



wwPDB EM Validation Summary Report ⓘ

Sep 9, 2026 – 04:20 pm BST

PDB ID : 9HEI / pdb_00009hei
EMDB ID : EMD-52077
Title : Universal Photosystem II Intermediate with Light-Dependent Water-Ferrocyanide Oxydo-reductase activity from Chlamydomonas reinhardtii
Authors : Nelson, N.; Klaiman, D.; Fadeeva, M.; Kandiah, E.
Deposited on : 2024-11-14
Resolution : 2.92 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:

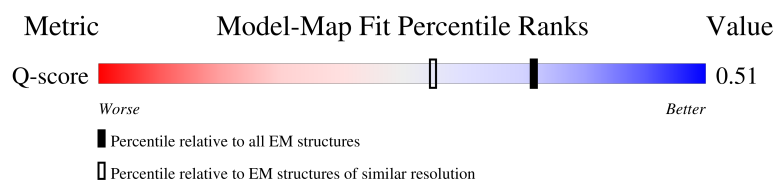
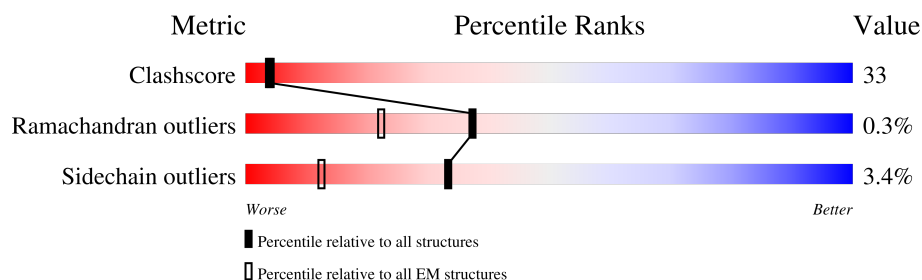
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.92 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.



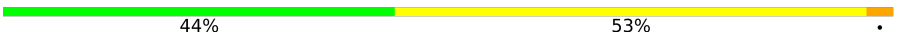
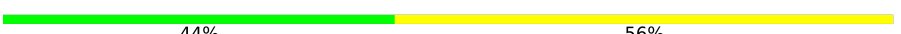
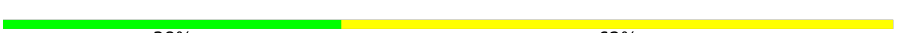
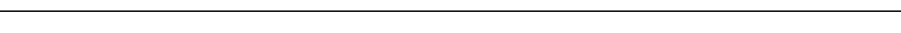
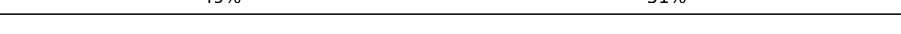
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13007 (2.42 - 3.42)

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	 43% 50% • 5%
2	B	480	 48% 48% •
3	V	32	 41% 56% •
4	C	449	 53% 45% •

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Mol	Chain	Length	Quality of chain
5	D	348	
6	E	75	
7	F	31	
8	H	66	
9	I	34	
10	J	36	
11	K	37	
12	L	35	
13	M	29	
14	O	240	
15	P	188	
16	Q	148	
17	T	30	
18	X	32	
19	Z	61	
20	U	23	
21	W	44	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	503	-	-	X	-
25	CLA	B	509	-	-	X	-
25	CLA	C	507	-	-	X	-
29	LMG	W	201	-	-	X	-

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 24697 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	318	Total	C	N	O	S	0	0
			2491	1635	409	432	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	480	Total	C	N	O	S	0	0
			3755	2462	630	651	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			224	147	37	40		

- 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
			3498	2288	584	609	17		

- 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
			2771	1828	456	475	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	75	Total	C	N	O	0	0
			610	399	101	110		

- 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
			251	171	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	66	Total	C	N	O	S	0	0
			501	336	74	89	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			275	189	41	43	2		

- 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
			262	178	40	44		

- 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	209	43	45		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	35	Total	C	N	O	0	0
			290	196	45	49		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	29	Total	C	N	O	0	0
			223	154	31	38		

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	240	Total	C	N	O	S	0	0
			1808	1150	291	363	4		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	188	Total	C	N	O	S	0	0
			1444	920	240	283	1		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O	S	0	0
			1192	746	214	232			

- Molecule 17 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	30	Total	C	N	O	S	0	0
			247	171	36	38	2		

- Molecule 18 is a protein called 4.1 kDa photosystem II subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	32	Total	C	N	O	S	0	0
			220	146	35	39			

- 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
			458	314	68	75	1		

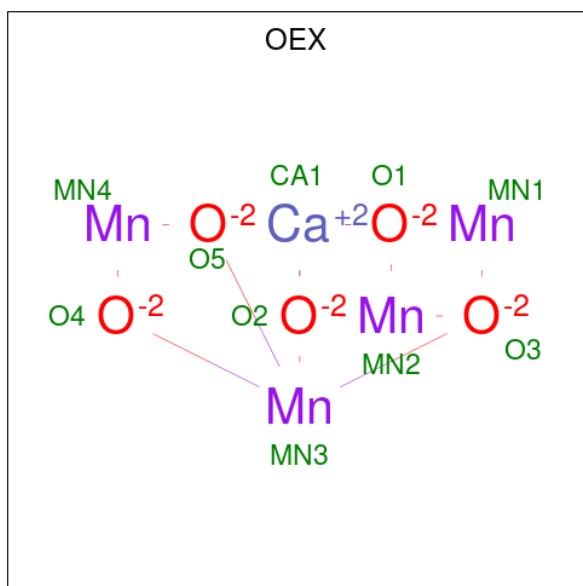
- Molecule 20 is a protein called Photosystem II reaction center protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	23	Total	C	N	O	S	0	0
			176	109	30	37			

- Molecule 21 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	44	Total	C	N	O	S	0	0
			344	226	57	59	2		

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).

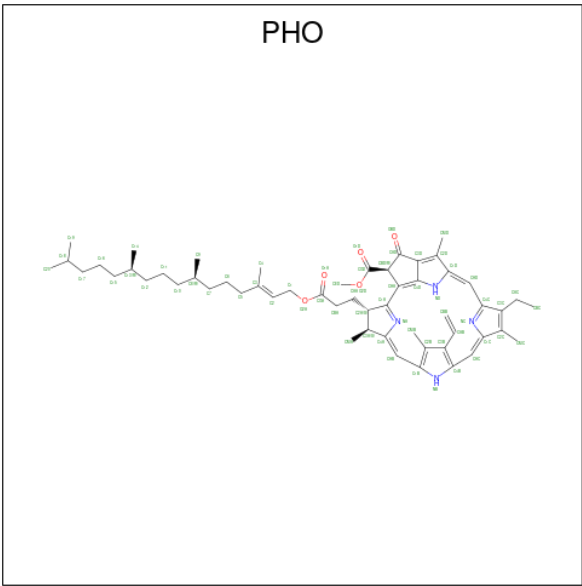


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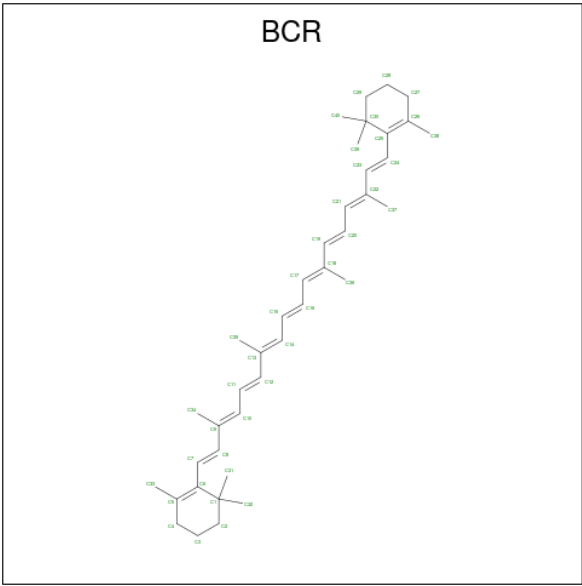
Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 52	C 42	Mg 1	N 4	O 5	0
25	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	H	1	Total 61	C 51	Mg 1	N 4	O 5	0

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



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

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



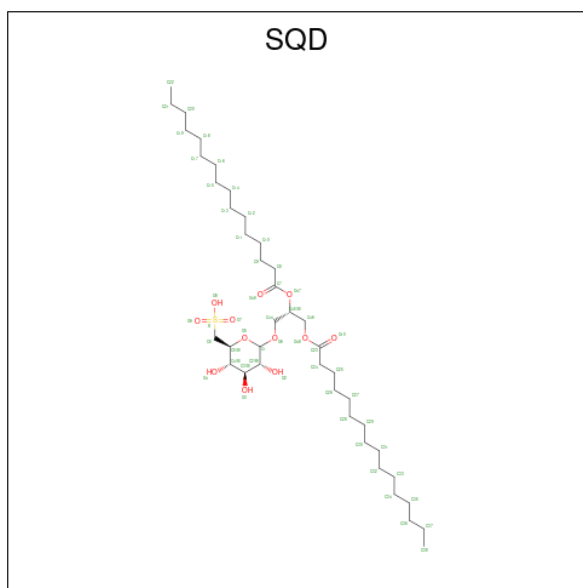
Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	C	0
			40	40	

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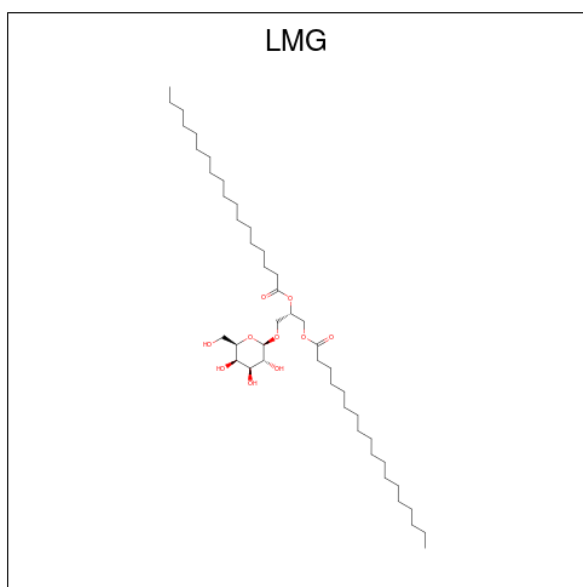
Mol	Chain	Residues	Atoms	AltConf
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	D	1	Total C 40 40	0
27	K	1	Total C 40 40	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



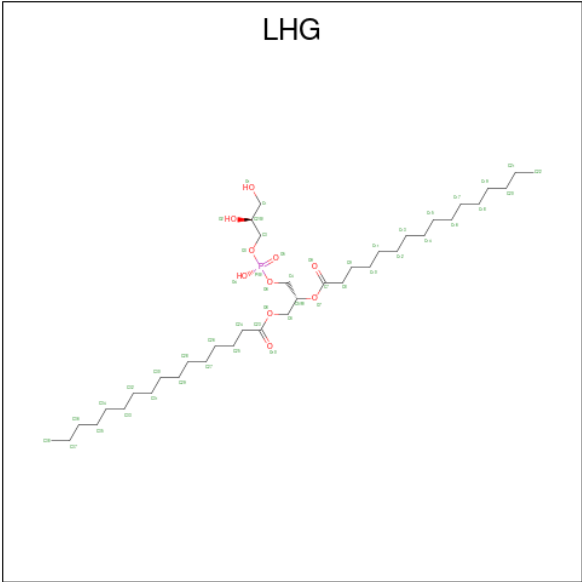
Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total C O S 51 38 12 1	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



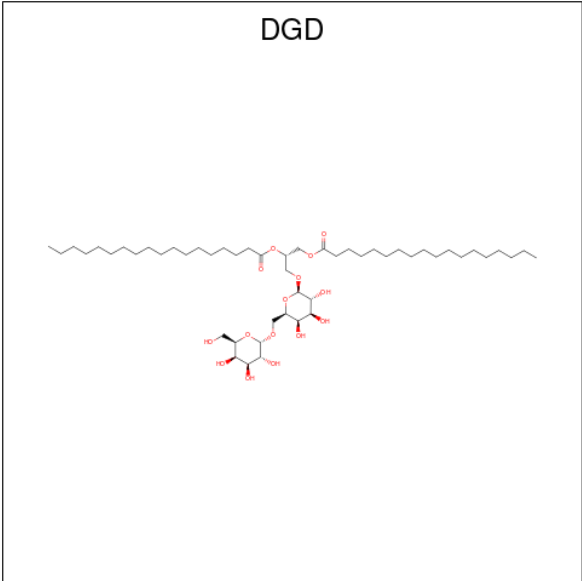
Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			43	33	10	
29	B	1	Total	C	O	0
			48	38	10	
29	C	1	Total	C	O	0
			51	41	10	
29	D	1	Total	C	O	0
			36	26	10	
29	W	1	Total	C	O	0
			48	38	10	

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



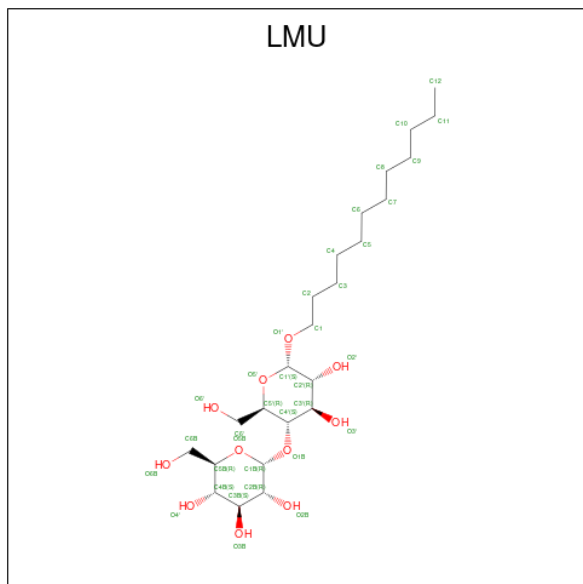
Mol	Chain	Residues	Atoms				AltConf
30	B	1	Total	C	O	P	0
			44	33	10	1	
30	B	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



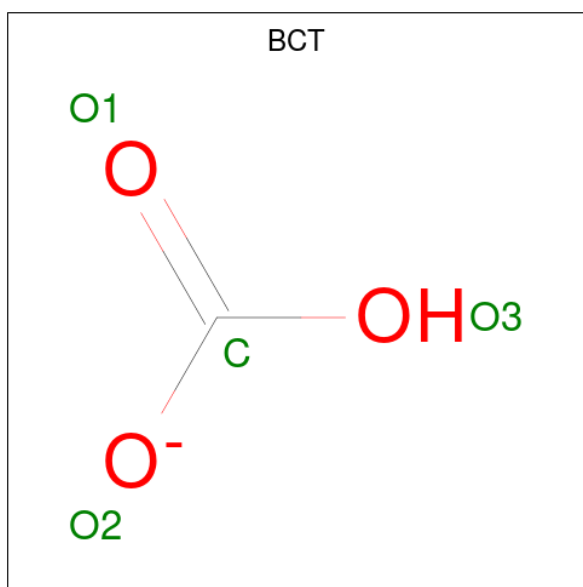
Mol	Chain	Residues	Atoms			AltConf
31	C	1	Total	C	O	0
			52	37	15	
31	C	1	Total	C	O	0
			54	39	15	
31	C	1	Total	C	O	0
			54	39	15	

- Molecule 32 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



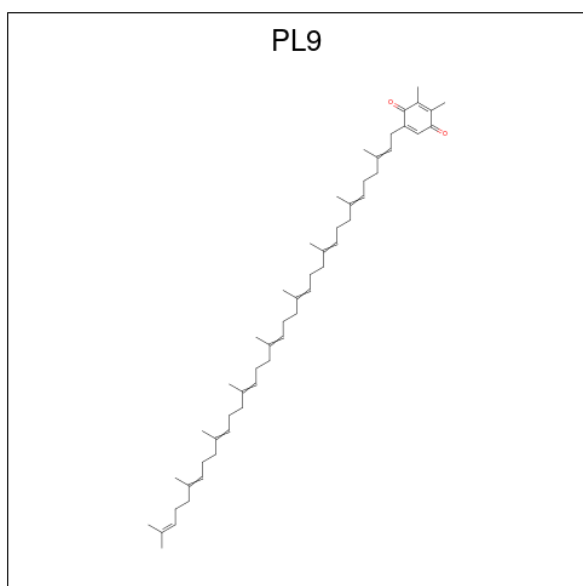
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			35	24	11	

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

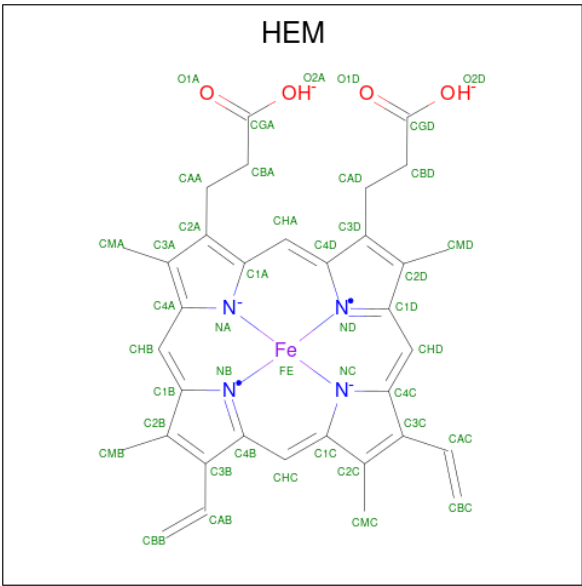
- Molecule 34 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

C₃₄H₃₂FeN₄O₄).



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

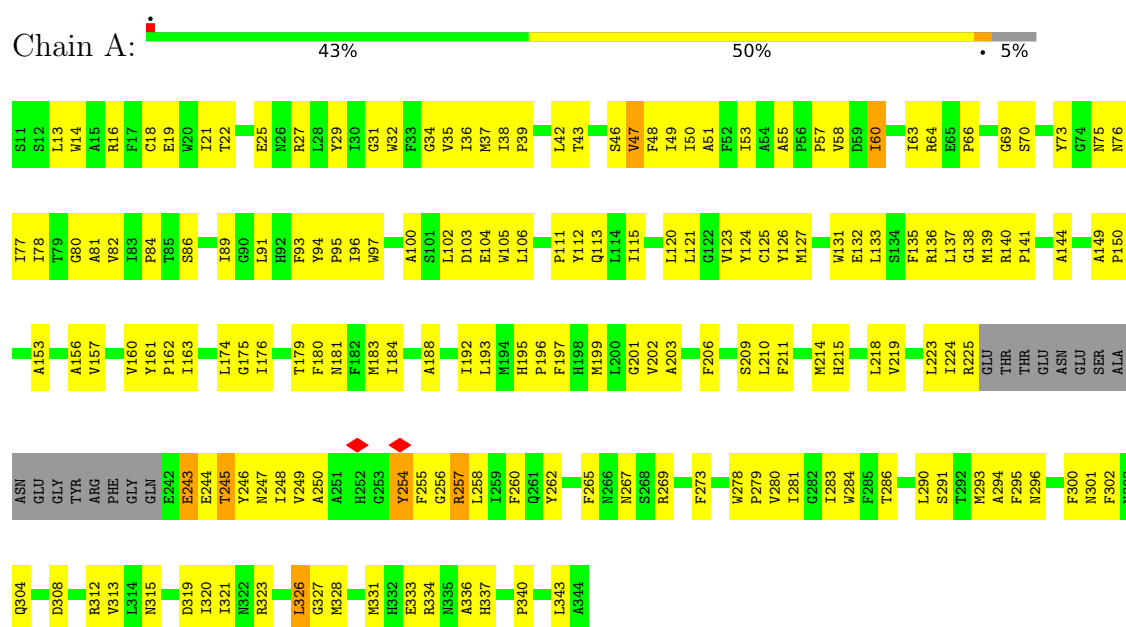
- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	A	2	Total	O	0
			2	2	
36	B	2	Total	O	0
			2	2	
36	C	2	Total	O	0
			2	2	
36	D	1	Total	O	0
			1	1	

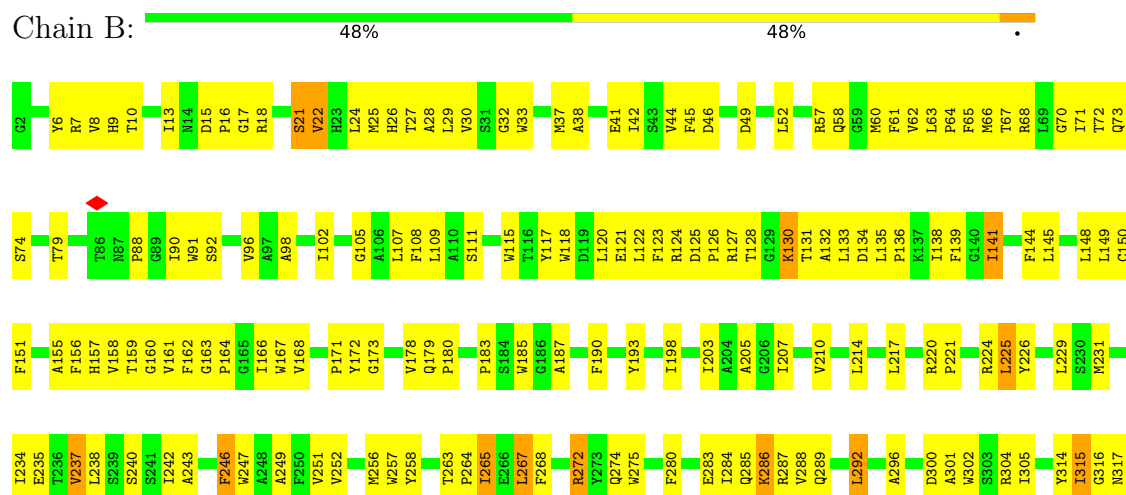
3 Residue-property plots

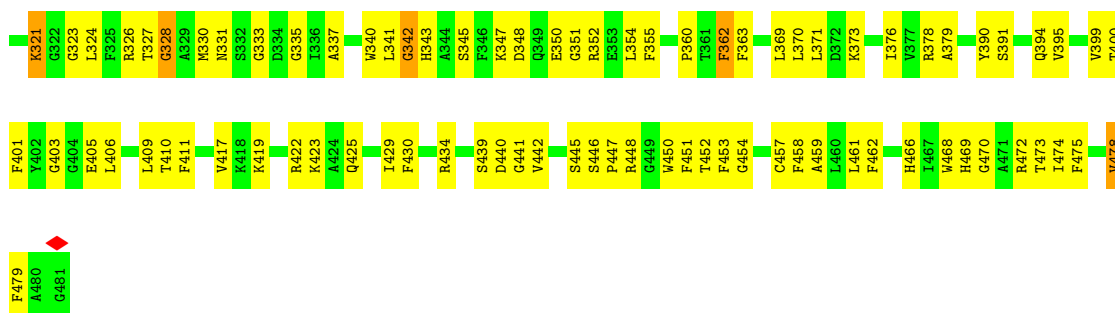
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

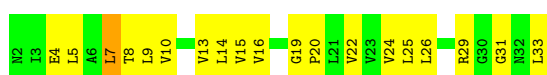


• Molecule 2: Photosystem II CP47 reaction center protein

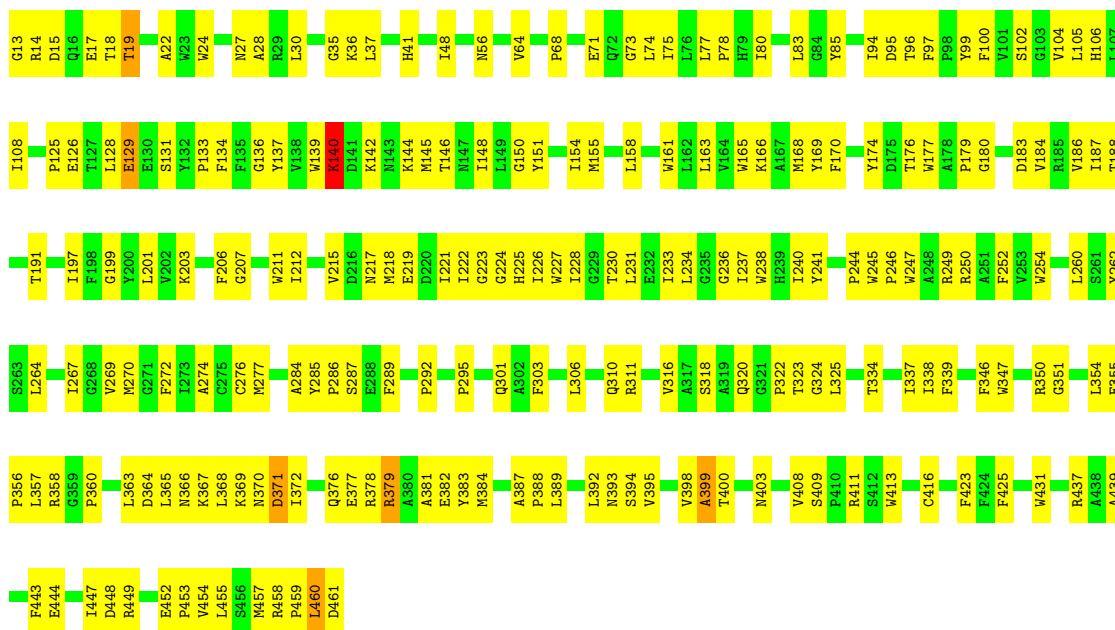




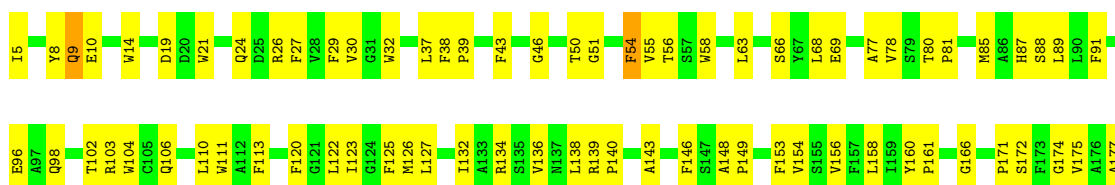
• Molecule 3: Photosystem II reaction center protein Psb30

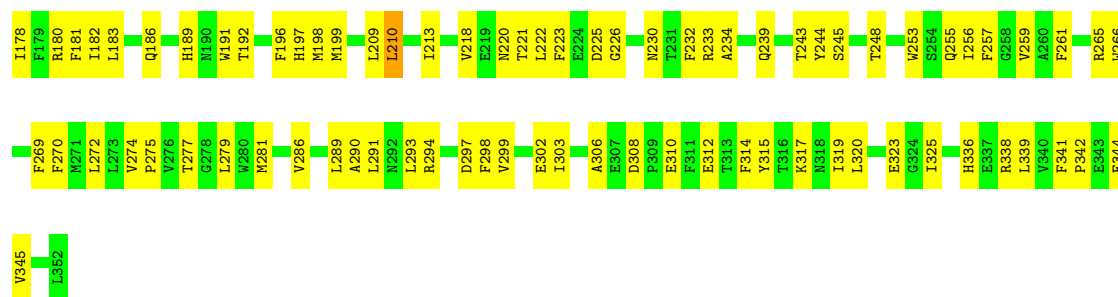


• Molecule 4: Photosystem II CP43 reaction center protein



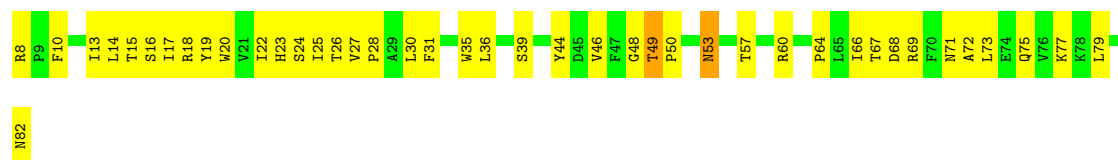
• Molecule 5: Photosystem II D2 protein





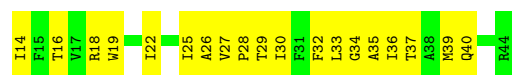
- Molecule 6: Cytochrome b559 subunit alpha

Chain E: 44% 53%



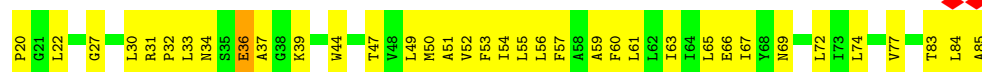
- Molecule 7: Cytochrome b559 subunit beta

Chain F: 39% 61%



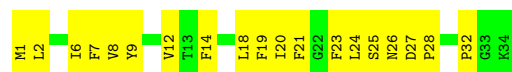
- Molecule 8: Photosystem II reaction center protein H

Chain H: 45% 53%



- Molecule 9: Photosystem II reaction center protein I

Chain I: 44% 56%

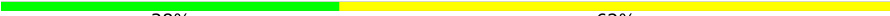


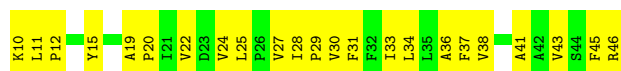
- Molecule 10: Photosystem II reaction center protein J

Chain J: 53% 44%



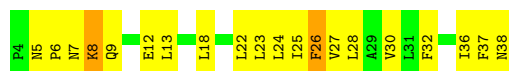
- Molecule 11: Photosystem II reaction center protein K

Chain K:  38% 62%



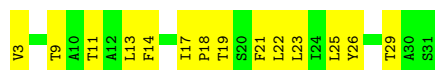
- Molecule 12: Photosystem II reaction center protein L

Chain L:  43% 51% 6%



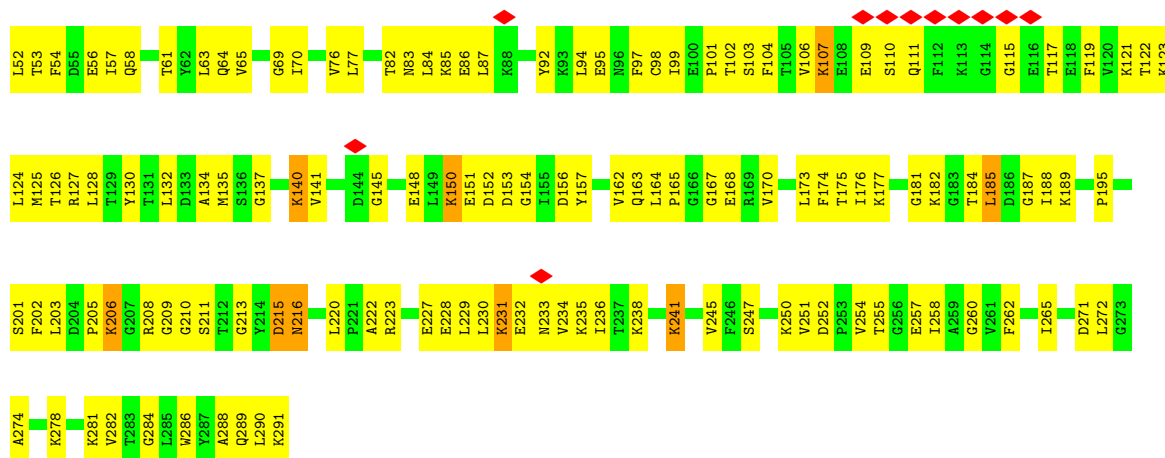
- Molecule 13: Photosystem II reaction center protein M

Chain M:  52% 48%



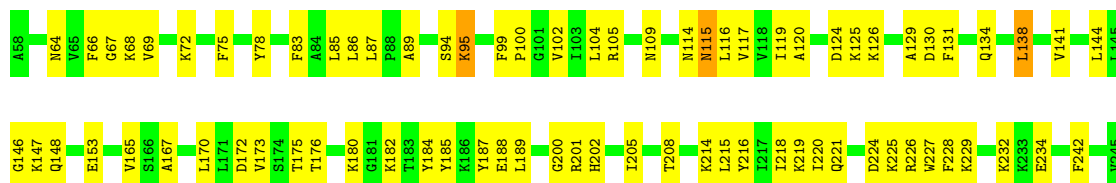
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O:  5% 45% 52%

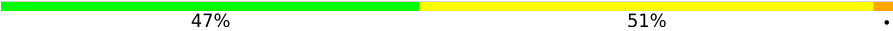


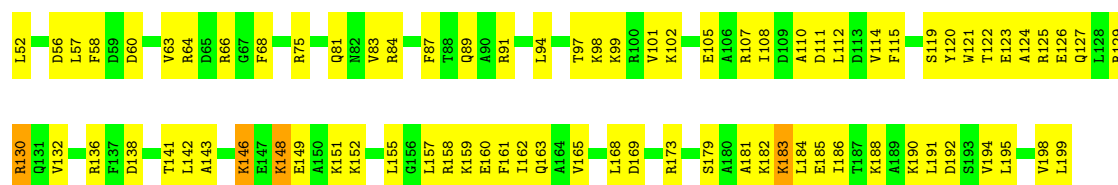
- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

Chain P:  60% 39%



- Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic

Chain Q:  47% 51%



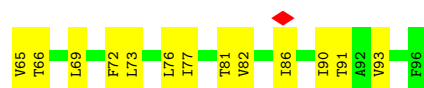
- Molecule 17: Photosystem II reaction center protein T

Chain T:  7% 67% 33%



- Molecule 18: 4.1 kDa photosystem II subunit

Chain X:  59% 41%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  49% 51%



- Molecule 20: Photosystem II reaction center protein U

Chain U:  35% 61%



- Molecule 21: Photosystem II reaction center W protein, chloroplastic

Chain W:  50% 39% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	361852	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.9	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.041	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	210.0, 210.0, 210.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.94	0/2570	1.14	0/3505
2	B	0.93	0/3883	1.13	3/5286 (0.1%)
3	V	0.98	0/224	1.29	0/307
4	C	0.92	0/3619	1.14	0/4931
5	D	0.92	0/2866	1.12	0/3909
6	E	0.92	0/628	1.16	0/857
7	F	0.91	0/258	1.16	0/349
8	H	0.93	0/512	1.18	0/701
9	I	0.89	0/283	1.13	0/383
10	J	0.93	0/268	1.19	0/366
11	K	0.92	0/309	1.08	0/425
12	L	0.90	0/298	1.09	0/405
13	M	0.93	0/227	1.18	0/311
14	O	0.98	0/1839	1.09	0/2482
15	P	0.97	0/1473	1.09	2/1987 (0.1%)
16	Q	0.90	0/1204	1.19	0/1616
17	T	0.90	0/254	1.15	0/343
18	X	0.95	0/222	1.31	0/301
19	Z	0.93	0/469	1.20	0/644
20	U	0.96	0/176	1.20	0/235
21	W	0.88	0/354	1.13	0/481
All	All	0.93	0/21936	1.14	5/29824 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	200	GLY	CA-C-O	-6.30	118.12	122.22
15	P	146	GLY	CA-C-O	-6.02	118.12	122.45
2	B	342	GLY	CA-C-O	-5.86	118.23	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	328	GLY	CA-C-O	-5.57	118.30	122.37
2	B	335	GLY	CA-C-O	-5.40	118.25	122.52

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	2491	0	2415	210	0
2	B	3755	0	3642	271	0
3	V	224	0	256	20	0
4	C	3498	0	3372	239	0
5	D	2771	0	2655	172	0
6	E	610	0	599	42	0
7	F	251	0	263	17	0
8	H	501	0	531	40	0
9	I	275	0	287	21	0
10	J	262	0	276	20	0
11	K	297	0	308	42	0
12	L	290	0	298	24	0
13	M	223	0	245	18	0
14	O	1808	0	1813	119	0
15	P	1444	0	1414	70	0
16	Q	1192	0	1216	88	0
17	T	247	0	260	12	0
18	X	220	0	244	13	0
19	Z	458	0	490	25	0
20	U	176	0	184	17	0
21	W	344	0	334	29	0
22	A	10	0	0	0	0
23	A	1	0	0	0	0
24	A	2	0	0	0	0
25	A	174	0	167	42	0
25	B	927	0	962	187	0
25	C	789	0	804	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	D	186	0	193	29	0
25	H	61	0	60	12	0
26	A	64	0	74	6	0
26	D	64	0	74	12	0
27	A	40	0	56	19	0
27	B	80	0	112	20	0
27	C	120	0	168	34	0
27	D	40	0	56	9	0
27	K	40	0	56	12	0
28	A	51	0	68	15	0
29	B	91	0	122	19	0
29	C	51	0	72	12	0
29	D	36	0	42	6	0
29	W	48	0	66	23	0
30	B	93	0	135	15	0
30	D	88	0	122	15	0
31	C	160	0	194	35	0
32	C	35	0	46	5	0
33	D	4	0	0	1	0
34	D	55	0	80	6	0
35	F	43	0	30	6	0
36	A	2	0	0	0	0
36	B	2	0	0	1	0
36	C	2	0	0	0	0
36	D	1	0	0	0	0
All	All	24697	0	24861	1619	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 33.

The worst 5 of 1619 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)
25:B:503:CLA:HAB	25:B:505:CLA:H172	1.36	1.07
1:A:333:GLU:HB3	1:A:336:ALA:HB3	1.39	1.00
2:B:157:HIS:CA	2:B:163:GLY:HA3	1.93	0.99
12:L:13:LEU:H	13:M:29:THR:HG21	1.25	0.98
2:B:157:HIS:HA	2:B:163:GLY:HA3	0.98	0.97

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	314/334 (94%)	295 (94%)	18 (6%)	1 (0%)	36	64
2	B	478/480 (100%)	458 (96%)	20 (4%)	0	100	100
3	V	30/32 (94%)	30 (100%)	0	0	100	100
4	C	447/449 (100%)	427 (96%)	17 (4%)	3 (1%)	18	46
5	D	346/348 (99%)	330 (95%)	14 (4%)	2 (1%)	21	50
6	E	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
8	H	64/66 (97%)	62 (97%)	2 (3%)	0	100	100
9	I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
10	J	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	L	33/35 (94%)	33 (100%)	0	0	100	100
13	M	27/29 (93%)	27 (100%)	0	0	100	100
14	O	238/240 (99%)	219 (92%)	18 (8%)	1 (0%)	30	58
15	P	186/188 (99%)	181 (97%)	5 (3%)	0	100	100
16	Q	146/148 (99%)	139 (95%)	7 (5%)	0	100	100
17	T	28/30 (93%)	28 (100%)	0	0	100	100
18	X	30/32 (94%)	30 (100%)	0	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100
20	U	21/23 (91%)	20 (95%)	1 (5%)	0	100	100
21	W	42/44 (96%)	42 (100%)	0	0	100	100
All	All	2692/2752 (98%)	2577 (96%)	108 (4%)	7 (0%)	37	64

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	8	TYR
4	C	140	LYS
1	A	141	PRO
4	C	371	ASP
4	C	399	ALA

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	259/272 (95%)	250 (96%)	9 (4%)	32	64
2	B	382/382 (100%)	363 (95%)	19 (5%)	22	52
3	V	26/26 (100%)	25 (96%)	1 (4%)	29	62
4	C	352/352 (100%)	347 (99%)	5 (1%)	59	83
5	D	278/278 (100%)	276 (99%)	2 (1%)	76	91
6	E	66/66 (100%)	63 (96%)	3 (4%)	24	56
7	F	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	55 (98%)	1 (2%)	51	79
9	I	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	26 (96%)	1 (4%)	30	63
11	K	31/31 (100%)	31 (100%)	0	100	100
12	L	33/33 (100%)	31 (94%)	2 (6%)	17	44
13	M	25/25 (100%)	25 (100%)	0	100	100
14	O	195/195 (100%)	181 (93%)	14 (7%)	13	37
15	P	150/150 (100%)	147 (98%)	3 (2%)	48	77
16	Q	126/126 (100%)	121 (96%)	5 (4%)	28	61
17	T	27/27 (100%)	27 (100%)	0	100	100
18	X	23/23 (100%)	22 (96%)	1 (4%)	26	58
19	Z	51/51 (100%)	49 (96%)	2 (4%)	28	61
20	U	20/20 (100%)	18 (90%)	2 (10%)	7	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	W	35/35 (100%)	30 (86%)	5 (14%)	3 10
All	All	2218/2231 (99%)	2143 (97%)	75 (3%)	33 65

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	P	95	LYS
21	W	77	ASN
15	P	138	LEU
18	X	65	VAL
2	B	321	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	236	ASN
14	O	178	GLN
5	D	239	GLN
12	L	5	ASN
14	O	266	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 3 are monoatomic - leaving 63 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	$\# Z > 2$
33	BCT	D	403	23	2,3,3	0.98	0	2,3,3	1.67	1 (50%)
22	OEX	A	401	1,4	0,14,14	-	-	-		
25	CLA	B	502	2	69,73,73	1.35	6 (8%)	83,113,113	1.97	21 (25%)
25	CLA	C	504	36	60,64,73	1.45	6 (10%)	72,102,113	2.08	18 (25%)
25	CLA	C	511	4	69,73,73	1.35	7 (10%)	83,113,113	1.99	19 (22%)
25	CLA	B	510	2	69,73,73	1.35	6 (8%)	83,113,113	1.96	19 (22%)
25	CLA	C	506	4	54,58,73	1.53	5 (9%)	65,95,113	2.04	17 (26%)
27	BCR	C	516	-	41,41,41	4.83	26 (63%)	56,56,56	2.50	22 (39%)
25	CLA	B	513	2	60,64,73	1.44	6 (10%)	72,102,113	2.06	20 (27%)
25	CLA	C	508	4	69,73,73	1.35	6 (8%)	83,113,113	1.96	21 (25%)
27	BCR	B	517	-	41,41,41	4.79	27 (65%)	56,56,56	2.26	18 (32%)
26	PHO	D	402	-	58,69,69	0.77	2 (3%)	56,99,99	0.98	3 (5%)
34	PL9	D	407	-	55,55,55	0.70	1 (1%)	68,69,69	0.59	1 (1%)
25	CLA	C	501	4	69,73,73	1.35	6 (8%)	83,113,113	1.91	19 (22%)
29	LMG	B	518	-	43,43,55	0.88	2 (4%)	51,51,63	1.10	3 (5%)
25	CLA	C	509	4	69,73,73	1.36	6 (8%)	83,113,113	1.90	20 (24%)
27	BCR	B	516	-	41,41,41	4.80	27 (65%)	56,56,56	2.28	21 (37%)
25	CLA	B	507	36	69,73,73	1.36	6 (8%)	83,113,113	1.96	18 (21%)
25	CLA	C	510	4	69,73,73	1.35	6 (8%)	83,113,113	1.99	19 (22%)
25	CLA	C	502	4	69,73,73	1.35	6 (8%)	83,113,113	1.95	21 (25%)
29	LMG	B	520	-	48,48,55	1.00	5 (10%)	56,56,63	1.11	2 (3%)
25	CLA	B	509	36	69,73,73	1.36	6 (8%)	83,113,113	1.91	18 (21%)
25	CLA	C	507	36	69,73,73	1.36	6 (8%)	83,113,113	1.95	19 (22%)
30	LHG	D	409	-	38,38,48	0.42	0	41,44,54	1.16	3 (7%)
25	CLA	D	405	5	60,64,73	1.44	6 (10%)	72,102,113	2.08	18 (25%)
25	CLA	B	515	2	54,58,73	1.53	6 (11%)	65,95,113	2.15	19 (29%)
25	CLA	B	511	2	69,73,73	1.35	6 (8%)	83,113,113	1.94	17 (20%)
35	HEM	F	101	6,7	50,50,50	1.57	7 (14%)	66,82,82	1.70	11 (16%)
29	LMG	C	520	-	51,51,55	1.06	5 (9%)	59,59,63	1.08	2 (3%)
25	CLA	A	408	1	64,68,73	1.40	7 (10%)	77,107,113	2.03	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DGD	C	519	-	55,55,67	0.94	3 (5%)	69,69,81	1.00	3 (4%)
25	CLA	C	513	4	50,54,73	1.62	7 (14%)	60,90,113	2.13	14 (23%)
28	SQD	A	410	-	50,51,54	0.81	0	59,62,65	0.93	3 (5%)
32	LMU	C	521	-	36,36,36	0.35	0	47,47,47	0.81	1 (2%)
31	DGD	C	518	-	55,55,67	0.99	4 (7%)	69,69,81	0.95	2 (2%)
25	CLA	A	405	1	69,73,73	1.34	6 (8%)	83,113,113	1.94	20 (24%)
25	CLA	B	508	2	69,73,73	1.35	7 (10%)	83,113,113	1.90	17 (20%)
25	CLA	H	101	-	65,69,73	1.39	7 (10%)	78,108,113	1.97	19 (24%)
25	CLA	B	503	2	69,73,73	1.34	7 (10%)	83,113,113	1.96	19 (22%)
25	CLA	B	505	2	69,73,73	1.35	7 (10%)	83,113,113	1.94	18 (21%)
26	PHO	A	407	-	58,69,69	0.77	2 (3%)	56,99,99	0.95	3 (5%)
29	LMG	W	201	-	48,48,55	0.99	5 (10%)	56,56,63	1.15	4 (7%)
27	BCR	K	101	-	41,41,41	4.79	27 (65%)	56,56,56	2.32	17 (30%)
25	CLA	B	512	2	69,73,73	1.36	7 (10%)	83,113,113	1.99	19 (22%)
25	CLA	B	501	-	69,73,73	1.35	7 (10%)	83,113,113	1.94	18 (21%)
30	LHG	D	408	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
25	CLA	C	503	4	69,73,73	1.35	6 (8%)	83,113,113	1.93	19 (22%)
30	LHG	B	519	-	43,43,48	0.40	0	46,49,54	1.11	3 (6%)
25	CLA	C	512	4	56,60,73	1.50	6 (10%)	67,97,113	2.18	19 (28%)
25	CLA	A	406	36	53,57,73	1.53	6 (11%)	62,93,113	2.19	17 (27%)
25	CLA	B	504	2	69,73,73	1.35	7 (10%)	83,113,113	1.94	19 (22%)
27	BCR	C	514	-	41,41,41	4.81	27 (65%)	56,56,56	2.27	22 (39%)
30	LHG	B	521	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
25	CLA	B	514	2	55,59,73	1.52	6 (10%)	66,96,113	2.14	18 (27%)
25	CLA	C	505	4	69,73,73	1.35	7 (10%)	83,113,113	1.94	18 (21%)
25	CLA	D	404	5	69,73,73	1.33	6 (8%)	83,113,113	1.95	19 (22%)
27	BCR	A	409	-	41,41,41	4.77	27 (65%)	56,56,56	2.36	21 (37%)
31	DGD	C	517	-	53,53,67	1.02	4 (7%)	67,67,81	1.00	3 (4%)
25	CLA	D	401	36	69,73,73	1.35	7 (10%)	83,113,113	1.94	19 (22%)
29	LMG	D	410	-	36,36,55	0.58	1 (2%)	44,44,63	1.04	3 (6%)
27	BCR	D	406	-	41,41,41	4.78	27 (65%)	56,56,56	2.46	21 (37%)
27	BCR	C	515	-	41,41,41	4.80	27 (65%)	56,56,56	2.46	20 (35%)
25	CLA	B	506	2	59,63,73	1.44	6 (10%)	71,101,113	2.12	19 (26%)

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
25	CLA	B	502	2	-	17/39/115/115	-
25	CLA	C	504	36	-	19/29/105/115	-
25	CLA	C	511	4	-	17/39/115/115	-
25	CLA	B	510	2	-	17/39/115/115	-
25	CLA	C	506	4	-	12/21/97/115	-
27	BCR	C	516	-	-	9/29/63/63	0/2/2/2
25	CLA	B	513	2	-	12/29/105/115	-
25	CLA	C	508	4	-	16/39/115/115	-
27	BCR	B	517	-	-	13/29/63/63	0/2/2/2
26	PHO	D	402	-	-	6/37/103/103	0/5/6/6
34	PL9	D	407	-	-	7/53/73/73	0/1/1/1
25	CLA	C	501	4	-	20/39/115/115	-
29	LMG	B	518	-	-	12/38/58/70	0/1/1/1
25	CLA	C	509	4	-	15/39/115/115	-
27	BCR	B	516	-	-	15/29/63/63	0/2/2/2
25	CLA	B	507	36	-	22/39/115/115	-
25	CLA	C	510	4	-	21/39/115/115	-
25	CLA	C	502	4	-	17/39/115/115	-
29	LMG	B	520	-	-	7/43/63/70	0/1/1/1
25	CLA	B	509	36	-	11/39/115/115	-
25	CLA	C	507	36	-	19/39/115/115	-
30	LHG	D	409	-	-	29/43/43/53	-
25	CLA	D	405	5	-	15/29/105/115	-
25	CLA	B	515	2	-	7/21/97/115	-
25	CLA	B	511	2	-	16/39/115/115	-
35	HEM	F	101	6,7	-	5/14/54/54	-
29	LMG	C	520	-	-	11/46/66/70	0/1/1/1
25	CLA	A	408	1	-	15/33/109/115	-
31	DGD	C	519	-	-	7/43/83/95	0/2/2/2
25	CLA	C	513	4	-	9/17/93/115	-
28	SQD	A	410	-	-	7/46/66/69	0/1/1/1
32	LMU	C	521	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	C	518	-	-	12/43/83/95	0/2/2/2
25	CLA	A	405	1	-	13/39/115/115	-
25	CLA	B	508	2	-	14/39/115/115	-
25	CLA	H	101	-	-	14/35/111/115	-
25	CLA	B	503	2	-	16/39/115/115	-
25	CLA	B	505	2	-	15/39/115/115	-
26	PHO	A	407	-	-	3/37/103/103	0/5/6/6
29	LMG	W	201	-	-	7/43/63/70	0/1/1/1
27	BCR	K	101	-	-	13/29/63/63	0/2/2/2
25	CLA	B	512	2	-	12/39/115/115	-
25	CLA	B	501	-	-	18/39/115/115	-
30	LHG	D	408	-	-	31/53/53/53	-
25	CLA	C	503	4	-	15/39/115/115	-
30	LHG	B	519	-	-	28/48/48/53	-
25	CLA	C	512	4	-	11/24/100/115	-
25	CLA	A	406	36	-	8/20/96/115	-
25	CLA	B	504	2	-	17/39/115/115	-
27	BCR	C	514	-	-	13/29/63/63	0/2/2/2
30	LHG	B	521	-	-	33/53/53/53	-
25	CLA	B	514	2	-	8/23/99/115	-
25	CLA	C	505	4	-	17/39/115/115	-
25	CLA	D	404	5	-	11/39/115/115	-
27	BCR	A	409	-	-	14/29/63/63	0/2/2/2
31	DGD	C	517	-	-	7/41/81/95	0/2/2/2
25	CLA	D	401	36	-	18/39/115/115	-
29	LMG	D	410	-	-	7/31/51/70	0/1/1/1
27	BCR	D	406	-	-	9/29/63/63	0/2/2/2
27	BCR	C	515	-	-	13/29/63/63	0/2/2/2
25	CLA	B	506	2	-	13/27/103/115	-

The worst 5 of 477 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	516	BCR	C26-C25	15.69	1.61	1.34
27	C	514	BCR	C26-C25	15.55	1.61	1.34
27	B	517	BCR	C26-C25	15.54	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	515	BCR	C26-C25	15.46	1.61	1.34
27	K	101	BCR	C26-C25	15.29	1.60	1.34

The worst 5 of 870 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	513	CLA	C4A-NA-C1A	9.71	111.07	106.71
25	C	504	CLA	C4A-NA-C1A	9.19	110.84	106.71
25	B	506	CLA	C4A-NA-C1A	9.15	110.82	106.71
25	A	408	CLA	C4A-NA-C1A	9.12	110.80	106.71
25	C	510	CLA	C4A-NA-C1A	9.09	110.79	106.71

There are no chirality outliers.

5 of 845 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	406	CLA	CBA-CGA-O2A-C1
25	A	406	CLA	O1A-CGA-O2A-C1
25	A	406	CLA	CHA-CBD-CGD-O2D
25	A	408	CLA	C3A-C2A-CAA-CBA
25	A	408	CLA	C2-C1-O2A-CGA

There are no ring outliers.

62 monomers are involved in 576 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	D	403	BCT	1	0
25	B	502	CLA	6	0
25	C	504	CLA	13	0
25	C	511	CLA	9	0
25	B	510	CLA	20	0
25	C	506	CLA	15	0
27	C	516	BCR	8	0
25	B	513	CLA	10	0
25	C	508	CLA	11	0
27	B	517	BCR	10	0
26	D	402	PHO	12	0
34	D	407	PL9	6	0
25	C	501	CLA	20	0
29	B	518	LMG	16	0
25	C	509	CLA	9	0

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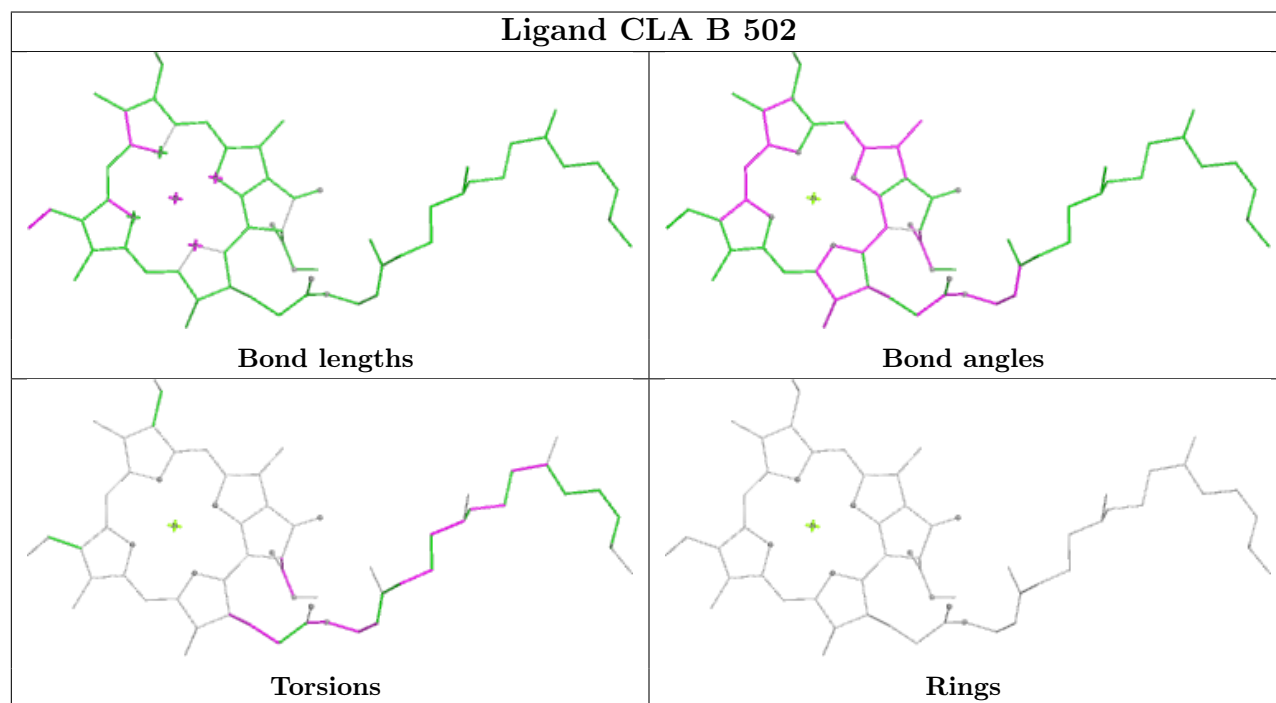
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	516	BCR	11	0
25	B	507	CLA	18	0
25	C	510	CLA	17	0
25	C	502	CLA	7	0
29	B	520	LMG	3	0
25	B	509	CLA	23	0
25	C	507	CLA	27	0
30	D	409	LHG	6	0
25	D	405	CLA	6	0
25	B	515	CLA	4	0
25	B	511	CLA	15	0
35	F	101	HEM	6	0
29	C	520	LMG	12	0
25	A	408	CLA	19	0
31	C	519	DGD	9	0
25	C	513	CLA	5	0
28	A	410	SQD	15	0
32	C	521	LMU	5	0
31	C	518	DGD	15	0
25	A	405	CLA	14	0
25	B	508	CLA	20	0
25	H	101	CLA	12	0
25	B	503	CLA	23	0
25	B	505	CLA	17	0
26	A	407	PHO	6	0
29	W	201	LMG	23	0
27	K	101	BCR	12	0
25	B	512	CLA	20	0
25	B	501	CLA	12	0
30	D	408	LHG	9	0
25	C	503	CLA	6	0
30	B	519	LHG	8	0
25	C	512	CLA	7	0
25	A	406	CLA	9	0
25	B	504	CLA	14	0
27	C	514	BCR	10	0
30	B	521	LHG	7	0
25	B	514	CLA	14	0
25	C	505	CLA	11	0
25	D	404	CLA	10	0
27	A	409	BCR	19	0
31	C	517	DGD	11	0

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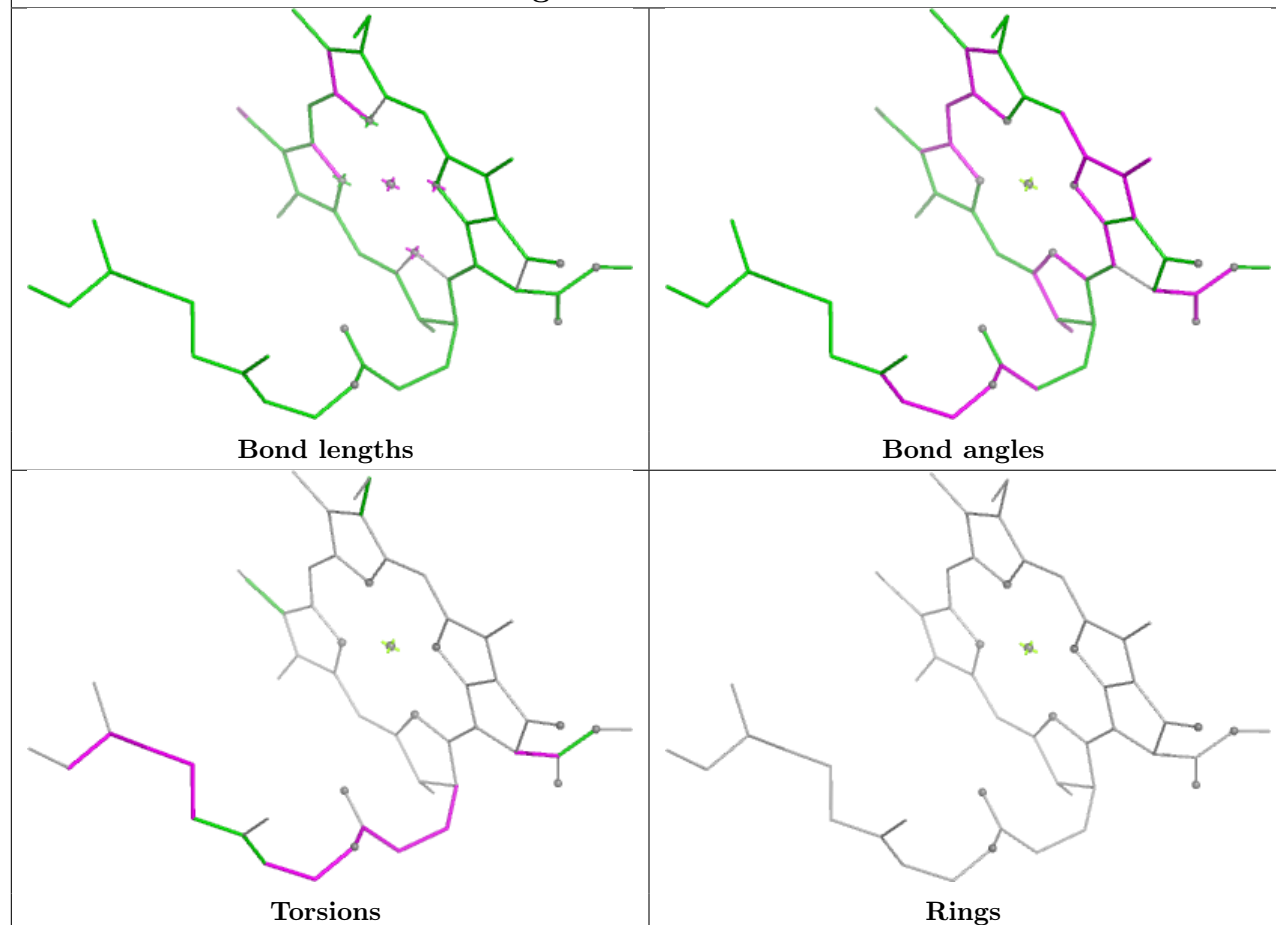
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	D	401	CLA	13	0
29	D	410	LMG	6	0
27	D	406	BCR	9	0
27	C	515	BCR	16	0
25	B	506	CLA	12	0

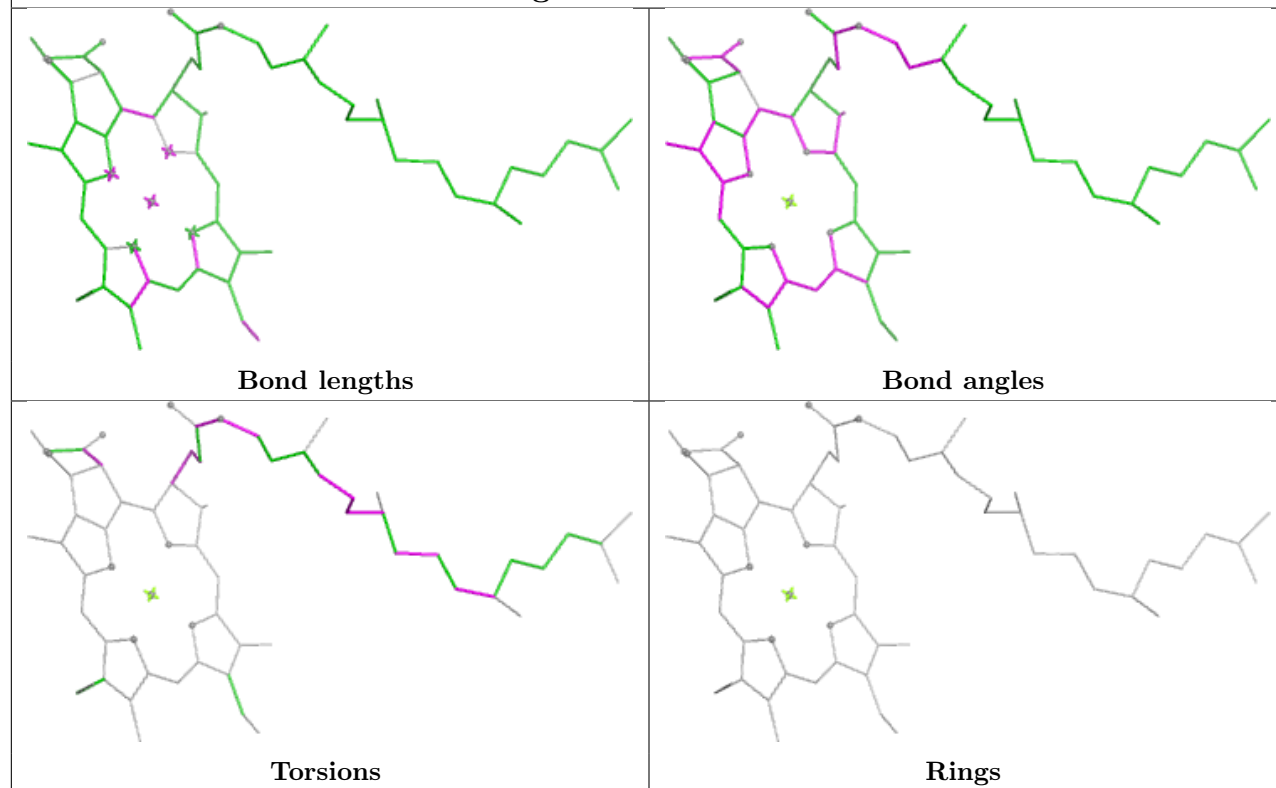
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

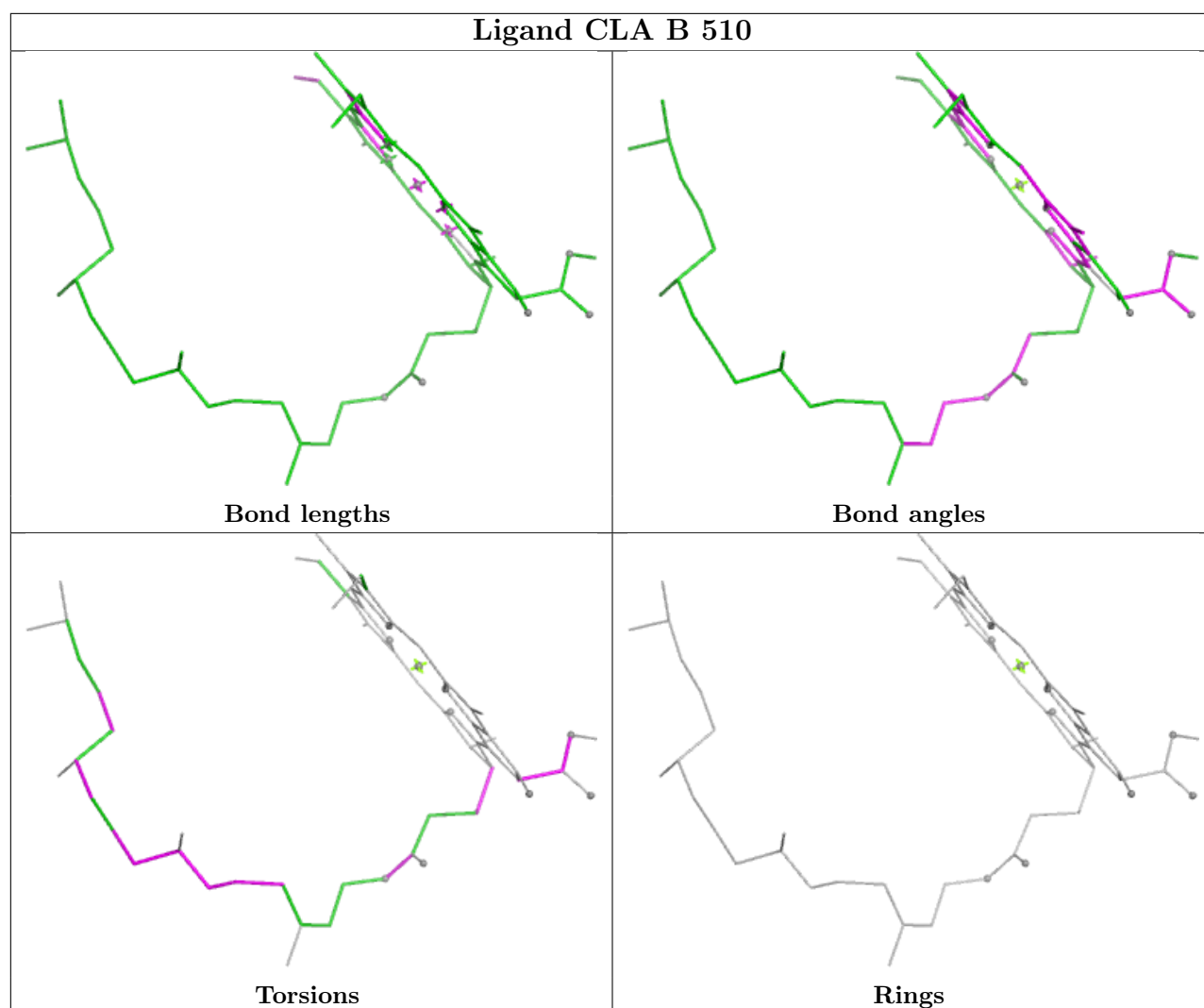


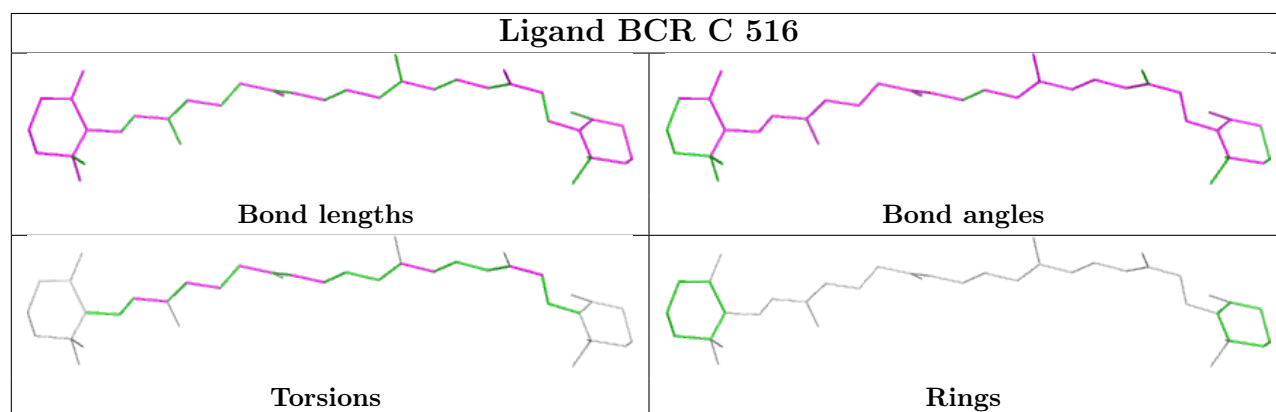
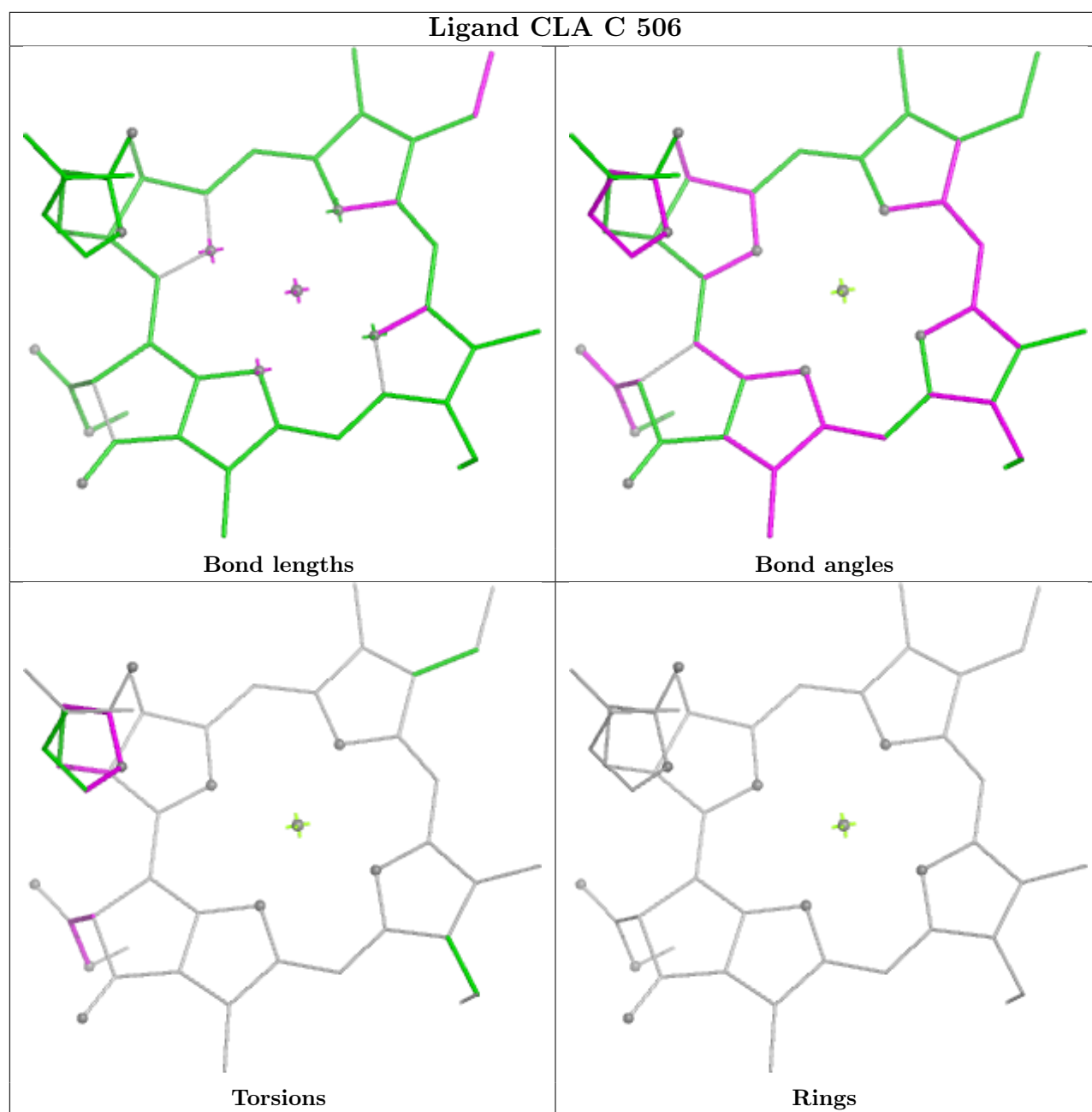
Ligand CLA C 504



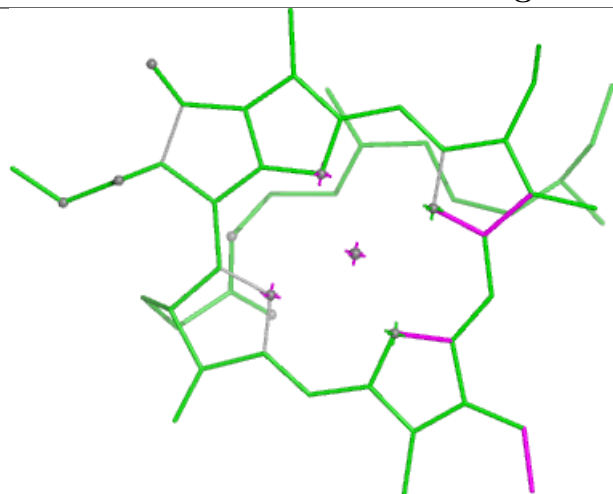
Ligand CLA C 511



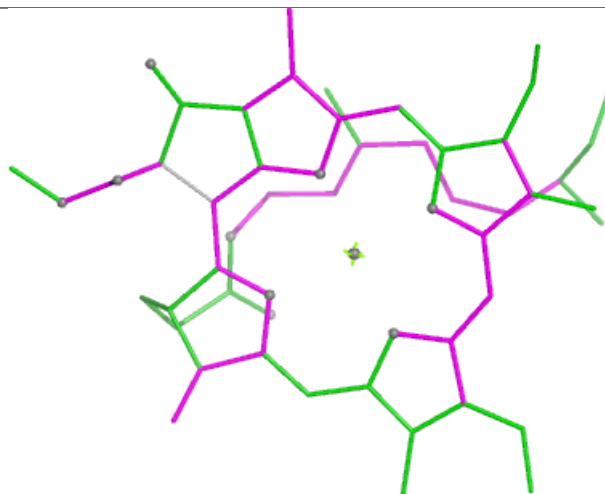




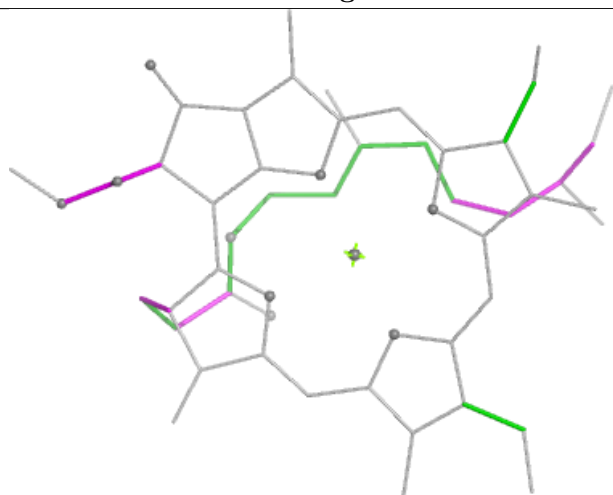
Ligand CLA B 513



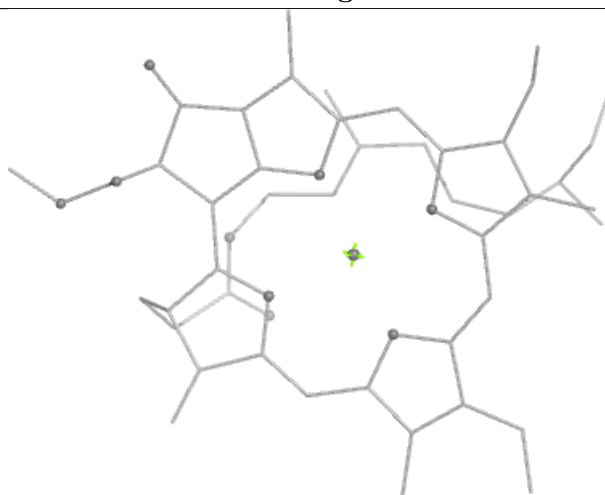
Bond lengths



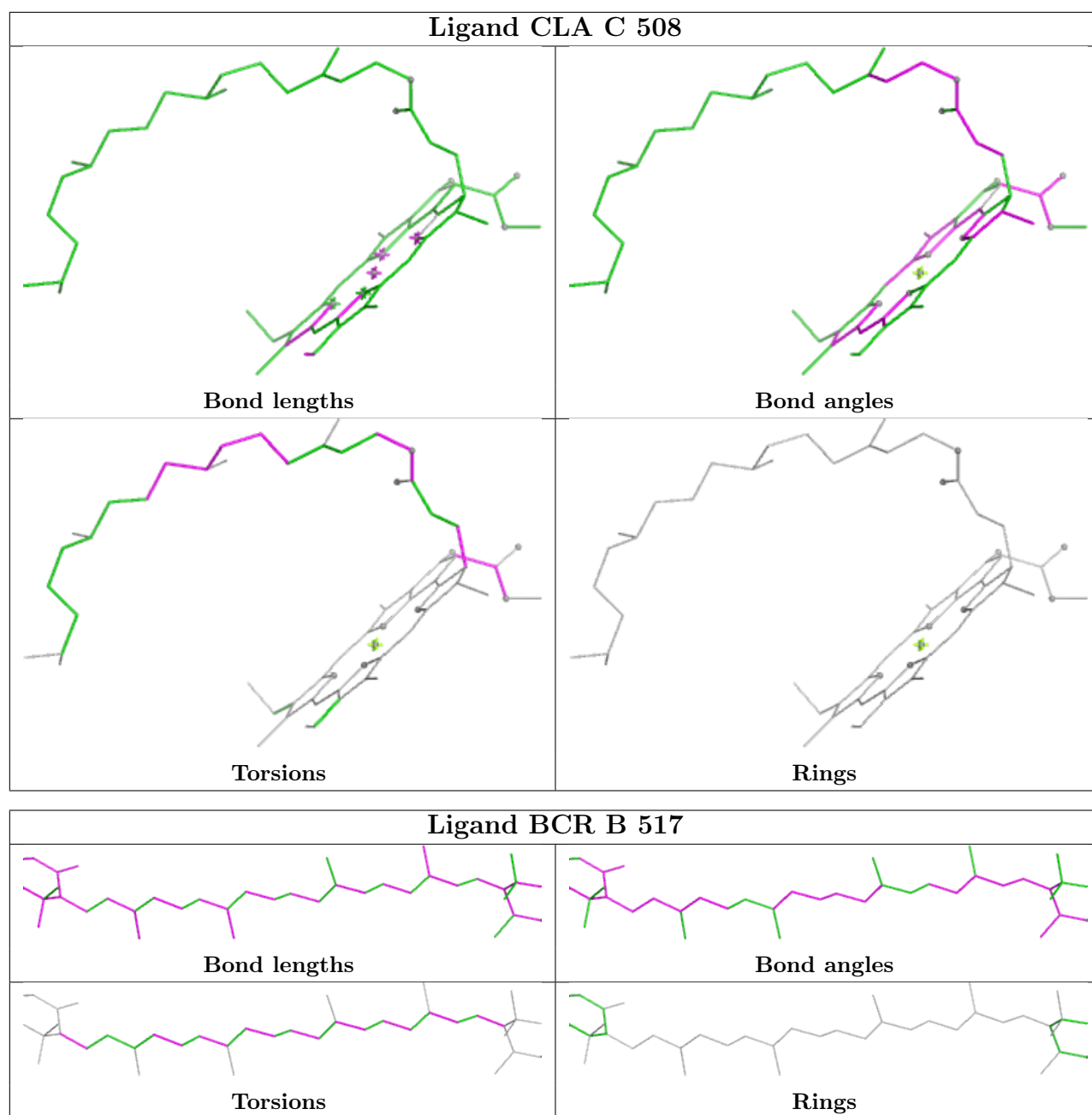
Bond angles

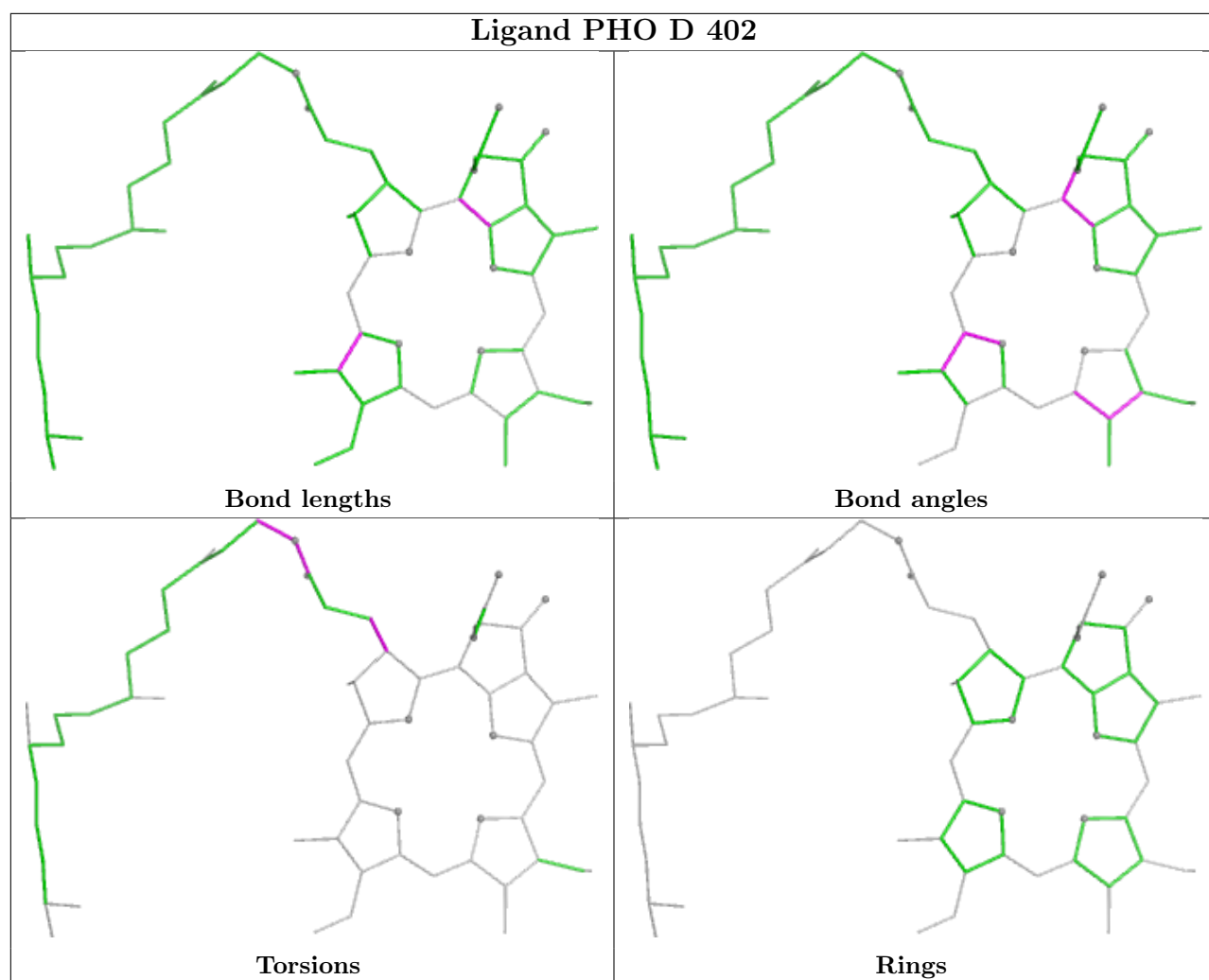


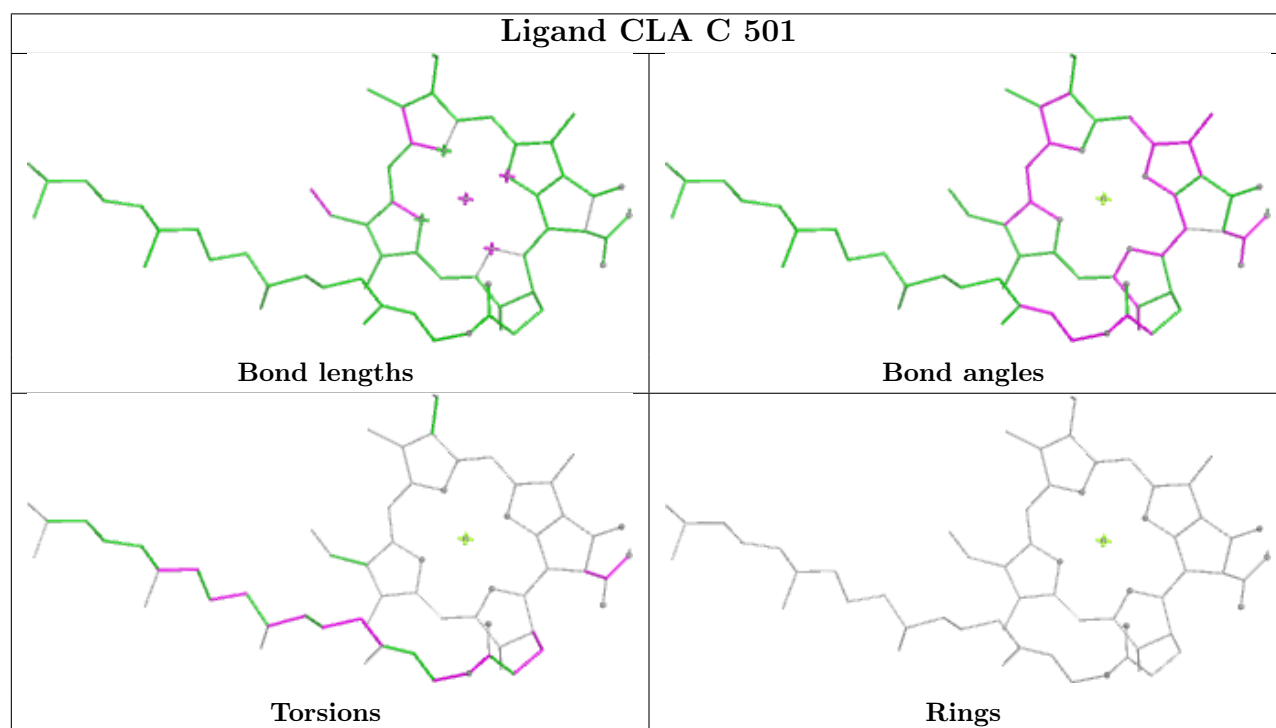
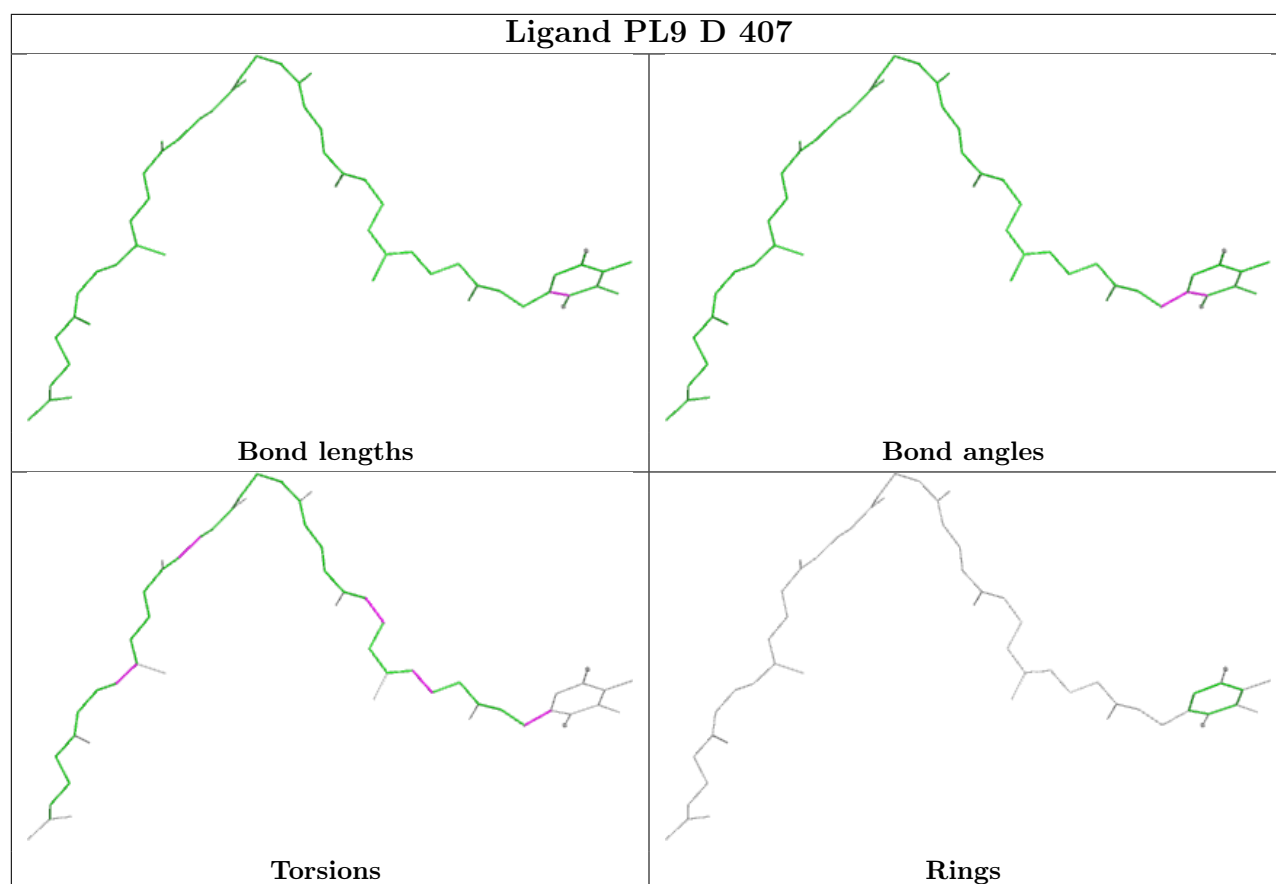
Torsions

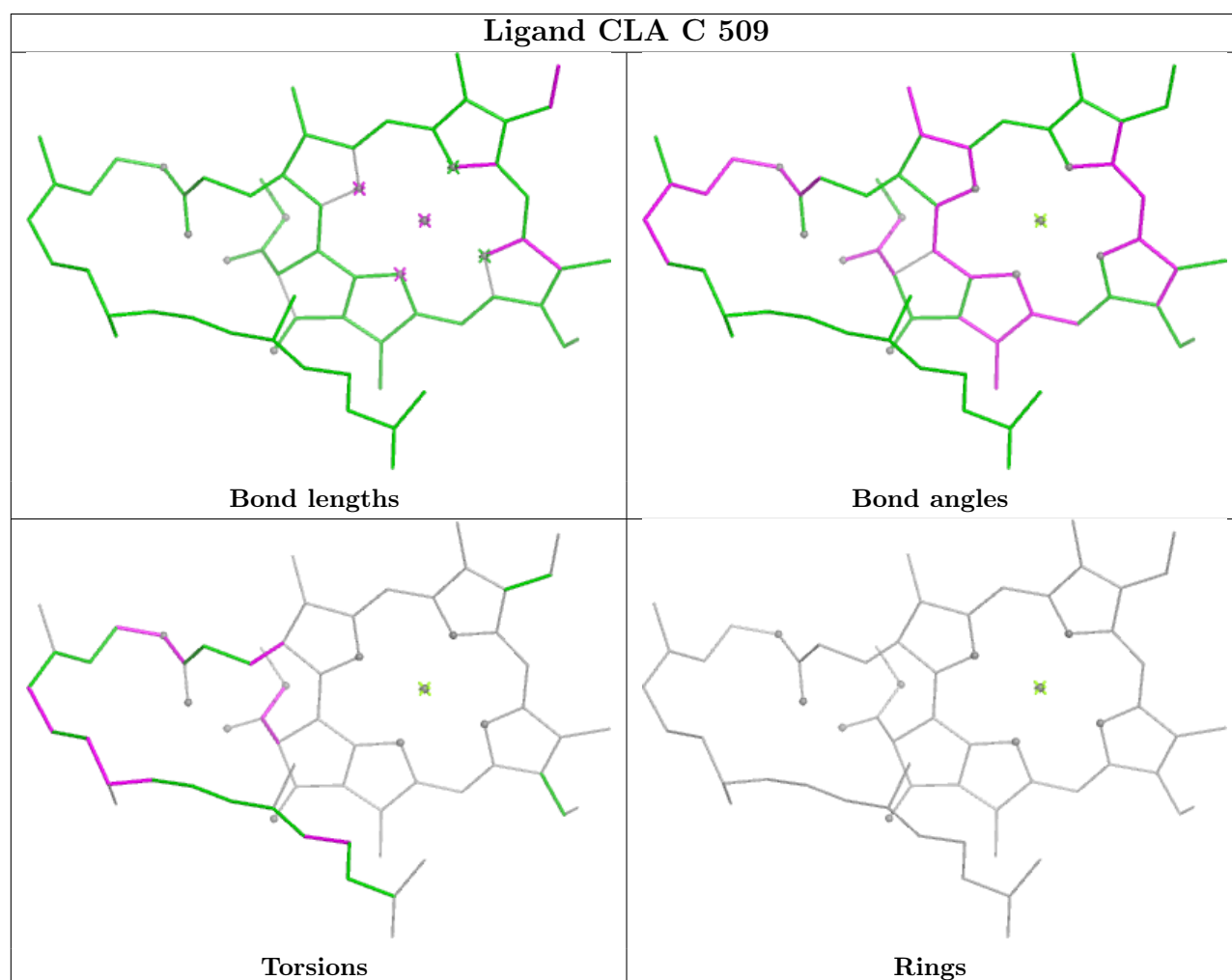
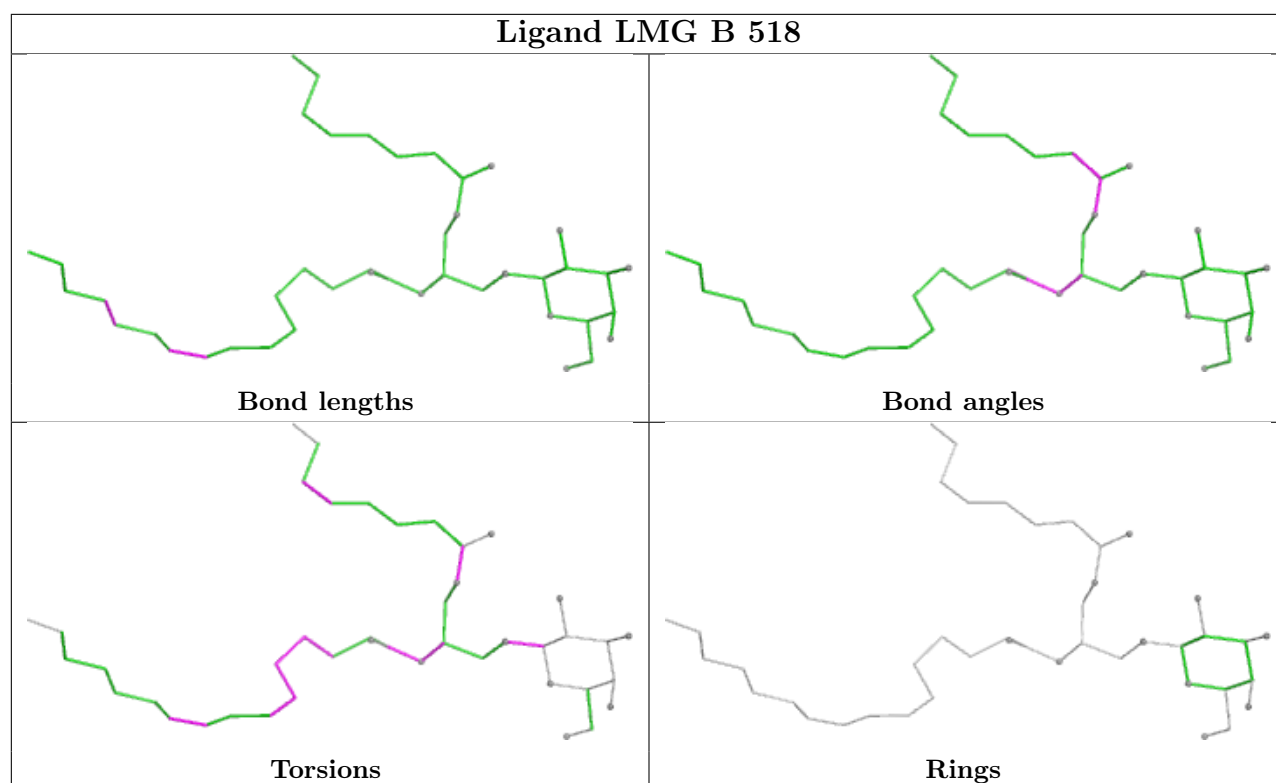


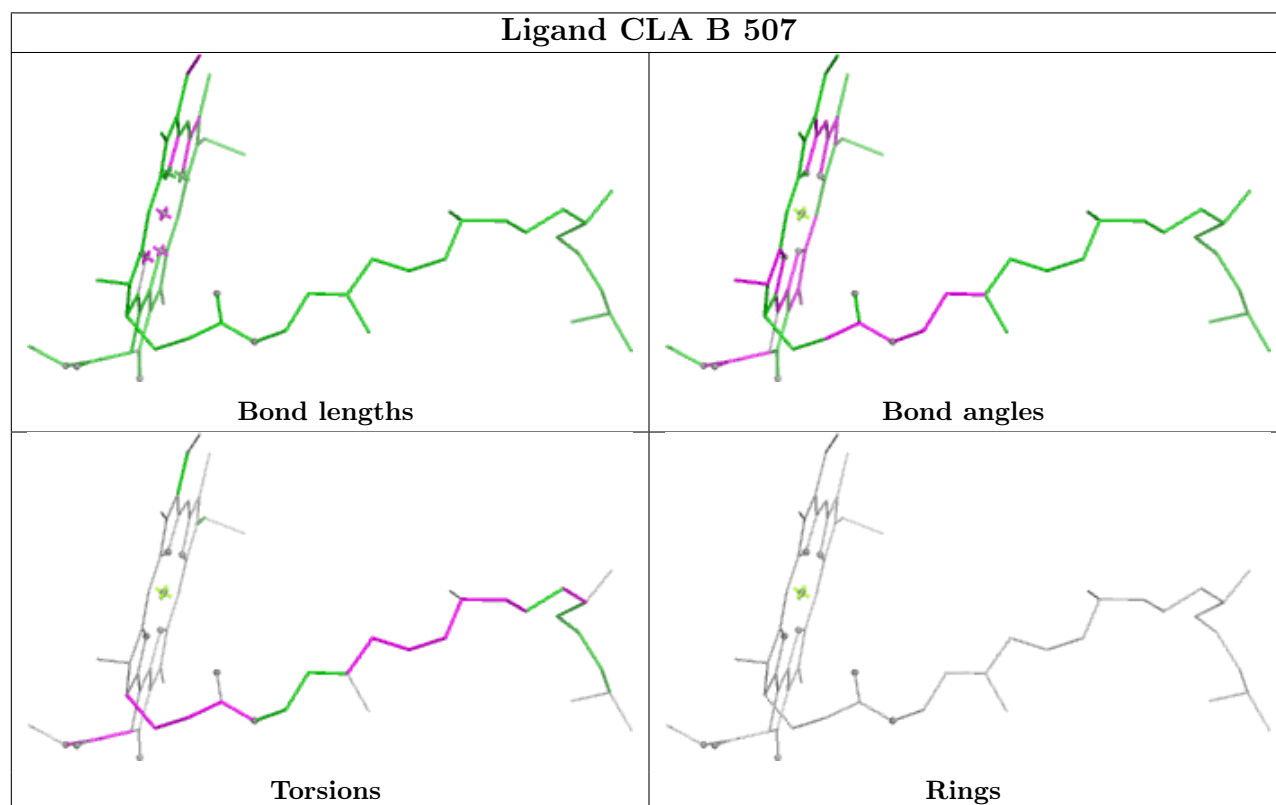
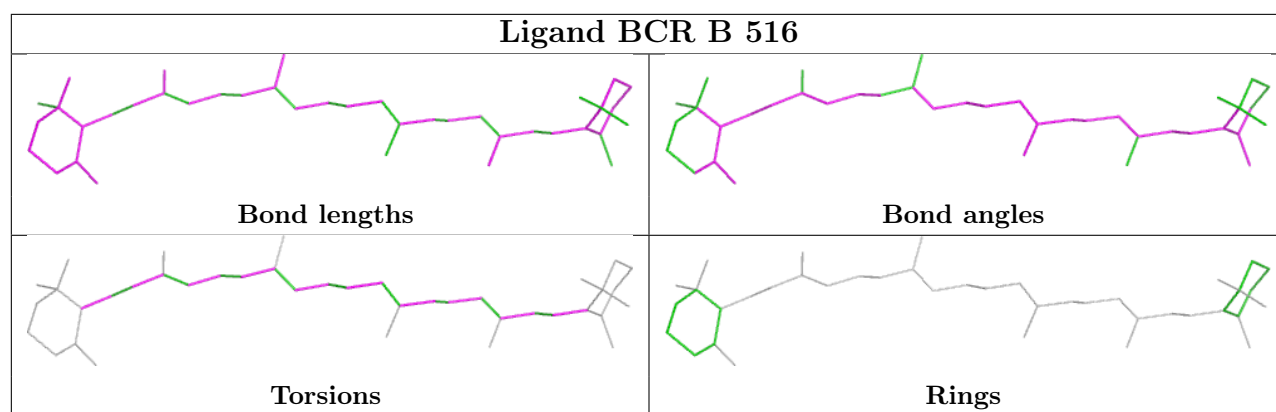
Rings



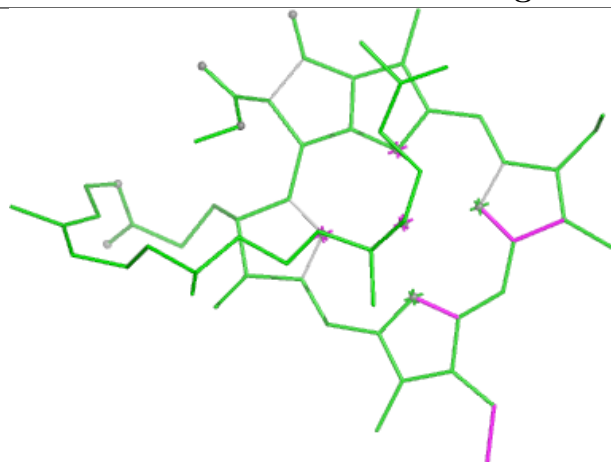




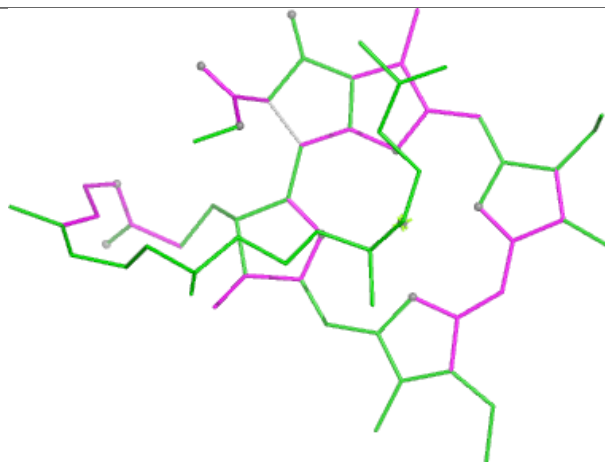




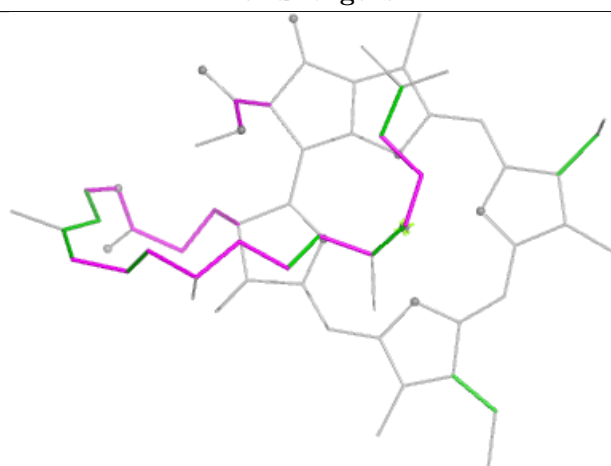
Ligand CLA C 510



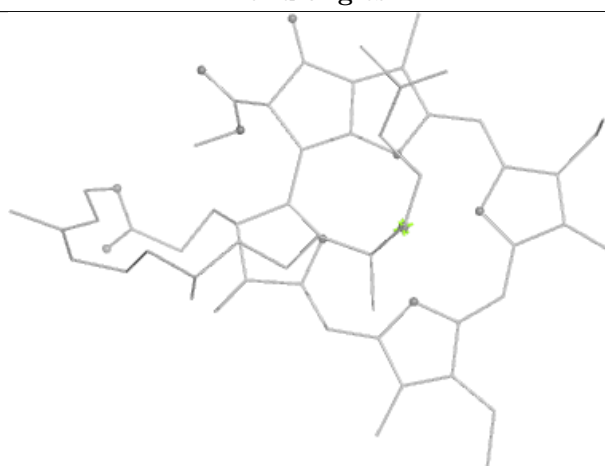
Bond lengths



Bond angles

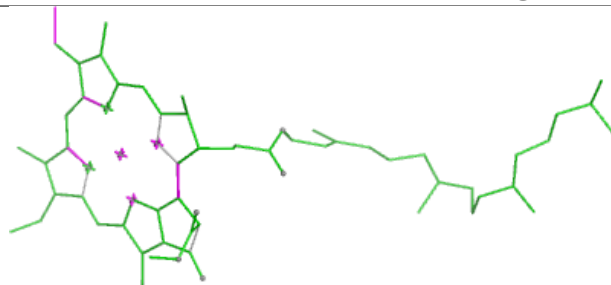


Torsions

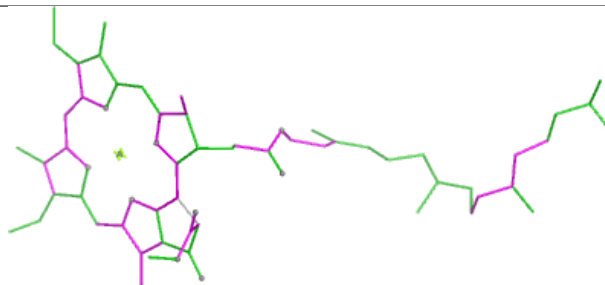


Rings

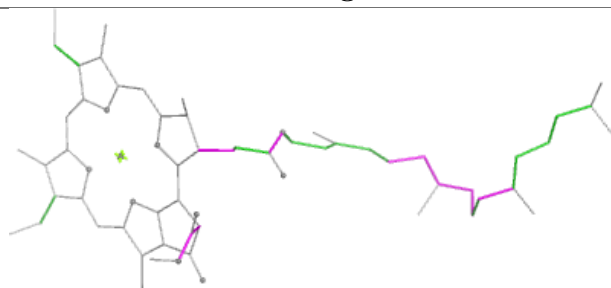
Ligand CLA C 502



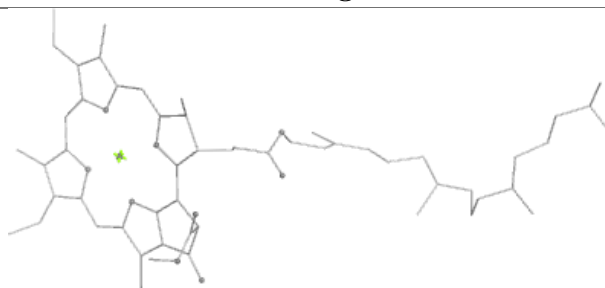
Bond lengths



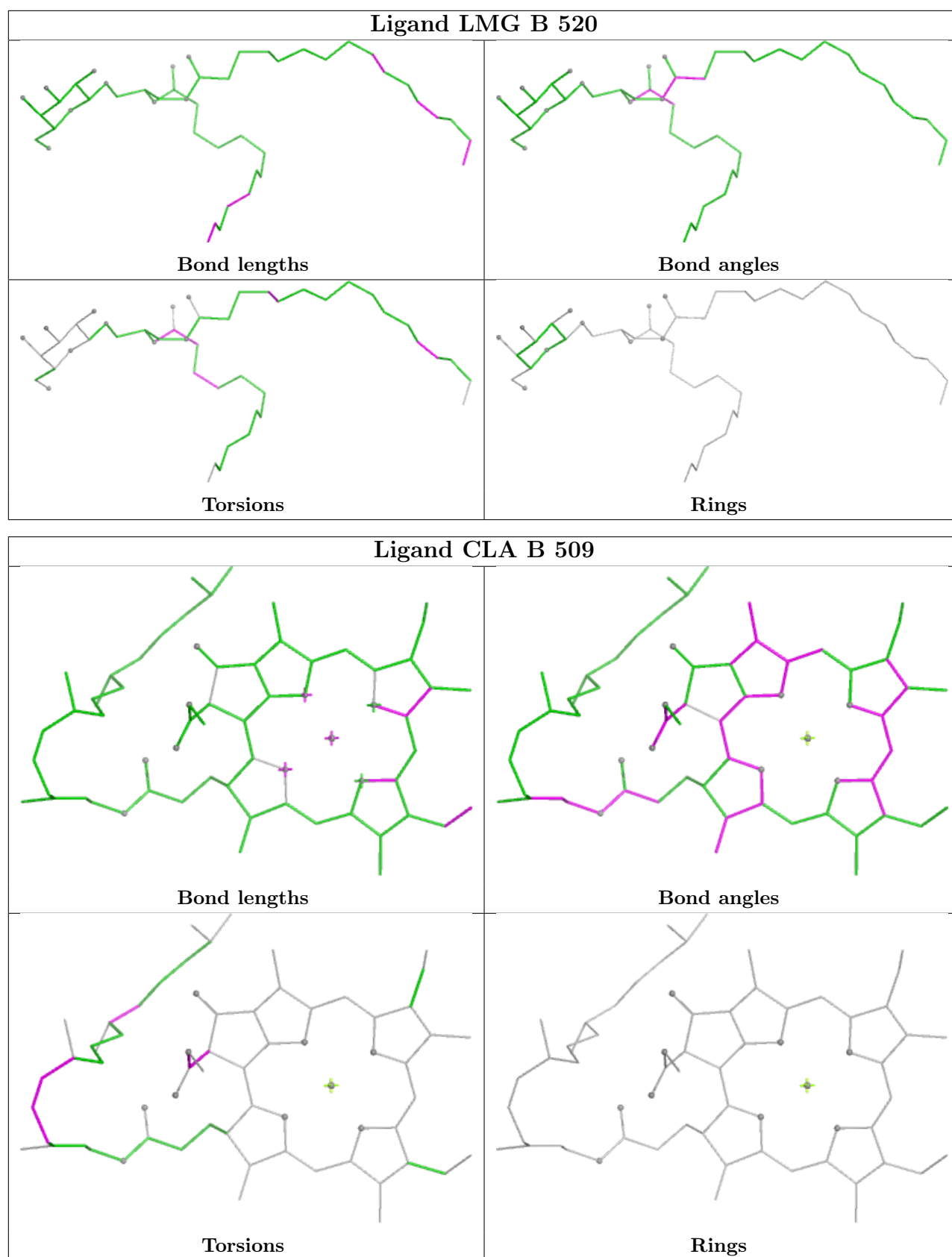
Bond angles

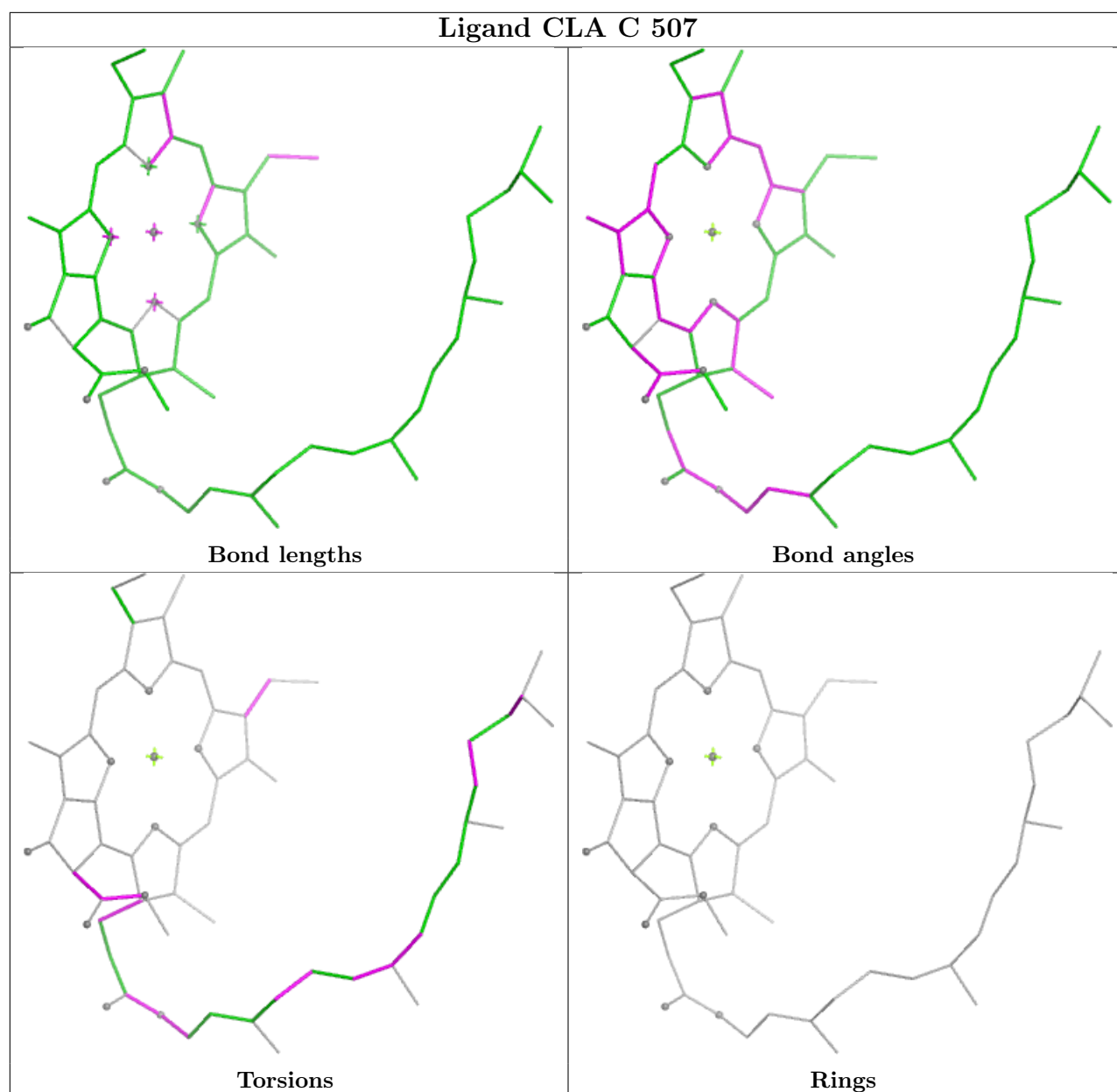


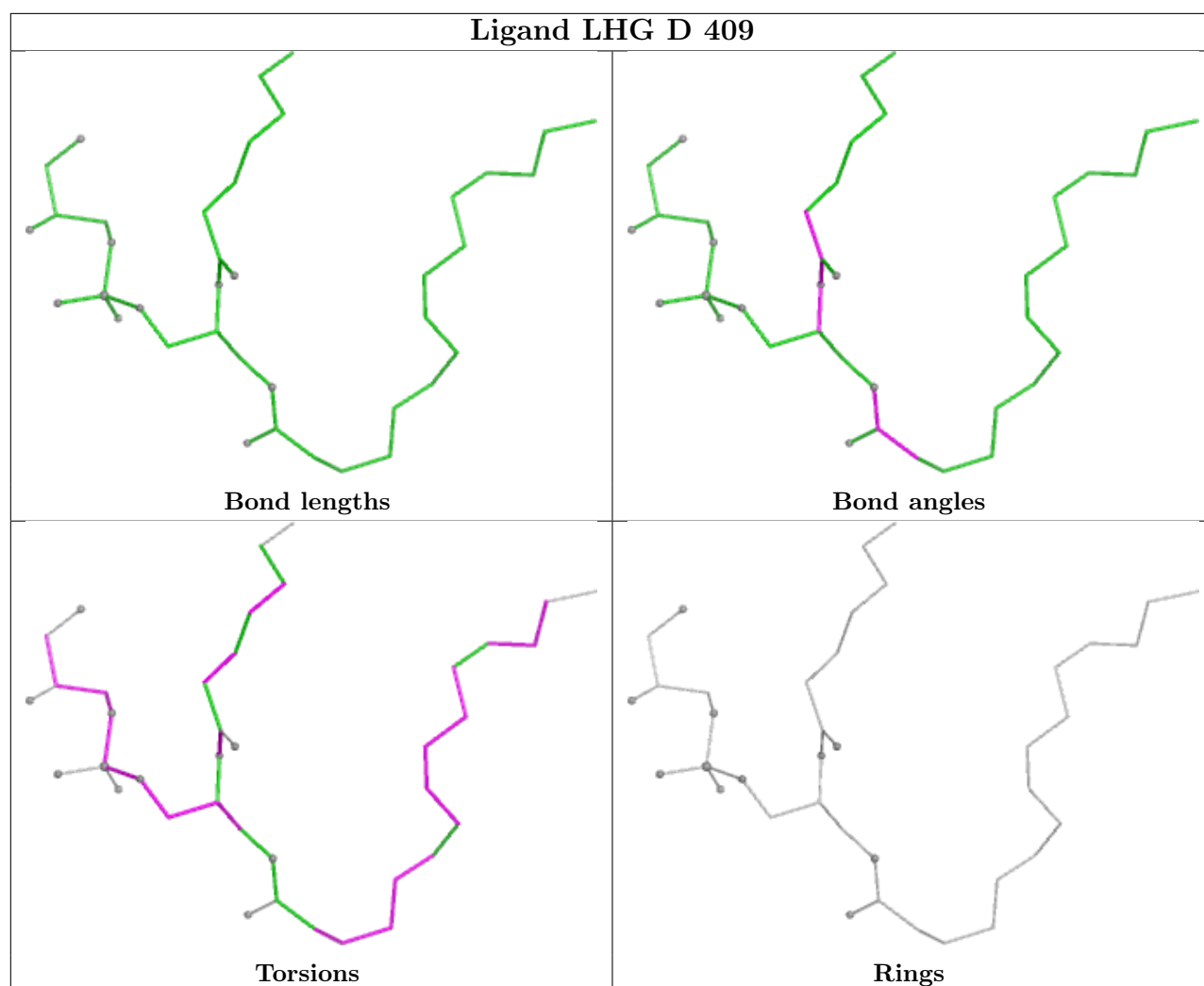
Torsions

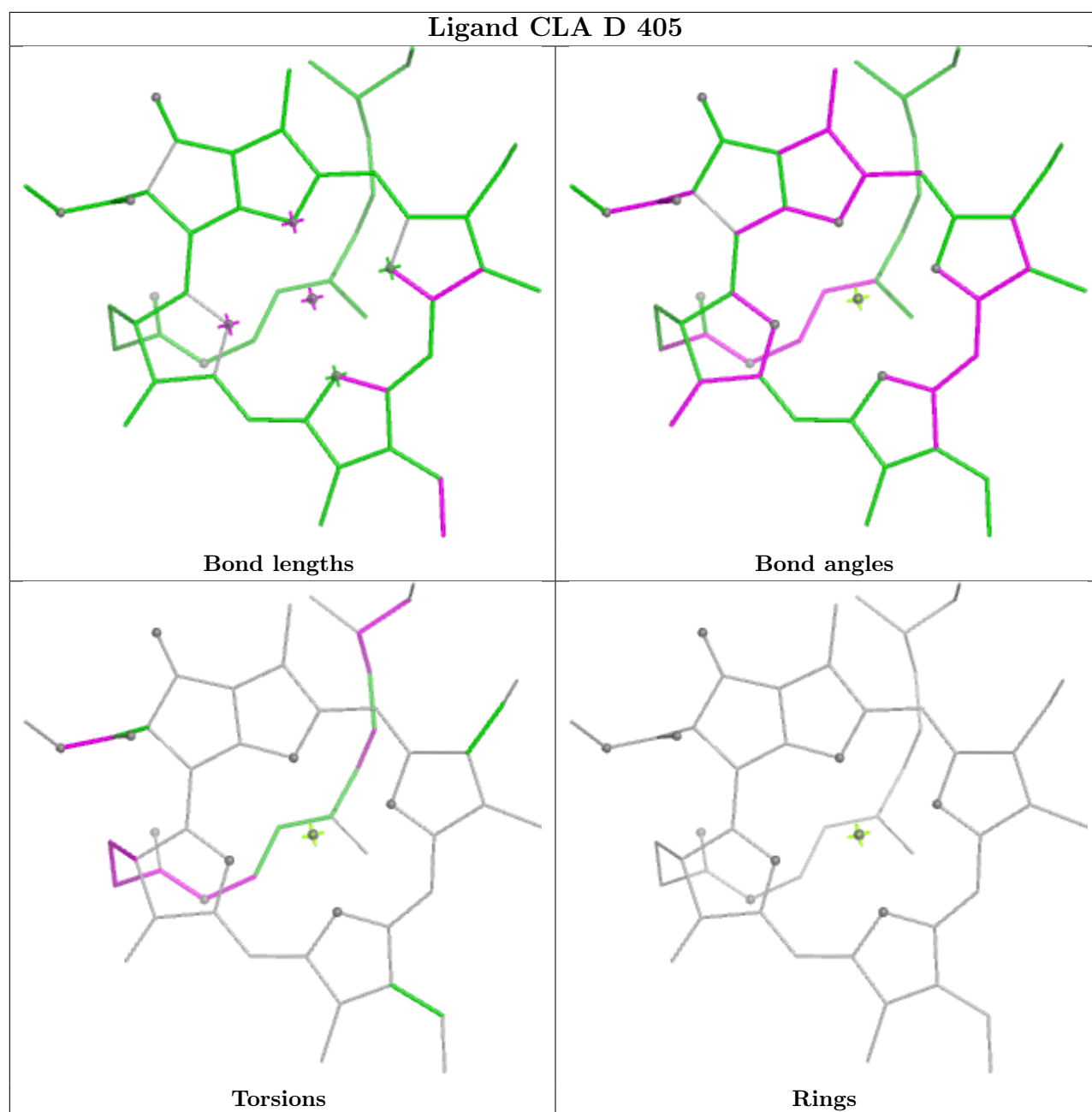


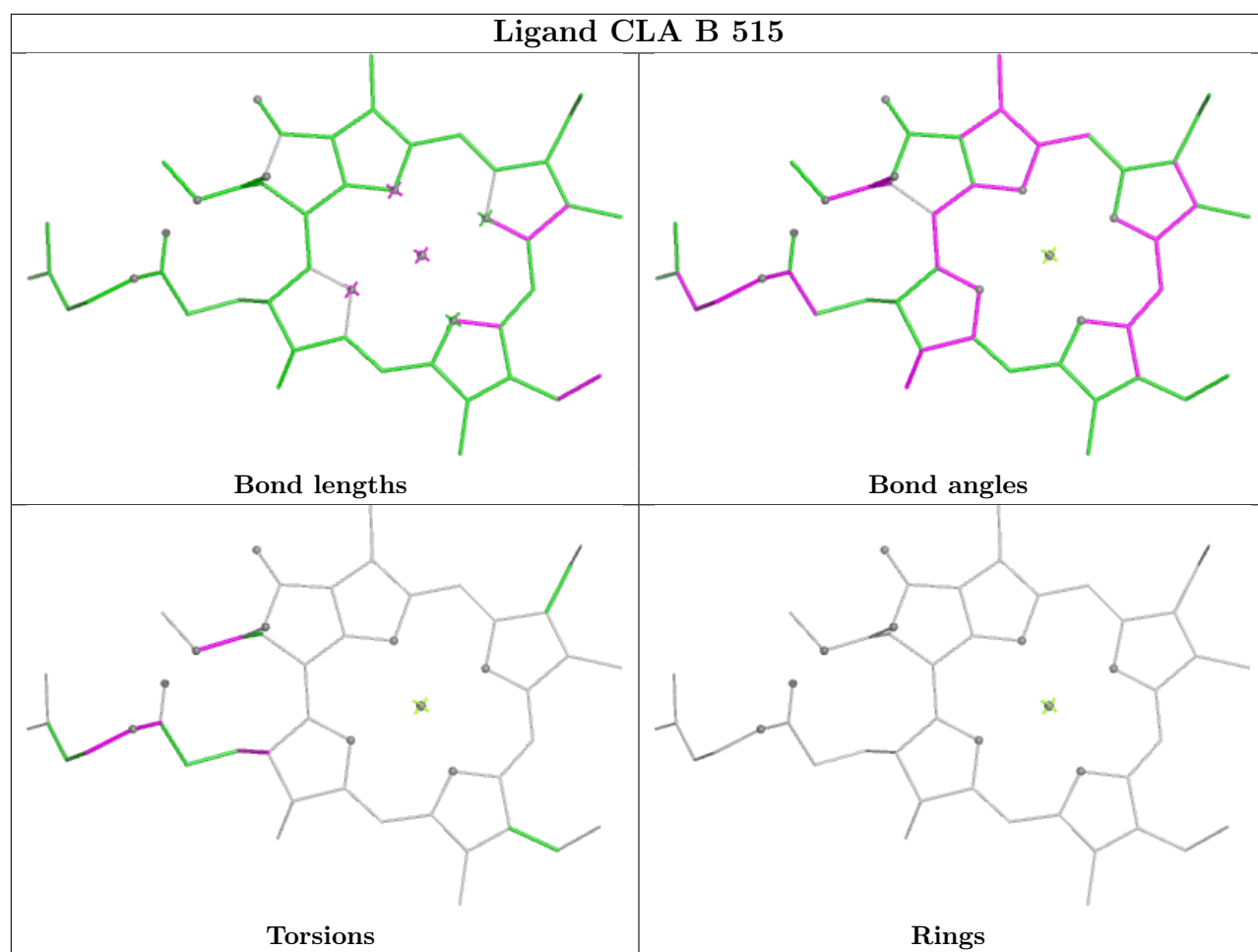
Rings

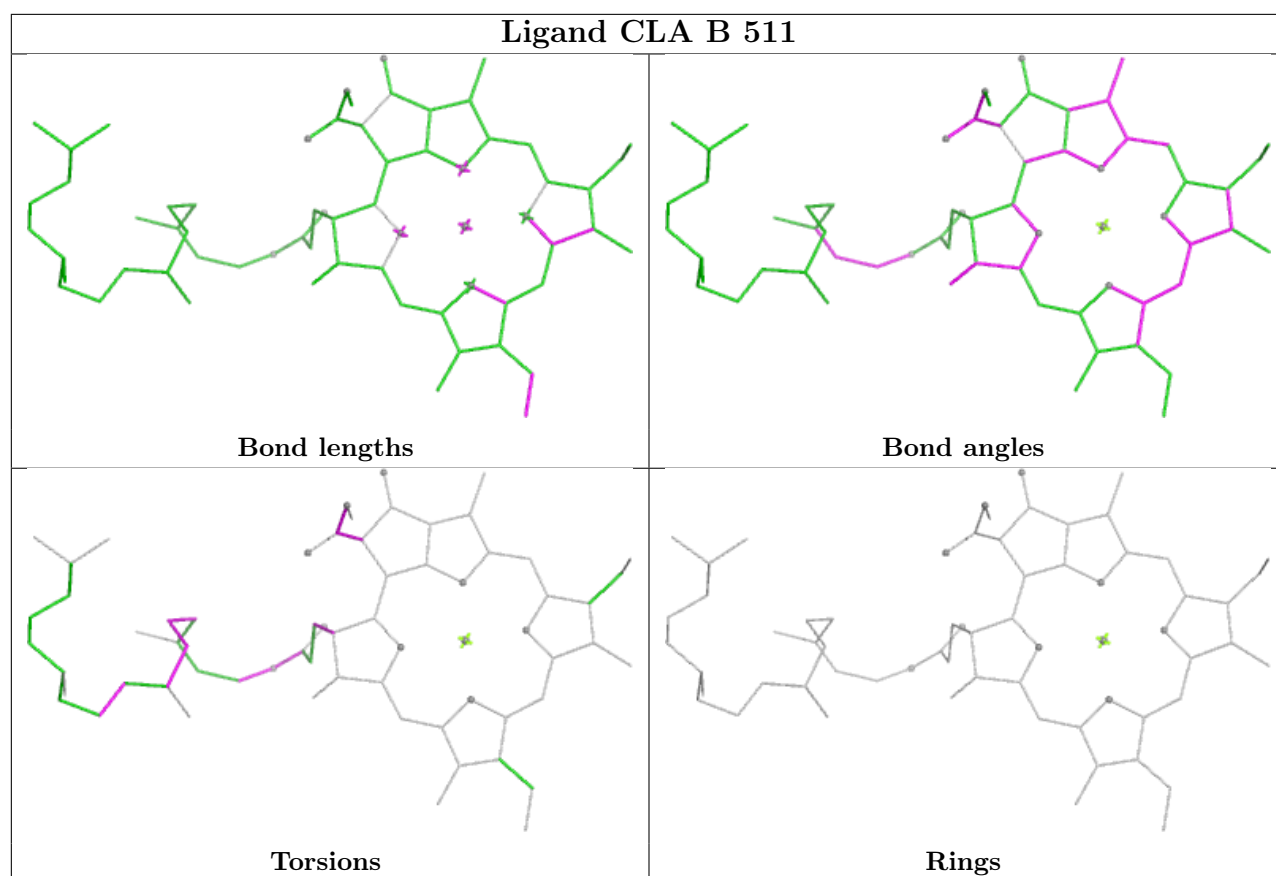


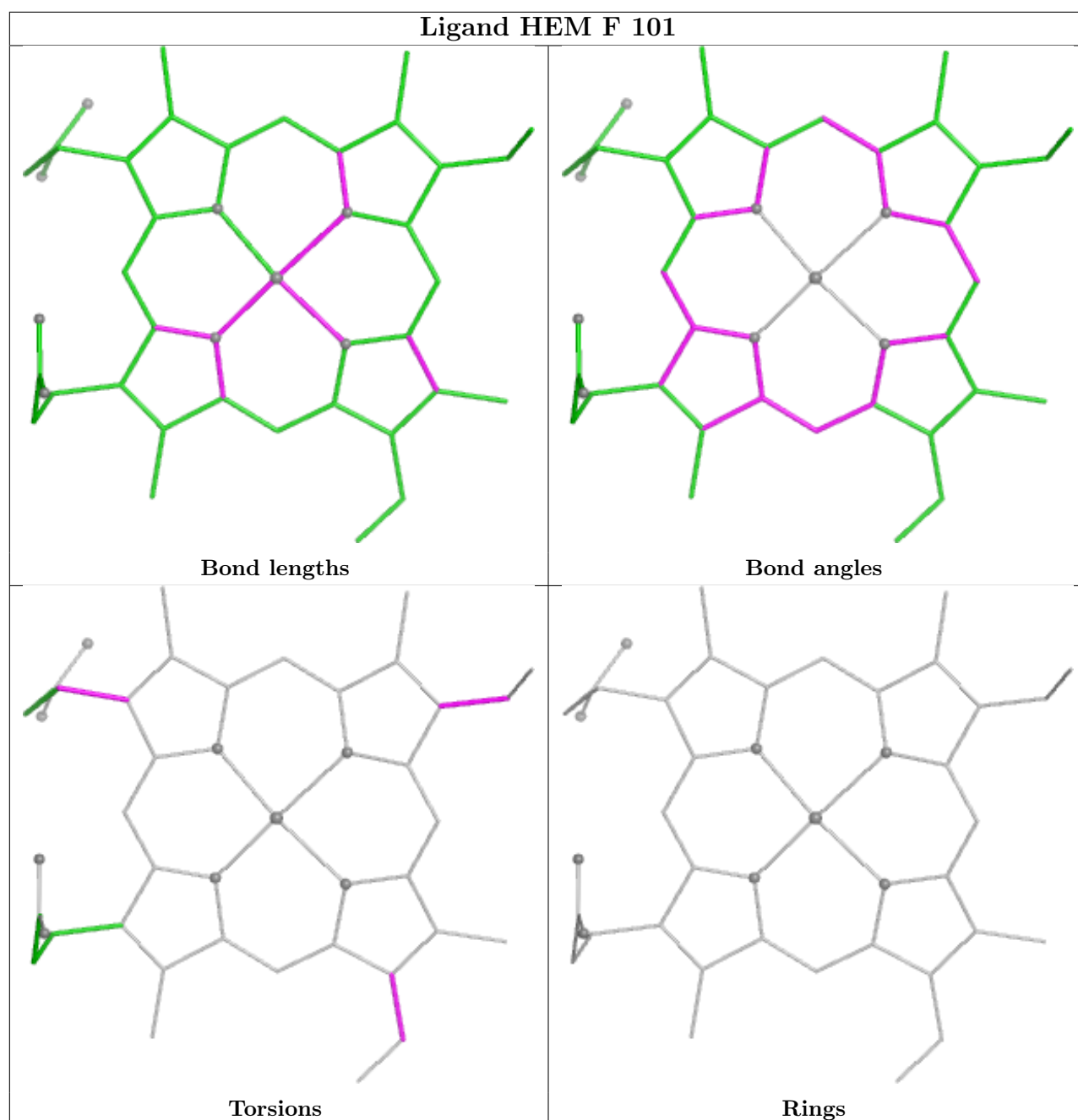


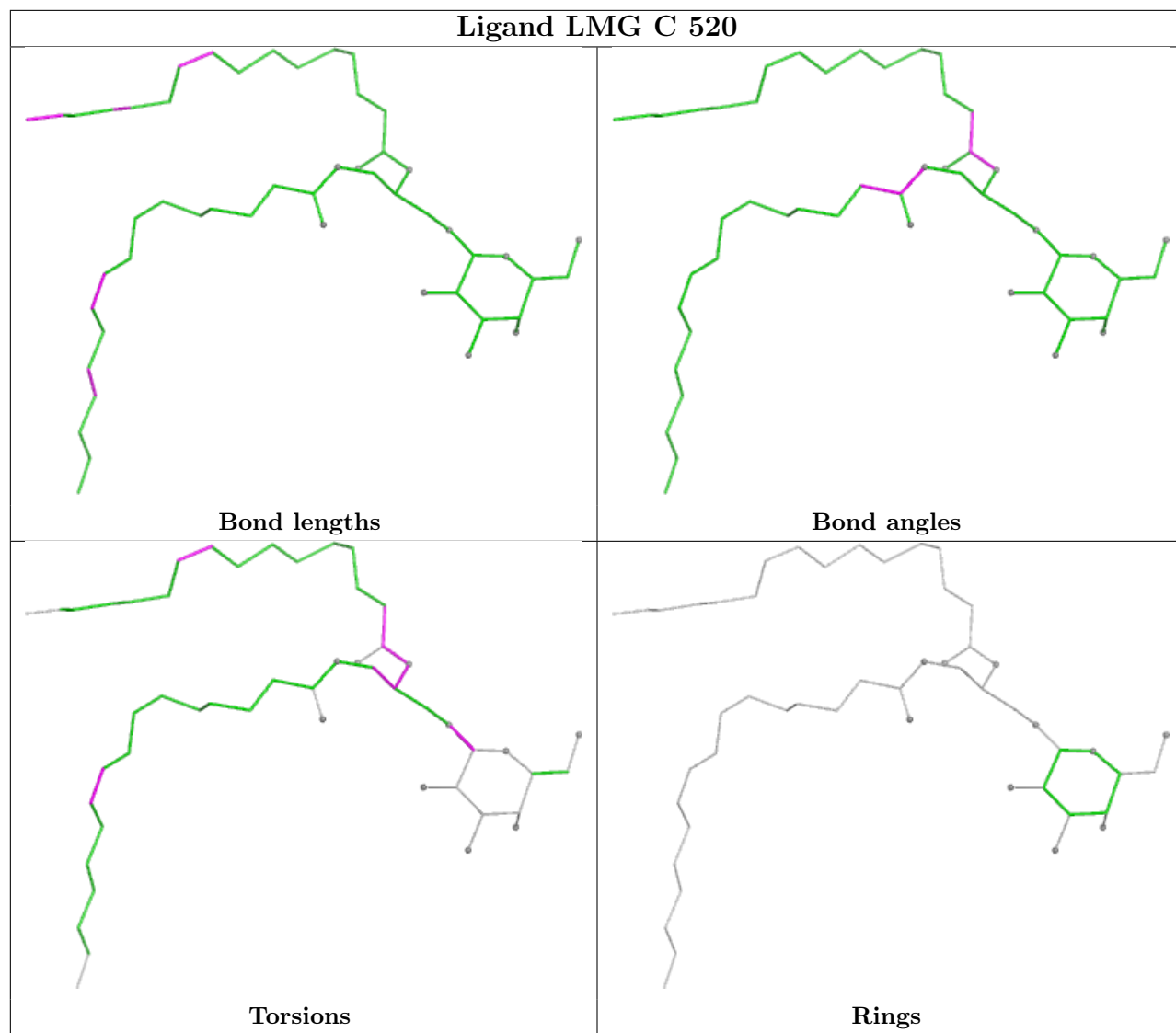




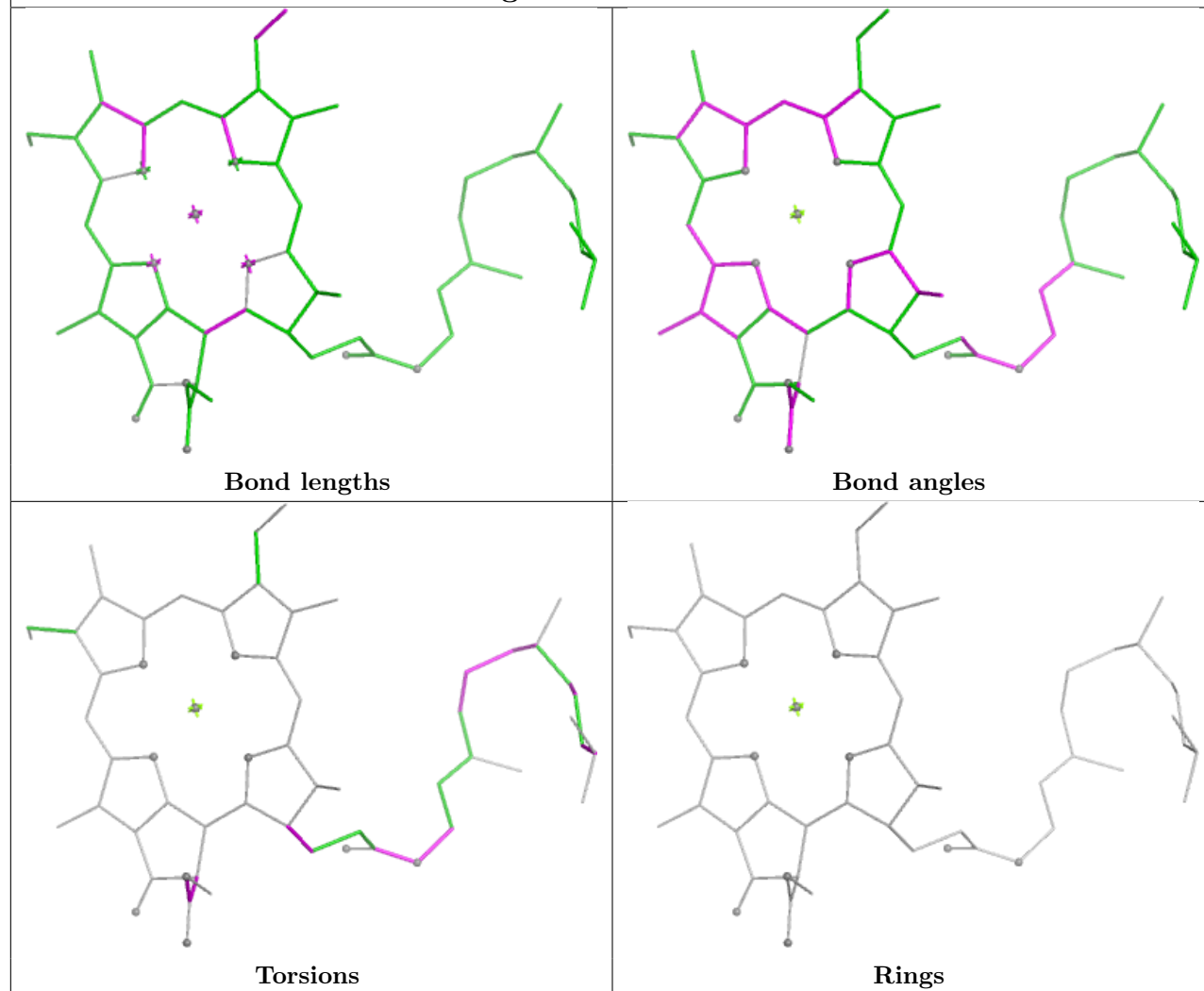




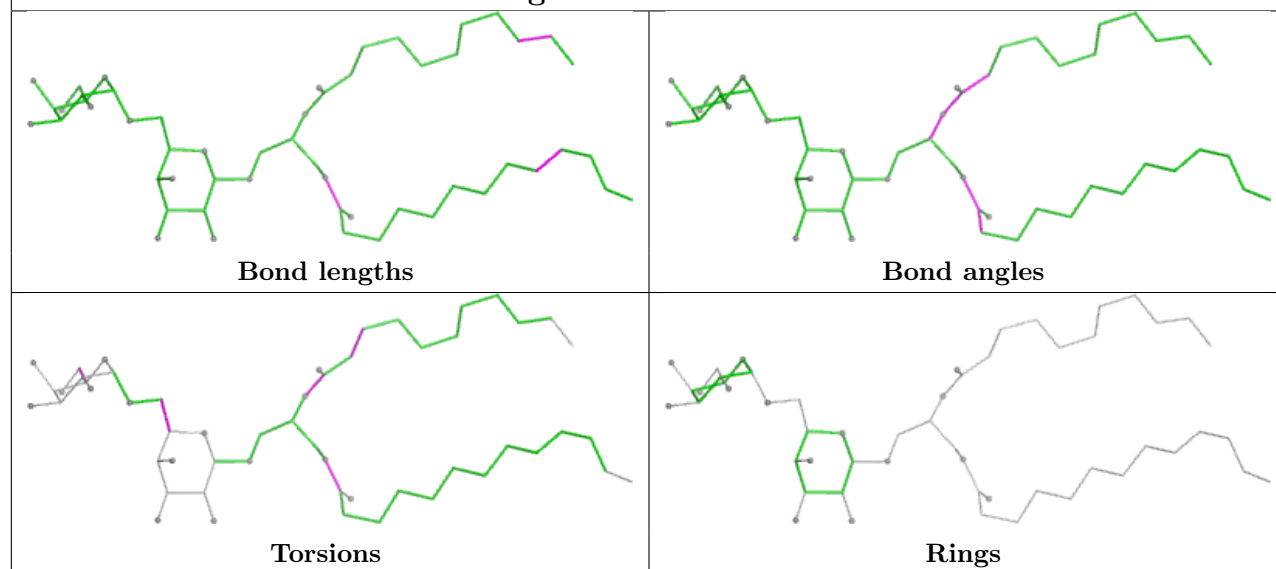


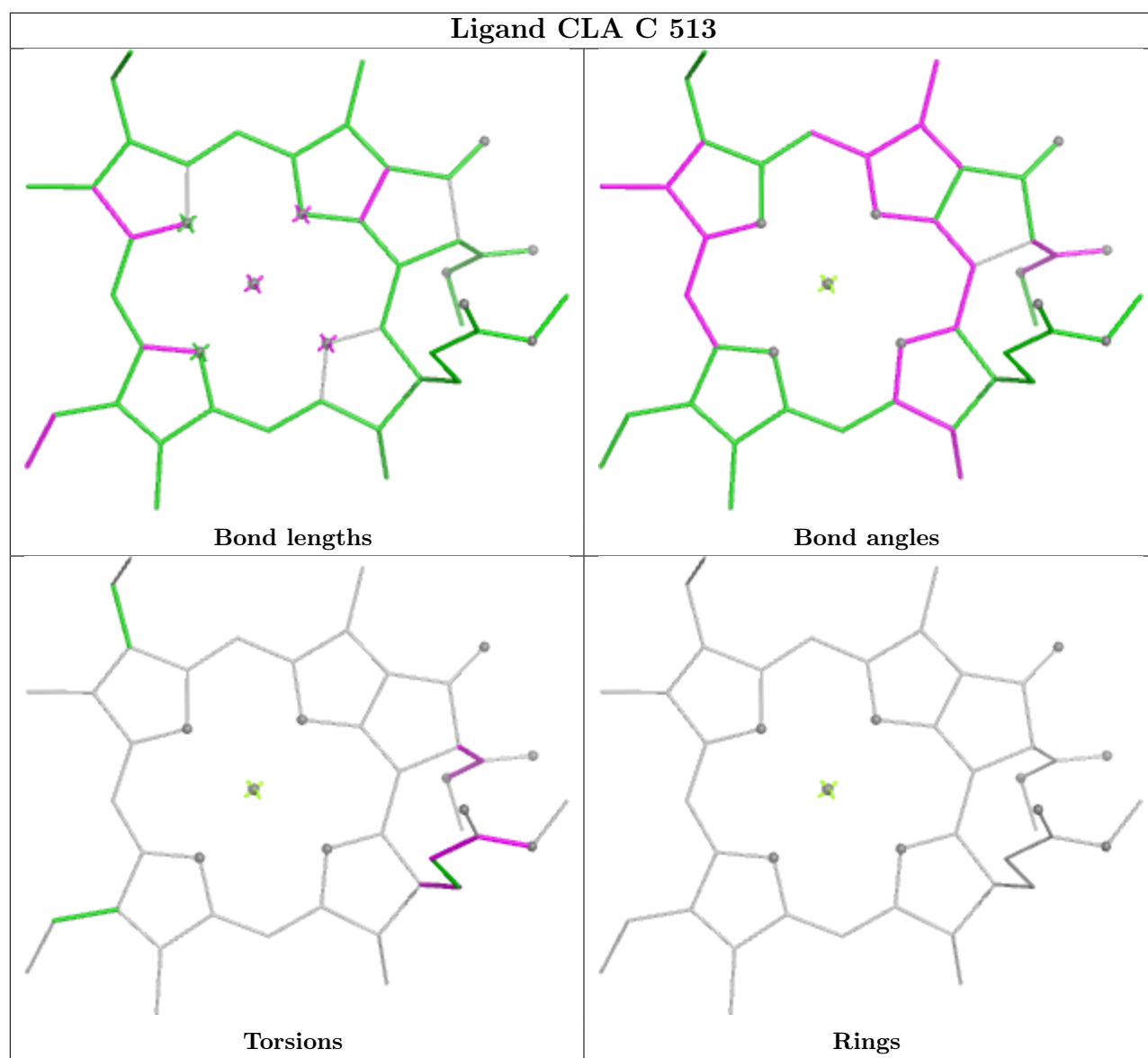


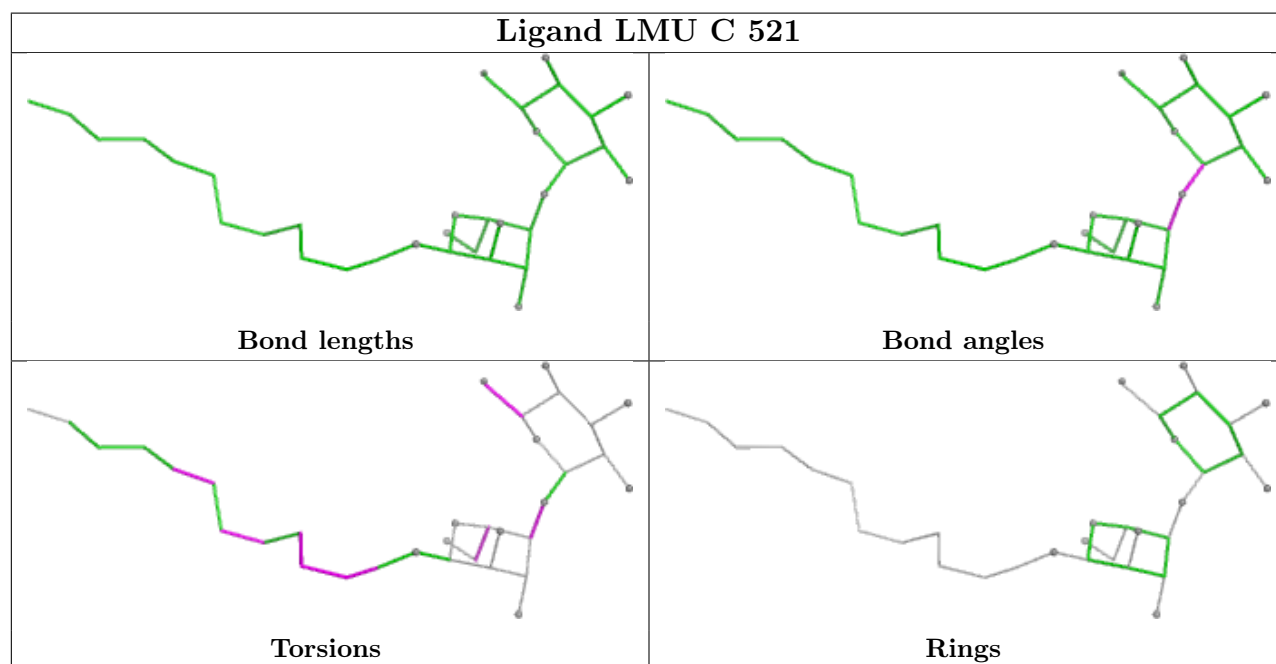
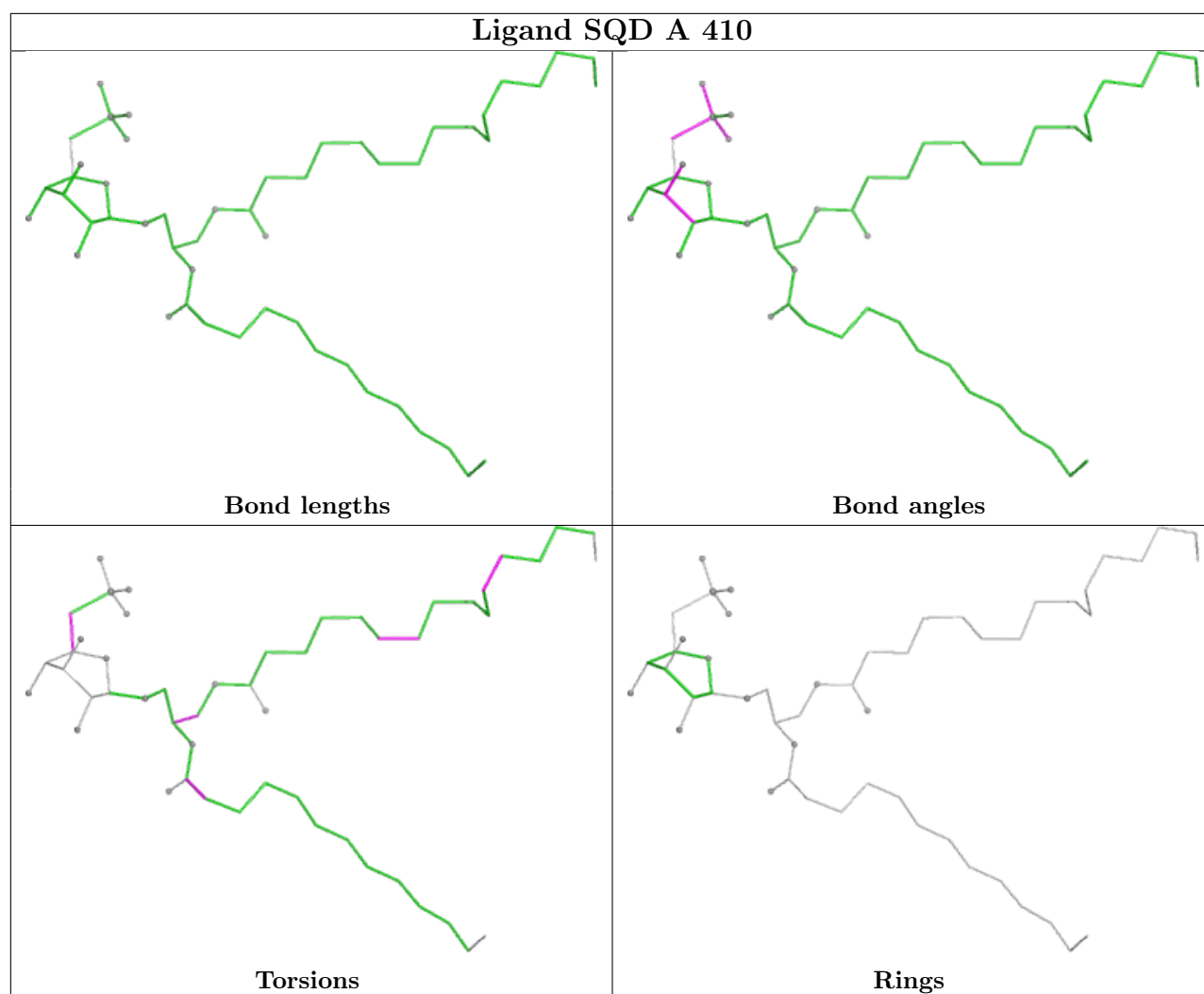
Ligand CLA A 408

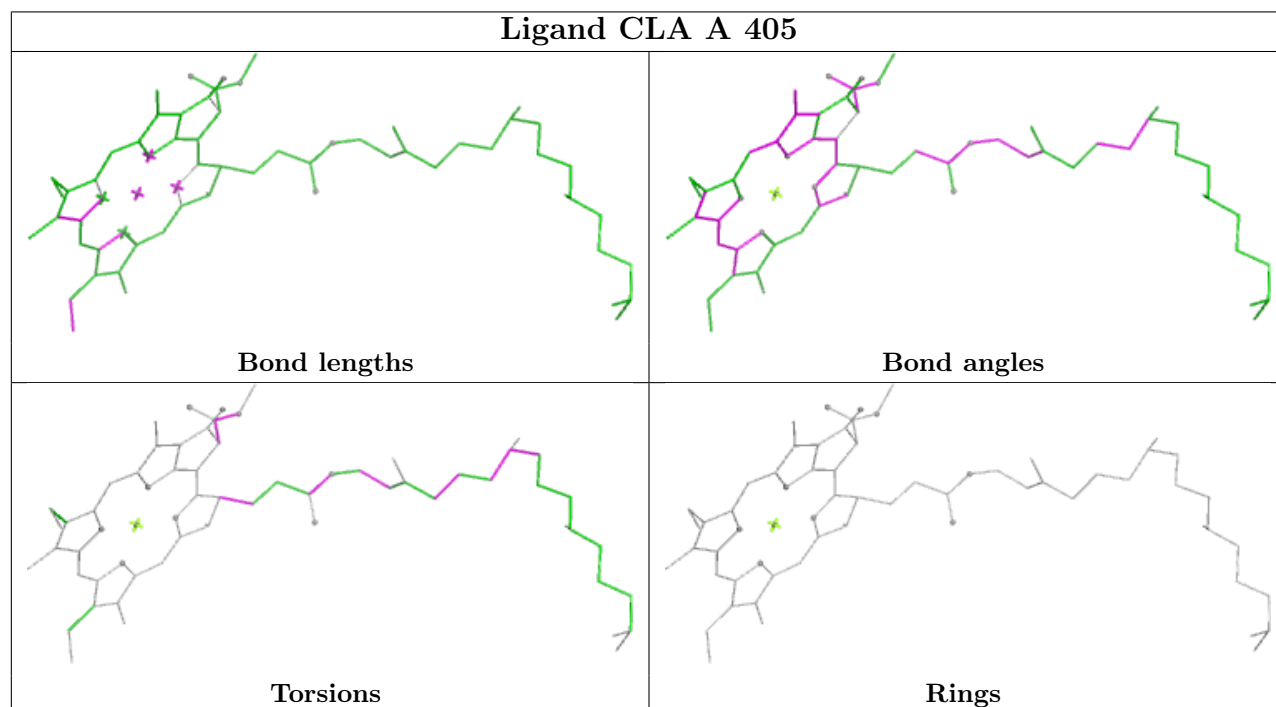
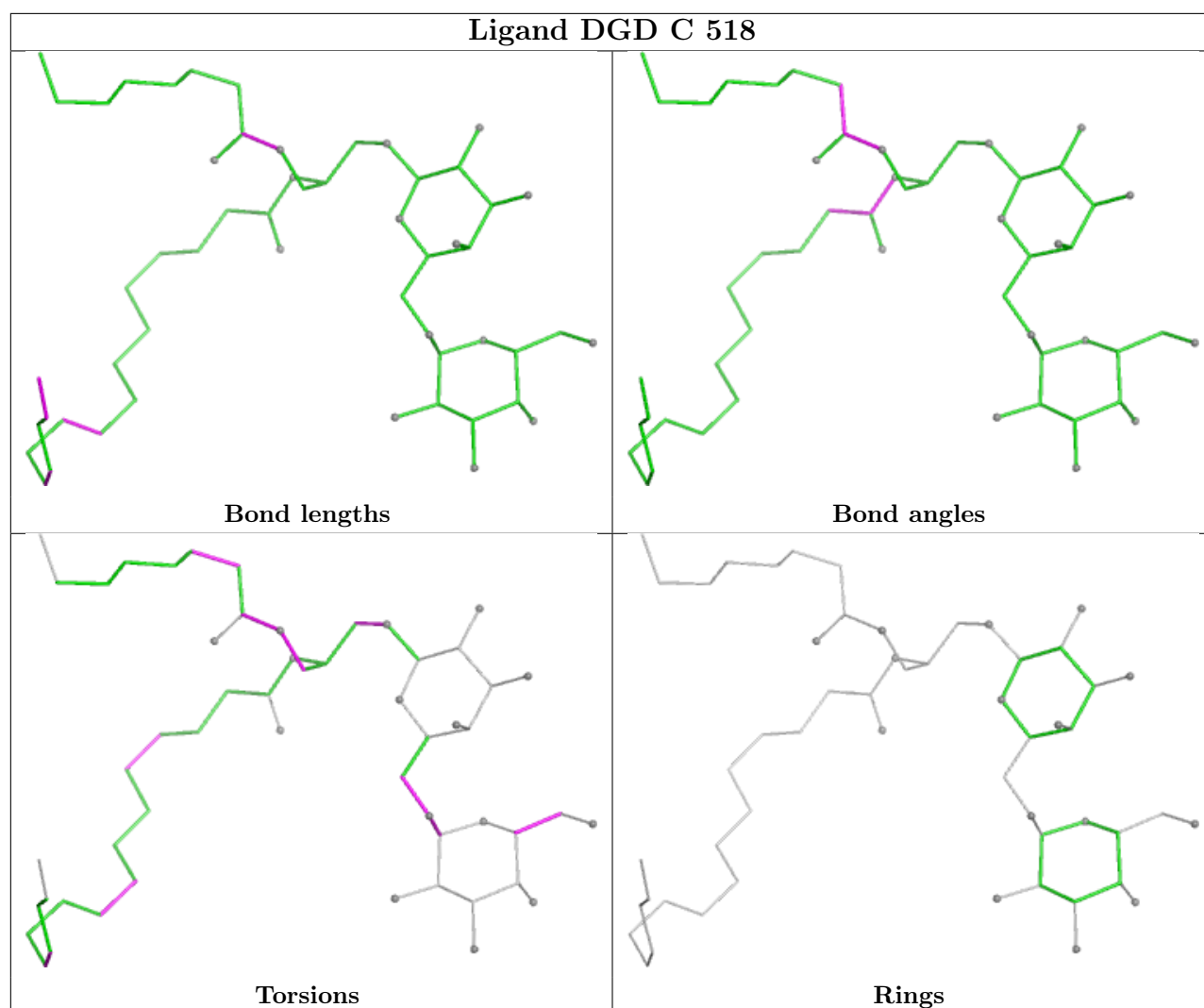


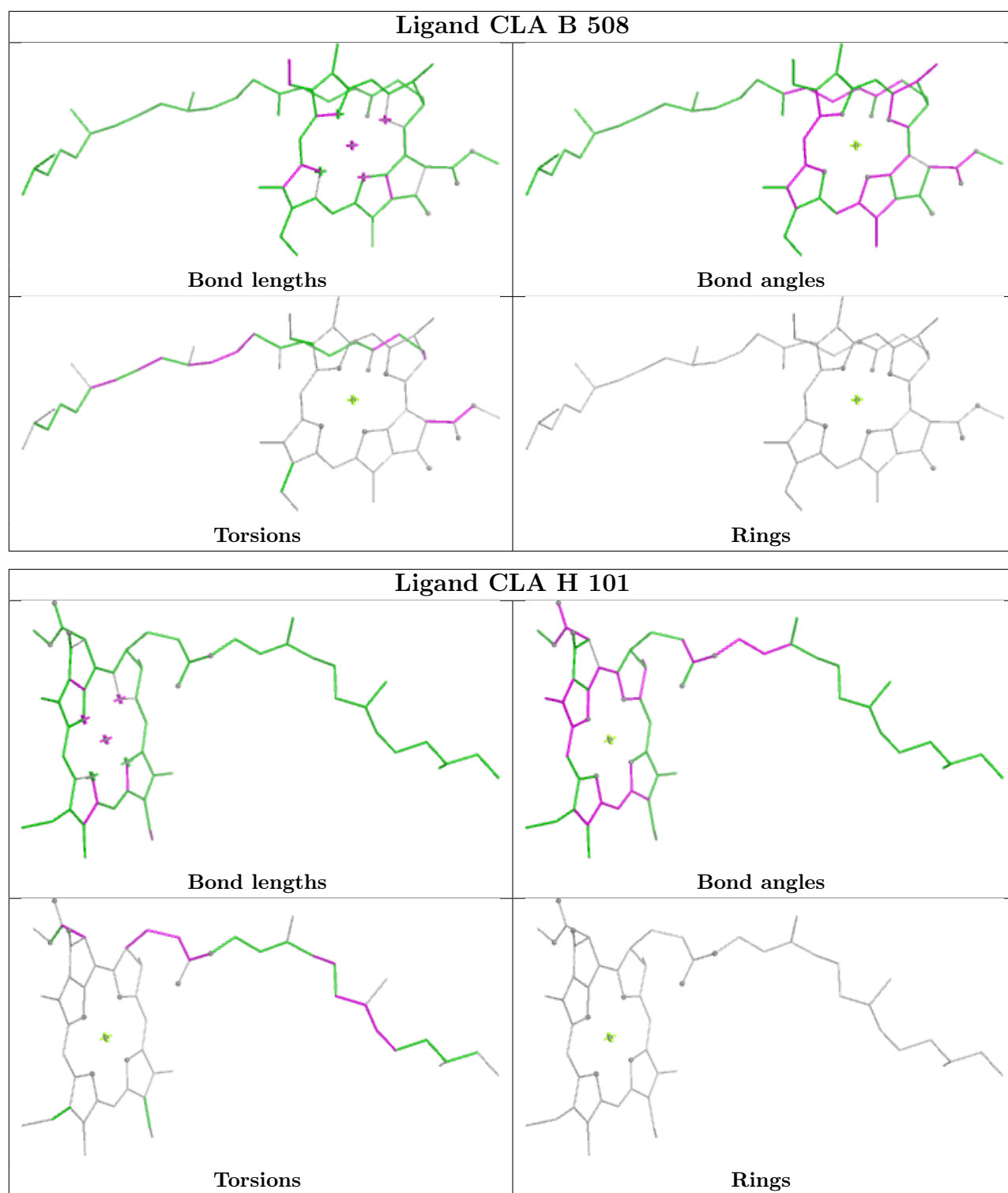
Ligand DGD C 519

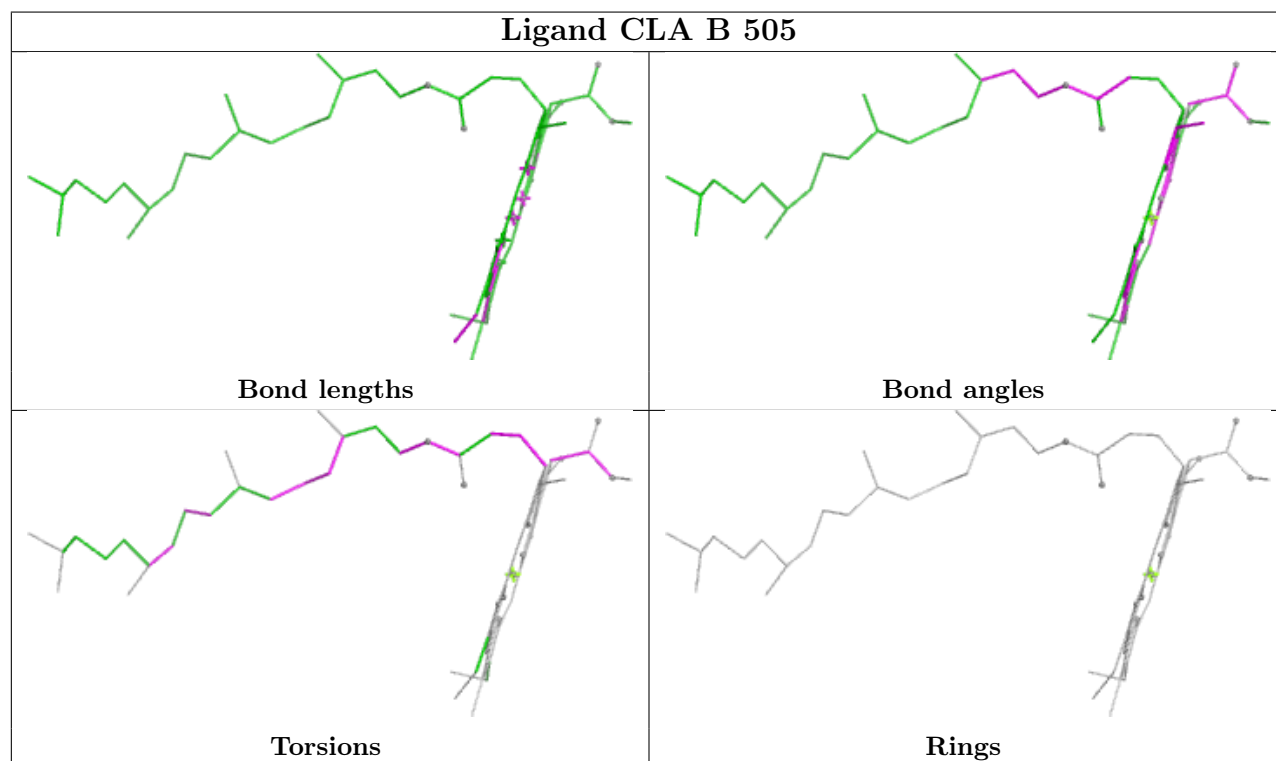
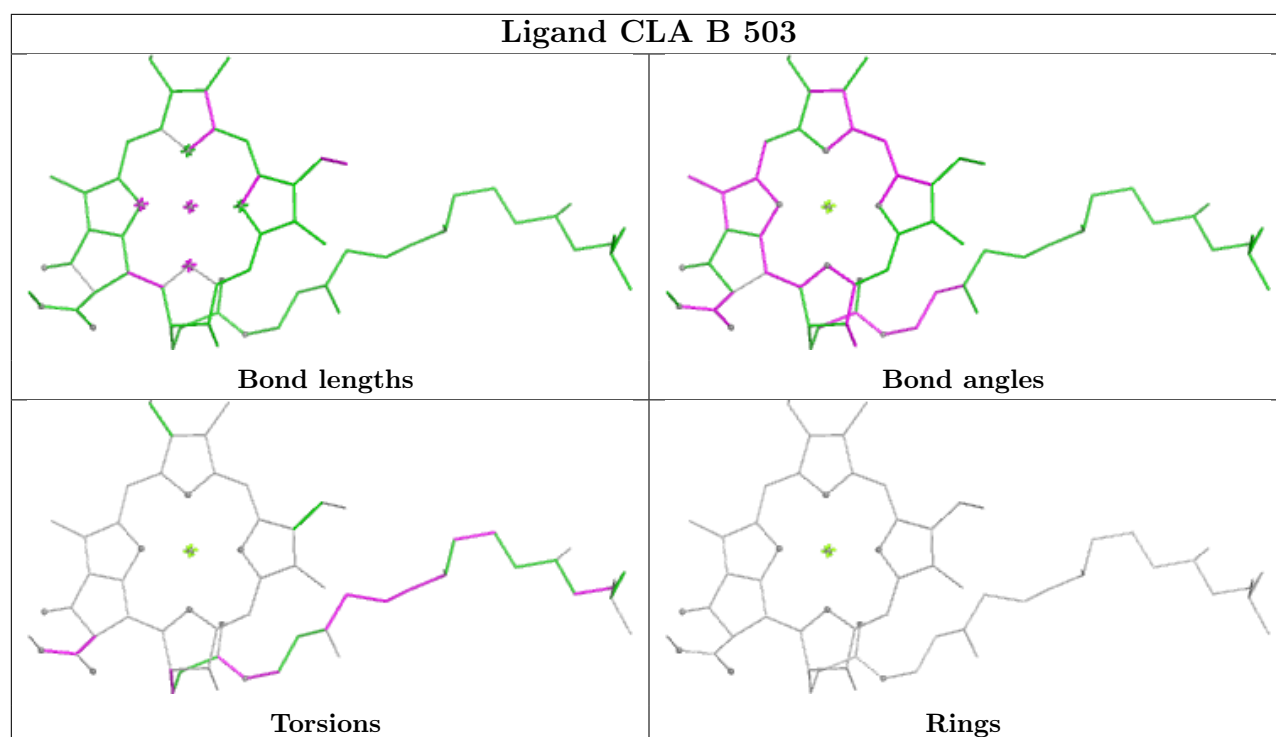


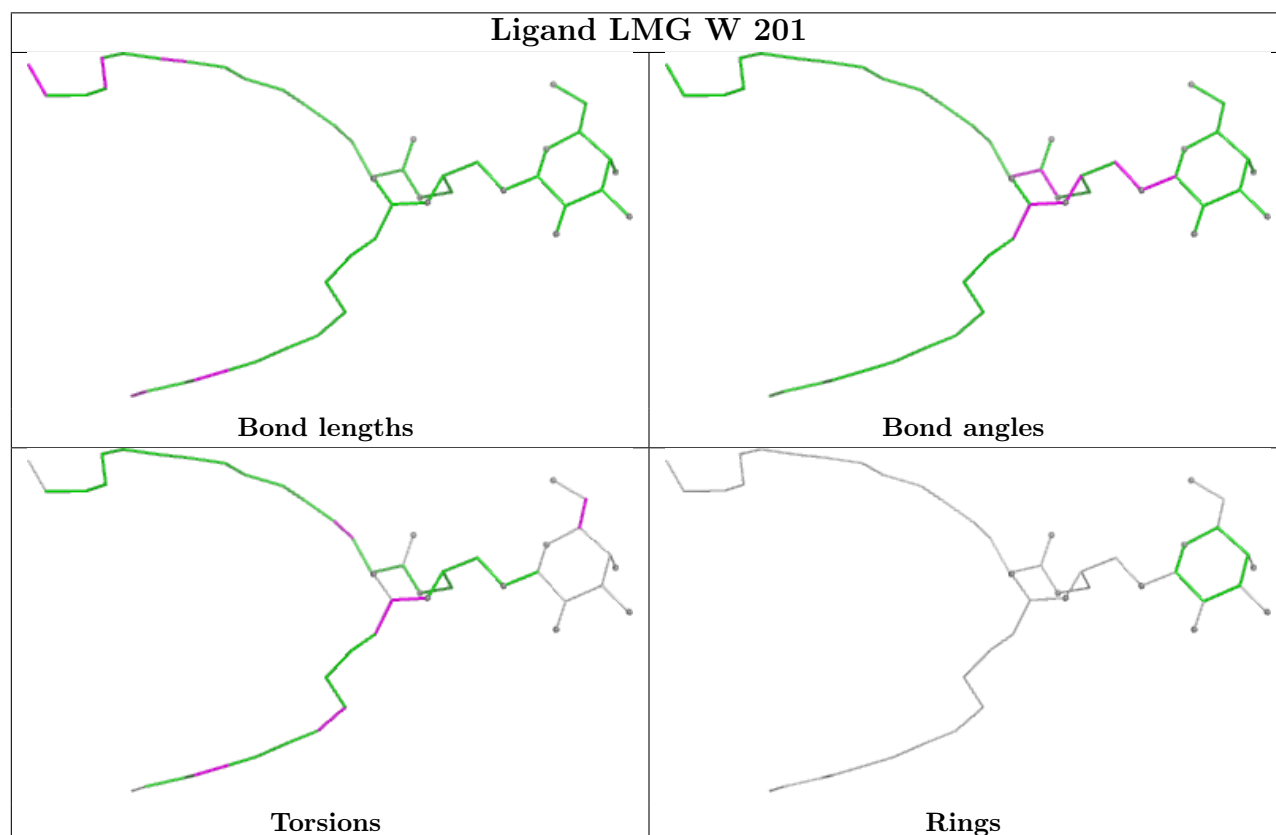
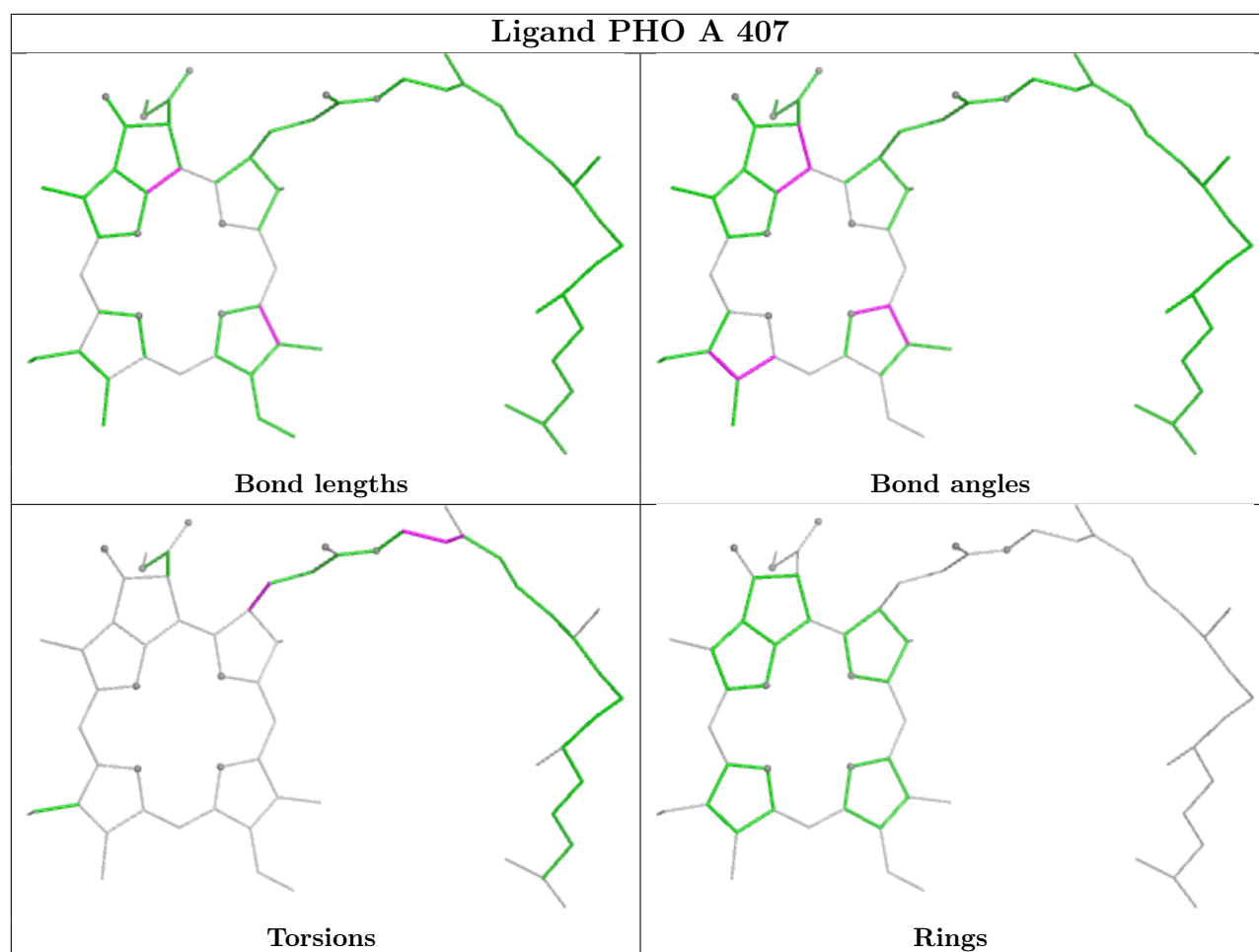


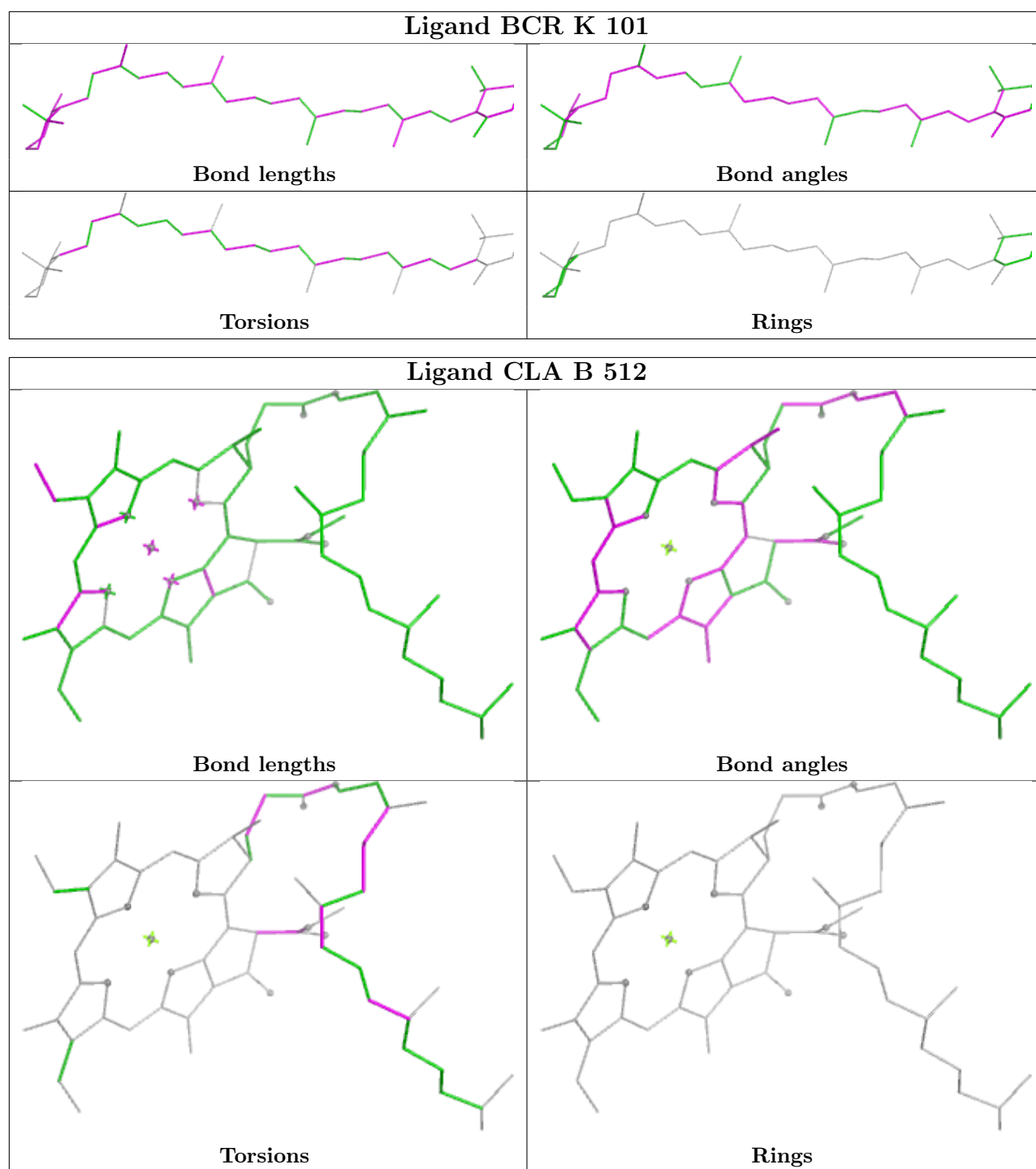


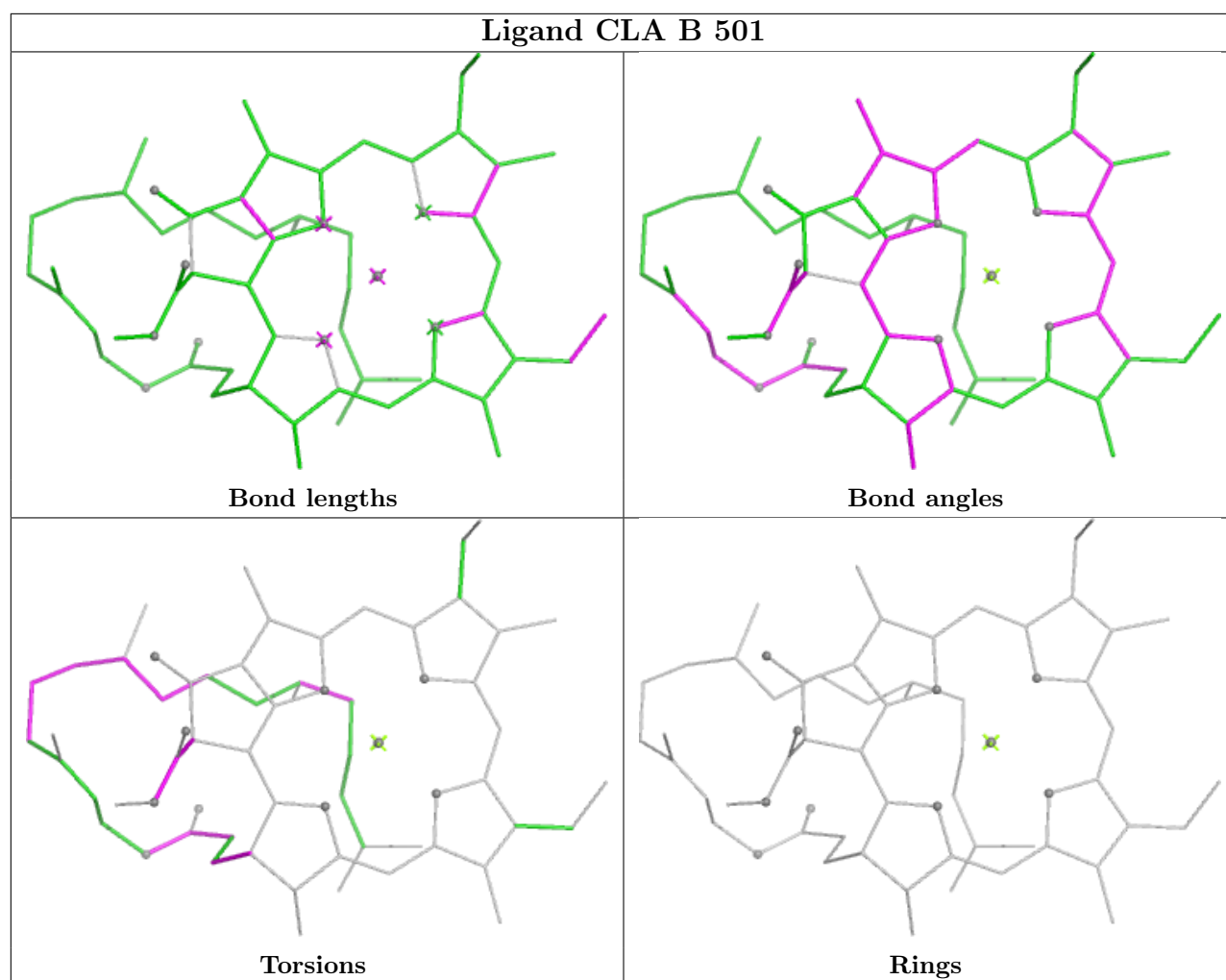


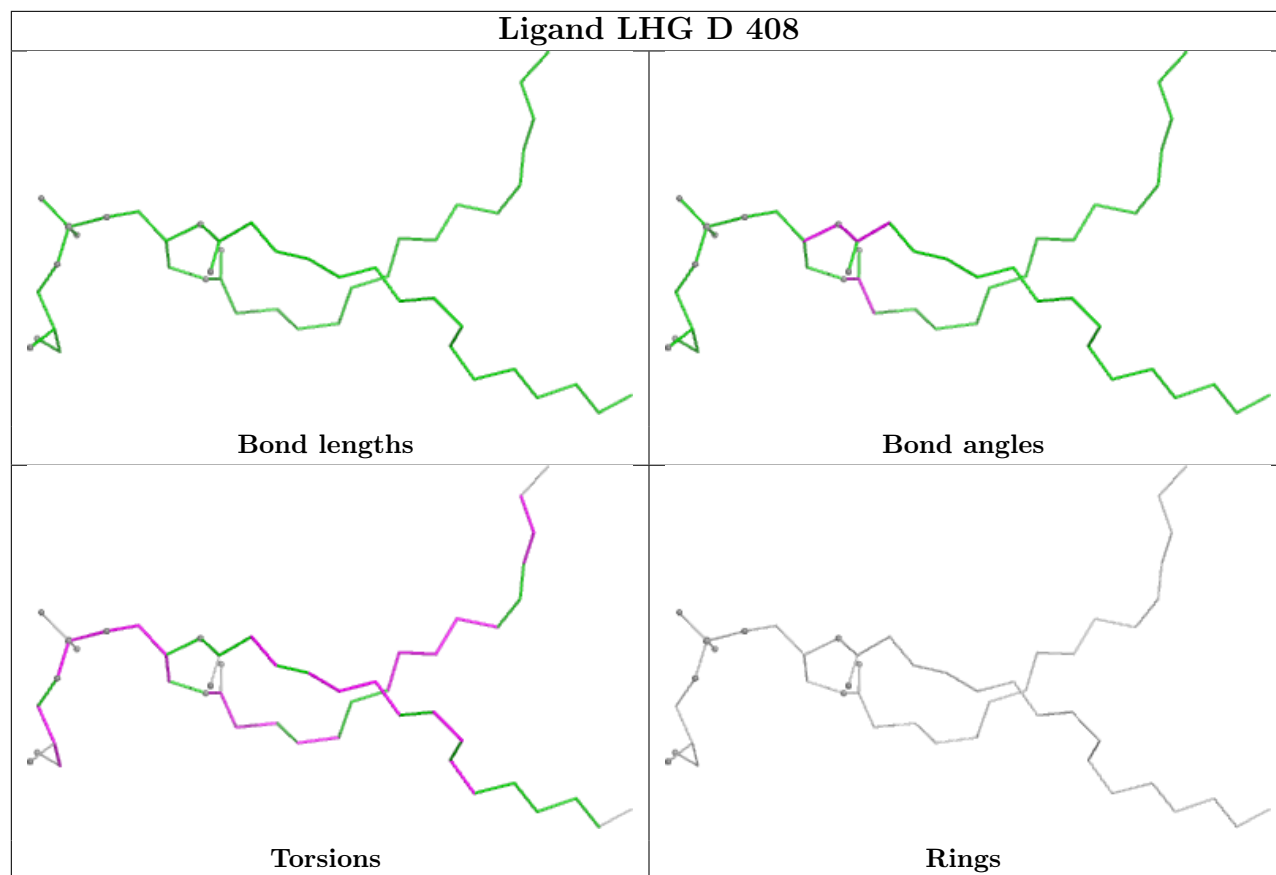


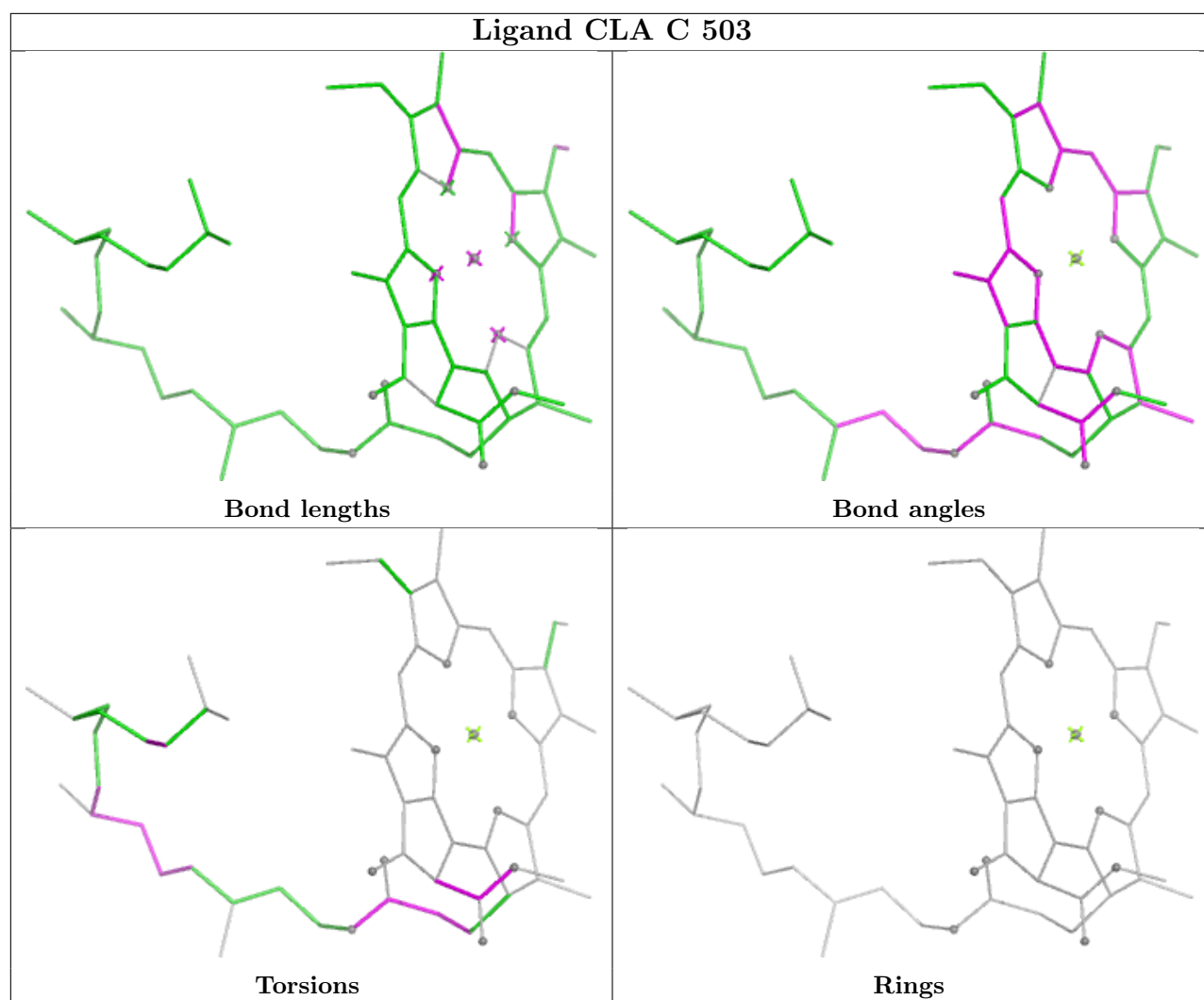


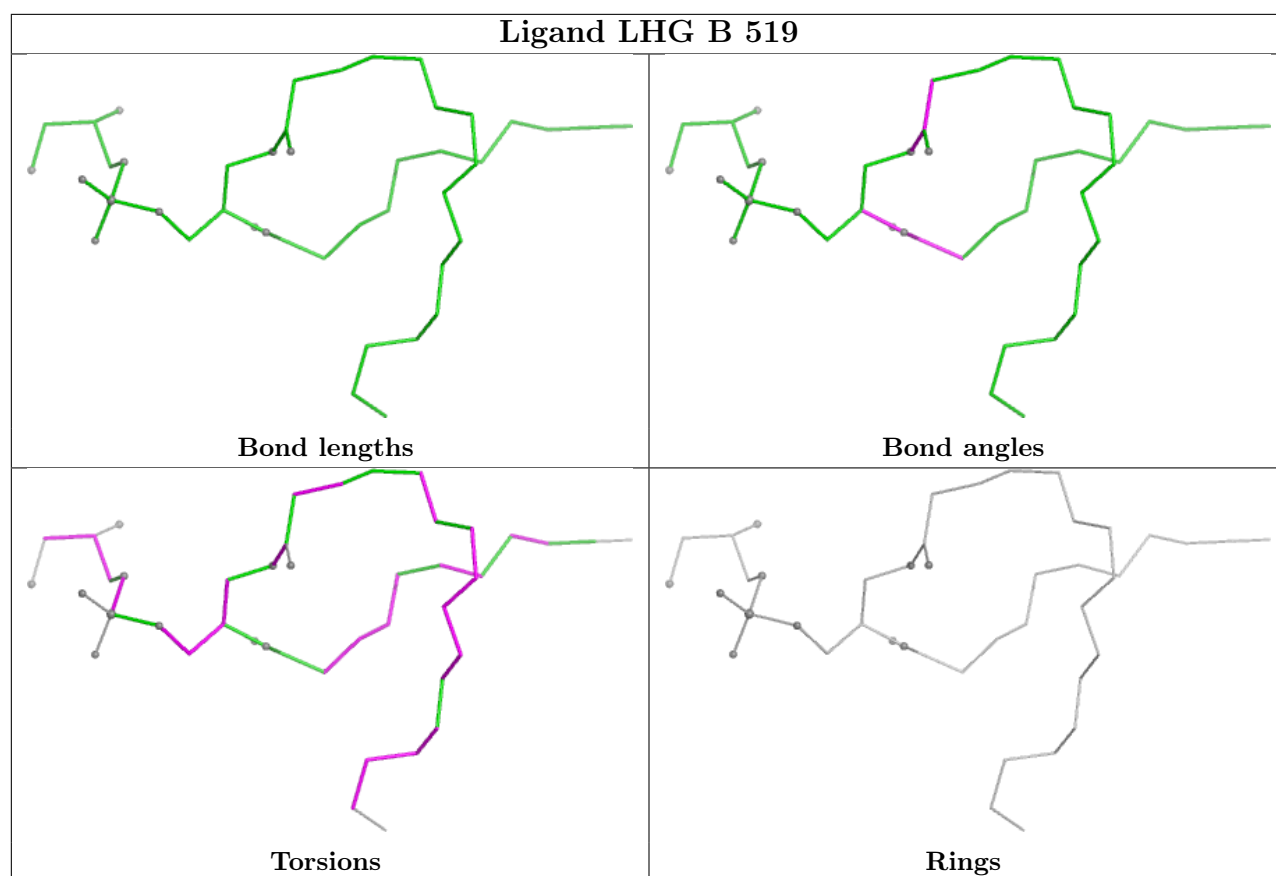


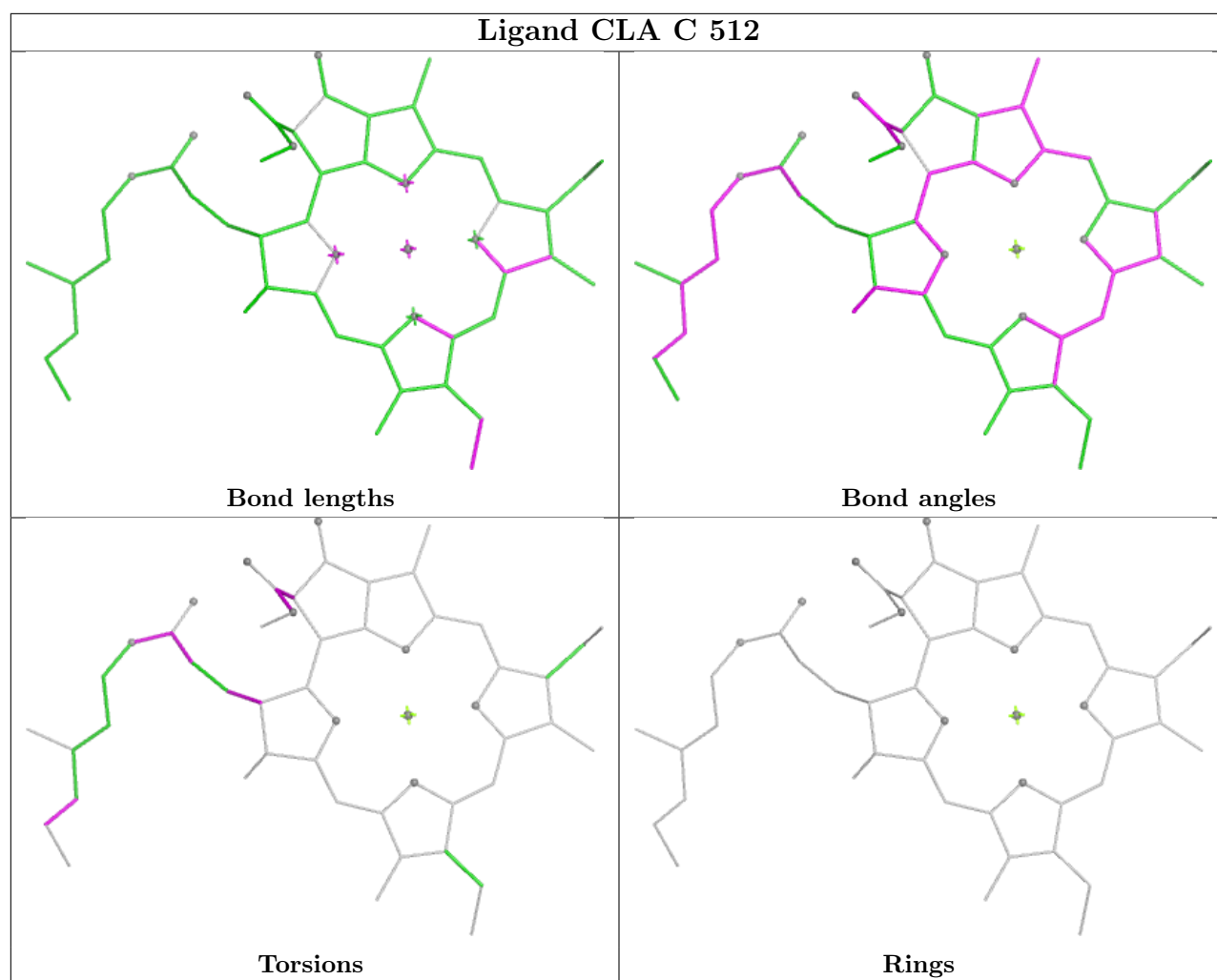


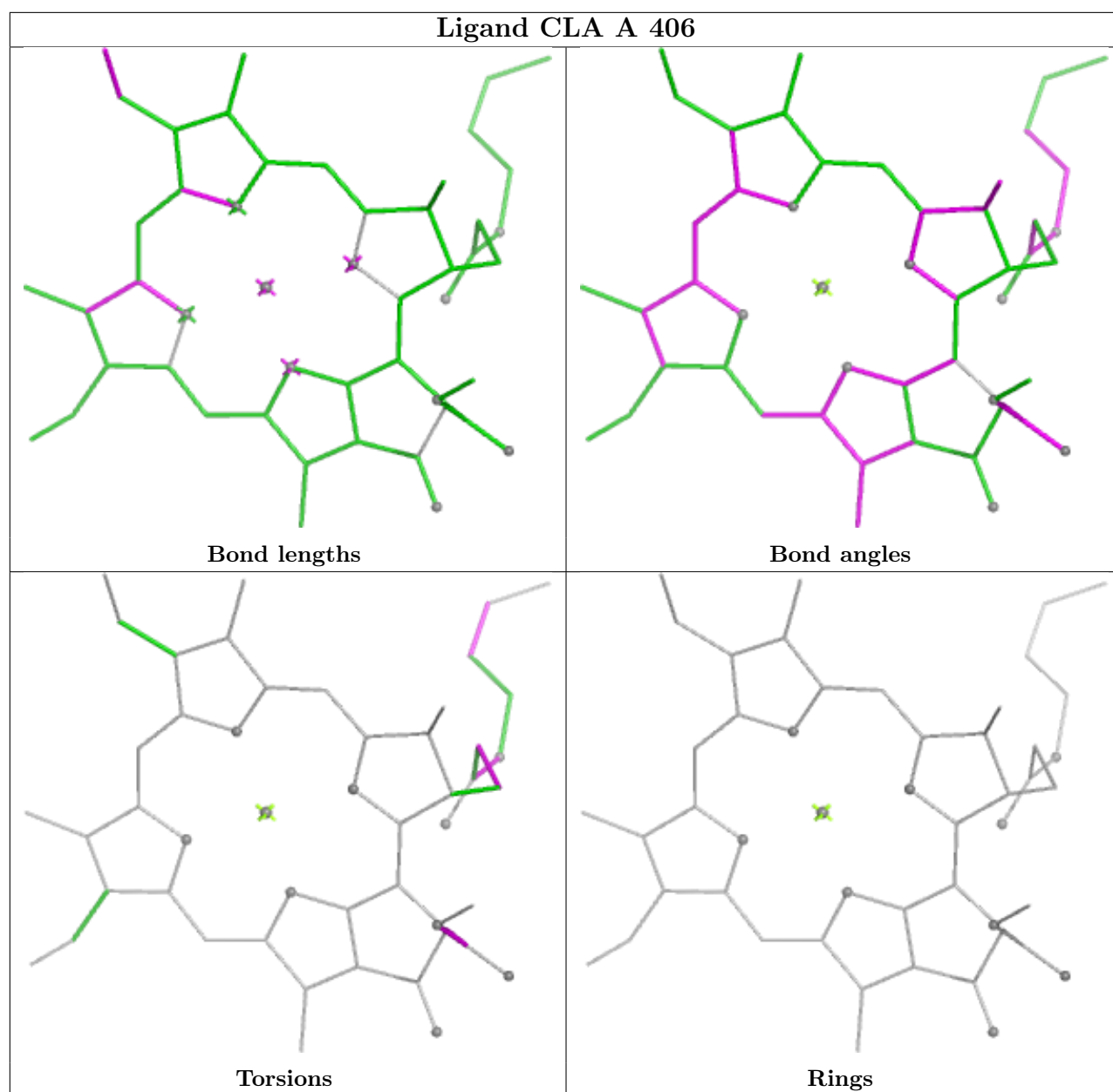


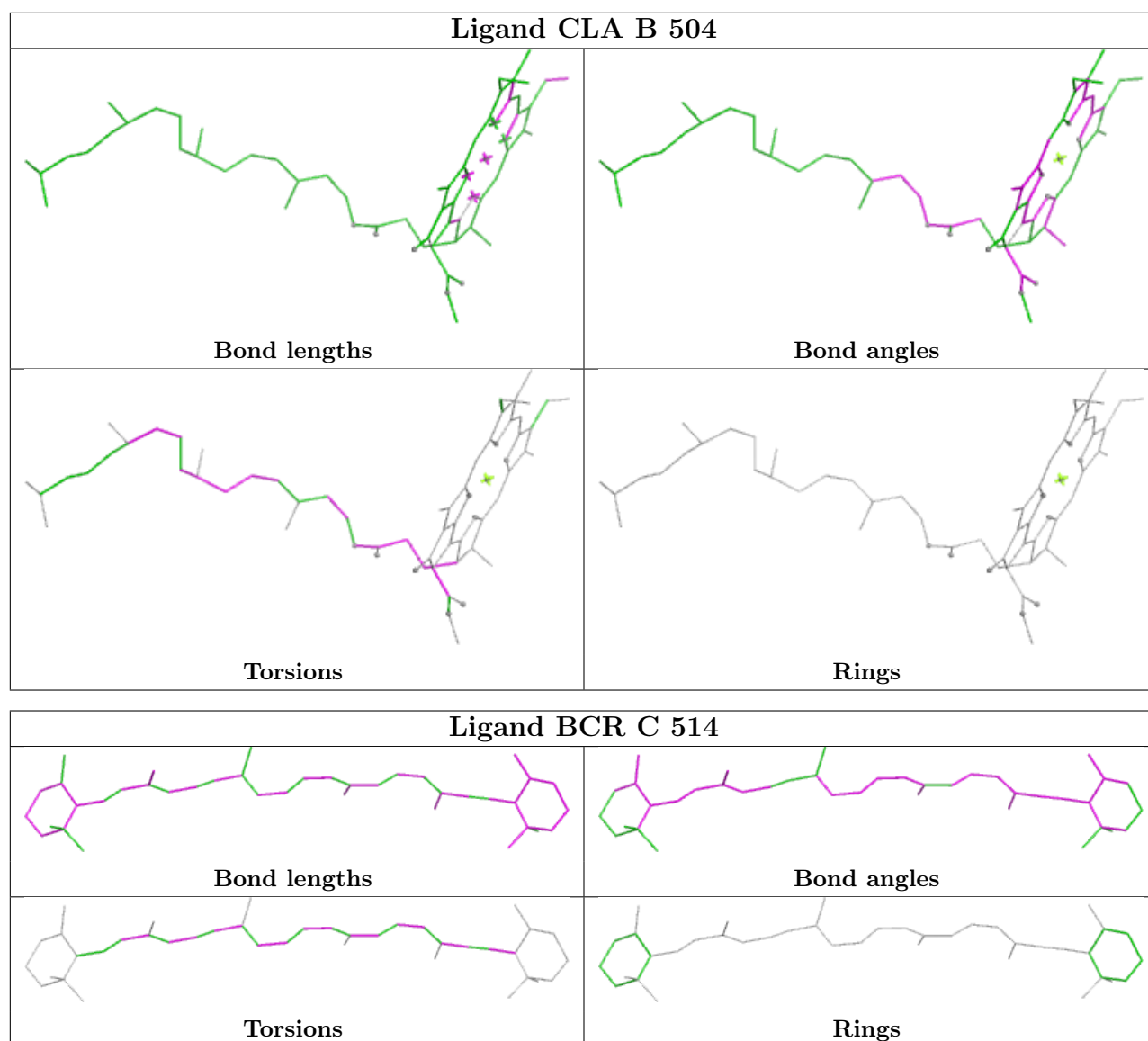


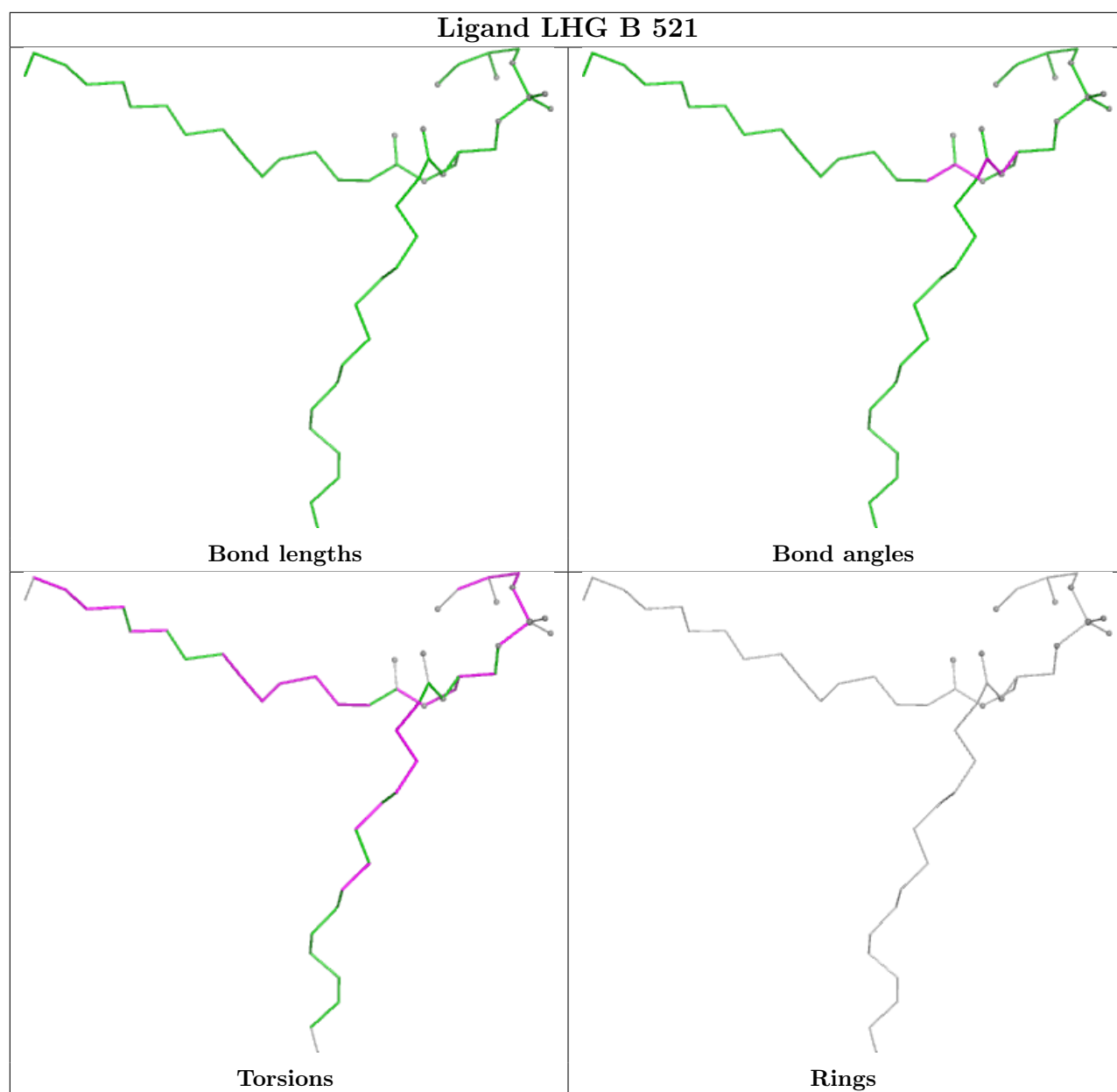




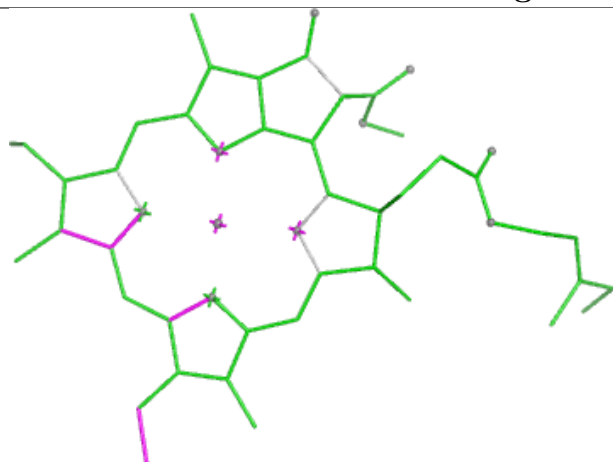




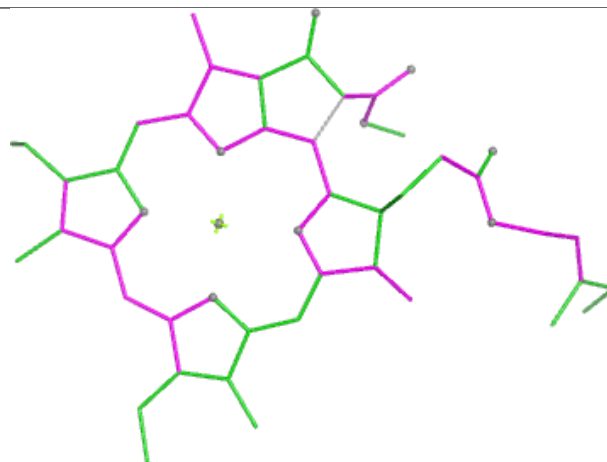




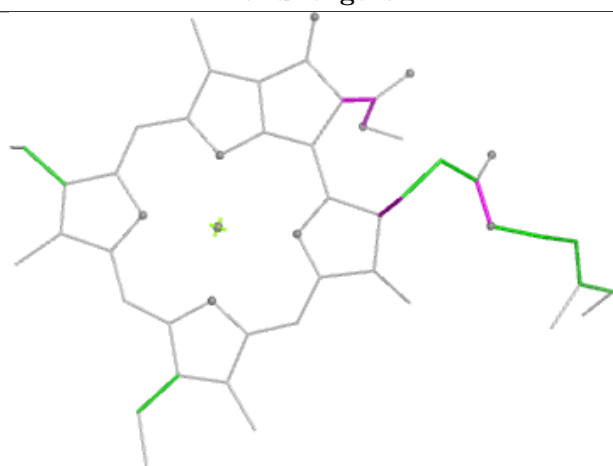
Ligand CLA B 514



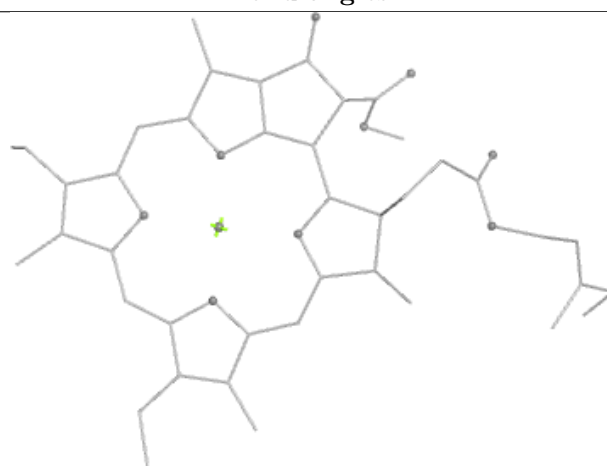
Bond lengths



Bond angles

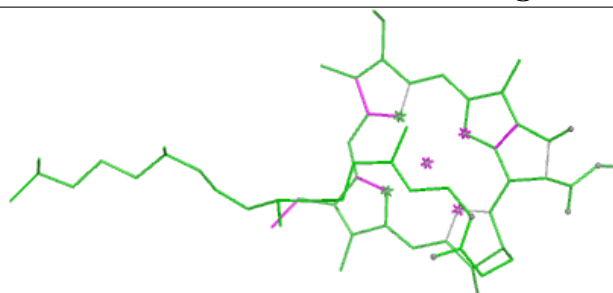


Torsions

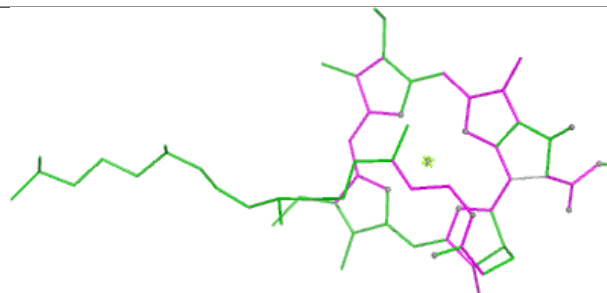


Rings

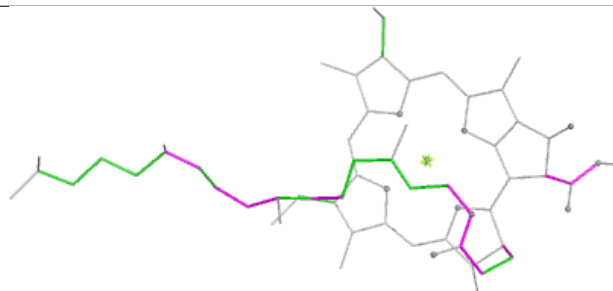
Ligand CLA C 505



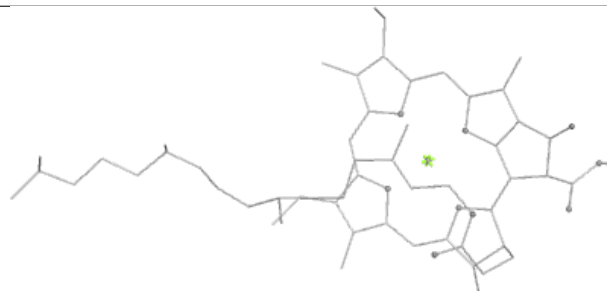
Bond lengths



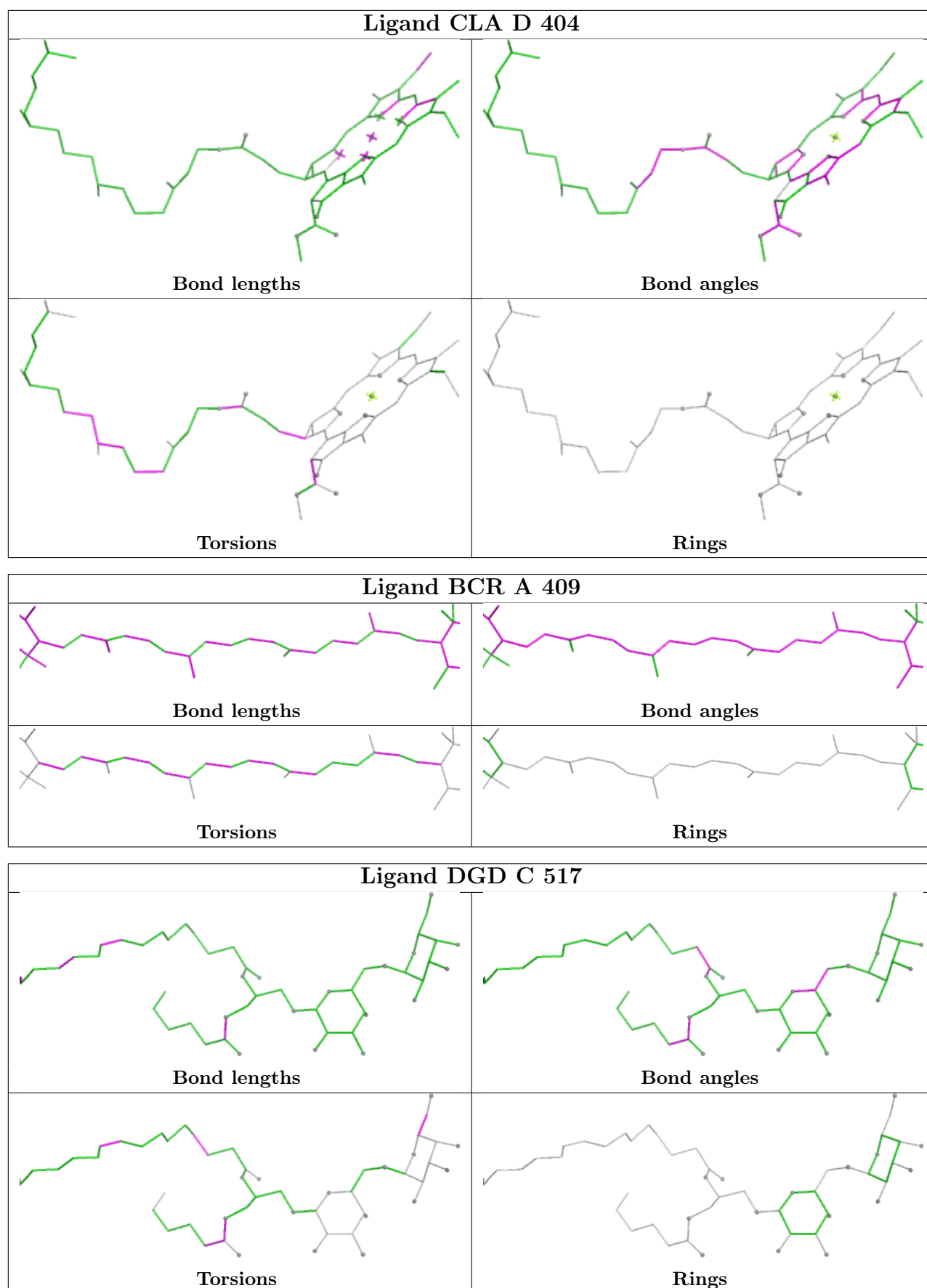
Bond angles

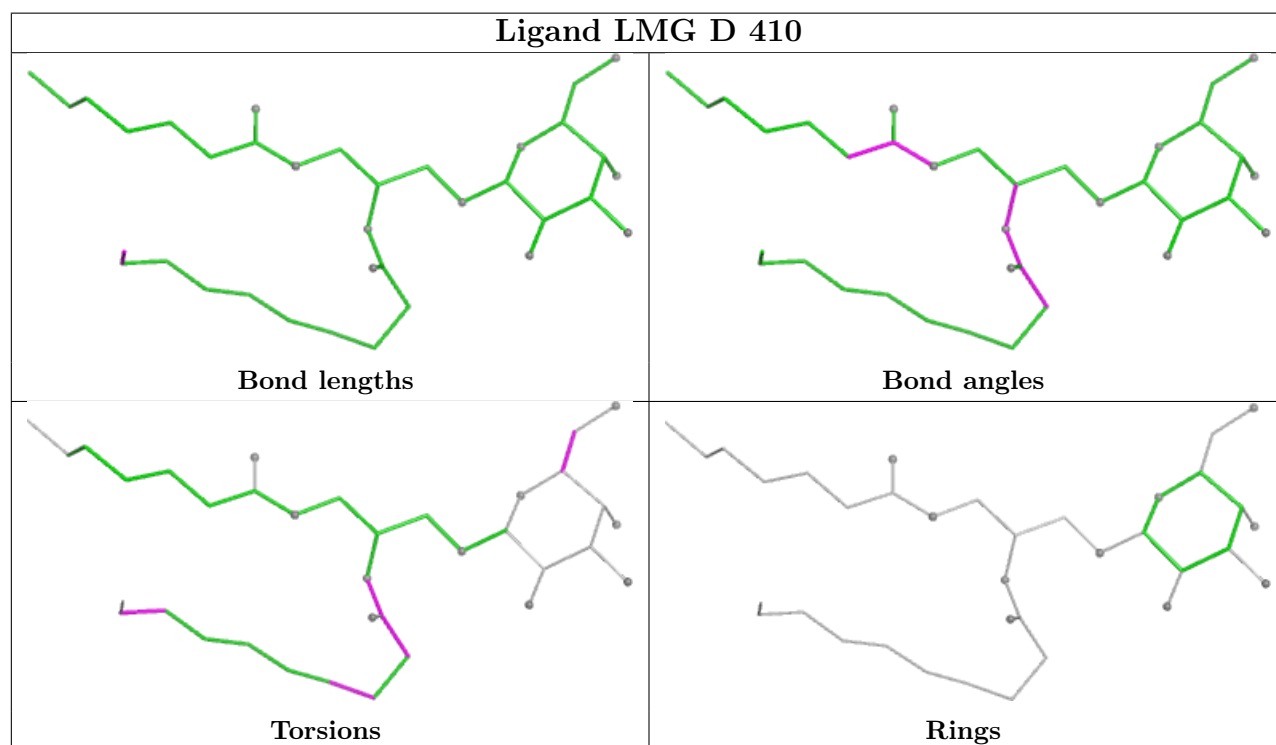
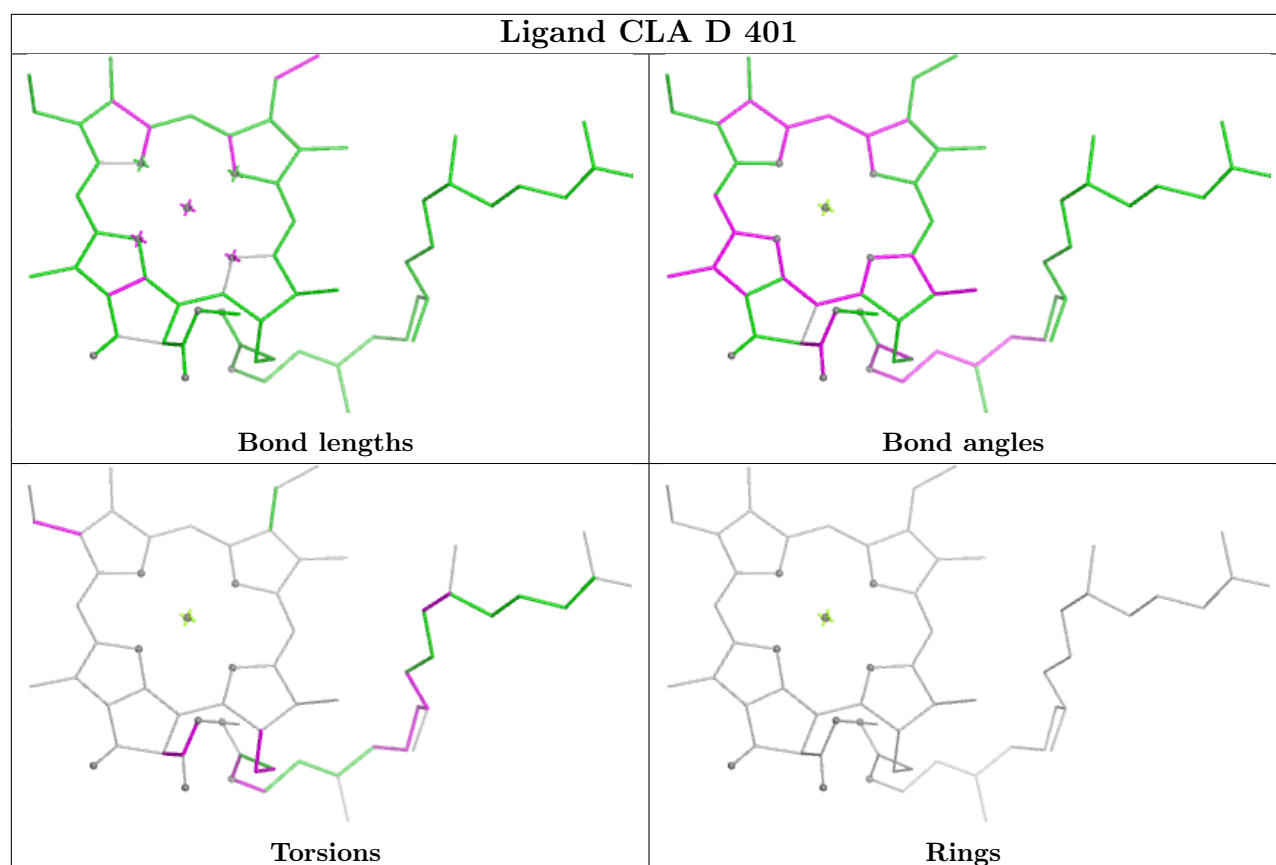


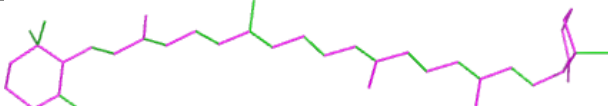
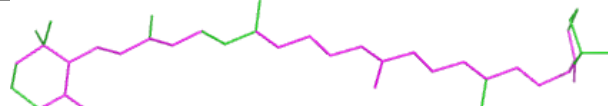
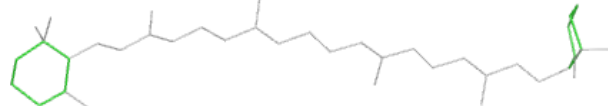
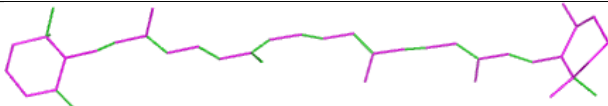
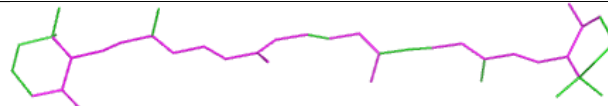
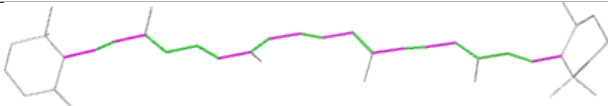
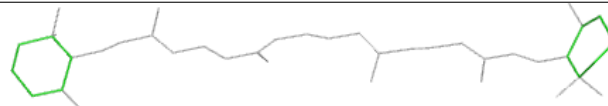
Torsions

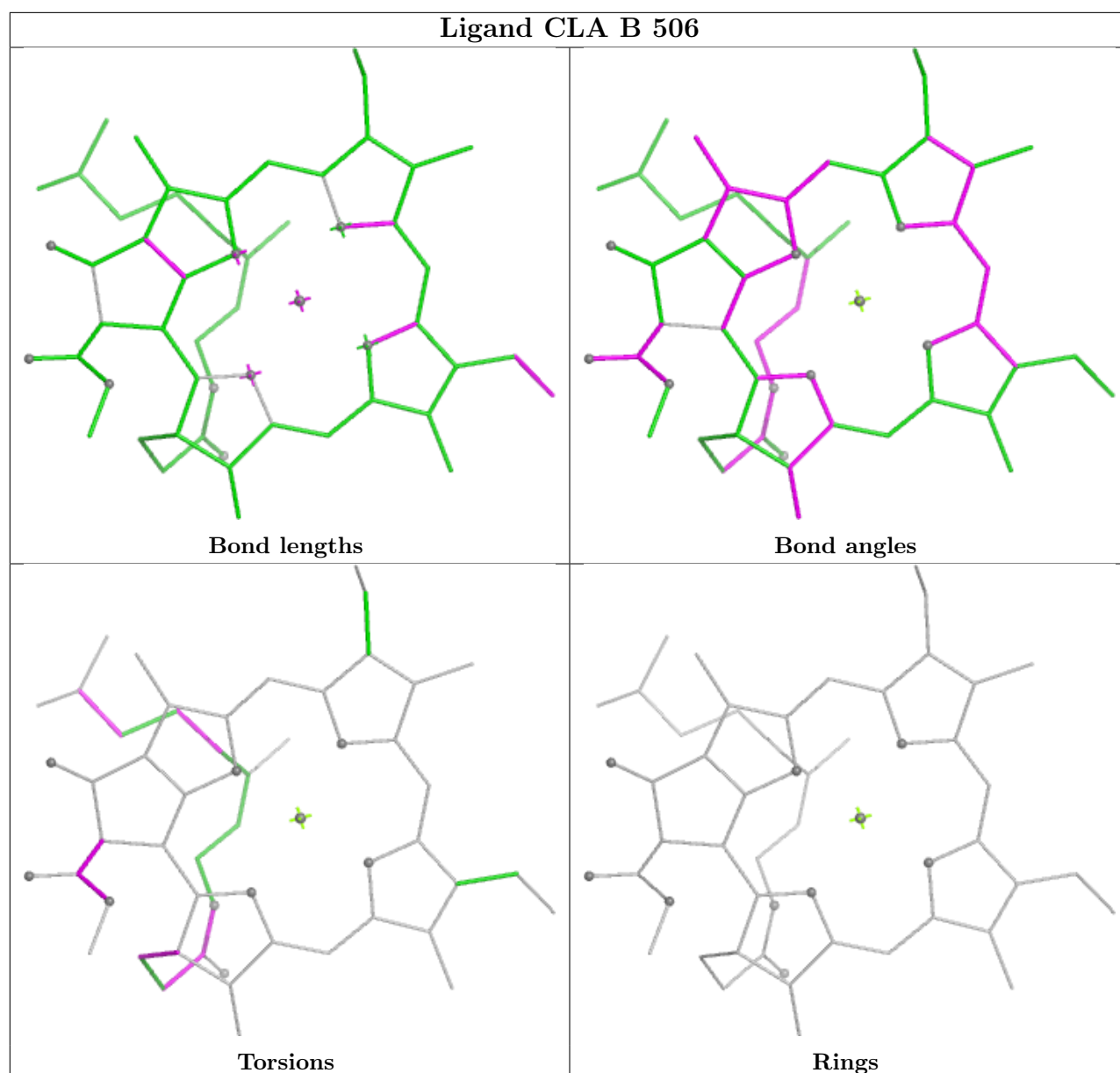


Rings





Ligand BCR D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 515	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

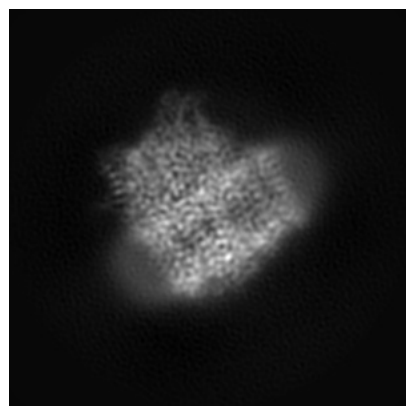
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52077. These allow visual inspection of the internal detail of the map and identification of artifacts.

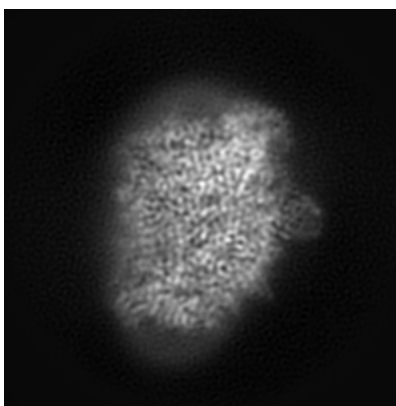
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

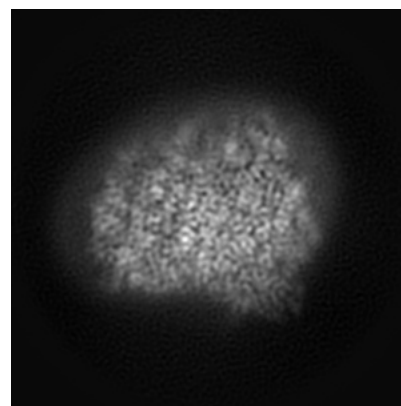
6.1.1 Primary map



X

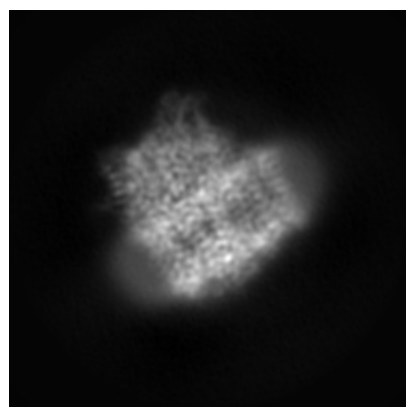


Y

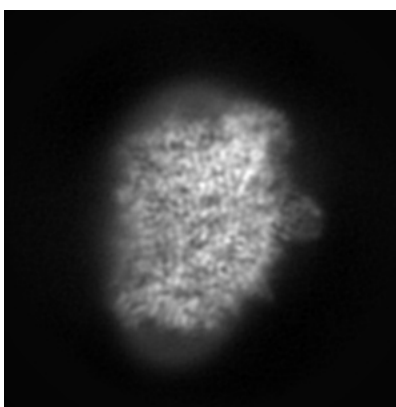


Z

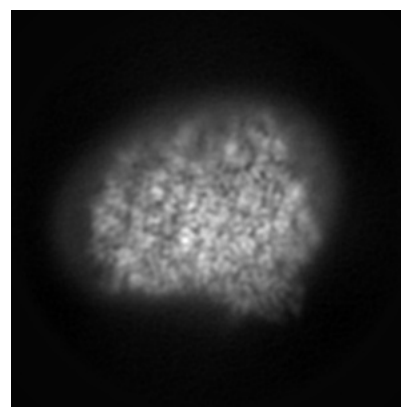
6.1.2 Raw map



X



Y

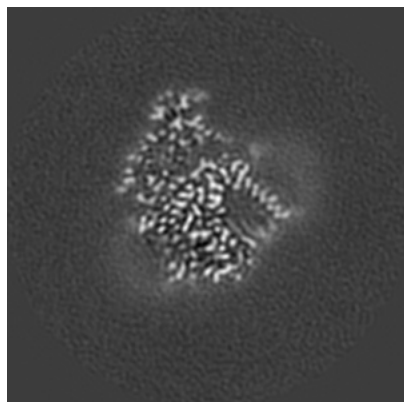


Z

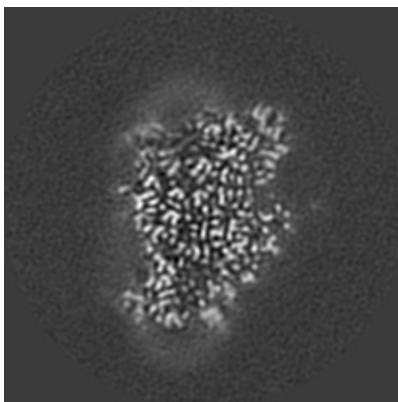
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

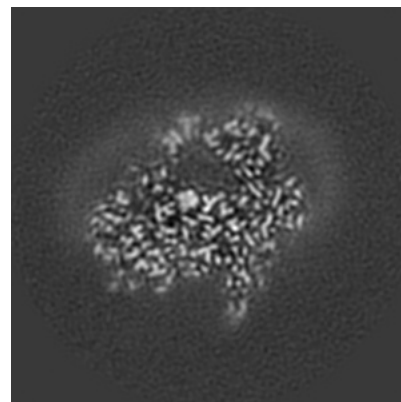
6.2.1 Primary map



X Index: 125

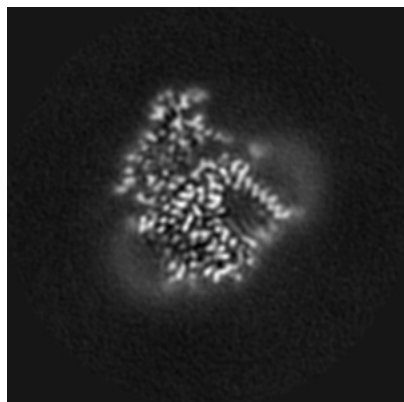


Y Index: 125

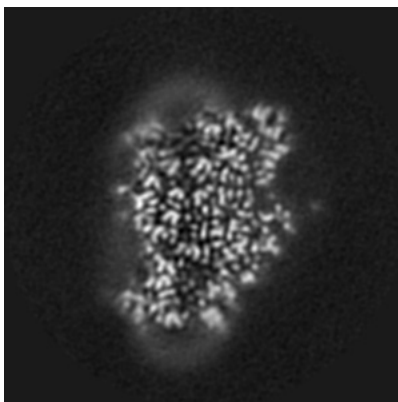


Z Index: 125

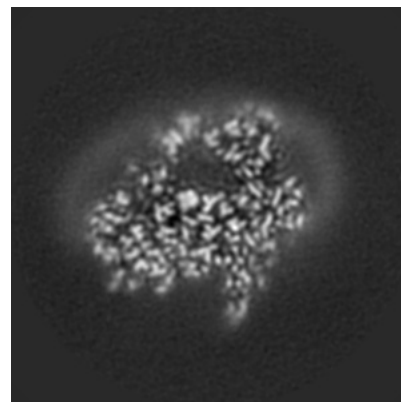
6.2.2 Raw map



X Index: 125



Y Index: 125

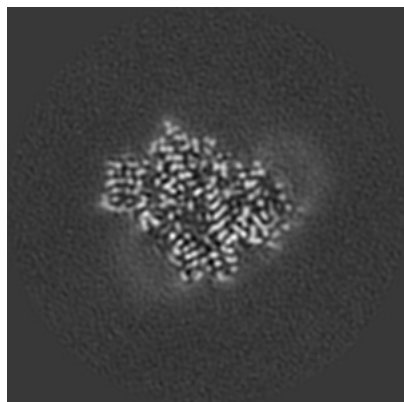


Z Index: 125

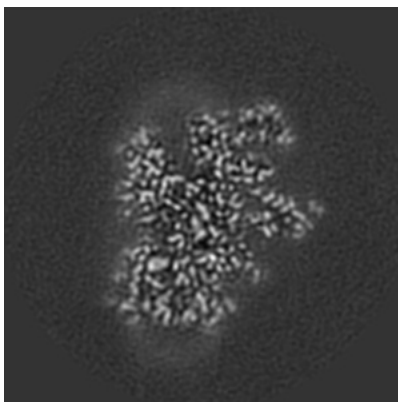
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

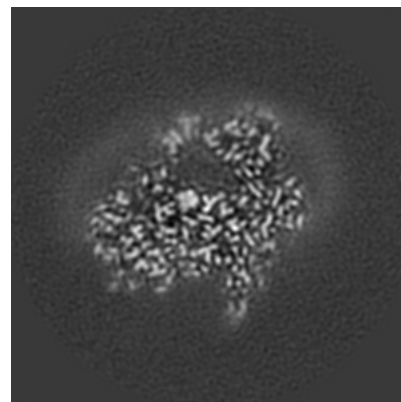
6.3.1 Primary map



X Index: 145

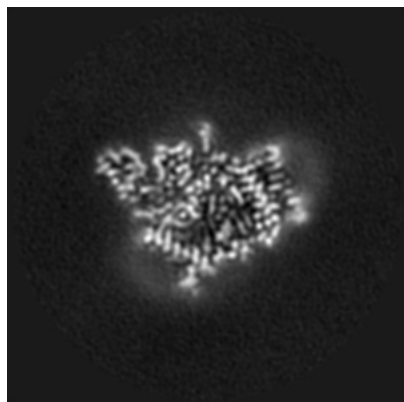


Y Index: 118

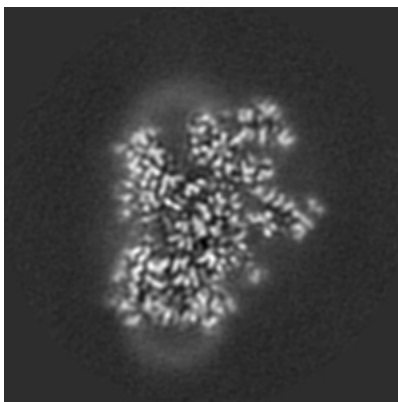


Z Index: 125

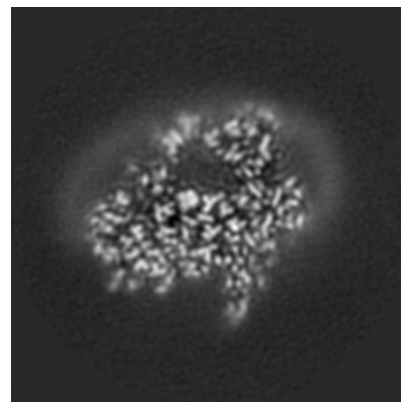
6.3.2 Raw map



X Index: 159



Y Index: 117

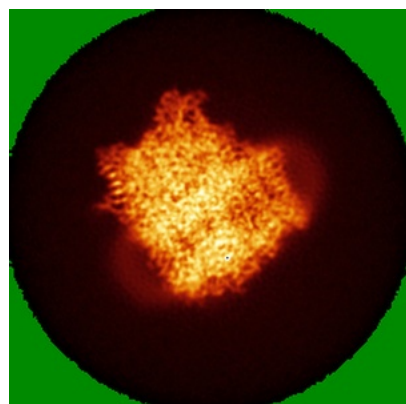


Z Index: 125

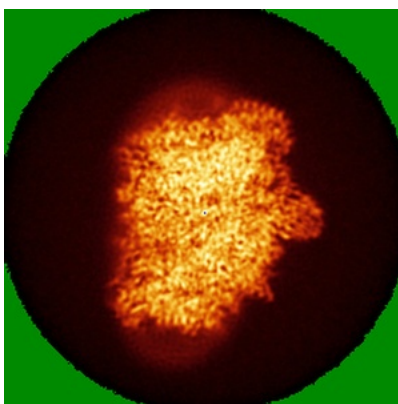
The images above show the largest variance slices of the map in three orthogonal directions.

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

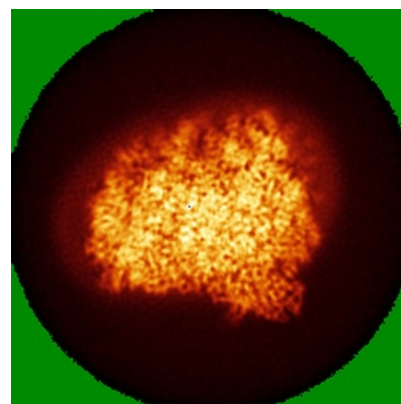
6.4.1 Primary map



X

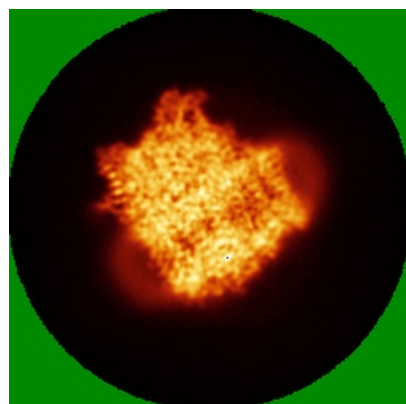


Y

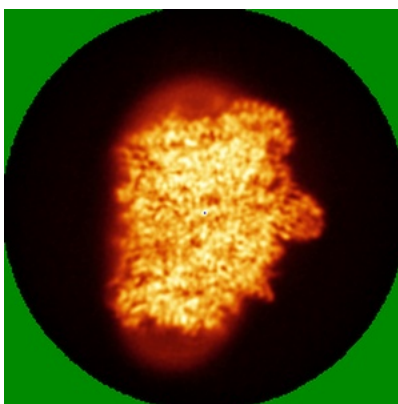


Z

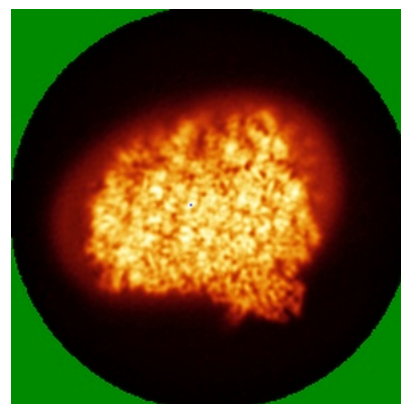
6.4.2 Raw map



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 0.007. 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.

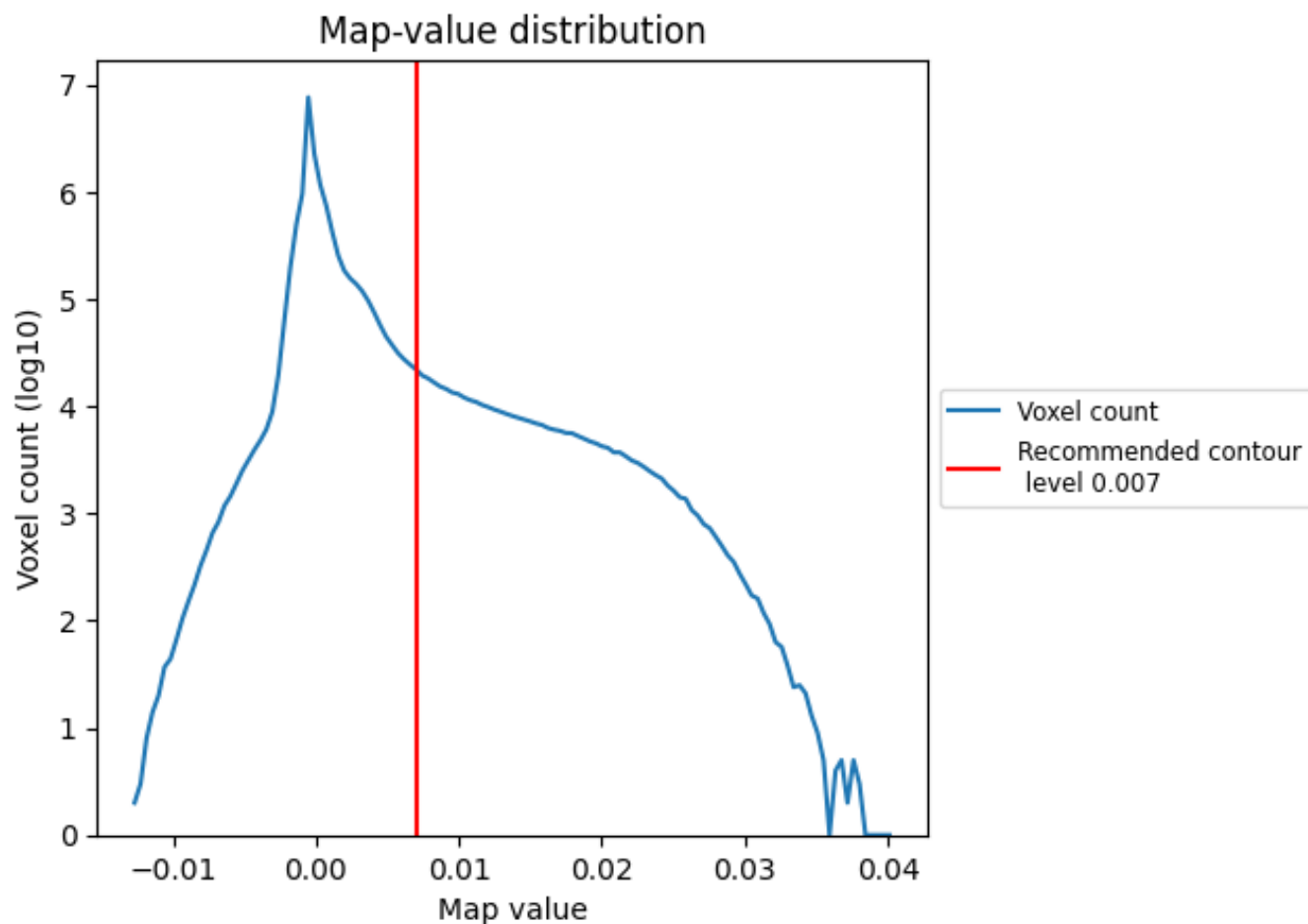
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

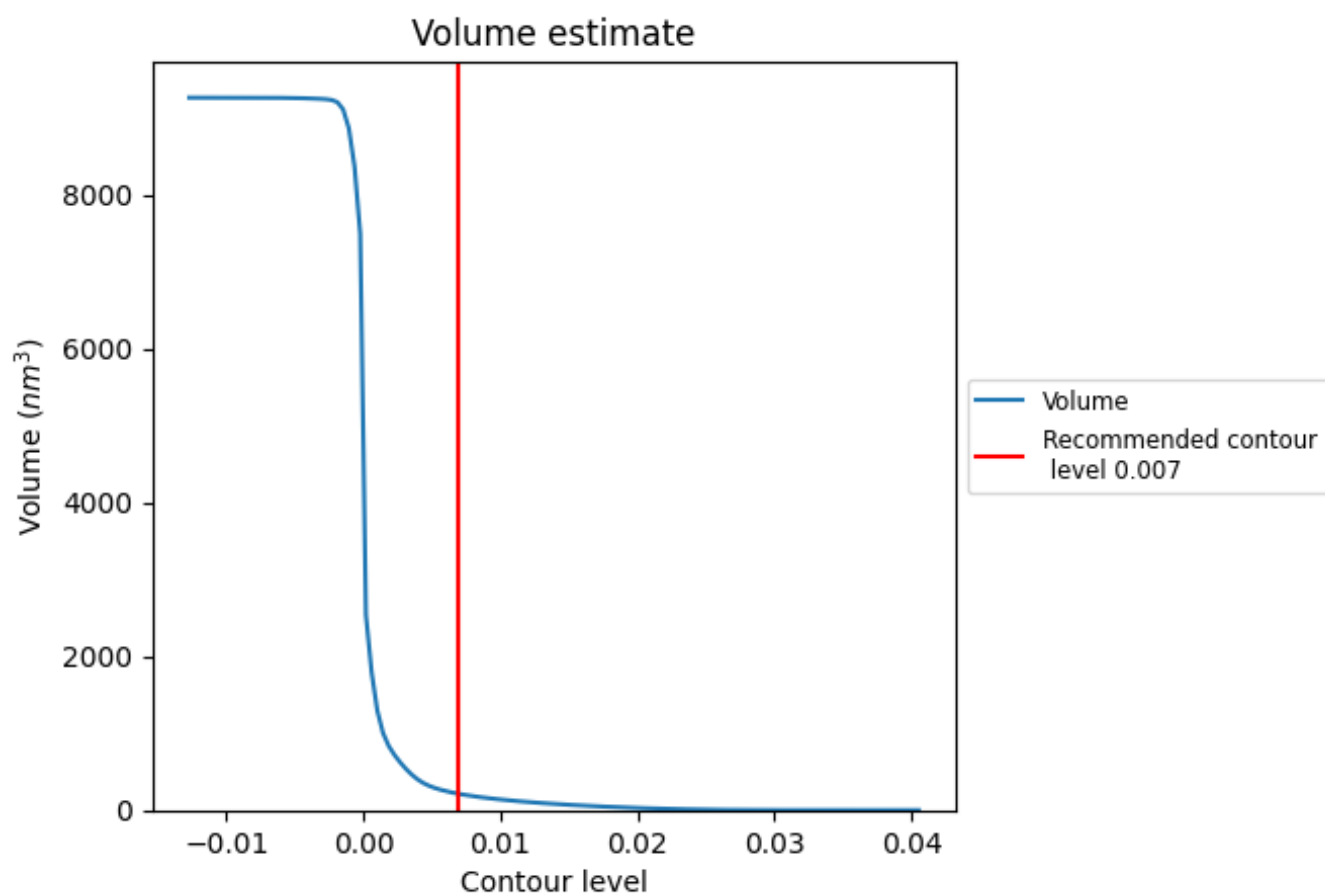
This section contains the results of statistical analysis of the map.

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.

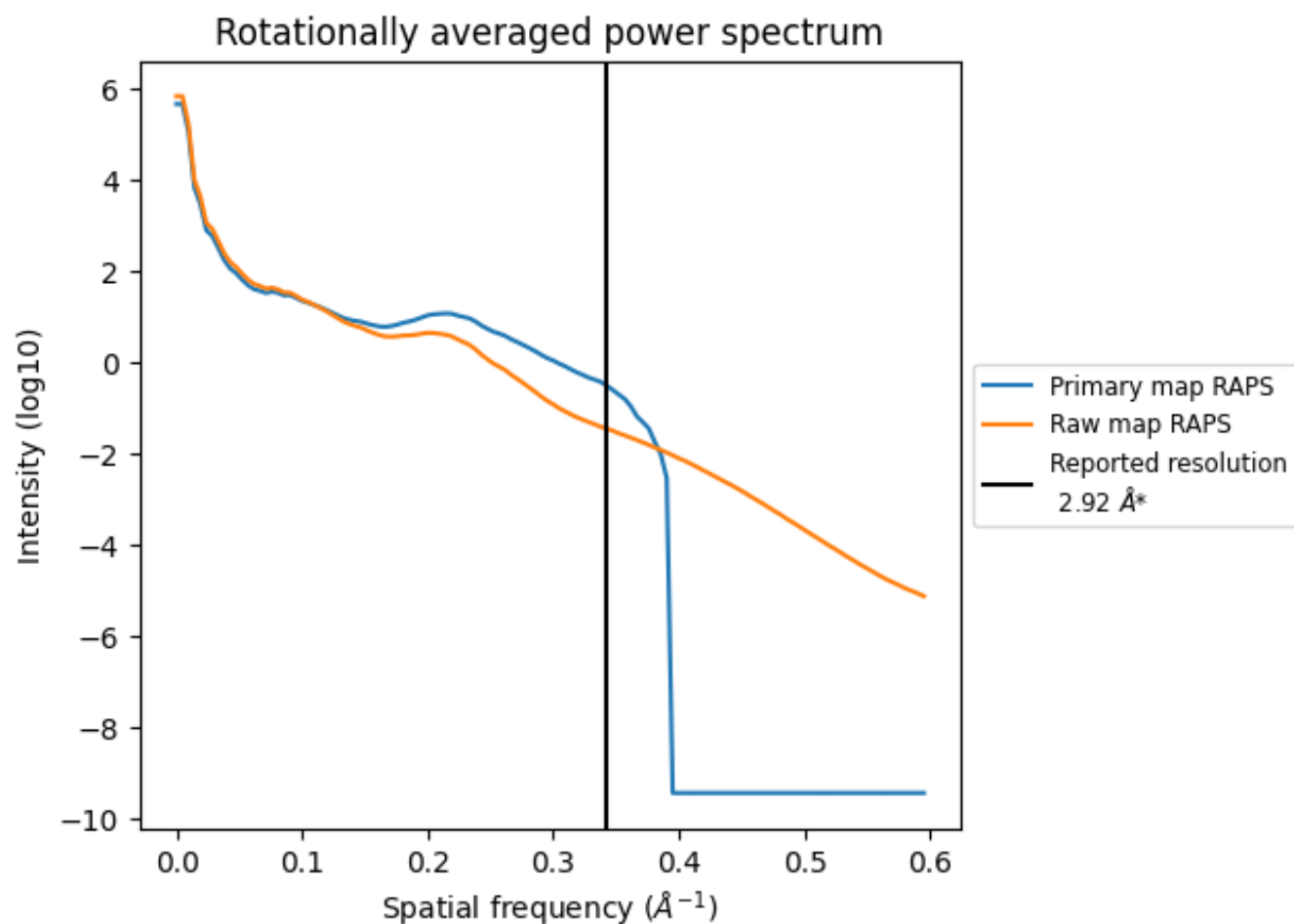
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm³; this corresponds to an approximate mass of 191 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 ⓘ

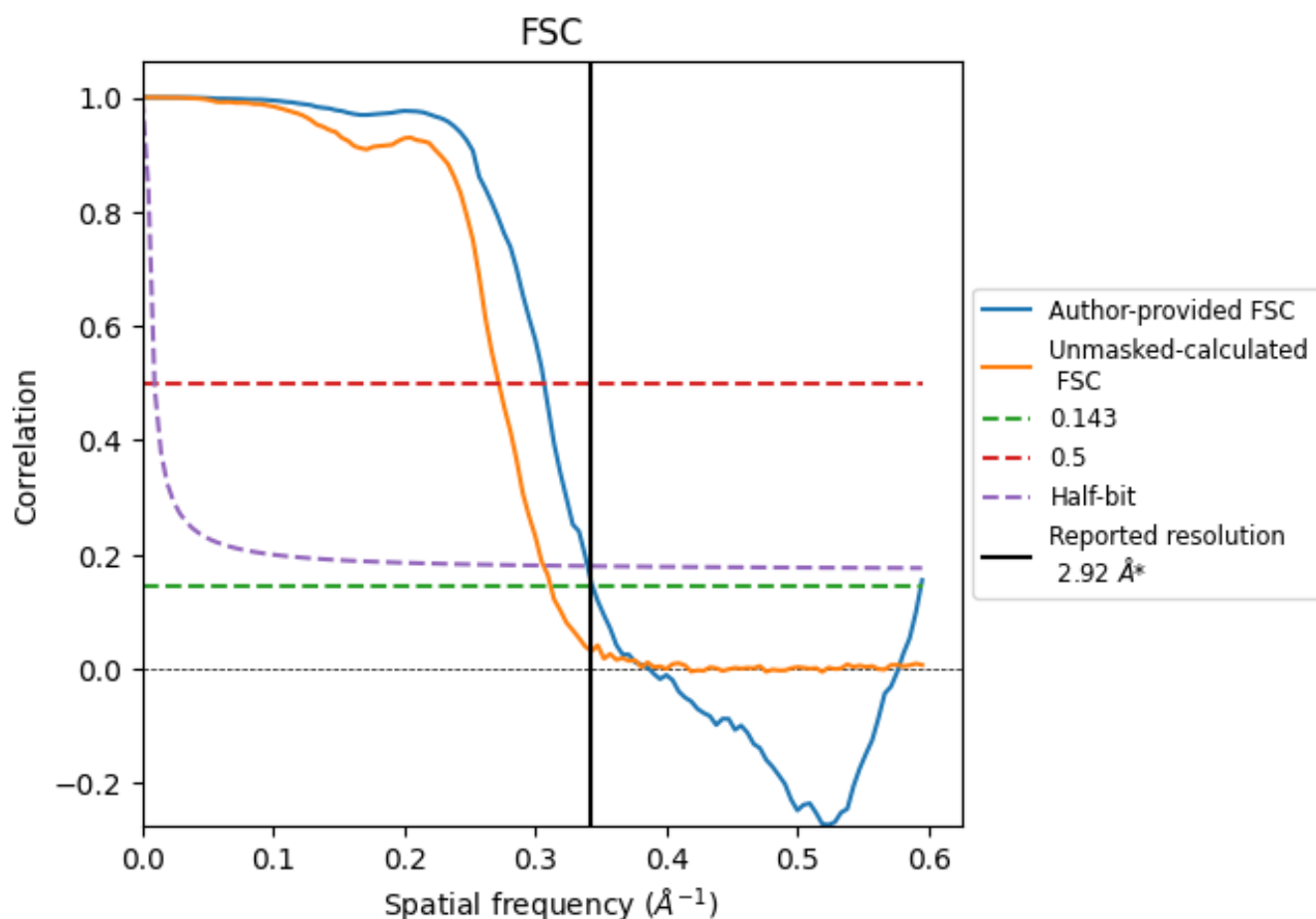


*Reported resolution corresponds to spatial frequency of 0.342 Å⁻¹

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 0.342 Å⁻¹

8.2 Resolution estimates [i](#)

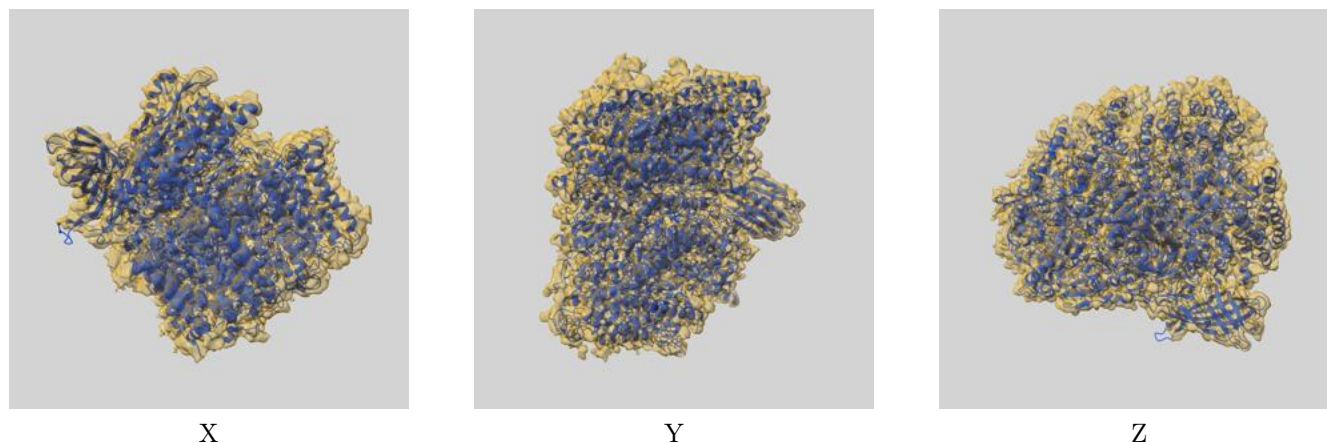
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.91	3.26	2.94
Unmasked-calculated*	3.21	3.68	3.27

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

9 Map-model fit [i](#)

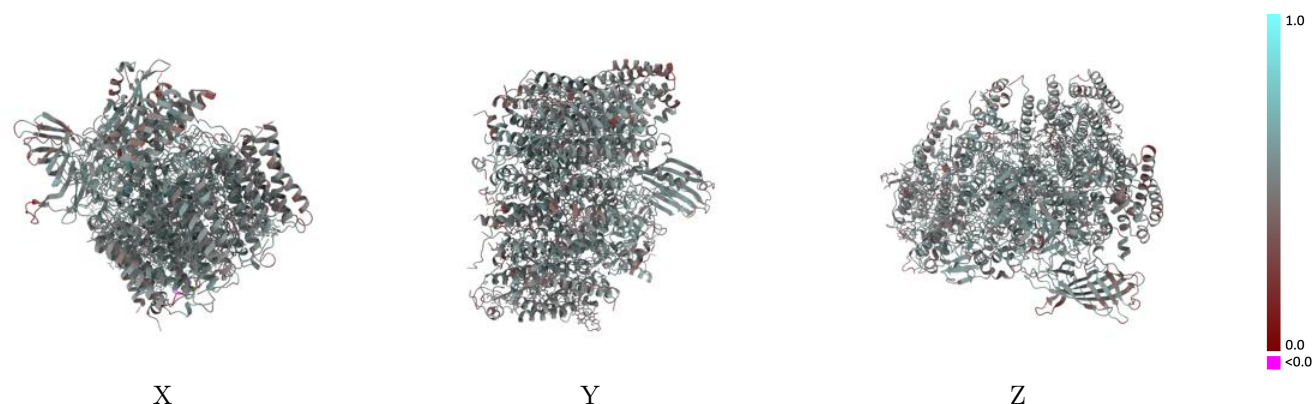
This section contains information regarding the fit between EMDB map EMD-52077 and PDB model 9HEI. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



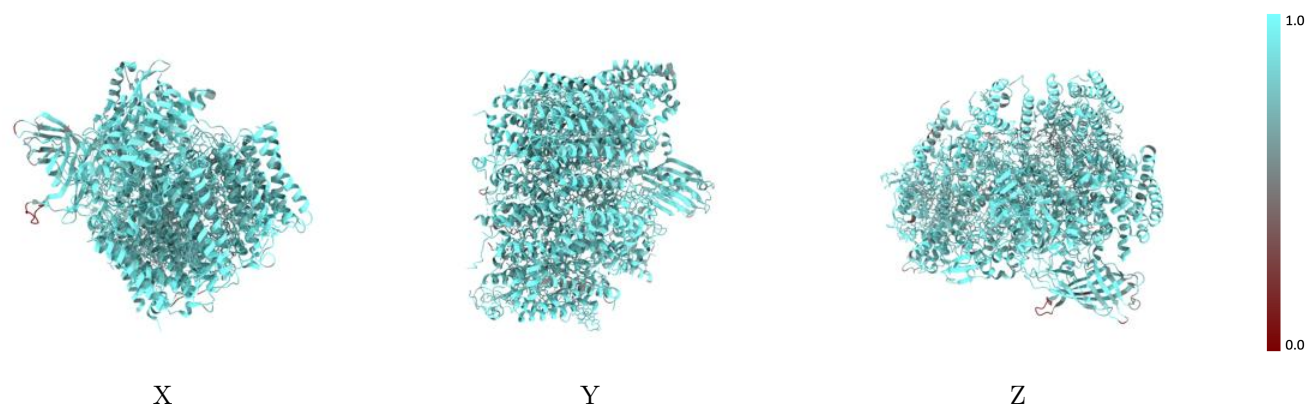
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



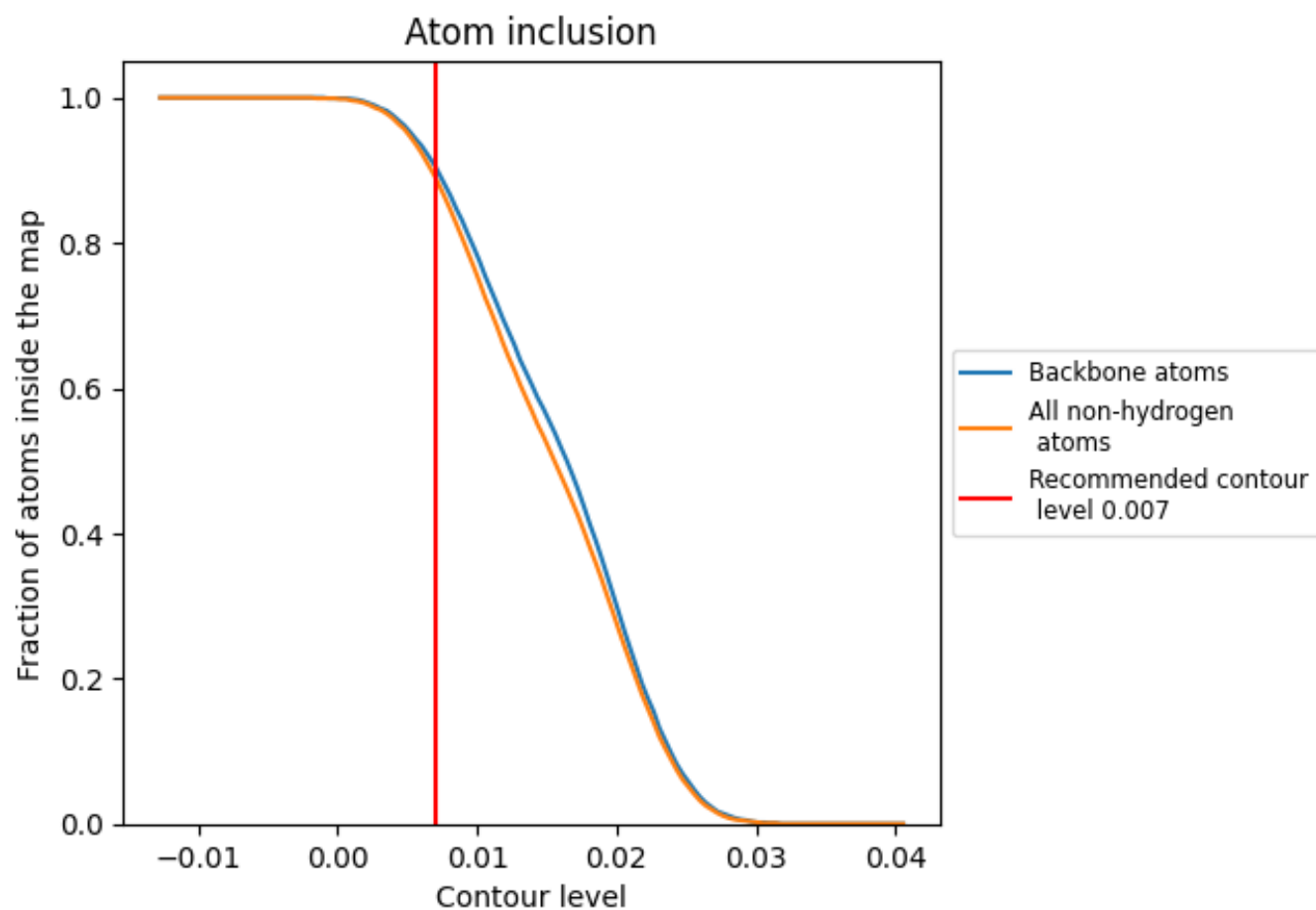
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.5100
A	 0.9240	 0.5290
B	 0.9020	 0.5140
C	 0.9010	 0.5220
D	 0.9240	 0.5440
E	 0.9160	 0.4760
F	 0.9020	 0.4870
H	 0.8590	 0.4820
I	 0.9230	 0.5160
J	 0.8910	 0.4990
K	 0.9280	 0.5190
L	 0.9370	 0.5200
M	 0.8370	 0.4570
O	 0.8160	 0.4860
P	 0.8800	 0.5130
Q	 0.8690	 0.4660
T	 0.8550	 0.4900
U	 0.7130	 0.4130
V	 0.9140	 0.4700
W	 0.8620	 0.4490
X	 0.7590	 0.4610
Z	 0.9060	 0.4630

