



## wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 04:38 PM JST

PDB ID : 7EDA / pdb\_00007eda  
EMDB ID : EMD-31062  
Title : Structure of monomeric photosystem II  
Authors : Yu, H.; Hamaguchi, T.; Nakajima, Y.; Kato, K.; kawakami, K.; Akita, F.;  
Yonekura, K.; Shen, J.R.  
Deposited on : 2021-03-15  
Resolution : 2.78 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

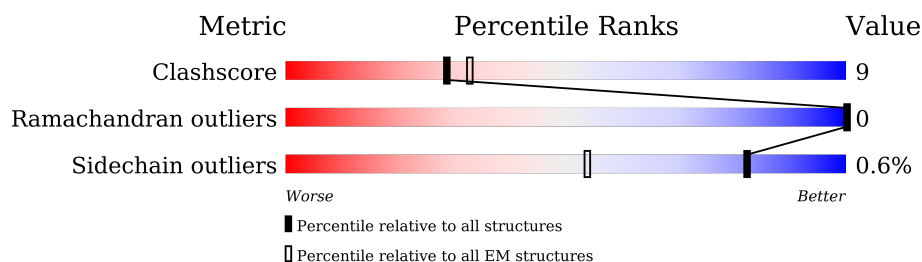
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.78 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	
2	B	504	
3	C	451	
4	D	341	
5	E	84	
6	F	45	
7	H	62	
8	I	38	

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Mol	Chain	Length	Quality of chain
9	J	40	
10	K	37	
11	L	37	
12	M	30	
13	O	244	
14	T	30	
15	U	104	
16	V	163	
17	Y	30	
18	X	40	
19	Z	62	
20	R	34	

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
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	410	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	617	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 22843 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2598	1708	429	446	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	504	Total	C	N	O	S	0	0
			3890	2560	652	665	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	451	Total	C	N	O	S	0	0
			3453	2268	583	589	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	2	0
			2699	1796	443	448	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	80	Total	C	N	O	0	0
			622	412	100	110		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	34	Total	C	N	O	S	0	0
			274	187	45	41	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	62	Total	C	N	O	S	0	0
			484	326	78	78	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	32	Total	C	N	O	S	0	0
			255	176	37	41	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	36	Total	C	N	O	S	0	0
			251	171	37	42	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			280	194	42	44		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	30	Total	C	N	O	0	0
			244	166	36	42		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	30	Total	C	N	O	0	0
			223	150	33	40		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	192	Total	C	N	O	S	0	0
			1415	907	237	267	4		

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	29	Total	C	N	O	S	0	0
			230	161	32	36	1		

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	U	84	Total	C	N	O	0	0
			629	409	110	110		

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	135	Total	C	N	O	S	0	0
			1016	651	171	190	4		

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0
			190	125	32	31	2		

- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	38	Total	C	N	O	0	0
			269	179	44	46		

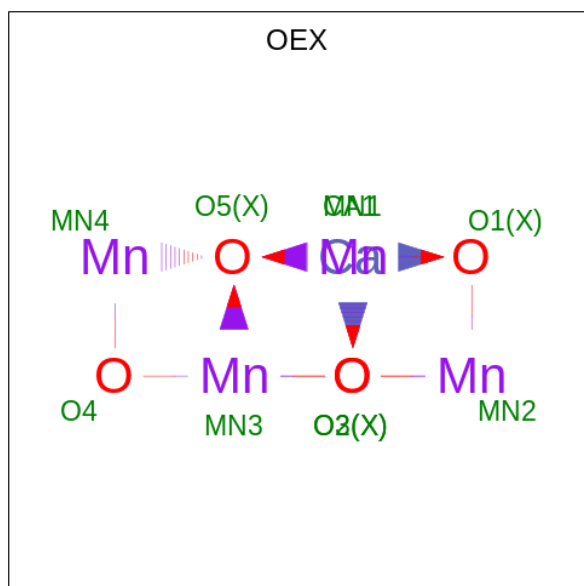
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	57	Total	C	N	O	S	0	0
			410	284	61	64	1		

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	34	Total	C	N	O	0	0
			186	115	36	35		

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



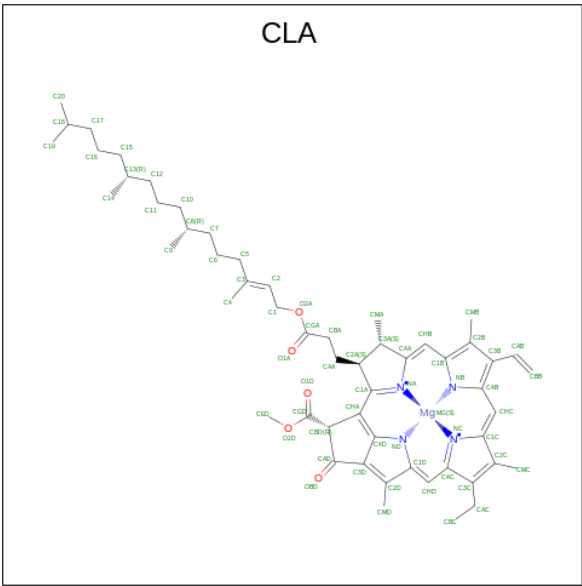
Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	Ca	Mn	O	0
			10	1	4	5	

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

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



- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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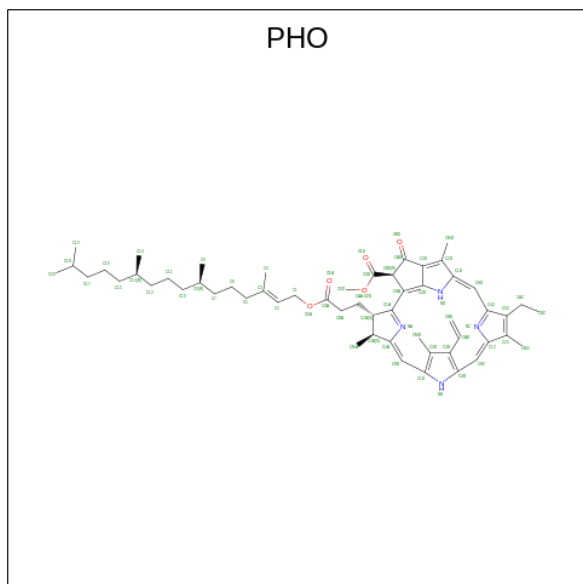
Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 62	C 52	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 57	C 47	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 52	C 42	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	C	1	Total 53	C 43	Mg 1	N 4	O 5	0
23	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	D	1	Total 60	C 50	Mg 1	N 4	O 5	0

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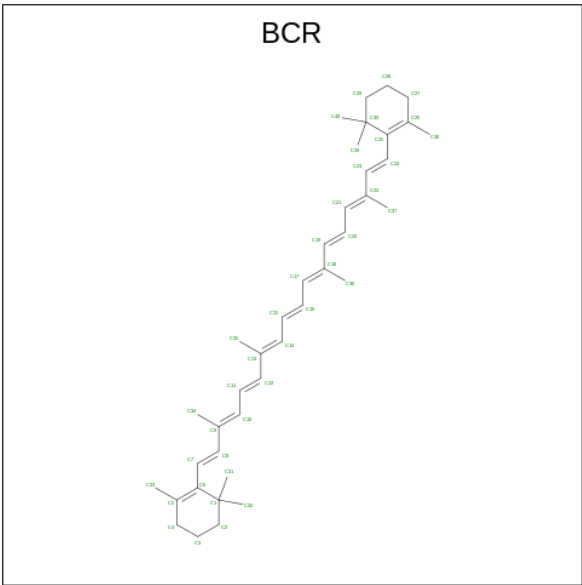
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	D	1	45	35	1	4	5	0

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



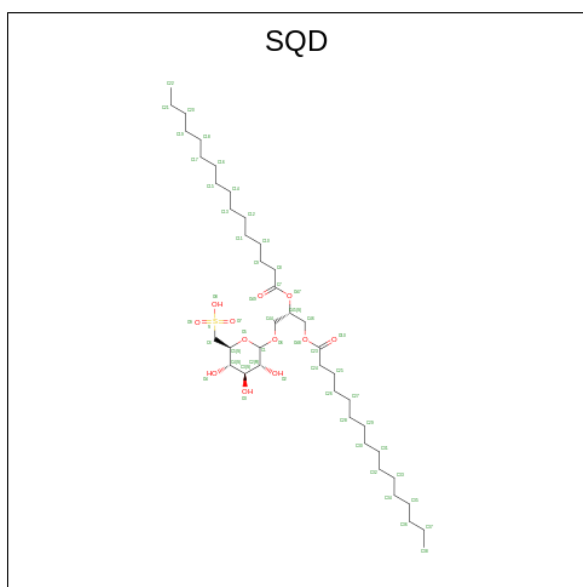
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
24	A	1	64	55	4	5	0
24	A	1	64	55	4	5	0

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ) (labeled as "Ligand of Interest" by depositor).



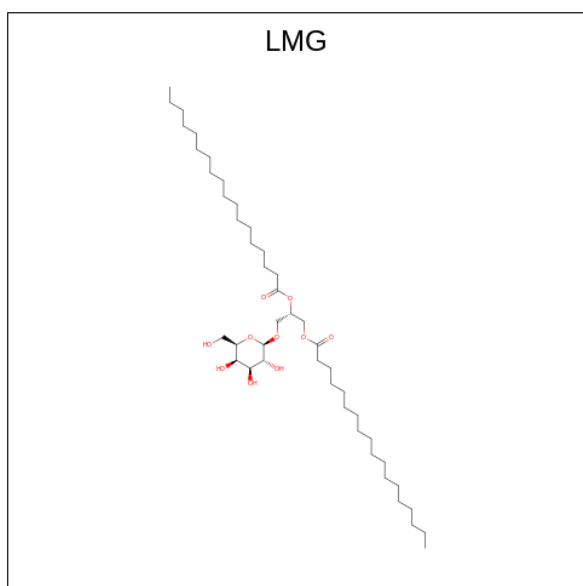
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	D	1	Total C 29 29	0
25	K	1	Total C 40 40	0
25	K	1	Total C 40 40	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			54	41	12	1	
26	D	1	Total	C	O	S	0
			24	13	10	1	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



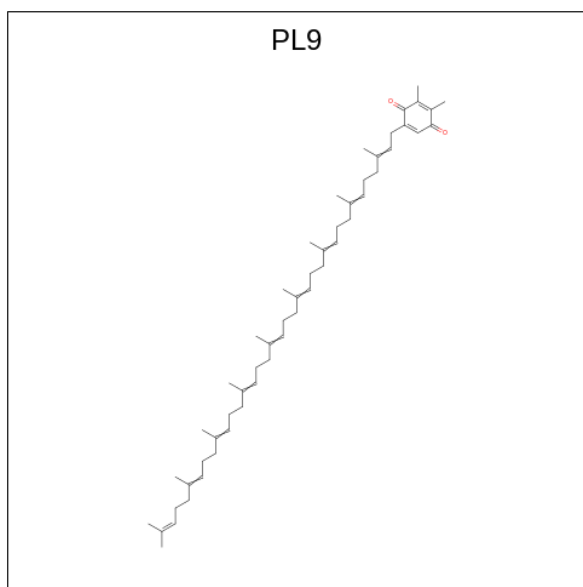
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			38	28	10	

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Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			39	29	10	
27	D	1	Total	C	O	0
			24	14	10	

- Molecule 28 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:  $C_{53}H_{80}O_2$ ).

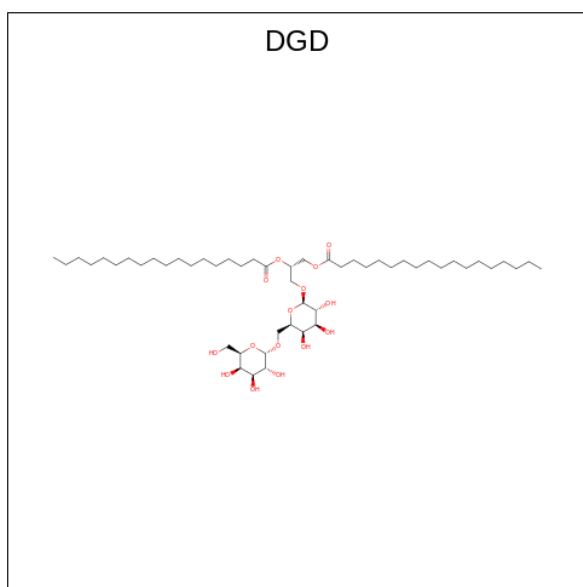


Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			51	49	2	
28	D	1	Total	C	O	0
			43	41	2	

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula: ) (labeled as "Ligand of Interest" by depositor).

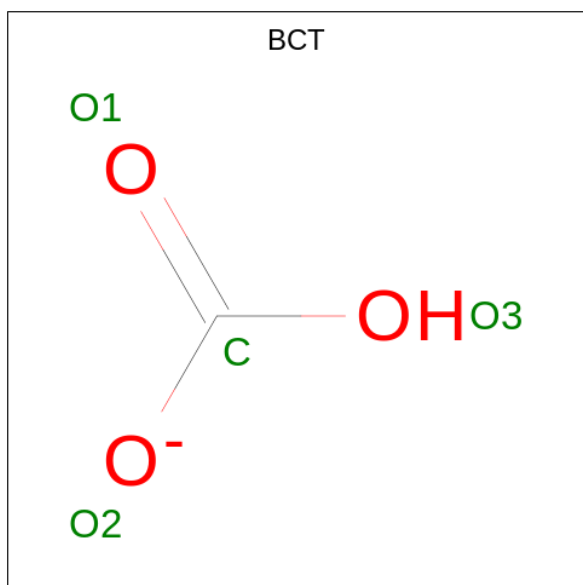
Mol	Chain	Residues	Atoms		AltConf
29	B	1	Total	C	0
			7	7	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



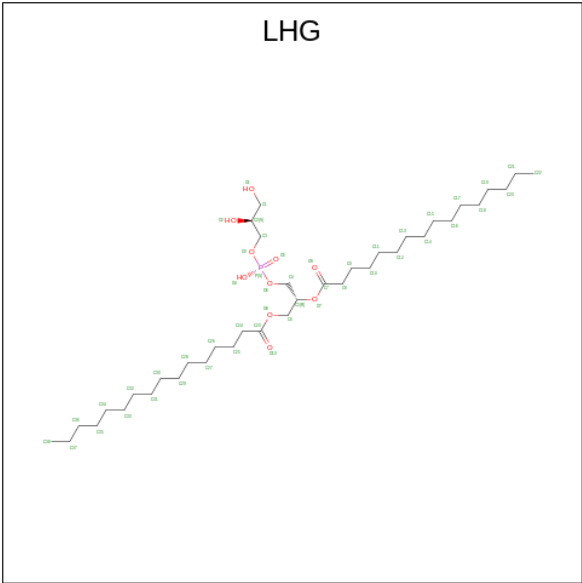
Mol	Chain	Residues	Atoms			AltConf
30	C	1	Total	C	O	0
			41	26	15	
30	C	1	Total	C	O	0
			49	34	15	
30	C	1	Total	C	O	0
			50	35	15	
30	H	1	Total	C	O	0
			50	35	15	

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3^-$ ).



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

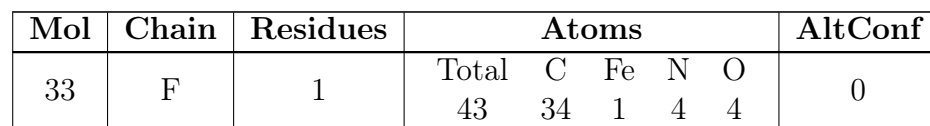
- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



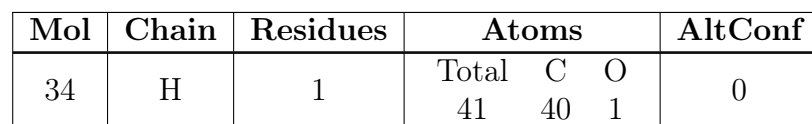
Mol	Chain	Residues	Atoms				AltConf
32	D	1	Total	C	O	P	0
			49	38	10	1	
32	D	1	Total	C	O	P	0
			32	21	10	1	
32	D	1	Total	C	O	P	0
			33	22	10	1	
32	L	1	Total	C	O	P	0
			40	29	10	1	

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).

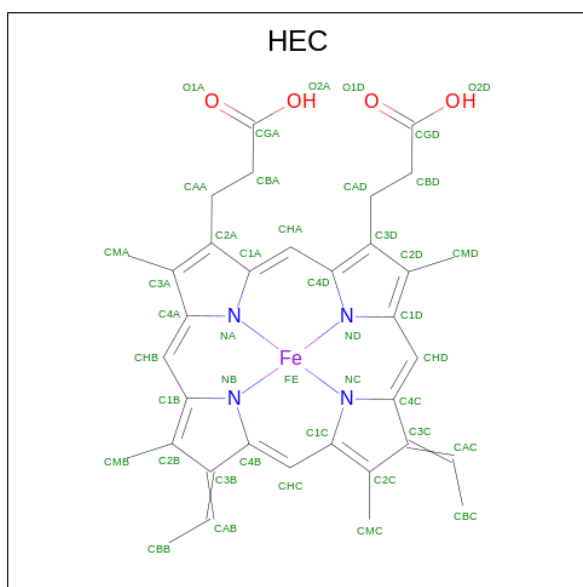




- Molecule 34 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O) (labeled as "Ligand of Interest" by depositor).



- Molecule 35 is HEME C (CCD ID: HEC) (formula:  $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$ ).



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

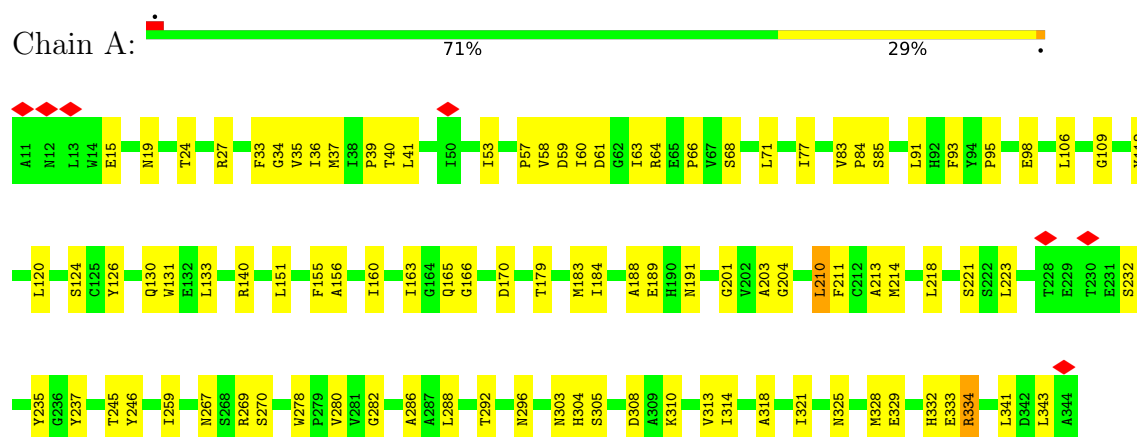
- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	A	7	Total O 7 7	0
36	B	5	Total O 5 5	0
36	C	4	Total O 4 4	0

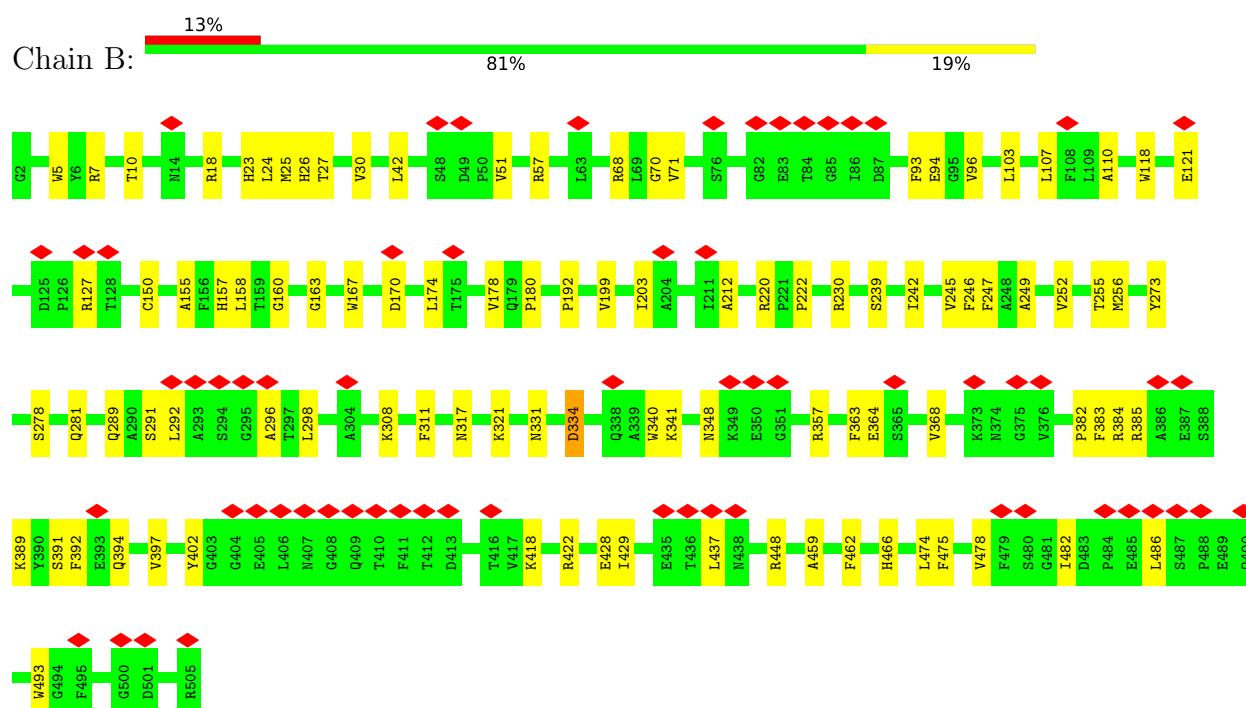
### 3 Residue-property plots

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

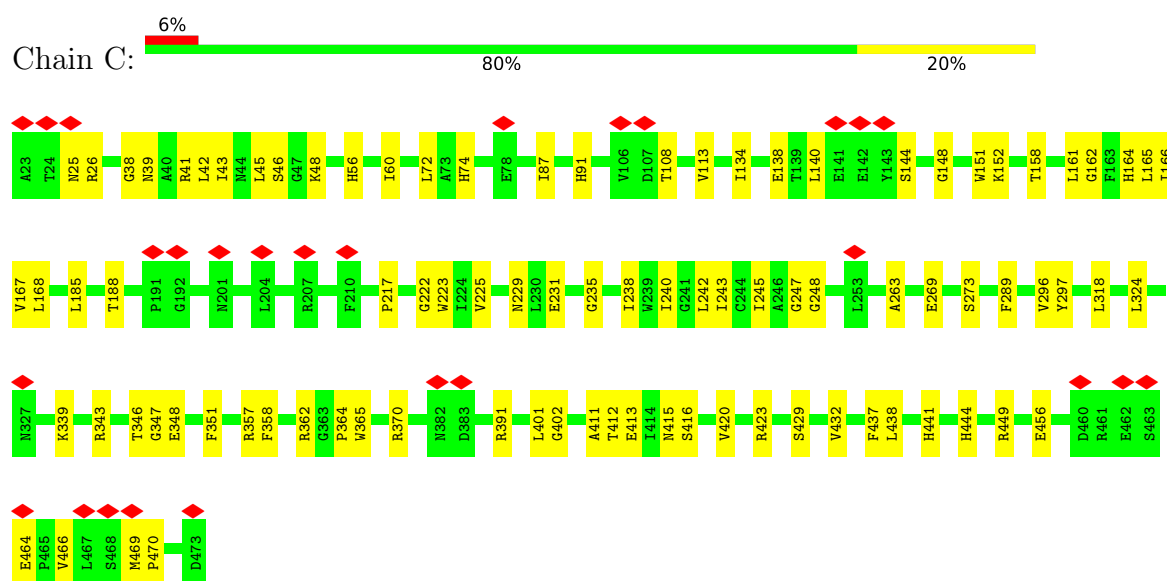
- Molecule 1: Photosystem II protein D1



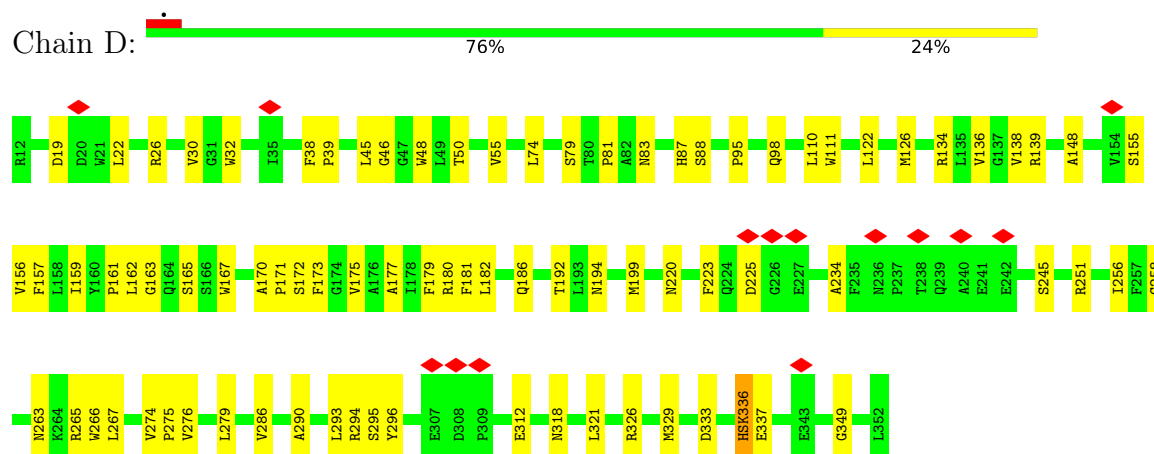
- Molecule 2: Photosystem II CP47 reaction center protein



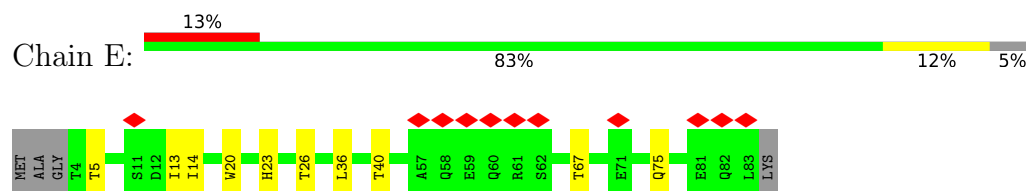
- Molecule 3: Photosystem II CP43 reaction center protein



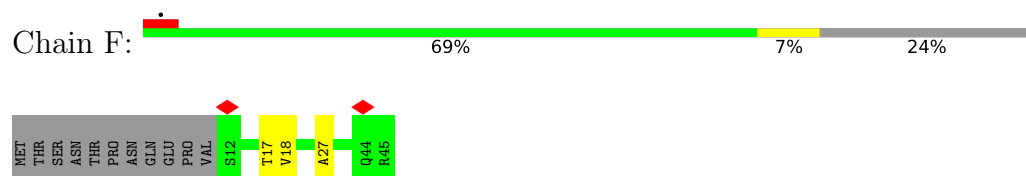
• Molecule 4: Photosystem II D2 protein



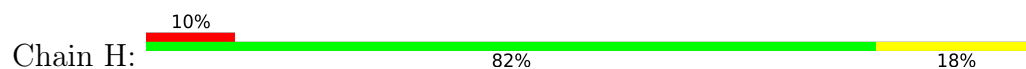
• Molecule 5: Cytochrome b559 subunit alpha

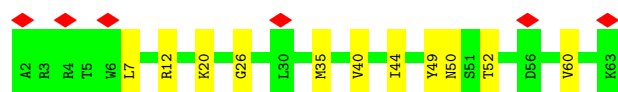


• Molecule 6: Cytochrome b559 subunit beta

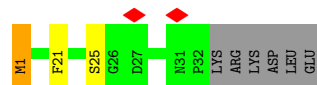
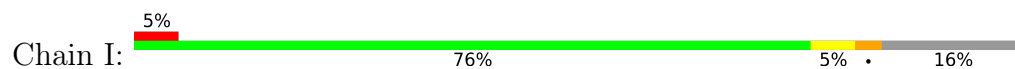


• Molecule 7: Photosystem II reaction center protein H

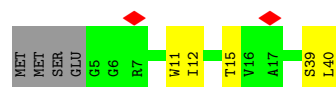
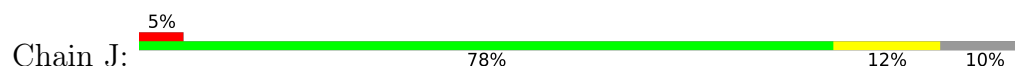




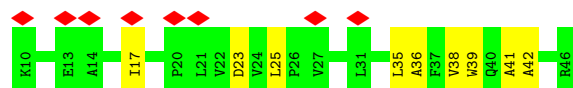
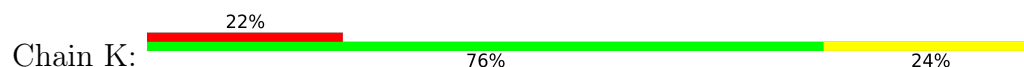
- Molecule 8: Photosystem II reaction center protein I



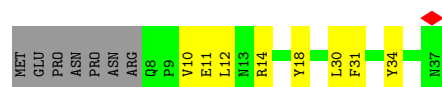
- Molecule 9: Photosystem II reaction center protein J



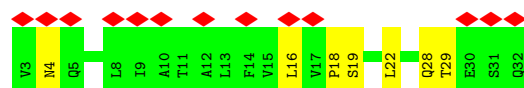
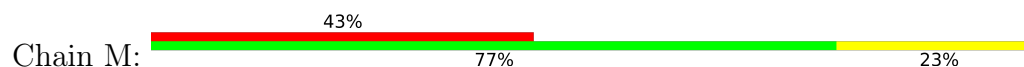
- Molecule 10: Photosystem II reaction center protein K



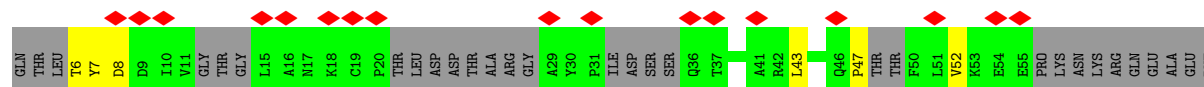
- Molecule 11: Photosystem II reaction center protein L

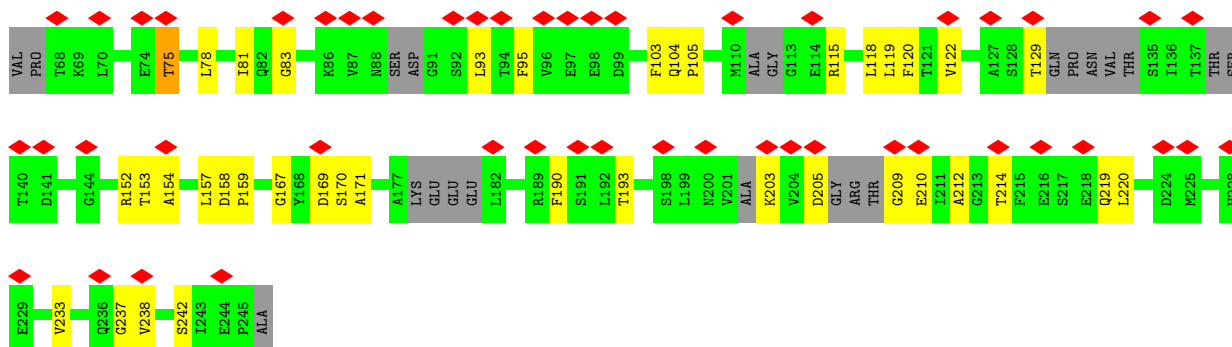


- Molecule 12: Photosystem II reaction center protein M

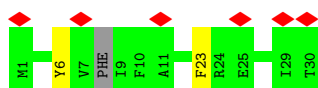


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

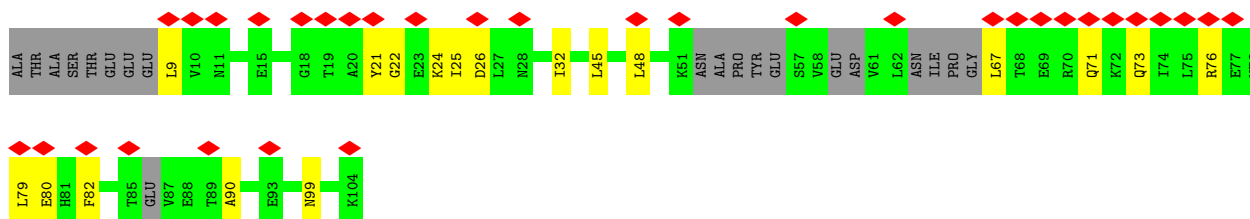




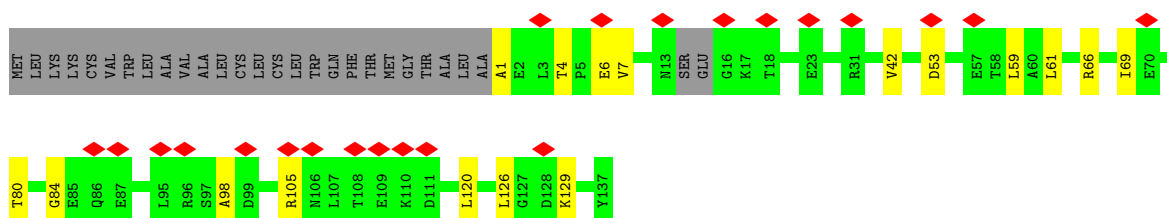
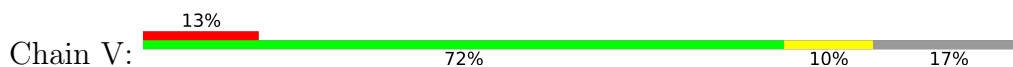
- Molecule 14: Photosystem II reaction center protein T



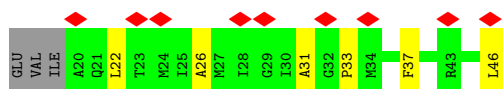
- Molecule 15: Photosystem II 12 kDa extrinsic protein



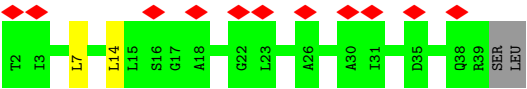
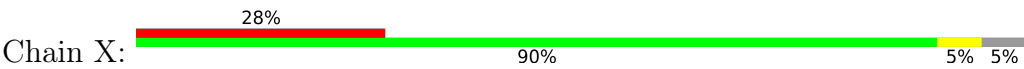
- Molecule 16: Cytochrome c-550



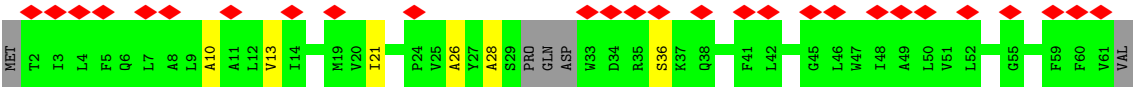
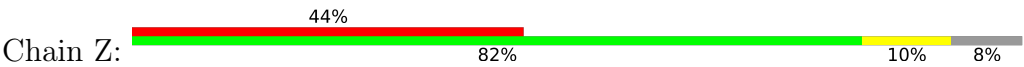
- Molecule 17: Photosystem II reaction center protein Ycf12



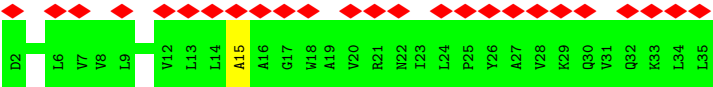
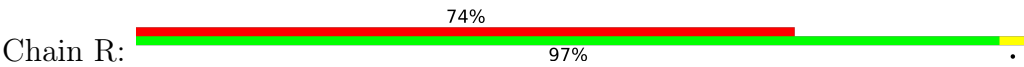
- Molecule 18: Photosystem II reaction center protein X



● Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	173875	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	70	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	0.180	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0316	Depositor
Map size ( $\text{\AA}$ )	197.26031, 197.26031, 197.26031	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.82191795, 0.82191795, 0.82191795	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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	0.48	0/2683	0.60	1/3660 (0.0%)
2	B	0.44	0/4028	0.55	0/5496
3	C	0.45	0/3566	0.55	0/4859
4	D	0.50	0/2777	0.61	2/3785 (0.1%)
5	E	0.38	0/641	0.52	0/880
6	F	0.38	0/283	0.53	0/386
7	H	0.36	0/497	0.61	0/679
8	I	0.36	0/252	0.52	0/344
9	J	0.34	0/257	0.56	0/349
10	K	0.48	0/290	0.64	0/399
11	L	0.45	0/249	0.55	0/337
12	M	0.38	0/226	0.61	0/310
13	O	0.36	0/1430	0.63	1/1928 (0.1%)
14	T	0.36	0/231	0.43	0/313
15	U	0.32	0/633	0.61	1/853 (0.1%)
16	V	0.35	0/1036	0.59	1/1410 (0.1%)
17	Y	0.28	0/191	0.54	0/256
18	X	0.30	0/271	0.56	0/367
19	Z	0.33	0/417	0.55	0/570
20	R	0.28	0/186	0.48	0/257
All	All	0.43	0/20144	0.58	6/27438 (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
3	C	0	1
4	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	I	0	2
All	All	0	4

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	61	LEU	CA-CB-CG	6.00	129.09	115.30
15	U	9	LEU	CA-CB-CG	5.44	127.80	115.30
4	D	267	LEU	CB-CG-CD1	-5.43	101.77	111.00
13	O	158	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	210	LEU	CA-CB-CG	5.10	127.02	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	222	GLY	Peptide
4	D	294	ARG	Peptide
8	I	1	FME	Mainchain,Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2598	0	2498	86	0
2	B	3890	0	3702	74	0
3	C	3453	0	3367	70	0
4	D	2699	0	2600	67	0
5	E	622	0	595	8	0
6	F	274	0	279	3	0
7	H	484	0	500	10	0
8	I	255	0	264	1	0
9	J	251	0	257	4	0
10	K	280	0	272	7	0
11	L	244	0	252	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	M	223	0	228	6	0
13	O	1415	0	1337	28	0
14	T	230	0	223	2	0
15	U	629	0	628	12	0
16	V	1016	0	1012	10	0
17	Y	190	0	203	6	0
18	X	269	0	294	2	0
19	Z	410	0	427	4	0
20	R	186	0	124	1	0
21	A	10	0	0	2	0
22	A	1	0	0	0	0
23	A	207	0	175	8	0
23	B	920	0	888	41	0
23	C	774	0	780	45	0
23	D	105	0	88	4	0
24	A	128	0	148	7	0
25	A	40	0	56	4	0
25	B	80	0	112	6	0
25	C	80	0	112	4	0
25	D	29	0	36	0	0
25	K	80	0	112	8	0
26	A	54	0	78	4	0
26	D	24	0	18	1	0
27	A	38	0	46	1	0
27	B	39	0	48	2	0
27	D	24	0	18	0	0
28	A	51	0	71	5	0
28	D	43	0	58	4	0
29	B	7	0	0	0	0
30	C	140	0	154	7	0
30	H	50	0	58	3	0
31	D	4	0	0	1	0
32	D	114	0	144	4	0
32	L	40	0	50	5	0
33	F	43	0	30	4	0
34	H	41	0	56	4	0
35	V	43	0	30	0	0
36	A	7	0	0	0	0
36	B	5	0	0	0	0
36	C	4	0	0	0	0
All	All	22843	0	22428	415	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 9.

The worst 5 of 415 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:343:LEU:O	3:C:401:LEU:HD11	1.65	0.96
1:A:334:ARG:HG3	13:O:157:LEU:HB2	1.51	0.92
1:A:334:ARG:HB2	13:O:157:LEU:HD12	1.53	0.88
23:B:610:CLA:H2	23:B:611:CLA:HBB2	1.66	0.76
2:B:30:VAL:HG12	23:B:606:CLA:HHD	1.71	0.72

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	332/334 (99%)	323 (97%)	9 (3%)	0	100	100
2	B	502/504 (100%)	484 (96%)	18 (4%)	0	100	100
3	C	449/451 (100%)	435 (97%)	14 (3%)	0	100	100
4	D	339/341 (99%)	326 (96%)	13 (4%)	0	100	100
5	E	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
7	H	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
8	I	30/38 (79%)	28 (93%)	2 (7%)	0	100	100
9	J	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	28/37 (76%)	28 (100%)	0	0	100	100
12	M	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
13	O	166/244 (68%)	156 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	T	25/30 (83%)	23 (92%)	2 (8%)	0	100	100
15	U	74/104 (71%)	71 (96%)	3 (4%)	0	100	100
16	V	131/163 (80%)	126 (96%)	5 (4%)	0	100	100
17	Y	25/30 (83%)	25 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	53/62 (86%)	52 (98%)	1 (2%)	0	100	100
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	2489/2710 (92%)	2403 (96%)	86 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	262/269 (97%)	261 (100%)	1 (0%)	89	96
2	B	379/402 (94%)	375 (99%)	4 (1%)	70	88
3	C	340/352 (97%)	340 (100%)	0	100	100
4	D	267/275 (97%)	264 (99%)	3 (1%)	70	88
5	E	63/73 (86%)	63 (100%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	100	100
7	H	50/53 (94%)	49 (98%)	1 (2%)	50	78
8	I	27/34 (79%)	27 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
10	K	26/30 (87%)	25 (96%)	1 (4%)	28	59
11	L	27/35 (77%)	27 (100%)	0	100	100
12	M	24/27 (89%)	24 (100%)	0	100	100
13	O	139/207 (67%)	137 (99%)	2 (1%)	62	85
14	T	22/26 (85%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	U	60/89 (67%)	60 (100%)	0	100	100
16	V	105/138 (76%)	105 (100%)	0	100	100
17	Y	17/23 (74%)	17 (100%)	0	100	100
18	X	28/33 (85%)	28 (100%)	0	100	100
19	Z	40/52 (77%)	40 (100%)	0	100	100
20	R	6/29 (21%)	6 (100%)	0	100	100
All	All	1932/2214 (87%)	1920 (99%)	12 (1%)	82	94

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	293[B]	LEU
7	H	49	TYR
13	O	118	LEU
10	K	25	LEU
2	B	334	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	415	ASN
4	D	142	ASN
16	V	68	ASN
5	E	75	GLN
2	B	285	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	HSK	D	336[A]	-	7,10,12	1.48	1 (14%)	3,12,16	1.14	0
14	FME	T	1	14	3,4,10	0.94	0	2,4,11	1.09	0
4	HSK	D	336[B]	-	7,11,12	1.41	1 (14%)	3,14,16	1.24	0
8	FME	I	1	8	8,9,10	0.69	0	7,9,11	1.37	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
14	FME	T	1	14	-	0/0/2/11	-
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
8	FME	I	1	8	-	0/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[A]	HSK	CE1-ND1	2.89	1.40	1.36
4	D	336[B]	HSK	CE1-ND1	2.70	1.40	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	O-C-CA	-2.46	118.33	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	336[A]	HSK	1	0
4	D	336[B]	HSK	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 67 ligands modelled in this entry, 1 is monoatomic and 1 is unknown - leaving 65 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	PHO	A	409	-	51,69,69	1.98	9 (17%)	47,99,99	2.17	15 (31%)
26	SQD	A	412	-	53,54,54	1.00	3 (5%)	62,65,65	1.60	8 (12%)
23	CLA	B	604	-	61,69,73	2.02	16 (26%)	71,108,113	2.78	27 (38%)
25	BCR	K	102	-	41,41,41	1.25	2 (4%)	56,56,56	1.82	16 (28%)
30	DGD	C	516	-	42,42,67	1.03	2 (4%)	56,56,81	1.38	7 (12%)
23	CLA	B	606	-	65,73,73	1.92	17 (26%)	76,113,113	2.82	29 (38%)
23	CLA	A	410	-	45,53,73	2.36	15 (33%)	52,89,113	3.18	24 (46%)
23	CLA	B	615	-	51,59,73	2.26	17 (33%)	59,96,113	2.99	29 (49%)
25	BCR	C	515	-	41,41,41	1.19	2 (4%)	56,56,56	1.77	15 (26%)
23	CLA	C	510	-	65,73,73	1.90	16 (24%)	76,113,113	2.76	28 (36%)
23	CLA	A	405	-	57,65,73	2.17	15 (26%)	66,103,113	2.85	28 (42%)
23	CLA	C	507	36	65,73,73	1.94	15 (23%)	76,113,113	2.87	25 (32%)
23	CLA	B	610	-	56,64,73	2.09	16 (28%)	65,102,113	2.95	29 (44%)
23	CLA	B	608	36	51,59,73	2.24	16 (31%)	59,96,113	2.93	27 (45%)
27	LMG	D	411	-	24,24,55	1.13	2 (8%)	32,32,63	1.43	6 (18%)
23	CLA	C	502	-	62,70,73	1.97	17 (27%)	72,109,113	2.73	26 (36%)
32	LHG	L	101	-	39,39,48	1.01	2 (5%)	42,45,54	1.18	4 (9%)
30	DGD	C	517	-	50,50,67	0.91	2 (4%)	64,64,81	1.36	8 (12%)
23	CLA	B	605	-	54,62,73	2.16	17 (31%)	62,99,113	2.97	29 (46%)
23	CLA	C	511	3	65,73,73	1.96	17 (26%)	76,113,113	2.65	28 (36%)
21	OEX	A	401	3,1,36	0,15,15	-	-	-	-	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	617	-	45,53,73	2.37	16 (35%)	52,89,113	3.12	23 (44%)
23	CLA	C	505	-	65,73,73	1.99	17 (26%)	76,113,113	2.65	29 (38%)
27	LMG	B	622	-	39,39,55	1.05	2 (5%)	47,47,63	1.53	9 (19%)
26	SQD	D	407	-	23,24,54	1.21	2 (8%)	30,33,65	2.06	9 (30%)
23	CLA	D	403	-	45,53,73	2.43	18 (40%)	52,89,113	3.25	26 (50%)
34	RRX	H	101	-	42,42,42	5.13	18 (42%)	57,58,58	5.04	32 (56%)
30	DGD	H	102	-	51,51,67	0.97	2 (3%)	65,65,81	1.39	10 (15%)
25	BCR	A	411	-	41,41,41	1.15	1 (2%)	56,56,56	1.78	15 (26%)
23	CLA	C	508	-	52,60,73	2.25	15 (28%)	60,97,113	3.08	30 (50%)
23	CLA	A	407	36	54,62,73	2.19	18 (33%)	62,99,113	3.10	28 (45%)
32	LHG	D	408	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
24	PHO	A	408	-	51,69,69	1.84	8 (15%)	47,99,99	1.91	13 (27%)
27	LMG	A	413	-	38,38,55	1.07	2 (5%)	46,46,63	1.37	6 (13%)
23	CLA	B	609	-	51,59,73	2.28	15 (29%)	59,96,113	2.92	26 (44%)
25	BCR	B	618	-	41,41,41	1.15	1 (2%)	56,56,56	1.90	12 (21%)
23	CLA	B	603	-	52,60,73	2.26	15 (28%)	60,97,113	3.10	29 (48%)
23	CLA	C	513	-	45,53,73	2.48	18 (40%)	52,89,113	3.27	26 (50%)
25	BCR	B	620	-	41,41,41	1.13	1 (2%)	56,56,56	1.87	15 (26%)
25	BCR	C	514	-	41,41,41	1.20	2 (4%)	56,56,56	1.85	15 (26%)
25	BCR	K	101	-	41,41,41	1.30	2 (4%)	56,56,56	2.23	22 (39%)
30	DGD	C	518	-	51,51,67	0.97	2 (3%)	65,65,81	0.98	3 (4%)
28	PL9	A	414	-	51,51,55	0.64	2 (3%)	63,64,69	1.69	21 (33%)
23	CLA	C	512	-	53,61,73	2.14	16 (30%)	61,98,113	3.09	25 (40%)
23	CLA	C	501	-	65,73,73	2.00	14 (21%)	76,113,113	2.77	28 (36%)
23	CLA	C	506	-	57,65,73	2.13	15 (26%)	66,103,113	2.80	26 (39%)
33	HEM	F	101	5,6	41,50,50	1.37	5 (12%)	45,82,82	1.82	11 (24%)
31	BCT	D	401	22	2,3,3	0.56	0	2,3,3	1.71	1 (50%)
23	CLA	C	509	-	65,73,73	1.93	16 (24%)	76,113,113	2.70	29 (38%)
23	CLA	C	503	-	65,73,73	1.94	14 (21%)	76,113,113	2.73	26 (34%)
23	CLA	B	607	-	55,63,73	2.12	17 (30%)	64,101,113	3.02	25 (39%)
23	CLA	B	611	36	65,73,73	1.96	18 (27%)	76,113,113	2.80	29 (38%)
23	CLA	B	612	-	65,73,73	2.07	18 (27%)	76,113,113	2.96	26 (34%)
23	CLA	B	614	-	54,62,73	2.17	16 (29%)	62,99,113	3.00	26 (41%)
35	HEC	V	201	16	32,50,50	1.61	4 (12%)	24,82,82	1.60	5 (20%)
25	BCR	D	404	-	29,29,41	0.65	0	37,37,56	1.74	8 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	PL9	D	405	-	43,43,55	0.71	1 (2%)	53,54,69	1.76	15 (28%)
23	CLA	B	602	36	65,73,73	2.02	17 (26%)	76,113,113	2.66	27 (35%)
23	CLA	B	616	-	65,73,73	1.96	17 (26%)	76,113,113	2.77	26 (34%)
23	CLA	A	406	36	51,59,73	2.25	15 (29%)	59,96,113	3.31	25 (42%)
23	CLA	D	402	-	59,67,73	2.04	15 (25%)	66,104,113	3.01	32 (48%)
32	LHG	D	410	-	32,32,48	1.11	2 (6%)	35,38,54	1.22	3 (8%)
23	CLA	B	613	-	65,73,73	2.26	20 (30%)	76,113,113	2.75	28 (36%)
23	CLA	C	504	36	50,58,73	2.38	15 (30%)	58,95,113	3.09	28 (48%)
32	LHG	D	409	-	31,31,48	1.10	2 (6%)	34,37,54	1.17	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	A	409	-	-	9/37/103/103	0/5/6/6
26	SQD	A	412	-	-	19/49/69/69	0/1/1/1
23	CLA	B	604	-	1/1/14/20	13/33/111/115	-
25	BCR	K	102	-	-	7/29/63/63	0/2/2/2
30	DGD	C	516	-	-	10/30/70/95	0/2/2/2
23	CLA	B	606	-	1/1/15/20	12/37/115/115	-
23	CLA	A	410	-	1/1/11/20	4/13/91/115	-
23	CLA	B	615	-	1/1/12/20	13/21/99/115	-
25	BCR	C	515	-	-	7/29/63/63	0/2/2/2
23	CLA	C	510	-	1/1/15/20	19/37/115/115	-
23	CLA	A	405	-	1/1/13/20	6/28/106/115	-
23	CLA	C	507	36	1/1/15/20	8/37/115/115	-
23	CLA	B	610	-	1/1/13/20	10/27/105/115	-
23	CLA	B	608	36	1/1/12/20	10/21/99/115	-
27	LMG	D	411	-	-	6/18/38/70	0/1/1/1
23	CLA	C	502	-	1/1/14/20	4/34/112/115	-
32	LHG	L	101	-	-	19/44/44/53	-
30	DGD	C	517	-	-	14/38/78/95	0/2/2/2
23	CLA	B	605	-	1/1/12/20	7/24/102/115	-
23	CLA	C	511	3	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	617	-	1/1/11/20	2/13/91/115	-
23	CLA	C	505	-	1/1/15/20	18/37/115/115	-
27	LMG	B	622	-	-	9/34/54/70	0/1/1/1
26	SQD	D	407	-	-	5/16/36/69	0/1/1/1
23	CLA	D	403	-	1/1/11/20	3/13/91/115	-
34	RRX	H	101	-	-	16/29/65/65	0/2/2/2
30	DGD	H	102	-	-	13/39/79/95	0/2/2/2
25	BCR	A	411	-	-	7/29/63/63	0/2/2/2
23	CLA	C	508	-	1/1/12/20	7/22/100/115	-
23	CLA	A	407	36	-	5/24/102/115	-
32	LHG	D	408	-	-	20/53/53/53	-
24	PHO	A	408	-	-	8/37/103/103	0/5/6/6
27	LMG	A	413	-	-	13/33/53/70	0/1/1/1
23	CLA	B	609	-	-	9/21/99/115	-
25	BCR	B	618	-	-	4/29/63/63	0/2/2/2
23	CLA	B	603	-	1/1/12/20	7/22/100/115	-
23	CLA	C	513	-	-	4/13/91/115	-
25	BCR	B	620	-	-	7/29/63/63	0/2/2/2
25	BCR	C	514	-	-	5/29/63/63	0/2/2/2
25	BCR	K	101	-	-	13/29/63/63	0/2/2/2
30	DGD	C	518	-	-	16/39/79/95	0/2/2/2
28	PL9	A	414	-	-	13/49/69/73	0/1/1/1
23	CLA	C	512	-	1/1/12/20	6/23/101/115	-
23	CLA	C	501	-	1/1/15/20	9/37/115/115	-
23	CLA	C	506	-	1/1/13/20	7/28/106/115	-
33	HEM	F	101	5,6	-	6/12/54/54	-
23	CLA	C	509	-	1/1/15/20	7/37/115/115	-
23	CLA	C	503	-	1/1/15/20	10/37/115/115	-
23	CLA	B	607	-	1/1/13/20	3/25/103/115	-
23	CLA	B	611	36	1/1/15/20	12/37/115/115	-
23	CLA	B	612	-	1/1/15/20	9/37/115/115	-
23	CLA	B	614	-	1/1/12/20	7/24/102/115	-
35	HEC	V	201	16	-	4/10/54/54	-
25	BCR	D	404	-	-	7/23/40/63	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	D	405	-	-	9/39/59/73	0/1/1/1
23	CLA	B	602	36	1/1/15/20	13/37/115/115	-
23	CLA	B	616	-	1/1/15/20	12/37/115/115	-
23	CLA	A	406	36	1/1/12/20	5/21/99/115	-
23	CLA	D	402	-	1/1/13/20	8/28/106/115	-
32	LHG	D	410	-	-	13/37/37/53	-
23	CLA	B	613	-	1/1/15/20	14/37/115/115	-
23	CLA	C	504	36	1/1/12/20	4/19/97/115	-
32	LHG	D	409	-	-	14/36/36/53	-

The worst 5 of 654 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	H	101	RRX	C21-C22	13.64	1.53	1.35
34	H	101	RRX	C17-C18	13.45	1.53	1.35
34	H	101	RRX	C10-C9	12.90	1.52	1.35
34	H	101	RRX	C14-C13	12.77	1.52	1.35
34	H	101	RRX	C26-C25	12.47	1.56	1.34

The worst 5 of 1260 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	H	101	RRX	C33-C5-C6	-11.40	111.73	124.53
23	B	612	CLA	C1D-ND-C4D	-11.38	98.25	106.33
23	B	612	CLA	C2D-C1D-ND	10.83	118.08	110.10
34	H	101	RRX	C16-C17-C18	-10.50	112.33	127.31
23	B	613	CLA	C1D-ND-C4D	-10.40	98.95	106.33

5 of 32 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	405	CLA	ND
23	A	406	CLA	ND
23	A	410	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND

5 of 593 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	405	CLA	CBD-CGD-O2D-CED
23	A	410	CLA	C1A-C2A-CAA-CBA
23	B	604	CLA	C2-C3-C5-C6
23	B	604	CLA	C4-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6

There are no ring outliers.

59 monomers are involved in 163 short contacts:

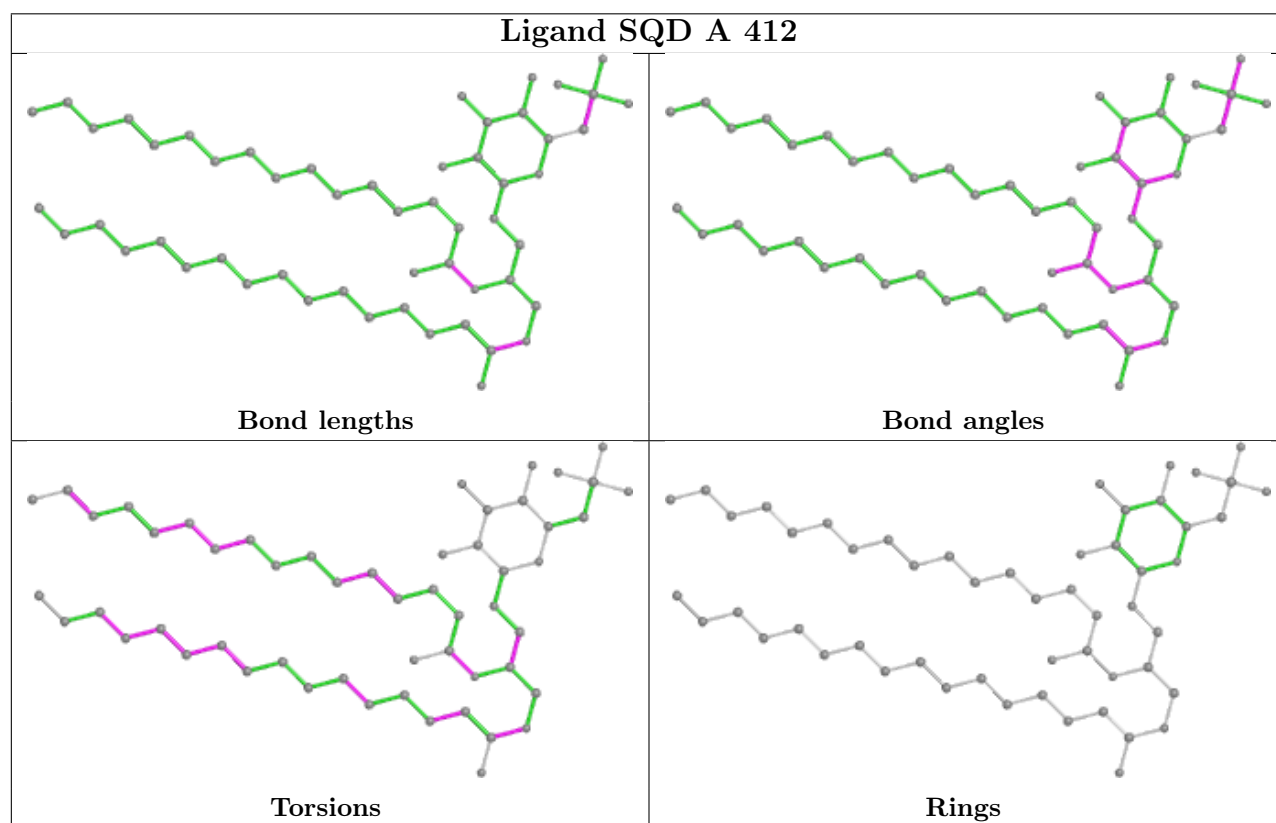
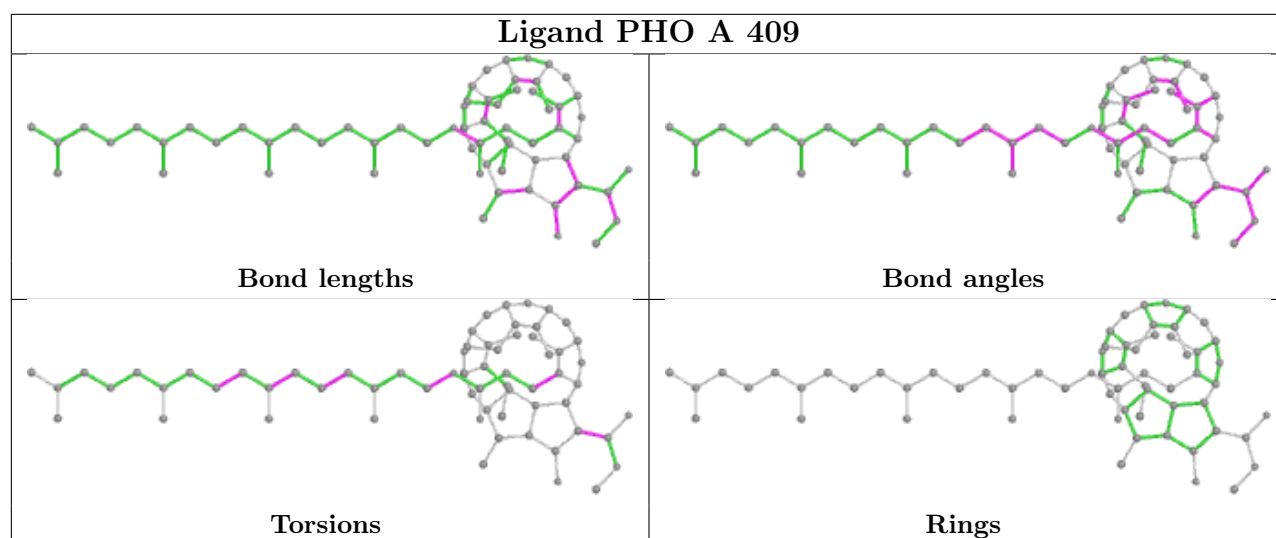
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	409	PHO	4	0
26	A	412	SQD	4	0
23	B	604	CLA	3	0
25	K	102	BCR	5	0
30	C	516	DGD	1	0
23	B	606	CLA	7	0
23	A	410	CLA	2	0
25	C	515	BCR	3	0
23	C	510	CLA	8	0
23	A	405	CLA	3	0
23	C	507	CLA	7	0
23	B	610	CLA	2	0
23	B	608	CLA	1	0
23	C	502	CLA	5	0
32	L	101	LHG	5	0
30	C	517	DGD	4	0
23	B	605	CLA	4	0
23	C	511	CLA	6	0
21	A	401	OEX	2	0
23	B	617	CLA	2	0
23	C	505	CLA	3	0
27	B	622	LMG	2	0
26	D	407	SQD	1	0
34	H	101	RRX	4	0
30	H	102	DGD	3	0
25	A	411	BCR	4	0
23	C	508	CLA	2	0
23	A	407	CLA	2	0
32	D	408	LHG	2	0
24	A	408	PHO	3	0
27	A	413	LMG	1	0
23	B	609	CLA	3	0
25	B	618	BCR	3	0

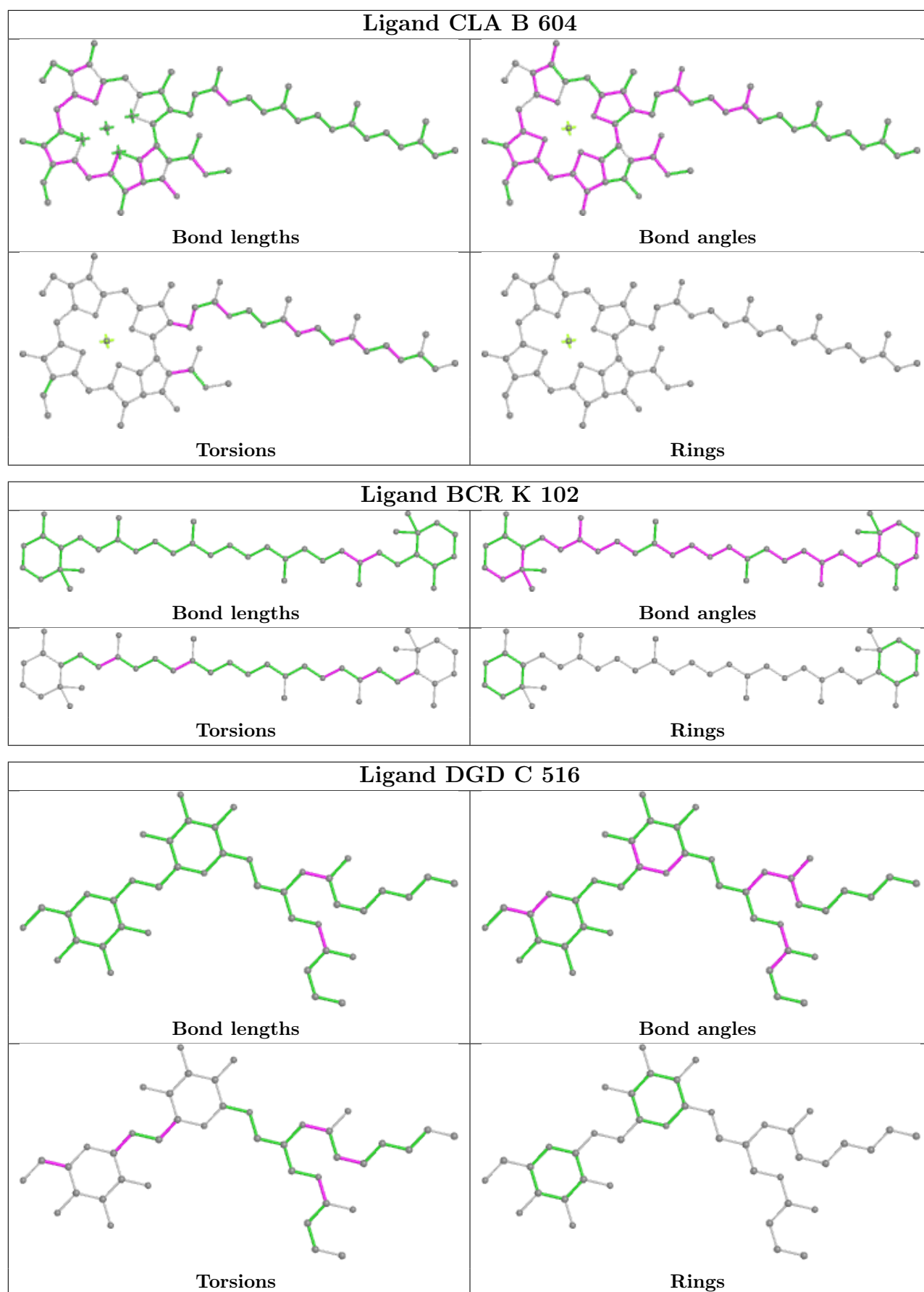
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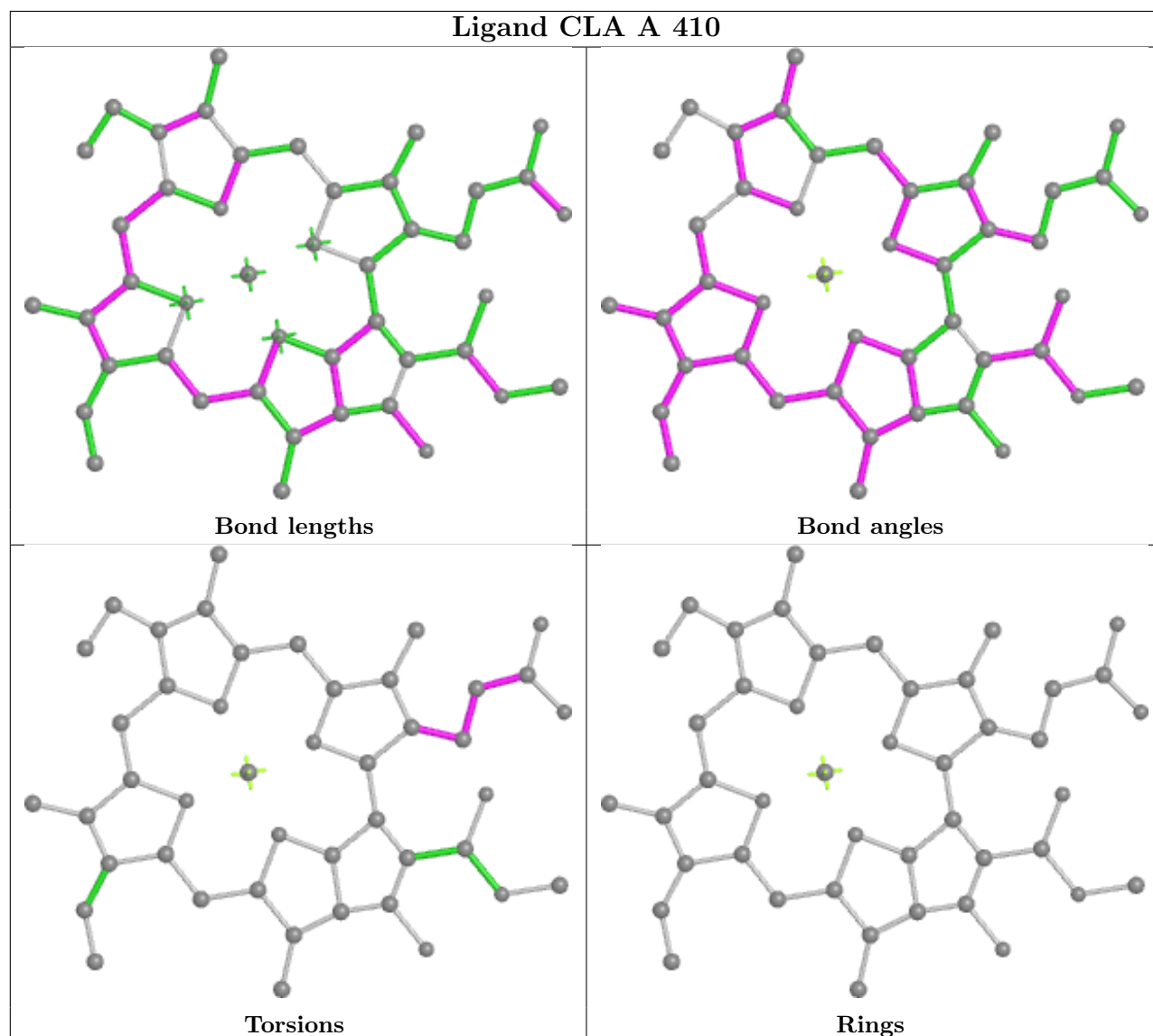
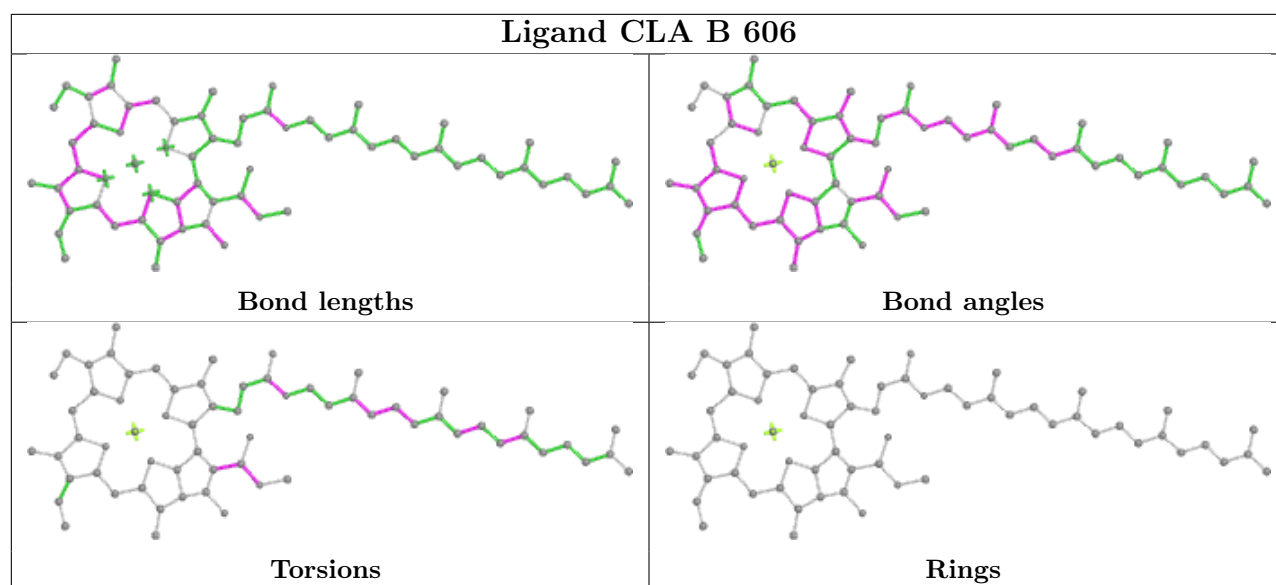
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	603	CLA	2	0
25	B	620	BCR	3	0
25	C	514	BCR	1	0
25	K	101	BCR	3	0
30	C	518	DGD	2	0
28	A	414	PL9	5	0
23	C	512	CLA	3	0
23	C	501	CLA	7	0
23	C	506	CLA	3	0
33	F	101	HEM	4	0
31	D	401	BCT	1	0
23	C	509	CLA	5	0
23	C	503	CLA	11	0
23	B	607	CLA	3	0
23	B	611	CLA	3	0
23	B	612	CLA	2	0
23	B	614	CLA	5	0
28	D	405	PL9	4	0
23	B	602	CLA	3	0
23	B	616	CLA	4	0
23	A	406	CLA	1	0
23	D	402	CLA	4	0
32	D	410	LHG	1	0
23	B	613	CLA	6	0
23	C	504	CLA	1	0
32	D	409	LHG	1	0

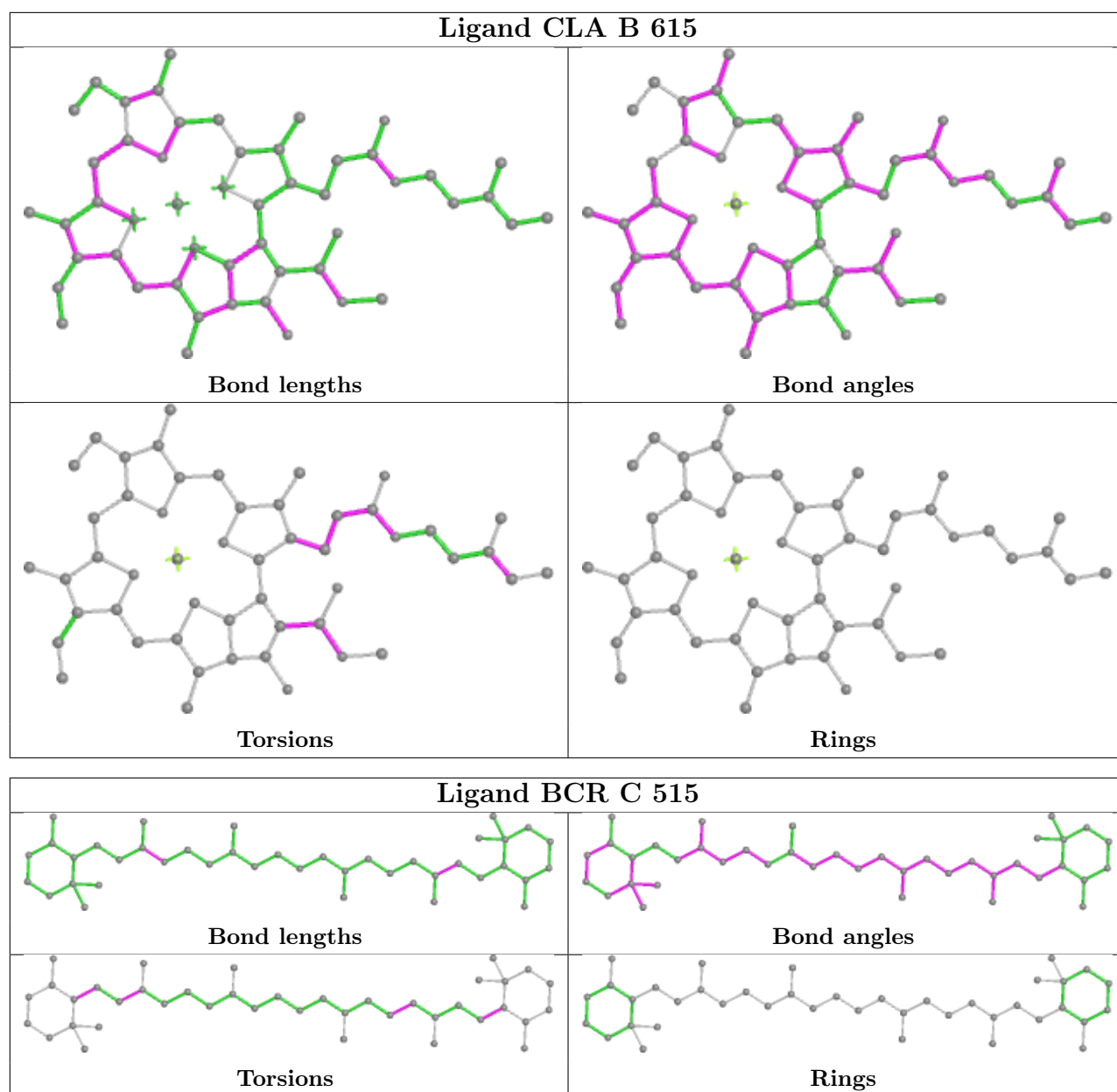
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

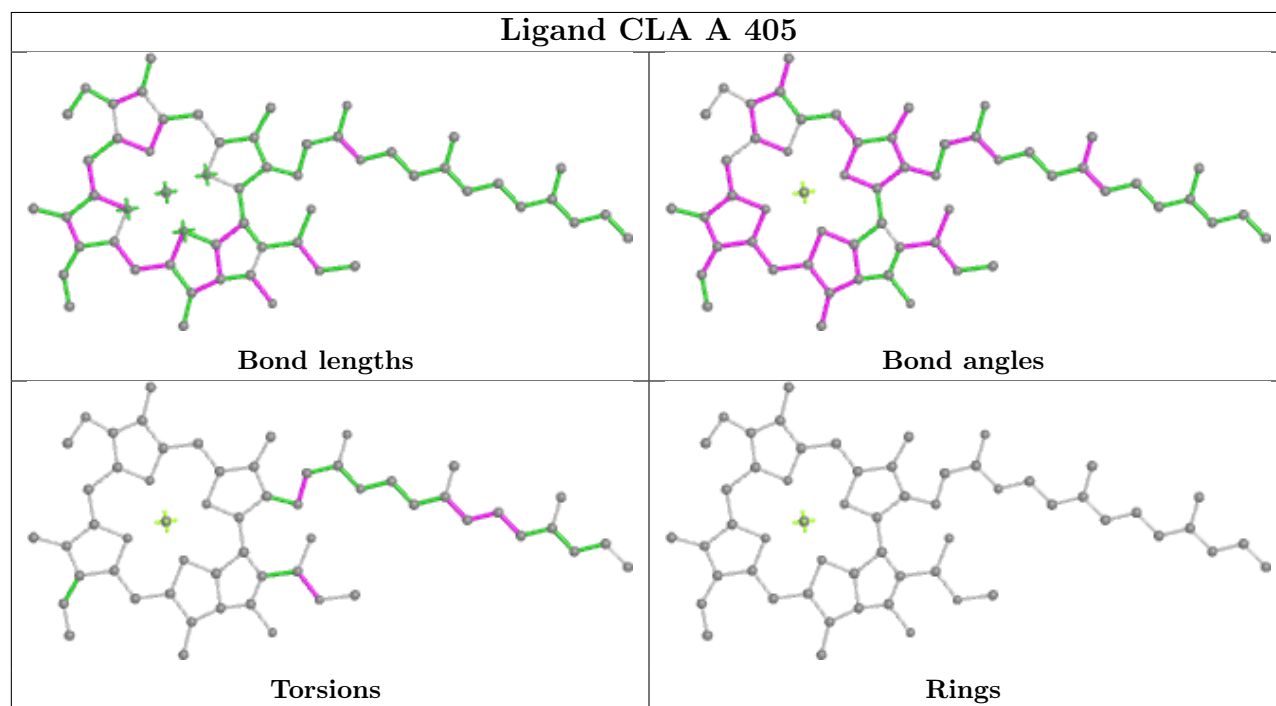
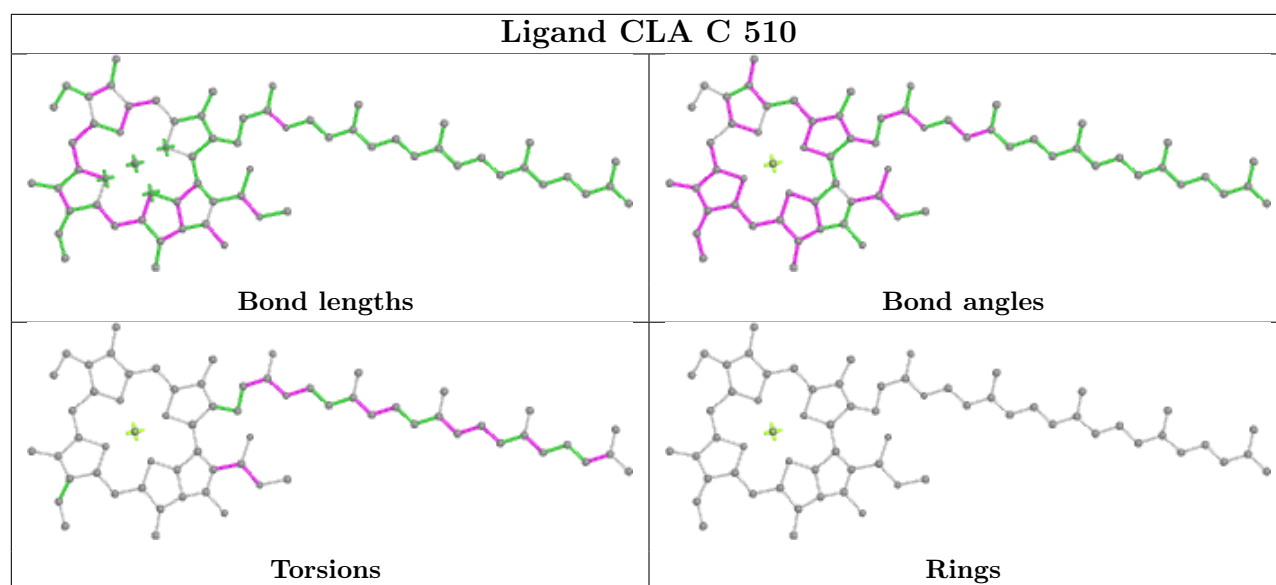


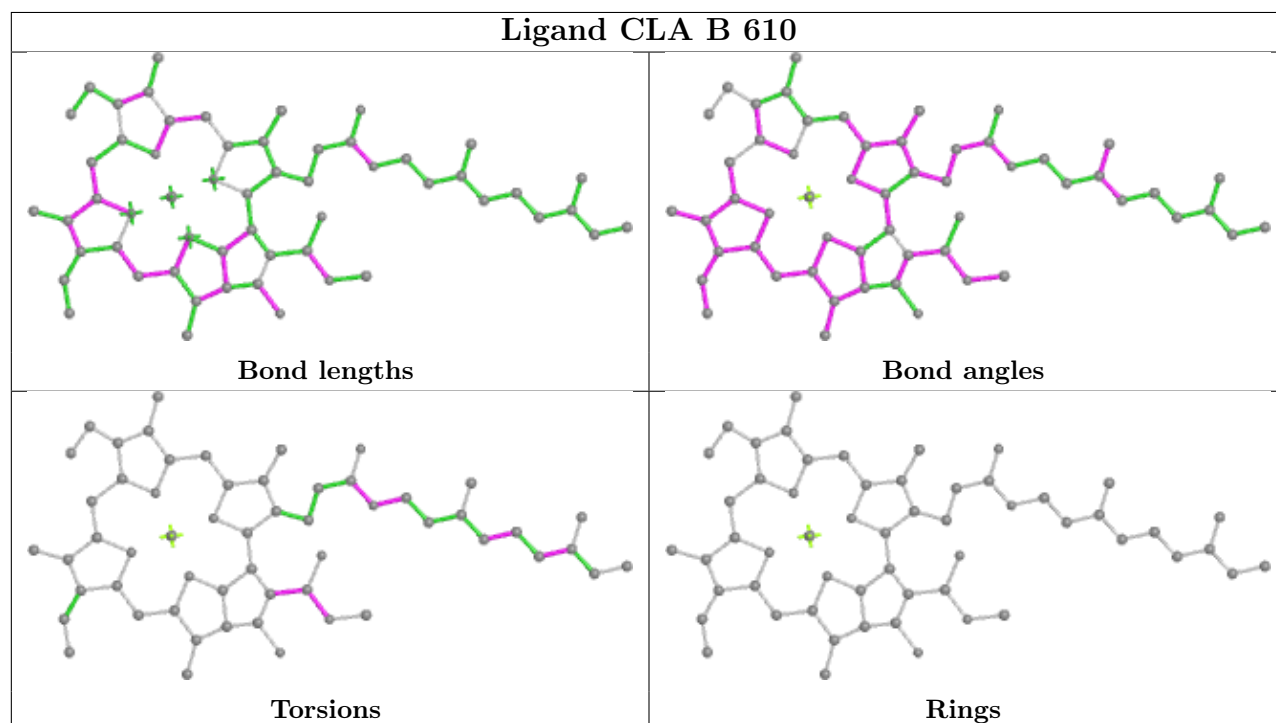
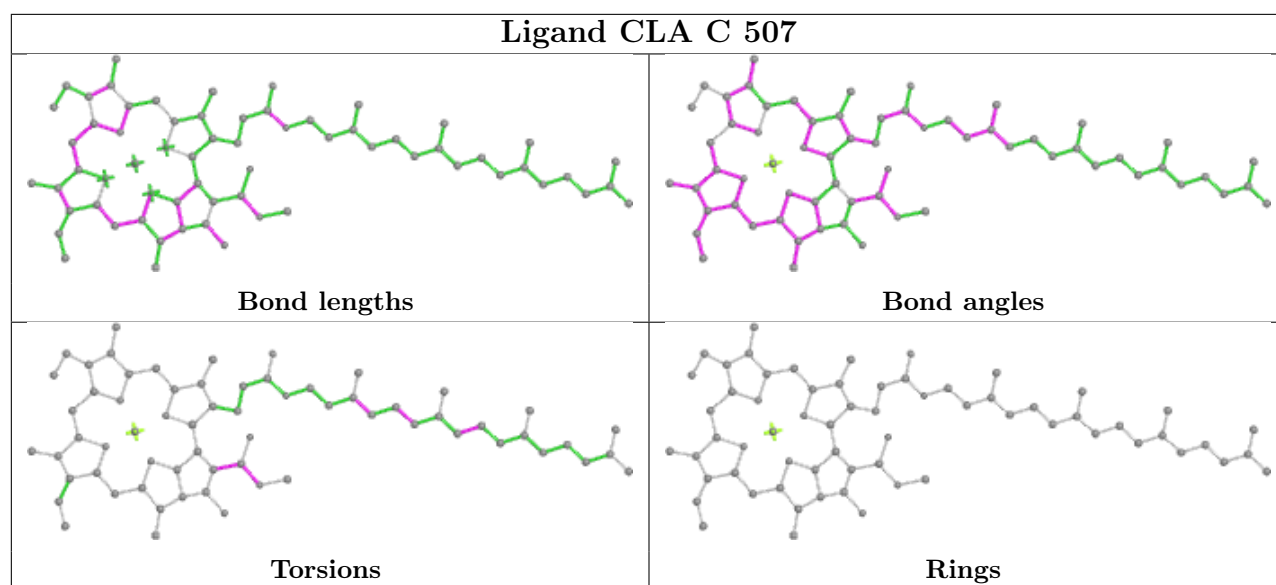


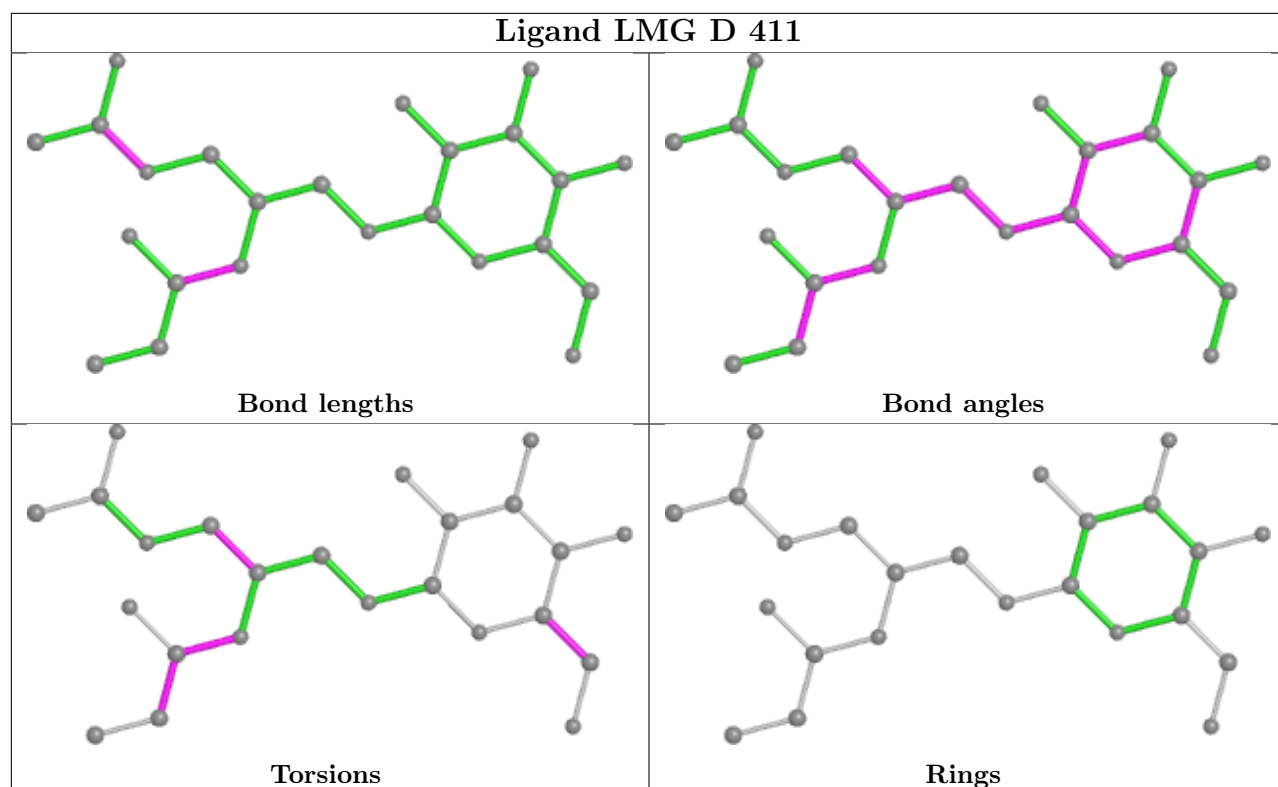
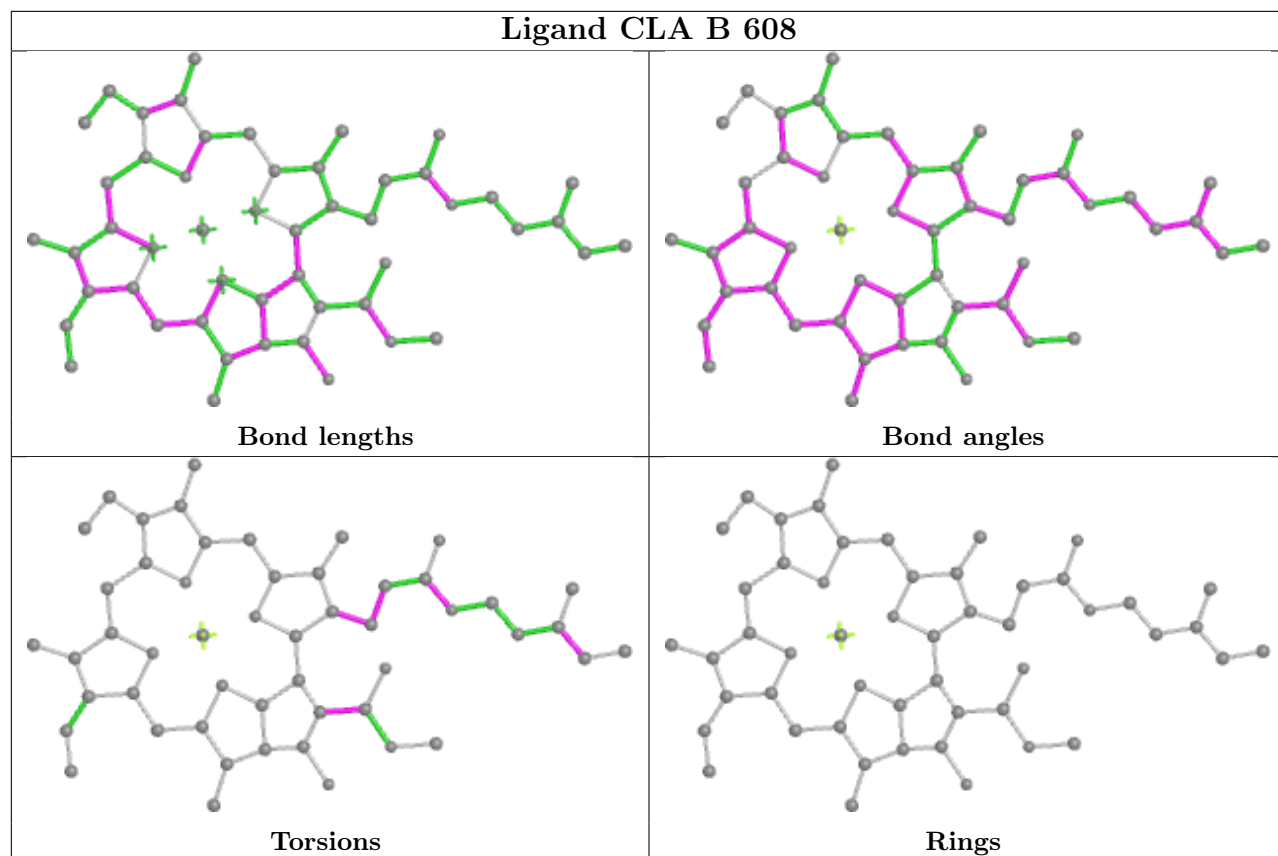


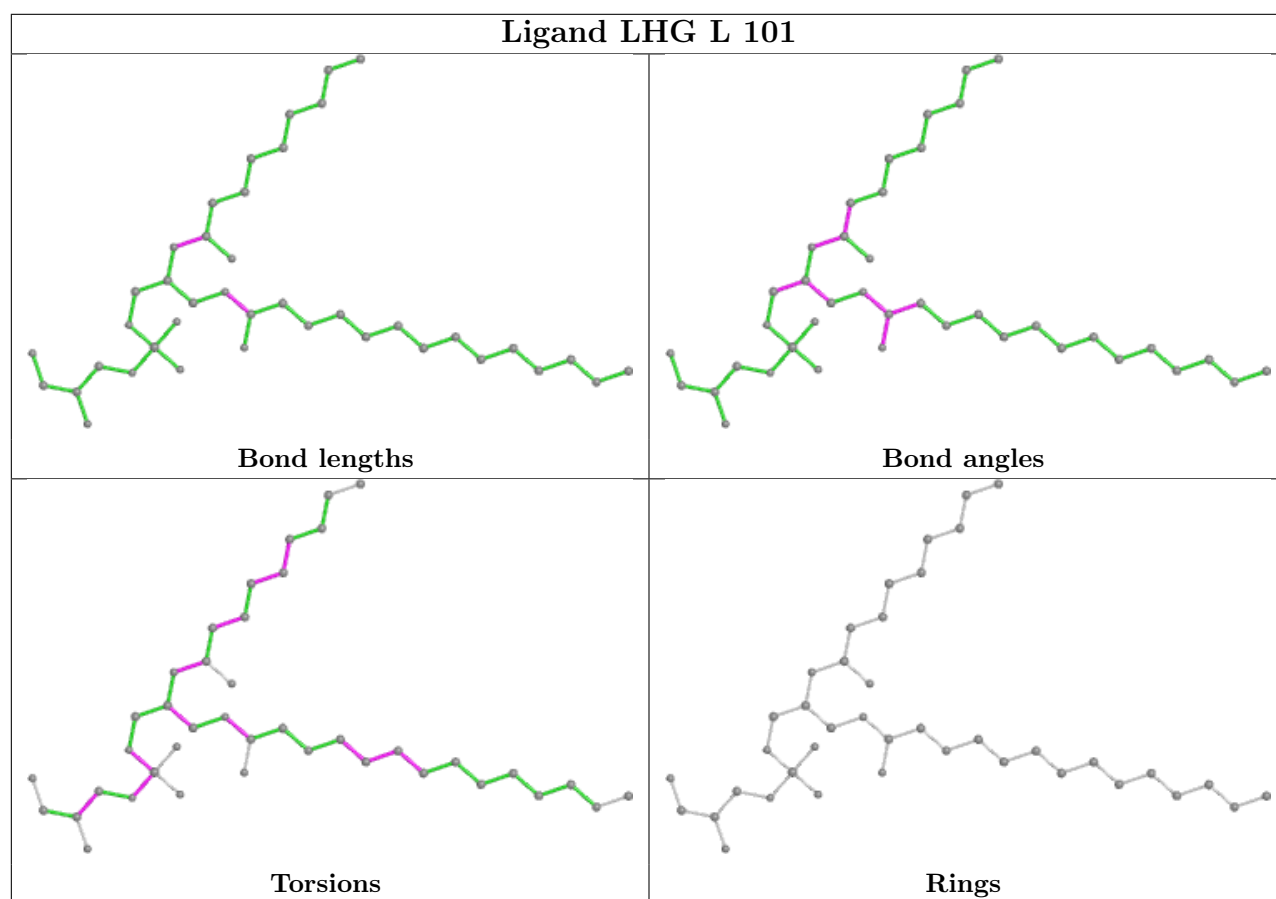
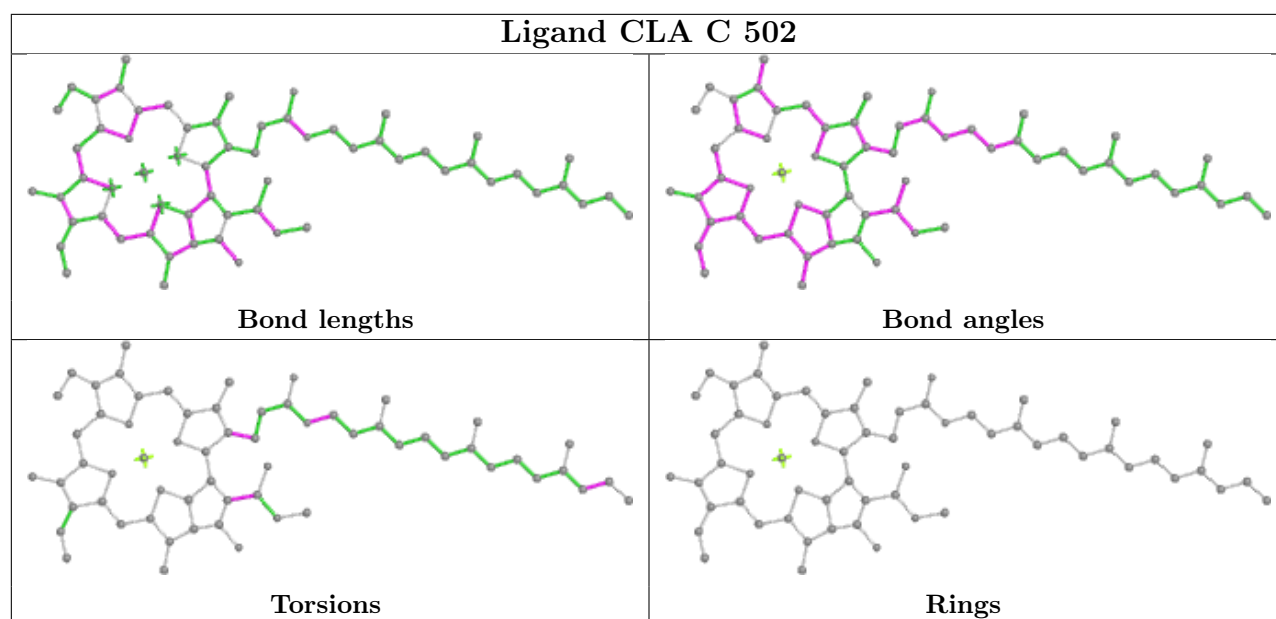


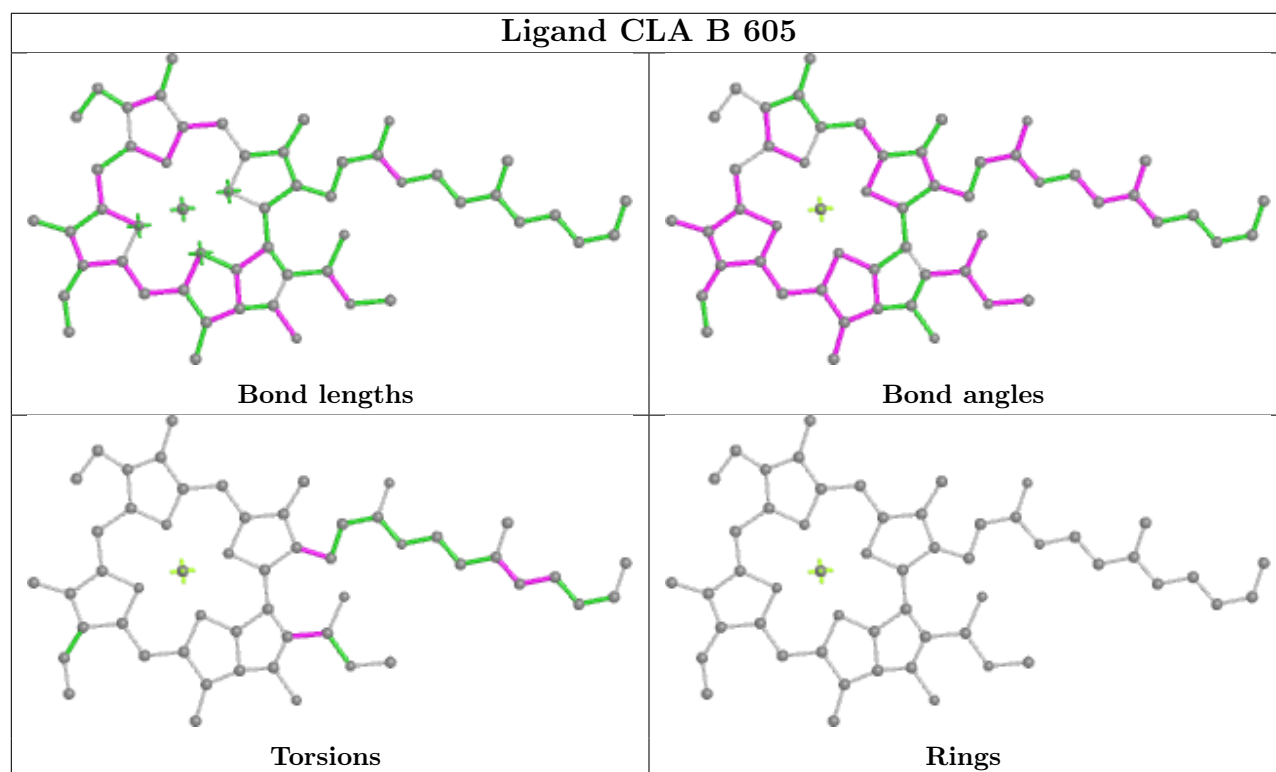
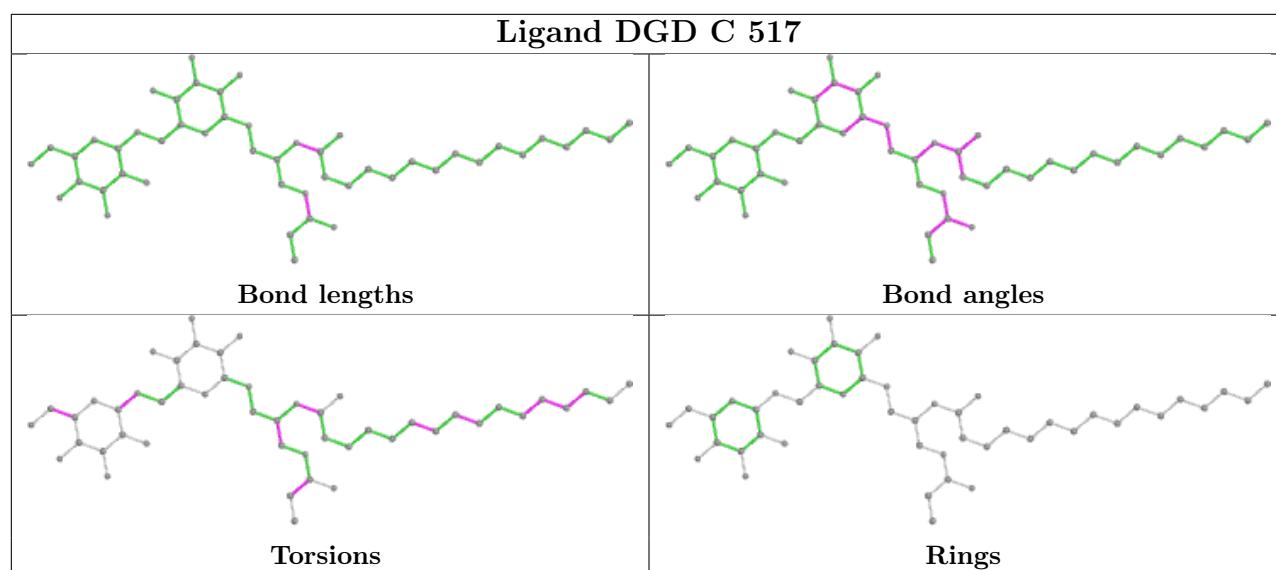




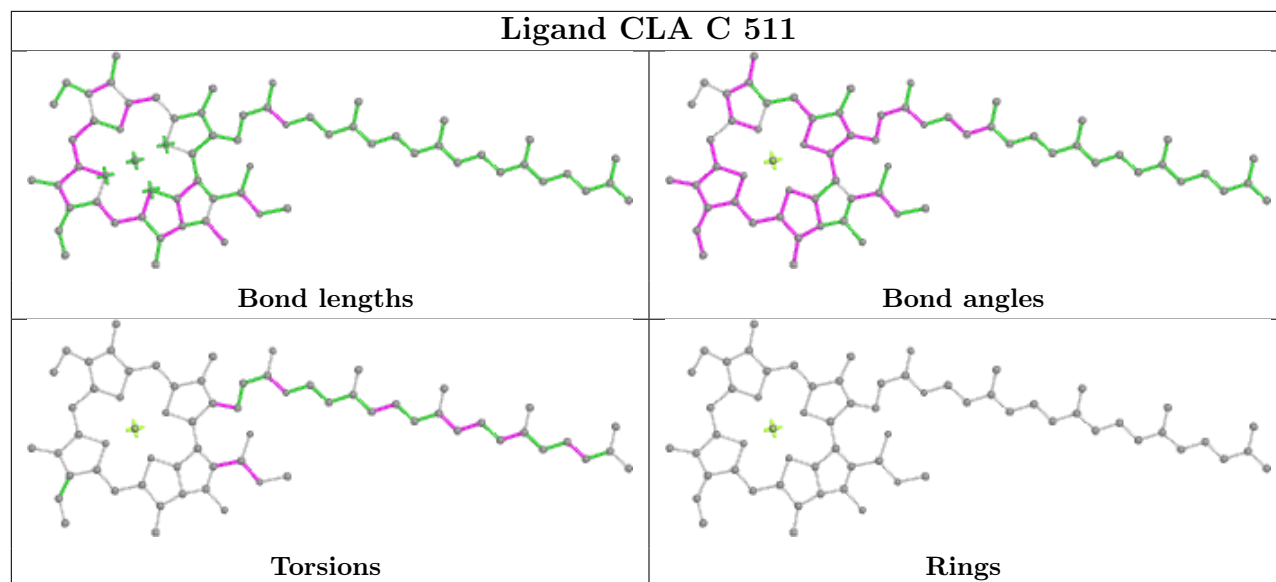




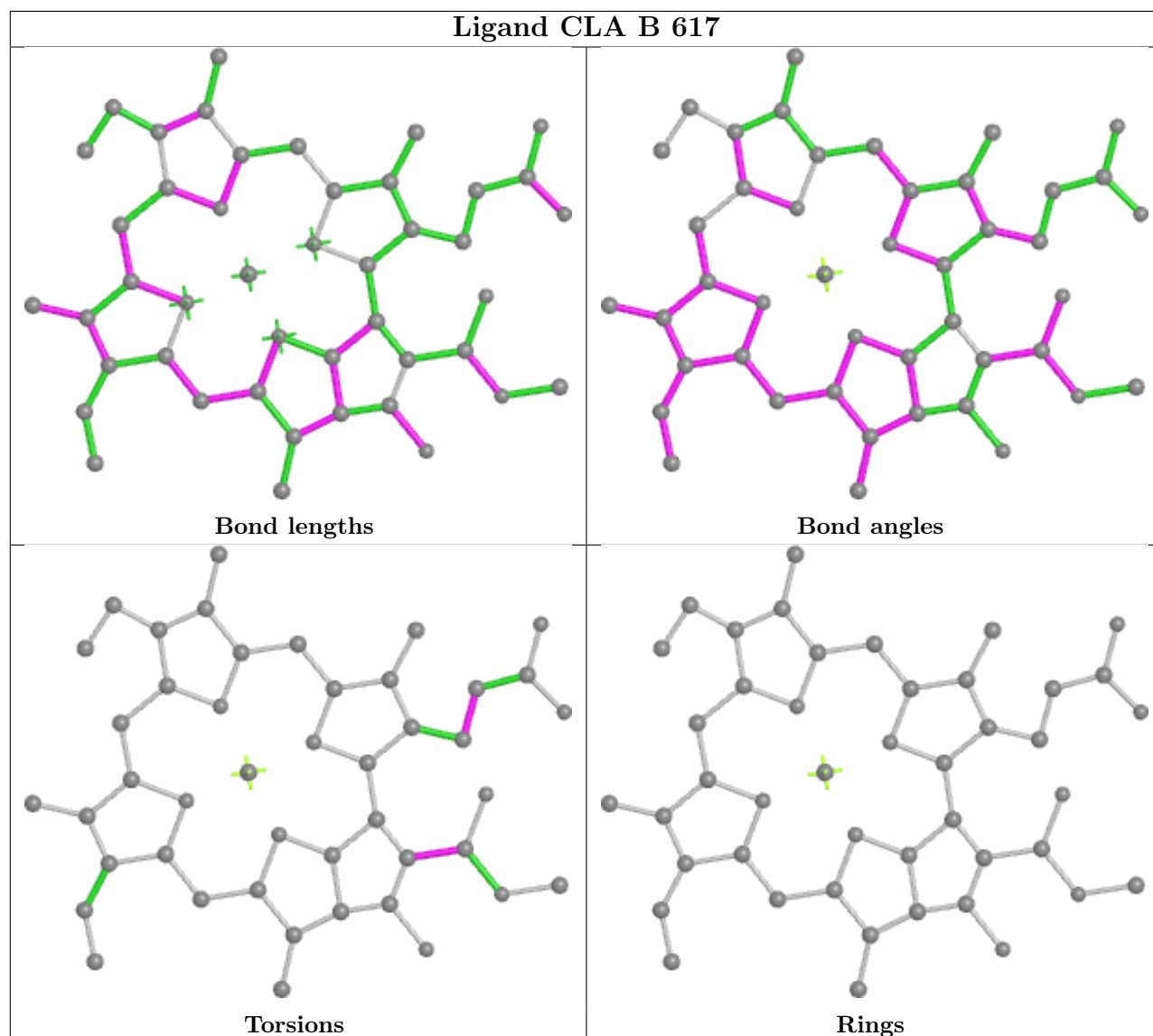




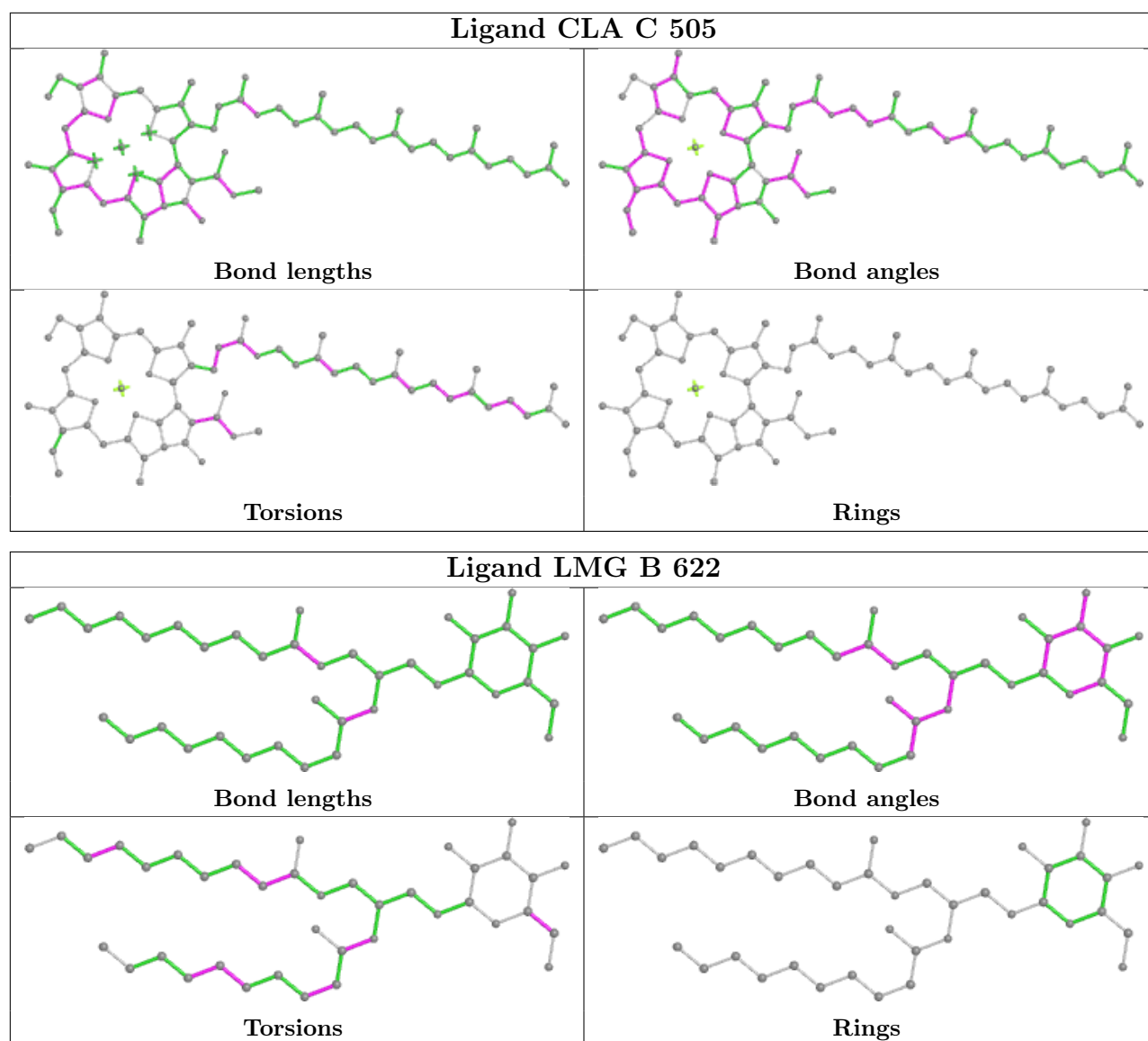
## Ligand CLA C 511

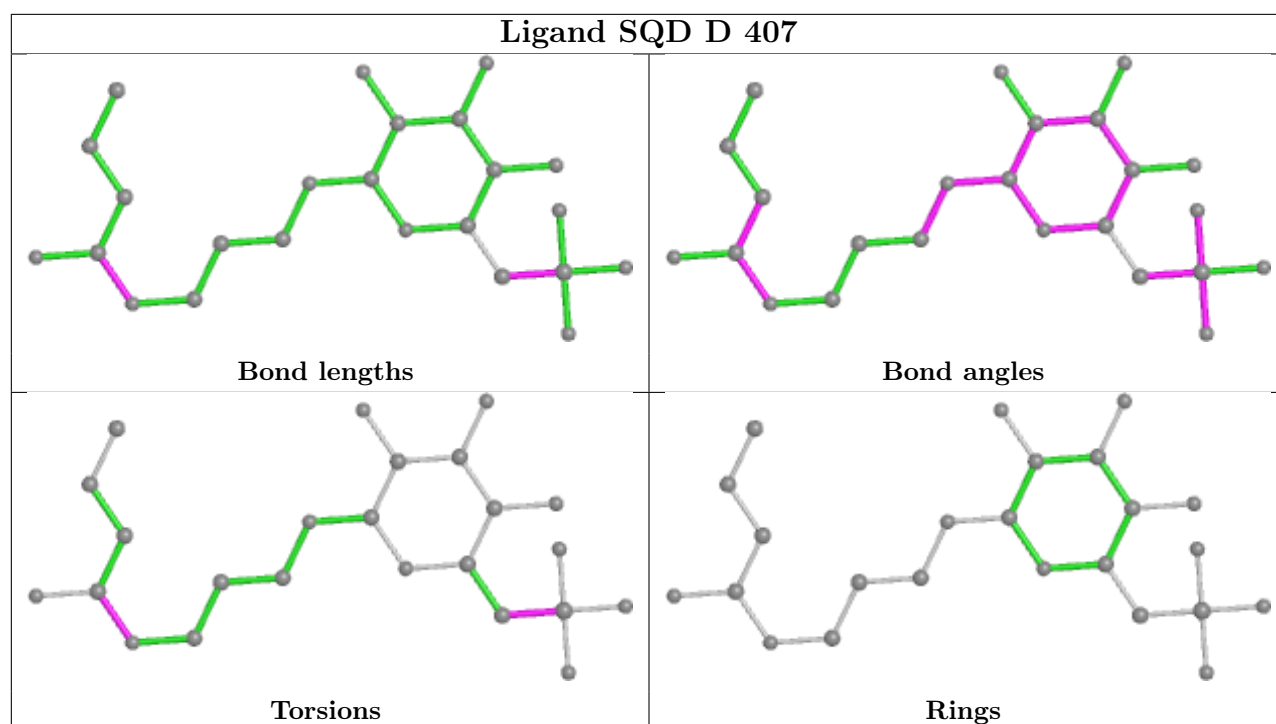


## Ligand CLA B 617

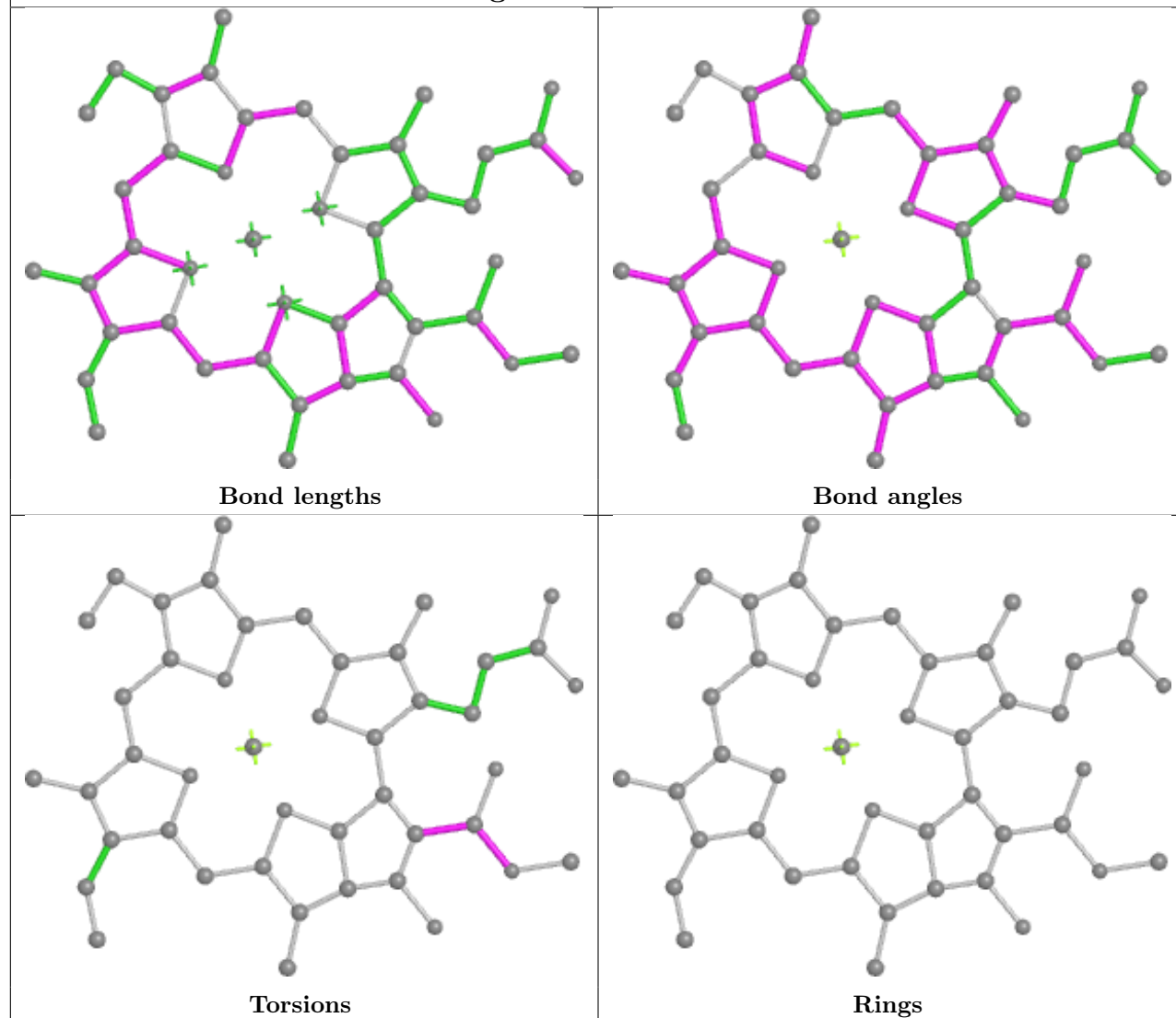




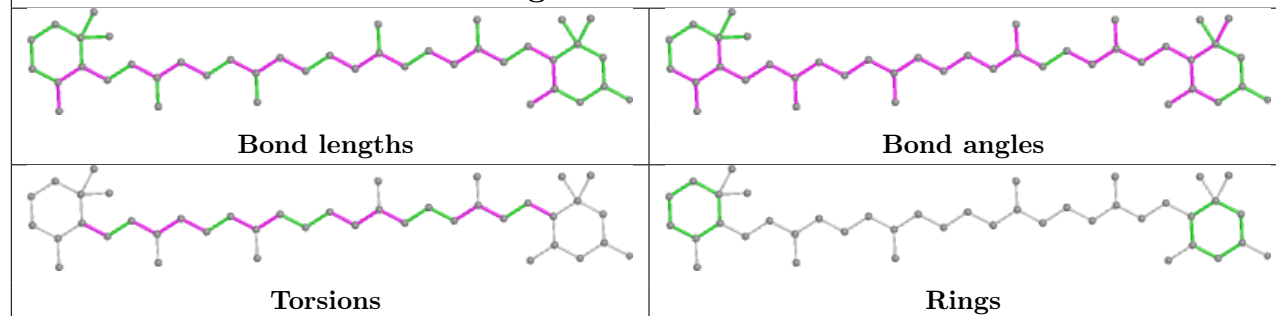


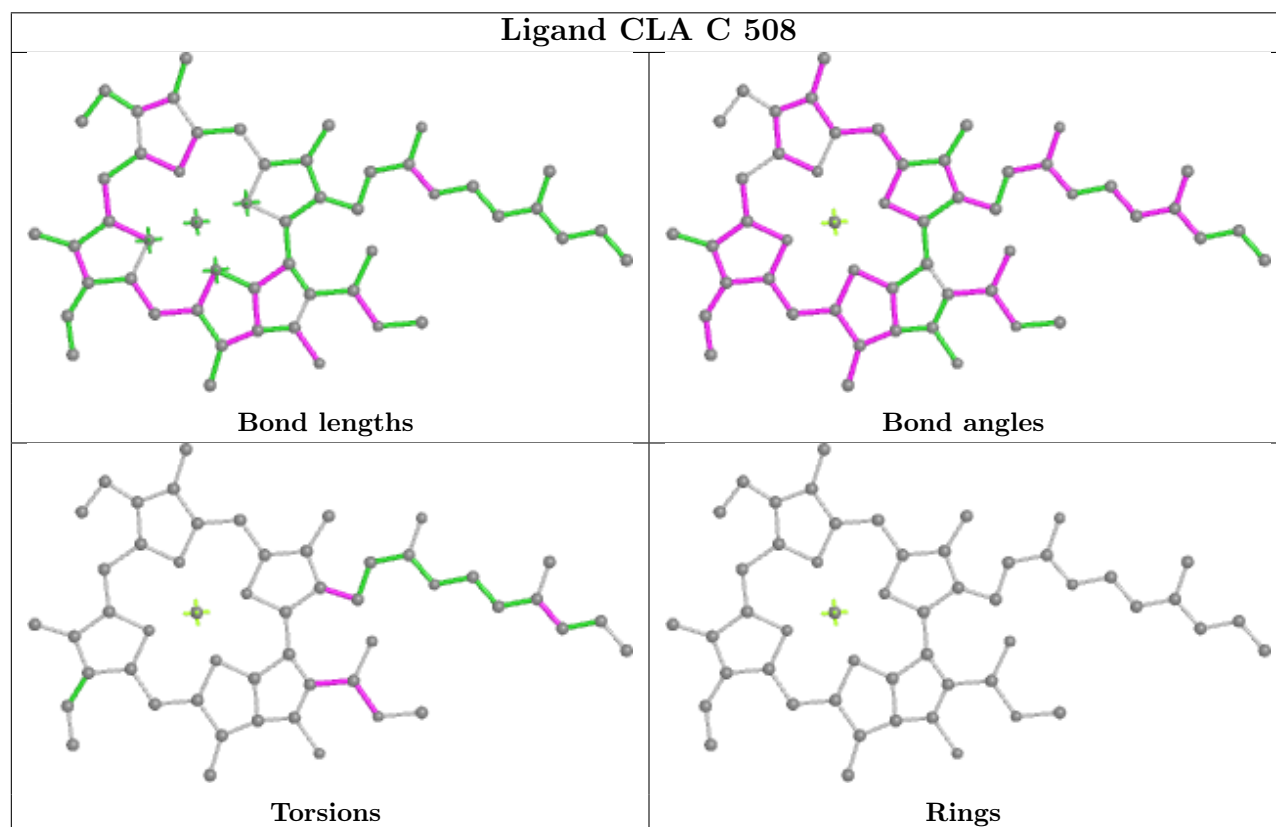
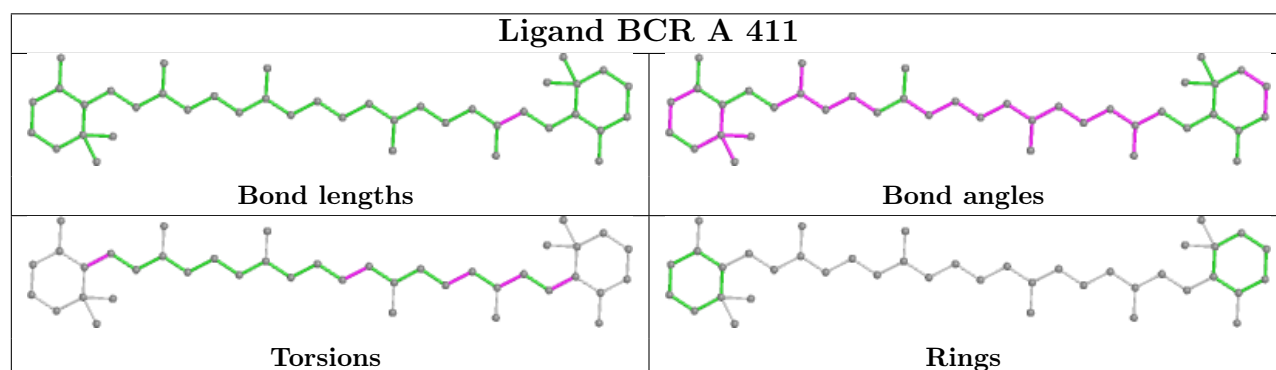
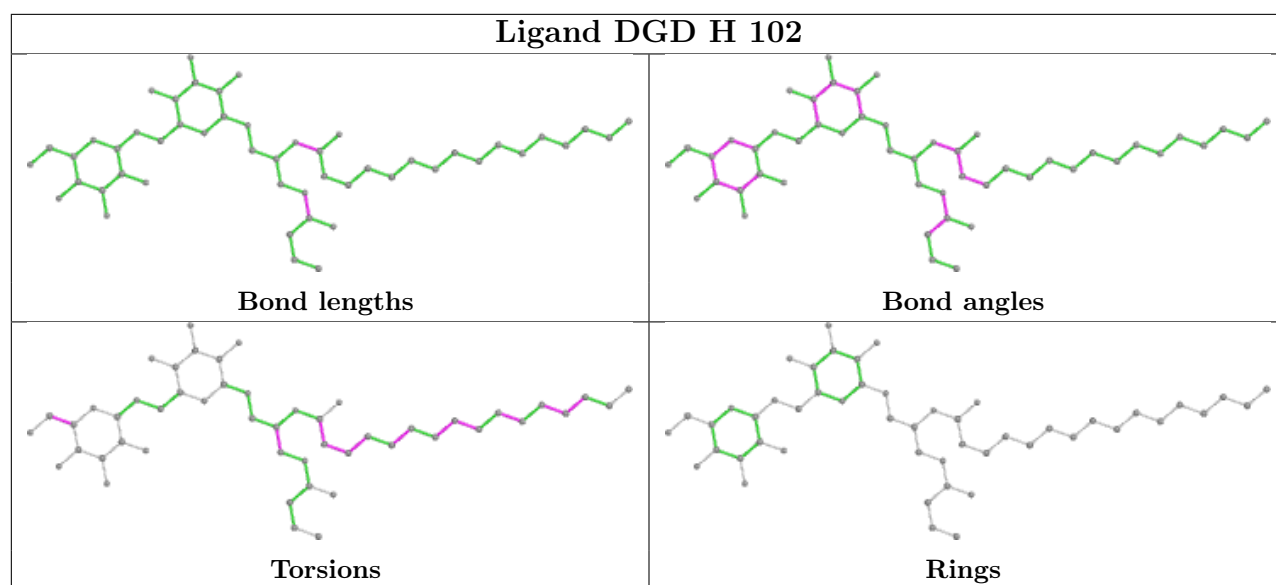


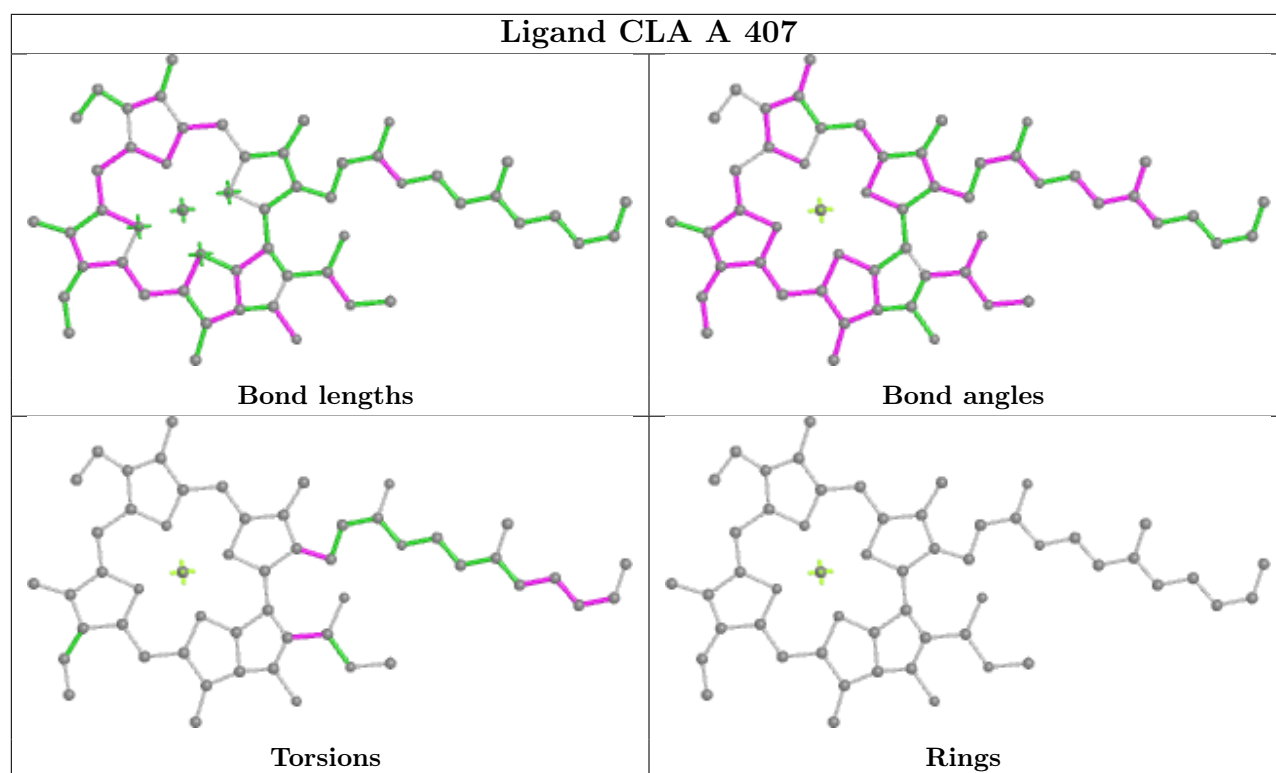
## Ligand CLA D 403

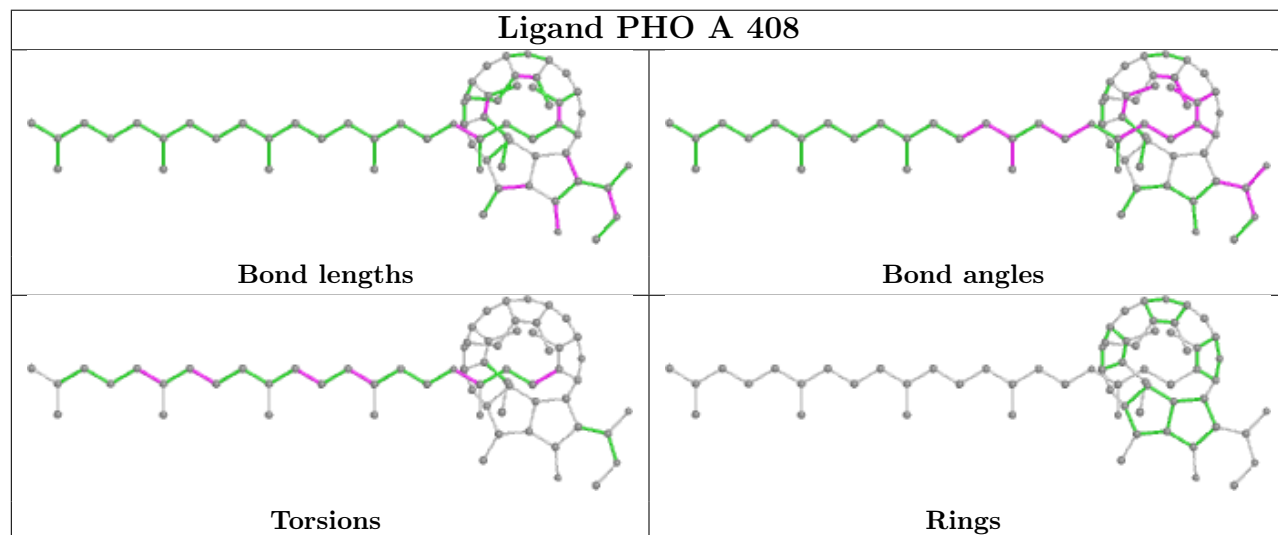
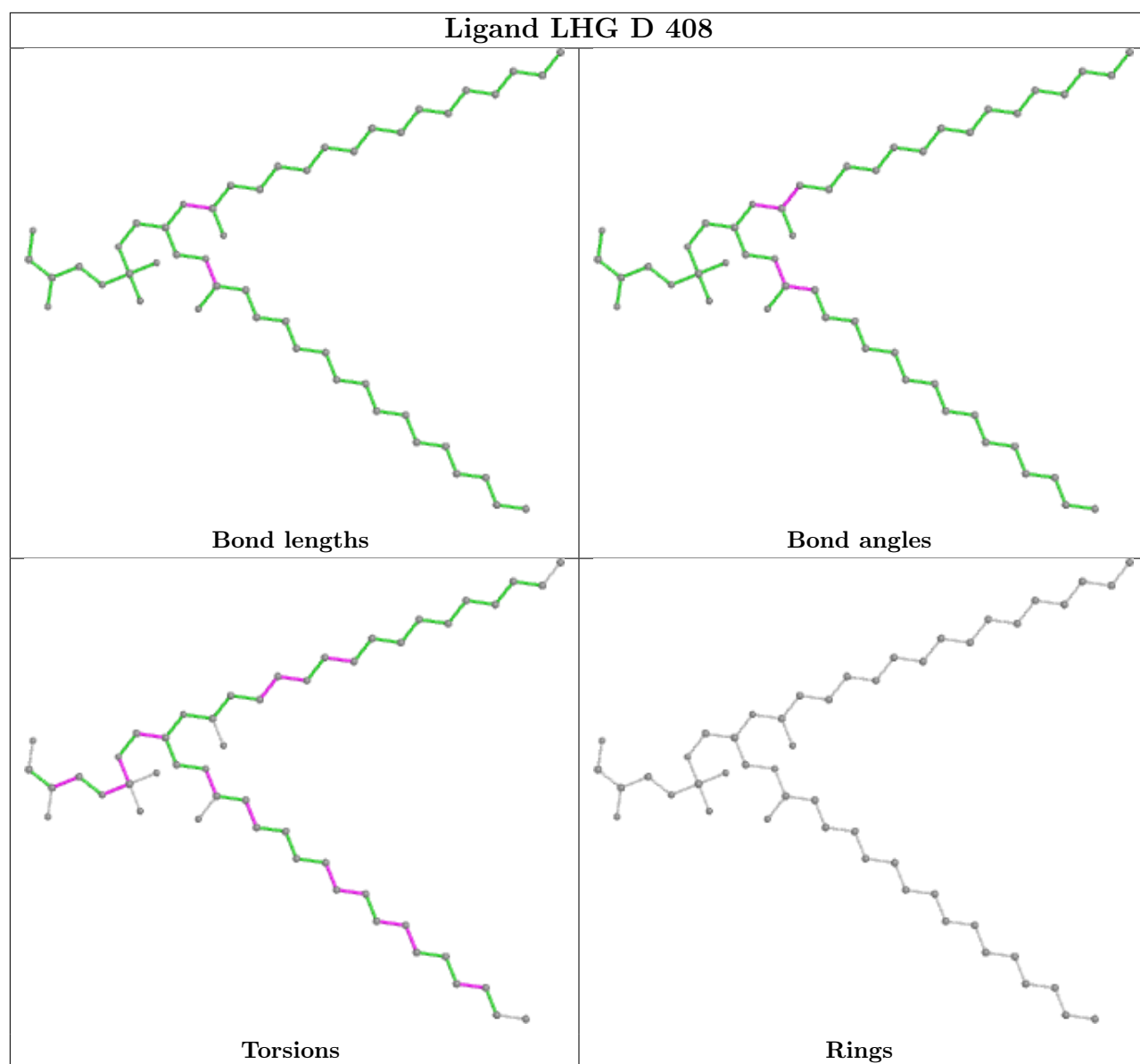


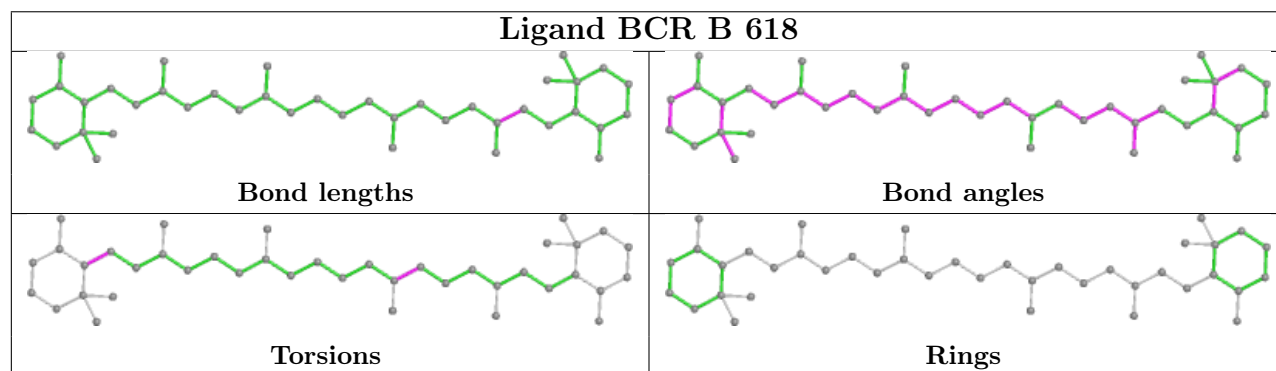
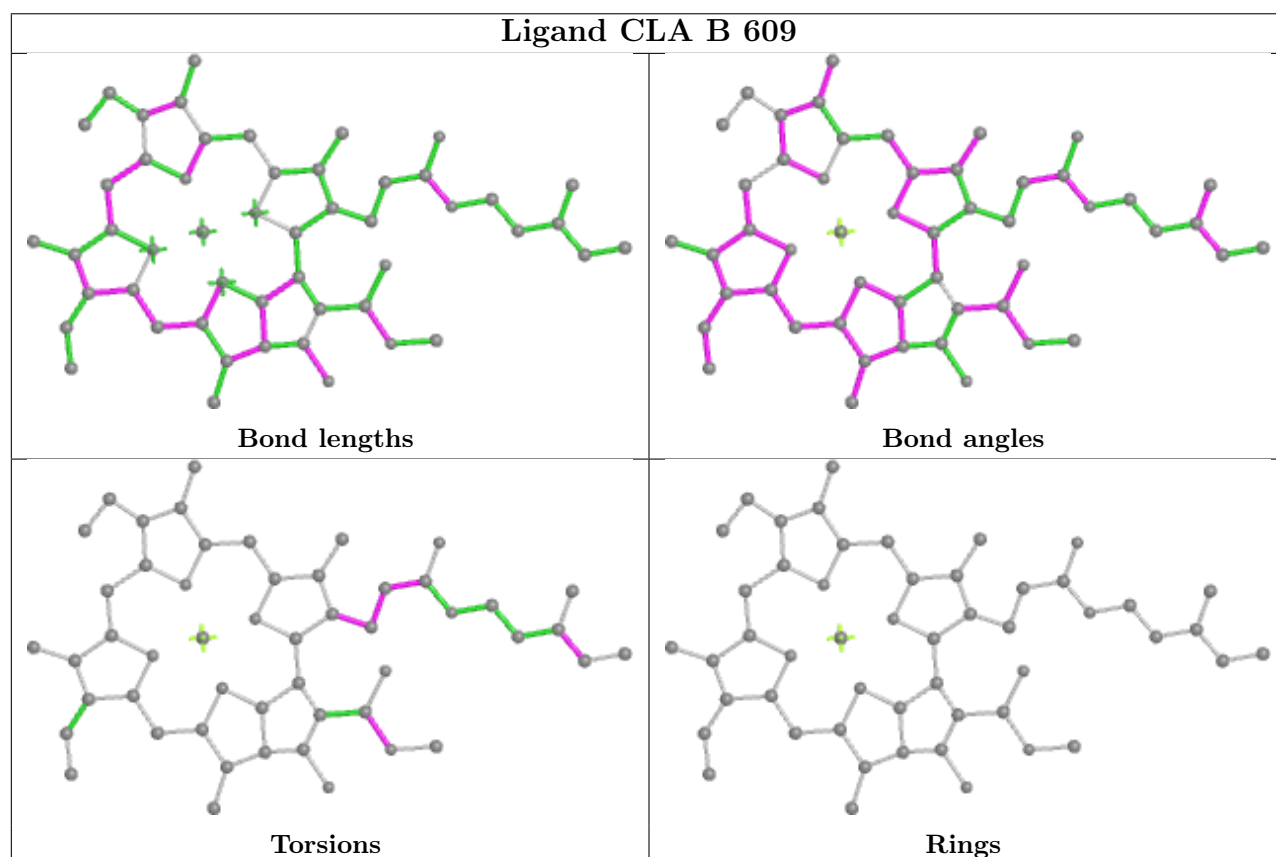
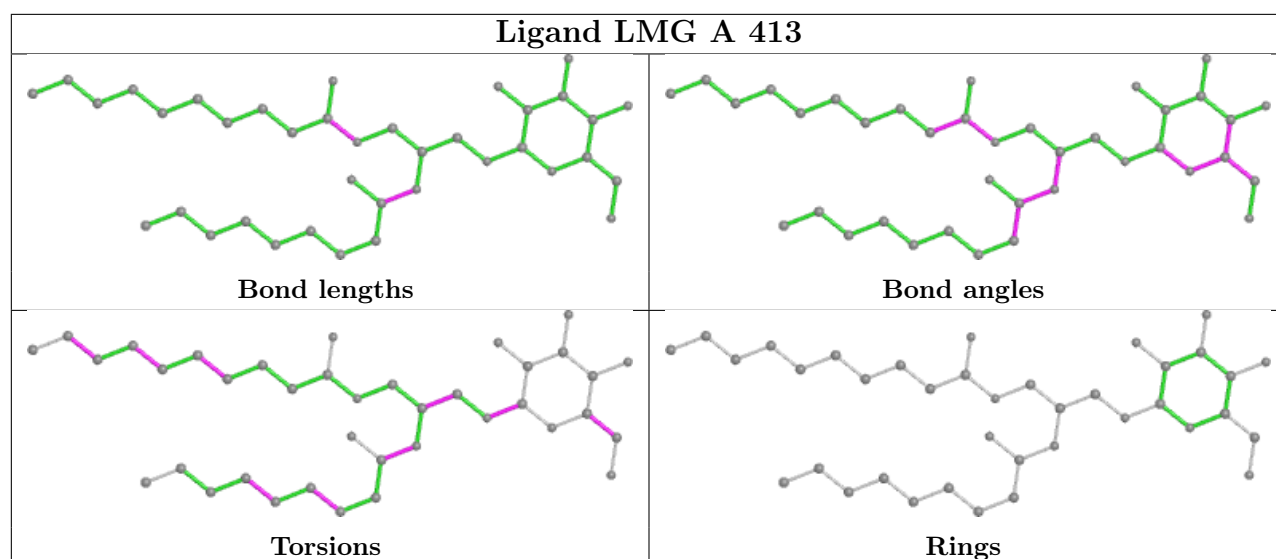
## Ligand RRX H 101

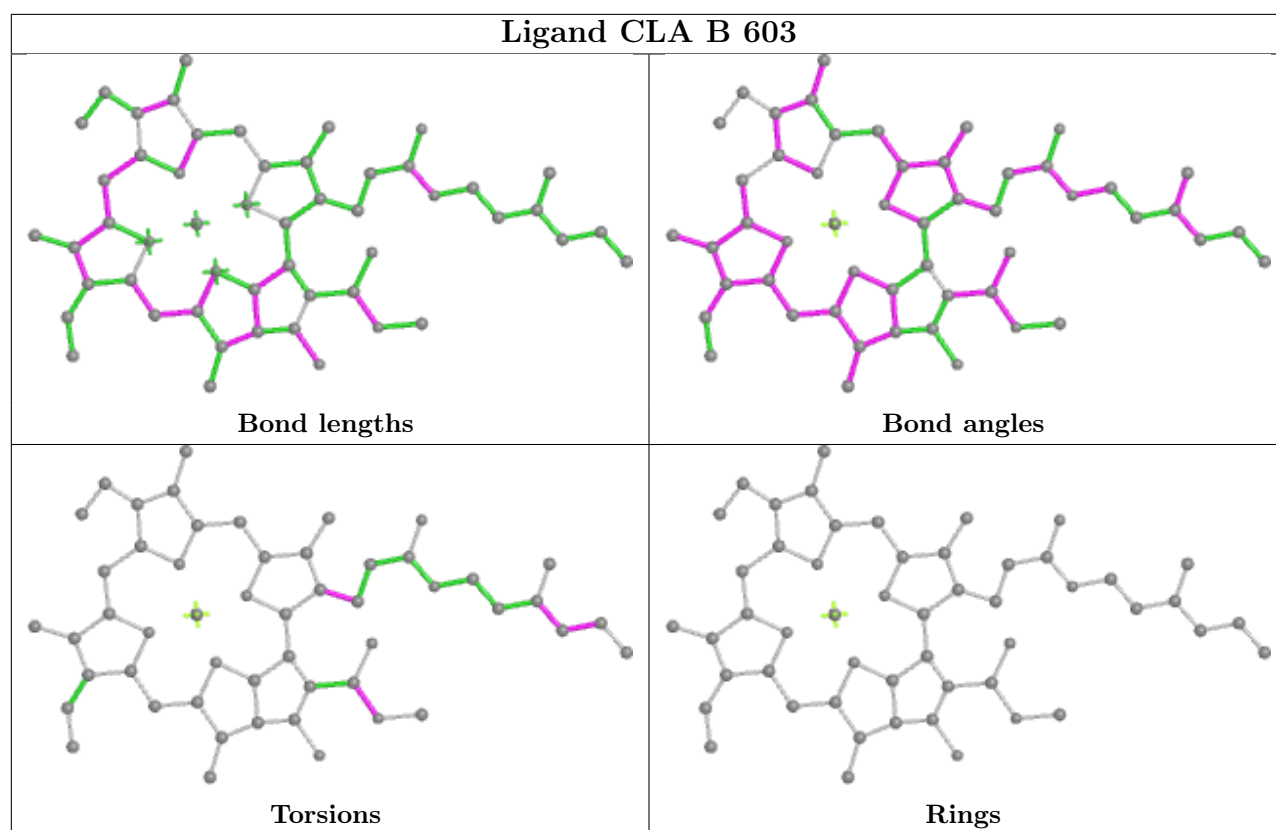






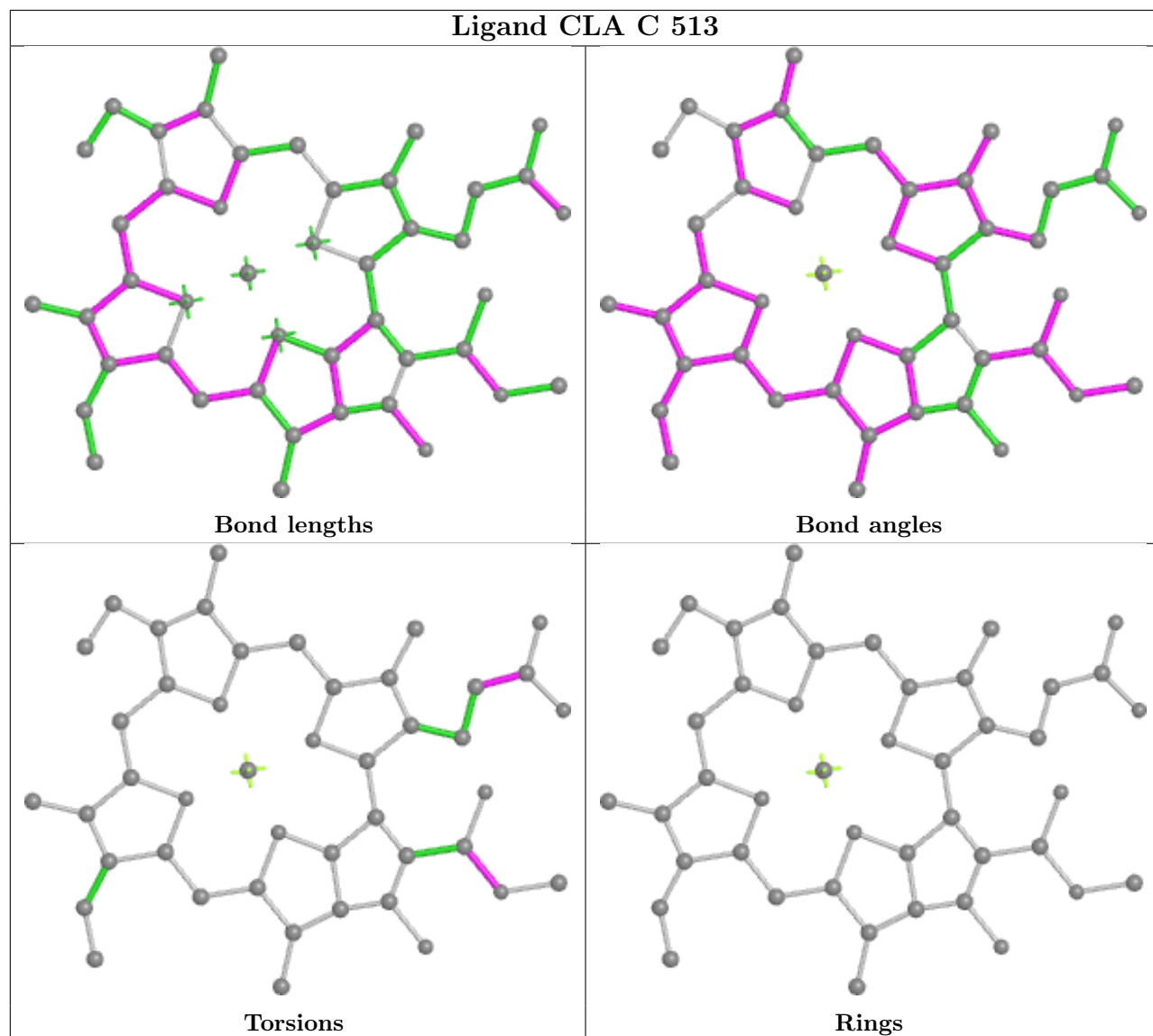




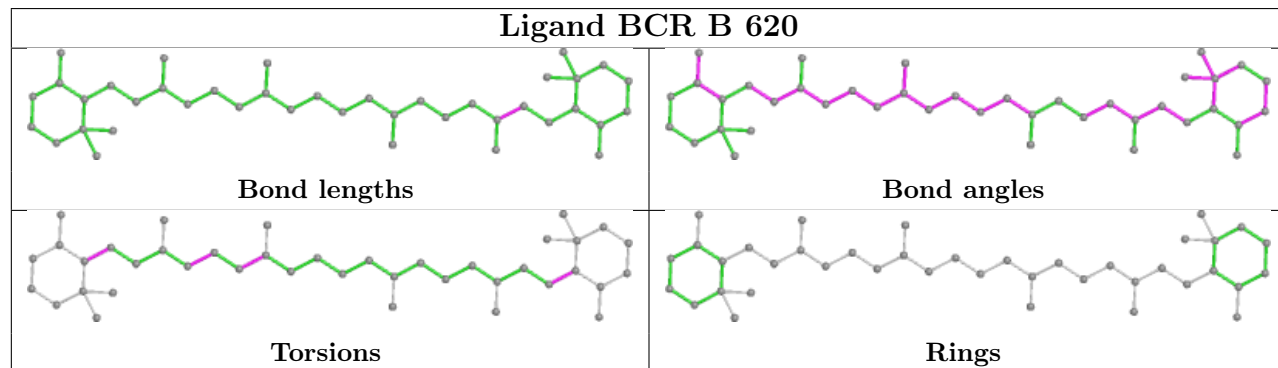


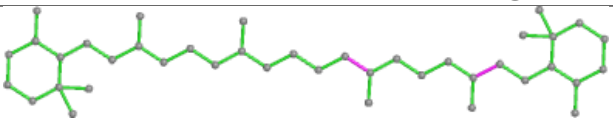
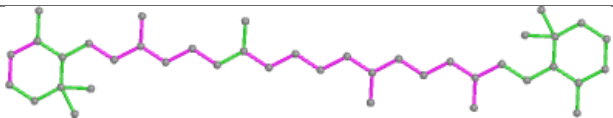
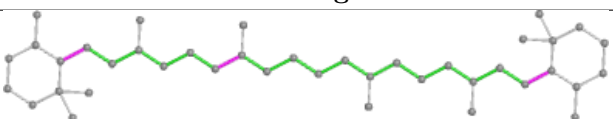
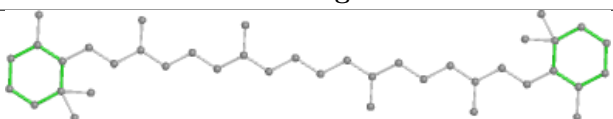


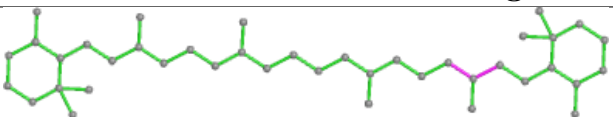
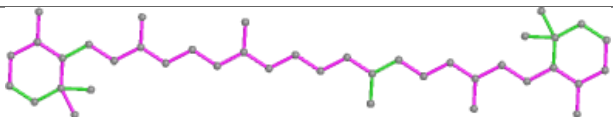
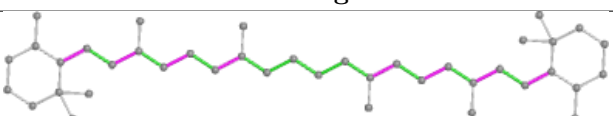
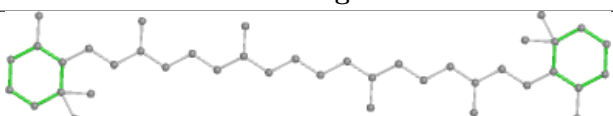
## Ligand CLA C 513

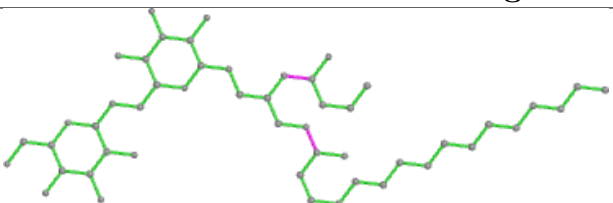
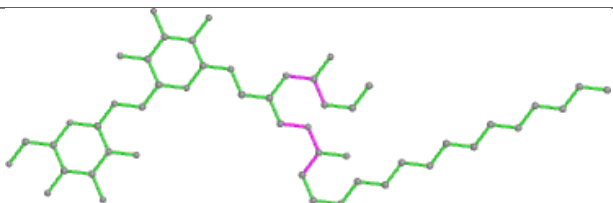
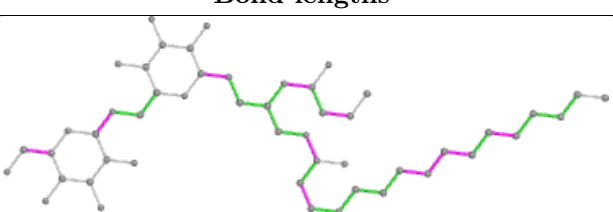
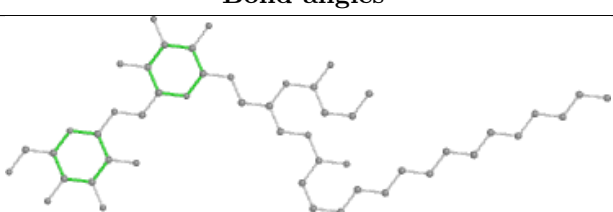


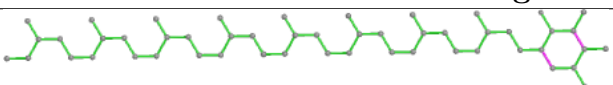
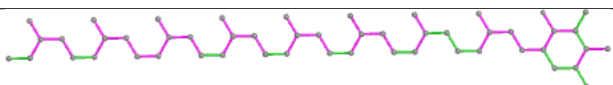
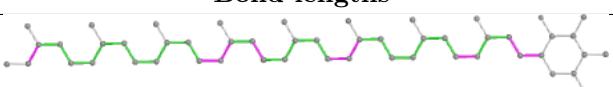
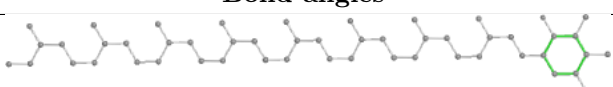
## Ligand BCR B 620

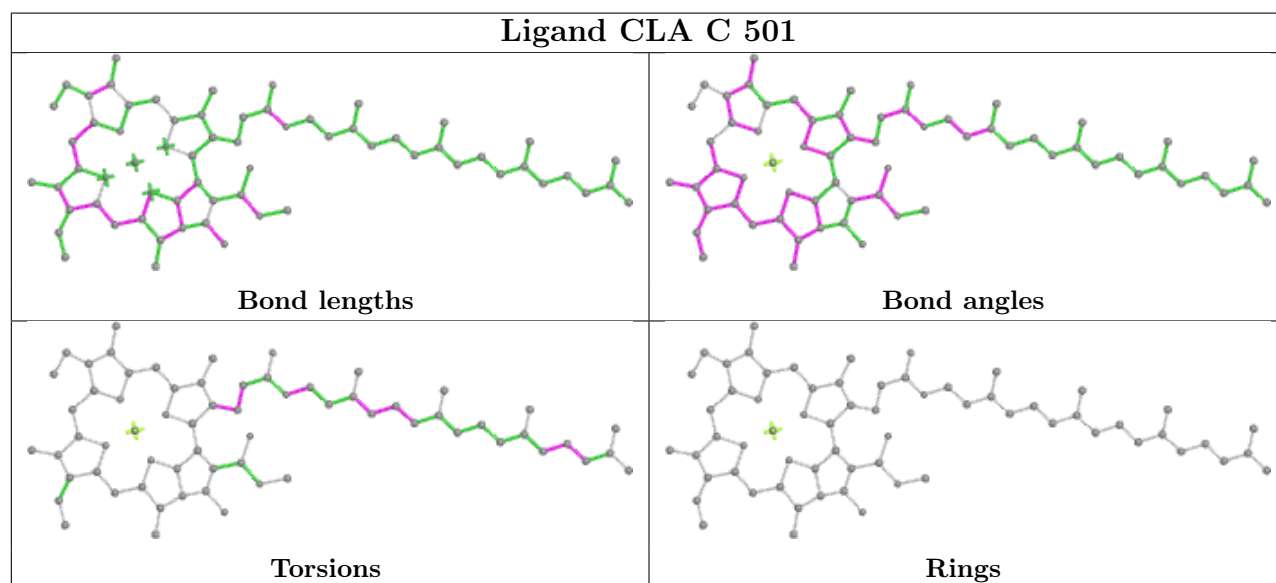
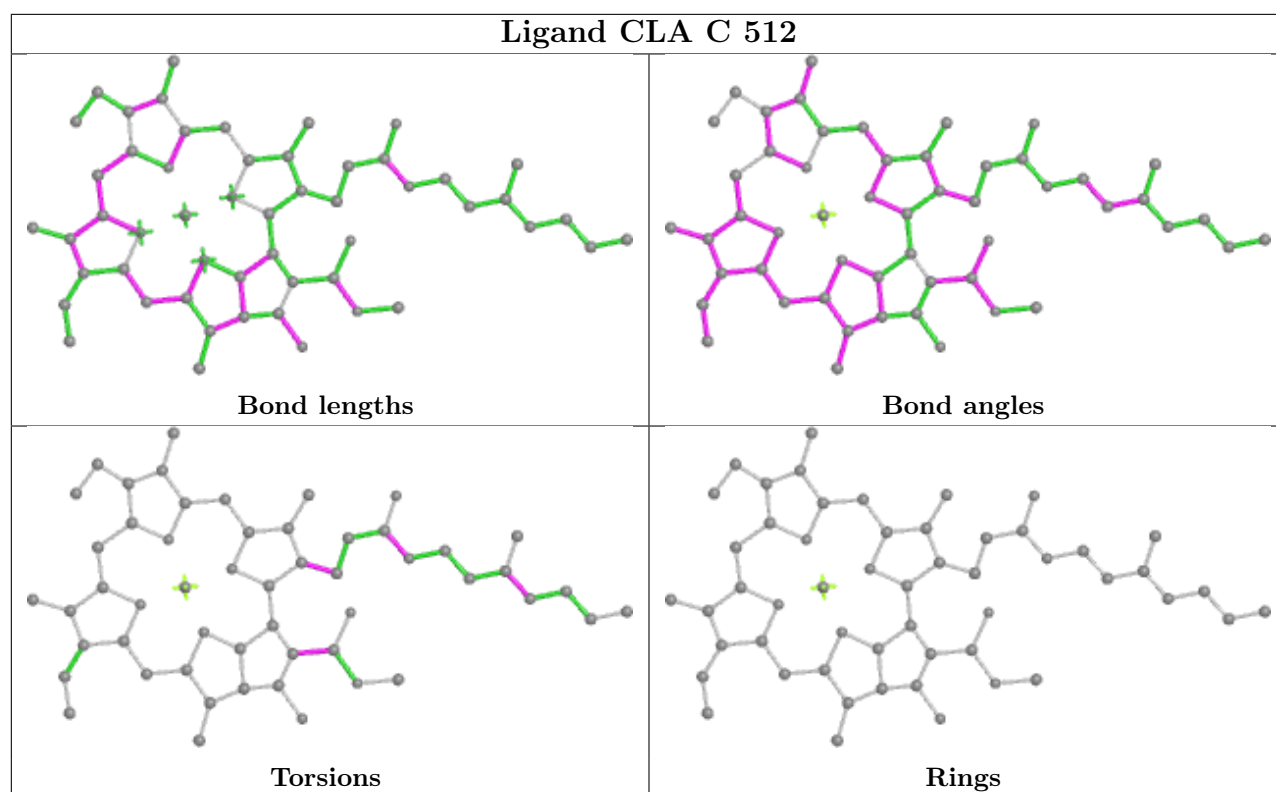


Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

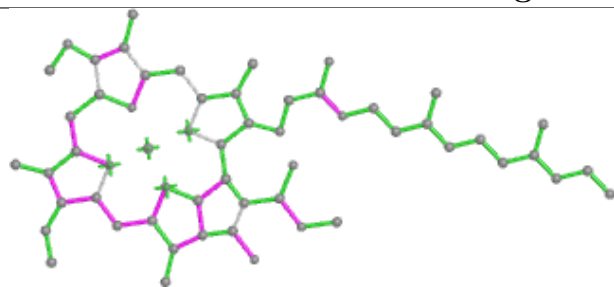
Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD C 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

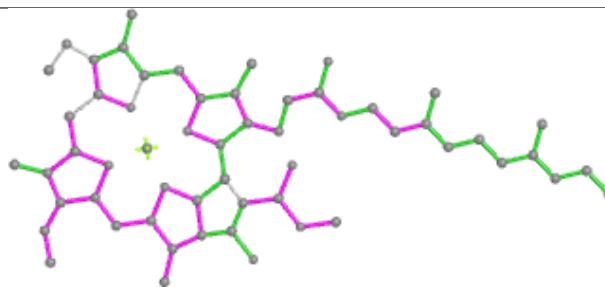
Ligand PL9 A 414	
	
Bond lengths	Bond angles
	
Torsions	Rings



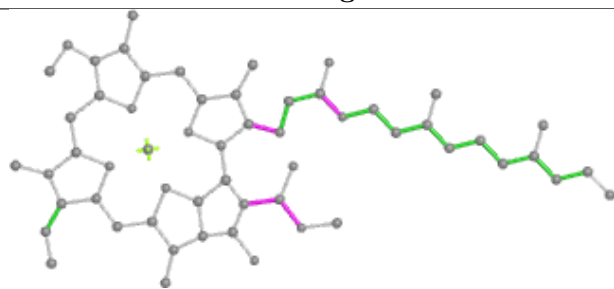
## Ligand CLA C 506



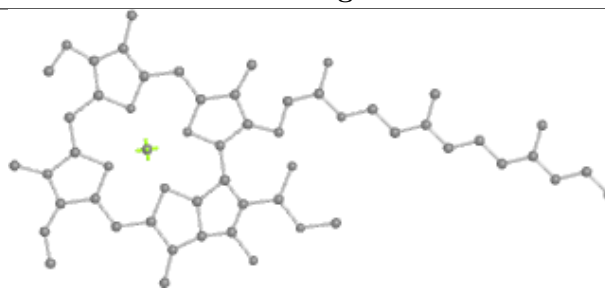
Bond lengths



Bond angles

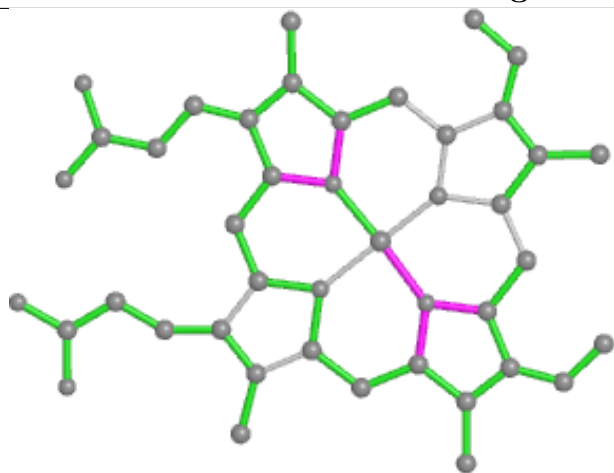


Torsions

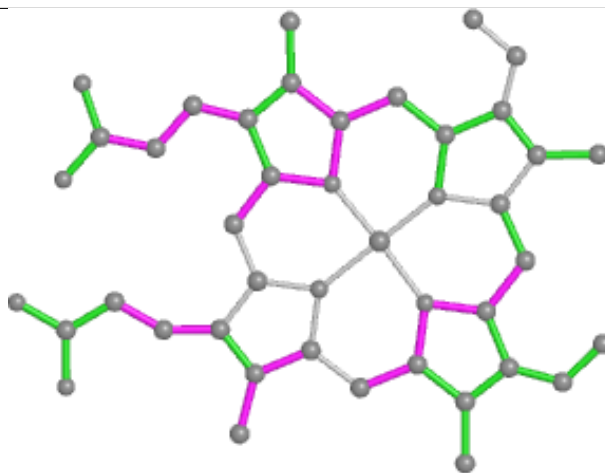


Rings

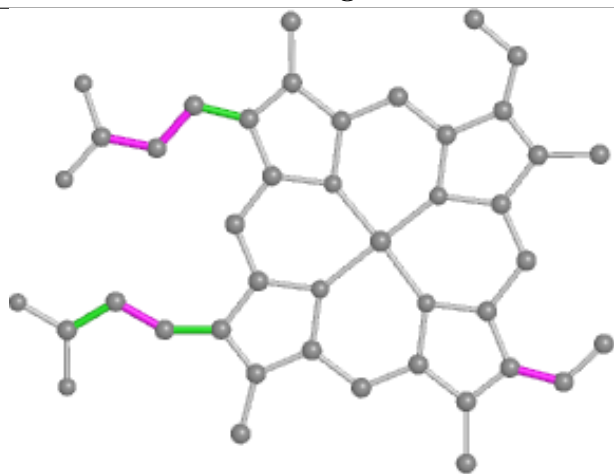
## Ligand HEM F 101



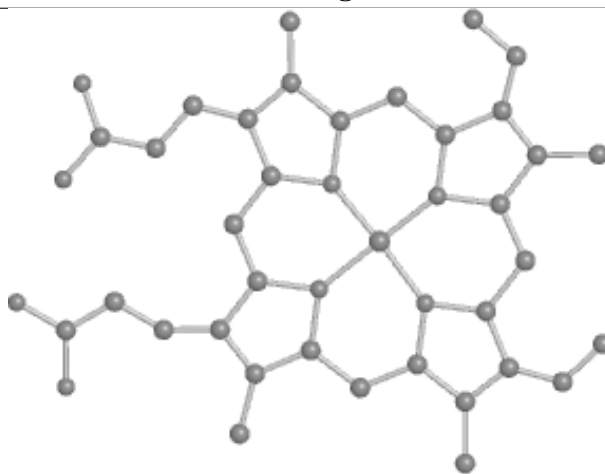
Bond lengths



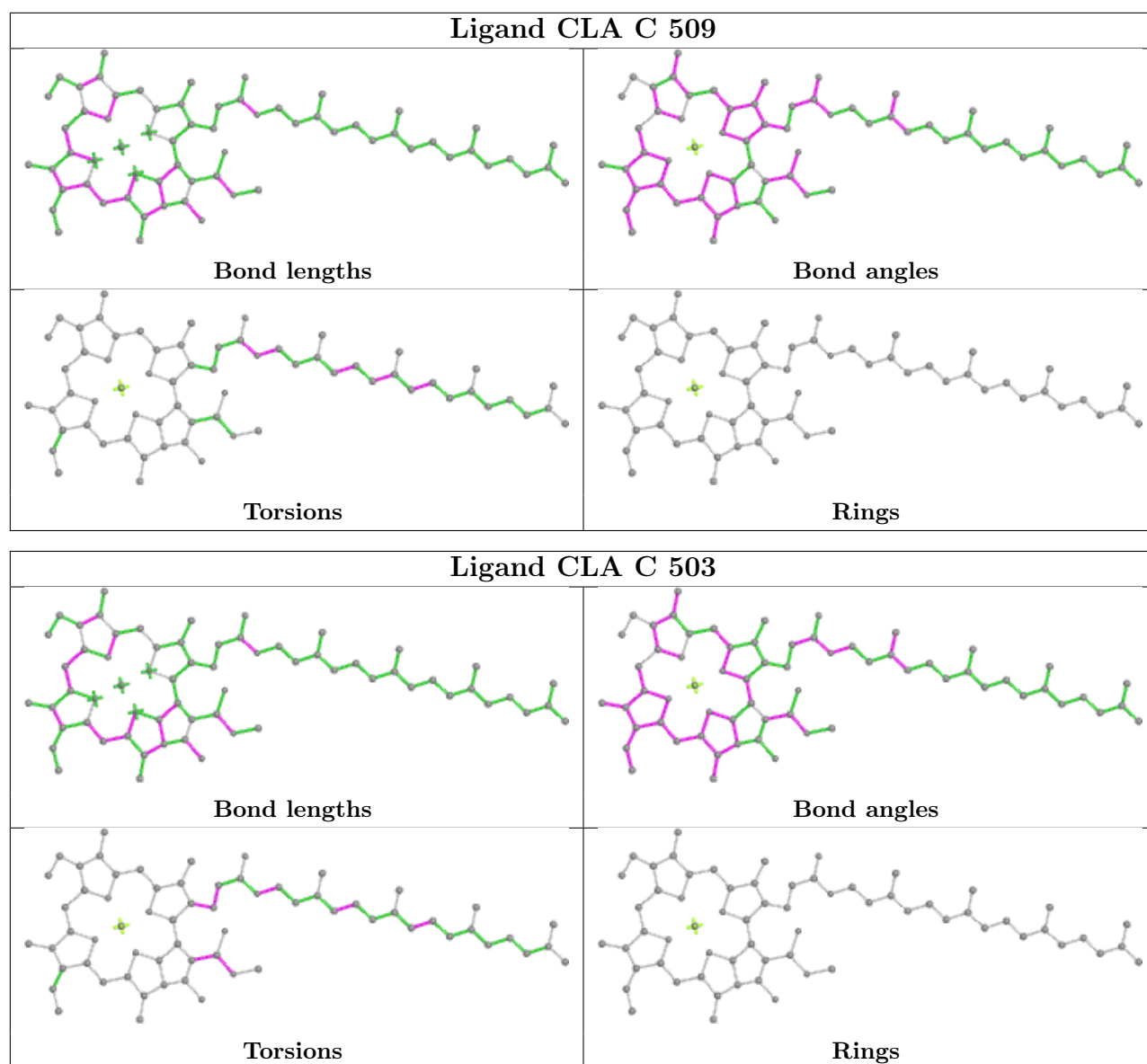
Bond angles



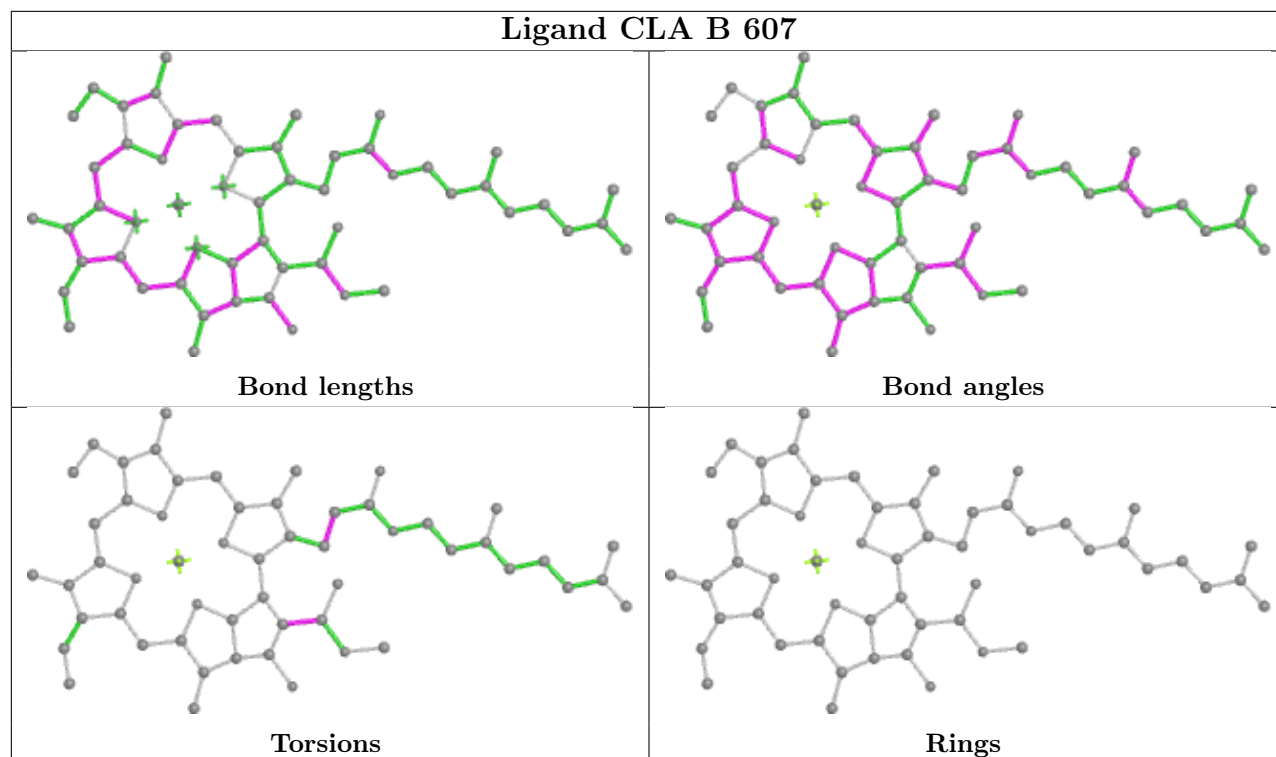
Torsions



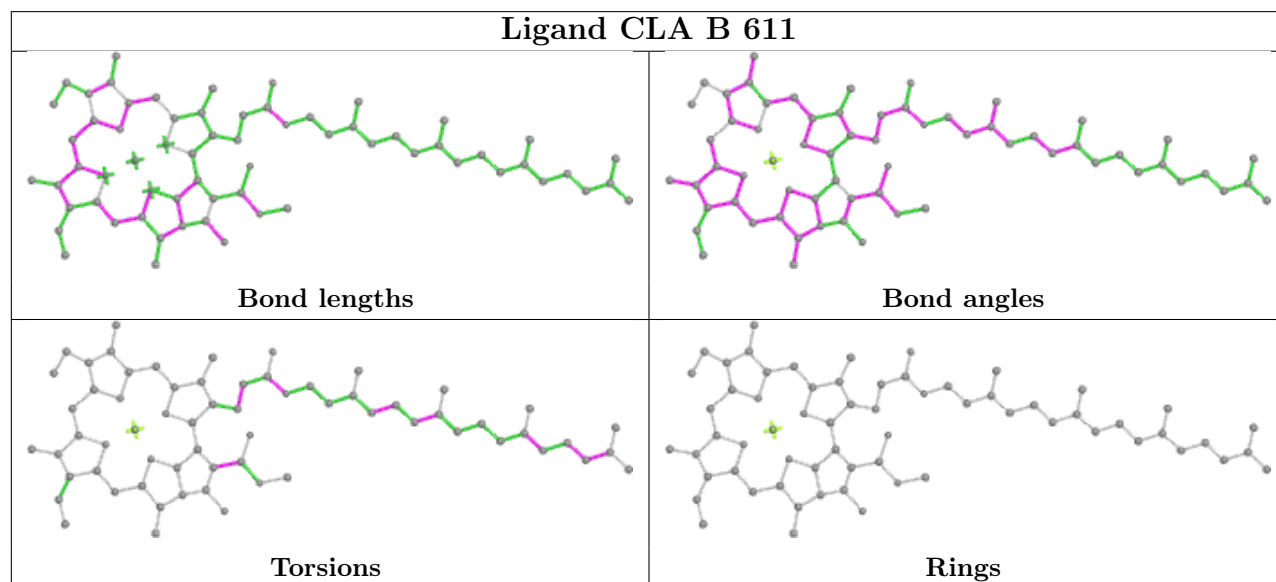
Rings

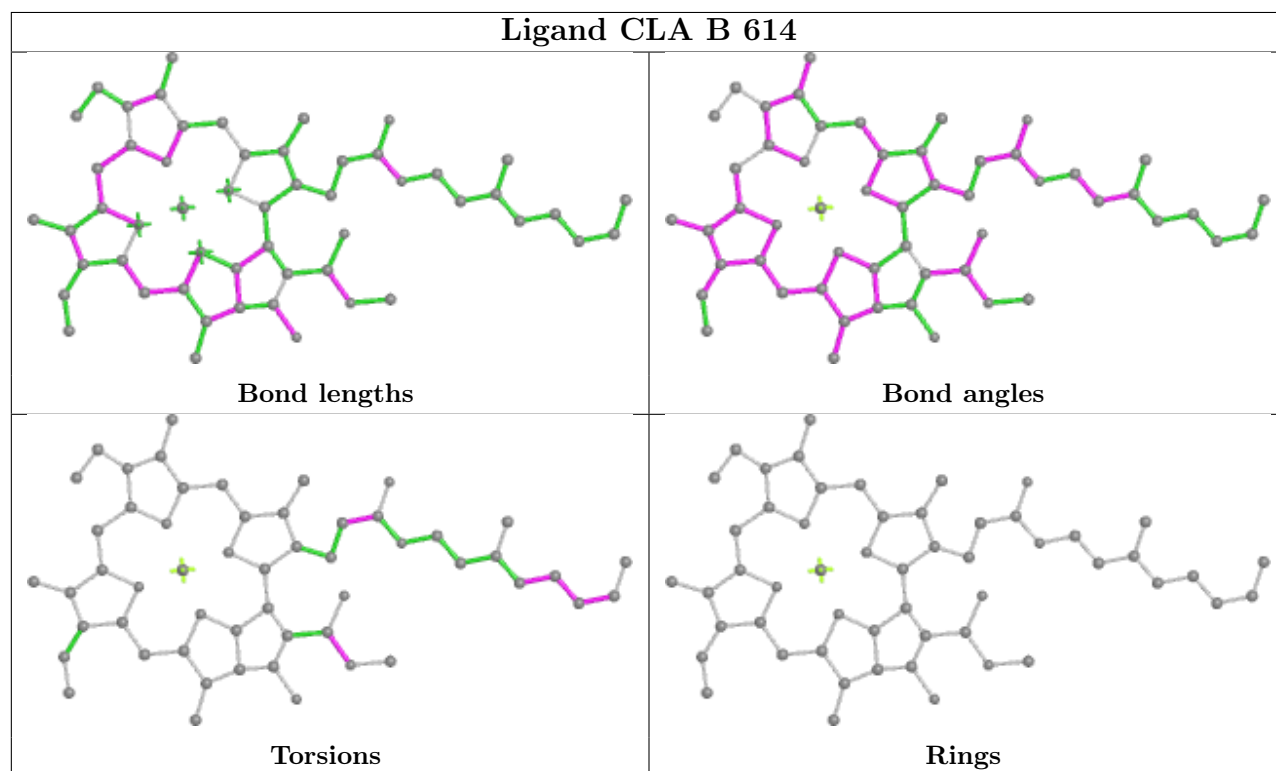
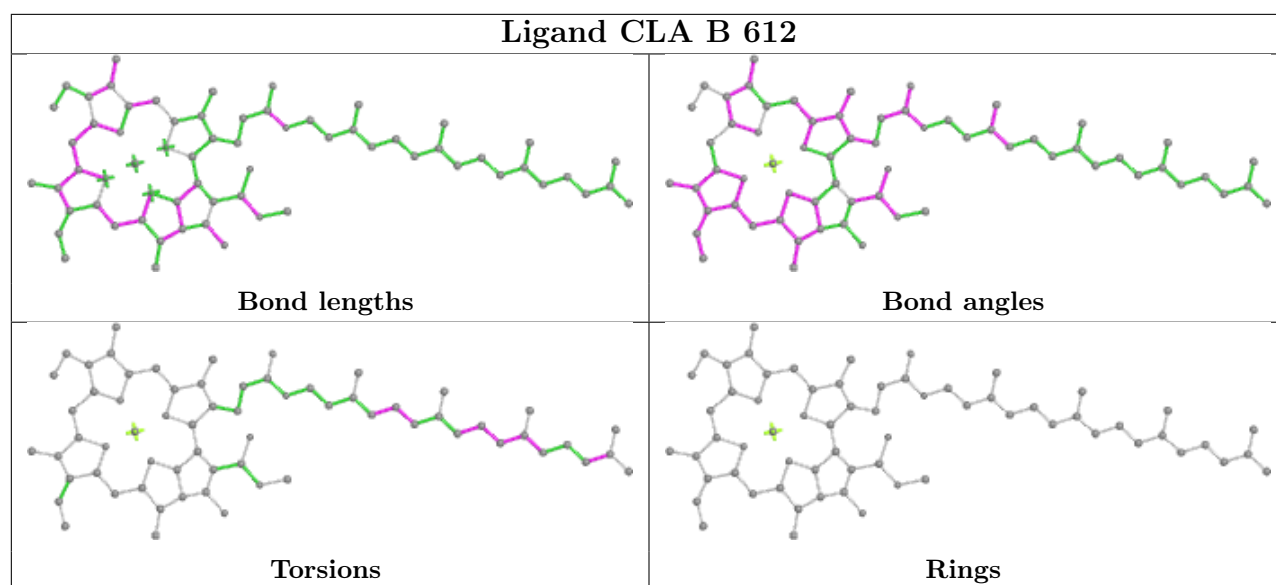


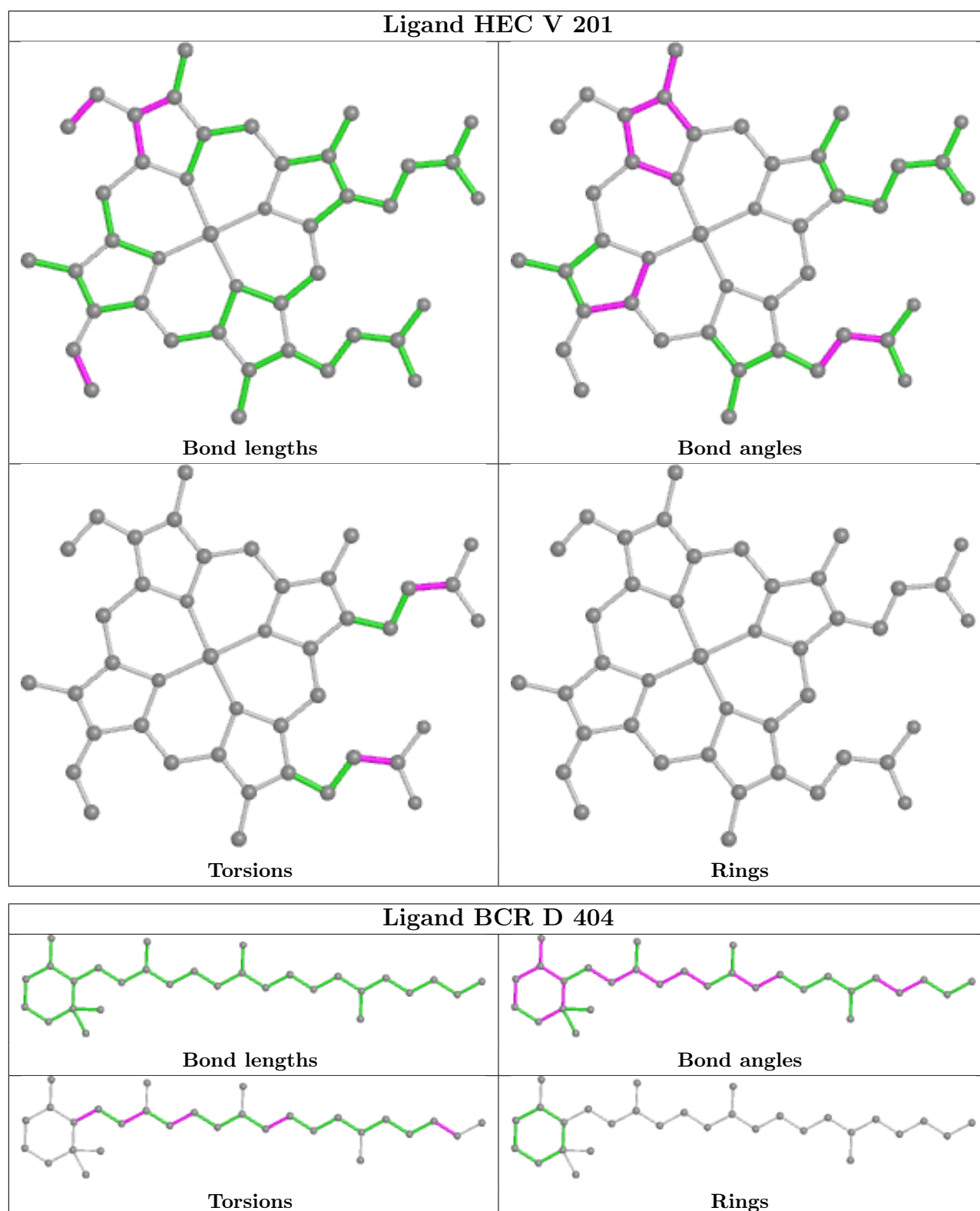
## Ligand CLA B 607



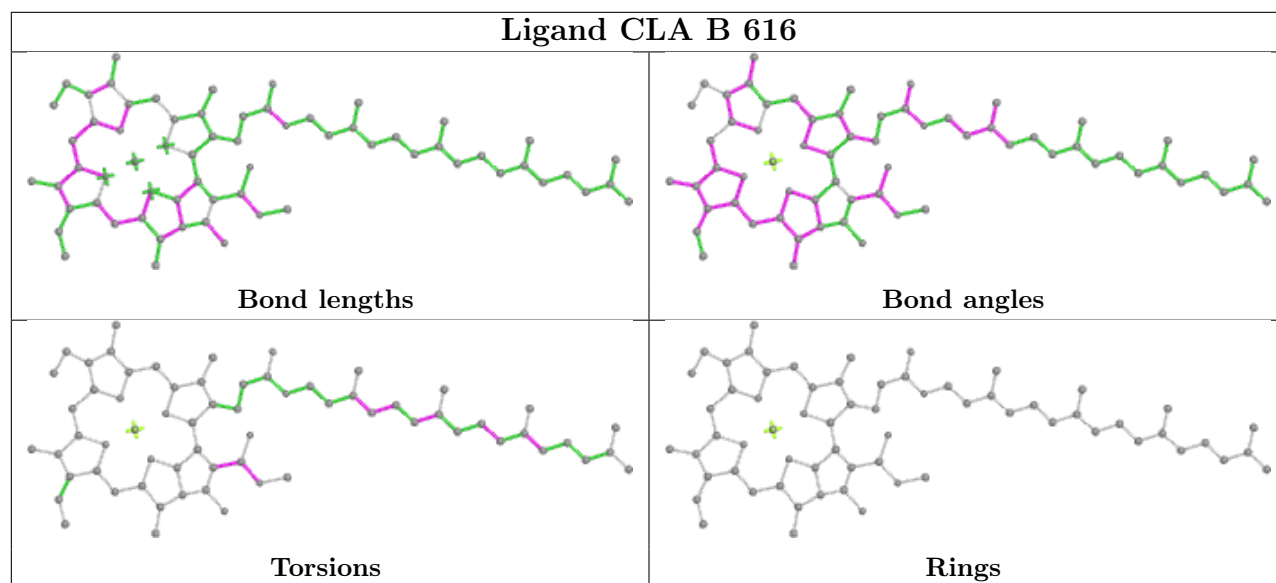
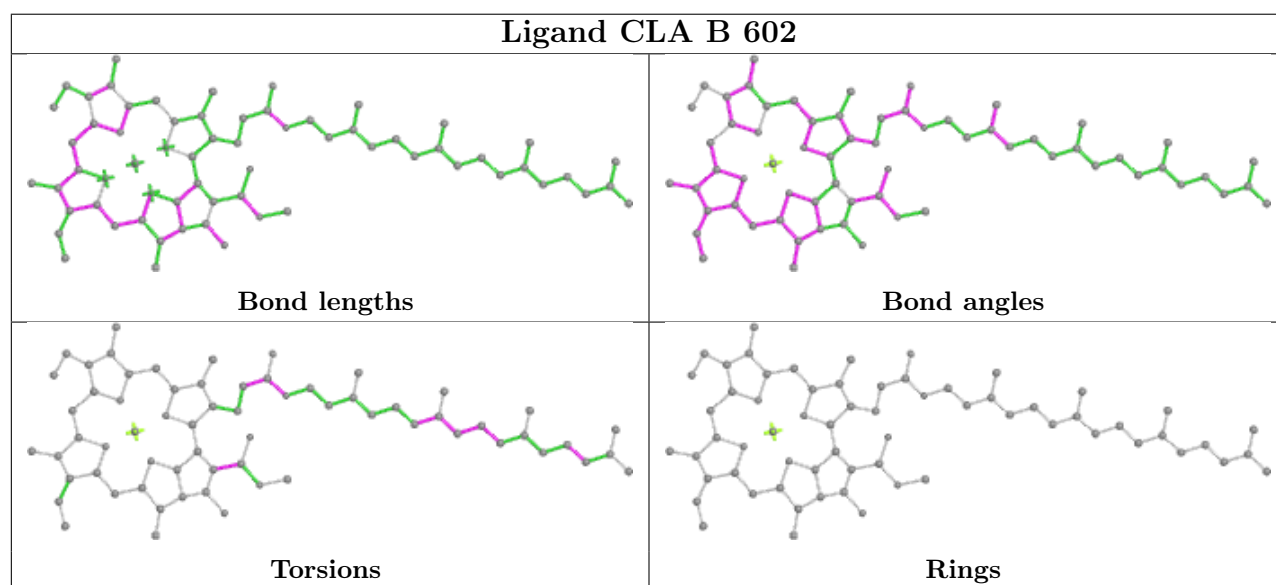
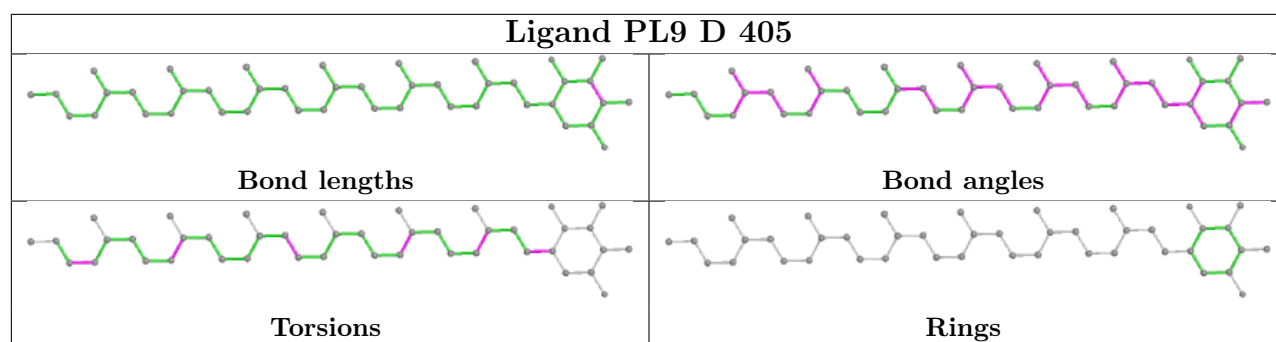
## Ligand CLA B 611

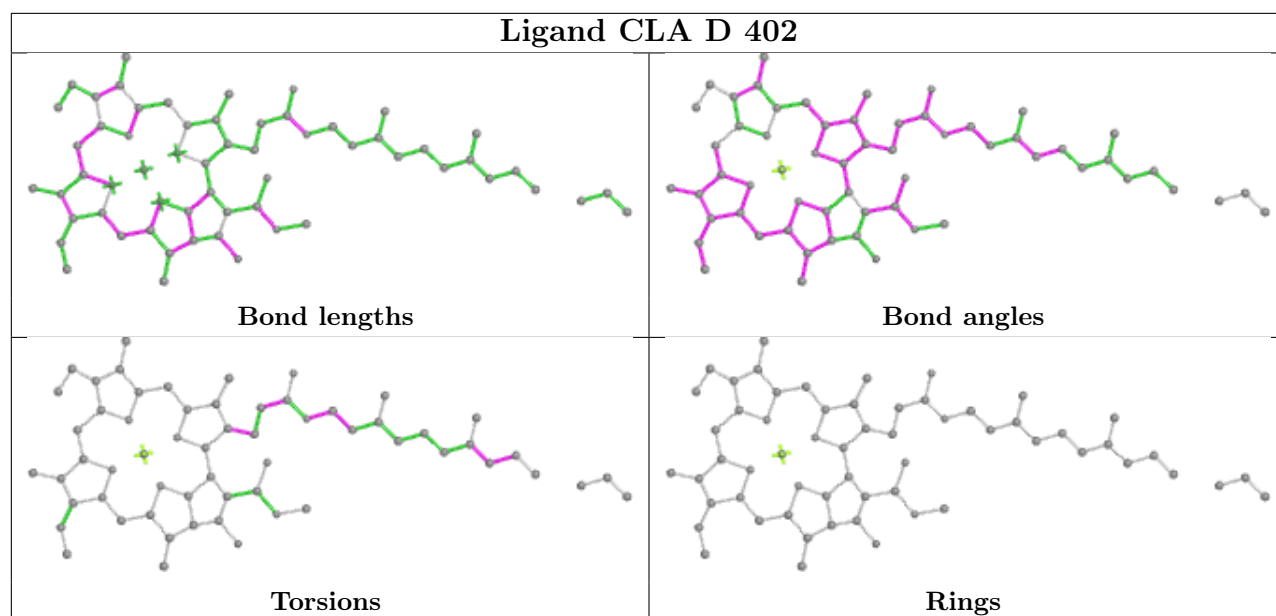
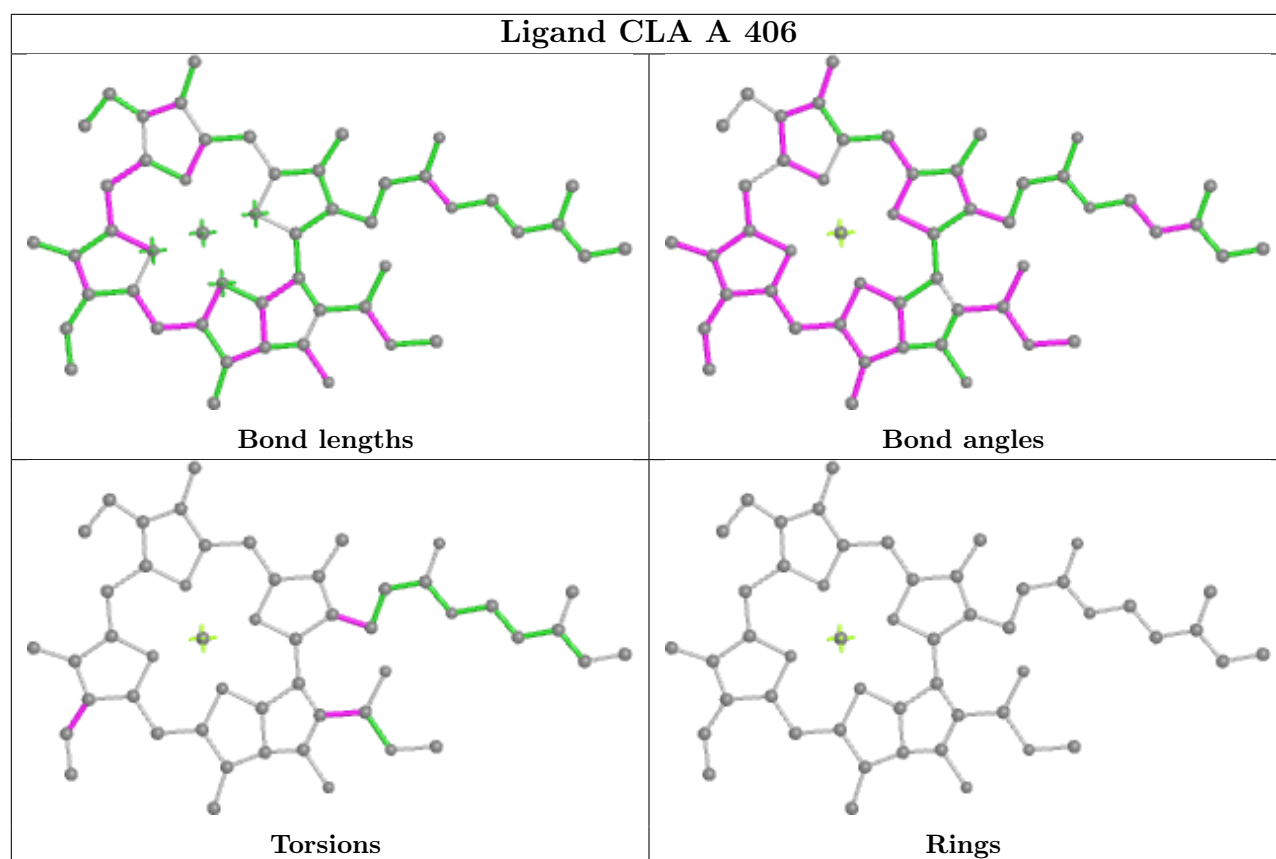


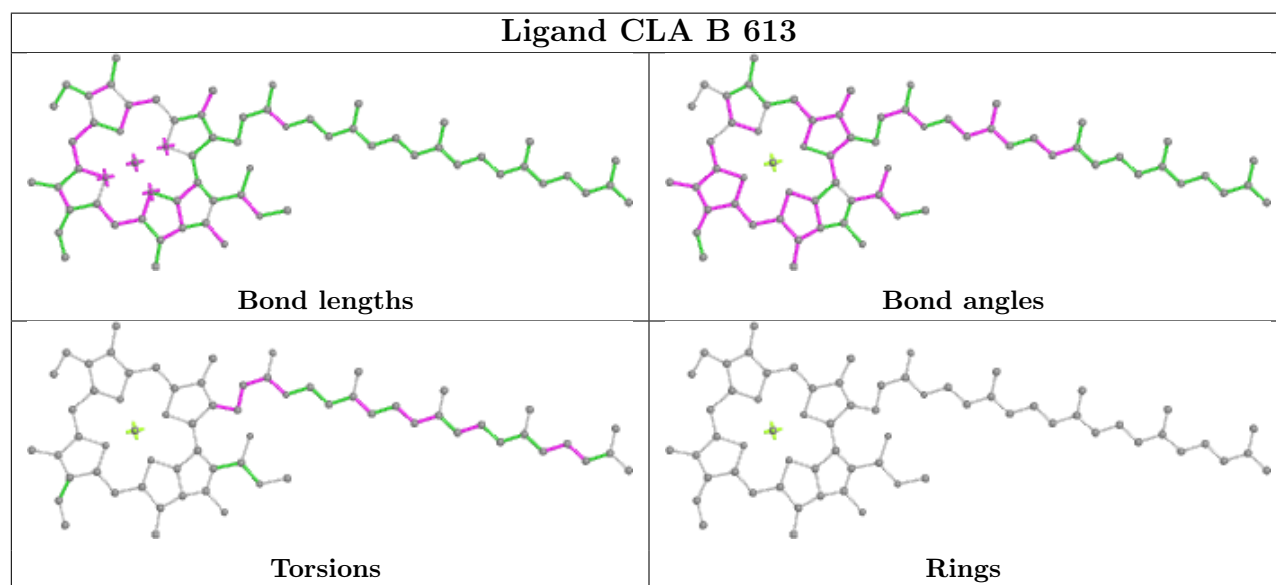
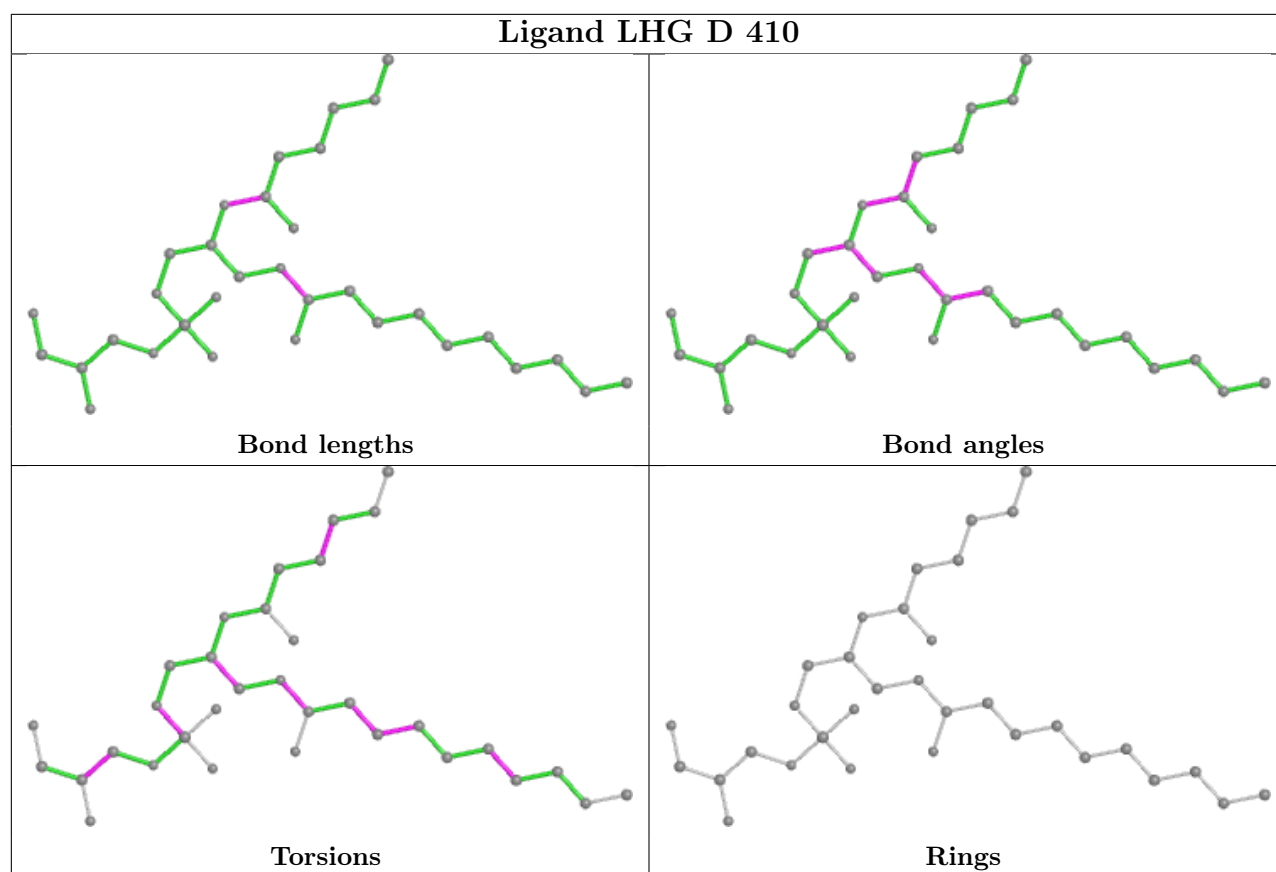




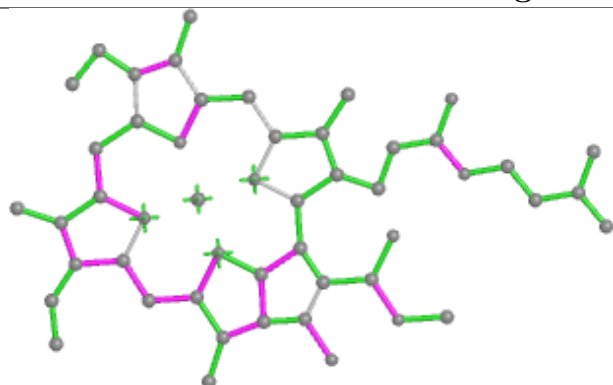




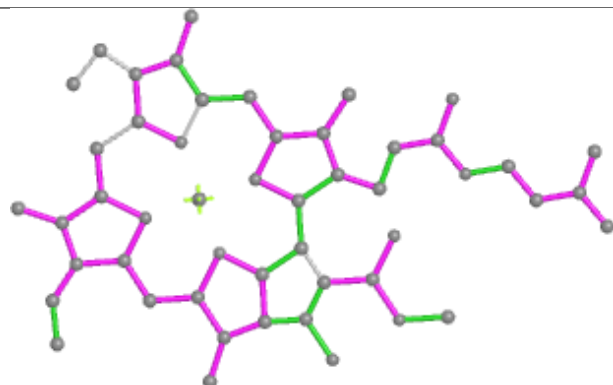




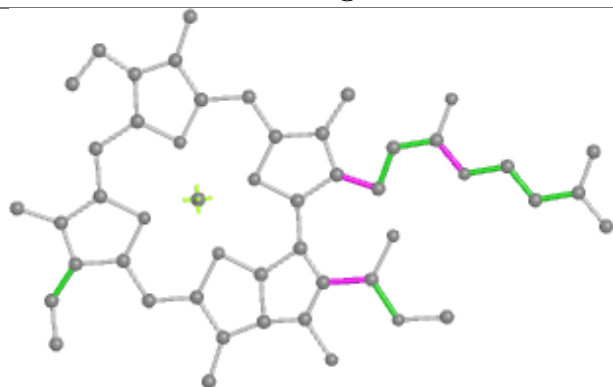
## Ligand CLA C 504



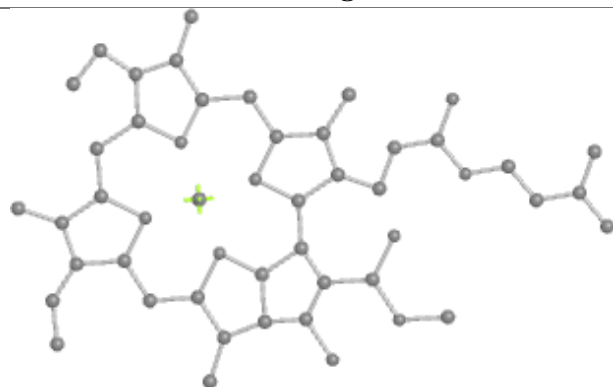
Bond lengths



Bond angles

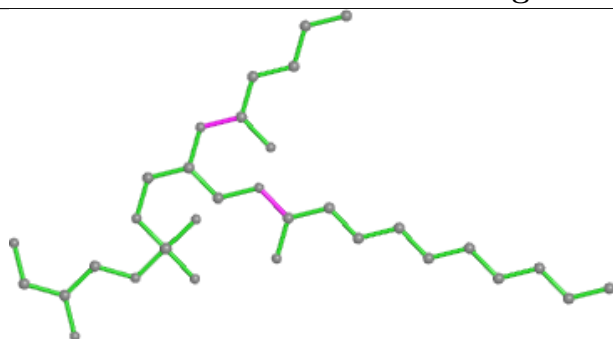


Torsions

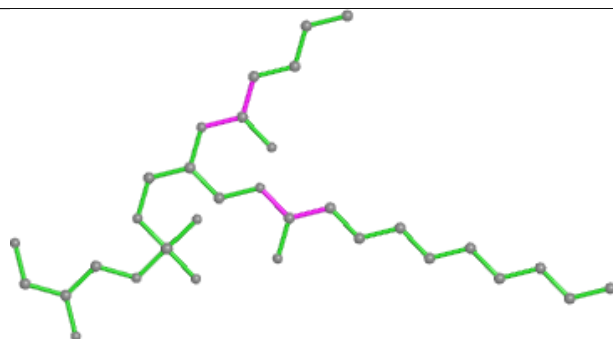


Rings

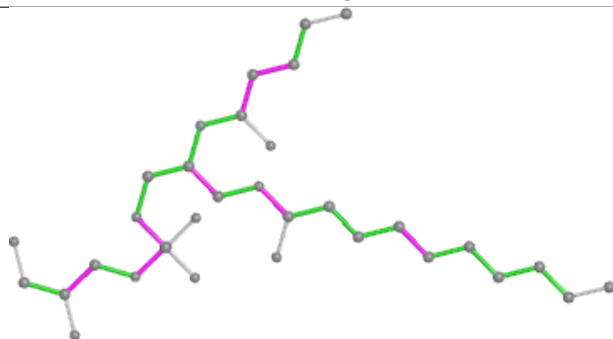
## Ligand LHG D 409



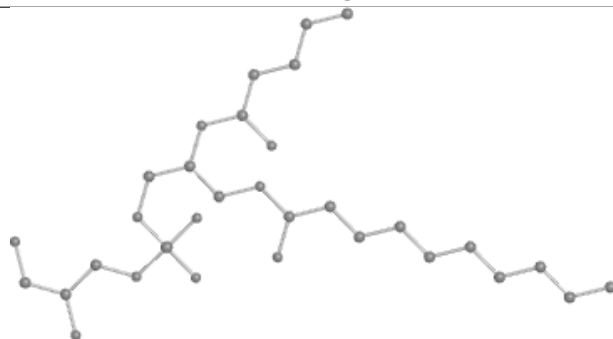
Bond lengths



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.

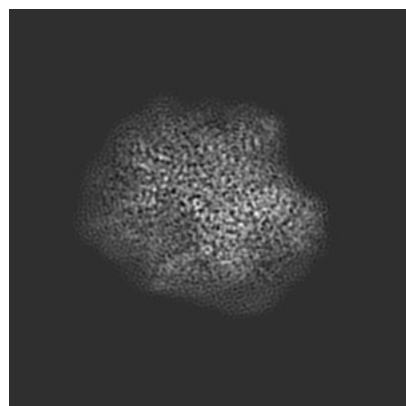
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31062. These allow visual inspection of the internal detail of the map and identification of artifacts.

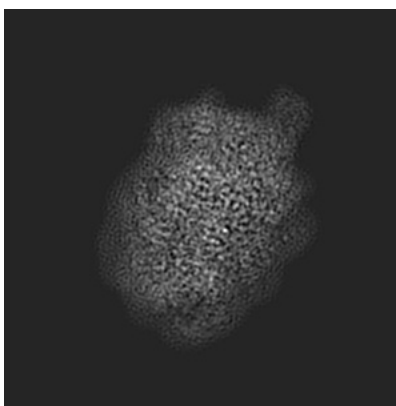
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

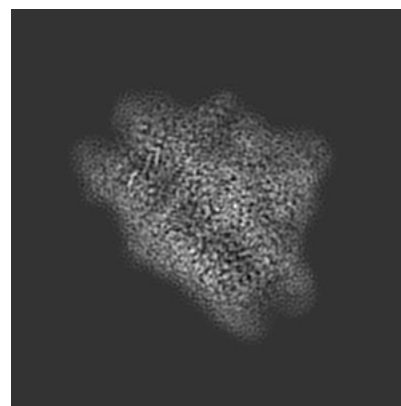
#### 6.1.1 Primary map



X

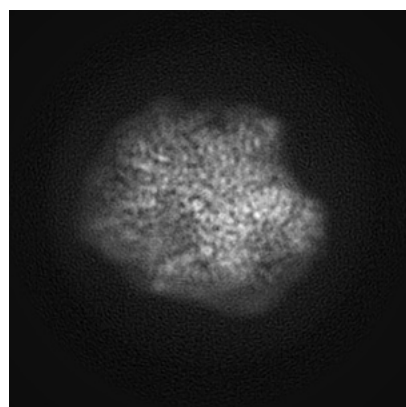


Y

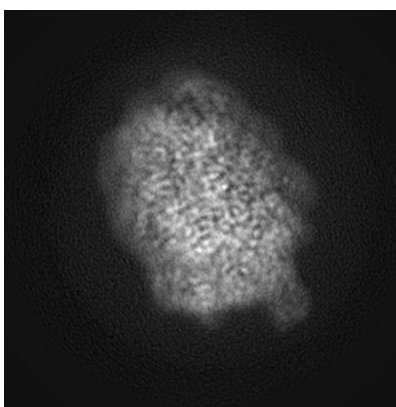


Z

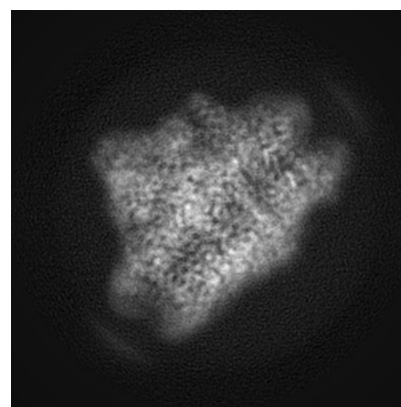
#### 6.1.2 Raw map



X



Y

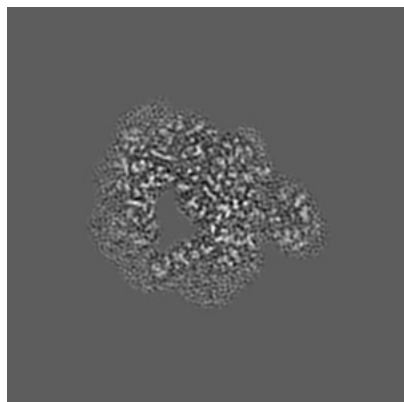


Z

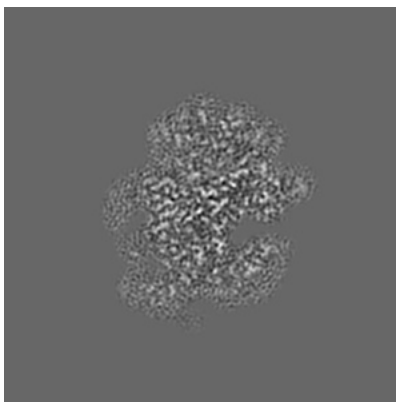
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

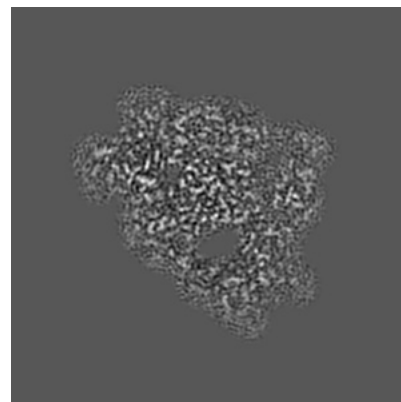
### 6.2.1 Primary map



X Index: 120

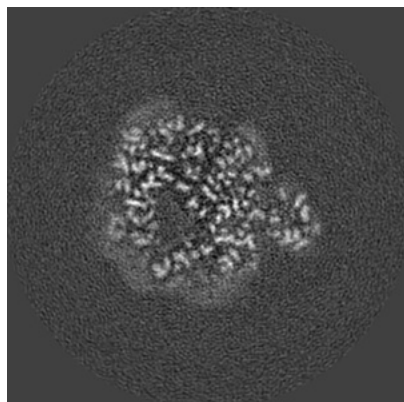


Y Index: 120

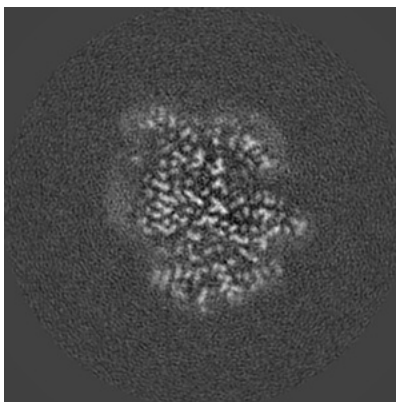


Z Index: 120

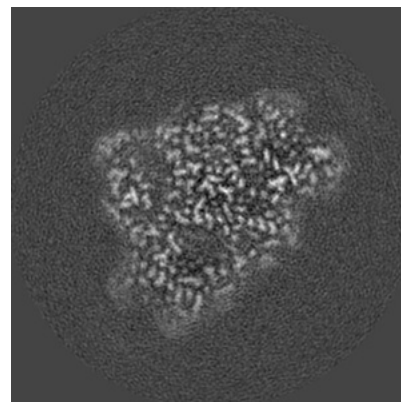
### 6.2.2 Raw map



X Index: 120



Y Index: 120

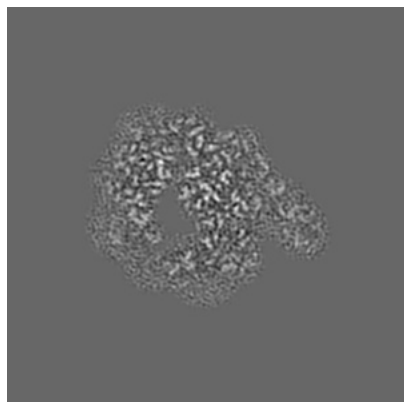


Z Index: 120

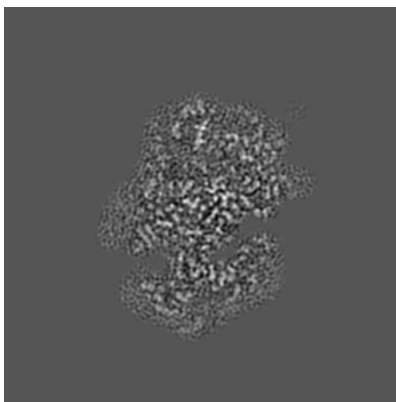
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

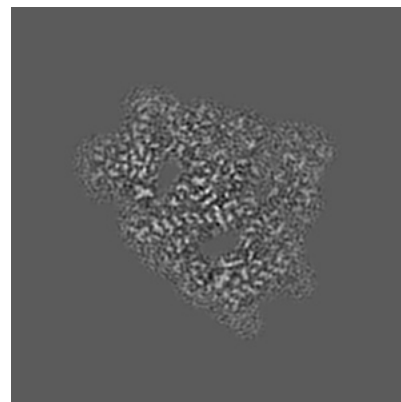
### 6.3.1 Primary map



X Index: 122

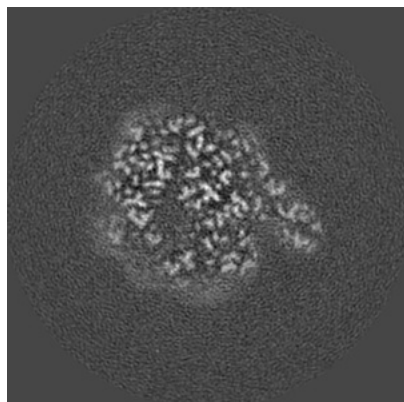


Y Index: 127

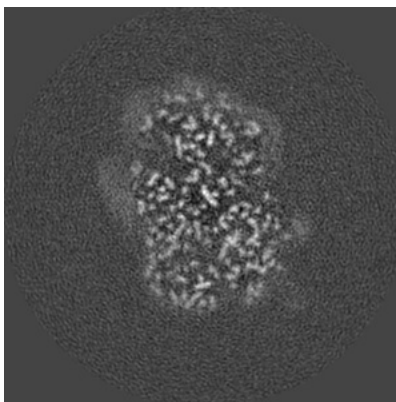


Z Index: 124

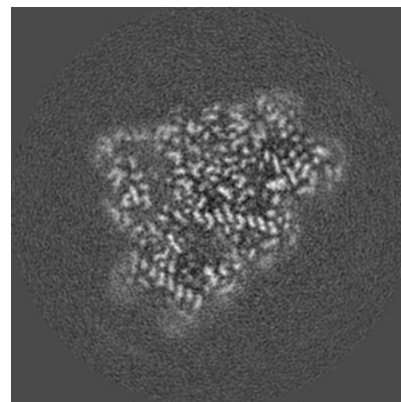
### 6.3.2 Raw map



X Index: 118



Y Index: 129



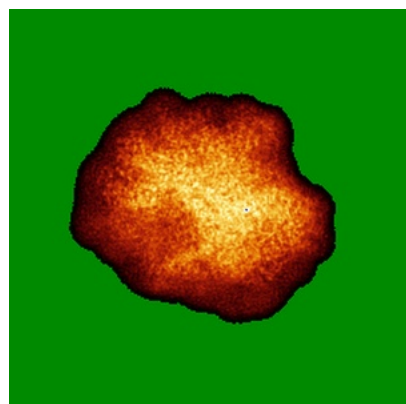
Z Index: 121

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

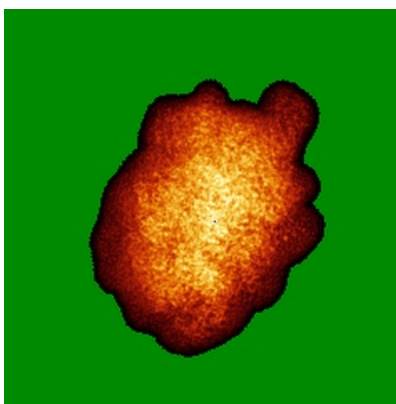


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

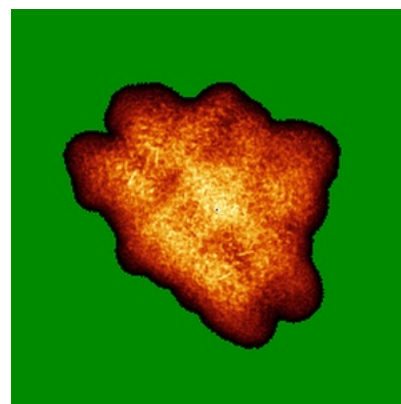
### 6.4.1 Primary map



X

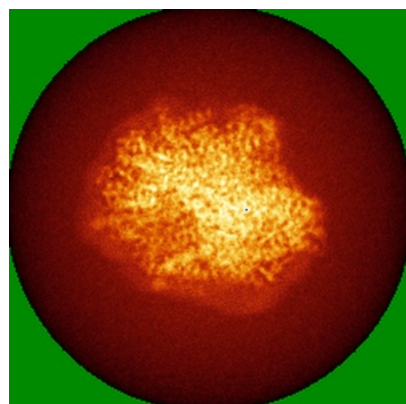


Y

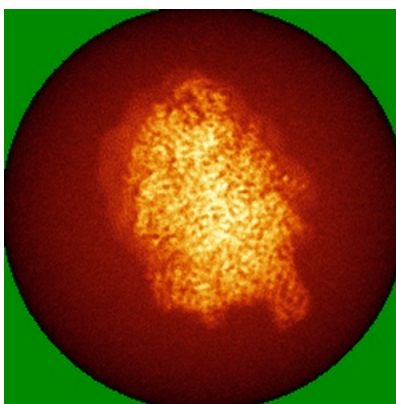


Z

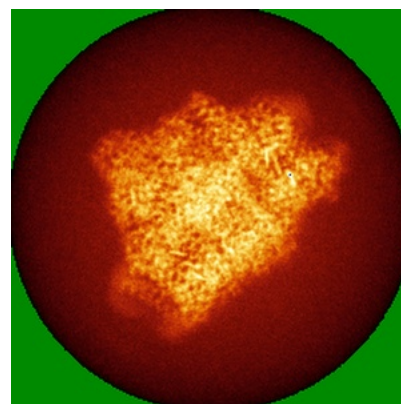
### 6.4.2 Raw map



X



Y

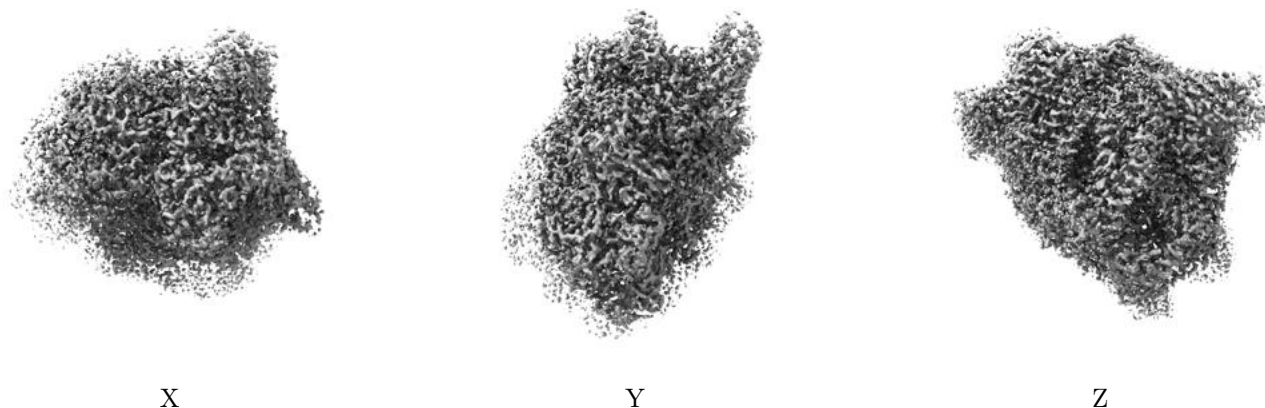


Z

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.

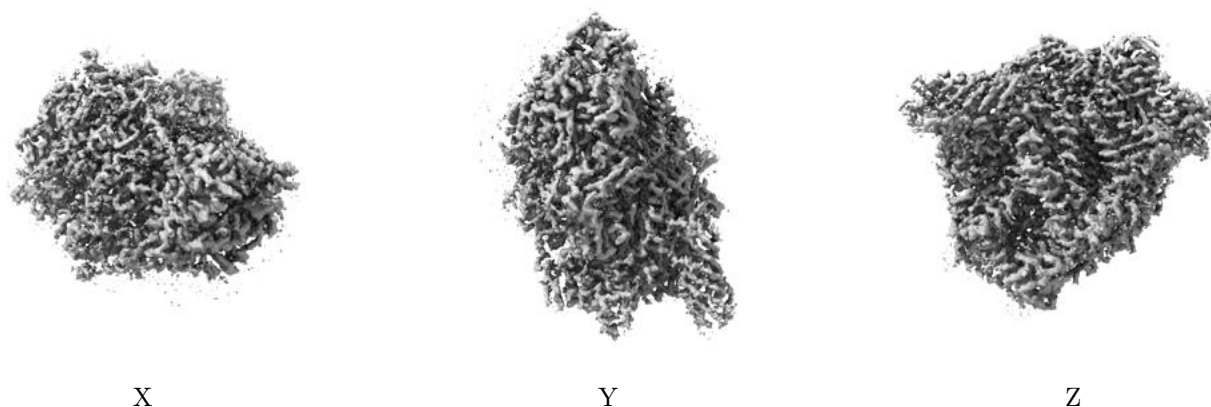
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0316. 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.

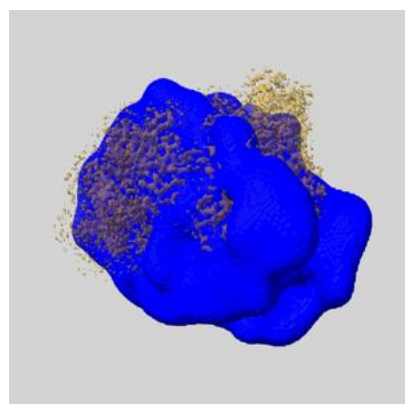
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

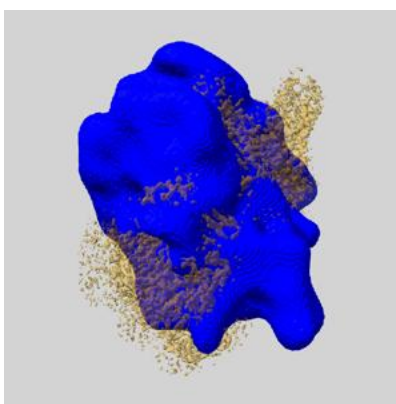
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

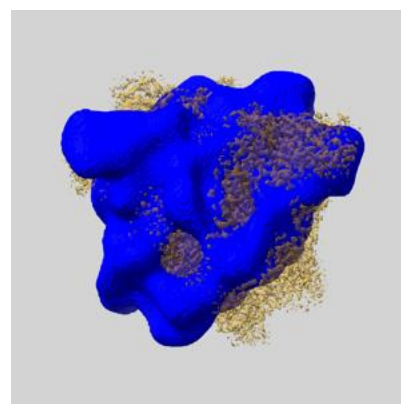
### 6.6.1 emd\_31062\_msk\_1.map [i](#)



X



Y

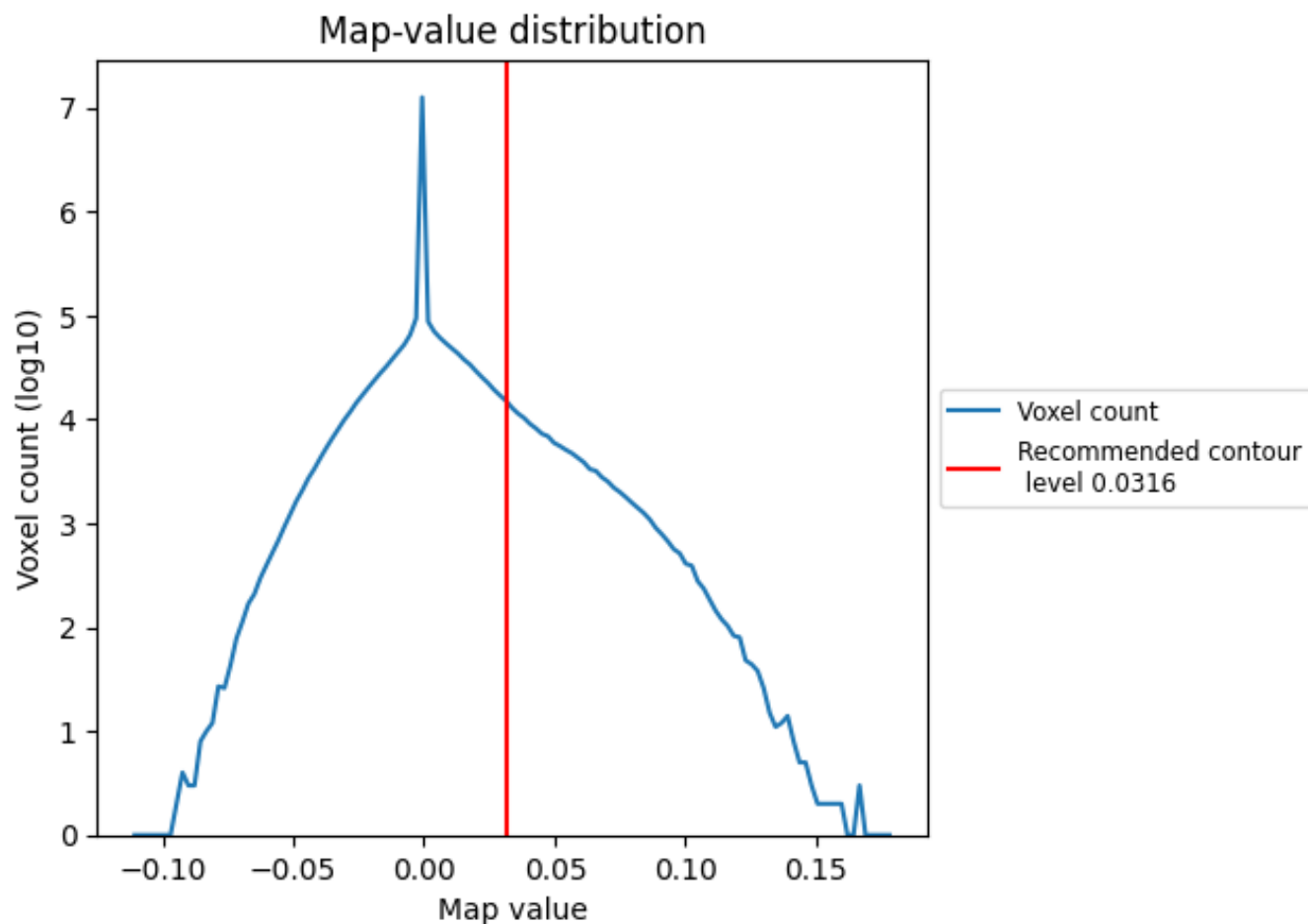


Z

## 7 Map analysis [i](#)

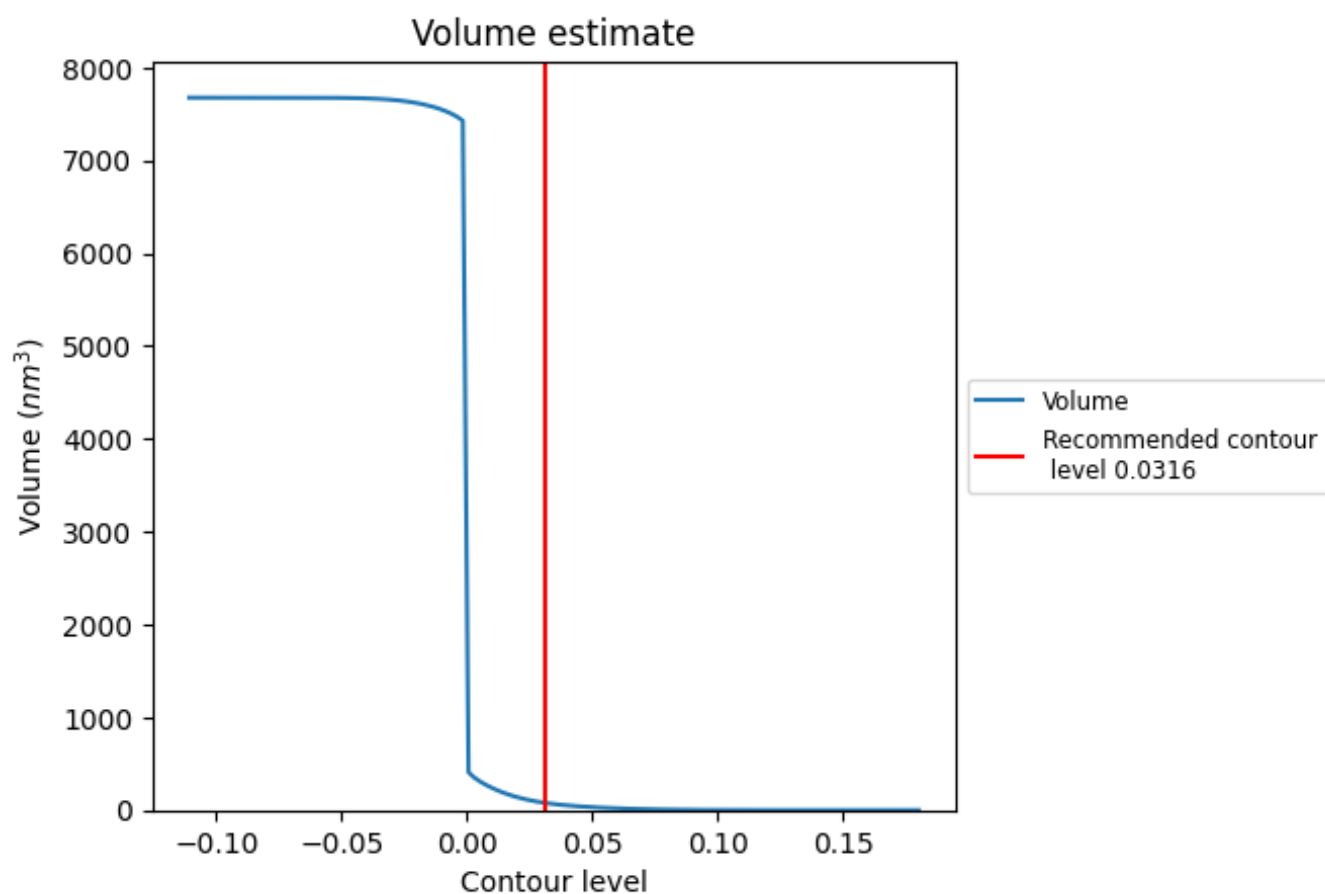
This section contains the results of statistical analysis of the map.

### 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.

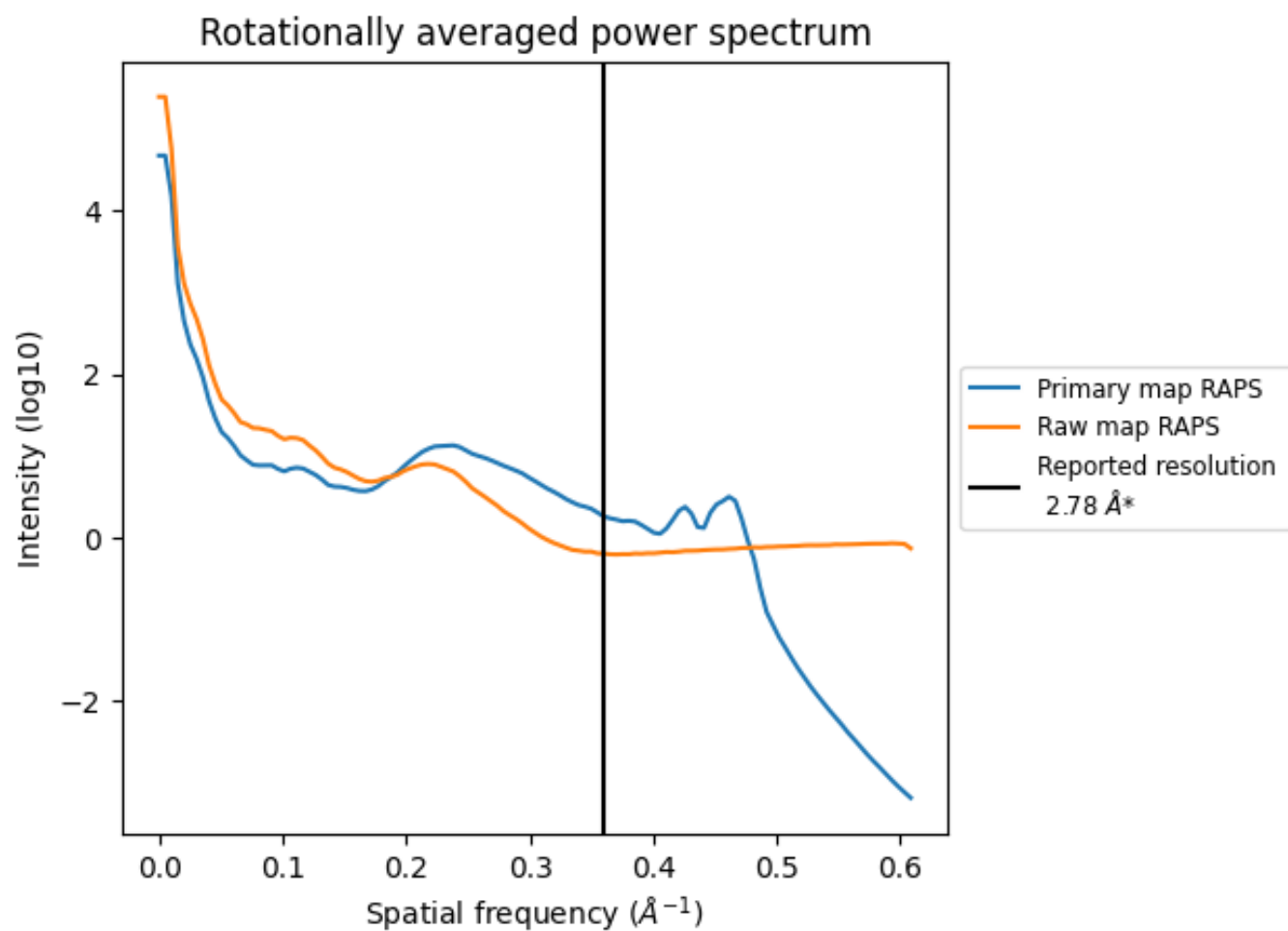
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77  $\text{nm}^3$ ; this corresponds to an approximate mass of 69 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 ⓘ

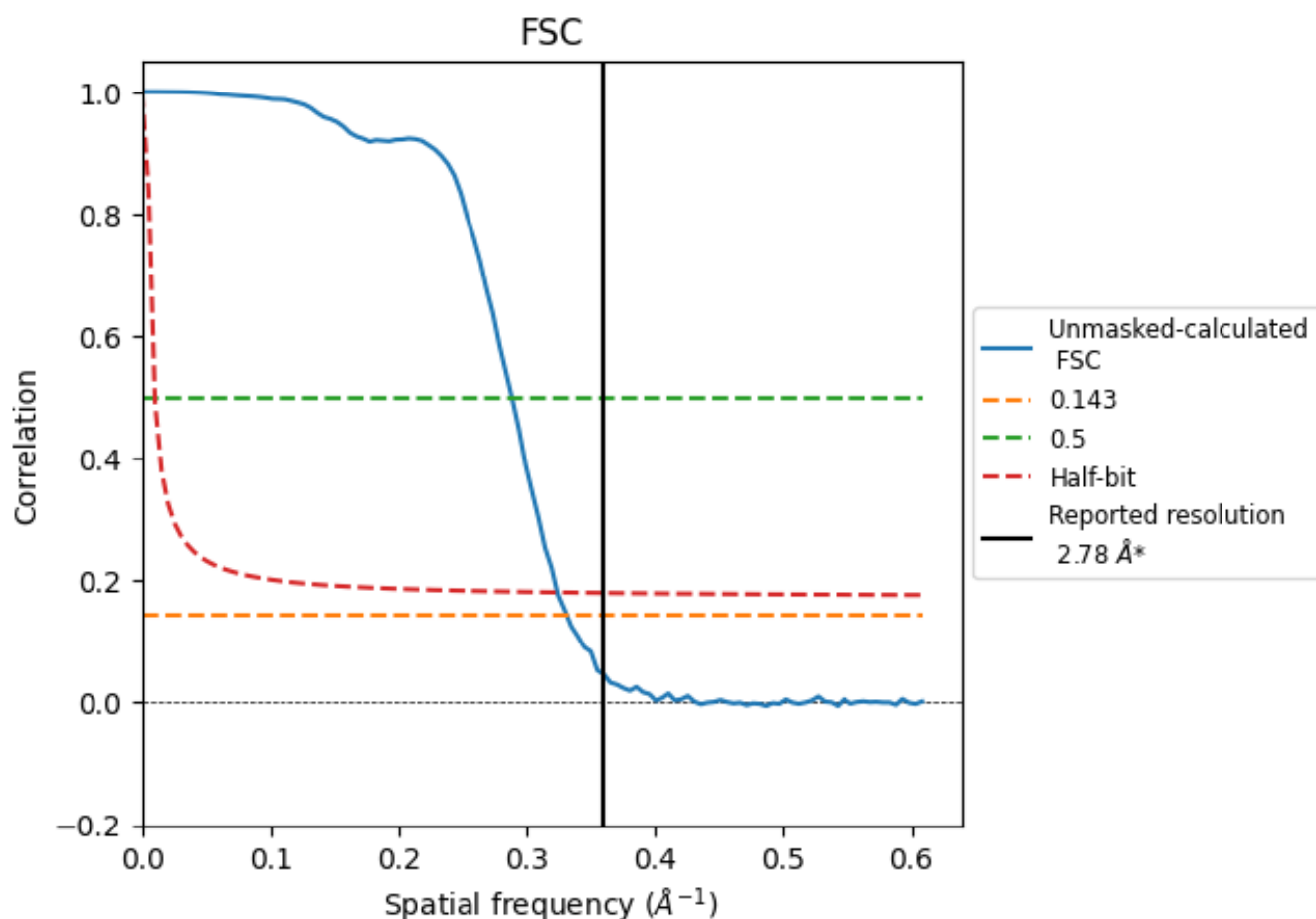


\*Reported resolution corresponds to spatial frequency of 0.360 Å<sup>-1</sup>

## 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 0.360 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.02	3.47	3.09

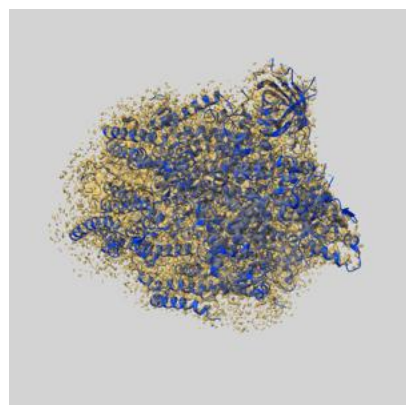
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



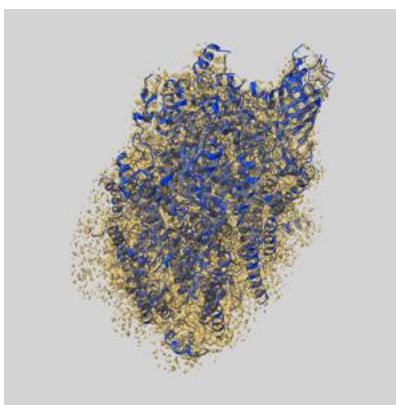
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31062 and PDB model 7EDA. Per-residue inclusion information can be found in section 3 on page 19.

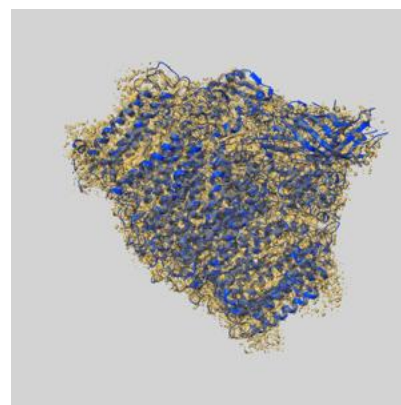
### 9.1 Map-model overlay [i](#)



X



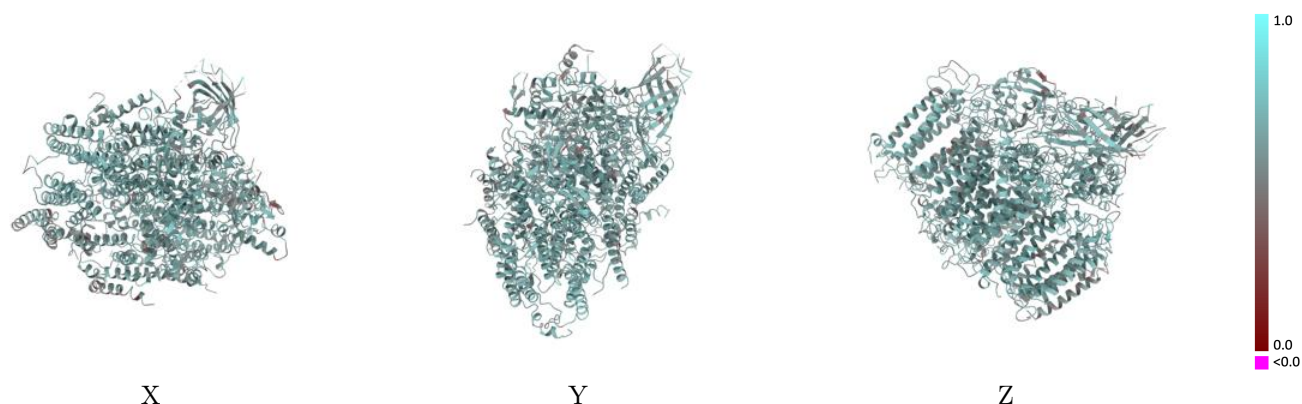
Y



Z

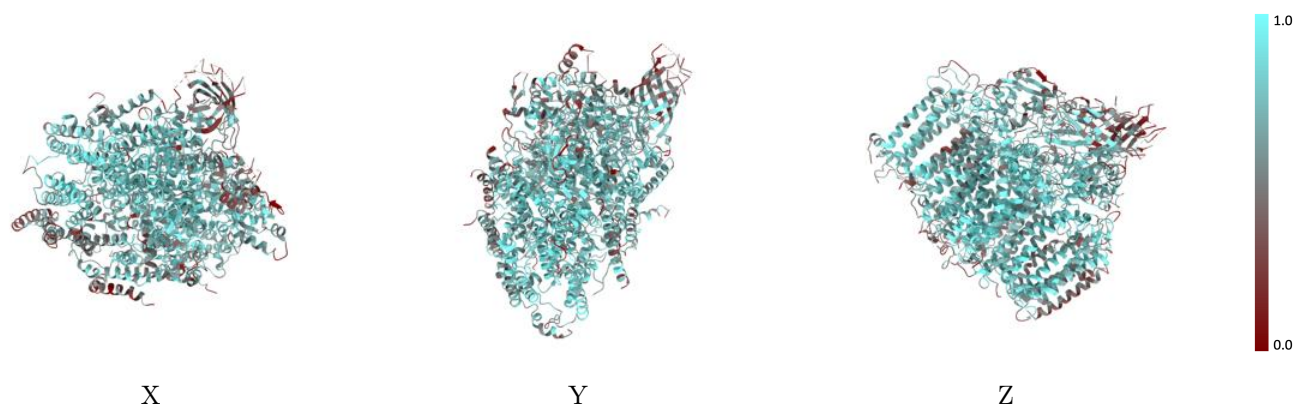
The images above show the 3D surface view of the map at the recommended contour level 0.0316 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



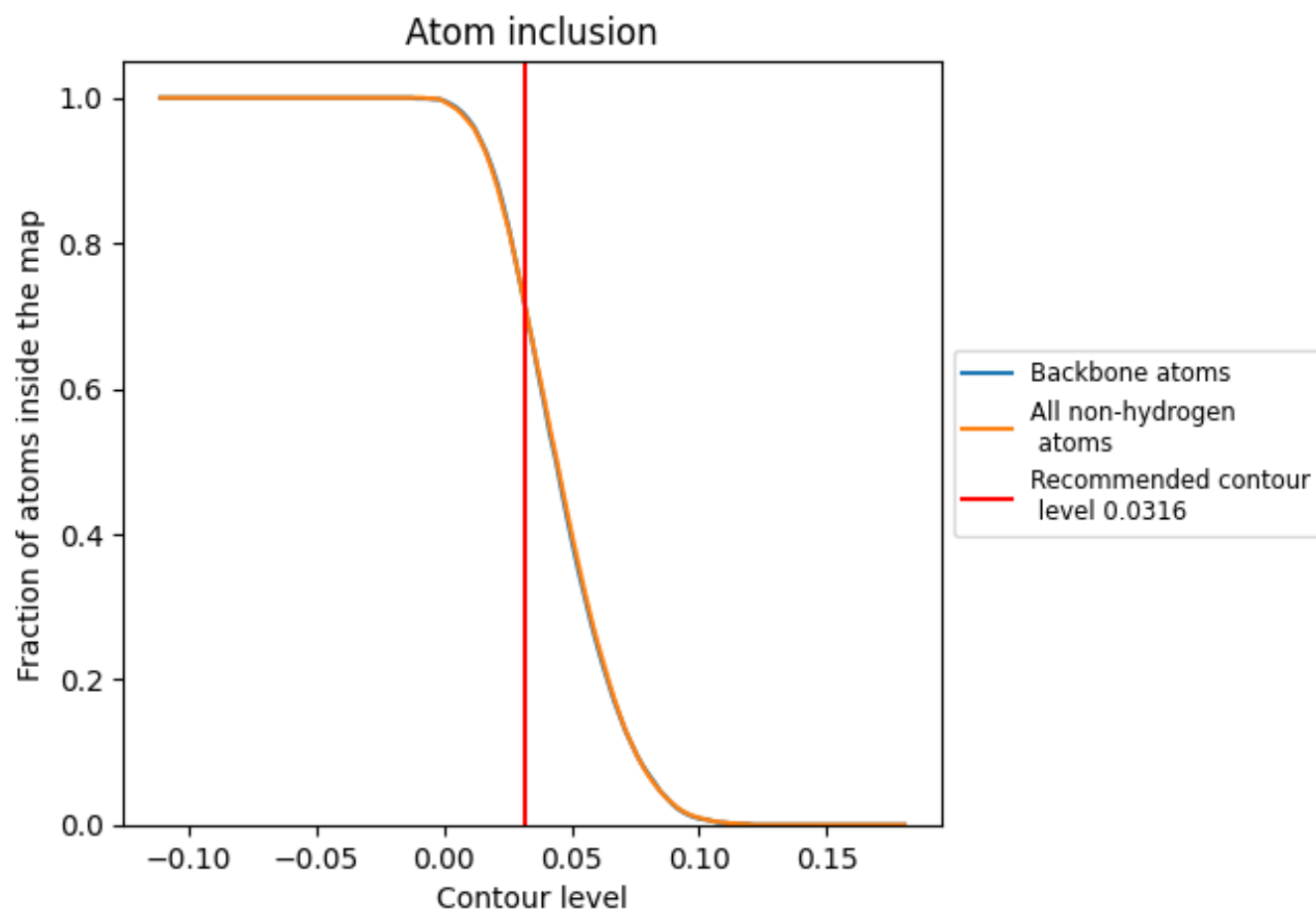
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0316).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.0316) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.6220
A	 0.8250	 0.6470
B	 0.7270	 0.6220
C	 0.7720	 0.6340
D	 0.8270	 0.6560
E	 0.6910	 0.6030
F	 0.7720	 0.6340
H	 0.6740	 0.6090
I	 0.6470	 0.6000
J	 0.6900	 0.6210
K	 0.6120	 0.5860
L	 0.7360	 0.6310
M	 0.5310	 0.5780
O	 0.5450	 0.5780
R	 0.3120	 0.5120
T	 0.5820	 0.5880
U	 0.5130	 0.5800
V	 0.6580	 0.6090
X	 0.5240	 0.5710
Y	 0.5000	 0.5650
Z	 0.4490	 0.5330

