



wwPDB EM Validation Summary Report ⓘ

Aug 3, 2026 – 02:35 pm BST

PDB ID : 9S3E / pdb_00009s3e
EMDB ID : EMD-54531
Title : Universal Photosystem II Intermediate with Light-Dependent Water-Ferrocyanide Oxydo-reductase activity from Pisum sativum
Authors : Nelson, N.; Klaiman, D.; Fadeeva, M.
Deposited on : 2025-07-24
Resolution : 2.10 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

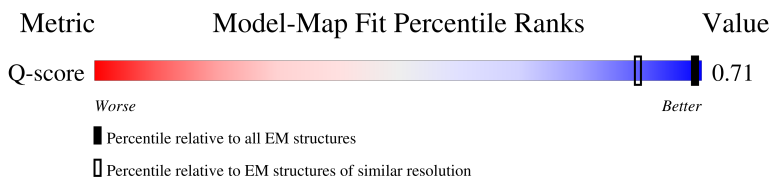
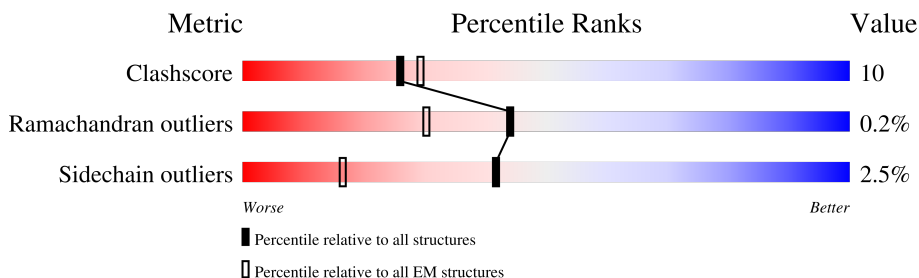
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.10 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.



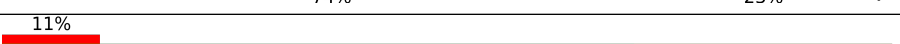
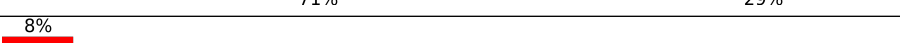
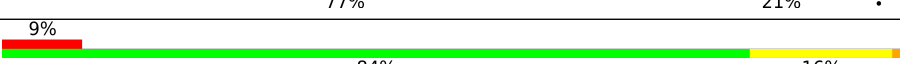
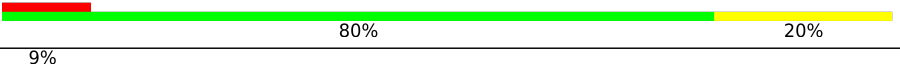
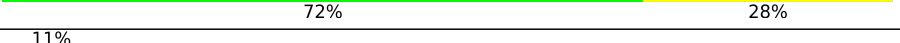
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2317 (1.60 - 2.60)

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	334	9% 76% 23% .
2	B	481	80% 19% .
3	C	449	80% 20% .
4	D	340	83% 16% .

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Mol	Chain	Length	Quality of chain
5	E	75	
6	F	30	
7	H	60	
8	I	33	
9	J	35	
10	K	37	
11	L	35	
12	M	28	
13	O	248	
14	P	186	
15	Q	148	
16	T	30	
17	W	47	
18	X	36	
19	U	28	

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 25160 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	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	481	Total	C	N	O	S	0	0
			3771	2471	639	649	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	449	Total	C	N	O	S	0	0
			3490	2296	582	602	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	340	Total	C	N	O	S	0	0
			2704	1786	442	464	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	75	Total	C	N	O	0	0
			612	400	100	112		

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	26	PHE	SER	conflict	UNP P62096

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	60	Total	C	N	O	S	0	0
			452	296	72	81	3		

- 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
			267	185	39	42	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	35	Total	C	N	O	S	0	0
			256	174	39	43			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	37	Total	C	N	O	S	0	0
			306	215	44	46	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	28	Total	C	N	O	S	0	0
			217	153	30	34			

- Molecule 13 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	186	Total	C	N	O	S	0	0
			1434	909	238	286	1		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	148	Total	C	N	O	S	0	0
			1157	742	197	218			

- 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
			245	172	34	38	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	47	Total	C	N	O	S	0	0
			368	245	54	68	1		

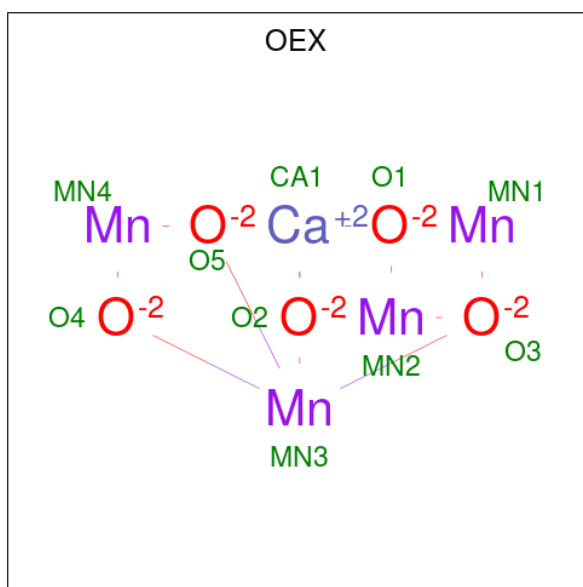
- Molecule 18 is a protein called Ultraviolet-B-repressible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	36	Total	C	N	O	S	0	0
			249	163	39	47			

- Molecule 19 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	28	Total	C	N	O	S	0	0
			212	131	41	37	3		

- Molecule 20 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

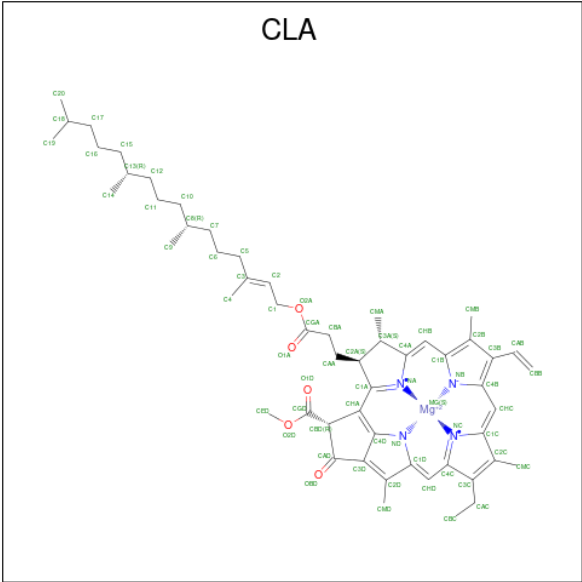
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



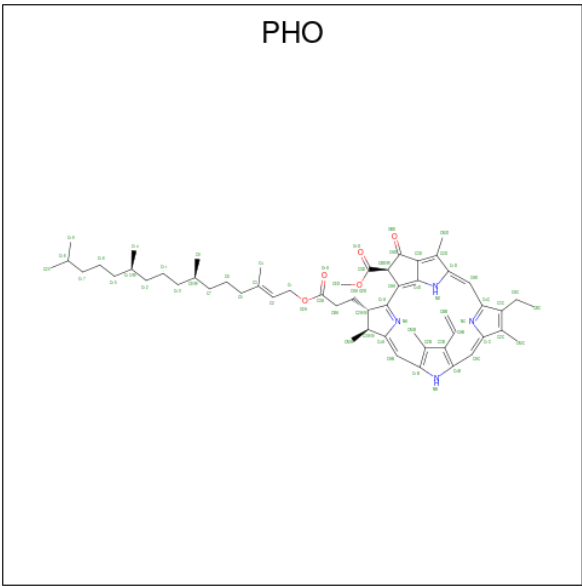
Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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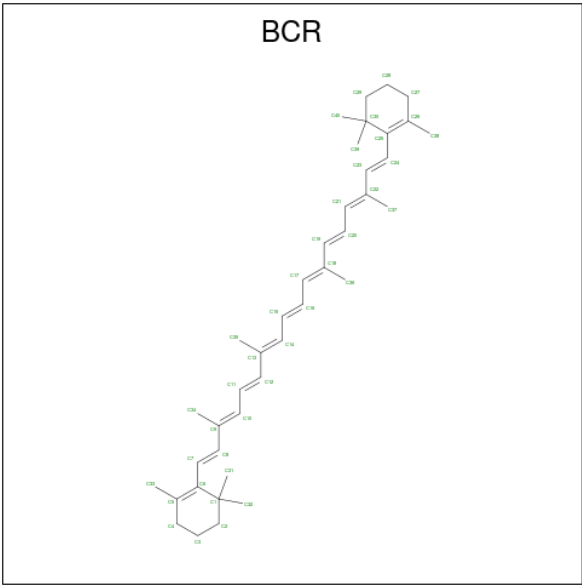
Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	C	1	Total 57	C 47	Mg 1	N 4	O 5	0
23	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



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

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



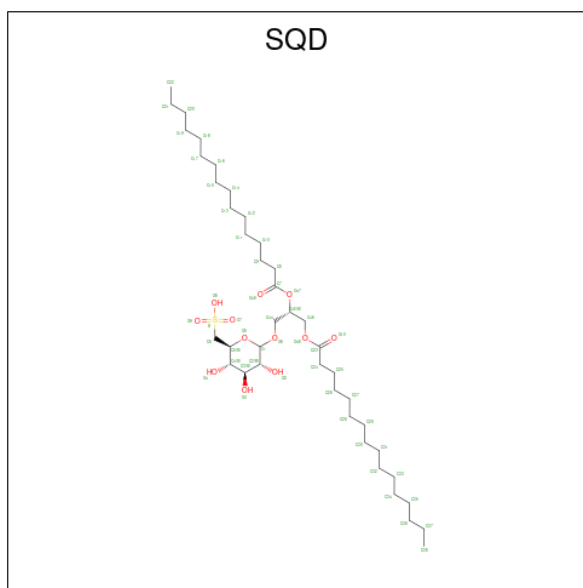
Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total	C	0
			40	40	

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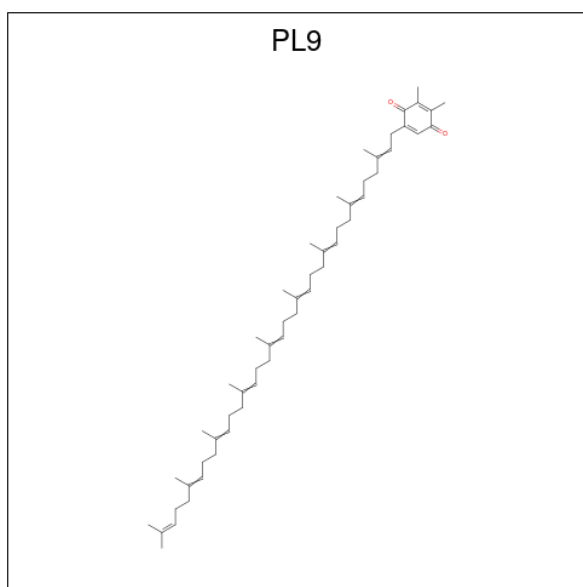
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	D	1	Total C 40 40	0
25	H	1	Total C 40 40	0
25	I	1	Total C 40 40	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



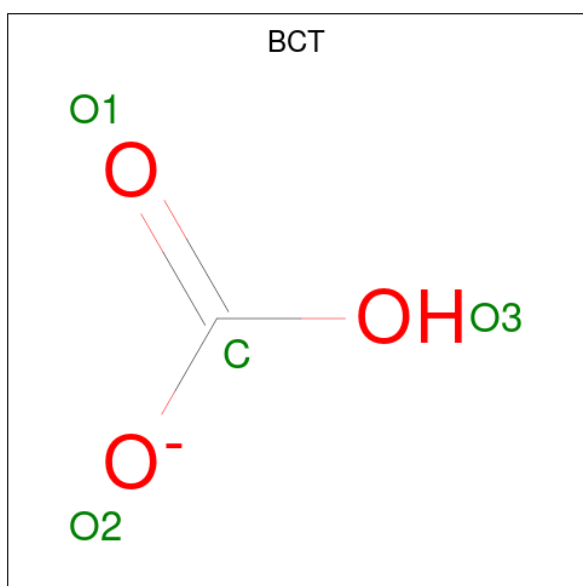
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C O S 50 37 12 1	0

- Molecule 27 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
27	A	1	Total	C	O	0
			13	11	2	
27	D	1	Total	C	O	0
			55	53	2	

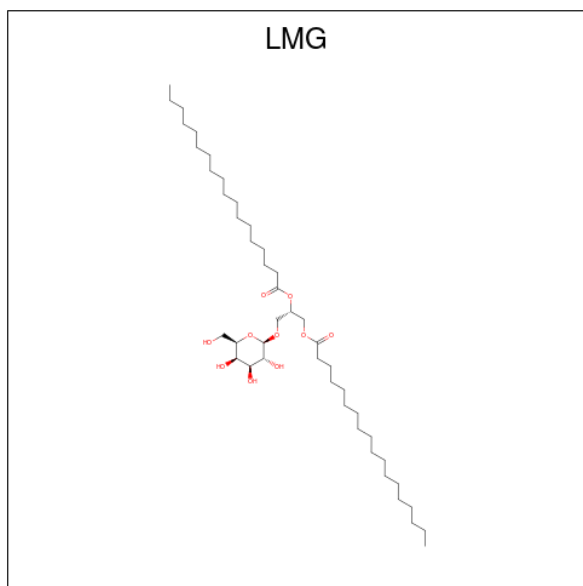
- Molecule 28 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



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

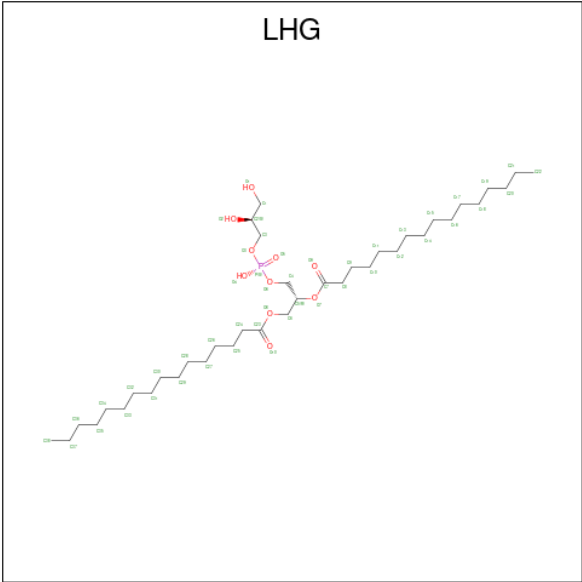
- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID:

LMG) (formula: $C_{45}H_{86}O_{10}$).



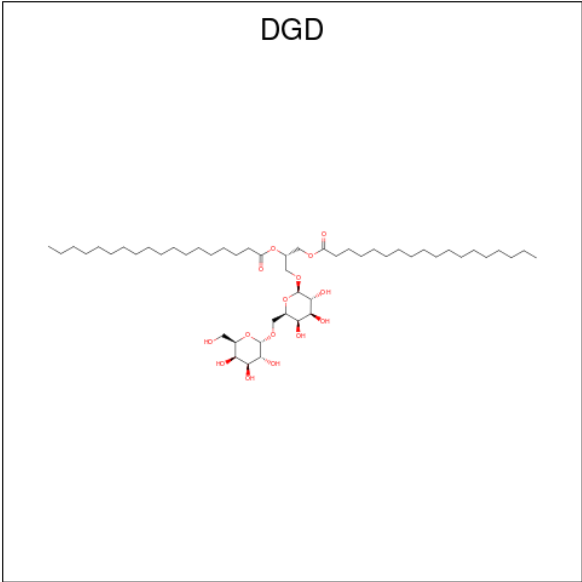
Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			51	41	10	
29	B	1	Total	C	O	0
			31	21	10	
29	C	1	Total	C	O	0
			51	41	10	
29	D	1	Total	C	O	0
			46	36	10	
29	I	1	Total	C	O	0
			40	30	10	
29	W	1	Total	C	O	0
			48	38	10	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



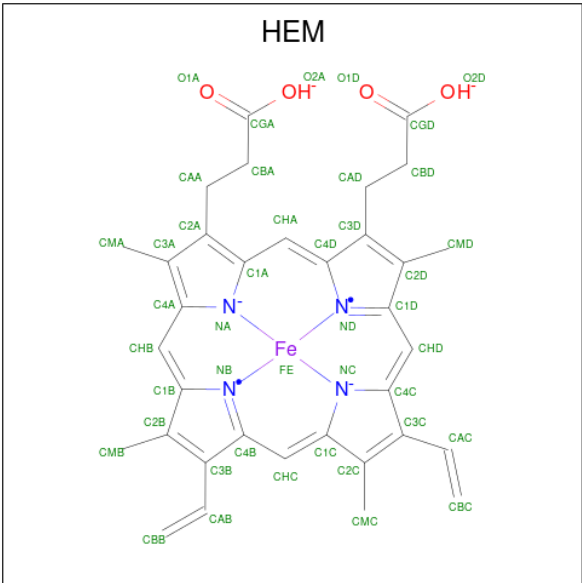
Mol	Chain	Residues	Atoms				AltConf
30	B	1	Total	C	O	P	0
			41	30	10	1	
30	B	1	Total	C	O	P	0
			46	35	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			43	32	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	W	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			55	40	15	
31	C	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			60	45	15	

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



Mol	Chain	Residues	Atoms					AltConf
32	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

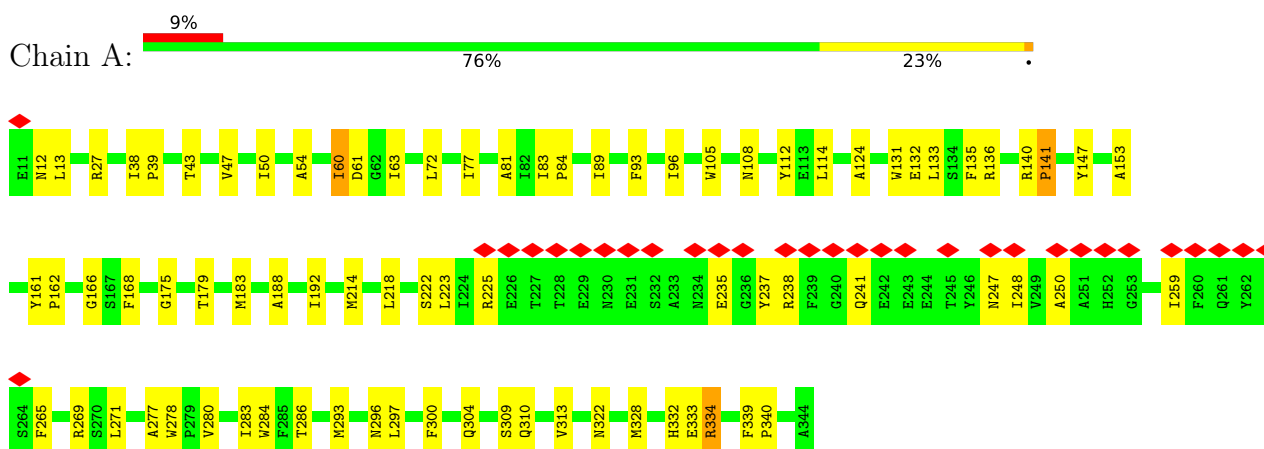
- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	A	121	Total	O	0
			121	121	
33	B	176	Total	O	0
			176	176	
33	C	159	Total	O	0
			159	159	
33	D	123	Total	O	0
			123	123	
33	E	18	Total	O	0
			18	18	
33	F	4	Total	O	0
			4	4	
33	H	14	Total	O	0
			14	14	
33	I	3	Total	O	0
			3	3	
33	J	4	Total	O	0
			4	4	
33	K	4	Total	O	0
			4	4	
33	L	10	Total	O	0
			10	10	
33	M	2	Total	O	0
			2	2	
33	O	54	Total	O	0
			54	54	
33	P	45	Total	O	0
			45	45	
33	Q	19	Total	O	0
			19	19	
33	T	6	Total	O	0
			6	6	
33	W	13	Total	O	0
			13	13	
33	X	1	Total	O	0
			1	1	
33	U	2	Total	O	0
			2	2	

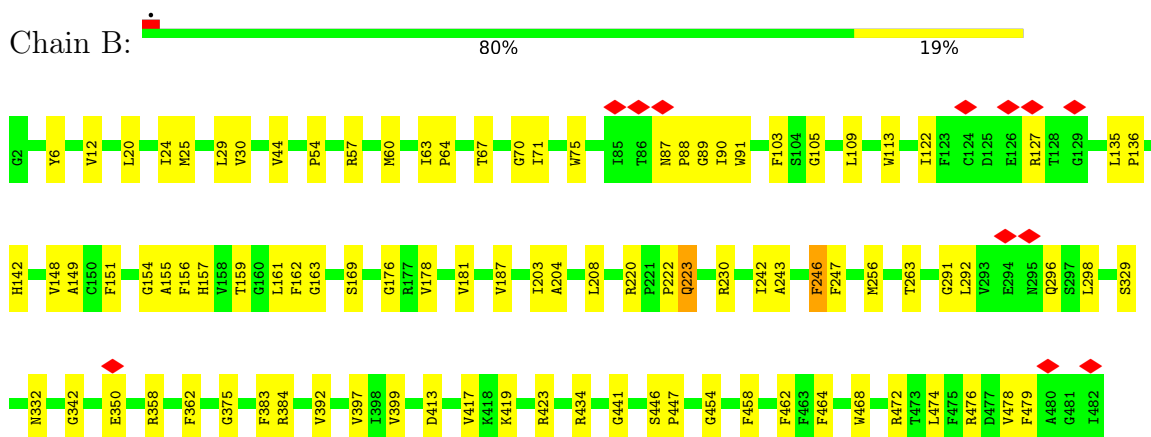
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

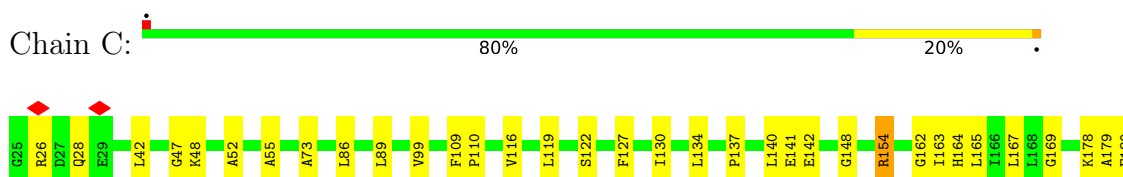
- Molecule 1: Photosystem II protein D1

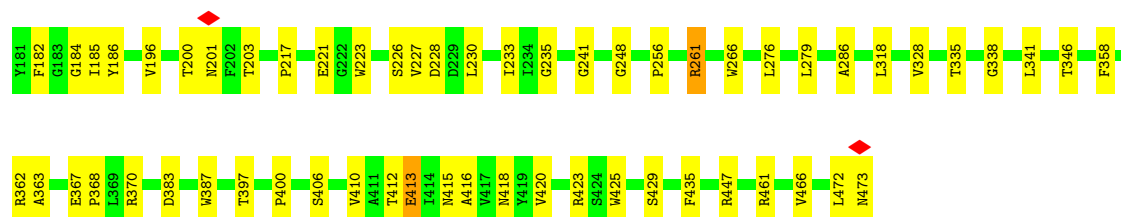


- Molecule 2: Photosystem II CP47 reaction center protein



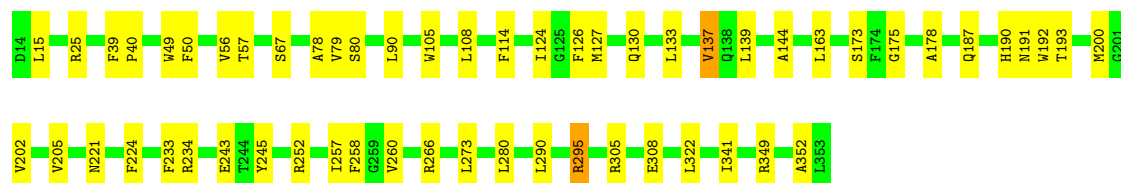
- Molecule 3: Photosystem II CP43 reaction center protein





• Molecule 4: Photosystem II D2 protein

Chain D: 83% 16% .



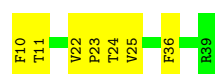
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 8% 84% 15% .



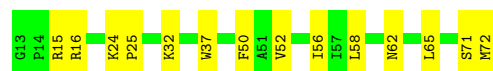
• Molecule 6: Cytochrome b559 subunit beta

Chain F: 77% 23%



• Molecule 7: Photosystem II reaction center protein H

Chain H: 77% 23%



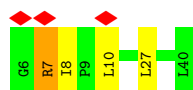
• Molecule 8: Photosystem II reaction center protein I

Chain I: 82% 18%

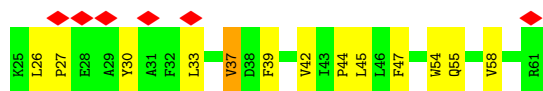


• Molecule 9: Photosystem II reaction center protein J

Chain J: 9% 89% 9% .



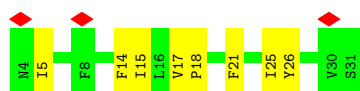
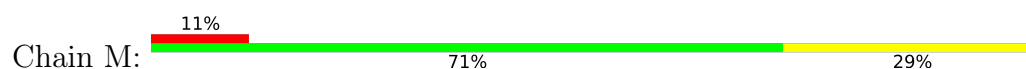
- Molecule 10: Photosystem II reaction center protein K



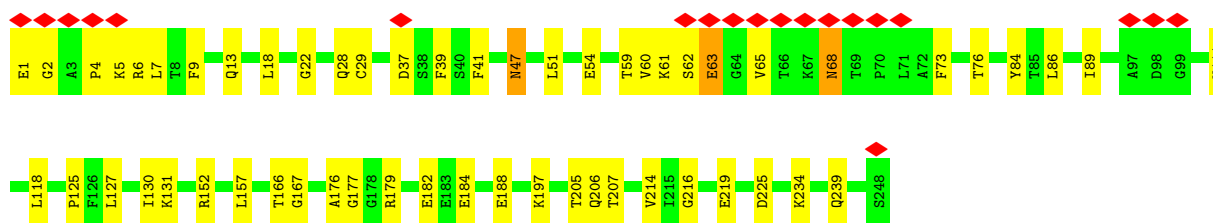
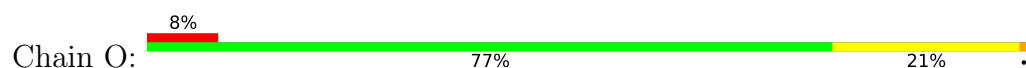
- Molecule 11: Photosystem II reaction center protein L



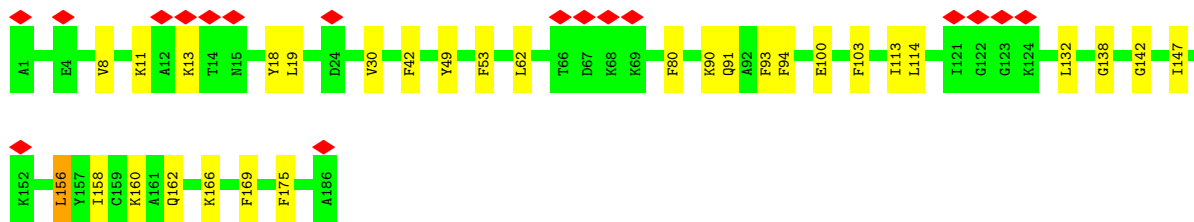
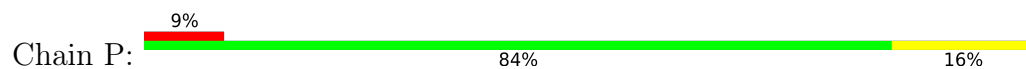
- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Oxygen-evolving enhancer protein 1, chloroplastic

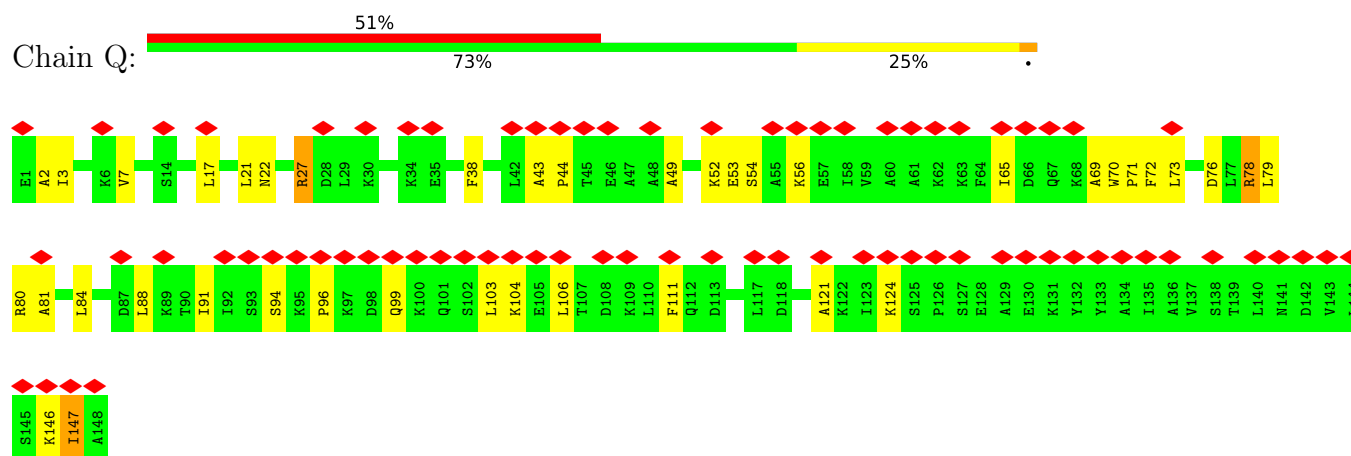


- Molecule 14: Oxygen-evolving enhancer protein 2, chloroplastic

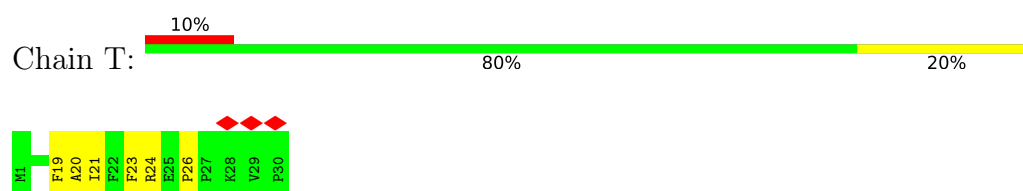


- Molecule 15: Oxygen-evolving enhancer protein 3

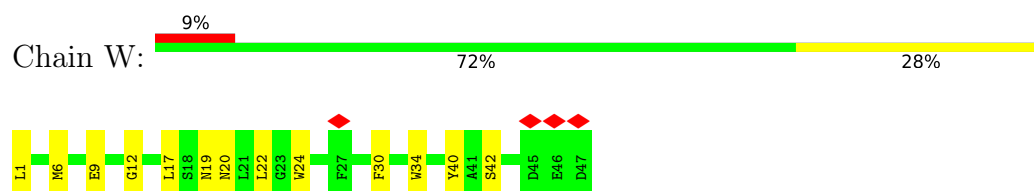




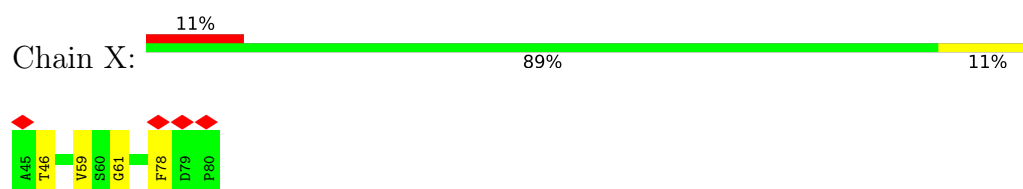
- Molecule 16: Photosystem II reaction center protein T



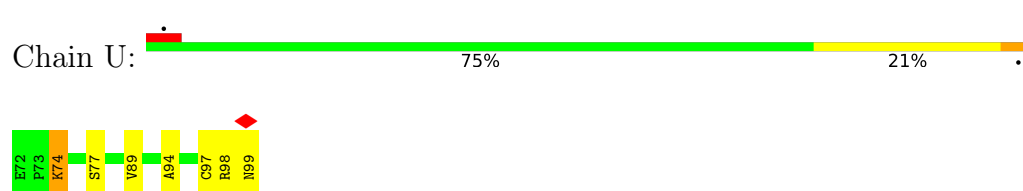
- Molecule 17: PSII 6.1 kDa protein



- Molecule 18: Ultraviolet-B-repressible protein



- Molecule 19: Photosystem II 5 kDa protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	323534	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.147	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	263.16, 263.16, 263.16	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, BCT, HEM, CL, PHO, FE2, BCR, DGD, PL9, CLA, LMG, OEX, 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	1.02	0/2697	1.16	1/3677 (0.0%)
2	B	1.02	0/3899	1.17	3/5308 (0.1%)
3	C	1.02	0/3607	1.15	0/4912
4	D	1.00	0/2796	1.16	0/3812
5	E	1.02	0/630	1.16	0/857
6	F	0.99	0/248	1.15	0/335
7	H	1.05	0/461	1.16	0/626
8	I	1.01	0/275	1.20	0/372
9	J	1.03	0/262	1.20	0/354
10	K	1.03	0/318	1.04	0/434
11	L	0.99	0/303	1.08	0/412
12	M	1.03	0/221	1.21	0/303
13	O	1.08	0/1906	1.15	1/2575 (0.0%)
14	P	1.05	0/1464	1.14	1/1978 (0.1%)
15	Q	1.04	0/1179	1.21	0/1591
16	T	0.99	0/253	1.12	0/344
17	W	0.98	0/378	1.14	0/514
18	X	1.06	0/252	1.29	0/345
19	U	1.03	0/216	1.22	0/291
All	All	1.03	0/21365	1.16	6/29040 (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	3
2	B	0	4
3	C	0	5
4	D	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	H	0	2
8	I	0	1
9	J	0	1
13	O	0	1
15	Q	0	3
All	All	0	24

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	342	GLY	CA-C-O	-6.04	118.10	122.45
13	O	2	GLY	CA-C-O	-5.53	118.16	122.52
2	B	89	GLY	CA-C-O	-5.40	118.26	122.52
14	P	142	GLY	CA-C-O	-5.34	118.30	122.52
2	B	246	PHE	CA-CB-CG	5.32	119.12	113.80

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	ARG	Sidechain
1	A	27	ARG	Sidechain
1	A	334	ARG	Sidechain
2	B	358	ARG	Sidechain
2	B	423	ARG	Sidechain

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	2616	0	2522	59	0
2	B	3771	0	3657	69	0
3	C	3490	0	3415	69	0
4	D	2704	0	2598	41	0
5	E	612	0	595	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	241	0	246	5	0
7	H	452	0	473	13	0
8	I	267	0	278	5	0
9	J	256	0	269	1	0
10	K	306	0	313	10	0
11	L	295	0	284	8	0
12	M	217	0	244	8	0
13	O	1870	0	1849	35	0
14	P	1434	0	1392	23	0
15	Q	1157	0	1210	30	0
16	T	245	0	260	4	0
17	W	368	0	355	10	0
18	X	249	0	266	2	0
19	U	212	0	220	5	0
20	A	10	0	0	0	0
21	A	1	0	0	0	0
22	A	2	0	0	0	0
23	A	175	0	169	10	0
23	B	1028	0	1119	71	0
23	C	813	0	857	63	0
23	D	195	0	214	17	0
24	A	64	0	74	2	0
24	D	64	0	74	3	0
25	A	40	0	56	5	0
25	B	120	0	168	22	0
25	C	40	0	56	5	0
25	D	40	0	56	6	0
25	H	40	0	56	4	0
25	I	40	0	56	4	0
26	A	50	0	66	4	0
27	A	13	0	7	1	0
27	D	55	0	80	1	0
28	A	4	0	0	0	0
29	B	82	0	104	10	0
29	C	51	0	72	9	0
29	D	46	0	62	8	0
29	I	40	0	50	2	0
29	W	48	0	66	6	0
30	B	87	0	120	11	0
30	D	92	0	130	5	0
30	L	49	0	74	2	0
30	W	49	0	74	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	B	62	0	82	6	0
31	C	177	0	228	21	0
32	E	43	0	30	4	0
33	A	121	0	0	1	0
33	B	176	0	0	0	0
33	C	159	0	0	0	0
33	D	123	0	0	0	0
33	E	18	0	0	0	0
33	F	4	0	0	0	0
33	H	14	0	0	0	0
33	I	3	0	0	0	0
33	J	4	0	0	0	0
33	K	4	0	0	0	0
33	L	10	0	0	0	0
33	M	2	0	0	0	0
33	O	54	0	0	0	0
33	P	45	0	0	0	0
33	Q	19	0	0	0	0
33	T	6	0	0	0	0
33	U	2	0	0	0	0
33	W	13	0	0	0	0
33	X	1	0	0	0	0
All	All	25160	0	24646	498	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 10.

The worst 5 of 498 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:165:LEU:HD21	23:C:506:CLA:HAB	1.54	0.88
23:C:508:CLA:H18	10:K:45:LEU:HD11	1.66	0.78
2:B:25:MET:HG2	25:B:517:BCR:H23C	1.67	0.77
30:D:407:LHG:HC62	11:L:16:THR:HG23	1.67	0.77
1:A:93:PHE:HZ	23:A:408:CLA:HAA1	1.50	0.76

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	332/334 (99%)	324 (98%)	6 (2%)	2 (1%)	21	18
2	B	479/481 (100%)	472 (98%)	7 (2%)	0	100	100
3	C	447/449 (100%)	434 (97%)	12 (3%)	1 (0%)	43	44
4	D	338/340 (99%)	329 (97%)	9 (3%)	0	100	100
5	E	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
6	F	28/30 (93%)	28 (100%)	0	0	100	100
7	H	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
8	I	31/33 (94%)	31 (100%)	0	0	100	100
9	J	33/35 (94%)	33 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	33/35 (94%)	33 (100%)	0	0	100	100
12	M	26/28 (93%)	26 (100%)	0	0	100	100
13	O	246/248 (99%)	232 (94%)	12 (5%)	2 (1%)	16	12
14	P	184/186 (99%)	180 (98%)	4 (2%)	0	100	100
15	Q	146/148 (99%)	144 (99%)	2 (1%)	0	100	100
16	T	28/30 (93%)	28 (100%)	0	0	100	100
17	W	45/47 (96%)	45 (100%)	0	0	100	100
18	X	34/36 (94%)	34 (100%)	0	0	100	100
19	U	26/28 (93%)	26 (100%)	0	0	100	100
All	All	2622/2660 (99%)	2561 (98%)	56 (2%)	5 (0%)	44	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	ALA
1	A	141	PRO

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Mol	Chain	Res	Type
1	A	259	ILE
13	O	65	VAL
13	O	68	ASN

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	270/270 (100%)	265 (98%)	5 (2%)	50	58
2	B	381/381 (100%)	373 (98%)	8 (2%)	47	54
3	C	351/351 (100%)	346 (99%)	5 (1%)	59	67
4	D	274/274 (100%)	266 (97%)	8 (3%)	37	42
5	E	67/67 (100%)	65 (97%)	2 (3%)	36	41
6	F	25/25 (100%)	25 (100%)	0	100	100
7	H	49/49 (100%)	48 (98%)	1 (2%)	48	56
8	I	30/30 (100%)	30 (100%)	0	100	100
9	J	26/26 (100%)	23 (88%)	3 (12%)	5	3
10	K	32/32 (100%)	31 (97%)	1 (3%)	35	39
11	L	33/33 (100%)	32 (97%)	1 (3%)	36	41
12	M	24/24 (100%)	24 (100%)	0	100	100
13	O	204/204 (100%)	197 (97%)	7 (3%)	32	35
14	P	150/150 (100%)	147 (98%)	3 (2%)	48	56
15	Q	125/125 (100%)	120 (96%)	5 (4%)	28	29
16	T	27/27 (100%)	27 (100%)	0	100	100
17	W	38/38 (100%)	36 (95%)	2 (5%)	20	19
18	X	29/29 (100%)	27 (93%)	2 (7%)	14	12
19	U	23/23 (100%)	21 (91%)	2 (9%)	9	7
All	All	2158/2158 (100%)	2103 (98%)	55 (2%)	42	48

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	H	65	LEU
13	O	47	ASN
19	U	97	CYS
17	W	9	GLU
9	J	7	ARG

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

Mol	Chain	Res	Type
15	Q	101	GLN
15	Q	141	ASN
4	D	84	ASN
3	C	418	ASN
17	W	20	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 3 are monoatomic - leaving 67 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
29	LMG	B	520	-	51,51,55	1.06	6 (11%)	59,59,63	1.09	3 (5%)
23	CLA	B	514	2	57,61,73	1.48	7 (12%)	68,98,113	2.10	18 (26%)
23	CLA	B	506	2	69,73,73	1.34	5 (7%)	83,113,113	1.95	21 (25%)
25	BCR	A	409	-	41,41,41	4.76	27 (65%)	56,56,56	2.25	18 (32%)
29	LMG	B	522	-	31,31,55	0.50	0	39,39,63	1.23	3 (7%)
23	CLA	A	406	33	54,58,73	1.53	7 (12%)	65,95,113	2.18	18 (27%)
23	CLA	B	516	2	69,73,73	1.35	5 (7%)	83,113,113	1.93	20 (24%)
23	CLA	C	505	3	69,73,73	1.35	7 (10%)	83,113,113	1.88	17 (20%)
23	CLA	C	507	33	69,73,73	1.35	7 (10%)	83,113,113	1.98	18 (21%)
25	BCR	B	519	-	41,41,41	4.81	27 (65%)	56,56,56	2.25	18 (32%)
32	HEM	E	101	6,5	50,50,50	1.99	15 (30%)	66,82,82	0.92	0
20	OEX	A	401	3,1,33	0,14,14	-	-	-	-	-
23	CLA	B	501	33	69,73,73	1.34	6 (8%)	83,113,113	1.91	19 (22%)
23	CLA	C	506	3	69,73,73	1.35	7 (10%)	83,113,113	1.96	20 (24%)
25	BCR	B	517	-	41,41,41	4.79	26 (63%)	56,56,56	2.26	22 (39%)
25	BCR	D	405	-	41,41,41	4.79	27 (65%)	56,56,56	2.35	19 (33%)
30	LHG	B	521	-	40,40,48	0.42	0	43,46,54	1.17	3 (6%)
23	CLA	D	401	33	69,73,73	1.34	7 (10%)	83,113,113	1.94	19 (22%)
30	LHG	B	523	-	45,45,48	0.40	0	48,51,54	0.95	2 (4%)
30	LHG	D	408	-	42,42,48	0.40	0	45,48,54	1.13	3 (6%)
23	CLA	B	511	2	69,73,73	1.34	6 (8%)	83,113,113	1.94	19 (22%)
23	CLA	B	504	2	69,73,73	1.35	6 (8%)	83,113,113	1.99	19 (22%)
23	CLA	B	503	2	69,73,73	1.35	6 (8%)	83,113,113	1.88	17 (20%)
23	CLA	C	501	3	69,73,73	1.35	7 (10%)	83,113,113	1.92	17 (20%)
30	LHG	D	407	-	48,48,48	0.39	0	51,54,54	1.01	3 (5%)
31	DGD	C	516	-	63,63,67	1.13	5 (7%)	77,77,81	0.96	2 (2%)
23	CLA	B	507	33	69,73,73	1.34	5 (7%)	83,113,113	2.01	19 (22%)
23	CLA	C	511	3	55,59,73	1.52	6 (10%)	66,96,113	2.14	19 (28%)
25	BCR	B	518	-	41,41,41	4.79	27 (65%)	56,56,56	2.16	18 (32%)
31	DGD	B	524	-	63,63,67	1.12	7 (11%)	77,77,81	0.92	2 (2%)
23	CLA	B	515	2	69,73,73	1.35	5 (7%)	83,113,113	1.89	18 (21%)
23	CLA	B	508	2	69,73,73	1.35	7 (10%)	83,113,113	1.87	18 (21%)
27	PL9	D	406	-	55,55,55	0.69	1 (1%)	68,69,69	0.64	2 (2%)
29	LMG	D	409	-	46,46,55	0.92	4 (8%)	54,54,63	1.03	3 (5%)
23	CLA	C	510	3	69,73,73	1.35	7 (10%)	83,113,113	1.90	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	509	-	69,73,73	1.34	5 (7%)	83,113,113	1.96	17 (20%)
23	CLA	C	508	3	69,73,73	1.35	6 (8%)	83,113,113	1.96	20 (24%)
25	BCR	C	514	-	41,41,41	4.81	27 (65%)	56,56,56	2.22	20 (35%)
29	LMG	I	101	-	40,40,55	0.92	3 (7%)	48,48,63	1.10	3 (6%)
30	LHG	L	101	-	48,48,48	0.39	0	51,54,54	0.94	2 (3%)
23	CLA	B	512	2	69,73,73	1.34	6 (8%)	83,113,113	1.97	18 (21%)
23	CLA	A	405	1	69,73,73	1.35	6 (8%)	83,113,113	1.89	19 (22%)
23	CLA	D	404	4	69,73,73	1.35	6 (8%)	83,113,113	1.95	20 (24%)
28	BCT	A	412	21	2,3,3	0.96	0	2,3,3	0.38	0
31	DGD	C	515	-	56,56,67	0.99	4 (7%)	70,70,81	0.98	3 (4%)
27	PL9	A	411	-	13,13,55	1.46	1 (7%)	17,17,69	1.08	1 (5%)
23	CLA	C	503	-	69,73,73	1.35	6 (8%)	83,113,113	1.94	19 (22%)
23	CLA	D	403	4	69,73,73	1.35	6 (8%)	83,113,113	1.90	18 (21%)
23	CLA	C	509	3	69,73,73	1.36	7 (10%)	83,113,113	1.92	19 (22%)
23	CLA	C	512	3	61,65,73	1.43	6 (9%)	73,103,113	2.05	19 (26%)
31	DGD	C	517	-	61,61,67	1.09	6 (9%)	75,75,81	0.96	2 (2%)
23	CLA	B	510	33	69,73,73	1.36	6 (8%)	83,113,113	1.90	19 (22%)
29	LMG	W	101	-	48,48,55	1.00	5 (10%)	56,56,63	1.20	4 (7%)
23	CLA	C	513	3	59,63,73	1.46	6 (10%)	71,101,113	2.06	19 (26%)
23	CLA	C	504	33	69,73,73	1.34	6 (8%)	83,113,113	1.94	17 (20%)
23	CLA	B	502	2	69,73,73	1.36	6 (8%)	83,113,113	1.92	20 (24%)
23	CLA	B	513	2	69,73,73	1.35	6 (8%)	83,113,113	1.88	18 (21%)
23	CLA	B	505	2	69,73,73	1.35	6 (8%)	83,113,113	1.95	19 (22%)
24	PHO	A	407	-	58,69,69	0.80	2 (3%)	56,99,99	1.00	3 (5%)
25	BCR	H	101	-	41,41,41	4.82	27 (65%)	56,56,56	2.23	18 (32%)
30	LHG	W	102	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
26	SQD	A	410	-	49,50,54	0.82	0	58,61,65	0.95	2 (3%)
29	LMG	C	518	-	51,51,55	1.07	6 (11%)	59,59,63	1.04	3 (5%)
23	CLA	A	408	1	64,68,73	1.40	6 (9%)	77,107,113	1.98	18 (23%)
24	PHO	D	402	-	58,69,69	0.78	2 (3%)	56,99,99	0.99	3 (5%)
23	CLA	C	502	3	69,73,73	1.34	7 (10%)	83,113,113	1.95	20 (24%)
25	BCR	I	102	-	41,41,41	4.83	27 (65%)	56,56,56	2.35	20 (35%)

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
29	LMG	B	520	-	-	13/46/66/70	0/1/1/1
23	CLA	B	514	2	-	6/25/101/115	-
23	CLA	B	506	2	-	15/39/115/115	-
25	BCR	A	409	-	-	13/29/63/63	0/2/2/2
29	LMG	B	522	-	-	7/26/46/70	0/1/1/1
23	CLA	A	406	33	-	11/21/97/115	-
23	CLA	B	516	2	-	10/39/115/115	-
23	CLA	C	505	3	-	13/39/115/115	-
23	CLA	C	507	33	-	12/39/115/115	-
25	BCR	B	519	-	-	9/29/63/63	0/2/2/2
32	HEM	E	101	6,5	-	3/14/54/54	-
25	BCR	B	517	-	-	13/29/63/63	0/2/2/2
23	CLA	B	501	33	-	13/39/115/115	-
23	CLA	C	506	3	-	17/39/115/115	-
25	BCR	D	405	-	-	11/29/63/63	0/2/2/2
30	LHG	B	521	-	-	29/45/45/53	-
23	CLA	D	401	33	-	15/39/115/115	-
30	LHG	B	523	-	-	30/50/50/53	-
30	LHG	D	408	-	-	23/47/47/53	-
23	CLA	B	511	2	-	10/39/115/115	-
23	CLA	B	504	2	-	12/39/115/115	-
23	CLA	B	503	2	-	11/39/115/115	-
23	CLA	C	501	3	-	12/39/115/115	-
30	LHG	D	407	-	-	33/53/53/53	-
31	DGD	C	516	-	-	11/51/91/95	0/2/2/2
23	CLA	B	507	33	-	24/39/115/115	-
23	CLA	C	511	3	-	5/23/99/115	-
25	BCR	B	518	-	-	12/29/63/63	0/2/2/2
31	DGD	B	524	-	-	8/51/91/95	0/2/2/2
23	CLA	B	515	2	-	12/39/115/115	-
23	CLA	B	508	2	-	14/39/115/115	-
27	PL9	D	406	-	-	3/53/73/73	0/1/1/1
29	LMG	D	409	-	-	10/41/61/70	0/1/1/1
23	CLA	C	510	3	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	509	-	-	18/39/115/115	-
23	CLA	C	508	3	-	17/39/115/115	-
25	BCR	C	514	-	-	14/29/63/63	0/2/2/2
29	LMG	I	101	-	-	7/35/55/70	0/1/1/1
30	LHG	L	101	-	-	28/53/53/53	-
23	CLA	B	512	2	-	12/39/115/115	-
23	CLA	A	405	1	-	9/39/115/115	-
23	CLA	D	404	4	-	16/39/115/115	-
31	DGD	C	515	-	-	8/44/84/95	0/2/2/2
27	PL9	A	411	-	-	0/5/18/73	0/1/1/1
23	CLA	C	503	-	-	12/39/115/115	-
23	CLA	D	403	4	-	14/39/115/115	-
23	CLA	C	509	3	-	13/39/115/115	-
23	CLA	C	512	3	-	20/30/106/115	-
31	DGD	C	517	-	-	11/49/89/95	0/2/2/2
23	CLA	B	510	33	-	8/39/115/115	-
29	LMG	W	101	-	-	6/43/63/70	0/1/1/1
23	CLA	C	513	3	-	8/27/103/115	-
23	CLA	C	504	33	-	14/39/115/115	-
23	CLA	B	502	2	-	16/39/115/115	-
23	CLA	B	513	2	-	11/39/115/115	-
23	CLA	B	505	2	-	21/39/115/115	-
24	PHO	A	407	-	-	4/37/103/103	0/5/6/6
25	BCR	H	101	-	-	10/29/63/63	0/2/2/2
30	LHG	W	102	-	-	35/53/53/53	-
26	SQD	A	410	-	-	10/45/65/69	0/1/1/1
29	LMG	C	518	-	-	3/46/66/70	0/1/1/1
23	CLA	A	408	1	-	11/33/109/115	-
24	PHO	D	402	-	-	0/37/103/103	0/5/6/6
23	CLA	C	502	3	-	12/39/115/115	-
25	BCR	I	102	-	-	14/29/63/63	0/2/2/2

The worst 5 of 498 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	518	BCR	C26-C25	15.64	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	514	BCR	C26-C25	15.59	1.61	1.34
25	H	101	BCR	C26-C25	15.50	1.61	1.34
25	B	519	BCR	C26-C25	15.49	1.61	1.34
25	I	102	BCR	C26-C25	15.40	1.61	1.34

The worst 5 of 861 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	504	CLA	C4A-NA-C1A	9.54	111.00	106.71
23	B	512	CLA	C4A-NA-C1A	9.53	110.99	106.71
23	B	507	CLA	C4A-NA-C1A	9.48	110.97	106.71
23	B	509	CLA	C4A-NA-C1A	9.38	110.92	106.71
23	C	507	CLA	C4A-NA-C1A	9.26	110.87	106.71

There are no chirality outliers.

5 of 836 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	405	CLA	CBD-CGD-O2D-CED
23	A	406	CLA	C1A-C2A-CAA-CBA
23	B	501	CLA	CBD-CGD-O2D-CED
23	B	502	CLA	CHA-CBD-CGD-O1D
23	B	502	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

65 monomers are involved in 264 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	520	LMG	5	0
23	B	514	CLA	1	0
23	B	506	CLA	7	0
25	A	409	BCR	5	0
29	B	522	LMG	5	0
23	A	406	CLA	1	0
23	B	516	CLA	8	0
23	C	505	CLA	8	0
23	C	507	CLA	9	0
25	B	519	BCR	12	0
32	E	101	HEM	4	0
23	B	501	CLA	7	0
23	C	506	CLA	6	0

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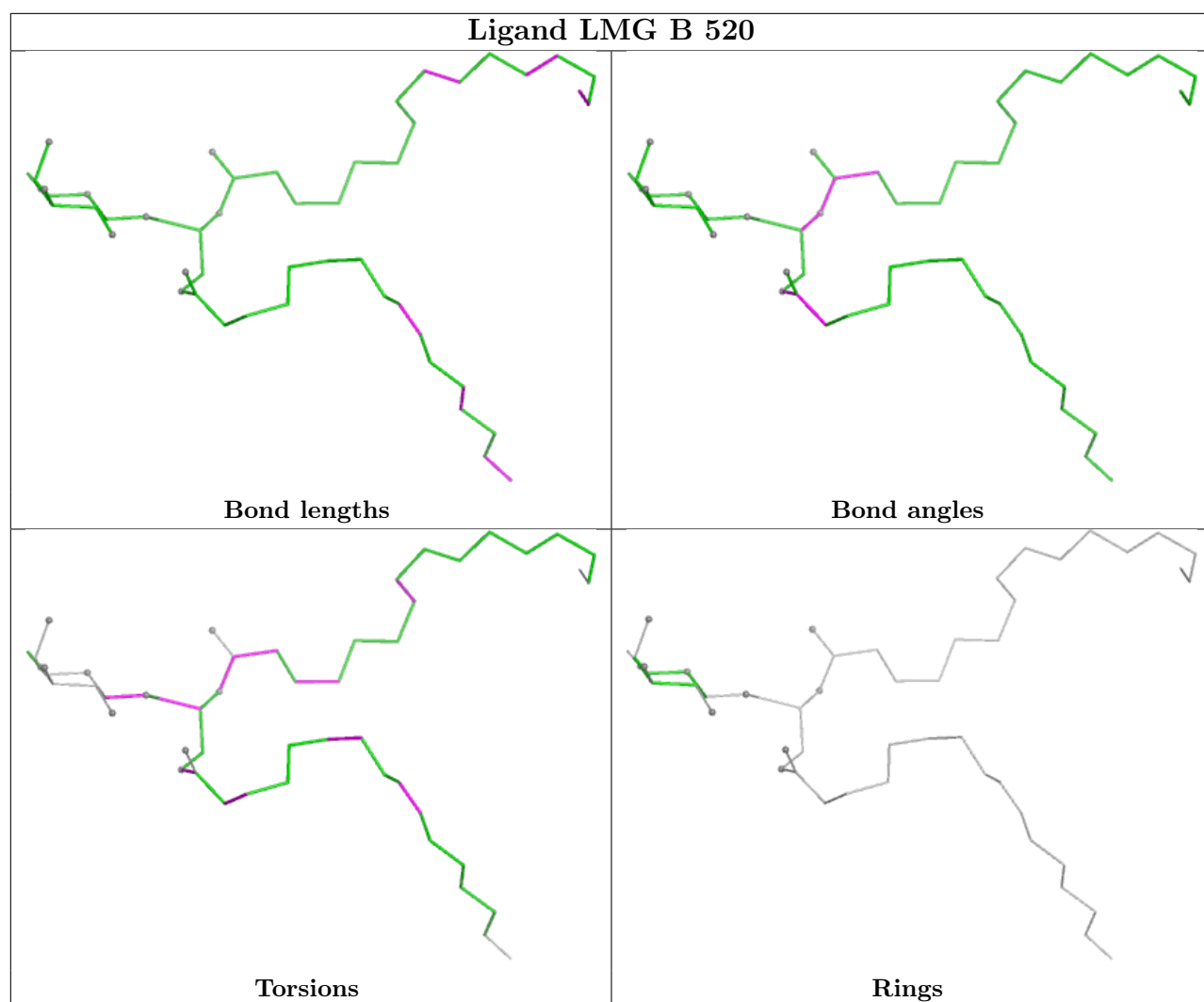
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	517	BCR	5	0
25	D	405	BCR	6	0
30	B	521	LHG	8	0
23	D	401	CLA	4	0
30	B	523	LHG	3	0
30	D	408	LHG	3	0
23	B	511	CLA	7	0
23	B	504	CLA	6	0
23	B	503	CLA	7	0
23	C	501	CLA	7	0
30	D	407	LHG	2	0
31	C	516	DGD	10	0
23	B	507	CLA	2	0
23	C	511	CLA	6	0
25	B	518	BCR	5	0
31	B	524	DGD	6	0
23	B	515	CLA	1	0
23	B	508	CLA	4	0
27	D	406	PL9	1	0
29	D	409	LMG	8	0
23	C	510	CLA	3	0
23	B	509	CLA	4	0
23	C	508	CLA	8	0
25	C	514	BCR	5	0
29	I	101	LMG	2	0
30	L	101	LHG	2	0
23	B	512	CLA	5	0
23	A	405	CLA	2	0
23	D	404	CLA	7	0
31	C	515	DGD	6	0
27	A	411	PL9	1	0
23	C	503	CLA	6	0
23	D	403	CLA	6	0
23	C	509	CLA	7	0
23	C	512	CLA	7	0
31	C	517	DGD	6	0
23	B	510	CLA	6	0
29	W	101	LMG	6	0
23	C	513	CLA	1	0
23	C	504	CLA	7	0
23	B	502	CLA	5	0
23	B	513	CLA	6	0

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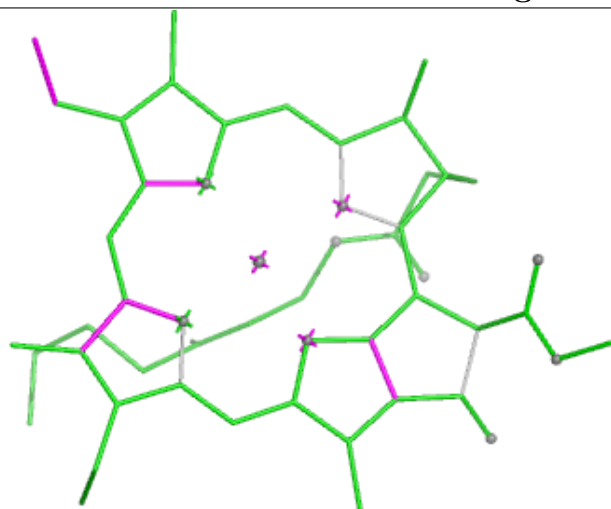
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	505	CLA	10	0
24	A	407	PHO	2	0
25	H	101	BCR	4	0
30	W	102	LHG	9	0
26	A	410	SQD	4	0
29	C	518	LMG	9	0
23	A	408	CLA	7	0
24	D	402	PHO	3	0
23	C	502	CLA	3	0
25	I	102	BCR	4	0

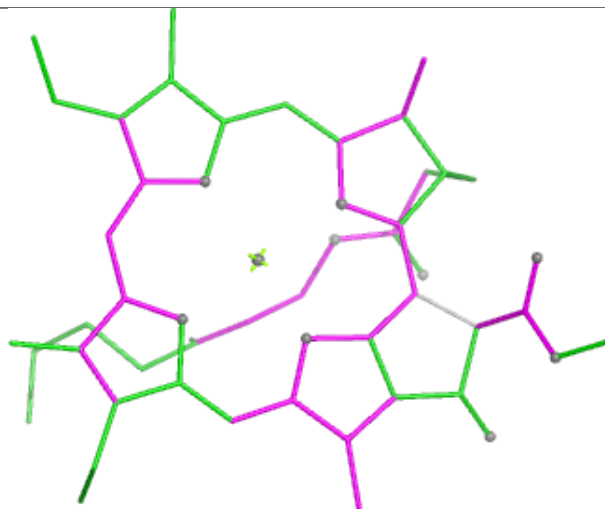
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



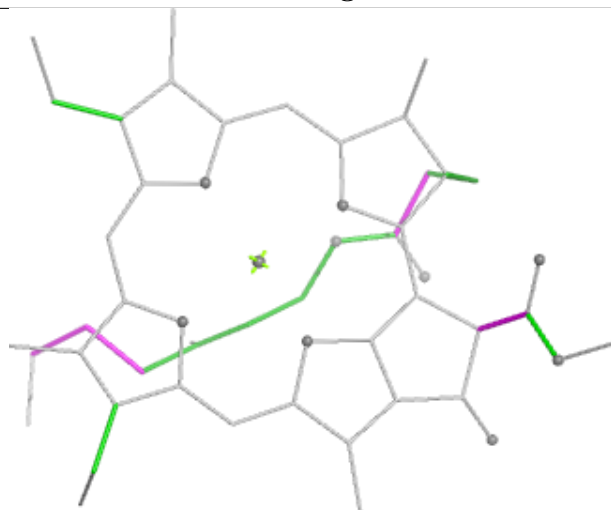
Ligand CLA B 514



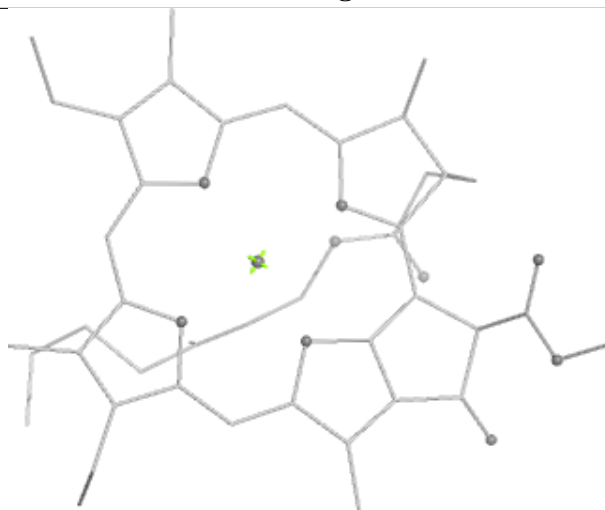
Bond lengths



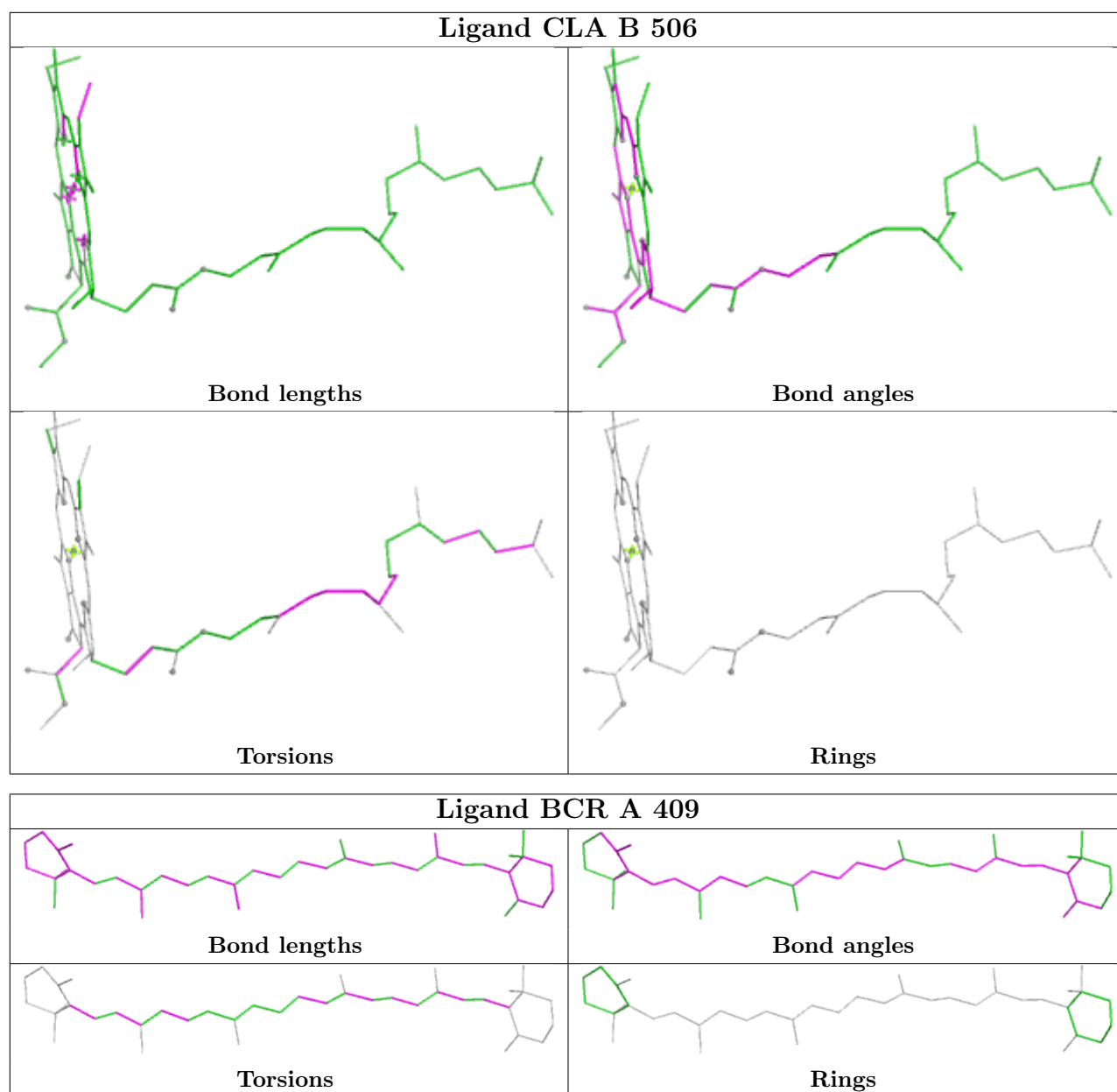
Bond angles

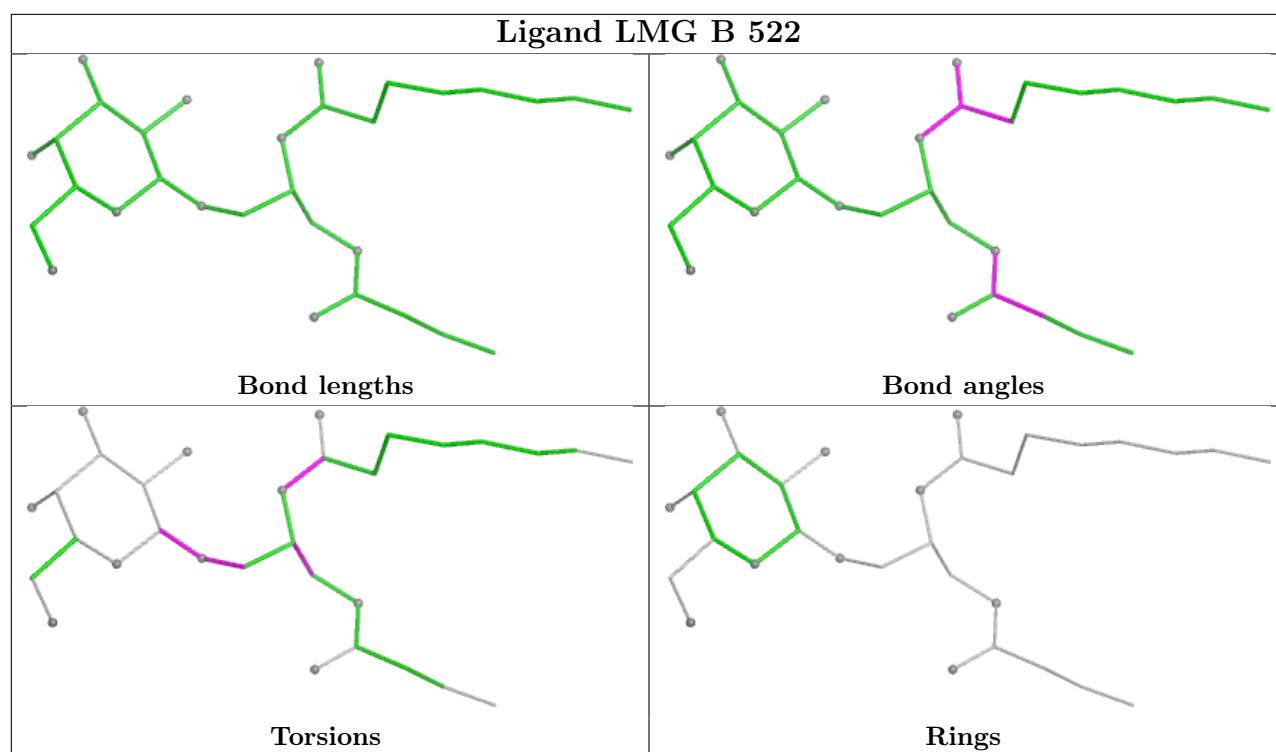


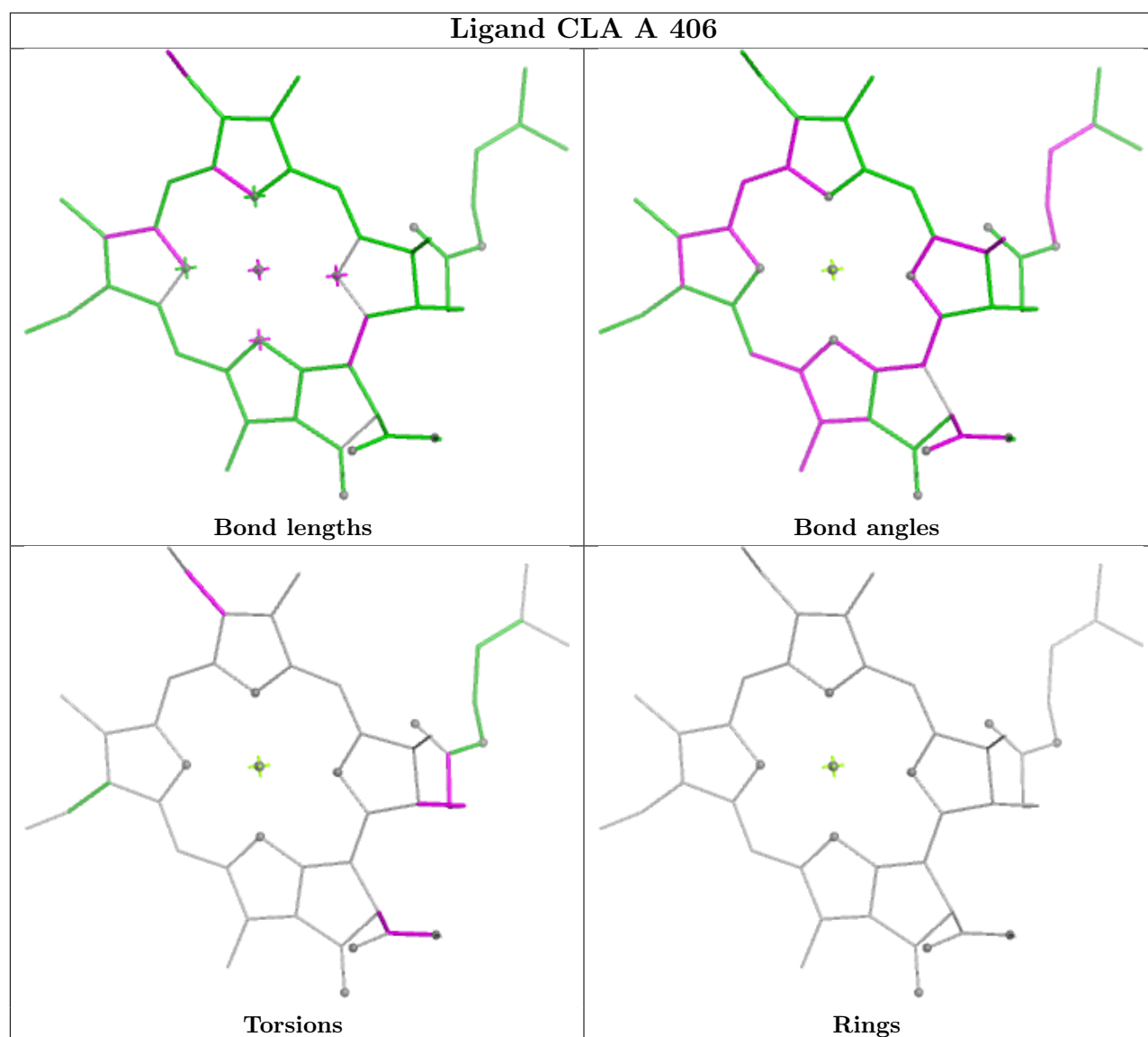
Torsions

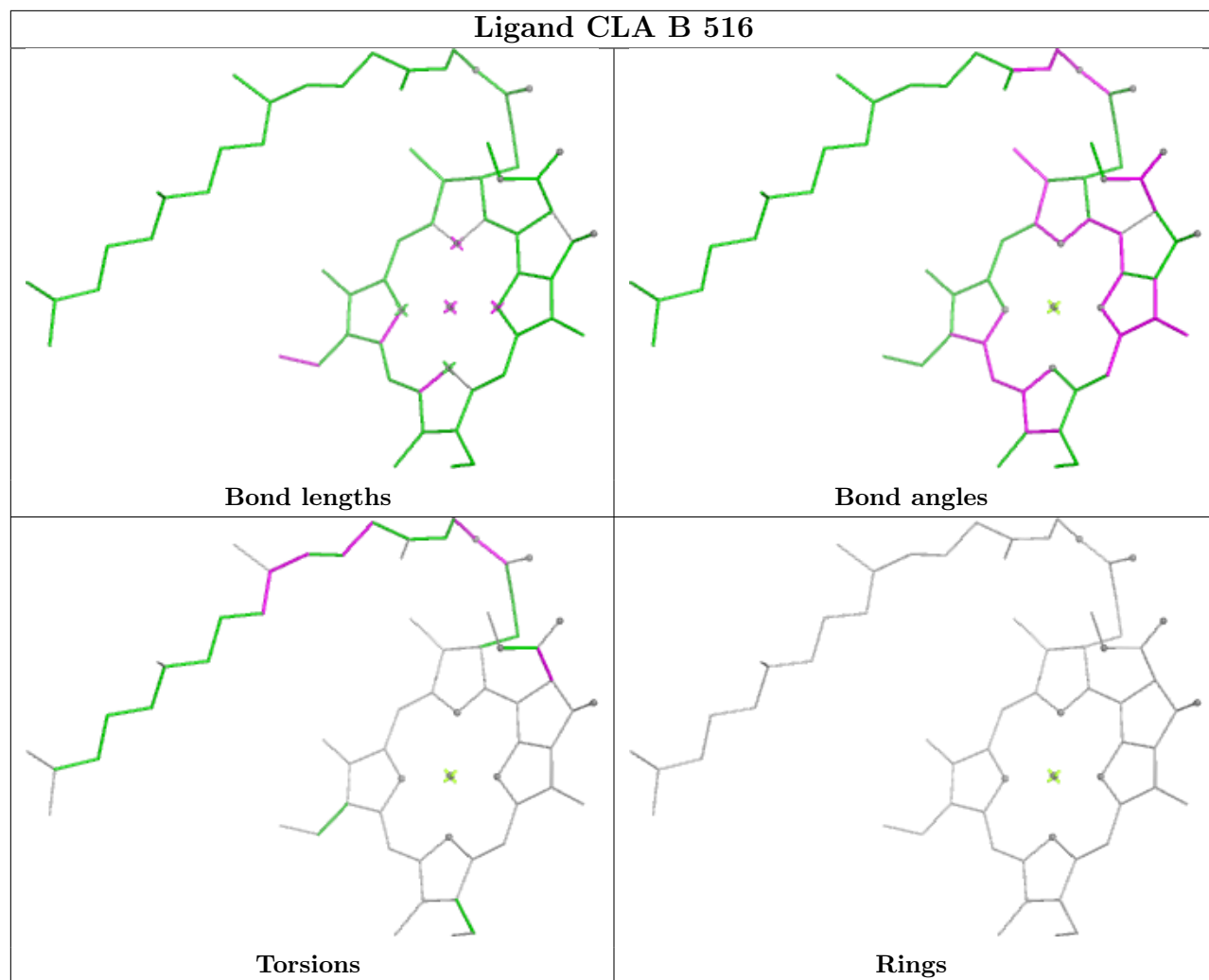


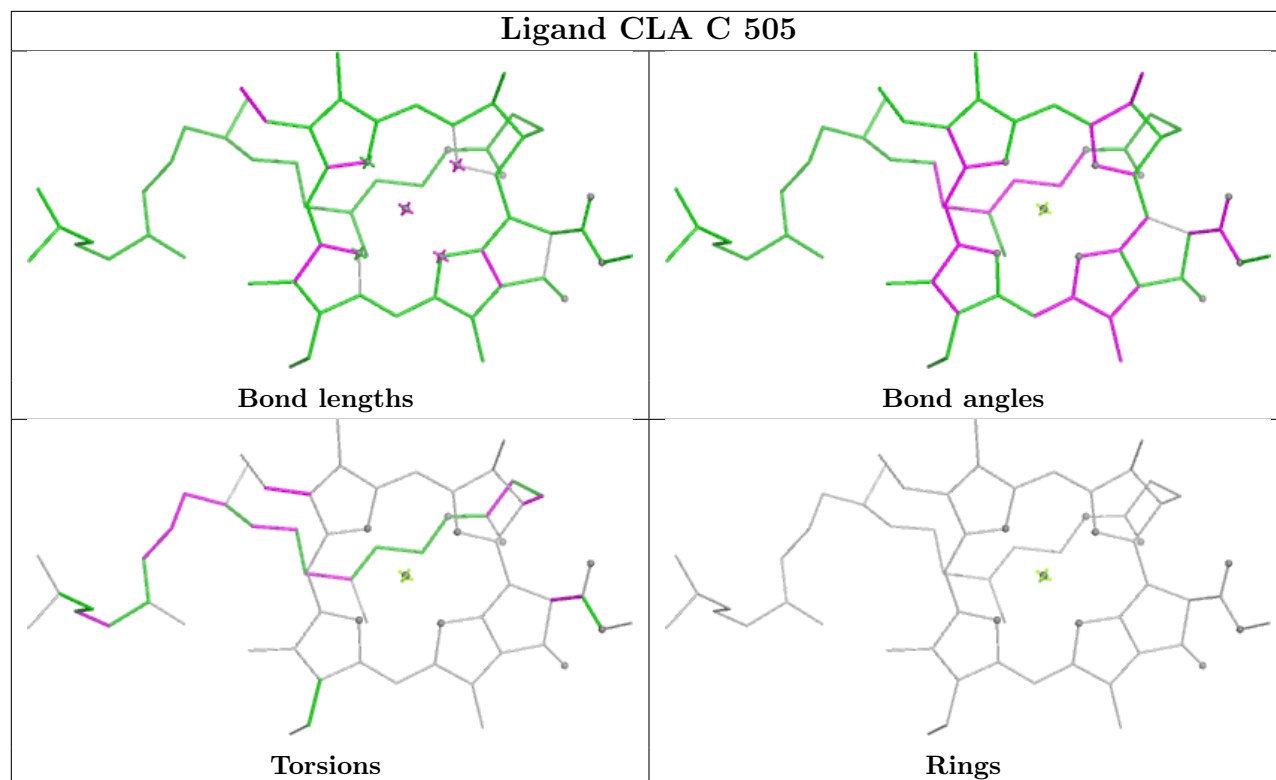
Rings

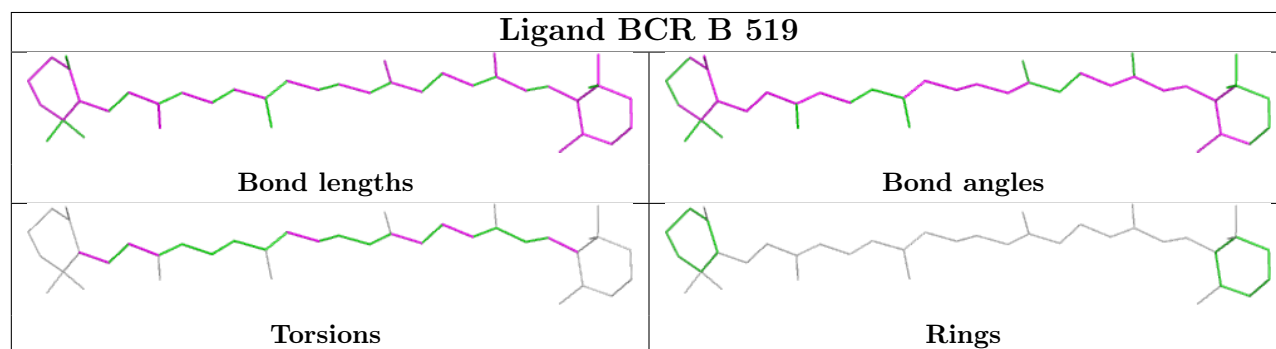
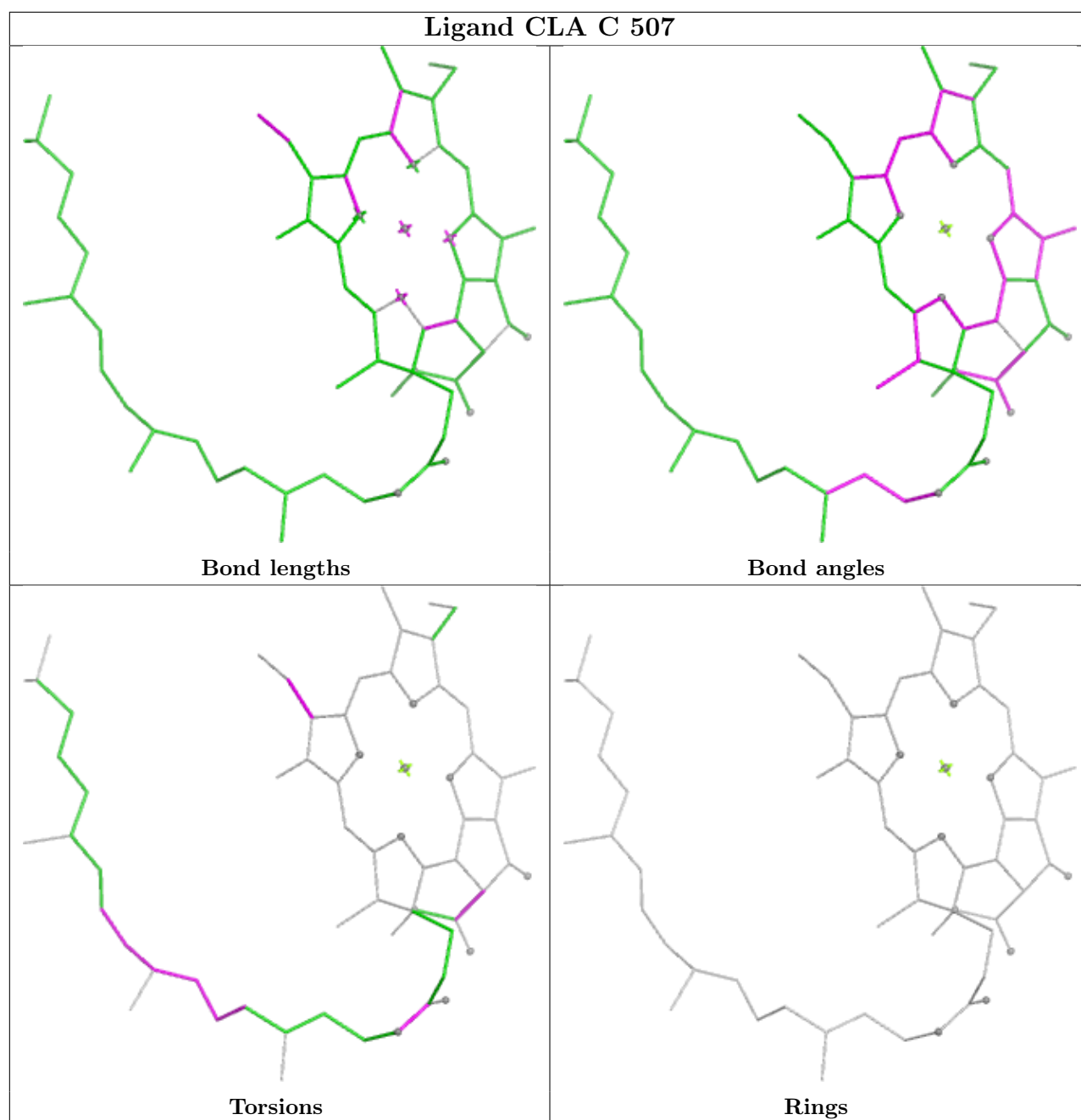


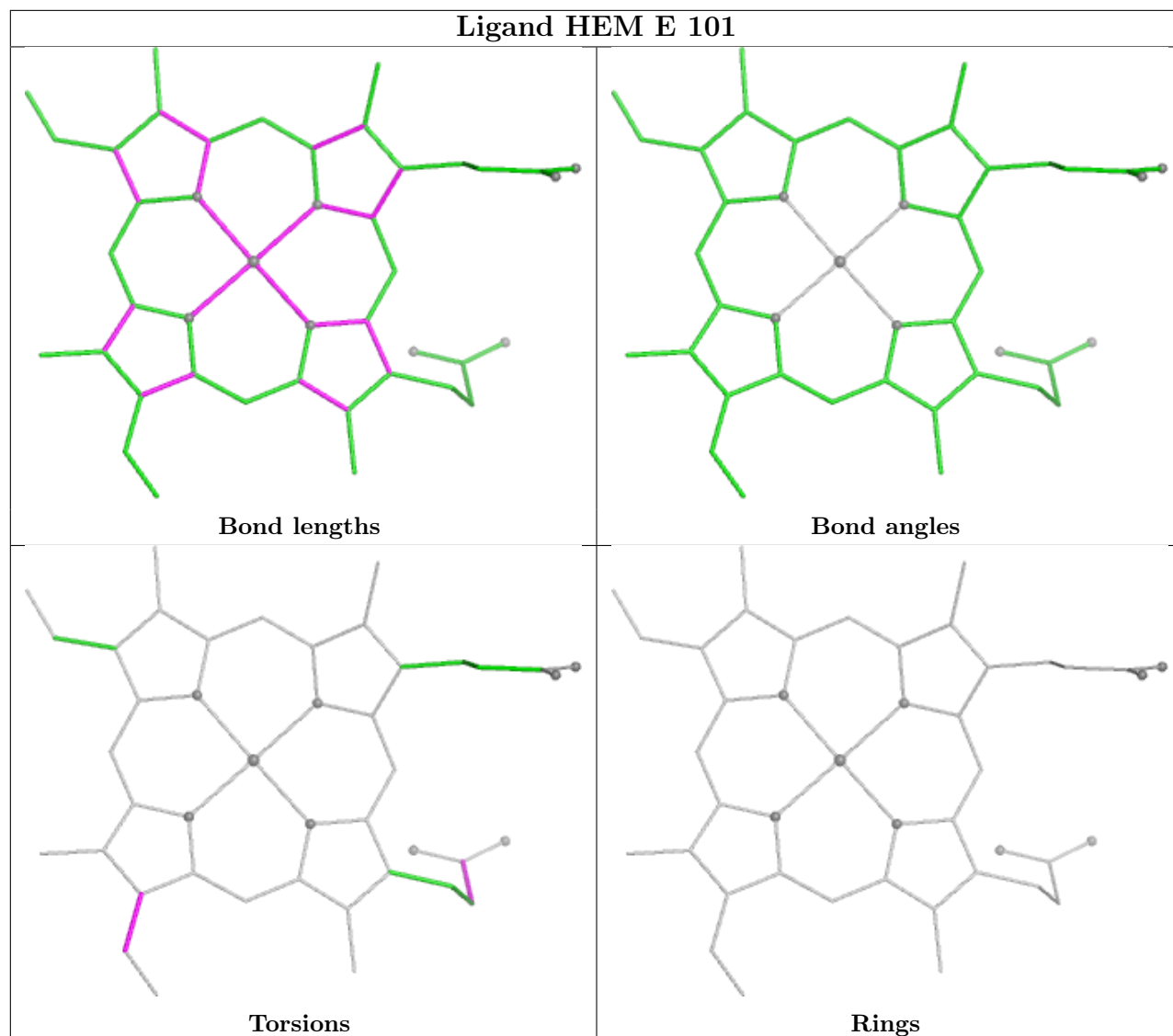




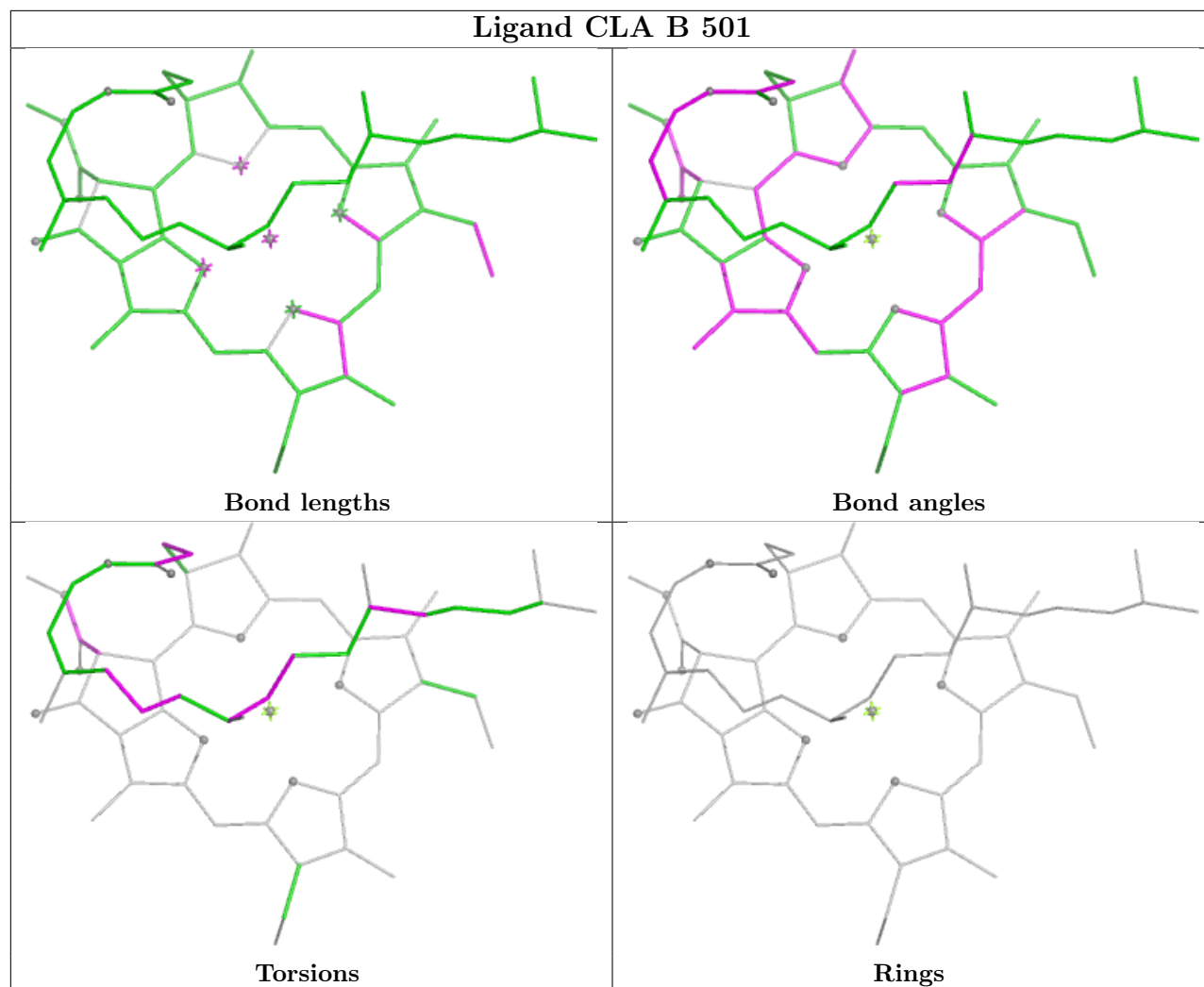


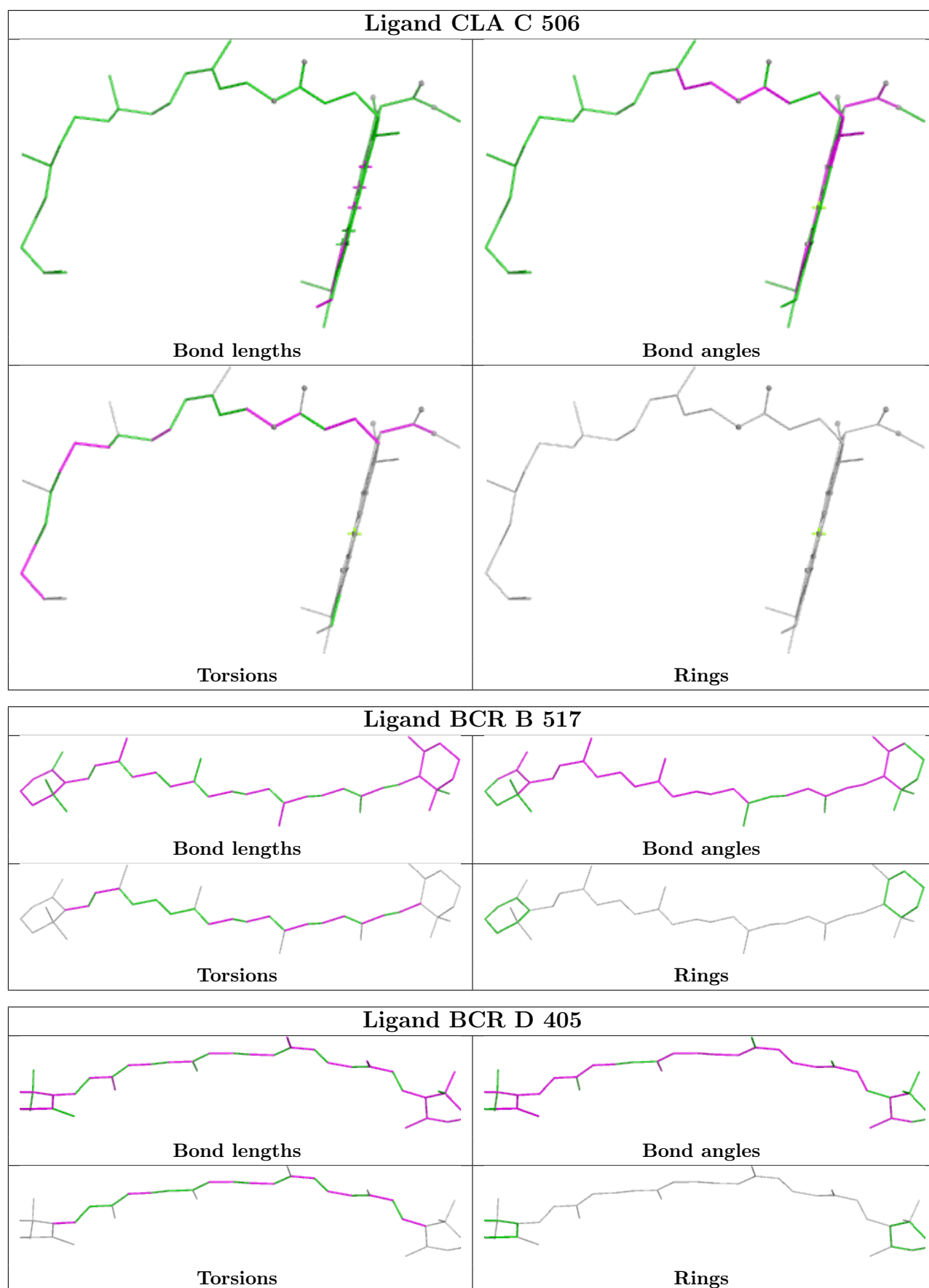


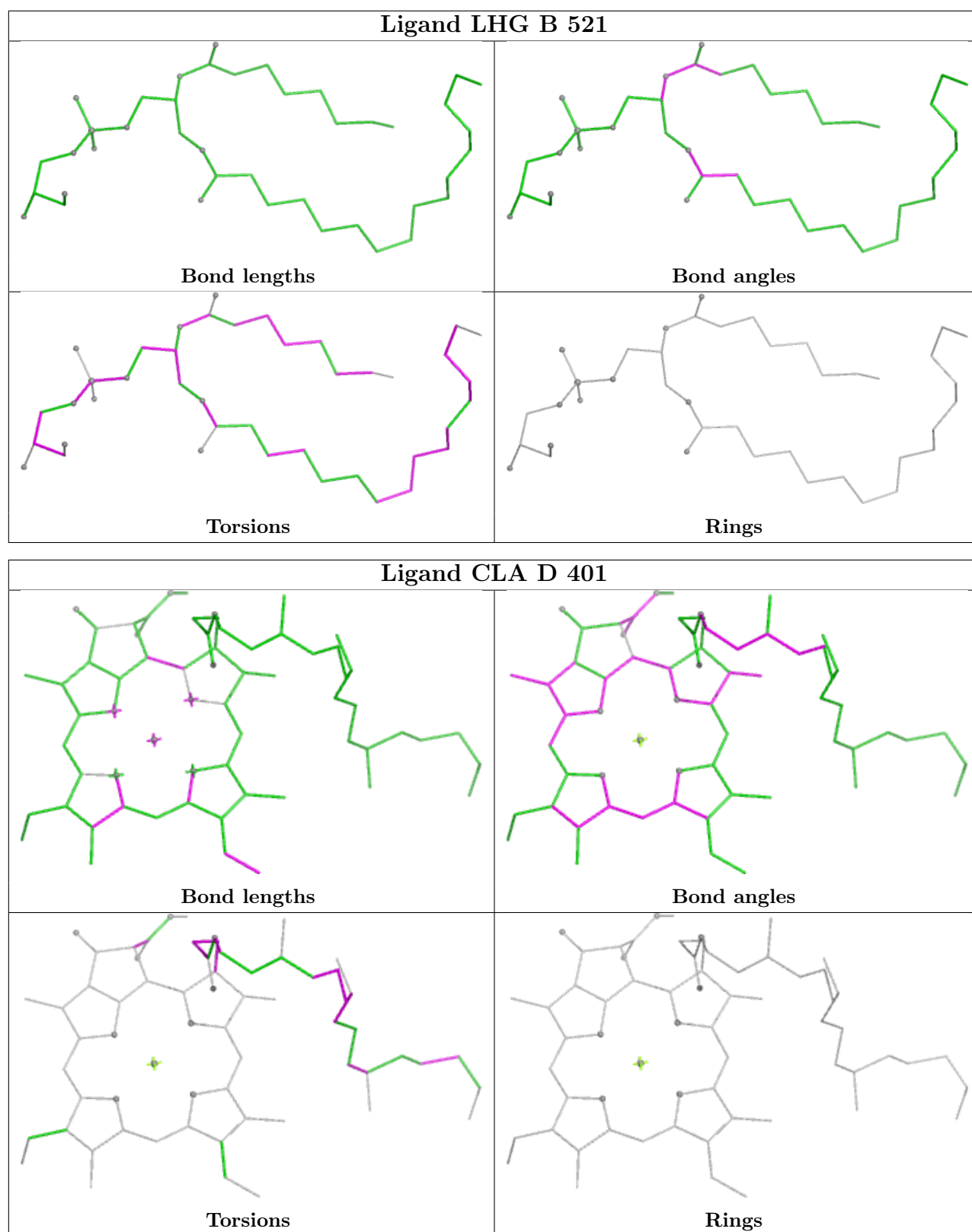


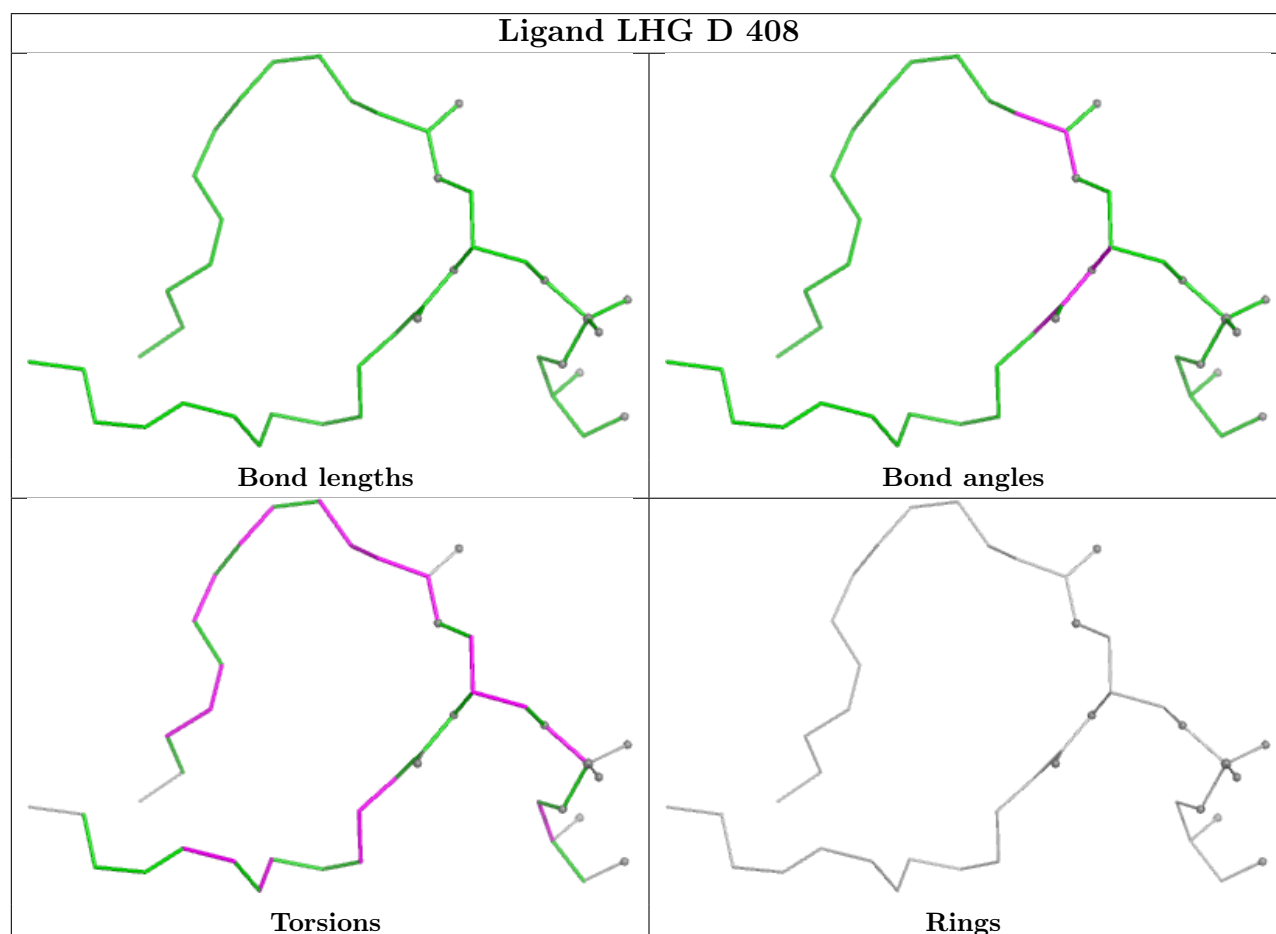
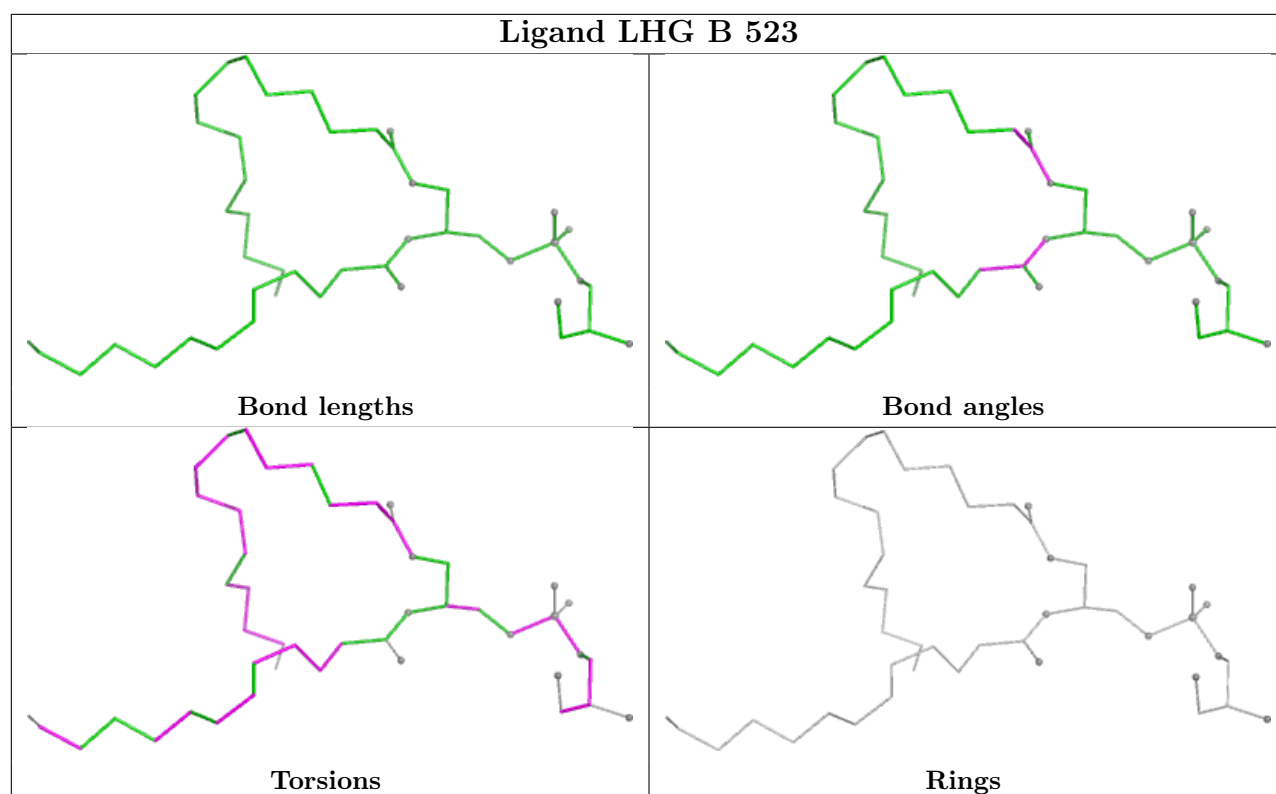


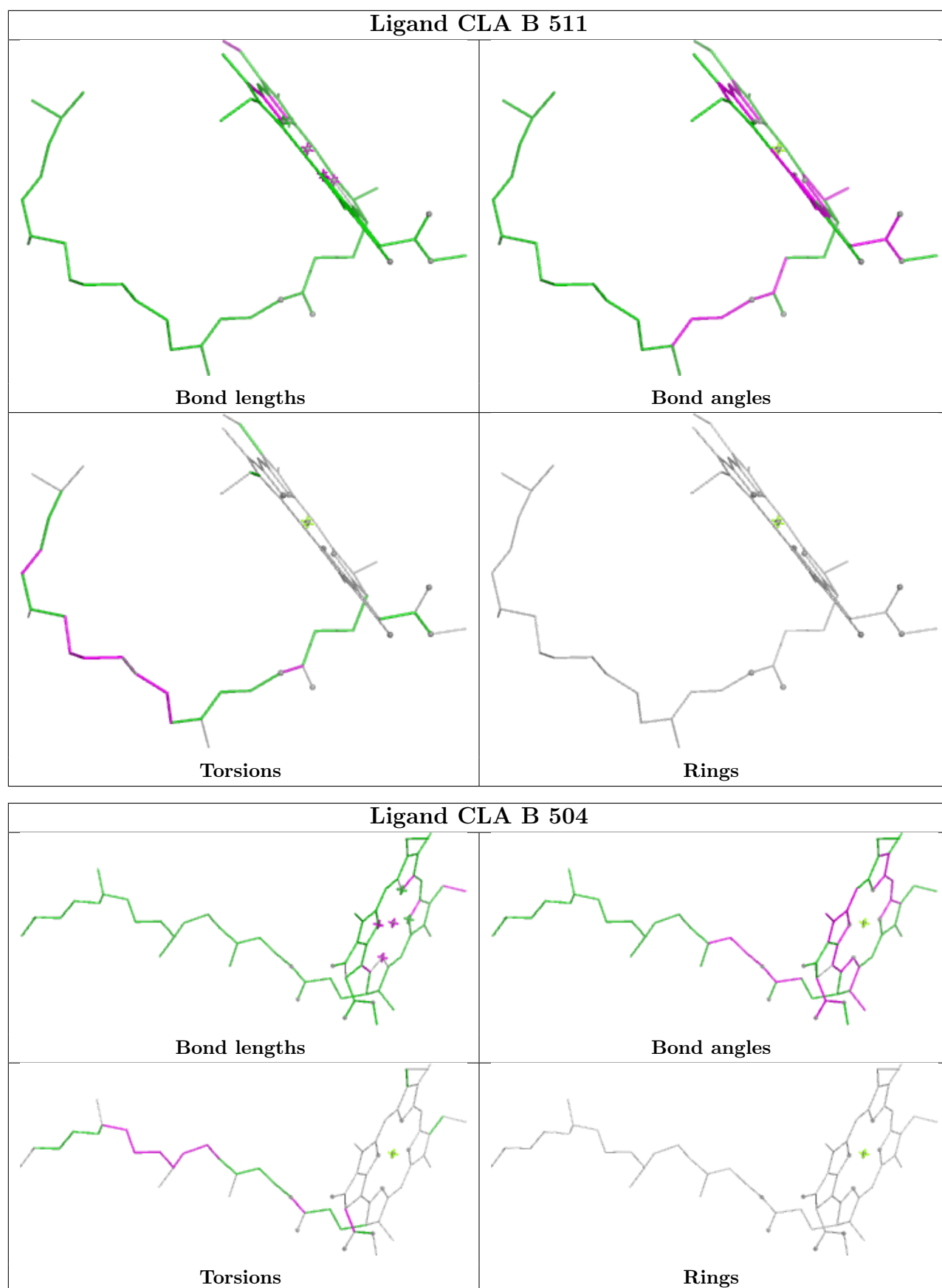
Ligand CLA B 501

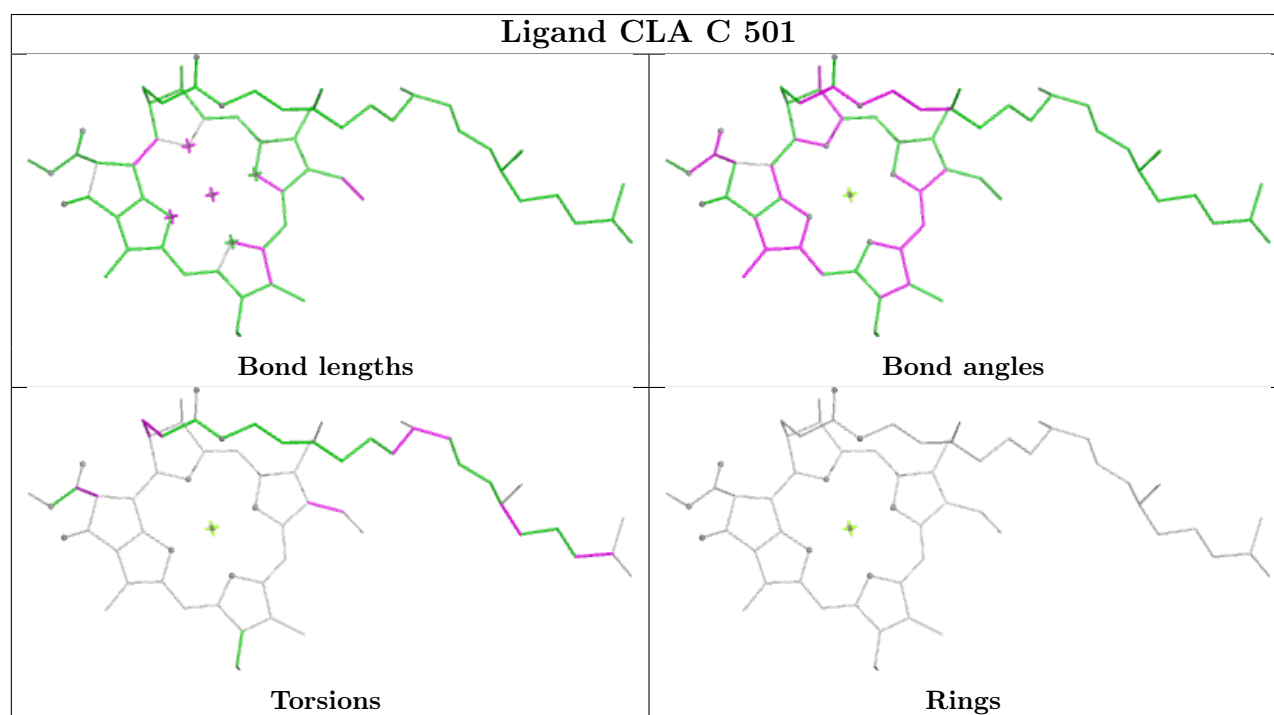
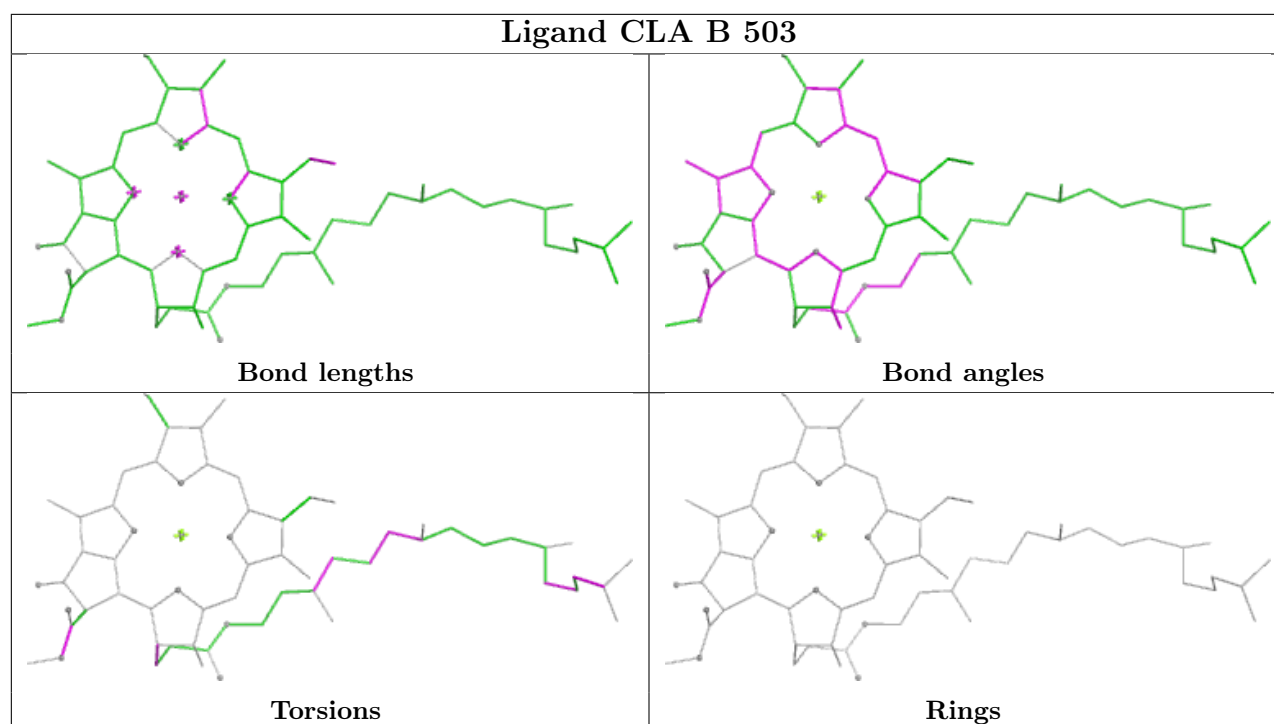


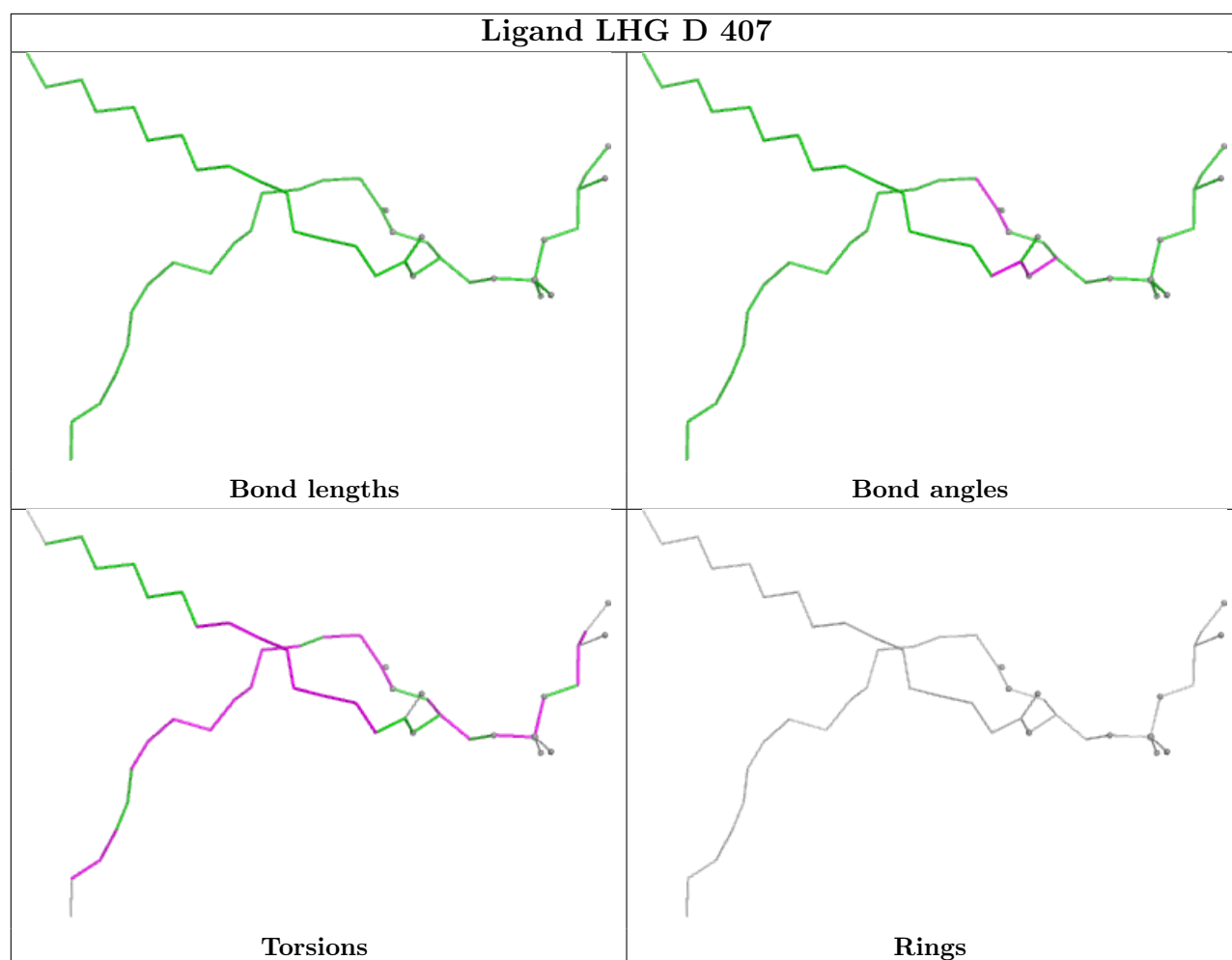


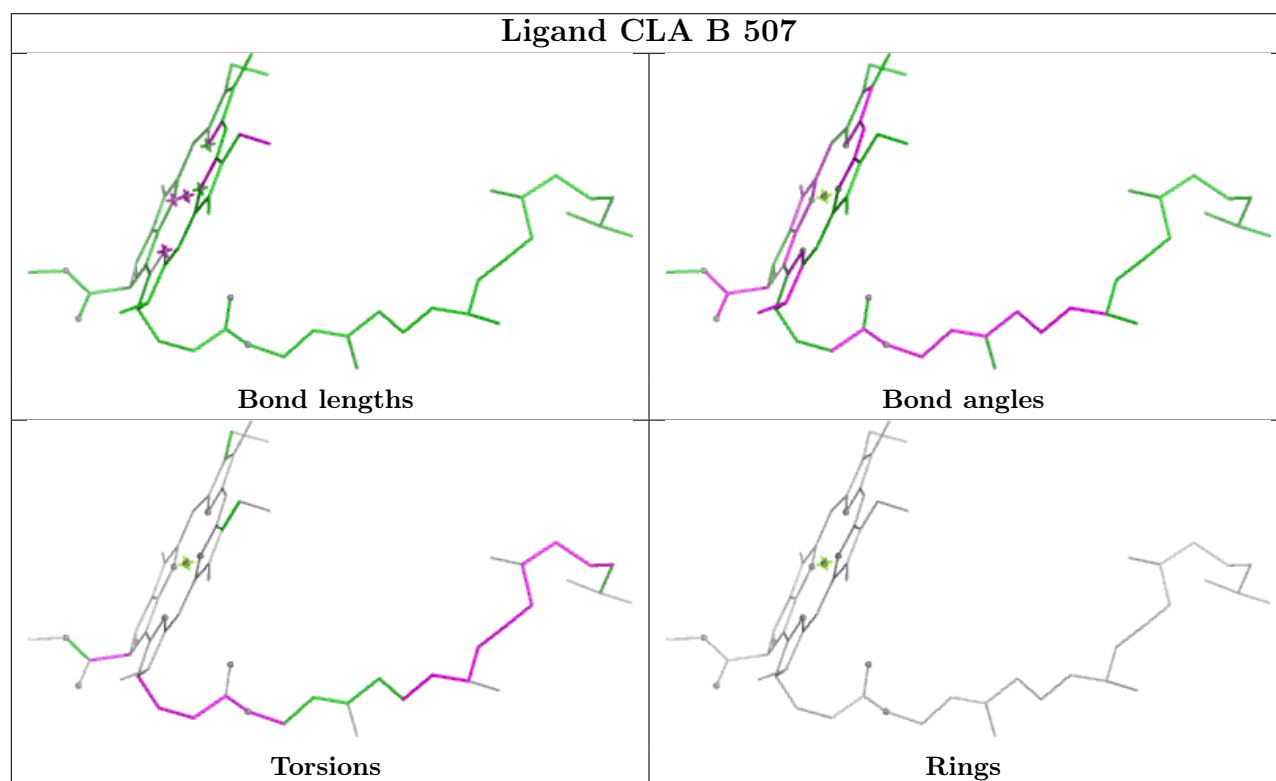
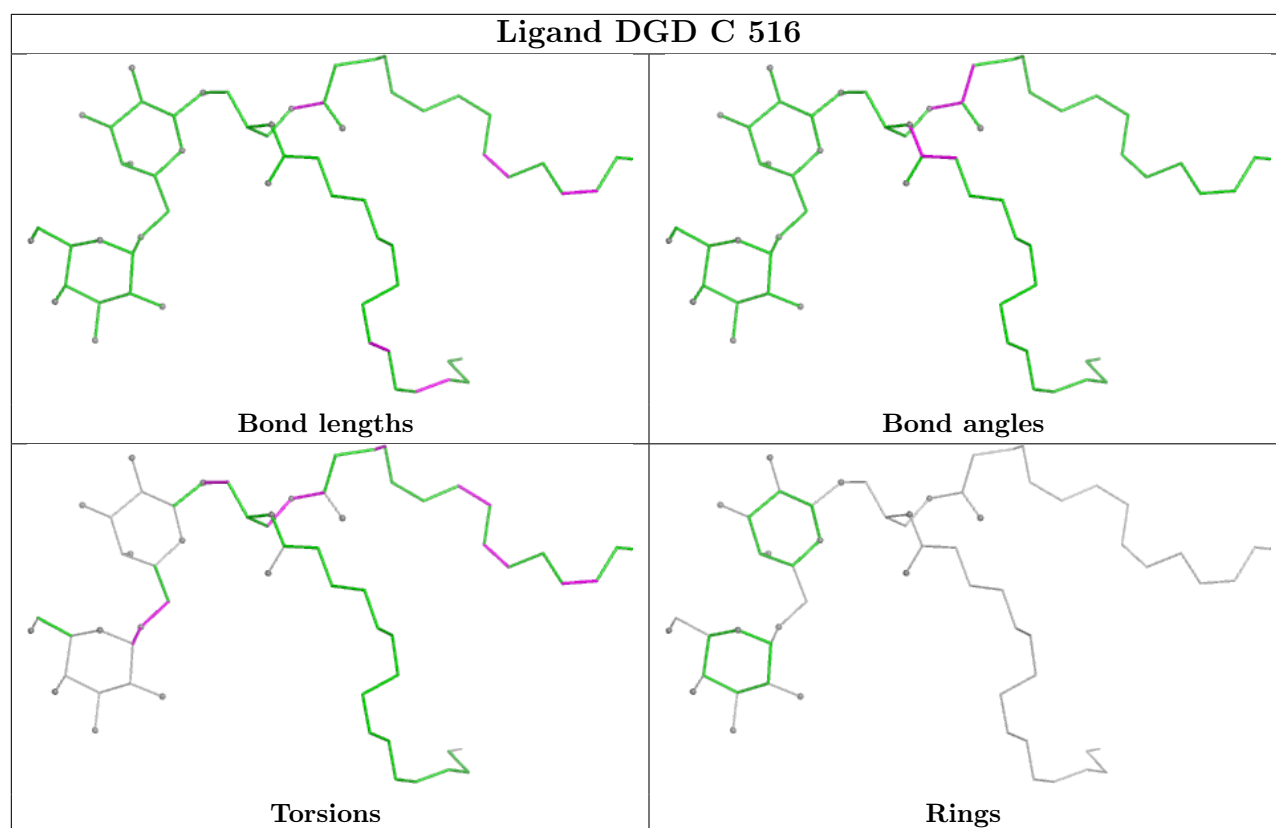


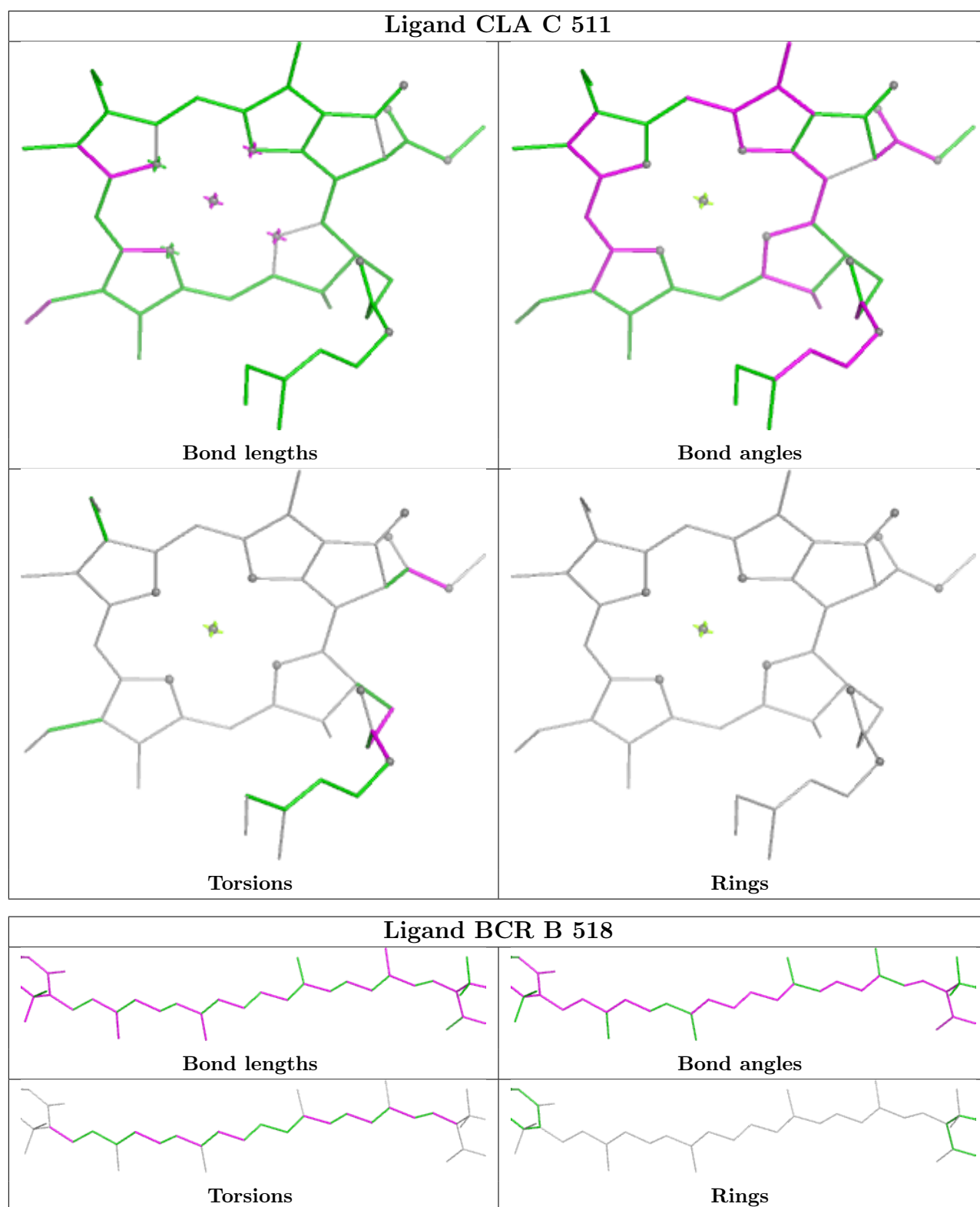


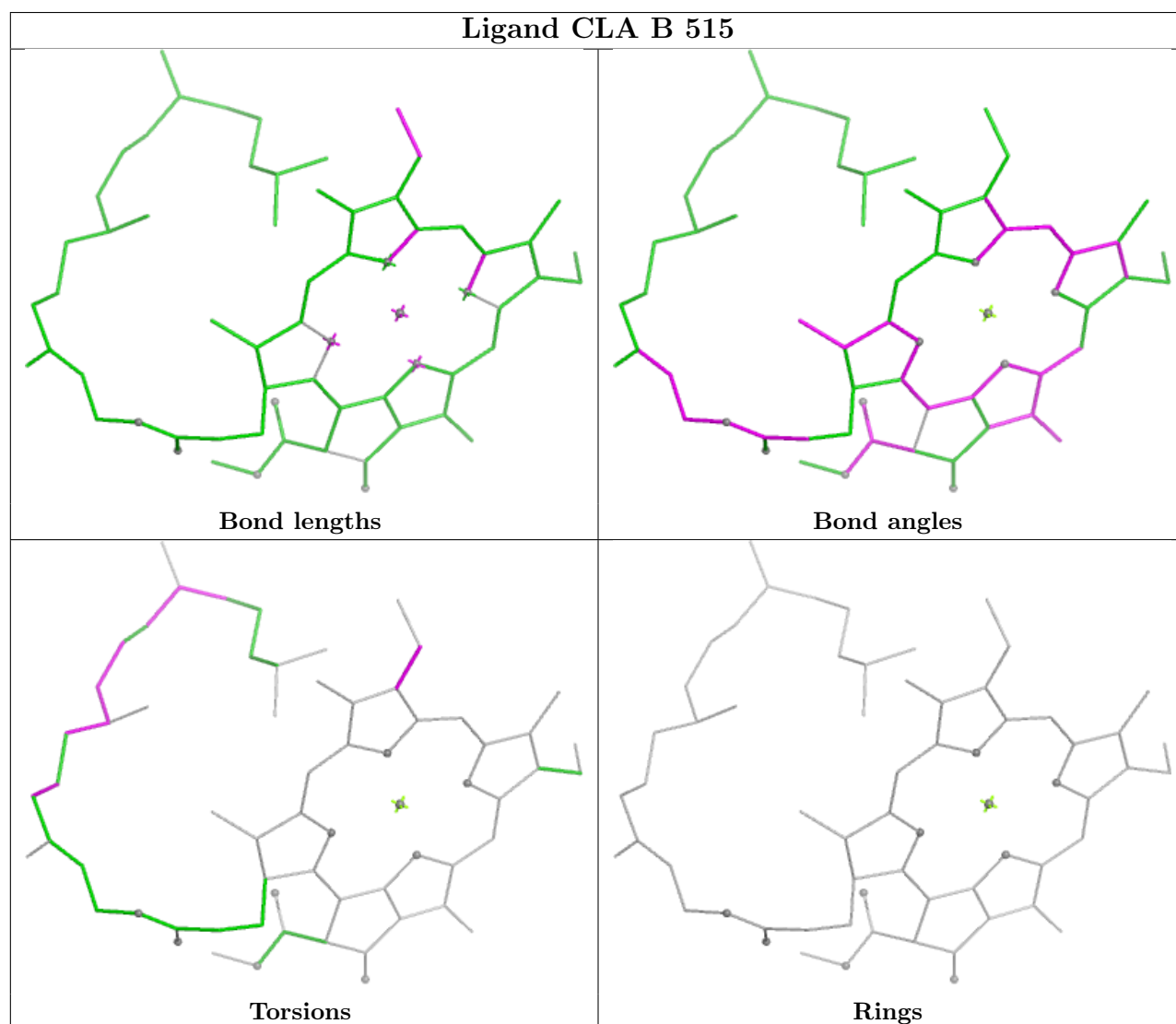
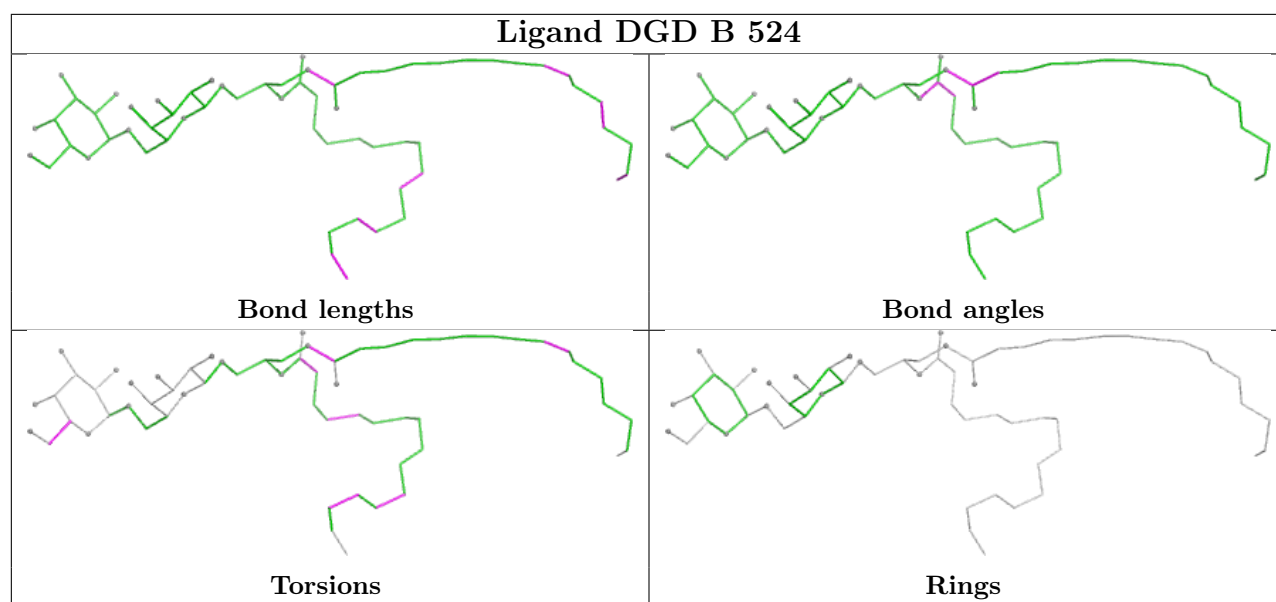


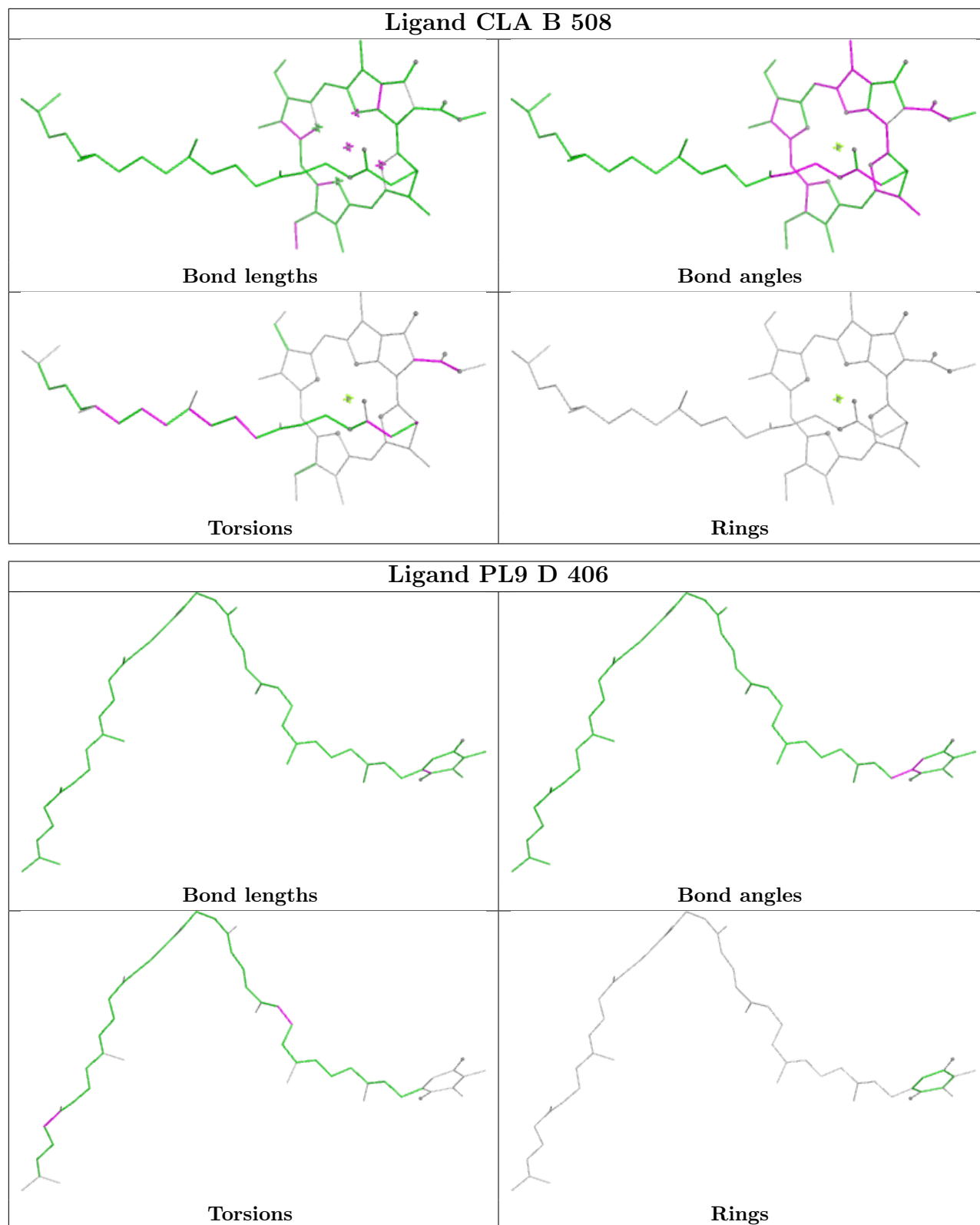


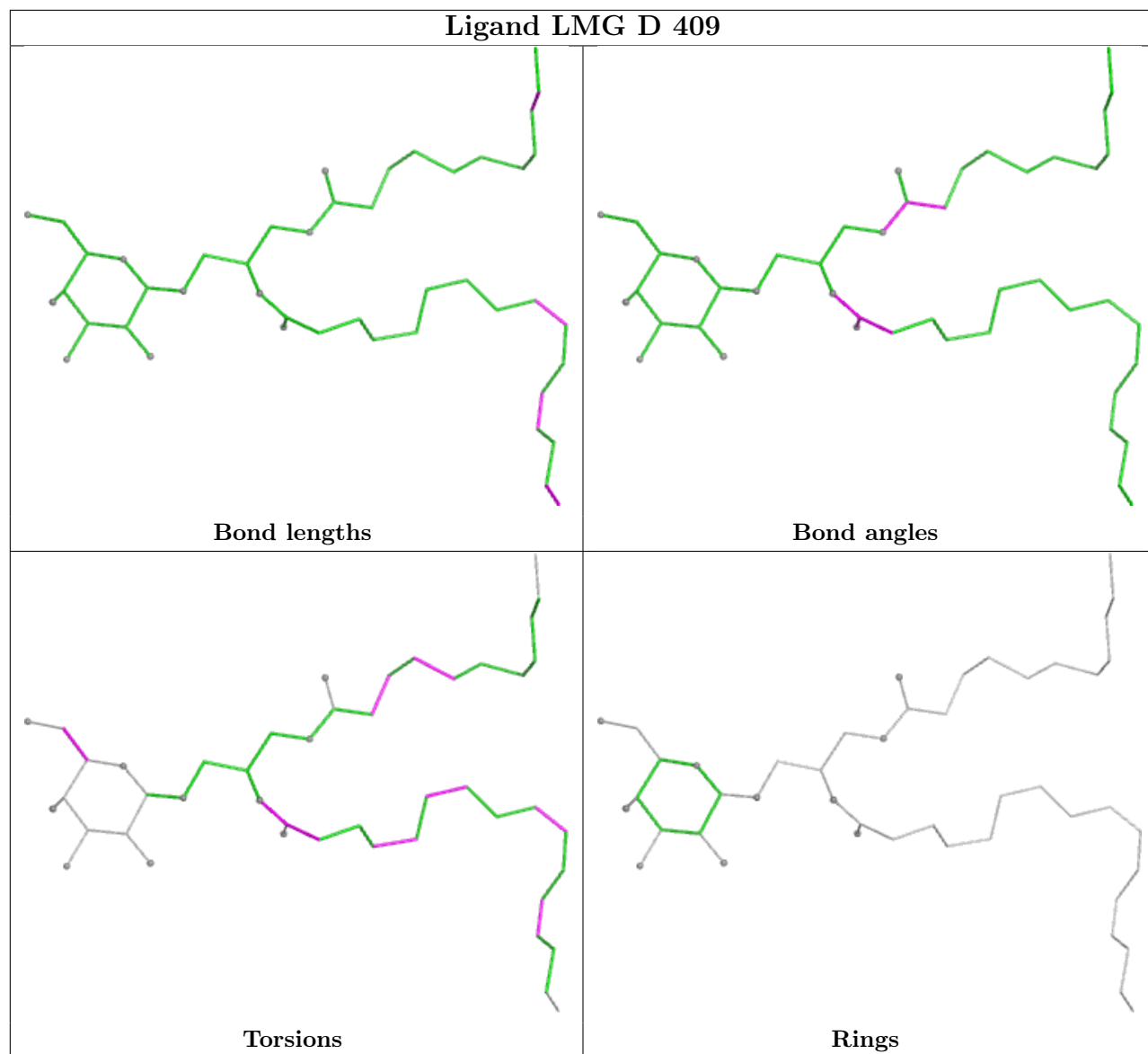


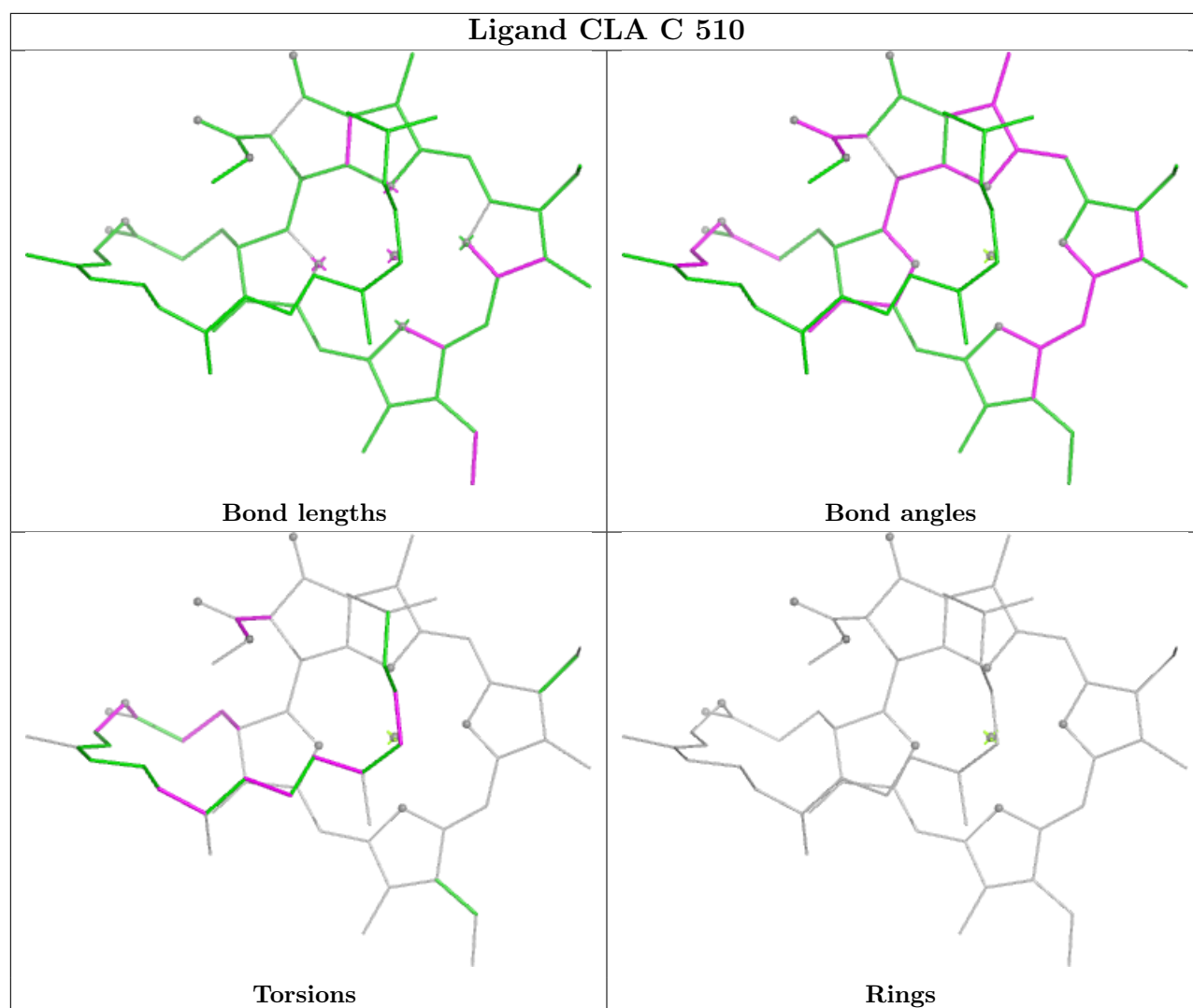


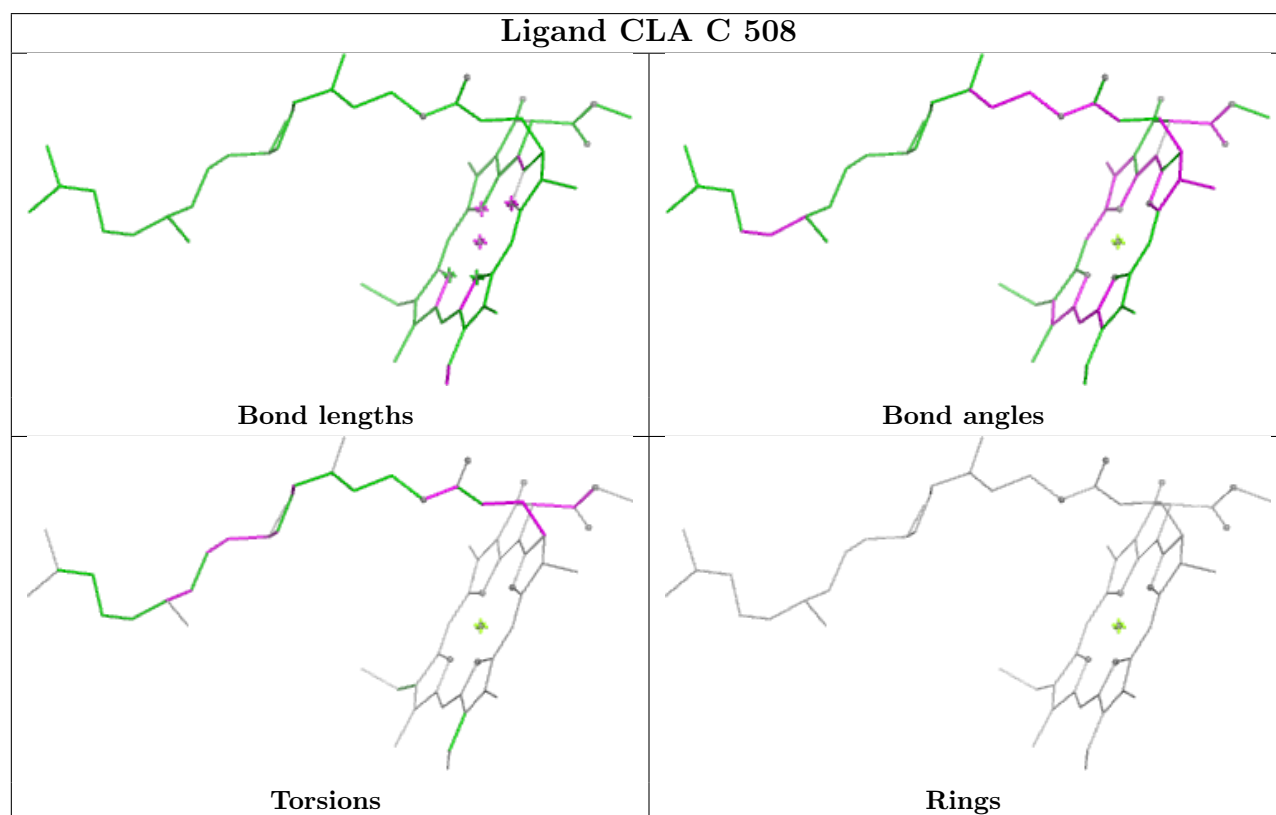
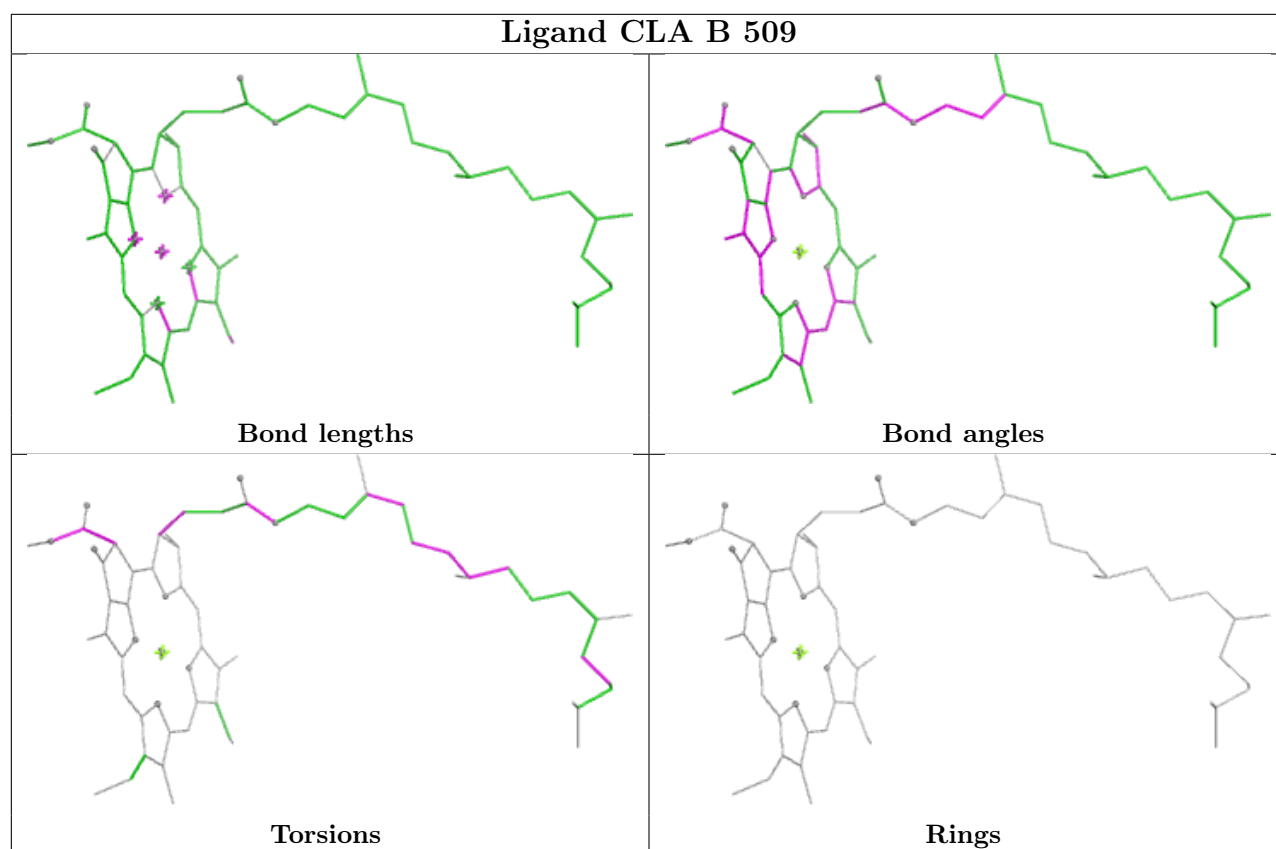


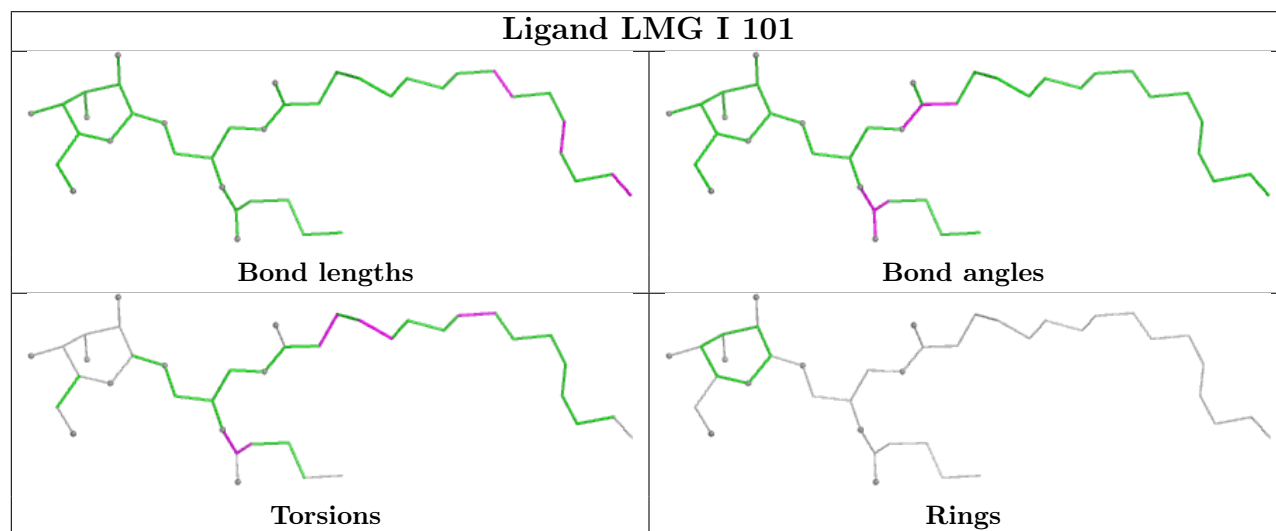
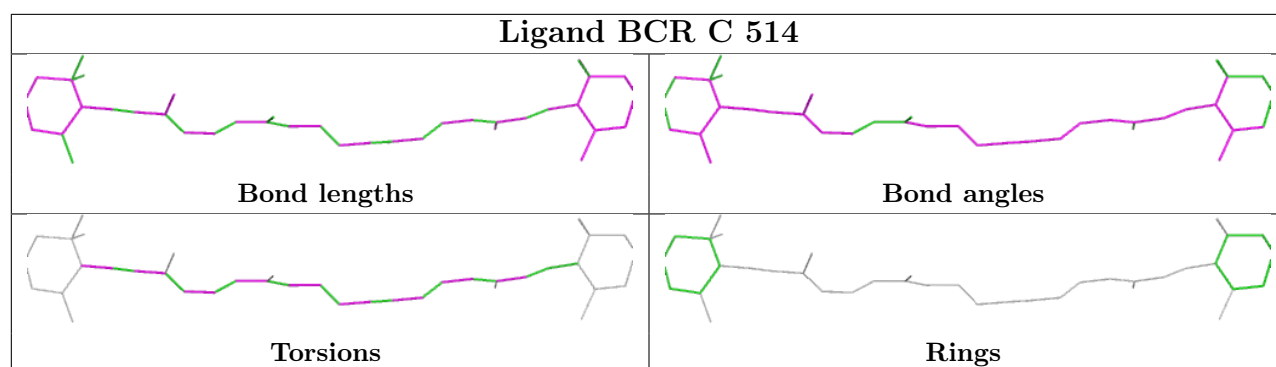


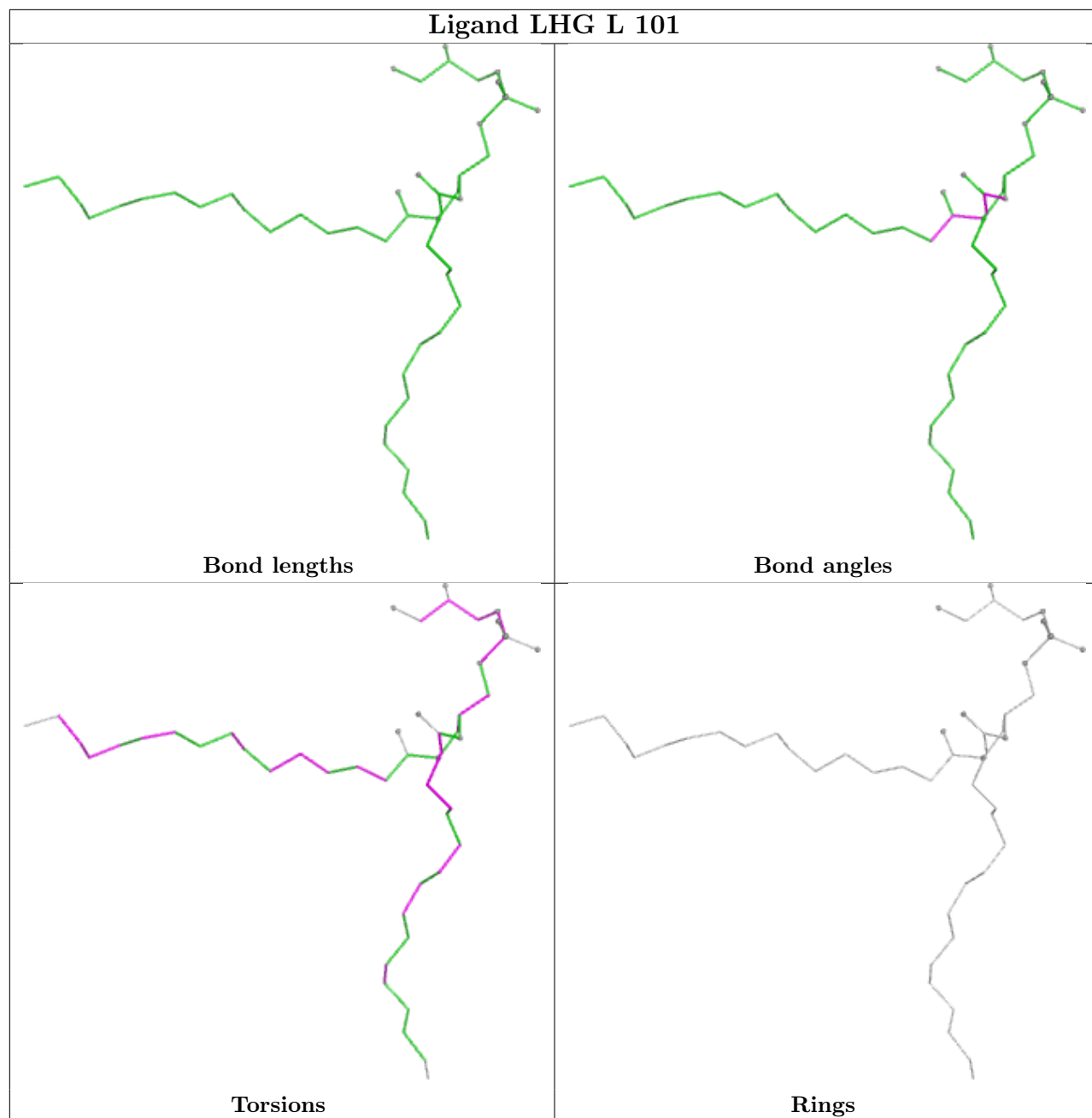


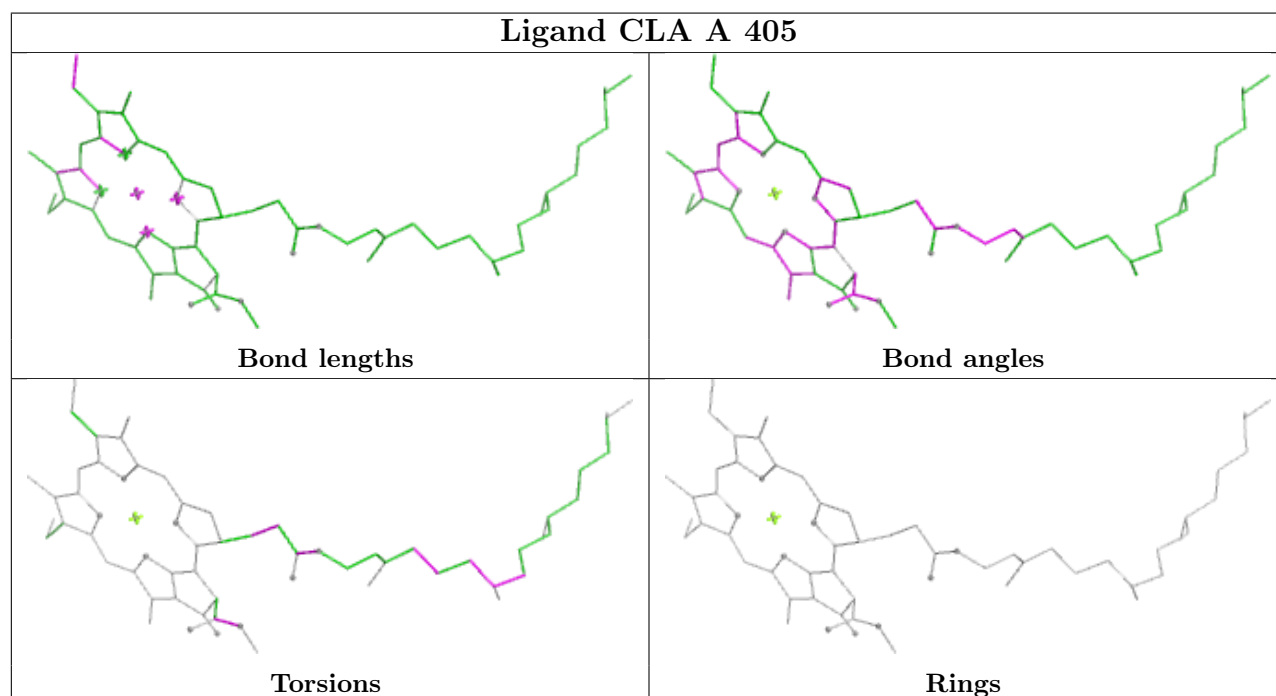
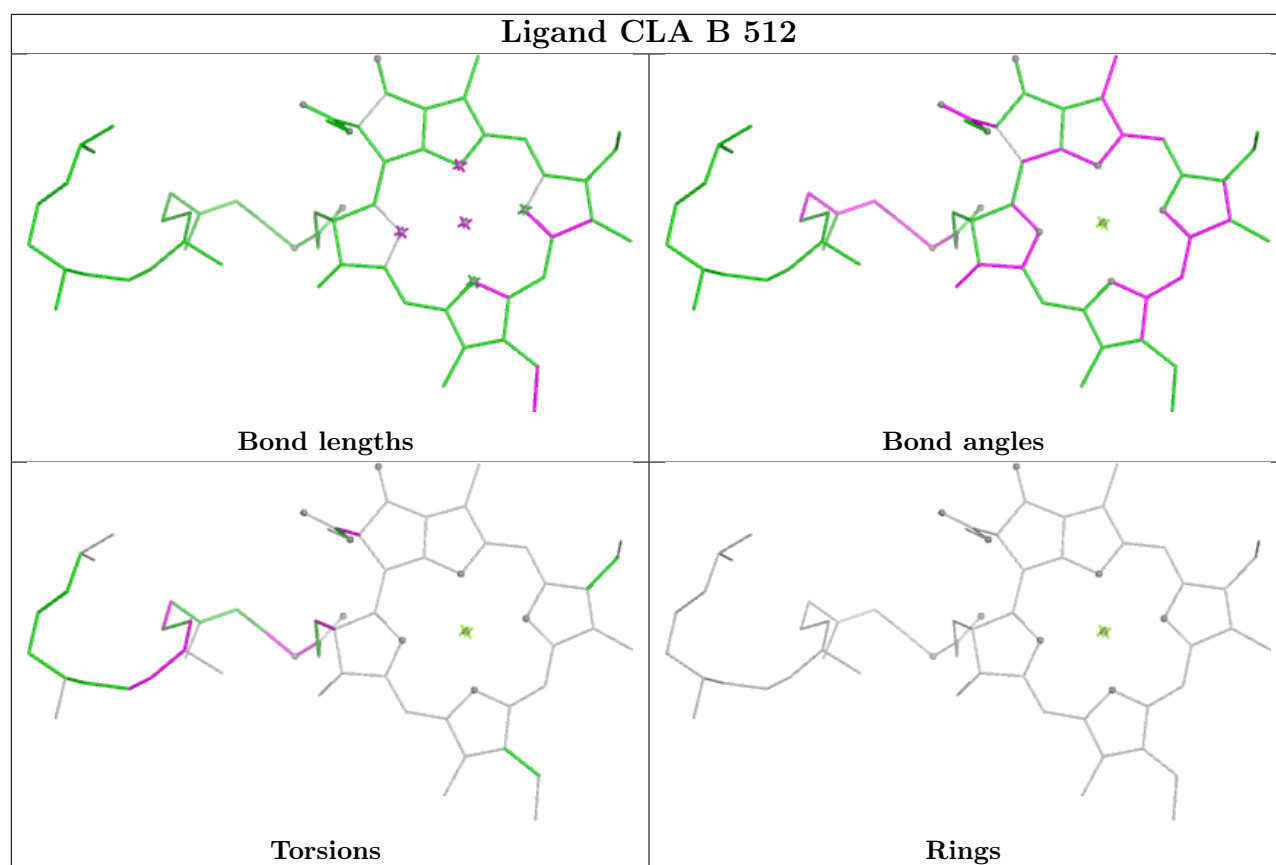


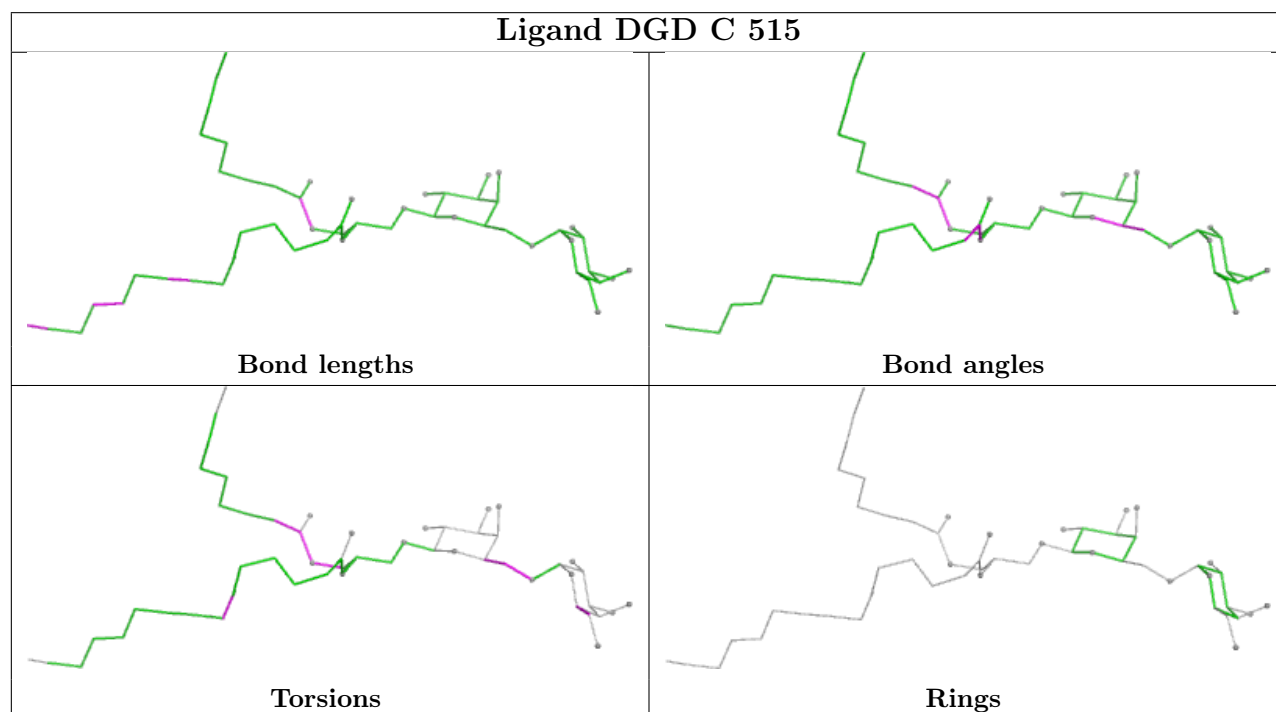
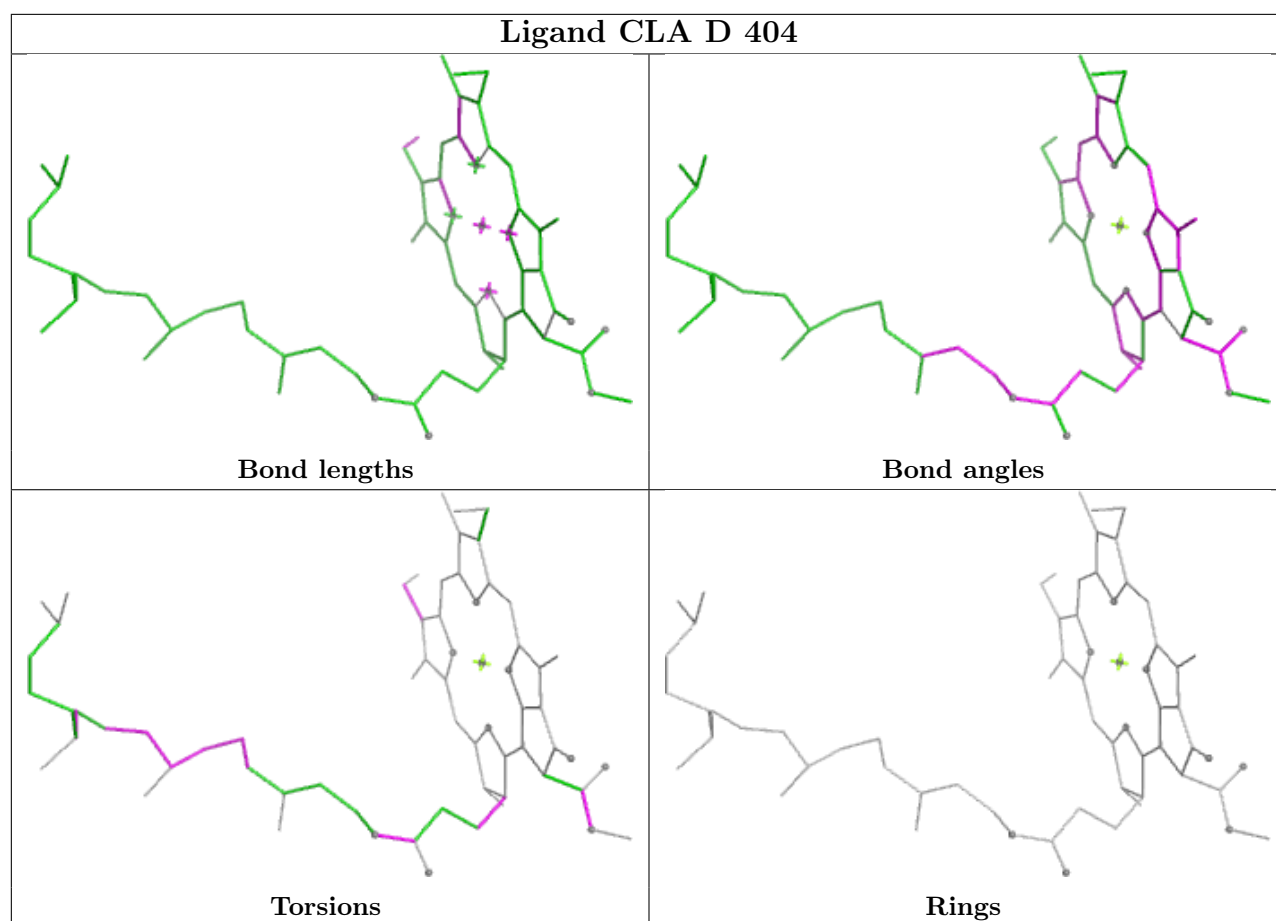




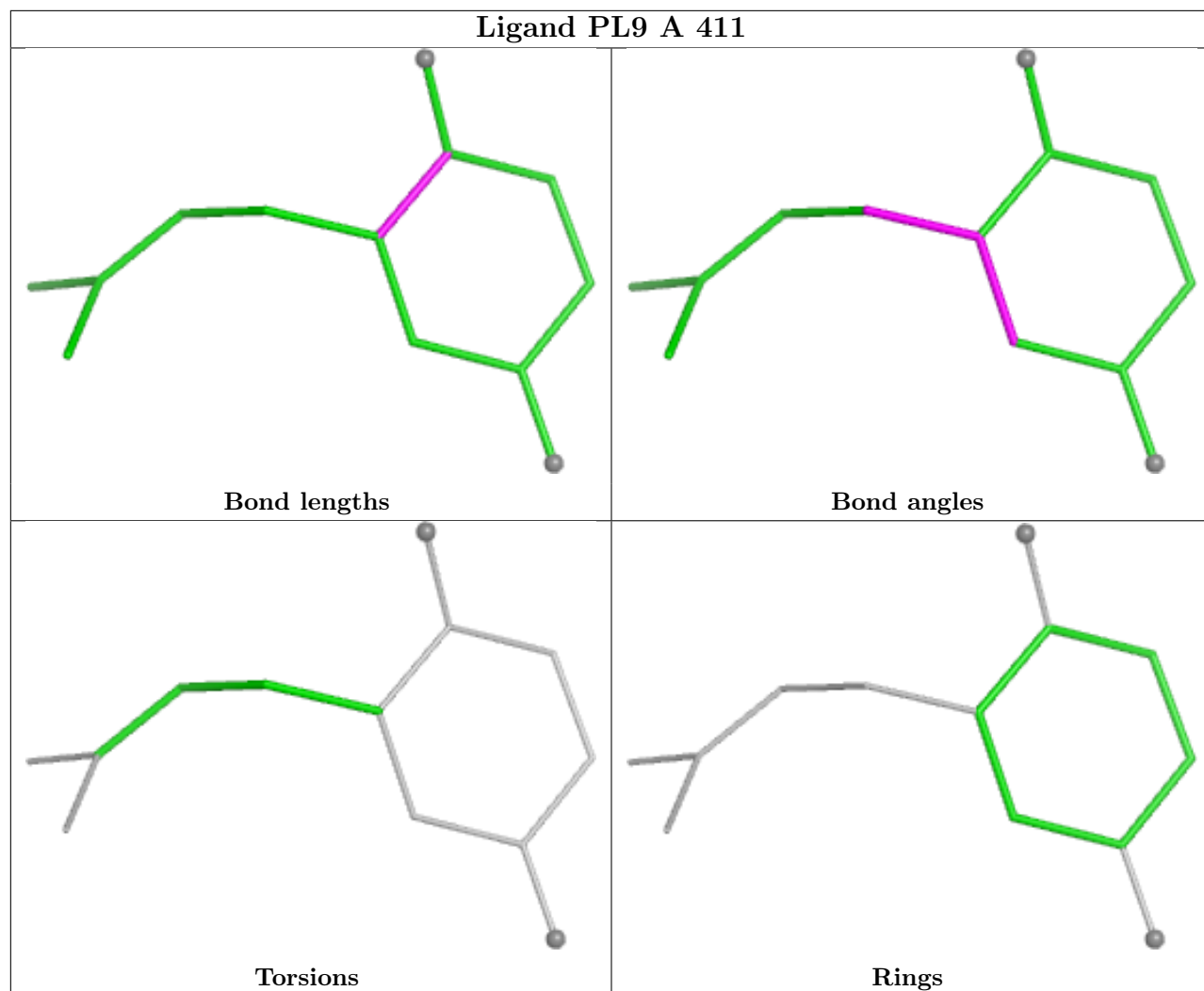


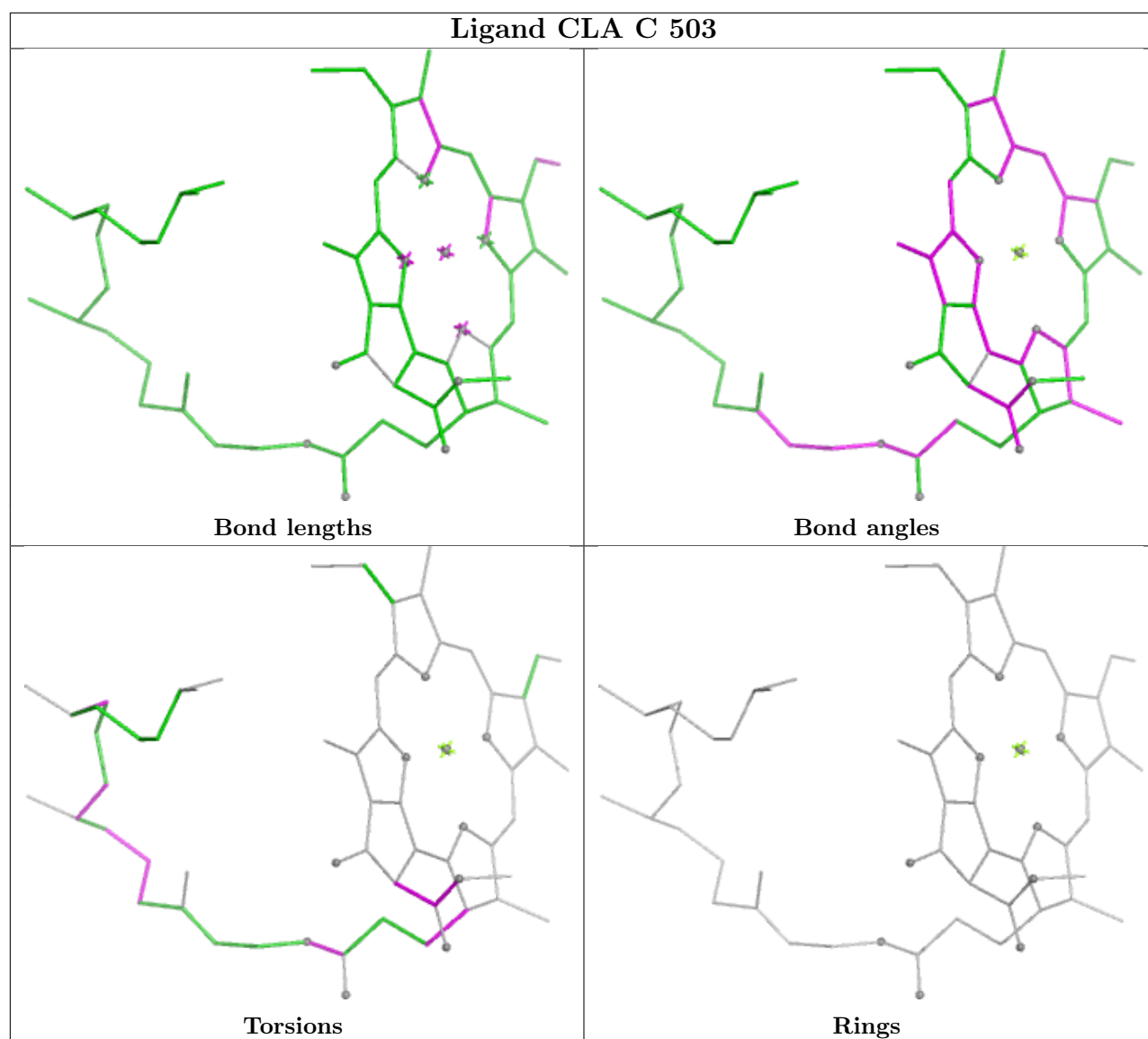


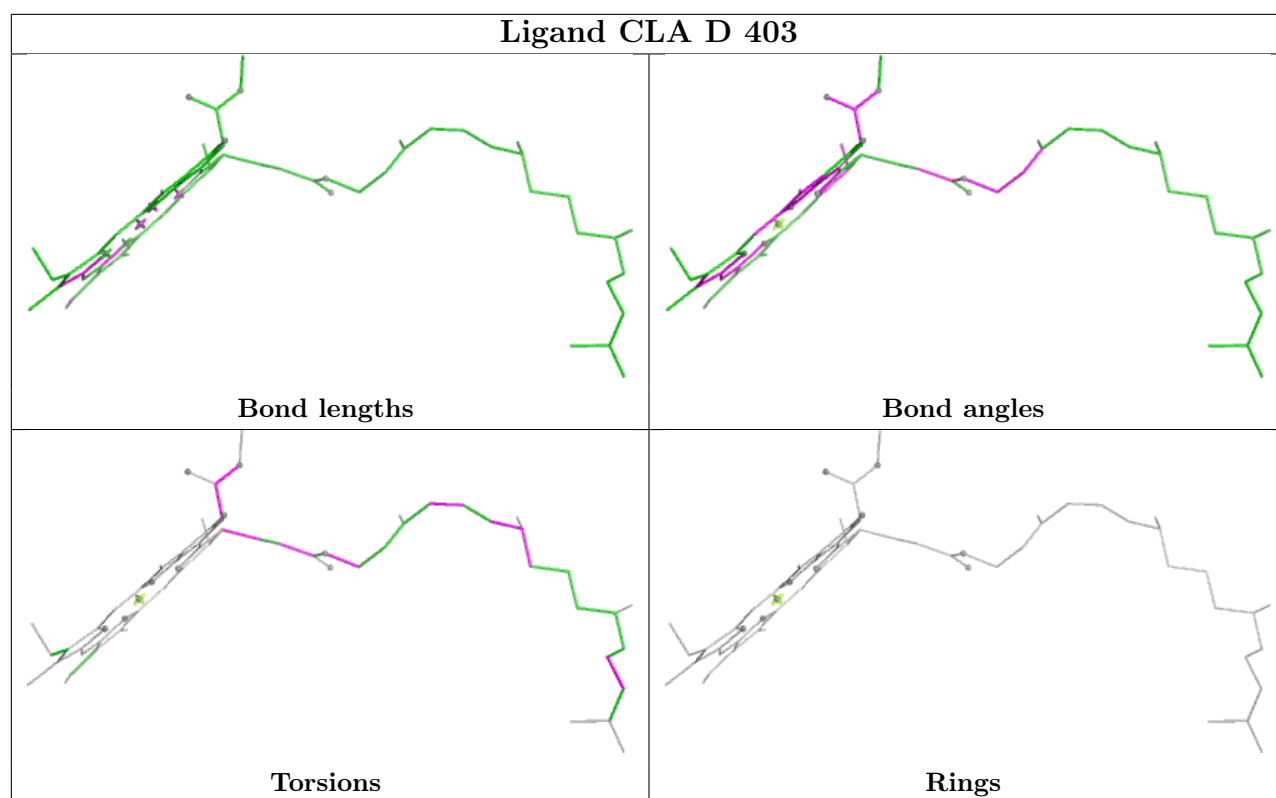


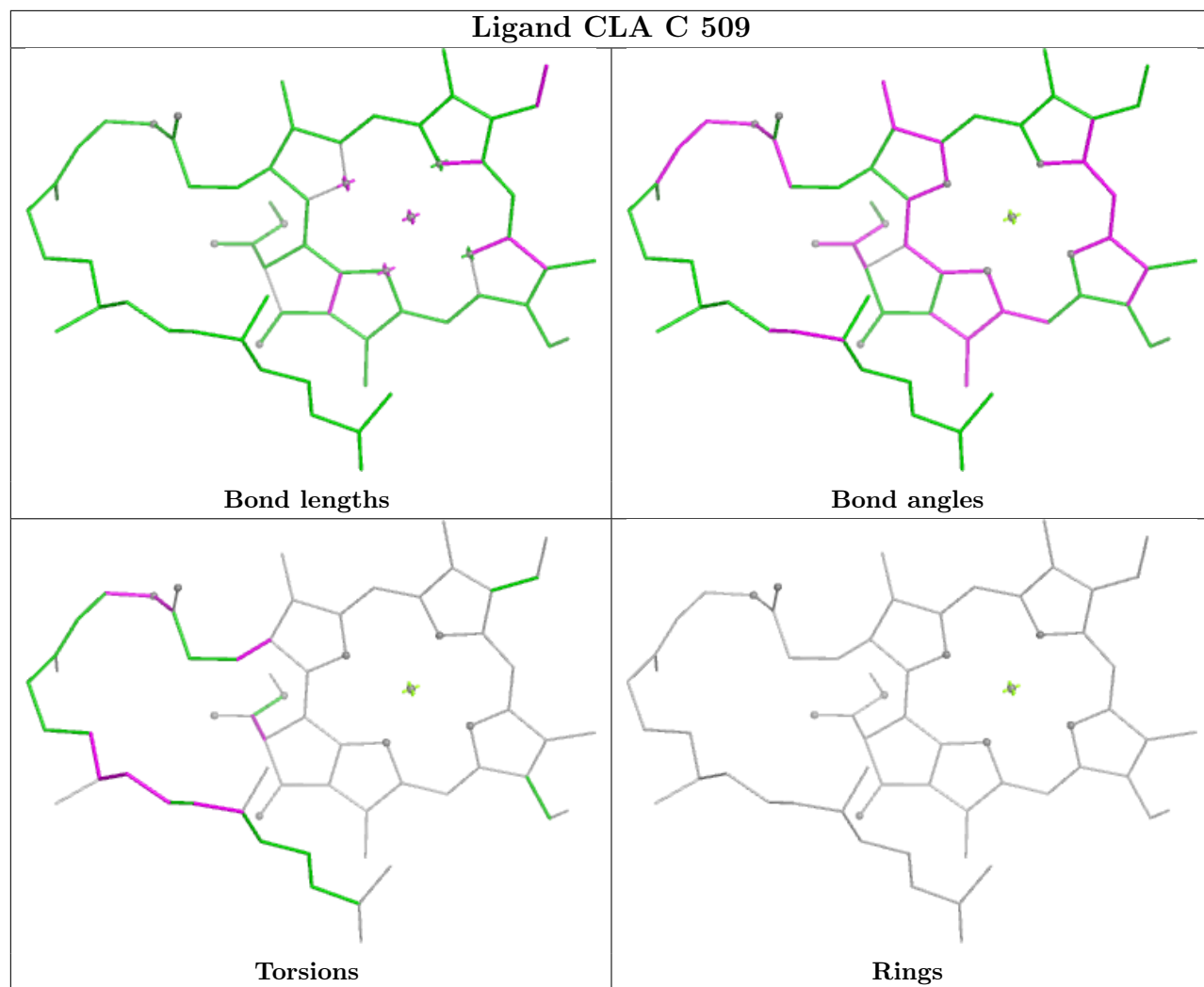


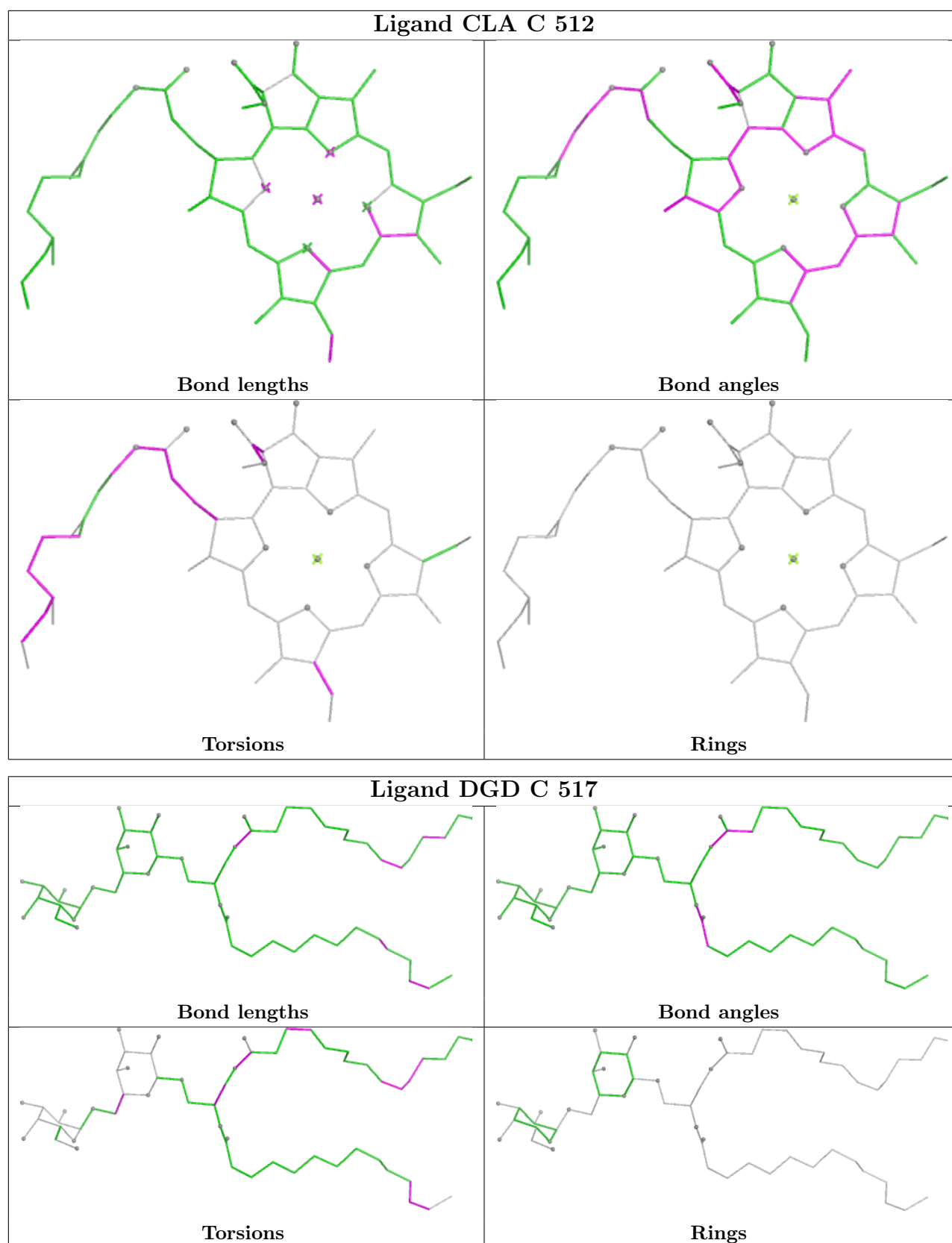
Ligand PL9 A 411

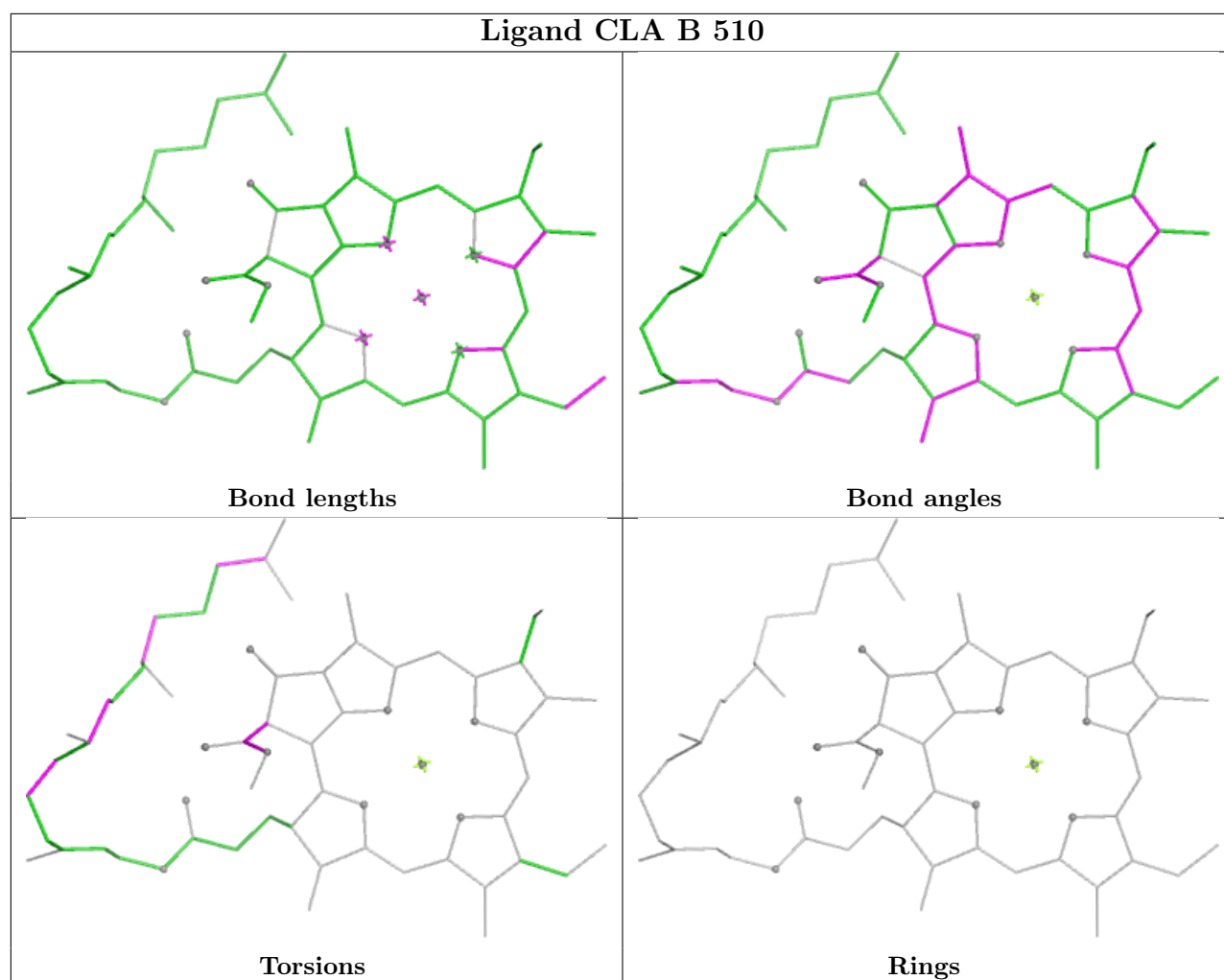


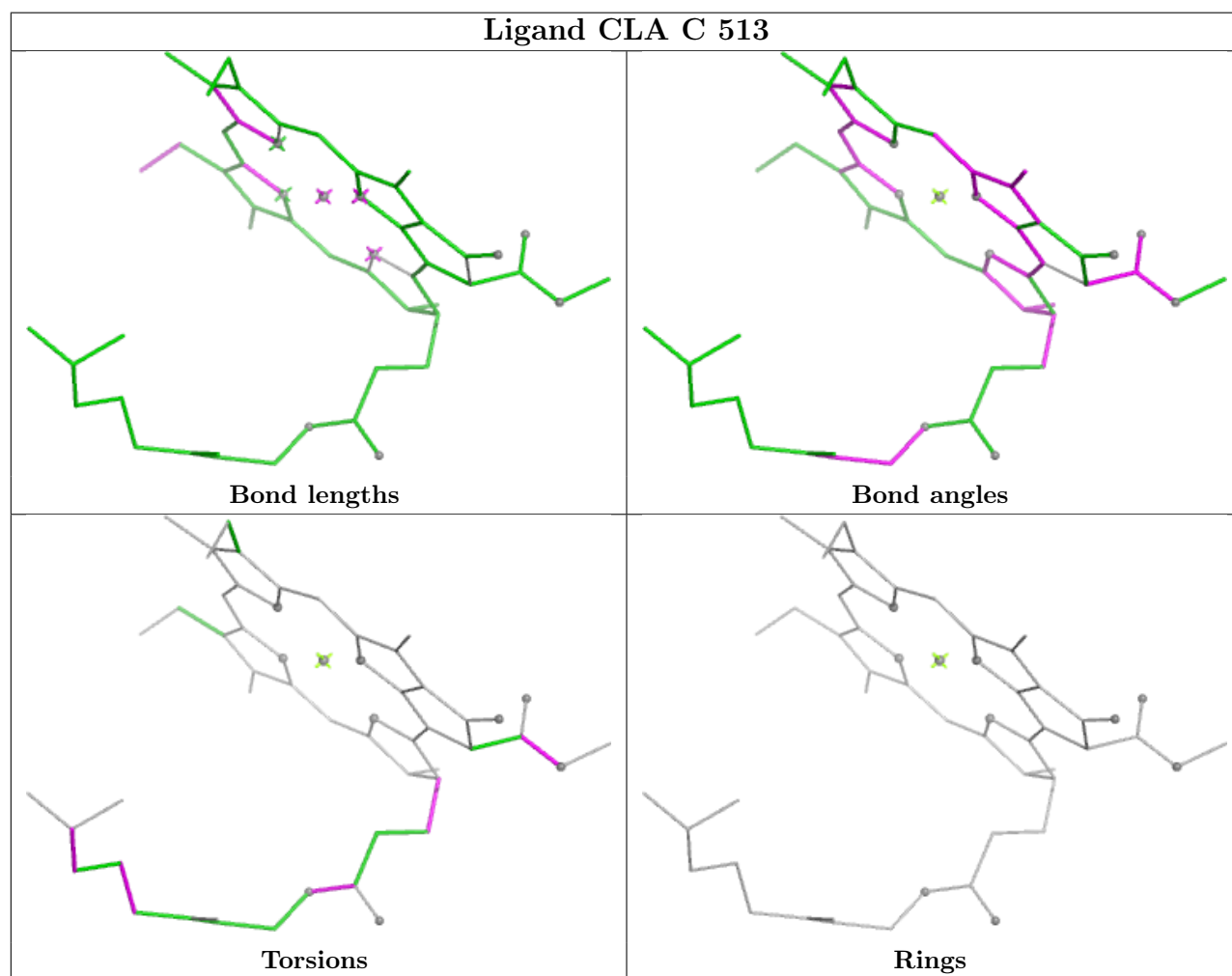
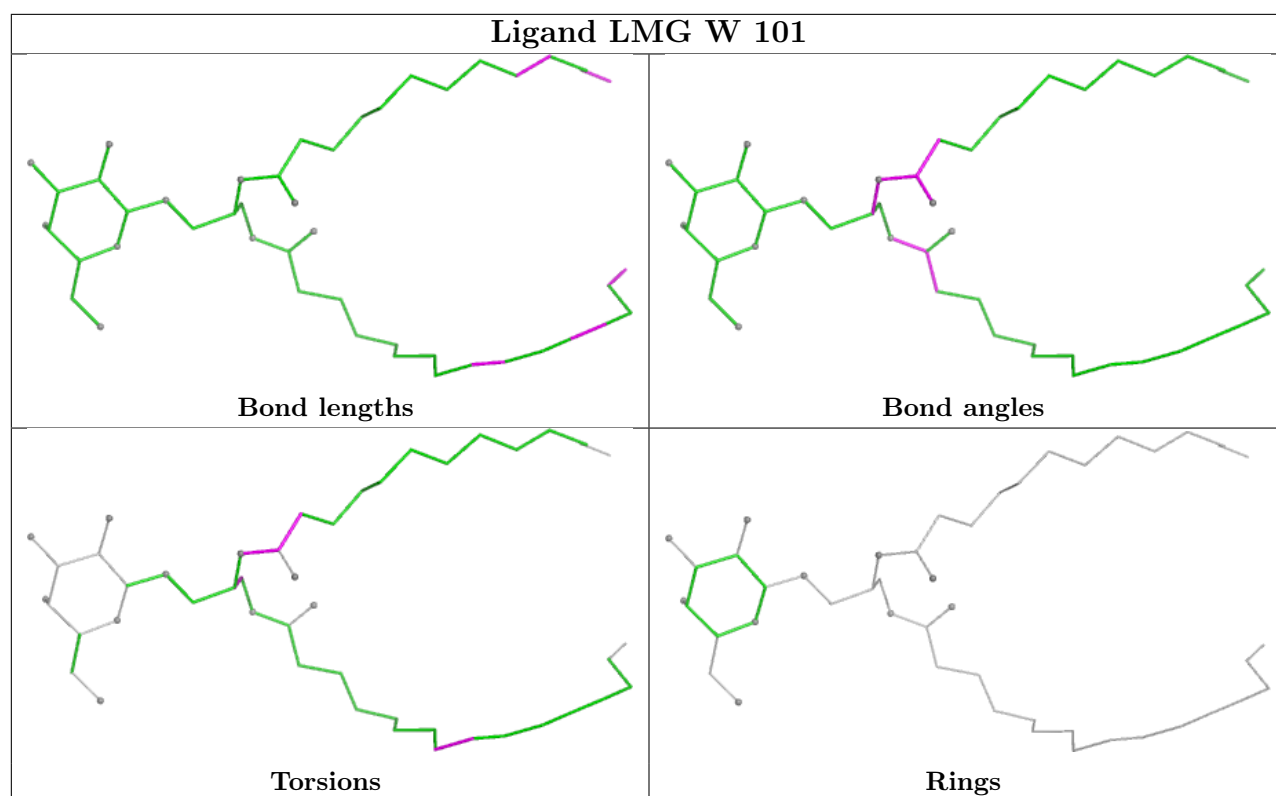


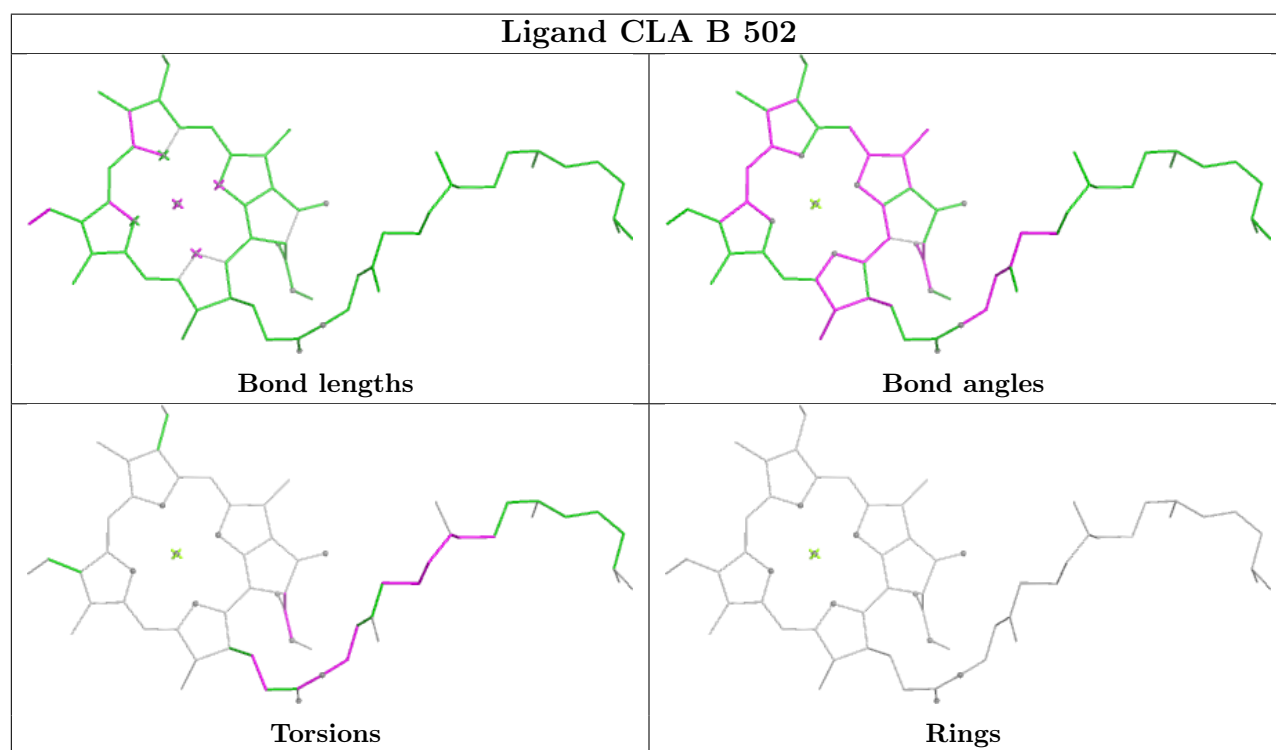
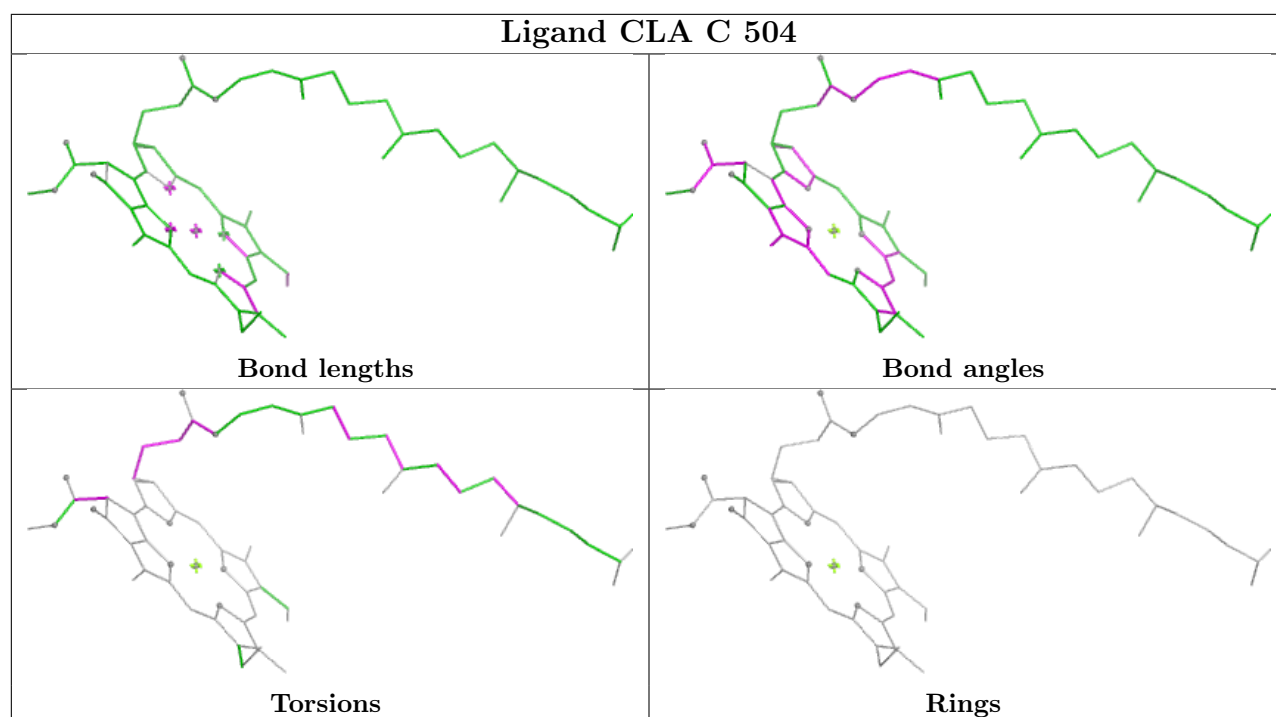


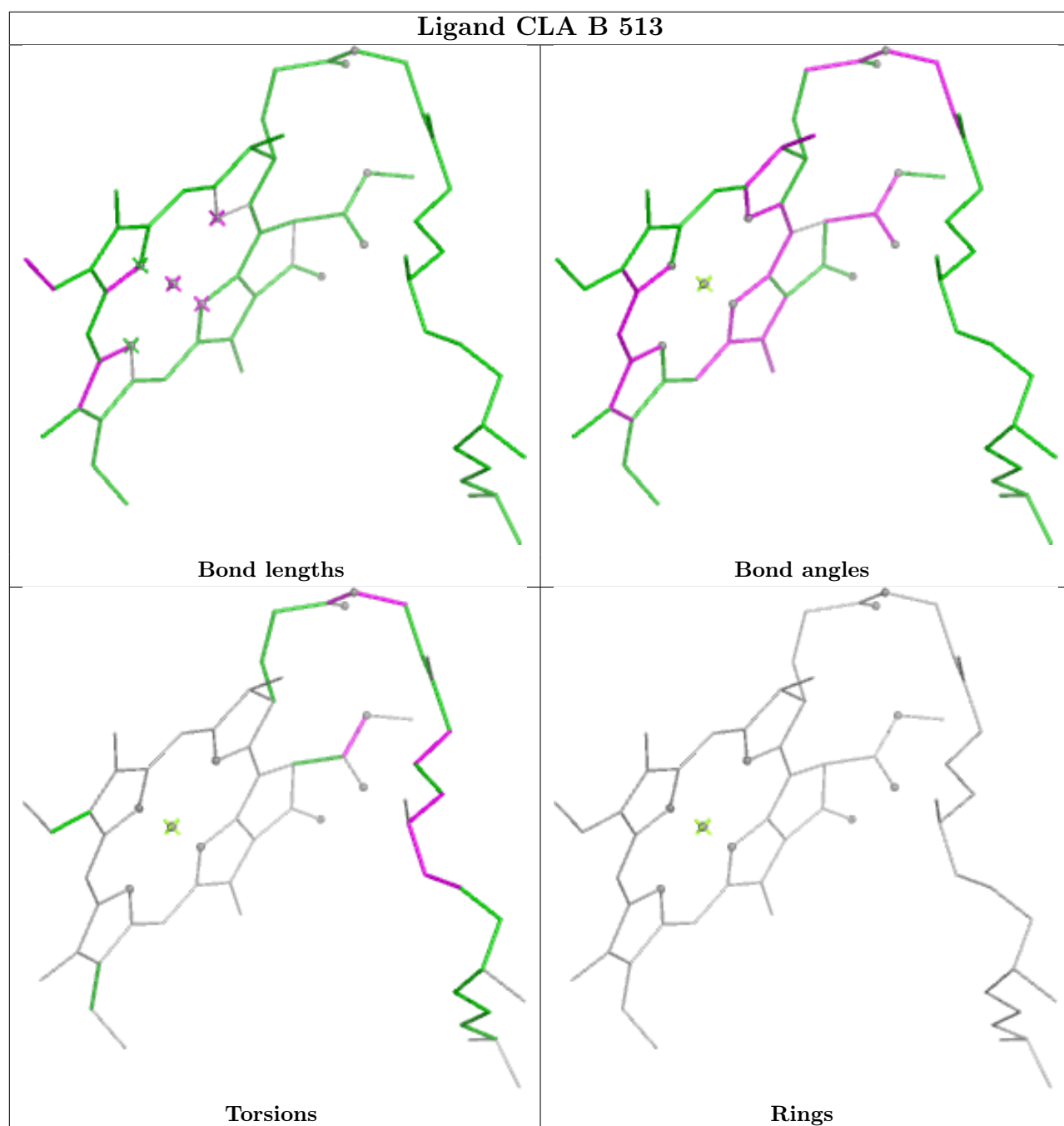


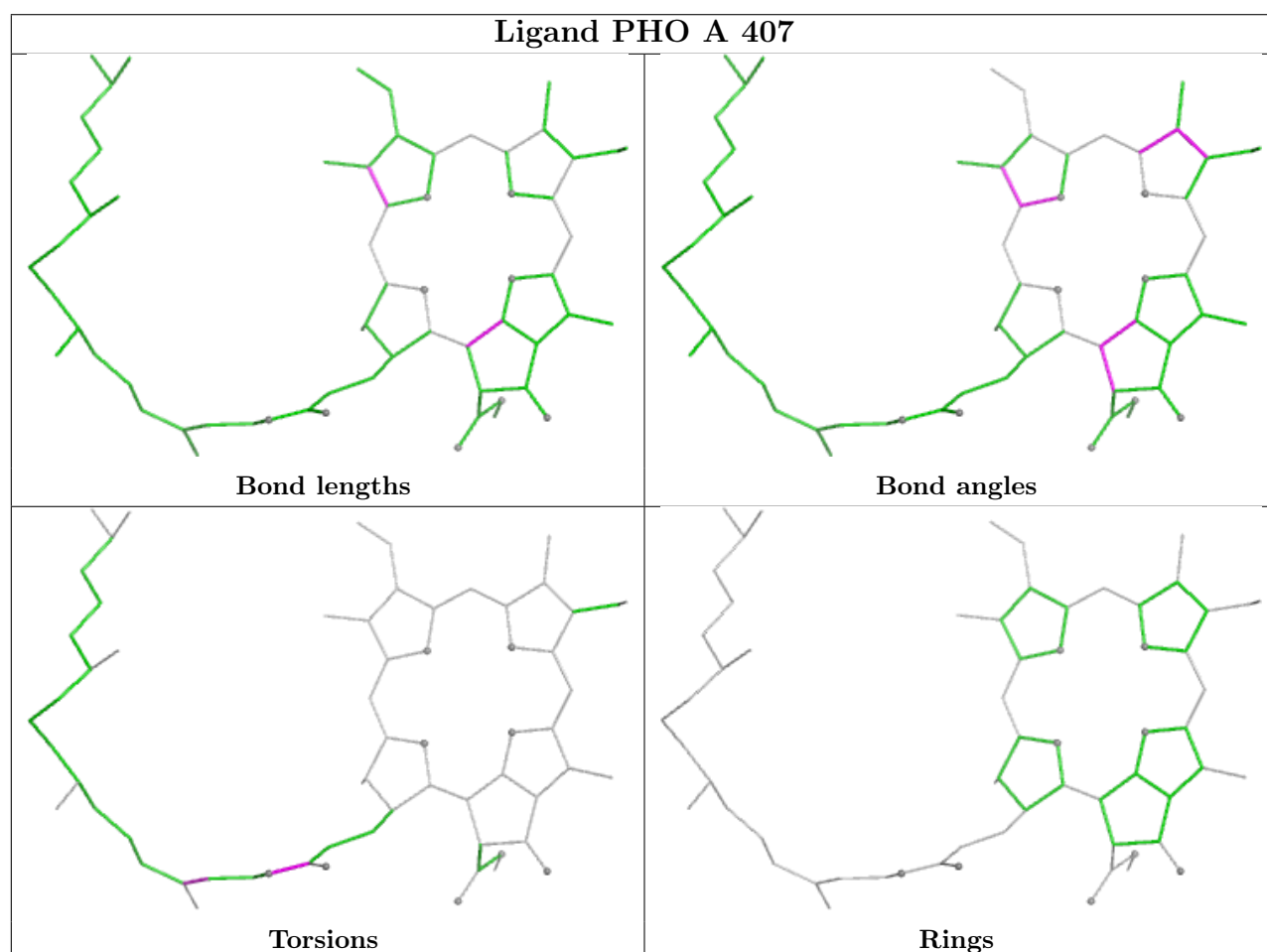
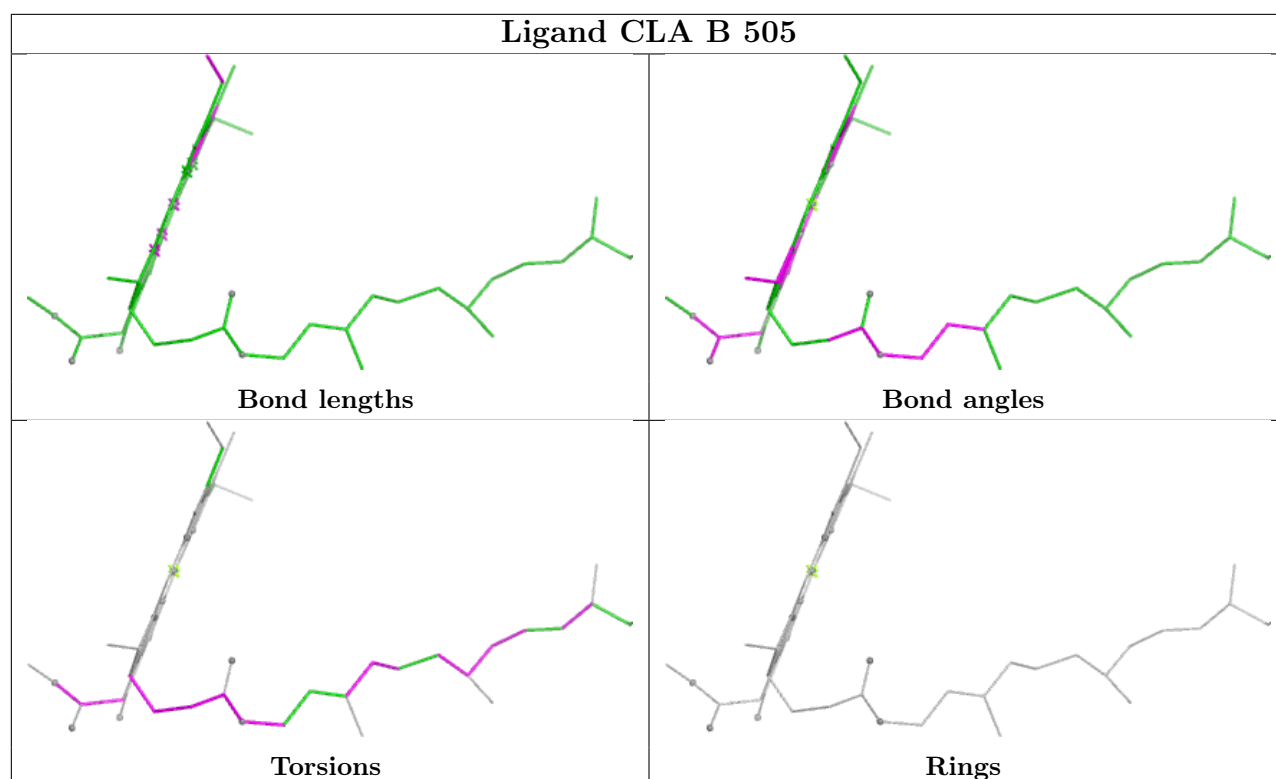


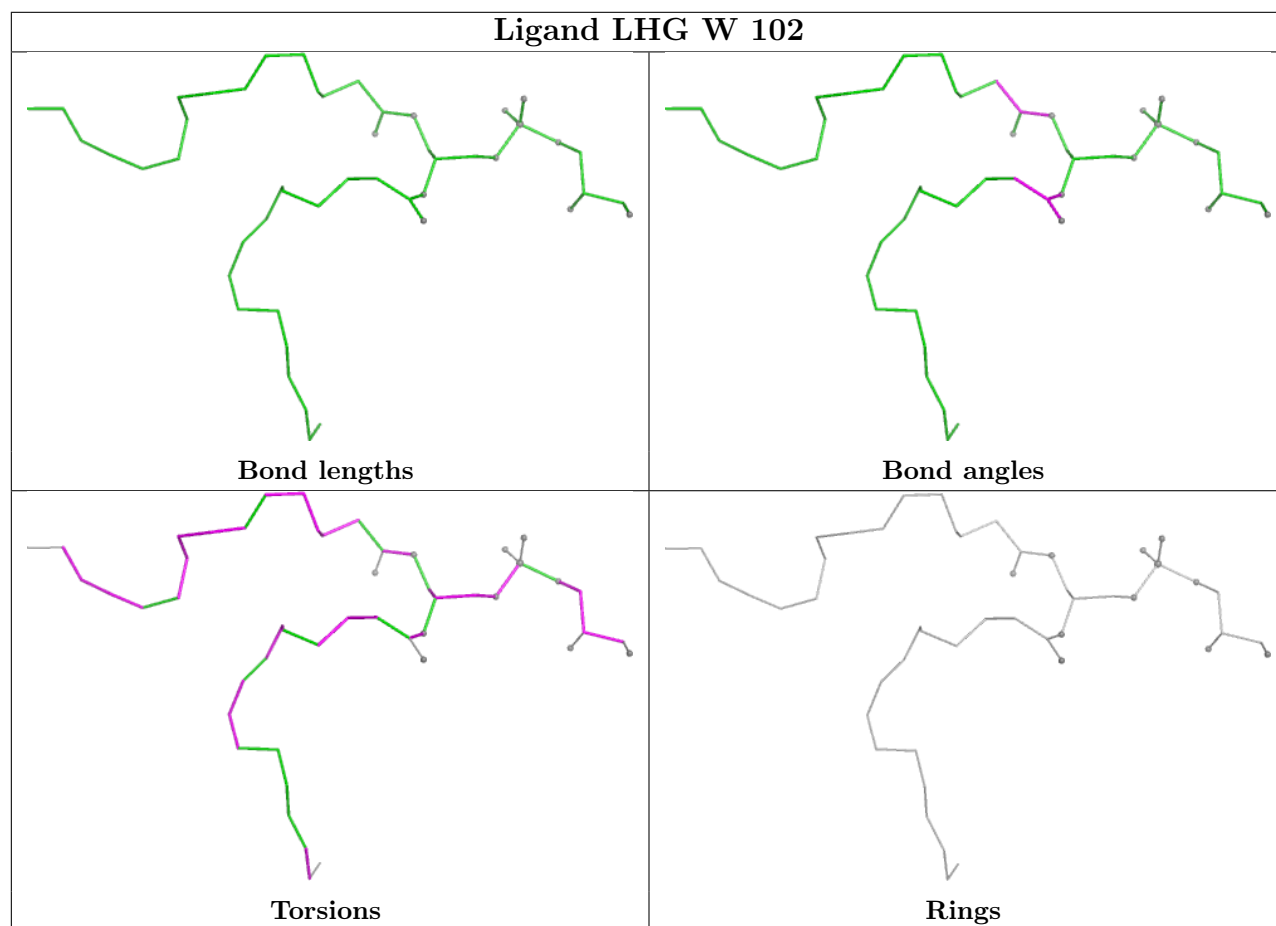
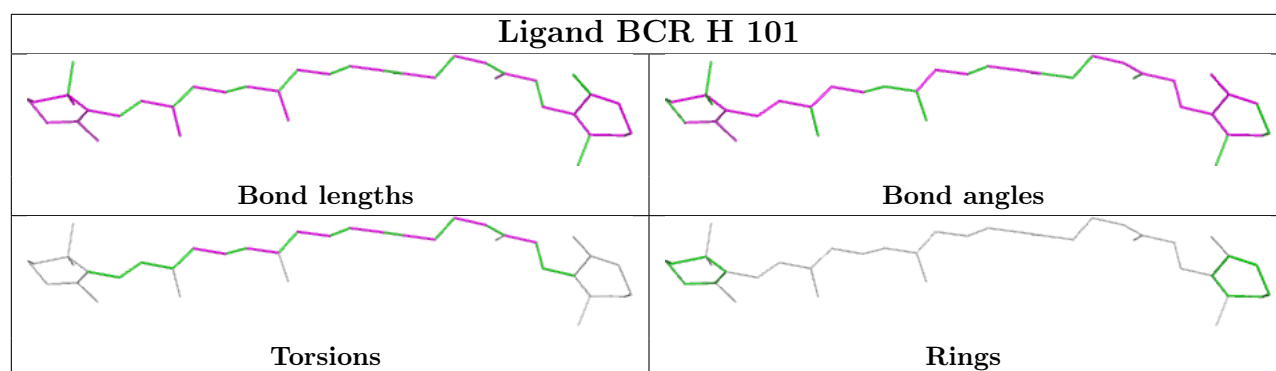


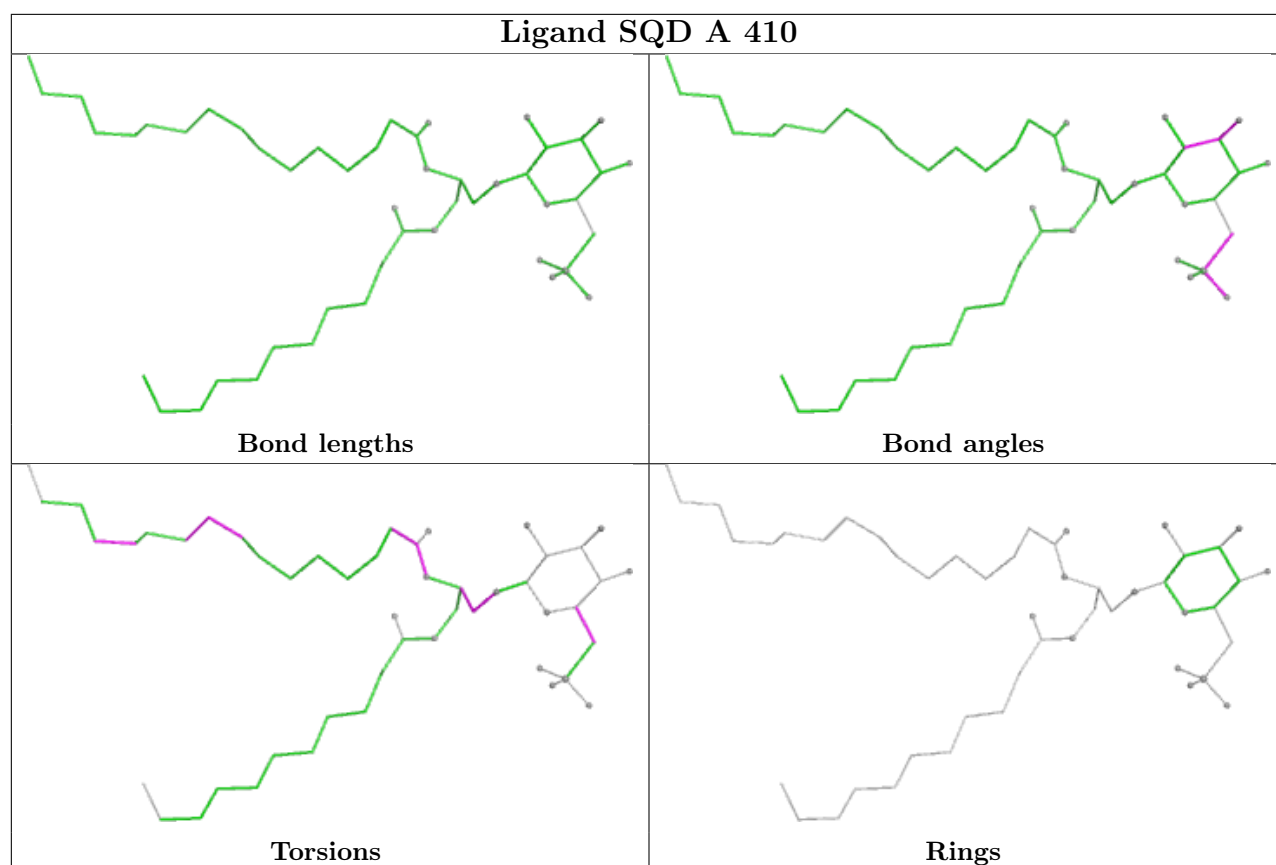


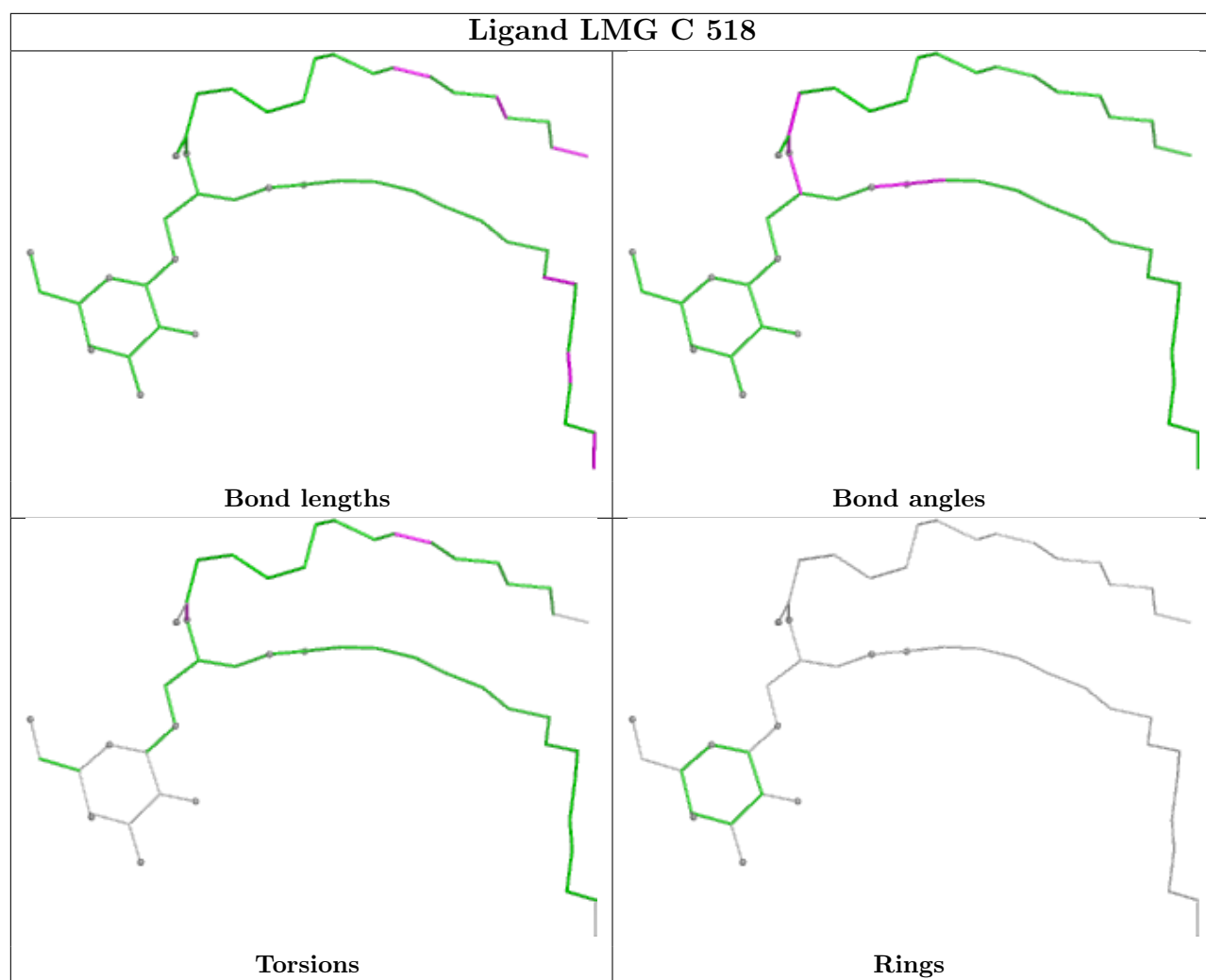


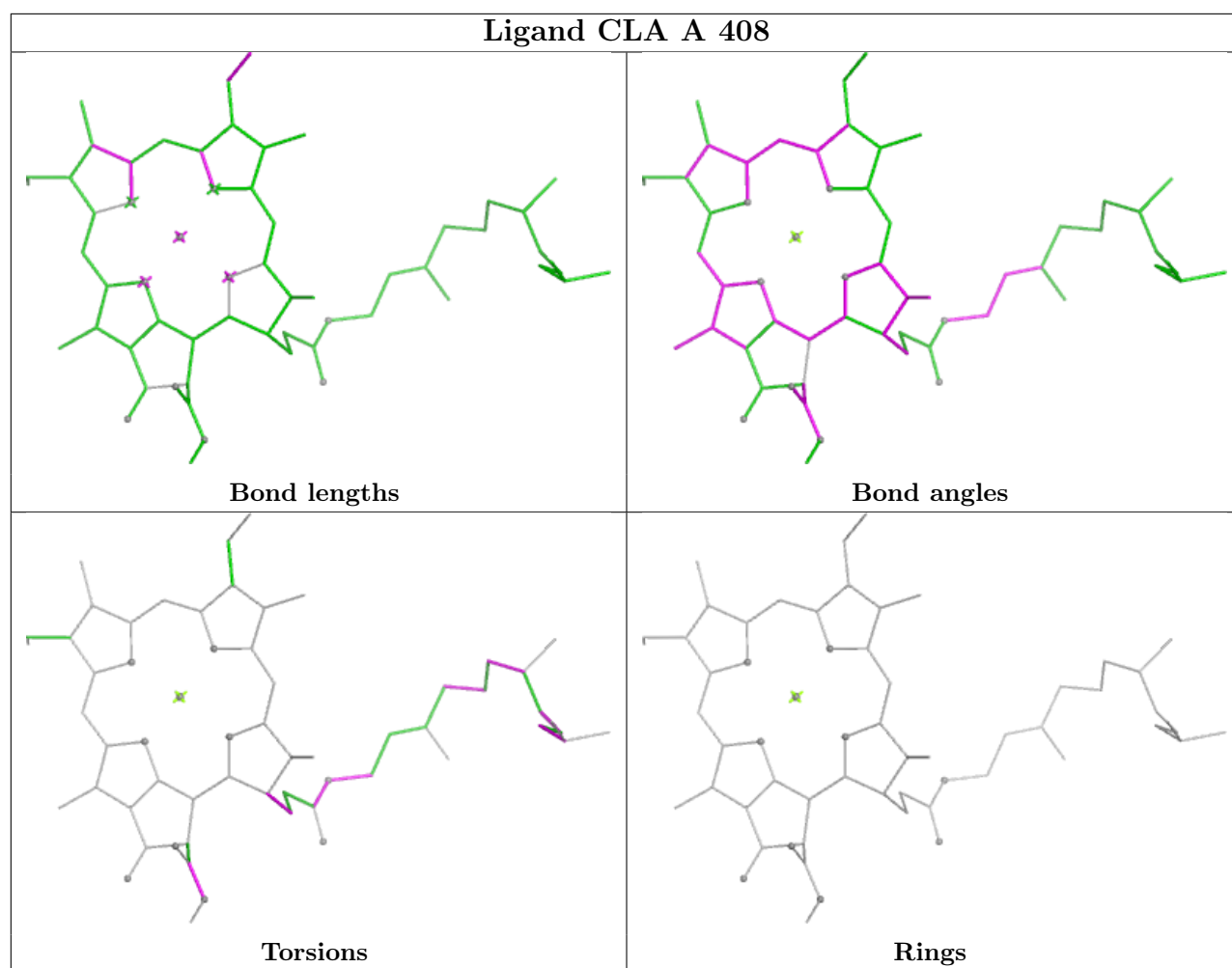


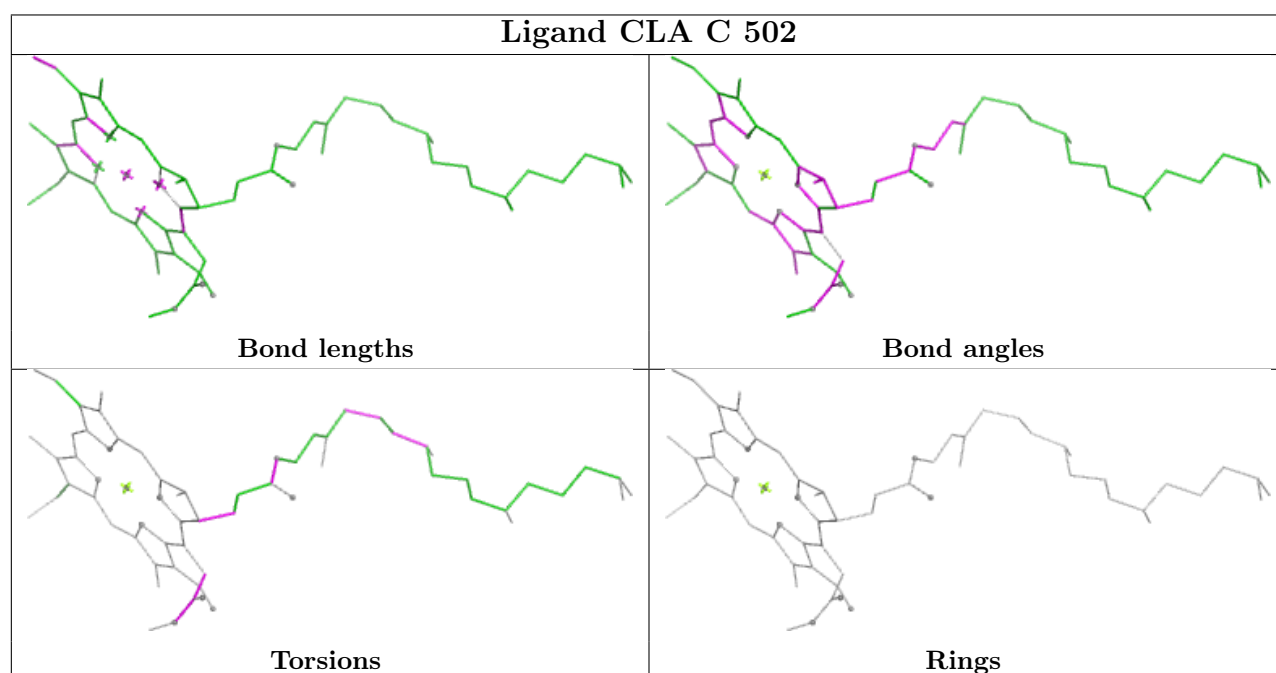
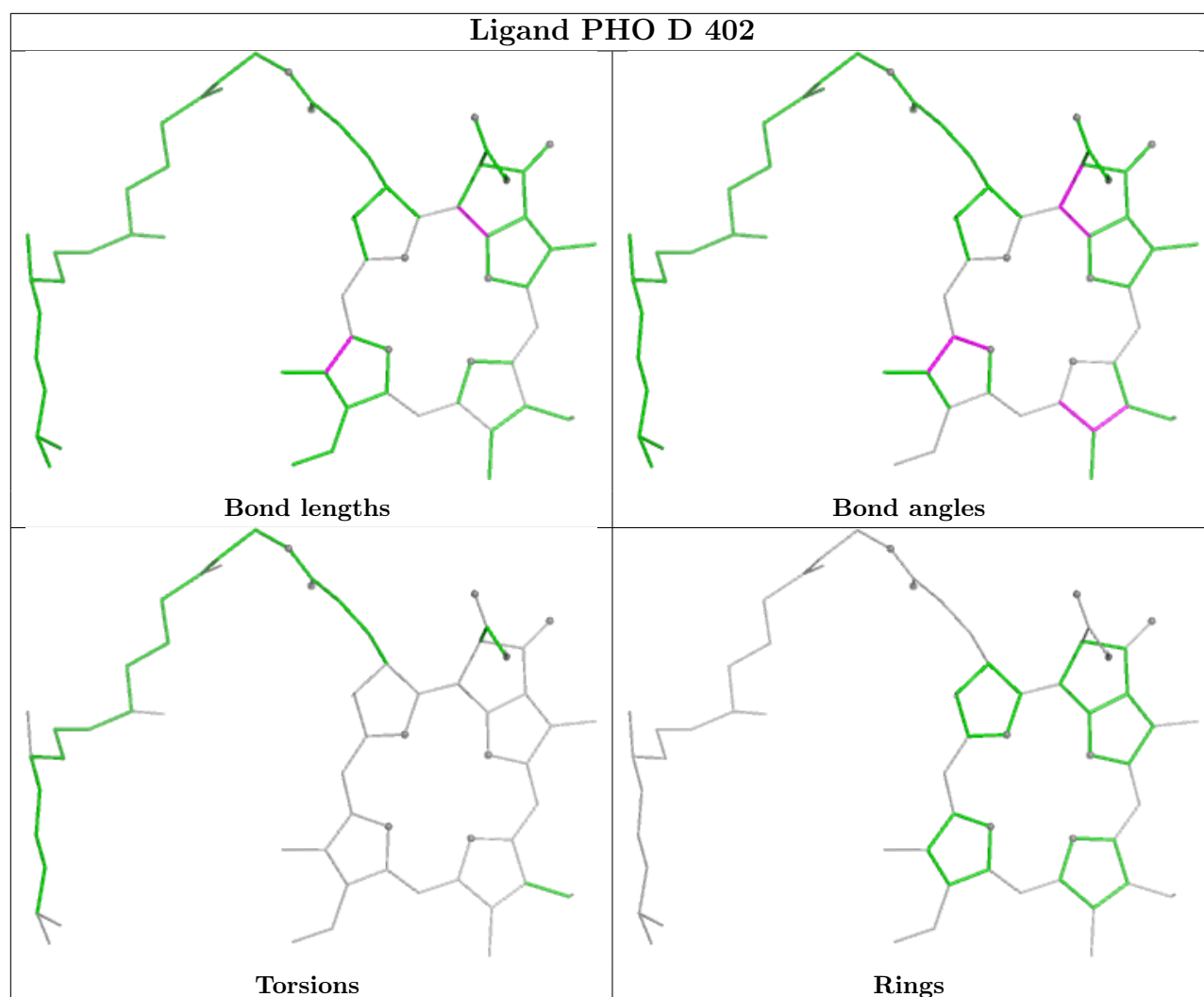


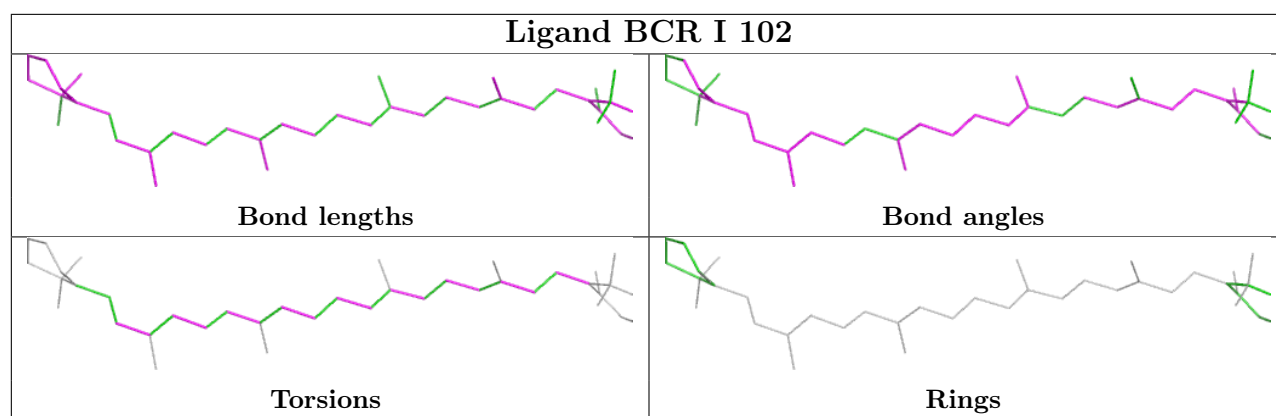












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

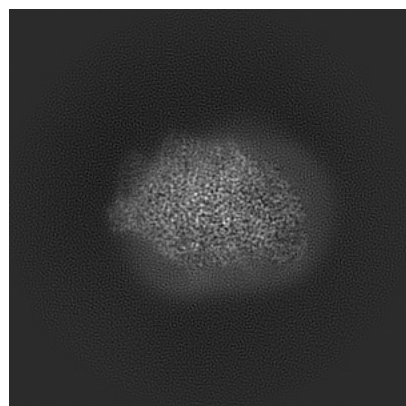
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54531. These allow visual inspection of the internal detail of the map and identification of artifacts.

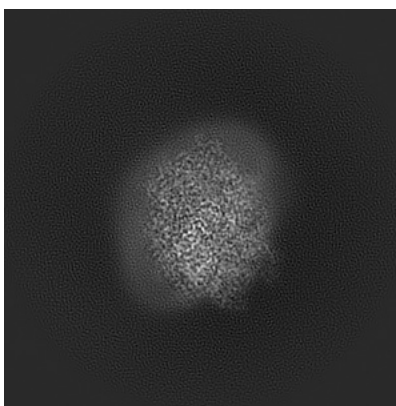
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

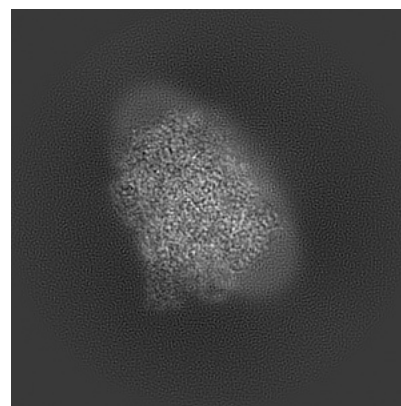
6.1.1 Primary map



X

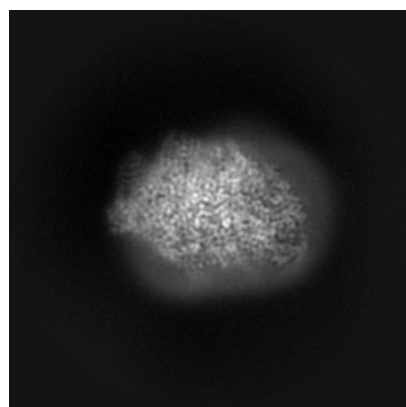


Y

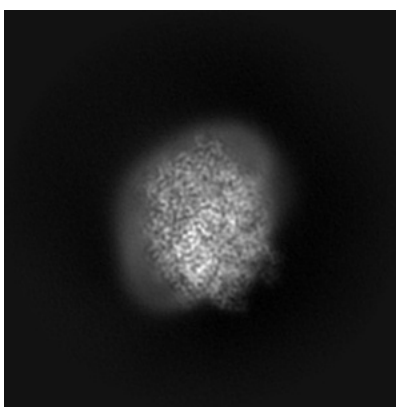


Z

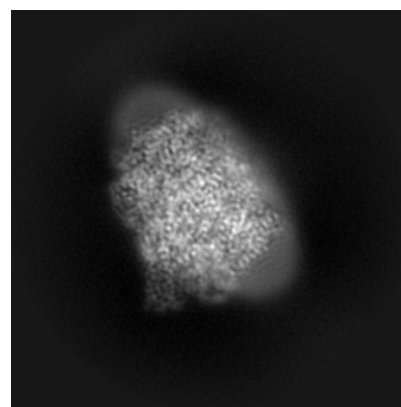
6.1.2 Raw map



X



Y

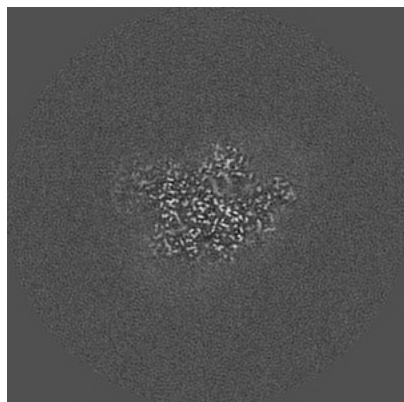


Z

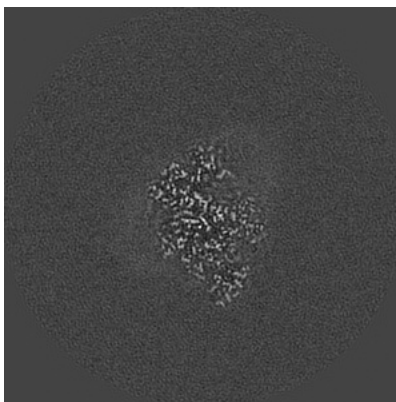
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

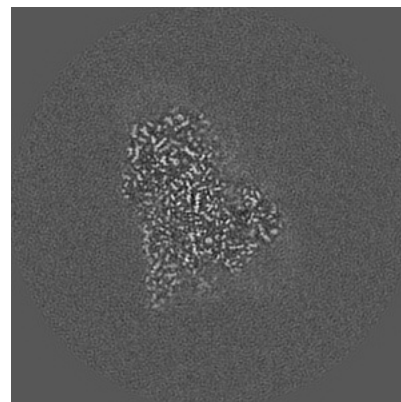
6.2.1 Primary map



X Index: 180

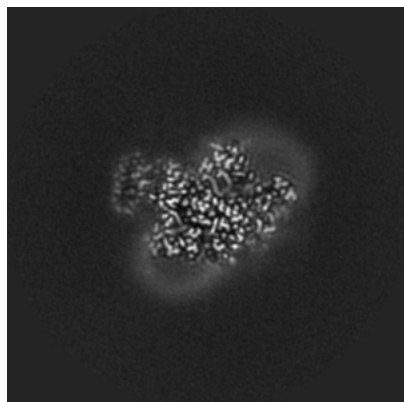


Y Index: 180

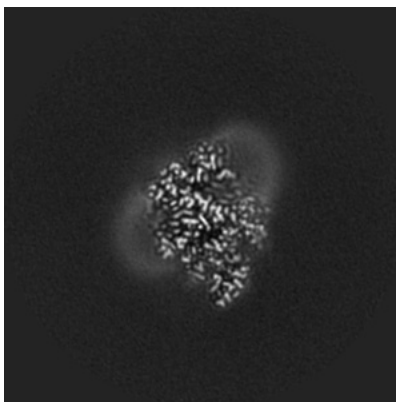


Z Index: 180

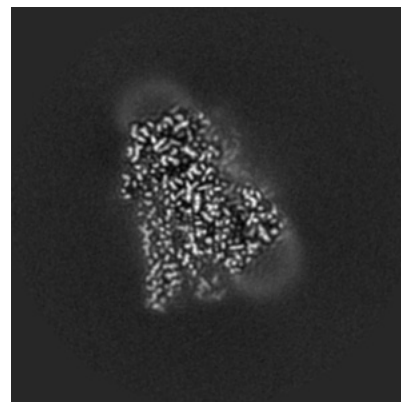
6.2.2 Raw map



X Index: 180



Y Index: 180

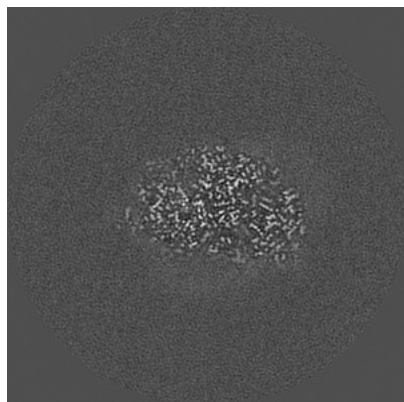


Z Index: 180

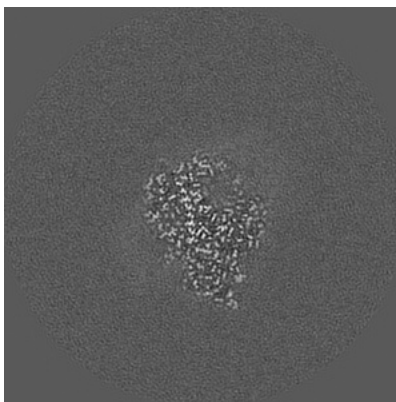
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

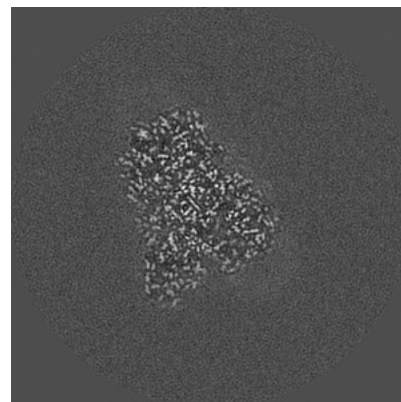
6.3.1 Primary map



X Index: 157

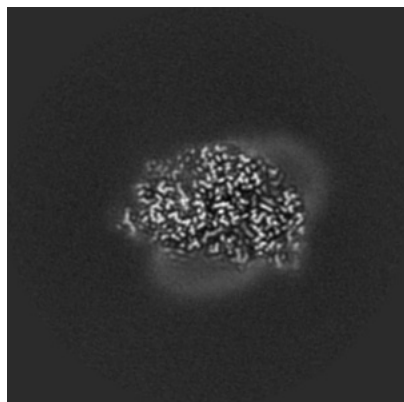


Y Index: 193

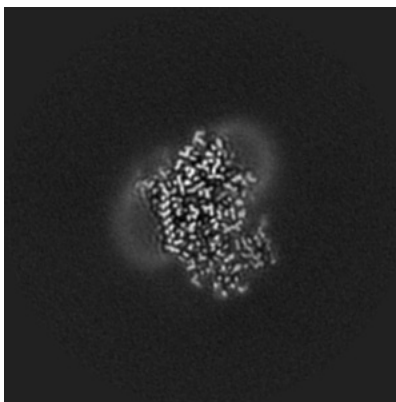


Z Index: 170

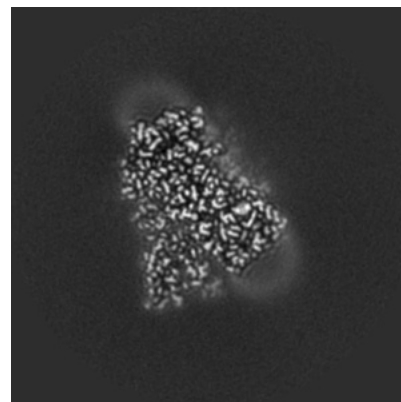
6.3.2 Raw map



X Index: 158



Y Index: 168

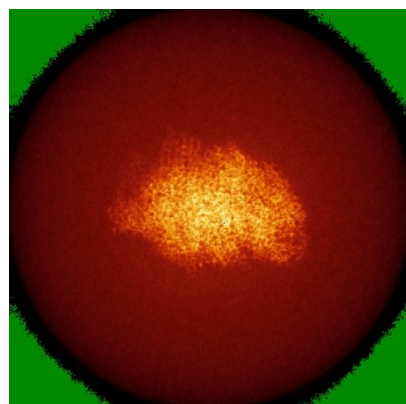


Z Index: 176

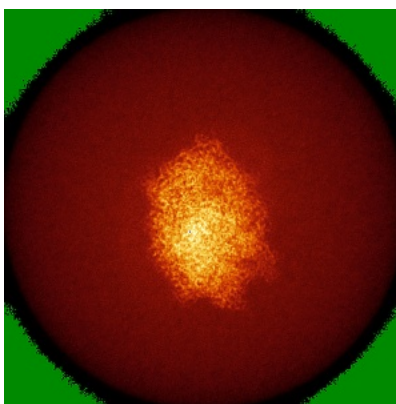
The images above show the largest variance slices of the map in three orthogonal directions.

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

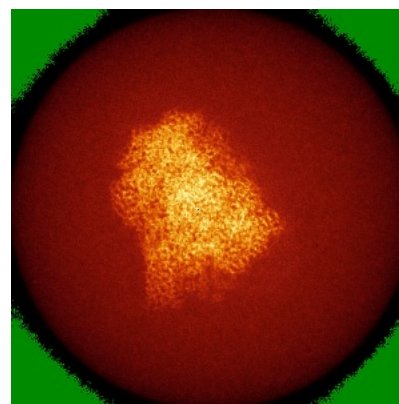
6.4.1 Primary map



X

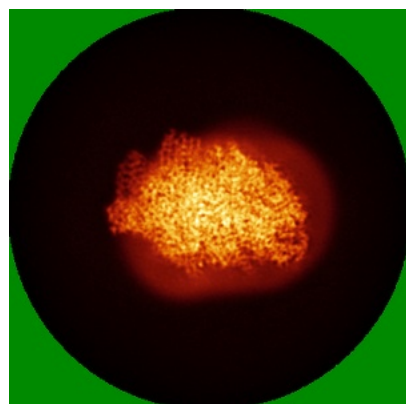


Y

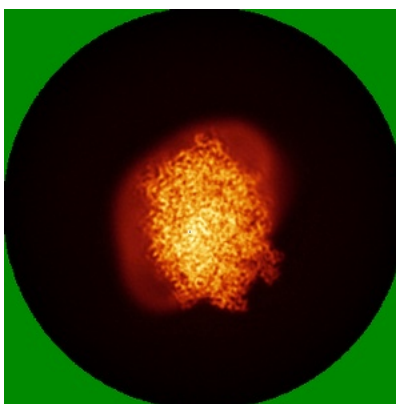


Z

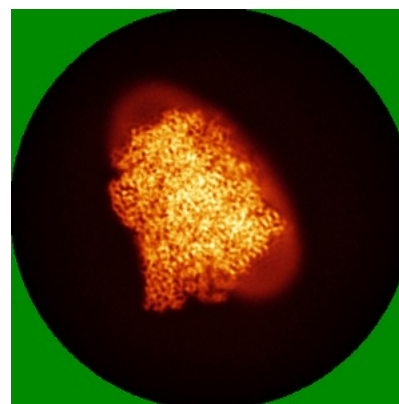
6.4.2 Raw map



X



Y

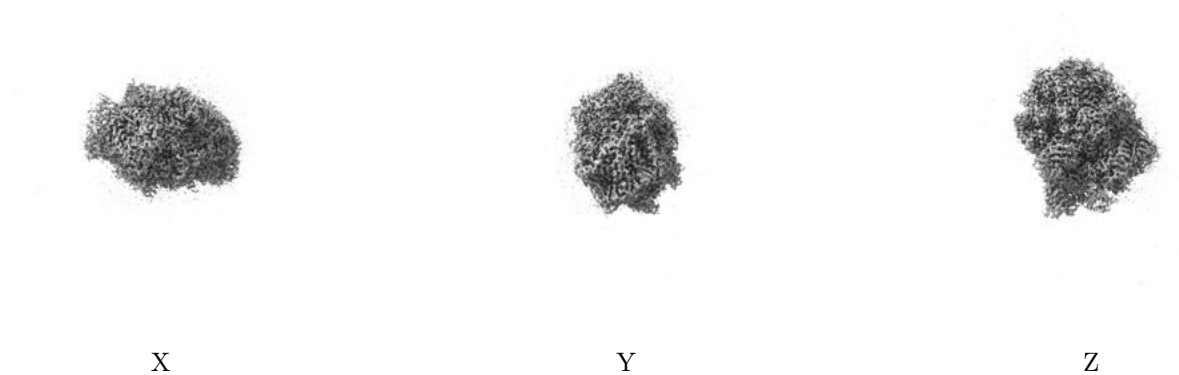


Z

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

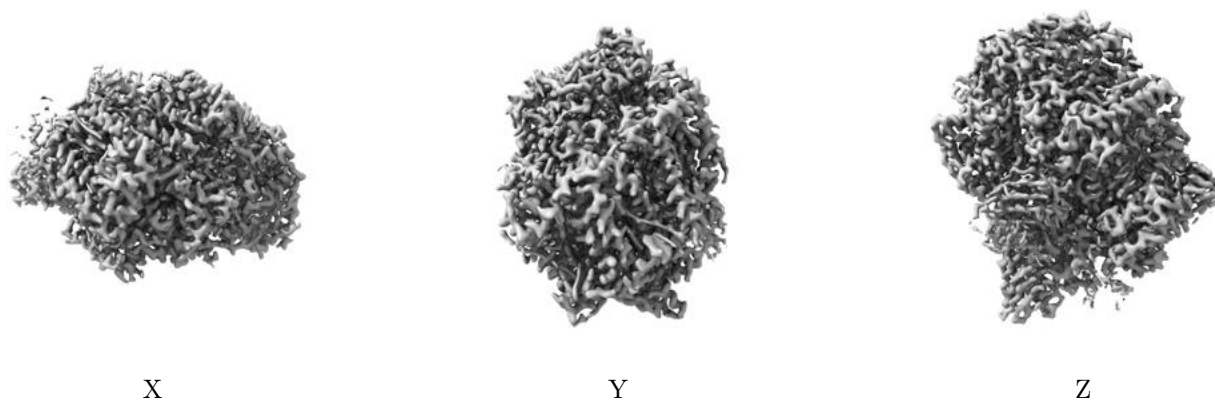
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

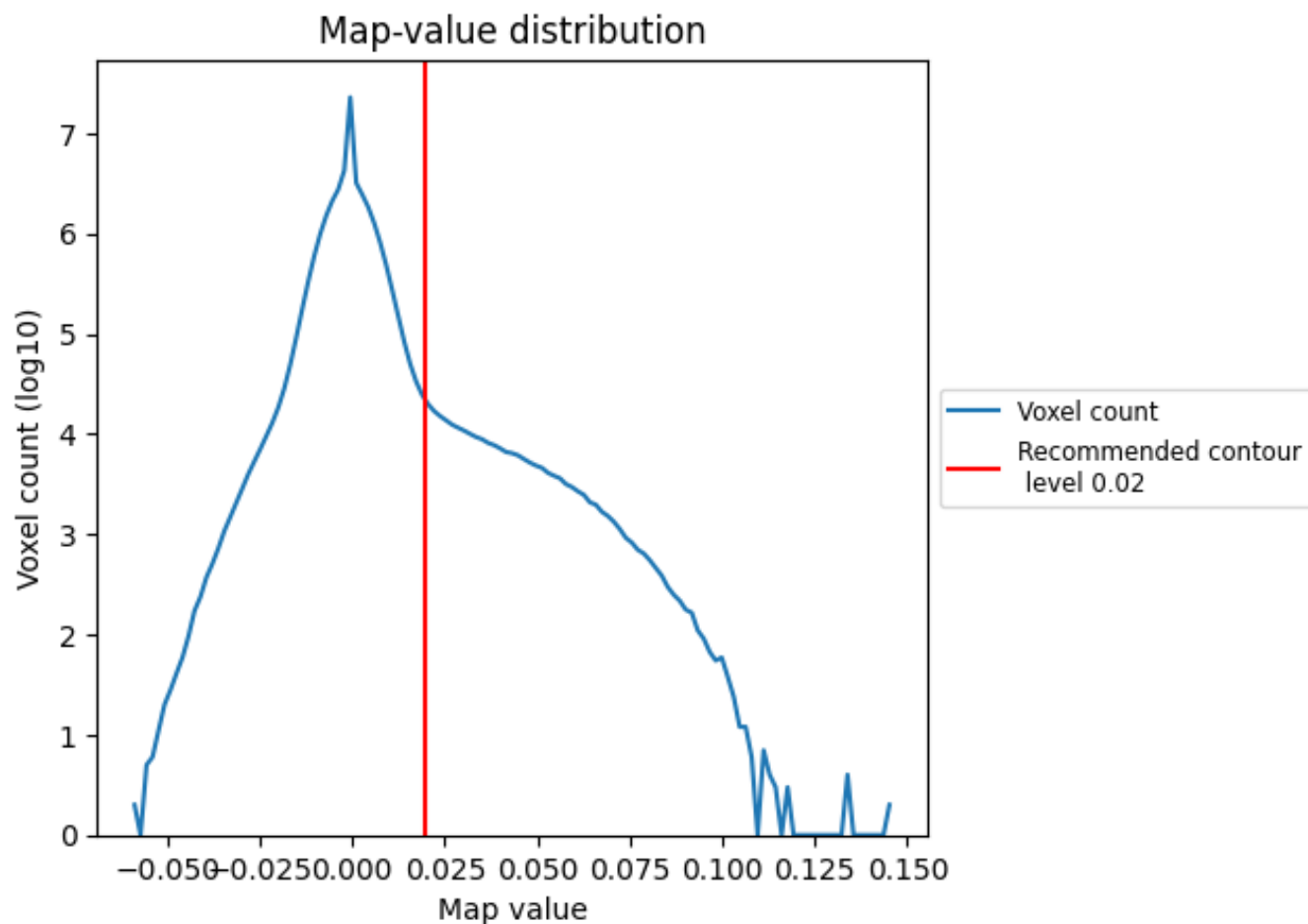
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

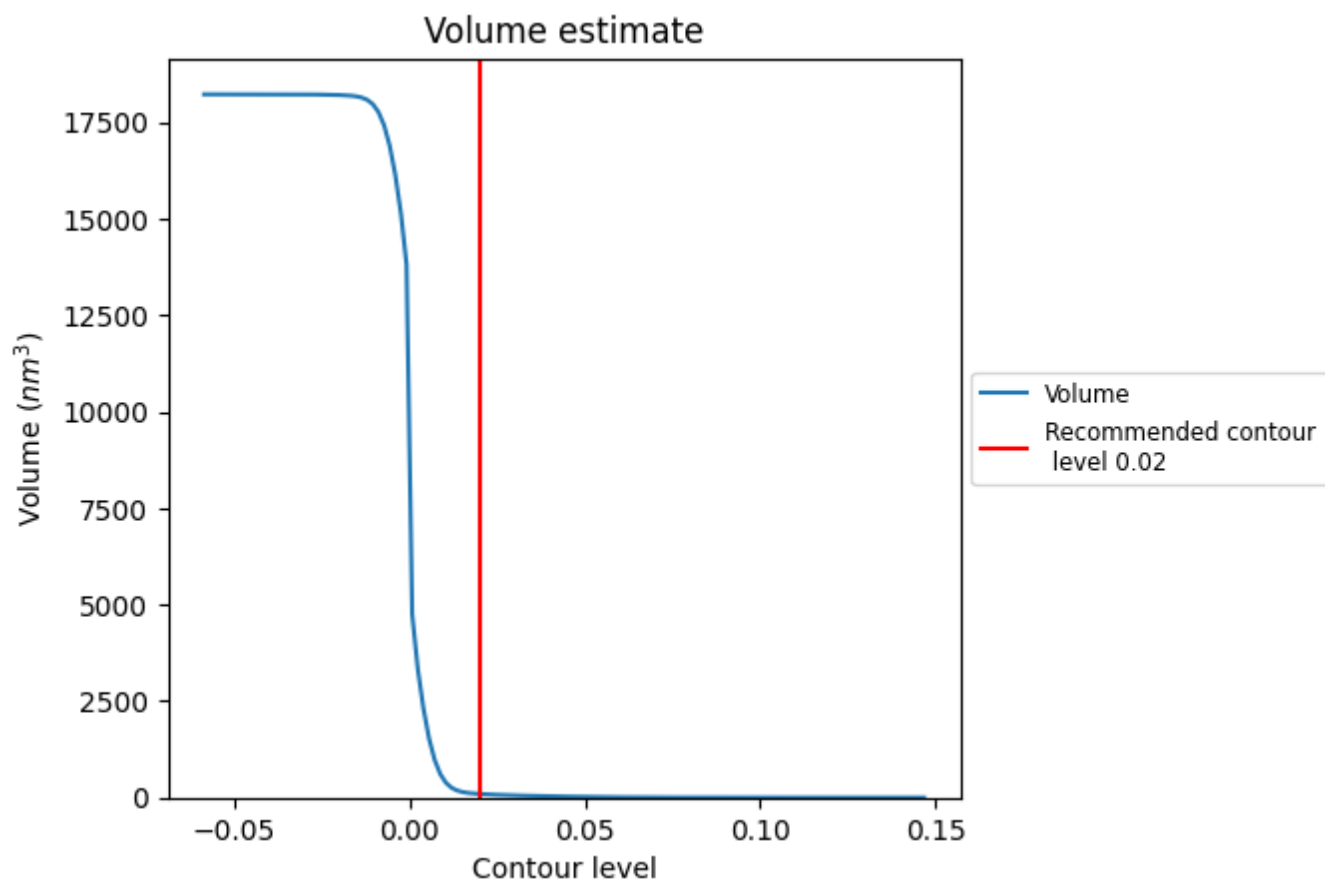
This section contains the results of statistical analysis of the map.

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.

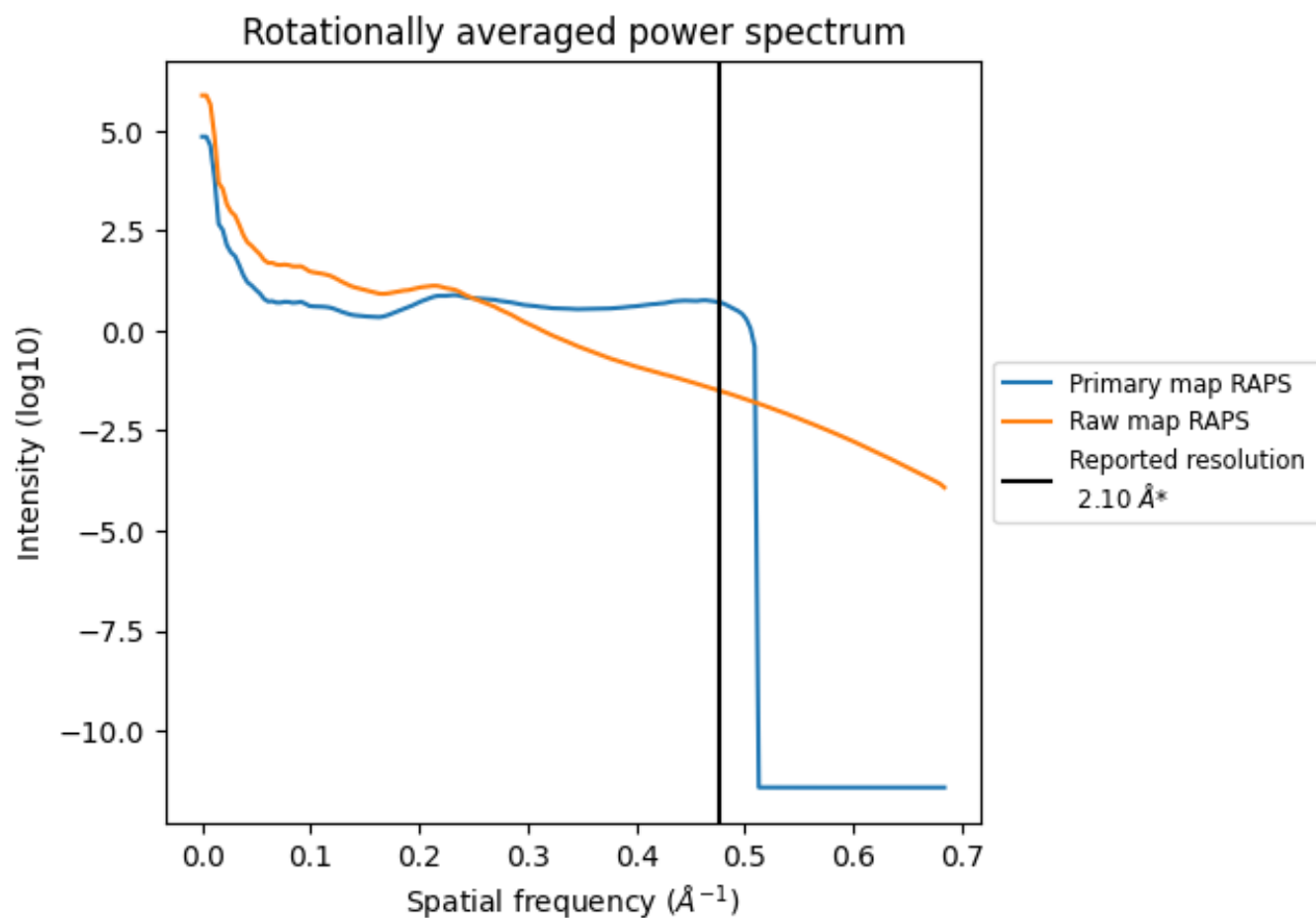
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm³; this corresponds to an approximate mass of 84 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 ⓘ

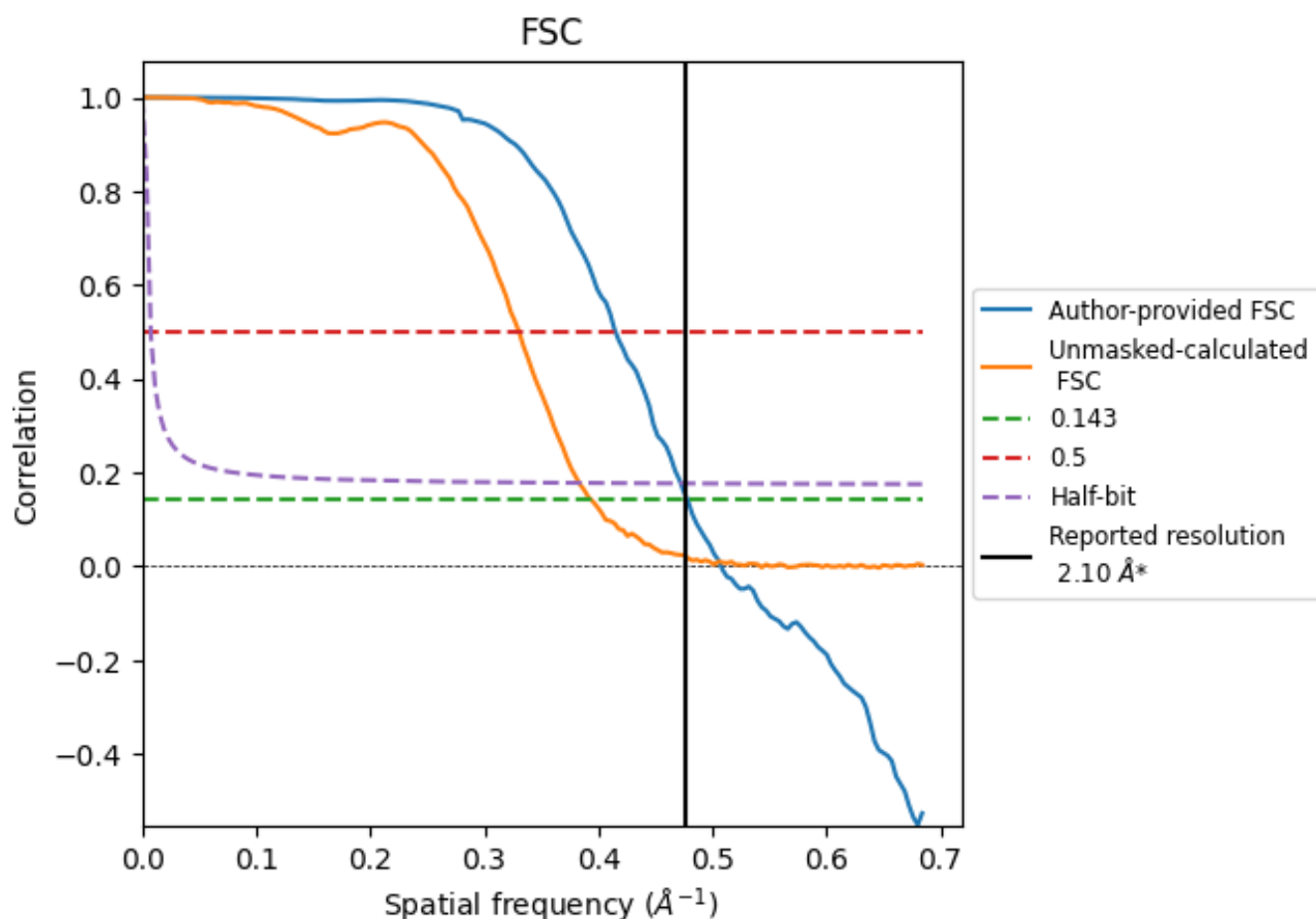


*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

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 0.476 Å⁻¹

8.2 Resolution estimates [i](#)

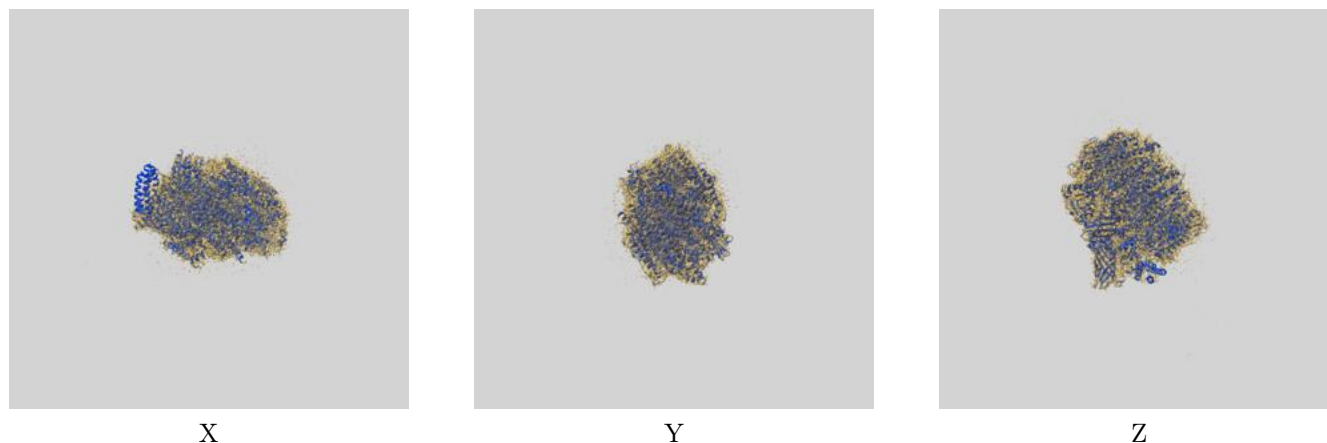
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.09	2.41	2.12
Unmasked-calculated*	2.54	3.03	2.61

*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 2.54 differs from the reported value 2.1 by more than 10 %

9 Map-model fit [i](#)

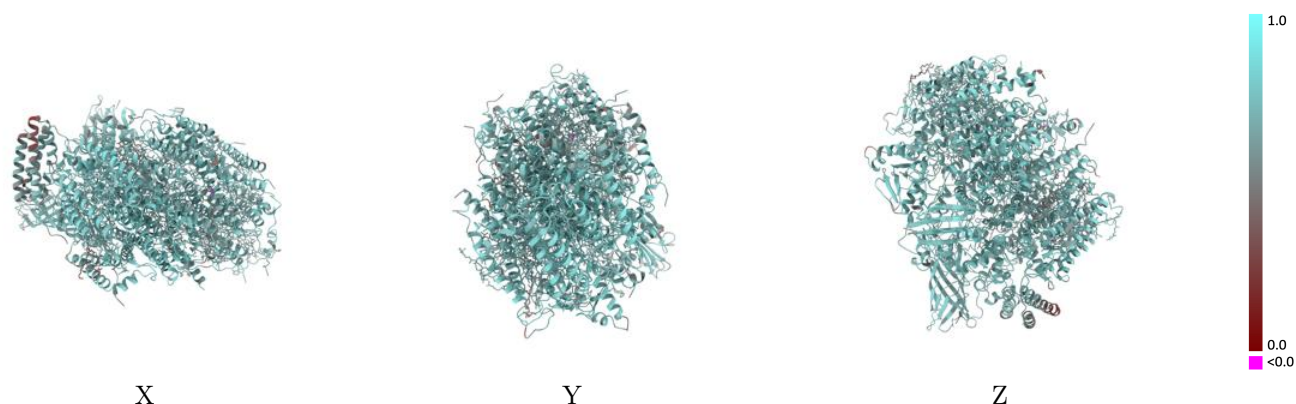
This section contains information regarding the fit between EMDB map EMD-54531 and PDB model 9S3E. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



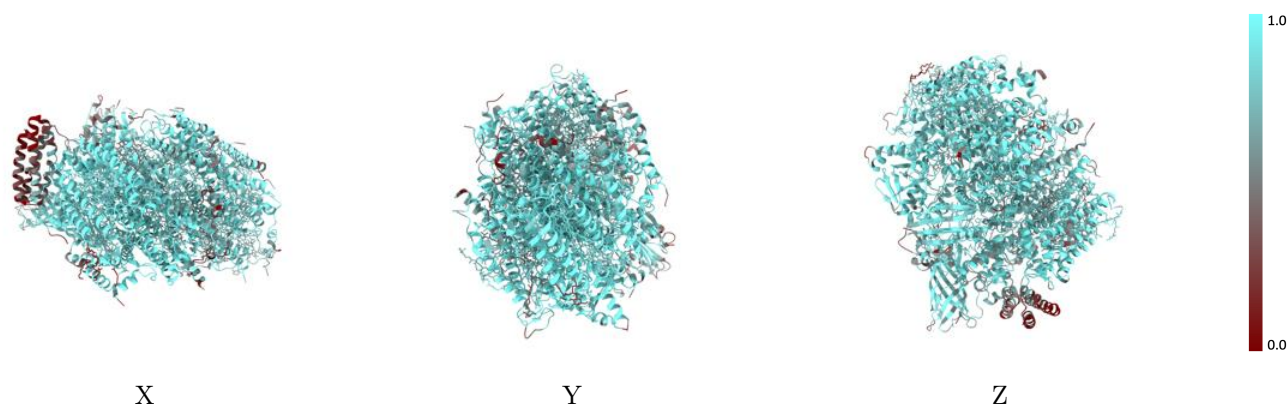
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



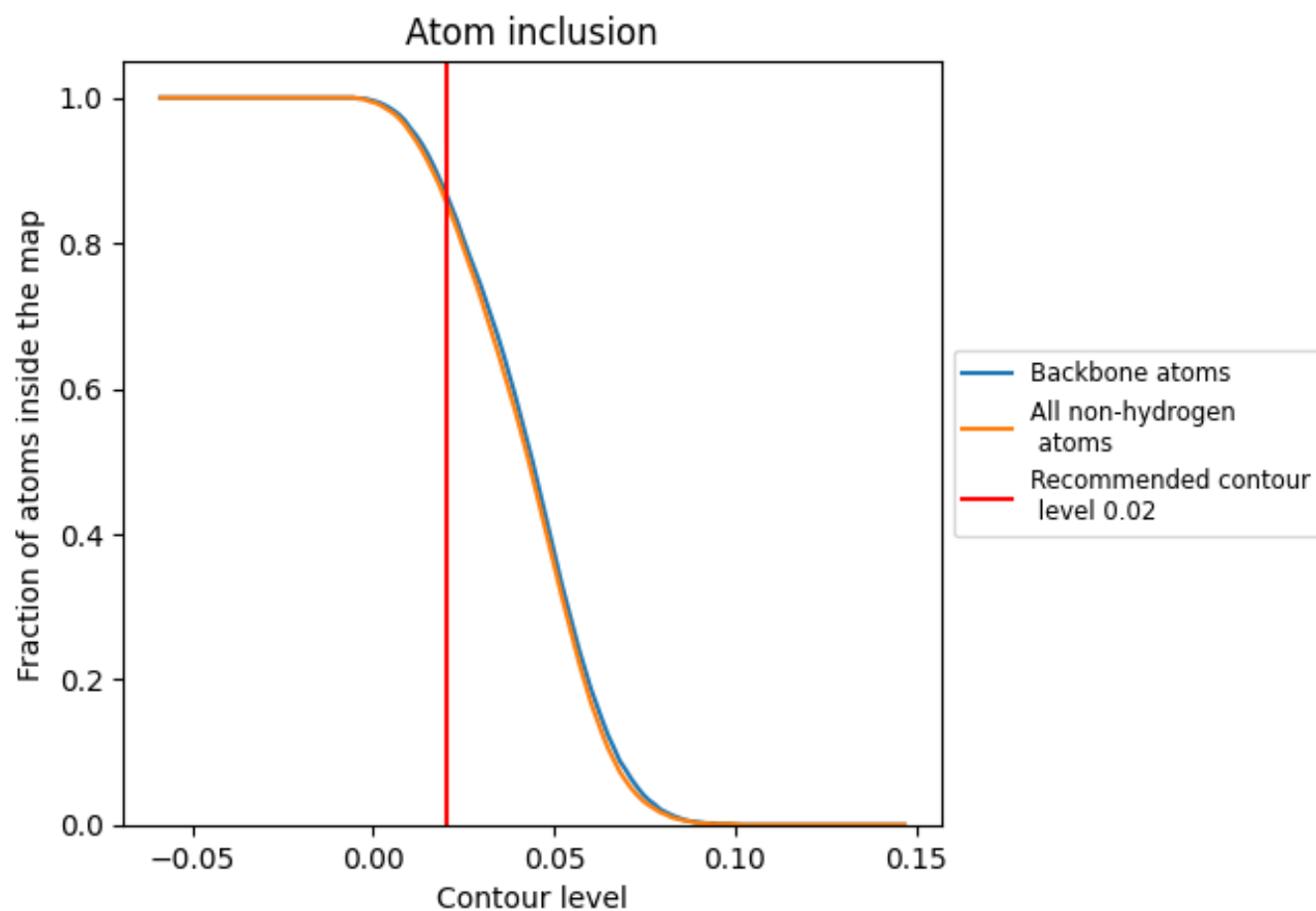
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8590	 0.7100
A	 0.8890	 0.7320
B	 0.8990	 0.7150
C	 0.9170	 0.7200
D	 0.9520	 0.7490
E	 0.8310	 0.6770
F	 0.9280	 0.7200
H	 0.9030	 0.7100
I	 0.8580	 0.6970
J	 0.7810	 0.6920
K	 0.7680	 0.6580
L	 0.9170	 0.7310
M	 0.6480	 0.6460
O	 0.8380	 0.6950
P	 0.7900	 0.7020
Q	 0.3970	 0.6010
T	 0.8550	 0.7170
U	 0.8290	 0.6470
W	 0.6670	 0.6190
X	 0.8430	 0.7000

