



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 10:46 PM EDT

PDB ID : 7SA3 / pdb_00007sa3
EMDB ID : EMD-24943
Title : Structure of a monomeric photosystem II core complex from a cyanobacterium acclimated to far-red light
Authors : Gisriel, C.J.; Bryant, D.A.; Brudvig, G.W.
Deposited on : 2021-09-22
Resolution : 2.25 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:

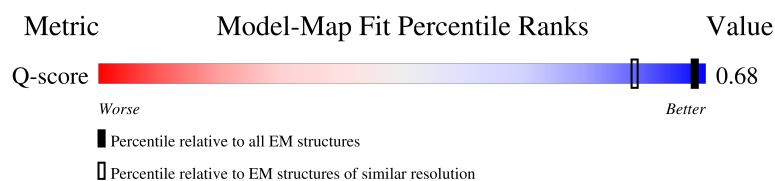
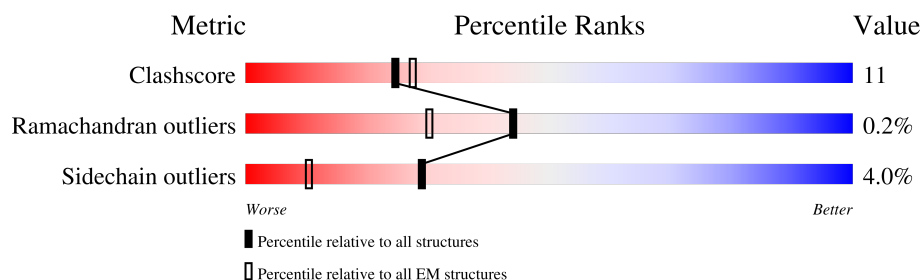
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.25 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.



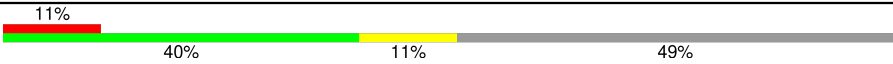
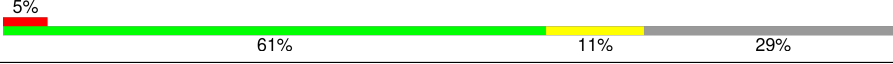
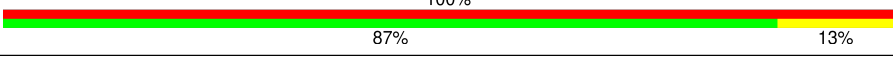
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3458 (1.75 - 2.75)

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	361	
2	B	509	
3	C	482	
4	D	352	

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Mol	Chain	Length	Quality of chain
5	E	80	
6	F	44	
7	I	38	
8	K	45	
9	N	23	

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
13	CL7	A	404	X	-	-	-
17	F6C	B	603	X	-	-	-
17	F6C	B	606	X	-	-	-
17	F6C	B	612	X	-	-	-
17	F6C	C	507	X	-	-	-

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 15960 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 q(B) protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	303	Total	C	N	O	S	0	0
			2382	1572	392	403	15		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	conflict	UNP B4WKH9
A	2	THR	-	conflict	UNP B4WKH9
A	3	THR	-	conflict	UNP B4WKH9
A	4	ILE	-	conflict	UNP B4WKH9
A	5	SER	-	conflict	UNP B4WKH9
A	6	THR	-	conflict	UNP B4WKH9
A	7	ARG	-	conflict	UNP B4WKH9
A	8	PRO	-	conflict	UNP B4WKH9
A	9	THR	-	conflict	UNP B4WKH9
A	10	SER	-	conflict	UNP B4WKH9
A	11	ARG	-	conflict	UNP B4WKH9
A	12	PHE	-	conflict	UNP B4WKH9
A	13	PRO	-	conflict	UNP B4WKH9
A	14	THR	-	conflict	UNP B4WKH9
A	15	TRP	-	conflict	UNP B4WKH9
A	16	ASP	-	conflict	UNP B4WKH9
A	17	ARG	-	conflict	UNP B4WKH9
A	18	PHE	-	conflict	UNP B4WKH9
A	19	CYS	-	conflict	UNP B4WKH9
A	20	ASN	-	conflict	UNP B4WKH9
A	21	TRP	-	conflict	UNP B4WKH9
A	22	VAL	-	conflict	UNP B4WKH9
A	23	THR	-	conflict	UNP B4WKH9
A	24	SER	-	conflict	UNP B4WKH9
A	25	THR	-	conflict	UNP B4WKH9
A	26	GLU	-	conflict	UNP B4WKH9
A	27	ASN	-	conflict	UNP B4WKH9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ARG	-	conflict	UNP B4WKH9
A	29	LEU	-	conflict	UNP B4WKH9
A	30	TYR	-	conflict	UNP B4WKH9
A	31	ILE	-	conflict	UNP B4WKH9
A	32	GLY	-	conflict	UNP B4WKH9
A	33	TRP	-	conflict	UNP B4WKH9
A	34	PHE	-	conflict	UNP B4WKH9
A	35	GLY	-	conflict	UNP B4WKH9
A	36	VAL	-	conflict	UNP B4WKH9
A	37	LEU	-	conflict	UNP B4WKH9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	450	Total	C	N	O	S	0	0
			3528	2316	593	607	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	420	Total	C	N	O	S	0	0
			3272	2154	553	554	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	336	Total	C	N	O	S	0	0
			2671	1770	435	452	14		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	41	Total	C	N	O	0	0
			330	225	49	56		

- 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
			243	165	41	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	27	Total	C	N	O	S	0	0
			213	150	28	34	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	37	Total	C	N	O	0	0
			294	206	45	43		

- Molecule 9 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	N	23	Total	C	N	O	0	0
			115	69	23	23		

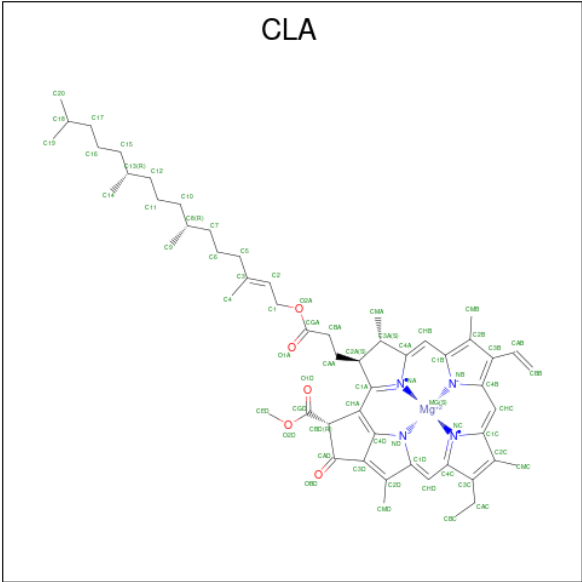
- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Ca	0
			1	1	

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Cl	0
			1	1	

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



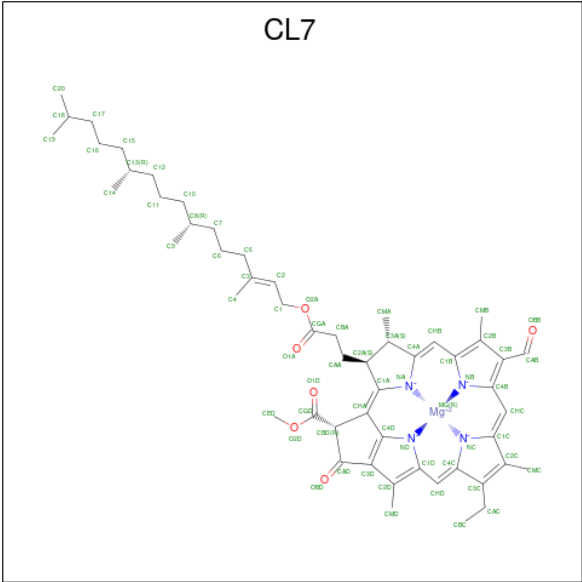
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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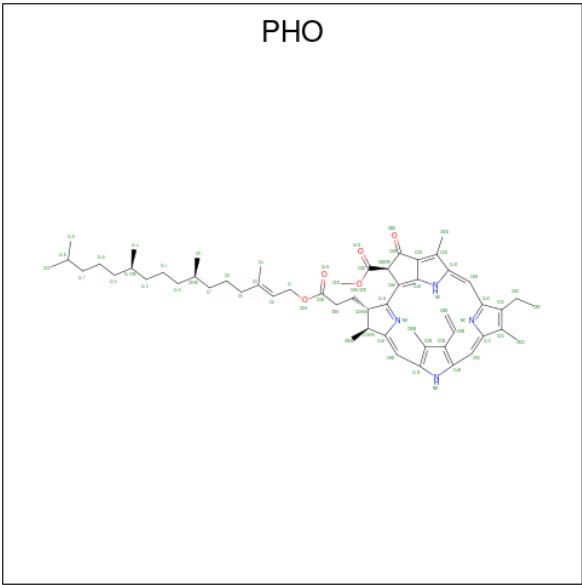
Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	C	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	D	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	D	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 13 is CHLOROPHYLL D (CCD ID: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



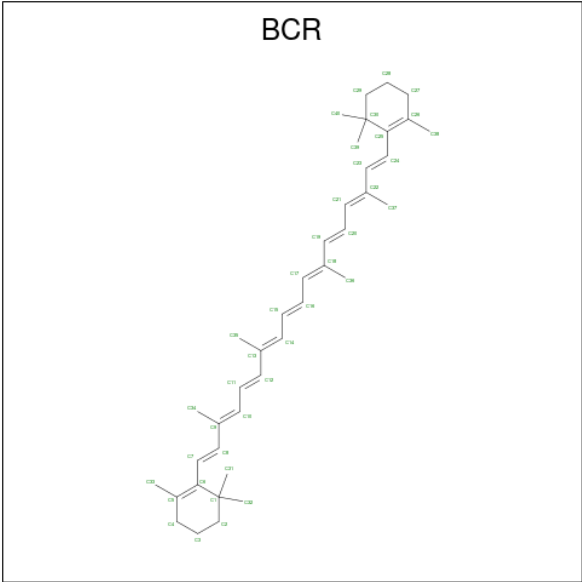
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

- Molecule 14 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



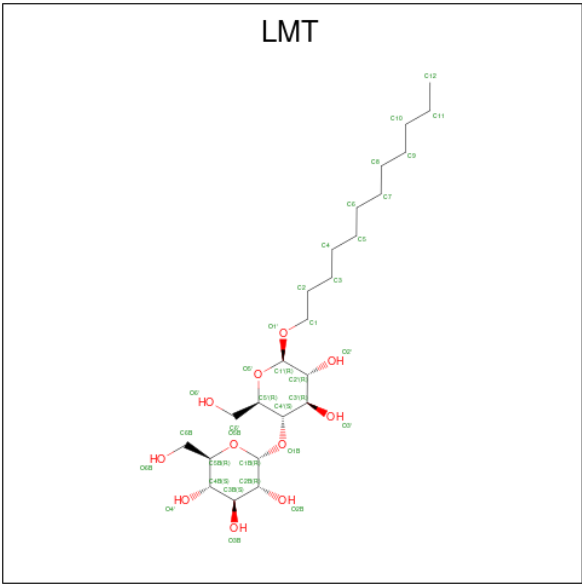
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	N	O	0
			64	55	4	5	
14	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



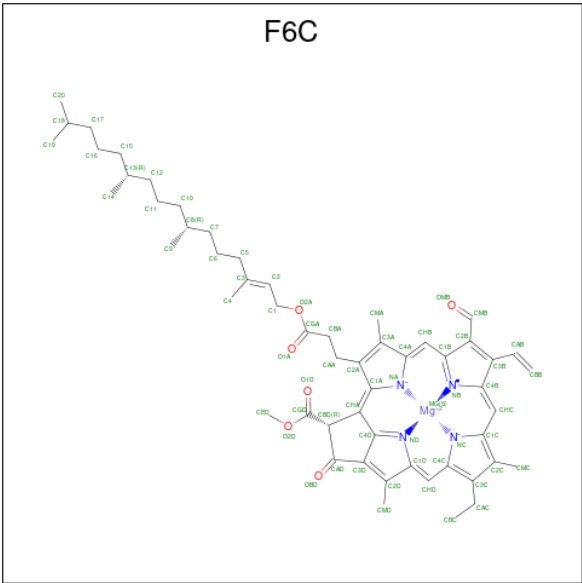
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	C	1	Total C 40 40	0
15	C	1	Total C 40 40	0
15	D	1	Total C 26 26	0

- Molecule 16 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



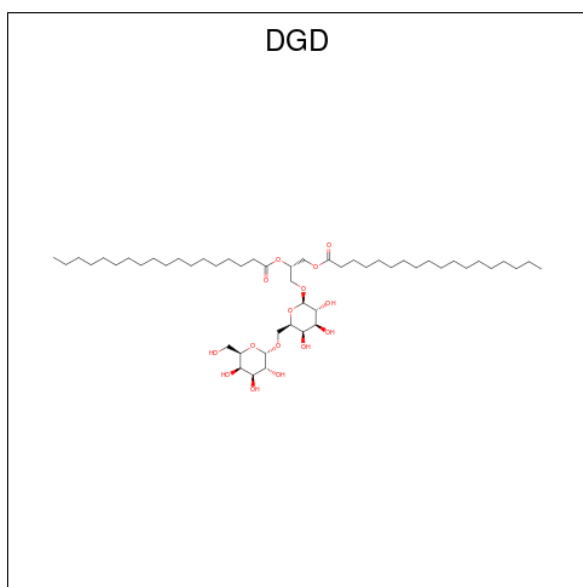
Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	O	0
			35	24	11	
16	A	1	Total	C	O	0
			31	20	11	
16	B	1	Total	C	O	0
			35	24	11	
16	B	1	Total	C	O	0
			30	19	11	
16	C	1	Total	C	O	0
			34	23	11	
16	D	1	Total	C	O	0
			20	15	5	

- Molecule 17 is Chlorophyll F (CCD ID: F6C) (formula: C₅₅H₆₈MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



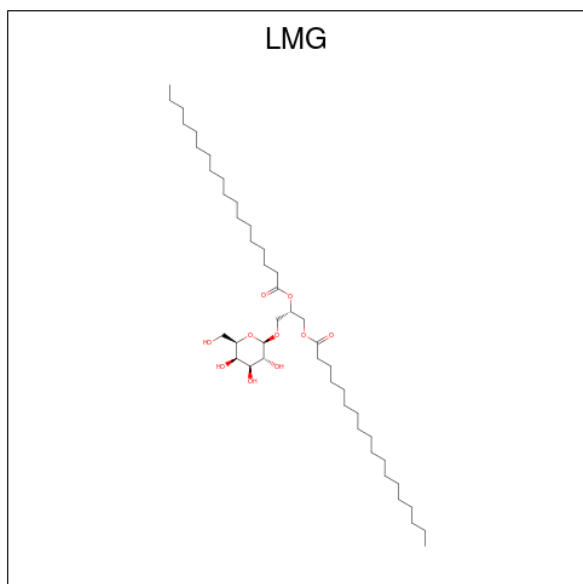
Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	B	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
17	B	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
17	C	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 18 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	C	O	0
			47	38	9	
18	C	1	Total	C	O	0
			47	32	15	

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total	C	O	0
			40	30	10	

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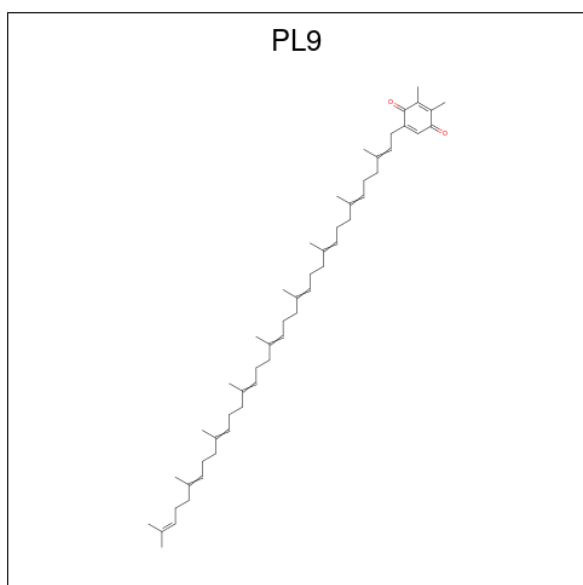
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Mol	Chain	Residues	Atoms			AltConf
19	D	1	Total	C	O	0
			33	23	10	

- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

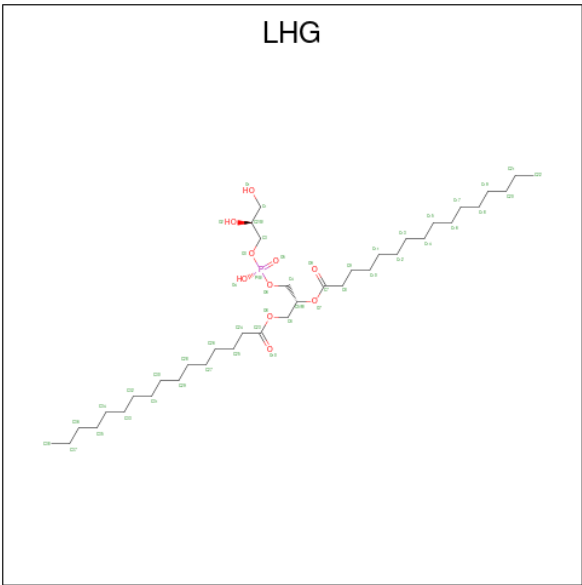
Mol	Chain	Residues	Atoms			AltConf
20	D	1	Total	Fe		0
			1	1		

- Molecule 21 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



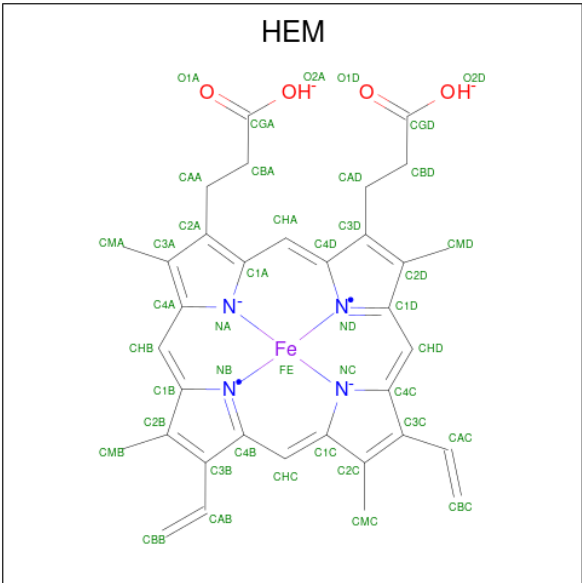
Mol	Chain	Residues	Atoms			AltConf
21	D	1	Total	C	O	0
			45	43	2	

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



Mol	Chain	Residues	Atoms				AltConf
22	D	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 23 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

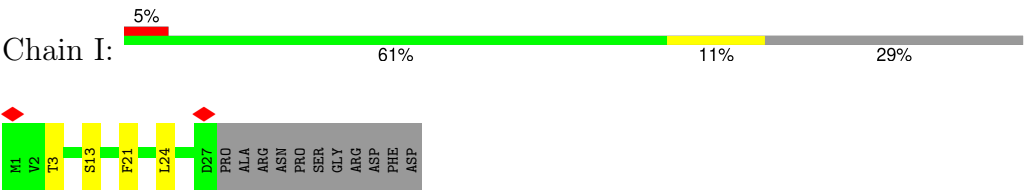


Mol	Chain	Residues	Atoms					AltConf
23	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

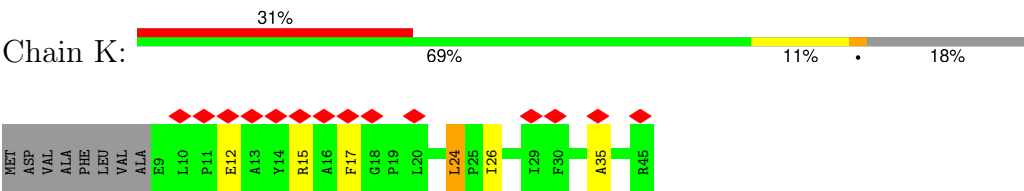
- Molecule 24 is water.

Mol	Chain	Residues	Atoms		AltConf
24	A	61	Total 61	O 61	0
24	B	59	Total 59	O 59	0
24	C	44	Total 44	O 44	0
24	D	65	Total 65	O 65	0
24	I	1	Total 1	O 1	0

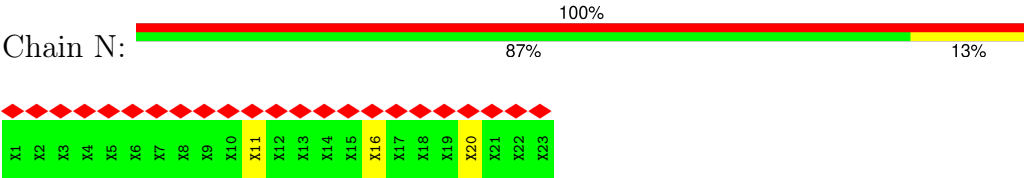
● Molecule 7: Photosystem II reaction center protein I



● Molecule 8: Photosystem II reaction center protein K



● Molecule 9: Unknown



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	315307	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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, LMG, CA, DGD, CLA, HEM, F6C, LMT, CL7, LHG, FE2, CL, PL9, BCR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/2462	0.56	0/3362
2	B	0.38	0/3651	0.57	1/4966 (0.0%)
3	C	0.36	0/3384	0.59	1/4608 (0.0%)
4	D	0.40	0/2760	0.56	0/3751
5	E	0.28	0/345	0.51	0/476
6	F	0.29	0/250	0.71	0/337
7	I	0.21	0/218	0.49	0/294
8	K	0.30	0/305	0.77	0/417
All	All	0.37	0/13375	0.58	2/18211 (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	2
2	B	0	6
8	K	0	1
All	All	0	9

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	19	LEU	N-CA-C	-6.11	106.37	113.88
3	C	226	TRP	N-CA-CB	-5.21	101.69	110.49

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	335	ARG	Peptide
1	A	340	PHE	Peptide
2	B	135	LEU	Peptide
2	B	384	ARG	Peptide
2	B	385	GLN	Peptide

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	2382	0	2311	75	0
2	B	3528	0	3377	49	0
3	C	3272	0	3190	66	0
4	D	2671	0	2592	83	0
5	E	330	0	310	6	0
6	F	243	0	252	6	0
7	I	213	0	226	3	0
8	K	294	0	301	4	0
9	N	115	0	25	2	0
10	A	1	0	0	0	0
11	A	1	0	0	0	0
12	A	175	0	170	12	0
12	B	610	0	562	38	0
12	C	695	0	688	40	0
12	D	105	0	92	3	0
13	A	65	0	70	3	0
14	A	64	0	74	5	0
14	D	64	0	74	2	0
15	A	40	0	49	5	0
15	B	40	0	49	2	0
15	C	80	0	98	6	0
15	D	26	0	29	1	0
16	A	66	0	78	3	0
16	B	65	0	78	1	0
16	C	34	0	40	2	0
16	D	20	0	24	0	0
17	B	168	0	0	8	0
17	C	61	0	0	2	0
18	B	47	0	66	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	C	47	0	52	2	0
19	B	40	0	50	1	0
19	D	33	0	36	2	0
20	D	1	0	0	0	0
21	D	45	0	61	4	0
22	D	46	0	65	7	0
23	F	43	0	30	4	0
24	A	61	0	0	6	0
24	B	59	0	0	1	0
24	C	44	0	0	6	0
24	D	65	0	0	2	0
24	I	1	0	0	0	0
All	All	15960	0	15119	327	0

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

The worst 5 of 327 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)
1:A:330:GLU:OE1	3:C:408:ASN:ND2	1.64	1.30
1:A:190:GLU:O	3:C:407:LEU:HG	1.30	1.29
24:A:556:HOH:O	3:C:407:LEU:HD23	1.55	1.05
1:A:335:ARG:NH2	24:A:501:HOH:O	1.89	1.03
2:B:388:SER:OG	2:B:394:GLN:NE2	2.01	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/361 (82%)	290 (98%)	7 (2%)	0	100	100
2	B	444/509 (87%)	427 (96%)	16 (4%)	1 (0%)	43	50
3	C	414/482 (86%)	391 (94%)	22 (5%)	1 (0%)	43	50
4	D	334/352 (95%)	324 (97%)	8 (2%)	2 (1%)	21	21
5	E	39/80 (49%)	37 (95%)	2 (5%)	0	100	100
6	F	28/44 (64%)	25 (89%)	3 (11%)	0	100	100
7	I	25/38 (66%)	25 (100%)	0	0	100	100
8	K	35/45 (78%)	33 (94%)	2 (6%)	0	100	100
All	All	1616/1911 (85%)	1552 (96%)	60 (4%)	4 (0%)	44	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	384	ARG
3	C	86	PRO
4	D	242	GLU
4	D	232	PHE

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	249/299 (83%)	243 (98%)	6 (2%)	43	54
2	B	358/410 (87%)	349 (98%)	9 (2%)	42	52
3	C	321/372 (86%)	303 (94%)	18 (6%)	19	20
4	D	273/290 (94%)	261 (96%)	12 (4%)	25	29
5	E	33/69 (48%)	30 (91%)	3 (9%)	9	7
6	F	24/37 (65%)	21 (88%)	3 (12%)	4	3
7	I	24/33 (73%)	23 (96%)	1 (4%)	26	31
8	K	29/37 (78%)	28 (97%)	1 (3%)	32	40
All	All	1311/1547 (85%)	1258 (96%)	53 (4%)	29	34

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	375	LYS
4	D	119	VAL
6	F	33	LEU
3	C	380	LEU
3	C	413	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	62	HIS
3	C	285	GLN
4	D	219	GLN
3	C	82	ASN
3	C	314	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 56 ligands modelled in this entry, 3 are monoatomic - leaving 53 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
12	CLA	C	501	3	69,73,73	2.20	21 (30%)	82,113,113	2.52	27 (32%)
15	BCR	A	408	-	41,41,41	2.74	6 (14%)	56,56,56	6.60	24 (42%)
12	CLA	D	404	4	49,53,73	2.51	22 (44%)	58,89,113	2.83	24 (41%)
12	CLA	C	503	3	69,73,73	2.19	21 (30%)	82,113,113	2.46	26 (31%)
15	BCR	C	517	-	41,41,41	2.64	6 (14%)	56,56,56	6.57	21 (37%)
12	CLA	B	604	2	59,63,73	2.43	22 (37%)	70,101,113	2.64	26 (37%)
14	PHO	A	406	-	58,69,69	2.09	9 (15%)	55,99,99	1.54	6 (10%)
12	CLA	C	502	3	69,73,73	2.21	21 (30%)	82,113,113	2.49	25 (30%)
12	CLA	C	513	-	49,53,73	2.54	21 (42%)	58,89,113	2.71	21 (36%)
18	DGD	C	515	-	48,48,67	1.16	4 (8%)	62,62,81	1.35	5 (8%)
15	BCR	C	514	-	41,41,41	2.68	6 (14%)	56,56,56	6.55	18 (32%)
17	F6C	B	603	2	57,59,74	3.08	30 (52%)	65,96,114	3.49	34 (52%)
12	CLA	A	405	24	54,58,73	2.52	22 (40%)	64,95,113	2.79	27 (42%)
12	CLA	B	602	2	59,63,73	2.41	20 (33%)	70,101,113	2.66	29 (41%)
13	CL7	A	404	24	69,73,73	2.27	22 (31%)	80,113,113	2.36	25 (31%)
16	LMT	D	409	-	20,20,36	1.42	4 (20%)	23,24,47	1.73	4 (17%)
17	F6C	B	612	2	62,64,74	2.93	30 (48%)	71,102,114	3.38	32 (45%)
12	CLA	C	506	3	59,63,73	2.44	22 (37%)	70,101,113	2.54	27 (38%)
19	LMG	B	617	-	40,40,55	1.20	4 (10%)	48,48,63	1.26	5 (10%)
12	CLA	B	607	2	69,73,73	2.25	21 (30%)	82,113,113	2.39	30 (36%)
12	CLA	B	608	2	49,53,73	2.53	23 (46%)	58,89,113	2.84	21 (36%)
17	F6C	C	507	24	67,69,74	2.83	30 (44%)	77,108,114	3.25	32 (41%)
21	PL9	D	406	-	45,45,55	1.54	5 (11%)	56,57,69	1.50	10 (17%)
17	F6C	B	606	24	67,69,74	2.84	27 (40%)	77,108,114	3.57	34 (44%)
23	HEM	F	101	5,6	50,50,50	1.41	9 (18%)	67,82,82	1.06	3 (4%)
12	CLA	B	605	2	59,63,73	2.41	20 (33%)	70,101,113	2.63	27 (38%)
19	LMG	D	408	-	33,33,55	1.15	2 (6%)	41,41,63	1.10	3 (7%)
16	LMT	A	409	-	36,36,36	1.17	6 (16%)	47,47,47	1.14	3 (6%)
12	CLA	C	511	3	49,53,73	2.50	21 (42%)	58,89,113	2.82	23 (39%)
12	CLA	C	512	3	49,53,73	2.50	19 (38%)	58,89,113	2.80	22 (37%)
12	CLA	B	609	-	49,53,73	2.51	21 (42%)	58,89,113	2.86	23 (39%)
12	CLA	C	505	3	69,73,73	2.23	20 (28%)	82,113,113	2.39	24 (29%)
12	CLA	B	610	2	59,63,73	2.39	19 (32%)	70,101,113	2.58	28 (40%)
12	CLA	A	407	1	64,68,73	2.30	20 (31%)	76,107,113	2.53	24 (31%)
22	LHG	D	407	-	45,45,48	0.92	2 (4%)	48,51,54	1.13	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	C	508	3	69,73,73	2.24	23 (33%)	82,113,113	2.48	26 (31%)
12	CLA	D	403	4	64,68,73	2.27	20 (31%)	76,107,113	2.74	25 (32%)
16	LMT	C	516	-	35,35,36	1.18	6 (17%)	46,46,47	0.96	0
12	CLA	B	611	2	69,73,73	2.20	20 (28%)	82,113,113	2.48	24 (29%)
12	CLA	C	504	24	54,58,73	2.49	21 (38%)	64,95,113	2.76	25 (39%)
12	CLA	B	614	2	54,58,73	2.49	23 (42%)	64,95,113	2.80	27 (42%)
12	CLA	A	403	1	69,73,73	2.19	20 (28%)	82,113,113	2.53	27 (32%)
16	LMT	A	410	-	32,32,36	1.29	5 (15%)	43,43,47	1.25	5 (11%)
14	PHO	D	402	-	58,69,69	2.15	9 (15%)	55,99,99	1.70	10 (18%)
12	CLA	C	510	3	69,73,73	2.21	21 (30%)	82,113,113	2.56	27 (32%)
15	BCR	B	615	-	41,41,41	2.76	6 (14%)	56,56,56	6.52	22 (39%)
16	LMT	B	618	-	36,36,36	1.13	4 (11%)	47,47,47	1.11	3 (6%)
15	BCR	D	405	-	25,26,41	3.08	5 (20%)	32,34,56	7.21	14 (43%)
18	DGD	B	616	-	47,47,67	0.96	4 (8%)	55,55,81	1.40	6 (10%)
16	LMT	B	619	-	31,31,36	1.36	7 (22%)	42,42,47	1.27	4 (9%)
12	CLA	C	509	3	69,73,73	2.25	22 (31%)	82,113,113	2.48	28 (34%)
12	CLA	B	613	-	69,73,73	2.22	20 (28%)	82,113,113	2.52	27 (32%)
12	CLA	B	601	2	59,63,73	2.40	21 (35%)	70,101,113	2.64	24 (34%)

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
12	CLA	C	501	3	-	11/39/115/115	-
15	BCR	A	408	-	-	10/29/63/63	0/2/2/2
12	CLA	D	404	4	-	4/15/91/115	-
12	CLA	C	503	3	-	12/39/115/115	-
15	BCR	C	517	-	-	11/29/63/63	0/2/2/2
12	CLA	B	604	2	-	13/27/103/115	-
14	PHO	A	406	-	-	9/37/103/103	0/5/6/6
12	CLA	C	502	3	-	17/39/115/115	-
12	CLA	C	513	-	-	3/15/91/115	-
18	DGD	C	515	-	-	15/36/76/95	0/2/2/2
15	BCR	C	514	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	F6C	B	603	2	1/1/7/16	9/23/79/97	-
12	CLA	A	405	24	-	7/21/97/115	-
12	CLA	B	602	2	-	10/27/103/115	-
13	CL7	A	404	24	2/2/15/20	21/39/115/115	-
16	LMT	D	409	-	-	9/12/28/61	0/1/1/2
17	F6C	B	612	2	1/1/8/16	13/29/85/97	-
12	CLA	C	506	3	-	8/27/103/115	-
19	LMG	B	617	-	-	9/35/55/70	0/1/1/1
17	F6C	C	507	24	1/1/9/16	17/35/91/97	-
12	CLA	B	607	2	-	13/39/115/115	-
12	CLA	B	608	2	-	11/15/91/115	-
21	PL9	D	406	-	-	14/41/61/73	0/1/1/1
17	F6C	B	606	24	1/1/9/16	17/35/91/97	-
23	HEM	F	101	5,6	-	3/14/54/54	-
12	CLA	B	605	2	-	9/27/103/115	-
19	LMG	D	408	-	-	5/28/48/70	0/1/1/1
16	LMT	A	409	-	-	8/21/61/61	0/2/2/2
12	CLA	C	511	3	-	3/15/91/115	-
12	CLA	C	512	3	-	8/15/91/115	-
12	CLA	B	609	-	-	7/15/91/115	-
12	CLA	C	505	3	-	19/39/115/115	-
12	CLA	B	610	2	-	11/27/103/115	-
12	CLA	A	407	1	-	12/33/109/115	-
22	LHG	D	407	-	-	21/50/50/53	-
12	CLA	C	508	3	-	18/39/115/115	-
12	CLA	D	403	4	-	6/33/109/115	-
16	LMT	C	516	-	-	12/20/60/61	0/2/2/2
12	CLA	B	611	2	-	15/39/115/115	-
12	CLA	C	504	24	-	6/21/97/115	-
12	CLA	B	614	2	-	2/21/97/115	-
12	CLA	A	403	1	-	8/39/115/115	-
16	LMT	A	410	-	-	7/17/57/61	0/2/2/2
14	PHO	D	402	-	-	6/37/103/103	0/5/6/6
12	CLA	C	510	3	-	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	B	615	-	-	9/29/63/63	0/2/2/2
16	LMT	B	618	-	-	11/21/61/61	0/2/2/2
15	BCR	D	405	-	-	10/20/37/63	0/1/1/2
18	DGD	B	616	-	-	19/41/61/95	0/1/1/2
16	LMT	B	619	-	-	6/16/56/61	0/2/2/2
12	CLA	C	509	3	-	10/39/115/115	-
12	CLA	B	613	-	-	17/39/115/115	-
12	CLA	B	601	2	-	9/27/103/115	-

The worst 5 of 835 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	606	F6C	C1A-CHA	10.21	1.51	1.35
14	D	402	PHO	C3B-C4B	9.60	1.51	1.41
14	A	406	PHO	C1B-C2B	9.53	1.50	1.39
17	B	603	F6C	MG-NA	9.33	2.24	2.05
17	C	507	F6C	MG-NA	9.24	2.24	2.05

The worst 5 of 1042 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	517	BCR	C20-C21-C22	21.29	157.14	127.28
15	B	615	BCR	C20-C21-C22	20.90	156.59	127.28
15	B	615	BCR	C15-C16-C17	20.83	166.15	123.52
15	A	408	BCR	C15-C16-C17	20.68	165.83	123.52
15	A	408	BCR	C20-C21-C22	20.67	156.27	127.28

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	404	CL7	NA
13	A	404	CL7	NC
17	B	603	F6C	NA
17	B	606	F6C	NA
17	B	612	F6C	NA

5 of 565 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	403	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	B	607	CLA	C2-C1-O2A-CGA
12	B	607	CLA	CBD-CGD-O2D-CED
12	B	608	CLA	C3A-C2A-CAA-CBA
12	B	608	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

47 monomers are involved in 142 short contacts:

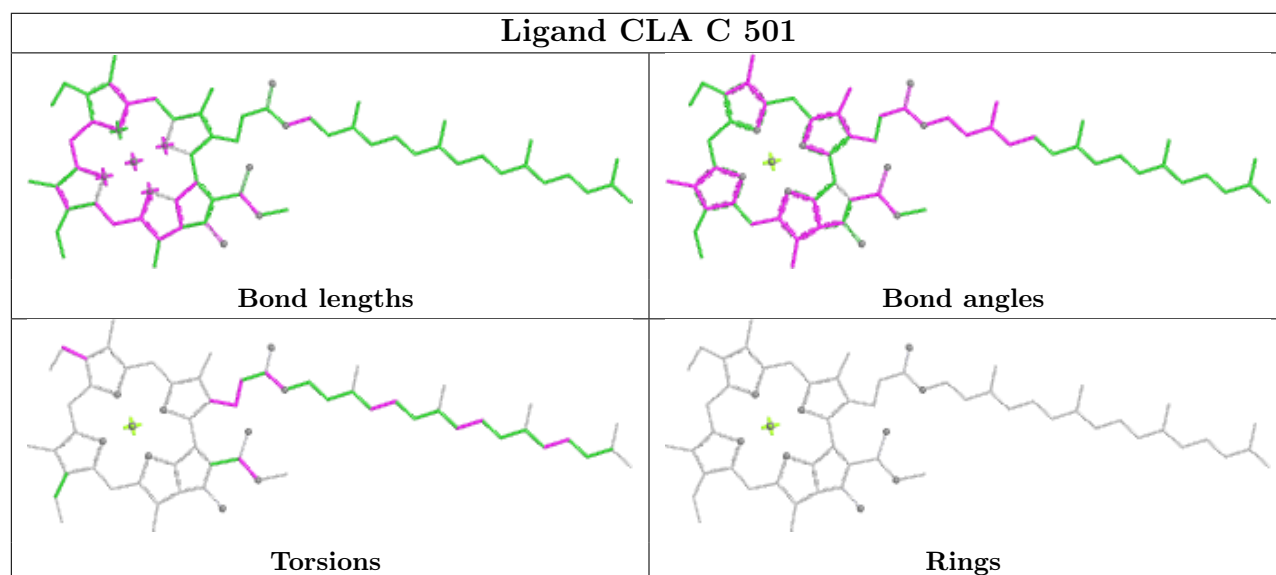
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	501	CLA	4	0
15	A	408	BCR	5	0
12	D	404	CLA	1	0
12	C	503	CLA	9	0
15	C	517	BCR	4	0
12	B	604	CLA	14	0
14	A	406	PHO	5	0
12	C	502	CLA	4	0
12	C	513	CLA	1	0
18	C	515	DGD	2	0
15	C	514	BCR	2	0
17	B	603	F6C	5	0
12	A	405	CLA	2	0
12	B	602	CLA	6	0
13	A	404	CL7	3	0
17	B	612	F6C	3	0
12	C	506	CLA	2	0
19	B	617	LMG	1	0
12	B	607	CLA	5	0
17	C	507	F6C	2	0
21	D	406	PL9	4	0
23	F	101	HEM	4	0
12	B	605	CLA	3	0
19	D	408	LMG	2	0
16	A	409	LMT	2	0
12	C	511	CLA	2	0
12	B	609	CLA	1	0
12	C	505	CLA	6	0
12	B	610	CLA	4	0
12	A	407	CLA	5	0
22	D	407	LHG	7	0
12	C	508	CLA	9	0
12	D	403	CLA	2	0

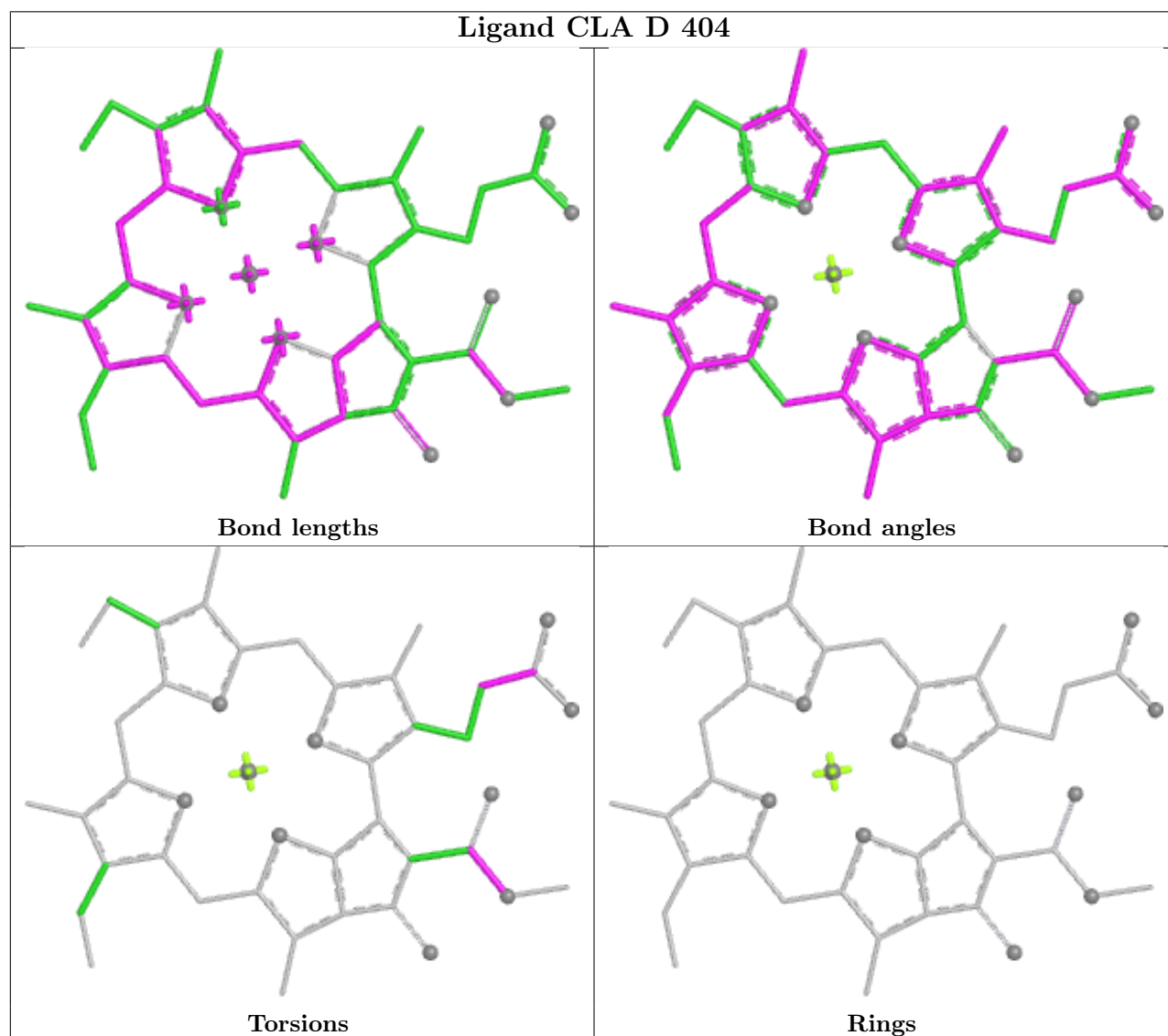
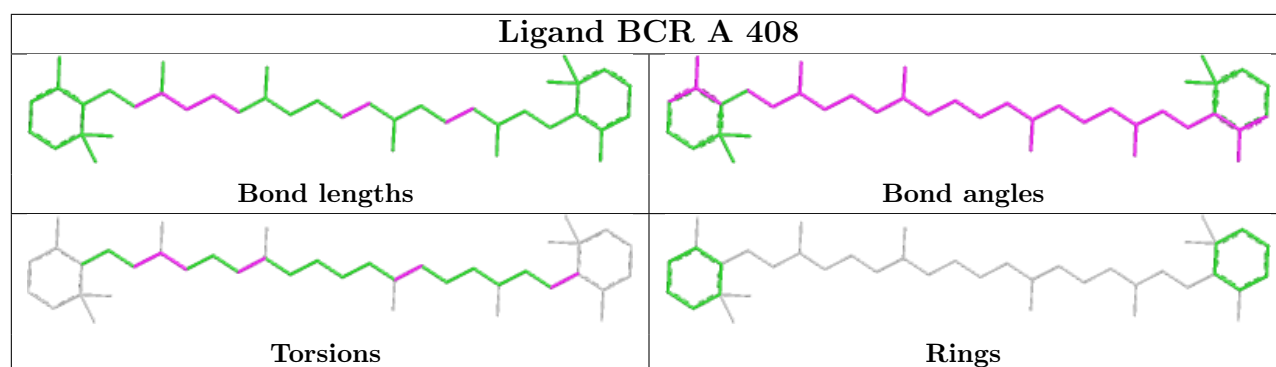
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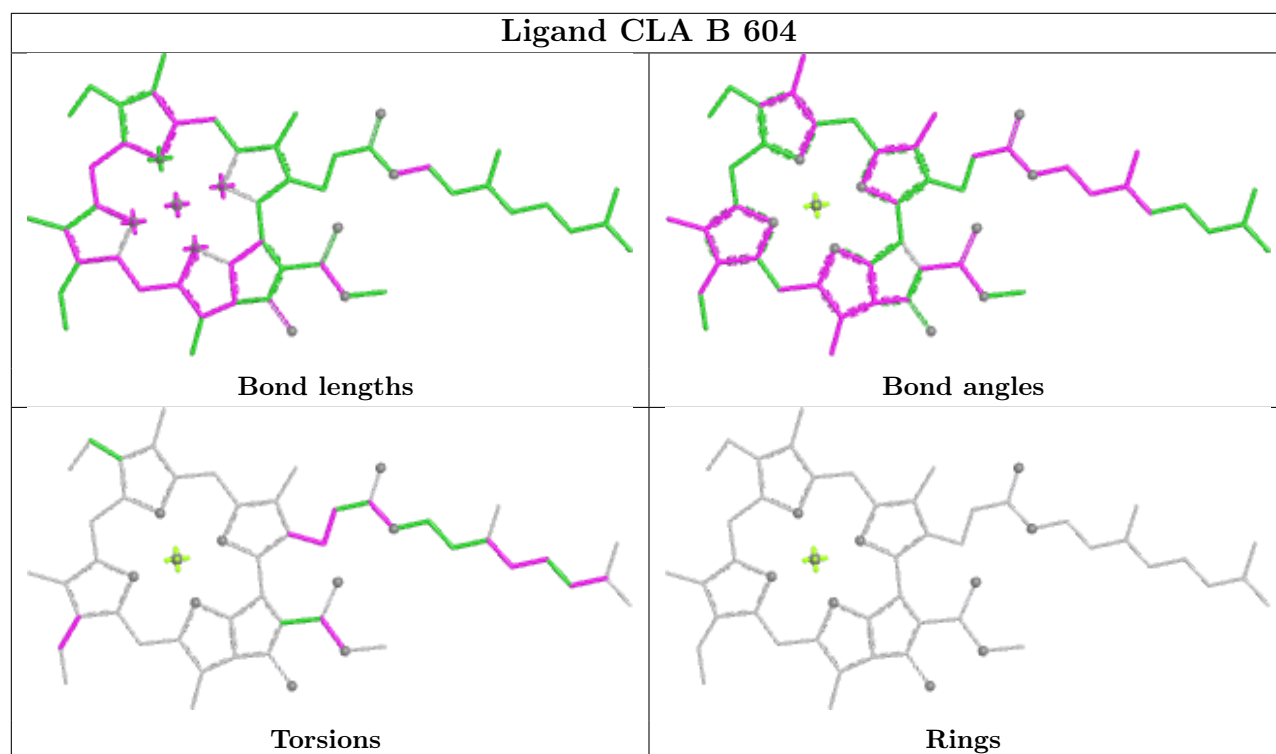
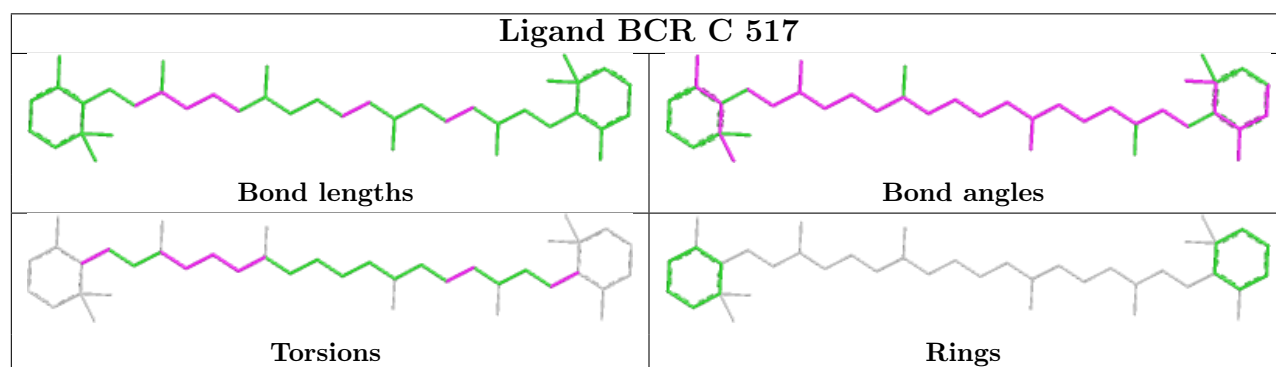
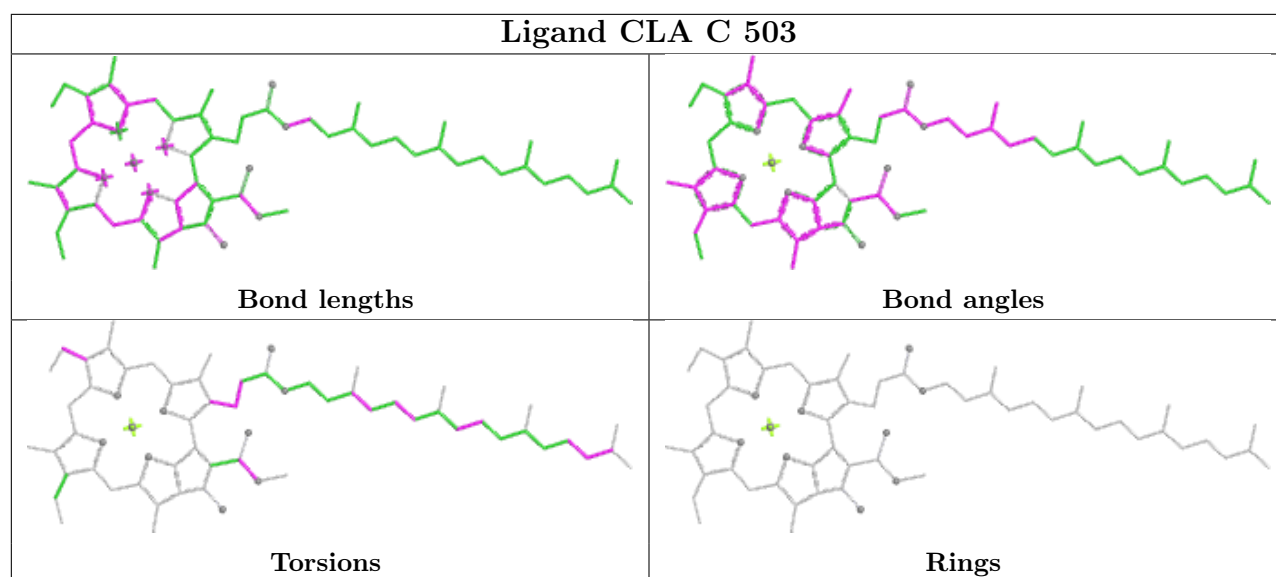
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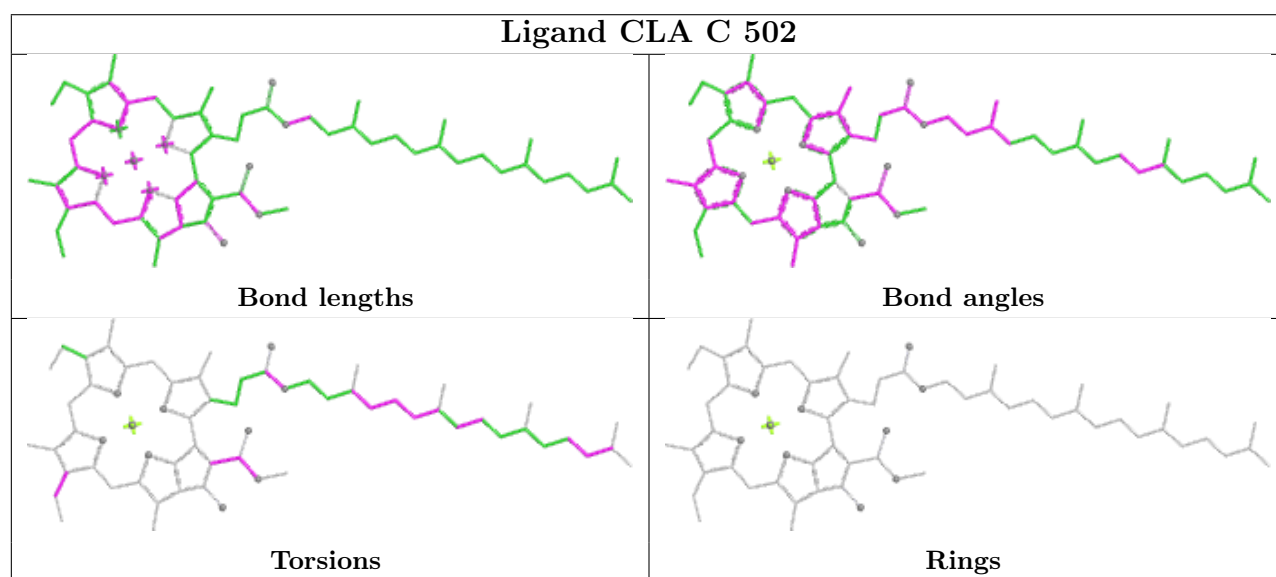
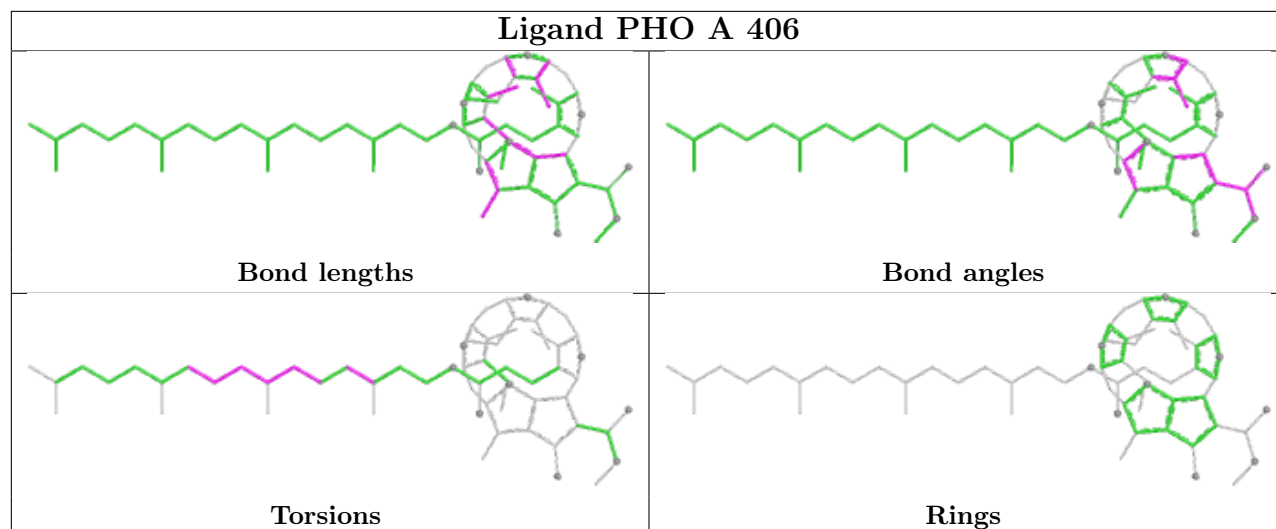
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	C	516	LMT	2	0
12	B	611	CLA	5	0
12	B	614	CLA	1	0
12	A	403	CLA	5	0
16	A	410	LMT	1	0
14	D	402	PHO	2	0
12	C	510	CLA	2	0
15	B	615	BCR	2	0
15	D	405	BCR	1	0
18	B	616	DGD	1	0
16	B	619	LMT	1	0
12	C	509	CLA	4	0
12	B	613	CLA	3	0
12	B	601	CLA	2	0

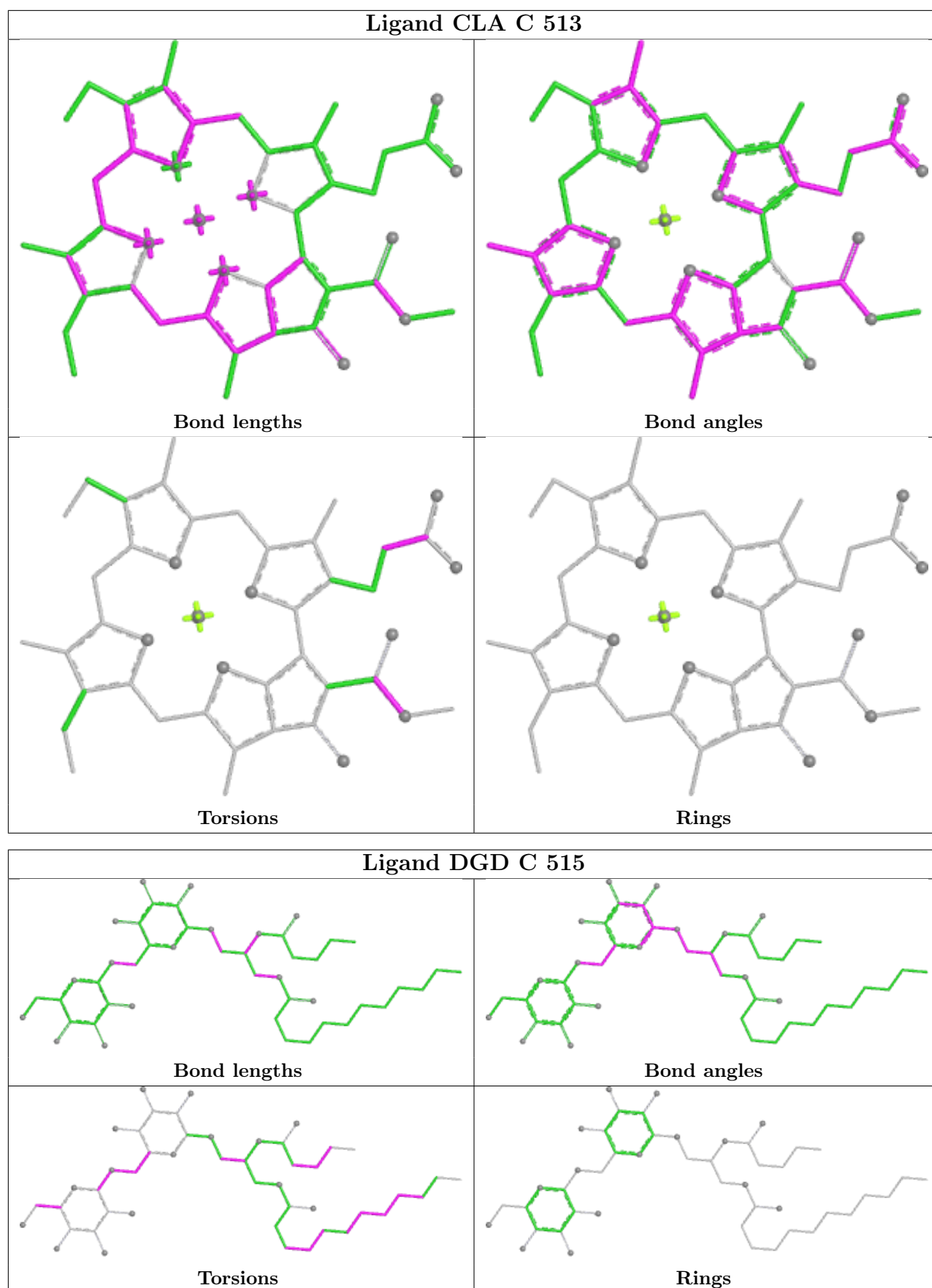
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

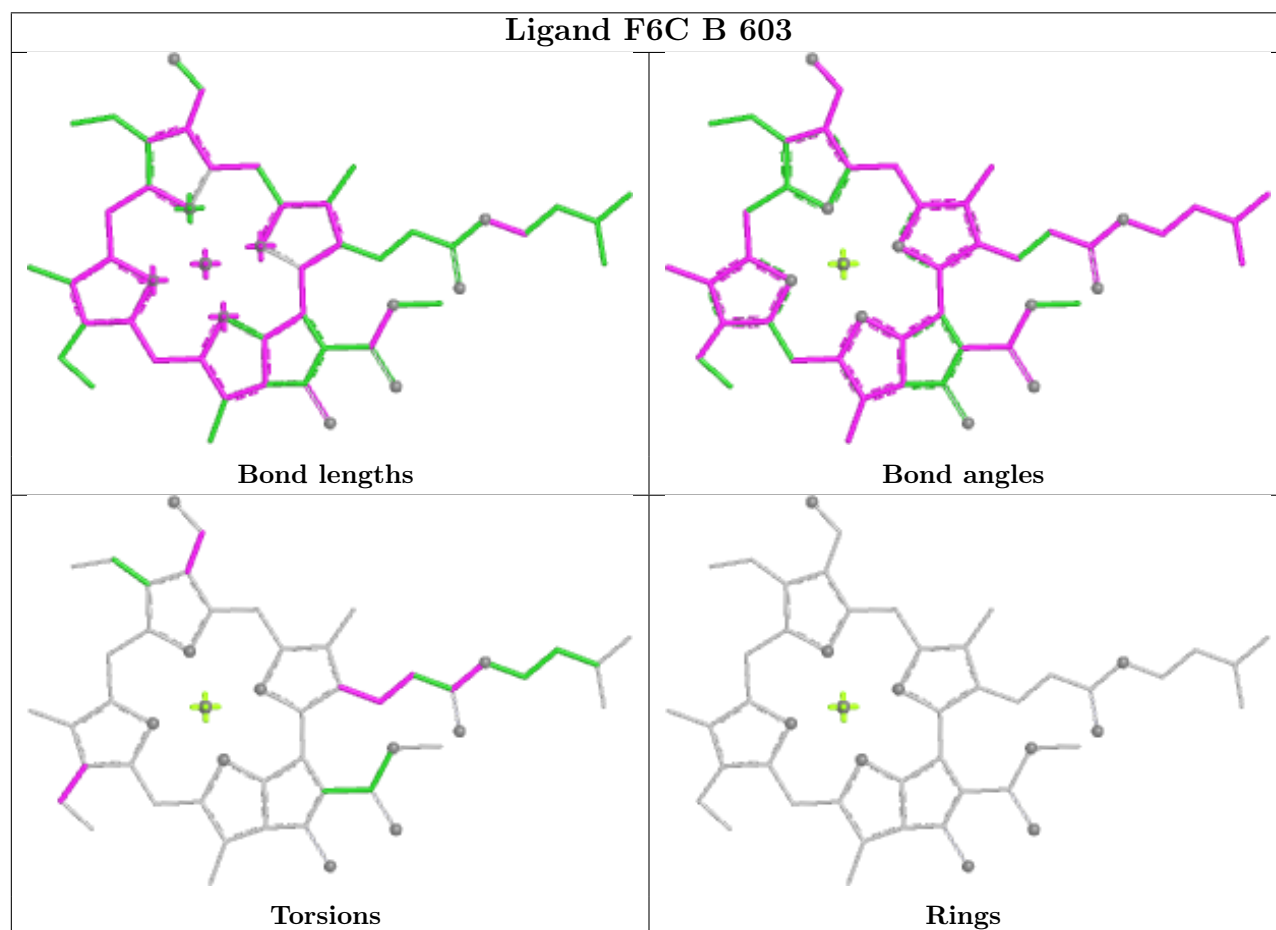
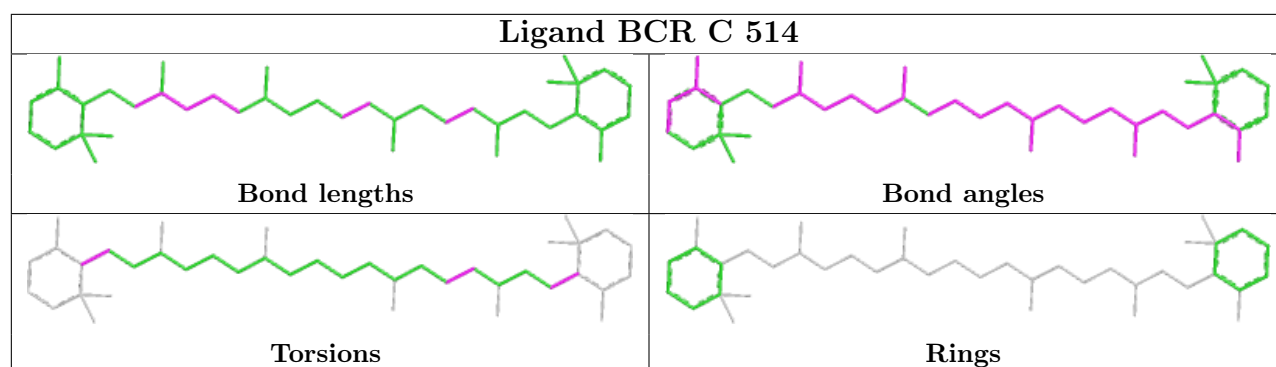




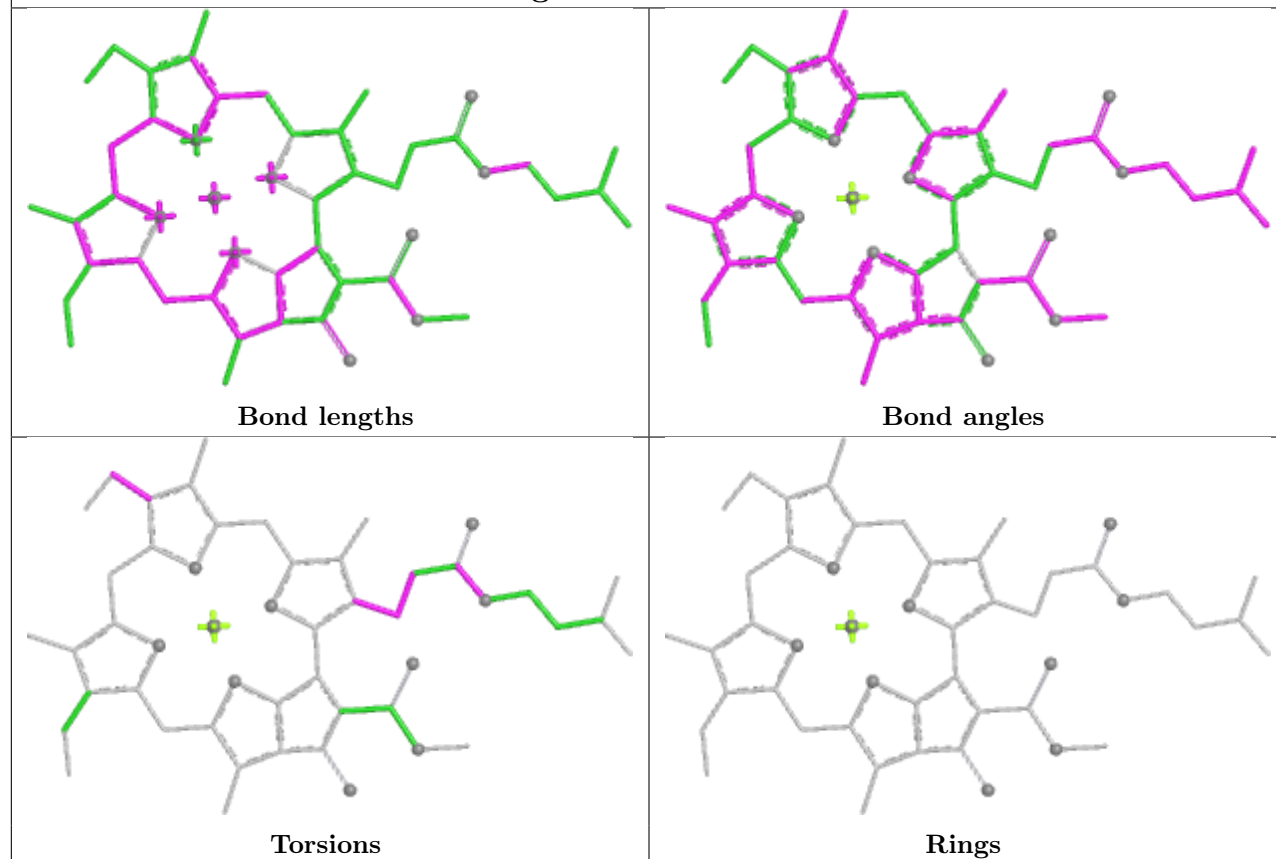




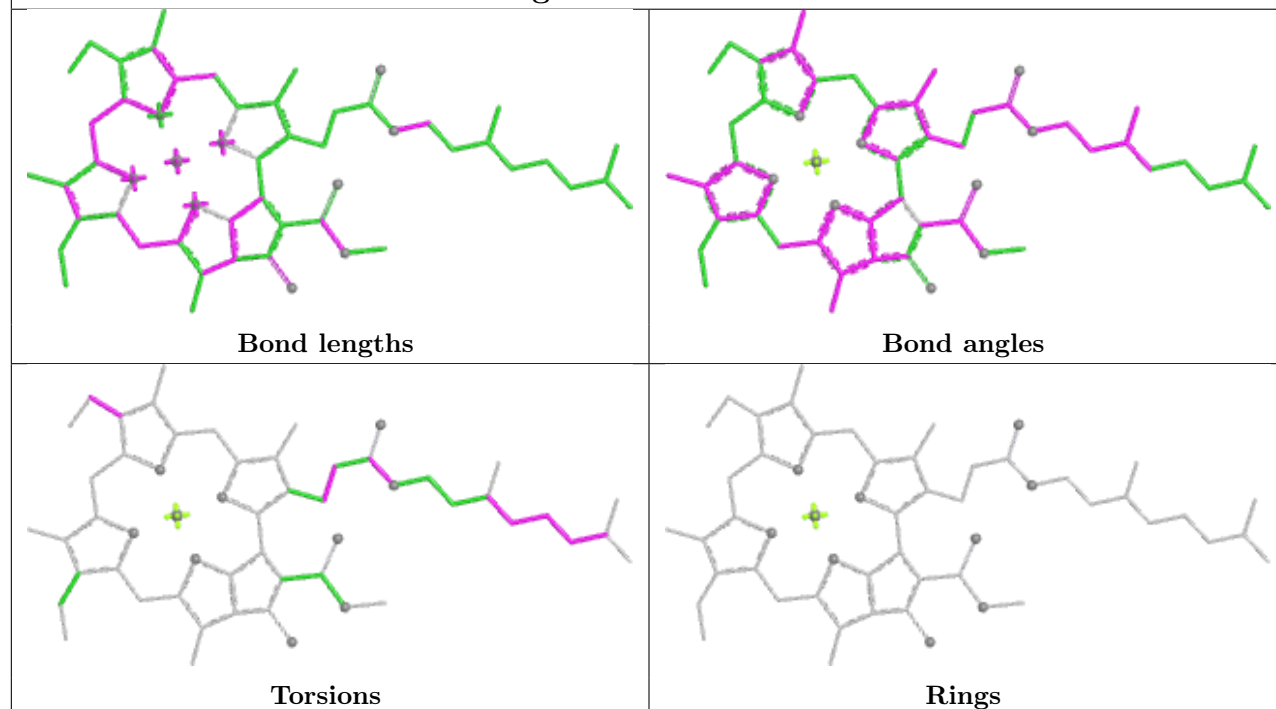


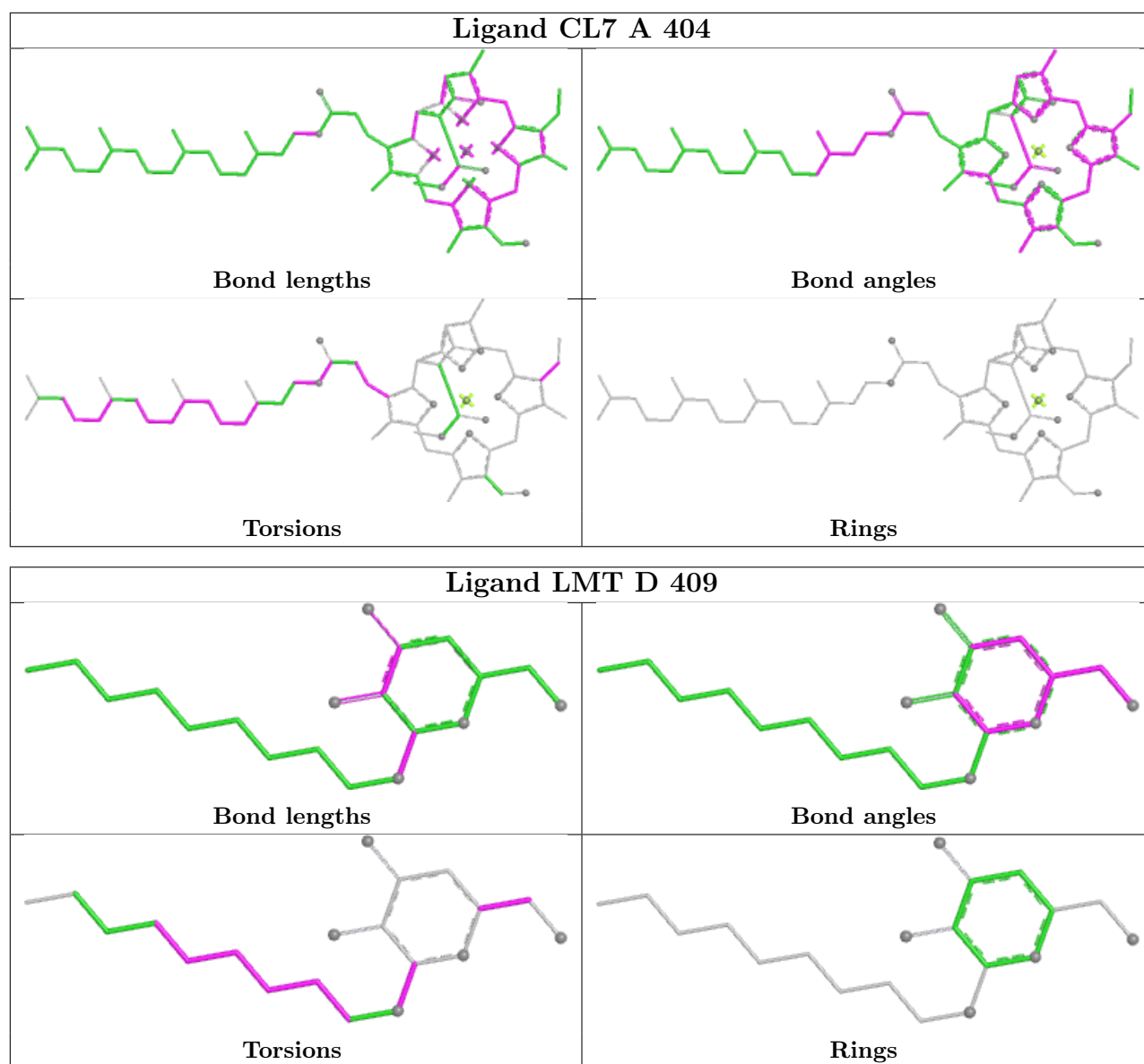


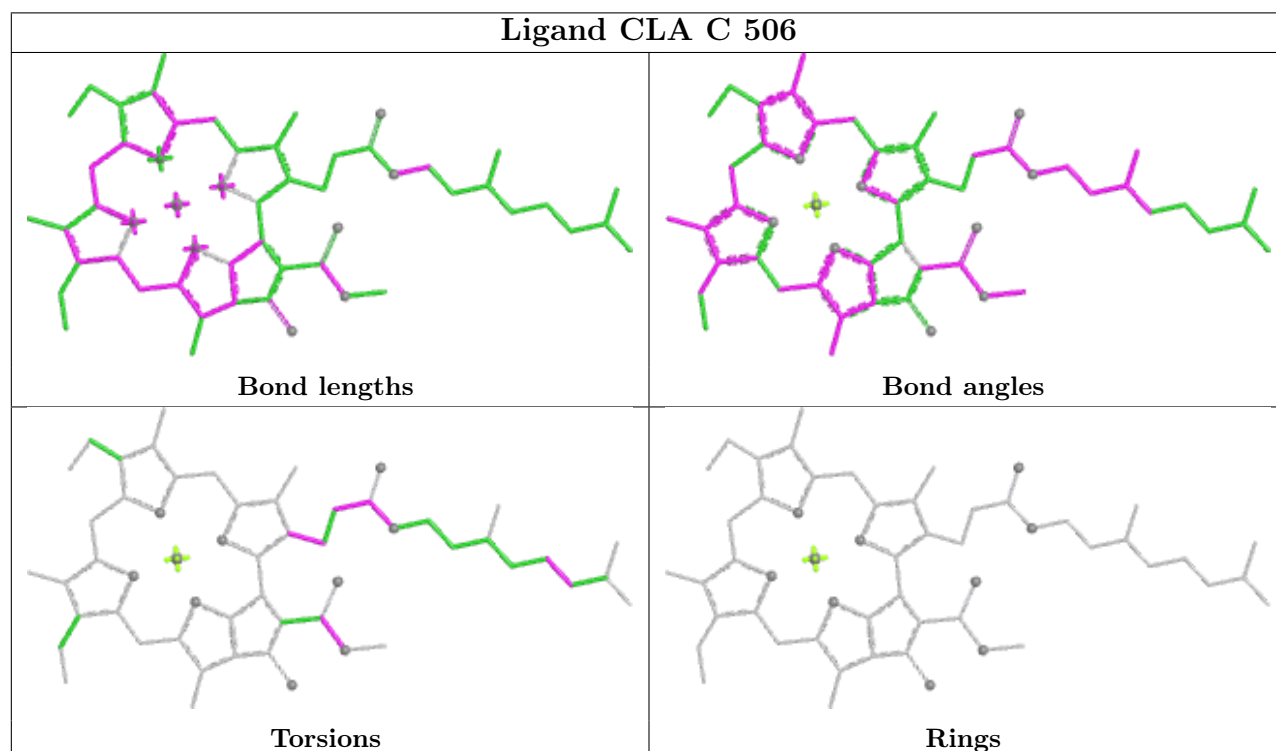
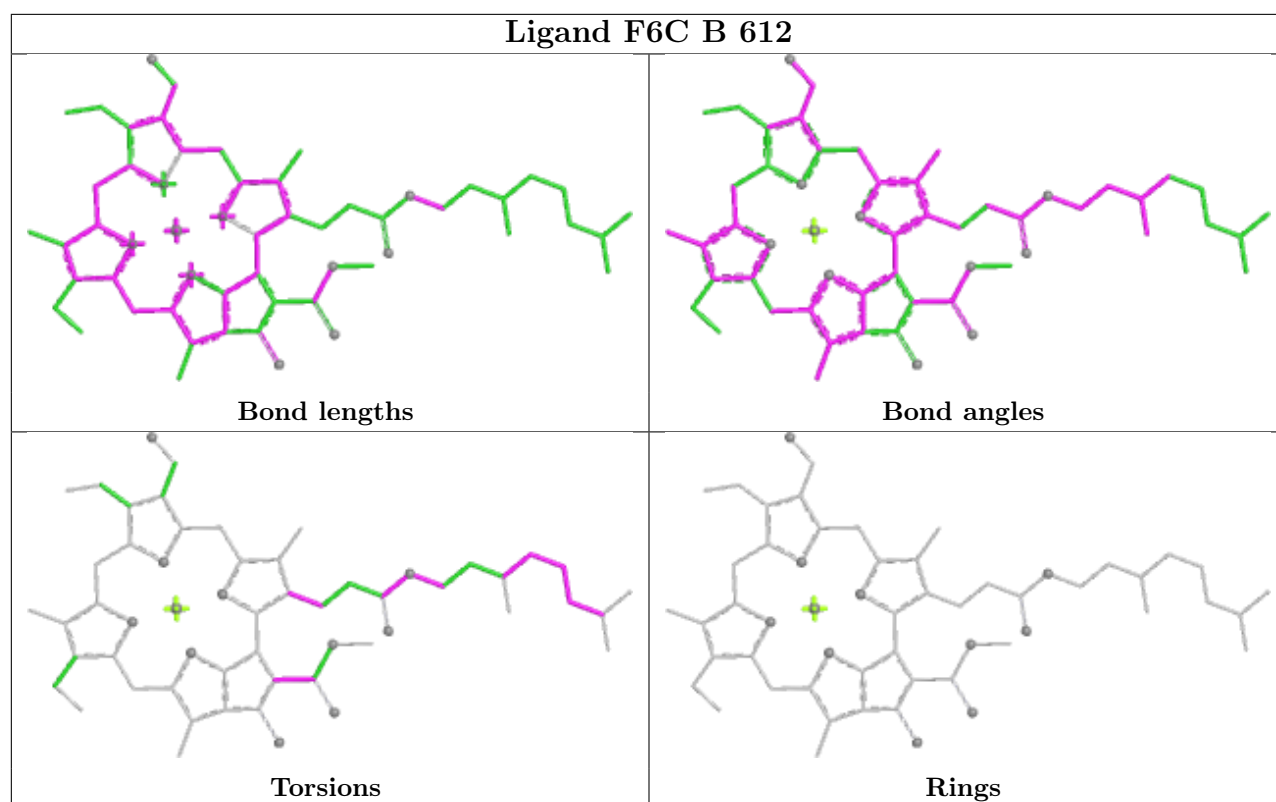
Ligand CLA A 405

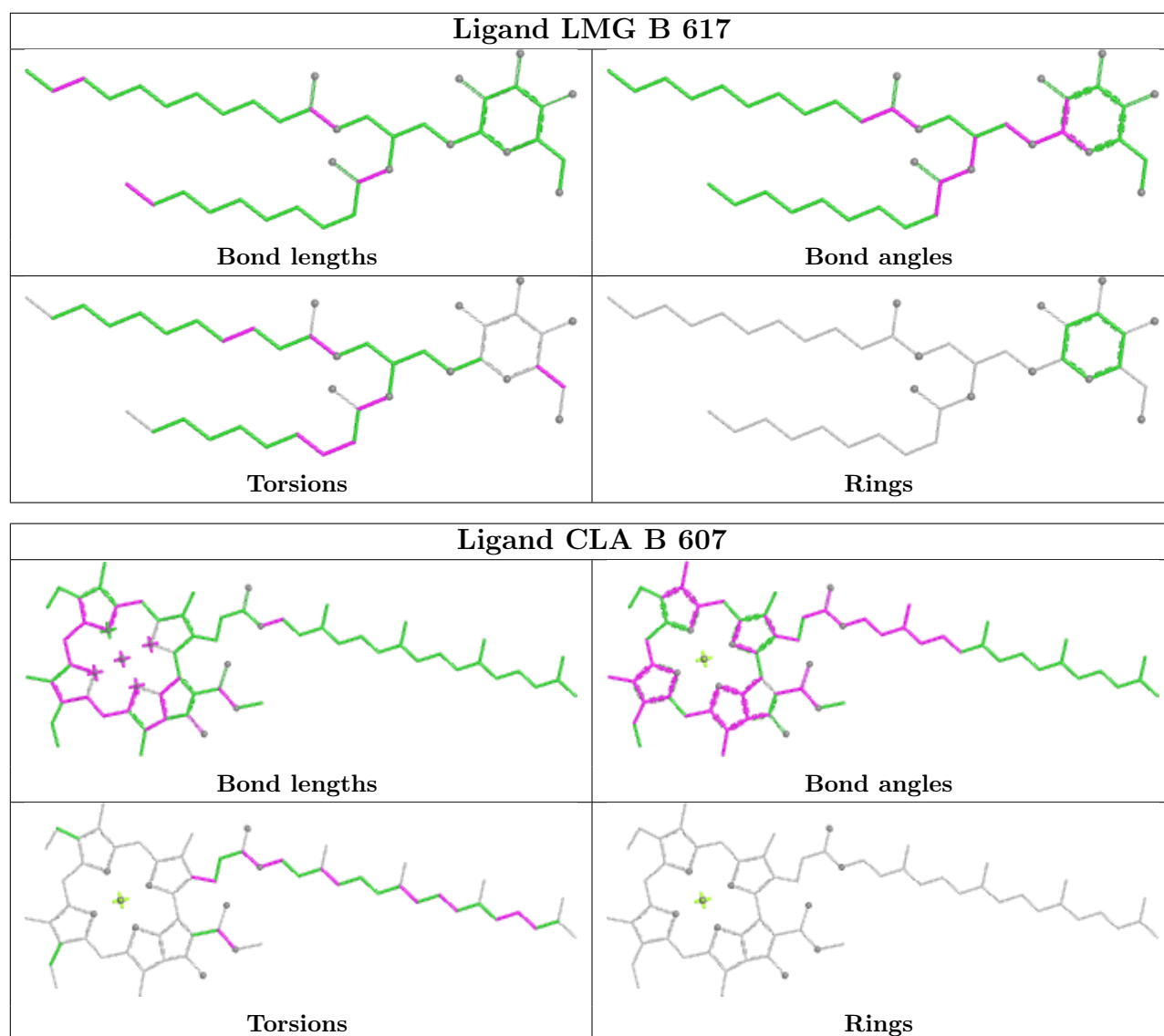


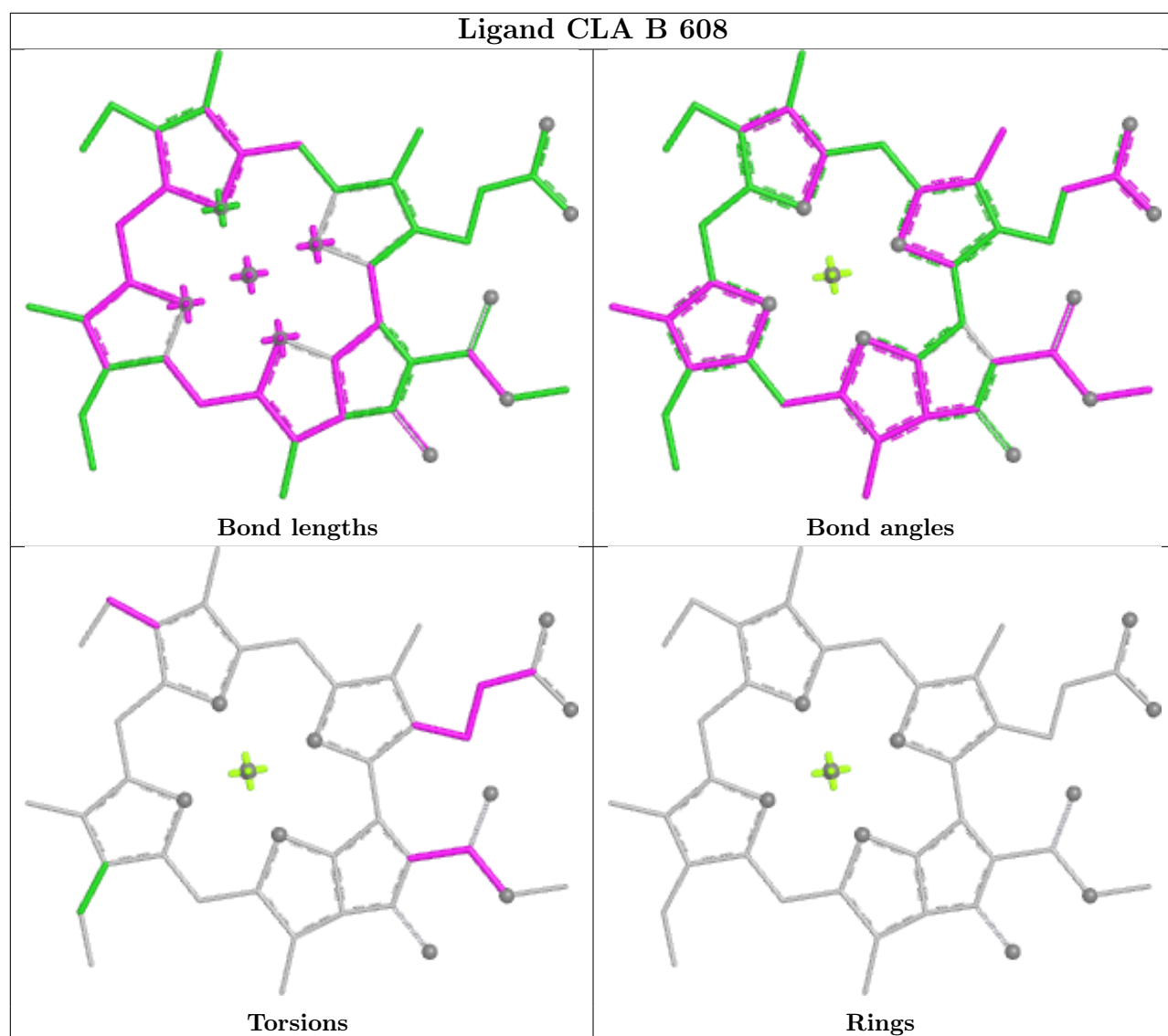
Ligand CLA B 602

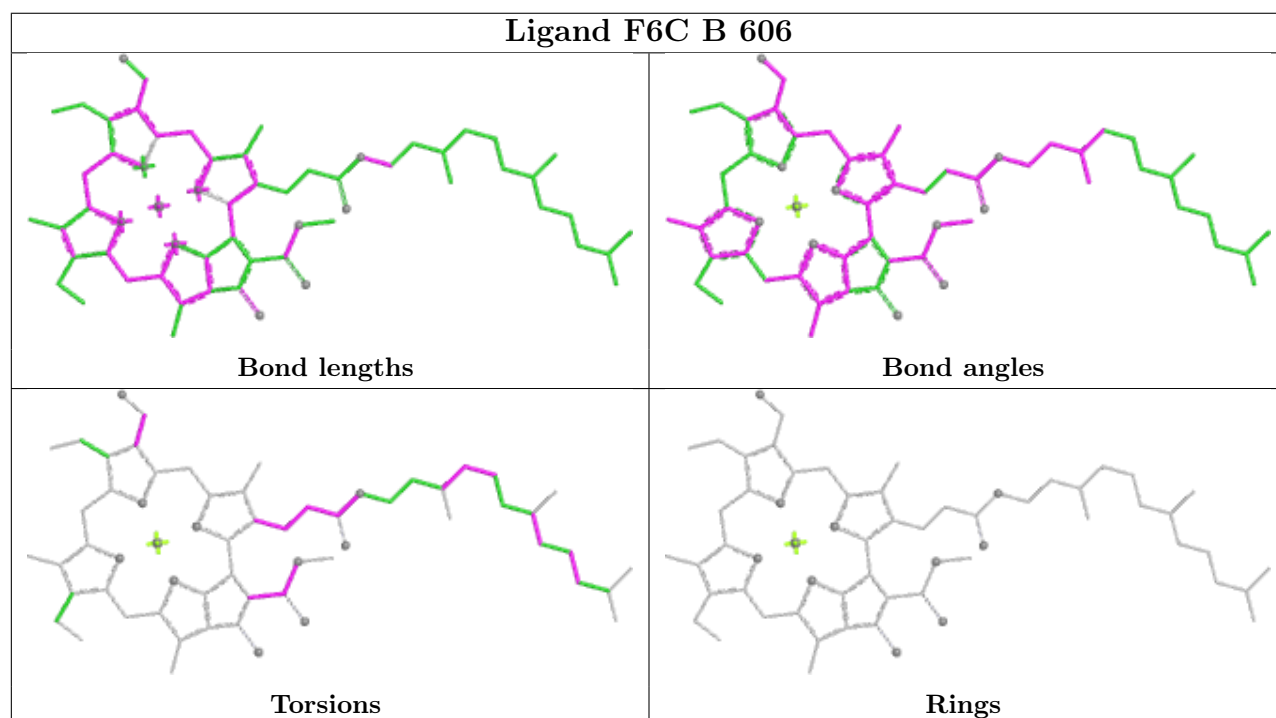
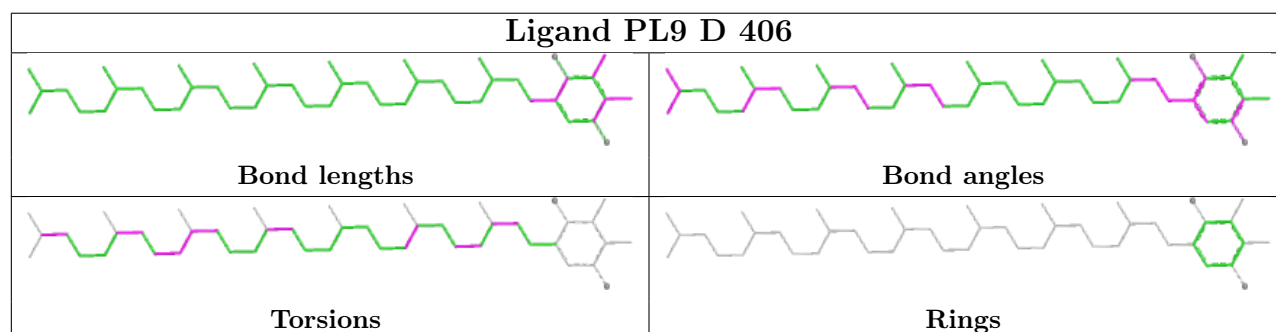
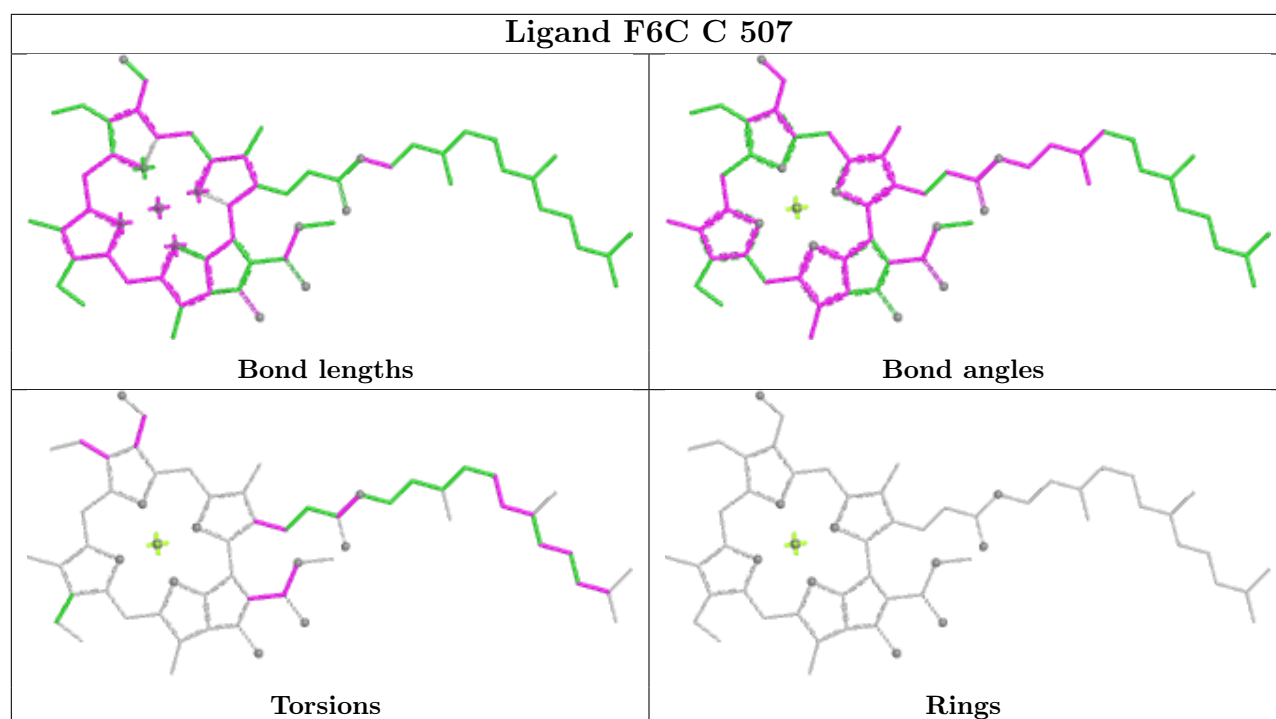


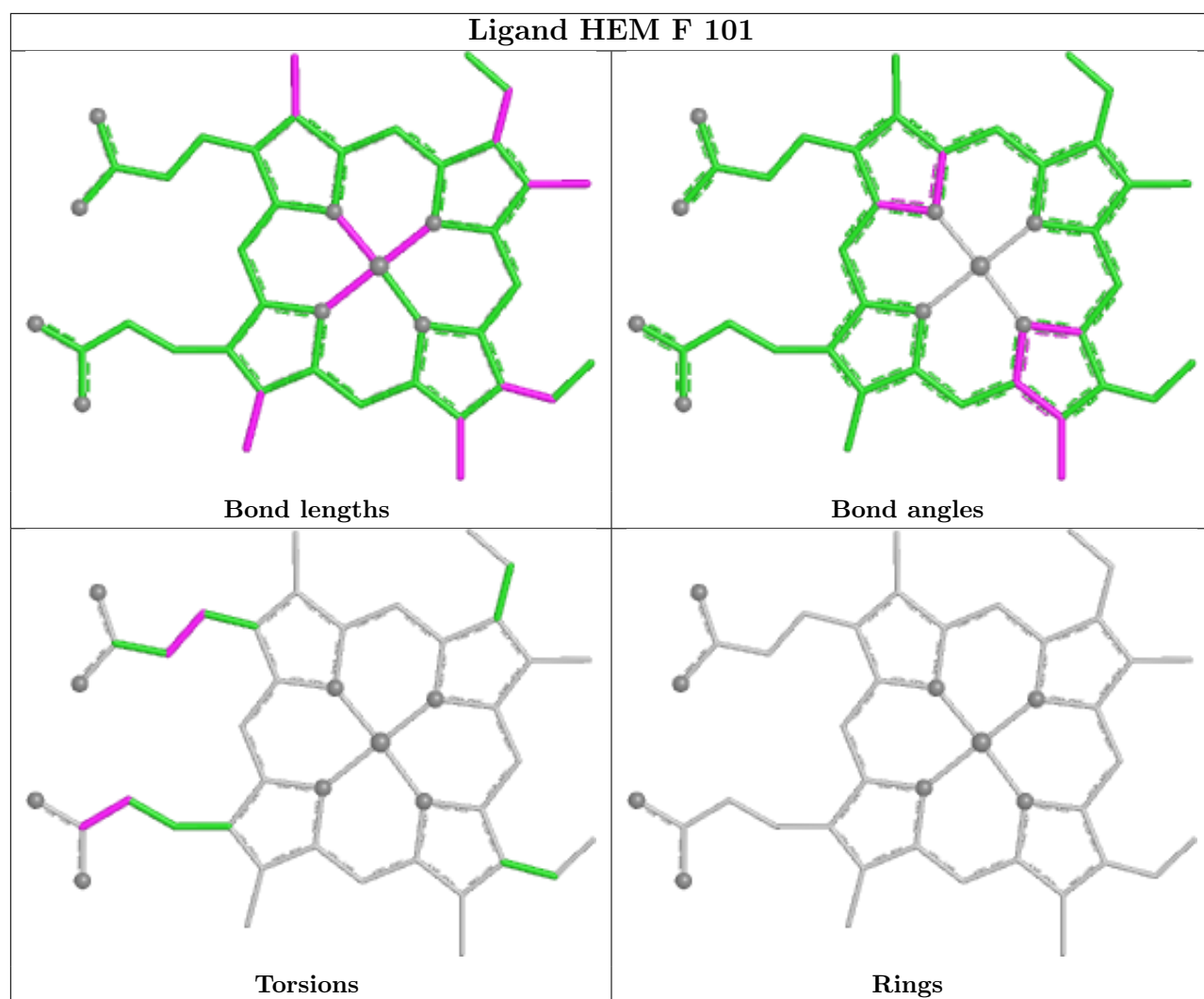


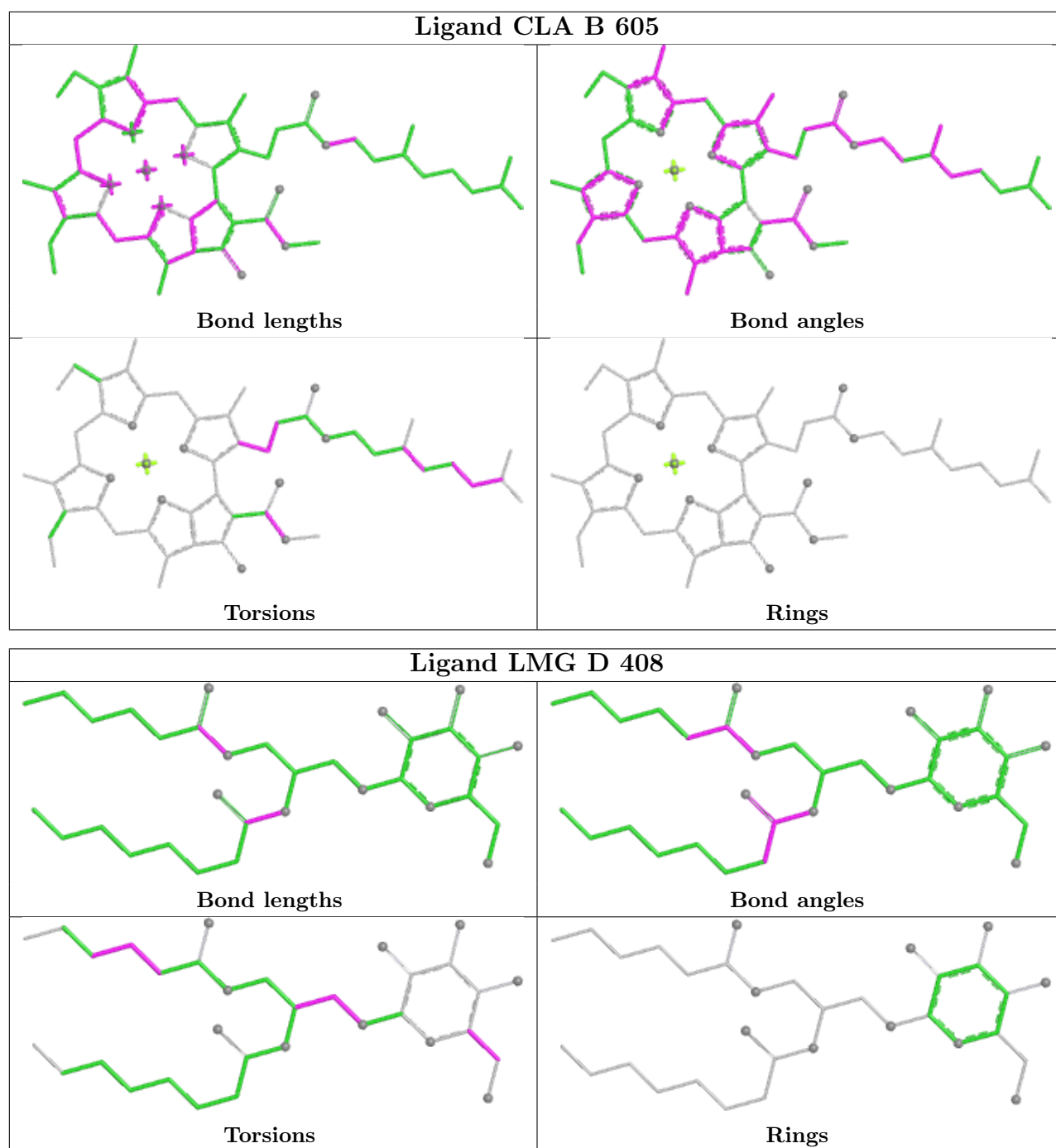


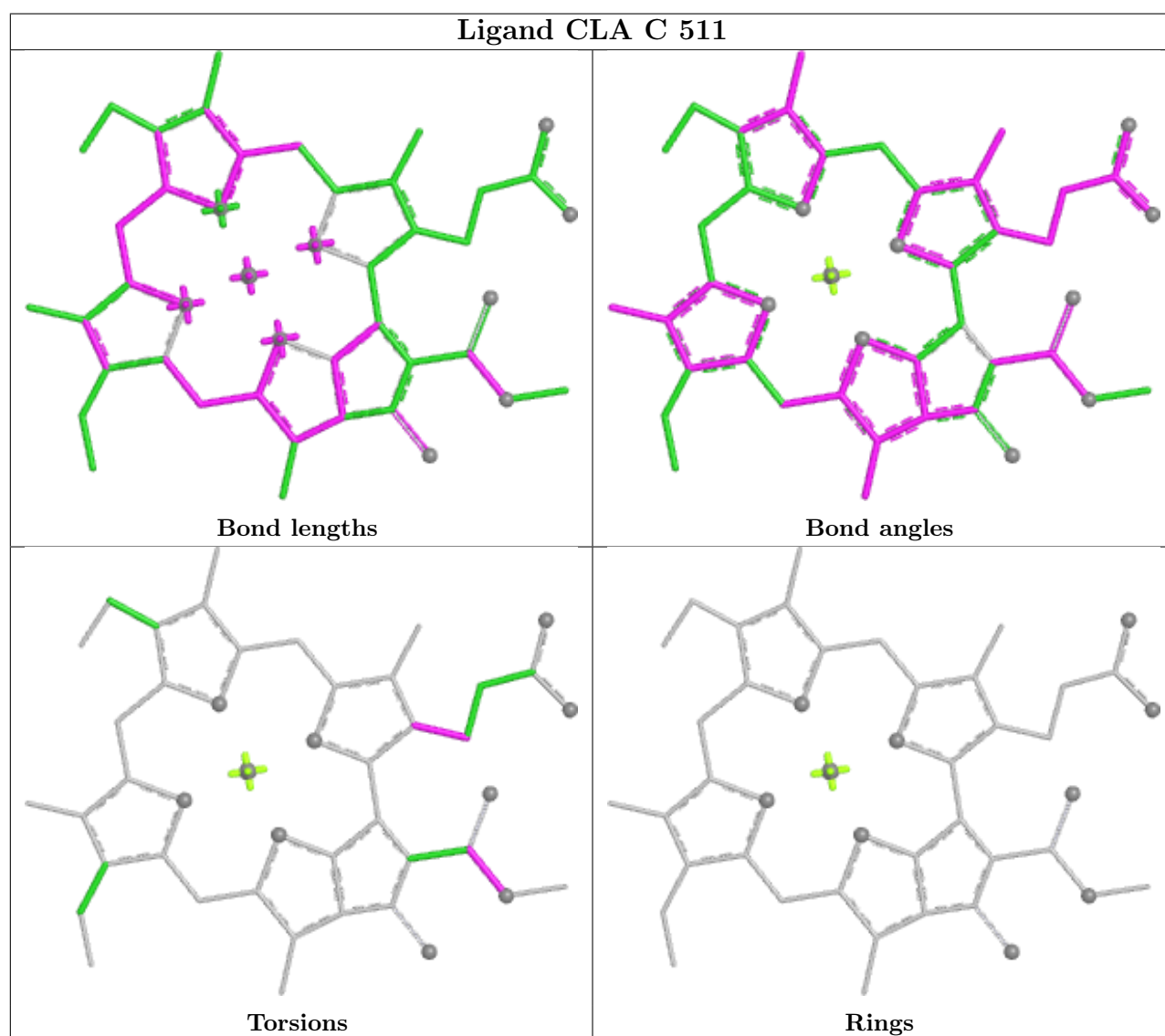
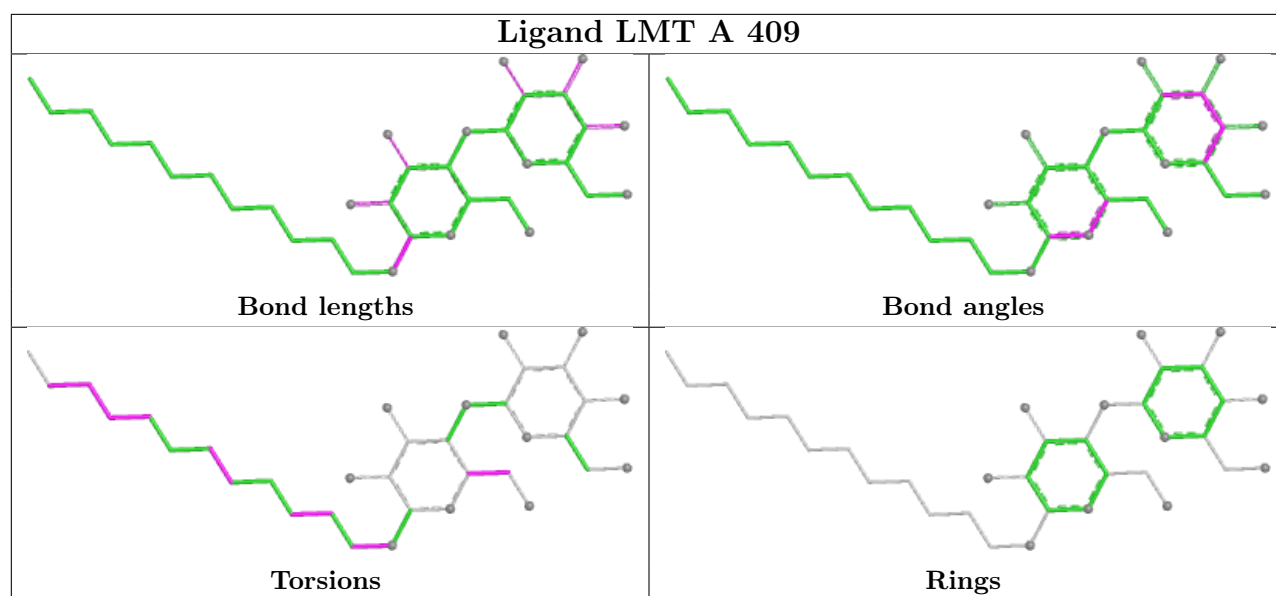


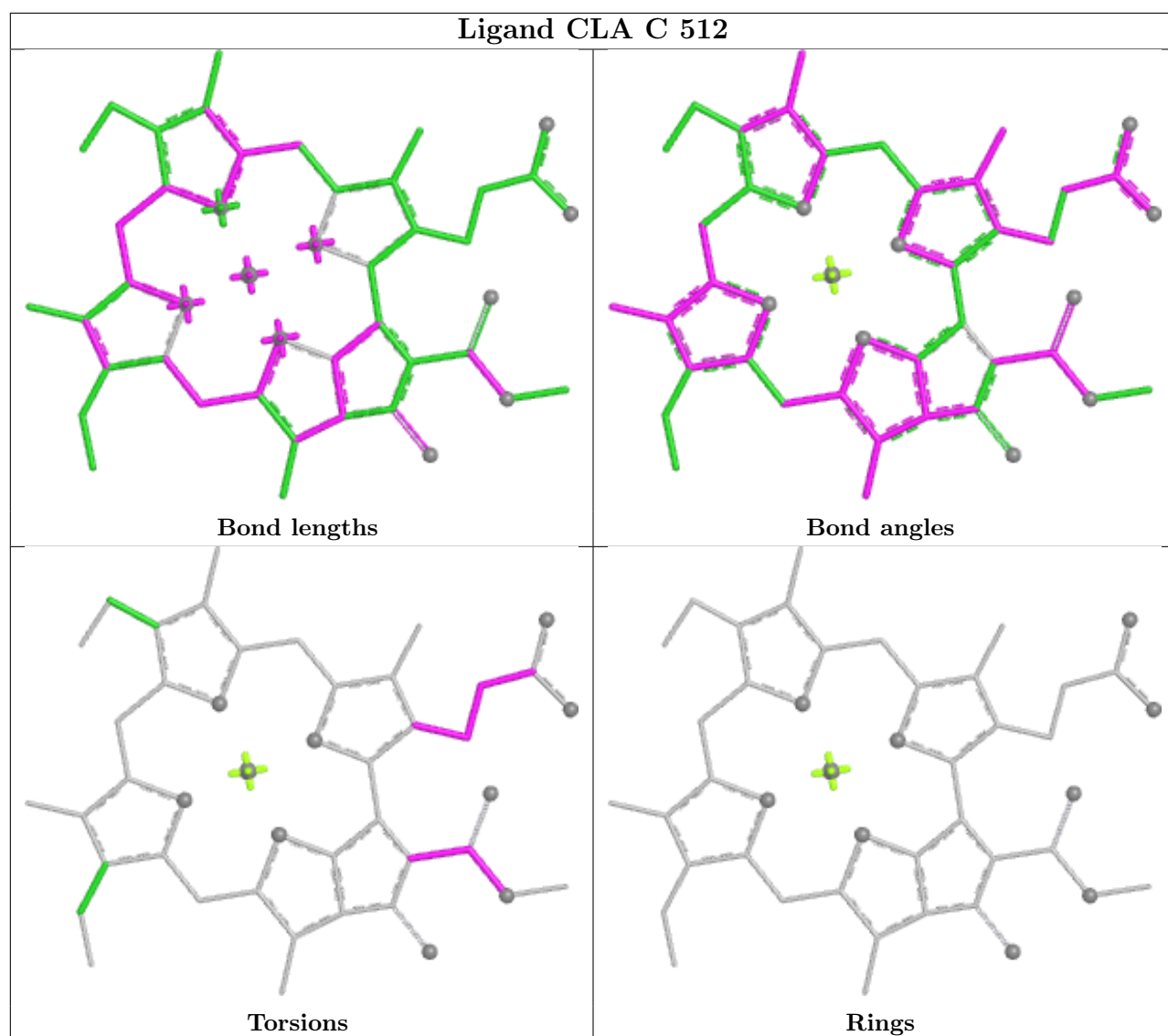




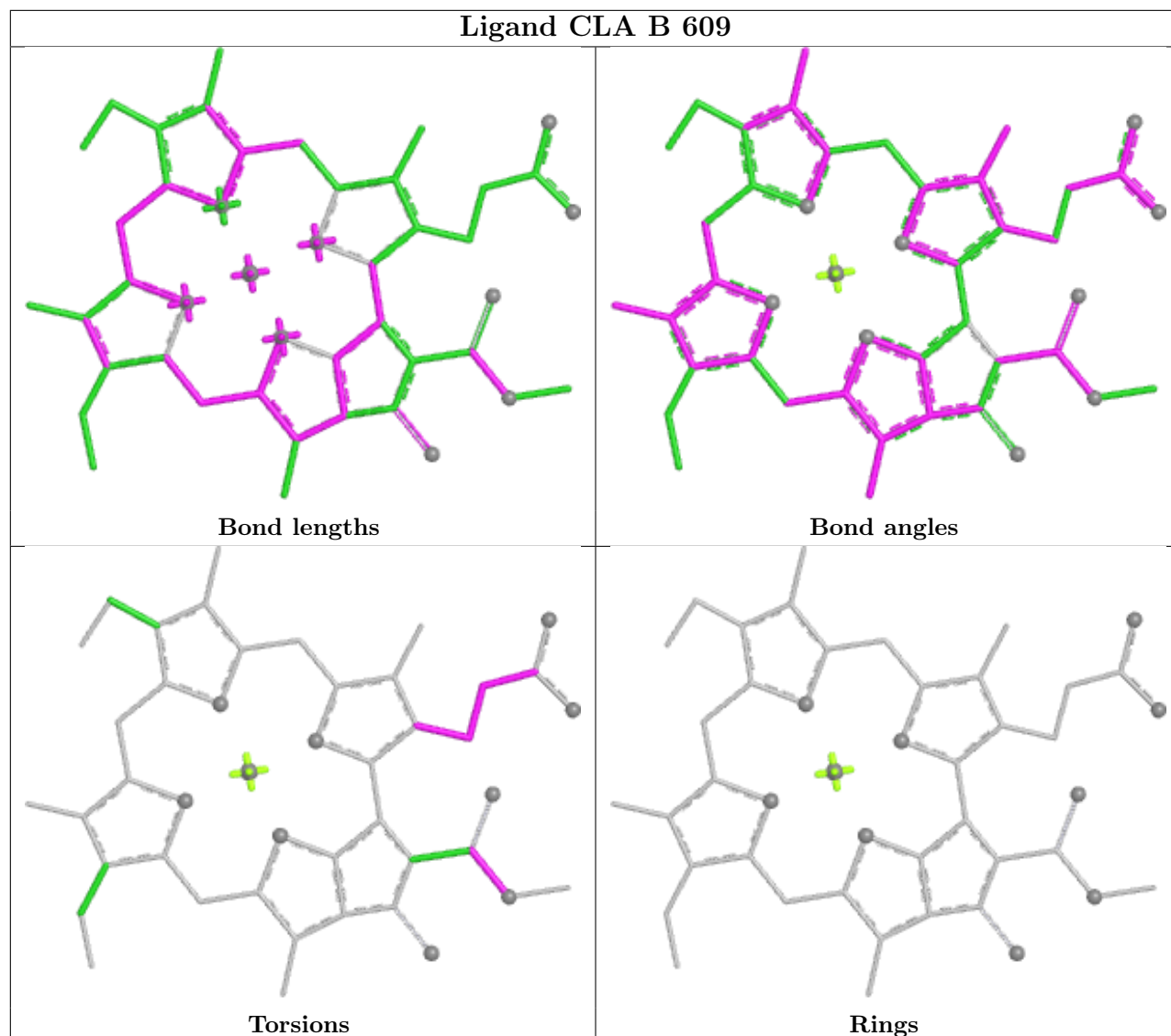




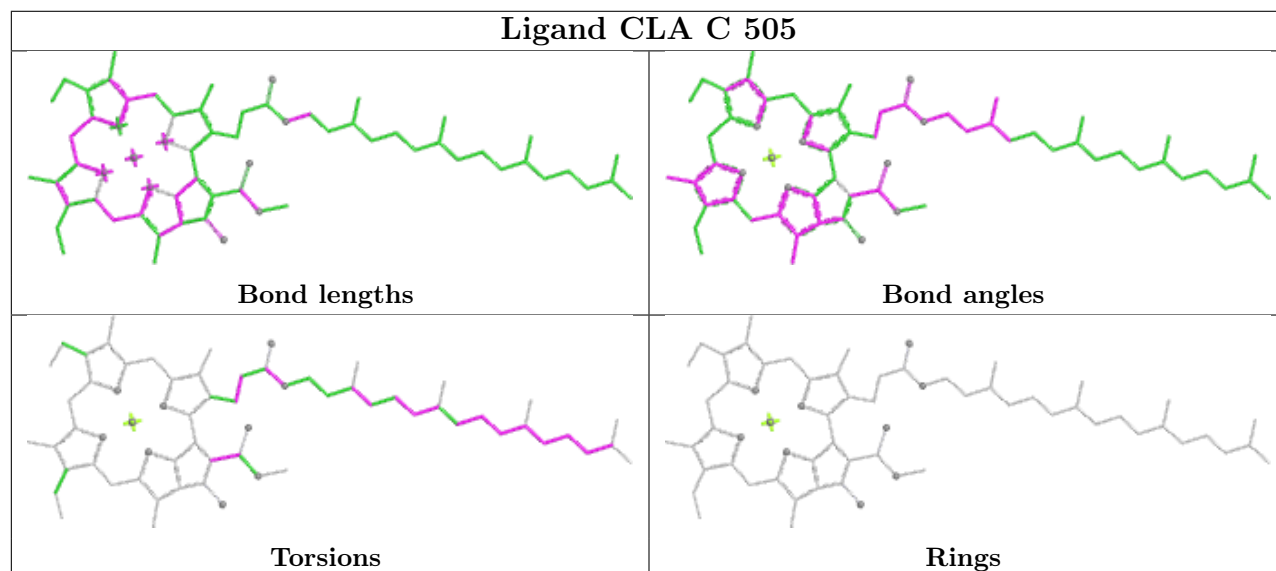




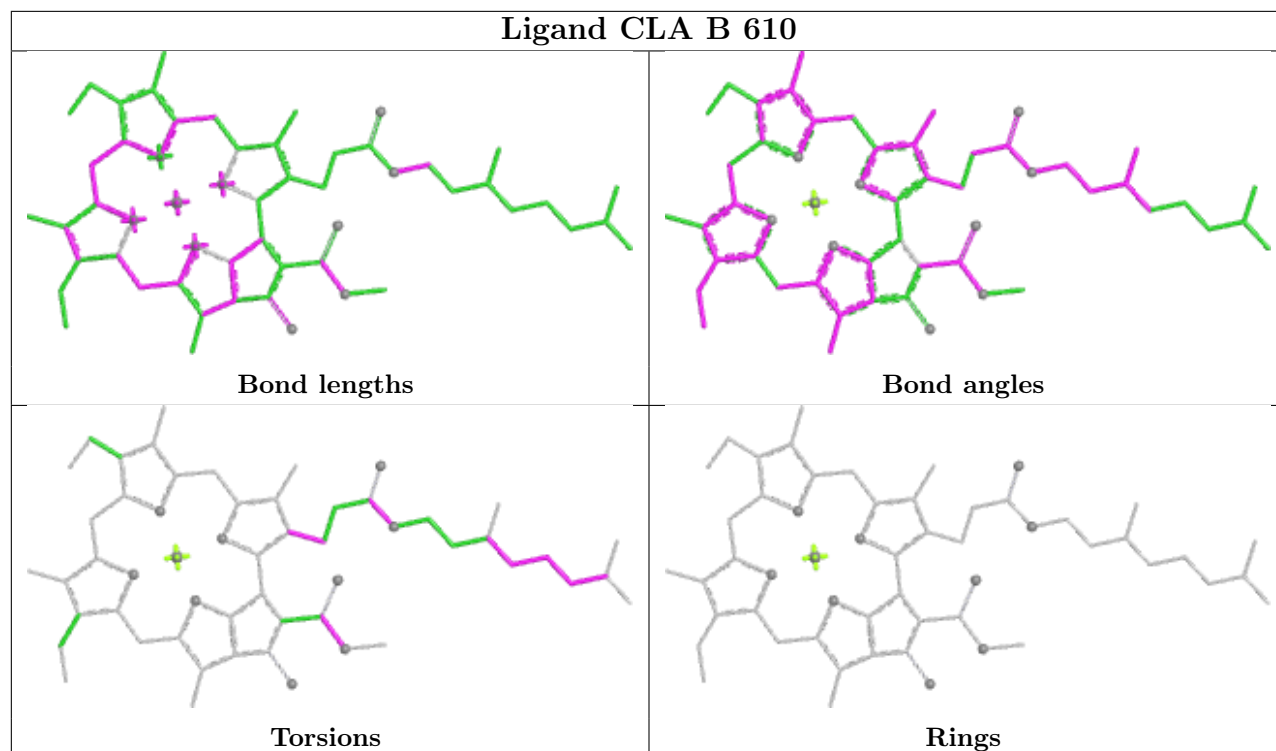
Ligand CLA B 609



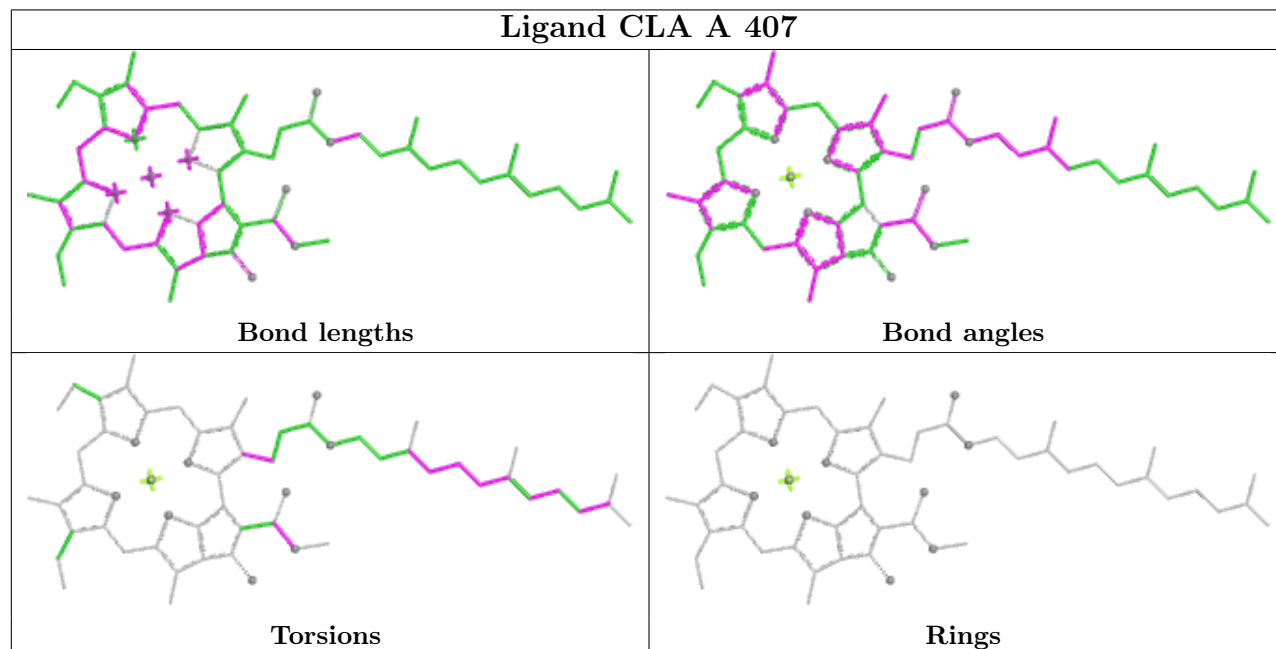
Ligand CLA C 505

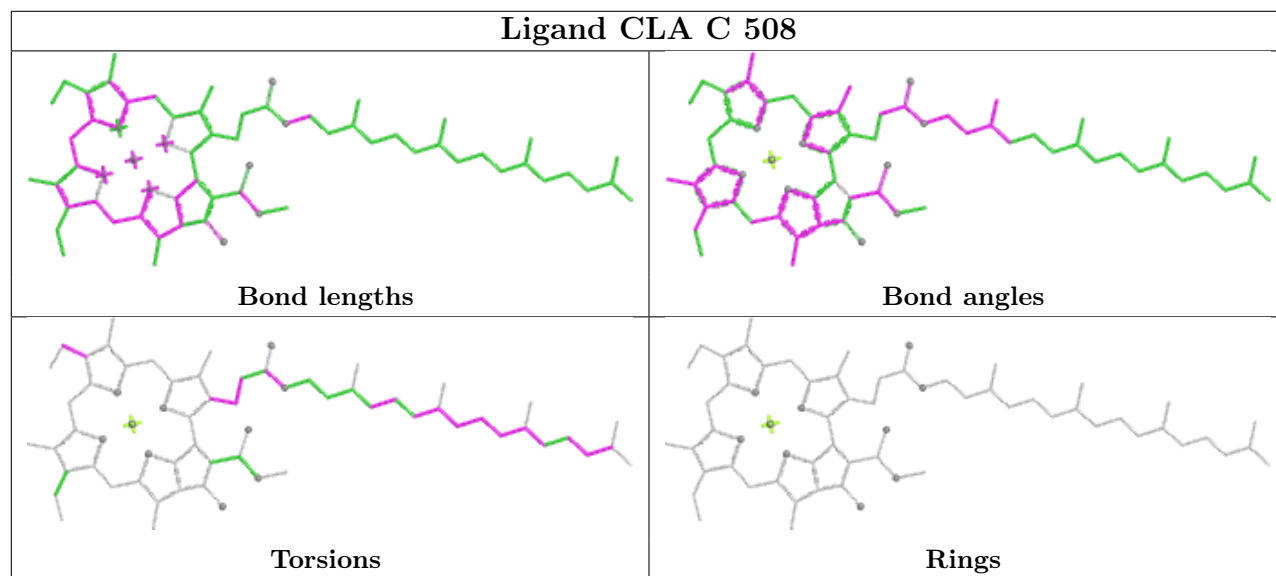
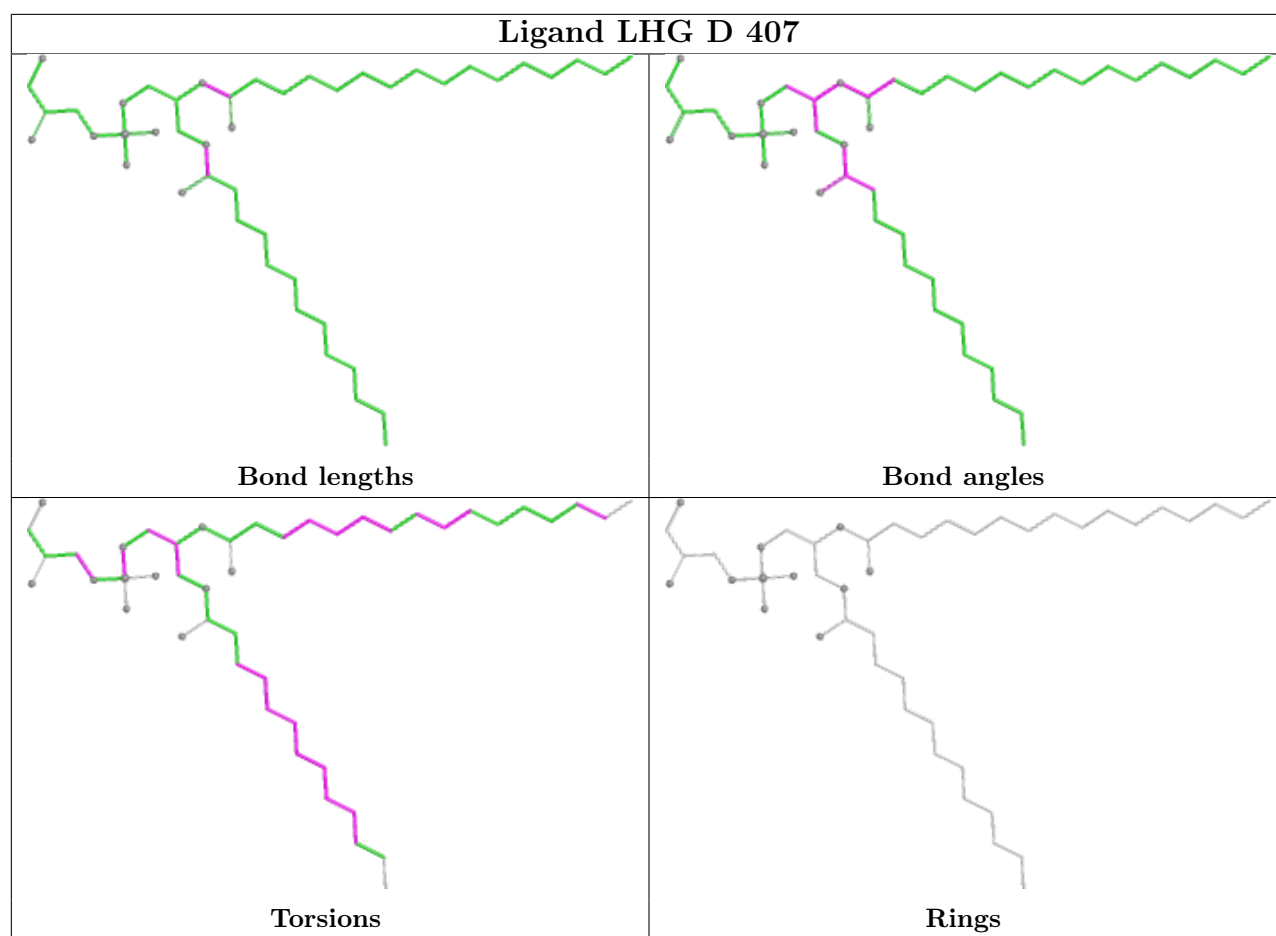


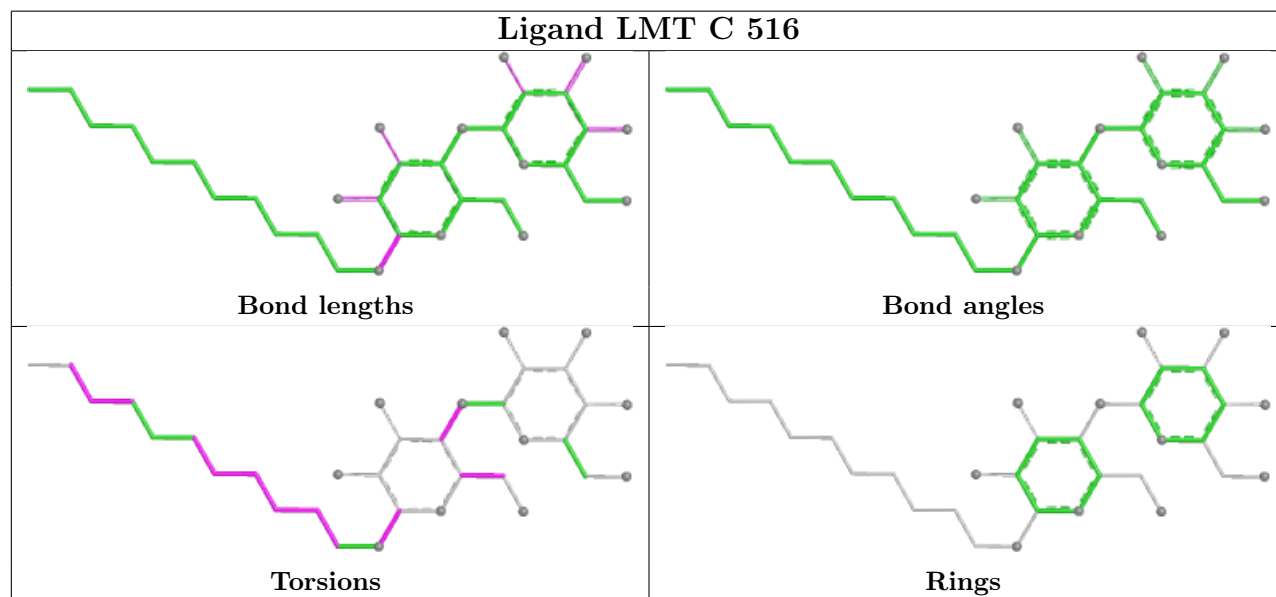
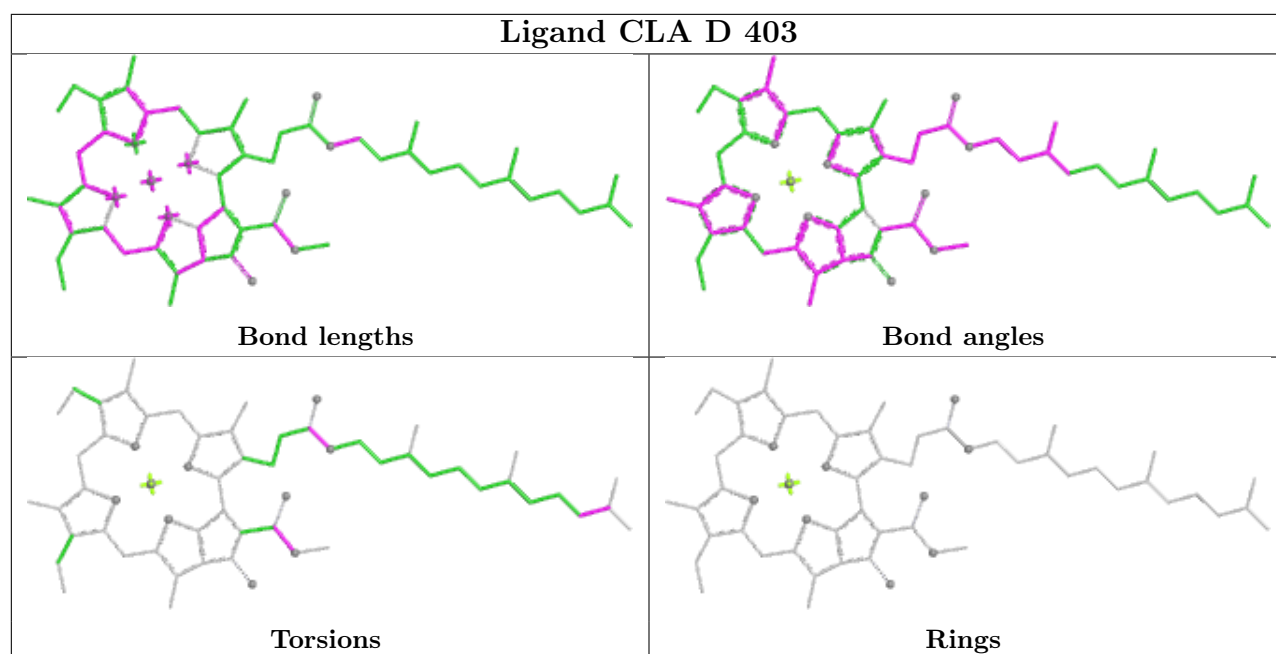
Ligand CLA B 610

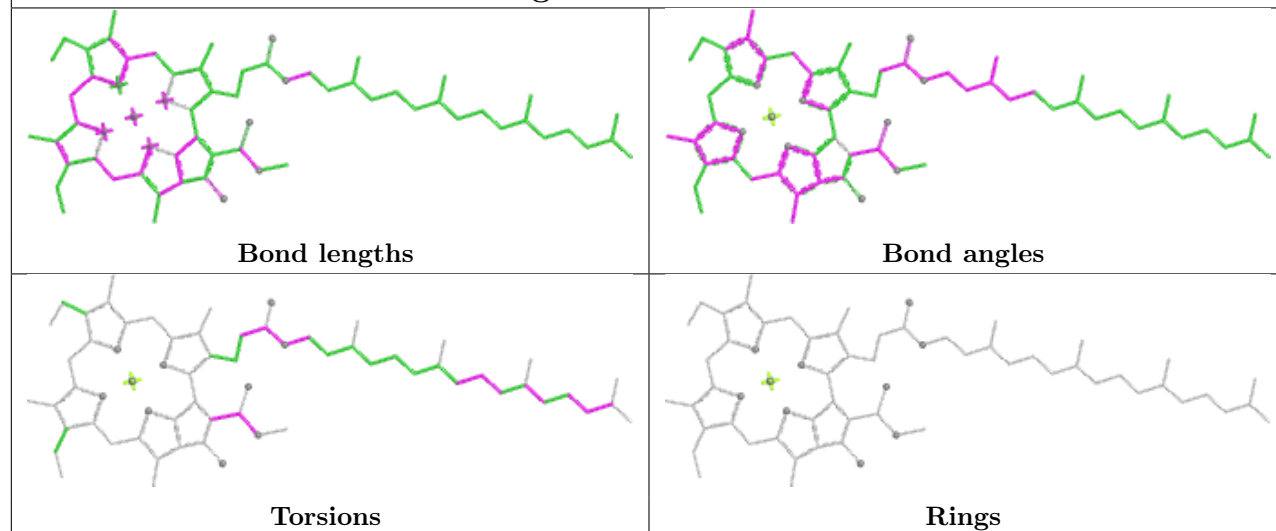
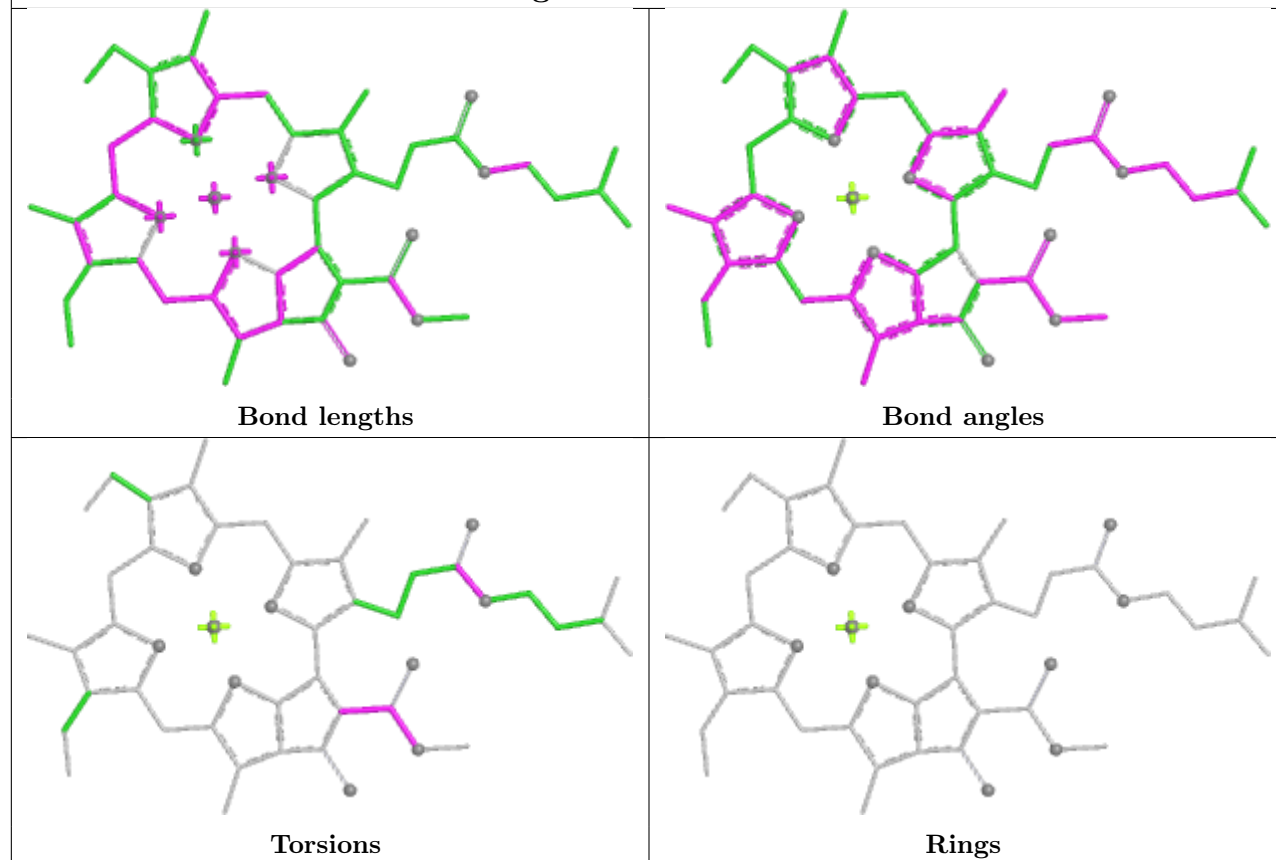


Ligand CLA A 407

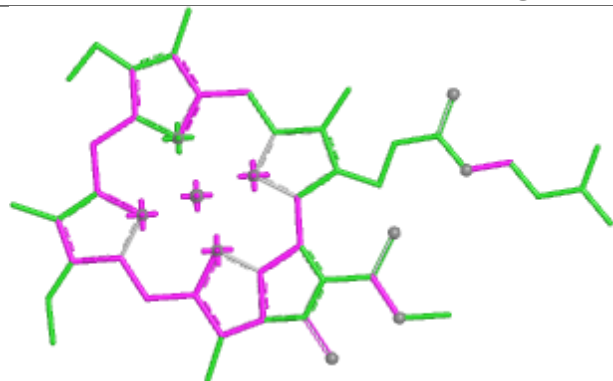




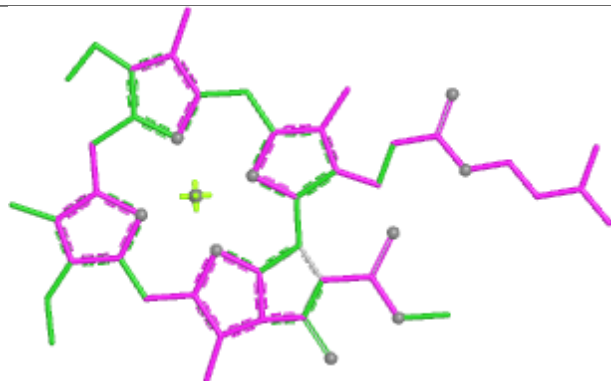


Ligand CLA B 611**Ligand CLA C 504**

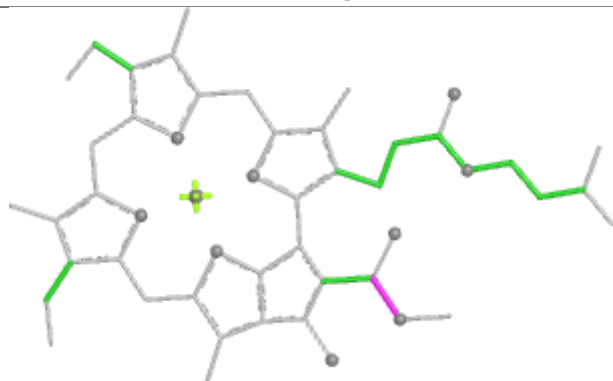
Ligand CLA B 614



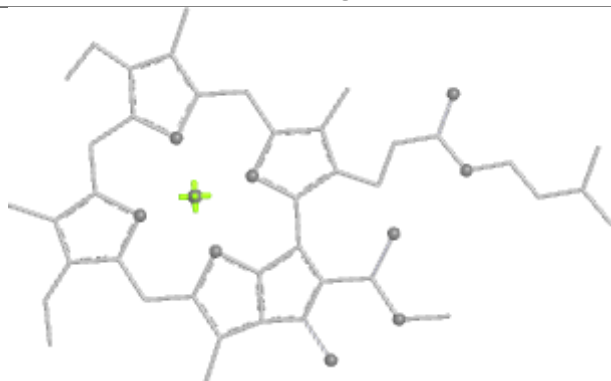
Bond lengths



Bond angles

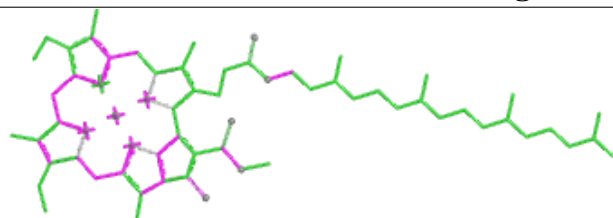


Torsions

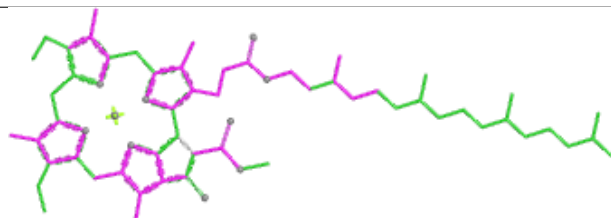


Rings

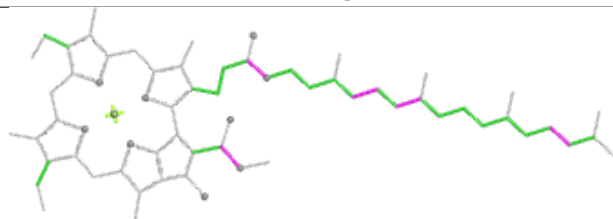
Ligand CLA A 403



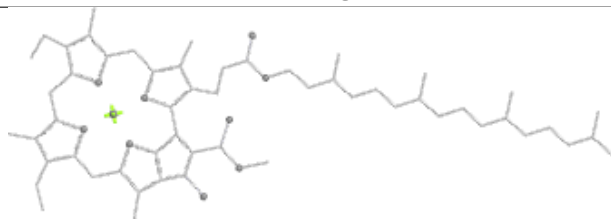
Bond lengths



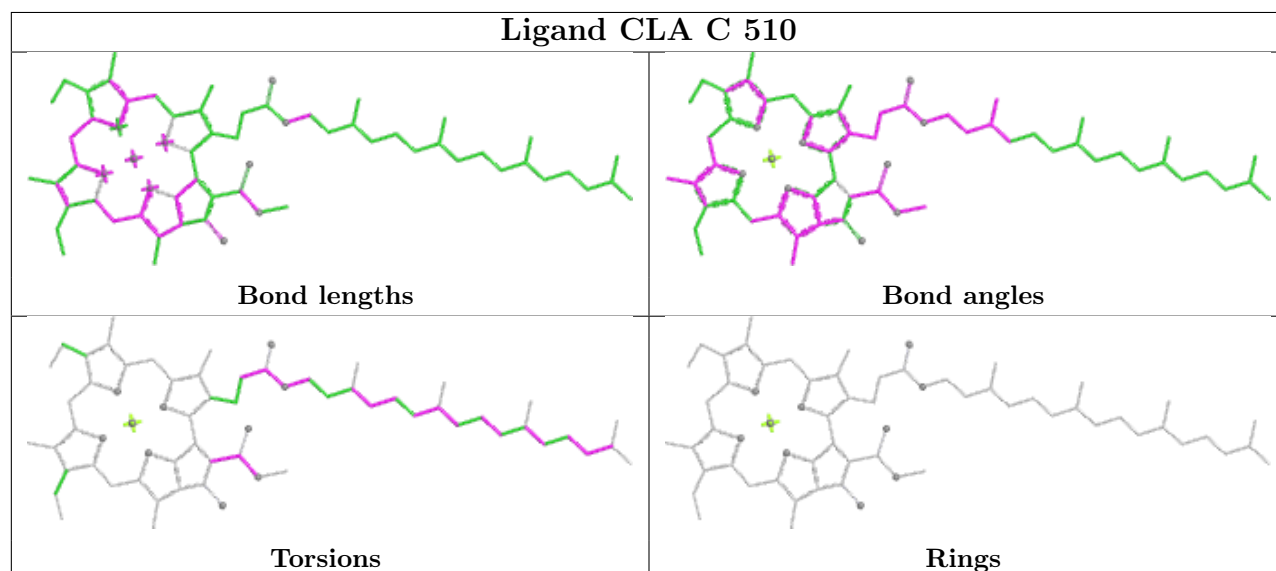
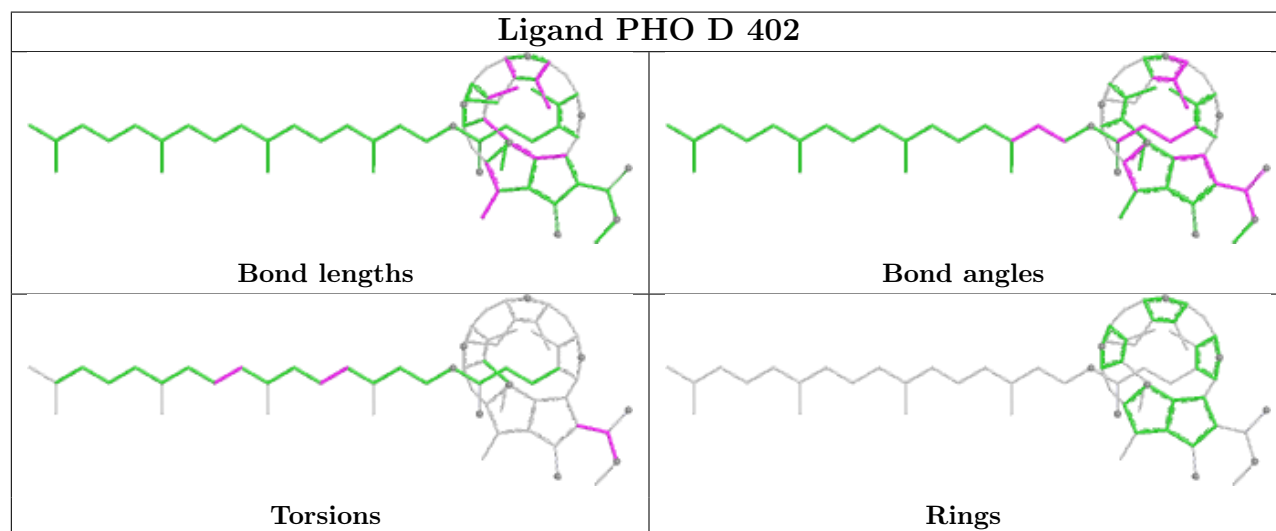
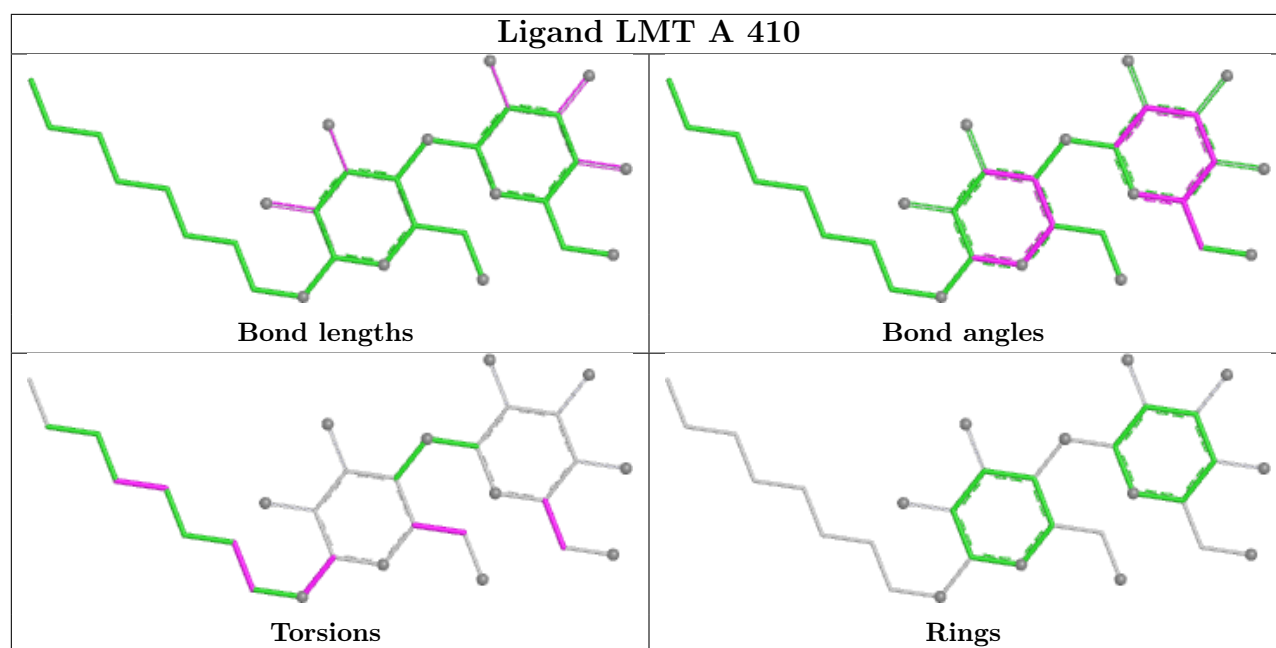
Bond angles

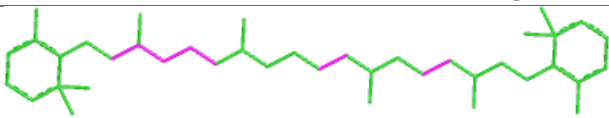
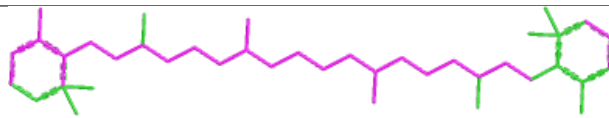
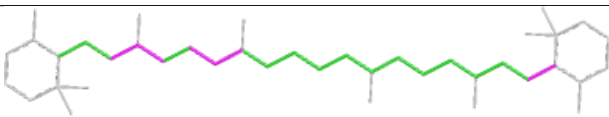
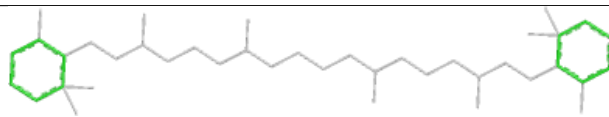


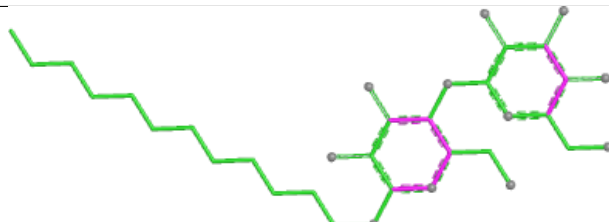
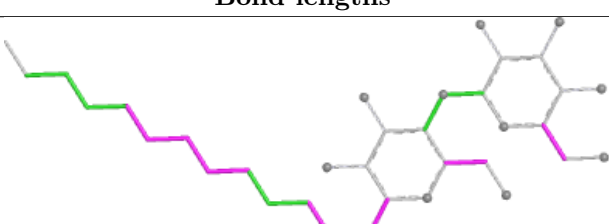
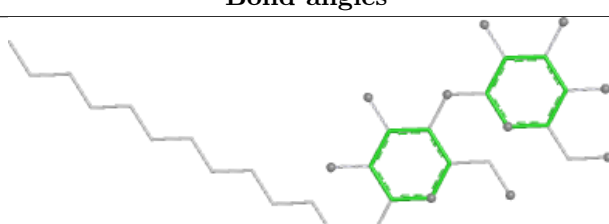
Torsions

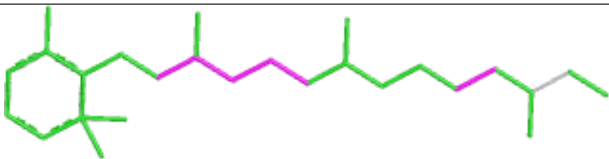
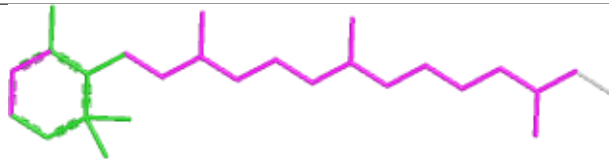
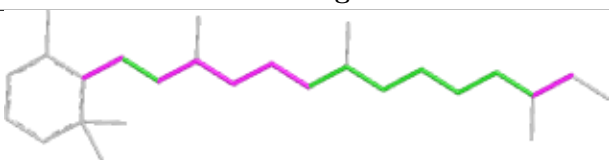
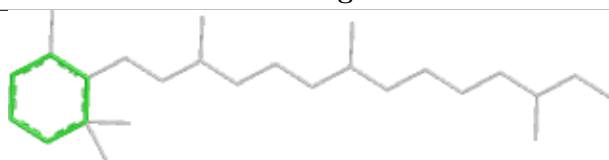


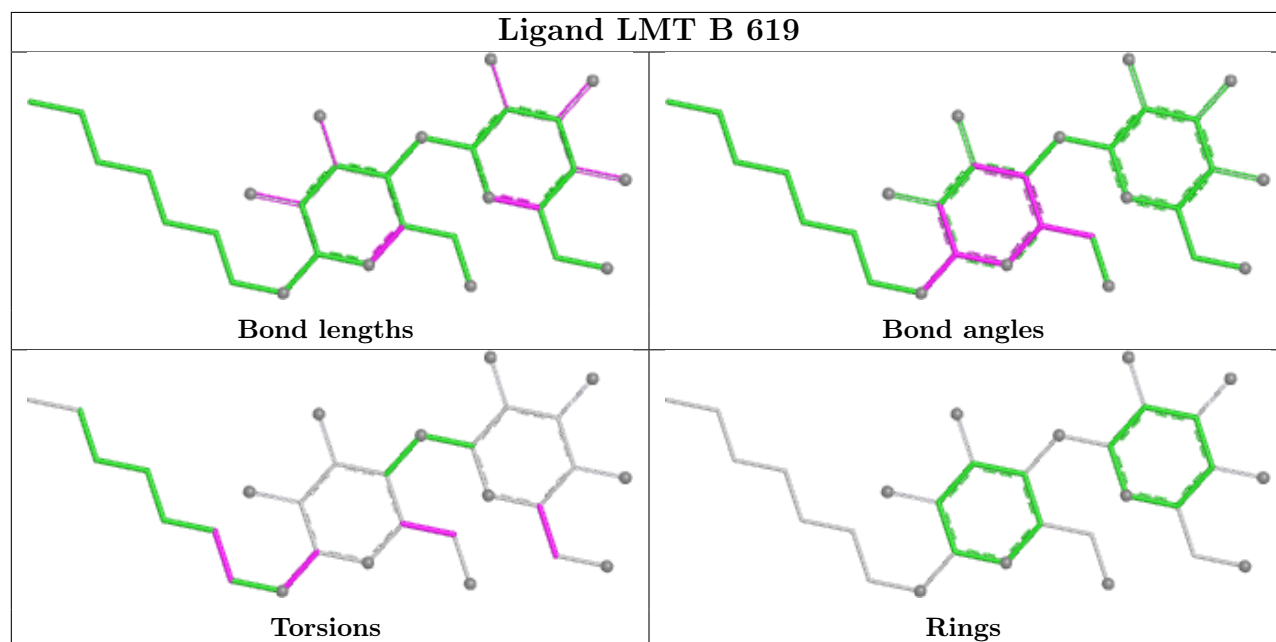
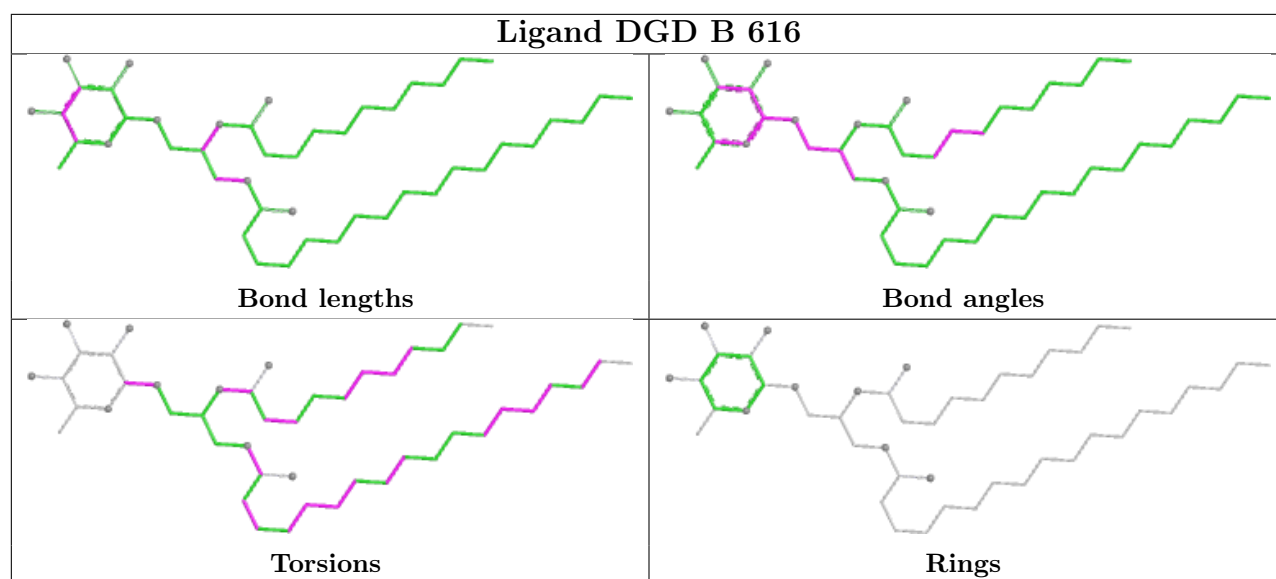
Rings

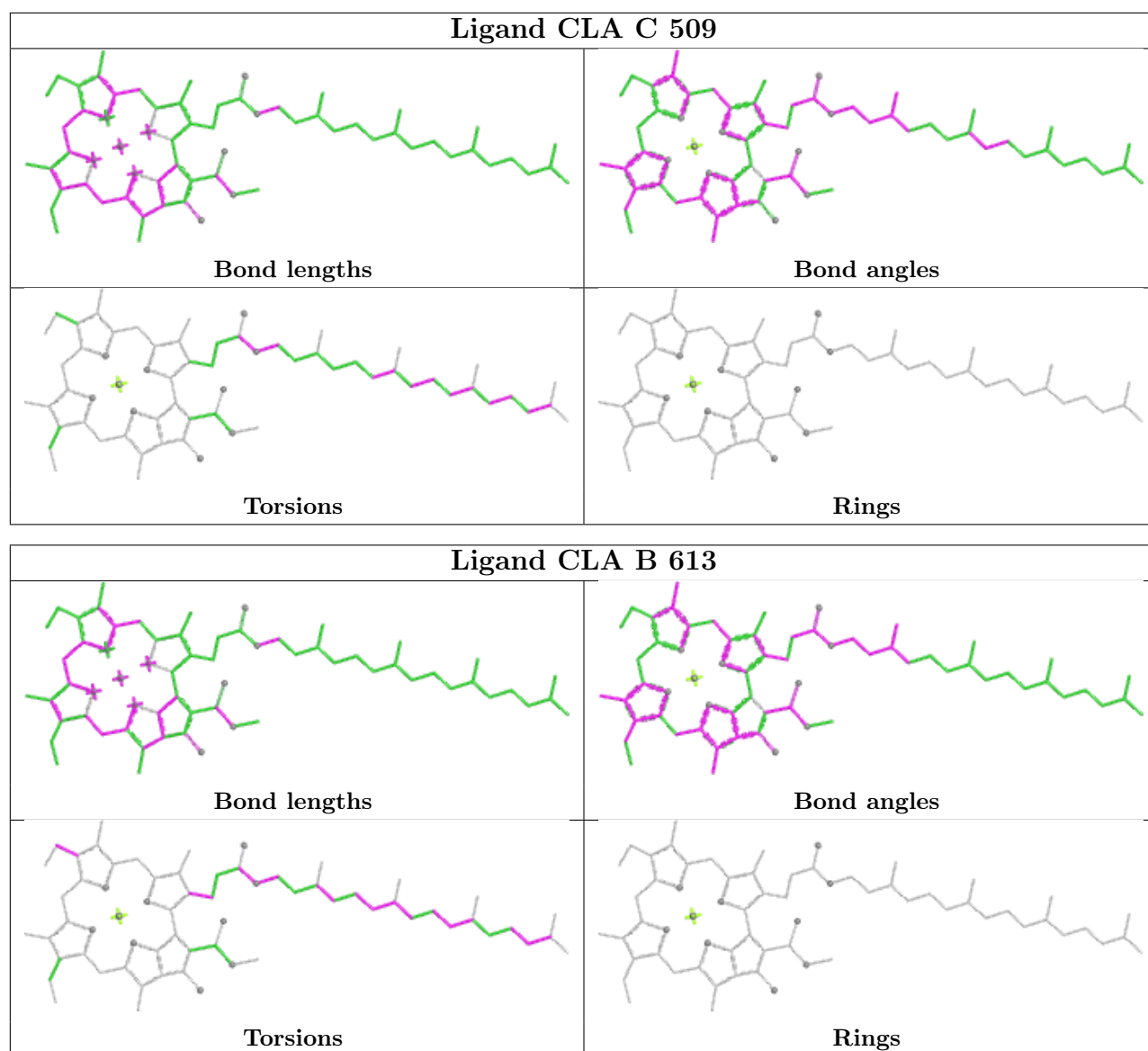


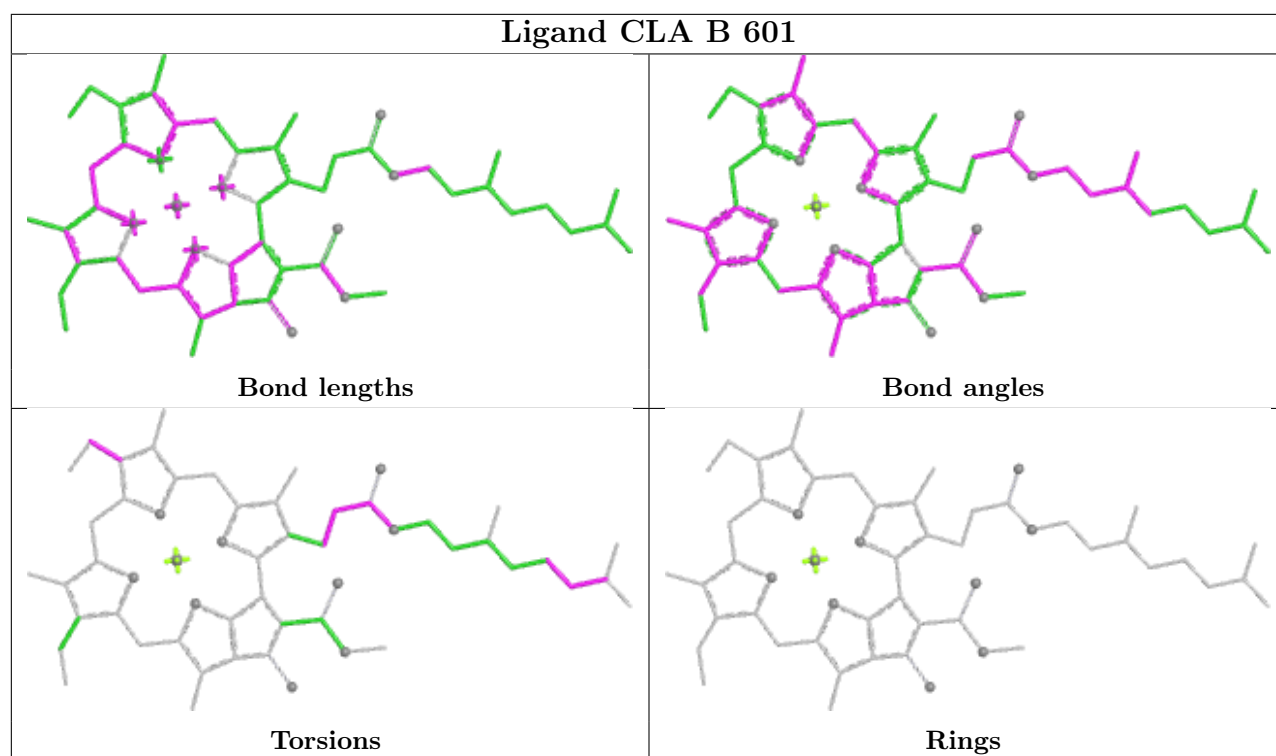
Ligand BCR B 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR D 405	
	
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.

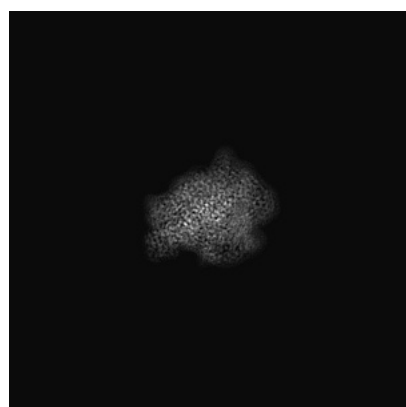
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24943. These allow visual inspection of the internal detail of the map and identification of artifacts.

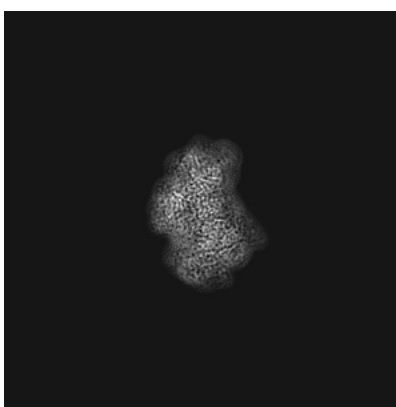
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

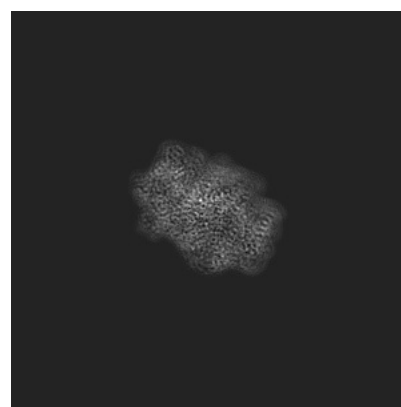
6.1.1 Primary map



X



Y



Z

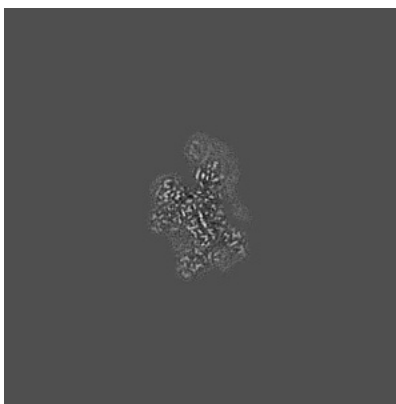
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

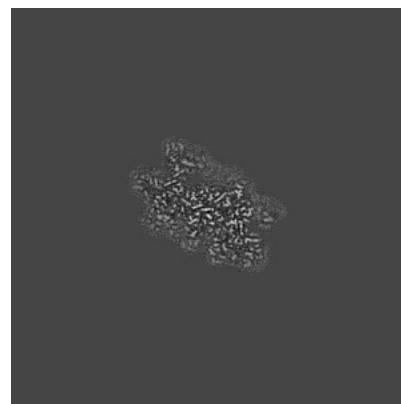
6.2.1 Primary map



X Index: 192



Y Index: 192

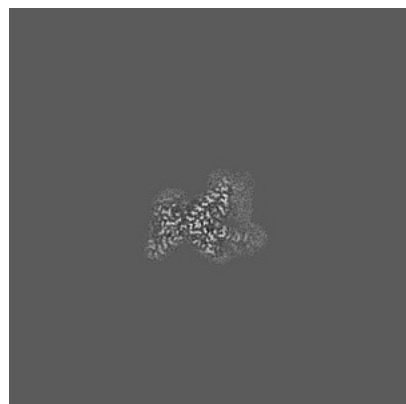


Z Index: 192

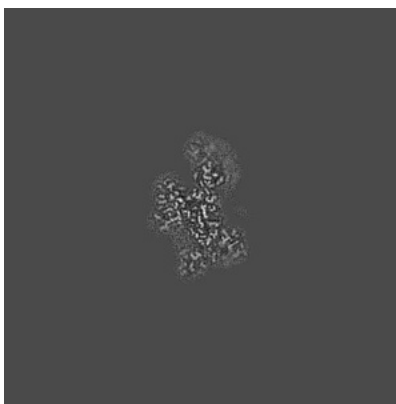
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

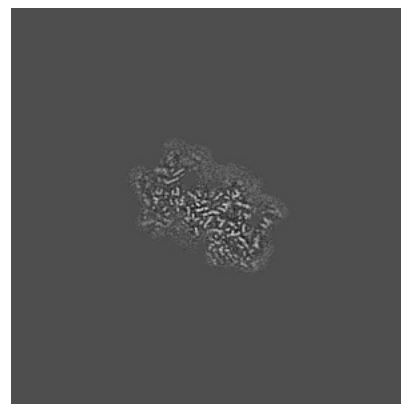
6.3.1 Primary map



X Index: 202



Y Index: 190

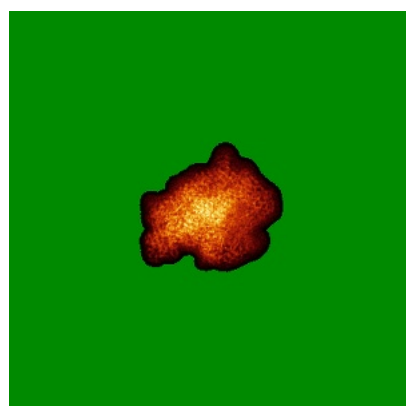


Z Index: 187

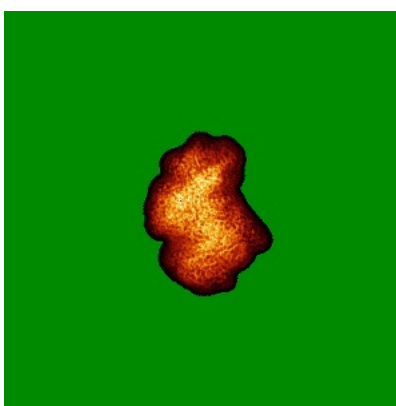
The images above show the largest variance slices of the map in three orthogonal directions.

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

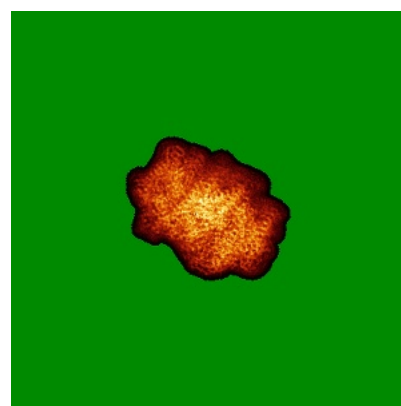
6.4.1 Primary map



X



Y

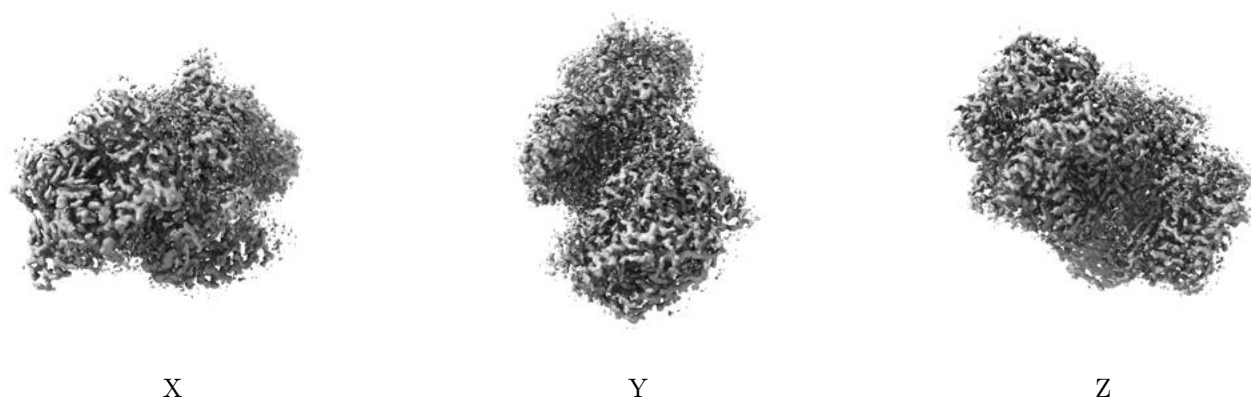


Z

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.

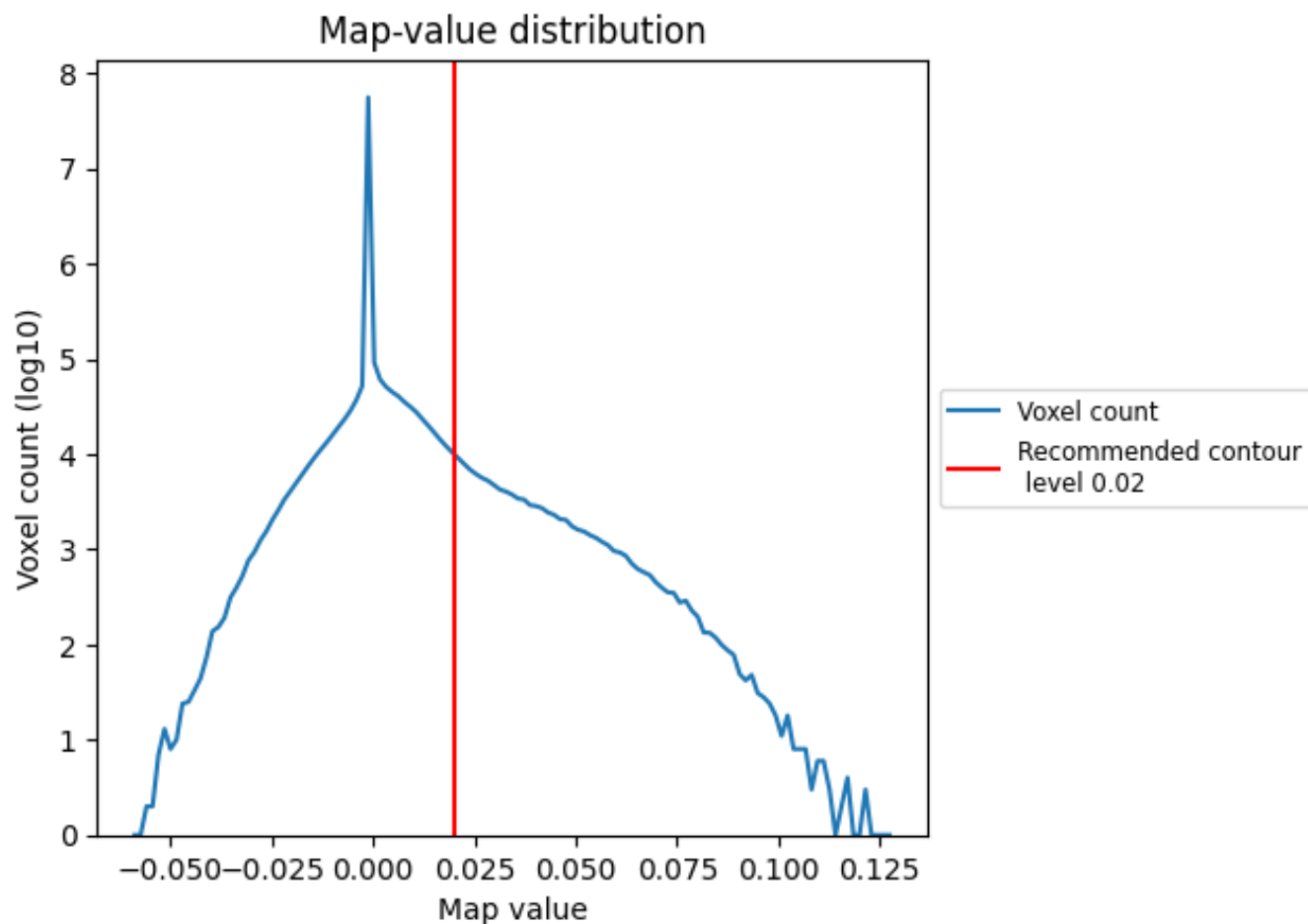
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

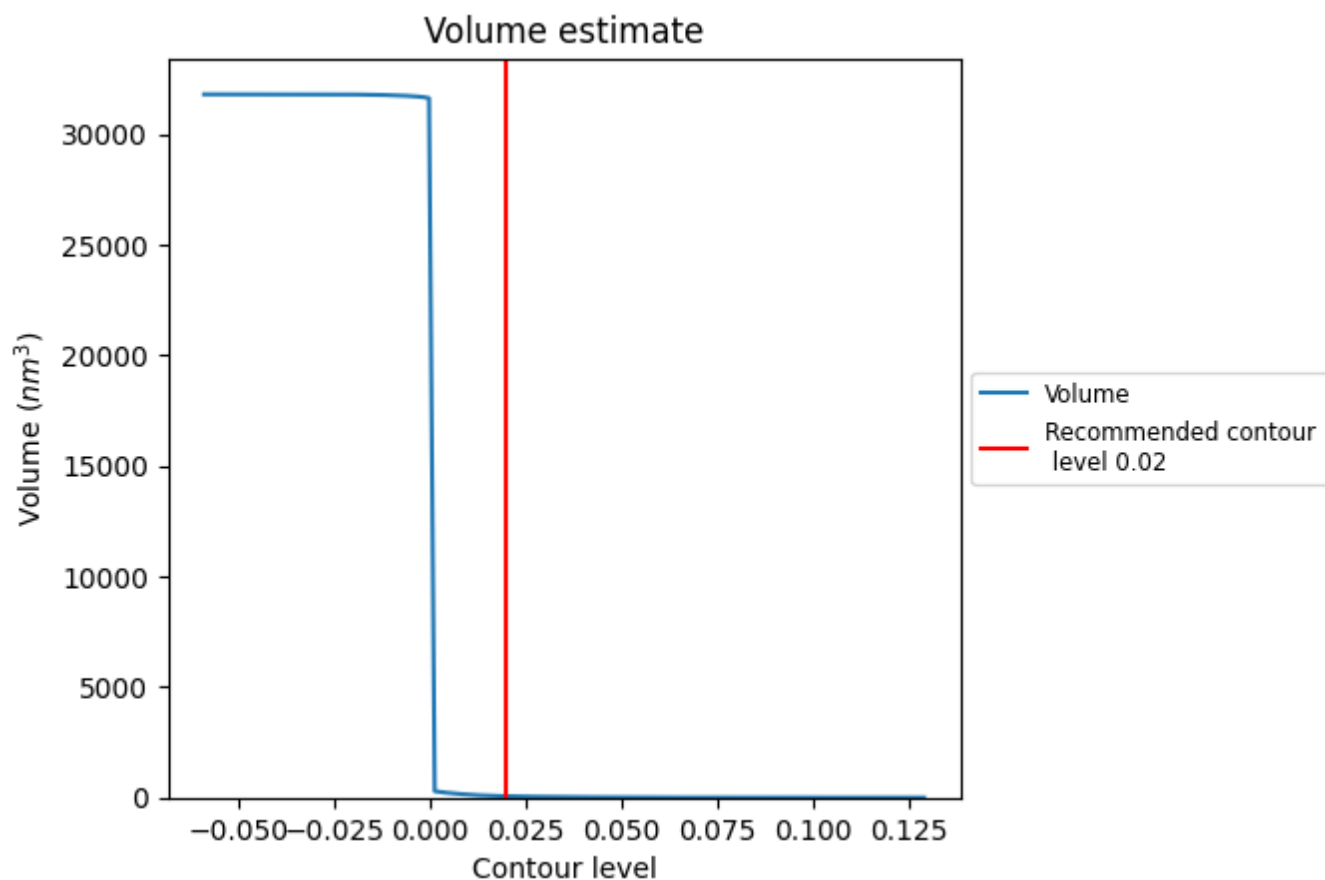
This section contains the results of statistical analysis of the map.

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.

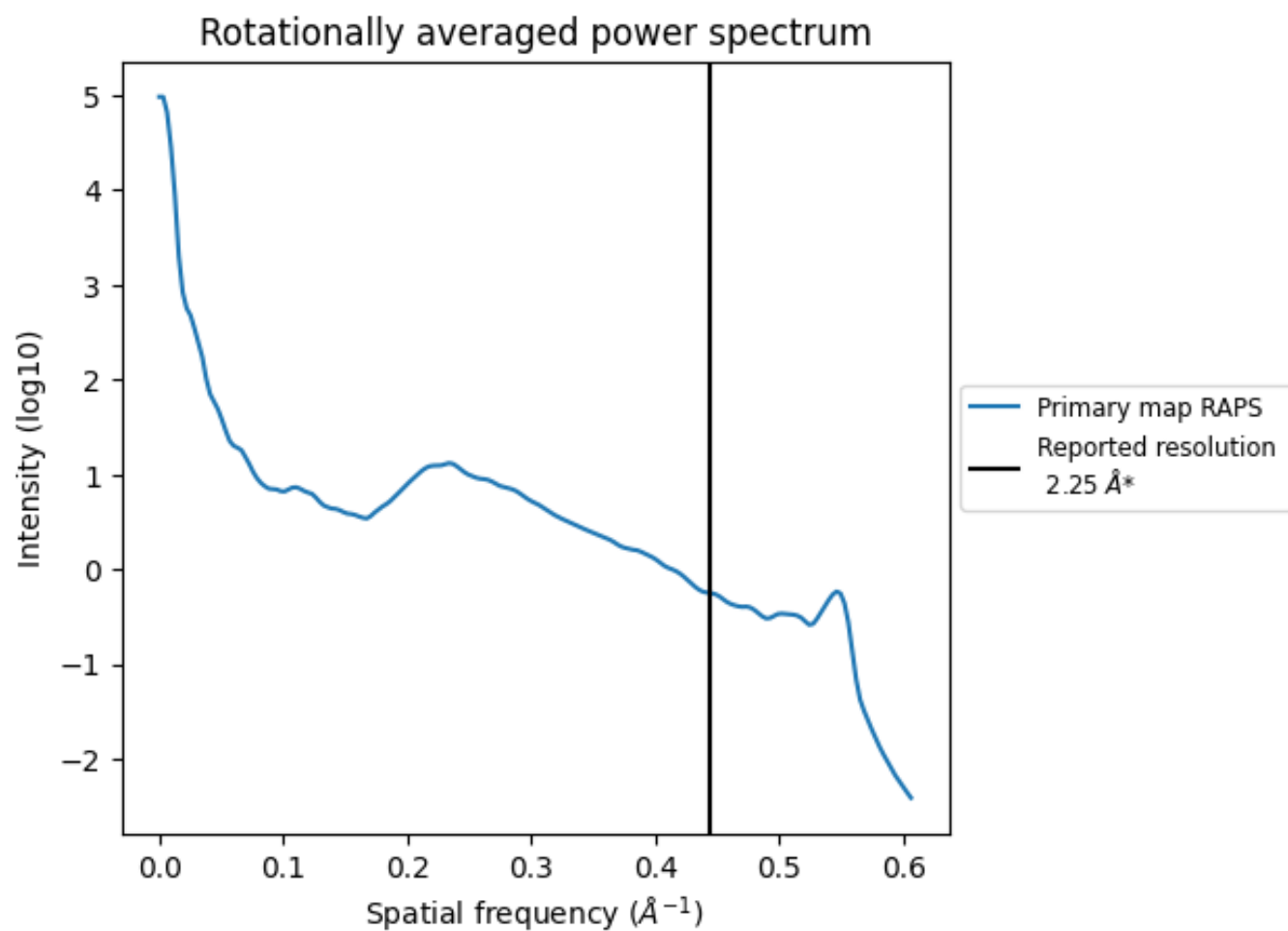
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm^3 ; this corresponds to an approximate mass of 54 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 ⓘ

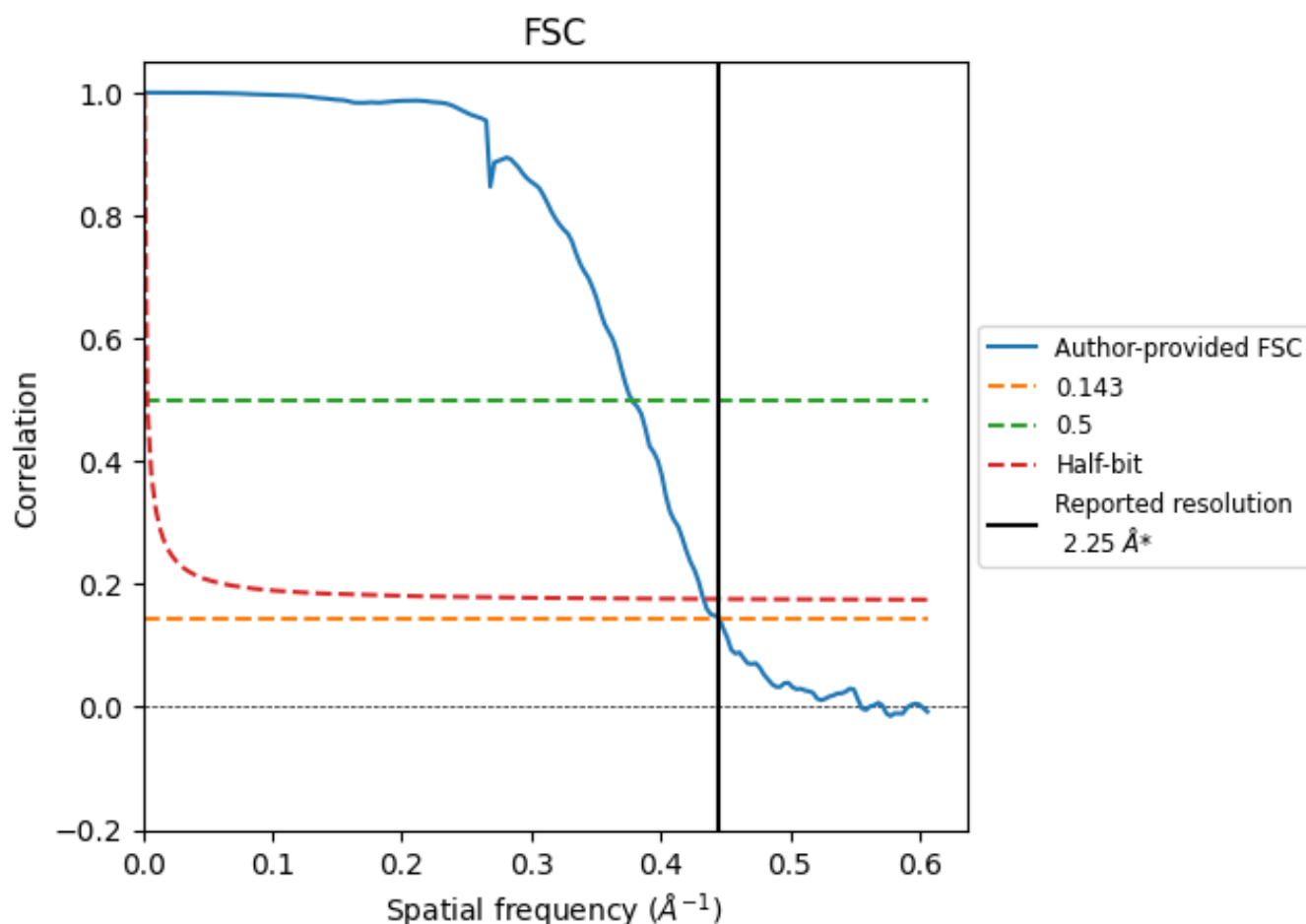


*Reported resolution corresponds to spatial frequency of 0.444 Å⁻¹

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 0.444 Å⁻¹

8.2 Resolution estimates [i](#)

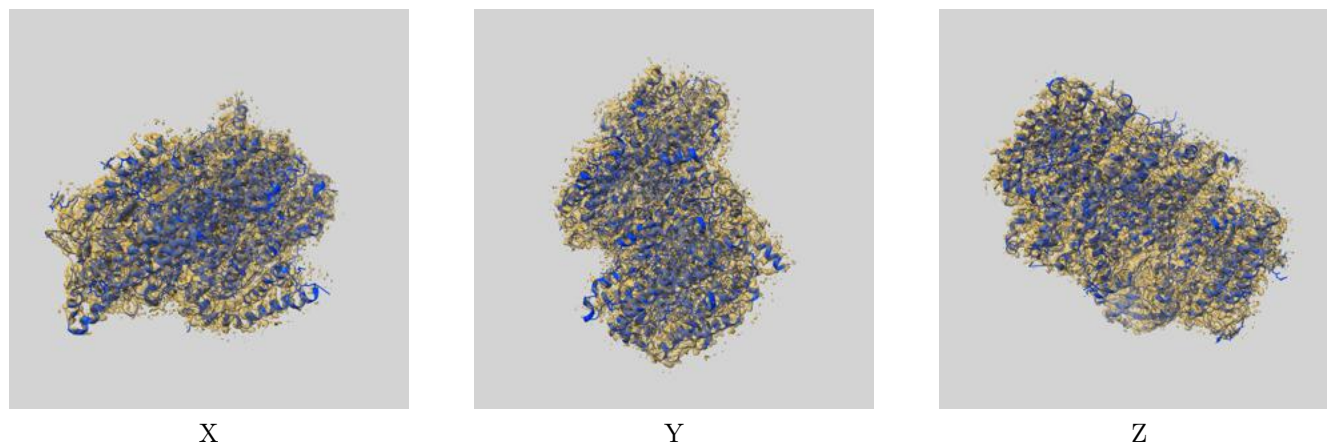
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.24	2.65	2.31
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

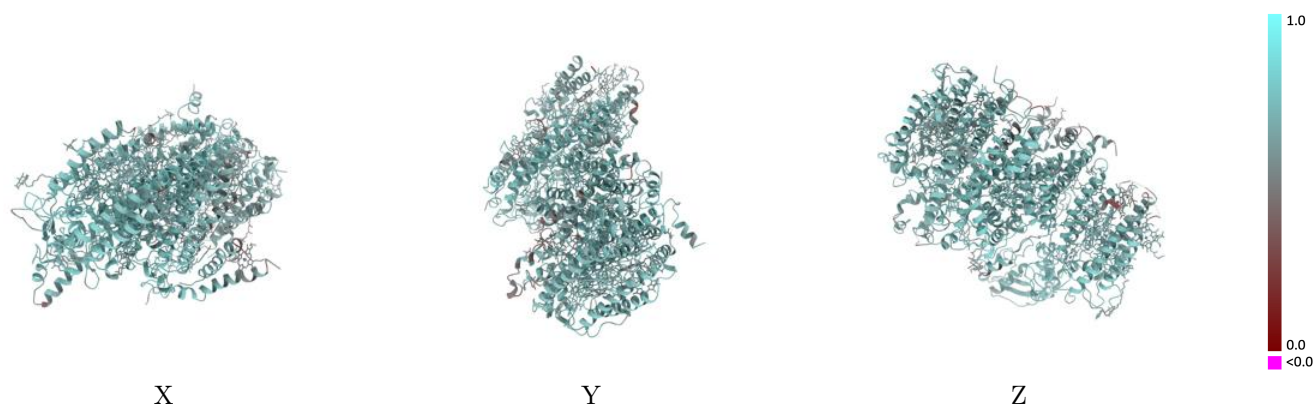
This section contains information regarding the fit between EMDB map EMD-24943 and PDB model 7SA3. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



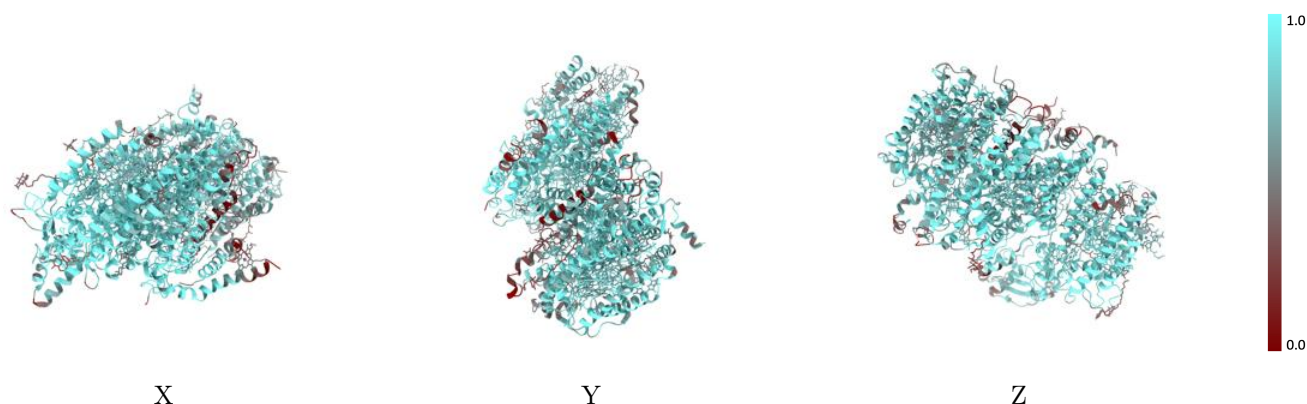
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



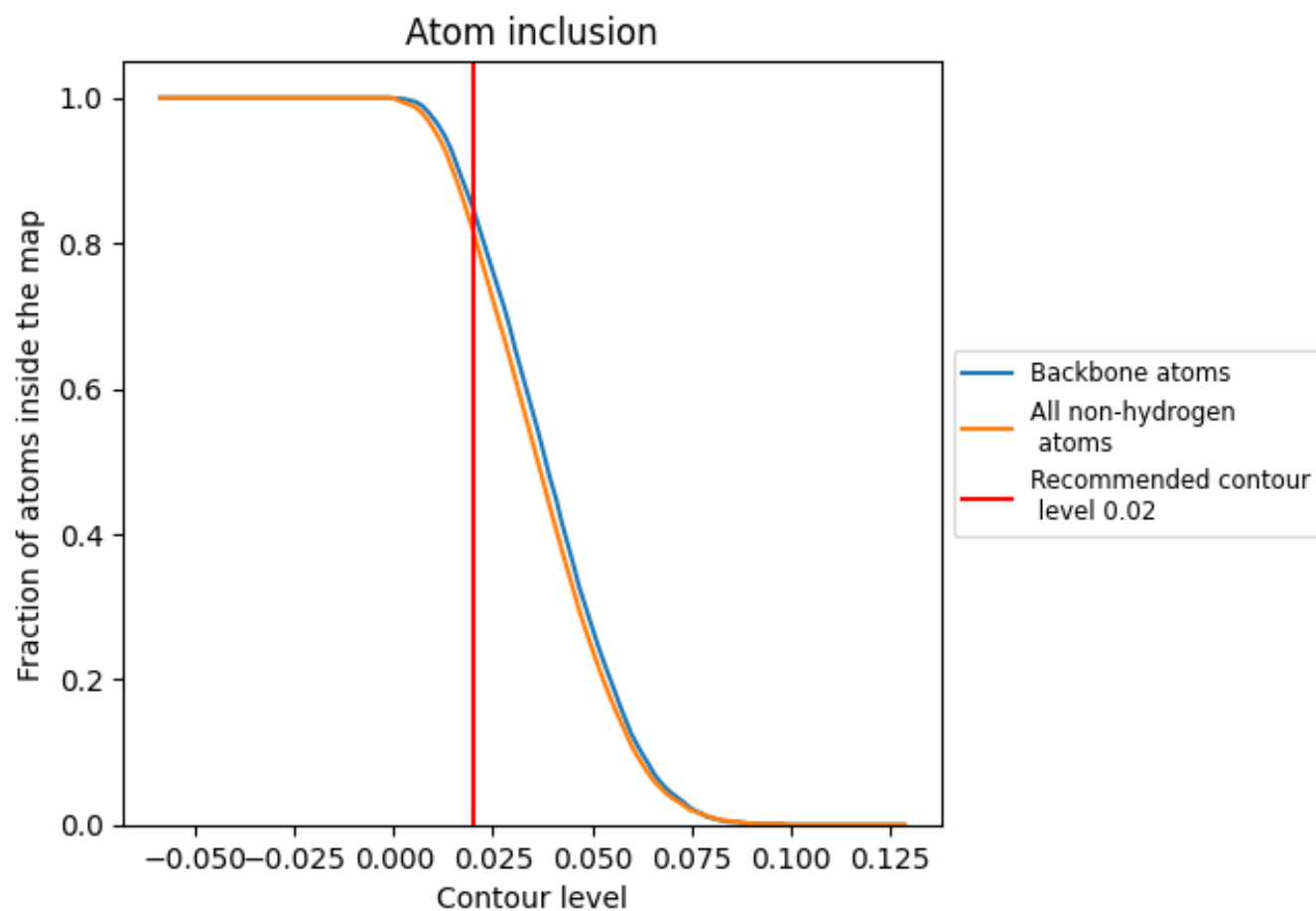
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 85% of all backbone atoms, 82% 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	0.8170	0.6800
A	0.8630	0.7030
B	0.8470	0.6850
C	0.7830	0.6650
D	0.8710	0.7060
E	0.7170	0.6340
F	0.6390	0.5940
I	0.7500	0.6480
K	0.4760	0.5710
N	0.1300	0.4730

1.0

0.0

<0.0