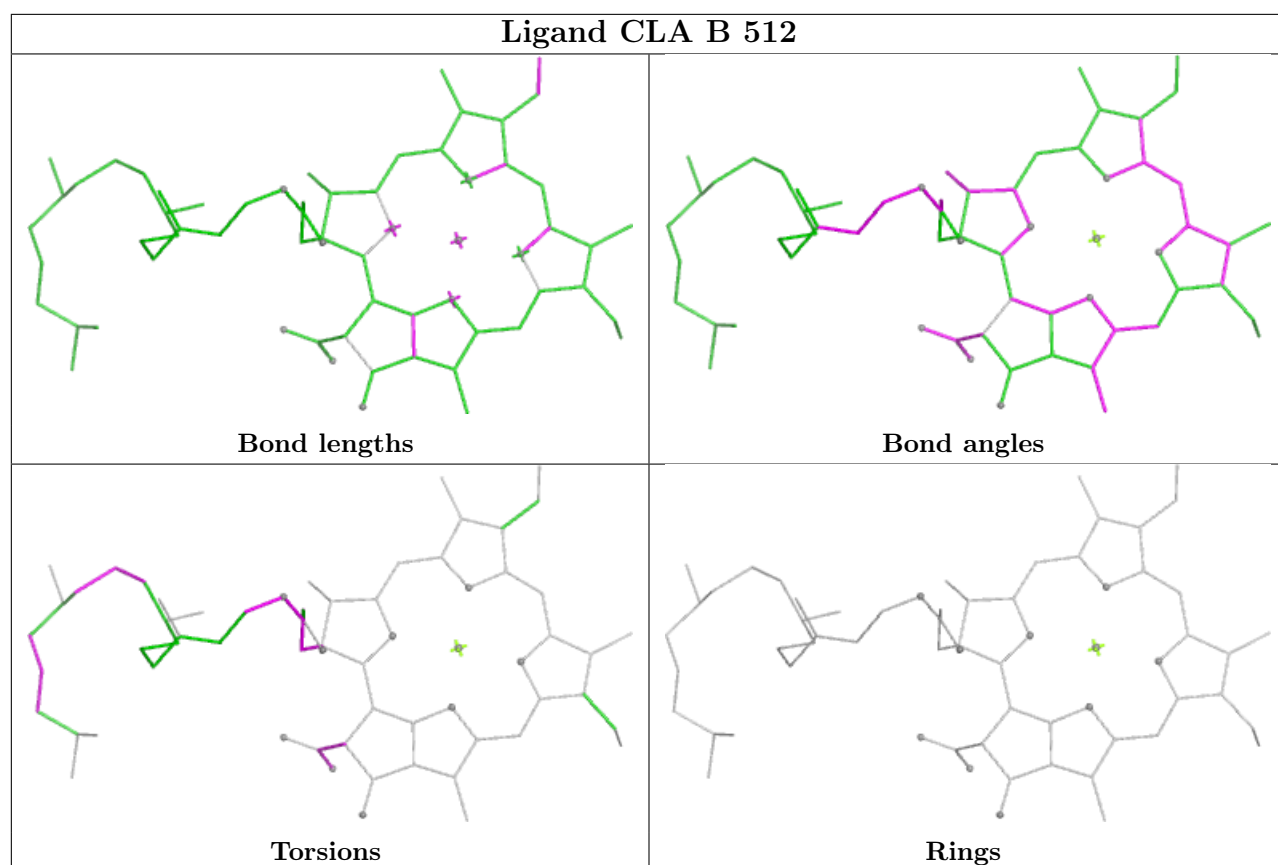
Ligand CLA C 511

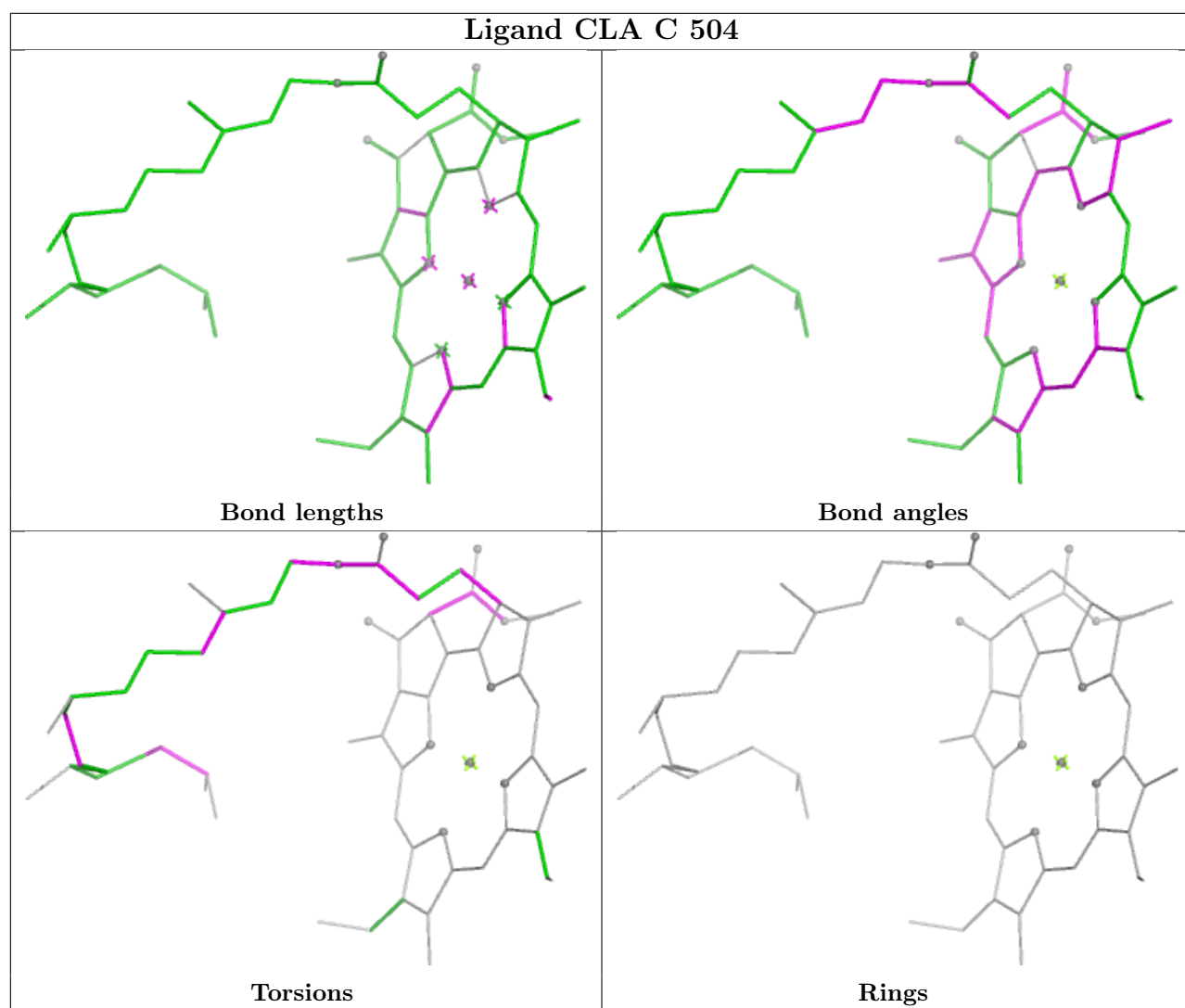


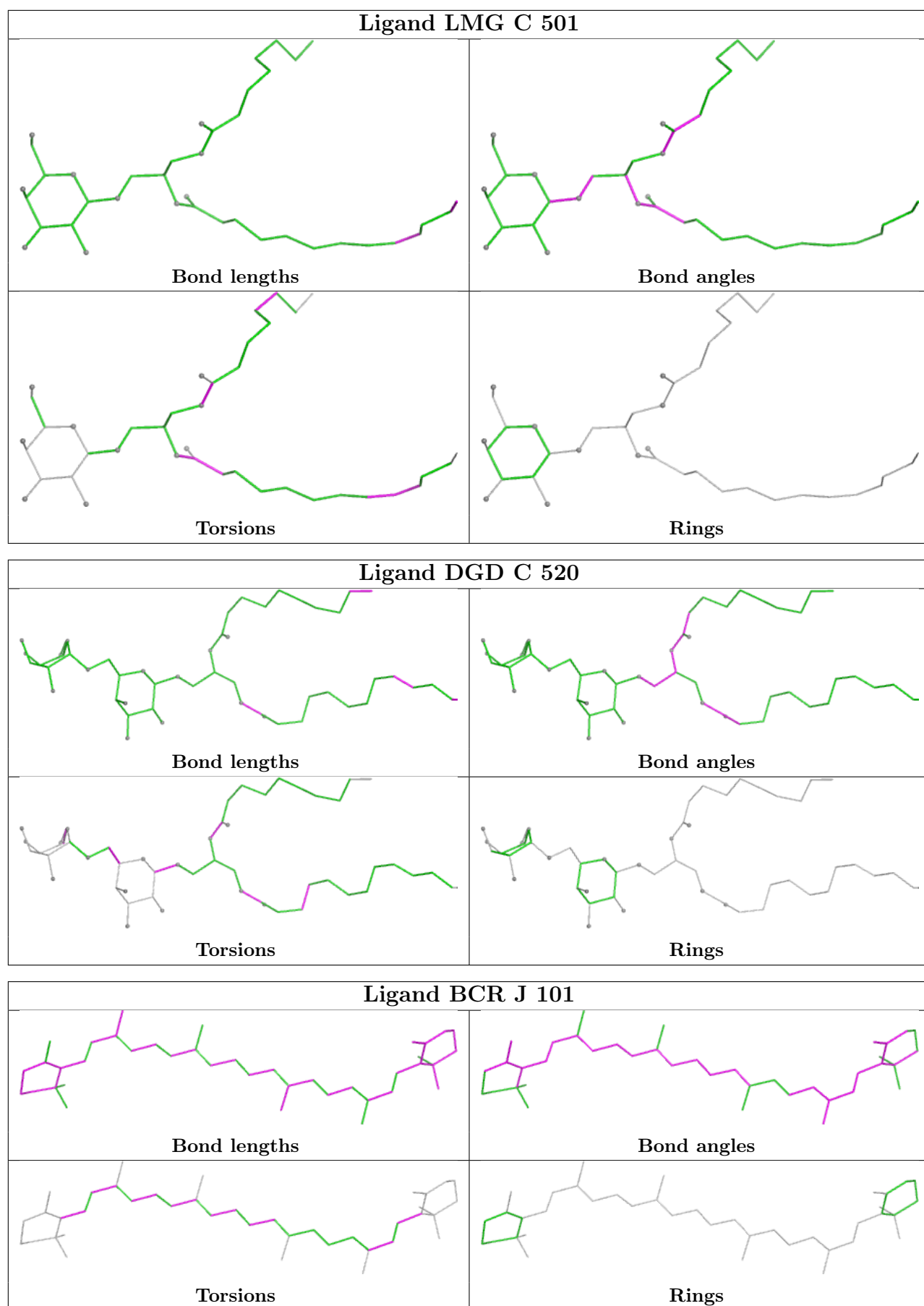


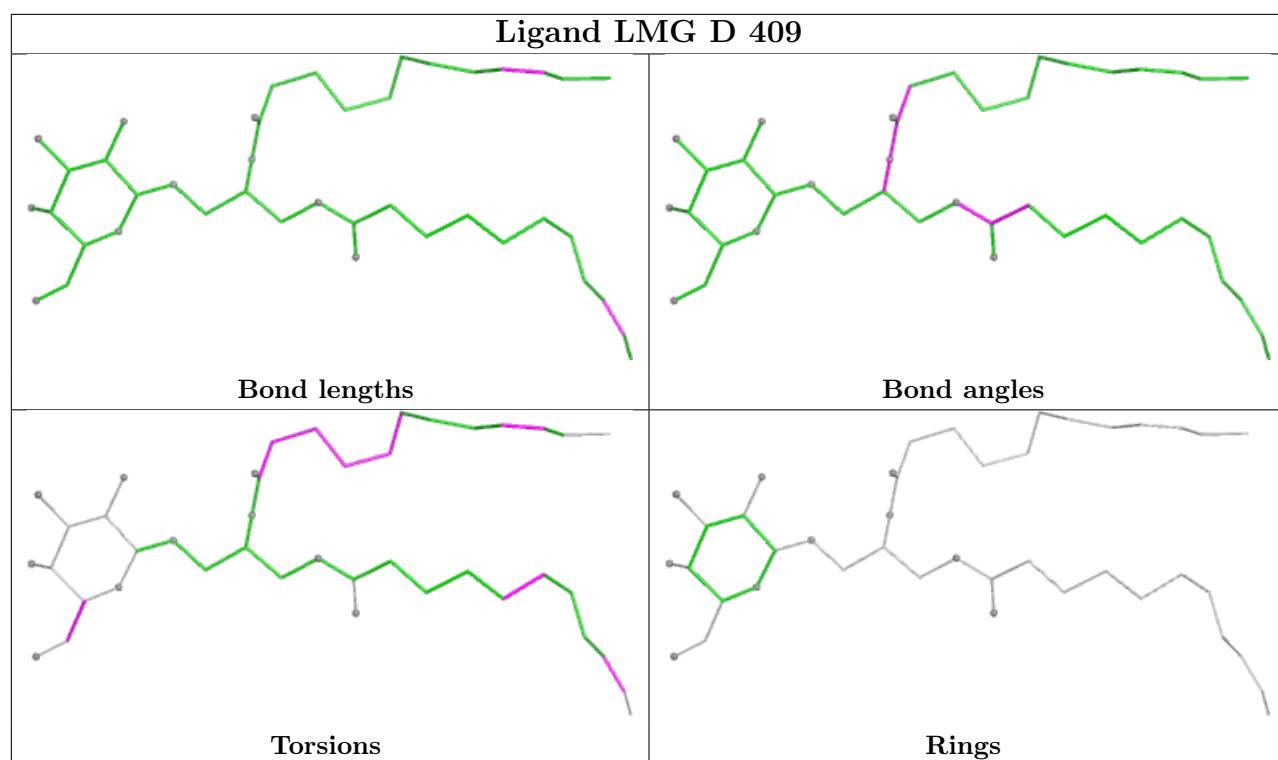


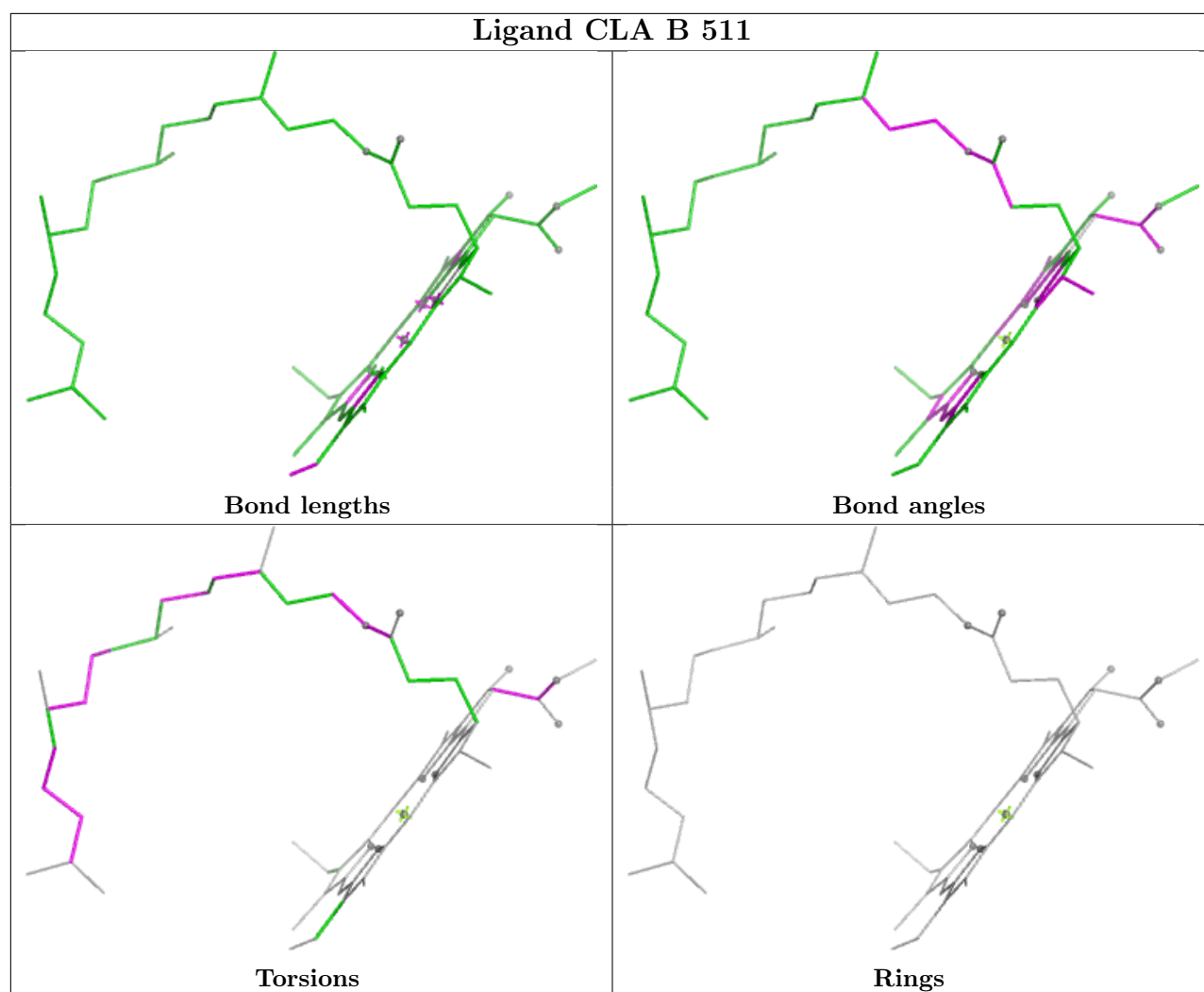


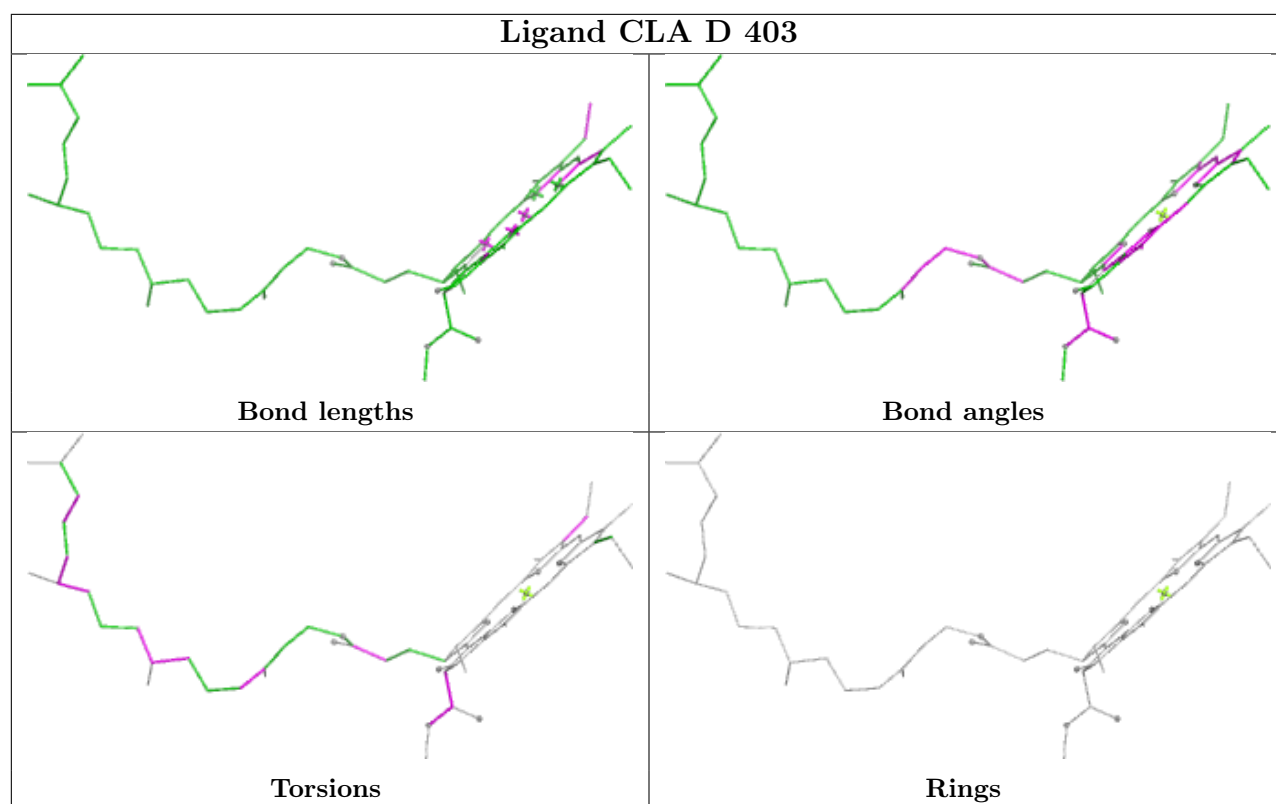


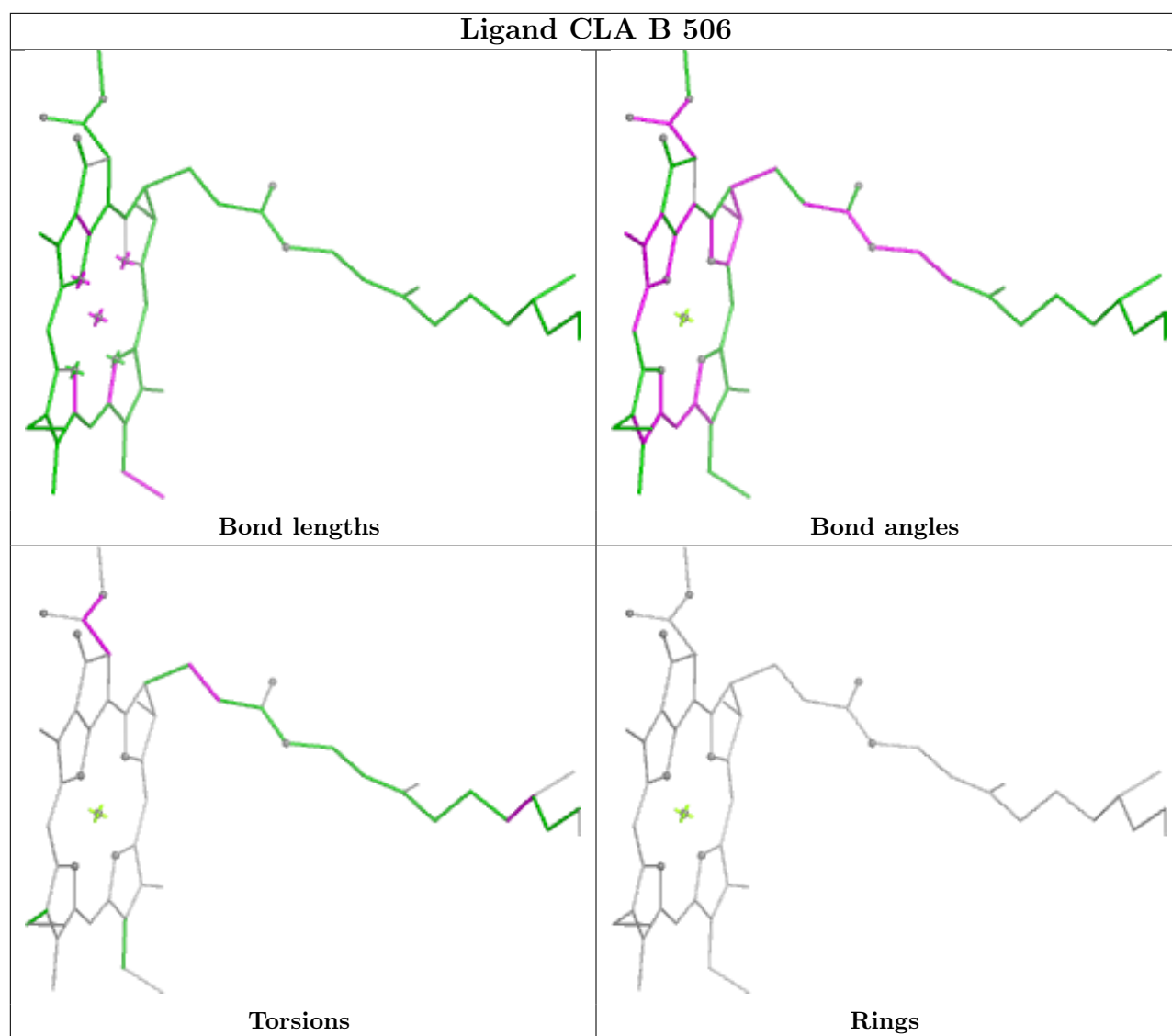


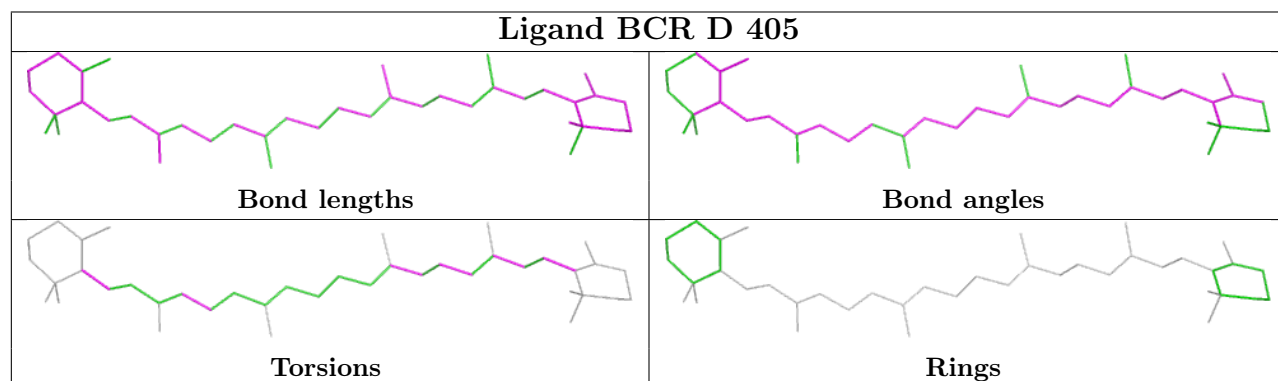
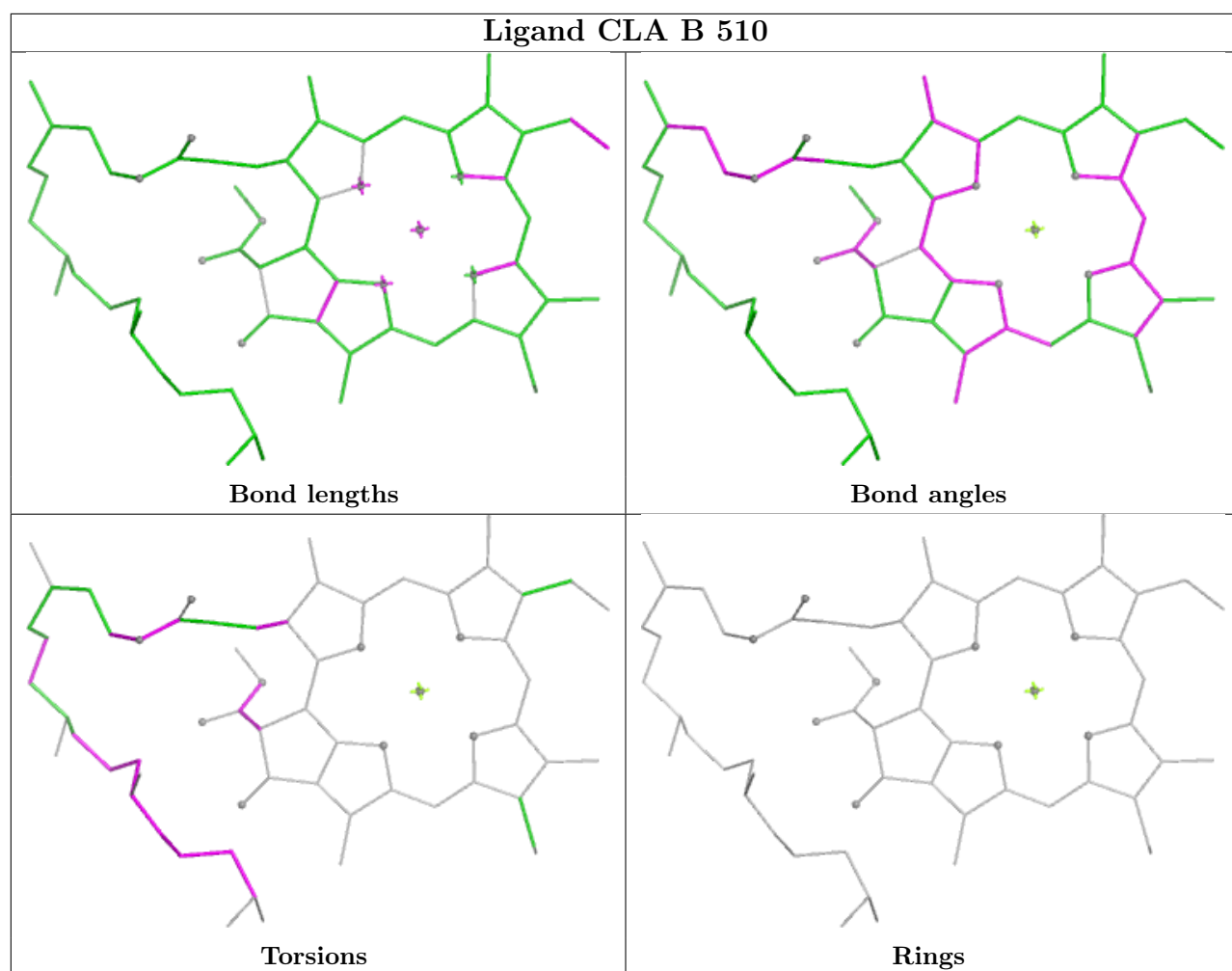


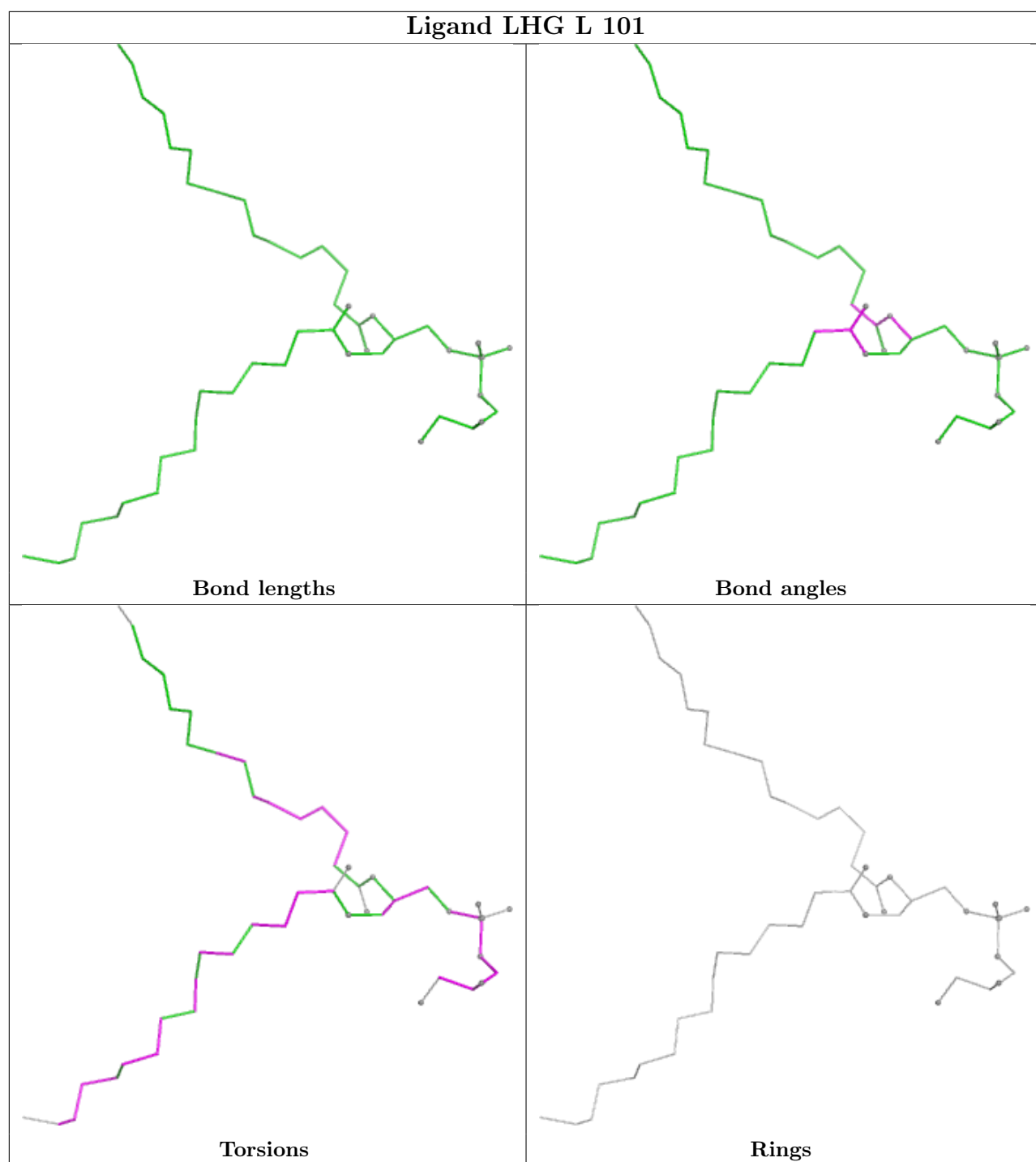


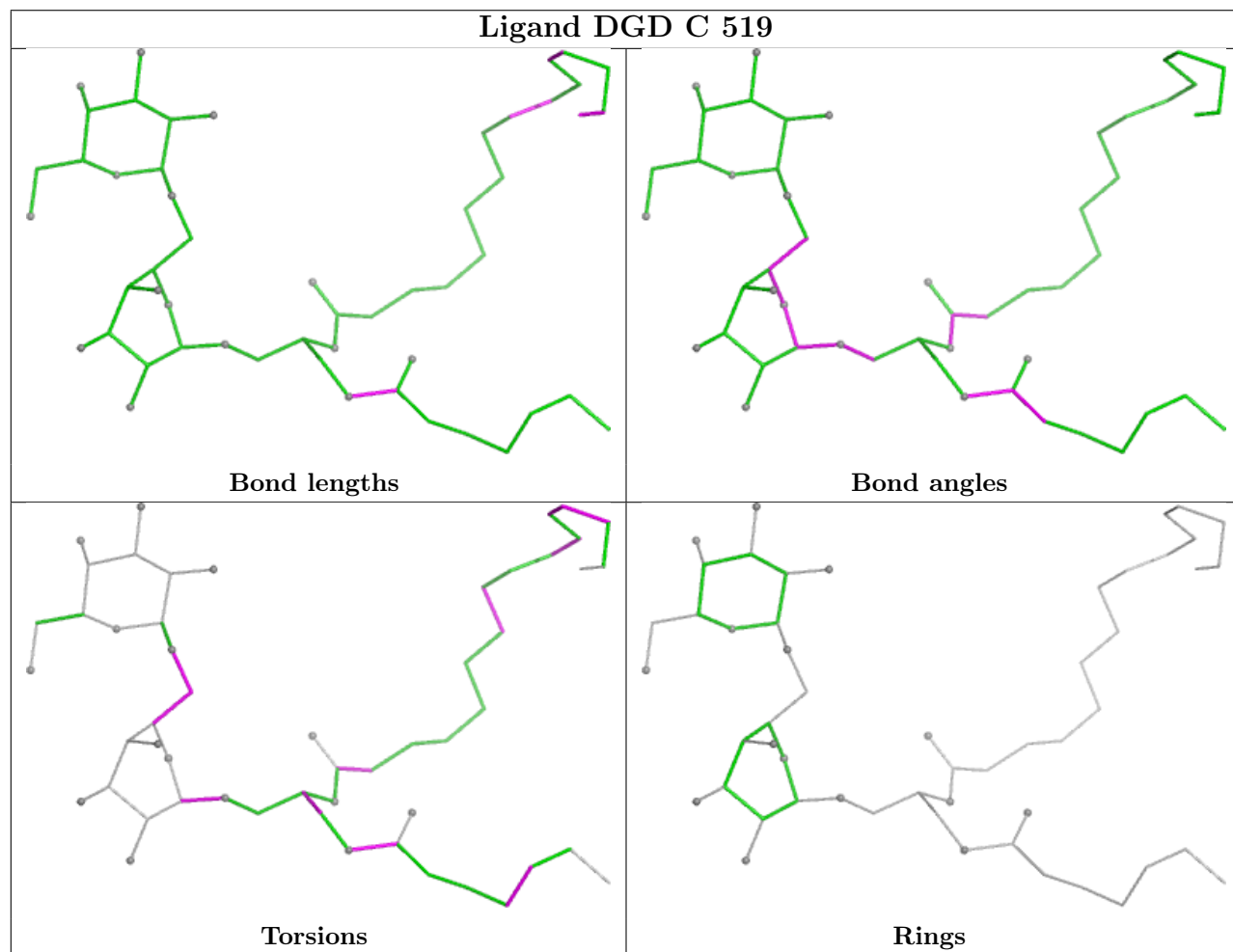
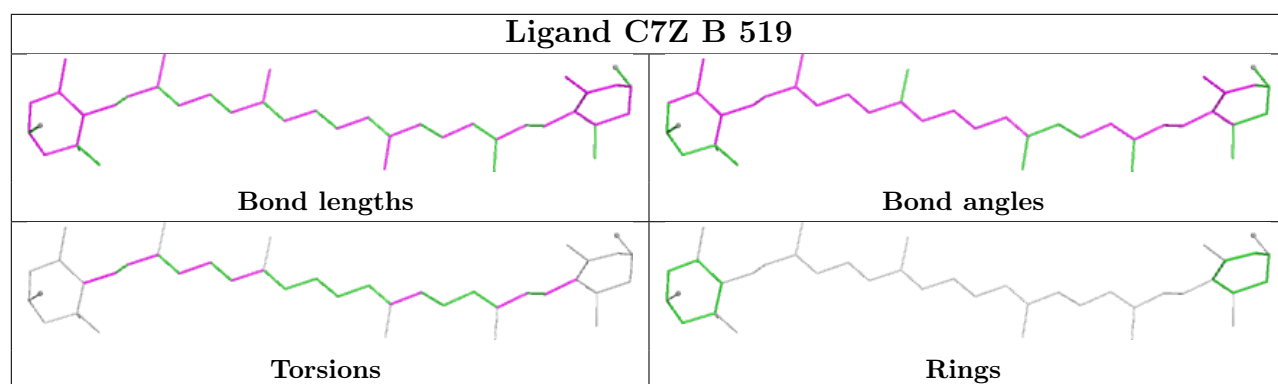


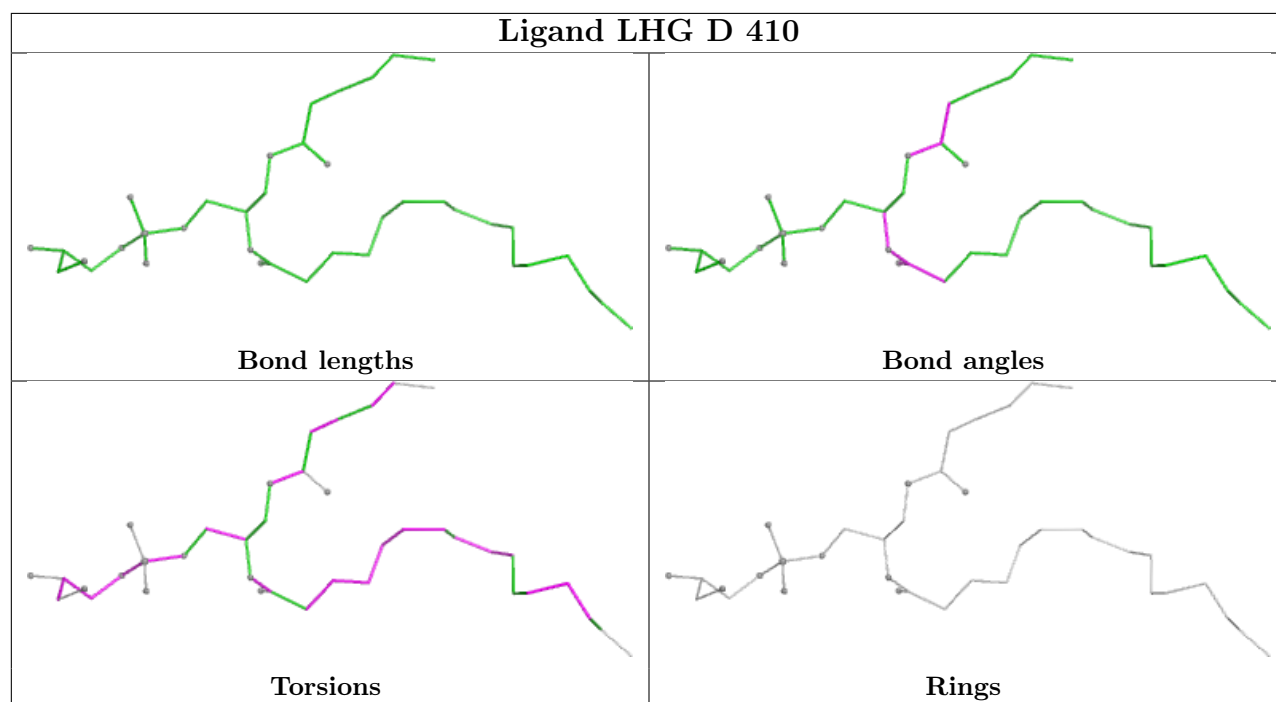
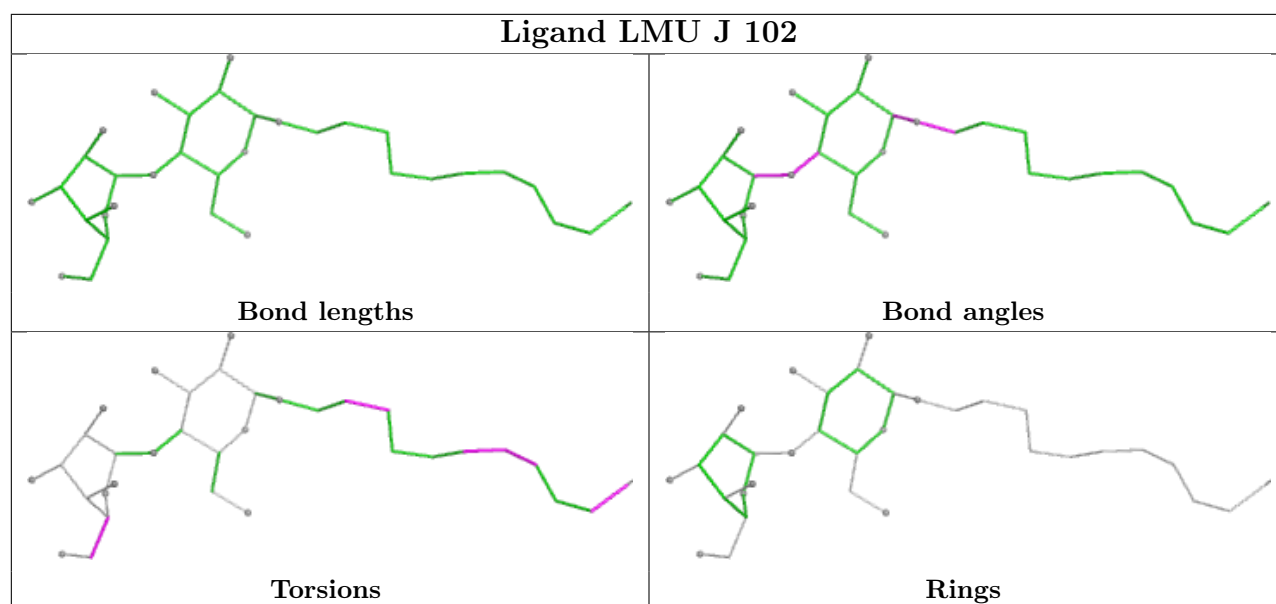


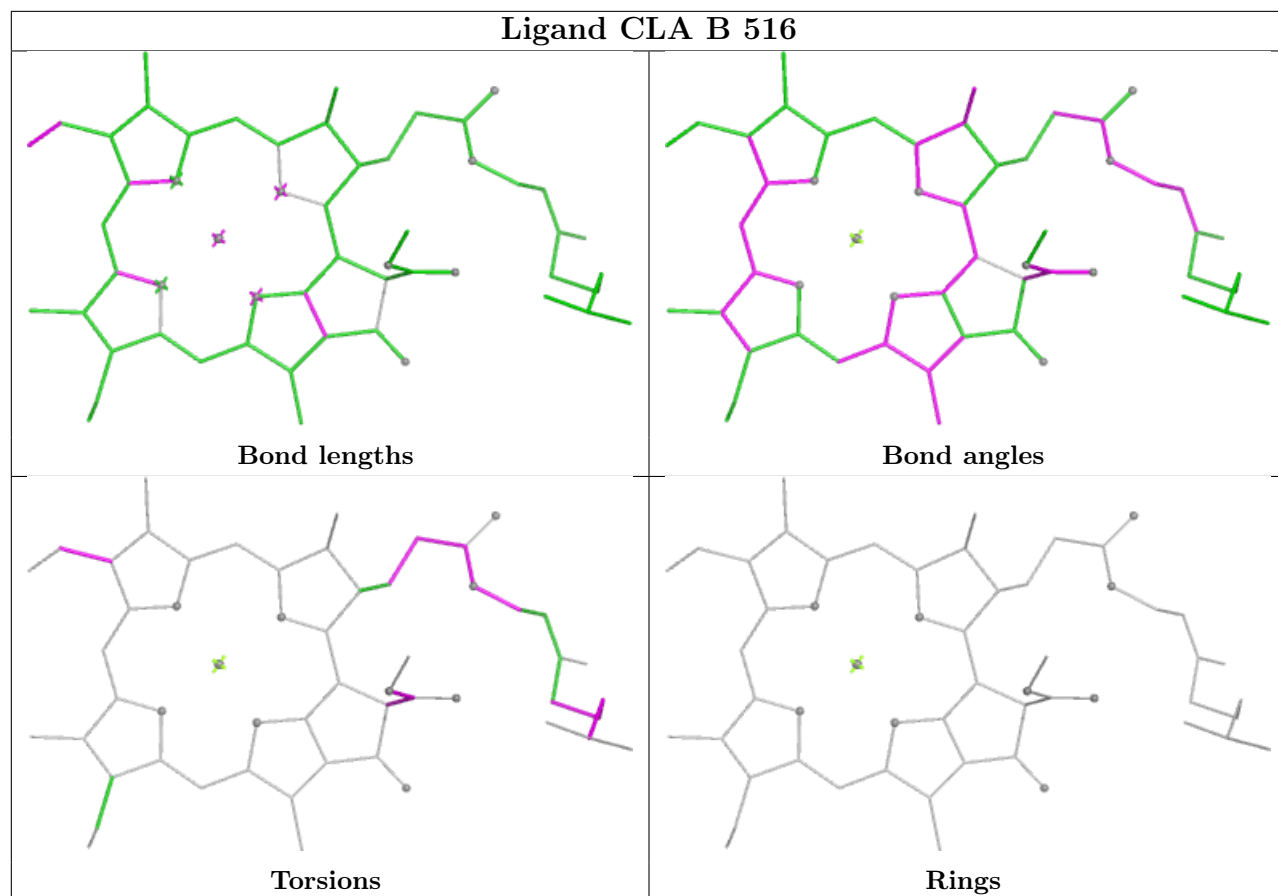


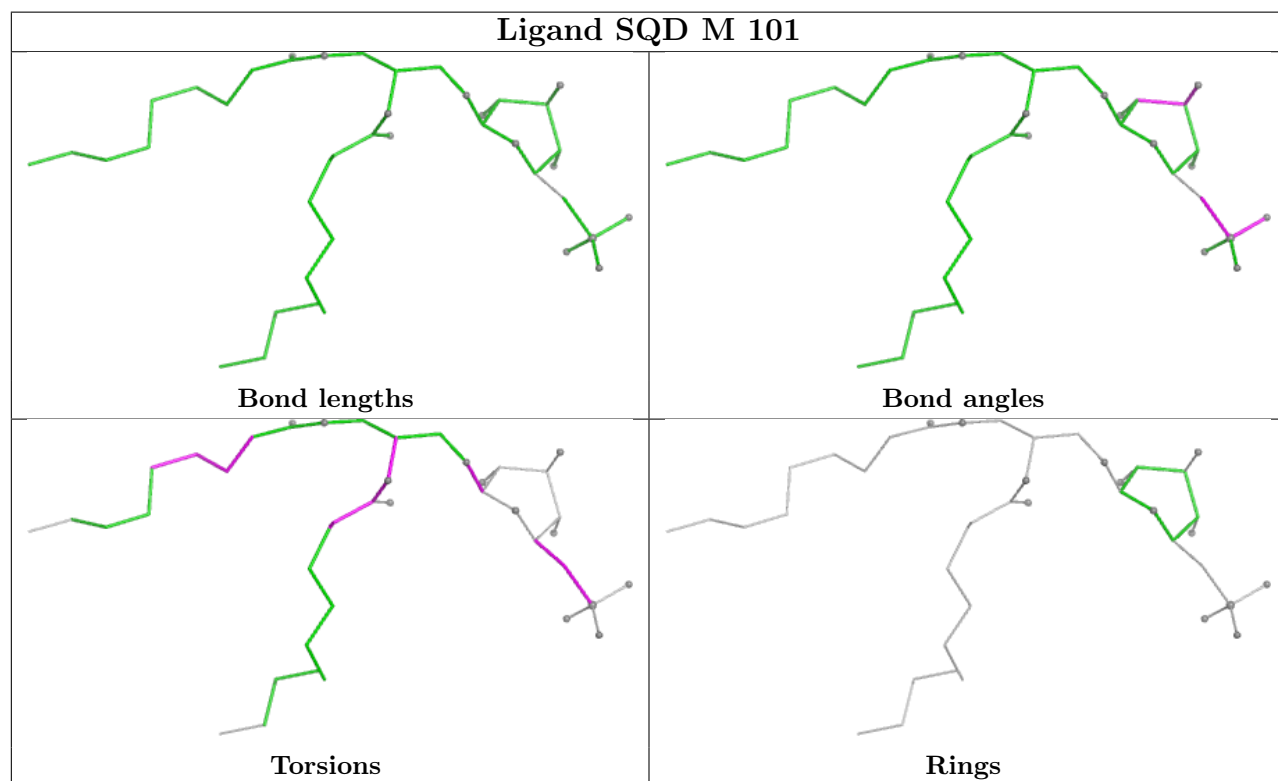
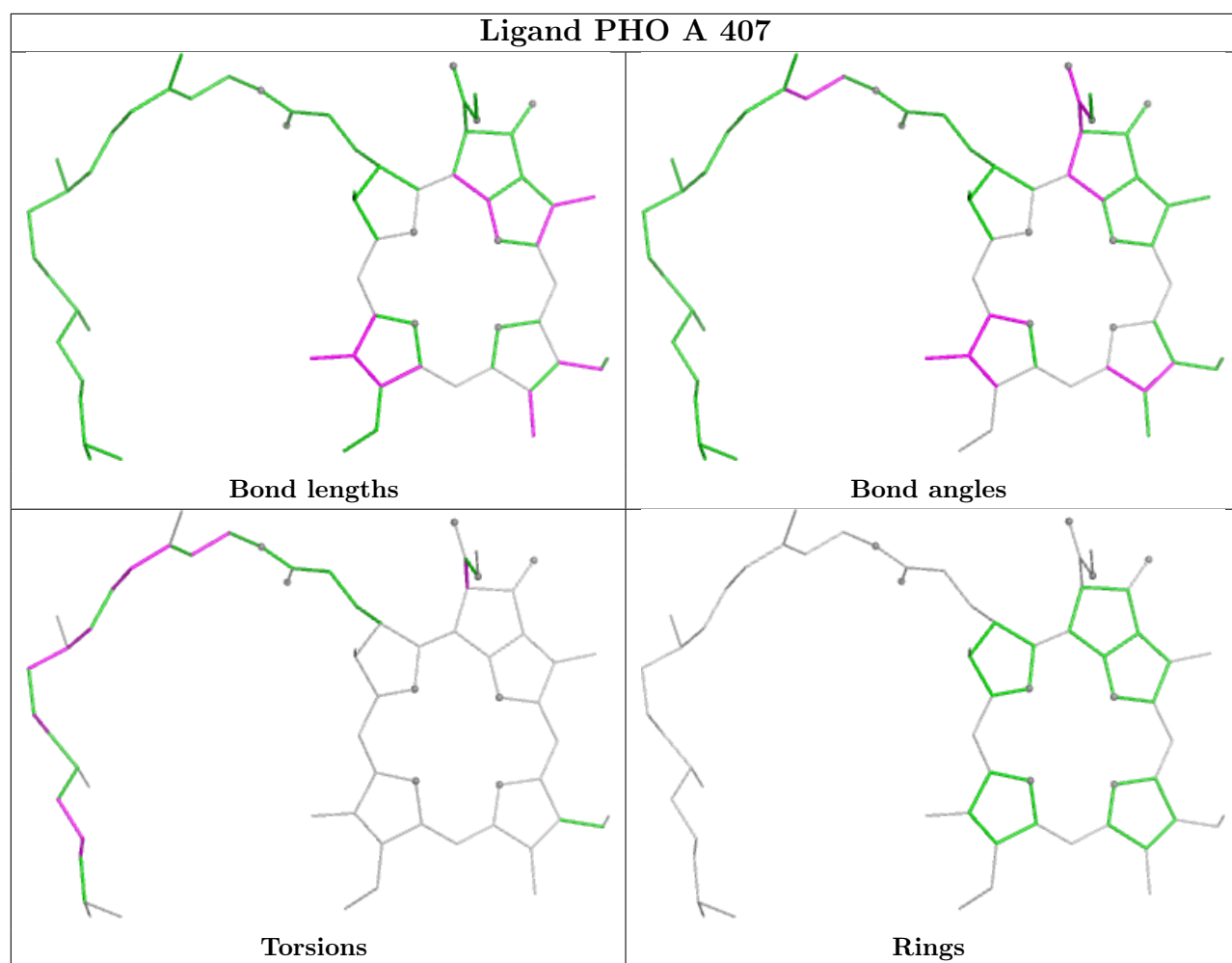


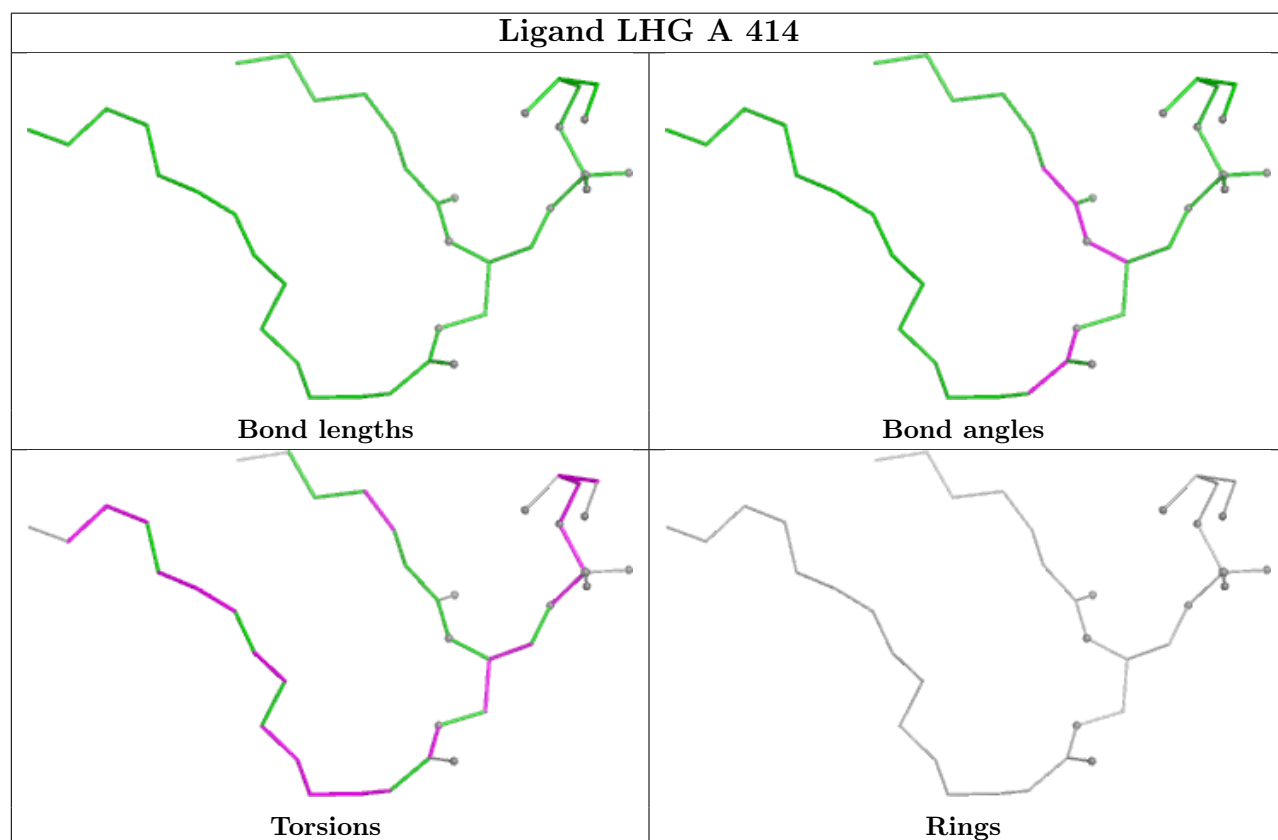
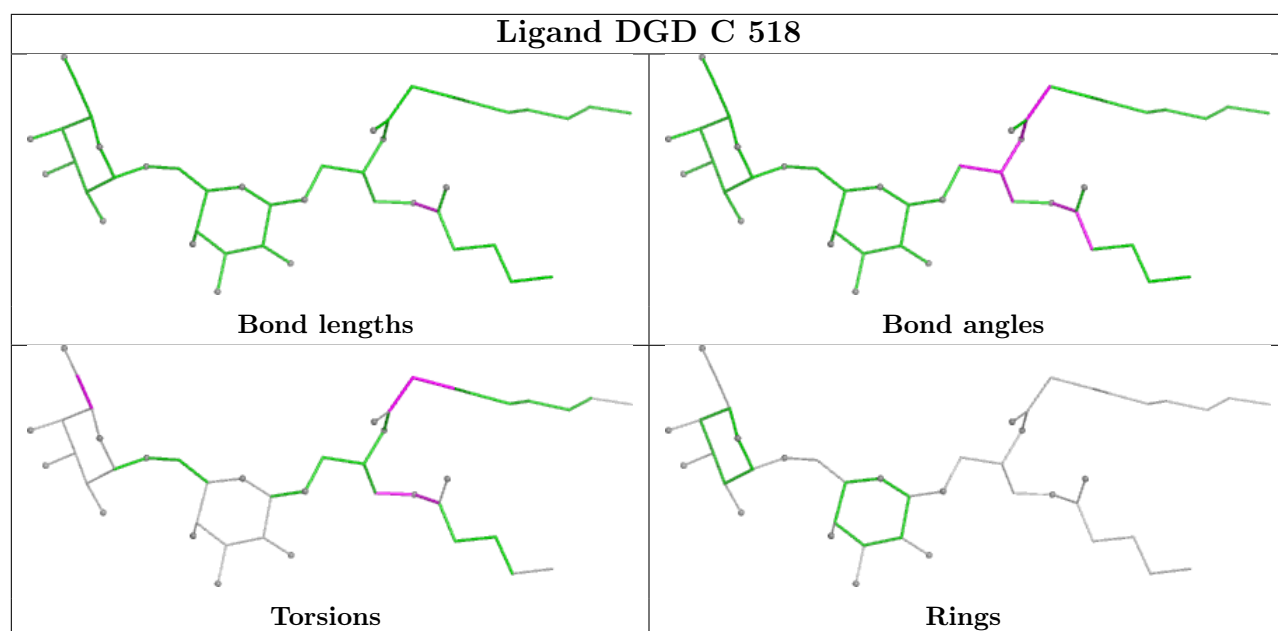


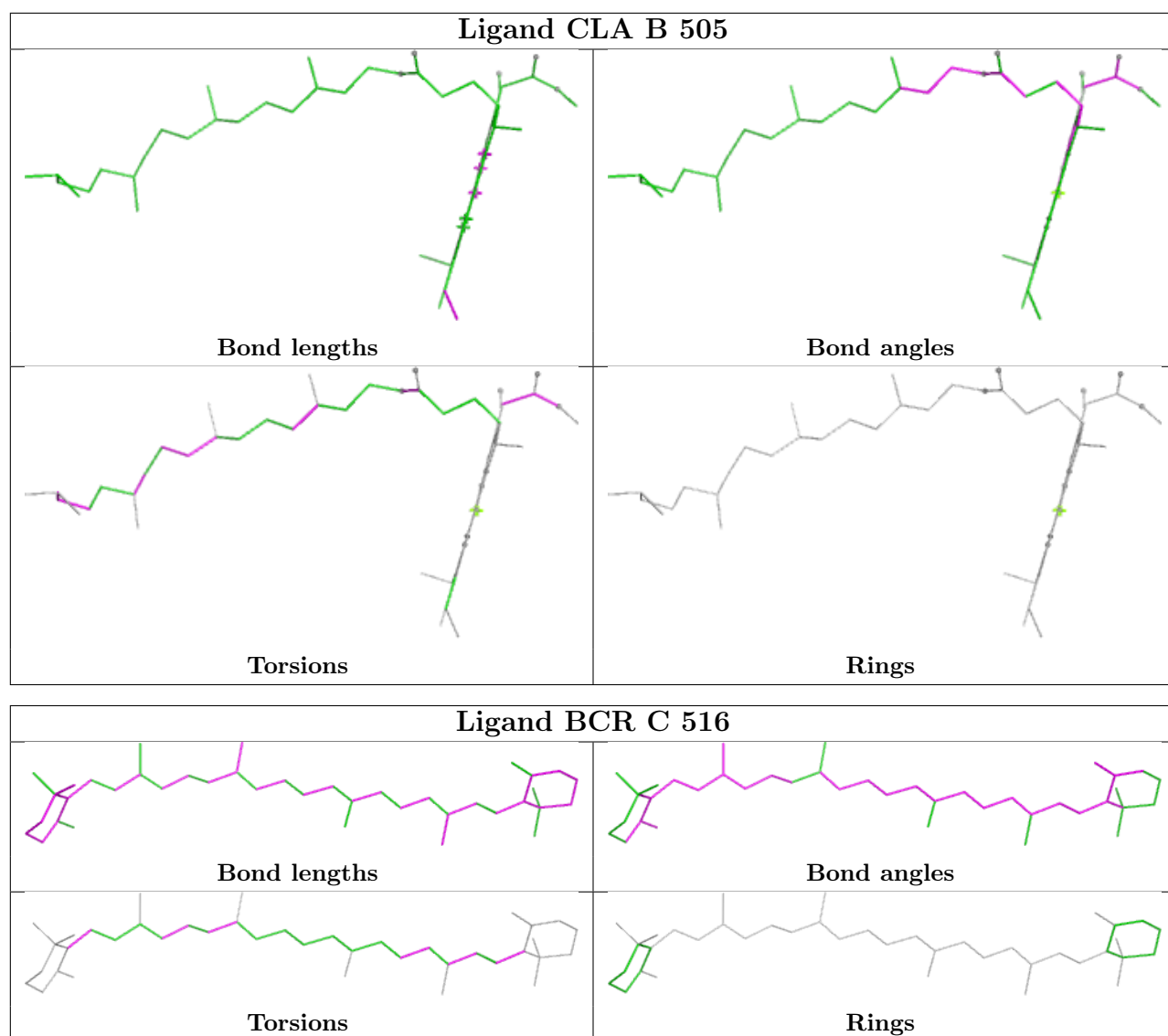


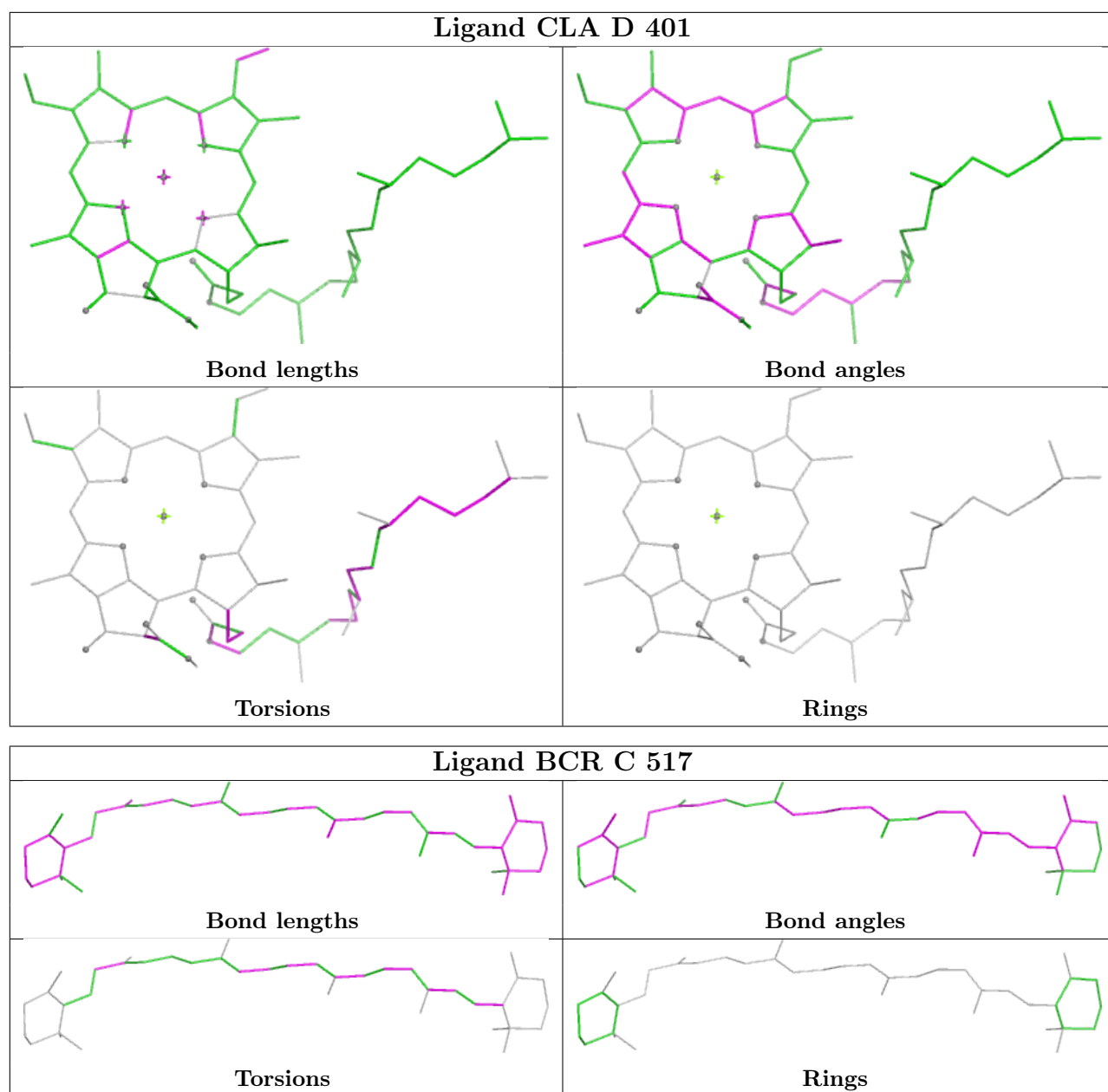


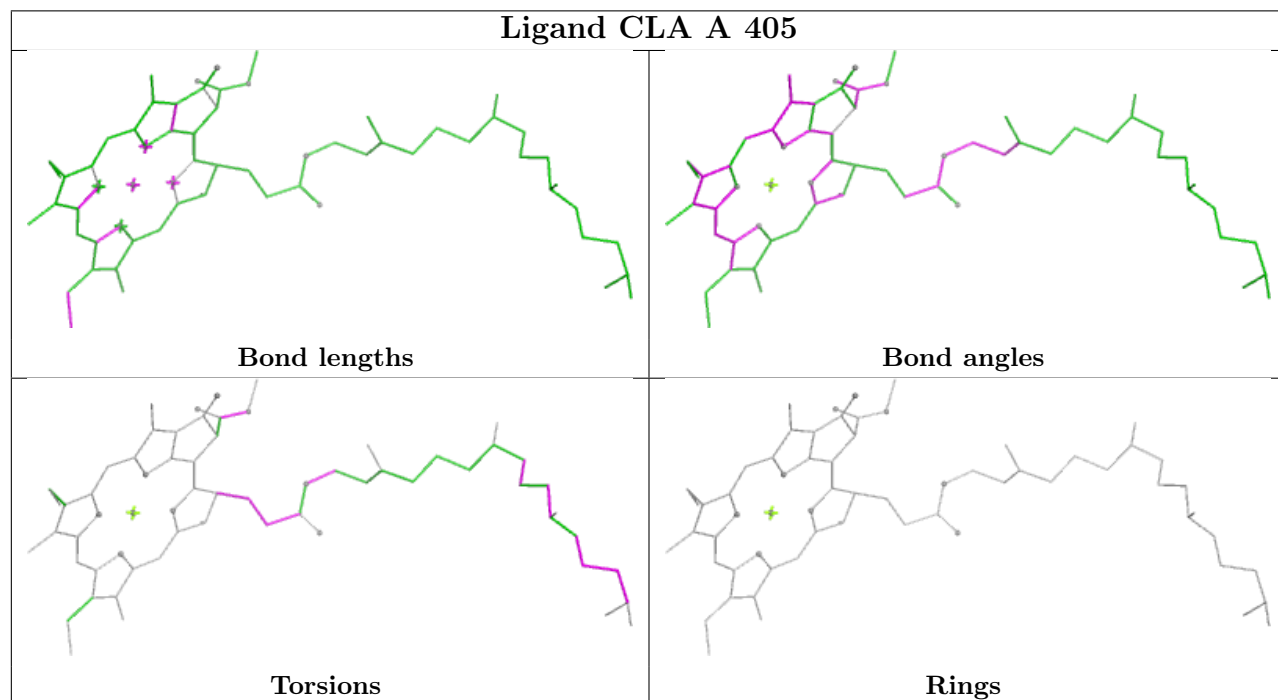
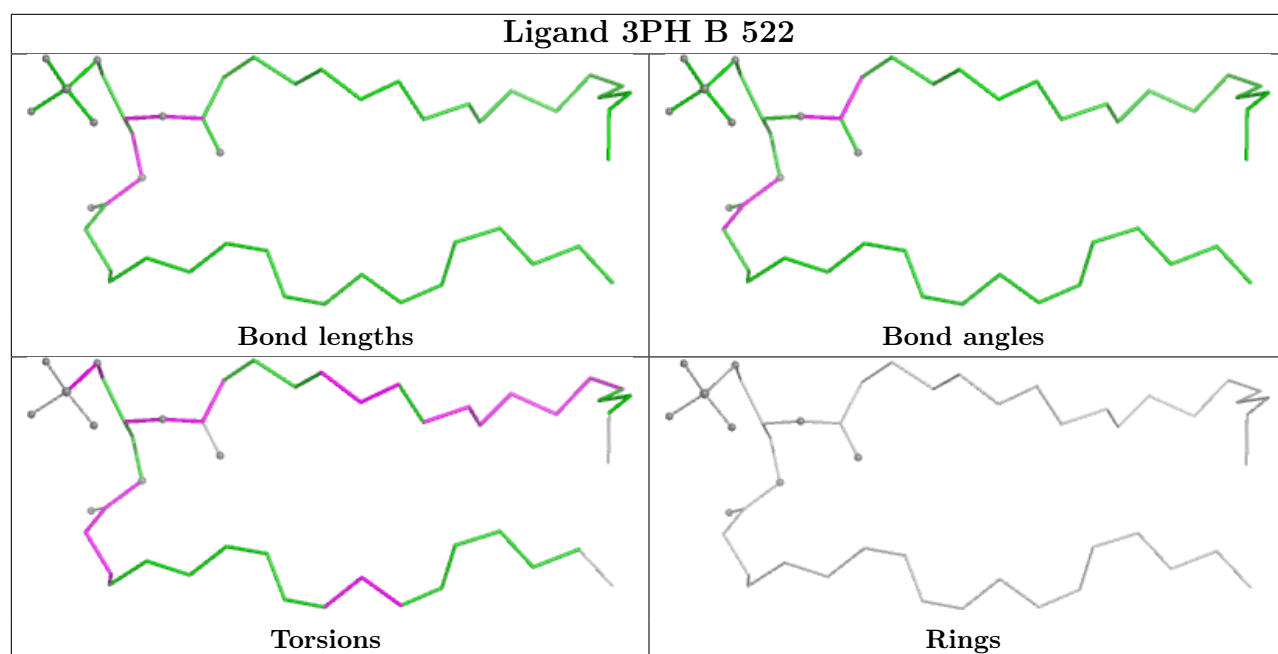


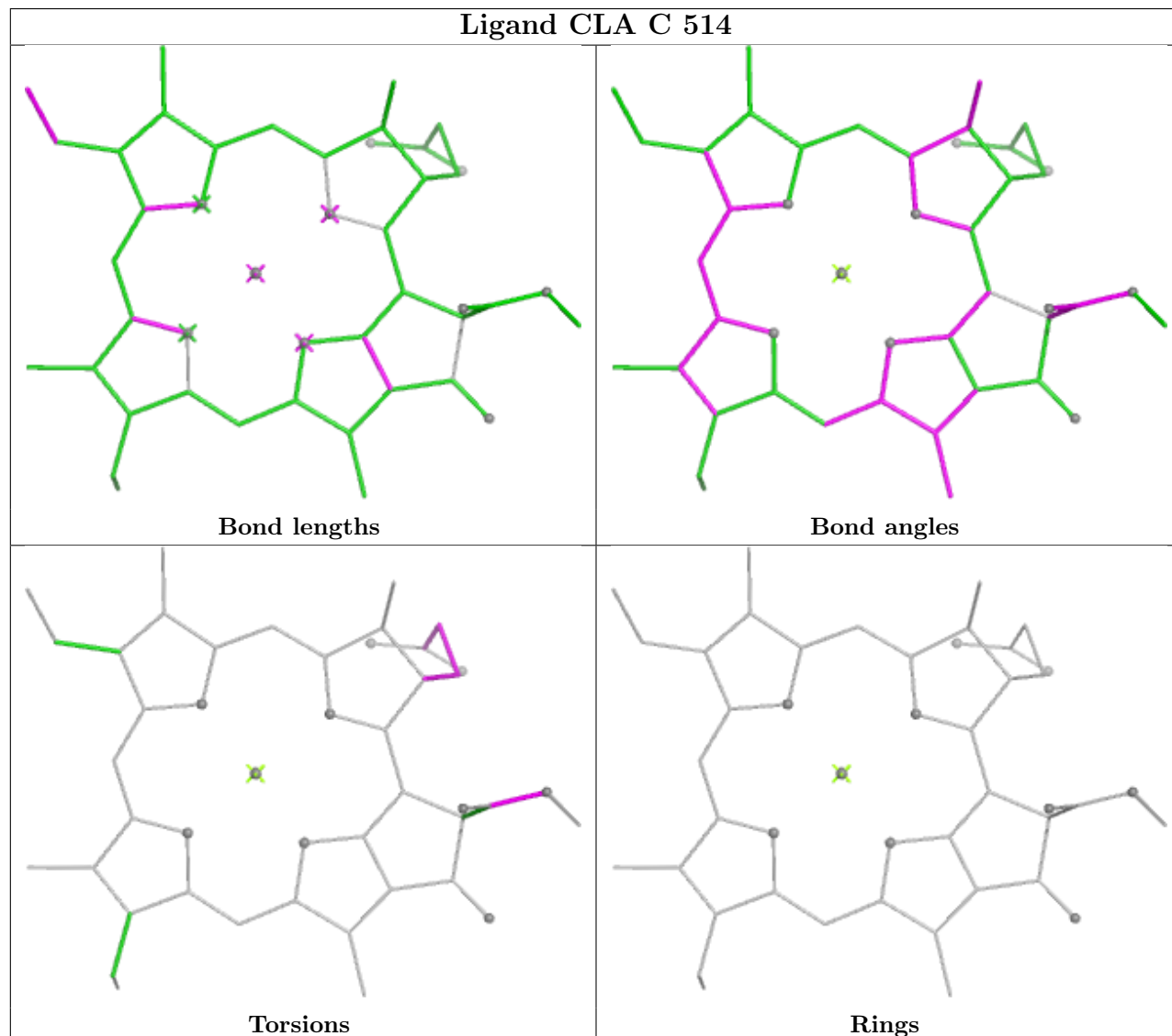
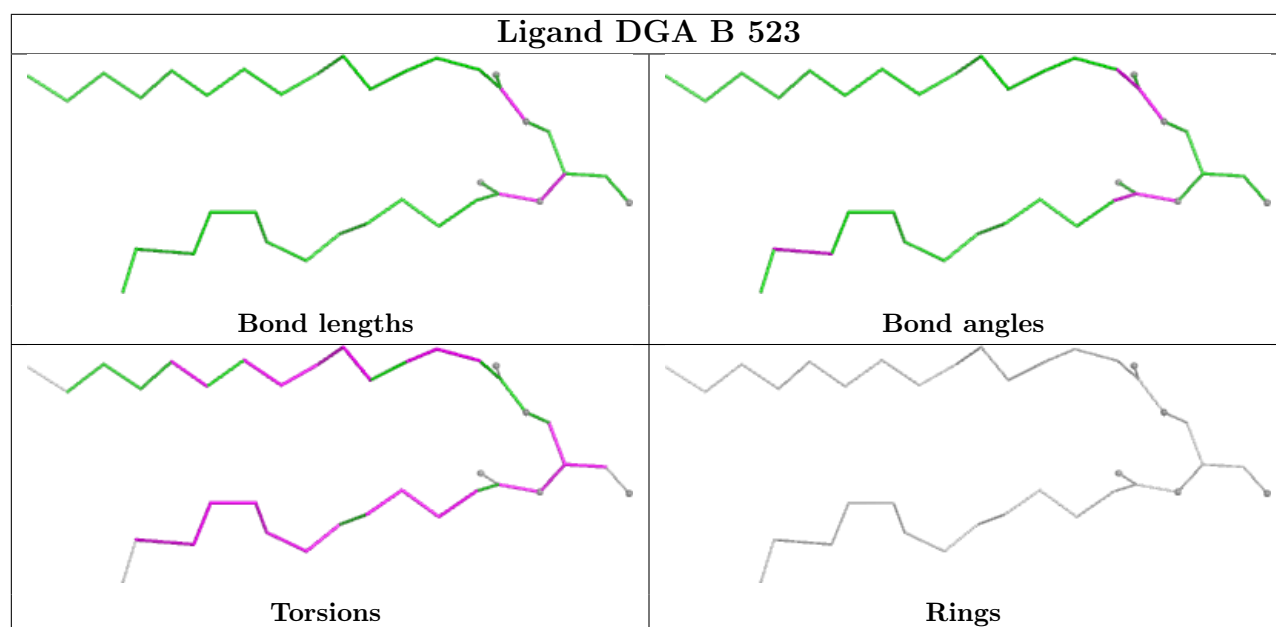


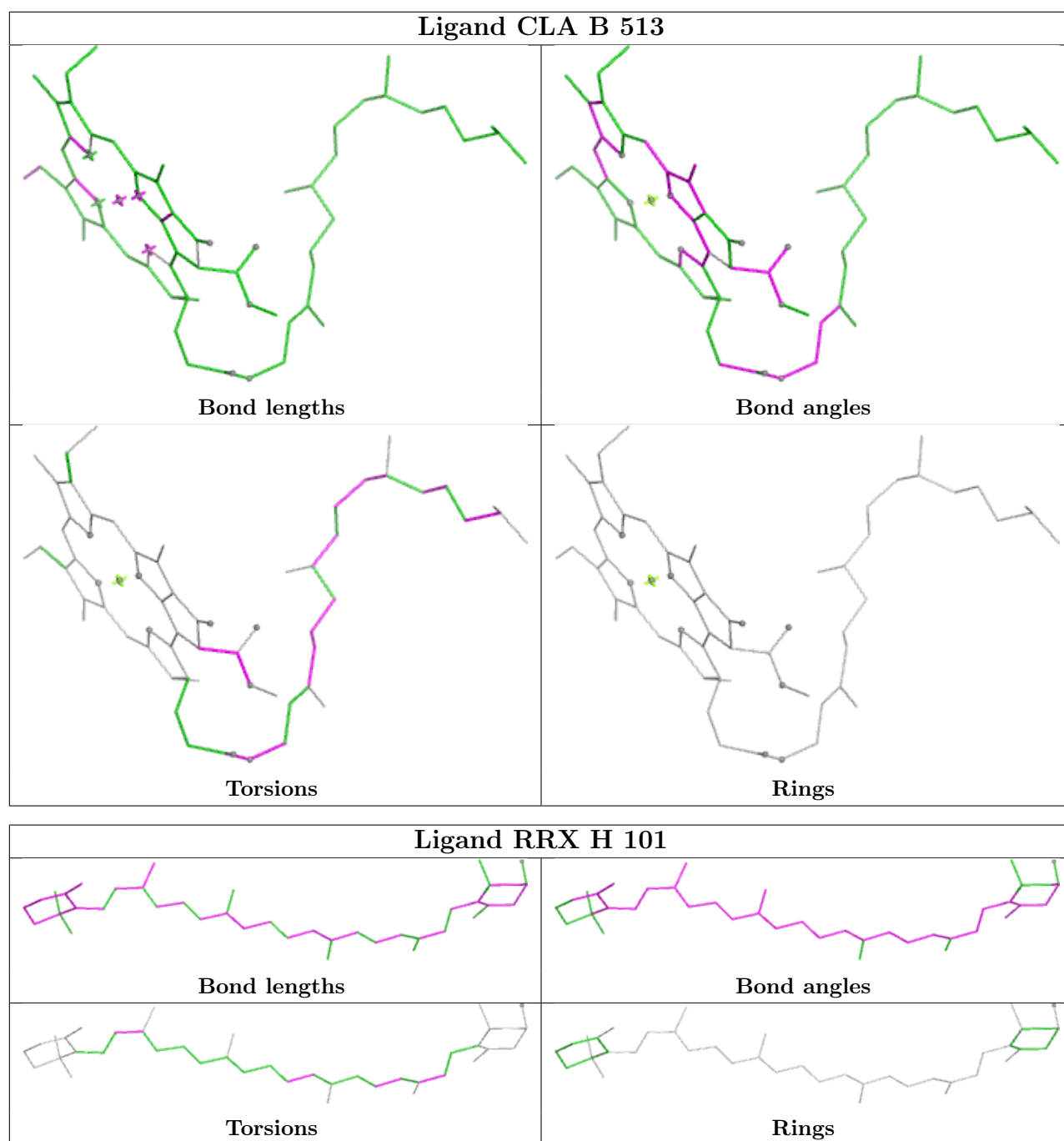


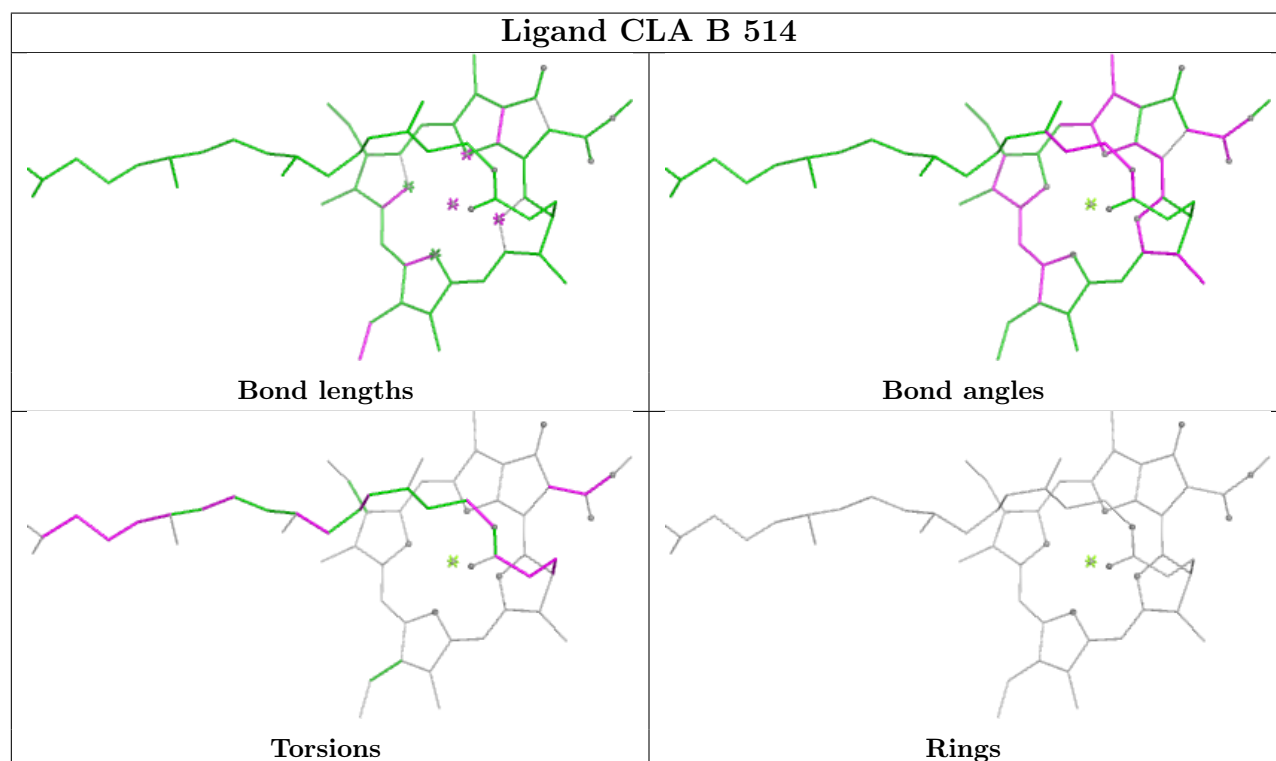
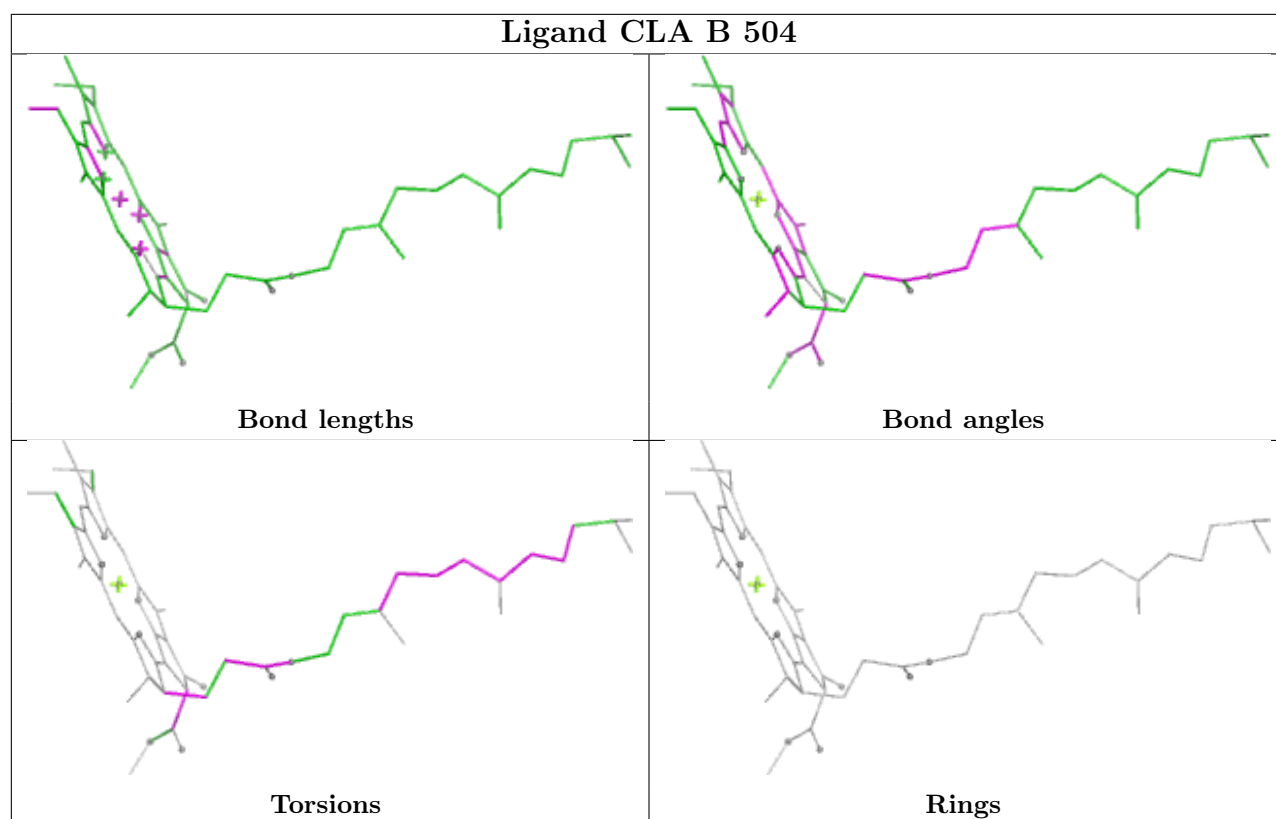


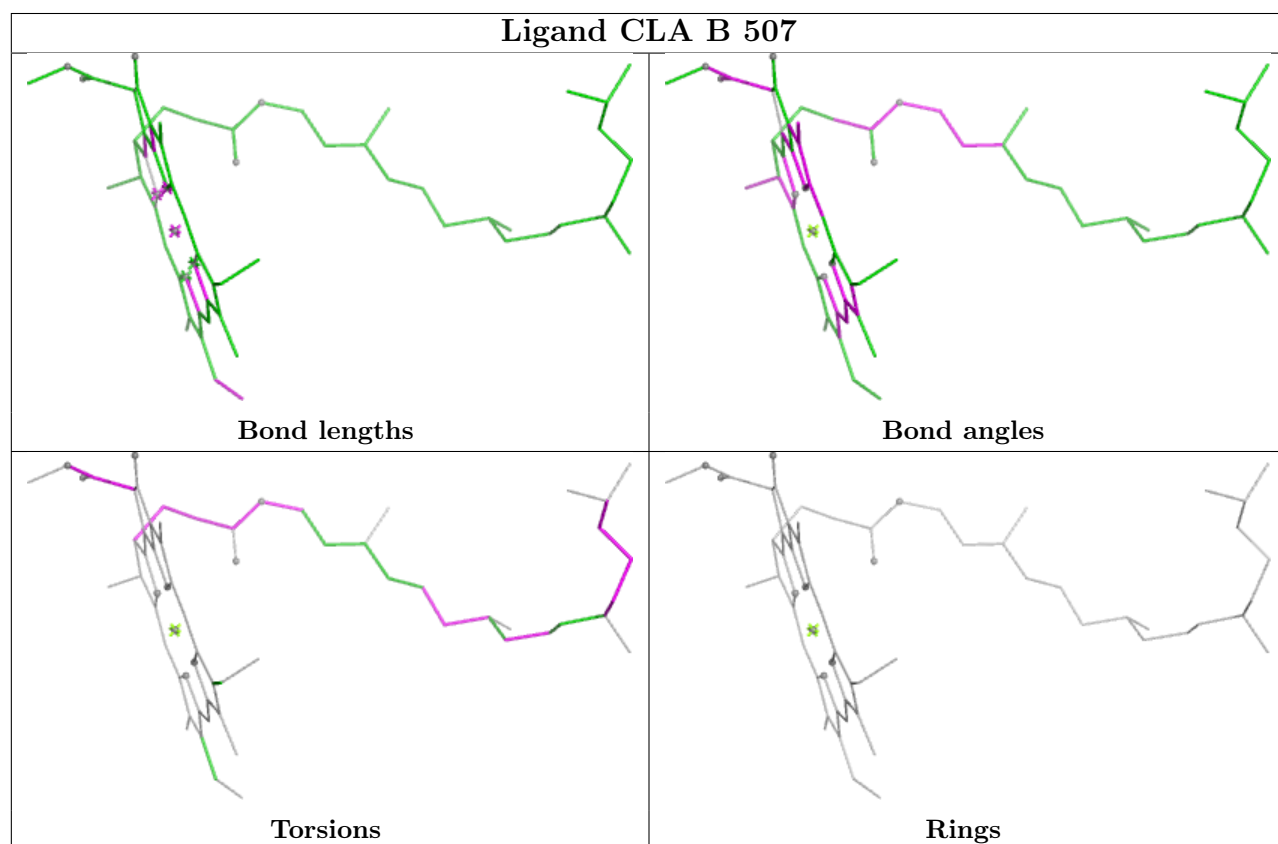
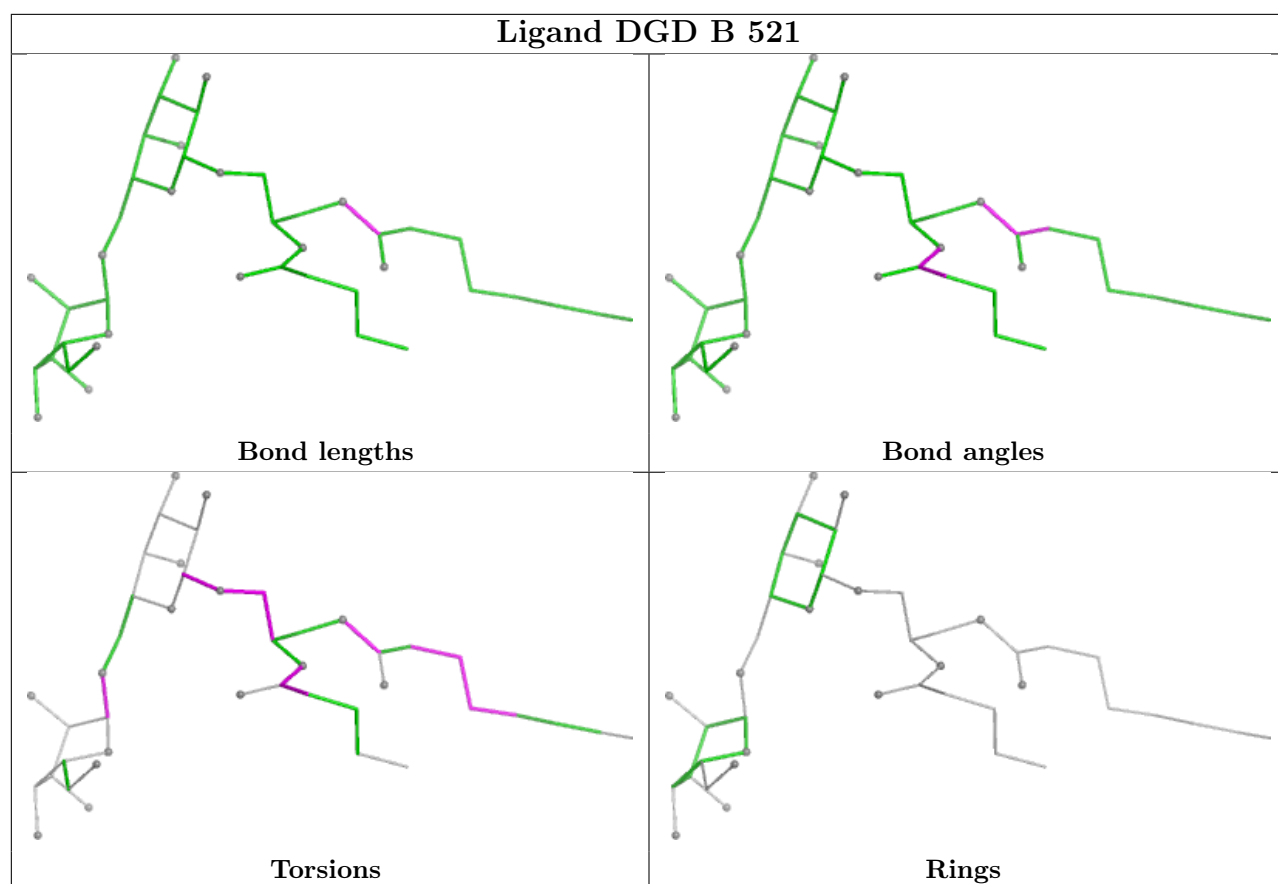


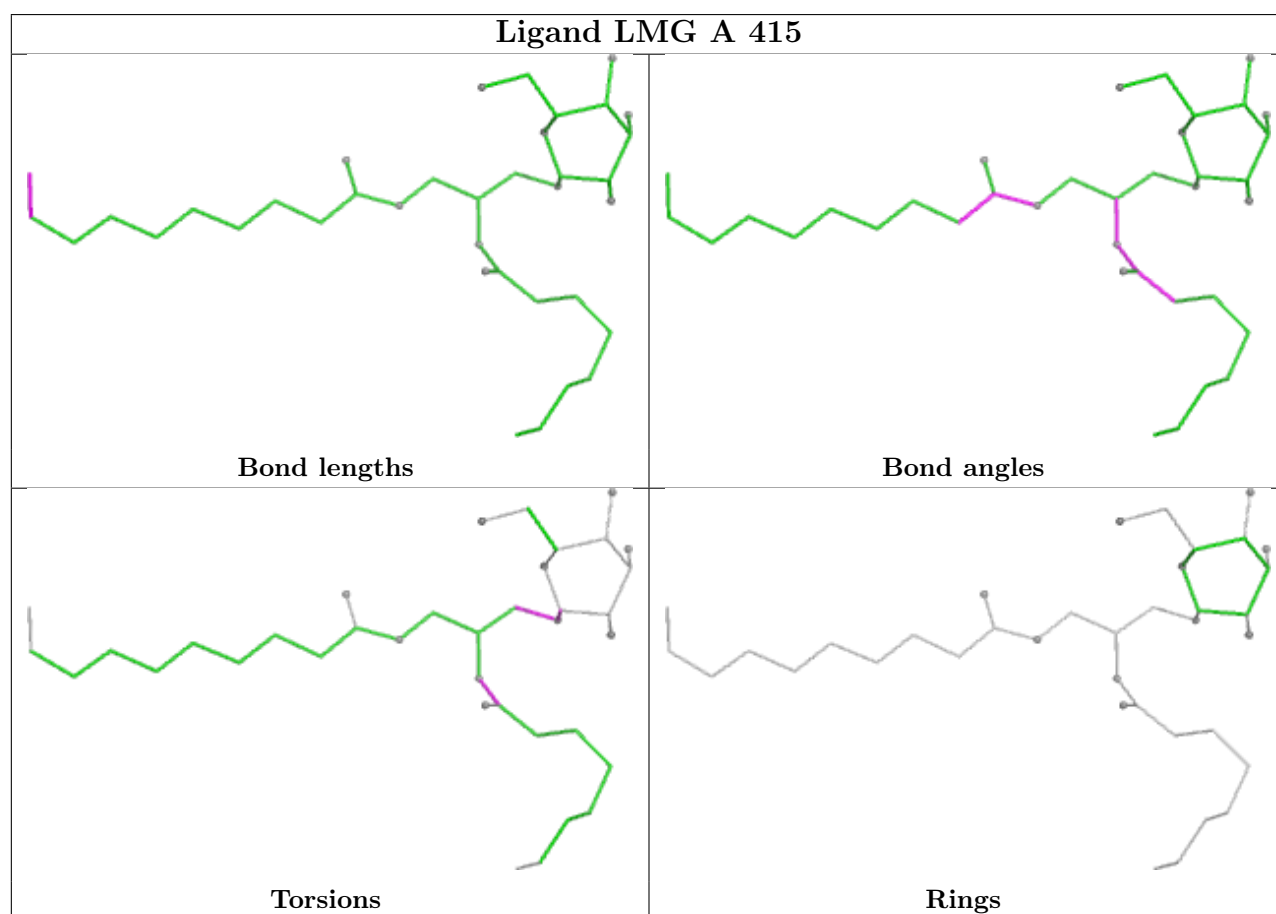
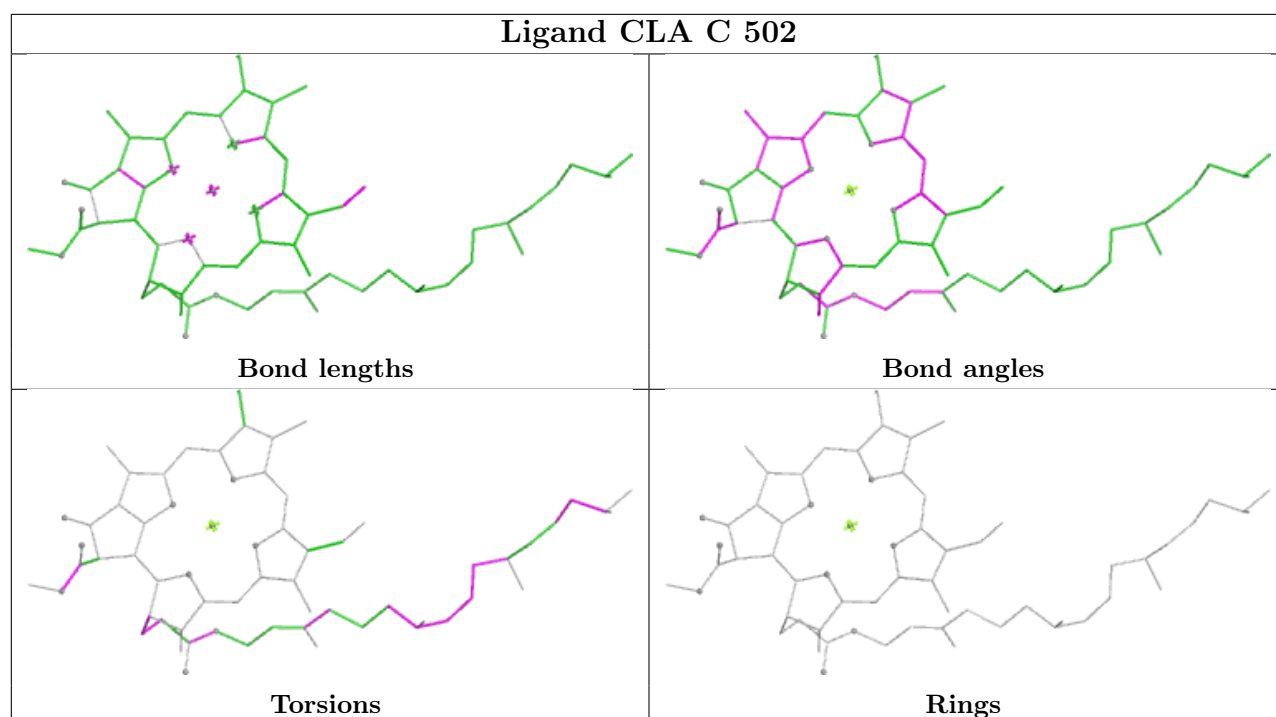


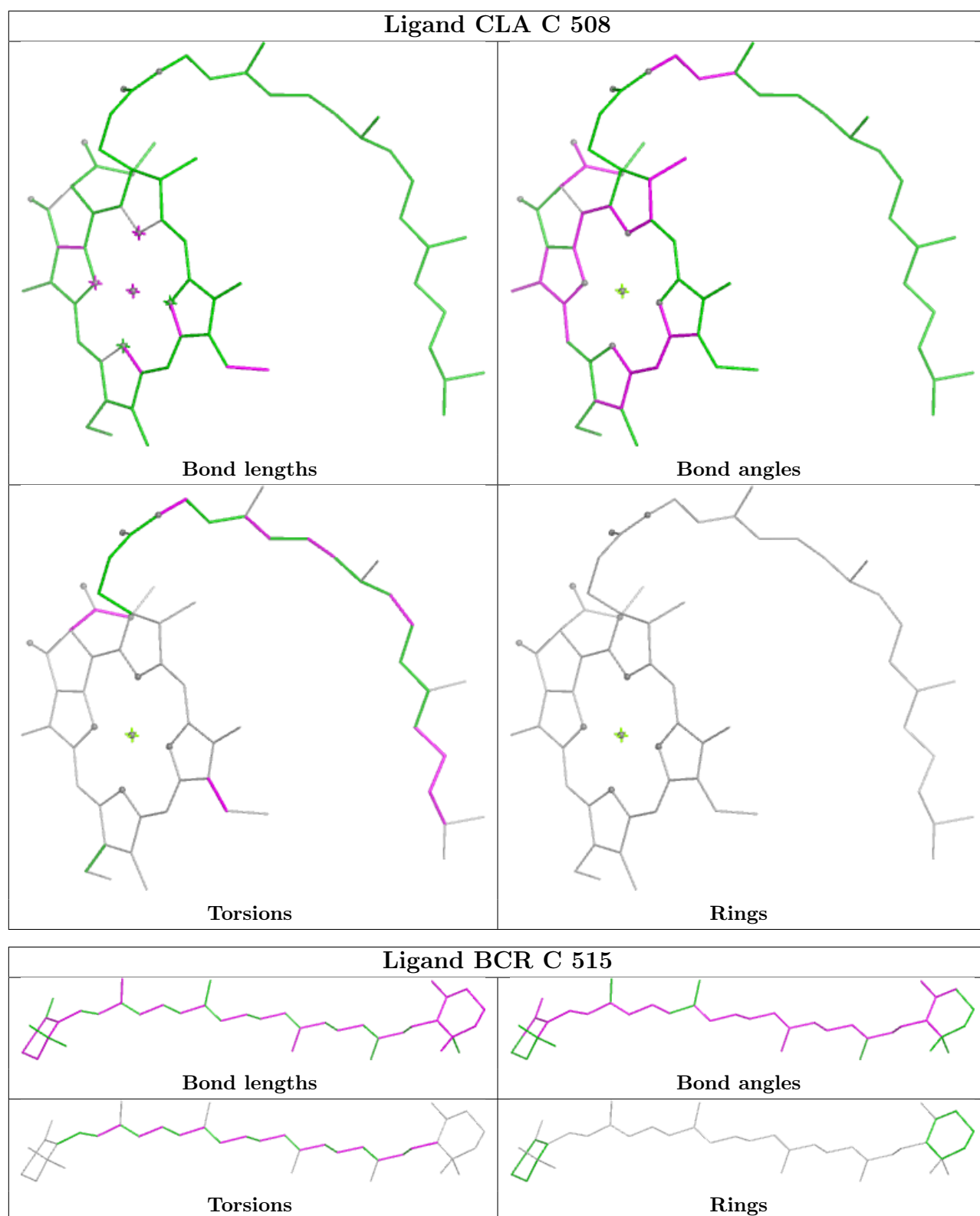


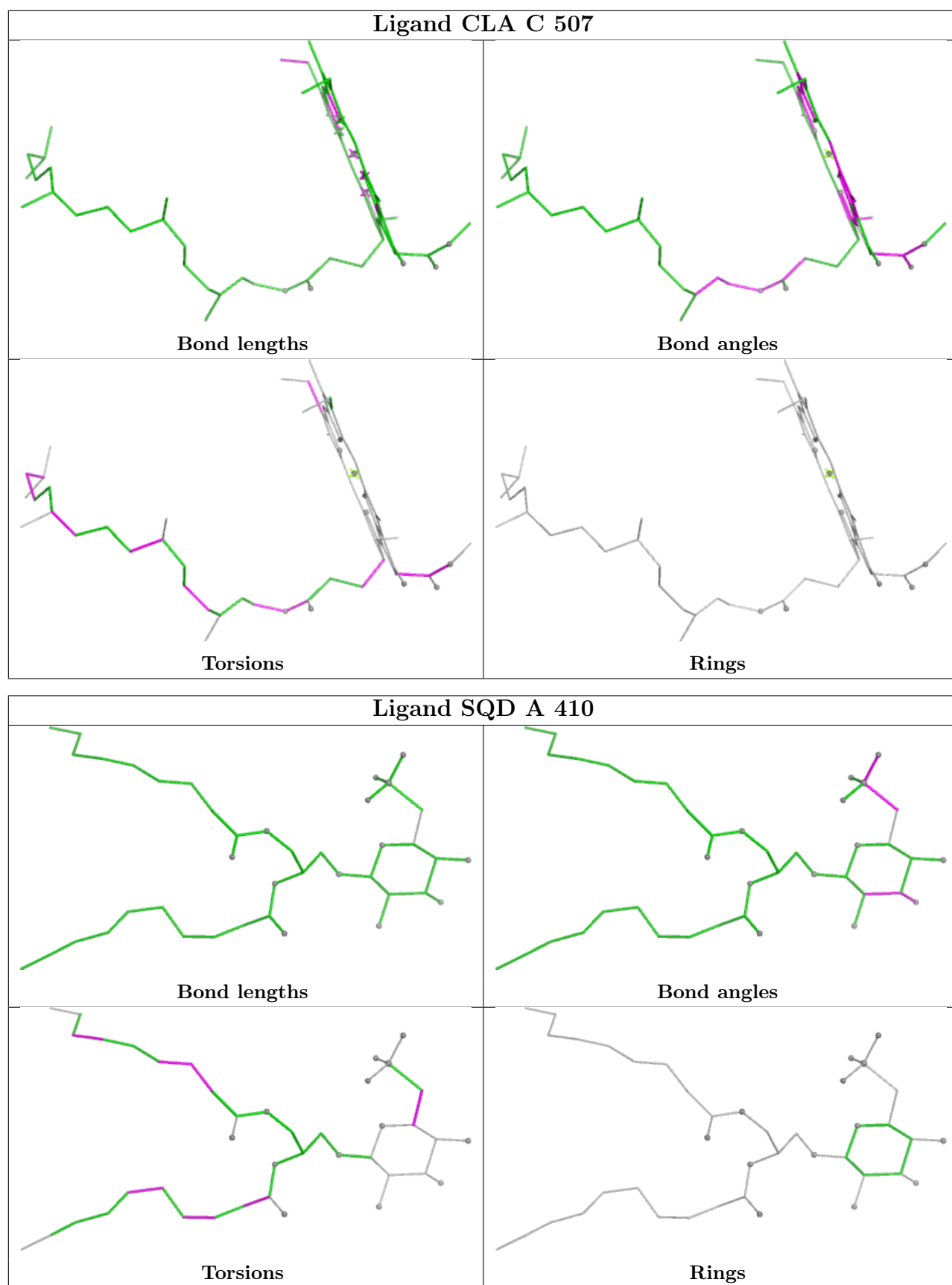


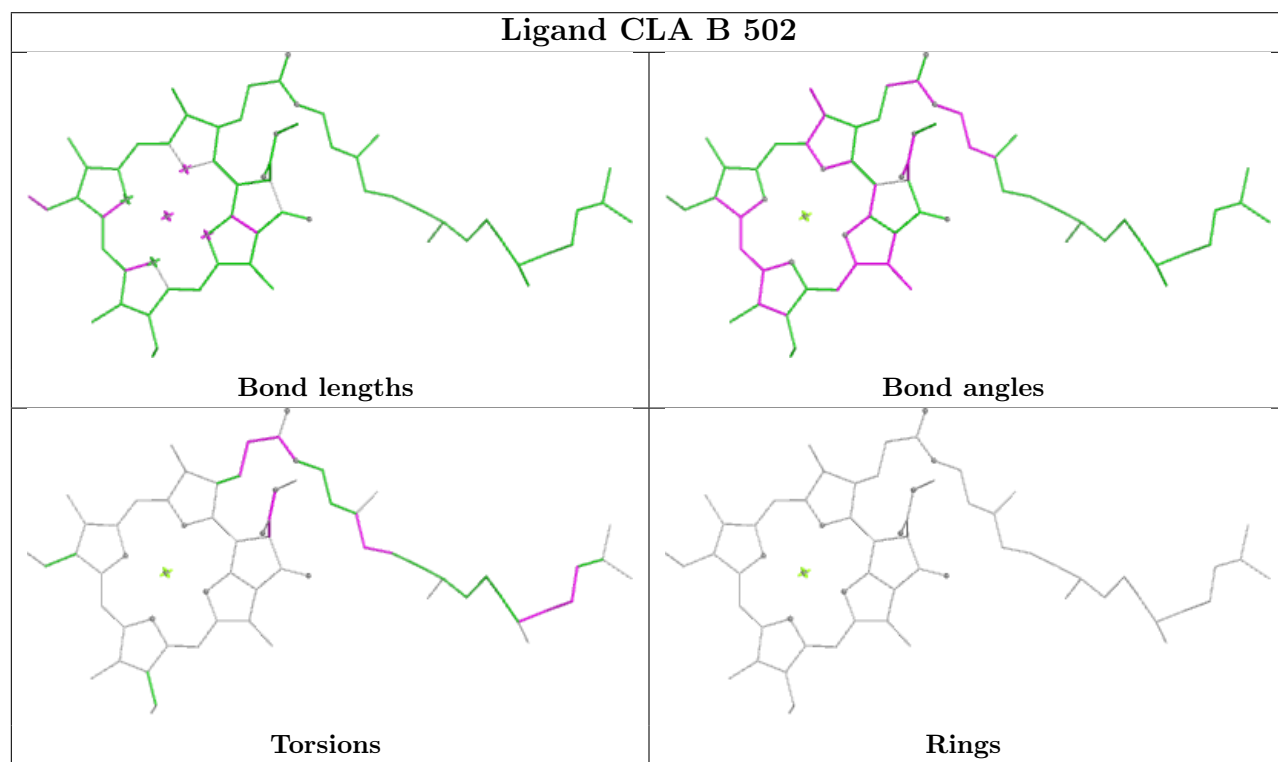
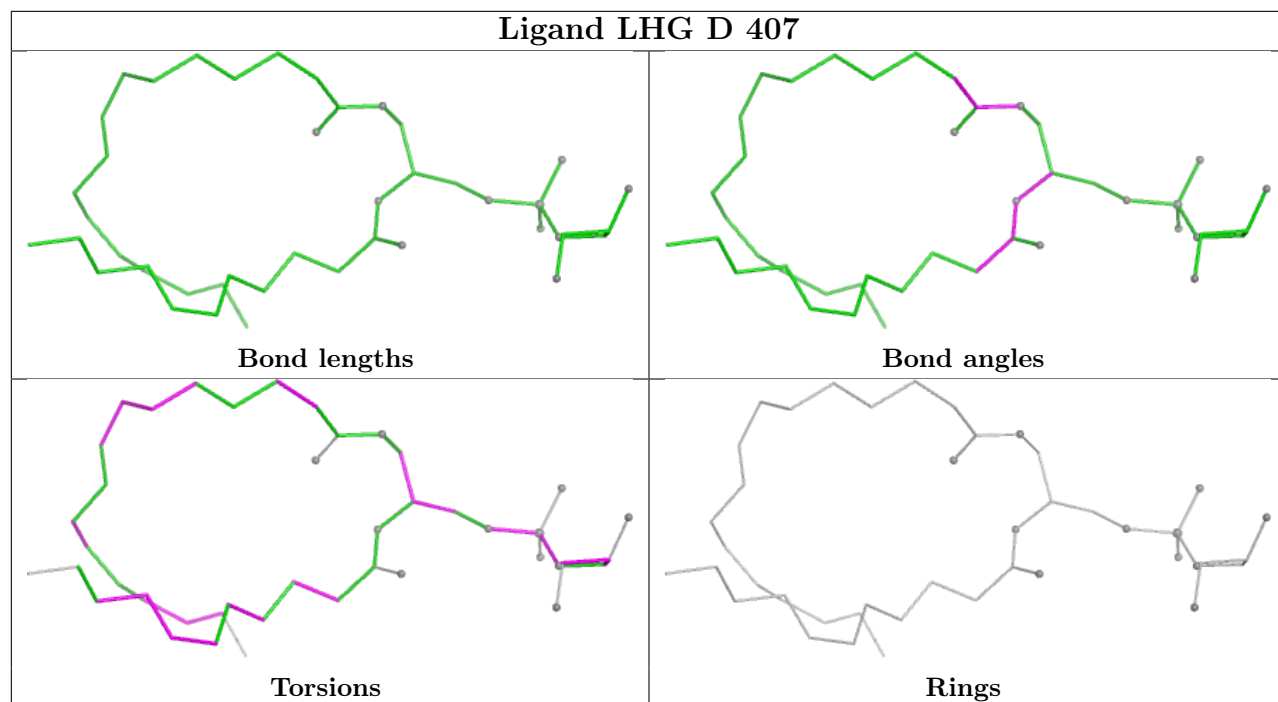


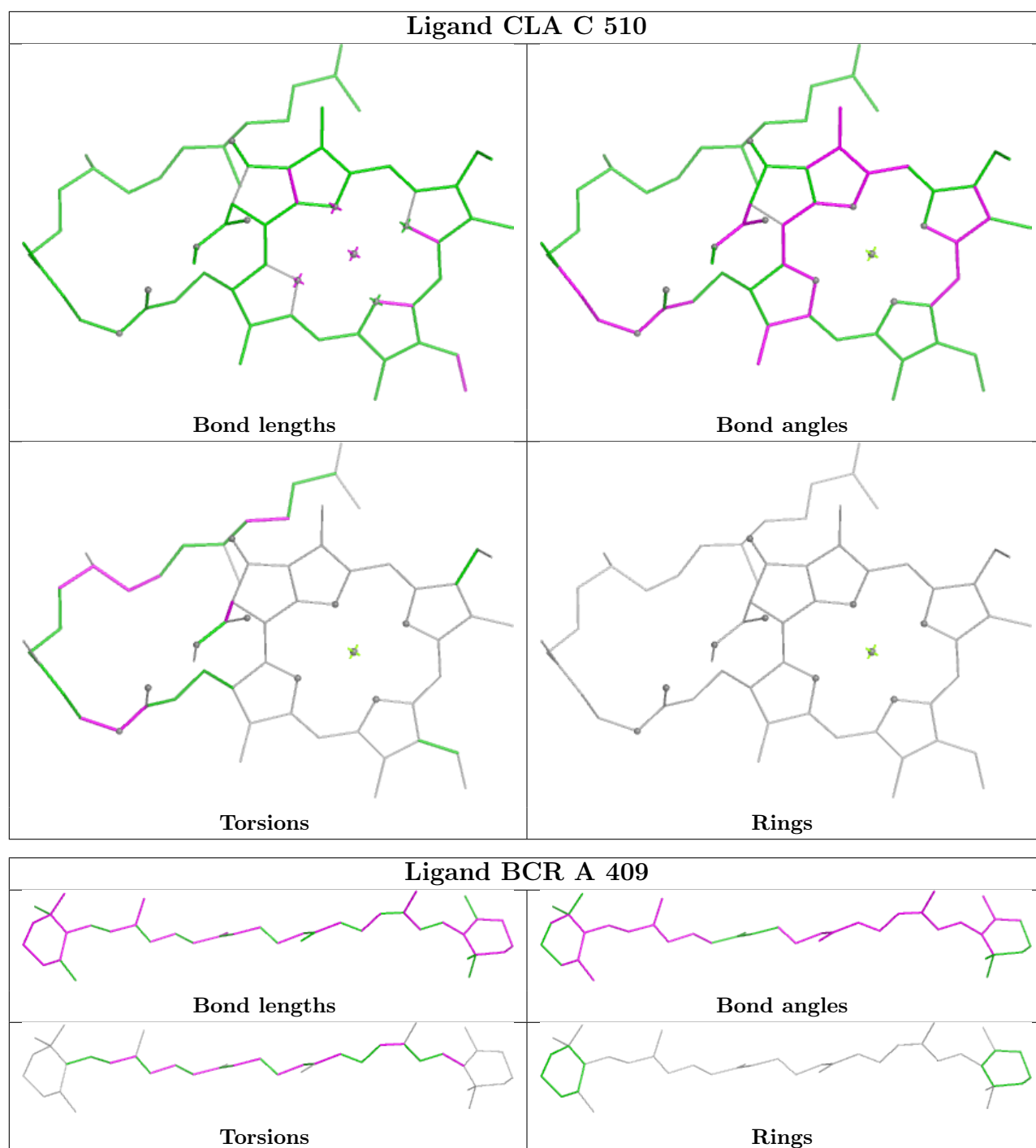












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

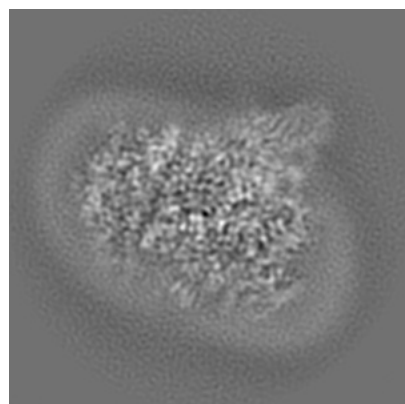
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51482. These allow visual inspection of the internal detail of the map and identification of artifacts.

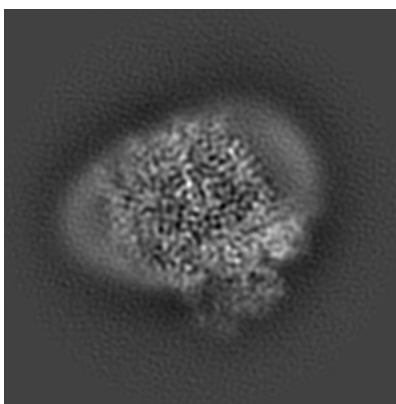
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

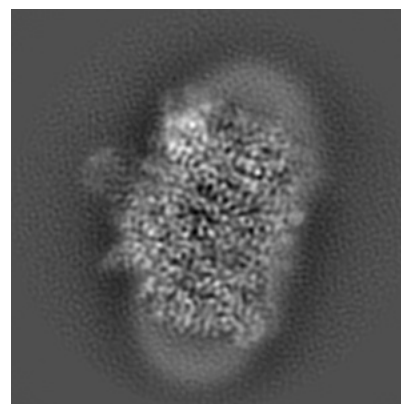
6.1.1 Primary map



X

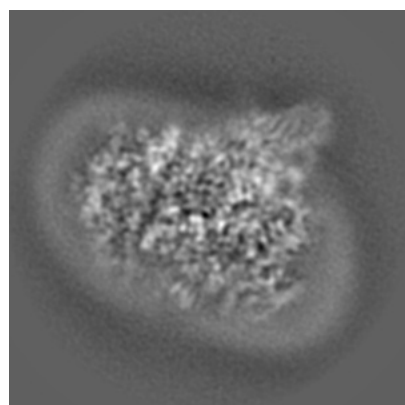


Y

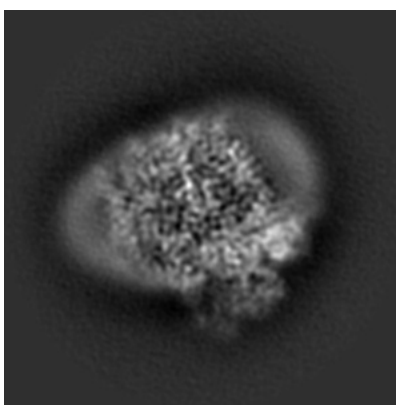


Z

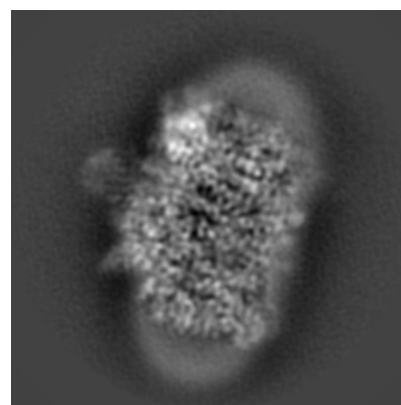
6.1.2 Raw map



X



Y

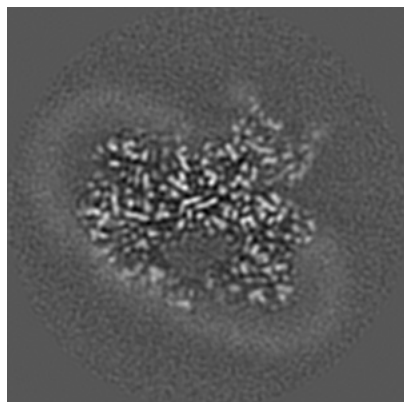


Z

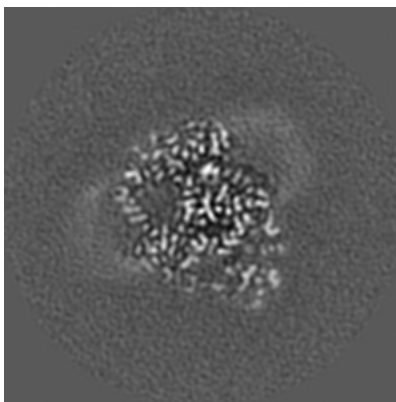
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

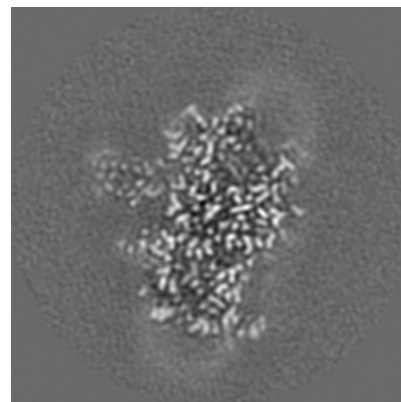
6.2.1 Primary map



X Index: 150

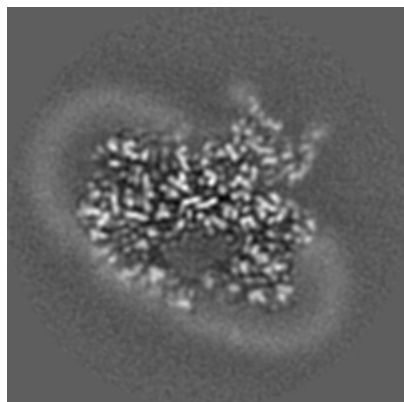


Y Index: 150

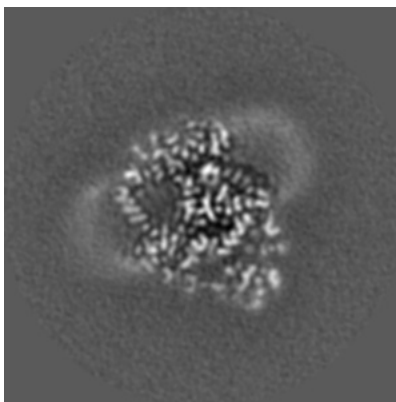


Z Index: 150

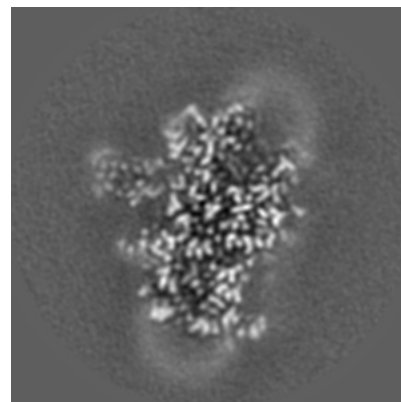
6.2.2 Raw map



X Index: 150



Y Index: 150

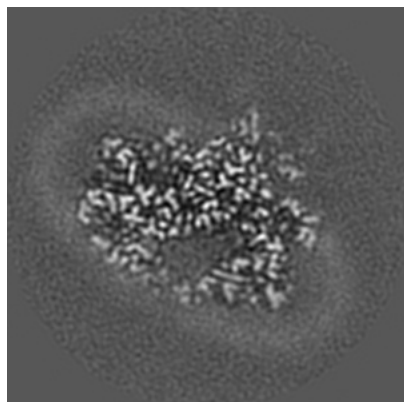


Z Index: 150

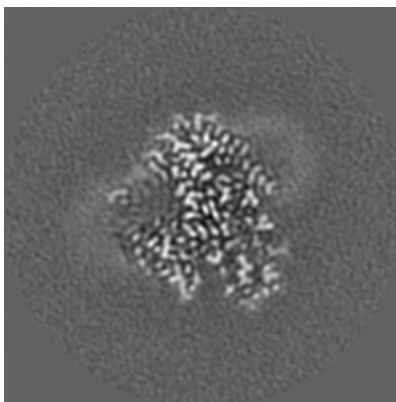
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

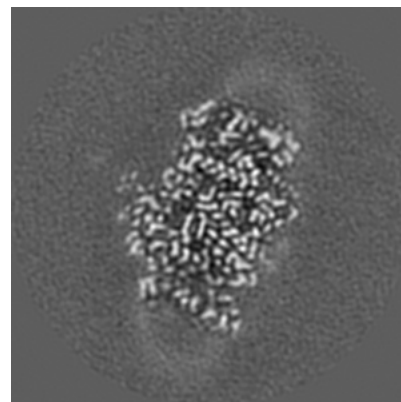
6.3.1 Primary map



X Index: 154

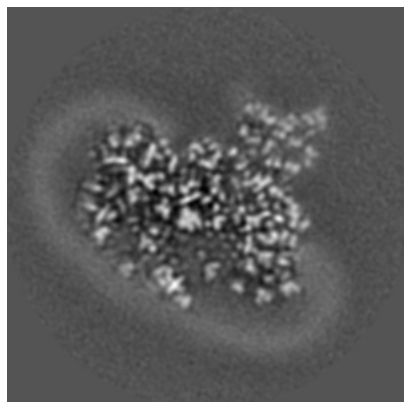


Y Index: 143

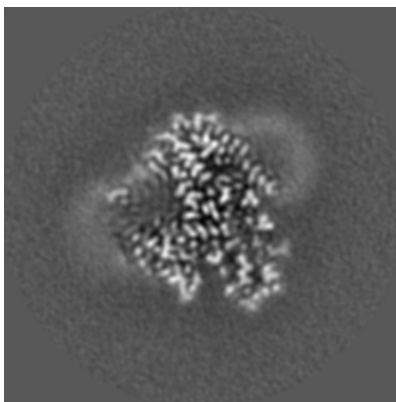


Z Index: 137

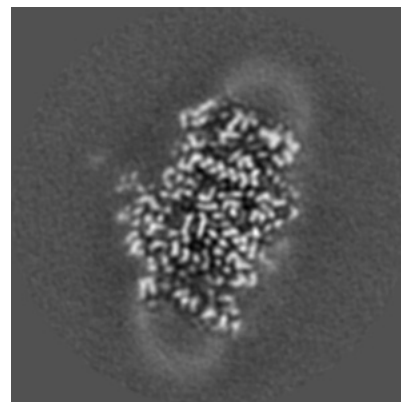
6.3.2 Raw map



X Index: 142



Y Index: 143

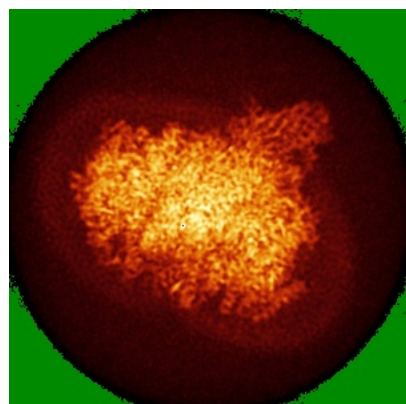


Z Index: 137

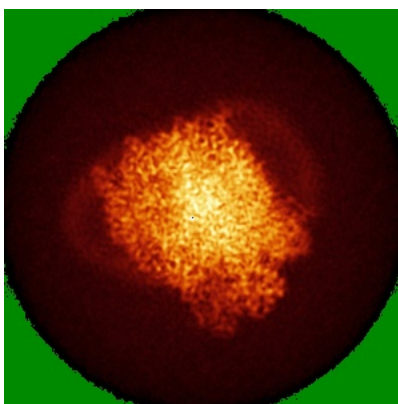
The images above show the largest variance slices of the map in three orthogonal directions.

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

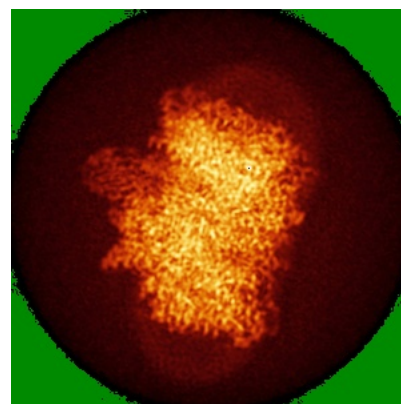
6.4.1 Primary map



X

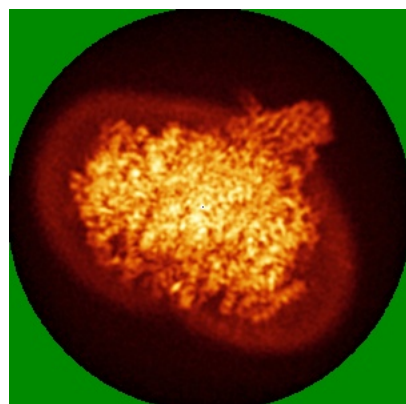


Y

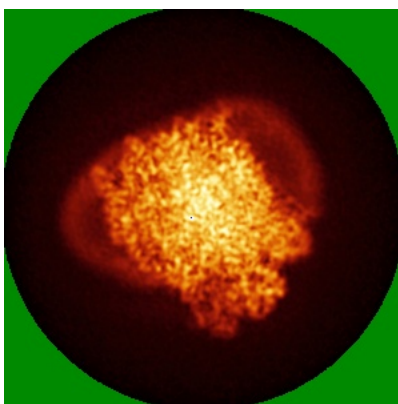


Z

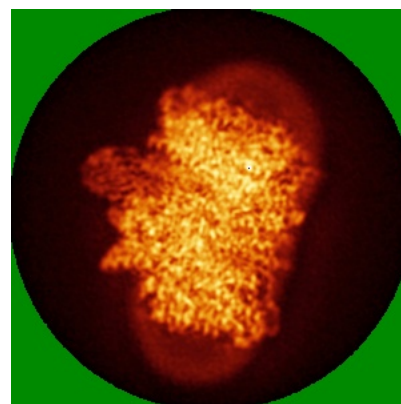
6.4.2 Raw map



X



Y

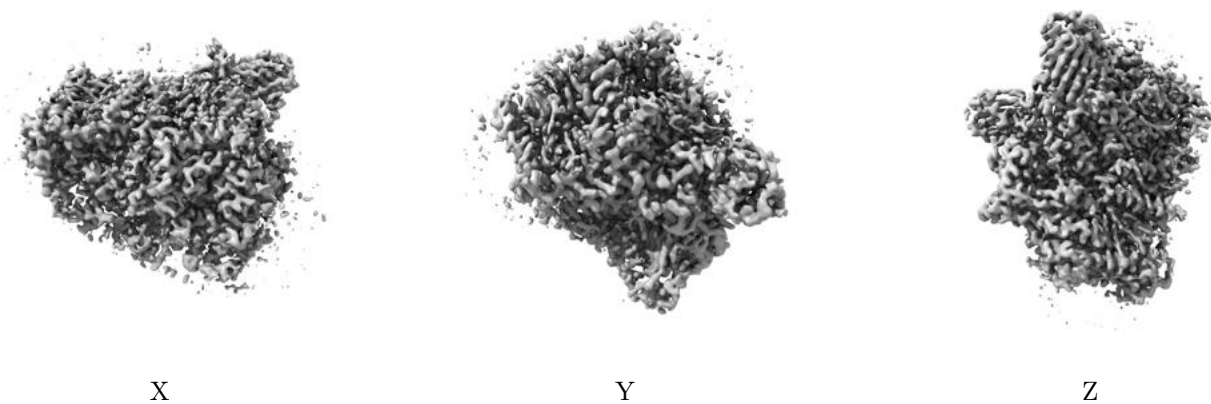


Z

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 0.0047. 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.

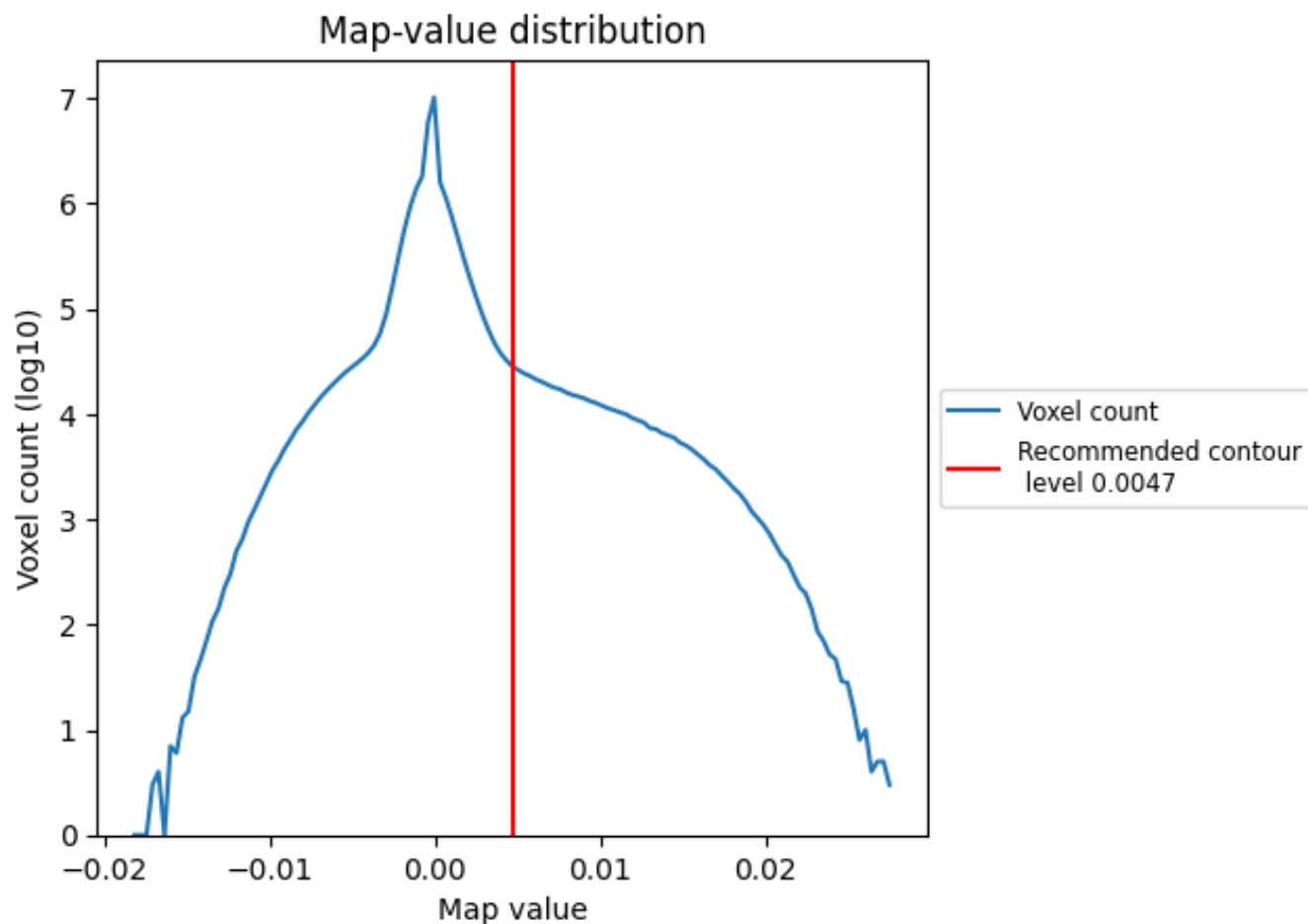
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

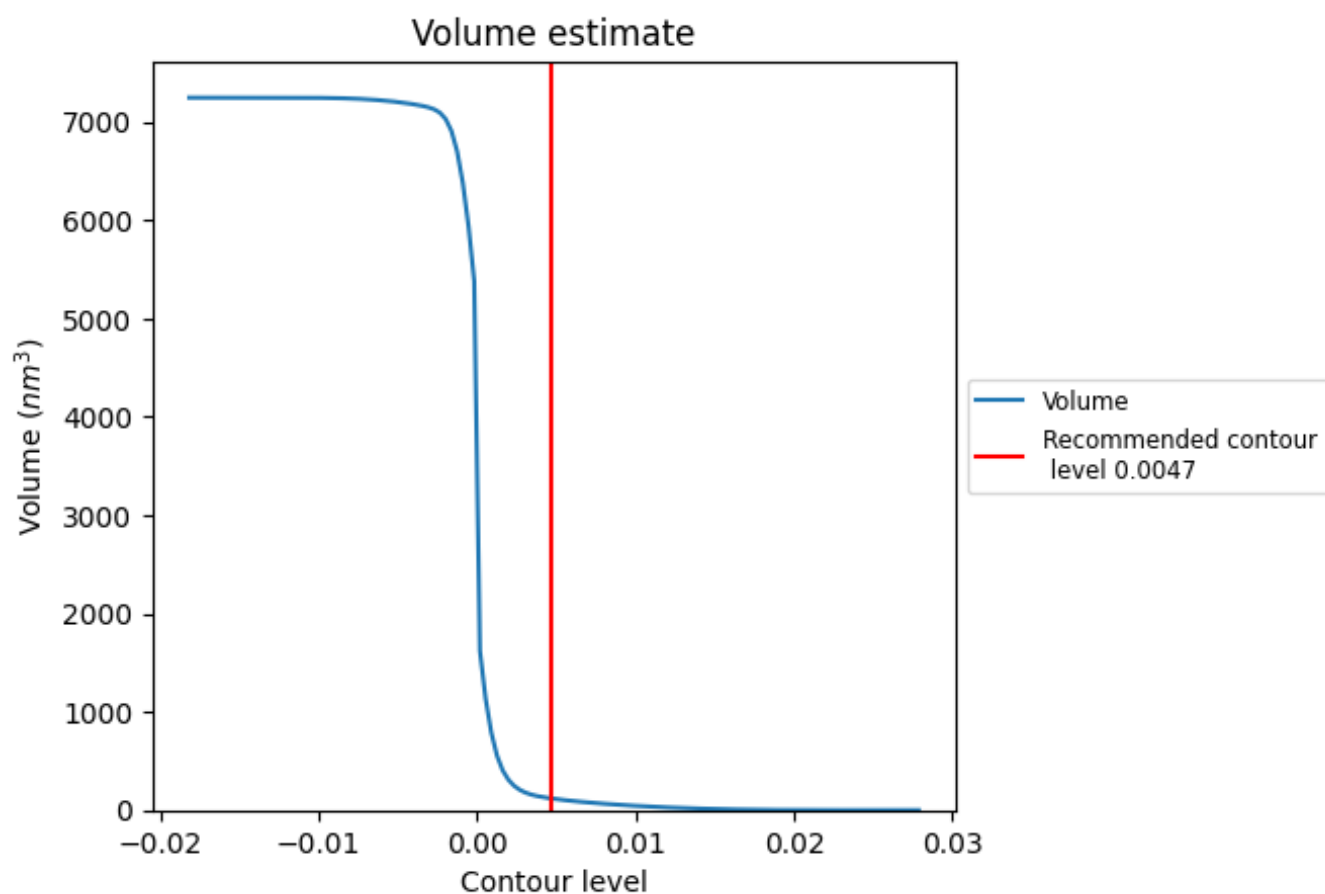
This section contains the results of statistical analysis of the map.

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.

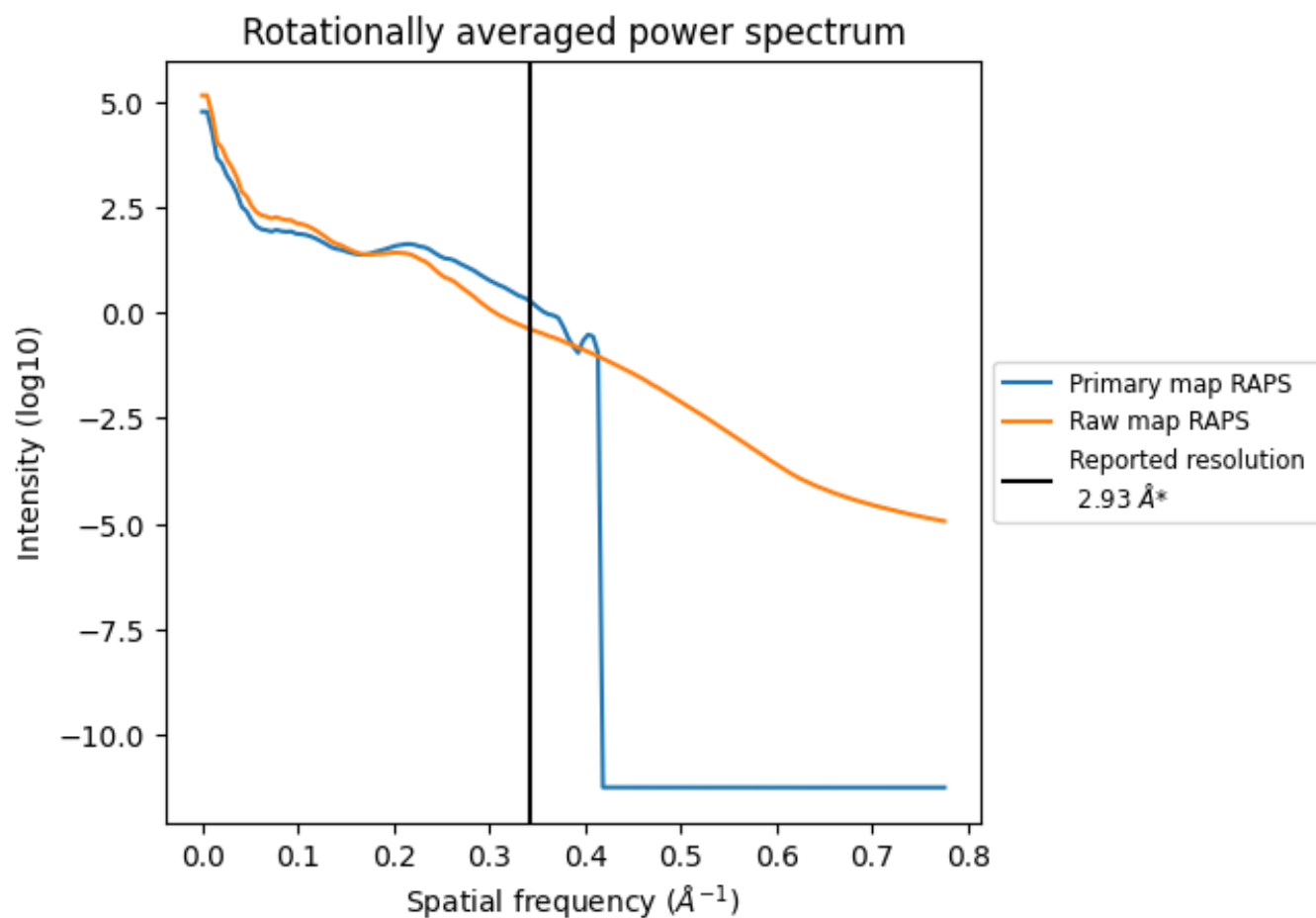
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm³; this corresponds to an approximate mass of 107 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 ⓘ

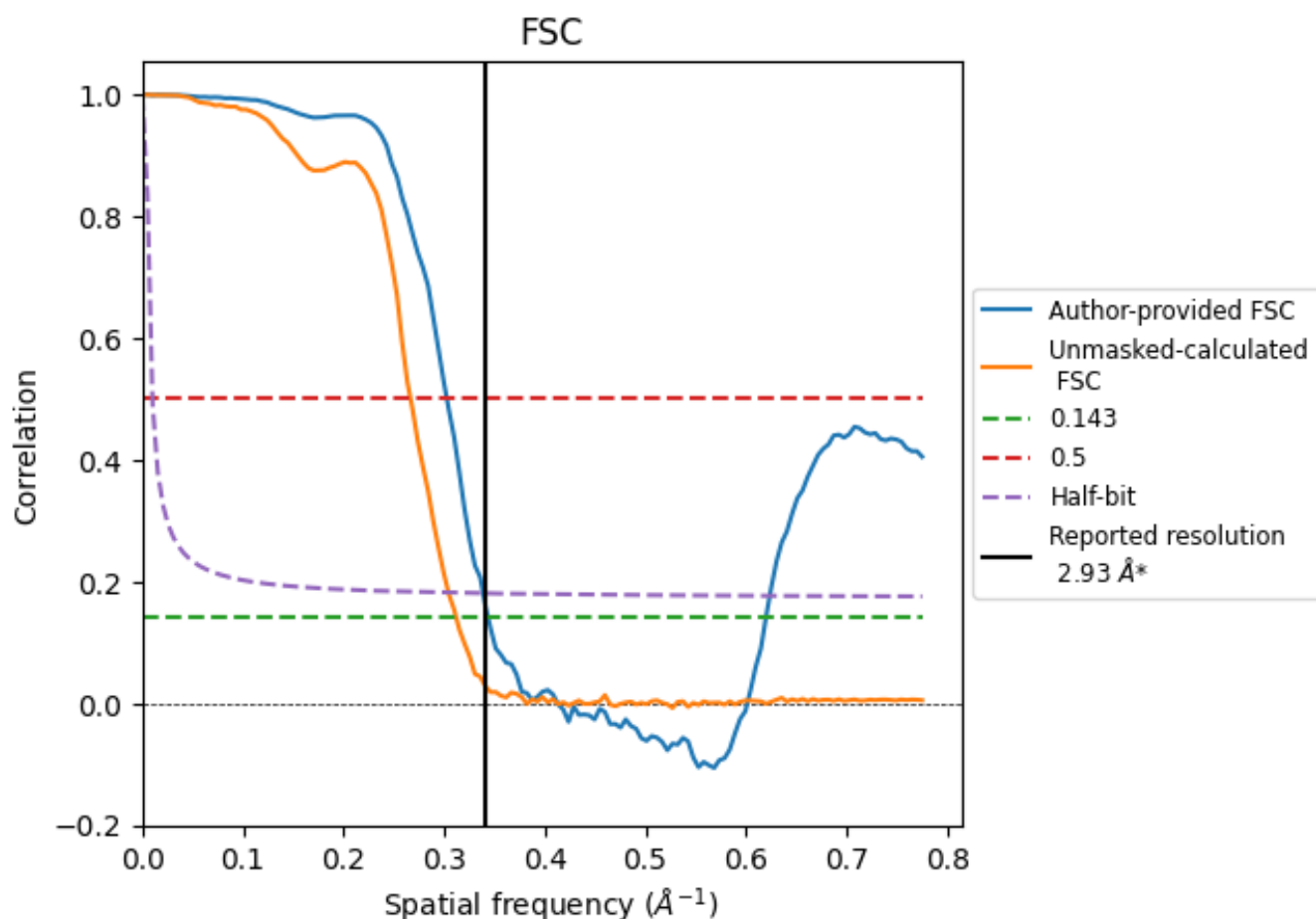


*Reported resolution corresponds to spatial frequency of 0.341 Å⁻¹

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 0.341 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

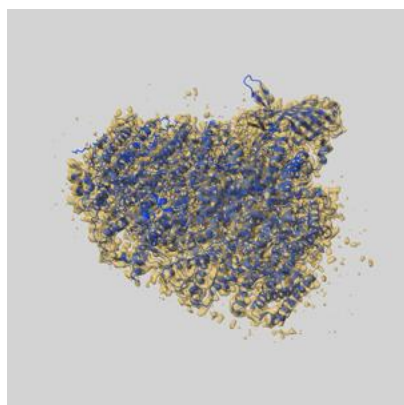
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.91	3.30	2.95
Unmasked-calculated*	3.21	3.75	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

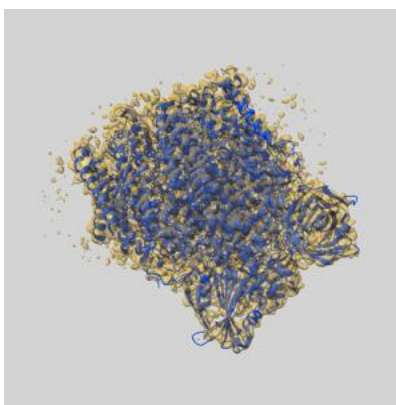
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51482 and PDB model 9GNW. Per-residue inclusion information can be found in section 3 on page 21.

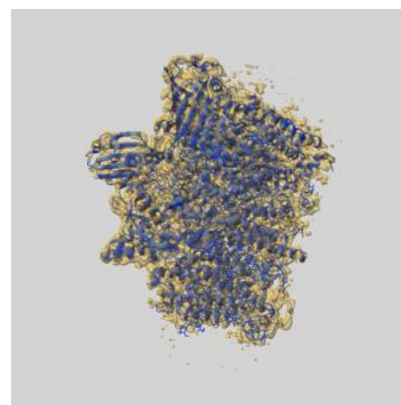
9.1 Map-model overlay [i](#)



X



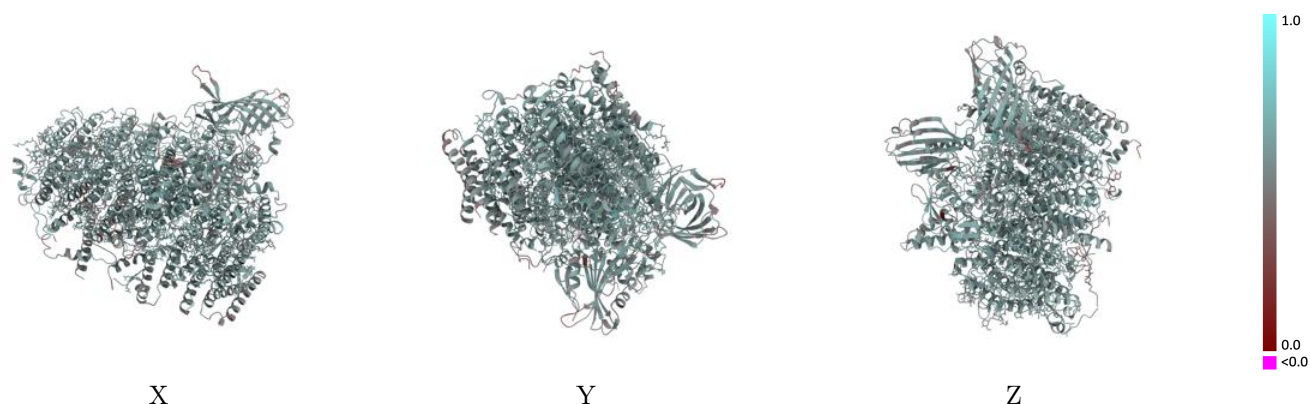
Y



Z

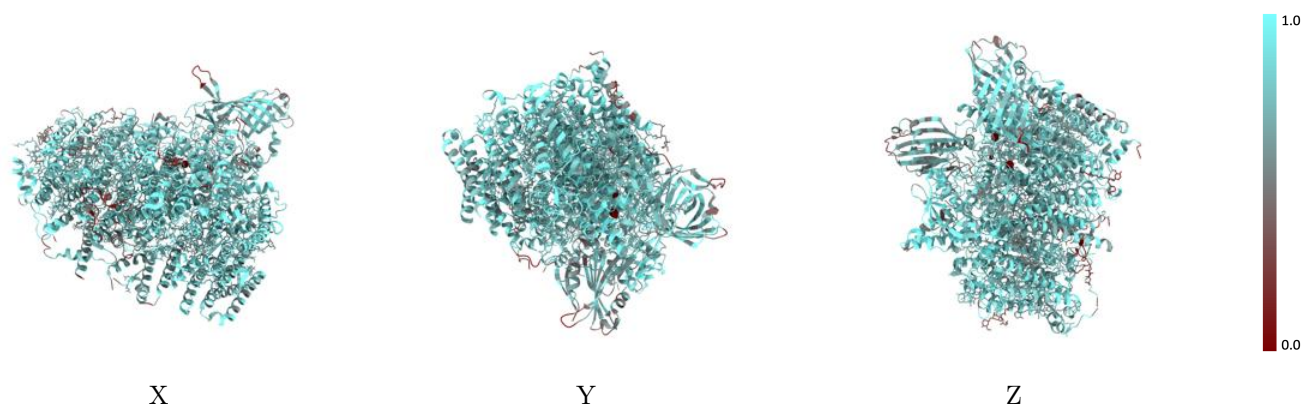
The images above show the 3D surface view of the map at the recommended contour level 0.0047 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



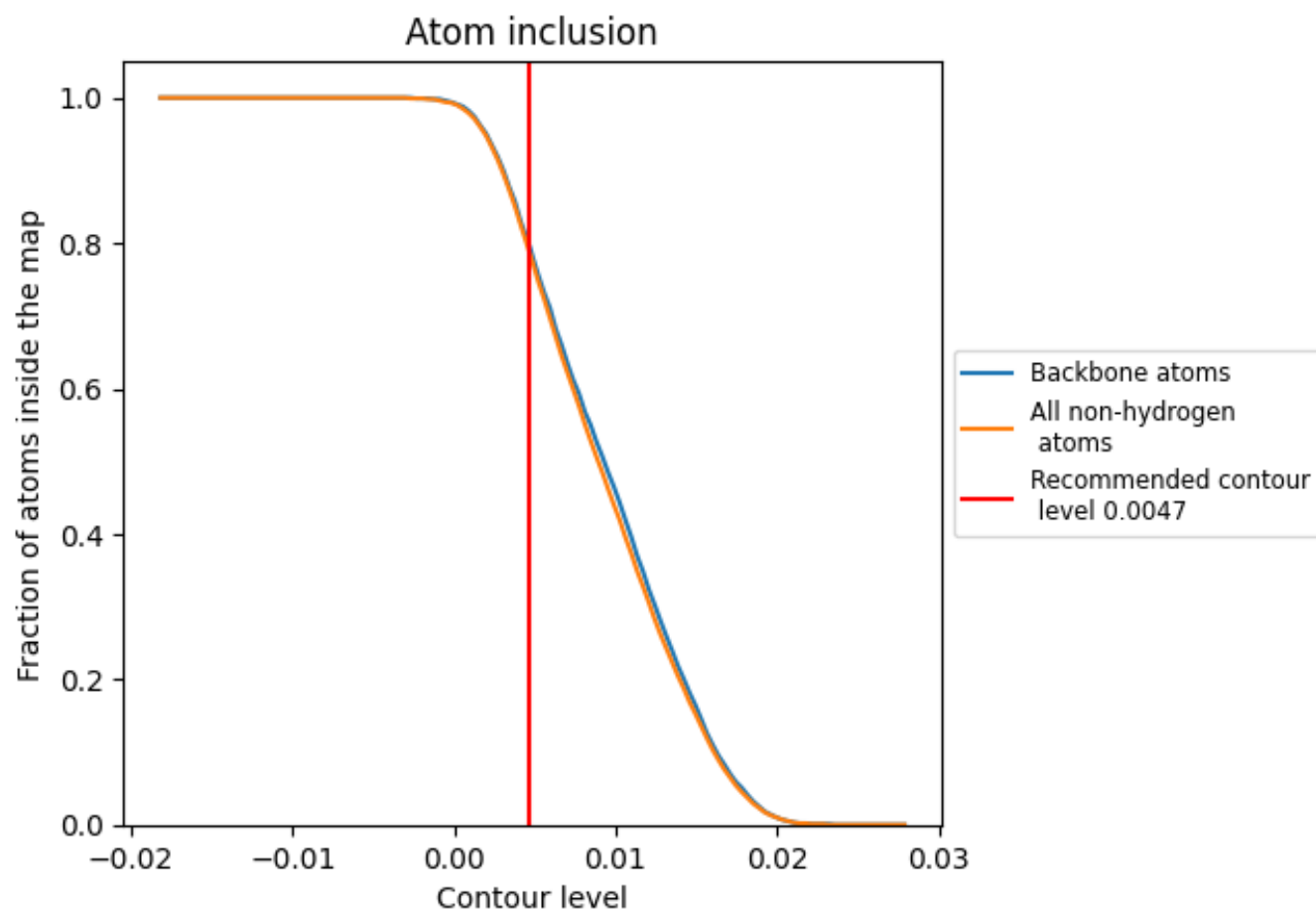
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0047).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.0047) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.5690
A	 0.7720	 0.5710
B	 0.8280	 0.5800
C	 0.8450	 0.5850
D	 0.8440	 0.5940
E	 0.8120	 0.5530
F	 0.7850	 0.5490
H	 0.8020	 0.5590
I	 0.8740	 0.5830
J	 0.7080	 0.5580
K	 0.8120	 0.5530
L	 0.8280	 0.5780
M	 0.6450	 0.5220
O	 0.7270	 0.5420
P	 0.5960	 0.5350
T	 0.7560	 0.5580
U	 0.6040	 0.4710
V	 0.7470	 0.5420
W	 0.5480	 0.5110
X	 0.7200	 0.5210
Z	 0.7280	 0.5050

