



## Full wwPDB EM Validation Report ⓘ

Jul 24, 2025 – 01:45 pm BST

PDB ID : 9G6F / pdb\_00009g6f  
EMDB ID : EMD-51100  
Title : Inactive PSII dimer from native Peak4 PSII dimers  
Authors : Zhao, Z.; Vercellino, I.; Nixon, P.J.; Sazanov, L.A.  
Deposited on : 2024-07-18  
Resolution : 2.20 Å (reported)  
Based on initial models : 3KZI, 7NHO

This is a Full wwPDB EM Validation 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.dev118  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.44

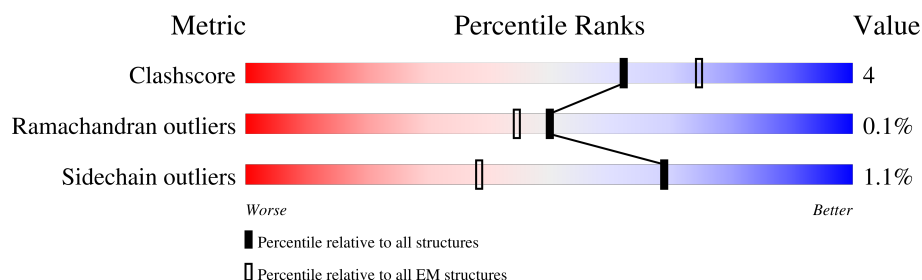
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.20 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	360	
1	a	360	
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	

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Mol	Chain	Length	Quality of chain
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	T	32	
13	t	32	
14	X	41	
14	x	41	
15	Y	46	
15	y	46	
16	Z	62	
16	z	62	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	403	X	-	-	-
19	CLA	A	404	X	-	-	-
19	CLA	A	405	X	-	-	-
19	CLA	A	407	X	-	-	-
19	CLA	B	601	X	-	-	-
19	CLA	B	602	X	-	-	-
19	CLA	B	603	X	-	-	-
19	CLA	B	604	X	-	-	-
19	CLA	B	605	X	-	-	-
19	CLA	B	606	X	-	-	-
19	CLA	B	607	X	-	-	-
19	CLA	B	608	X	-	-	-
19	CLA	B	609	X	-	-	-
19	CLA	B	610	X	-	-	-
19	CLA	B	611	X	-	-	-
19	CLA	B	612	X	-	-	-
19	CLA	B	613	X	-	-	-
19	CLA	B	614	X	-	-	-
19	CLA	B	615	X	-	-	-
19	CLA	B	616	X	-	-	-
19	CLA	C	503	X	-	-	-
19	CLA	C	504	X	-	-	-
19	CLA	C	505	X	-	-	-
19	CLA	C	506	X	-	-	-
19	CLA	C	507	X	-	-	-
19	CLA	C	508	X	-	-	-
19	CLA	C	509	X	-	-	-
19	CLA	C	510	X	-	-	-
19	CLA	C	511	X	-	-	-
19	CLA	C	512	X	-	-	-
19	CLA	C	513	X	-	-	-
19	CLA	C	514	X	-	-	-
19	CLA	C	515	X	-	-	-
19	CLA	D	408	X	-	-	-
19	CLA	D	409	X	-	-	-
19	CLA	a	404	X	-	-	-
19	CLA	a	405	X	-	-	-
19	CLA	a	406	X	-	-	-
19	CLA	a	408	X	-	-	-
19	CLA	b	603	X	-	-	-
19	CLA	b	604	X	-	-	-
19	CLA	b	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	b	606	X	-	-	-
19	CLA	b	607	X	-	-	-
19	CLA	b	608	X	-	-	-
19	CLA	b	609	X	-	-	-
19	CLA	b	610	X	-	-	-
19	CLA	b	611	X	-	-	-
19	CLA	b	612	X	-	-	-
19	CLA	b	613	X	-	-	-
19	CLA	b	614	X	-	-	-
19	CLA	b	615	X	-	-	-
19	CLA	b	616	X	-	-	-
19	CLA	b	617	X	-	-	-
19	CLA	b	618	X	-	-	-
19	CLA	c	502	X	-	-	-
19	CLA	c	503	X	-	-	-
19	CLA	c	504	X	-	-	-
19	CLA	c	505	X	-	-	-
19	CLA	c	506	X	-	-	-
19	CLA	c	507	X	-	-	-
19	CLA	c	508	X	-	-	-
19	CLA	c	509	X	-	-	-
19	CLA	c	510	X	-	-	-
19	CLA	c	511	X	-	-	-
19	CLA	c	512	X	-	-	-
19	CLA	c	513	X	-	-	-
19	CLA	c	514	X	-	-	-
19	CLA	d	404	X	-	-	-
19	CLA	d	405	X	-	-	-

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 42670 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	324	Total	C	N	O	S	0	0
			2544	1667	417	445	15		
1	a	324	Total	C	N	O	S	0	0
			2544	1667	417	445	15		

- 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
			3961	2601	661	686	13		
2	b	505	Total	C	N	O	S	0	0
			3968	2605	664	686	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	436	Total	C	N	O	S	0	0
			3377	2214	565	585	13		
3	c	436	Total	C	N	O	S	0	0
			3377	2214	565	585	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	0	0
			2712	1798	444	458	12		
4	d	341	Total	C	N	O	S	0	0
			2712	1798	444	458	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	81	Total	C	N	O	0	0
			657	430	107	120		
5	e	81	Total	C	N	O	0	0
			650	427	106	117		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	33	Total	C	N	O	S	0	0
			265	182	43	39	1		
6	f	33	Total	C	N	O	S	0	0
			269	184	44	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	64	Total	C	N	O	S	0	0
			506	339	81	84	2		
7	h	64	Total	C	N	O	S	0	0
			506	339	81	84	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			288	196	45	46	1		
8	i	35	Total	C	N	O	S	0	0
			288	196	45	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	28	Total	C	N	O	S	0	0
			206	145	29	31	1		
9	j	28	Total	C	N	O	S	0	0
			206	145	29	31	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
			285	199	42	44		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total	C	N	O	0	0
			285	199	42	44		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	35	Total	C	N	O	0	0
			287	192	46	49		
11	l	35	Total	C	N	O	0	0
			287	192	46	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	33	Total	C	N	O	S	0	0
			258	172	38	47	1		
12	m	33	Total	C	N	O	S	0	0
			258	172	38	47	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	30	Total	C	N	O	S	0	0
			258	181	36	39	2		
13	t	30	Total	C	N	O	S	0	0
			258	181	36	39	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	X	35	Total	C	N	O	0	0
			254	172	38	44		
14	x	35	Total	C	N	O	0	0
			254	172	38	44		

- Molecule 15 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Y	28	Total	C	N	O	S	0	0
			205	134	36	32	3		
15	y	28	Total	C	N	O	S	0	0
			196	131	30	32	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	61	Total	C	N	O	S	0	0
			467	321	70	74	2		
16	z	61	Total	C	N	O	S	0	0
			458	317	67	72	2		

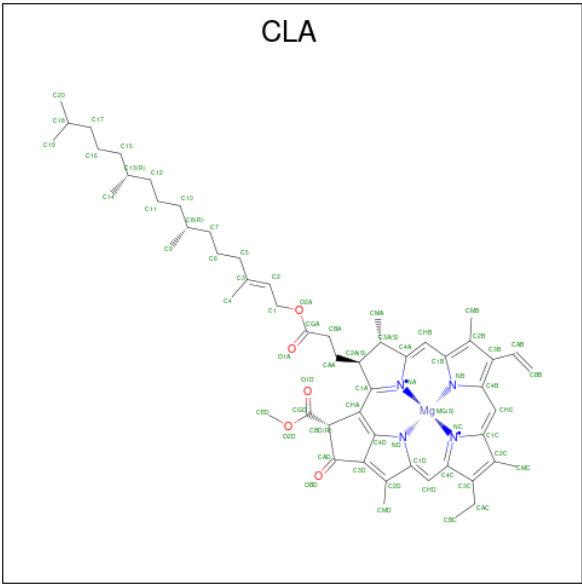
- Molecule 17 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Fe	0
			1	1	
17	a	1	Total	Fe	0
			1	1	

- Molecule 18 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Cl	0
			1	1	
18	a	1	Total	Cl	0
			1	1	

- Molecule 19 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
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

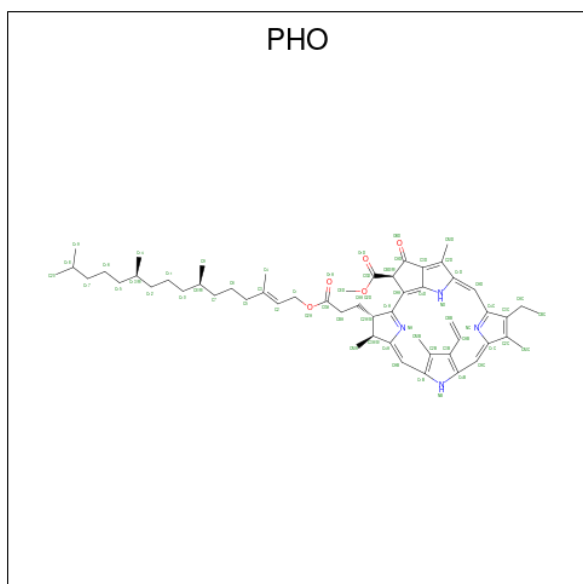
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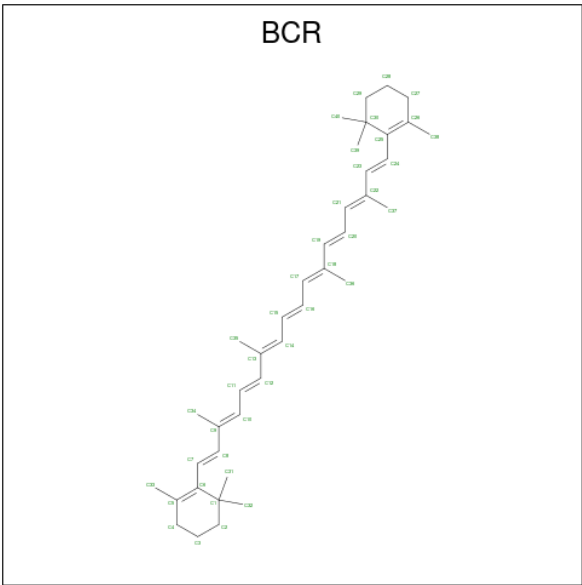
Mol	Chain	Residues	Atoms					AltConf
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 20 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



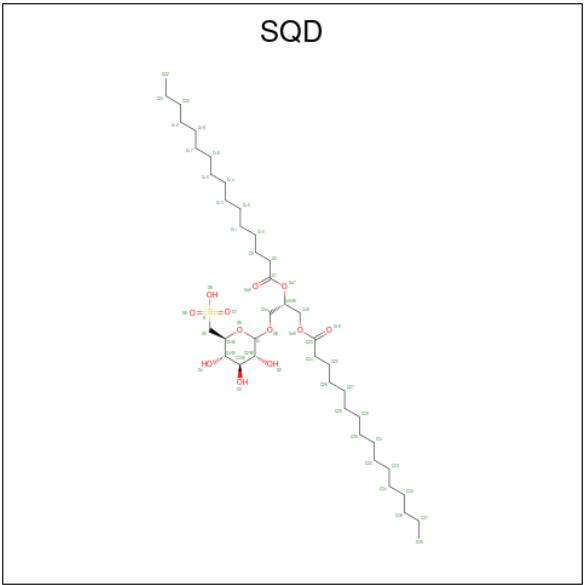
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	D	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	Y	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
21	b	1	Total C 40 40	0
21	c	1	Total C 40 40	0
21	c	1	Total C 40 40	0
21	d	1	Total C 40 40	0
21	k	1	Total C 40 40	0
21	y	1	Total C 40 40	0

- Molecule 22 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).



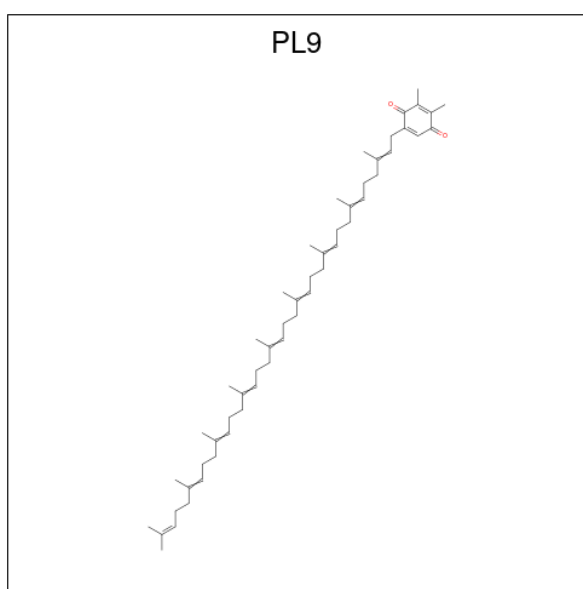
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C O S 50 37 12 1	0
22	A	1	Total C O S 54 41 12 1	0
22	F	1	Total C O S 33 23 9 1	0
22	L	1	Total C O S 54 41 12 1	0
22	a	1	Total C O S 54 41 12 1	0

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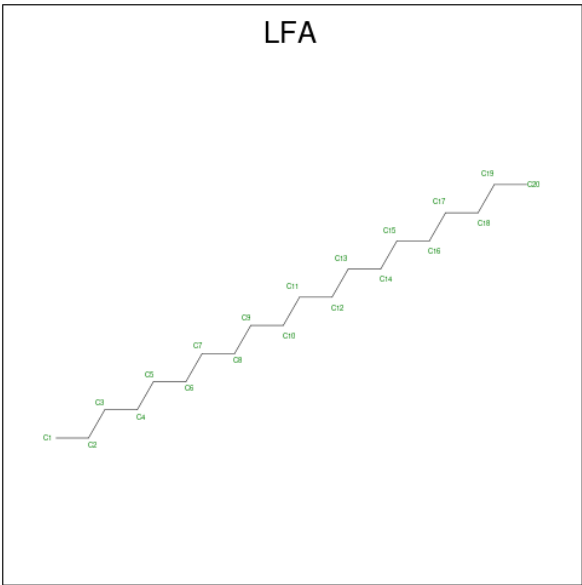
Mol	Chain	Residues	Atoms				AltConf
22	a	1	Total	C	O	S	0
			43	30	12	1	
22	f	1	Total	C	O	S	0
			45	32	12	1	
22	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 23 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<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O		0
			55	53	2		
23	D	1	Total	C	O		0
			55	53	2		
23	a	1	Total	C	O		0
			55	53	2		
23	d	1	Total	C	O		0
			55	53	2		

- Molecule 24 is EICOSANE (CCD ID: LFA) (formula: C<sub>20</sub>H<sub>42</sub>).



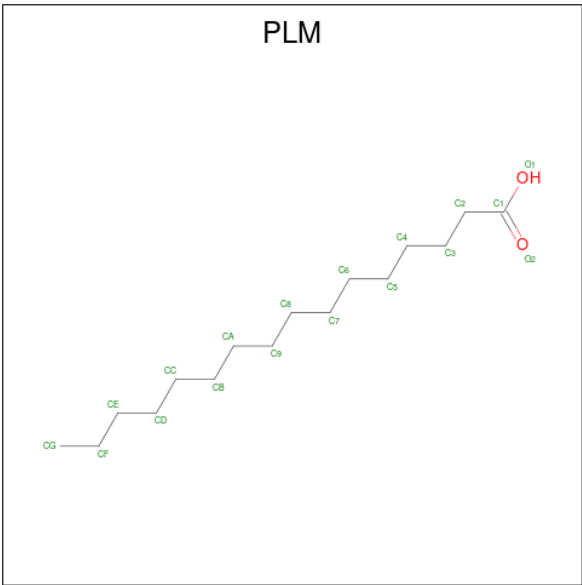
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	C	0
			15	15	
24	A	1	Total	C	0
			13	13	
24	B	1	Total	C	0
			13	13	
24	B	1	Total	C	0
			7	7	
24	B	1	Total	C	0
			11	11	
24	B	1	Total	C	0
			7	7	
24	C	1	Total	C	0
			7	7	
24	D	1	Total	C	0
			16	16	
24	D	1	Total	C	0
			13	13	
24	D	1	Total	C	0
			9	9	
24	H	1	Total	C	0
			14	14	
24	H	1	Total	C	0
			6	6	
24	I	1	Total	C	0
			7	7	
24	J	1	Total	C	0
			17	17	

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Mol	Chain	Residues	Atoms	AltConf
24	K	1	Total C 7 7	0
24	M	1	Total C 10 10	0
24	X	1	Total C 13 13	0
24	Z	1	Total C 8 8	0
24	a	1	Total C 11 11	0
24	b	1	Total C 12 12	0
24	b	1	Total C 11 11	0
24	b	1	Total C 9 9	0
24	b	1	Total C 9 9	0
24	b	1	Total C 7 7	0
24	d	1	Total C 15 15	0
24	d	1	Total C 8 8	0
24	h	1	Total C 8 8	0
24	h	1	Total C 6 6	0
24	h	1	Total C 7 7	0
24	i	1	Total C 11 11	0
24	k	1	Total C 7 7	0
24	m	1	Total C 9 9	0
24	x	1	Total C 13 13	0

- Molecule 25 is PALMITIC ACID (CCD ID: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



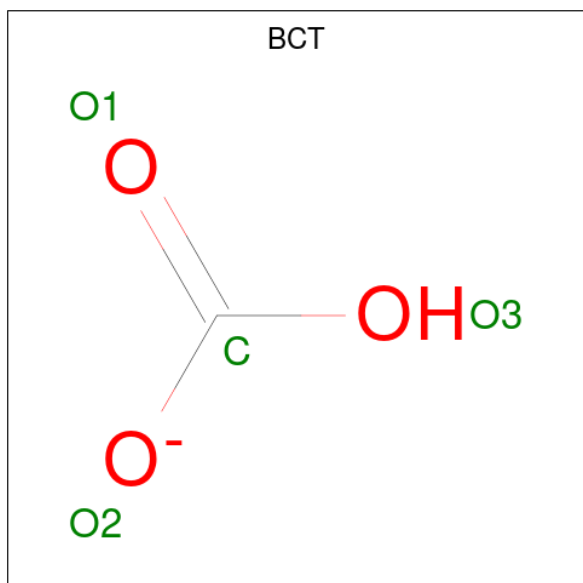
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			18	16	2	
25	A	1	Total	C	O	0
			11	9	2	
25	B	1	Total	C	O	0
			8	6	2	
25	B	1	Total	C	O	0
			12	10	2	
25	B	1	Total	C	O	0
			13	11	2	
25	B	1	Total	C	O	0
			16	14	2	
25	C	1	Total	C	O	0
			9	7	2	
25	D	1	Total	C	O	0
			18	16	2	
25	E	1	Total	C	O	0
			18	16	2	
25	H	1	Total	C	O	0
			10	8	2	
25	I	1	Total	C	O	0
			16	14	2	
25	I	1	Total	C	O	0
			18	16	2	
25	I	1	Total	C	O	0
			11	9	2	
25	a	1	Total	C	O	0
			17	15	2	

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Mol	Chain	Residues	Atoms			AltConf
25	a	1	Total	C	O	0
			12	10	2	
25	b	1	Total	C	O	0
			18	16	2	
25	b	1	Total	C	O	0
			9	7	2	
25	b	1	Total	C	O	0
			14	12	2	
25	b	1	Total	C	O	0
			13	11	2	
25	b	1	Total	C	O	0
			16	14	2	
25	e	1	Total	C	O	0
			18	16	2	
25	i	1	Total	C	O	0
			16	14	2	
25	i	1	Total	C	O	0
			13	11	2	
25	i	1	Total	C	O	0
			13	11	2	

- Molecule 26 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).



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

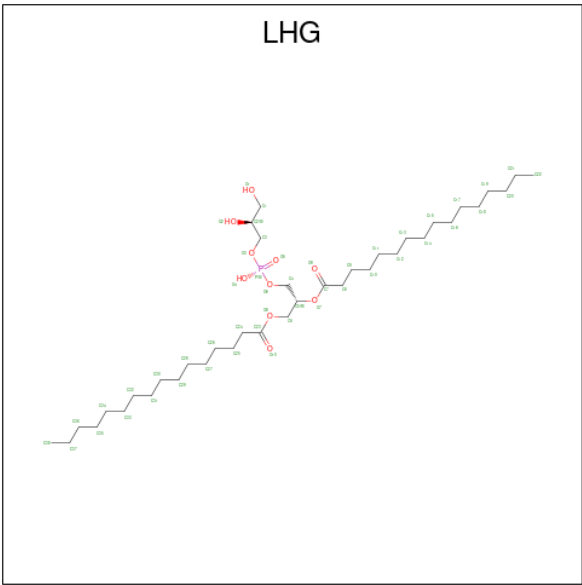
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Mol	Chain	Residues	Atoms			AltConf
26	d	1	Total	C	O	0
			4	1	3	

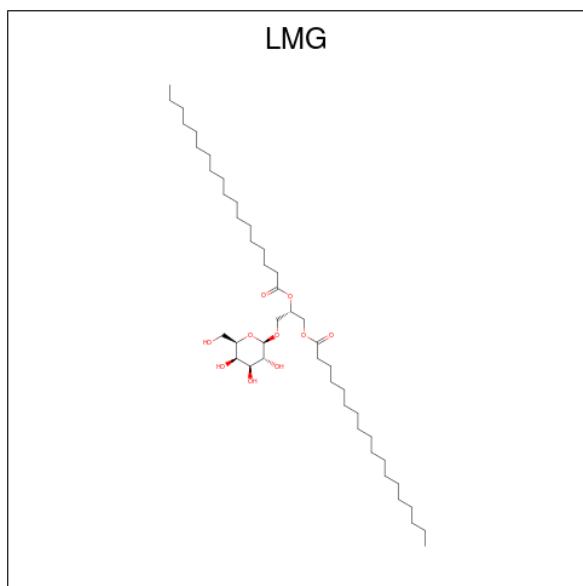
- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	P	0
			46	35	10	1	
27	D	1	Total	C	O	P	0
			49	38	10	1	
27	D	1	Total	C	O	P	0
			49	38	10	1	
27	L	1	Total	C	O	P	0
			49	38	10	1	
27	a	1	Total	C	O	P	0
			46	35	10	1	
27	a	1	Total	C	O	P	0
			49	38	10	1	
27	d	1	Total	C	O	P	0
			49	38	10	1	
27	d	1	Total	C	O	P	0
			49	38	10	1	
27	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID:

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



Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			51	41	10	
28	C	1	Total	C	O	0
			51	41	10	
28	C	1	Total	C	O	0
			42	32	10	
28	D	1	Total	C	O	0
			48	38	10	
28	b	1	Total	C	O	0
			51	41	10	
28	c	1	Total	C	O	0
			51	41	10	
28	c	1	Total	C	O	0
			51	41	10	
28	d	1	Total	C	O	0
			51	41	10	

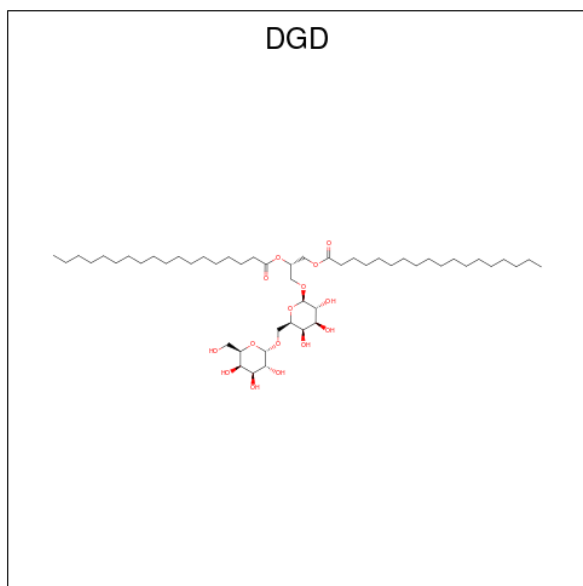
- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			AltCon
29	C	1	Total 30	C 19	O 11	0
29	D	1	Total 35	C 24	O 11	0
29	D	1	Total 24	C 18	O 6	0
29	M	1	Total 35	C 24	O 11	0
29	M	1	Total 35	C 24	O 11	0
29	b	1	Total 20	C 14	O 6	0
29	d	1	Total 34	C 23	O 11	0
29	d	1	Total 24	C 18	O 6	0
29	i	1	Total 35	C 24	O 11	0
29	m	1	Total 35	C 24	O 11	0
29	m	1	Total 35	C 24	O 11	0
29	t	1	Total 24	C 18	O 6	0
29	z	1	Total 35	C 24	O 11	0

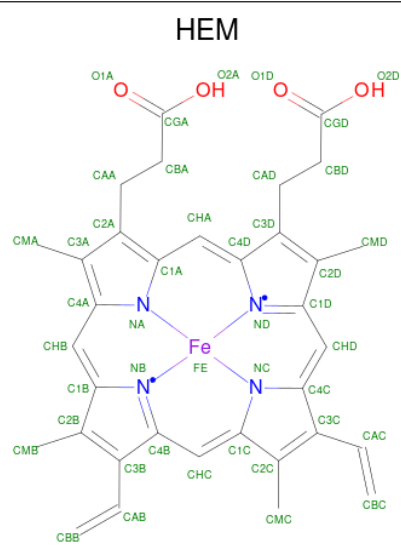
- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:

C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



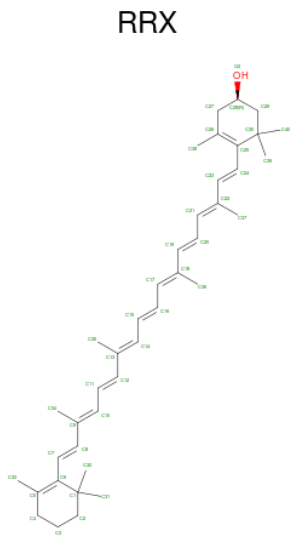
Mol	Chain	Residues	Atoms			AltConf
30	C	1	Total	C	O	0
			62	47	15	
30	D	1	Total	C	O	0
			44	35	9	
30	H	1	Total	C	O	0
			62	47	15	
30	J	1	Total	C	O	0
			54	39	15	
30	c	1	Total	C	O	0
			62	47	15	
30	c	1	Total	C	O	0
			62	47	15	
30	c	1	Total	C	O	0
			62	47	15	
30	d	1	Total	C	O	0
			47	36	11	
30	h	1	Total	C	O	0
			62	47	15	

- Molecule 31 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>).



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

- Molecule 32 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula:  $C_{40}H_{56}O$ ).



Mol	Chain	Residues	Atoms			AltConf
32	H	1	Total 41	C 40	O 1	0
32	x	1	Total 41	C 40	O 1	0

- Molecule 33 is water.

Mol	Chain	Residues	Atoms	AltConf
33	A	72	Total O 72 72	1
33	B	137	Total O 137 137	1
33	C	59	Total O 59 59	0
33	D	87	Total O 87 87	0
33	E	8	Total O 8 8	0
33	H	22	Total O 22 22	0
33	K	2	Total O 2 2	0
33	L	5	Total O 5 5	0
33	M	2	Total O 2 2	0
33	T	4	Total O 4 4	0
33	X	3	Total O 3 3	0
33	a	70	Total O 70 70	1
33	b	146	Total O 146 146	1
33	c	61	Total O 61 61	0
33	d	86	Total O 86 86	0
33	e	7	Total O 7 7	0
33	f	1	Total O 1 1	0
33	h	19	Total O 19 19	0
33	k	1	Total O 1 1	0
33	l	7	Total O 7 7	0
33	m	2	Total O 2 2	0

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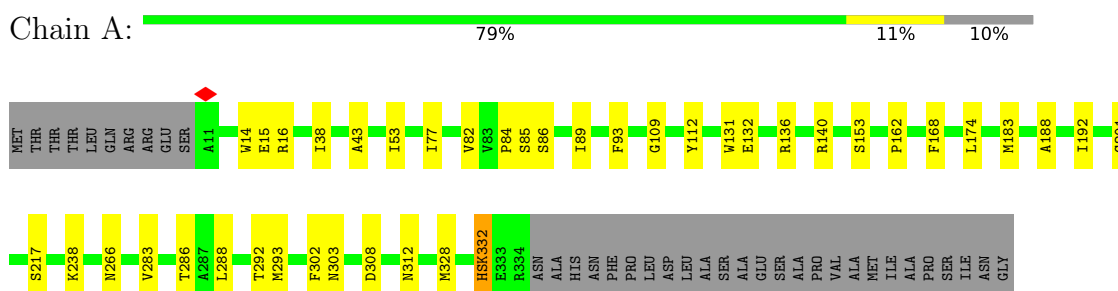
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Mol	Chain	Residues	Atoms		AltConf
33	t	3	Total	O	0
			3	3	
33	x	5	Total	O	0
			5	5	

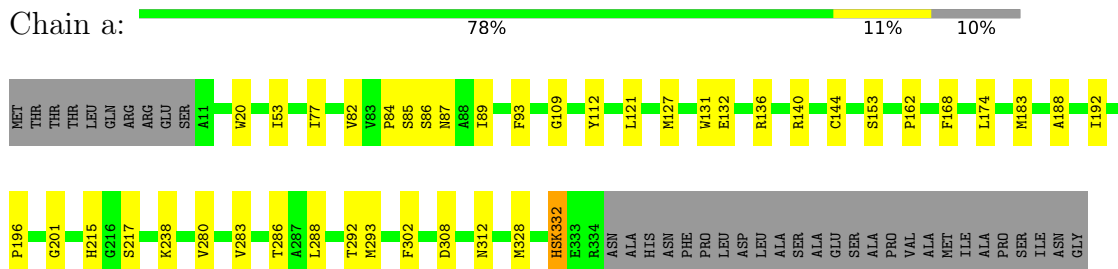
### 3 Residue-property plots

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.

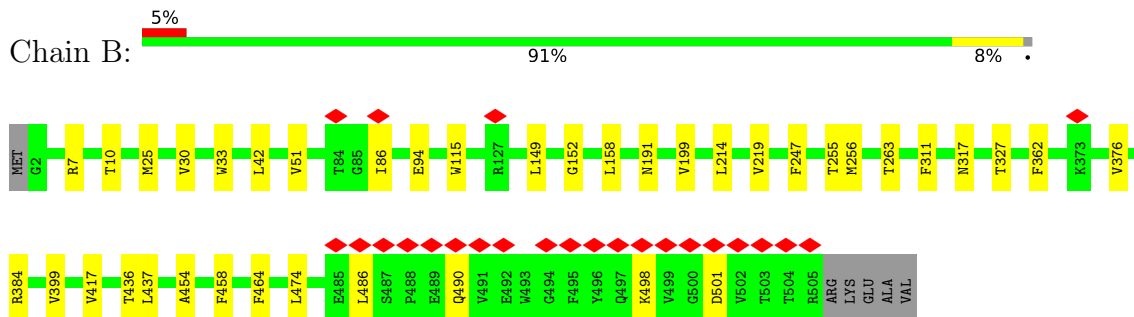
- Molecule 1: Photosystem II protein D1 1



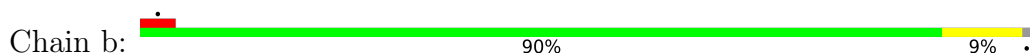
- Molecule 1: Photosystem II protein D1 1



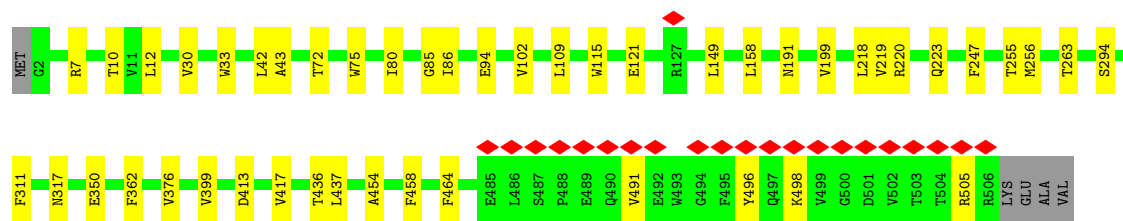
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein

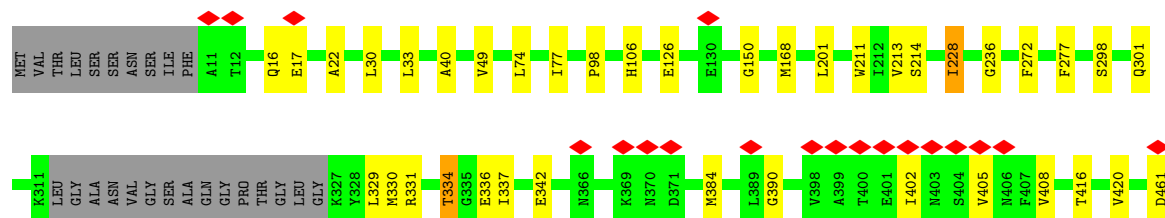






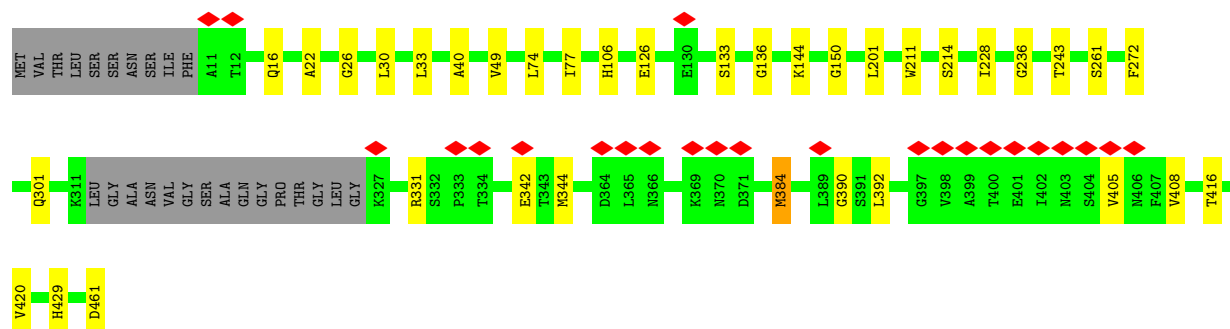
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 86% 8% 5%



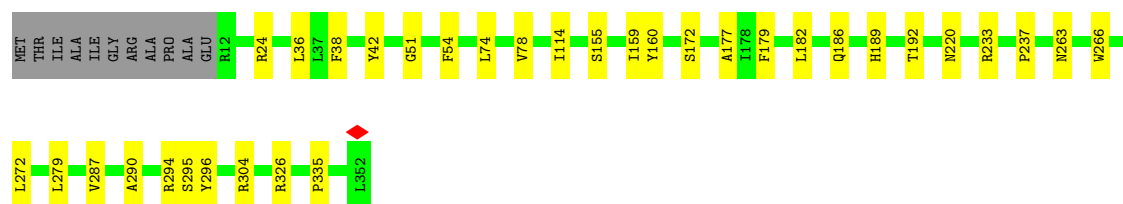
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 87% 8% 5%



• Molecule 4: Photosystem II D2 protein

Chain D: 87% 10%



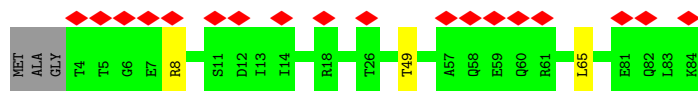
• Molecule 4: Photosystem II D2 protein

Chain d: 88% 9%

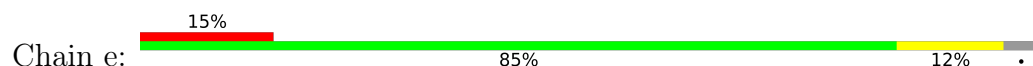




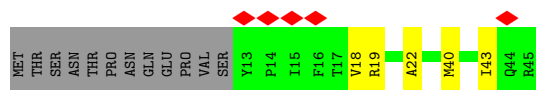
- Molecule 5: Cytochrome b559 subunit alpha



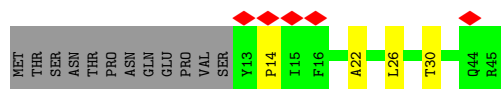
- Molecule 5: Cytochrome b559 subunit alpha



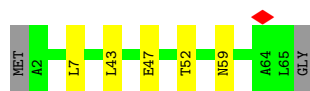
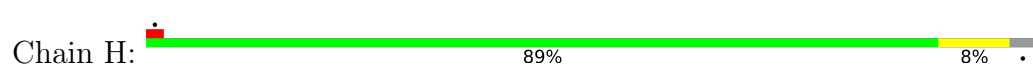
- Molecule 6: Cytochrome b559 subunit beta



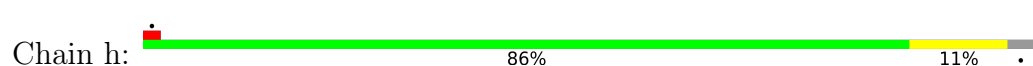
- Molecule 6: Cytochrome b559 subunit beta



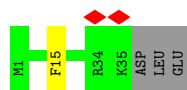
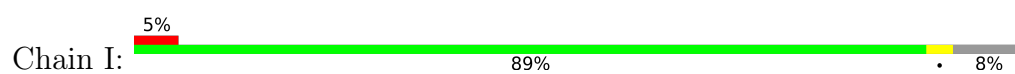
- Molecule 7: Photosystem II reaction center protein H



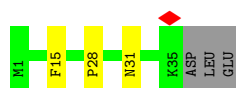
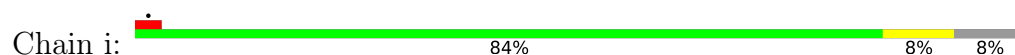
- Molecule 7: Photosystem II reaction center protein H



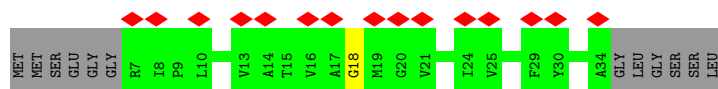
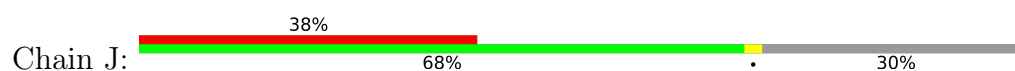
- Molecule 8: Photosystem II reaction center protein I



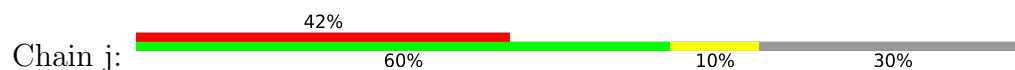
- Molecule 8: Photosystem II reaction center protein I



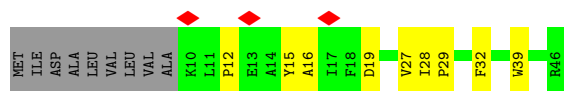
- Molecule 9: Photosystem II reaction center protein J



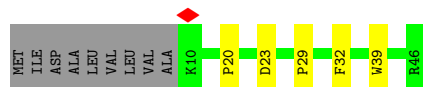
- Molecule 9: Photosystem II reaction center protein J



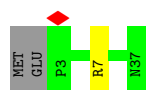
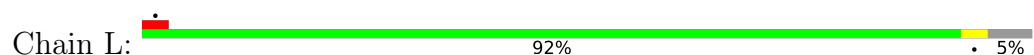
- Molecule 10: Photosystem II reaction center protein K




- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L

Chain l:  89% 5% 5%




- Molecule 12: Photosystem II reaction center protein M

Chain M:  75% 17% 8%




- Molecule 12: Photosystem II reaction center protein M

Chain m:  81% 11% 8%




- Molecule 13: Photosystem II reaction center protein T

Chain T:  75% 19% 6%




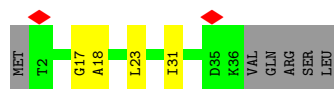
- Molecule 13: Photosystem II reaction center protein T

Chain t:  78% 16% 6%



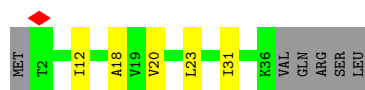
- Molecule 14: Photosystem II reaction center X protein

Chain X:  5% 76% 10% 15%

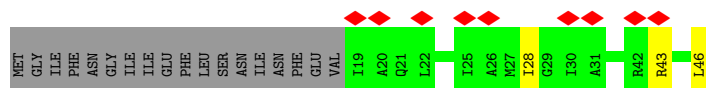


- Molecule 14: Photosystem II reaction center X protein

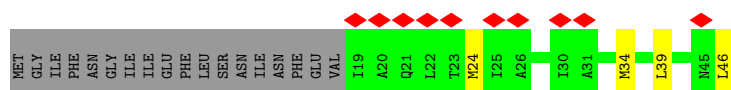
Chain x:  73% 12% 15%



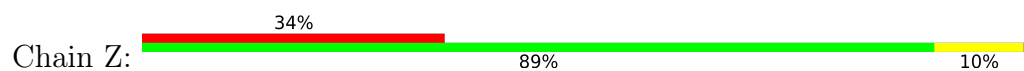
- Molecule 15: Photosystem II reaction center protein Ycf12



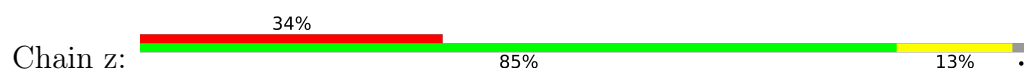
- Molecule 15: Photosystem II reaction center protein Ycf12



- Molecule 16: Photosystem II reaction center protein Z



- Molecule 16: Photosystem II reaction center protein Z



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	417537	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.387	Depositor
Minimum map value	-0.150	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.037	Depositor
Map size (Å)	137.5, 208.5, 104.5	wwPDB
Map dimensions	209, 417, 275	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.22	0/2613	0.45	0/3562
1	a	0.22	0/2613	0.44	0/3562
2	B	0.21	0/4101	0.42	0/5590
2	b	0.20	0/4108	0.43	2/5599 (0.0%)
3	C	0.21	0/3487	0.42	0/4750
3	c	0.20	0/3487	0.40	0/4750
4	D	0.22	0/2807	0.42	0/3827
4	d	0.23	0/2807	0.42	0/3827
5	E	0.21	0/676	0.46	0/923
5	e	0.19	0/669	0.43	0/914
6	F	0.27	0/274	0.58	0/374
6	f	0.26	0/278	0.57	0/379
7	H	0.21	0/519	0.46	0/708
7	h	0.21	0/519	0.47	0/708
8	I	0.21	0/285	0.50	0/385
8	i	0.20	0/285	0.47	0/385
9	J	0.18	0/212	0.36	0/291
9	j	0.18	0/212	0.38	0/291
10	K	0.30	0/295	0.72	2/407 (0.5%)
10	k	0.28	0/295	0.51	0/407
11	L	0.15	0/294	0.32	0/399
11	l	0.15	0/294	0.31	0/399
12	M	0.34	0/261	0.59	0/356
12	m	0.34	0/261	0.61	0/356
13	T	0.21	0/257	0.40	0/349
13	t	0.20	0/257	0.38	0/349
14	X	0.19	0/257	0.38	0/348
14	x	0.18	0/257	0.37	0/348
15	Y	0.19	0/206	0.50	0/275
15	y	0.23	0/197	0.58	0/265
16	Z	0.19	0/478	0.41	0/654

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	z	0.19	0/469	0.34	0/643
All	All	0.21	0/34030	0.44	4/46380 (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	1
1	a	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	27	VAL	CA-C-N	7.20	124.77	120.24
10	K	27	VAL	C-N-CA	7.20	124.77	120.24
2	b	85	GLY	CA-C-N	5.41	131.72	121.97
2	b	85	GLY	C-N-CA	5.41	131.72	121.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	HSK	Mainchain
1	a	332	HSK	Mainchain

## 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	2544	0	2447	33	0
1	a	2544	0	2447	32	0
2	B	3961	0	3820	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	3968	0	3827	34	0
3	C	3377	0	3286	26	0
3	c	3377	0	3286	24	0
4	D	2712	0	2617	27	0
4	d	2712	0	2617	23	0
5	E	657	0	644	3	0
5	e	650	0	636	6	0
6	F	265	0	271	5	0
6	f	269	0	277	4	0
7	H	506	0	529	4	0
7	h	506	0	529	6	0
8	I	288	0	307	1	0
8	i	288	0	307	2	0
9	J	206	0	213	1	0
9	j	206	0	213	2	0
10	K	285	0	290	5	0
10	k	285	0	290	3	0
11	L	287	0	299	2	0
11	l	287	0	299	2	0
12	M	258	0	276	5	0
12	m	258	0	276	2	0
13	T	258	0	261	4	0
13	t	258	0	261	4	0
14	X	254	0	282	2	0
14	x	254	0	282	2	0
15	Y	205	0	228	3	0
15	y	196	0	215	3	0
16	Z	467	0	501	2	0
16	z	458	0	488	5	0
17	A	1	0	0	0	0
17	a	1	0	0	0	0
18	A	1	0	0	0	0
18	a	1	0	0	0	0
19	A	260	0	288	6	0
19	B	1040	0	1152	21	0
19	C	845	0	936	17	0
19	D	130	0	144	5	0
19	a	260	0	288	6	0
19	b	1040	0	1152	25	0
19	c	845	0	936	17	0
19	d	130	0	144	5	0
20	A	64	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	D	64	0	74	3	0
20	a	64	0	74	0	0
20	d	64	0	74	2	0
21	A	40	0	56	1	0
21	B	160	0	224	5	0
21	C	80	0	112	2	0
21	D	40	0	56	0	0
21	K	40	0	56	2	0
21	Y	40	0	56	2	0
21	a	40	0	56	2	0
21	b	160	0	224	8	0
21	c	80	0	112	1	0
21	d	40	0	56	0	0
21	k	40	0	56	0	0
21	y	40	0	56	1	0
22	A	104	0	145	3	0
22	F	33	0	39	3	0
22	L	54	0	78	2	0
22	a	97	0	128	2	0
22	f	45	0	57	2	0
22	l	54	0	78	1	0
23	A	55	0	80	3	0
23	D	55	0	80	0	0
23	a	55	0	80	5	0
23	d	55	0	80	1	0
24	A	28	0	51	0	0
24	B	38	0	63	2	0
24	C	7	0	10	0	0
24	D	38	0	70	3	0
24	H	20	0	32	0	0
24	I	7	0	10	0	0
24	J	17	0	33	0	0
24	K	7	0	10	0	0
24	M	10	0	16	0	0
24	X	13	0	22	1	0
24	Z	8	0	12	0	0
24	a	11	0	18	0	0
24	b	48	0	76	1	0
24	d	23	0	41	1	0
24	h	21	0	30	0	0
24	i	11	0	18	0	0
24	k	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	m	9	0	14	0	0
24	x	13	0	25	0	0
25	A	29	0	45	1	0
25	B	49	0	66	0	0
25	C	9	0	10	1	0
25	D	18	0	31	2	0
25	E	18	0	31	0	0
25	H	10	0	12	0	0
25	I	45	0	69	0	0
25	a	29	0	42	2	0
25	b	70	0	103	1	0
25	e	18	0	31	0	0
25	i	42	0	60	0	0
26	A	4	0	0	0	0
26	d	4	0	0	0	0
27	A	46	0	65	1	0
27	D	98	0	148	1	0
27	L	49	0	74	2	0
27	a	95	0	139	4	0
27	d	98	0	148	0	0
27	l	49	0	74	1	0
28	B	51	0	72	2	0
28	C	93	0	126	3	0
28	D	48	0	66	1	0
28	b	51	0	72	4	0
28	c	102	0	144	1	0
28	d	51	0	72	3	0
29	C	30	0	33	2	0
29	D	59	0	81	3	0
29	M	70	0	92	1	0
29	b	20	0	24	1	0
29	d	58	0	76	1	0
29	i	35	0	46	0	0
29	m	70	0	92	1	0
29	t	24	0	35	1	0
29	z	35	0	46	3	0
30	C	62	0	82	1	0
30	D	44	0	57	1	0
30	H	62	0	82	0	0
30	J	54	0	66	4	0
30	c	186	0	246	4	0
30	d	47	0	59	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	h	62	0	82	2	0
31	F	43	0	30	1	0
31	f	43	0	30	0	0
32	H	41	0	56	0	0
32	x	41	0	56	0	0
33	A	72	0	0	0	0
33	B	137	0	0	0	0
33	C	59	0	0	0	0
33	D	87	0	0	1	0
33	E	8	0	0	0	0
33	H	22	0	0	0	0
33	K	2	0	0	0	0
33	L	5	0	0	1	0
33	M	2	0	0	0	0
33	T	4	0	0	0	0
33	X	3	0	0	0	0
33	a	70	0	0	0	0
33	b	146	0	0	0	0
33	c	61	0	0	0	0
33	d	86	0	0	0	0
33	e	7	0	0	0	0
33	f	1	0	0	0	0
33	h	19	0	0	0	0
33	k	1	0	0	0	0
33	l	7	0	0	1	0
33	m	2	0	0	0	0
33	t	3	0	0	0	0
33	x	5	0	0	0	0
All	All	42670	0	43454	350	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 4.

All (350) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:30:LEU:HD21	19:c:512:CLA:H2A	1.74	0.68
3:C:30:LEU:HD21	19:C:513:CLA:H2A	1.75	0.68
23:A:410:PL9:H33	4:D:42:TYR:HB2	1.76	0.68
27:a:416:LHG:HC32	5:e:9:PRO:HA	1.77	0.66
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:16:GLN:OE1	4:d:233:ARG:NH1	2.31	0.63
4:d:192:THR:HG23	19:d:404:CLA:HBC2	1.80	0.62
3:C:16:GLN:OE1	4:D:233:ARG:NH1	2.31	0.61
21:b:619:BCR:H332	28:b:622:LMG:H111	1.83	0.61
4:D:192:THR:HG23	19:D:408:CLA:HBC2	1.82	0.60
19:B:615:CLA:H71	19:B:616:CLA:H18	1.83	0.60
19:b:617:CLA:H71	19:b:618:CLA:H18	1.84	0.59
4:d:186:GLN:HB2	19:d:404:CLA:HBC1	1.83	0.59
20:d:402:PHO:HBA2	19:d:404:CLA:H142	1.85	0.59
4:D:186:GLN:HB2	19:D:408:CLA:HBC1	1.85	0.58
2:b:12:LEU:HB2	19:b:614:CLA:HMC2	1.84	0.58
2:B:454:ALA:HB2	28:B:620:LMG:H172	1.86	0.58
3:c:390:GLY:HA3	3:c:408:VAL:HG22	1.86	0.57
1:A:16:ARG:HB3	25:A:413:PLM:H21	1.87	0.57
3:C:301:GLN:HA	3:C:384:MET:HG3	1.86	0.57
5:E:8:ARG:O	6:F:19:ARG:NH2	2.31	0.57
2:b:454:ALA:HB2	28:b:622:LMG:H172	1.86	0.57
19:B:606:CLA:HBC1	24:B:625:LFA:H152	1.87	0.57
3:c:301:GLN:HA	3:c:384:MET:HG3	1.87	0.57
10:k:39:TRP:NE1	15:y:46:LEU:O	2.35	0.57
4:D:335:PRO:HB2	5:E:65:LEU:HD11	1.87	0.57
19:c:503:CLA:H61	19:c:513:CLA:H42	1.87	0.57
4:d:36:LEU:HB2	24:d:411:LFA:H41	1.87	0.57
19:B:602:CLA:H101	19:B:609:CLA:H193	1.86	0.56
21:b:619:BCR:HC31	28:b:622:LMG:H291	1.87	0.56
3:C:272:PHE:HB3	30:C:517:DGD:HB61	1.87	0.56
1:A:85:SER:HA	1:A:109:GLY:HA3	1.87	0.56
10:K:29:PRO:O	10:K:32:PHE:HB2	2.05	0.56
1:a:85:SER:HA	1:a:109:GLY:HA3	1.88	0.56
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.86	0.56
3:c:342:GLU:OE2	3:c:342:GLU:N	2.39	0.56
20:D:401:PHO:HBA2	19:D:408:CLA:H142	1.88	0.56
3:C:390:GLY:HA3	3:C:408:VAL:HG22	1.88	0.56
10:K:39:TRP:NE1	15:Y:46:LEU:O	2.37	0.56
25:a:401:PLM:H62	21:a:409:BCR:H291	1.86	0.56
19:C:504:CLA:H61	19:C:514:CLA:H42	1.87	0.55
19:c:505:CLA:H72	30:c:517:DGD:HB92	1.88	0.55
7:h:47:GLU:HB3	7:h:52:THR:HB	1.87	0.55
13:t:7:VAL:HG12	29:t:101:LMT:H122	1.87	0.55
12:M:3:VAL:HG11	13:T:2:GLU:HG2	1.89	0.55
3:C:342:GLU:OE2	3:C:342:GLU:N	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:C:509:CLA:H142	21:C:516:BCR:H362	1.89	0.55
3:c:16:GLN:HG3	3:c:22:ALA:HA	1.89	0.55
10:k:29:PRO:O	10:k:32:PHE:HB2	2.06	0.55
1:a:20:TRP:HE1	22:a:412:SQD:H3	1.72	0.55
23:a:411:PL9:H403	6:f:22:ALA:HB2	1.89	0.55
21:B:618:BCR:H382	21:B:629:BCR:H11C	1.89	0.54
2:b:149:LEU:HD22	19:b:606:CLA:H152	1.89	0.54
3:c:272:PHE:HB3	30:c:516:DGD:HB61	1.88	0.54
2:b:149:LEU:HD23	19:b:605:CLA:HBC1	1.89	0.54
8:i:28:PRO:O	8:i:31:ASN:ND2	2.40	0.54
16:z:26:ALA:HB1	16:z:36:SER:HB3	1.90	0.54
27:a:416:LHG:H221	4:d:37:LEU:HD21	1.88	0.54
1:A:266:ASN:HD22	4:D:237:PRO:HG3	1.73	0.54
12:M:18:PRO:O	12:M:21:PHE:HB3	2.07	0.54
1:a:308:ASP:OD1	1:a:312:ASN:N	2.42	0.53
22:f:102:SQD:H371	14:x:20:VAL:HG22	1.91	0.53
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.91	0.53
1:A:15:GLU:HG3	29:C:502:LMT:H6'2	1.90	0.53
2:B:498:LYS:HD3	2:B:501:ASP:HB2	1.90	0.53
1:a:53:ILE:HG21	29:d:401:LMT:H82	1.90	0.53
2:b:191:ASN:ND2	7:h:59:ASN:O	2.39	0.53
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.91	0.53
1:a:153:SER:HB3	19:a:404:CLA:HED1	1.91	0.53
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.90	0.53
2:b:247:PHE:HB2	19:b:610:CLA:HBC1	1.91	0.53
19:B:615:CLA:H2	19:B:616:CLA:HBB2	1.91	0.52
2:B:149:LEU:HD23	19:B:603:CLA:HBC1	1.92	0.52
13:t:29:ILE:HG22	13:t:30:THR:HG23	1.91	0.52
2:B:247:PHE:HB2	19:B:608:CLA:HBC1	1.91	0.52
28:C:518:LMG:H131	28:C:518:LMG:HC91	1.91	0.52
3:c:26:GLY:HA3	19:c:512:CLA:HMD2	1.91	0.52
19:C:515:CLA:HAB	21:K:101:BCR:H371	1.92	0.52
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.52
3:C:16:GLN:HG3	3:C:22:ALA:HA	1.91	0.52
19:D:409:CLA:H42	7:H:43:LEU:HD11	1.91	0.52
1:A:153:SER:HB3	19:A:403:CLA:HED1	1.90	0.52
10:K:16:ALA:O	10:K:19:ASP:HB2	2.10	0.51
3:C:334:THR:OG1	3:C:336:GLU:OE2	2.27	0.51
27:D:413:LHG:H311	13:T:21:ILE:HD11	1.92	0.51
1:a:84:PRO:HA	1:a:112:TYR:CG	2.45	0.51
1:A:53:ILE:HG21	29:D:402:LMT:H82	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:PHE:O	2:B:317:ASN:ND2	2.42	0.51
1:a:292:THR:HG21	30:c:517:DGD:HBH1	1.91	0.51
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.92	0.51
13:T:29:ILE:HG22	13:T:30:THR:HG23	1.92	0.51
5:e:8:ARG:HH22	5:e:16:SER:HB2	1.76	0.51
2:B:498:LYS:HA	4:D:24:ARG:HA	1.93	0.50
2:b:158:LEU:HB3	2:b:199:VAL:HG22	1.93	0.50
19:b:617:CLA:H2	19:b:618:CLA:CBB	2.42	0.50
10:k:20:PRO:O	10:k:23:ASP:HB2	2.11	0.50
2:b:7:ARG:O	2:b:10:THR:OG1	2.29	0.50
2:b:350:GLU:N	2:b:350:GLU:OE1	2.44	0.50
12:m:18:PRO:O	12:m:21:PHE:HB3	2.12	0.50
19:b:617:CLA:H2	19:b:618:CLA:HBB2	1.91	0.50
2:B:399:VAL:HG12	2:B:417:VAL:HG22	1.92	0.50
1:a:87:ASN:HD22	3:c:344:MET:HE3	1.77	0.50
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.94	0.49
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.92	0.49
3:C:330:MET:HG2	3:C:331:ARG:H	1.76	0.49
19:C:515:CLA:H2	25:C:520:PLM:H52	1.93	0.49
25:D:405:PLM:HF1	24:D:406:LFA:H162	1.93	0.49
2:b:42:LEU:HD13	2:b:94:GLU:HG3	1.94	0.49
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.93	0.49
30:J:101:DGD:O5D	30:J:101:DGD:O4D	2.25	0.49
3:c:201:LEU:HD22	19:c:507:CLA:H202	1.94	0.49
19:c:502:CLA:C3D	19:c:504:CLA:H2	2.42	0.49
19:C:503:CLA:C3D	19:C:505:CLA:H2	2.42	0.49
1:A:308:ASP:OD1	1:A:312:ASN:N	2.42	0.49
19:c:507:CLA:H18	19:c:507:CLA:H122	1.93	0.49
19:B:615:CLA:H2	19:B:616:CLA:CBB	2.43	0.49
11:L:7:ARG:NH1	33:L:202:HOH:O	2.45	0.49
4:d:54:PHE:O	5:e:49:THR:OG1	2.25	0.49
2:b:413:ASP:OD2	2:b:413:ASP:N	2.40	0.48
3:C:201:LEU:HD22	19:C:508:CLA:H202	1.94	0.48
4:D:159:ILE:HG21	4:D:287:VAL:HG22	1.94	0.48
19:D:409:CLA:H121	14:X:18:ALA:HB2	1.96	0.48
2:b:115:TRP:HZ2	11:l:7:ARG:HH22	1.61	0.48
1:A:201:GLY:HA3	1:A:286:THR:HB	1.95	0.48
12:M:31:SER:OG	12:m:31:SER:OG	2.32	0.48
2:b:311:PHE:O	2:b:317:ASN:ND2	2.45	0.48
3:c:211:TRP:O	3:c:214:SER:OG	2.31	0.48
1:A:14:TRP:HD1	29:C:502:LMT:H6'1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:MET:HB3	19:A:403:CLA:HBC2	1.95	0.48
3:C:98:PRO:HB3	28:C:518:LMG:H112	1.95	0.48
23:a:411:PL9:H371	23:a:411:PL9:H351	1.50	0.48
4:d:159:ILE:HG21	4:d:287:VAL:HG22	1.94	0.48
15:Y:28:ILE:HG23	21:Y:101:BCR:H10C	1.95	0.48
1:A:38:ILE:HG12	22:A:411:SQD:H142	1.95	0.48
4:D:294:ARG:NH2	33:D:508:HOH:O	2.46	0.48
2:B:256:MET:HA	2:B:263:THR:HG21	1.97	0.47
1:a:93:PHE:HZ	19:a:408:CLA:HAA1	1.79	0.47
1:a:183:MET:HB3	19:a:404:CLA:HBC2	1.95	0.47
19:b:613:CLA:H142	27:l:101:LHG:H361	1.96	0.47
3:C:33:LEU:HD22	3:C:126:GLU:HG2	1.95	0.47
1:a:201:GLY:HA3	1:a:286:THR:HB	1.95	0.47
19:b:618:CLA:HED2	19:b:618:CLA:H43	1.95	0.47
3:c:49:VAL:HG13	3:c:106:HIS:HD2	1.79	0.47
15:y:39:LEU:HD21	16:z:25:VAL:HA	1.96	0.47
30:D:415:DGD:HA21	30:D:415:DGD:HA52	1.71	0.47
19:d:405:CLA:H121	14:x:18:ALA:HB2	1.95	0.47
2:B:42:LEU:HD13	2:B:94:GLU:HG3	1.95	0.47
3:C:17:GLU:N	3:C:17:GLU:OE2	2.47	0.47
19:B:616:CLA:HED2	19:B:616:CLA:H43	1.95	0.47
4:D:294:ARG:HG3	4:D:296:TYR:HB2	1.97	0.47
2:b:256:MET:HA	2:b:263:THR:HG21	1.96	0.47
19:C:509:CLA:H142	19:C:509:CLA:H111	1.78	0.47
4:D:279:LEU:HD22	20:D:401:PHO:HBC3	1.96	0.47
1:A:77:ILE:HD11	13:T:6:TYR:HB3	1.97	0.47
22:A:411:SQD:H272	2:b:109:LEU:HD13	1.95	0.47
2:B:191:ASN:ND2	7:H:59:ASN:O	2.46	0.47
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.96	0.47
2:b:33:TRP:CD1	21:b:601:BCR:H381	2.50	0.47
2:B:33:TRP:CD1	21:B:629:BCR:H381	2.49	0.47
2:B:255:THR:HG21	19:B:602:CLA:HED1	1.96	0.47
19:C:508:CLA:H72	21:C:516:BCR:H10C	1.97	0.47
2:b:255:THR:HG21	19:b:604:CLA:HED1	1.95	0.47
4:d:279:LEU:HD22	20:d:402:PHO:HBC3	1.96	0.47
1:A:93:PHE:HZ	19:A:407:CLA:HAA1	1.80	0.47
1:A:217:SER:HA	4:D:272:LEU:HD12	1.97	0.47
4:d:49:LEU:HD21	28:d:410:LMG:H351	1.96	0.47
1:A:303:ASN:HD22	3:C:402:ILE:HG22	1.80	0.46
23:a:411:PL9:H272	23:a:411:PL9:H251	1.72	0.46
23:A:410:PL9:H372	4:D:38:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:408:CLA:H152	19:c:507:CLA:H13	1.96	0.46
2:b:496:TYR:HE1	2:b:505:ARG:HD2	1.81	0.46
2:B:436:THR:HG23	2:B:437:LEU:HG	1.97	0.46
19:B:611:CLA:H142	27:L:101:LHG:H361	1.97	0.46
30:J:101:DGD:HD2	30:J:101:DGD:HG32	1.68	0.46
1:a:280:VAL:HG11	27:a:415:LHG:H282	1.97	0.46
3:C:211:TRP:O	3:C:214:SER:OG	2.33	0.46
4:D:304:ARG:NH2	29:D:402:LMT:O3B	2.45	0.46
4:D:296:TYR:OH	4:D:326:ARG:NH1	2.43	0.46
1:a:86:SER:HB3	1:a:89:ILE:HG12	1.97	0.46
19:d:405:CLA:H42	7:h:43:LEU:HD11	1.97	0.46
19:b:604:CLA:H112	19:b:604:CLA:H152	1.73	0.46
1:A:86:SER:HB3	1:A:89:ILE:HG12	1.98	0.46
1:a:215:HIS:ND1	23:a:411:PL9:O1	2.39	0.46
2:B:115:TRP:HZ2	11:L:7:ARG:HH22	1.64	0.45
3:c:461:ASP:OD1	3:c:461:ASP:N	2.48	0.45
30:J:101:DGD:HB61	30:J:101:DGD:HB92	1.82	0.45
1:A:131:TRP:CZ3	19:C:507:CLA:HAA2	2.52	0.45
2:B:327:THR:HG22	19:B:607:CLA:H12	1.98	0.45
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.99	0.45
28:d:410:LMG:H412	6:f:30:THR:HG21	1.98	0.45
3:C:461:ASP:OD1	3:C:461:ASP:N	2.50	0.45
19:A:407:CLA:H152	19:C:508:CLA:H13	1.98	0.45
3:C:49:VAL:HG13	3:C:106:HIS:HD2	1.80	0.45
22:L:102:SQD:H311	22:L:102:SQD:H341	1.65	0.45
3:c:331:ARG:HA	3:c:331:ARG:HD2	1.82	0.45
1:A:183:MET:HA	19:A:403:CLA:HMD1	1.99	0.45
19:b:615:CLA:H72	19:b:615:CLA:H112	1.68	0.45
5:e:32:ILE:HD13	5:e:32:ILE:HA	1.84	0.45
2:B:25:MET:HG2	21:B:617:BCR:H23C	1.98	0.45
6:F:40:MET:HA	6:F:43:ILE:HD12	1.99	0.45
22:F:102:SQD:H282	22:F:102:SQD:H311	1.77	0.45
4:d:160:TYR:HA	4:d:290:ALA:HB2	1.99	0.45
2:B:464:PHE:HD2	19:B:611:CLA:HAC2	1.82	0.44
4:D:54:PHE:O	5:E:49:THR:OG1	2.25	0.44
22:L:102:SQD:H201	21:b:601:BCR:H351	1.98	0.44
19:C:515:CLA:H141	19:C:515:CLA:H162	1.80	0.44
19:B:613:CLA:H72	19:B:613:CLA:H112	1.69	0.44
19:B:615:CLA:H161	7:H:7:LEU:HD21	1.99	0.44
3:C:168:MET:HE2	3:C:168:MET:HB3	1.82	0.44
19:C:508:CLA:H122	19:C:508:CLA:H18	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:c:514:CLA:H172	28:c:518:LMG:H411	2.00	0.44
1:A:292:THR:HG21	30:J:101:DGD:HBf1	1.99	0.44
19:B:607:CLA:H92	28:B:620:LMG:H321	2.00	0.44
2:b:30:VAL:HG12	19:b:607:CLA:HHD	2.00	0.44
2:B:7:ARG:O	2:B:10:THR:OG1	2.28	0.44
1:a:196:PRO:HB3	30:c:519:DGD:HA71	1.99	0.44
1:a:288:LEU:HD13	3:c:420:VAL:HG13	2.00	0.44
11:l:7:ARG:NH1	33:l:202:HOH:O	2.49	0.44
23:A:410:PL9:H403	6:F:22:ALA:HB2	2.00	0.44
1:a:121:LEU:HD21	19:c:506:CLA:H172	1.99	0.44
2:B:30:VAL:HG12	19:B:605:CLA:HHD	2.00	0.44
5:e:18:ARG:HA	5:e:21:VAL:HG12	1.99	0.44
2:B:474:LEU:HD13	24:D:404:LFA:H21	2.00	0.44
2:b:43:ALA:HB1	29:b:602:LMT:H12	2.00	0.44
4:d:51:GLY:HA3	4:d:78:VAL:HG22	2.00	0.44
16:z:37:LYS:HE2	29:z:101:LMT:H1B	1.99	0.44
16:z:58:ASN:HA	16:z:61:VAL:HG12	1.98	0.44
6:f:14:PRO:HG3	22:f:102:SQD:H4	1.99	0.44
19:A:407:CLA:HAB	8:I:15:PHE:CD2	2.53	0.43
2:b:72:THR:HG22	2:b:80:ILE:HD11	1.98	0.43
28:D:414:LMG:H192	28:D:414:LMG:H161	1.79	0.43
1:a:217:SER:HA	4:d:272:LEU:HD12	2.01	0.43
3:c:33:LEU:HD22	3:c:126:GLU:HG2	1.99	0.43
1:A:292:THR:HA	3:C:416:THR:HG22	2.01	0.43
6:F:19:ARG:NH2	31:F:101:HEM:O2D	2.48	0.43
1:a:131:TRP:CZ3	19:c:506:CLA:HAA2	2.52	0.43
19:c:507:CLA:H72	21:c:515:BCR:H10C	2.00	0.43
1:A:283:VAL:HA	1:A:286:THR:HG22	2.00	0.43
7:H:47:GLU:HB3	7:H:52:THR:HB	2.00	0.43
22:l:102:SQD:H341	22:l:102:SQD:H311	1.66	0.43
19:a:408:CLA:HAB	8:i:15:PHE:CD2	2.53	0.43
2:b:464:PHE:HD2	19:b:613:CLA:HAC2	1.83	0.43
19:b:609:CLA:H92	28:b:622:LMG:H321	2.00	0.43
19:b:617:CLA:H92	19:b:617:CLA:H61	1.85	0.43
22:A:409:SQD:H262	27:A:417:LHG:H142	2.01	0.43
1:a:82:VAL:HB	1:a:174:LEU:HB2	2.01	0.43
1:a:283:VAL:HA	1:a:286:THR:HG22	2.00	0.43
19:b:608:CLA:H61	19:b:608:CLA:H102	1.85	0.43
3:c:136:GLY:O	3:c:144:LYS:NZ	2.48	0.43
4:d:148:ALA:HB2	4:d:276:VAL:HG13	2.01	0.43
2:B:486:LEU:HD11	2:B:490:GLN:HE21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:179:PHE:HA	4:D:182:LEU:HD12	2.00	0.43
2:b:458:PHE:HB3	19:b:606:CLA:HBC2	2.01	0.43
2:B:458:PHE:HB3	19:B:604:CLA:HBC2	2.01	0.43
4:D:36:LEU:HB2	24:D:404:LFA:H131	2.01	0.43
16:Z:23:VAL:HG22	16:Z:40:ILE:HG12	2.00	0.43
1:a:127:MET:HG3	1:a:144:CYS:HB2	2.01	0.43
2:b:399:VAL:HG12	2:b:417:VAL:HG22	2.01	0.43
19:b:617:CLA:H161	7:h:7:LEU:HD21	2.00	0.43
21:b:619:BCR:H311	29:m:101:LMT:H72	2.01	0.43
4:d:123:ILE:HD11	30:h:102:DGD:HAE1	2.00	0.43
4:d:179:PHE:HA	4:d:182:LEU:HD12	2.00	0.43
1:a:302:PHE:HE2	4:d:74:LEU:HD12	1.84	0.42
3:c:261:SER:O	3:c:429:HIS:ND1	2.43	0.42
1:a:131:TRP:CH2	19:c:506:CLA:HAA2	2.55	0.42
2:b:149:LEU:HD13	19:b:606:CLA:H171	2.01	0.42
1:A:302:PHE:HE2	4:D:74:LEU:HD12	1.83	0.42
1:a:77:ILE:HD11	13:t:6:TYR:HB3	2.00	0.42
19:b:607:CLA:H62	19:b:607:CLA:H41	1.85	0.42
19:b:614:CLA:H171	19:b:615:CLA:HBB2	2.01	0.42
4:d:123:ILE:HD11	30:h:102:DGD:HAH2	2.02	0.42
19:B:604:CLA:H91	19:B:604:CLA:H111	1.87	0.42
1:a:238:LYS:HA	1:a:238:LYS:HD3	1.82	0.42
3:c:74:LEU:HD13	3:c:77:ILE:HD12	2.01	0.42
4:d:263:ASN:HB3	4:d:266:TRP:HB3	2.00	0.42
3:C:74:LEU:HD13	3:C:77:ILE:HD12	2.01	0.42
20:D:401:PHO:H62	20:D:401:PHO:H41	1.81	0.42
9:J:18:GLY:HA3	21:Y:101:BCR:H371	2.01	0.42
1:a:132:GLU:O	1:a:136:ARG:HG2	2.20	0.42
1:a:292:THR:HA	3:c:416:THR:HG22	2.00	0.42
2:b:102:VAL:HA	21:b:620:BCR:H402	2.02	0.42
3:C:150:GLY:HA2	3:C:236:GLY:HA2	2.00	0.42
3:C:228:ILE:HD13	3:C:228:ILE:HA	1.82	0.42
19:C:504:CLA:H161	19:C:504:CLA:H141	1.78	0.42
10:K:12:PRO:HB2	10:K:15:TYR:HD1	1.85	0.42
21:K:101:BCR:H20C	21:K:101:BCR:H361	1.93	0.42
21:B:629:BCR:HC8	13:t:18:PHE:HD1	1.85	0.42
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.01	0.42
6:F:18:VAL:HG22	22:F:102:SQD:H252	2.02	0.42
19:b:606:CLA:H93	19:b:607:CLA:HAB	2.02	0.42
12:M:33:GLN:HE21	12:M:33:GLN:HB2	1.73	0.41
2:b:436:THR:HG23	2:b:437:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:150:GLY:HA2	3:c:236:GLY:HA2	2.01	0.41
1:A:288:LEU:HD13	3:C:420:VAL:HG13	2.02	0.41
19:B:604:CLA:HBA2	19:B:612:CLA:H152	2.02	0.41
19:B:612:CLA:H171	19:B:613:CLA:HBB2	2.01	0.41
14:X:17:GLY:HA2	24:X:101:LFA:H121	2.02	0.41
19:c:512:CLA:H191	29:z:101:LMT:H122	2.02	0.41
15:y:24:MET:HE2	15:y:24:MET:HB2	1.79	0.41
16:z:47:TRP:CE2	29:z:101:LMT:H112	2.55	0.41
12:M:6:LEU:HD11	29:M:101:LMT:H21	2.02	0.41
2:b:75:TRP:CD2	25:b:631:PLM:H62	2.55	0.41
19:c:505:CLA:H92	19:c:505:CLA:H62	1.86	0.41
4:d:51:GLY:HA2	4:d:55:VAL:HB	2.02	0.41
28:d:410:LMG:H192	28:d:410:LMG:H161	1.75	0.41
4:D:155:SER:HA	4:D:159:ILE:HB	2.03	0.41
25:a:414:PLM:H72	25:a:414:PLM:H41	1.84	0.41
1:A:82:VAL:HB	1:A:174:LEU:HB2	2.03	0.41
3:C:213:VAL:HG13	3:C:277:PHE:HA	2.02	0.41
22:F:102:SQD:H242	22:F:102:SQD:H271	1.80	0.41
23:d:407:PL9:H43	23:d:407:PL9:H471	1.85	0.41
2:B:247:PHE:HE1	19:B:602:CLA:H102	1.86	0.41
27:a:416:LHG:O4	5:e:10:PHE:N	2.53	0.41
19:b:607:CLA:H141	19:b:607:CLA:H161	1.86	0.41
4:D:263:ASN:HB3	4:D:266:TRP:HB3	2.03	0.41
2:b:498:LYS:HA	4:d:24:ARG:HA	2.03	0.41
21:b:620:BCR:H20C	21:b:620:BCR:H361	1.90	0.41
3:c:40:ALA:HB2	19:c:512:CLA:HMA2	2.03	0.41
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.02	0.41
3:C:329:LEU:HD12	3:C:337:ILE:HG23	2.02	0.41
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.02	0.41
10:K:28:ILE:HD11	15:Y:28:ILE:HD13	2.02	0.41
19:a:404:CLA:H192	19:a:404:CLA:H161	1.88	0.41
2:b:33:TRP:HD1	21:b:601:BCR:H381	1.86	0.41
2:b:218:LEU:HB3	24:b:626:LFA:H102	2.03	0.41
2:b:220:ARG:HD2	7:h:20:LYS:HG2	2.03	0.41
1:A:132:GLU:O	1:A:136:ARG:HG2	2.21	0.41
2:B:152:GLY:HA3	24:B:625:LFA:H191	2.03	0.41
29:D:403:LMT:H111	25:D:405:PLM:HG3	2.03	0.41
23:a:411:PL9:H321	6:f:26:LEU:HD21	2.03	0.41
2:b:121:GLU:O	7:h:12:ARG:NH1	2.54	0.41
19:b:606:CLA:HBA2	19:b:614:CLA:H152	2.02	0.41
3:c:392:LEU:HD12	3:c:392:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:ALA:HB2	19:C:513:CLA:HMA2	2.04	0.40
2:b:491:VAL:HG12	4:d:136:VAL:HG13	2.02	0.40
19:c:503:CLA:H161	19:c:503:CLA:H141	1.76	0.40
9:j:18:GLY:HA3	21:y:101:BCR:H371	2.02	0.40
1:A:131:TRP:CH2	19:C:507:CLA:HAA2	2.55	0.40
2:B:214:LEU:HD23	2:B:214:LEU:HA	1.95	0.40
21:B:629:BCR:HC41	22:a:412:SQD:H141	2.03	0.40
27:L:101:LHG:H142	27:L:101:LHG:H171	1.91	0.40
16:Z:17:PHE:O	16:Z:21:ILE:HG22	2.22	0.40
3:c:228:ILE:HD13	3:c:228:ILE:HA	1.96	0.40
1:A:238:LYS:HA	1:A:238:LYS:HD3	1.87	0.40
1:a:140:ARG:HB2	4:d:220:ASN:HA	2.02	0.40
21:a:409:BCR:H24C	21:a:409:BCR:H371	1.94	0.40
1:A:43:ALA:HB1	21:A:408:BCR:H362	2.03	0.40
28:C:501:LMG:H161	28:C:501:LMG:H132	1.95	0.40
19:C:510:CLA:H162	19:C:510:CLA:H122	1.95	0.40
9:j:24:ILE:HD12	9:j:24:ILE:HA	1.90	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/360 (89%)	315 (98%)	6 (2%)	0	100	100
1	a	321/360 (89%)	316 (98%)	5 (2%)	0	100	100
2	B	502/510 (98%)	495 (99%)	5 (1%)	2 (0%)	30	34
2	b	503/510 (99%)	495 (98%)	7 (1%)	1 (0%)	44	52
3	C	432/461 (94%)	423 (98%)	9 (2%)	0	100	100
3	c	432/461 (94%)	425 (98%)	7 (2%)	0	100	100
4	D	339/352 (96%)	334 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	339/352 (96%)	333 (98%)	6 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
6	F	31/45 (69%)	30 (97%)	1 (3%)	0	100	100
6	f	31/45 (69%)	30 (97%)	1 (3%)	0	100	100
7	H	62/66 (94%)	62 (100%)	0	0	100	100
7	h	62/66 (94%)	61 (98%)	1 (2%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	26/40 (65%)	26 (100%)	0	0	100	100
9	j	26/40 (65%)	26 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	33/37 (89%)	33 (100%)	0	0	100	100
11	l	33/37 (89%)	33 (100%)	0	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	31/36 (86%)	31 (100%)	0	0	100	100
13	T	28/32 (88%)	28 (100%)	0	0	100	100
13	t	28/32 (88%)	28 (100%)	0	0	100	100
14	X	33/41 (80%)	33 (100%)	0	0	100	100
14	x	33/41 (80%)	33 (100%)	0	0	100	100
15	Y	26/46 (56%)	26 (100%)	0	0	100	100
15	y	26/46 (56%)	26 (100%)	0	0	100	100
16	Z	59/62 (95%)	59 (100%)	0	0	100	100
16	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
All	All	4141/4512 (92%)	4079 (98%)	59 (1%)	3 (0%)	50	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	86	ILE
2	b	86	ILE
2	B	384	ARG

### 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	261/290 (90%)	261 (100%)	0	100	100
1	a	261/290 (90%)	261 (100%)	0	100	100
2	B	400/407 (98%)	396 (99%)	4 (1%)	73	84
2	b	400/407 (98%)	395 (99%)	5 (1%)	65	78
3	C	340/362 (94%)	336 (99%)	4 (1%)	67	80
3	c	340/362 (94%)	336 (99%)	4 (1%)	67	80
4	D	275/283 (97%)	274 (100%)	1 (0%)	89	95
4	d	275/283 (97%)	272 (99%)	3 (1%)	70	82
5	E	71/73 (97%)	71 (100%)	0	100	100
5	e	69/73 (94%)	67 (97%)	2 (3%)	37	50
6	F	26/39 (67%)	26 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	54/55 (98%)	54 (100%)	0	100	100
8	I	31/34 (91%)	31 (100%)	0	100	100
8	i	31/34 (91%)	31 (100%)	0	100	100
9	J	19/28 (68%)	19 (100%)	0	100	100
9	j	19/28 (68%)	17 (90%)	2 (10%)	5	5
10	K	28/37 (76%)	28 (100%)	0	100	100
10	k	28/37 (76%)	28 (100%)	0	100	100
11	L	33/35 (94%)	33 (100%)	0	100	100
11	l	33/35 (94%)	32 (97%)	1 (3%)	36	48
12	M	30/33 (91%)	30 (100%)	0	100	100
12	m	30/33 (91%)	29 (97%)	1 (3%)	33	44
13	T	26/28 (93%)	26 (100%)	0	100	100
13	t	26/28 (93%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	X	28/34 (82%)	26 (93%)	2 (7%)	12	13
14	x	28/34 (82%)	25 (89%)	3 (11%)	5	5
15	Y	20/37 (54%)	19 (95%)	1 (5%)	20	26
15	y	19/37 (51%)	18 (95%)	1 (5%)	19	24
16	Z	50/52 (96%)	48 (96%)	2 (4%)	27	35
16	z	48/52 (92%)	47 (98%)	1 (2%)	48	63
All	All	3380/3654 (92%)	3343 (99%)	37 (1%)	69	82

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	219	VAL
2	B	362	PHE
2	B	376	VAL
3	C	228	ILE
3	C	298	SER
3	C	334	THR
3	C	405	VAL
4	D	295	SER
14	X	23	LEU
14	X	31	ILE
15	Y	43	ARG
16	Z	25	VAL
16	Z	38	GLN
2	b	219	VAL
2	b	223	GLN
2	b	294	SER
2	b	362	PHE
2	b	376	VAL
3	c	133	SER
3	c	243	THR
3	c	384	MET
3	c	405	VAL
4	d	90	LEU
4	d	294	ARG
4	d	352	LEU
5	e	4	THR
5	e	65	LEU
9	j	21	VAL

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Mol	Chain	Res	Type
9	j	22	ILE
11	l	12	LEU
12	m	9	ILE
14	x	12	ILE
14	x	23	LEU
14	x	31	ILE
15	y	34	MET
16	z	20	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	261	GLN
1	A	266	ASN
1	A	312	ASN
2	B	14	ASN
2	B	282	GLN
2	B	289	GLN
2	B	395	GLN
2	B	438	ASN
2	B	490	GLN
2	B	497	GLN
3	C	44	HIS
3	C	299	GLN
3	C	361	ASN
3	C	370	ASN
3	C	373	GLN
4	D	250	ASN
7	H	59	ASN
11	L	6	ASN
12	M	33	GLN
14	X	33	GLN
16	Z	6	GLN
1	a	261	GLN
1	a	266	ASN
1	a	312	ASN
2	b	14	ASN
2	b	179	GLN
2	b	282	GLN
2	b	289	GLN
2	b	374	ASN

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Mol	Chain	Res	Type
2	b	438	ASN
3	c	44	HIS
3	c	361	ASN
3	c	370	ASN
3	c	373	GLN
4	d	250	ASN
7	h	59	ASN
10	k	40	GLN
11	l	6	ASN
11	l	8	GLN
12	m	4	ASN
14	x	33	GLN
16	z	58	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\# Z  > 2$
13	FME	t	1	13	8,9,10	0.36	0	7,9,11	0.92	0
1	HSK	a	332	1	7,11,12	1.31	1 (14%)	3,14,16	0.91	0
8	FME	i	1	8	8,9,10	0.36	0	7,9,11	0.73	0
1	HSK	A	332	1	7,11,12	1.33	1 (14%)	3,14,16	0.89	0
8	FME	I	1	8	8,9,10	0.36	0	7,9,11	0.76	0
13	FME	T	1	13	8,9,10	0.38	0	7,9,11	1.38	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
13	FME	t	1	13	-	4/7/9/11	-
1	HSK	a	332	1	-	2/5/6/8	0/1/1/1
8	FME	i	1	8	-	2/7/9/11	-
1	HSK	A	332	1	-	2/5/6/8	0/1/1/1
8	FME	I	1	8	-	3/7/9/11	-
13	FME	T	1	13	-	3/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	HSK	CE1-ND1	-2.18	1.34	1.36
1	a	332	HSK	CE1-ND1	-2.17	1.34	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	1	FME	CA-N-CN	2.89	127.26	122.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	332	HSK	C-CA-CB-CG
1	A	332	HSK	N-CA-CB-CG
8	I	1	FME	C-CA-CB-CG
1	a	332	HSK	C-CA-CB-CG
1	a	332	HSK	N-CA-CB-CG
8	i	1	FME	C-CA-CB-CG
13	t	1	FME	C-CA-CB-CG
8	I	1	FME	CA-CB-CG-SD
13	T	1	FME	CA-CB-CG-SD
8	i	1	FME	CA-CB-CG-SD
13	t	1	FME	CA-CB-CG-SD
13	t	1	FME	N-CA-CB-CG
13	T	1	FME	C-CA-CB-CG
13	T	1	FME	CB-CA-N-CN
13	t	1	FME	CB-CA-N-CN
8	I	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 212 ligands modelled in this entry, 4 are monoatomic - leaving 208 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
31	HEM	f	101	6,5	41,50,50	1.47	4 (9%)	45,82,82	1.40	5 (11%)
24	LFA	B	624	-	6,6,19	0.26	0	5,5,18	0.17	0
19	CLA	B	604	-	65,73,73	1.48	6 (9%)	76,113,113	1.56	11 (14%)
30	DGD	d	414	-	47,47,67	0.52	0	54,55,81	0.66	0
19	CLA	B	613	-	65,73,73	1.42	7 (10%)	76,113,113	1.46	7 (9%)
19	CLA	B	603	-	65,73,73	1.43	6 (9%)	76,113,113	1.40	9 (11%)
21	BCR	B	618	-	41,41,41	0.37	0	56,56,56	0.78	0
19	CLA	c	511	-	65,73,73	1.45	7 (10%)	76,113,113	1.37	6 (7%)
21	BCR	C	521	-	41,41,41	0.37	0	56,56,56	1.11	5 (8%)
29	LMT	d	412	-	24,24,36	0.52	0	29,29,47	0.69	0
28	LMG	C	501	-	51,51,55	0.51	0	59,59,63	0.62	0
29	LMT	t	101	-	24,24,36	0.53	0	29,29,47	1.09	3 (10%)
25	PLM	i	102	-	12,12,17	0.77	0	12,12,17	0.70	0
19	CLA	b	608	-	65,73,73	1.44	7 (10%)	76,113,113	1.54	8 (10%)
19	CLA	c	503	-	65,73,73	1.43	7 (10%)	76,113,113	1.46	6 (7%)
24	LFA	D	407	-	8,8,19	0.25	0	7,7,18	0.21	0
24	LFA	Z	101	-	7,7,19	0.25	0	6,6,18	0.20	0
25	PLM	i	101	-	15,15,17	0.67	0	15,15,17	0.67	0
28	LMG	B	620	-	51,51,55	0.51	0	59,59,63	0.61	0
19	CLA	b	613	-	65,73,73	1.43	7 (10%)	76,113,113	1.50	9 (11%)
25	PLM	C	520	-	8,8,17	0.91	0	8,8,17	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	BCR	B	619	-	41,41,41	0.32	0	56,56,56	0.75	0
24	LFA	M	103	-	9,9,19	0.23	0	8,8,18	0.21	0
24	LFA	A	412	-	14,14,19	0.24	0	13,13,18	0.20	0
24	LFA	b	624	-	11,11,19	0.21	0	10,10,18	0.23	0
31	HEM	F	101	6,5	41,50,50	1.47	5 (12%)	45,82,82	1.40	6 (13%)
19	CLA	c	508	33	65,73,73	1.42	6 (9%)	76,113,113	1.49	8 (10%)
24	LFA	a	413	-	10,10,19	0.23	0	9,9,18	0.21	0
19	CLA	c	514	-	65,73,73	1.40	7 (10%)	76,113,113	1.50	7 (9%)
29	LMT	d	401	-	35,35,36	0.53	0	46,46,47	0.74	0
27	LHG	a	415	-	45,45,48	0.53	0	48,51,54	0.52	0
19	CLA	b	617	-	65,73,73	1.42	7 (10%)	76,113,113	1.41	6 (7%)
24	LFA	D	406	-	12,12,19	0.23	0	11,11,18	0.28	0
24	LFA	K	102	-	6,6,19	0.25	0	5,5,18	0.20	0
19	CLA	B	607	33	65,73,73	1.44	5 (7%)	76,113,113	1.51	7 (9%)
24	LFA	B	621	-	12,12,19	0.22	0	11,11,18	0.19	0
19	CLA	D	409	-	65,73,73	1.43	7 (10%)	76,113,113	1.43	6 (7%)
25	PLM	a	414	-	11,11,17	0.78	0	11,11,17	0.75	0
24	LFA	J	102	-	16,16,19	0.24	0	15,15,18	0.20	0
19	CLA	b	603	33	65,73,73	1.48	5 (7%)	76,113,113	1.38	6 (7%)
21	BCR	b	601	-	41,41,41	0.31	0	56,56,56	1.44	9 (16%)
21	BCR	B	629	-	41,41,41	0.34	0	56,56,56	0.88	2 (3%)
19	CLA	B	605	-	65,73,73	1.46	7 (10%)	76,113,113	1.45	7 (9%)
27	LHG	A	417	-	45,45,48	0.54	0	48,51,54	0.50	0
24	LFA	b	629	-	8,8,19	0.23	0	7,7,18	0.21	0
27	LHG	D	413	-	48,48,48	0.51	0	51,54,54	0.49	0
28	LMG	b	622	-	51,51,55	0.50	0	59,59,63	0.61	0
25	PLM	A	413	-	17,17,17	0.65	0	17,17,17	0.62	0
19	CLA	d	404	-	65,73,73	1.44	7 (10%)	76,113,113	1.38	6 (7%)
30	DGD	c	517	-	63,63,67	0.55	0	77,77,81	0.78	2 (2%)
20	PHO	D	401	-	51,69,69	0.63	0	47,99,99	1.04	3 (6%)
19	CLA	D	408	-	65,73,73	1.44	7 (10%)	76,113,113	1.38	6 (7%)
19	CLA	a	408	-	65,73,73	1.43	7 (10%)	76,113,113	1.48	9 (11%)
19	CLA	d	405	-	65,73,73	1.44	7 (10%)	76,113,113	1.42	6 (7%)
21	BCR	D	410	-	41,41,41	0.34	0	56,56,56	0.71	0
25	PLM	b	628	-	13,13,17	0.73	0	13,13,17	0.69	0
27	LHG	d	408	-	48,48,48	0.52	0	51,54,54	0.51	0
29	LMT	D	403	-	24,24,36	0.49	0	29,29,47	0.68	0
24	LFA	i	105	-	10,10,19	0.24	0	9,9,18	0.19	0
19	CLA	B	601	33	65,73,73	1.49	5 (7%)	76,113,113	1.38	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	SQD	a	410	-	53,54,54	1.49	6 (11%)	62,65,65	1.51	7 (11%)
19	CLA	B	609	-	65,73,73	1.49	7 (10%)	76,113,113	1.37	7 (9%)
25	PLM	I	104	-	10,10,17	0.84	0	10,10,17	0.81	0
19	CLA	A	403	-	65,73,73	1.42	6 (9%)	76,113,113	1.50	8 (10%)
19	CLA	C	514	-	65,73,73	1.43	6 (9%)	76,113,113	1.48	6 (7%)
19	CLA	b	618	-	65,73,73	1.41	7 (10%)	76,113,113	1.52	6 (7%)
30	DGD	D	415	-	44,44,67	0.55	0	52,52,81	0.68	1 (1%)
28	LMG	c	518	-	51,51,55	0.48	0	59,59,63	0.58	0
19	CLA	B	608	-	65,73,73	1.43	7 (10%)	76,113,113	1.45	8 (10%)
19	CLA	C	506	33	65,73,73	1.44	7 (10%)	76,113,113	1.50	7 (9%)
24	LFA	H	101	-	13,13,19	0.21	0	12,12,18	0.27	0
25	PLM	A	415	-	10,10,17	0.83	0	10,10,17	0.77	0
25	PLM	a	401	-	16,16,17	0.68	0	16,16,17	0.60	0
19	CLA	c	506	-	65,73,73	1.45	7 (10%)	76,113,113	1.46	8 (10%)
22	SQD	L	102	-	53,54,54	1.52	9 (16%)	62,65,65	1.53	9 (14%)
19	CLA	c	510	-	65,73,73	1.41	6 (9%)	76,113,113	1.50	6 (7%)
25	PLM	b	625	-	8,8,17	0.93	0	8,8,17	0.82	0
19	CLA	B	612	-	65,73,73	1.41	7 (10%)	76,113,113	1.54	7 (9%)
19	CLA	C	503	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	9 (11%)
28	LMG	c	501	-	51,51,55	0.50	0	59,59,63	0.63	0
19	CLA	A	405	33	65,73,73	1.40	6 (9%)	76,113,113	1.51	10 (13%)
19	CLA	b	605	-	65,73,73	1.43	6 (9%)	76,113,113	1.40	8 (10%)
25	PLM	B	626	-	12,12,17	0.76	0	12,12,17	0.71	0
22	SQD	A	409	-	49,50,54	1.53	6 (12%)	58,61,65	1.54	7 (12%)
19	CLA	b	610	-	65,73,73	1.43	7 (10%)	76,113,113	1.48	8 (10%)
19	CLA	B	602	-	65,73,73	1.43	6 (9%)	76,113,113	1.47	9 (11%)
22	SQD	a	412	-	42,43,54	1.67	7 (16%)	51,54,65	1.43	6 (11%)
22	SQD	A	411	-	53,54,54	1.54	7 (13%)	62,65,65	1.32	6 (9%)
25	PLM	b	631	-	15,15,17	0.69	0	15,15,17	0.63	0
19	CLA	B	614	-	65,73,73	1.43	7 (10%)	76,113,113	1.45	8 (10%)
20	PHO	a	407	-	51,69,69	0.69	0	47,99,99	0.91	3 (6%)
19	CLA	b	609	33	65,73,73	1.43	5 (7%)	76,113,113	1.49	7 (9%)
24	LFA	I	103	-	6,6,19	0.26	0	5,5,18	0.18	0
30	DGD	J	101	-	55,55,67	0.54	0	69,69,81	0.86	2 (2%)
24	LFA	x	101	-	12,12,19	0.22	0	11,11,18	0.24	0
21	BCR	c	515	-	41,41,41	0.32	0	56,56,56	0.68	0
25	PLM	D	405	-	17,17,17	0.64	0	17,17,17	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LHG	D	412	-	48,48,48	0.52	0	51,54,54	0.51	0
27	LHG	a	416	-	48,48,48	0.51	0	51,54,54	0.49	0
32	RRX	H	102	-	42,42,42	0.20	0	57,58,58	0.39	0
21	BCR	a	409	-	41,41,41	0.32	0	56,56,56	0.71	0
21	BCR	y	101	-	41,41,41	0.34	0	56,56,56	1.06	4 (7%)
29	LMT	m	102	-	36,36,36	0.55	0	47,47,47	0.69	0
19	CLA	b	612	33	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
23	PL9	D	411	-	55,55,55	1.30	6 (10%)	68,69,69	1.51	14 (20%)
29	LMT	i	103	-	36,36,36	0.52	0	47,47,47	1.02	2 (4%)
24	LFA	X	101	-	12,12,19	0.22	0	11,11,18	0.25	0
22	SQD	f	102	-	44,45,54	1.63	9 (20%)	53,56,65	1.56	8 (15%)
30	DGD	H	103	-	63,63,67	0.59	0	77,77,81	0.75	0
19	CLA	c	504	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	7 (9%)
25	PLM	B	623	-	11,11,17	0.79	0	11,11,17	0.74	0
26	BCT	A	416	17	2,3,3	0.89	0	2,3,3	3.22	2 (100%)
19	CLA	c	502	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
19	CLA	C	512	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	6 (7%)
21	BCR	b	619	-	41,41,41	0.32	0	56,56,56	0.85	2 (3%)
21	BCR	C	516	-	41,41,41	0.33	0	56,56,56	0.69	0
19	CLA	b	607	-	65,73,73	1.45	7 (10%)	76,113,113	1.47	7 (9%)
19	CLA	b	614	-	65,73,73	1.39	7 (10%)	76,113,113	1.54	7 (9%)
24	LFA	B	628	-	6,6,19	0.26	0	5,5,18	0.15	0
24	LFA	d	413	-	7,7,19	0.25	0	6,6,18	0.20	0
20	PHO	d	402	-	51,69,69	0.63	0	47,99,99	1.02	2 (4%)
21	BCR	b	620	-	41,41,41	0.36	0	56,56,56	0.92	3 (5%)
30	DGD	c	516	-	63,63,67	0.58	0	77,77,81	0.75	2 (2%)
19	CLA	C	509	33	65,73,73	1.43	6 (9%)	76,113,113	1.49	8 (10%)
30	DGD	c	519	-	63,63,67	0.55	0	77,77,81	0.71	1 (1%)
21	BCR	B	617	-	41,41,41	0.33	0	56,56,56	0.78	1 (1%)
25	PLM	B	622	-	7,7,17	1.00	0	7,7,17	0.93	0
21	BCR	k	101	-	41,41,41	0.32	0	56,56,56	0.56	0
22	SQD	F	102	-	31,32,54	2.37	8 (25%)	34,36,65	1.67	6 (17%)
24	LFA	d	411	-	14,14,19	0.20	0	13,13,18	0.25	0
19	CLA	C	511	-	65,73,73	1.41	6 (9%)	76,113,113	1.49	6 (7%)
19	CLA	C	515	-	65,73,73	1.43	6 (9%)	76,113,113	1.47	8 (10%)
19	CLA	a	406	33	65,73,73	1.40	6 (9%)	76,113,113	1.52	10 (13%)
24	LFA	A	414	-	12,12,19	0.23	0	11,11,18	0.21	0
29	LMT	m	101	-	36,36,36	0.53	0	47,47,47	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	c	513	-	65,73,73	1.43	6 (9%)	76,113,113	1.48	6 (7%)
19	CLA	B	616	-	65,73,73	1.42	7 (10%)	76,113,113	1.53	6 (7%)
24	LFA	C	519	-	6,6,19	0.27	0	5,5,18	0.16	0
19	CLA	C	508	-	65,73,73	1.46	6 (9%)	76,113,113	1.47	8 (10%)
19	CLA	C	510	-	65,73,73	1.43	6 (9%)	76,113,113	1.51	8 (10%)
21	BCR	c	520	-	41,41,41	0.37	0	56,56,56	1.16	5 (8%)
24	LFA	h	101	-	7,7,19	0.26	0	6,6,18	0.18	0
25	PLM	b	623	-	17,17,17	0.64	0	17,17,17	0.66	0
28	LMG	D	414	-	48,48,55	0.53	0	56,56,63	0.62	0
24	LFA	b	626	-	10,10,19	0.24	0	9,9,18	0.21	0
25	PLM	H	105	-	9,9,17	0.90	0	9,9,17	0.79	0
19	CLA	b	604	-	65,73,73	1.43	7 (10%)	76,113,113	1.46	9 (11%)
25	PLM	I	102	-	17,17,17	0.66	0	17,17,17	0.65	0
24	LFA	H	104	-	5,5,19	0.27	0	4,4,18	0.16	0
19	CLA	b	606	-	65,73,73	1.48	6 (9%)	76,113,113	1.54	10 (13%)
21	BCR	K	101	-	41,41,41	0.32	0	56,56,56	0.59	0
24	LFA	m	103	-	8,8,19	0.24	0	7,7,18	0.19	0
24	LFA	D	404	-	15,15,19	0.17	0	14,14,18	0.37	0
25	PLM	E	101	-	17,17,17	0.64	0	17,17,17	0.58	0
25	PLM	b	630	-	12,12,17	0.74	0	12,12,17	0.74	0
19	CLA	c	509	-	65,73,73	1.42	7 (10%)	76,113,113	1.51	9 (11%)
29	LMT	C	502	-	31,31,36	0.64	0	42,42,47	0.85	1 (2%)
24	LFA	k	102	-	6,6,19	0.25	0	5,5,18	0.21	0
19	CLA	a	405	33	65,73,73	1.41	6 (9%)	76,113,113	1.55	9 (11%)
19	CLA	B	611	-	65,73,73	1.43	7 (10%)	76,113,113	1.49	9 (11%)
19	CLA	B	615	-	65,73,73	1.43	7 (10%)	76,113,113	1.41	7 (9%)
19	CLA	C	505	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
21	BCR	Y	101	-	41,41,41	0.35	0	56,56,56	1.00	2 (3%)
19	CLA	b	615	-	65,73,73	1.43	7 (10%)	76,113,113	1.45	7 (9%)
28	LMG	d	410	-	51,51,55	0.53	0	59,59,63	0.59	0
29	LMT	M	101	-	36,36,36	0.52	0	47,47,47	0.79	0
25	PLM	B	627	-	15,15,17	0.70	0	15,15,17	0.61	0
20	PHO	A	406	-	51,69,69	0.69	1 (1%)	47,99,99	0.90	3 (6%)
19	CLA	c	505	33	65,73,73	1.44	7 (10%)	76,113,113	1.51	7 (9%)
19	CLA	C	507	-	65,73,73	1.45	7 (10%)	76,113,113	1.45	8 (10%)
23	PL9	a	411	-	55,55,55	1.08	3 (5%)	68,69,69	1.56	13 (19%)
21	BCR	d	406	-	41,41,41	0.34	0	56,56,56	0.71	0
24	LFA	B	625	-	10,10,19	0.24	0	9,9,18	0.18	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	LFA	h	103	-	5,5,19	0.26	0	4,4,18	0.16	0
29	LMT	D	402	-	36,36,36	0.53	0	47,47,47	0.72	0
29	LMT	z	101	-	36,36,36	0.52	0	47,47,47	0.97	4 (8%)
24	LFA	b	632	-	6,6,19	0.27	0	5,5,18	0.18	0
19	CLA	C	504	-	65,73,73	1.43	7 (10%)	76,113,113	1.46	6 (7%)
32	RRX	x	102	-	42,42,42	0.20	0	57,58,58	0.40	0
30	DGD	h	102	-	63,63,67	0.59	0	77,77,81	0.75	1 (1%)
19	CLA	c	507	-	65,73,73	1.46	6 (9%)	76,113,113	1.48	8 (10%)
21	BCR	b	621	-	41,41,41	0.32	0	56,56,56	0.75	0
23	PL9	A	410	-	55,55,55	1.07	3 (5%)	68,69,69	1.48	12 (17%)
24	LFA	h	104	-	6,6,19	0.25	0	5,5,18	0.19	0
25	PLM	i	104	-	12,12,17	0.76	0	12,12,17	0.69	0
25	PLM	I	101	-	15,15,17	0.68	0	15,15,17	0.64	0
19	CLA	B	610	33	65,73,73	1.47	6 (9%)	76,113,113	1.36	7 (9%)
19	CLA	C	513	3	65,73,73	1.45	7 (10%)	76,113,113	1.50	7 (9%)
27	LHG	L	101	-	48,48,48	0.51	0	51,54,54	0.54	0
28	LMG	C	518	-	42,42,55	0.53	0	50,50,63	0.70	0
19	CLA	A	407	-	65,73,73	1.45	7 (10%)	76,113,113	1.45	9 (11%)
19	CLA	c	512	3	65,73,73	1.44	7 (10%)	76,113,113	1.51	8 (10%)
19	CLA	b	611	-	65,73,73	1.49	7 (10%)	76,113,113	1.37	7 (9%)
24	LFA	b	627	-	8,8,19	0.25	0	7,7,18	0.18	0
27	LHG	l	101	-	48,48,48	0.51	0	51,54,54	0.53	0
29	LMT	M	102	-	36,36,36	0.55	0	47,47,47	0.73	0
25	PLM	e	101	-	17,17,17	0.64	0	17,17,17	0.61	0
19	CLA	a	404	-	65,73,73	1.43	6 (9%)	76,113,113	1.51	8 (10%)
19	CLA	B	606	-	65,73,73	1.43	7 (10%)	76,113,113	1.53	8 (10%)
19	CLA	A	404	33	65,73,73	1.41	6 (9%)	76,113,113	1.55	9 (11%)
30	DGD	C	517	-	63,63,67	0.59	0	77,77,81	0.74	2 (2%)
22	SQD	l	102	-	53,54,54	1.52	9 (16%)	62,65,65	1.51	8 (12%)
29	LMT	b	602	-	20,20,36	0.50	0	25,25,47	0.86	1 (4%)
23	PL9	d	407	-	55,55,55	1.31	6 (10%)	68,69,69	1.51	13 (19%)
19	CLA	b	616	-	65,73,73	1.42	7 (10%)	76,113,113	1.45	8 (10%)
27	LHG	d	409	-	48,48,48	0.51	0	51,54,54	0.49	0
21	BCR	A	408	-	41,41,41	0.32	0	56,56,56	0.73	0
26	BCT	d	403	17	2,3,3	0.88	0	2,3,3	3.21	2 (100%)

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
31	HEM	f	101	6,5	-	5/12/54/54	-
24	LFA	B	624	-	-	0/4/4/17	-
19	CLA	B	604	-	1/1/15/20	12/37/115/115	-
30	DGD	d	414	-	-	13/41/62/95	0/1/1/2
19	CLA	B	613	-	1/1/15/20	8/37/115/115	-
19	CLA	B	603	-	1/1/15/20	12/37/115/115	-
21	BCR	B	618	-	-	0/29/63/63	0/2/2/2
19	CLA	c	511	-	1/1/15/20	7/37/115/115	-
21	BCR	C	521	-	-	5/29/63/63	0/2/2/2
29	LMT	d	412	-	-	1/15/35/61	0/1/1/2
28	LMG	C	501	-	-	22/46/66/70	0/1/1/1
29	LMT	t	101	-	-	7/15/35/61	0/1/1/2
25	PLM	i	102	-	-	3/10/10/15	-
19	CLA	b	608	-	1/1/15/20	3/37/115/115	-
19	CLA	c	503	-	1/1/15/20	10/37/115/115	-
24	LFA	D	407	-	-	0/6/6/17	-
24	LFA	Z	101	-	-	1/5/5/17	-
25	PLM	i	101	-	-	3/13/13/15	-
28	LMG	B	620	-	-	18/46/66/70	0/1/1/1
19	CLA	b	613	-	1/1/15/20	3/37/115/115	-
25	PLM	C	520	-	-	0/6/6/15	-
21	BCR	B	619	-	-	3/29/63/63	0/2/2/2
24	LFA	M	103	-	-	1/7/7/17	-
24	LFA	A	412	-	-	2/12/12/17	-
24	LFA	b	624	-	-	1/9/9/17	-
31	HEM	F	101	6,5	-	2/12/54/54	-
19	CLA	c	508	33	1/1/15/20	6/37/115/115	-
24	LFA	a	413	-	-	1/8/8/17	-
19	CLA	c	514	-	1/1/15/20	4/37/115/115	-
29	LMT	d	401	-	-	2/20/60/61	0/2/2/2
27	LHG	a	415	-	-	15/50/50/53	-
19	CLA	b	617	-	1/1/15/20	7/37/115/115	-
24	LFA	D	406	-	-	3/10/10/17	-
24	LFA	K	102	-	-	0/4/4/17	-
19	CLA	B	607	33	1/1/15/20	4/37/115/115	-
24	LFA	B	621	-	-	4/10/10/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	D	409	-	1/1/15/20	11/37/115/115	-
25	PLM	a	414	-	-	6/9/9/15	-
24	LFA	J	102	-	-	2/14/14/17	-
19	CLA	b	603	33	1/1/15/20	15/37/115/115	-
21	BCR	b	601	-	-	9/29/63/63	0/2/2/2
21	BCR	B	629	-	-	10/29/63/63	0/2/2/2
19	CLA	B	605	-	1/1/15/20	8/37/115/115	-
27	LHG	A	417	-	-	16/50/50/53	-
24	LFA	b	629	-	-	1/6/6/17	-
27	LHG	D	413	-	-	14/53/53/53	-
28	LMG	b	622	-	-	23/46/66/70	0/1/1/1
25	PLM	A	413	-	-	4/15/15/15	-
19	CLA	d	404	-	1/1/15/20	4/37/115/115	-
30	DGD	c	517	-	-	18/51/91/95	0/2/2/2
20	PHO	D	401	-	-	4/37/103/103	0/5/6/6
19	CLA	D	408	-	1/1/15/20	4/37/115/115	-
19	CLA	a	408	-	1/1/15/20	10/37/115/115	-
19	CLA	d	405	-	1/1/15/20	9/37/115/115	-
21	BCR	D	410	-	-	8/29/63/63	0/2/2/2
25	PLM	b	628	-	-	2/11/11/15	-
27	LHG	d	408	-	-	8/53/53/53	-
29	LMT	D	403	-	-	7/15/35/61	0/1/1/2
24	LFA	i	105	-	-	0/8/8/17	-
19	CLA	B	601	33	1/1/15/20	15/37/115/115	-
22	SQD	a	410	-	-	21/49/69/69	0/1/1/1
19	CLA	B	609	-	1/1/15/20	4/37/115/115	-
25	PLM	I	104	-	-	5/8/8/15	-
19	CLA	A	403	-	1/1/15/20	7/37/115/115	-
19	CLA	C	514	-	1/1/15/20	8/37/115/115	-
19	CLA	b	618	-	1/1/15/20	14/37/115/115	-
30	DGD	D	415	-	-	16/38/58/95	0/1/1/2
28	LMG	c	518	-	-	15/46/66/70	0/1/1/1
19	CLA	B	608	-	1/1/15/20	8/37/115/115	-
19	CLA	C	506	33	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LFA	H	101	-	-	5/11/11/17	-
25	PLM	A	415	-	-	5/8/8/15	-
25	PLM	a	401	-	-	5/14/14/15	-
19	CLA	c	506	-	1/1/15/20	7/37/115/115	-
22	SQD	L	102	-	-	25/49/69/69	0/1/1/1
19	CLA	c	510	-	1/1/15/20	7/37/115/115	-
25	PLM	b	625	-	-	3/6/6/15	-
19	CLA	B	612	-	1/1/15/20	6/37/115/115	-
19	CLA	C	503	-	1/1/15/20	6/37/115/115	-
28	LMG	c	501	-	-	18/46/66/70	0/1/1/1
19	CLA	A	405	33	1/1/15/20	12/37/115/115	-
19	CLA	b	605	-	1/1/15/20	12/37/115/115	-
25	PLM	B	626	-	-	3/10/10/15	-
22	SQD	A	409	-	-	22/45/65/69	0/1/1/1
19	CLA	b	610	-	1/1/15/20	7/37/115/115	-
19	CLA	B	602	-	1/1/15/20	1/37/115/115	-
22	SQD	a	412	-	-	17/38/58/69	0/1/1/1
22	SQD	A	411	-	-	22/49/69/69	0/1/1/1
25	PLM	b	631	-	-	5/13/13/15	-
19	CLA	B	614	-	1/1/15/20	16/37/115/115	-
20	PHO	a	407	-	-	5/37/103/103	0/5/6/6
19	CLA	b	609	33	1/1/15/20	4/37/115/115	-
24	LFA	I	103	-	-	1/4/4/17	-
30	DGD	J	101	-	-	18/43/83/95	0/2/2/2
24	LFA	x	101	-	-	0/10/10/17	-
21	BCR	c	515	-	-	6/29/63/63	0/2/2/2
25	PLM	D	405	-	-	3/15/15/15	-
27	LHG	D	412	-	-	8/53/53/53	-
27	LHG	a	416	-	-	21/53/53/53	-
32	RRX	H	102	-	-	2/29/65/65	0/2/2/2
21	BCR	a	409	-	-	3/29/63/63	0/2/2/2
21	BCR	y	101	-	-	8/29/63/63	0/2/2/2
29	LMT	m	102	-	-	4/21/61/61	0/2/2/2
19	CLA	b	612	33	1/1/15/20	7/37/115/115	-
23	PL9	D	411	-	-	11/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	i	103	-	-	7/21/61/61	0/2/2/2
24	LFA	X	101	-	-	3/10/10/17	-
22	SQD	f	102	-	-	18/40/60/69	0/1/1/1
30	DGD	H	103	-	-	12/51/91/95	0/2/2/2
19	CLA	c	504	-	1/1/15/20	7/37/115/115	-
25	PLM	B	623	-	-	0/9/9/15	-
19	CLA	c	502	-	1/1/15/20	6/37/115/115	-
19	CLA	C	512	-	1/1/15/20	7/37/115/115	-
21	BCR	b	619	-	-	5/29/63/63	0/2/2/2
21	BCR	C	516	-	-	6/29/63/63	0/2/2/2
19	CLA	b	607	-	1/1/15/20	8/37/115/115	-
19	CLA	b	614	-	1/1/15/20	6/37/115/115	-
24	LFA	B	628	-	-	2/4/4/17	-
24	LFA	d	413	-	-	0/5/5/17	-
20	PHO	d	402	-	-	4/37/103/103	0/5/6/6
21	BCR	b	620	-	-	1/29/63/63	0/2/2/2
30	DGD	c	516	-	-	21/51/91/95	0/2/2/2
19	CLA	C	509	33	1/1/15/20	12/37/115/115	-
30	DGD	c	519	-	-	11/51/91/95	0/2/2/2
21	BCR	B	617	-	-	5/29/63/63	0/2/2/2
25	PLM	B	622	-	-	2/5/5/15	-
21	BCR	k	101	-	-	7/29/63/63	0/2/2/2
22	SQD	F	102	-	-	20/33/33/69	-
24	LFA	d	411	-	-	0/12/12/17	-
19	CLA	C	511	-	1/1/15/20	8/37/115/115	-
19	CLA	C	515	-	1/1/15/20	4/37/115/115	-
19	CLA	a	406	33	1/1/15/20	11/37/115/115	-
24	LFA	A	414	-	-	2/10/10/17	-
29	LMT	m	101	-	-	11/21/61/61	0/2/2/2
19	CLA	c	513	-	1/1/15/20	8/37/115/115	-
19	CLA	B	616	-	1/1/15/20	14/37/115/115	-
24	LFA	C	519	-	-	0/4/4/17	-
19	CLA	C	508	-	1/1/15/20	18/37/115/115	-
19	CLA	C	510	-	1/1/15/20	5/37/115/115	-
21	BCR	c	520	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LFA	h	101	-	-	0/5/5/17	-
25	PLM	b	623	-	-	3/15/15/15	-
28	LMG	D	414	-	-	12/43/63/70	0/1/1/1
24	LFA	b	626	-	-	2/8/8/17	-
25	PLM	H	105	-	-	2/7/7/15	-
19	CLA	b	604	-	1/1/15/20	6/37/115/115	-
25	PLM	I	102	-	-	4/15/15/15	-
24	LFA	H	104	-	-	0/3/3/17	-
19	CLA	b	606	-	1/1/15/20	5/37/115/115	-
21	BCR	K	101	-	-	7/29/63/63	0/2/2/2
24	LFA	m	103	-	-	1/6/6/17	-
24	LFA	D	404	-	-	4/13/13/17	-
25	PLM	E	101	-	-	7/15/15/15	-
25	PLM	b	630	-	-	2/10/10/15	-
19	CLA	c	509	-	1/1/15/20	6/37/115/115	-
29	LMT	C	502	-	-	4/16/56/61	0/2/2/2
24	LFA	k	102	-	-	0/4/4/17	-
19	CLA	a	405	33	1/1/15/20	3/37/115/115	-
19	CLA	B	611	-	1/1/15/20	3/37/115/115	-
19	CLA	B	615	-	1/1/15/20	6/37/115/115	-
19	CLA	C	505	-	1/1/15/20	6/37/115/115	-
21	BCR	Y	101	-	-	7/29/63/63	0/2/2/2
19	CLA	b	615	-	1/1/15/20	8/37/115/115	-
28	LMG	d	410	-	-	14/46/66/70	0/1/1/1
29	LMT	M	101	-	-	7/21/61/61	0/2/2/2
25	PLM	B	627	-	-	3/13/13/15	-
20	PHO	A	406	-	-	4/37/103/103	0/5/6/6
19	CLA	c	505	33	1/1/15/20	8/37/115/115	-
19	CLA	C	507	-	1/1/15/20	7/37/115/115	-
23	PL9	a	411	-	-	30/53/73/73	0/1/1/1
21	BCR	d	406	-	-	8/29/63/63	0/2/2/2
24	LFA	B	625	-	-	3/8/8/17	-
24	LFA	h	103	-	-	0/3/3/17	-
29	LMT	D	402	-	-	6/21/61/61	0/2/2/2
29	LMT	z	101	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LFA	b	632	-	-	2/4/4/17	-
19	CLA	C	504	-	1/1/15/20	10/37/115/115	-
32	RRX	x	102	-	-	2/29/65/65	0/2/2/2
30	DGD	h	102	-	-	13/51/91/95	0/2/2/2
19	CLA	c	507	-	1/1/15/20	18/37/115/115	-
21	BCR	b	621	-	-	3/29/63/63	0/2/2/2
23	PL9	A	410	-	-	21/53/73/73	0/1/1/1
24	LFA	h	104	-	-	1/4/4/17	-
25	PLM	i	104	-	-	5/10/10/15	-
25	PLM	I	101	-	-	6/13/13/15	-
19	CLA	B	610	33	1/1/15/20	7/37/115/115	-
19	CLA	C	513	3	1/1/15/20	6/37/115/115	-
27	LHG	L	101	-	-	18/53/53/53	-
28	LMG	C	518	-	-	19/37/57/70	0/1/1/1
19	CLA	A	407	-	1/1/15/20	10/37/115/115	-
19	CLA	c	512	3	1/1/15/20	6/37/115/115	-
19	CLA	b	611	-	1/1/15/20	4/37/115/115	-
24	LFA	b	627	-	-	0/6/6/17	-
27	LHG	l	101	-	-	25/53/53/53	-
29	LMT	M	102	-	-	4/21/61/61	0/2/2/2
25	PLM	e	101	-	-	3/15/15/15	-
19	CLA	a	404	-	1/1/15/20	7/37/115/115	-
19	CLA	B	606	-	1/1/15/20	3/37/115/115	-
19	CLA	A	404	33	1/1/15/20	3/37/115/115	-
30	DGD	C	517	-	-	22/51/91/95	0/2/2/2
22	SQD	l	102	-	-	26/49/69/69	0/1/1/1
29	LMT	b	602	-	-	8/11/31/61	0/1/1/2
23	PL9	d	407	-	-	6/53/73/73	0/1/1/1
19	CLA	b	616	-	1/1/15/20	14/37/115/115	-
27	LHG	d	409	-	-	14/53/53/53	-
21	BCR	A	408	-	-	3/29/63/63	0/2/2/2

All (543) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	601	CLA	C4B-NB	7.42	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	612	CLA	C4B-NB	7.36	1.41	1.35
19	B	610	CLA	C4B-NB	7.35	1.41	1.35
19	B	609	CLA	C4B-NB	7.34	1.41	1.35
19	b	611	CLA	C4B-NB	7.34	1.41	1.35
19	c	502	CLA	C4B-NB	7.33	1.41	1.35
19	C	503	CLA	C4B-NB	7.33	1.41	1.35
19	b	603	CLA	C4B-NB	7.30	1.41	1.35
19	B	605	CLA	C4B-NB	7.21	1.41	1.35
19	C	505	CLA	C4B-NB	7.17	1.41	1.35
19	b	607	CLA	C4B-NB	7.17	1.41	1.35
19	B	604	CLA	C4B-NB	7.16	1.41	1.35
19	b	606	CLA	C4B-NB	7.12	1.41	1.35
19	C	514	CLA	C4B-NB	7.11	1.41	1.35
19	b	608	CLA	C4B-NB	7.09	1.41	1.35
19	C	507	CLA	C4B-NB	7.09	1.41	1.35
19	c	506	CLA	C4B-NB	7.09	1.41	1.35
19	c	507	CLA	C4B-NB	7.08	1.41	1.35
22	F	102	SQD	O47-C45	-7.07	1.38	1.46
19	C	506	CLA	C4B-NB	7.07	1.41	1.35
19	c	505	CLA	C4B-NB	7.06	1.41	1.35
19	C	512	CLA	C4B-NB	7.06	1.41	1.35
19	c	513	CLA	C4B-NB	7.06	1.41	1.35
19	B	607	CLA	C4B-NB	7.05	1.41	1.35
19	c	504	CLA	C4B-NB	7.05	1.41	1.35
19	C	513	CLA	C4B-NB	7.03	1.41	1.35
19	b	609	CLA	C4B-NB	7.02	1.41	1.35
19	c	512	CLA	C4B-NB	7.01	1.41	1.35
19	d	404	CLA	C4B-NB	6.99	1.41	1.35
19	C	508	CLA	C4B-NB	6.99	1.41	1.35
19	B	611	CLA	C4B-NB	6.98	1.41	1.35
19	c	511	CLA	C4B-NB	6.96	1.41	1.35
19	c	509	CLA	C4B-NB	6.96	1.41	1.35
19	C	510	CLA	C4B-NB	6.95	1.41	1.35
19	B	615	CLA	C4B-NB	6.93	1.41	1.35
19	B	603	CLA	C4B-NB	6.93	1.41	1.35
19	b	605	CLA	C4B-NB	6.93	1.41	1.35
19	D	408	CLA	C4B-NB	6.93	1.41	1.35
19	b	613	CLA	C4B-NB	6.92	1.41	1.35
19	B	606	CLA	C4B-NB	6.91	1.41	1.35
19	A	407	CLA	C4B-NB	6.91	1.41	1.35
19	B	602	CLA	C4B-NB	6.89	1.41	1.35
19	b	604	CLA	C4B-NB	6.89	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	610	CLA	C4B-NB	6.89	1.41	1.35
19	B	614	CLA	C4B-NB	6.87	1.41	1.35
19	C	509	CLA	C4B-NB	6.86	1.41	1.35
19	d	405	CLA	C4B-NB	6.85	1.41	1.35
19	C	515	CLA	C4B-NB	6.85	1.41	1.35
19	D	409	CLA	C4B-NB	6.85	1.41	1.35
19	B	608	CLA	C4B-NB	6.84	1.41	1.35
19	C	504	CLA	C4B-NB	6.83	1.41	1.35
19	b	617	CLA	C4B-NB	6.83	1.41	1.35
19	a	408	CLA	C4B-NB	6.81	1.41	1.35
19	C	511	CLA	C4B-NB	6.79	1.41	1.35
19	c	510	CLA	C4B-NB	6.77	1.41	1.35
19	b	615	CLA	C4B-NB	6.76	1.41	1.35
19	b	616	CLA	C4B-NB	6.75	1.41	1.35
19	A	403	CLA	C4B-NB	6.74	1.41	1.35
19	c	503	CLA	C4B-NB	6.74	1.41	1.35
19	a	405	CLA	C4B-NB	6.72	1.41	1.35
19	B	613	CLA	C4B-NB	6.71	1.41	1.35
19	a	404	CLA	C4B-NB	6.69	1.41	1.35
19	c	508	CLA	C4B-NB	6.68	1.41	1.35
19	B	612	CLA	C4B-NB	6.67	1.41	1.35
19	A	404	CLA	C4B-NB	6.63	1.41	1.35
19	A	405	CLA	C4B-NB	6.58	1.41	1.35
19	b	614	CLA	C4B-NB	6.58	1.41	1.35
19	c	514	CLA	C4B-NB	6.57	1.41	1.35
19	a	406	CLA	C4B-NB	6.57	1.41	1.35
19	B	616	CLA	C4B-NB	6.53	1.41	1.35
19	b	618	CLA	C4B-NB	6.48	1.41	1.35
22	F	102	SQD	C6-S	4.94	1.84	1.77
22	f	102	SQD	O48-C23	4.80	1.47	1.33
22	F	102	SQD	O47-C7	4.77	1.43	1.33
23	d	407	PL9	C7-C3	-4.74	1.46	1.51
23	D	411	PL9	C7-C3	-4.71	1.46	1.51
22	F	102	SQD	O48-C23	4.69	1.47	1.33
22	A	411	SQD	O48-C23	4.69	1.47	1.33
22	a	410	SQD	O48-C23	4.63	1.46	1.33
22	A	409	SQD	O48-C23	4.62	1.46	1.33
22	a	412	SQD	O48-C23	4.57	1.46	1.33
22	l	102	SQD	O48-C23	4.45	1.46	1.33
22	L	102	SQD	O48-C23	4.44	1.46	1.33
23	a	411	PL9	C7-C3	-4.05	1.47	1.51
31	f	101	HEM	C3C-CAC	4.01	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	F	101	HEM	C3C-CAC	3.95	1.55	1.47
19	B	601	CLA	C1D-ND	3.92	1.42	1.37
19	b	603	CLA	C1D-ND	3.91	1.42	1.37
19	C	505	CLA	C1D-ND	3.77	1.42	1.37
19	B	616	CLA	C1D-ND	3.77	1.42	1.37
23	d	407	PL9	C3-C4	-3.76	1.43	1.49
23	D	411	PL9	C3-C4	-3.75	1.43	1.49
19	C	515	CLA	C1D-ND	3.71	1.42	1.37
19	b	615	CLA	C1D-ND	3.71	1.42	1.37
19	c	504	CLA	C1D-ND	3.70	1.42	1.37
19	A	405	CLA	C1D-ND	3.70	1.42	1.37
19	b	618	CLA	C1D-ND	3.70	1.42	1.37
31	f	101	HEM	C3C-C2C	-3.69	1.35	1.40
19	c	503	CLA	C1D-ND	3.68	1.42	1.37
19	a	406	CLA	C1D-ND	3.67	1.42	1.37
19	b	606	CLA	C1D-ND	3.65	1.42	1.37
19	c	512	CLA	C1D-ND	3.64	1.42	1.37
19	A	407	CLA	C1D-ND	3.64	1.42	1.37
19	C	513	CLA	C1D-ND	3.64	1.42	1.37
19	B	602	CLA	C1D-ND	3.64	1.42	1.37
19	b	604	CLA	C1D-ND	3.63	1.42	1.37
19	B	605	CLA	C1D-ND	3.63	1.42	1.37
19	C	509	CLA	C1D-ND	3.62	1.42	1.37
19	d	405	CLA	C1D-ND	3.62	1.42	1.37
19	B	613	CLA	C1D-ND	3.61	1.42	1.37
19	b	611	CLA	C1D-ND	3.61	1.42	1.37
19	c	508	CLA	C1D-ND	3.61	1.42	1.37
19	c	505	CLA	C1D-ND	3.60	1.42	1.37
19	B	604	CLA	C1D-ND	3.60	1.42	1.37
19	C	512	CLA	C1D-ND	3.59	1.42	1.37
19	C	508	CLA	C1D-ND	3.59	1.42	1.37
19	C	506	CLA	C1D-ND	3.59	1.42	1.37
19	a	408	CLA	C1D-ND	3.58	1.42	1.37
19	b	607	CLA	C1D-ND	3.58	1.42	1.37
19	c	511	CLA	C1D-ND	3.58	1.42	1.37
19	C	503	CLA	C1D-ND	3.58	1.42	1.37
31	F	101	HEM	C3C-C2C	-3.57	1.35	1.40
19	A	404	CLA	C1D-ND	3.56	1.42	1.37
19	B	606	CLA	C1D-ND	3.56	1.42	1.37
19	B	609	CLA	C1D-ND	3.56	1.42	1.37
19	c	502	CLA	C1D-ND	3.55	1.42	1.37
19	b	616	CLA	C1D-ND	3.55	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	102	SQD	O47-C7	3.55	1.44	1.34
19	B	614	CLA	C1D-ND	3.55	1.42	1.37
19	a	405	CLA	C1D-ND	3.55	1.42	1.37
19	c	509	CLA	C1D-ND	3.55	1.42	1.37
19	c	514	CLA	C1D-ND	3.54	1.42	1.37
19	D	409	CLA	C1D-ND	3.53	1.42	1.37
19	a	404	CLA	C1D-ND	3.53	1.42	1.37
22	l	102	SQD	O47-C7	3.53	1.44	1.34
19	b	612	CLA	C1D-ND	3.52	1.42	1.37
22	a	410	SQD	O47-C45	-3.52	1.37	1.46
22	F	102	SQD	O5-C1	3.51	1.50	1.40
19	B	607	CLA	C1D-ND	3.51	1.42	1.37
22	A	409	SQD	O47-C45	-3.51	1.37	1.46
19	C	504	CLA	C1D-ND	3.50	1.42	1.37
22	A	411	SQD	O47-C45	-3.50	1.37	1.46
19	C	510	CLA	C1D-ND	3.50	1.42	1.37
19	b	608	CLA	C1D-ND	3.49	1.42	1.37
19	B	608	CLA	C1D-ND	3.49	1.42	1.37
19	B	611	CLA	C4D-ND	-3.49	1.32	1.37
19	b	613	CLA	C4D-ND	-3.49	1.32	1.37
19	b	609	CLA	C1D-ND	3.47	1.42	1.37
19	B	615	CLA	C1D-ND	3.47	1.42	1.37
19	b	613	CLA	C1D-ND	3.46	1.42	1.37
22	a	412	SQD	O5-C1	3.45	1.50	1.41
19	B	610	CLA	C1D-ND	3.44	1.42	1.37
22	A	411	SQD	O5-C1	3.44	1.50	1.41
19	C	511	CLA	C1D-ND	3.43	1.42	1.37
22	f	102	SQD	O47-C45	-3.43	1.38	1.46
19	c	507	CLA	C1D-ND	3.43	1.42	1.37
19	b	617	CLA	C1D-ND	3.43	1.42	1.37
19	A	403	CLA	C1D-ND	3.42	1.42	1.37
19	b	610	CLA	C1D-ND	3.41	1.42	1.37
22	a	412	SQD	O47-C45	-3.40	1.38	1.46
19	B	611	CLA	C1D-ND	3.40	1.42	1.37
19	b	610	CLA	C4D-ND	-3.39	1.33	1.37
19	c	510	CLA	C1D-ND	3.39	1.42	1.37
19	b	614	CLA	C4D-ND	-3.39	1.33	1.37
23	A	410	PL9	C7-C3	-3.38	1.47	1.51
19	c	513	CLA	C1D-ND	3.38	1.41	1.37
22	f	102	SQD	O47-C7	3.38	1.43	1.34
19	B	612	CLA	C4D-ND	-3.34	1.33	1.37
19	c	511	CLA	C4D-ND	-3.33	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	408	CLA	C4D-ND	-3.32	1.33	1.37
19	B	616	CLA	C4D-ND	-3.32	1.33	1.37
19	B	608	CLA	C4D-ND	-3.32	1.33	1.37
19	d	404	CLA	C4D-ND	-3.31	1.33	1.37
22	f	102	SQD	O5-C1	3.31	1.50	1.41
19	B	607	CLA	C4D-ND	-3.31	1.33	1.37
19	C	514	CLA	C1D-ND	3.30	1.41	1.37
19	c	503	CLA	C4D-ND	-3.30	1.33	1.37
19	b	618	CLA	C4D-ND	-3.30	1.33	1.37
19	B	610	CLA	C4D-ND	-3.30	1.33	1.37
19	a	406	CLA	C4D-ND	-3.30	1.33	1.37
19	A	405	CLA	C4D-ND	-3.29	1.33	1.37
22	l	102	SQD	O5-C1	3.29	1.50	1.41
22	a	412	SQD	O47-C7	3.29	1.43	1.34
19	b	615	CLA	C4D-ND	-3.28	1.33	1.37
19	C	504	CLA	C4D-ND	-3.28	1.33	1.37
19	b	607	CLA	C4D-ND	-3.28	1.33	1.37
19	c	509	CLA	C4D-ND	-3.27	1.33	1.37
19	B	614	CLA	C4D-ND	-3.27	1.33	1.37
19	B	606	CLA	C4D-ND	-3.26	1.33	1.37
19	b	616	CLA	C4D-ND	-3.26	1.33	1.37
19	B	613	CLA	C4D-ND	-3.26	1.33	1.37
19	b	608	CLA	C4D-ND	-3.26	1.33	1.37
19	a	405	CLA	C4D-ND	-3.26	1.33	1.37
19	C	507	CLA	C1D-ND	3.24	1.41	1.37
19	b	612	CLA	C4D-ND	-3.24	1.33	1.37
19	B	603	CLA	C1D-ND	3.24	1.41	1.37
19	c	506	CLA	C1D-ND	3.24	1.41	1.37
19	A	404	CLA	C4D-ND	-3.24	1.33	1.37
19	C	510	CLA	C4D-ND	-3.24	1.33	1.37
19	b	609	CLA	C4D-ND	-3.23	1.33	1.37
19	c	504	CLA	C4D-ND	-3.23	1.33	1.37
22	L	102	SQD	O5-C1	3.22	1.50	1.41
19	B	605	CLA	C4D-ND	-3.22	1.33	1.37
19	C	509	CLA	C4D-ND	-3.22	1.33	1.37
19	b	604	CLA	C4D-ND	-3.22	1.33	1.37
19	C	512	CLA	C4D-ND	-3.21	1.33	1.37
22	A	411	SQD	O47-C7	3.21	1.43	1.34
19	C	505	CLA	C4D-ND	-3.20	1.33	1.37
19	c	508	CLA	C4D-ND	-3.20	1.33	1.37
19	C	506	CLA	C4D-ND	-3.19	1.33	1.37
22	A	409	SQD	O47-C7	3.18	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	c	510	CLA	CHC-C1C	3.18	1.43	1.35
19	C	507	CLA	C4D-ND	-3.17	1.33	1.37
22	f	102	SQD	C24-C23	3.17	1.60	1.50
22	a	410	SQD	O47-C7	3.17	1.43	1.34
19	b	605	CLA	C1D-ND	3.17	1.41	1.37
19	C	510	CLA	CHC-C1C	3.17	1.43	1.35
31	F	101	HEM	CAB-C3B	3.17	1.56	1.47
19	c	505	CLA	C4D-ND	-3.16	1.33	1.37
19	a	404	CLA	C4D-ND	-3.15	1.33	1.37
19	b	611	CLA	C4D-ND	-3.15	1.33	1.37
19	C	515	CLA	CHC-C1C	3.15	1.43	1.35
19	A	403	CLA	C4D-ND	-3.15	1.33	1.37
19	A	407	CLA	C4D-ND	-3.15	1.33	1.37
19	C	511	CLA	CHC-C1C	3.15	1.43	1.35
31	f	101	HEM	CAB-C3B	3.14	1.56	1.47
19	c	502	CLA	CHC-C1C	3.14	1.43	1.35
19	b	617	CLA	C4D-ND	-3.14	1.33	1.37
19	D	409	CLA	C4D-ND	-3.13	1.33	1.37
19	c	507	CLA	C4D-ND	-3.13	1.33	1.37
19	c	506	CLA	C4D-ND	-3.12	1.33	1.37
19	B	602	CLA	C4D-ND	-3.12	1.33	1.37
19	B	609	CLA	C4D-ND	-3.12	1.33	1.37
19	A	407	CLA	CHC-C1C	3.12	1.43	1.35
19	C	505	CLA	CHC-C1C	3.12	1.43	1.35
19	C	508	CLA	C4D-ND	-3.11	1.33	1.37
19	C	514	CLA	CHC-C1C	3.11	1.42	1.35
19	c	514	CLA	C4D-ND	-3.11	1.33	1.37
19	c	509	CLA	CHC-C1C	3.11	1.42	1.35
19	B	602	CLA	CHC-C1C	3.11	1.42	1.35
19	c	513	CLA	CHC-C1C	3.10	1.42	1.35
19	b	616	CLA	CHC-C1C	3.10	1.42	1.35
19	b	604	CLA	CHC-C1C	3.10	1.42	1.35
19	B	615	CLA	C4D-ND	-3.09	1.33	1.37
19	d	405	CLA	C4D-ND	-3.09	1.33	1.37
19	a	408	CLA	CHC-C1C	3.09	1.42	1.35
19	B	614	CLA	CHC-C1C	3.09	1.42	1.35
19	c	504	CLA	CHC-C1C	3.08	1.42	1.35
19	b	612	CLA	CHC-C1C	3.08	1.42	1.35
19	B	603	CLA	CHC-C1C	3.08	1.42	1.35
19	C	507	CLA	CHC-C1C	3.08	1.42	1.35
19	B	613	CLA	CHC-C1C	3.08	1.42	1.35
19	D	408	CLA	C1D-ND	3.08	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	409	CLA	CHC-C1C	3.08	1.42	1.35
19	d	405	CLA	CHC-C1C	3.07	1.42	1.35
19	C	513	CLA	CHC-C1C	3.07	1.42	1.35
19	a	408	CLA	C4D-ND	-3.07	1.33	1.37
19	C	503	CLA	CHC-C1C	3.07	1.42	1.35
19	c	514	CLA	CHC-C1C	3.07	1.42	1.35
19	B	607	CLA	CHC-C1C	3.06	1.42	1.35
19	b	610	CLA	CHC-C1C	3.06	1.42	1.35
19	b	614	CLA	CHC-C1C	3.06	1.42	1.35
19	B	609	CLA	CHC-C1C	3.06	1.42	1.35
19	b	615	CLA	CHC-C1C	3.05	1.42	1.35
19	b	606	CLA	C4D-ND	-3.05	1.33	1.37
19	b	609	CLA	CHC-C1C	3.05	1.42	1.35
19	b	605	CLA	CHC-C1C	3.05	1.42	1.35
22	A	411	SQD	C24-C23	3.05	1.59	1.50
19	c	506	CLA	CHC-C1C	3.05	1.42	1.35
19	c	507	CLA	CHC-C1C	3.05	1.42	1.35
19	C	508	CLA	CHC-C1C	3.05	1.42	1.35
19	c	502	CLA	C4D-ND	-3.04	1.33	1.37
19	C	514	CLA	C4D-ND	-3.04	1.33	1.37
22	a	410	SQD	C24-C23	3.04	1.59	1.50
19	C	515	CLA	C4D-ND	-3.04	1.33	1.37
19	b	603	CLA	CHC-C1C	3.04	1.42	1.35
19	B	610	CLA	CHC-C1C	3.04	1.42	1.35
19	B	601	CLA	CHC-C1C	3.04	1.42	1.35
19	B	604	CLA	C4D-ND	-3.03	1.33	1.37
19	c	512	CLA	C4D-ND	-3.03	1.33	1.37
19	b	611	CLA	CHC-C1C	3.03	1.42	1.35
22	a	412	SQD	C24-C23	3.03	1.59	1.50
19	B	606	CLA	CHC-C1C	3.03	1.42	1.35
19	B	612	CLA	CHC-C1C	3.03	1.42	1.35
19	C	511	CLA	C4D-ND	-3.03	1.33	1.37
19	d	404	CLA	CHC-C1C	3.02	1.42	1.35
19	b	608	CLA	CHC-C1C	3.02	1.42	1.35
19	B	608	CLA	CHC-C1C	3.02	1.42	1.35
19	B	611	CLA	CHC-C1C	3.02	1.42	1.35
19	c	513	CLA	C4D-ND	-3.02	1.33	1.37
19	D	408	CLA	CHC-C1C	3.02	1.42	1.35
19	C	513	CLA	C4D-ND	-3.01	1.33	1.37
19	b	613	CLA	CHC-C1C	3.00	1.42	1.35
22	a	410	SQD	O5-C1	3.00	1.49	1.41
19	B	612	CLA	C1D-ND	3.00	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	409	SQD	C24-C23	3.00	1.59	1.50
22	F	102	SQD	C24-C23	2.99	1.59	1.50
19	c	510	CLA	C4D-ND	-2.99	1.33	1.37
19	A	403	CLA	CHC-C1C	2.99	1.42	1.35
19	A	405	CLA	CHC-C1C	2.99	1.42	1.35
19	a	404	CLA	CHC-C1C	2.99	1.42	1.35
22	l	102	SQD	O47-C45	-2.99	1.39	1.46
19	b	607	CLA	CHC-C1C	2.99	1.42	1.35
19	C	512	CLA	CHC-C1C	2.98	1.42	1.35
19	C	503	CLA	C4D-ND	-2.98	1.33	1.37
19	d	404	CLA	C1D-ND	2.98	1.41	1.37
19	c	511	CLA	CHC-C1C	2.98	1.42	1.35
19	a	406	CLA	CHC-C1C	2.98	1.42	1.35
19	c	512	CLA	CHC-C1C	2.98	1.42	1.35
19	C	504	CLA	CHC-C1C	2.96	1.42	1.35
19	b	617	CLA	CHC-C1C	2.96	1.42	1.35
22	L	102	SQD	O47-C45	-2.96	1.39	1.46
19	B	605	CLA	CHC-C1C	2.95	1.42	1.35
19	B	603	CLA	C4D-ND	-2.95	1.33	1.37
19	c	503	CLA	CHC-C1C	2.95	1.42	1.35
19	B	616	CLA	CHC-C1C	2.95	1.42	1.35
19	C	506	CLA	CHC-C1C	2.95	1.42	1.35
19	B	601	CLA	C4D-ND	-2.95	1.33	1.37
22	l	102	SQD	C24-C23	2.94	1.59	1.50
19	b	605	CLA	C4D-ND	-2.94	1.33	1.37
19	c	505	CLA	CHC-C1C	2.94	1.42	1.35
19	b	618	CLA	CHC-C1C	2.94	1.42	1.35
22	A	409	SQD	O5-C1	2.93	1.49	1.41
22	L	102	SQD	C24-C23	2.93	1.59	1.50
23	A	410	PL9	C3-C4	-2.92	1.44	1.49
19	B	615	CLA	CHC-C1C	2.92	1.42	1.35
23	a	411	PL9	C3-C4	-2.92	1.44	1.49
19	b	614	CLA	C1D-ND	2.91	1.41	1.37
19	b	603	CLA	C4D-ND	-2.90	1.33	1.37
19	c	508	CLA	CHC-C1C	2.89	1.42	1.35
19	A	404	CLA	CHC-C1C	2.88	1.42	1.35
19	C	509	CLA	CHC-C1C	2.87	1.42	1.35
19	a	405	CLA	CHC-C1C	2.86	1.42	1.35
19	b	606	CLA	CMB-C2B	-2.85	1.45	1.51
19	B	604	CLA	CMB-C2B	-2.83	1.45	1.51
19	C	508	CLA	CMB-C2B	-2.81	1.45	1.51
19	b	606	CLA	CHC-C1C	2.81	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	c	507	CLA	CMB-C2B	-2.77	1.45	1.51
19	B	604	CLA	CHC-C1C	2.77	1.42	1.35
19	b	605	CLA	CMB-C2B	-2.65	1.46	1.51
23	D	411	PL9	C6-C1	-2.63	1.43	1.48
19	C	507	CLA	CMD-C2D	-2.63	1.45	1.50
19	B	609	CLA	CMB-C2B	-2.62	1.46	1.51
19	b	611	CLA	CMB-C2B	-2.62	1.46	1.51
19	B	603	CLA	CMB-C2B	-2.61	1.46	1.51
23	d	407	PL9	C6-C1	-2.60	1.44	1.48
19	c	506	CLA	CMD-C2D	-2.58	1.45	1.50
19	c	502	CLA	CMB-C2B	-2.57	1.46	1.51
19	b	614	CLA	CMD-C2D	-2.57	1.45	1.50
19	A	404	CLA	CMB-C2B	-2.57	1.46	1.51
19	b	610	CLA	CMB-C2B	-2.57	1.46	1.51
19	b	613	CLA	CMB-C2B	-2.57	1.46	1.51
19	B	612	CLA	CMD-C2D	-2.55	1.45	1.50
19	b	615	CLA	CMB-C2B	-2.54	1.46	1.51
19	B	608	CLA	CMB-C2B	-2.54	1.46	1.51
19	B	613	CLA	CMB-C2B	-2.54	1.46	1.51
19	c	511	CLA	CMB-C2B	-2.53	1.46	1.51
19	a	404	CLA	CMD-C2D	-2.52	1.45	1.50
19	C	512	CLA	CMB-C2B	-2.52	1.46	1.51
19	D	408	CLA	CMD-C2D	-2.52	1.45	1.50
19	b	618	CLA	CMC-C2C	-2.52	1.45	1.50
19	A	407	CLA	CMB-C2B	-2.52	1.46	1.51
19	B	603	CLA	CMD-C2D	-2.52	1.45	1.50
19	B	616	CLA	CMC-C2C	-2.51	1.45	1.50
19	a	405	CLA	CMB-C2B	-2.51	1.46	1.51
19	A	403	CLA	CMD-C2D	-2.51	1.45	1.50
19	B	610	CLA	CMB-C2B	-2.50	1.46	1.51
19	b	612	CLA	CMB-C2B	-2.50	1.46	1.51
19	B	611	CLA	CMB-C2B	-2.50	1.46	1.51
19	b	607	CLA	CMB-C2B	-2.50	1.46	1.51
19	C	503	CLA	CMB-C2B	-2.50	1.46	1.51
19	b	616	CLA	CMB-C2B	-2.50	1.46	1.51
19	a	404	CLA	CMB-C2B	-2.49	1.46	1.51
19	c	508	CLA	CMB-C2B	-2.49	1.46	1.51
19	b	605	CLA	CMD-C2D	-2.49	1.45	1.50
19	c	509	CLA	CMB-C2B	-2.49	1.46	1.51
19	A	403	CLA	CMB-C2B	-2.48	1.46	1.51
19	c	503	CLA	CMB-C2B	-2.48	1.46	1.51
19	d	404	CLA	CMD-C2D	-2.48	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	604	CLA	CMD-C2D	-2.47	1.45	1.50
19	C	507	CLA	CMB-C2B	-2.47	1.46	1.51
19	b	603	CLA	CMB-C2B	-2.47	1.46	1.51
19	c	506	CLA	CMB-C2B	-2.45	1.46	1.51
19	B	606	CLA	CMB-C2B	-2.45	1.46	1.51
19	B	615	CLA	CMB-C2B	-2.45	1.46	1.51
19	C	509	CLA	CMB-C2B	-2.45	1.46	1.51
19	B	601	CLA	CMB-C2B	-2.45	1.46	1.51
19	b	614	CLA	CMB-C2B	-2.45	1.46	1.51
19	b	617	CLA	CMB-C2B	-2.45	1.46	1.51
19	c	512	CLA	CMB-C2B	-2.45	1.46	1.51
19	C	510	CLA	CMB-C2B	-2.45	1.46	1.51
19	c	505	CLA	CMB-C2B	-2.45	1.46	1.51
19	B	605	CLA	CMB-C2B	-2.44	1.46	1.51
19	D	408	CLA	CMB-C2B	-2.44	1.46	1.51
19	d	404	CLA	CMB-C2B	-2.44	1.46	1.51
19	a	408	CLA	CMB-C2B	-2.44	1.46	1.51
19	C	506	CLA	CMB-C2B	-2.43	1.46	1.51
19	C	504	CLA	CMB-C2B	-2.43	1.46	1.51
19	B	614	CLA	CMB-C2B	-2.43	1.46	1.51
19	b	606	CLA	CMD-C2D	-2.43	1.45	1.50
19	C	513	CLA	CMB-C2B	-2.42	1.46	1.51
19	d	405	CLA	CMB-C2B	-2.42	1.46	1.51
19	D	409	CLA	CMB-C2B	-2.42	1.46	1.51
19	c	504	CLA	CMB-C2B	-2.41	1.46	1.51
19	C	514	CLA	CMB-C2B	-2.41	1.46	1.51
19	B	607	CLA	CMB-C2B	-2.41	1.46	1.51
19	B	612	CLA	CMB-C2B	-2.41	1.46	1.51
19	c	513	CLA	CMB-C2B	-2.41	1.46	1.51
19	B	602	CLA	CMB-C2B	-2.40	1.46	1.51
19	b	609	CLA	CMB-C2B	-2.39	1.46	1.51
19	C	505	CLA	CMB-C2B	-2.39	1.46	1.51
23	d	407	PL9	C52-C5	-2.39	1.45	1.50
19	b	608	CLA	CMB-C2B	-2.38	1.46	1.51
23	D	411	PL9	C52-C5	-2.37	1.45	1.50
19	b	604	CLA	CMB-C2B	-2.36	1.46	1.51
19	a	406	CLA	CMB-C2B	-2.35	1.46	1.51
19	C	512	CLA	CMD-C2D	-2.34	1.45	1.50
19	C	504	CLA	CMC-C2C	-2.33	1.45	1.50
19	b	618	CLA	CMB-C2B	-2.32	1.46	1.51
19	c	511	CLA	CMD-C2D	-2.32	1.45	1.50
19	C	511	CLA	CMB-C2B	-2.32	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	410	PL9	C53-C6	-2.32	1.45	1.50
19	c	503	CLA	CMC-C2C	-2.31	1.45	1.50
19	B	616	CLA	CMB-C2B	-2.31	1.46	1.51
19	A	405	CLA	CMB-C2B	-2.29	1.46	1.51
19	C	515	CLA	CMB-C2B	-2.29	1.46	1.51
19	b	610	CLA	CMD-C2D	-2.29	1.46	1.50
19	b	608	CLA	CMC-C2C	-2.27	1.46	1.50
19	B	608	CLA	CMD-C2D	-2.25	1.46	1.50
23	a	411	PL9	C53-C6	-2.24	1.46	1.50
19	C	510	CLA	CMC-C2C	-2.24	1.46	1.50
19	c	509	CLA	CMC-C2C	-2.24	1.46	1.50
23	D	411	PL9	C53-C6	-2.24	1.46	1.50
19	c	510	CLA	CMB-C2B	-2.23	1.47	1.51
19	c	514	CLA	CMB-C2B	-2.22	1.47	1.51
19	B	612	CLA	CMC-C2C	-2.22	1.46	1.50
23	d	407	PL9	C53-C6	-2.22	1.46	1.50
22	L	102	SQD	C8-C7	2.22	1.57	1.50
19	c	510	CLA	CMD-C2D	-2.21	1.46	1.50
22	A	411	SQD	O9-S	2.21	1.51	1.45
19	c	514	CLA	CMD-C2D	-2.20	1.46	1.50
19	B	606	CLA	CMC-C2C	-2.20	1.46	1.50
19	C	511	CLA	CMD-C2D	-2.20	1.46	1.50
22	l	102	SQD	C8-C7	2.19	1.57	1.50
19	b	614	CLA	CMC-C2C	-2.19	1.46	1.50
19	b	607	CLA	CMD-C2D	-2.18	1.46	1.50
19	b	617	CLA	CMD-C2D	-2.18	1.46	1.50
19	B	611	CLA	CMC-C2C	-2.17	1.46	1.50
19	B	614	CLA	CMD-C2D	-2.17	1.46	1.50
19	b	617	CLA	CMC-C2C	-2.16	1.46	1.50
22	f	102	SQD	O9-S	2.15	1.51	1.45
19	B	615	CLA	CMC-C2C	-2.15	1.46	1.50
19	c	512	CLA	CMC-C2C	-2.15	1.46	1.50
22	a	412	SQD	O7-S	2.15	1.51	1.45
19	B	615	CLA	CMD-C2D	-2.14	1.46	1.50
19	C	514	CLA	CMD-C2D	-2.14	1.46	1.50
22	F	102	SQD	O9-S	2.14	1.51	1.45
19	b	616	CLA	CMD-C2D	-2.14	1.46	1.50
19	c	507	CLA	CMD-C2D	-2.14	1.46	1.50
19	b	608	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	613	CLA	CMC-C2C	-2.13	1.46	1.50
22	L	102	SQD	O9-S	2.13	1.51	1.45
23	d	407	PL9	C7-C8	-2.13	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	404	CLA	CMD-C2D	-2.13	1.46	1.50
19	c	513	CLA	CMD-C2D	-2.12	1.46	1.50
22	l	102	SQD	O9-S	2.12	1.51	1.45
19	C	505	CLA	CMD-C2D	-2.12	1.46	1.50
19	d	405	CLA	CMD-C2D	-2.12	1.46	1.50
19	B	605	CLA	CMD-C2D	-2.12	1.46	1.50
19	B	606	CLA	CMD-C2D	-2.12	1.46	1.50
19	c	502	CLA	CMD-C2D	-2.12	1.46	1.50
19	B	610	CLA	CMD-C2D	-2.11	1.46	1.50
22	a	412	SQD	O9-S	2.11	1.51	1.45
19	C	503	CLA	CMD-C2D	-2.11	1.46	1.50
19	a	406	CLA	CMD-C2D	-2.11	1.46	1.50
22	A	411	SQD	O7-S	2.11	1.51	1.45
19	D	409	CLA	CMD-C2D	-2.11	1.46	1.50
19	C	513	CLA	CMC-C2C	-2.11	1.46	1.50
22	l	102	SQD	O7-S	2.10	1.51	1.45
19	c	508	CLA	CMD-C2D	-2.09	1.46	1.50
31	F	101	HEM	FE-ND	2.09	2.07	1.96
19	a	405	CLA	CMD-C2D	-2.09	1.46	1.50
22	L	102	SQD	O7-S	2.09	1.51	1.45
22	a	410	SQD	O9-S	2.08	1.51	1.45
23	D	411	PL9	C7-C8	-2.08	1.47	1.50
19	B	613	CLA	CMC-C2C	-2.08	1.46	1.50
19	B	616	CLA	CMD-C2D	-2.08	1.46	1.50
22	l	102	SQD	C6-S	2.08	1.85	1.77
19	b	612	CLA	CMD-C2D	-2.08	1.46	1.50
19	C	508	CLA	CMD-C2D	-2.08	1.46	1.50
19	c	506	CLA	CMC-C2C	-2.08	1.46	1.50
19	b	616	CLA	CMC-C2C	-2.07	1.46	1.50
19	C	506	CLA	CMD-C2D	-2.07	1.46	1.50
19	B	614	CLA	CMC-C2C	-2.07	1.46	1.50
19	C	506	CLA	CMC-C2C	-2.07	1.46	1.50
19	B	609	CLA	C3B-C2B	-2.07	1.37	1.40
19	b	615	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	618	CLA	CMD-C2D	-2.07	1.46	1.50
22	f	102	SQD	O7-S	2.07	1.51	1.45
19	C	513	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	607	CLA	CMC-C2C	-2.06	1.46	1.50
19	c	512	CLA	CMD-C2D	-2.06	1.46	1.50
19	C	509	CLA	CMD-C2D	-2.06	1.46	1.50
19	D	409	CLA	CMC-C2C	-2.06	1.46	1.50
19	a	408	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	602	CLA	CMD-C2D	-2.06	1.46	1.50
19	c	505	CLA	CMC-C2C	-2.05	1.46	1.50
22	L	102	SQD	C6-S	2.05	1.84	1.77
19	B	611	CLA	CMD-C2D	-2.05	1.46	1.50
19	c	514	CLA	CMC-C2C	-2.05	1.46	1.50
19	c	504	CLA	CMD-C2D	-2.05	1.46	1.50
19	C	507	CLA	CMC-C2C	-2.05	1.46	1.50
19	c	505	CLA	CMD-C2D	-2.05	1.46	1.50
19	A	407	CLA	CMC-C2C	-2.05	1.46	1.50
19	D	408	CLA	CMC-C2C	-2.05	1.46	1.50
22	A	409	SQD	O9-S	2.05	1.51	1.45
19	A	407	CLA	CMD-C2D	-2.05	1.46	1.50
31	f	101	HEM	CMB-C2B	2.05	1.55	1.50
19	b	613	CLA	CMD-C2D	-2.04	1.46	1.50
22	F	102	SQD	O7-S	2.04	1.51	1.45
22	f	102	SQD	C6-S	2.03	1.84	1.77
19	b	604	CLA	CMD-C2D	-2.03	1.46	1.50
19	B	605	CLA	CMC-C2C	-2.03	1.46	1.50
19	b	610	CLA	CMC-C2C	-2.03	1.46	1.50
19	b	615	CLA	CMC-C2C	-2.02	1.46	1.50
19	A	405	CLA	CMD-C2D	-2.02	1.46	1.50
19	B	608	CLA	CMC-C2C	-2.02	1.46	1.50
31	F	101	HEM	CMB-C2B	2.02	1.55	1.50
19	B	613	CLA	CMD-C2D	-2.02	1.46	1.50
19	b	611	CLA	C3B-C2B	-2.02	1.37	1.40
22	f	102	SQD	C8-C7	2.02	1.56	1.50
19	C	515	CLA	CMD-C2D	-2.02	1.46	1.50
19	C	504	CLA	CMD-C2D	-2.01	1.46	1.50
19	c	503	CLA	CMD-C2D	-2.01	1.46	1.50
20	A	406	PHO	C3B-C2B	-2.01	1.37	1.40
19	d	404	CLA	CMC-C2C	-2.01	1.46	1.50
19	d	405	CLA	CMC-C2C	-2.01	1.46	1.50
19	a	408	CLA	CMC-C2C	-2.01	1.46	1.50
19	b	611	CLA	CMC-C2C	-2.01	1.46	1.50
19	B	609	CLA	CMC-C2C	-2.01	1.46	1.50
19	c	509	CLA	CMD-C2D	-2.00	1.46	1.50
19	c	511	CLA	CMC-C2C	-2.00	1.46	1.50
19	b	604	CLA	CMC-C2C	-2.00	1.46	1.50

All (717) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	606	CLA	C4A-NA-C1A	8.07	110.33	106.71
19	B	604	CLA	C4A-NA-C1A	8.06	110.33	106.71
19	B	612	CLA	C4A-NA-C1A	8.04	110.32	106.71
19	B	607	CLA	C4A-NA-C1A	7.94	110.28	106.71
19	b	614	CLA	C4A-NA-C1A	7.93	110.27	106.71
19	b	609	CLA	C4A-NA-C1A	7.77	110.20	106.71
19	c	508	CLA	C4A-NA-C1A	7.65	110.14	106.71
19	C	509	CLA	C4A-NA-C1A	7.57	110.11	106.71
19	c	506	CLA	C4A-NA-C1A	7.46	110.06	106.71
19	B	605	CLA	C4A-NA-C1A	7.46	110.06	106.71
19	b	607	CLA	C4A-NA-C1A	7.45	110.06	106.71
19	C	507	CLA	C4A-NA-C1A	7.44	110.05	106.71
19	b	608	CLA	C4A-NA-C1A	7.40	110.03	106.71
19	B	606	CLA	C4A-NA-C1A	7.40	110.03	106.71
19	C	510	CLA	C4A-NA-C1A	7.40	110.03	106.71
19	b	613	CLA	C4A-NA-C1A	7.38	110.02	106.71
19	C	504	CLA	C4A-NA-C1A	7.36	110.02	106.71
19	c	512	CLA	C4A-NA-C1A	7.31	109.99	106.71
19	c	503	CLA	C4A-NA-C1A	7.30	109.99	106.71
19	c	509	CLA	C4A-NA-C1A	7.30	109.99	106.71
19	B	611	CLA	C4A-NA-C1A	7.30	109.99	106.71
19	C	513	CLA	C4A-NA-C1A	7.28	109.98	106.71
19	C	506	CLA	C4A-NA-C1A	7.25	109.97	106.71
19	B	614	CLA	C4A-NA-C1A	7.20	109.94	106.71
19	c	505	CLA	C4A-NA-C1A	7.19	109.94	106.71
19	a	408	CLA	C4A-NA-C1A	7.17	109.93	106.71
19	B	616	CLA	C4A-NA-C1A	7.16	109.92	106.71
19	B	615	CLA	C4A-NA-C1A	7.14	109.92	106.71
19	c	507	CLA	C4A-NA-C1A	7.12	109.91	106.71
19	b	616	CLA	C4A-NA-C1A	7.10	109.90	106.71
19	A	407	CLA	C4A-NA-C1A	7.10	109.90	106.71
19	b	617	CLA	C4A-NA-C1A	7.05	109.87	106.71
19	C	508	CLA	C4A-NA-C1A	7.04	109.87	106.71
19	b	618	CLA	C4A-NA-C1A	7.02	109.86	106.71
19	d	404	CLA	C4A-NA-C1A	7.01	109.86	106.71
19	B	613	CLA	C4A-NA-C1A	7.00	109.85	106.71
19	D	408	CLA	C4A-NA-C1A	7.00	109.85	106.71
19	a	404	CLA	C4A-NA-C1A	6.94	109.83	106.71
19	A	403	CLA	C4A-NA-C1A	6.93	109.82	106.71
19	b	615	CLA	C4A-NA-C1A	6.92	109.82	106.71
19	C	514	CLA	C4A-NA-C1A	6.91	109.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	601	CLA	C4A-NA-C1A	6.87	109.79	106.71
19	D	409	CLA	C4A-NA-C1A	6.83	109.78	106.71
19	b	603	CLA	C4A-NA-C1A	6.82	109.77	106.71
19	c	510	CLA	C4A-NA-C1A	6.82	109.77	106.71
19	B	602	CLA	C4A-NA-C1A	6.81	109.77	106.71
19	b	610	CLA	C4A-NA-C1A	6.78	109.76	106.71
19	c	513	CLA	C4A-NA-C1A	6.78	109.76	106.71
19	c	514	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	A	404	CLA	C4A-NA-C1A	6.76	109.75	106.71
19	B	608	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	d	405	CLA	C4A-NA-C1A	6.72	109.72	106.71
19	a	405	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	a	406	CLA	C4A-NA-C1A	6.66	109.70	106.71
19	C	512	CLA	C4A-NA-C1A	6.65	109.70	106.71
19	A	405	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	c	511	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	b	604	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	C	511	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	b	611	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	B	609	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	C	505	CLA	C4A-NA-C1A	6.58	109.66	106.71
19	C	515	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	C	503	CLA	C4A-NA-C1A	6.43	109.60	106.71
19	c	504	CLA	C4A-NA-C1A	6.43	109.60	106.71
19	b	605	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	c	502	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	B	603	CLA	C4A-NA-C1A	6.38	109.57	106.71
19	b	612	CLA	C4A-NA-C1A	6.17	109.48	106.71
19	B	610	CLA	C4A-NA-C1A	6.02	109.41	106.71
22	f	102	SQD	O9-S-C6	5.80	113.84	106.94
23	a	411	PL9	C7-C3-C4	5.39	121.26	116.88
19	b	608	CLA	CMB-C2B-C1B	-5.05	120.70	128.46
21	b	601	BCR	C15-C14-C13	5.02	134.47	127.31
19	c	507	CLA	CMB-C2B-C1B	-4.94	120.87	128.46
19	c	510	CLA	CMB-C2B-C1B	-4.90	120.94	128.46
19	c	509	CLA	CMB-C2B-C1B	-4.89	120.94	128.46
19	a	405	CLA	CMB-C2B-C1B	-4.89	120.95	128.46
19	c	514	CLA	CMB-C2B-C1B	-4.88	120.97	128.46
19	A	404	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
19	B	616	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
19	b	618	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
19	C	510	CLA	CMB-C2B-C1B	-4.86	120.99	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	511	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
19	C	508	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
22	L	102	SQD	O9-S-C6	4.85	112.70	106.94
19	B	606	CLA	CMB-C2B-C1B	-4.83	121.05	128.46
19	c	505	CLA	CMB-C2B-C1B	-4.80	121.08	128.46
22	l	102	SQD	O9-S-C6	4.77	112.61	106.94
23	A	410	PL9	C7-C3-C4	4.76	120.75	116.88
19	a	406	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
19	A	405	CLA	CMB-C2B-C1B	-4.72	121.20	128.46
19	B	612	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
19	b	614	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
19	B	613	CLA	CMB-C2B-C1B	-4.71	121.23	128.46
19	b	615	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
19	a	404	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
19	A	403	CLA	CMB-C2B-C1B	-4.65	121.32	128.46
19	B	611	CLA	CMB-C2B-C1B	-4.62	121.37	128.46
19	b	610	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
23	D	411	PL9	C7-C3-C4	4.60	120.61	116.88
19	b	613	CLA	CMB-C2B-C1B	-4.59	121.40	128.46
19	C	506	CLA	CMB-C2B-C1B	-4.59	121.41	128.46
19	B	608	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
23	d	407	PL9	C7-C3-C4	4.54	120.57	116.88
19	C	515	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
19	C	513	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
19	C	514	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
19	b	616	CLA	CMB-C2B-C1B	-4.49	121.56	128.46
19	c	513	CLA	CMB-C2B-C1B	-4.48	121.57	128.46
19	c	512	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
19	c	514	CLA	CMB-C2B-C3B	4.41	132.93	124.68
19	B	614	CLA	CMB-C2B-C1B	-4.38	121.72	128.46
19	b	609	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
19	B	607	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
19	C	509	CLA	CMB-C2B-C1B	-4.30	121.85	128.46
22	l	102	SQD	O7-S-C6	4.30	112.05	106.94
22	L	102	SQD	O7-S-C6	4.26	112.01	106.94
19	c	510	CLA	CMB-C2B-C3B	4.24	132.62	124.68
22	F	102	SQD	O47-C7-O49	-4.23	120.18	125.57
19	C	511	CLA	CMB-C2B-C3B	4.23	132.59	124.68
19	B	616	CLA	CMB-C2B-C3B	4.22	132.58	124.68
19	c	508	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
19	b	618	CLA	CMB-C2B-C3B	4.20	132.53	124.68
19	B	603	CLA	CMB-C2B-C1B	-4.16	122.07	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	604	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
19	b	608	CLA	CMB-C2B-C3B	4.15	132.44	124.68
19	C	505	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
22	L	102	SQD	O47-C7-C8	4.12	120.38	111.50
19	b	605	CLA	CMB-C2B-C1B	-4.12	122.14	128.46
19	a	406	CLA	CMB-C2B-C3B	4.12	132.38	124.68
19	B	602	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
19	C	504	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
22	l	102	SQD	O47-C7-C8	4.10	120.34	111.50
19	C	515	CLA	CMB-C2B-C3B	4.08	132.31	124.68
19	A	405	CLA	CMB-C2B-C3B	4.07	132.28	124.68
19	c	503	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
19	a	405	CLA	CMB-C2B-C3B	4.03	132.23	124.68
19	c	509	CLA	CMB-C2B-C3B	4.03	132.23	124.68
19	b	614	CLA	CMB-C2B-C3B	4.03	132.22	124.68
19	c	505	CLA	CMB-C2B-C3B	4.02	132.21	124.68
22	a	410	SQD	O9-S-O7	-4.02	100.03	113.95
22	A	409	SQD	O8-S-C6	4.01	112.14	105.74
19	A	404	CLA	CMB-C2B-C3B	4.01	132.19	124.68
19	C	512	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
19	B	612	CLA	CMB-C2B-C3B	4.00	132.17	124.68
22	a	412	SQD	O47-C7-C8	4.00	120.12	111.50
19	B	606	CLA	CMB-C2B-C3B	4.00	132.16	124.68
26	A	416	BCT	O2-C-O1	3.98	129.87	119.55
19	C	510	CLA	CMB-C2B-C3B	3.98	132.12	124.68
26	d	403	BCT	O2-C-O1	3.97	129.84	119.55
19	d	405	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
19	c	511	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
19	a	408	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
22	A	409	SQD	O9-S-O7	-3.96	100.25	113.95
19	c	504	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
21	b	601	BCR	C15-C16-C17	-3.94	115.40	123.47
19	D	409	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
22	a	410	SQD	O8-S-C6	3.92	111.98	105.74
22	f	102	SQD	O9-S-O7	-3.91	100.41	113.95
19	B	613	CLA	CMB-C2B-C3B	3.90	131.98	124.68
22	F	102	SQD	O9-S-C6	3.90	111.61	106.92
19	B	610	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
19	A	403	CLA	CMB-C2B-C3B	3.89	131.96	124.68
19	b	615	CLA	CMB-C2B-C3B	3.89	131.95	124.68
19	C	506	CLA	CMB-C2B-C3B	3.88	131.94	124.68
19	a	404	CLA	CMB-C2B-C3B	3.88	131.94	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	607	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
19	b	612	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
22	a	410	SQD	O47-C7-C8	3.86	119.83	111.50
22	f	102	SQD	O47-C7-C8	3.84	119.78	111.50
19	c	513	CLA	CMB-C2B-C3B	3.83	131.85	124.68
22	A	409	SQD	O47-C7-C8	3.82	119.73	111.50
19	C	514	CLA	CMB-C2B-C3B	3.82	131.82	124.68
19	c	506	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
22	F	102	SQD	O9-S-O7	-3.80	100.80	113.95
19	b	610	CLA	CMB-C2B-C3B	3.79	131.77	124.68
19	C	507	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
19	c	512	CLA	CMB-C2B-C3B	3.78	131.75	124.68
22	A	411	SQD	O47-C7-C8	3.77	119.64	111.50
19	b	616	CLA	CMB-C2B-C3B	3.77	131.72	124.68
19	c	507	CLA	CMB-C2B-C3B	3.77	131.72	124.68
19	B	608	CLA	CMB-C2B-C3B	3.77	131.72	124.68
19	C	513	CLA	CMB-C2B-C3B	3.76	131.72	124.68
19	b	613	CLA	CMB-C2B-C3B	3.75	131.69	124.68
22	l	102	SQD	O9-S-O7	-3.74	100.99	113.95
19	d	404	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
19	C	508	CLA	CMB-C2B-C3B	3.74	131.67	124.68
19	A	407	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
19	B	611	CLA	CMB-C2B-C3B	3.73	131.66	124.68
19	B	605	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
22	a	410	SQD	O7-S-C6	3.72	111.36	106.94
19	C	509	CLA	CMB-C2B-C3B	3.72	131.63	124.68
19	D	408	CLA	CMB-C2B-C1B	-3.71	122.75	128.46
22	L	102	SQD	O9-S-O7	-3.71	101.11	113.95
19	B	609	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
19	b	611	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
23	a	411	PL9	C7-C3-C2	-3.68	118.46	123.30
19	c	508	CLA	CMB-C2B-C3B	3.67	131.54	124.68
19	B	607	CLA	CMB-C2B-C3B	3.66	131.53	124.68
19	B	614	CLA	CMB-C2B-C3B	3.65	131.51	124.68
22	a	412	SQD	O9-S-O7	-3.65	101.32	113.95
19	b	609	CLA	CMB-C2B-C3B	3.65	131.50	124.68
19	B	615	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
19	b	617	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
22	F	102	SQD	O7-S-C6	3.60	111.25	106.92
21	b	601	BCR	C16-C15-C14	3.59	130.83	123.47
22	A	409	SQD	O7-S-C6	3.58	111.19	106.94
19	B	602	CLA	CMB-C2B-C3B	3.58	131.38	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	409	SQD	O9-S-C6	3.56	111.17	106.94
19	b	604	CLA	CMB-C2B-C3B	3.56	131.33	124.68
19	C	503	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
22	a	410	SQD	O9-S-C6	3.54	111.14	106.94
22	A	411	SQD	O9-S-O7	-3.53	101.73	113.95
22	a	412	SQD	O7-S-C6	3.52	111.12	106.94
19	B	601	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
19	c	502	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
22	A	411	SQD	O7-S-C6	3.48	111.07	106.94
19	C	505	CLA	CMB-C2B-C3B	3.47	131.17	124.68
19	b	603	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
19	a	408	CLA	CMB-C2B-C3B	3.47	131.16	124.68
29	t	101	LMT	C1'-O5'-C5'	3.46	120.48	113.69
19	C	504	CLA	CMB-C2B-C3B	3.45	131.13	124.68
19	B	604	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
19	B	603	CLA	CMB-C2B-C3B	3.41	131.06	124.68
31	f	101	HEM	CMC-C2C-C3C	3.41	131.06	124.68
19	b	606	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
19	d	405	CLA	CMB-C2B-C3B	3.40	131.04	124.68
19	c	503	CLA	CMB-C2B-C3B	3.39	131.03	124.68
19	b	605	CLA	CMB-C2B-C3B	3.39	131.01	124.68
19	D	409	CLA	CMB-C2B-C3B	3.35	130.94	124.68
19	b	604	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
20	D	401	PHO	CMB-C2B-C3B	3.31	130.88	124.68
31	F	101	HEM	CMC-C2C-C3C	3.31	130.87	124.68
19	c	504	CLA	CMB-C2B-C3B	3.31	130.87	124.68
19	c	506	CLA	CMB-C2B-C3B	3.31	130.87	124.68
19	B	602	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
20	d	402	PHO	CMB-C2B-C3B	3.28	130.82	124.68
19	C	507	CLA	CMB-C2B-C3B	3.27	130.80	124.68
19	c	508	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
22	f	102	SQD	O7-S-C6	3.25	110.80	106.94
22	a	412	SQD	O9-S-C6	3.25	110.80	106.94
22	A	411	SQD	O9-S-C6	3.24	110.79	106.94
21	b	601	BCR	C16-C17-C18	3.24	131.93	127.31
19	C	512	CLA	CMB-C2B-C3B	3.23	130.72	124.68
19	c	511	CLA	CMB-C2B-C3B	3.21	130.69	124.68
19	A	407	CLA	CMB-C2B-C3B	3.21	130.69	124.68
19	b	607	CLA	CMB-C2B-C3B	3.21	130.68	124.68
19	C	509	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
30	c	517	DGD	C3D-C4D-C5D	-3.17	104.59	110.24
19	d	404	CLA	CMB-C2B-C3B	3.16	130.60	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	608	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
19	D	408	CLA	CMB-C2B-C3B	3.15	130.57	124.68
19	b	617	CLA	CMB-C2B-C3B	3.15	130.57	124.68
23	A	410	PL9	C7-C3-C2	-3.14	119.17	123.30
23	D	411	PL9	C7-C3-C2	-3.14	119.17	123.30
23	d	407	PL9	C7-C3-C2	-3.14	119.18	123.30
22	A	409	SQD	O6-C1-C2	3.13	113.18	108.30
19	B	615	CLA	CMB-C2B-C3B	3.13	130.53	124.68
19	B	605	CLA	CMB-C2B-C3B	3.12	130.52	124.68
19	B	603	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
19	B	606	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
19	b	605	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
22	a	410	SQD	O6-C1-C2	3.09	113.13	108.30
19	c	514	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
19	B	610	CLA	CMB-C2B-C3B	3.07	130.43	124.68
19	c	503	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
19	B	614	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
19	b	612	CLA	CMB-C2B-C3B	3.06	130.40	124.68
23	d	407	PL9	C7-C8-C9	-3.06	121.70	126.79
19	b	616	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
19	A	407	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
19	C	504	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
19	B	615	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	a	412	SQD	O8-S-C6	3.04	110.58	105.74
19	C	514	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
19	C	515	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
23	D	411	PL9	C7-C8-C9	-3.04	121.74	126.79
19	a	408	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
31	F	101	HEM	CBA-CAA-C2A	-3.03	107.44	112.62
19	c	506	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
19	b	617	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
19	b	606	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
19	C	507	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
31	F	101	HEM	C4B-CHC-C1C	2.99	126.51	122.56
19	b	611	CLA	CMB-C2B-C3B	2.99	130.28	124.68
19	D	409	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	a	405	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
19	B	604	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
19	B	609	CLA	CMB-C2B-C3B	2.98	130.25	124.68
21	b	601	BCR	C12-C13-C14	-2.98	114.37	118.94
19	a	406	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
19	d	405	CLA	O2D-CGD-O1D	-2.96	118.05	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	101	HEM	CBA-CAA-C2A	-2.96	107.56	112.62
19	A	404	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
19	A	405	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
19	c	502	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
19	B	611	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
19	C	510	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
19	C	503	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
19	C	511	CLA	CHB-C4A-NA	2.93	128.57	124.51
19	c	513	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
19	c	509	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
19	C	503	CLA	CMB-C2B-C3B	2.93	130.15	124.68
19	c	510	CLA	CHB-C4A-NA	2.92	128.56	124.51
19	b	618	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
19	C	505	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
19	B	612	CLA	CHB-C4A-NA	2.91	128.53	124.51
19	b	614	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
19	c	504	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
19	b	613	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
19	c	502	CLA	CMB-C2B-C3B	2.89	130.09	124.68
19	D	408	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
19	B	604	CLA	C1-C2-C3	-2.89	121.04	126.04
19	d	404	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
19	B	612	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
19	b	614	CLA	CHB-C4A-NA	2.87	128.48	124.51
19	B	616	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
19	a	408	CLA	CHB-C4A-NA	2.85	128.46	124.51
19	A	403	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	b	615	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	a	404	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	B	613	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	F	102	SQD	O8-S-C6	2.84	110.36	105.77
19	B	601	CLA	CMB-C2B-C3B	2.84	129.99	124.68
22	A	411	SQD	O8-S-C6	2.84	110.26	105.74
19	b	603	CLA	CMB-C2B-C3B	2.83	129.98	124.68
19	B	610	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	c	505	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	C	514	CLA	CHB-C4A-NA	2.81	128.40	124.51
23	d	407	PL9	C40-C39-C41	2.81	120.00	115.27
19	b	612	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
19	B	607	CLA	CHB-C4A-NA	2.81	128.39	124.51
30	J	101	DGD	C3G-O3G-C1D	2.80	119.22	113.74
19	C	511	CLA	O2D-CGD-O1D	-2.80	118.36	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	410	PL9	C40-C39-C41	2.80	119.97	115.27
31	f	101	HEM	C4B-CHC-C1C	2.80	126.25	122.56
23	a	411	PL9	C27-C28-C29	-2.79	120.93	127.66
19	C	513	CLA	CHB-C4A-NA	2.79	128.37	124.51
19	c	513	CLA	CHB-C4A-NA	2.79	128.36	124.51
19	C	506	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
22	a	412	SQD	O48-C23-C24	2.78	120.64	111.91
19	c	512	CLA	CHB-C4A-NA	2.78	128.35	124.51
19	b	609	CLA	CHB-C4A-NA	2.78	128.35	124.51
29	i	103	LMT	C1B-O5B-C5B	2.77	119.13	113.69
19	B	601	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
19	C	513	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
19	D	409	CLA	CHB-C4A-NA	2.76	128.33	124.51
19	c	512	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
19	B	608	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
19	b	606	CLA	CHB-C4A-NA	2.75	128.31	124.51
19	b	610	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
19	B	607	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
19	d	405	CLA	CHB-C4A-NA	2.74	128.30	124.51
19	A	407	CLA	CHB-C4A-NA	2.74	128.30	124.51
19	b	603	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
19	b	609	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
19	B	604	CLA	CHB-C4A-NA	2.72	128.28	124.51
19	C	515	CLA	CHB-C4A-NA	2.72	128.28	124.51
19	c	510	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
19	c	514	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	L	102	SQD	C3-C4-C5	2.72	115.08	110.24
22	A	411	SQD	O48-C23-C24	2.71	120.41	111.91
19	b	617	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	B	605	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
21	c	520	BCR	C33-C5-C4	-2.70	108.43	113.62
19	b	607	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
19	B	615	CLA	CHB-C4A-NA	2.69	128.24	124.51
19	C	508	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
19	B	602	CLA	CHB-C4A-NA	2.67	128.21	124.51
19	C	509	CLA	CHB-C4A-NA	2.67	128.21	124.51
19	b	611	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
23	a	411	PL9	C35-C34-C36	2.66	119.75	115.27
22	F	102	SQD	O48-C23-C24	2.66	120.26	111.91
22	f	102	SQD	O48-C23-C24	2.66	120.26	111.91
19	c	508	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	l	102	SQD	O48-C23-C24	2.65	120.24	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	611	CLA	O2D-CGD-CBD	2.65	115.98	111.27
19	B	601	CLA	CHB-C4A-NA	2.65	128.18	124.51
19	c	507	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
23	a	411	PL9	C22-C23-C24	-2.65	121.29	127.66
19	C	506	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	L	102	SQD	O48-C23-C24	2.64	120.18	111.91
21	y	101	BCR	C8-C9-C10	-2.63	114.91	118.94
19	C	510	CLA	CHB-C4A-NA	2.63	128.15	124.51
19	b	604	CLA	CHB-C4A-NA	2.62	128.14	124.51
19	c	507	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	l	102	SQD	C4-C3-C2	2.61	115.39	110.82
19	b	613	CLA	O2D-CGD-CBD	2.61	115.91	111.27
22	A	409	SQD	O48-C23-C24	2.61	120.10	111.91
19	b	603	CLA	CHB-C4A-NA	2.60	128.11	124.51
19	C	508	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
19	c	505	CLA	CHB-C4A-NA	2.60	128.11	124.51
19	c	509	CLA	CHB-C4A-NA	2.60	128.11	124.51
19	B	609	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
20	a	407	PHO	CMB-C2B-C3B	2.60	129.54	124.68
23	A	410	PL9	C27-C28-C29	-2.59	121.43	127.66
19	C	508	CLA	CHB-C4A-NA	2.59	128.09	124.51
31	F	101	HEM	CBD-CAD-C3D	-2.59	105.44	112.63
23	D	411	PL9	C36-C34-C33	-2.58	115.89	121.12
23	A	410	PL9	C22-C23-C24	-2.58	121.44	127.66
20	A	406	PHO	CMB-C2B-C3B	2.58	129.51	124.68
19	c	507	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
19	B	616	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	a	405	CLA	CHD-C1D-ND	-2.57	122.09	124.45
19	c	506	CLA	O2D-CGD-CBD	2.57	115.83	111.27
19	C	505	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	a	406	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	B	606	CLA	CHB-C4A-NA	2.56	128.06	124.51
22	a	410	SQD	O48-C23-C24	2.56	119.95	111.91
19	A	405	CLA	CHB-C4A-NA	2.56	128.05	124.51
19	c	504	CLA	CHB-C4A-NA	2.56	128.05	124.51
19	B	604	CLA	CMB-C2B-C3B	2.55	129.46	124.68
19	A	404	CLA	CHD-C1D-ND	-2.55	122.11	124.45
19	a	408	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
23	d	407	PL9	C22-C23-C24	-2.55	121.53	127.66
19	C	515	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
29	t	101	LMT	C4'-C3'-C2'	2.54	115.26	110.82
19	b	618	CLA	CHB-C4A-NA	2.54	128.02	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	504	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	b	608	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	B	607	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
19	b	609	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
19	C	512	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
19	A	404	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	a	405	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	b	616	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	C	507	CLA	O2D-CGD-CBD	2.53	115.76	111.27
19	c	511	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
23	D	411	PL9	C22-C23-C24	-2.52	121.59	127.66
23	A	410	PL9	C7-C8-C9	-2.52	122.60	126.79
31	F	101	HEM	C4D-ND-C1D	2.51	107.67	105.07
19	b	607	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	B	614	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	d	402	PHO	C1B-NB-C4B	2.51	112.24	107.09
19	B	605	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	B	613	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	b	606	CLA	CMB-C2B-C3B	2.50	129.36	124.68
31	f	101	HEM	C4D-ND-C1D	2.50	107.66	105.07
19	A	407	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
19	c	514	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
19	a	404	CLA	CHB-C4A-NA	2.50	127.96	124.51
23	d	407	PL9	C36-C34-C33	-2.49	116.07	121.12
21	y	101	BCR	C7-C8-C9	2.49	130.00	126.23
23	a	411	PL9	C40-C39-C41	2.49	119.46	115.27
21	c	520	BCR	C7-C8-C9	-2.49	122.48	126.23
22	L	102	SQD	O6-C1-C2	2.48	112.18	108.30
19	c	503	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	b	613	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	c	502	CLA	CHB-C4A-NA	2.47	127.93	124.51
21	c	520	BCR	C4-C5-C6	-2.47	119.14	122.73
19	b	615	CLA	CHB-C4A-NA	2.47	127.92	124.51
19	A	403	CLA	CHB-C4A-NA	2.47	127.92	124.51
23	D	411	PL9	O1-C4-C3	-2.46	118.01	120.72
19	C	503	CLA	CHB-C4A-NA	2.46	127.92	124.51
20	D	401	PHO	C1B-NB-C4B	2.46	112.14	107.09
21	b	601	BCR	C35-C13-C14	2.46	126.37	122.92
19	B	608	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	A	406	PHO	C1B-NB-C4B	2.46	112.14	107.09
20	a	407	PHO	C1B-NB-C4B	2.45	112.13	107.09
19	b	605	CLA	O2A-CGA-O1A	-2.45	117.42	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	610	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	a	411	PL9	C20-C19-C21	2.44	119.38	115.27
23	d	407	PL9	O1-C4-C3	-2.44	118.03	120.72
21	C	521	BCR	C7-C8-C9	-2.44	122.55	126.23
19	d	405	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
19	b	606	CLA	O2D-CGD-CBD	2.44	115.60	111.27
19	B	603	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
19	B	609	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	B	604	CLA	O2D-CGD-CBD	2.42	115.57	111.27
21	b	620	BCR	C33-C5-C4	-2.42	108.97	113.62
22	f	102	SQD	O8-S-C6	2.41	109.59	105.74
19	D	409	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
19	C	507	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	A	404	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
19	b	605	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
19	c	506	CLA	CHB-C4A-NA	2.41	127.84	124.51
31	f	101	HEM	C1B-NB-C4B	2.41	107.56	105.07
19	b	610	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
19	B	608	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
19	B	610	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
19	B	607	CLA	CHD-C1D-ND	-2.40	122.25	124.45
19	b	611	CLA	CHB-C4A-NA	2.40	127.82	124.51
19	a	406	CLA	O2D-CGD-CBD	2.39	115.52	111.27
19	a	404	CLA	C2D-C1D-ND	-2.39	108.34	110.10
19	B	611	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	c	505	CLA	CHD-C1D-ND	-2.39	122.26	124.45
23	A	410	PL9	C20-C19-C21	2.39	119.29	115.27
21	C	521	BCR	C33-C5-C4	-2.39	109.03	113.62
31	F	101	HEM	C1B-NB-C4B	2.38	107.54	105.07
19	B	602	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
19	b	612	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
21	Y	101	BCR	C8-C9-C10	-2.38	115.29	118.94
19	B	603	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
23	a	411	PL9	C7-C8-C9	-2.38	122.83	126.79
19	A	403	CLA	C2D-C1D-ND	-2.37	108.35	110.10
19	C	506	CLA	CHD-C1D-ND	-2.37	122.27	124.45
19	a	405	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	c	506	CLA	C1-C2-C3	-2.37	121.95	126.04
23	a	411	PL9	C32-C33-C34	-2.36	121.97	127.66
19	b	604	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
19	C	510	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
29	t	101	LMT	O5'-C1'-C2'	2.35	115.33	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	l	102	SQD	O6-C1-C2	2.35	111.97	108.30
19	B	610	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	b	612	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	c	509	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
19	B	616	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
19	B	604	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
19	b	605	CLA	CHB-C4A-NA	2.33	127.73	124.51
19	a	404	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	C	503	CLA	CHD-C1D-ND	-2.32	122.32	124.45
30	c	517	DGD	C6D-O5D-C1E	2.32	118.28	113.74
19	c	504	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
29	z	101	LMT	C1'-O5'-C5'	2.32	118.25	113.69
19	b	618	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
23	d	407	PL9	C20-C19-C21	2.32	119.18	115.27
19	A	403	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
21	b	601	BCR	C37-C22-C21	2.31	126.17	122.92
19	C	509	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
19	a	408	CLA	CHD-C1D-ND	-2.31	122.33	124.45
19	C	512	CLA	CHB-C4A-NA	2.31	127.71	124.51
19	b	616	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
19	B	603	CLA	CHB-C4A-NA	2.31	127.70	124.51
21	B	629	BCR	C37-C22-C21	2.30	126.15	122.92
21	b	601	BCR	C19-C18-C17	-2.30	115.41	118.94
19	b	608	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
19	b	611	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
19	B	609	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
19	c	511	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	A	405	CLA	O2D-CGD-CBD	2.29	115.34	111.27
19	c	505	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	B	606	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
19	c	506	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
19	C	508	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
19	b	609	CLA	CHD-C1D-ND	-2.29	122.35	124.45
19	C	507	CLA	C1-C2-C3	-2.29	122.09	126.04
19	B	614	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
21	b	620	BCR	C4-C5-C6	-2.29	119.41	122.73
19	b	613	CLA	C1-C2-C3	-2.29	122.09	126.04
19	b	607	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
19	C	507	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
23	D	411	PL9	C20-C19-C21	2.28	119.11	115.27
19	c	508	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
19	a	406	CLA	C1B-CHB-C4A	-2.28	125.60	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	c	502	CLA	CHD-C1D-ND	-2.28	122.36	124.45
19	b	606	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
23	a	411	PL9	O2-C1-C6	2.27	124.52	120.59
21	b	601	BCR	C20-C21-C22	2.27	130.55	127.31
19	B	605	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
19	C	503	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
21	c	520	BCR	C29-C28-C27	2.27	116.45	111.38
19	B	611	CLA	C1-C2-C3	-2.27	122.12	126.04
19	B	601	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
19	C	505	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
19	c	502	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
29	C	502	LMT	C6B-C5B-C4B	2.26	118.31	113.00
19	B	612	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
23	D	411	PL9	C27-C28-C29	-2.26	122.21	127.66
22	l	102	SQD	O8-S-C6	2.26	109.34	105.74
23	d	407	PL9	C27-C28-C29	-2.26	122.22	127.66
29	z	101	LMT	O5'-C1'-O1'	-2.26	104.63	109.97
19	C	515	CLA	CHD-C1D-ND	-2.26	122.38	124.45
19	C	506	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
19	A	405	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
19	C	512	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
19	B	610	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
19	b	612	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
19	C	504	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
19	c	510	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
19	b	614	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
19	B	612	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
19	c	508	CLA	O2D-CGD-CBD	2.24	115.25	111.27
19	B	606	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	b	603	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	b	614	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
29	z	101	LMT	C1-O1'-C1'	2.23	117.55	113.84
19	D	408	CLA	CHB-C4A-NA	2.23	127.60	124.51
19	b	608	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
19	c	503	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
19	a	406	CLA	CHD-C1D-ND	-2.23	122.41	124.45
19	C	511	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
30	D	415	DGD	C3G-O3G-C1D	2.22	118.08	113.74
19	b	613	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
21	Y	101	BCR	C7-C8-C9	2.22	129.58	126.23
19	d	404	CLA	CHB-C4A-NA	2.21	127.57	124.51
19	C	514	CLA	C1B-CHB-C4A	-2.21	125.74	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	410	PL9	O2-C1-C6	2.20	124.41	120.59
26	d	403	BCT	O3-C-O1	-2.20	113.83	119.55
19	c	513	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
26	A	416	BCT	O3-C-O1	-2.20	113.84	119.55
19	A	407	CLA	CHD-C1D-ND	-2.20	122.43	124.45
21	C	521	BCR	C29-C28-C27	2.20	116.29	111.38
19	b	606	CLA	CBC-CAC-C3C	2.20	118.48	112.43
19	C	509	CLA	O2D-CGD-CBD	2.19	115.16	111.27
19	B	605	CLA	CHD-C1D-ND	-2.18	122.45	124.45
19	A	405	CLA	CHD-C1D-ND	-2.18	122.45	124.45
19	c	511	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
19	B	611	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
19	D	408	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
19	B	604	CLA	CBC-CAC-C3C	2.17	118.41	112.43
30	C	517	DGD	C3G-O3G-C1D	2.17	117.97	113.74
19	c	509	CLA	O2D-CGD-CBD	2.16	115.11	111.27
19	C	509	CLA	C2A-C1A-CHA	2.16	127.64	123.86
19	C	510	CLA	O2D-CGD-CBD	2.16	115.10	111.27
19	d	404	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
19	c	507	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
20	A	406	PHO	CMC-C2C-C3C	2.16	129.01	124.94
19	b	617	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
19	C	505	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
19	b	616	CLA	CHD-C1D-ND	-2.14	122.48	124.45
19	b	610	CLA	CHD-C1D-ND	-2.14	122.49	124.45
23	a	411	PL9	O2-C1-C2	-2.14	116.89	121.78
21	C	521	BCR	C4-C5-C6	-2.13	119.63	122.73
19	B	608	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
19	b	608	CLA	O2D-CGD-CBD	2.13	115.06	111.27
19	c	504	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
19	B	615	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
19	c	508	CLA	C2A-C1A-CHA	2.13	127.58	123.86
23	a	411	PL9	C12-C13-C14	-2.12	122.55	127.66
19	B	602	CLA	O2D-CGD-CBD	2.12	115.04	111.27
19	b	604	CLA	O2D-CGD-CBD	2.12	115.04	111.27
29	b	602	LMT	O1'-C1'-C2'	2.12	111.62	108.30
19	B	608	CLA	CHD-C1D-ND	-2.12	122.50	124.45
21	b	619	BCR	C29-C30-C25	2.12	113.74	110.48
19	B	603	CLA	C2D-C1D-ND	-2.12	108.54	110.10
19	C	503	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
19	a	406	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
19	C	510	CLA	O2A-CGA-O1A	-2.12	118.25	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	606	CLA	O2D-CGD-CBD	2.12	115.03	111.27
23	D	411	PL9	O2-C1-C2	-2.12	116.93	121.78
19	A	404	CLA	O2D-CGD-CBD	2.11	115.03	111.27
19	C	513	CLA	CHD-C1D-ND	-2.11	122.51	124.45
19	A	407	CLA	O2D-CGD-CBD	2.11	115.03	111.27
22	L	102	SQD	O5-C5-C4	2.11	113.53	109.69
21	y	101	BCR	C33-C5-C6	-2.11	122.16	124.53
19	a	408	CLA	O2D-CGD-CBD	2.11	115.02	111.27
23	A	410	PL9	O2-C1-C2	-2.11	116.94	121.78
29	z	101	LMT	C1B-O5B-C5B	2.11	117.83	113.69
19	b	607	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	d	407	PL9	O2-C1-C2	-2.11	116.95	121.78
23	D	411	PL9	C50-C49-C48	-2.11	116.56	122.65
19	b	616	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
20	a	407	PHO	CMC-C2C-C3C	2.10	128.91	124.94
19	b	606	CLA	C2D-C1D-ND	-2.10	108.56	110.10
19	c	502	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
19	B	613	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
19	b	610	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
23	A	410	PL9	C36-C34-C33	-2.10	116.87	121.12
19	B	614	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
19	A	405	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
19	b	615	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
23	a	411	PL9	C37-C38-C39	-2.09	122.62	127.66
21	B	629	BCR	C20-C21-C22	2.09	130.30	127.31
19	a	405	CLA	O2D-CGD-CBD	2.09	114.98	111.27
21	b	620	BCR	C29-C30-C25	2.09	113.70	110.48
19	c	512	CLA	CHD-C1D-ND	-2.09	122.53	124.45
22	f	102	SQD	C3-C4-C5	2.09	113.96	110.24
19	B	604	CLA	C2D-C1D-ND	-2.09	108.57	110.10
23	d	407	PL9	O2-C1-C6	2.08	124.20	120.59
22	L	102	SQD	O8-S-C6	2.08	109.06	105.74
19	c	512	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
19	c	509	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
19	B	614	CLA	CHD-C1D-ND	-2.08	122.54	124.45
30	c	516	DGD	C3G-O3G-C1D	2.08	117.79	113.74
20	D	401	PHO	C1-C2-C3	-2.07	122.46	126.04
19	b	604	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	D	411	PL9	C41-C39-C38	-2.07	116.94	121.12
19	C	513	CLA	C1B-CHB-C4A	-2.07	126.03	130.12
23	d	407	PL9	C50-C49-C48	-2.06	116.68	122.65
23	A	410	PL9	C32-C33-C34	-2.06	122.69	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	408	CLA	C1-C2-C3	-2.06	122.48	126.04
23	D	411	PL9	C42-C43-C44	-2.06	122.70	127.66
19	c	509	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	D	411	PL9	O2-C1-C6	2.06	124.15	120.59
19	B	602	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	d	407	PL9	C8-C7-C3	2.05	117.78	111.98
19	A	405	CLA	C1-C2-C3	-2.05	122.50	126.04
19	a	404	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	b	604	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	a	406	CLA	C1-C2-C3	-2.05	122.50	126.04
30	C	517	DGD	C6D-O5D-C1E	2.05	117.74	113.74
29	i	103	LMT	O5B-C5B-C4B	2.05	113.41	109.69
23	D	411	PL9	C8-C7-C3	2.05	117.76	111.98
19	b	605	CLA	C2D-C1D-ND	-2.04	108.60	110.10
23	A	410	PL9	O1-C4-C3	-2.04	118.47	120.72
30	J	101	DGD	C6D-O5D-C1E	2.04	117.72	113.74
19	A	403	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
21	C	521	BCR	C24-C23-C22	-2.04	123.16	126.23
21	B	617	BCR	C23-C22-C21	-2.04	115.81	118.94
21	b	619	BCR	C33-C5-C6	-2.04	122.24	124.53
19	B	602	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
19	b	606	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
21	c	520	BCR	C29-C30-C25	2.03	113.61	110.48
19	b	611	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
19	B	609	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
21	y	101	BCR	C2-C1-C6	2.03	113.60	110.48
30	h	102	DGD	C6D-O5D-C1E	2.03	117.70	113.74
19	B	604	CLA	C1B-CHB-C4A	-2.03	126.11	130.12
22	f	102	SQD	O6-C1-C2	2.03	111.47	108.30
19	B	613	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
19	c	507	CLA	CHD-C1D-ND	-2.02	122.59	124.45
19	C	503	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
19	A	404	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
19	B	603	CLA	O2D-CGD-CBD	2.02	114.86	111.27
30	c	516	DGD	C6D-O5D-C1E	2.02	117.68	113.74
19	c	514	CLA	CAA-C2A-C3A	-2.02	107.26	112.78
19	B	615	CLA	C2A-C1A-CHA	2.02	127.38	123.86
19	C	515	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
19	b	615	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
19	C	508	CLA	CHD-C1D-ND	-2.01	122.61	124.45
19	a	405	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
19	B	611	CLA	O2A-CGA-O1A	-2.01	118.52	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	407	CLA	C1-C2-C3	-2.01	122.57	126.04
19	c	512	CLA	C2A-C1A-CHA	2.01	127.37	123.86
30	c	519	DGD	C1E-O6E-C5E	2.00	117.62	113.69
19	b	613	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	403	CLA	ND
19	A	404	CLA	ND
19	A	405	CLA	ND
19	A	407	CLA	ND
19	B	601	CLA	ND
19	B	602	CLA	ND
19	B	603	CLA	ND
19	B	604	CLA	ND
19	B	605	CLA	ND
19	B	606	CLA	ND
19	B	607	CLA	ND
19	B	608	CLA	ND
19	B	609	CLA	ND
19	B	610	CLA	ND
19	B	611	CLA	ND
19	B	612	CLA	ND
19	B	613	CLA	ND
19	B	614	CLA	ND
19	B	615	CLA	ND
19	B	616	CLA	ND
19	C	503	CLA	ND
19	C	504	CLA	ND
19	C	505	CLA	ND
19	C	506	CLA	ND
19	C	507	CLA	ND
19	C	508	CLA	ND
19	C	509	CLA	ND
19	C	510	CLA	ND
19	C	511	CLA	ND
19	C	512	CLA	ND
19	C	513	CLA	ND
19	C	514	CLA	ND
19	C	515	CLA	ND
19	D	408	CLA	ND

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Mol	Chain	Res	Type	Atom
19	D	409	CLA	ND
19	a	404	CLA	ND
19	a	405	CLA	ND
19	a	406	CLA	ND
19	a	408	CLA	ND
19	b	603	CLA	ND
19	b	604	CLA	ND
19	b	605	CLA	ND
19	b	606	CLA	ND
19	b	607	CLA	ND
19	b	608	CLA	ND
19	b	609	CLA	ND
19	b	610	CLA	ND
19	b	611	CLA	ND
19	b	612	CLA	ND
19	b	613	CLA	ND
19	b	614	CLA	ND
19	b	615	CLA	ND
19	b	616	CLA	ND
19	b	617	CLA	ND
19	b	618	CLA	ND
19	c	502	CLA	ND
19	c	503	CLA	ND
19	c	504	CLA	ND
19	c	505	CLA	ND
19	c	506	CLA	ND
19	c	507	CLA	ND
19	c	508	CLA	ND
19	c	509	CLA	ND
19	c	510	CLA	ND
19	c	511	CLA	ND
19	c	512	CLA	ND
19	c	513	CLA	ND
19	c	514	CLA	ND
19	d	404	CLA	ND
19	d	405	CLA	ND

All (1545) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	403	CLA	CBD-CGD-O2D-CED
19	A	404	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	A	404	CLA	CHA-CBD-CGD-O2D
19	B	601	CLA	CHA-CBD-CGD-O1D
19	B	601	CLA	CHA-CBD-CGD-O2D
19	B	601	CLA	CAD-CBD-CGD-O1D
19	B	603	CLA	C4-C3-C5-C6
19	B	605	CLA	C2-C3-C5-C6
19	B	605	CLA	C4-C3-C5-C6
19	B	606	CLA	CHA-CBD-CGD-O1D
19	B	606	CLA	CHA-CBD-CGD-O2D
19	B	608	CLA	C14-C13-C15-C16
19	B	614	CLA	CHA-CBD-CGD-O1D
19	B	614	CLA	CHA-CBD-CGD-O2D
19	B	614	CLA	CAD-CBD-CGD-O1D
19	C	504	CLA	CHA-CBD-CGD-O1D
19	C	504	CLA	CHA-CBD-CGD-O2D
19	C	504	CLA	CAD-CBD-CGD-O1D
19	C	505	CLA	CBD-CGD-O2D-CED
19	C	510	CLA	CHA-CBD-CGD-O1D
19	C	510	CLA	CHA-CBD-CGD-O2D
19	C	514	CLA	C1A-C2A-CAA-CBA
19	C	514	CLA	C3A-C2A-CAA-CBA
19	a	404	CLA	CBD-CGD-O2D-CED
19	a	405	CLA	CHA-CBD-CGD-O1D
19	a	405	CLA	CHA-CBD-CGD-O2D
19	b	603	CLA	CHA-CBD-CGD-O1D
19	b	603	CLA	CHA-CBD-CGD-O2D
19	b	603	CLA	CAD-CBD-CGD-O1D
19	b	603	CLA	C11-C10-C8-C9
19	b	605	CLA	C2-C3-C5-C6
19	b	605	CLA	C4-C3-C5-C6
19	b	607	CLA	C2-C3-C5-C6
19	b	607	CLA	C4-C3-C5-C6
19	b	608	CLA	CHA-CBD-CGD-O1D
19	b	608	CLA	CHA-CBD-CGD-O2D
19	b	616	CLA	CHA-CBD-CGD-O1D
19	b	616	CLA	CHA-CBD-CGD-O2D
19	b	616	CLA	CAD-CBD-CGD-O1D
19	c	503	CLA	CHA-CBD-CGD-O1D
19	c	503	CLA	CHA-CBD-CGD-O2D
19	c	503	CLA	CAD-CBD-CGD-O1D
19	c	504	CLA	CHA-CBD-CGD-O1D
19	c	504	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	c	509	CLA	CHA-CBD-CGD-O1D
19	c	509	CLA	CHA-CBD-CGD-O2D
19	c	513	CLA	C1A-C2A-CAA-CBA
19	c	513	CLA	C3A-C2A-CAA-CBA
21	B	617	BCR	C1-C6-C7-C8
21	B	617	BCR	C36-C18-C19-C20
21	B	619	BCR	C21-C22-C23-C24
21	B	619	BCR	C37-C22-C23-C24
21	B	629	BCR	C7-C8-C9-C10
21	B	629	BCR	C7-C8-C9-C34
21	B	629	BCR	C11-C12-C13-C14
21	C	521	BCR	C7-C8-C9-C10
21	C	521	BCR	C7-C8-C9-C34
21	D	410	BCR	C1-C6-C7-C8
21	D	410	BCR	C7-C8-C9-C10
21	D	410	BCR	C7-C8-C9-C34
21	D	410	BCR	C23-C24-C25-C26
21	D	410	BCR	C23-C24-C25-C30
21	Y	101	BCR	C7-C8-C9-C10
21	Y	101	BCR	C7-C8-C9-C34
21	Y	101	BCR	C17-C18-C19-C20
21	Y	101	BCR	C36-C18-C19-C20
21	b	601	BCR	C1-C6-C7-C8
21	b	621	BCR	C21-C22-C23-C24
21	b	621	BCR	C37-C22-C23-C24
21	c	515	BCR	C7-C8-C9-C34
21	c	520	BCR	C7-C8-C9-C10
21	c	520	BCR	C7-C8-C9-C34
21	d	406	BCR	C1-C6-C7-C8
21	d	406	BCR	C23-C24-C25-C26
21	d	406	BCR	C23-C24-C25-C30
21	y	101	BCR	C7-C8-C9-C34
21	y	101	BCR	C17-C18-C19-C20
21	y	101	BCR	C36-C18-C19-C20
22	A	411	SQD	O5-C5-C6-S
22	F	102	SQD	C44-C45-O47-C7
22	F	102	SQD	O49-C7-O47-C45
22	F	102	SQD	O6-C1-O5-C5
22	F	102	SQD	O5-C5-C6-S
22	L	102	SQD	C8-C7-O47-C45
22	L	102	SQD	O5-C5-C6-S
22	a	412	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
22	f	102	SQD	C5-C6-S-O7
22	f	102	SQD	C5-C6-S-O8
22	f	102	SQD	C5-C6-S-O9
22	l	102	SQD	O5-C1-O6-C44
22	l	102	SQD	C46-C45-O47-C7
22	l	102	SQD	C8-C7-O47-C45
22	l	102	SQD	O5-C5-C6-S
23	A	410	PL9	C12-C13-C14-C16
23	A	410	PL9	C18-C19-C21-C22
23	A	410	PL9	C19-C21-C22-C23
23	A	410	PL9	C22-C23-C24-C25
23	A	410	PL9	C22-C23-C24-C26
23	A	410	PL9	C27-C28-C29-C31
23	A	410	PL9	C32-C33-C34-C36
23	A	410	PL9	C34-C36-C37-C38
23	A	410	PL9	C37-C38-C39-C40
23	D	411	PL9	C37-C38-C39-C40
23	D	411	PL9	C37-C38-C39-C41
23	a	411	PL9	C7-C8-C9-C10
23	a	411	PL9	C7-C8-C9-C11
23	a	411	PL9	C12-C13-C14-C16
23	a	411	PL9	C17-C18-C19-C20
23	a	411	PL9	C17-C18-C19-C21
23	a	411	PL9	C22-C23-C24-C25
23	a	411	PL9	C22-C23-C24-C26
23	a	411	PL9	C28-C29-C31-C32
23	a	411	PL9	C32-C33-C34-C36
27	D	413	LHG	O1-C1-C2-C3
27	D	413	LHG	C3-O3-P-O4
27	D	413	LHG	C4-O6-P-O4
27	L	101	LHG	C4-O6-P-O4
27	d	409	LHG	O1-C1-C2-C3
27	d	409	LHG	C3-O3-P-O4
27	d	409	LHG	C4-O6-P-O4
27	l	101	LHG	O1-C1-C2-C3
27	l	101	LHG	C1-C2-C3-O3
27	l	101	LHG	C3-O3-P-O4
27	l	101	LHG	C4-O6-P-O4
28	C	501	LMG	C2-C1-O1-C7
29	C	502	LMT	C2'-C1'-O1'-C1
29	C	502	LMT	O5'-C1'-O1'-C1
29	D	403	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
29	D	403	LMT	O5'-C1'-O1'-C1
29	D	403	LMT	C2-C1-O1'-C1'
29	b	602	LMT	C2'-C1'-O1'-C1
29	b	602	LMT	O5'-C1'-O1'-C1
29	z	101	LMT	C2'-C1'-O1'-C1
29	z	101	LMT	O5'-C1'-O1'-C1
30	D	415	DGD	O1G-C1G-C2G-O2G
30	D	415	DGD	O6D-C1D-O3G-C3G
30	J	101	DGD	C2B-C1B-O2G-C2G
30	J	101	DGD	O6D-C1D-O3G-C3G
30	d	414	DGD	C2B-C1B-O2G-C2G
31	f	101	HEM	C3D-CAD-CBD-CGD
19	C	505	CLA	O1D-CGD-O2D-CED
19	A	403	CLA	O1D-CGD-O2D-CED
19	a	404	CLA	O1D-CGD-O2D-CED
19	c	504	CLA	O1D-CGD-O2D-CED
19	C	515	CLA	CBD-CGD-O2D-CED
22	f	102	SQD	C24-C23-O48-C46
19	B	603	CLA	CBD-CGD-O2D-CED
19	C	504	CLA	CBD-CGD-O2D-CED
19	b	605	CLA	CBD-CGD-O2D-CED
19	c	503	CLA	CBD-CGD-O2D-CED
19	c	514	CLA	CBD-CGD-O2D-CED
22	f	102	SQD	O10-C23-O48-C46
28	C	518	LMG	O10-C28-O8-C9
19	c	512	CLA	CBD-CGD-O2D-CED
22	L	102	SQD	O49-C7-O47-C45
30	d	414	DGD	O1B-C1B-O2G-C2G
19	B	614	CLA	C3-C5-C6-C7
19	b	616	CLA	C3-C5-C6-C7
28	C	518	LMG	C29-C28-O8-C9
19	C	513	CLA	CBD-CGD-O2D-CED
19	b	616	CLA	CBD-CGD-O2D-CED
30	J	101	DGD	O1A-C1A-O1G-C1G
19	B	603	CLA	C2-C3-C5-C6
19	B	614	CLA	CBD-CGD-O2D-CED
19	B	616	CLA	CBD-CGD-O2D-CED
19	b	618	CLA	CBD-CGD-O2D-CED
19	B	606	CLA	C2A-CAA-CBA-CGA
19	C	509	CLA	C2A-CAA-CBA-CGA
19	b	608	CLA	C2A-CAA-CBA-CGA
19	c	508	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	F	102	SQD	C24-C23-O48-C46
28	C	501	LMG	O6-C5-C6-O5
28	c	501	LMG	O6-C5-C6-O5
30	J	101	DGD	C6B-C7B-C8B-C9B
23	a	411	PL9	C27-C28-C29-C30
22	l	102	SQD	O49-C7-O47-C45
30	J	101	DGD	O1B-C1B-O2G-C2G
23	A	410	PL9	C37-C38-C39-C41
23	a	411	PL9	C27-C28-C29-C31
22	F	102	SQD	O10-C23-O48-C46
19	B	608	CLA	CBD-CGD-O2D-CED
19	C	508	CLA	CBD-CGD-O2D-CED
19	b	610	CLA	CBD-CGD-O2D-CED
19	c	507	CLA	CBD-CGD-O2D-CED
27	D	412	LHG	O2-C2-C3-O3
27	d	408	LHG	O2-C2-C3-O3
30	J	101	DGD	C2A-C1A-O1G-C1G
30	d	414	DGD	C2A-C1A-O1G-C1G
30	J	101	DGD	C4A-C5A-C6A-C7A
29	C	502	LMT	O5B-C5B-C6B-O6B
30	J	101	DGD	O6E-C5E-C6E-O5E
29	i	103	LMT	C3'-C4'-O1B-C1B
19	B	610	CLA	CBD-CGD-O2D-CED
19	b	611	CLA	CBD-CGD-O2D-CED
19	b	612	CLA	CBD-CGD-O2D-CED
28	c	518	LMG	O6-C5-C6-O5
30	h	102	DGD	C6B-C7B-C8B-C9B
28	c	501	LMG	C4-C5-C6-O5
30	c	519	DGD	O6E-C5E-C6E-O5E
30	H	103	DGD	C6B-C7B-C8B-C9B
30	d	414	DGD	O1A-C1A-O1G-C1G
23	a	411	PL9	C35-C34-C36-C37
23	a	411	PL9	C23-C24-C26-C27
23	a	411	PL9	C33-C34-C36-C37
30	J	101	DGD	C4D-C5D-C6D-O5D
28	C	501	LMG	C4-C5-C6-O5
29	t	101	LMT	C4'-C5'-C6'-O6'
22	L	102	SQD	O5-C1-O6-C44
22	f	102	SQD	O5-C1-O6-C44
28	C	501	LMG	O6-C1-O1-C7
19	C	515	CLA	O1D-CGD-O2D-CED
23	A	410	PL9	C14-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	D	411	PL9	C39-C41-C42-C43
23	a	411	PL9	C9-C11-C12-C13
23	a	411	PL9	C34-C36-C37-C38
23	d	407	PL9	C39-C41-C42-C43
30	c	517	DGD	O6E-C5E-C6E-O5E
23	A	410	PL9	C12-C13-C14-C15
23	A	410	PL9	C27-C28-C29-C30
19	B	609	CLA	CBD-CGD-O2D-CED
19	C	504	CLA	O1D-CGD-O2D-CED
19	c	503	CLA	O1D-CGD-O2D-CED
27	D	412	LHG	C1-C2-C3-O3
27	d	408	LHG	C1-C2-C3-O3
30	c	519	DGD	C4E-C5E-C6E-O5E
19	b	603	CLA	C3-C5-C6-C7
19	C	504	CLA	CBA-CGA-O2A-C1
19	C	507	CLA	CBA-CGA-O2A-C1
19	C	508	CLA	CBA-CGA-O2A-C1
19	c	503	CLA	CBA-CGA-O2A-C1
19	c	506	CLA	CBA-CGA-O2A-C1
22	L	102	SQD	C24-C23-O48-C46
22	l	102	SQD	C24-C23-O48-C46
28	c	518	LMG	C29-C28-O8-C9
28	B	620	LMG	O6-C5-C6-O5
19	B	607	CLA	CBD-CGD-O2D-CED
21	b	601	BCR	C13-C14-C15-C16
19	C	514	CLA	C10-C11-C12-C13
29	C	502	LMT	C4B-C5B-C6B-O6B
19	c	503	CLA	C13-C15-C16-C17
30	c	517	DGD	C1B-C2B-C3B-C4B
30	D	415	DGD	C2D-C1D-O3G-C3G
30	J	101	DGD	C2D-C1D-O3G-C3G
22	F	102	SQD	O47-C45-C46-O48
28	b	622	LMG	O6-C5-C6-O5
29	t	101	LMT	O5'-C5'-C6'-O6'
19	A	405	CLA	C11-C12-C13-C14
19	B	601	CLA	C11-C10-C8-C9
19	C	511	CLA	C6-C7-C8-C9
19	a	406	CLA	C11-C12-C13-C14
19	c	510	CLA	C6-C7-C8-C9
19	B	614	CLA	C5-C6-C7-C8
21	B	629	BCR	C11-C12-C13-C35
21	C	516	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
21	D	410	BCR	C37-C22-C23-C24
21	b	601	BCR	C37-C22-C23-C24
21	d	406	BCR	C7-C8-C9-C34
21	d	406	BCR	C37-C22-C23-C24
21	D	410	BCR	C21-C22-C23-C24
21	b	601	BCR	C7-C8-C9-C10
21	d	406	BCR	C21-C22-C23-C24
19	c	514	CLA	O1D-CGD-O2D-CED
22	f	102	SQD	C8-C7-O47-C45
28	C	518	LMG	C11-C10-O7-C8
23	D	411	PL9	C47-C48-C49-C51
19	c	506	CLA	O1A-CGA-O2A-C1
19	A	407	CLA	C13-C15-C16-C17
19	C	504	CLA	C13-C15-C16-C17
30	J	101	DGD	C4E-C5E-C6E-O5E
19	C	509	CLA	C13-C15-C16-C17
27	D	412	LHG	C23-C24-C25-C26
19	C	504	CLA	O1A-CGA-O2A-C1
28	c	518	LMG	O10-C28-O8-C9
25	i	104	PLM	C4-C5-C6-C7
19	A	407	CLA	C10-C11-C12-C13
19	a	408	CLA	C10-C11-C12-C13
19	a	408	CLA	C13-C15-C16-C17
19	C	507	CLA	O1A-CGA-O2A-C1
22	A	409	SQD	C23-C24-C25-C26
22	a	410	SQD	C23-C24-C25-C26
25	A	413	PLM	C1-C2-C3-C4
27	d	408	LHG	C23-C24-C25-C26
28	c	501	LMG	C28-C29-C30-C31
30	D	415	DGD	C1A-C2A-C3A-C4A
19	A	407	CLA	C15-C16-C17-C18
19	a	408	CLA	C15-C16-C17-C18
30	c	516	DGD	C2A-C3A-C4A-C5A
19	b	616	CLA	C5-C6-C7-C8
30	c	516	DGD	C1B-C2B-C3B-C4B
19	b	609	CLA	CBD-CGD-O2D-CED
22	A	411	SQD	C16-C17-C18-C19
27	A	417	LHG	C15-C16-C17-C18
19	c	507	CLA	C5-C6-C7-C8
19	B	604	CLA	C6-C7-C8-C10
19	B	604	CLA	C11-C12-C13-C15
19	C	510	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	a	408	CLA	C6-C7-C8-C10
19	b	613	CLA	C12-C13-C15-C16
19	C	508	CLA	O1A-CGA-O2A-C1
19	c	503	CLA	O1A-CGA-O2A-C1
21	B	629	BCR	C13-C14-C15-C16
19	B	603	CLA	O1D-CGD-O2D-CED
19	b	605	CLA	O1D-CGD-O2D-CED
19	B	615	CLA	C10-C11-C12-C13
19	b	617	CLA	C10-C11-C12-C13
22	l	102	SQD	O10-C23-O48-C46
22	a	412	SQD	O5-C1-O6-C44
28	c	501	LMG	O6-C1-O1-C7
23	A	410	PL9	C24-C26-C27-C28
23	A	410	PL9	C29-C31-C32-C33
23	D	411	PL9	C34-C36-C37-C38
23	a	411	PL9	C19-C21-C22-C23
29	m	101	LMT	O1'-C1-C2-C3
27	a	416	LHG	O2-C2-C3-O3
27	l	101	LHG	O2-C2-C3-O3
22	f	102	SQD	O49-C7-O47-C45
28	C	518	LMG	O9-C10-O7-C8
28	B	620	LMG	C4-C5-C6-O5
19	B	616	CLA	C8-C10-C11-C12
19	C	509	CLA	C10-C11-C12-C13
19	D	409	CLA	C10-C11-C12-C13
19	b	604	CLA	C15-C16-C17-C18
19	b	618	CLA	C8-C10-C11-C12
22	L	102	SQD	O10-C23-O48-C46
19	B	601	CLA	C10-C11-C12-C13
19	c	507	CLA	C10-C11-C12-C13
19	c	512	CLA	O1D-CGD-O2D-CED
28	C	501	LMG	C11-C10-O7-C8
19	B	613	CLA	C8-C10-C11-C12
19	C	508	CLA	C5-C6-C7-C8
19	b	603	CLA	C10-C11-C12-C13
19	b	615	CLA	C8-C10-C11-C12
19	d	405	CLA	C10-C11-C12-C13
27	D	413	LHG	C3-O3-P-O6
27	D	413	LHG	C4-O6-P-O3
27	a	416	LHG	C3-O3-P-O6
27	d	409	LHG	C3-O3-P-O6
27	d	409	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
27	l	101	LHG	C3-O3-P-O6
19	a	408	CLA	CBA-CGA-O2A-C1
19	C	513	CLA	O1D-CGD-O2D-CED
30	J	101	DGD	O6D-C5D-C6D-O5D
19	b	616	CLA	O1D-CGD-O2D-CED
28	C	501	LMG	O9-C10-O7-C8
28	d	410	LMG	C16-C17-C18-C19
30	C	517	DGD	C2A-C3A-C4A-C5A
19	B	610	CLA	C16-C17-C18-C20
19	b	612	CLA	C16-C17-C18-C20
19	c	507	CLA	C16-C17-C18-C19
19	B	601	CLA	C3-C5-C6-C7
19	b	618	CLA	O1D-CGD-O2D-CED
19	A	407	CLA	CBA-CGA-O2A-C1
19	B	608	CLA	CBA-CGA-O2A-C1
19	c	507	CLA	CBA-CGA-O2A-C1
27	a	416	LHG	C24-C23-O8-C6
19	B	613	CLA	C13-C15-C16-C17
21	B	629	BCR	C9-C10-C11-C12
25	e	101	PLM	C6-C7-C8-C9
30	D	415	DGD	C2B-C1B-O2G-C2G
22	A	409	SQD	C24-C25-C26-C27
22	A	409	SQD	C27-C28-C29-C30
22	L	102	SQD	C11-C12-C13-C14
24	A	414	LFA	C11-C12-C13-C14
25	b	623	PLM	C5-C6-C7-C8
25	b	631	PLM	C6-C7-C8-C9
27	A	417	LHG	C30-C31-C32-C33
27	L	101	LHG	C25-C26-C27-C28
27	d	409	LHG	C15-C16-C17-C18
27	l	101	LHG	C33-C34-C35-C36
28	C	501	LMG	C35-C36-C37-C38
29	t	101	LMT	C6-C7-C8-C9
30	c	516	DGD	C4B-C5B-C6B-C7B
19	B	614	CLA	O1D-CGD-O2D-CED
19	B	616	CLA	O1D-CGD-O2D-CED
19	B	616	CLA	C16-C17-C18-C19
19	b	618	CLA	C16-C17-C18-C19
22	A	409	SQD	C12-C13-C14-C15
22	A	409	SQD	C30-C31-C32-C33
22	a	410	SQD	C16-C17-C18-C19
22	a	410	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
25	E	101	PLM	C5-C6-C7-C8
27	D	412	LHG	C25-C26-C27-C28
28	c	518	LMG	C15-C16-C17-C18
30	C	517	DGD	CAB-CBB-CCB-CDB
30	H	103	DGD	CBA-CCA-CDA-CEA
30	c	516	DGD	CAB-CBB-CCB-CDB
22	L	102	SQD	C46-C45-O47-C7
30	D	415	DGD	O1B-C1B-O2G-C2G
19	C	508	CLA	C10-C11-C12-C13
22	a	410	SQD	C7-C8-C9-C10
30	c	517	DGD	C4E-C5E-C6E-O5E
22	l	102	SQD	C15-C16-C17-C18
27	A	417	LHG	C10-C11-C12-C13
27	L	101	LHG	C33-C34-C35-C36
30	C	517	DGD	C4B-C5B-C6B-C7B
22	A	409	SQD	C16-C17-C18-C19
25	I	101	PLM	C2-C3-C4-C5
30	D	415	DGD	C7B-C8B-C9B-CAB
30	c	516	DGD	C3B-C4B-C5B-C6B
24	H	101	LFA	C10-C11-C12-C13
25	b	631	PLM	C2-C3-C4-C5
27	d	408	LHG	C25-C26-C27-C28
22	a	412	SQD	C2-C1-O6-C44
28	c	501	LMG	C2-C1-O1-C7
22	a	410	SQD	C24-C25-C26-C27
22	a	410	SQD	C30-C31-C32-C33
28	c	518	LMG	C38-C39-C40-C41
30	J	101	DGD	C7B-C8B-C9B-CAB
19	b	615	CLA	C13-C15-C16-C17
19	A	407	CLA	O1A-CGA-O2A-C1
19	B	604	CLA	C16-C17-C18-C20
19	b	617	CLA	C16-C17-C18-C19
23	d	407	PL9	C15-C14-C16-C17
22	A	409	SQD	C10-C11-C12-C13
22	a	410	SQD	C34-C35-C36-C37
25	a	401	PLM	CB-CC-CD-CE
25	i	102	PLM	C6-C7-C8-C9
28	B	620	LMG	C35-C36-C37-C38
28	b	622	LMG	C29-C30-C31-C32
28	c	501	LMG	C13-C14-C15-C16
29	t	101	LMT	C5-C6-C7-C8
19	A	405	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B	608	CLA	C11-C12-C13-C14
19	a	406	CLA	C6-C7-C8-C9
19	a	408	CLA	C6-C7-C8-C9
19	b	606	CLA	C11-C12-C13-C14
19	B	608	CLA	O1D-CGD-O2D-CED
19	b	610	CLA	O1D-CGD-O2D-CED
22	a	410	SQD	C11-C12-C13-C14
22	a	412	SQD	C10-C11-C12-C13
24	D	406	LFA	C16-C17-C18-C19
25	b	625	PLM	C3-C4-C5-C6
27	A	417	LHG	C24-C25-C26-C27
28	d	410	LMG	C19-C20-C21-C22
29	M	102	LMT	C2-C3-C4-C5
30	D	415	DGD	C4B-C5B-C6B-C7B
30	d	414	DGD	C2B-C3B-C4B-C5B
21	B	629	BCR	C37-C22-C23-C24
21	b	601	BCR	C7-C8-C9-C34
24	B	628	LFA	C7-C8-C9-C10
25	E	101	PLM	C6-C7-C8-C9
28	D	414	LMG	C37-C38-C39-C40
27	A	417	LHG	O1-C1-C2-C3
27	D	412	LHG	O1-C1-C2-C3
27	a	415	LHG	O1-C1-C2-C3
27	a	416	LHG	O1-C1-C2-C3
27	d	408	LHG	O1-C1-C2-C3
22	A	411	SQD	C11-C12-C13-C14
22	A	411	SQD	C14-C15-C16-C17
22	A	411	SQD	C30-C31-C32-C33
22	a	410	SQD	C15-C16-C17-C18
22	a	410	SQD	C31-C32-C33-C34
27	L	101	LHG	C31-C32-C33-C34
27	a	415	LHG	C30-C31-C32-C33
28	c	518	LMG	C16-C17-C18-C19
30	h	102	DGD	C7A-C8A-C9A-CAA
28	c	518	LMG	C4-C5-C6-O5
29	m	101	LMT	C4'-C5'-C6'-O6'
30	d	414	DGD	C1B-C2B-C3B-C4B
19	c	507	CLA	O1D-CGD-O2D-CED
22	A	409	SQD	C11-C10-C9-C8
22	F	102	SQD	C25-C26-C27-C28
25	B	626	PLM	C5-C6-C7-C8
27	l	101	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
28	B	620	LMG	C32-C33-C34-C35
28	B	620	LMG	C33-C34-C35-C36
28	C	501	LMG	C16-C17-C18-C19
28	C	501	LMG	C18-C19-C20-C21
29	i	103	LMT	C6-C7-C8-C9
29	m	101	LMT	C3-C4-C5-C6
30	H	103	DGD	C7A-C8A-C9A-CAA
30	c	517	DGD	C2A-C3A-C4A-C5A
30	d	414	DGD	C7B-C8B-C9B-CAB
19	B	610	CLA	C16-C17-C18-C19
19	B	615	CLA	C16-C17-C18-C19
19	B	616	CLA	C16-C17-C18-C20
19	C	508	CLA	C16-C17-C18-C19
19	C	508	CLA	C16-C17-C18-C20
19	C	509	CLA	C16-C17-C18-C19
19	C	509	CLA	C16-C17-C18-C20
19	b	612	CLA	C16-C17-C18-C19
19	b	617	CLA	C16-C17-C18-C20
19	b	618	CLA	C16-C17-C18-C20
22	L	102	SQD	C31-C32-C33-C34
27	l	101	LHG	C25-C26-C27-C28
30	C	517	DGD	C3B-C4B-C5B-C6B
30	c	517	DGD	C6B-C7B-C8B-C9B
30	c	517	DGD	CAB-CBB-CCB-CDB
24	H	101	LFA	C7-C8-C9-C10
24	J	102	LFA	C12-C13-C14-C15
27	a	415	LHG	C10-C11-C12-C13
28	C	501	LMG	C31-C32-C33-C34
25	a	414	PLM	C1-C2-C3-C4
28	D	414	LMG	C28-C29-C30-C31
19	a	408	CLA	O1A-CGA-O2A-C1
22	A	411	SQD	C25-C26-C27-C28
27	A	417	LHG	C11-C12-C13-C14
30	c	516	DGD	C4A-C5A-C6A-C7A
19	b	610	CLA	CBA-CGA-O2A-C1
25	I	104	PLM	C4-C5-C6-C7
28	b	622	LMG	C18-C19-C20-C21
30	C	517	DGD	C5B-C6B-C7B-C8B
30	c	516	DGD	C5B-C6B-C7B-C8B
29	b	602	LMT	O5'-C5'-C6'-O6'
29	t	101	LMT	C2-C1-O1'-C1'
28	b	622	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
29	D	403	LMT	C2-C3-C4-C5
30	H	103	DGD	C9B-CAB-CBB-CCB
30	h	102	DGD	C9B-CAB-CBB-CCB
19	C	508	CLA	O1D-CGD-O2D-CED
19	c	507	CLA	C16-C17-C18-C20
22	l	102	SQD	C11-C12-C13-C14
22	l	102	SQD	C31-C32-C33-C34
28	b	622	LMG	C33-C34-C35-C36
30	c	516	DGD	C8A-C9A-CAA-CBA
30	c	517	DGD	C9A-CAA-CBA-CCA
30	h	102	DGD	CBA-CCA-CDA-CEA
28	B	620	LMG	C18-C19-C20-C21
23	d	407	PL9	C45-C44-C46-C47
24	D	404	LFA	C11-C10-C9-C8
22	F	102	SQD	O5-C1-O6-C44
27	D	413	LHG	O1-C1-C2-O2
22	A	411	SQD	C28-C29-C30-C31
27	a	416	LHG	O10-C23-O8-C6
28	d	410	LMG	C28-C29-C30-C31
19	B	615	CLA	C16-C17-C18-C20
22	L	102	SQD	C15-C16-C17-C18
30	C	517	DGD	C8A-C9A-CAA-CBA
19	B	610	CLA	C13-C15-C16-C17
19	b	612	CLA	C13-C15-C16-C17
22	A	411	SQD	C33-C34-C35-C36
29	i	103	LMT	C3-C4-C5-C6
19	B	608	CLA	O1A-CGA-O2A-C1
19	b	610	CLA	C13-C15-C16-C17
22	A	411	SQD	C26-C27-C28-C29
27	A	417	LHG	C13-C14-C15-C16
27	D	413	LHG	C14-C15-C16-C17
23	a	411	PL9	C37-C38-C39-C41
29	b	602	LMT	C3-C4-C5-C6
19	B	614	CLA	C10-C11-C12-C13
19	c	507	CLA	O1A-CGA-O2A-C1
22	L	102	SQD	C9-C10-C11-C12
22	l	102	SQD	C32-C33-C34-C35
25	i	102	PLM	C5-C6-C7-C8
27	d	409	LHG	C32-C33-C34-C35
28	B	620	LMG	C31-C32-C33-C34
25	b	625	PLM	C1-C2-C3-C4
21	A	408	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
21	B	617	BCR	C5-C6-C7-C8
21	B	619	BCR	C23-C24-C25-C26
21	C	516	BCR	C5-C6-C7-C8
21	C	521	BCR	C5-C6-C7-C8
21	D	410	BCR	C5-C6-C7-C8
21	K	101	BCR	C1-C6-C7-C8
21	K	101	BCR	C5-C6-C7-C8
21	Y	101	BCR	C5-C6-C7-C8
21	a	409	BCR	C23-C24-C25-C26
21	b	601	BCR	C5-C6-C7-C8
21	b	621	BCR	C23-C24-C25-C26
21	c	515	BCR	C5-C6-C7-C8
21	c	520	BCR	C5-C6-C7-C8
21	d	406	BCR	C5-C6-C7-C8
21	y	101	BCR	C5-C6-C7-C8
22	f	102	SQD	C30-C31-C32-C33
19	b	611	CLA	O1D-CGD-O2D-CED
30	D	415	DGD	C2A-C1A-O1G-C1G
19	B	603	CLA	C5-C6-C7-C8
19	C	508	CLA	C13-C15-C16-C17
19	b	605	CLA	C5-C6-C7-C8
22	A	409	SQD	C8-C7-O47-C45
22	L	102	SQD	C32-C33-C34-C35
25	I	101	PLM	C5-C6-C7-C8
27	A	417	LHG	C28-C29-C30-C31
28	B	620	LMG	C29-C30-C31-C32
28	c	518	LMG	C39-C40-C41-C42
22	A	409	SQD	C15-C16-C17-C18
28	D	414	LMG	C16-C17-C18-C19
19	c	507	CLA	C13-C15-C16-C17
29	i	103	LMT	O5B-C5B-C6B-O6B
30	H	103	DGD	C7B-C8B-C9B-CAB
30	J	101	DGD	C4B-C5B-C6B-C7B
30	h	102	DGD	CCB-CDB-CEB-CFB
23	D	411	PL9	C15-C14-C16-C17
19	A	405	CLA	C6-C7-C8-C10
19	B	611	CLA	C12-C13-C15-C16
19	B	613	CLA	C11-C10-C8-C7
19	a	406	CLA	C6-C7-C8-C10
19	b	615	CLA	C11-C10-C8-C7
19	c	509	CLA	C11-C10-C8-C7
23	d	407	PL9	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
19	b	610	CLA	O1A-CGA-O2A-C1
30	D	415	DGD	O1A-C1A-O1G-C1G
29	m	101	LMT	O5'-C5'-C6'-O6'
22	A	411	SQD	O49-C7-O47-C45
27	d	408	LHG	C16-C17-C18-C19
19	B	610	CLA	C2A-CAA-CBA-CGA
19	b	612	CLA	C2A-CAA-CBA-CGA
19	B	610	CLA	O1D-CGD-O2D-CED
19	b	613	CLA	C15-C16-C17-C18
19	c	509	CLA	C5-C6-C7-C8
25	D	405	PLM	C8-C9-CA-CB
27	D	412	LHG	C16-C17-C18-C19
30	c	517	DGD	CBA-CCA-CDA-CEA
22	F	102	SQD	C33-C34-C35-C36
27	A	417	LHG	C26-C27-C28-C29
19	b	612	CLA	O1D-CGD-O2D-CED
19	C	510	CLA	C5-C6-C7-C8
22	f	102	SQD	C24-C25-C26-C27
29	m	102	LMT	O1'-C1-C2-C3
23	a	411	PL9	C32-C33-C34-C35
19	b	616	CLA	C10-C11-C12-C13
22	a	410	SQD	C29-C30-C31-C32
28	C	501	LMG	C29-C30-C31-C32
28	b	622	LMG	C20-C21-C22-C23
29	D	403	LMT	C11-C10-C9-C8
29	d	412	LMT	C7-C8-C9-C10
30	h	102	DGD	C7B-C8B-C9B-CAB
28	C	518	LMG	C10-C11-C12-C13
22	A	411	SQD	C8-C7-O47-C45
22	a	410	SQD	C33-C34-C35-C36
30	d	414	DGD	C6B-C7B-C8B-C9B
28	b	622	LMG	C4-C5-C6-O5
22	f	102	SQD	C9-C10-C11-C12
30	H	103	DGD	CCB-CDB-CEB-CFB
22	F	102	SQD	C32-C33-C34-C35
27	a	415	LHG	C27-C28-C29-C30
28	C	518	LMG	C2-C1-O1-C7
24	B	625	LFA	C14-C15-C16-C17
30	J	101	DGD	CBB-CCB-CDB-CEB
30	c	516	DGD	CBA-CCA-CDA-CEA
22	A	411	SQD	C24-C25-C26-C27
25	a	401	PLM	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	i	104	PLM	C3-C4-C5-C6
28	B	620	LMG	C20-C21-C22-C23
28	D	414	LMG	C31-C32-C33-C34
30	c	516	DGD	O6E-C5E-C6E-O5E
23	A	410	PL9	C20-C19-C21-C22
28	C	518	LMG	C11-C12-C13-C14
29	m	101	LMT	C2-C3-C4-C5
19	A	407	CLA	C6-C7-C8-C9
19	B	604	CLA	C11-C12-C13-C14
19	B	611	CLA	C14-C13-C15-C16
19	C	510	CLA	C11-C10-C8-C9
19	C	513	CLA	C6-C7-C8-C9
19	b	613	CLA	C14-C13-C15-C16
19	c	509	CLA	C11-C10-C8-C9
19	c	512	CLA	C6-C7-C8-C9
19	c	513	CLA	C14-C13-C15-C16
23	A	410	PL9	C47-C48-C49-C51
19	C	511	CLA	C8-C10-C11-C12
30	C	517	DGD	C6A-C7A-C8A-C9A
30	C	517	DGD	O6E-C5E-C6E-O5E
22	l	102	SQD	C11-C10-C9-C8
25	a	401	PLM	C2-C3-C4-C5
21	c	515	BCR	C7-C8-C9-C10
21	d	406	BCR	C7-C8-C9-C10
19	A	404	CLA	C1A-C2A-CAA-CBA
19	A	405	CLA	C1A-C2A-CAA-CBA
19	a	405	CLA	C1A-C2A-CAA-CBA
19	a	406	CLA	C1A-C2A-CAA-CBA
19	B	604	CLA	C16-C17-C18-C19
22	A	409	SQD	O49-C7-O47-C45
28	C	518	LMG	C12-C13-C14-C15
29	i	103	LMT	C5-C6-C7-C8
21	C	521	BCR	C19-C20-C21-C22
19	B	609	CLA	O1D-CGD-O2D-CED
19	B	611	CLA	C15-C16-C17-C18
27	L	101	LHG	C4-O6-P-O3
30	C	517	DGD	C9A-CAA-CBA-CCA
25	i	101	PLM	C1-C2-C3-C4
28	B	620	LMG	C19-C20-C21-C22
22	F	102	SQD	C31-C32-C33-C34
28	c	518	LMG	C34-C35-C36-C37
29	M	101	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
28	C	518	LMG	O6-C5-C6-O5
28	b	622	LMG	C19-C20-C21-C22
29	D	403	LMT	C7-C8-C9-C10
19	d	405	CLA	C13-C15-C16-C17
29	M	101	LMT	O1'-C1-C2-C3
27	a	415	LHG	C16-C17-C18-C19
19	b	617	CLA	C5-C6-C7-C8
30	d	414	DGD	O6D-C5D-C6D-O5D
30	c	516	DGD	C9A-CAA-CBA-CCA
22	A	409	SQD	C25-C26-C27-C28
25	B	626	PLM	C7-C8-C9-CA
29	M	101	LMT	C7-C8-C9-C10
19	B	607	CLA	O1D-CGD-O2D-CED
22	F	102	SQD	O6-C44-C45-C46
22	F	102	SQD	C44-C45-C46-O48
22	L	102	SQD	C44-C45-C46-O48
22	l	102	SQD	C44-C45-C46-O48
30	D	415	DGD	C5B-C6B-C7B-C8B
30	d	414	DGD	O1G-C1G-C2G-C3G
19	C	511	CLA	C10-C11-C12-C13
25	i	101	PLM	C3-C4-C5-C6
27	a	415	LHG	C32-C33-C34-C35
30	C	517	DGD	CBA-CCA-CDA-CEA
28	c	518	LMG	C8-C7-O1-C1
30	c	517	DGD	C5D-C6D-O5D-C1E
25	B	622	PLM	C3-C4-C5-C6
19	D	409	CLA	C13-C15-C16-C17
22	a	412	SQD	C15-C16-C17-C18
25	a	401	PLM	C9-CA-CB-CC
25	i	104	PLM	C8-C9-CA-CB
22	l	102	SQD	O48-C23-C24-C25
24	a	413	LFA	C9-C10-C11-C12
28	b	622	LMG	C15-C16-C17-C18
29	D	403	LMT	C3-C4-C5-C6
27	d	409	LHG	O1-C1-C2-O2
22	f	102	SQD	C33-C34-C35-C36
25	i	102	PLM	C4-C5-C6-C7
30	c	517	DGD	C3B-C4B-C5B-C6B
28	D	414	LMG	O6-C5-C6-O5
22	A	411	SQD	C23-C24-C25-C26
28	d	410	LMG	O6-C5-C6-O5
24	H	101	LFA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	a	401	PLM	CC-CD-CE-CF
28	c	518	LMG	C37-C38-C39-C40
29	i	103	LMT	C5'-C4'-O1B-C1B
19	D	408	CLA	C2-C1-O2A-CGA
20	D	401	PHO	C2-C1-O2A-CGA
20	d	402	PHO	C2-C1-O2A-CGA
28	c	501	LMG	C21-C22-C23-C24
28	d	410	LMG	C34-C35-C36-C37
23	d	407	PL9	C47-C48-C49-C51
22	L	102	SQD	O48-C23-C24-C25
22	a	412	SQD	C13-C14-C15-C16
27	d	409	LHG	C14-C15-C16-C17
29	i	103	LMT	O1'-C1-C2-C3
19	b	609	CLA	O1D-CGD-O2D-CED
30	D	415	DGD	C9B-CAB-CBB-CCB
27	L	101	LHG	C11-C12-C13-C14
27	a	416	LHG	C13-C14-C15-C16
30	J	101	DGD	O2G-C2G-C3G-O3G
30	c	516	DGD	O6D-C5D-C6D-O5D
22	l	102	SQD	C12-C13-C14-C15
27	l	101	LHG	C11-C12-C13-C14
29	M	101	LMT	C2-C3-C4-C5
30	C	517	DGD	C4A-C5A-C6A-C7A
29	m	101	LMT	O5B-C5B-C6B-O6B
29	z	101	LMT	O5'-C5'-C6'-O6'
23	a	411	PL9	C12-C13-C14-C15
19	C	509	CLA	C15-C16-C17-C18
19	A	407	CLA	C6-C7-C8-C10
19	A	407	CLA	C11-C10-C8-C7
19	B	601	CLA	C6-C7-C8-C10
19	B	603	CLA	C6-C7-C8-C10
19	B	603	CLA	C11-C10-C8-C7
19	B	616	CLA	C11-C12-C13-C15
19	B	616	CLA	C12-C13-C15-C16
19	C	506	CLA	C12-C13-C15-C16
19	C	512	CLA	C6-C7-C8-C10
19	C	513	CLA	C6-C7-C8-C10
19	C	514	CLA	C12-C13-C15-C16
19	D	409	CLA	C11-C10-C8-C7
19	b	603	CLA	C11-C10-C8-C7
19	b	603	CLA	C11-C12-C13-C15
19	b	605	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	b	605	CLA	C11-C10-C8-C7
19	b	616	CLA	C12-C13-C15-C16
19	b	618	CLA	C11-C12-C13-C15
19	b	618	CLA	C12-C13-C15-C16
19	c	505	CLA	C12-C13-C15-C16
19	c	507	CLA	C11-C12-C13-C15
19	c	510	CLA	C6-C7-C8-C10
19	c	511	CLA	C6-C7-C8-C10
19	c	512	CLA	C6-C7-C8-C10
19	c	513	CLA	C12-C13-C15-C16
19	d	404	CLA	C11-C12-C13-C15
19	d	405	CLA	C11-C10-C8-C7
23	A	410	PL9	C43-C44-C46-C47
28	C	518	LMG	C14-C15-C16-C17
19	A	407	CLA	C11-C10-C8-C9
19	B	603	CLA	C6-C7-C8-C9
19	B	614	CLA	C14-C13-C15-C16
19	B	616	CLA	C11-C12-C13-C14
19	B	616	CLA	C14-C13-C15-C16
19	C	508	CLA	C11-C12-C13-C14
19	C	512	CLA	C6-C7-C8-C9
19	D	409	CLA	C11-C10-C8-C9
19	b	605	CLA	C6-C7-C8-C9
19	b	615	CLA	C11-C12-C13-C14
19	b	616	CLA	C14-C13-C15-C16
19	b	618	CLA	C11-C12-C13-C14
19	b	618	CLA	C14-C13-C15-C16
19	c	508	CLA	C11-C10-C8-C9
19	c	511	CLA	C6-C7-C8-C9
19	d	405	CLA	C11-C10-C8-C9
30	C	517	DGD	O6D-C5D-C6D-O5D
19	C	503	CLA	C2A-CAA-CBA-CGA
25	H	105	PLM	C5-C6-C7-C8
19	b	607	CLA	CBD-CGD-O2D-CED
21	B	617	BCR	C17-C18-C19-C20
21	y	101	BCR	C7-C8-C9-C10
25	I	104	PLM	C6-C7-C8-C9
27	a	416	LHG	C1-C2-C3-O3
22	L	102	SQD	C16-C17-C18-C19
19	C	513	CLA	CBA-CGA-O2A-C1
29	m	101	LMT	C1-C2-C3-C4
22	a	412	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
19	B	615	CLA	C5-C6-C7-C8
28	B	620	LMG	C15-C16-C17-C18
23	A	410	PL9	C39-C41-C42-C43
24	J	102	LFA	C13-C14-C15-C16
25	b	631	PLM	C5-C6-C7-C8
25	B	627	PLM	C1-C2-C3-C4
28	b	622	LMG	C28-C29-C30-C31
30	c	517	DGD	CAA-CBA-CCA-CDA
25	A	415	PLM	C3-C4-C5-C6
28	d	410	LMG	C21-C22-C23-C24
23	D	411	PL9	C45-C44-C46-C47
28	b	622	LMG	C30-C31-C32-C33
22	A	411	SQD	C9-C10-C11-C12
29	b	602	LMT	C4-C5-C6-C7
24	B	628	LFA	C11-C10-C9-C8
19	c	504	CLA	C8-C10-C11-C12
30	C	517	DGD	C1B-C2B-C3B-C4B
28	B	620	LMG	C17-C18-C19-C20
21	c	520	BCR	C19-C20-C21-C22
29	D	402	LMT	C2-C1-O1'-C1'
29	M	101	LMT	C2-C1-O1'-C1'
29	m	101	LMT	C2-C1-O1'-C1'
29	z	101	LMT	C2-C1-O1'-C1'
25	e	101	PLM	CD-CE-CF-CG
28	c	501	LMG	C12-C13-C14-C15
22	L	102	SQD	C33-C34-C35-C36
28	D	414	LMG	C38-C39-C40-C41
28	b	622	LMG	C17-C18-C19-C20
19	c	510	CLA	C15-C16-C17-C18
29	M	102	LMT	O1'-C1-C2-C3
22	l	102	SQD	C33-C34-C35-C36
30	h	102	DGD	O2G-C1B-C2B-C3B
29	m	101	LMT	O5B-C1B-O1B-C4'
22	A	409	SQD	C31-C32-C33-C34
27	l	101	LHG	C30-C31-C32-C33
30	c	519	DGD	C8A-C9A-CAA-CBA
30	h	102	DGD	CDA-CEA-CFA-CGA
22	L	102	SQD	C25-C26-C27-C28
29	m	101	LMT	C4-C5-C6-C7
19	c	502	CLA	C2A-CAA-CBA-CGA
19	C	505	CLA	C8-C10-C11-C12
30	c	516	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
19	B	605	CLA	CBD-CGD-O2D-CED
30	C	517	DGD	C4D-C5D-C6D-O5D
30	c	516	DGD	C4D-C5D-C6D-O5D
28	c	501	LMG	C22-C23-C24-C25
24	A	412	LFA	C7-C8-C9-C10
27	a	415	LHG	C13-C14-C15-C16
24	B	621	LFA	C7-C8-C9-C10
22	F	102	SQD	O6-C44-C45-O47
30	d	414	DGD	O1G-C1G-C2G-O2G
22	l	102	SQD	C25-C26-C27-C28
22	a	410	SQD	C25-C26-C27-C28
28	c	518	LMG	C12-C13-C14-C15
23	a	411	PL9	C29-C31-C32-C33
28	d	410	LMG	C13-C14-C15-C16
19	A	403	CLA	C2-C1-O2A-CGA
19	B	613	CLA	C2-C1-O2A-CGA
19	a	404	CLA	C2-C1-O2A-CGA
19	b	615	CLA	C2-C1-O2A-CGA
19	d	404	CLA	C2-C1-O2A-CGA
28	c	501	LMG	C16-C17-C18-C19
25	A	415	PLM	C1-C2-C3-C4
19	B	613	CLA	C11-C12-C13-C14
19	B	614	CLA	C11-C12-C13-C14
19	C	509	CLA	C11-C12-C13-C14
19	C	514	CLA	C14-C13-C15-C16
19	a	406	CLA	C11-C10-C8-C9
19	b	604	CLA	C11-C10-C8-C9
19	b	616	CLA	C11-C12-C13-C14
19	c	507	CLA	C11-C12-C13-C14
30	c	516	DGD	C8B-C9B-CAB-CBB
19	c	511	CLA	CBD-CGD-O2D-CED
22	A	411	SQD	C27-C28-C29-C30
25	i	101	PLM	CA-CB-CC-CD
29	m	102	LMT	C5-C6-C7-C8
19	C	507	CLA	C2A-CAA-CBA-CGA
19	c	506	CLA	C2A-CAA-CBA-CGA
21	A	408	BCR	C23-C24-C25-C30
21	B	617	BCR	C23-C24-C25-C26
21	B	629	BCR	C5-C6-C7-C8
21	K	101	BCR	C23-C24-C25-C26
21	Y	101	BCR	C1-C6-C7-C8
21	a	409	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
21	c	515	BCR	C23-C24-C25-C26
21	k	101	BCR	C1-C6-C7-C8
21	k	101	BCR	C5-C6-C7-C8
21	k	101	BCR	C23-C24-C25-C26
21	y	101	BCR	C1-C6-C7-C8
32	H	102	RRX	C23-C24-C25-C30
32	H	102	RRX	C23-C24-C25-C26
28	C	501	LMG	C20-C21-C22-C23
28	b	622	LMG	C38-C39-C40-C41
21	k	101	BCR	C37-C22-C23-C24
29	z	101	LMT	C4'-C5'-C6'-O6'
28	D	414	LMG	C19-C20-C21-C22
30	c	517	DGD	C3A-C4A-C5A-C6A
21	B	629	BCR	C21-C22-C23-C24
21	C	516	BCR	C7-C8-C9-C10
21	b	601	BCR	C21-C22-C23-C24
19	B	616	CLA	C10-C11-C12-C13
19	b	606	CLA	C8-C10-C11-C12
19	b	618	CLA	C10-C11-C12-C13
19	c	502	CLA	C13-C15-C16-C17
27	a	415	LHG	C26-C27-C28-C29
27	d	409	LHG	C12-C13-C14-C15
27	l	101	LHG	C23-C24-C25-C26
27	a	415	LHG	C15-C16-C17-C18
28	c	501	LMG	C38-C39-C40-C41
28	d	410	LMG	C35-C36-C37-C38
29	m	101	LMT	C2B-C1B-O1B-C4'
30	H	103	DGD	O2G-C1B-C2B-C3B
19	A	405	CLA	C11-C10-C8-C7
19	B	601	CLA	C11-C10-C8-C7
19	B	614	CLA	C11-C12-C13-C15
19	C	506	CLA	C11-C10-C8-C7
19	C	507	CLA	C11-C12-C13-C15
19	C	508	CLA	C11-C12-C13-C15
19	C	511	CLA	C11-C12-C13-C15
19	D	409	CLA	C12-C13-C15-C16
19	a	406	CLA	C11-C10-C8-C7
19	a	408	CLA	C11-C10-C8-C7
19	b	604	CLA	C11-C10-C8-C7
19	b	606	CLA	C11-C12-C13-C15
19	b	616	CLA	C11-C12-C13-C15
19	c	505	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	c	506	CLA	C11-C12-C13-C15
19	c	508	CLA	C11-C10-C8-C7
19	c	514	CLA	C11-C10-C8-C7
19	d	405	CLA	C12-C13-C15-C16
23	D	411	PL9	C43-C44-C46-C47
23	a	411	PL9	C43-C44-C46-C47
28	b	622	LMG	C31-C32-C33-C34
30	c	517	DGD	CBB-CCB-CDB-CEB
21	b	601	BCR	C15-C16-C17-C18
21	c	520	BCR	C9-C10-C11-C12
20	d	402	PHO	CBA-CGA-O2A-C1
24	B	625	LFA	C17-C18-C19-C20
19	C	514	CLA	C5-C6-C7-C8
19	B	601	CLA	C2A-CAA-CBA-CGA
19	B	607	CLA	C2A-CAA-CBA-CGA
19	b	609	CLA	C2A-CAA-CBA-CGA
24	b	632	LFA	C10-C11-C12-C13
28	C	501	LMG	C17-C18-C19-C20
28	B	620	LMG	C11-C10-O7-C8
28	b	622	LMG	C11-C10-O7-C8
22	A	411	SQD	C15-C16-C17-C18
30	c	519	DGD	CAA-CBA-CCA-CDA
28	c	501	LMG	C10-C11-C12-C13
22	l	102	SQD	C17-C18-C19-C20
19	B	601	CLA	C8-C10-C11-C12
19	c	512	CLA	CBA-CGA-O2A-C1
22	f	102	SQD	C23-C24-C25-C26
27	A	417	LHG	C14-C15-C16-C17
28	C	518	LMG	C13-C14-C15-C16
28	C	518	LMG	C16-C17-C18-C19
27	l	101	LHG	C29-C30-C31-C32
30	c	519	DGD	C9B-CAB-CBB-CCB
30	h	102	DGD	CAA-CBA-CCA-CDA
19	B	614	CLA	CAD-CBD-CGD-O2D
19	C	511	CLA	CAD-CBD-CGD-O2D
19	C	514	CLA	CAD-CBD-CGD-O2D
19	D	409	CLA	CAD-CBD-CGD-O2D
19	b	616	CLA	CAD-CBD-CGD-O2D
19	c	510	CLA	CAD-CBD-CGD-O2D
19	c	513	CLA	CAD-CBD-CGD-O2D
19	d	405	CLA	CAD-CBD-CGD-O2D
19	B	604	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	A	410	PL9	C45-C44-C46-C47
25	I	104	PLM	C2-C3-C4-C5
22	a	412	SQD	O6-C44-C45-C46
30	D	415	DGD	O1G-C1G-C2G-C3G
30	c	519	DGD	O1G-C1G-C2G-C3G
19	b	603	CLA	C8-C10-C11-C12
19	b	615	CLA	C5-C6-C7-C8
19	c	510	CLA	C13-C15-C16-C17
25	B	627	PLM	CB-CC-CD-CE
25	a	414	PLM	C5-C6-C7-C8
28	c	518	LMG	C17-C18-C19-C20
19	A	403	CLA	C2A-CAA-CBA-CGA
19	a	404	CLA	C2A-CAA-CBA-CGA
22	f	102	SQD	C31-C32-C33-C34
30	d	414	DGD	C8B-C9B-CAB-CBB
25	I	102	PLM	CD-CE-CF-CG
28	B	620	LMG	O9-C10-O7-C8
28	b	622	LMG	O9-C10-O7-C8
19	C	505	CLA	CHA-CBD-CGD-O1D
19	C	505	CLA	CHA-CBD-CGD-O2D
19	C	506	CLA	CHA-CBD-CGD-O1D
19	C	506	CLA	CHA-CBD-CGD-O2D
19	C	508	CLA	CHA-CBD-CGD-O1D
19	c	504	CLA	CHA-CBD-CGD-O2D
19	c	505	CLA	CHA-CBD-CGD-O1D
19	c	507	CLA	CHA-CBD-CGD-O1D
19	c	510	CLA	CHA-CBD-CGD-O1D
19	C	513	CLA	O1A-CGA-O2A-C1
22	F	102	SQD	C24-C25-C26-C27
28	d	410	LMG	C32-C33-C34-C35
22	L	102	SQD	O47-C45-C46-O48
22	l	102	SQD	O47-C45-C46-O48
28	C	501	LMG	O1-C7-C8-O7
28	c	501	LMG	O1-C7-C8-O7
27	D	412	LHG	O1-C1-C2-O2
27	a	416	LHG	O1-C1-C2-O2
27	d	408	LHG	O1-C1-C2-O2
23	D	411	PL9	C13-C14-C16-C17
19	B	613	CLA	C5-C6-C7-C8
19	A	405	CLA	C11-C10-C8-C9
19	C	507	CLA	C11-C12-C13-C14
19	a	408	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	l	102	SQD	C10-C11-C12-C13
19	b	607	CLA	O1D-CGD-O2D-CED
29	d	401	LMT	C1-C2-C3-C4
22	f	102	SQD	C29-C30-C31-C32
29	t	101	LMT	C4-C5-C6-C7
24	b	626	LFA	C7-C8-C9-C10
19	c	512	CLA	O1A-CGA-O2A-C1
20	d	402	PHO	O1A-CGA-O2A-C1
21	K	101	BCR	C37-C22-C23-C24
27	L	101	LHG	O1-C1-C2-C3
25	I	104	PLM	C5-C6-C7-C8
27	a	415	LHG	C31-C32-C33-C34
19	B	605	CLA	O1D-CGD-O2D-CED
19	C	503	CLA	C1A-C2A-CAA-CBA
19	c	502	CLA	C1A-C2A-CAA-CBA
30	c	519	DGD	CDA-CEA-CFA-CGA
29	m	102	LMT	C1-C2-C3-C4
19	D	409	CLA	CBA-CGA-O2A-C1
22	l	102	SQD	C9-C10-C11-C12
27	L	101	LHG	C30-C31-C32-C33
19	c	511	CLA	O1D-CGD-O2D-CED
29	M	101	LMT	O5B-C1B-O1B-C4'
22	L	102	SQD	C10-C11-C12-C13
22	a	410	SQD	C10-C11-C12-C13
27	A	417	LHG	C2-C3-O3-P
27	a	415	LHG	C2-C3-O3-P
22	A	411	SQD	C12-C13-C14-C15
27	D	413	LHG	C4-O6-P-O5
27	a	416	LHG	C3-O3-P-O5
27	d	409	LHG	C4-O6-P-O5
27	l	101	LHG	C3-O3-P-O5
28	D	414	LMG	C35-C36-C37-C38
30	c	517	DGD	O6E-C1E-O5D-C6D
19	a	406	CLA	C10-C11-C12-C13
27	a	415	LHG	C24-C25-C26-C27
30	c	517	DGD	CDB-CEB-CFB-CGB
19	A	407	CLA	C3-C5-C6-C7
24	b	626	LFA	C10-C11-C12-C13
28	c	518	LMG	C33-C34-C35-C36
30	H	103	DGD	CDA-CEA-CFA-CGA
19	C	505	CLA	CAD-CBD-CGD-O1D
19	C	506	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	C	508	CLA	CAD-CBD-CGD-O1D
19	c	504	CLA	CAD-CBD-CGD-O1D
19	c	507	CLA	CAD-CBD-CGD-O1D
22	a	412	SQD	C5-C6-S-O7
28	c	501	LMG	C14-C15-C16-C17
28	c	501	LMG	C20-C21-C22-C23
28	B	620	LMG	C30-C31-C32-C33
24	B	625	LFA	C11-C12-C13-C14
29	M	102	LMT	C5-C6-C7-C8
19	B	612	CLA	CBA-CGA-O2A-C1
19	b	614	CLA	CBA-CGA-O2A-C1
30	C	517	DGD	C2A-C1A-O1G-C1G
24	B	621	LFA	C11-C10-C9-C8
19	A	405	CLA	C11-C12-C13-C15
19	B	601	CLA	C11-C12-C13-C15
19	B	608	CLA	C12-C13-C15-C16
19	B	614	CLA	C12-C13-C15-C16
19	B	615	CLA	C12-C13-C15-C16
19	C	511	CLA	C6-C7-C8-C10
19	D	408	CLA	C11-C12-C13-C15
19	a	406	CLA	C11-C12-C13-C15
19	b	603	CLA	C6-C7-C8-C10
19	b	617	CLA	C12-C13-C15-C16
19	c	507	CLA	C6-C7-C8-C10
23	d	407	PL9	C13-C14-C16-C17
25	D	405	PLM	C1-C2-C3-C4
29	m	102	LMT	O5'-C5'-C6'-O6'
25	I	101	PLM	C1-C2-C3-C4
19	B	612	CLA	O1A-CGA-O2A-C1
19	D	409	CLA	O1A-CGA-O2A-C1
19	b	614	CLA	O1A-CGA-O2A-C1
19	b	603	CLA	C2A-CAA-CBA-CGA
22	F	102	SQD	C30-C31-C32-C33
28	C	501	LMG	C40-C41-C42-C43
30	h	102	DGD	C9A-CAA-CBA-CCA
28	C	501	LMG	O1-C7-C8-C9
30	J	101	DGD	C1G-C2G-C3G-O3G
22	a	412	SQD	C26-C27-C28-C29
27	a	416	LHG	C29-C30-C31-C32
27	D	413	LHG	C30-C31-C32-C33
30	C	517	DGD	C8B-C9B-CAB-CBB
27	D	413	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
30	D	415	DGD	C8B-C9B-CAB-CBB
30	h	102	DGD	CCA-CDA-CEA-CFA
28	C	518	LMG	C15-C16-C17-C18
19	B	604	CLA	CBA-CGA-O2A-C1
22	l	102	SQD	C29-C30-C31-C32
19	B	601	CLA	C11-C12-C13-C14
19	C	506	CLA	C11-C10-C8-C9
19	C	509	CLA	C14-C13-C15-C16
19	C	511	CLA	C11-C12-C13-C14
19	D	409	CLA	C14-C13-C15-C16
19	c	505	CLA	C11-C10-C8-C9
19	c	506	CLA	C11-C12-C13-C14
19	d	405	CLA	C14-C13-C15-C16
22	l	102	SQD	C28-C29-C30-C31
22	L	102	SQD	C29-C30-C31-C32
27	L	101	LHG	C11-C10-C9-C8
30	J	101	DGD	C2A-C3A-C4A-C5A
25	H	105	PLM	C4-C5-C6-C7
30	C	517	DGD	O1A-C1A-O1G-C1G
22	A	411	SQD	C13-C14-C15-C16
27	A	417	LHG	C32-C33-C34-C35
30	c	516	DGD	CDA-CEA-CFA-CGA
24	B	621	LFA	C16-C17-C18-C19
22	A	411	SQD	C17-C18-C19-C20
27	l	101	LHG	C9-C10-C11-C12
19	C	512	CLA	CBD-CGD-O2D-CED
22	a	410	SQD	O49-C7-O47-C45
22	A	409	SQD	C29-C30-C31-C32
25	I	102	PLM	C4-C5-C6-C7
27	L	101	LHG	C9-C10-C11-C12
24	X	101	LFA	C12-C13-C14-C15
25	D	405	PLM	C7-C8-C9-CA
27	A	417	LHG	C29-C30-C31-C32
22	L	102	SQD	C28-C29-C30-C31
22	f	102	SQD	C46-C45-O47-C7
22	a	412	SQD	C24-C23-O48-C46
27	L	101	LHG	C24-C25-C26-C27
19	B	604	CLA	O1A-CGA-O2A-C1
22	a	412	SQD	O10-C23-O48-C46
27	D	413	LHG	C35-C36-C37-C38
27	l	101	LHG	C11-C10-C9-C8
30	D	415	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
30	d	414	DGD	C2A-C3A-C4A-C5A
19	B	604	CLA	C15-C16-C17-C18
27	L	101	LHG	C17-C18-C19-C20
27	l	101	LHG	C24-C25-C26-C27
20	D	401	PHO	O1A-CGA-O2A-C1
30	c	516	DGD	O1A-C1A-O1G-C1G
21	B	629	BCR	C1-C6-C7-C8
21	C	516	BCR	C23-C24-C25-C26
21	C	516	BCR	C23-C24-C25-C30
21	b	619	BCR	C23-C24-C25-C26
21	c	515	BCR	C23-C24-C25-C30
32	x	102	RRX	C23-C24-C25-C30
32	x	102	RRX	C23-C24-C25-C26
29	M	101	LMT	C2B-C1B-O1B-C4'
19	C	512	CLA	O1D-CGD-O2D-CED
27	a	416	LHG	C7-C8-C9-C10
30	c	516	DGD	C2A-C1A-O1G-C1G
27	a	416	LHG	C25-C26-C27-C28
28	C	518	LMG	C17-C18-C19-C20
22	a	410	SQD	C8-C7-O47-C45
30	C	517	DGD	O6E-C1E-O5D-C6D
30	c	516	DGD	O6E-C1E-O5D-C6D
19	d	405	CLA	C8-C10-C11-C12
30	C	517	DGD	C2E-C1E-O5D-C6D
30	c	516	DGD	C2E-C1E-O5D-C6D
30	c	517	DGD	C2E-C1E-O5D-C6D
28	C	518	LMG	O1-C7-C8-O7
30	c	519	DGD	O1G-C1G-C2G-O2G
27	l	101	LHG	C4-O6-P-O3
27	D	412	LHG	C27-C28-C29-C30
24	D	406	LFA	C15-C16-C17-C18
24	m	103	LFA	C9-C10-C11-C12
28	c	501	LMG	O1-C7-C8-C9
19	B	608	CLA	C11-C12-C13-C15
28	C	501	LMG	C21-C22-C23-C24
28	d	410	LMG	C39-C40-C41-C42
22	l	102	SQD	C7-C8-C9-C10
19	B	601	CLA	C6-C7-C8-C9
19	B	603	CLA	C11-C10-C8-C9
19	B	604	CLA	C6-C7-C8-C9
19	C	506	CLA	C14-C13-C15-C16
19	b	603	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	b	605	CLA	C11-C10-C8-C9
19	c	505	CLA	C14-C13-C15-C16
19	c	507	CLA	C6-C7-C8-C9
19	d	404	CLA	C11-C12-C13-C14
22	L	102	SQD	C12-C13-C14-C15
28	D	414	LMG	C13-C14-C15-C16
20	D	401	PHO	CBA-CGA-O2A-C1
19	B	612	CLA	C10-C11-C12-C13
19	b	614	CLA	C10-C11-C12-C13
19	b	618	CLA	O1A-CGA-O2A-C1
22	l	102	SQD	O10-C23-C24-C25
27	d	409	LHG	C11-C12-C13-C14
19	B	616	CLA	O1A-CGA-O2A-C1
28	c	518	LMG	C31-C32-C33-C34
19	D	409	CLA	C8-C10-C11-C12
23	a	411	PL9	C47-C48-C49-C51
28	C	501	LMG	C38-C39-C40-C41
19	B	616	CLA	CBA-CGA-O2A-C1
28	B	620	LMG	C29-C28-O8-C9
24	D	404	LFA	C10-C11-C12-C13
27	l	101	LHG	C17-C18-C19-C20
22	A	409	SQD	C19-C20-C21-C22
19	b	618	CLA	CBA-CGA-O2A-C1
28	b	622	LMG	C29-C28-O8-C9
28	C	501	LMG	C10-C11-C12-C13
21	C	516	BCR	C19-C20-C21-C22
21	C	521	BCR	C9-C10-C11-C12
21	a	409	BCR	C19-C20-C21-C22
21	b	601	BCR	C9-C10-C11-C12
27	a	416	LHG	C35-C36-C37-C38
28	B	620	LMG	C16-C17-C18-C19
19	B	614	CLA	C4-C3-C5-C6
28	B	620	LMG	O10-C28-O8-C9
28	b	622	LMG	O10-C28-O8-C9
25	b	631	PLM	O1-C1-C2-C3
28	b	622	LMG	C16-C17-C18-C19
28	b	622	LMG	C40-C41-C42-C43
19	c	507	CLA	C3A-C2A-CAA-CBA
25	B	627	PLM	C3-C4-C5-C6
30	H	103	DGD	CCA-CDA-CEA-CFA
24	D	404	LFA	C6-C7-C8-C9
25	I	101	PLM	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
22	A	409	SQD	C17-C18-C19-C20
23	a	411	PL9	C4-C3-C7-C8
27	a	416	LHG	C24-C25-C26-C27
28	d	410	LMG	C30-C31-C32-C33
19	C	504	CLA	C6-C7-C8-C9
19	b	611	CLA	C6-C7-C8-C9
19	c	503	CLA	C6-C7-C8-C9
27	D	413	LHG	C29-C30-C31-C32
29	M	102	LMT	O5'-C5'-C6'-O6'
27	a	415	LHG	C28-C29-C30-C31
25	a	414	PLM	C6-C7-C8-C9
27	L	101	LHG	C1-C2-C3-O3
27	a	416	LHG	C4-C5-C6-O8
27	a	415	LHG	C11-C12-C13-C14
25	I	101	PLM	O1-C1-C2-C3
24	D	404	LFA	C13-C14-C15-C16
21	b	619	BCR	C7-C8-C9-C34
21	b	619	BCR	C36-C18-C19-C20
24	H	101	LFA	C3-C4-C5-C6
29	t	101	LMT	C2-C3-C4-C5
30	H	103	DGD	C2B-C3B-C4B-C5B
22	a	412	SQD	C7-C8-C9-C10
22	a	410	SQD	C19-C20-C21-C22
29	D	402	LMT	C2-C3-C4-C5
23	a	411	PL9	C20-C19-C21-C22
19	D	409	CLA	C1A-C2A-CAA-CBA
19	d	405	CLA	C1A-C2A-CAA-CBA
22	A	409	SQD	C11-C12-C13-C14
30	h	102	DGD	C2B-C3B-C4B-C5B
19	C	503	CLA	C16-C17-C18-C20
19	C	507	CLA	C12-C13-C15-C16
19	C	515	CLA	C11-C10-C8-C7
19	c	506	CLA	C12-C13-C15-C16
19	A	405	CLA	C13-C15-C16-C17
25	A	415	PLM	O1-C1-C2-C3
27	A	417	LHG	C17-C18-C19-C20
21	c	515	BCR	C19-C20-C21-C22
29	b	602	LMT	C5-C6-C7-C8
27	d	408	LHG	C27-C28-C29-C30
22	L	102	SQD	O10-C23-C24-C25
27	a	415	LHG	C25-C26-C27-C28
27	a	416	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	d	401	LMT	C7-C8-C9-C10
27	a	416	LHG	C2-C3-O3-P
19	B	614	CLA	C2A-CAA-CBA-CGA
19	b	616	CLA	C2A-CAA-CBA-CGA
19	A	405	CLA	C10-C11-C12-C13
19	c	510	CLA	C8-C10-C11-C12
25	A	415	PLM	O2-C1-C2-C3
25	a	414	PLM	O1-C1-C2-C3
19	b	604	CLA	C5-C6-C7-C8
24	B	621	LFA	C13-C14-C15-C16
27	D	413	LHG	C34-C35-C36-C37
19	C	509	CLA	C8-C10-C11-C12
25	I	102	PLM	O1-C1-C2-C3
23	a	411	PL9	C45-C44-C46-C47
25	E	101	PLM	C9-CA-CB-CC
31	F	101	HEM	CAA-CBA-CGA-O2A
24	Z	101	LFA	C9-C10-C11-C12
19	a	404	CLA	C15-C16-C17-C18
27	a	416	LHG	O7-C5-C6-O8
22	A	411	SQD	C34-C35-C36-C37
21	Y	101	BCR	C19-C20-C21-C22
25	E	101	PLM	CC-CD-CE-CF
28	C	501	LMG	C15-C16-C17-C18
29	D	402	LMT	O5'-C1'-O1'-C1
24	A	414	LFA	C6-C7-C8-C9
25	b	631	PLM	O2-C1-C2-C3
31	f	101	HEM	CAA-CBA-CGA-O2A
28	d	410	LMG	C20-C21-C22-C23
25	I	102	PLM	O2-C1-C2-C3
25	b	628	PLM	O1-C1-C2-C3
19	b	604	CLA	C14-C13-C15-C16
30	C	517	DGD	CDA-CEA-CFA-CGA
19	B	612	CLA	C8-C10-C11-C12
19	b	614	CLA	C8-C10-C11-C12
19	c	508	CLA	C5-C6-C7-C8
28	D	414	LMG	C36-C37-C38-C39
21	K	101	BCR	C23-C24-C25-C30
21	b	620	BCR	C23-C24-C25-C26
21	k	101	BCR	C23-C24-C25-C30
25	i	104	PLM	C2-C3-C4-C5
28	C	518	LMG	O1-C7-C8-C9
27	d	409	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	a	414	PLM	O2-C1-C2-C3
31	F	101	HEM	CAA-CBA-CGA-O1A
21	K	101	BCR	C15-C16-C17-C18
21	k	101	BCR	C15-C16-C17-C18
21	y	101	BCR	C19-C20-C21-C22
19	C	506	CLA	C4-C3-C5-C6
19	C	503	CLA	C13-C15-C16-C17
22	L	102	SQD	C45-C44-O6-C1
22	l	102	SQD	C45-C44-O6-C1
30	C	517	DGD	C5D-C6D-O5D-C1E
30	c	516	DGD	C5D-C6D-O5D-C1E
30	c	519	DGD	C5D-C6D-O5D-C1E
22	f	102	SQD	C11-C10-C9-C8
19	c	509	CLA	C16-C17-C18-C19
19	B	605	CLA	C13-C15-C16-C17
19	a	404	CLA	C13-C15-C16-C17
19	b	607	CLA	C13-C15-C16-C17
27	D	413	LHG	C7-C8-C9-C10
25	a	414	PLM	C4-C5-C6-C7
25	B	626	PLM	C6-C7-C8-C9
27	A	417	LHG	C27-C28-C29-C30
19	c	505	CLA	C4-C3-C5-C6
23	a	411	PL9	C25-C24-C26-C27
23	a	411	PL9	C30-C29-C31-C32
30	h	102	DGD	O1B-C1B-C2B-C3B
19	C	509	CLA	C12-C13-C15-C16
23	D	411	PL9	C28-C29-C31-C32
25	E	101	PLM	O1-C1-C2-C3
25	A	415	PLM	C5-C6-C7-C8
30	C	517	DGD	C2B-C3B-C4B-C5B
27	l	101	LHG	O1-C1-C2-O2
21	A	408	BCR	C19-C20-C21-C22
23	a	411	PL9	C42-C43-C44-C46
24	b	632	LFA	C9-C10-C11-C12
19	B	613	CLA	CAA-CBA-CGA-O2A
19	b	615	CLA	CAA-CBA-CGA-O2A
23	D	411	PL9	C35-C34-C36-C37
23	a	411	PL9	C15-C14-C16-C17
19	A	403	CLA	C15-C16-C17-C18
19	B	609	CLA	C6-C7-C8-C9
19	B	615	CLA	C14-C13-C15-C16
19	C	515	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	D	408	CLA	C11-C12-C13-C14
19	b	603	CLA	C6-C7-C8-C9
19	b	617	CLA	C14-C13-C15-C16
19	c	514	CLA	C11-C10-C8-C9
25	b	628	PLM	O2-C1-C2-C3
28	b	622	LMG	C34-C35-C36-C37
19	C	508	CLA	C3A-C2A-CAA-CBA
27	L	101	LHG	O2-C2-C3-O3
22	A	409	SQD	C14-C15-C16-C17
27	L	101	LHG	C14-C15-C16-C17
27	l	101	LHG	C14-C15-C16-C17
31	f	101	HEM	CAA-CBA-CGA-O1A
19	B	601	CLA	CAD-CBD-CGD-O2D
19	B	603	CLA	CAD-CBD-CGD-O2D
19	B	604	CLA	CAD-CBD-CGD-O2D
19	B	607	CLA	CAD-CBD-CGD-O2D
19	B	610	CLA	CAD-CBD-CGD-O2D
19	C	503	CLA	CAD-CBD-CGD-O2D
19	C	504	CLA	CAD-CBD-CGD-O2D
19	b	603	CLA	CAD-CBD-CGD-O2D
19	b	605	CLA	CAD-CBD-CGD-O2D
19	b	606	CLA	CAD-CBD-CGD-O2D
19	b	609	CLA	CAD-CBD-CGD-O2D
19	b	612	CLA	CAD-CBD-CGD-O2D
19	c	502	CLA	CAD-CBD-CGD-O2D
19	c	503	CLA	CAD-CBD-CGD-O2D
24	M	103	LFA	C11-C12-C13-C14
25	A	413	PLM	O1-C1-C2-C3
31	f	101	HEM	CAD-CBD-CGD-O2D
19	B	604	CLA	C4-C3-C5-C6
19	B	612	CLA	CAA-CBA-CGA-O2A
19	C	512	CLA	CAA-CBA-CGA-O2A
19	b	614	CLA	CAA-CBA-CGA-O2A
22	A	409	SQD	O47-C7-C8-C9
22	a	412	SQD	O48-C23-C24-C25
21	K	101	BCR	C21-C22-C23-C24
21	k	101	BCR	C21-C22-C23-C24
27	a	416	LHG	C23-C24-C25-C26
19	c	511	CLA	CAA-CBA-CGA-O2A
22	a	412	SQD	C9-C10-C11-C12
25	A	413	PLM	C9-CA-CB-CC
28	c	501	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
19	C	511	CLA	O2A-C1-C2-C3
19	D	408	CLA	O2A-C1-C2-C3
19	d	404	CLA	O2A-C1-C2-C3
20	a	407	PHO	O2A-C1-C2-C3
24	b	624	LFA	C11-C12-C13-C14
28	D	414	LMG	C17-C18-C19-C20
24	b	629	LFA	C7-C8-C9-C10
25	i	104	PLM	C6-C7-C8-C9
19	A	405	CLA	CHA-CBD-CGD-O1D
19	A	405	CLA	CHA-CBD-CGD-O2D
19	B	605	CLA	CHA-CBD-CGD-O1D
19	C	508	CLA	CHA-CBD-CGD-O2D
19	C	509	CLA	CHA-CBD-CGD-O2D
19	a	406	CLA	CHA-CBD-CGD-O1D
19	a	406	CLA	CHA-CBD-CGD-O2D
19	b	607	CLA	CHA-CBD-CGD-O1D
19	c	505	CLA	CHA-CBD-CGD-O2D
19	c	507	CLA	CHA-CBD-CGD-O2D
19	c	508	CLA	CHA-CBD-CGD-O1D
19	c	508	CLA	CHA-CBD-CGD-O2D
19	B	616	CLA	CAA-CBA-CGA-O2A
30	c	517	DGD	O1G-C1G-C2G-O2G
28	c	501	LMG	C18-C19-C20-C21
19	b	618	CLA	CAA-CBA-CGA-O2A
28	C	501	LMG	O7-C10-C11-C12
22	F	102	SQD	C35-C36-C37-C38
25	A	413	PLM	O2-C1-C2-C3
20	A	406	PHO	CHA-CBD-CGD-O1D
20	A	406	PHO	CHA-CBD-CGD-O2D
20	D	401	PHO	CHA-CBD-CGD-O1D
20	a	407	PHO	CHA-CBD-CGD-O1D
20	a	407	PHO	CHA-CBD-CGD-O2D
20	d	402	PHO	CHA-CBD-CGD-O1D
30	H	103	DGD	CAA-CBA-CCA-CDA
30	H	103	DGD	O1B-C1B-C2B-C3B
22	A	411	SQD	O48-C23-C24-C25
28	C	518	LMG	O8-C28-C29-C30
29	D	402	LMT	C4'-C5'-C6'-O6'
25	b	623	PLM	O2-C1-C2-C3
19	C	508	CLA	C6-C7-C8-C10
23	A	410	PL9	C4-C3-C7-C8
19	C	507	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	C	508	CLA	C6-C7-C8-C9
19	c	506	CLA	C14-C13-C15-C16
22	a	412	SQD	C5-C6-S-O8
19	B	603	CLA	C2A-CAA-CBA-CGA
19	b	605	CLA	C2A-CAA-CBA-CGA
24	H	101	LFA	C11-C10-C9-C8
25	E	101	PLM	C7-C8-C9-CA
30	c	517	DGD	C1A-C2A-C3A-C4A
19	C	512	CLA	CAA-CBA-CGA-O1A
24	X	101	LFA	C6-C7-C8-C9
22	F	102	SQD	C27-C28-C29-C30
22	a	410	SQD	C32-C33-C34-C35
27	A	417	LHG	C31-C32-C33-C34
19	c	513	CLA	CAA-CBA-CGA-O2A
25	E	101	PLM	O2-C1-C2-C3
19	c	511	CLA	CAA-CBA-CGA-O1A
21	b	619	BCR	C7-C8-C9-C10
19	C	508	CLA	C1A-C2A-CAA-CBA
19	a	408	CLA	C1A-C2A-CAA-CBA
19	c	504	CLA	C1A-C2A-CAA-CBA
19	c	507	CLA	C1A-C2A-CAA-CBA
19	c	502	CLA	C16-C17-C18-C20
19	b	615	CLA	CAA-CBA-CGA-O1A
19	B	602	CLA	C8-C10-C11-C12
19	B	613	CLA	CAA-CBA-CGA-O1A
31	f	101	HEM	CAD-CBD-CGD-O1D
28	C	518	LMG	C7-C8-C9-O8
24	A	412	LFA	C10-C11-C12-C13
24	I	103	LFA	C11-C12-C13-C14
24	h	104	LFA	C7-C8-C9-C10
25	e	101	PLM	C8-C9-CA-CB
28	b	622	LMG	C10-C11-C12-C13
28	b	622	LMG	C36-C37-C38-C39
22	A	409	SQD	C9-C10-C11-C12
27	l	101	LHG	C10-C11-C12-C13
22	A	409	SQD	O49-C7-C8-C9
24	X	101	LFA	C10-C11-C12-C13
25	b	625	PLM	O1-C1-C2-C3
19	A	403	CLA	C13-C15-C16-C17
27	L	101	LHG	C4-O6-P-O5
27	l	101	LHG	C4-O6-P-O5
22	a	412	SQD	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
24	D	406	LFA	C14-C15-C16-C17
19	B	612	CLA	CAA-CBA-CGA-O1A
19	b	614	CLA	CAA-CBA-CGA-O1A
30	D	415	DGD	C7A-C8A-C9A-CAA
27	d	409	LHG	C35-C36-C37-C38
29	D	402	LMT	C6-C7-C8-C9
25	b	630	PLM	O1-C1-C2-C3
19	A	405	CLA	CAD-CBD-CGD-O1D
19	B	605	CLA	CAD-CBD-CGD-O1D
19	B	609	CLA	CAD-CBD-CGD-O1D
19	b	607	CLA	CAD-CBD-CGD-O1D
19	b	611	CLA	CAD-CBD-CGD-O1D
19	c	505	CLA	CAD-CBD-CGD-O1D
22	A	409	SQD	O5-C5-C6-S
22	a	410	SQD	O5-C5-C6-S
22	a	410	SQD	C5-C6-S-O7
19	B	616	CLA	CAA-CBA-CGA-O1A
19	b	618	CLA	CAA-CBA-CGA-O1A
28	C	501	LMG	O9-C10-C11-C12
28	C	518	LMG	O10-C28-C29-C30
19	C	514	CLA	CAA-CBA-CGA-O2A
30	c	519	DGD	O1G-C1A-C2A-C3A
19	B	605	CLA	C11-C12-C13-C14
19	C	512	CLA	C11-C10-C8-C9
19	b	607	CLA	C11-C12-C13-C14
19	b	610	CLA	C6-C7-C8-C9
19	c	511	CLA	C11-C10-C8-C9
19	b	603	CLA	CAA-CBA-CGA-O2A
27	l	101	LHG	O7-C7-C8-C9
22	L	102	SQD	C14-C15-C16-C17
25	b	623	PLM	O1-C1-C2-C3
20	A	406	PHO	C10-C11-C12-C13
22	F	102	SQD	C6-C5-O5-C1
29	D	402	LMT	C3-C4-C5-C6
19	B	601	CLA	CAA-CBA-CGA-O2A
19	C	503	CLA	CAA-CBA-CGA-O2A
19	c	502	CLA	CAA-CBA-CGA-O2A
27	L	101	LHG	O7-C7-C8-C9
25	B	622	PLM	O1-C1-C2-C3
19	A	403	CLA	C4-C3-C5-C6
19	a	404	CLA	C4-C3-C5-C6
19	B	614	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	C	509	CLA	C6-C7-C8-C10
19	b	604	CLA	C12-C13-C15-C16
19	b	610	CLA	C6-C7-C8-C10
19	b	617	CLA	C11-C12-C13-C15
20	A	406	PHO	C3A-C2A-CAA-CBA
20	a	407	PHO	C3A-C2A-CAA-CBA
22	f	102	SQD	C27-C28-C29-C30
22	a	410	SQD	O47-C7-C8-C9
28	d	410	LMG	O7-C10-C11-C12
25	I	101	PLM	C9-CA-CB-CC
21	b	619	BCR	C17-C18-C19-C20
21	y	101	BCR	C21-C22-C23-C24
19	c	513	CLA	CAA-CBA-CGA-O1A
27	a	416	LHG	C30-C31-C32-C33
29	b	602	LMT	C2-C1-O1'-C1'
19	c	513	CLA	C5-C6-C7-C8
30	c	519	DGD	O1A-C1A-C2A-C3A
19	B	603	CLA	C13-C15-C16-C17
19	a	406	CLA	C13-C15-C16-C17
28	D	414	LMG	O7-C10-C11-C12
19	b	605	CLA	C13-C15-C16-C17
22	A	411	SQD	O10-C23-C24-C25
27	L	101	LHG	O9-C7-C8-C9
27	l	101	LHG	O9-C7-C8-C9
20	a	407	PHO	C2A-CAA-CBA-CGA
25	I	104	PLM	O2-C1-C2-C3
19	b	606	CLA	C13-C15-C16-C17
27	a	416	LHG	C5-C6-O8-C23
28	d	410	LMG	O9-C10-C11-C12
29	b	602	LMT	C4'-C5'-C6'-O6'
25	b	630	PLM	O2-C1-C2-C3

There are no ring outliers.

119 monomers are involved in 191 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	604	CLA	3	0
19	B	613	CLA	2	0
19	B	603	CLA	1	0
21	B	618	BCR	1	0
28	C	501	LMG	1	0
29	t	101	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	b	608	CLA	1	0
19	c	503	CLA	2	0
28	B	620	LMG	2	0
19	b	613	CLA	2	0
25	C	520	PLM	1	0
31	F	101	HEM	1	0
19	c	514	CLA	1	0
29	d	401	LMT	1	0
27	a	415	LHG	1	0
19	b	617	CLA	5	0
24	D	406	LFA	1	0
19	B	607	CLA	2	0
19	D	409	CLA	2	0
25	a	414	PLM	1	0
21	b	601	BCR	3	0
21	B	629	BCR	4	0
19	B	605	CLA	1	0
27	A	417	LHG	1	0
27	D	413	LHG	1	0
28	b	622	LMG	4	0
25	A	413	PLM	1	0
19	d	404	CLA	3	0
30	c	517	DGD	2	0
20	D	401	PHO	3	0
19	D	408	CLA	3	0
19	a	408	CLA	3	0
19	d	405	CLA	2	0
29	D	403	LMT	1	0
19	B	609	CLA	1	0
19	A	403	CLA	3	0
19	C	514	CLA	1	0
19	b	618	CLA	4	0
30	D	415	DGD	1	0
28	c	518	LMG	1	0
19	B	608	CLA	1	0
25	a	401	PLM	1	0
19	c	506	CLA	3	0
22	L	102	SQD	2	0
19	B	612	CLA	2	0
19	C	503	CLA	1	0
19	b	605	CLA	1	0
22	A	409	SQD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	b	610	CLA	1	0
19	B	602	CLA	3	0
22	a	412	SQD	2	0
22	A	411	SQD	2	0
25	b	631	PLM	1	0
19	b	609	CLA	1	0
30	J	101	DGD	4	0
21	c	515	BCR	1	0
25	D	405	PLM	2	0
27	a	416	LHG	3	0
21	a	409	BCR	2	0
21	y	101	BCR	1	0
24	X	101	LFA	1	0
22	f	102	SQD	2	0
19	c	504	CLA	1	0
19	c	502	CLA	1	0
21	b	619	BCR	3	0
21	C	516	BCR	2	0
19	b	607	CLA	4	0
19	b	614	CLA	3	0
20	d	402	PHO	2	0
21	b	620	BCR	2	0
30	c	516	DGD	1	0
19	C	509	CLA	2	0
30	c	519	DGD	1	0
21	B	617	BCR	1	0
22	F	102	SQD	3	0
24	d	411	LFA	1	0
19	C	515	CLA	3	0
29	m	101	LMT	1	0
19	c	513	CLA	1	0
19	B	616	CLA	4	0
19	C	508	CLA	4	0
19	C	510	CLA	1	0
28	D	414	LMG	1	0
24	b	626	LFA	1	0
19	b	604	CLA	2	0
19	b	606	CLA	5	0
21	K	101	BCR	2	0
24	D	404	LFA	2	0
29	C	502	LMT	2	0
19	B	611	CLA	2	0

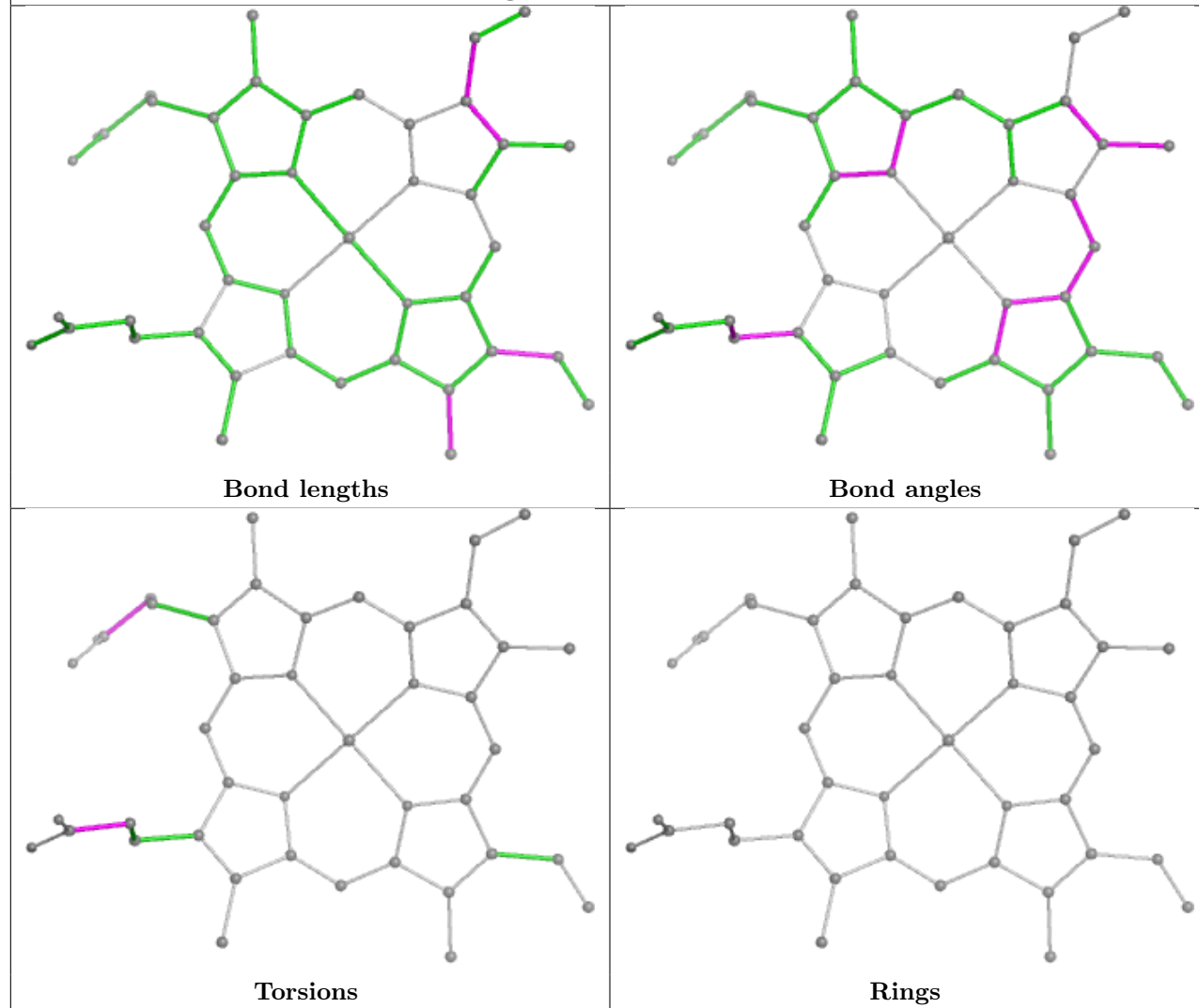
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	615	CLA	4	0
19	C	505	CLA	1	0
21	Y	101	BCR	2	0
19	b	615	CLA	2	0
28	d	410	LMG	3	0
29	M	101	LMT	1	0
19	c	505	CLA	2	0
19	C	507	CLA	2	0
23	a	411	PL9	5	0
24	B	625	LFA	2	0
29	D	402	LMT	2	0
29	z	101	LMT	3	0
19	C	504	CLA	2	0
30	h	102	DGD	2	0
19	c	507	CLA	4	0
23	A	410	PL9	3	0
19	C	513	CLA	2	0
27	L	101	LHG	2	0
28	C	518	LMG	2	0
19	A	407	CLA	3	0
19	c	512	CLA	4	0
27	l	101	LHG	1	0
19	a	404	CLA	3	0
19	B	606	CLA	1	0
30	C	517	DGD	1	0
22	l	102	SQD	1	0
29	b	602	LMT	1	0
23	d	407	PL9	1	0
21	A	408	BCR	1	0

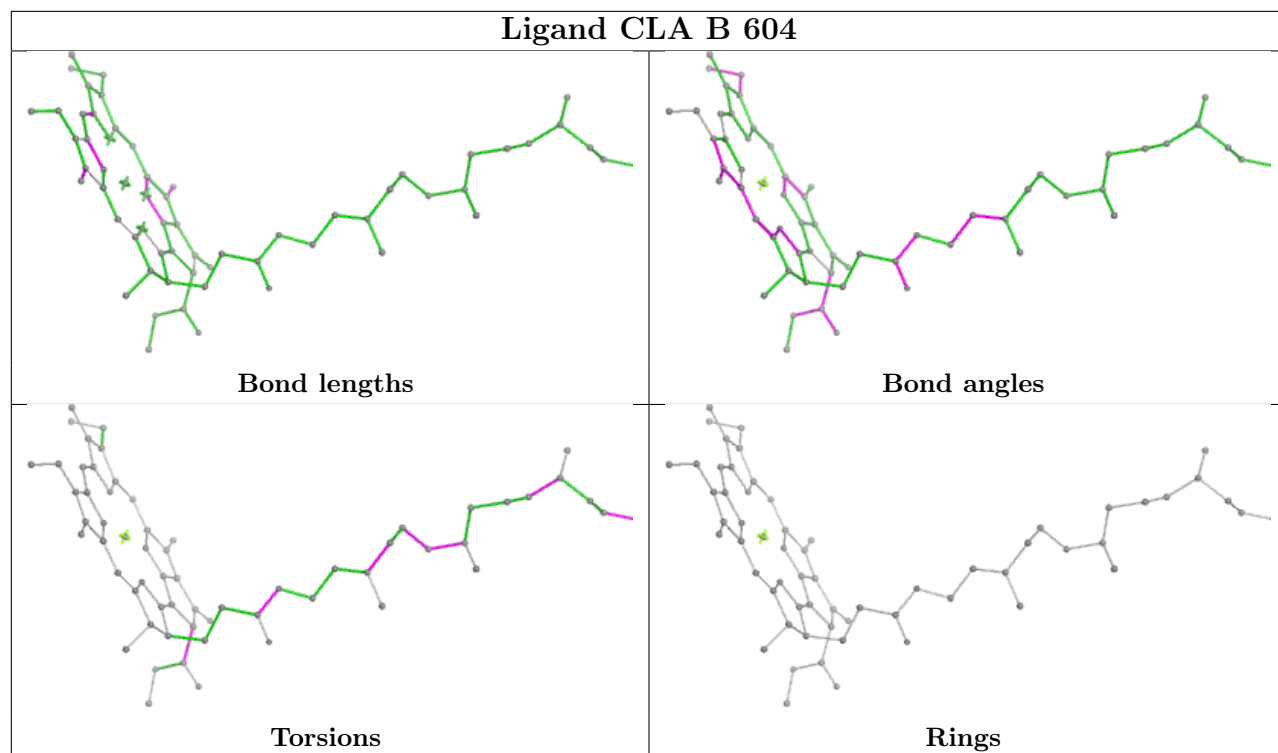
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 HEM f 101

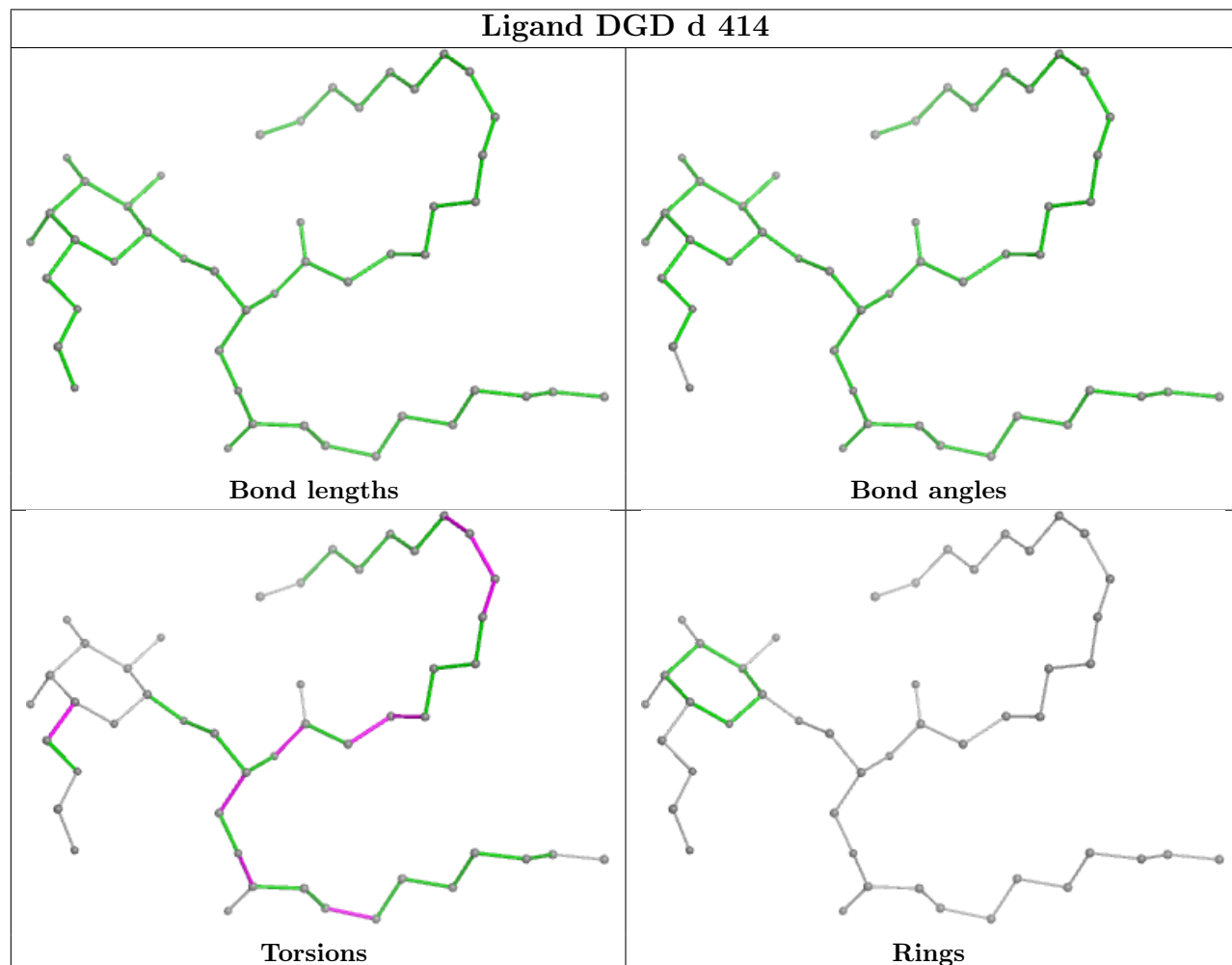


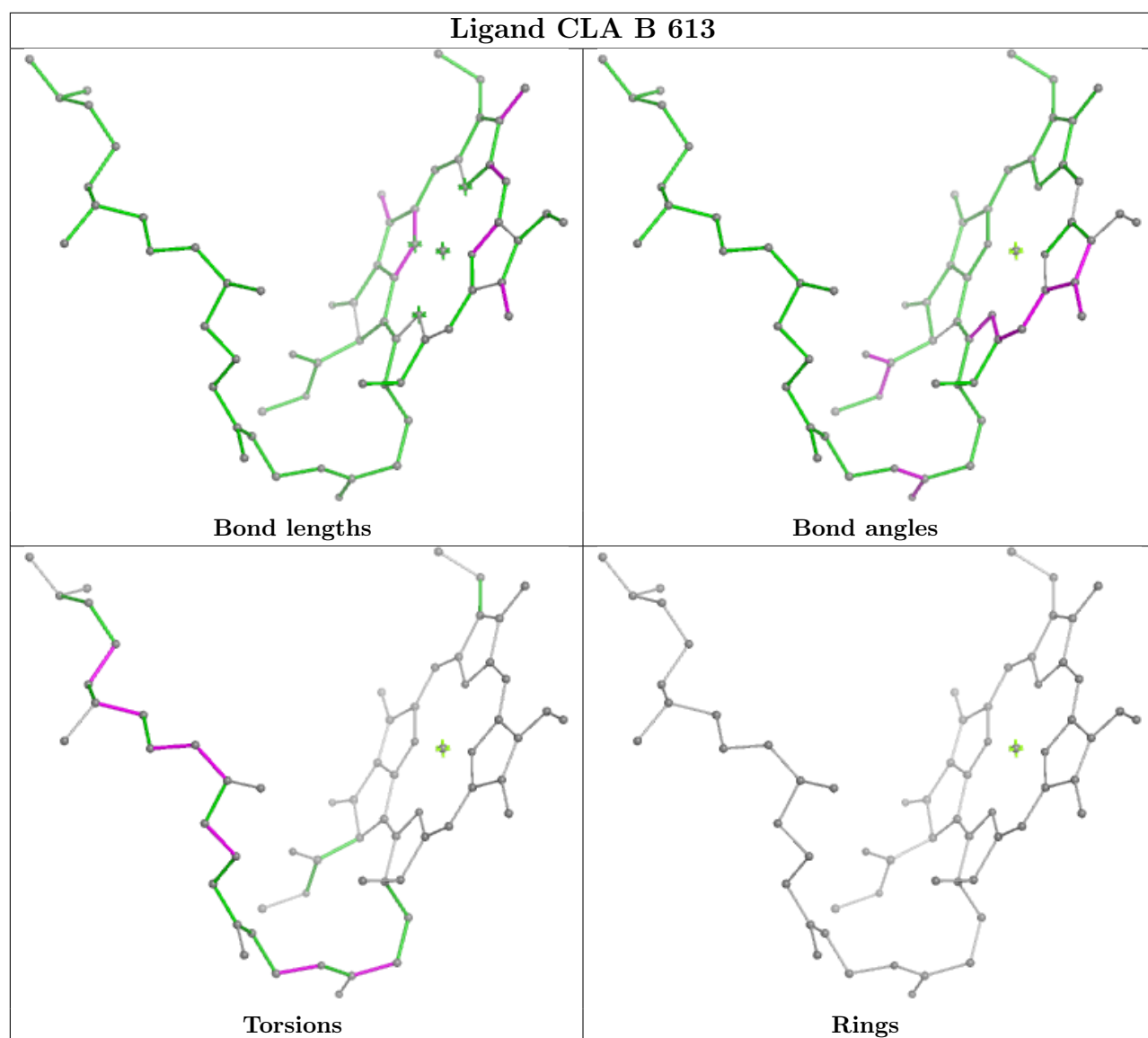


## Ligand CLA B 604

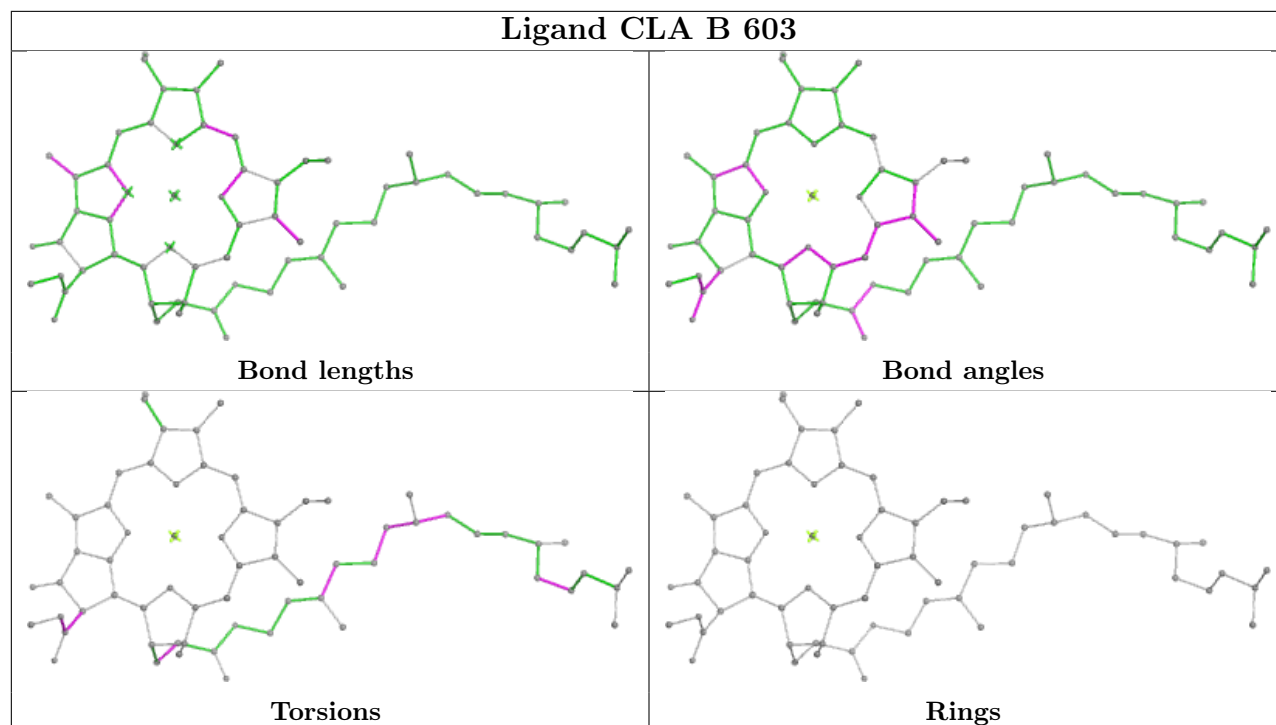


## Ligand DGD d 414

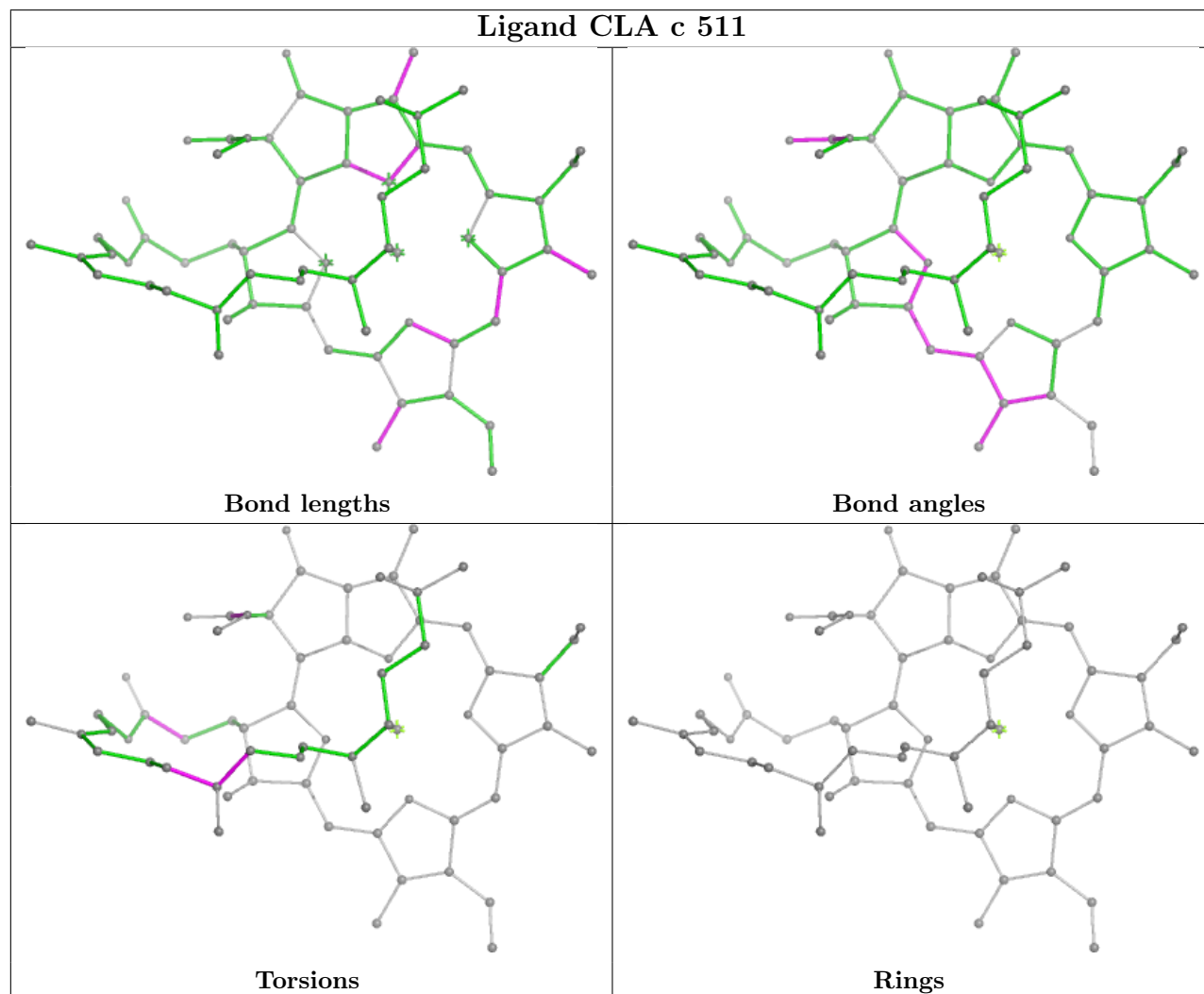


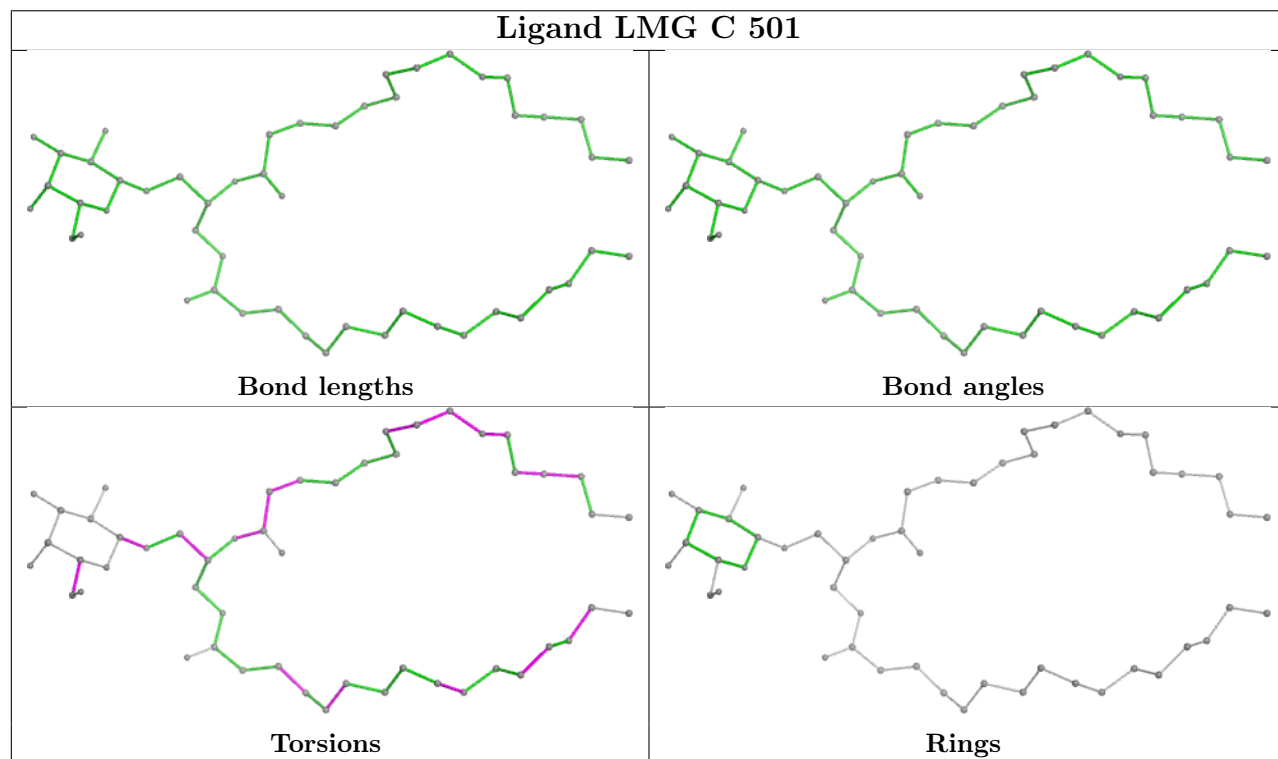
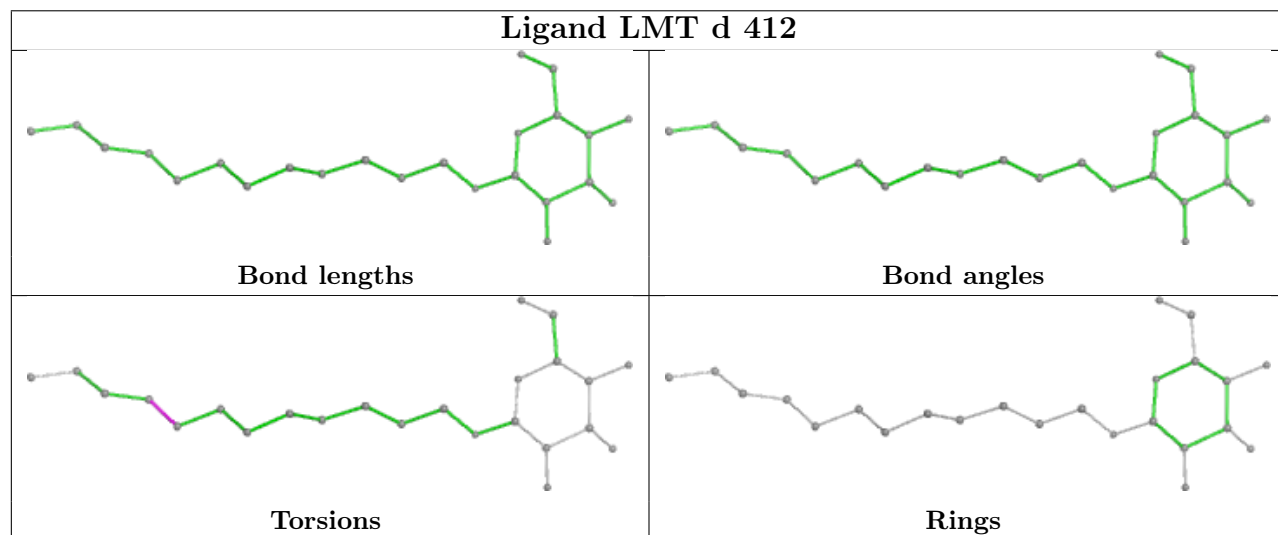
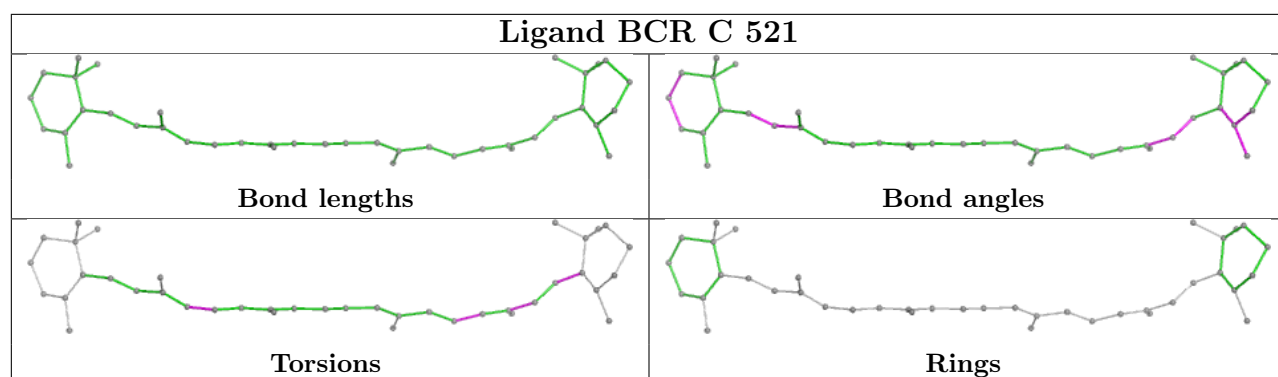


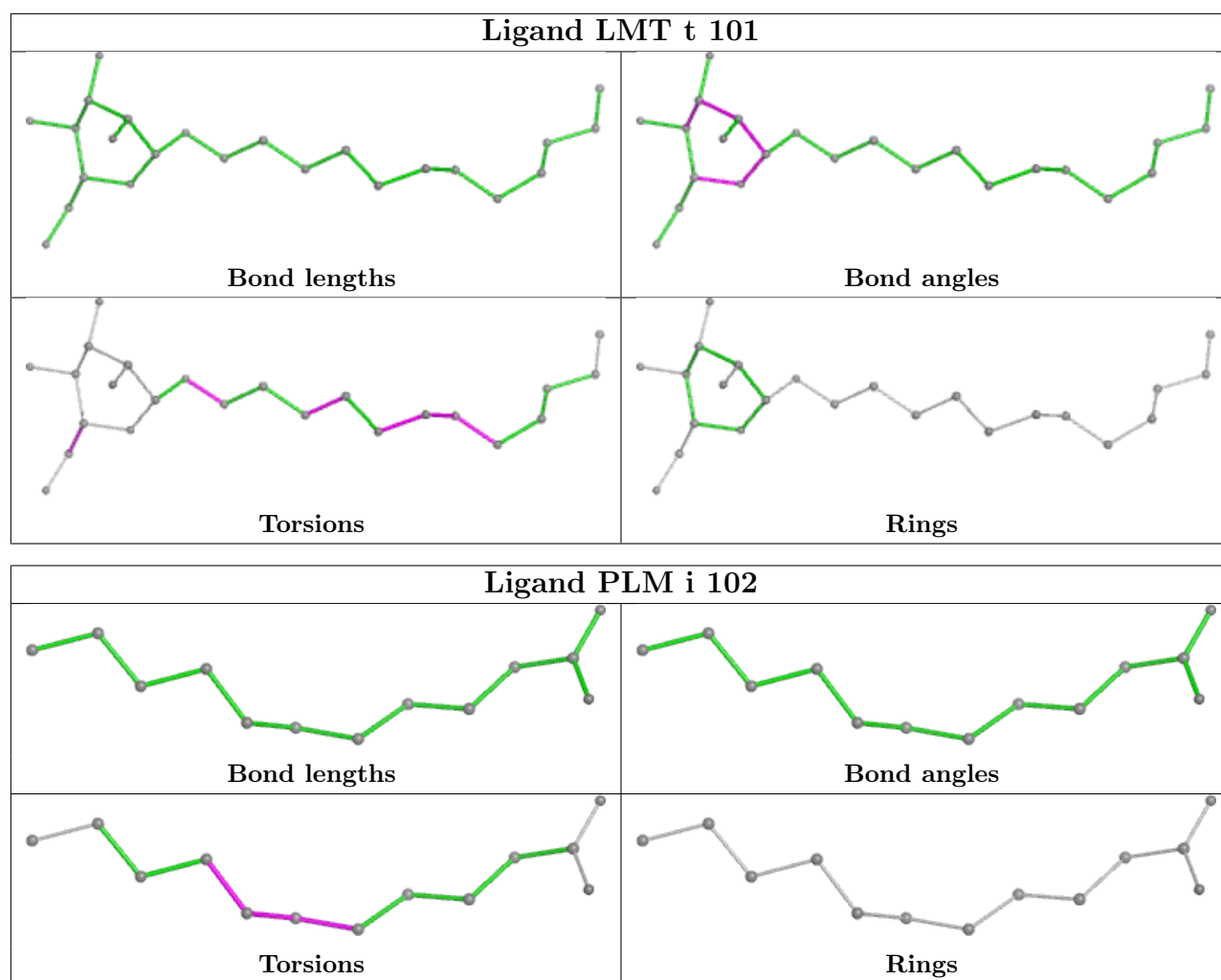
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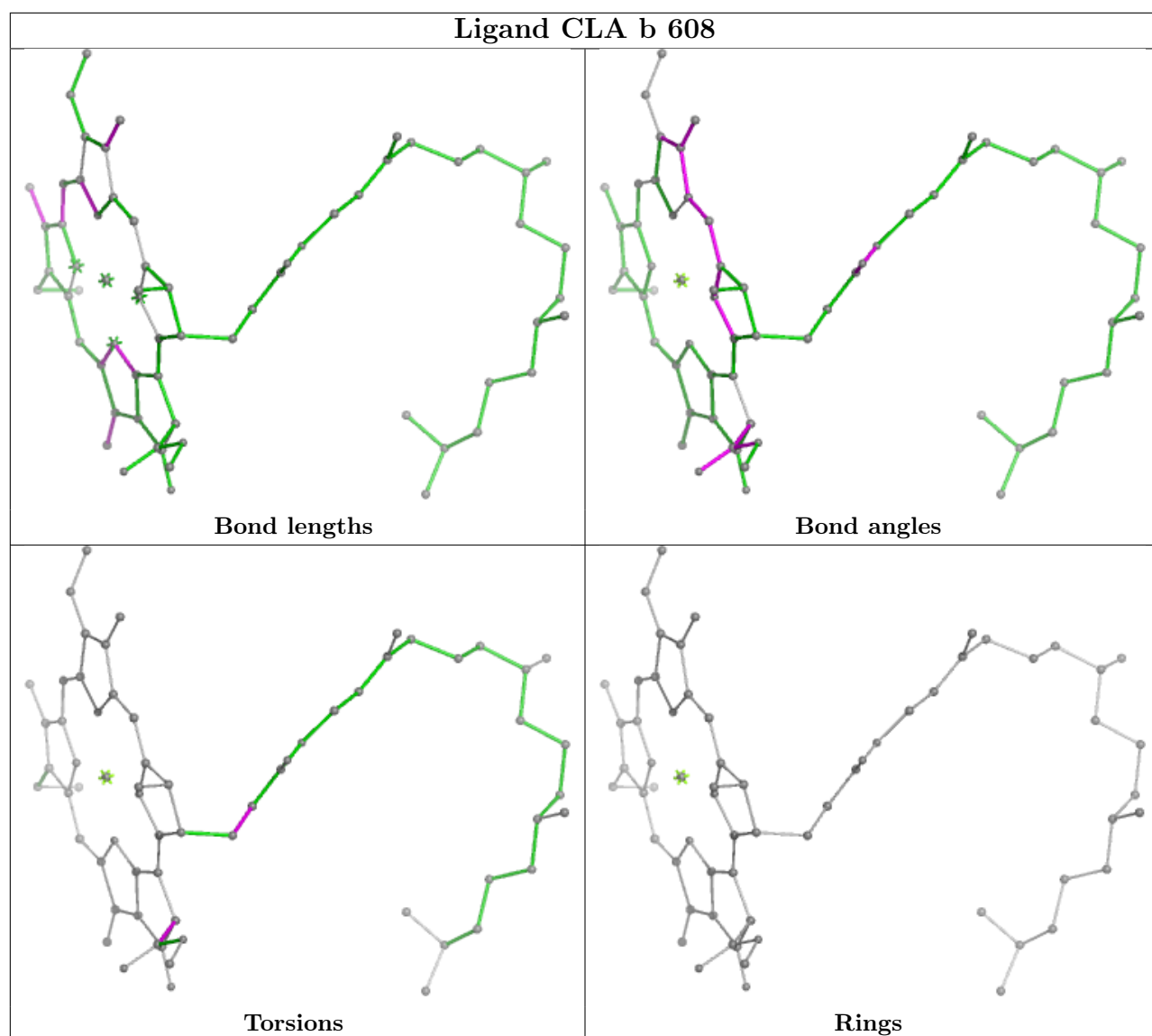


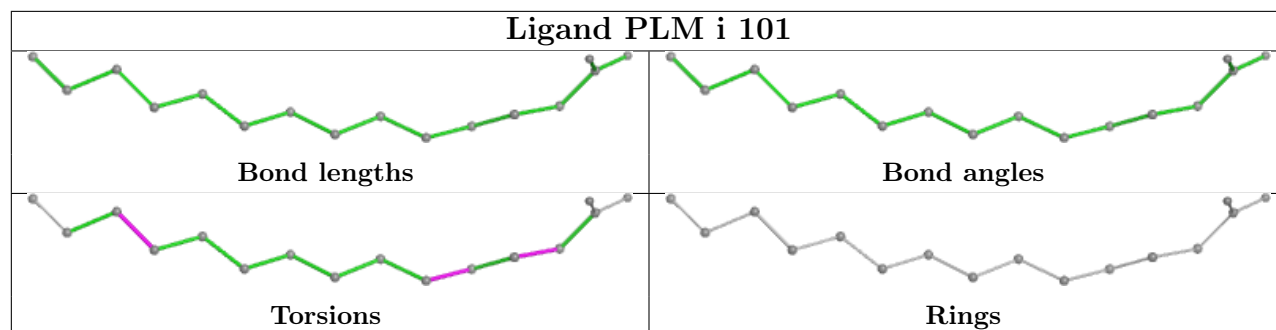
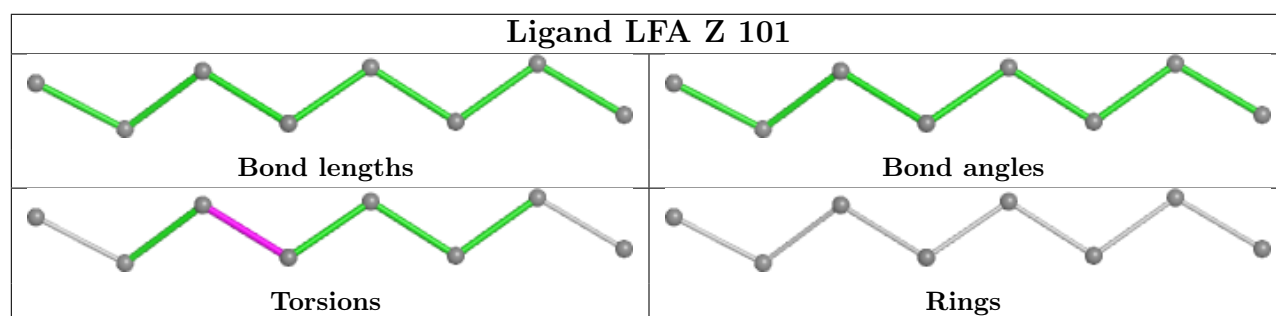
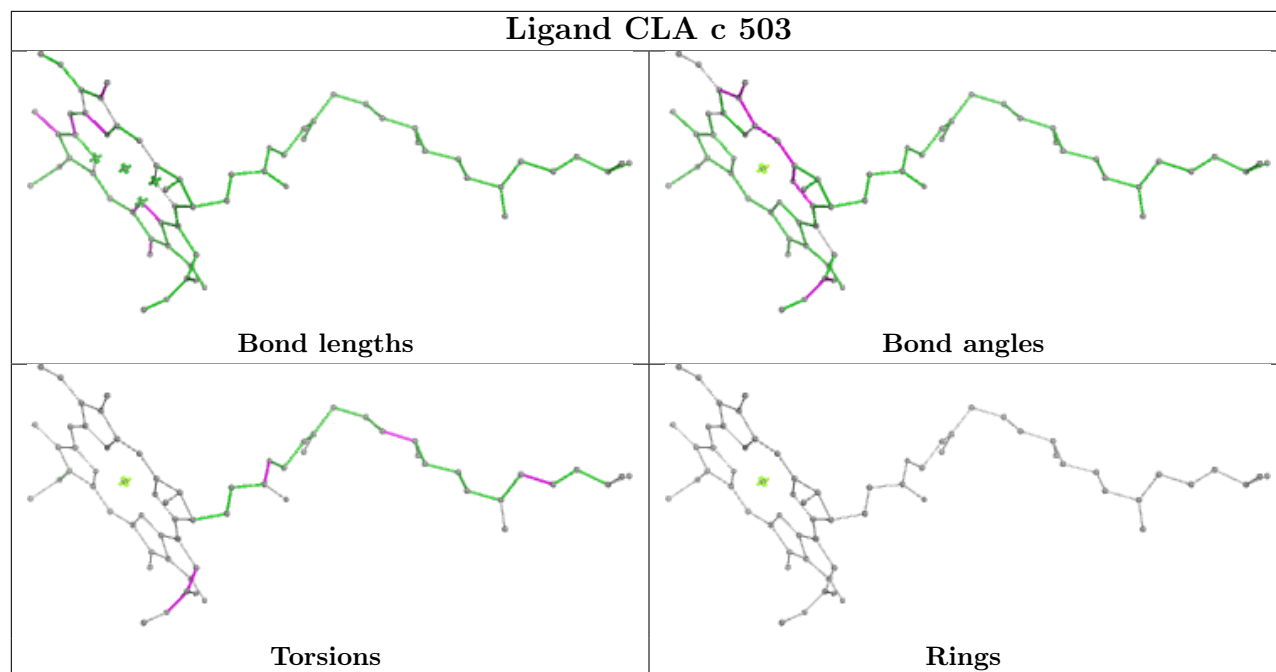
## Ligand CLA c 511

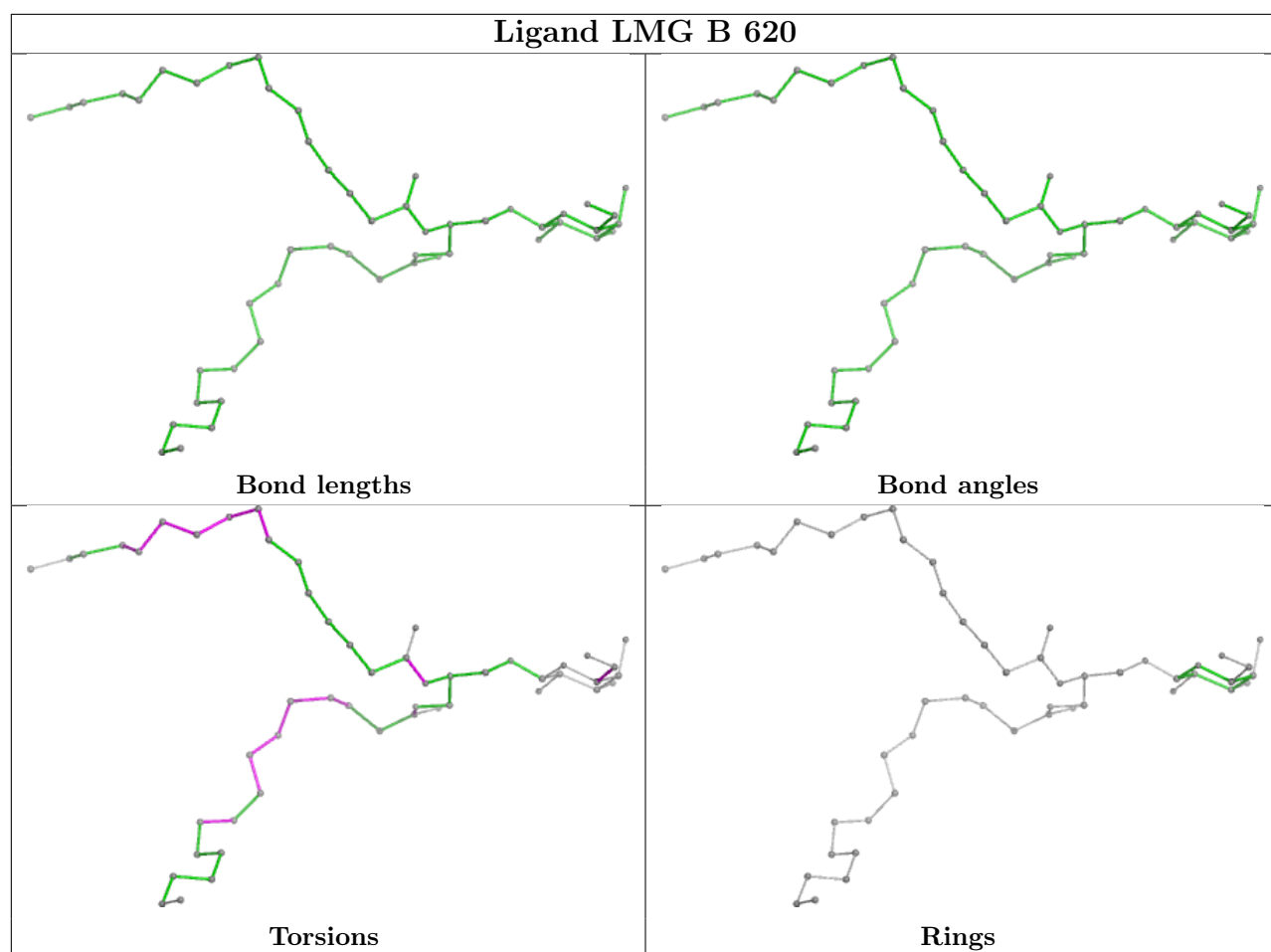




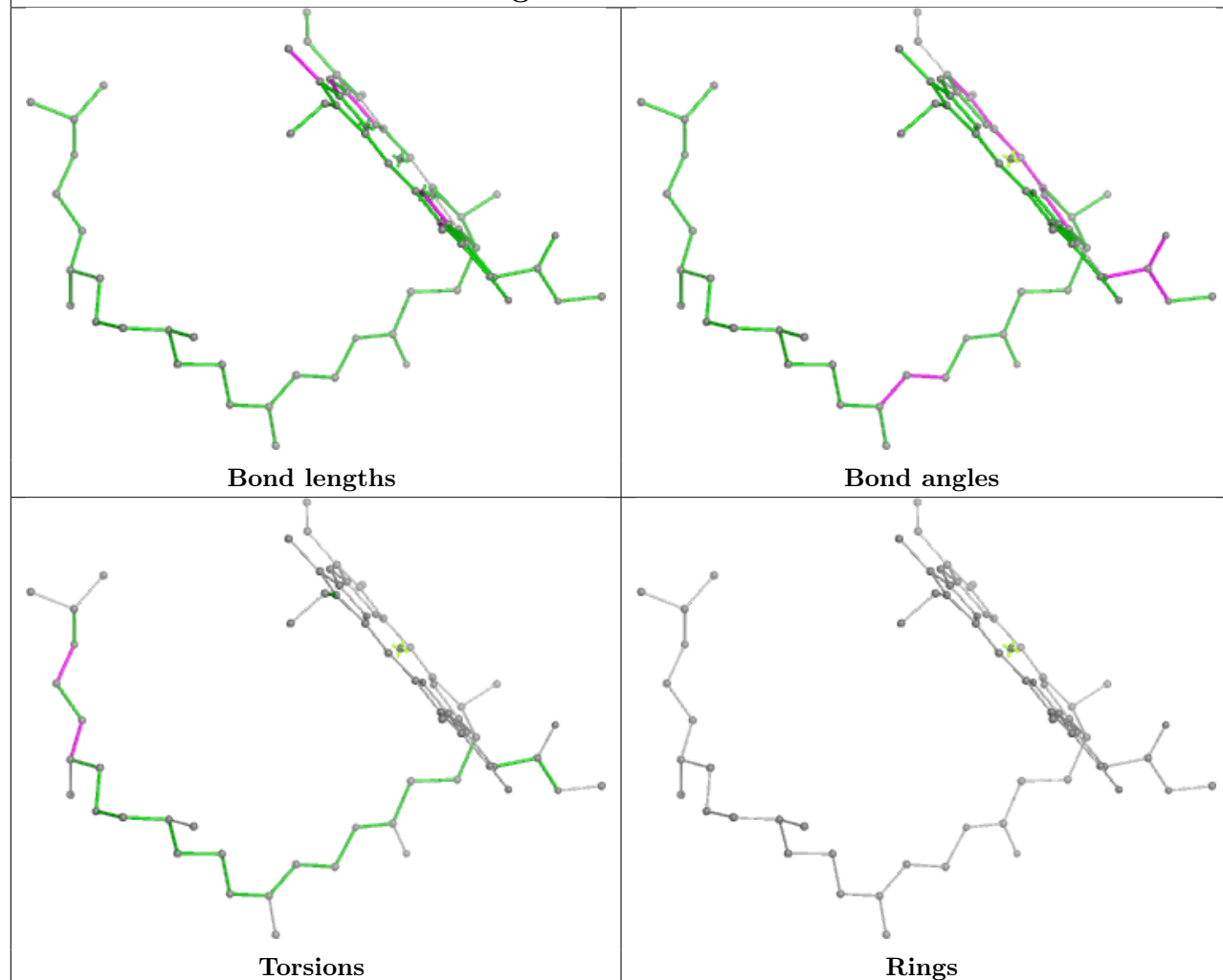
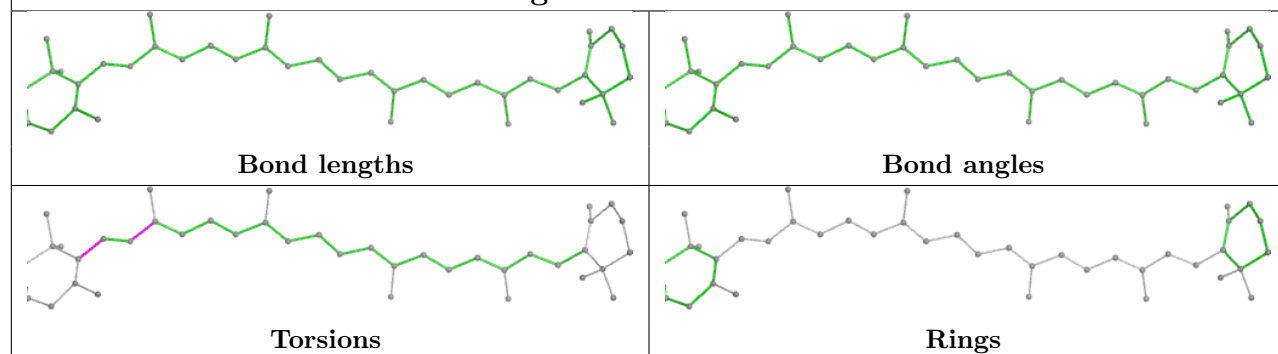


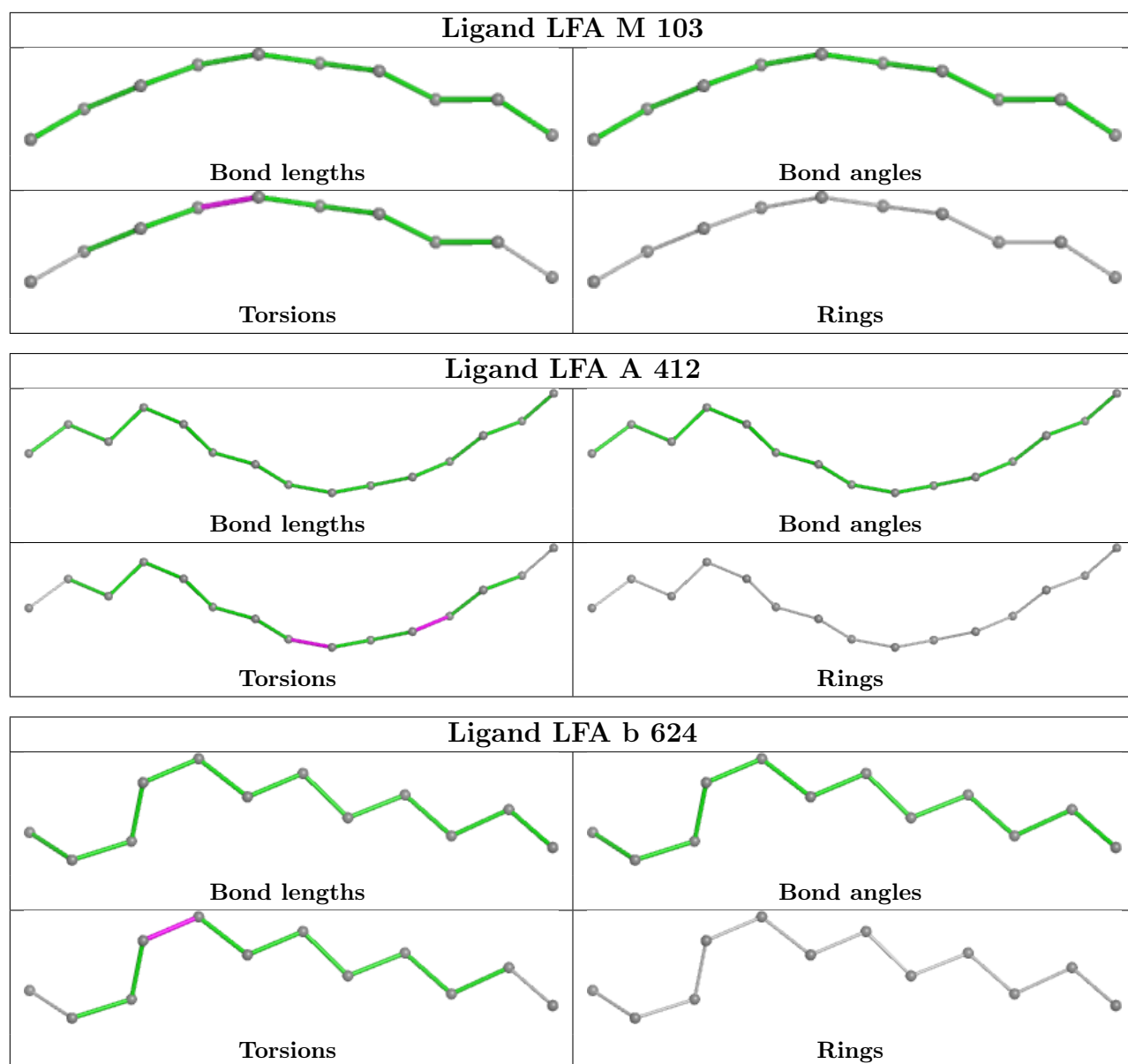


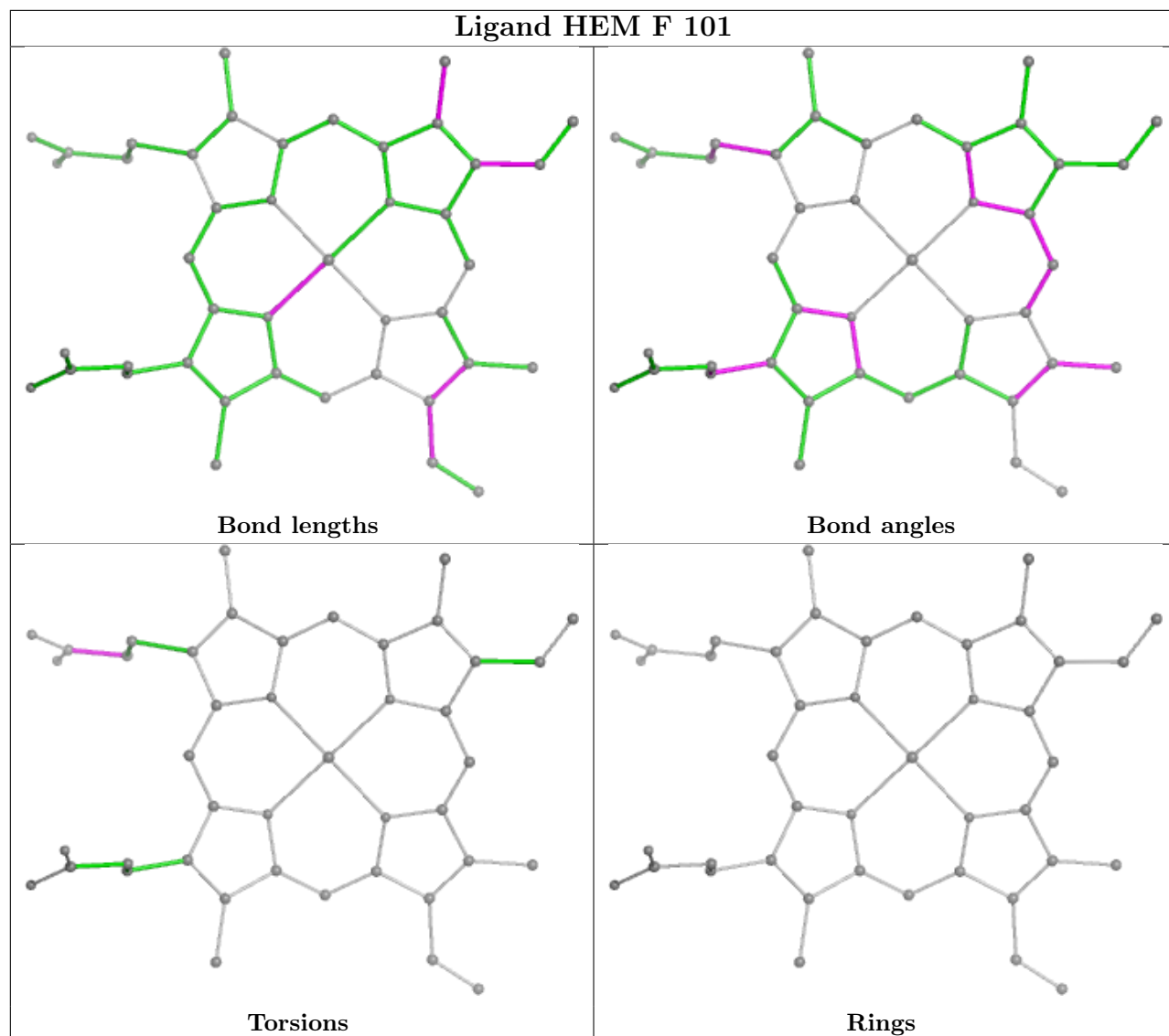


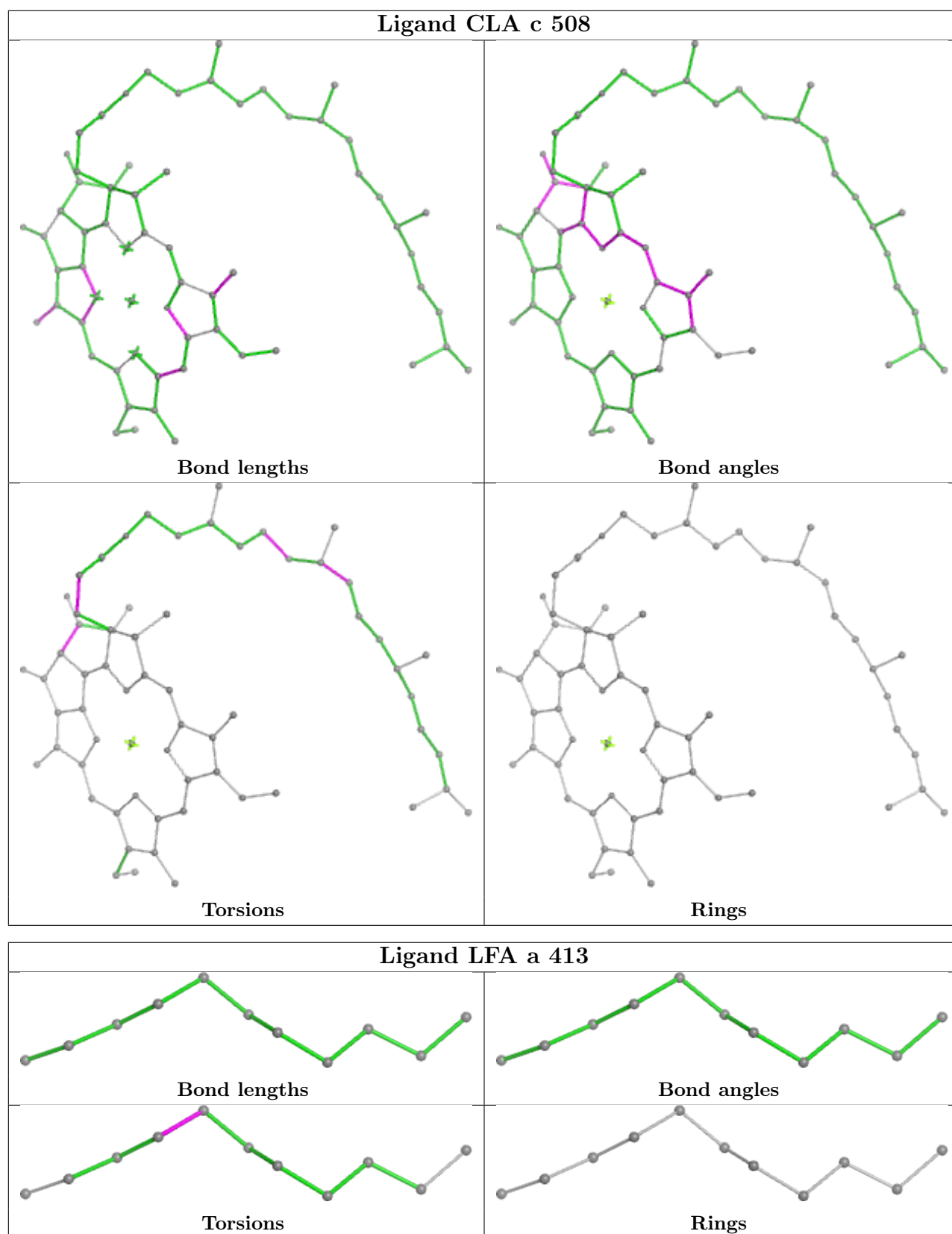


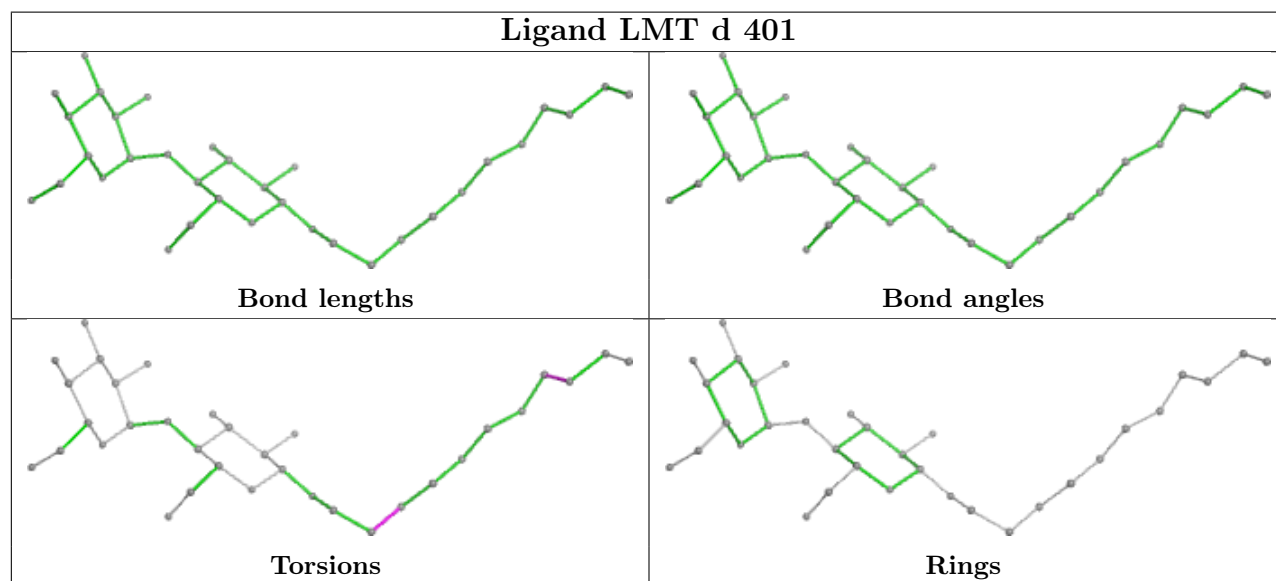
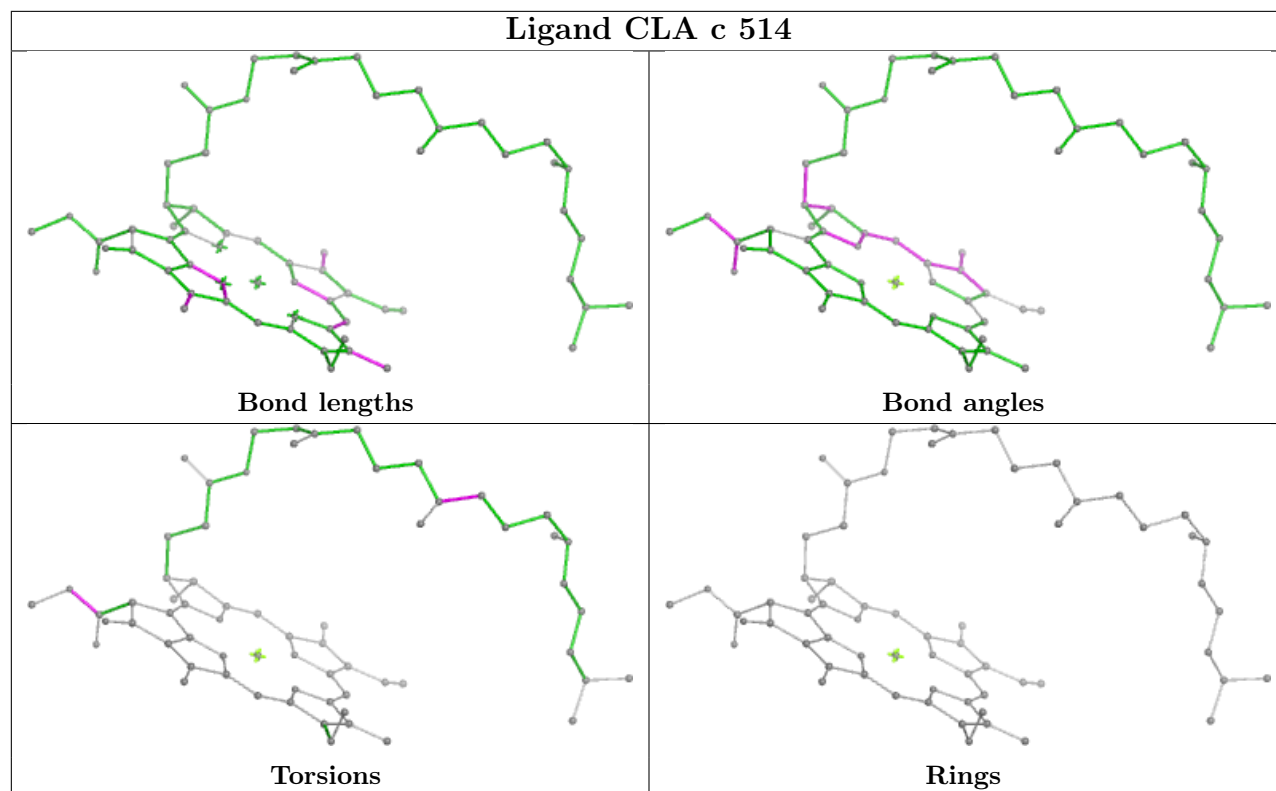


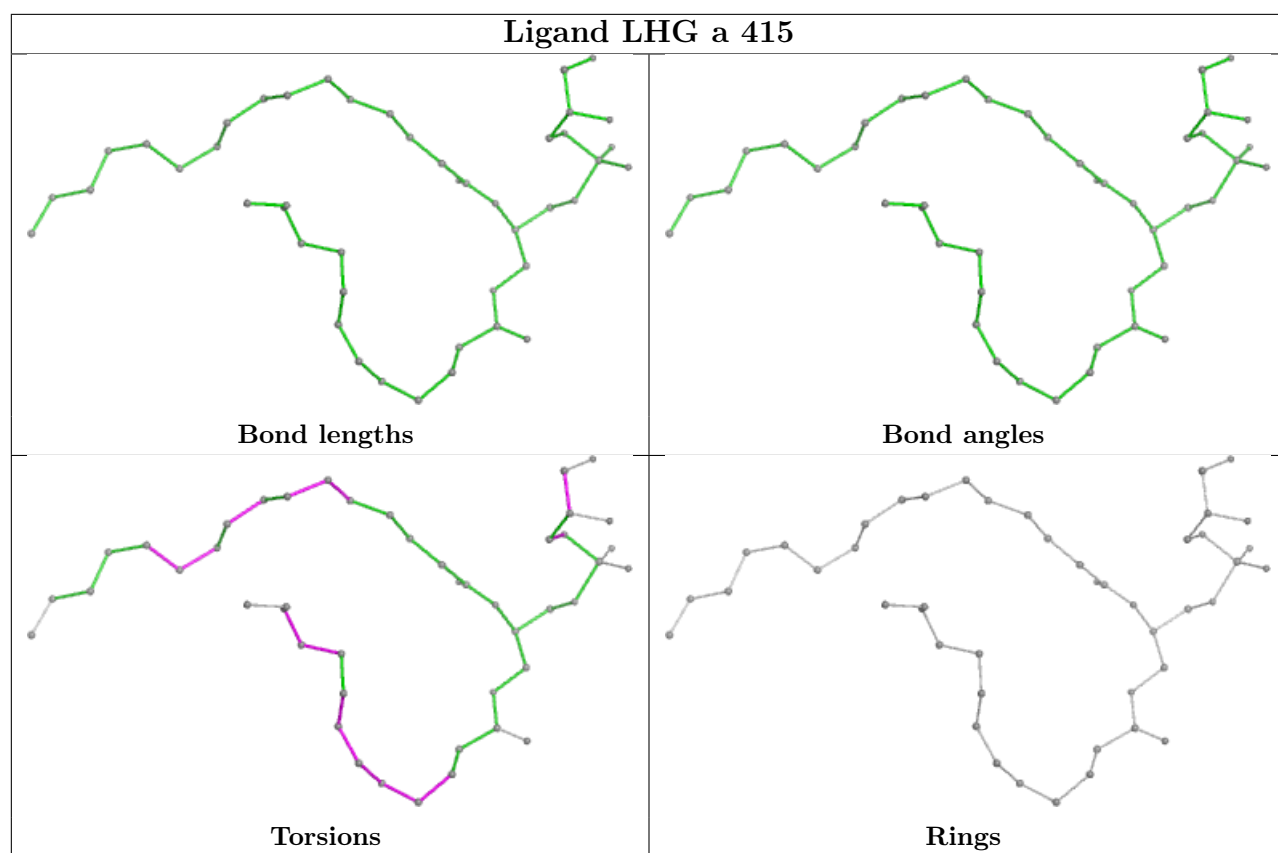
**Ligand CLA b 613****Ligand BCR B 619**



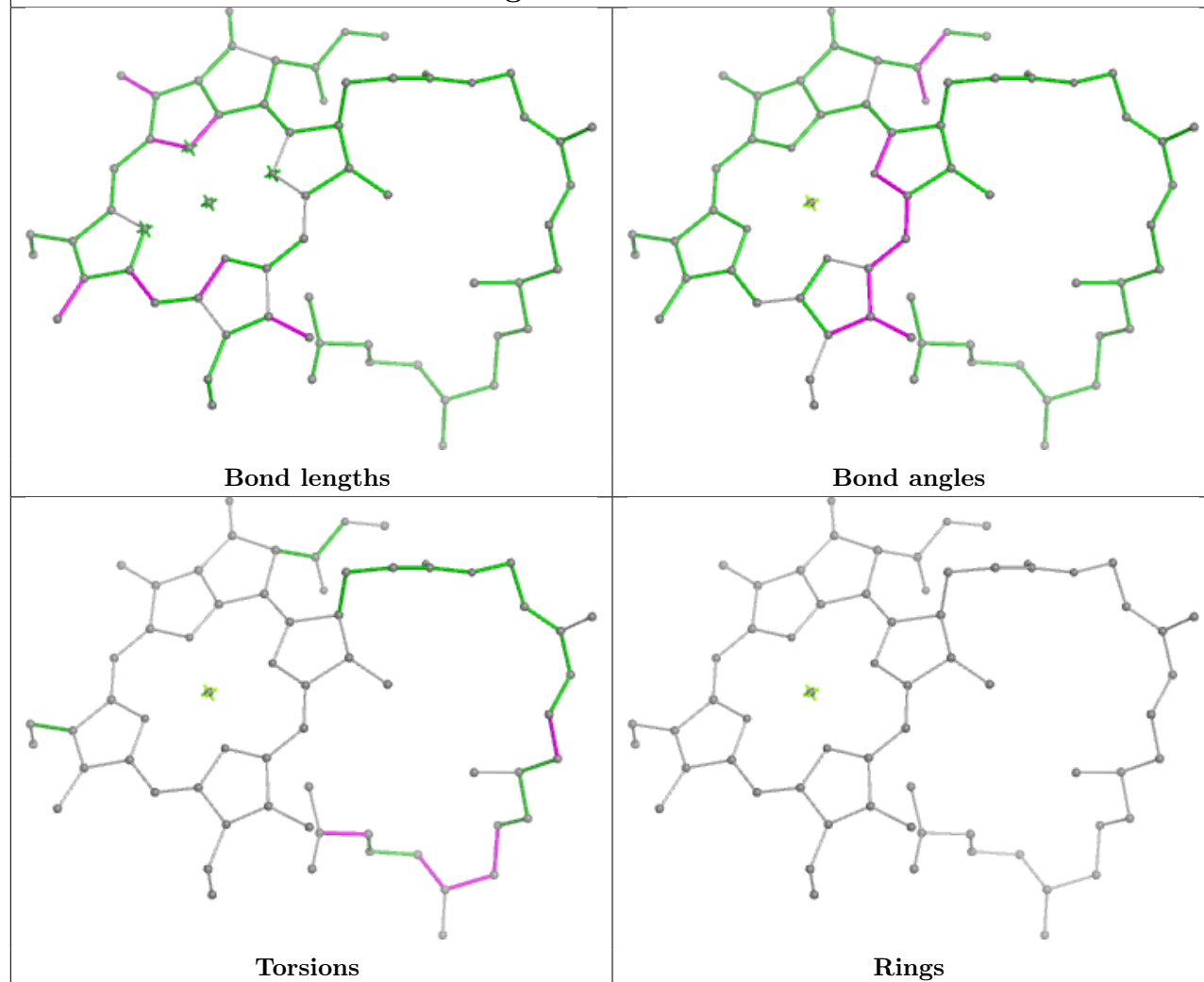




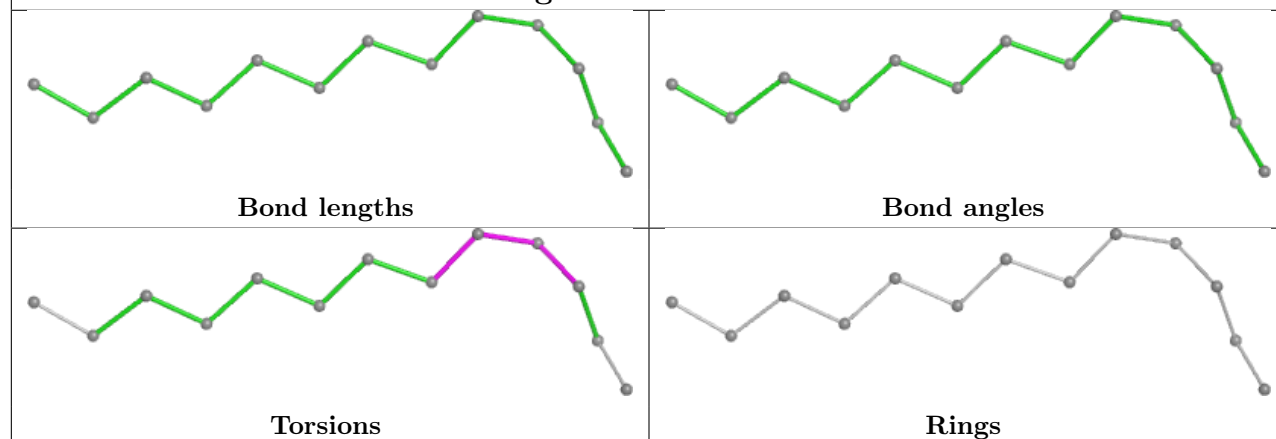


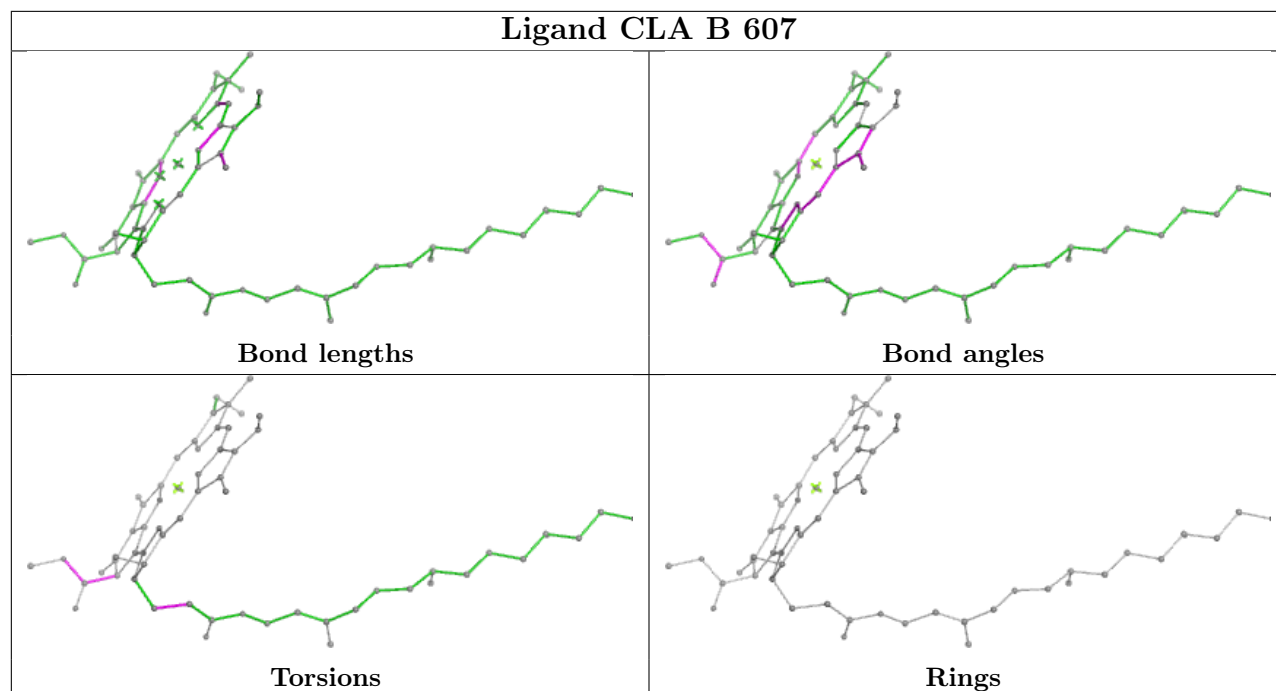
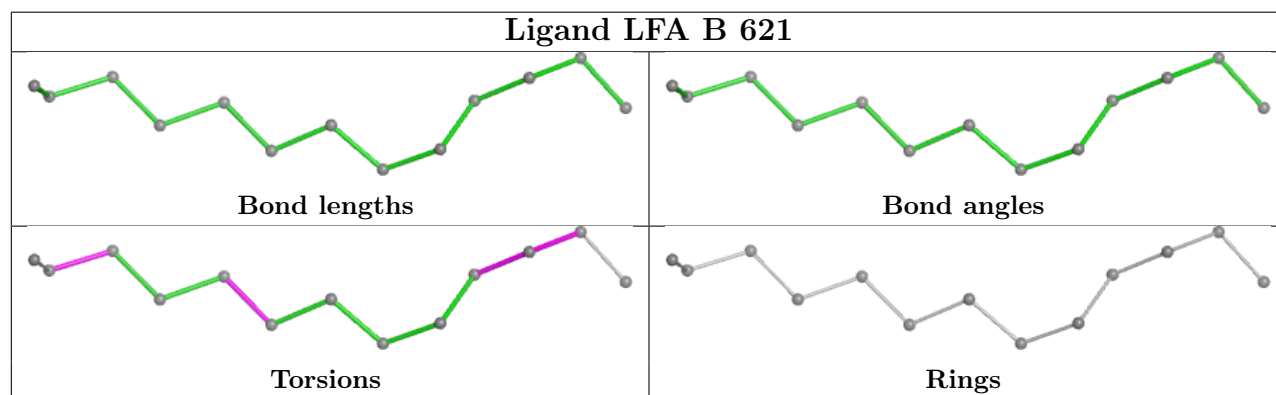


## Ligand CLA b 617

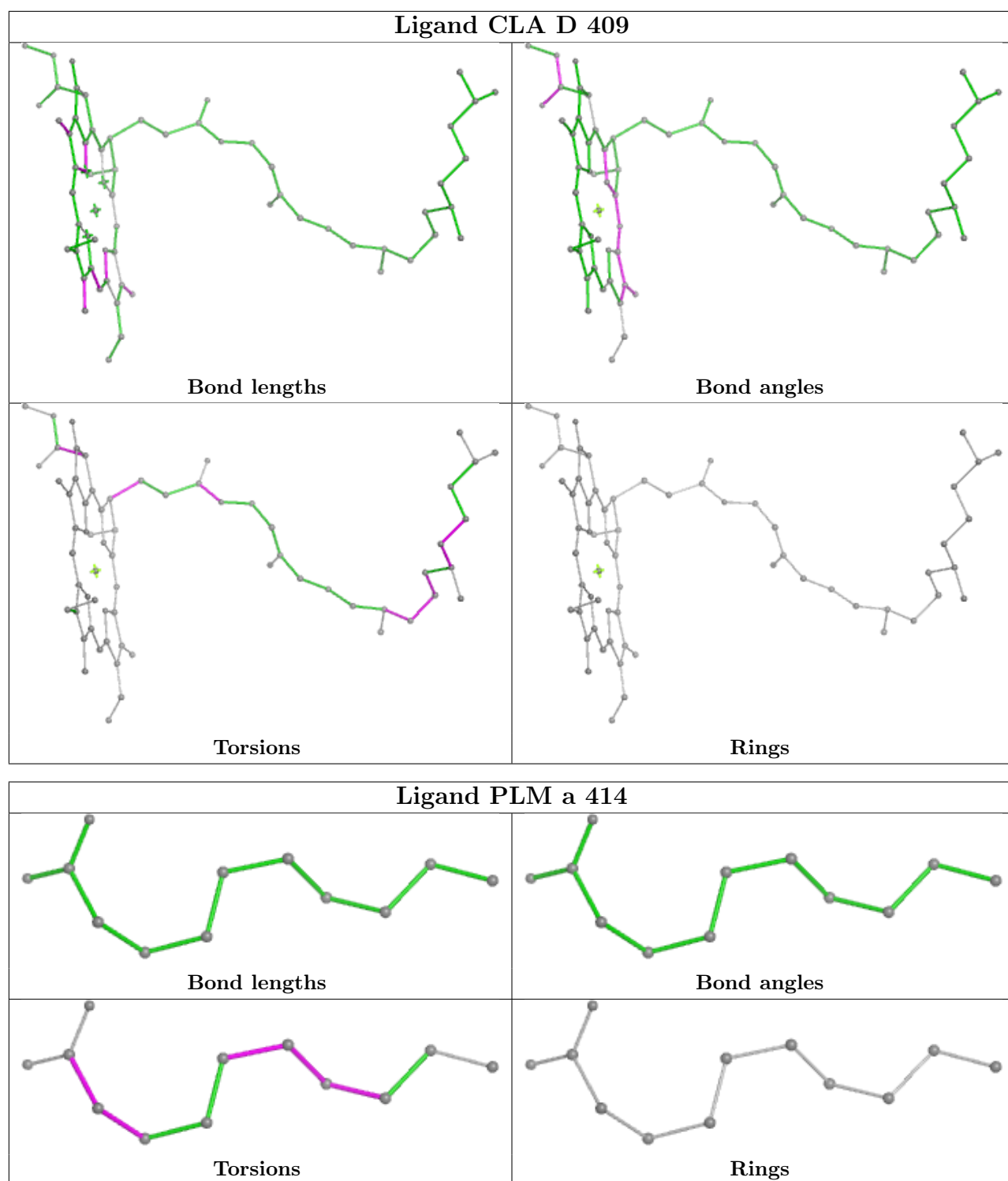


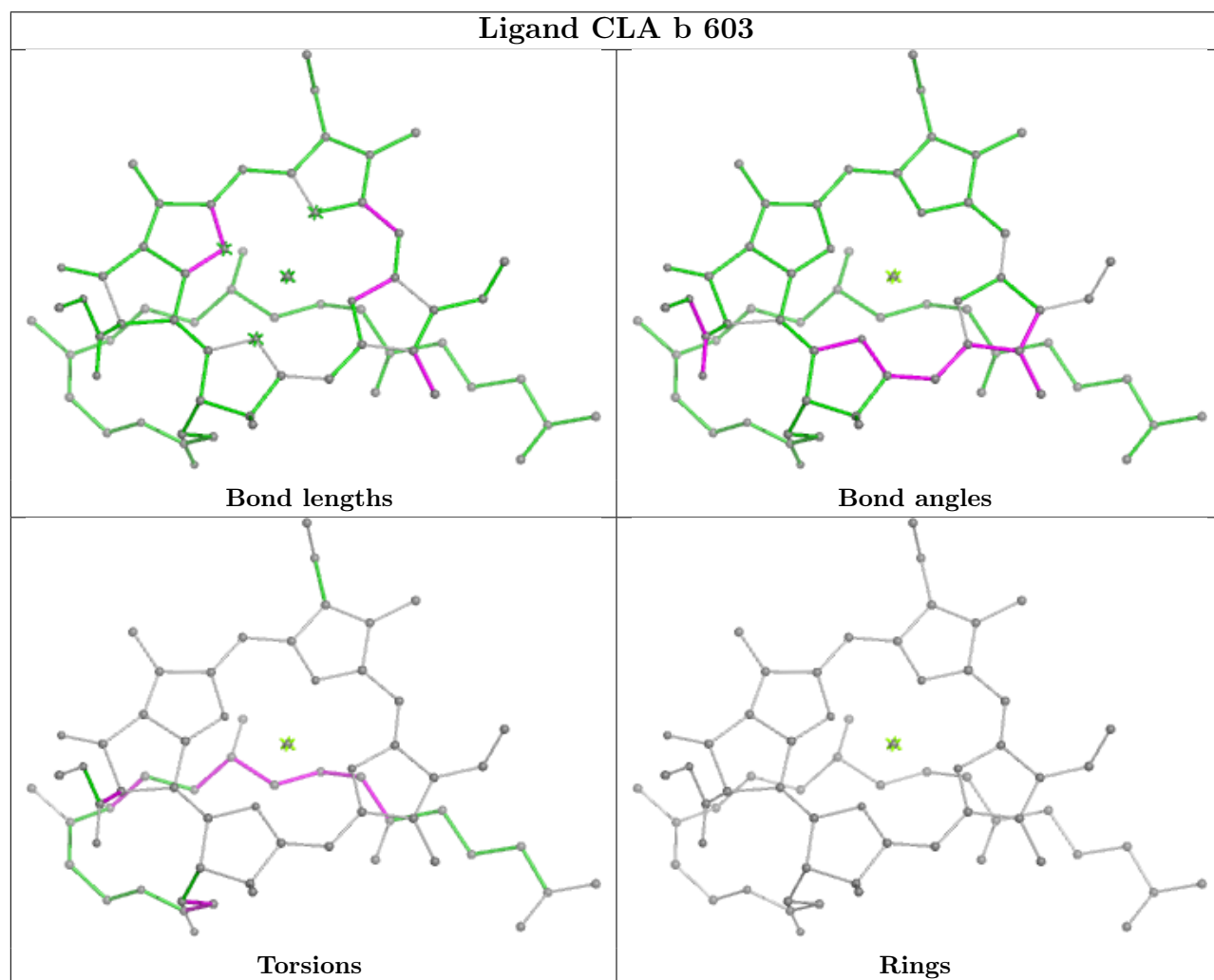
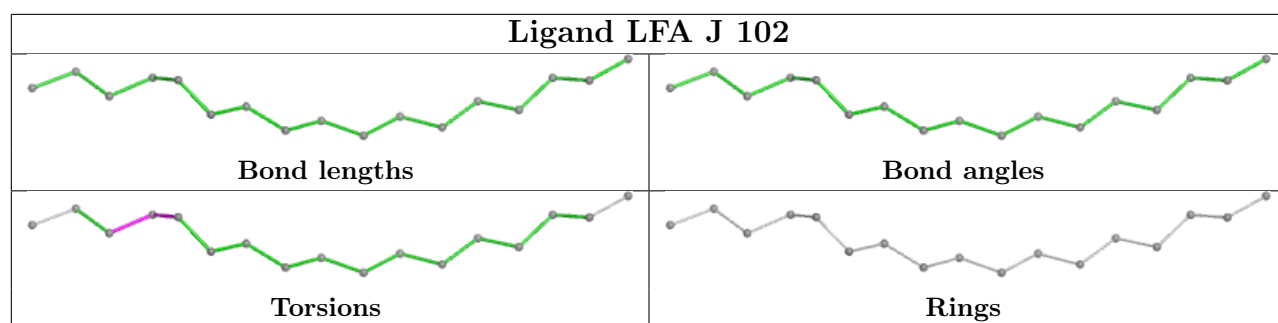
## Ligand LFA D 406

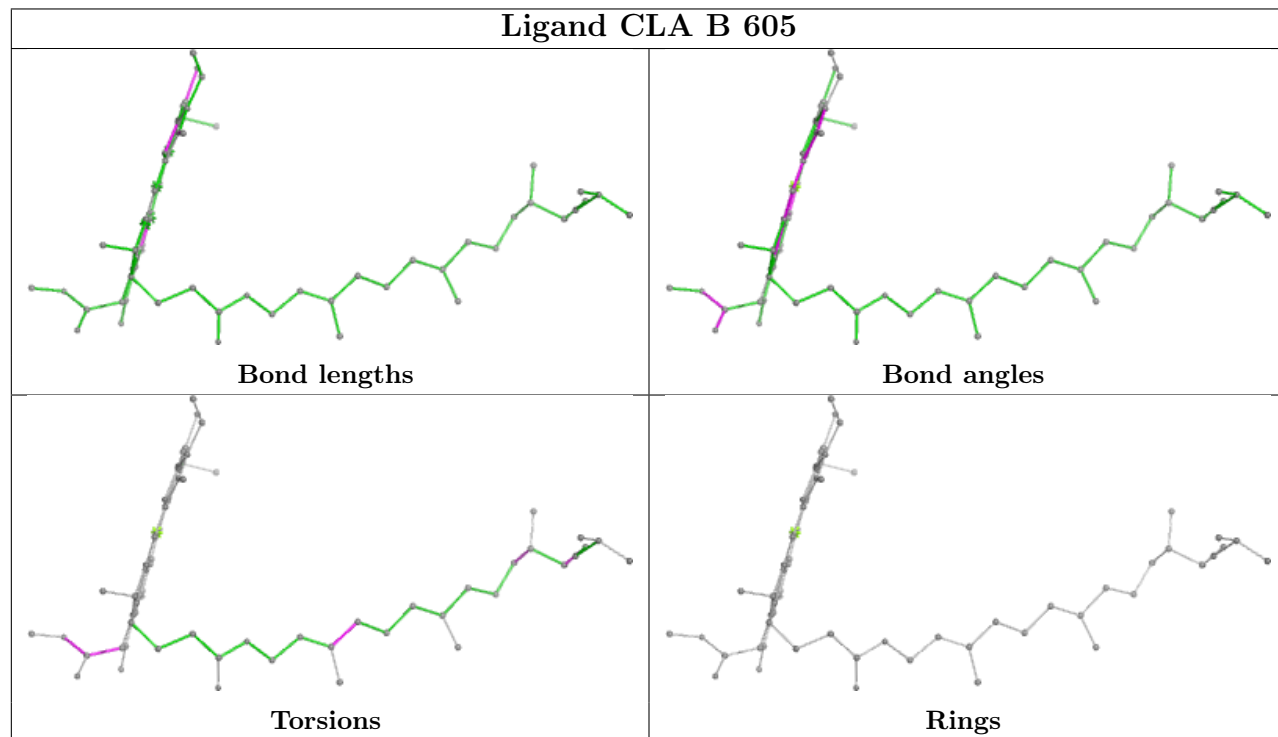
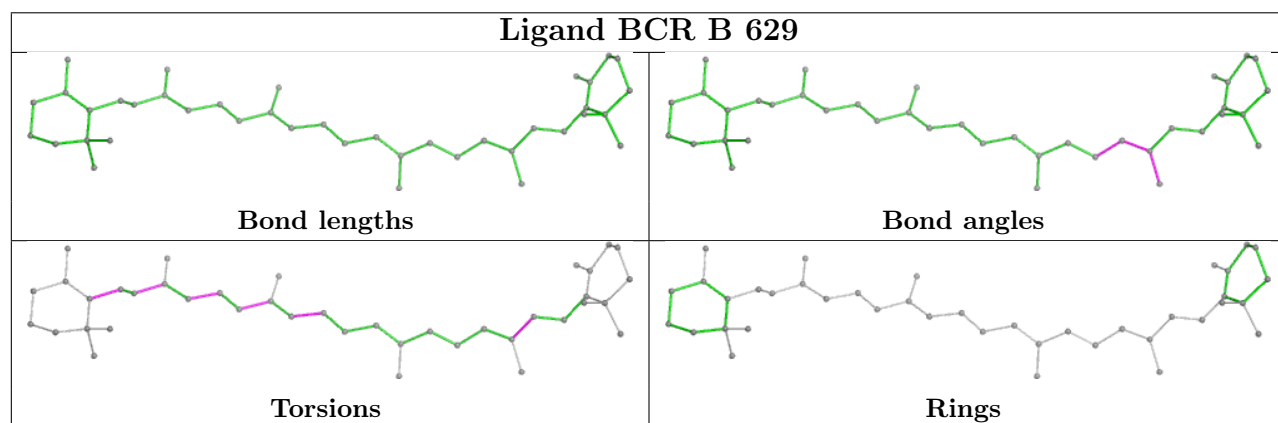
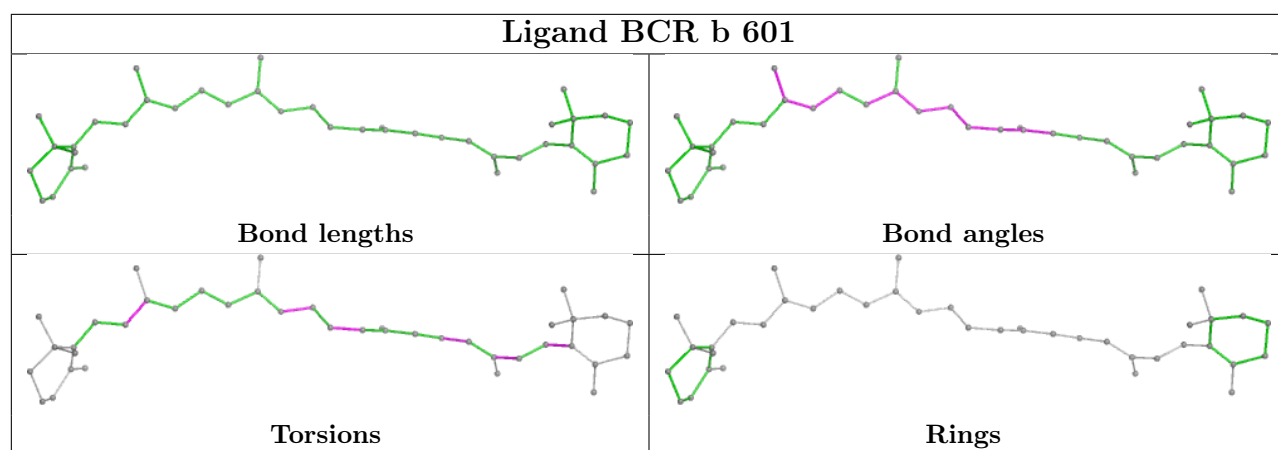


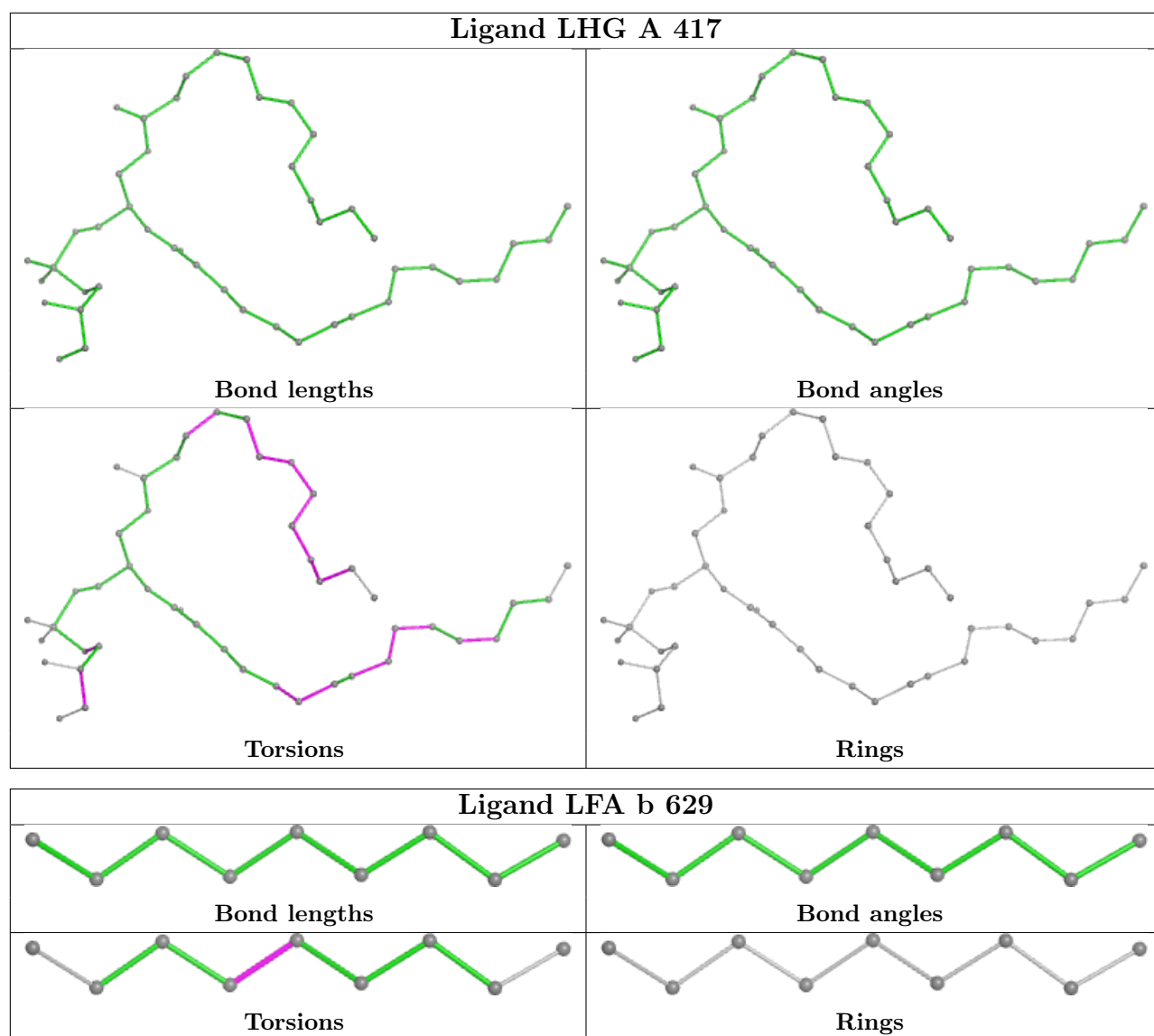
**Ligand CLA B 607****Ligand LFA B 621**

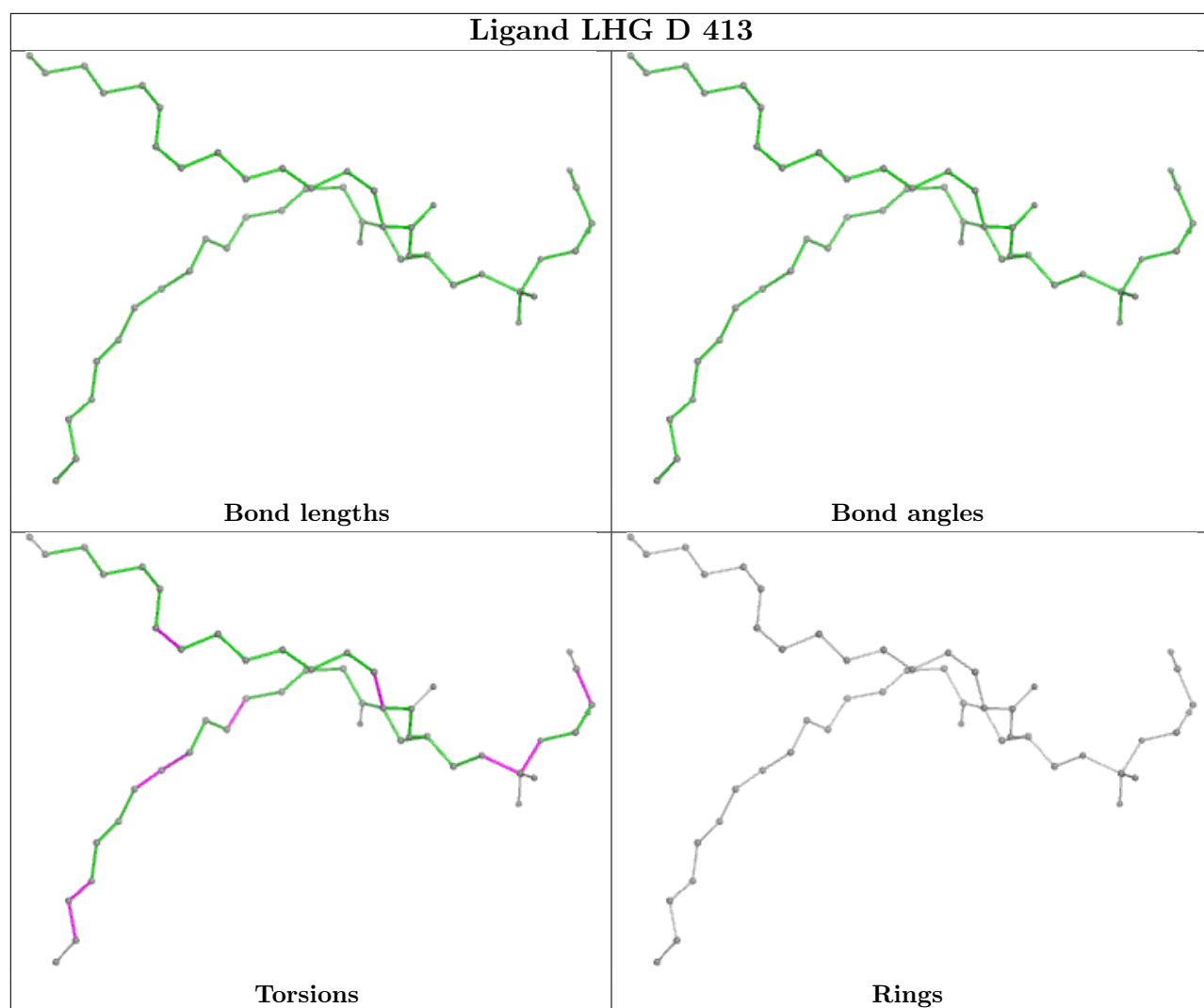


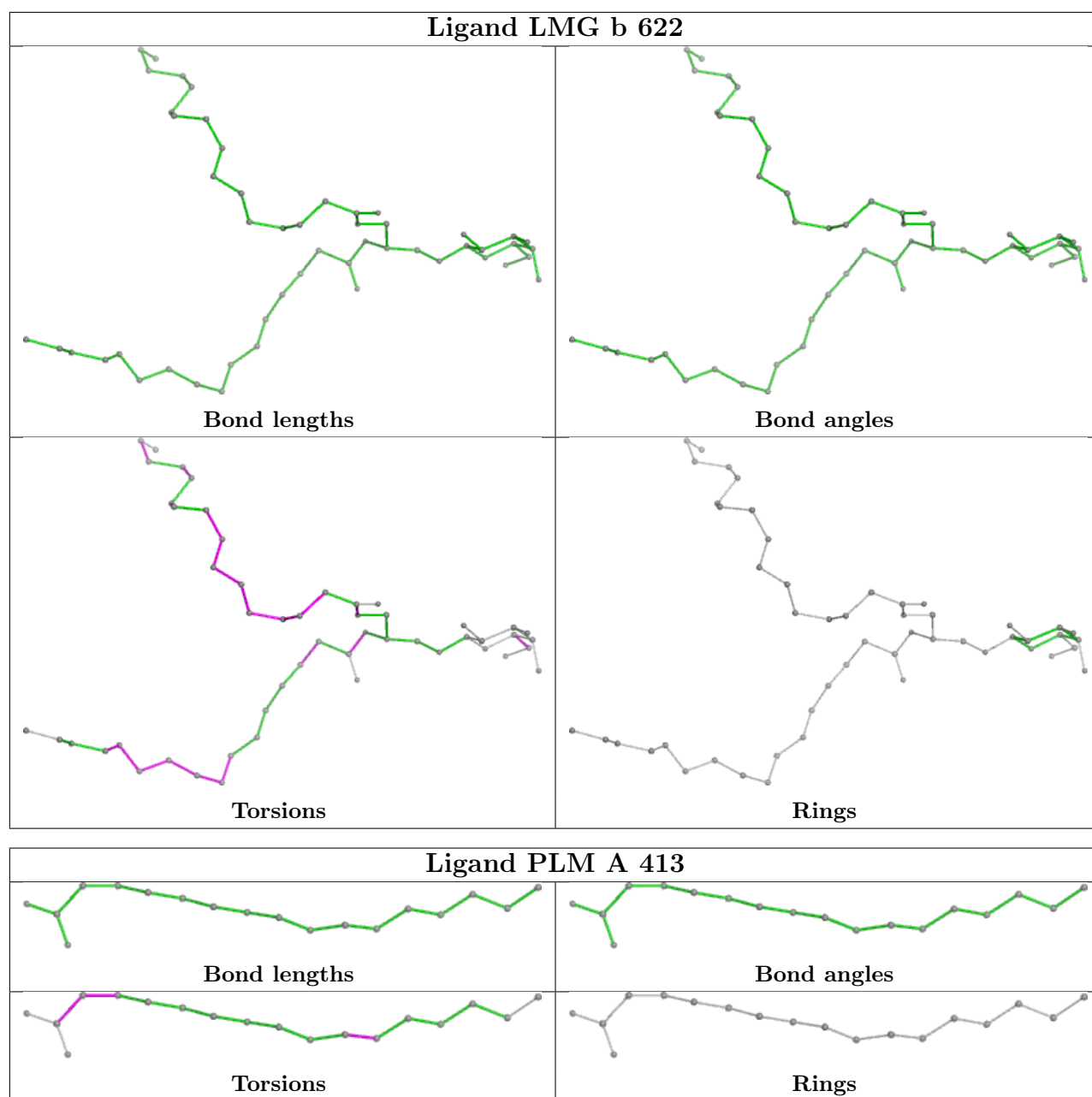


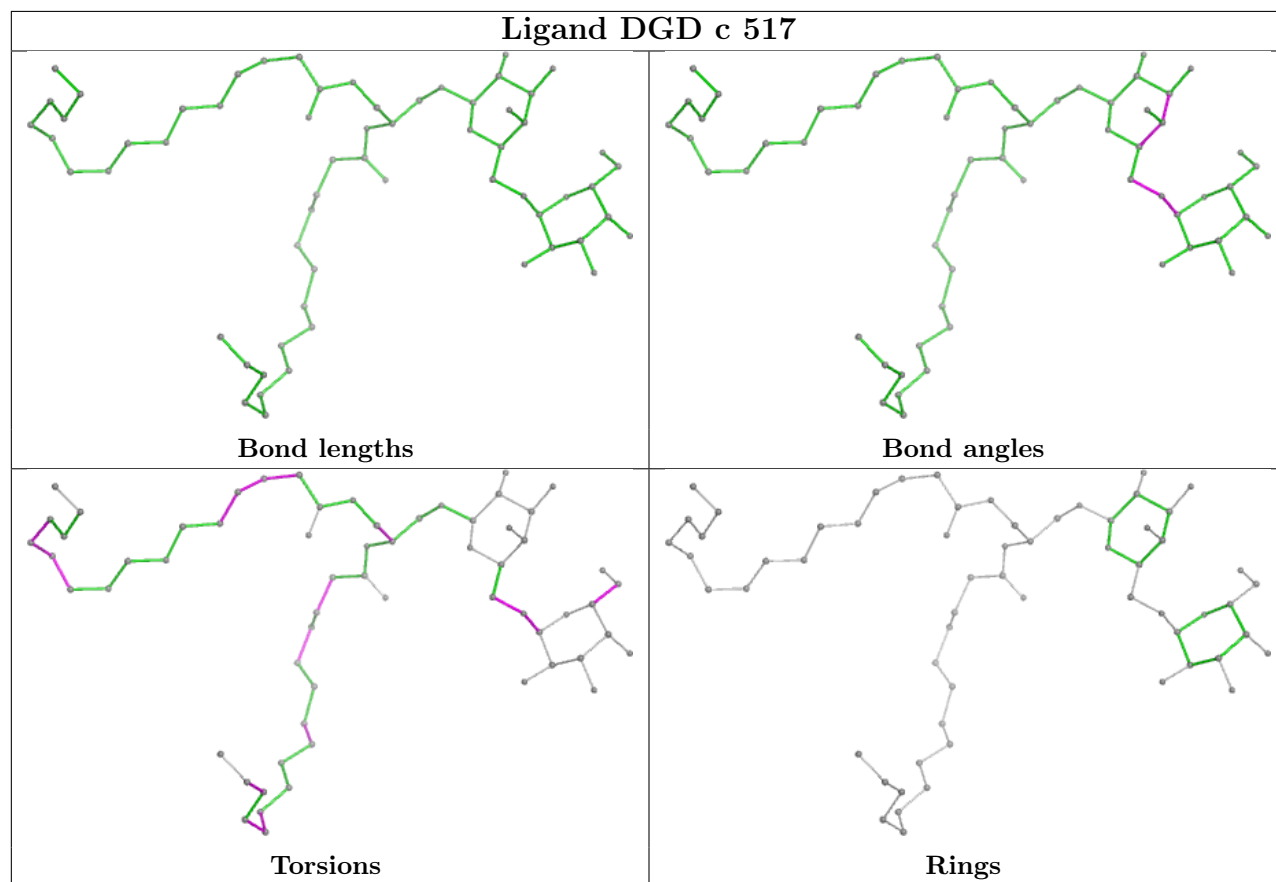
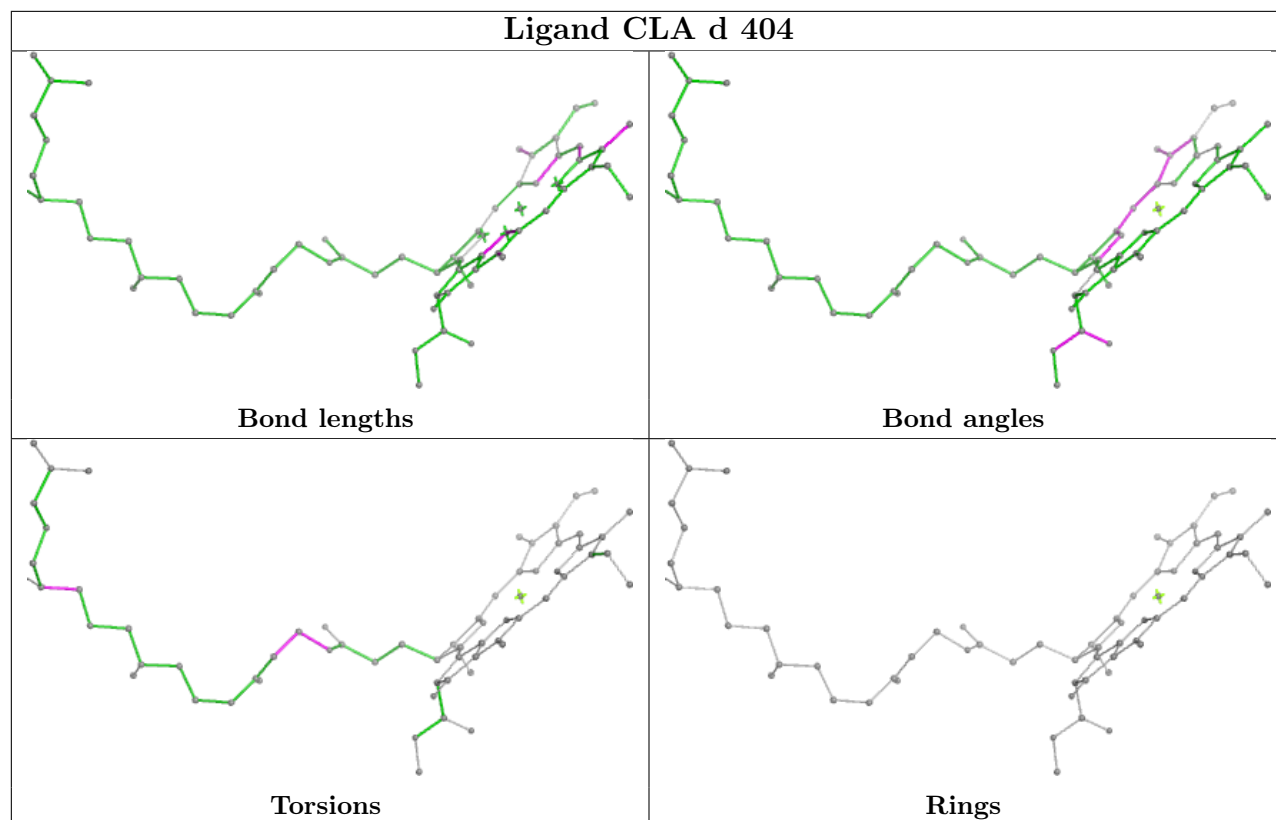


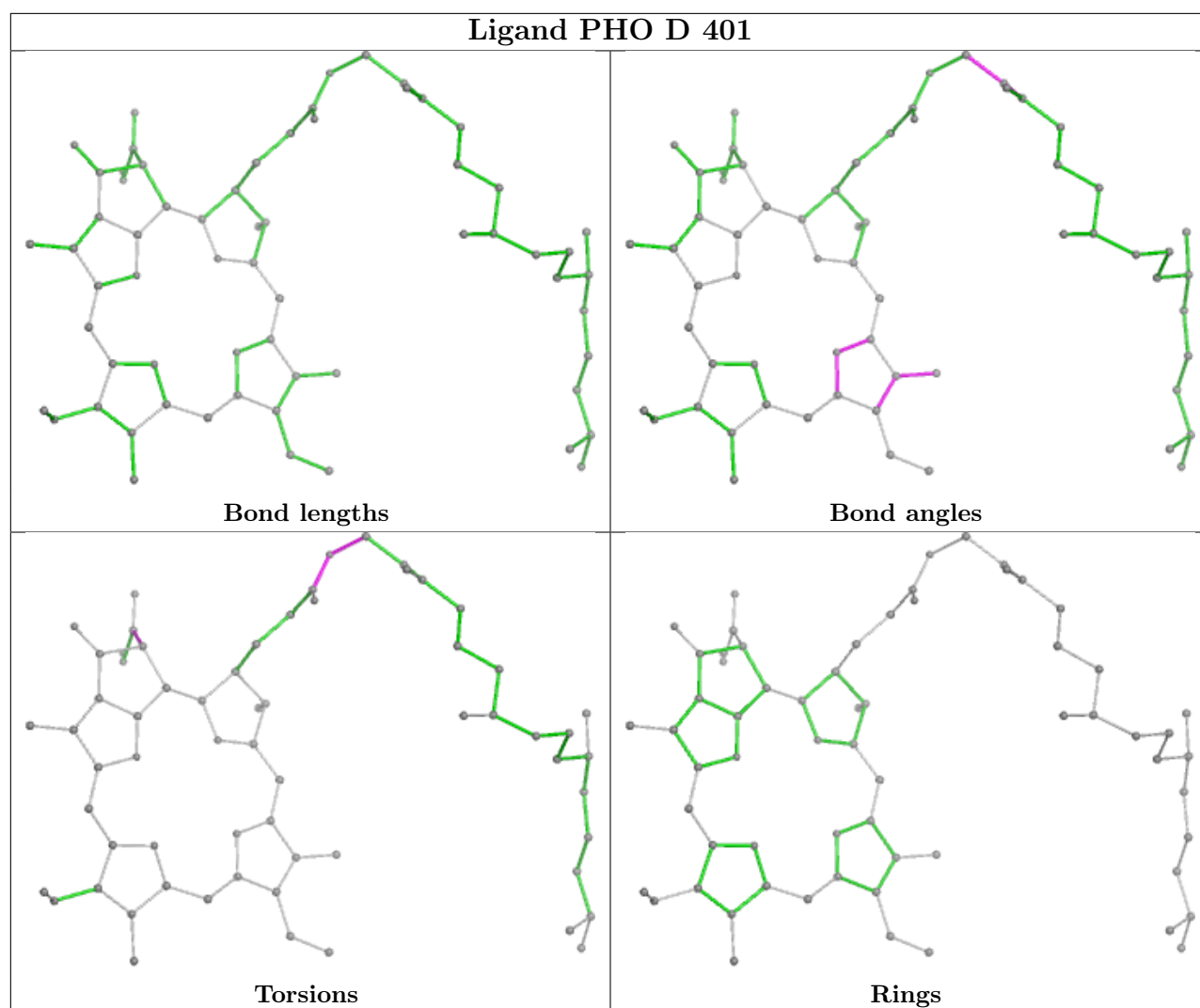




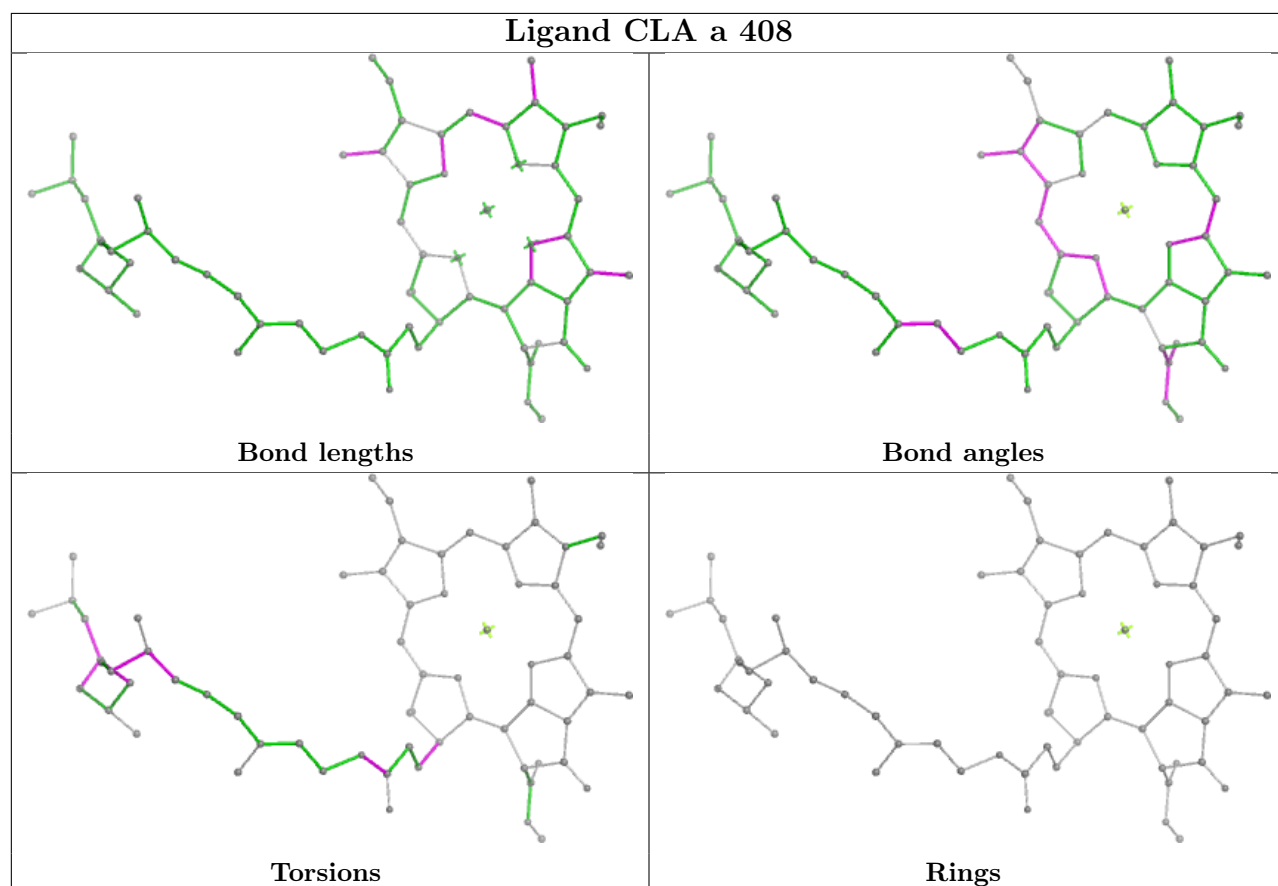
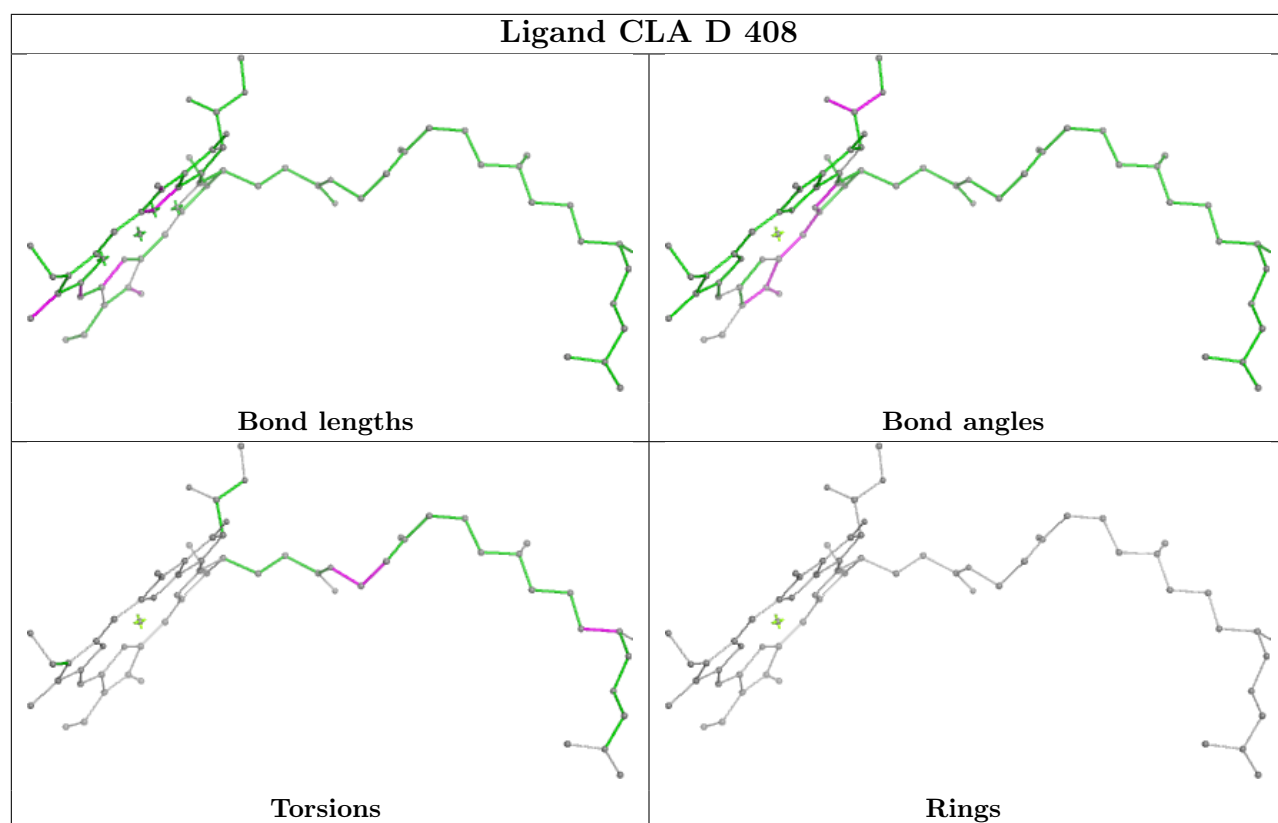




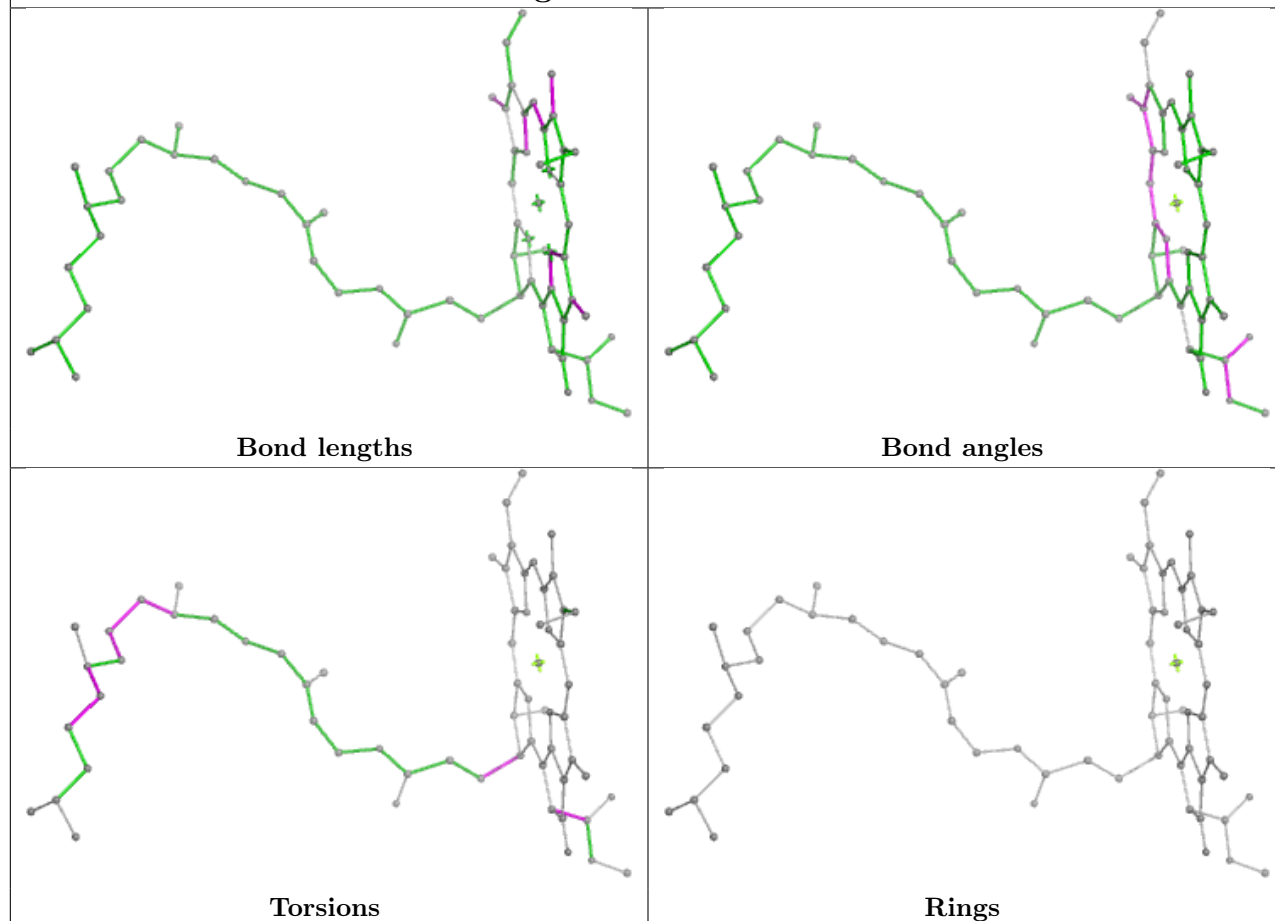




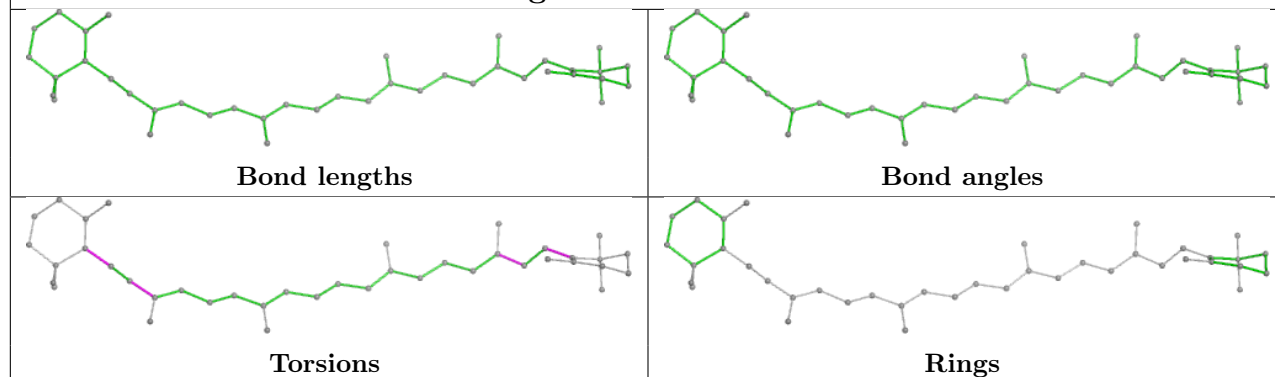


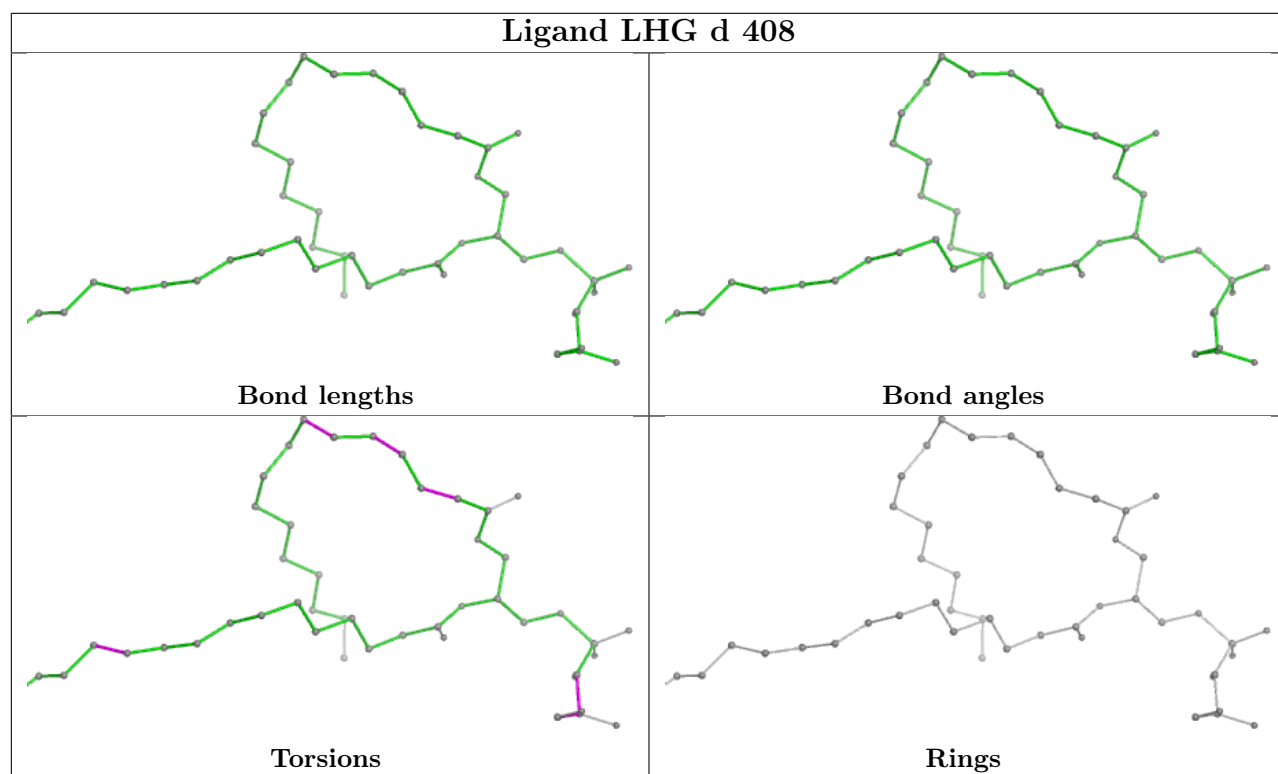
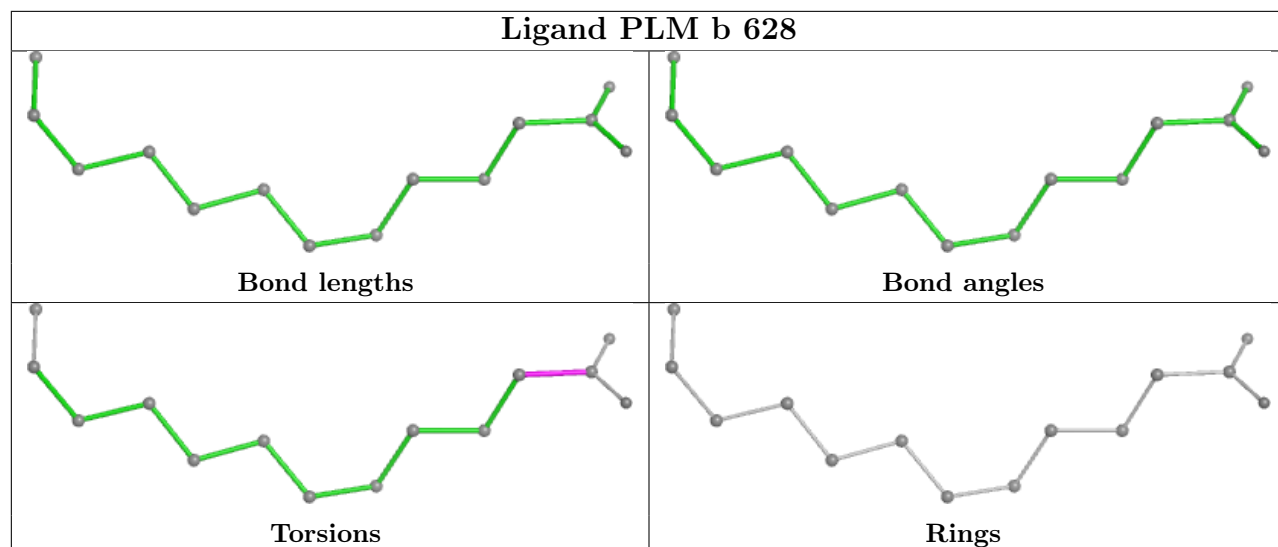


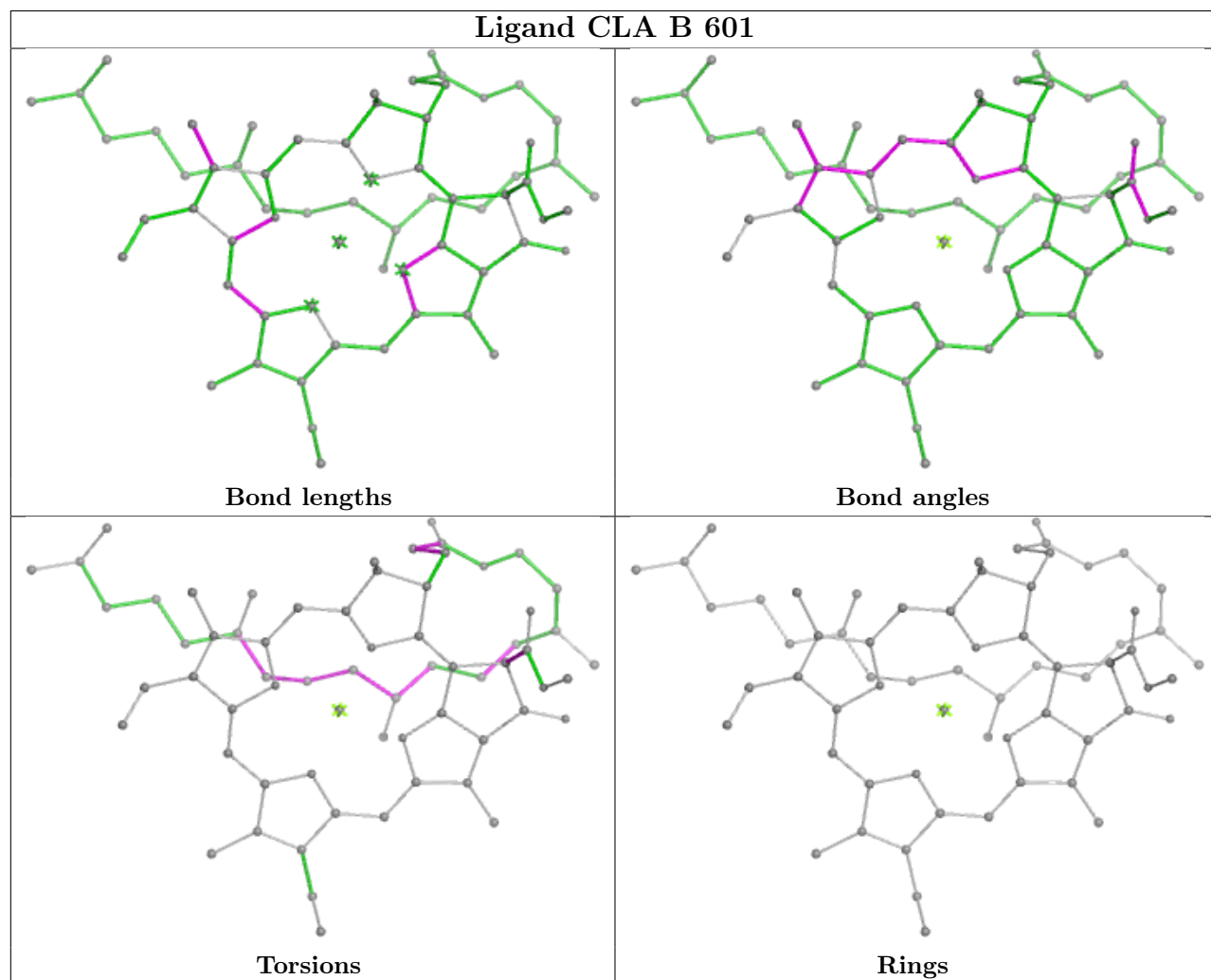
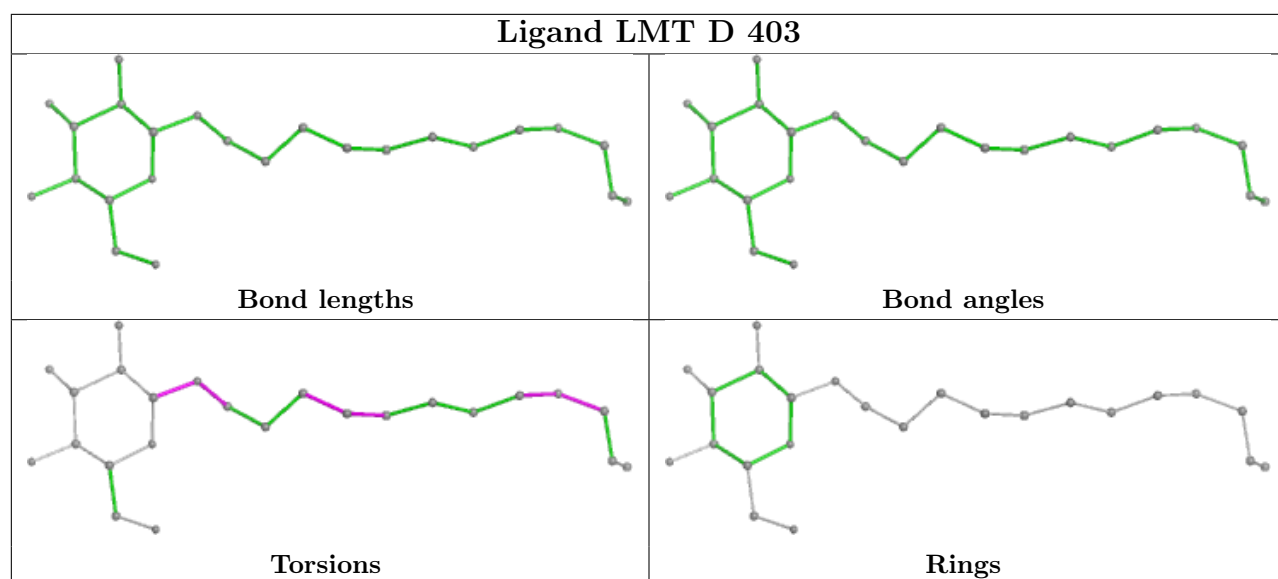
## Ligand CLA d 405

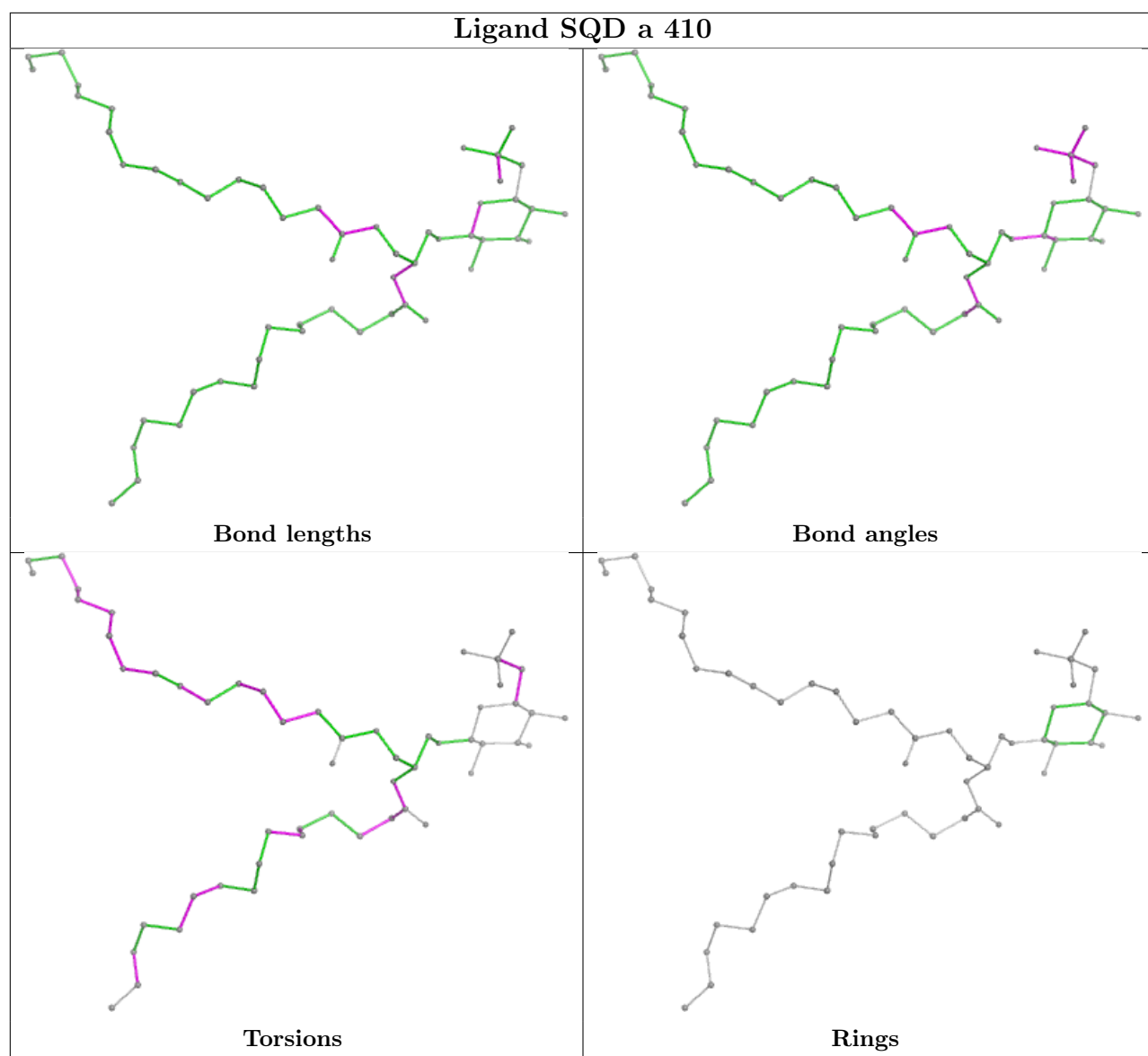


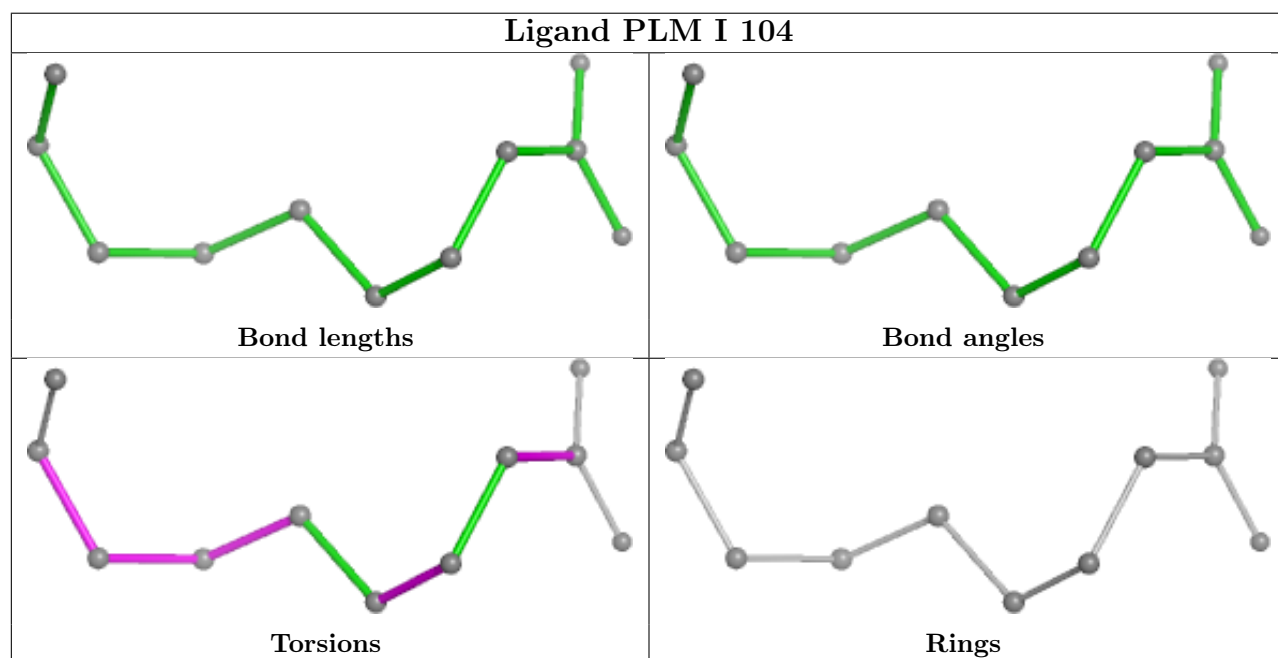
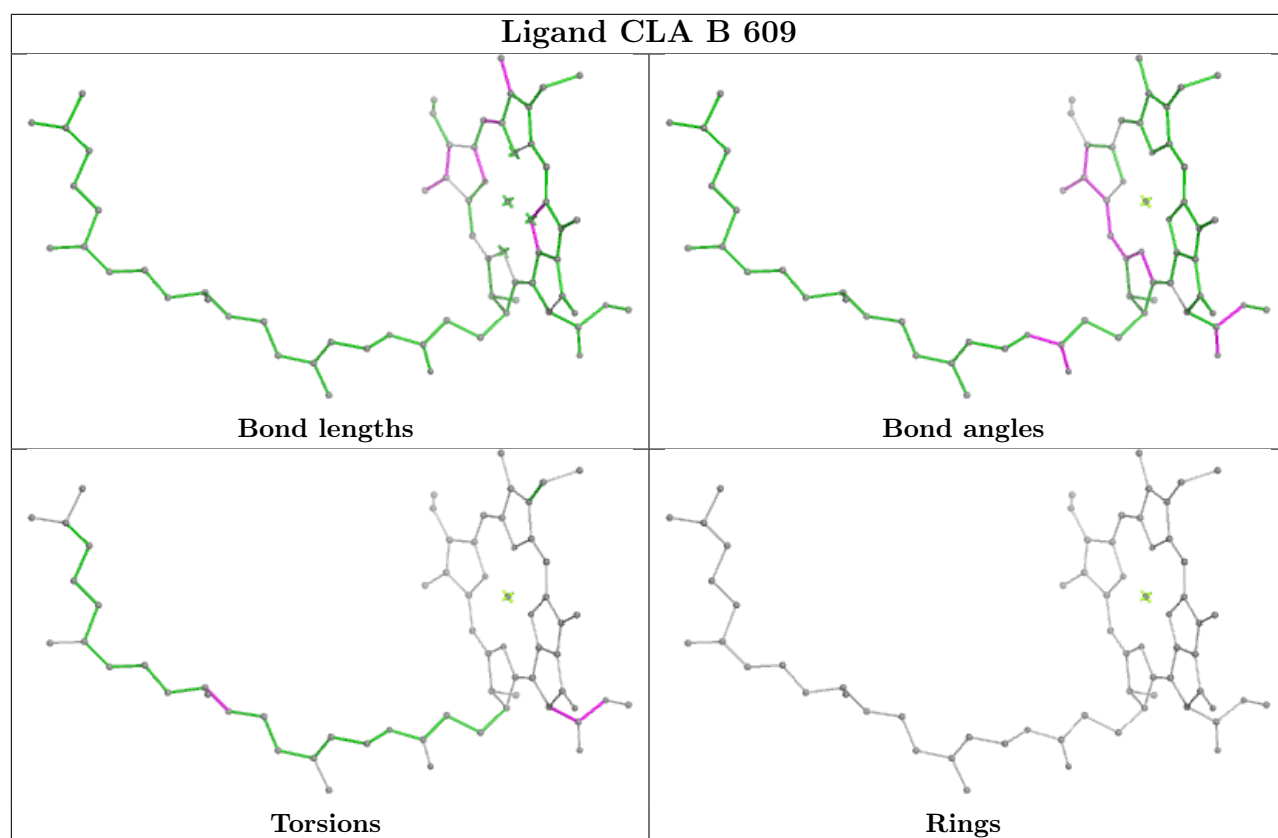
## Ligand BCR D 410

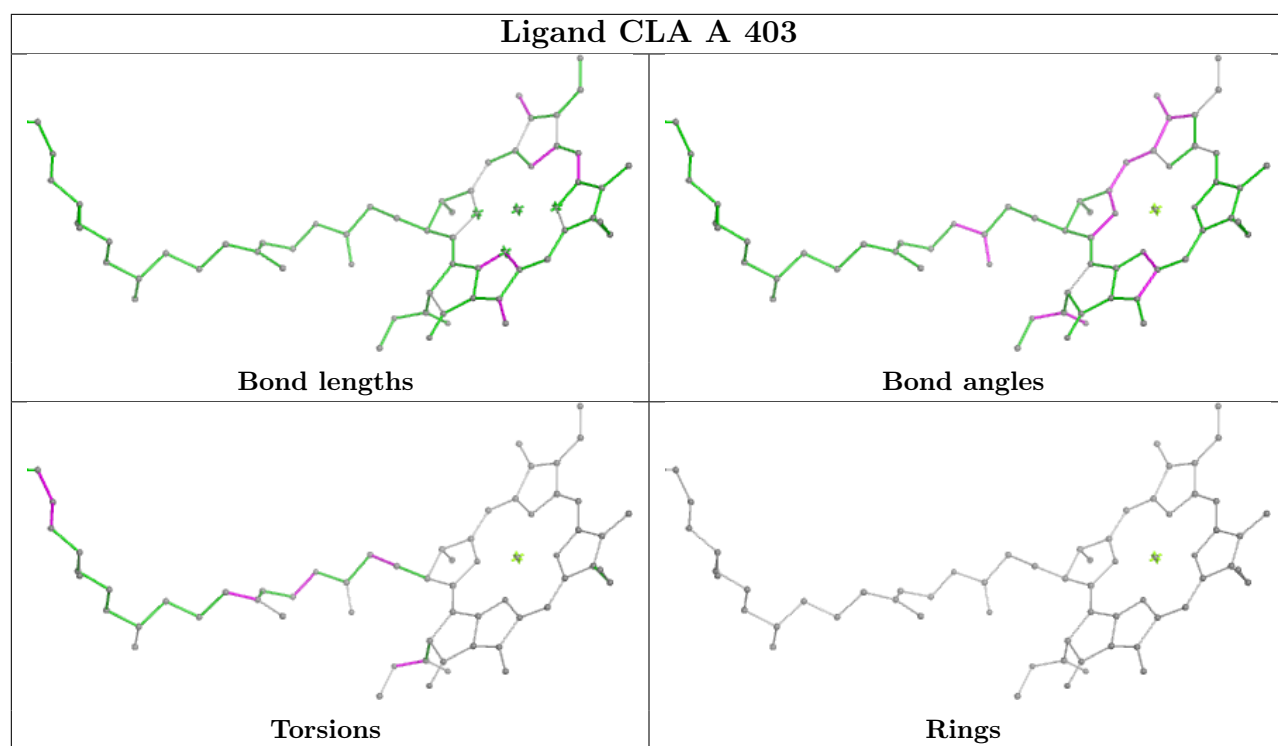


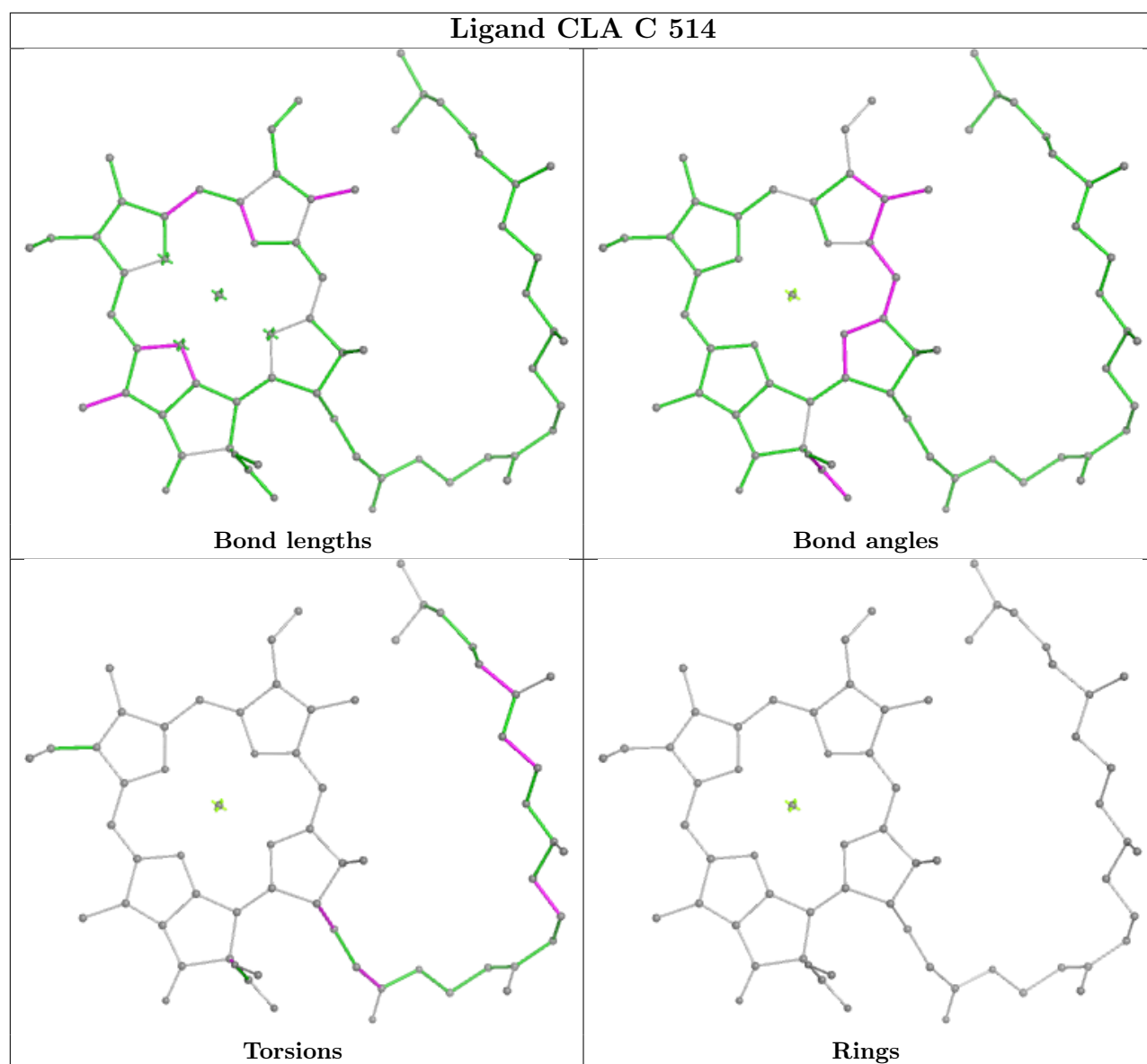




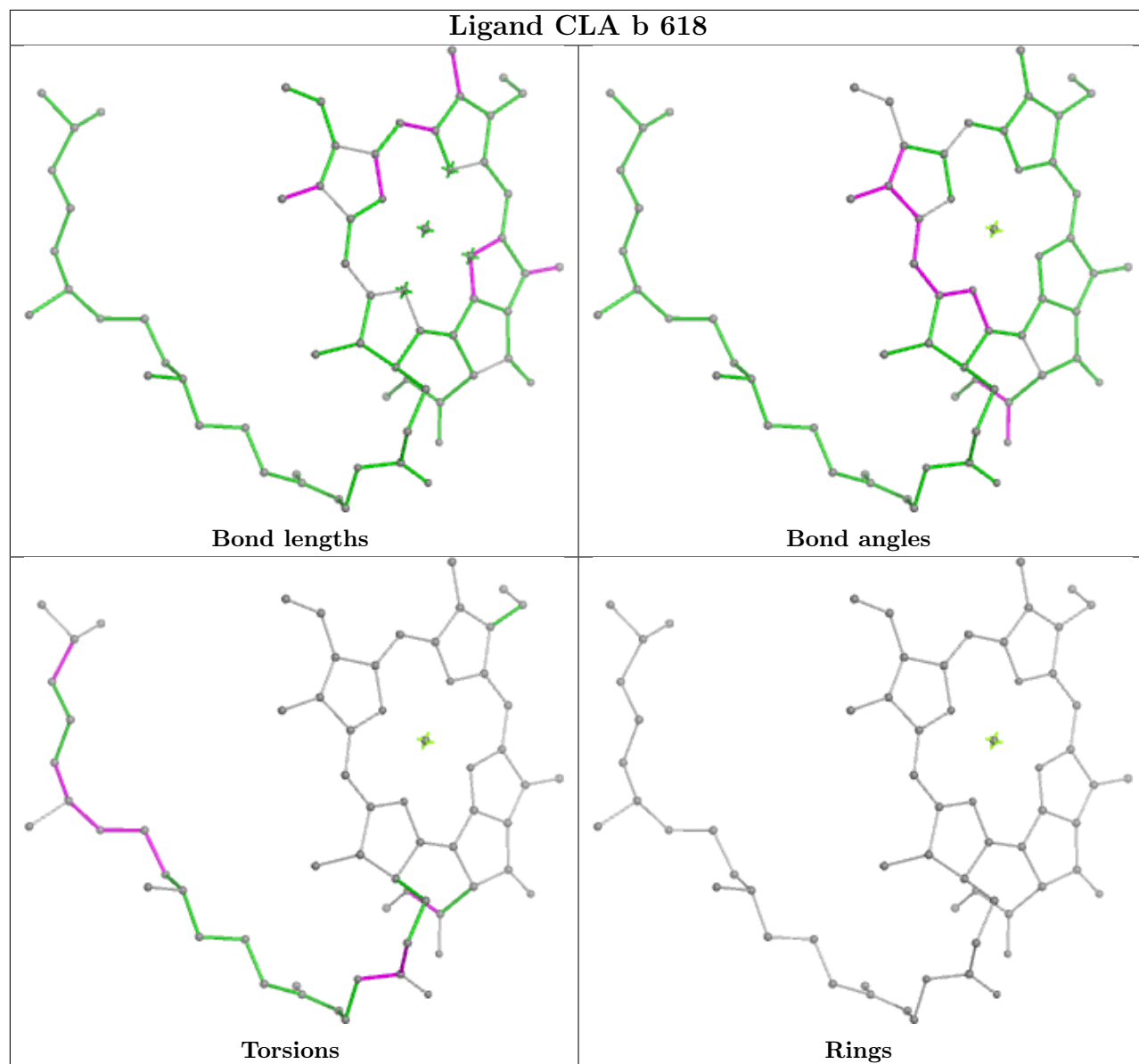


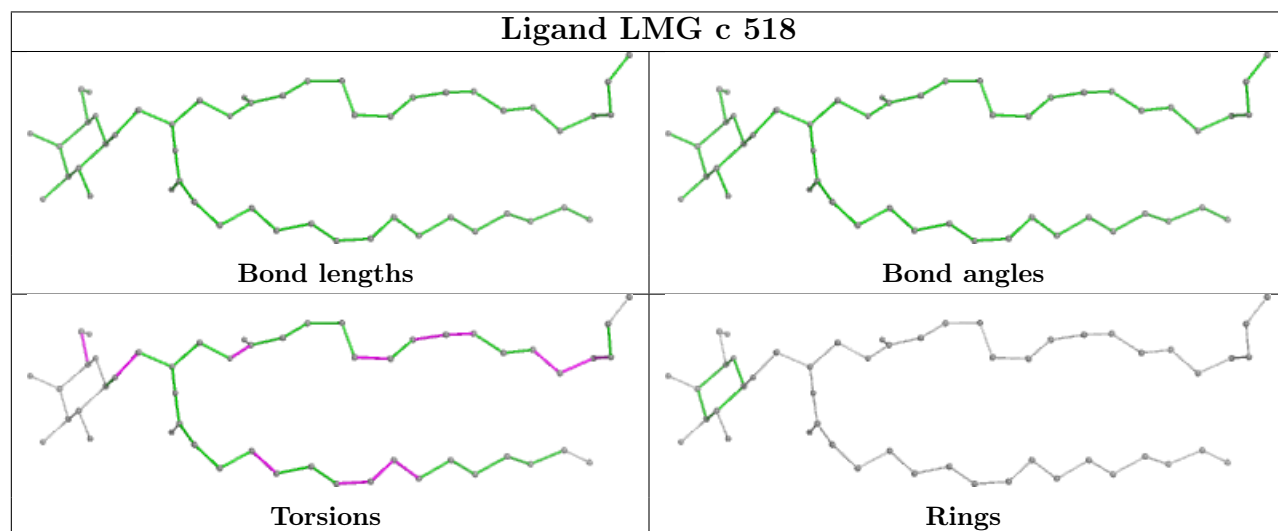
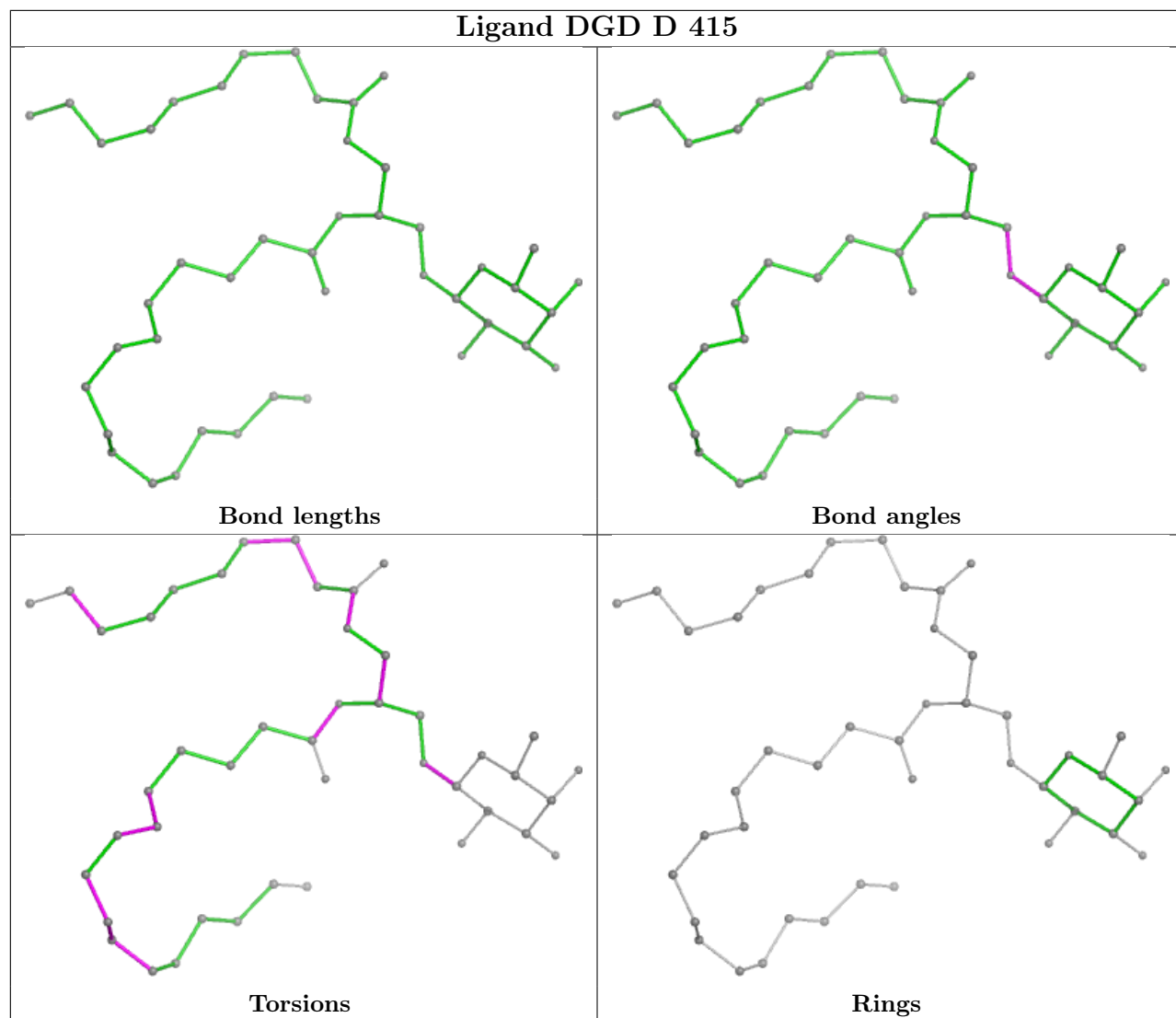




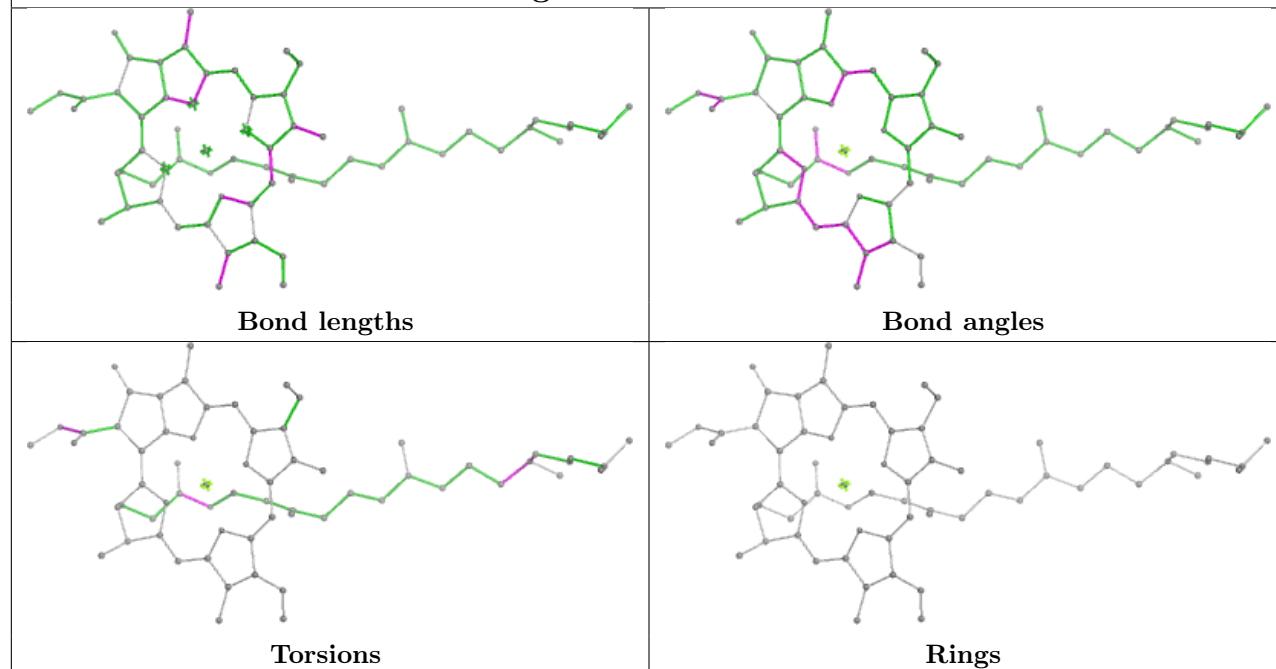




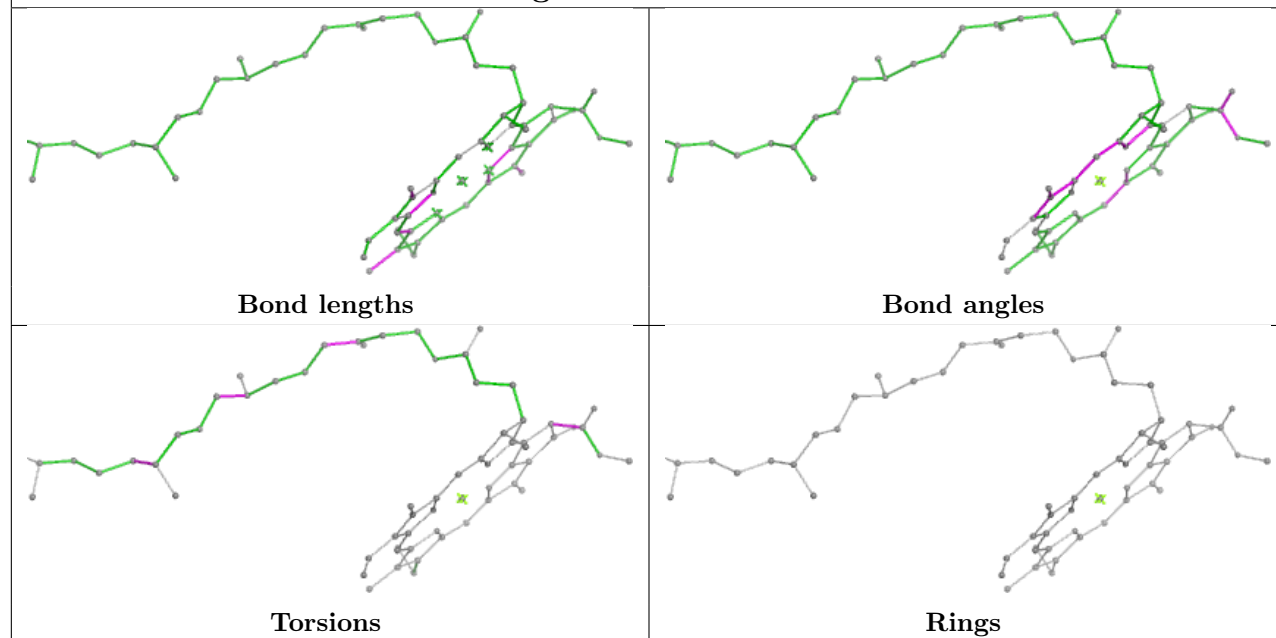


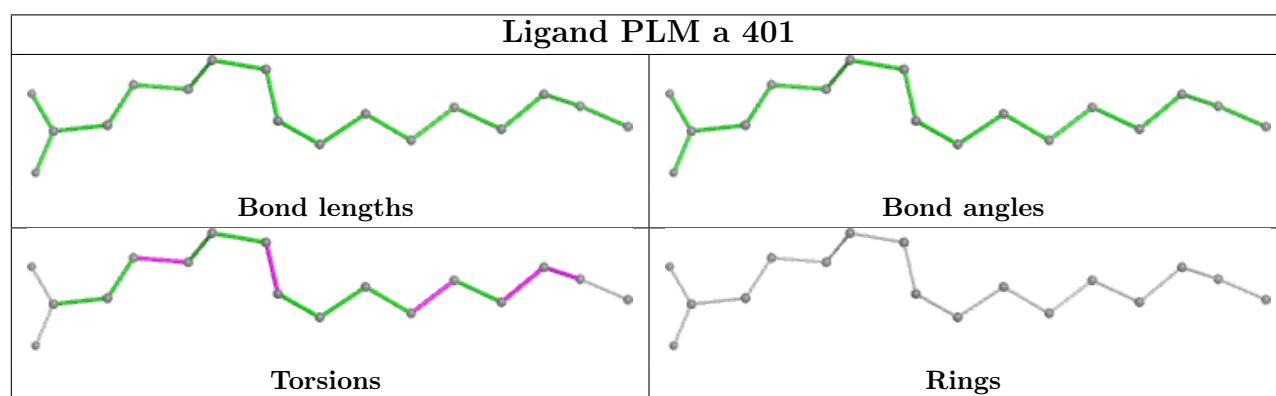
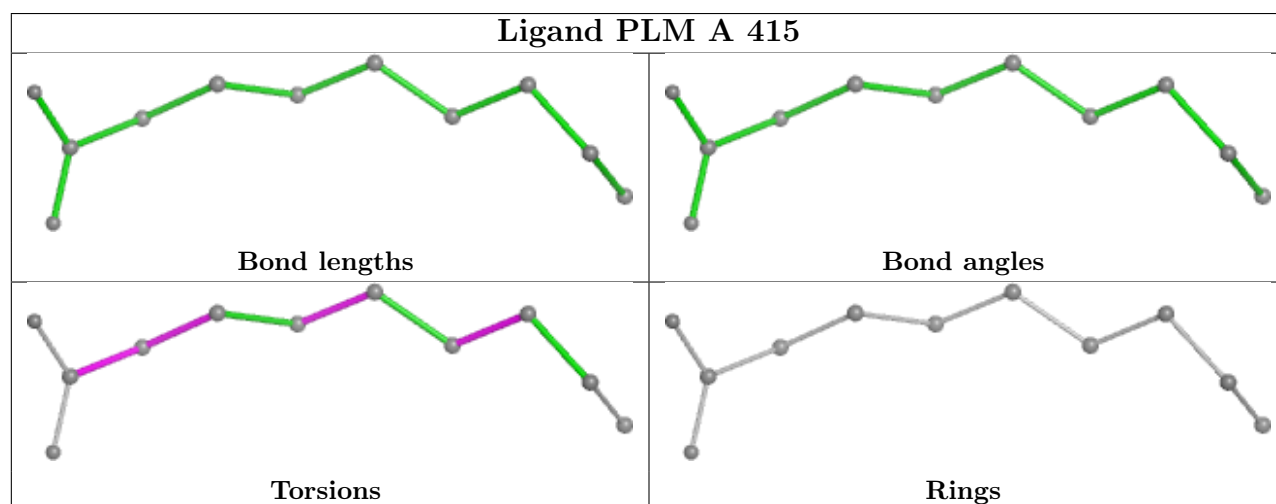
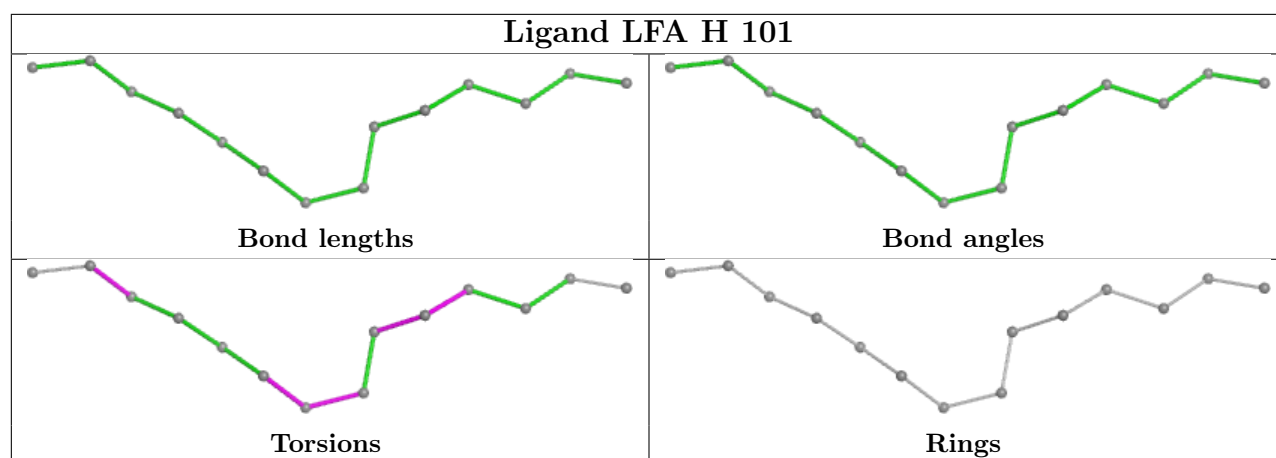


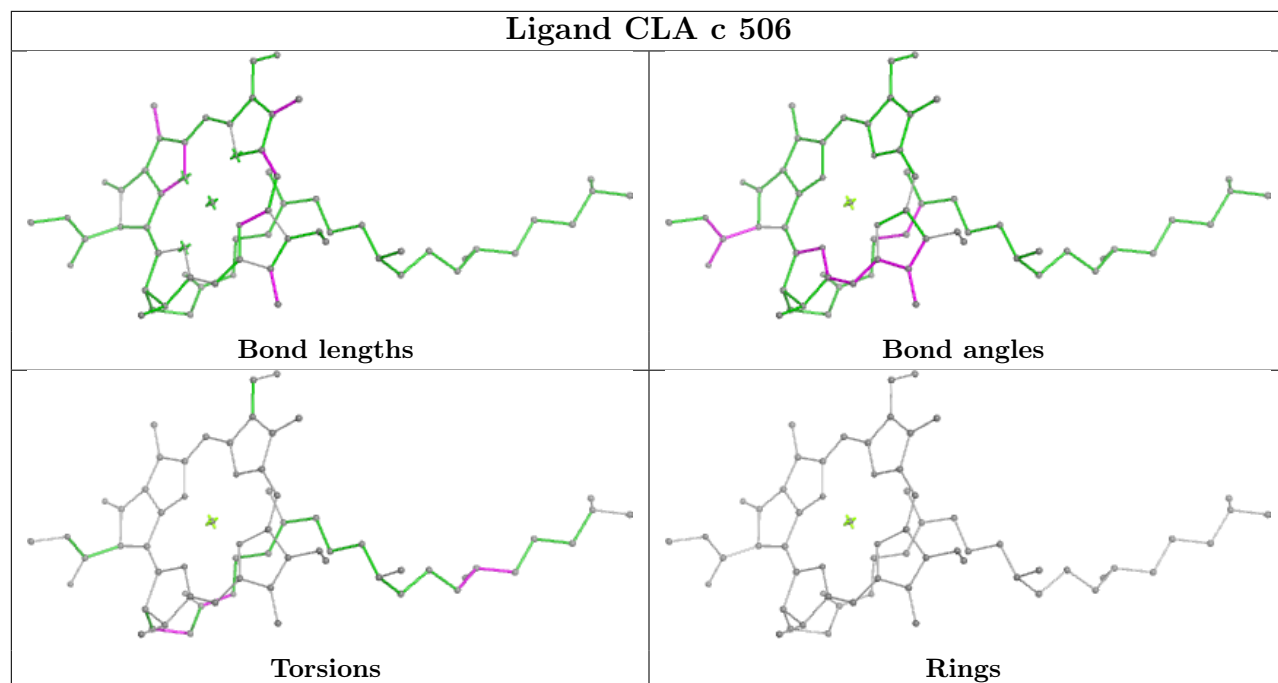
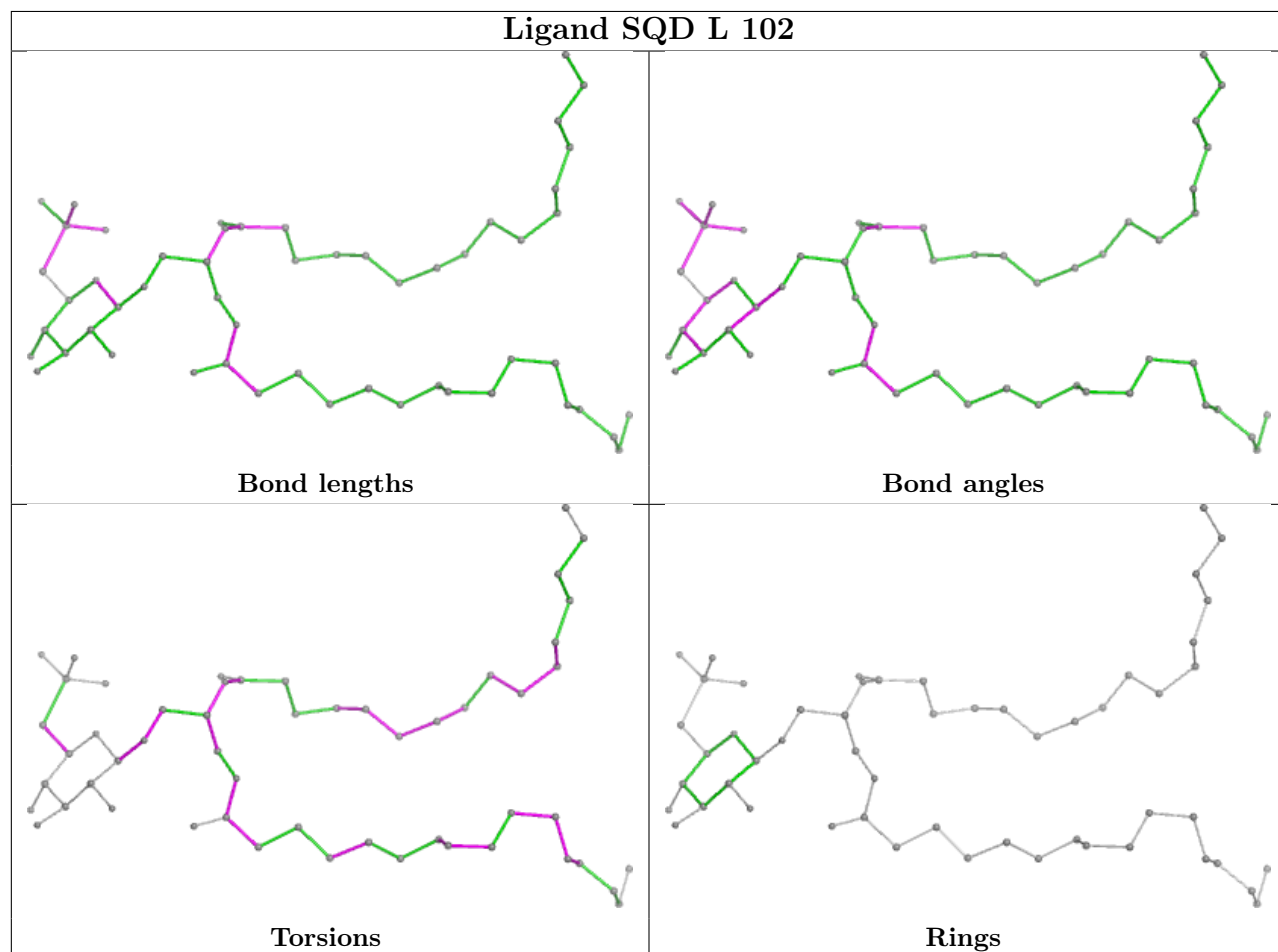
## Ligand CLA B 608



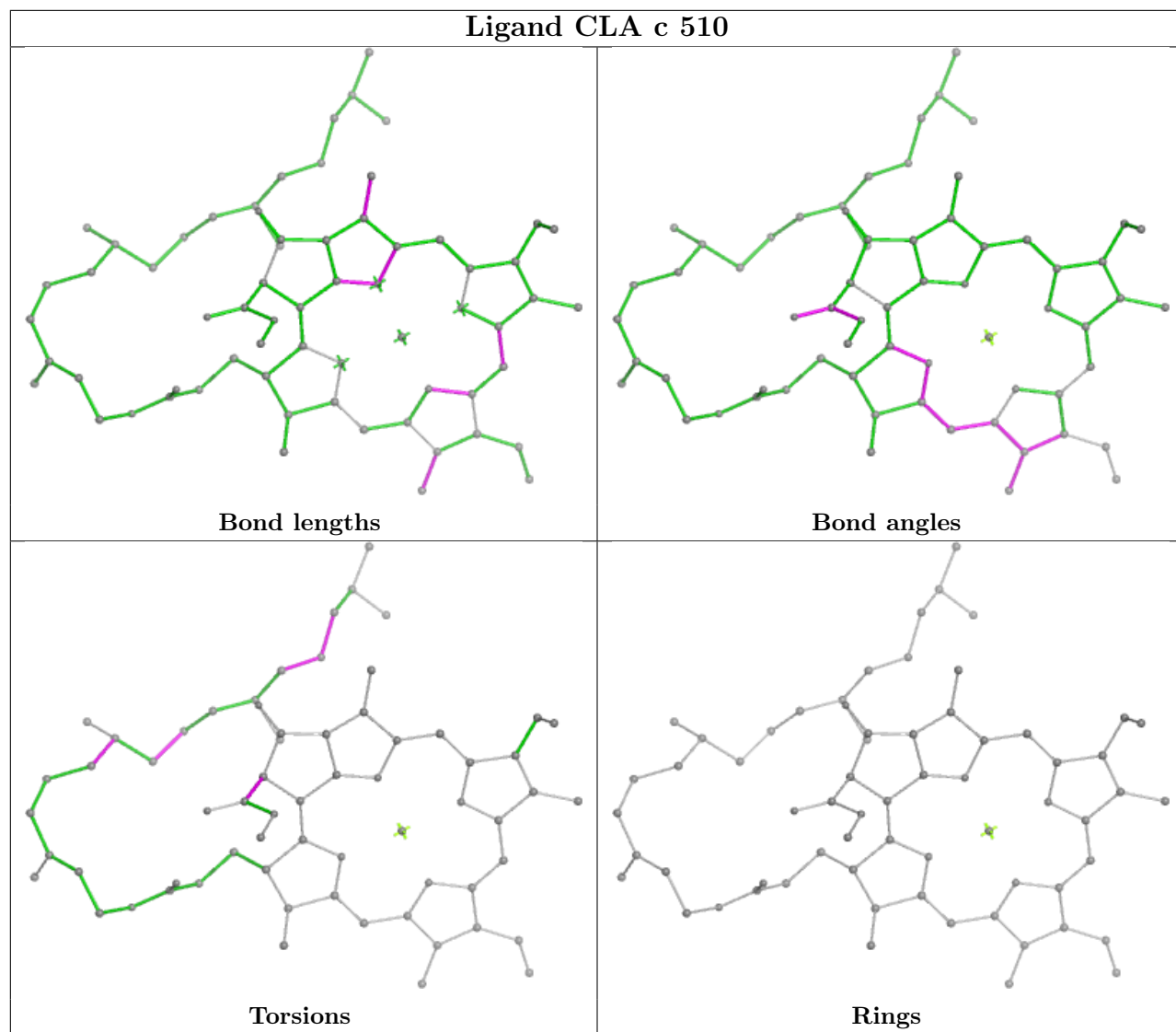
## Ligand CLA C 506

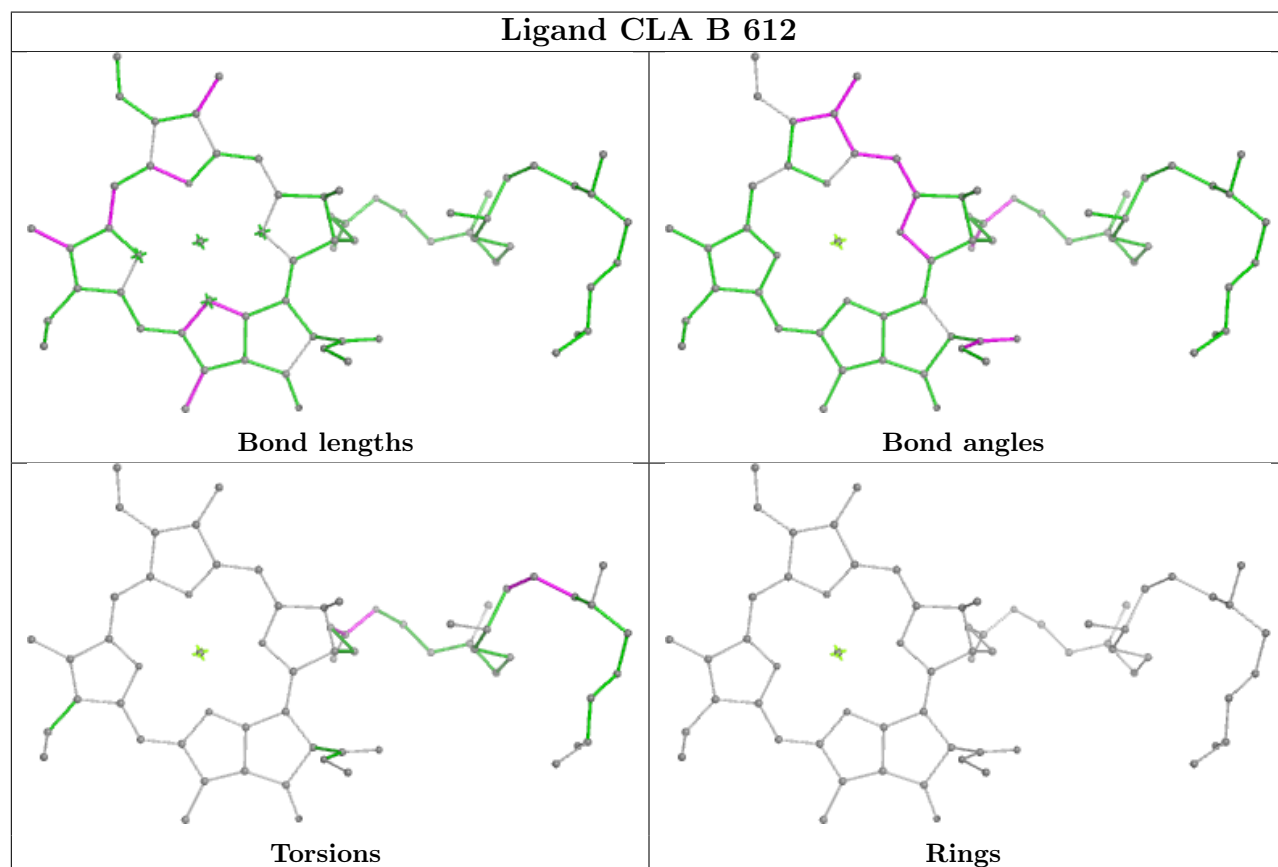
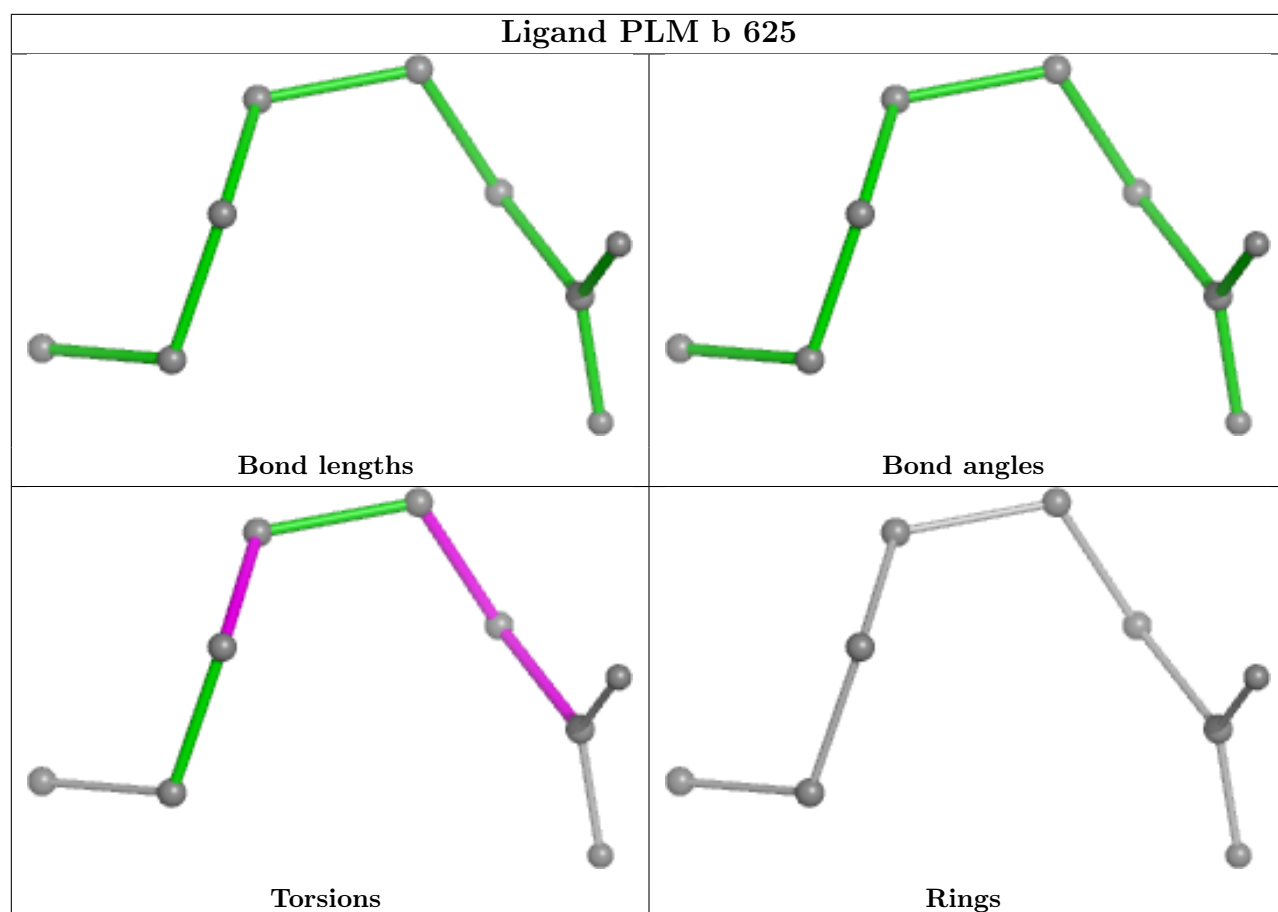




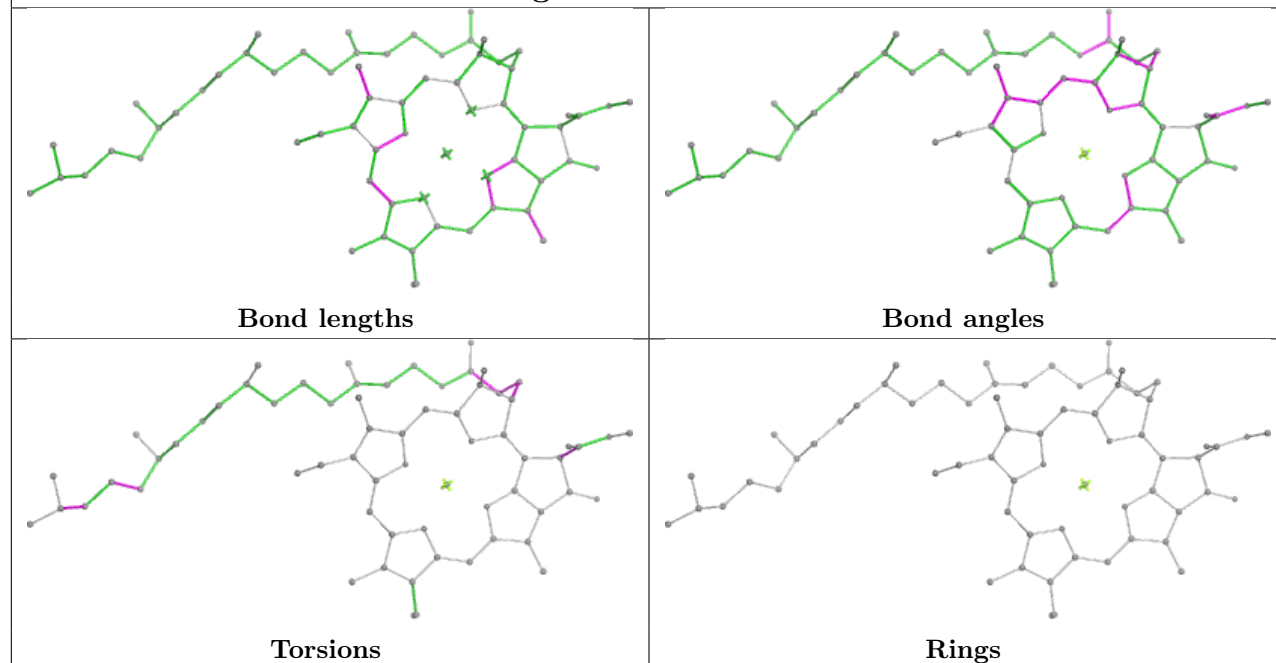
**Ligand CLA c 506****Ligand SQD L 102**

## Ligand CLA c 510

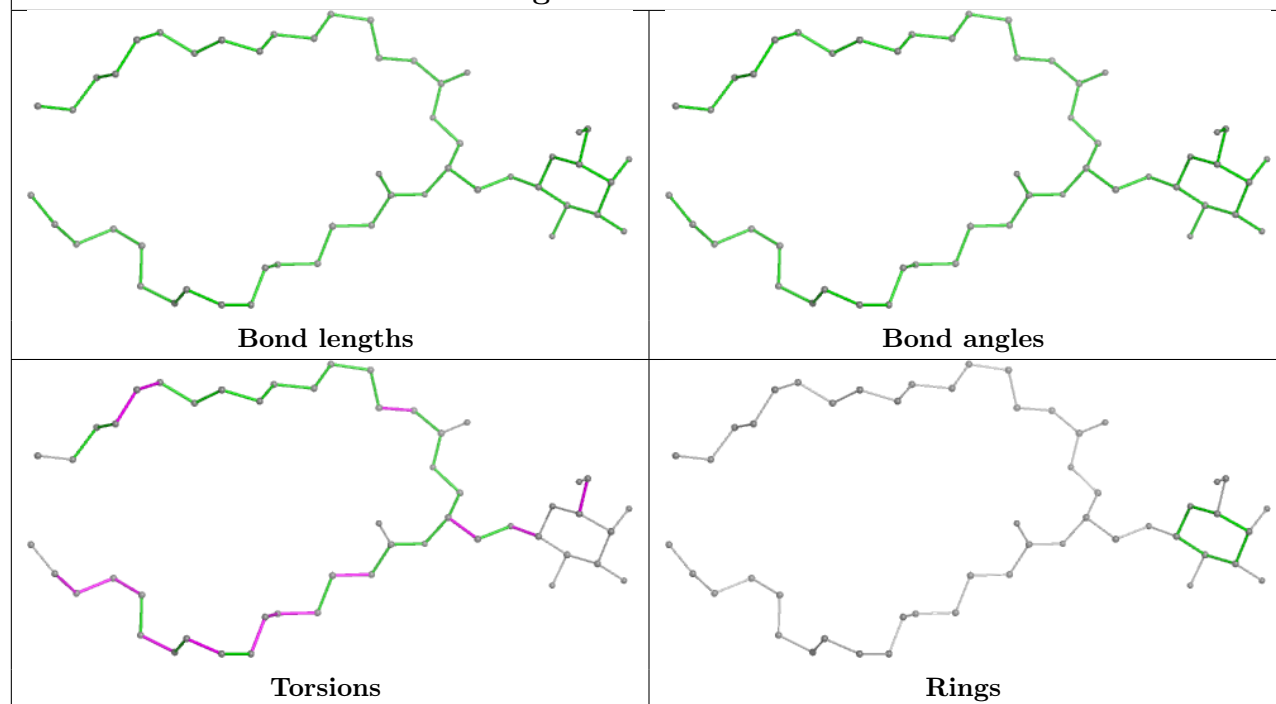




## Ligand CLA C 503

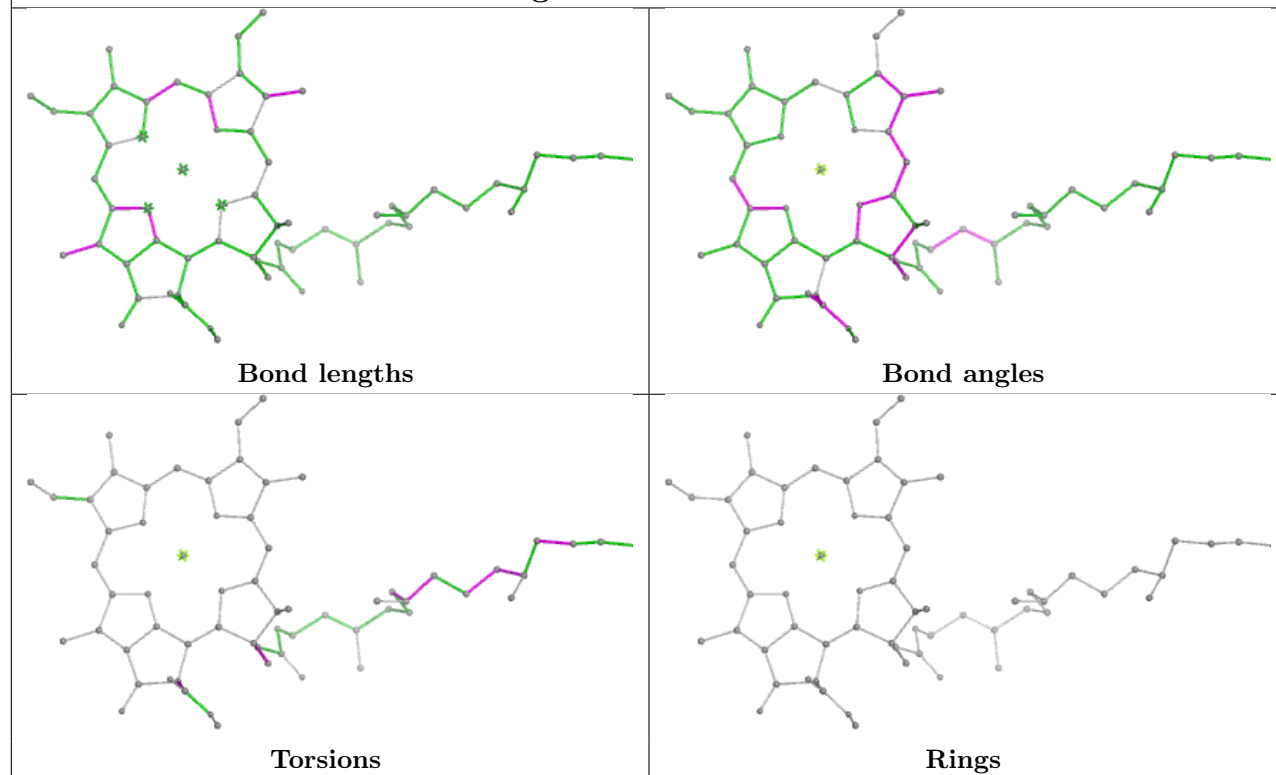


## Ligand LMG c 501

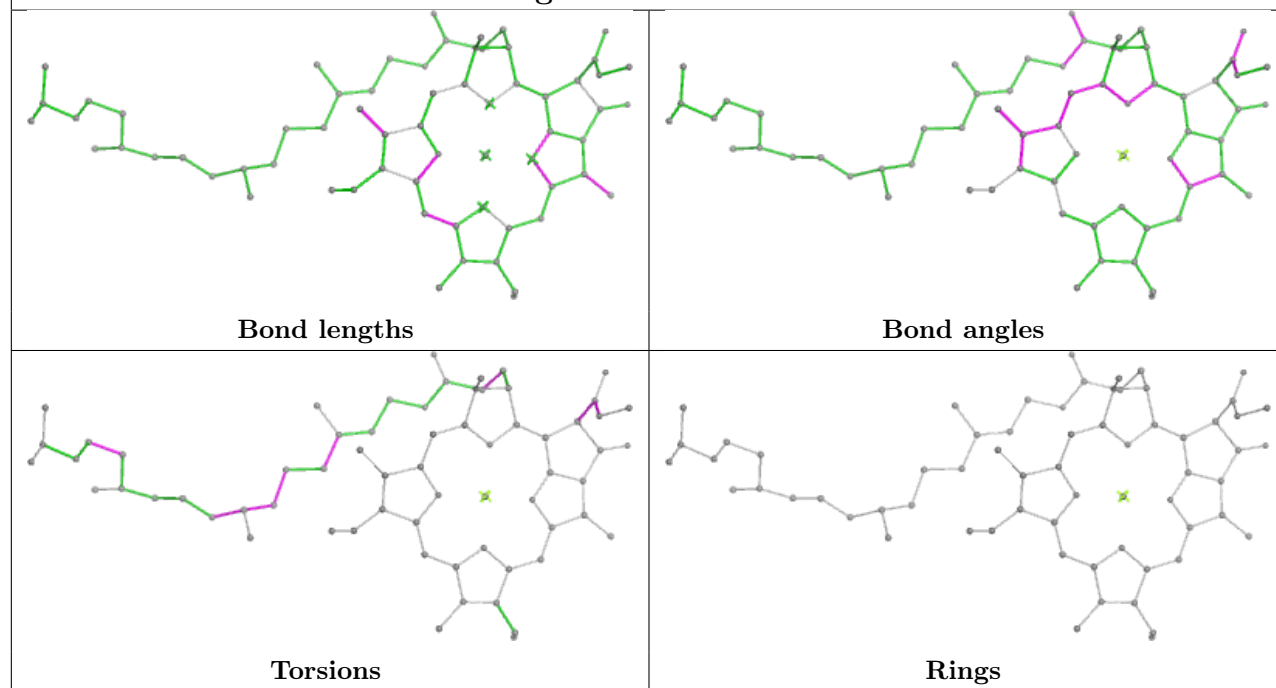


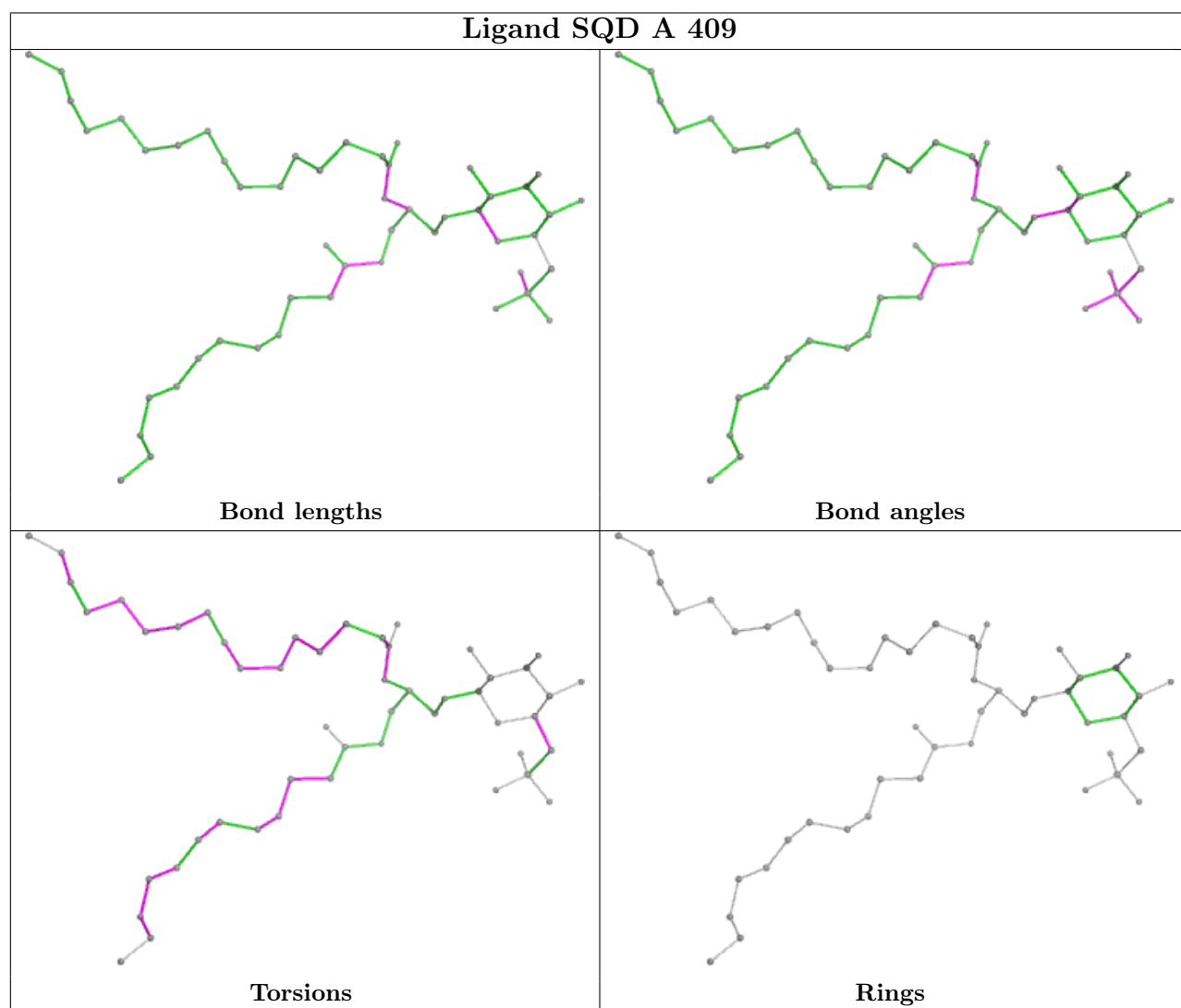
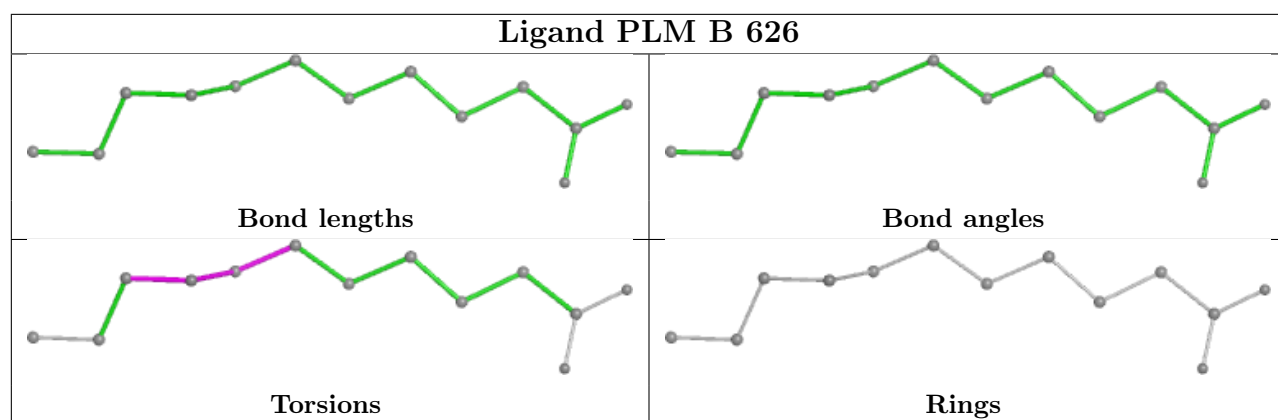


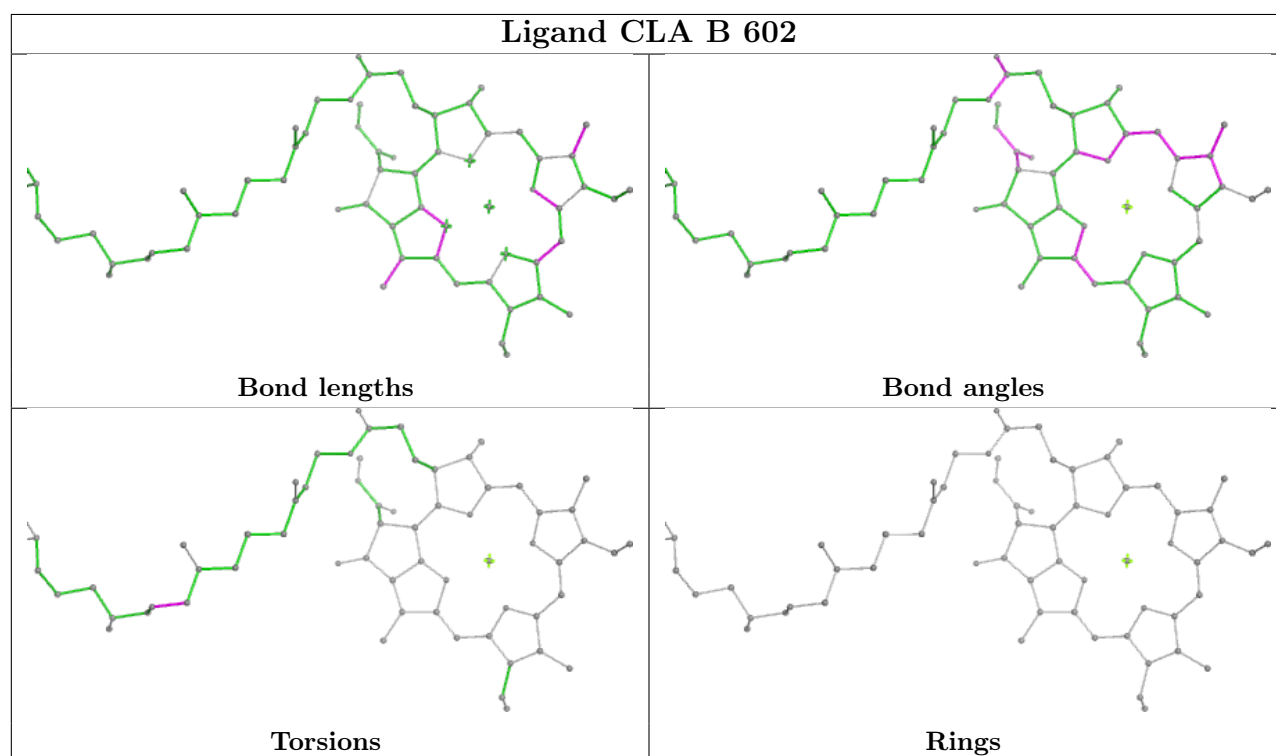
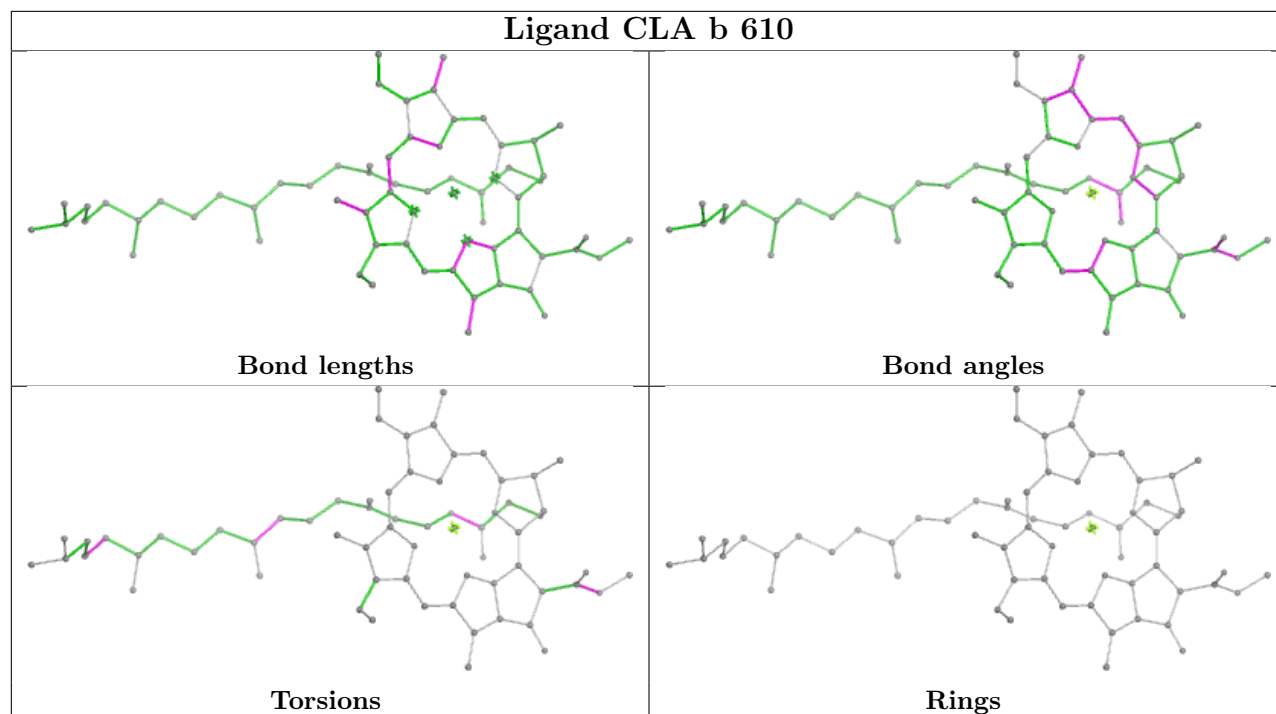
## Ligand CLA A 405

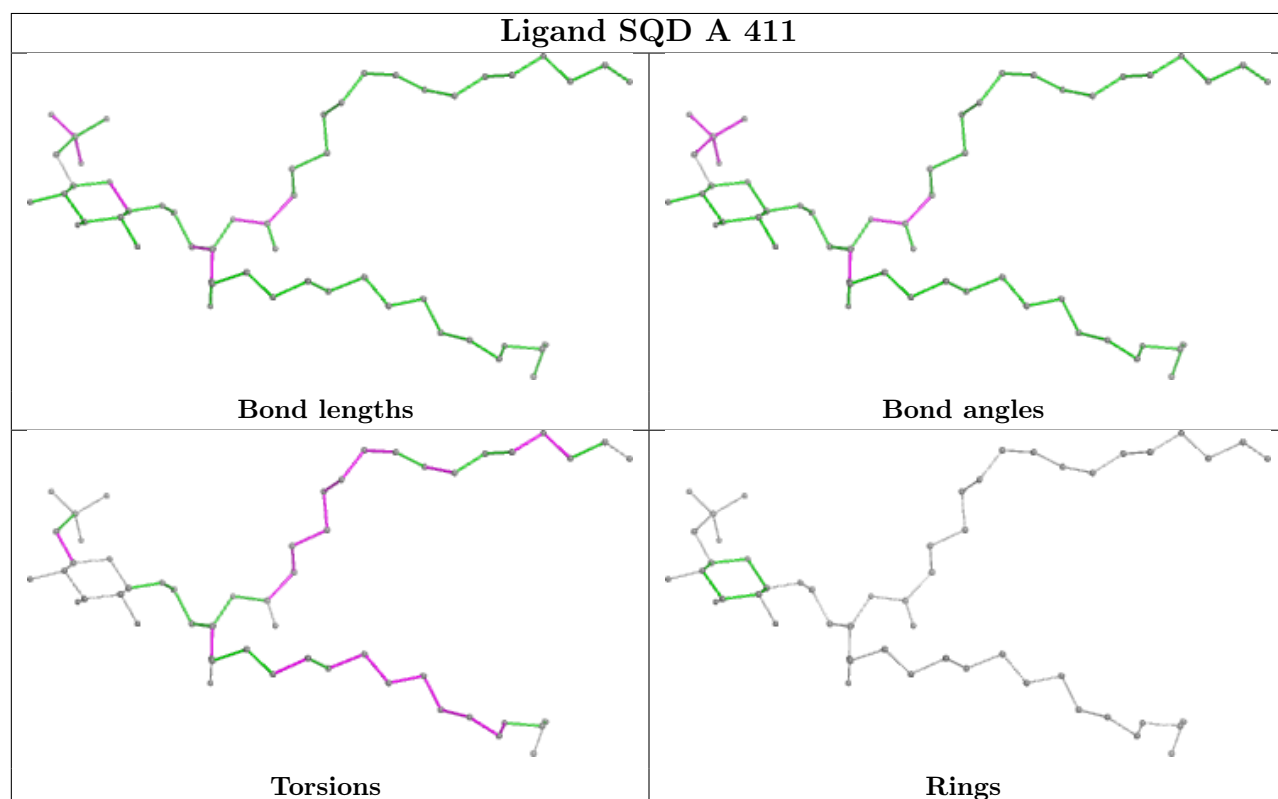
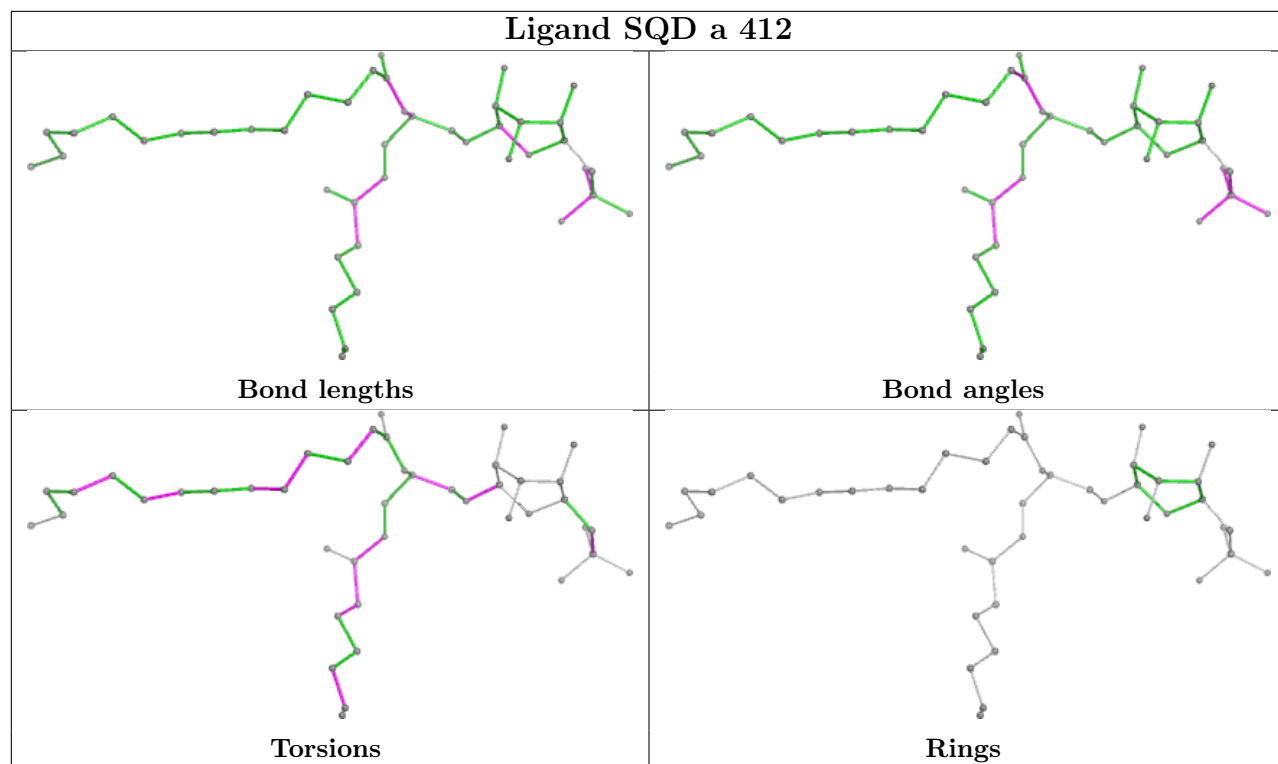


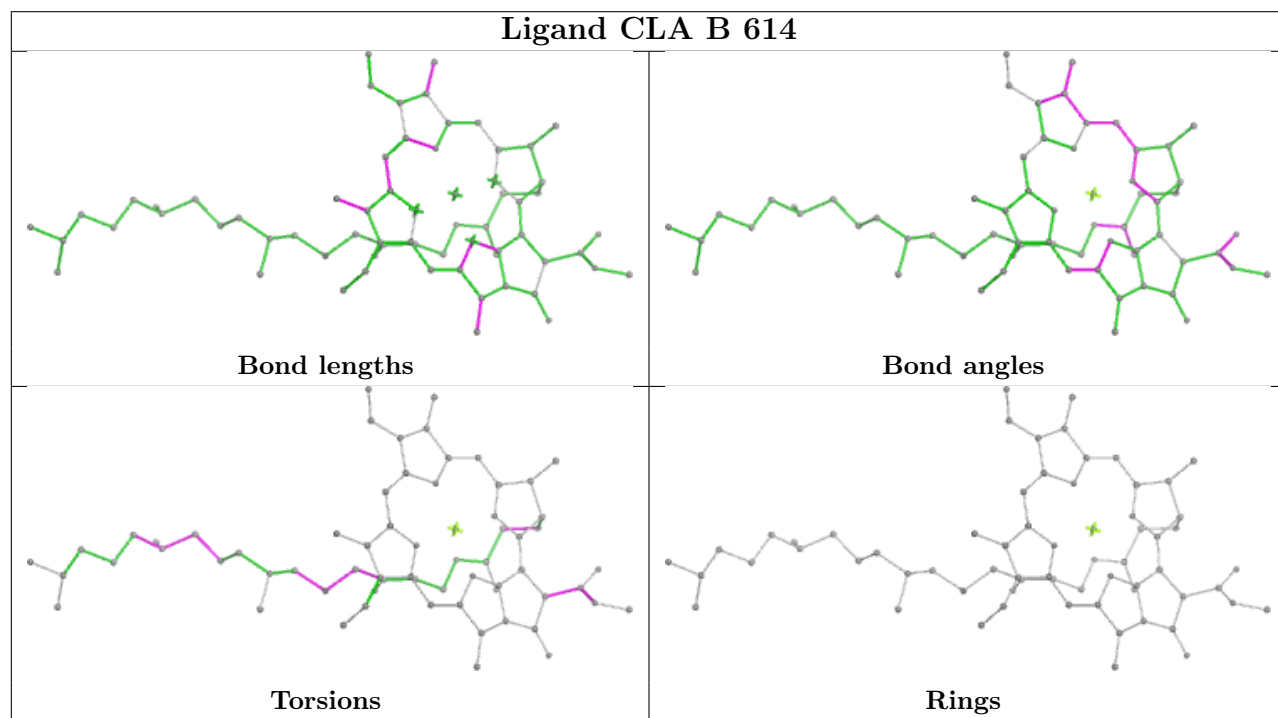
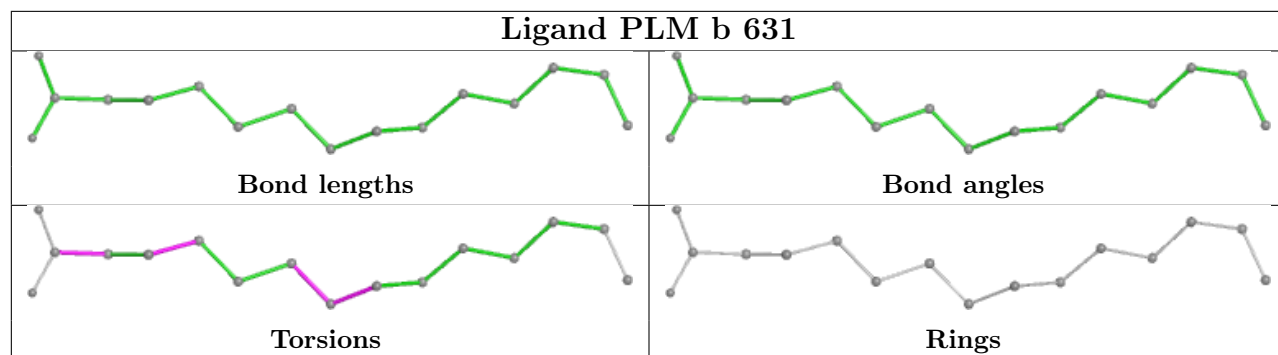
## Ligand CLA b 605



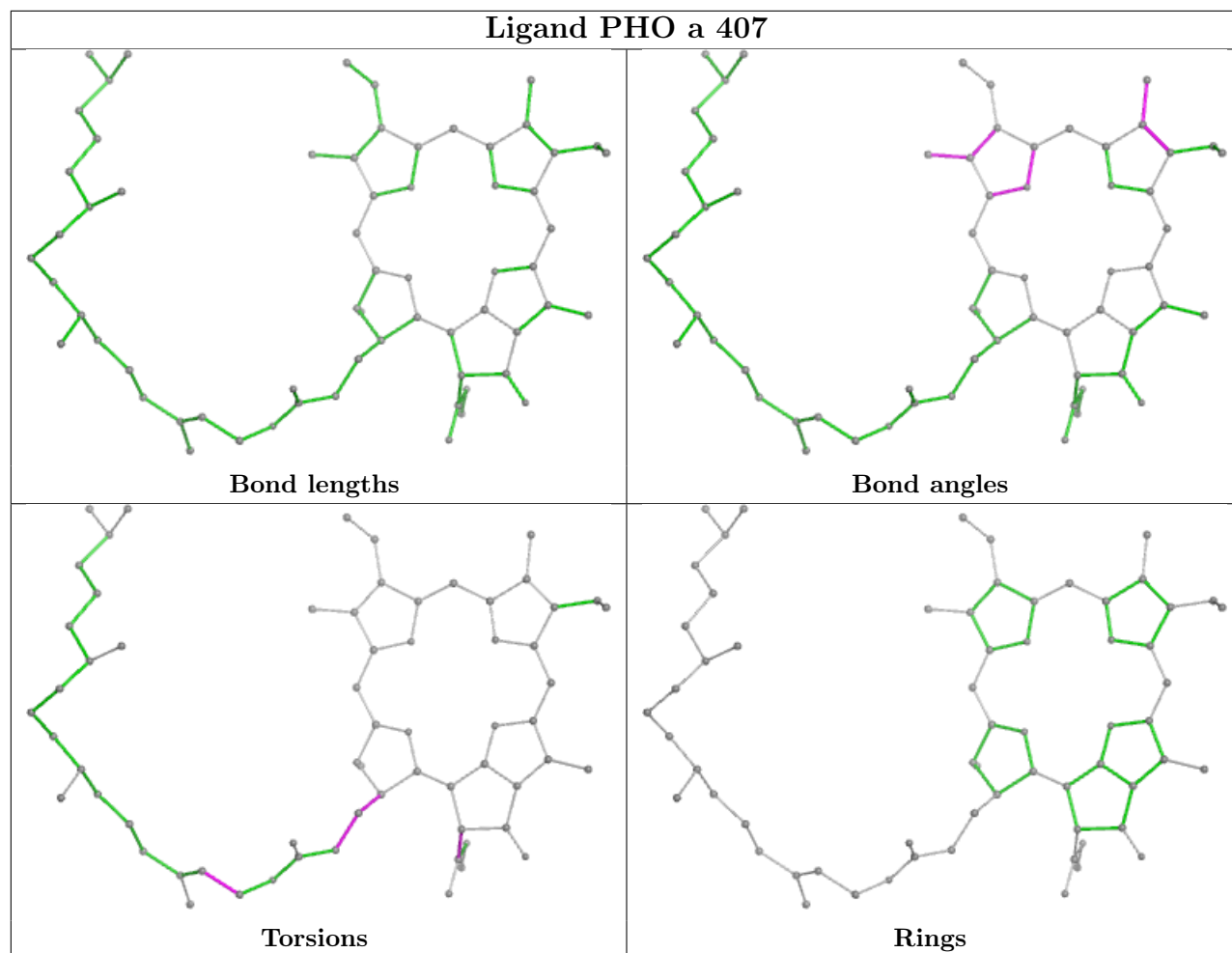




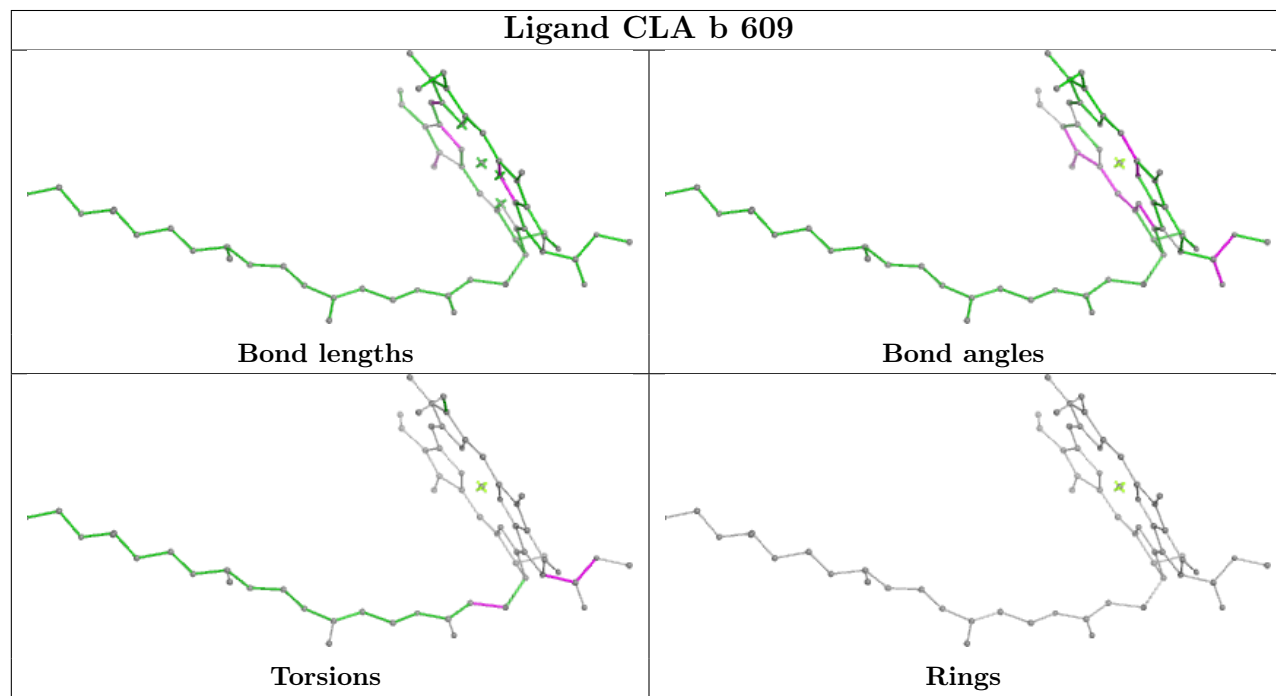


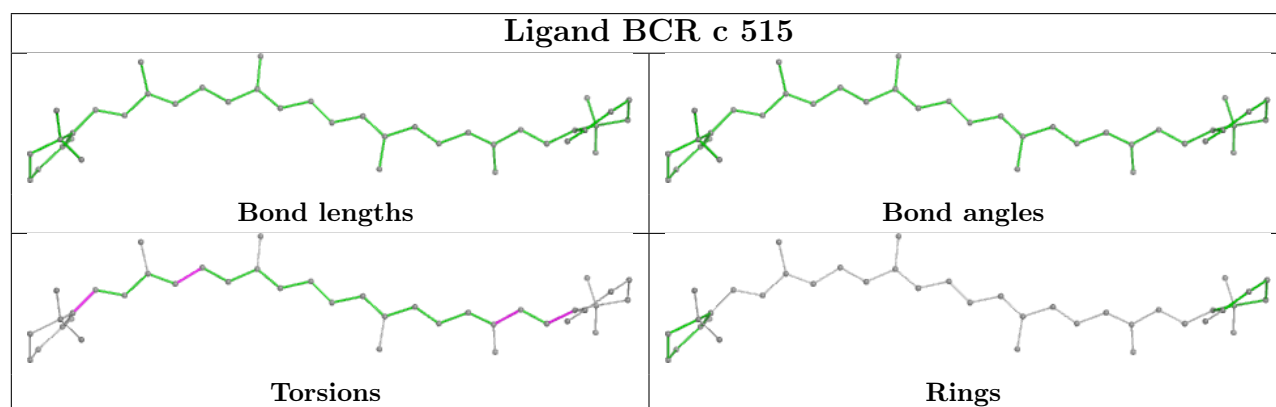
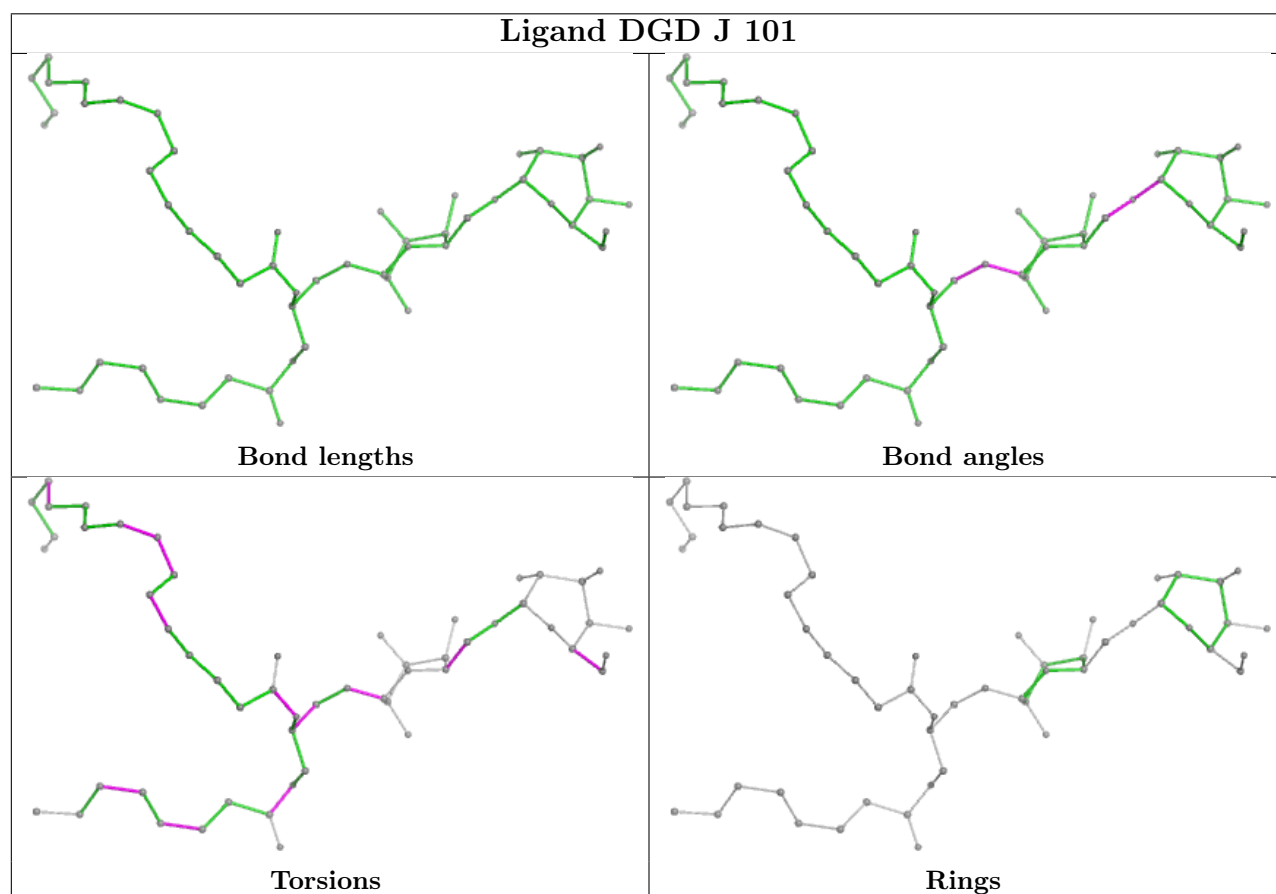
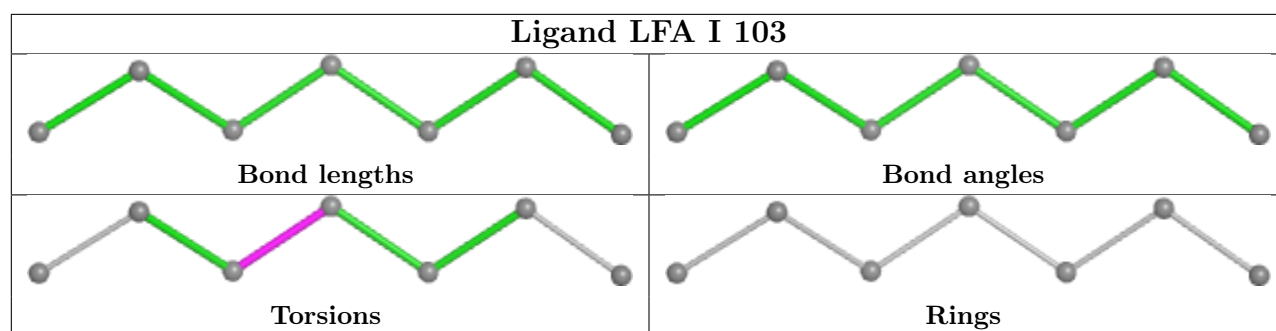


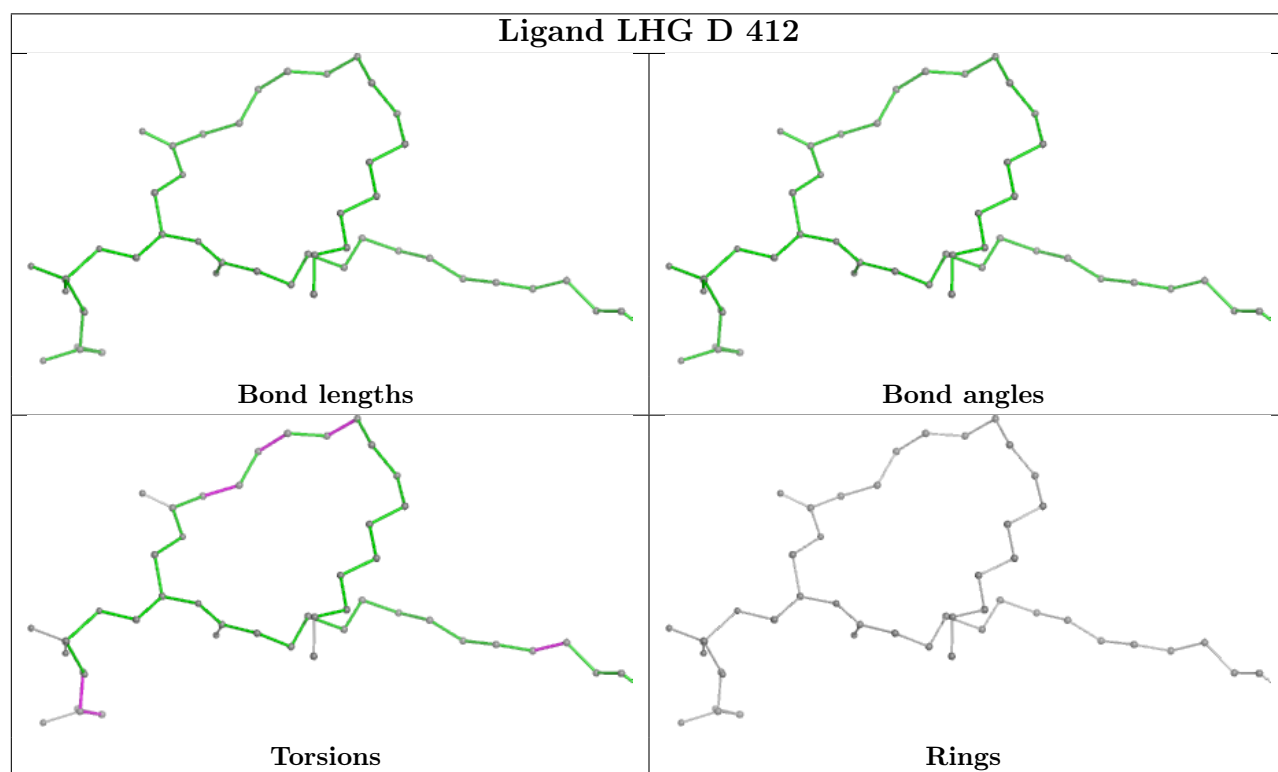
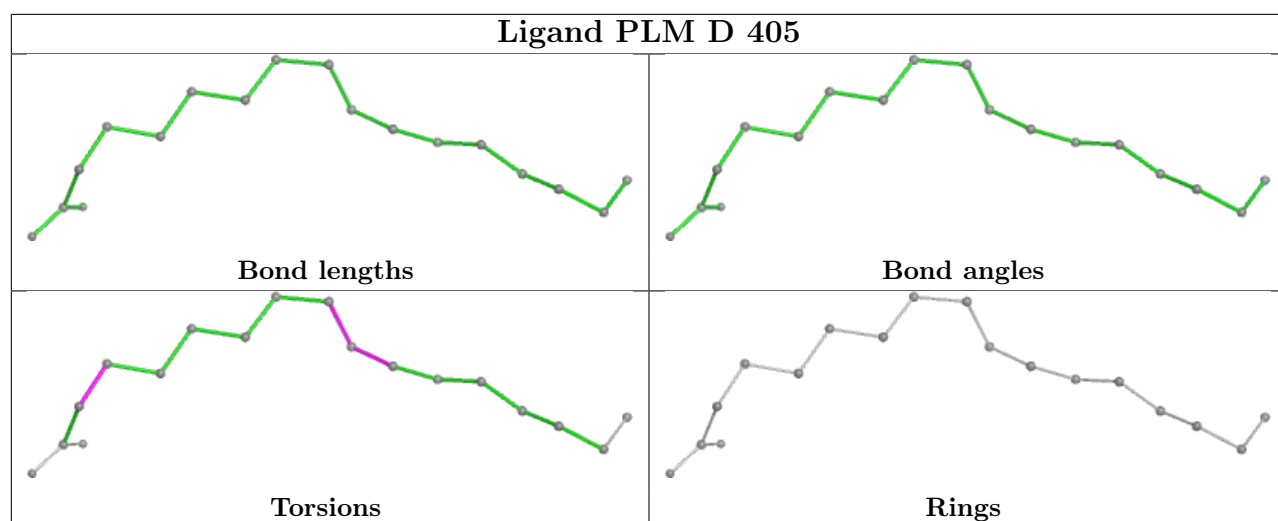
## Ligand PHO a 407



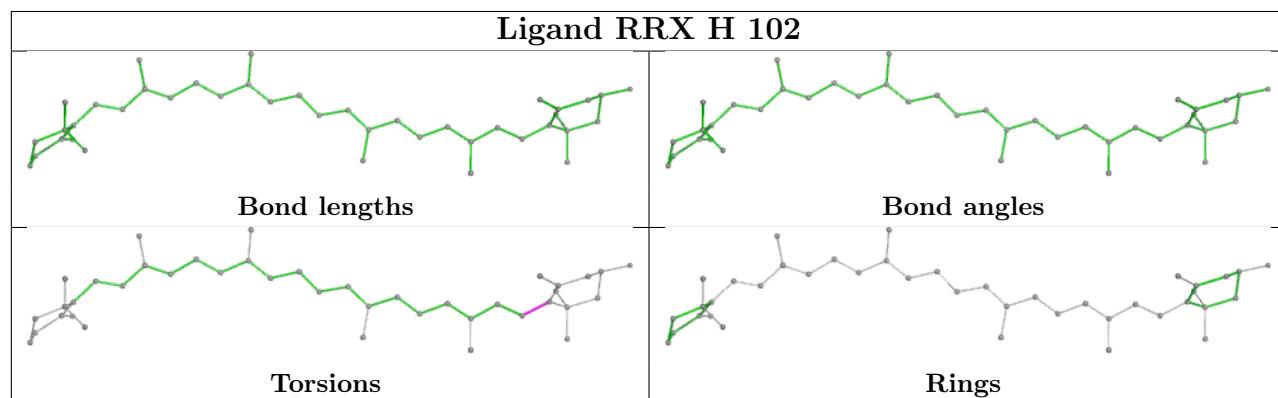
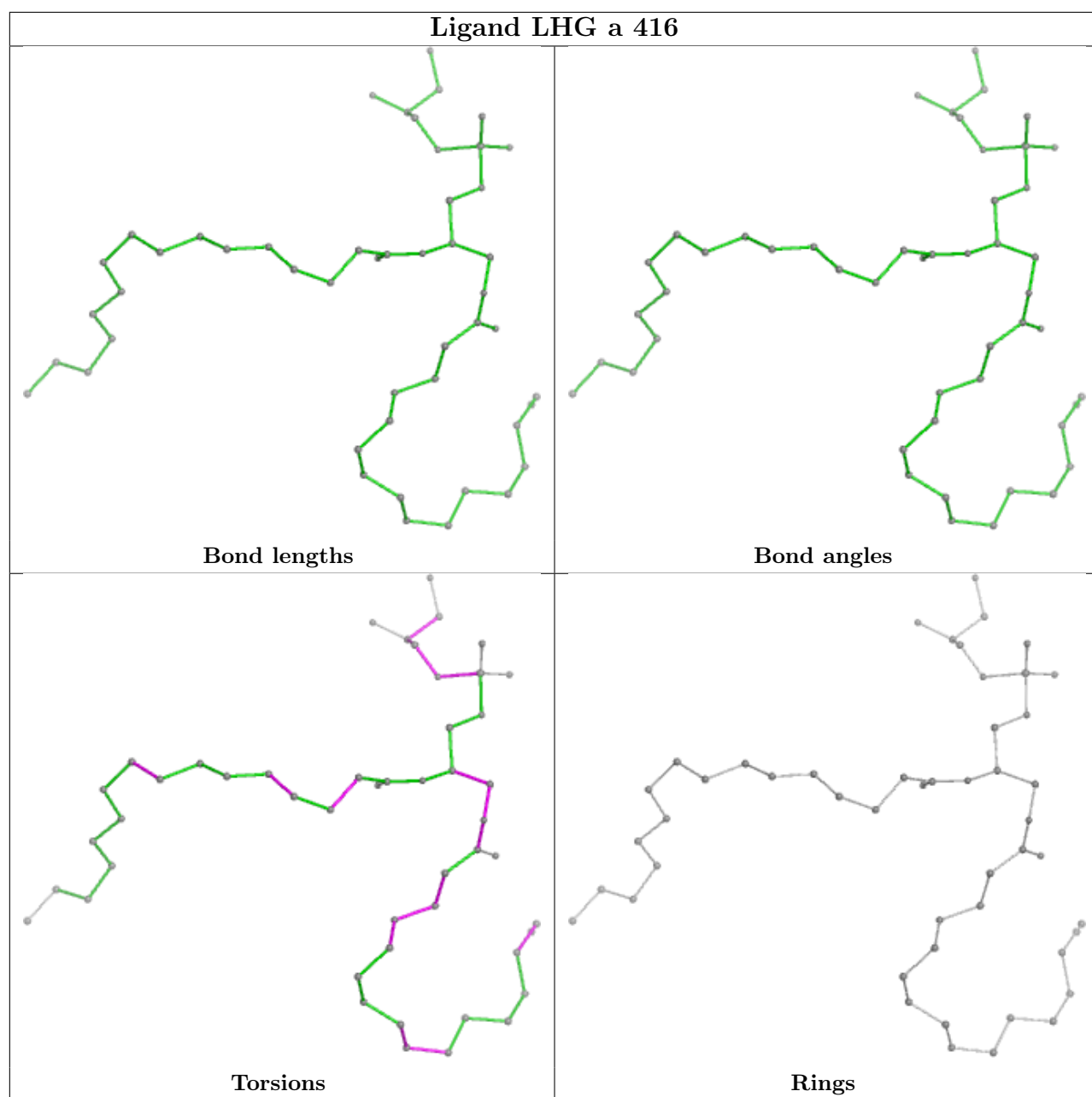
## Ligand CLA b 609

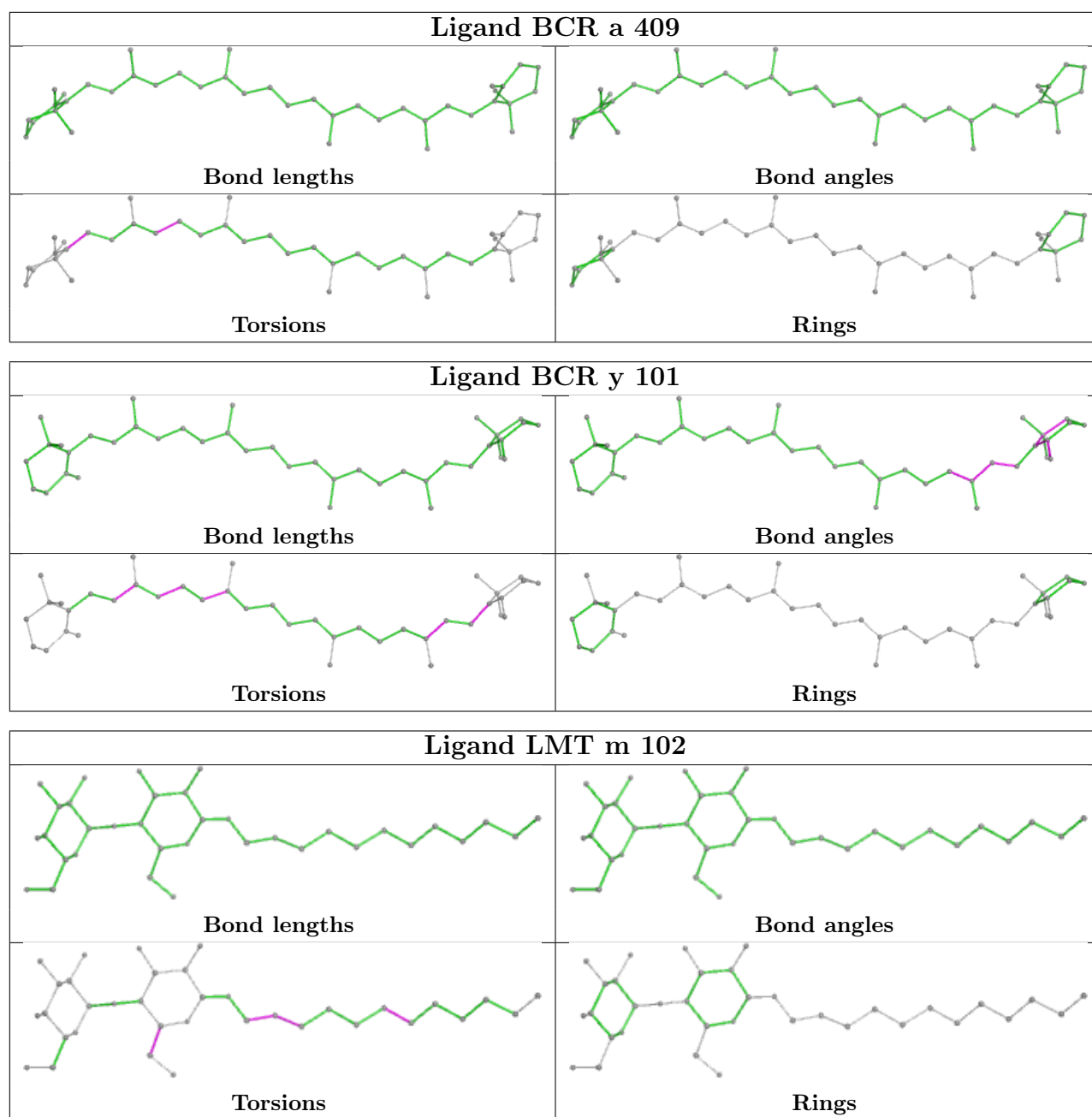




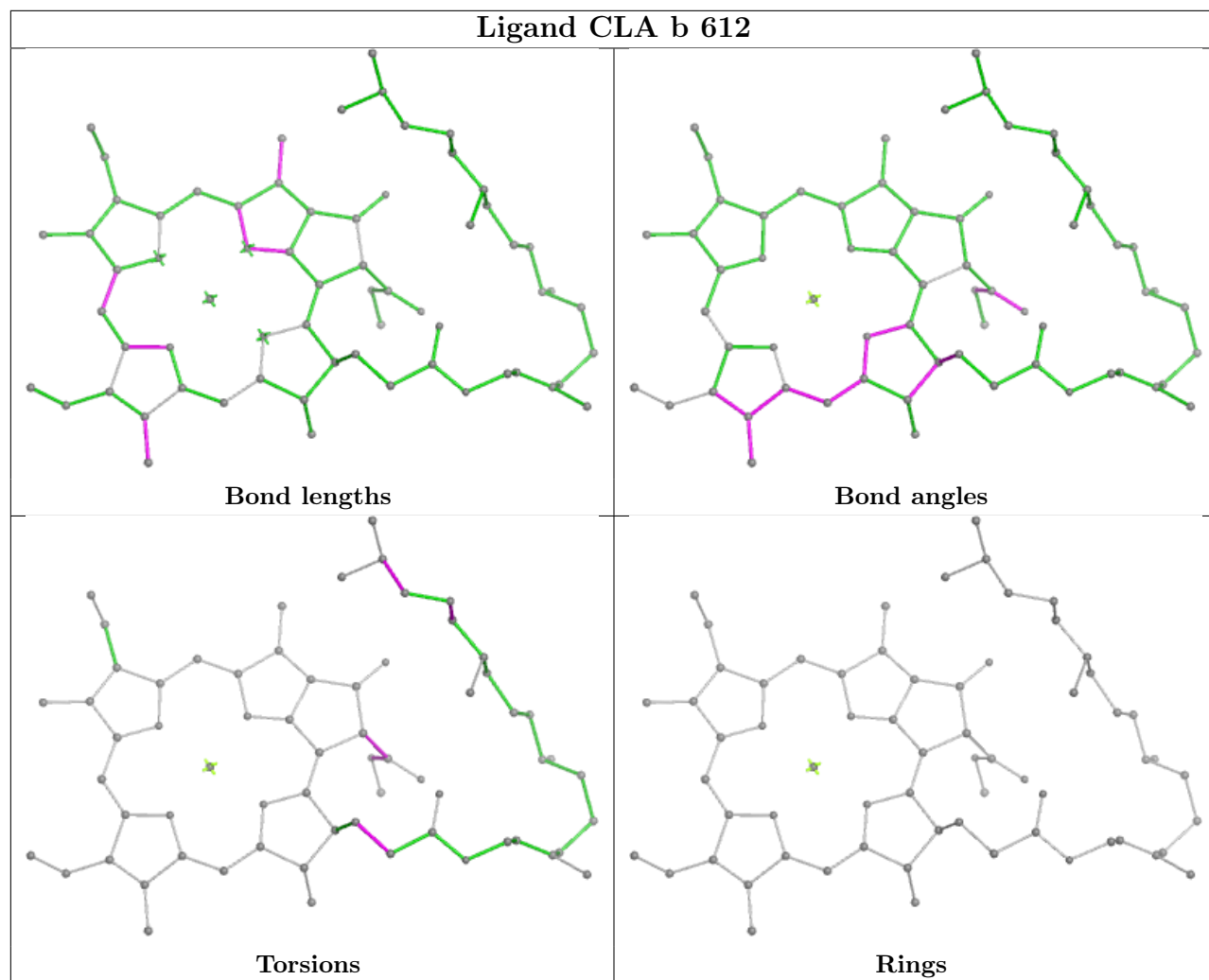


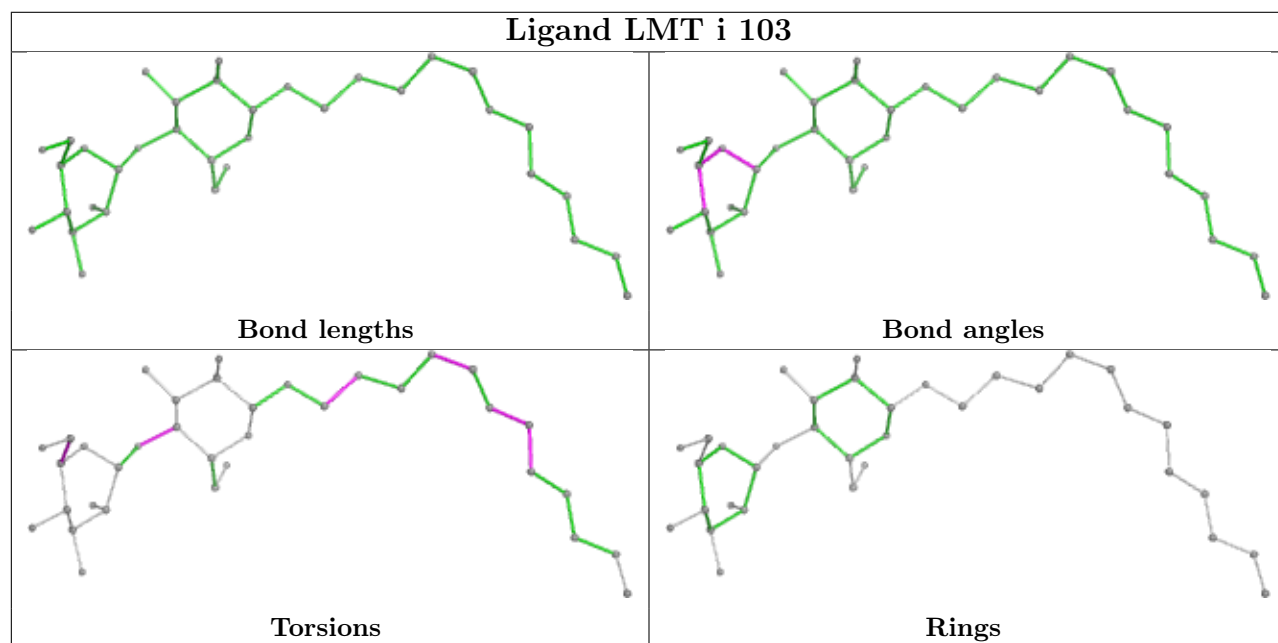
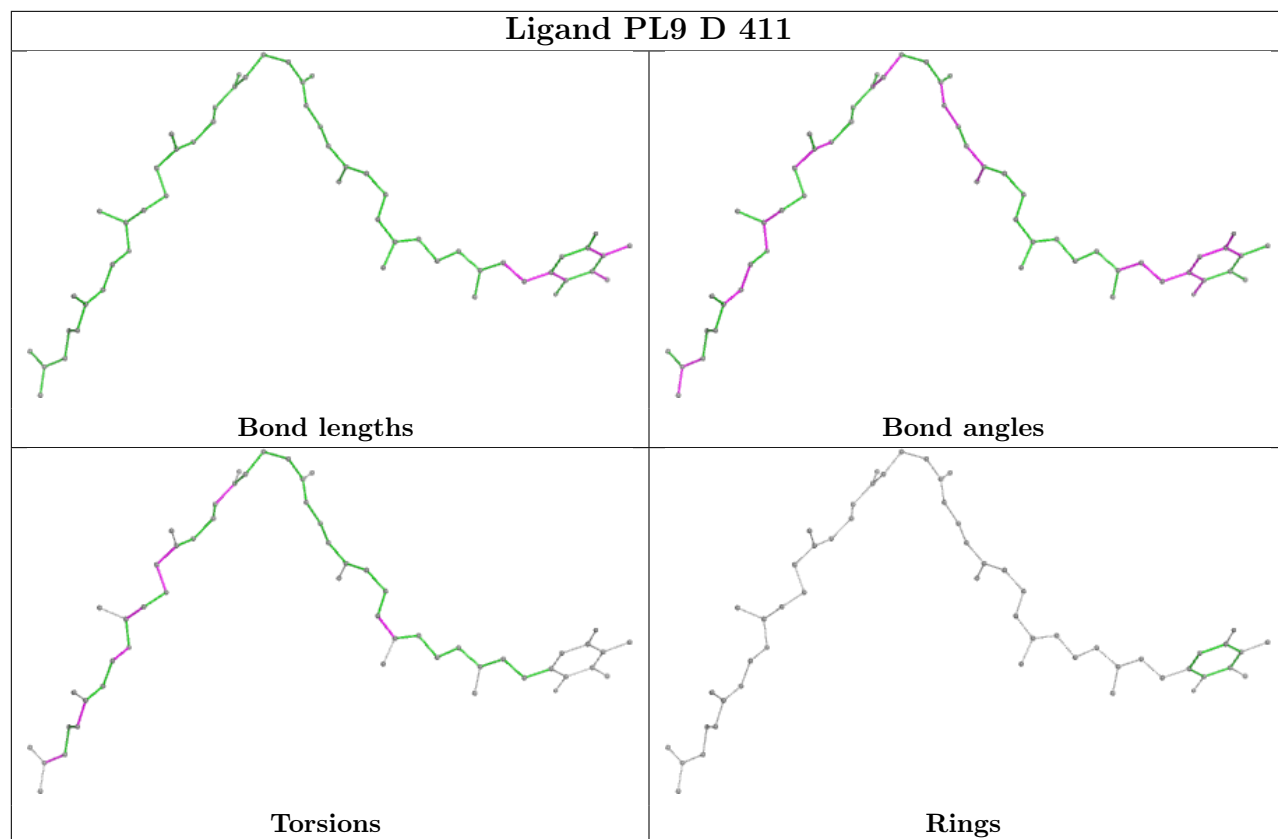


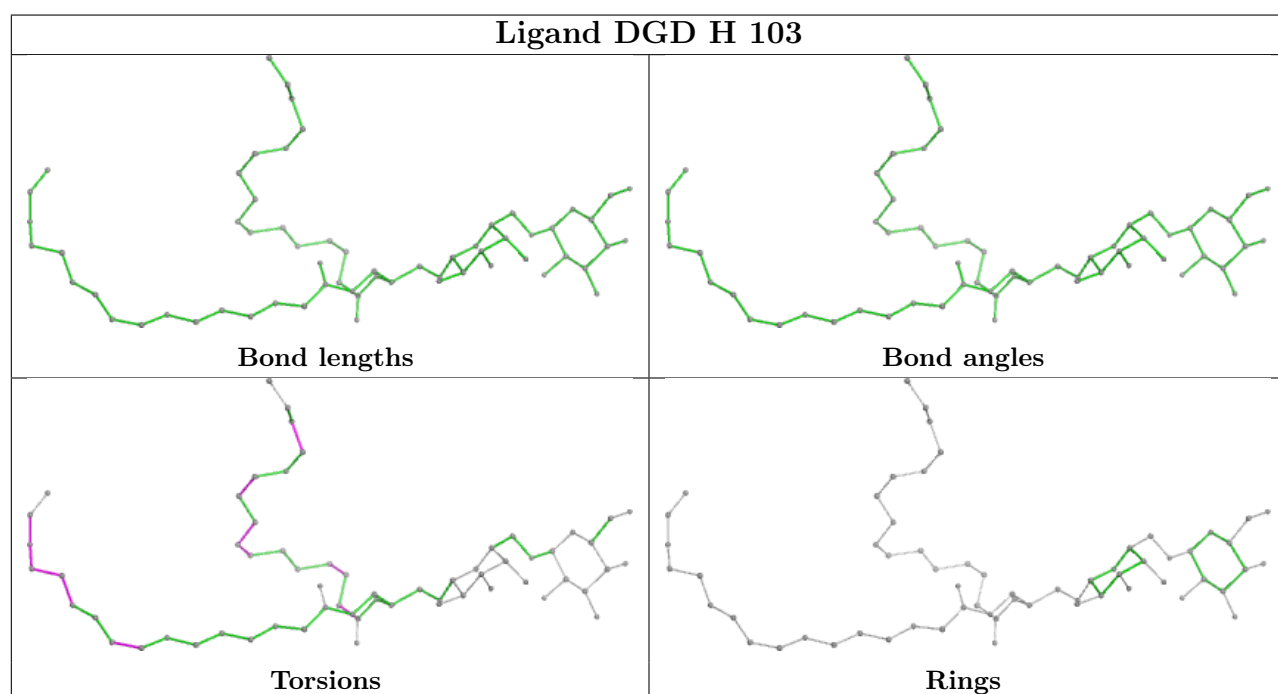
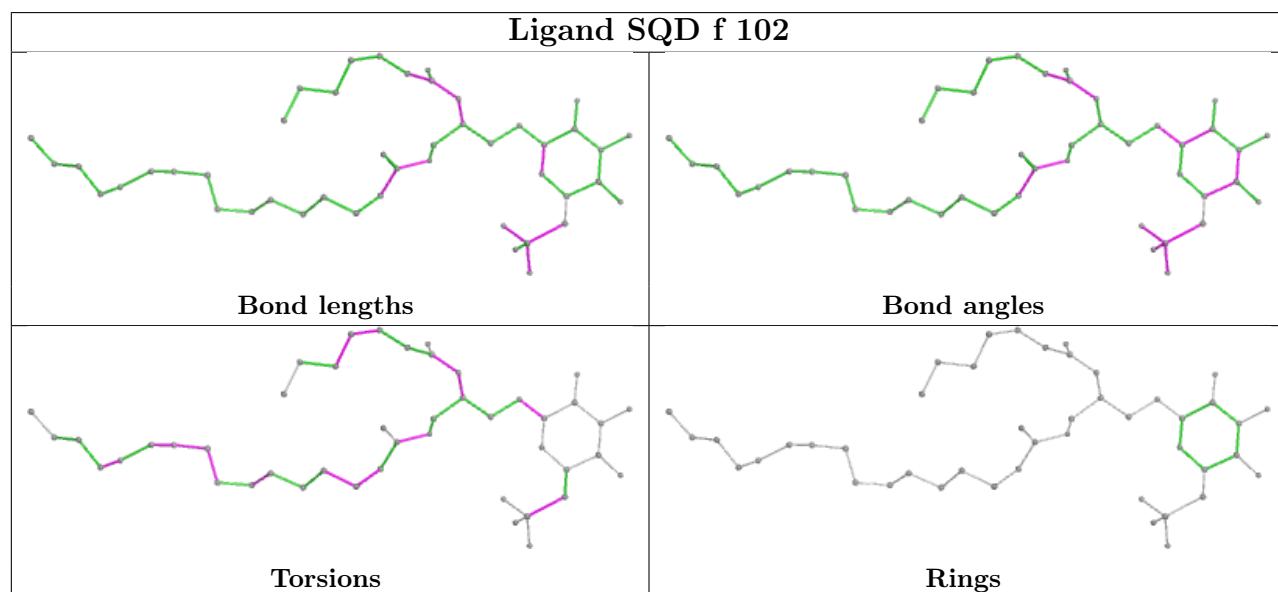
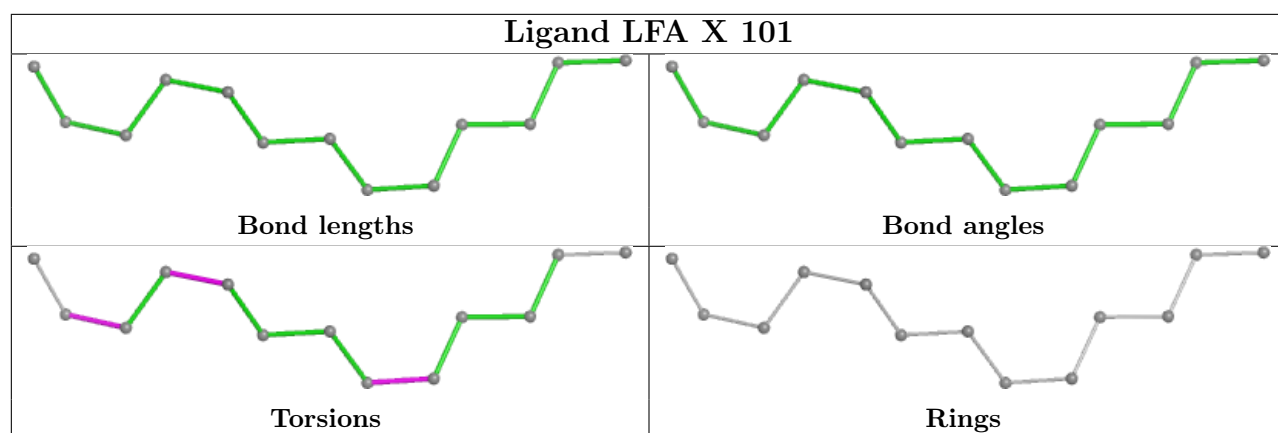




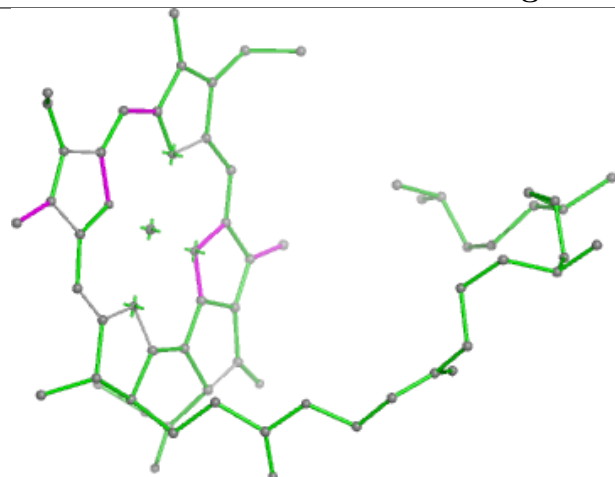
## Ligand CLA b 612



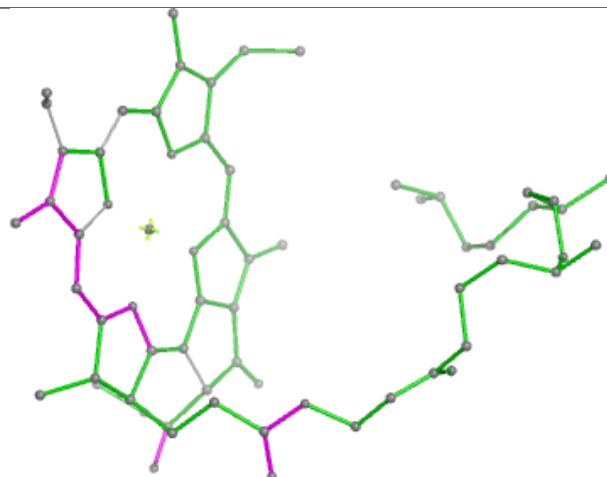




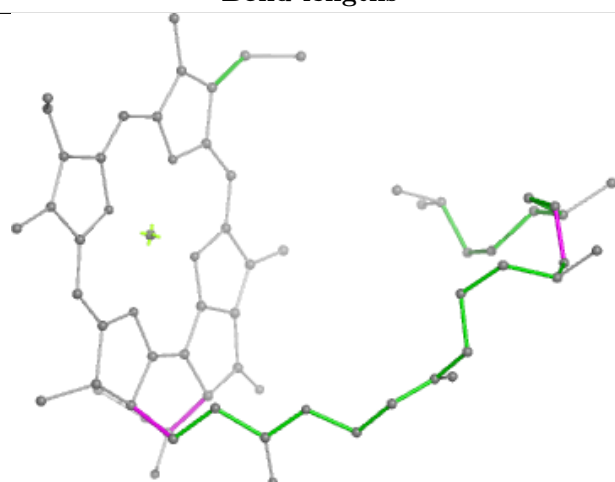
## Ligand CLA c 504



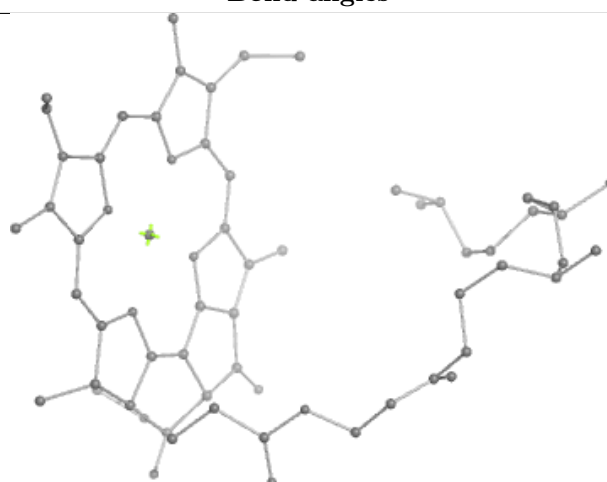
Bond lengths



Bond angles

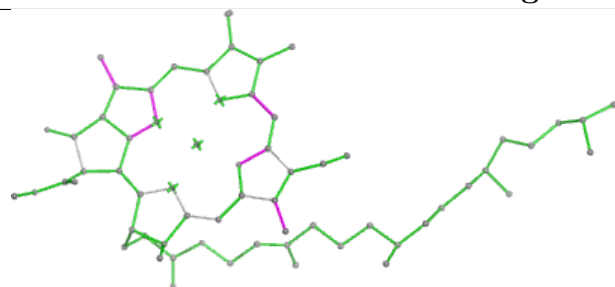


Torsions

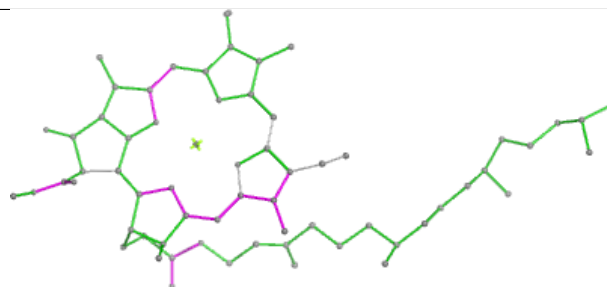


Rings

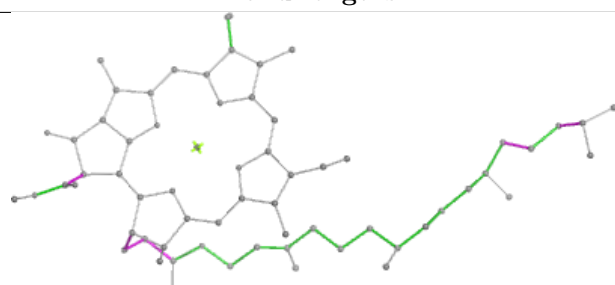
## Ligand CLA c 502



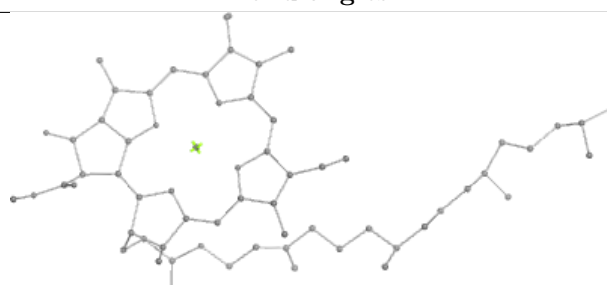
Bond lengths



Bond angles

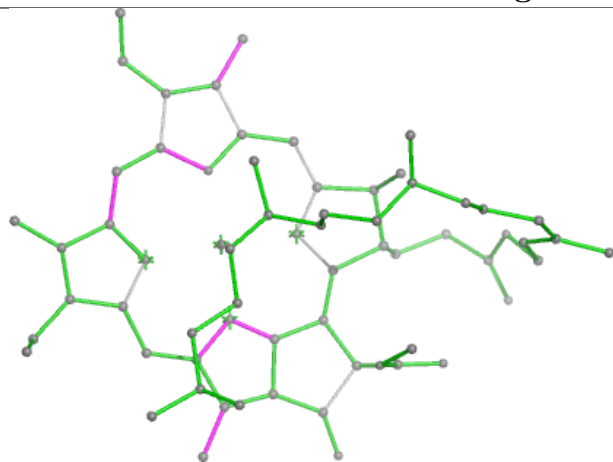


Torsions

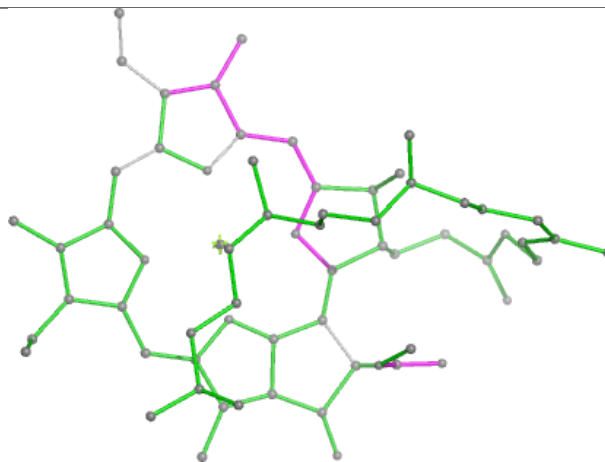


Rings

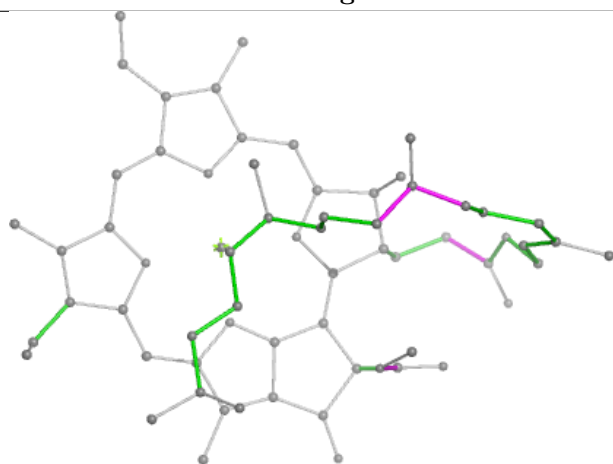
## Ligand CLA C 512



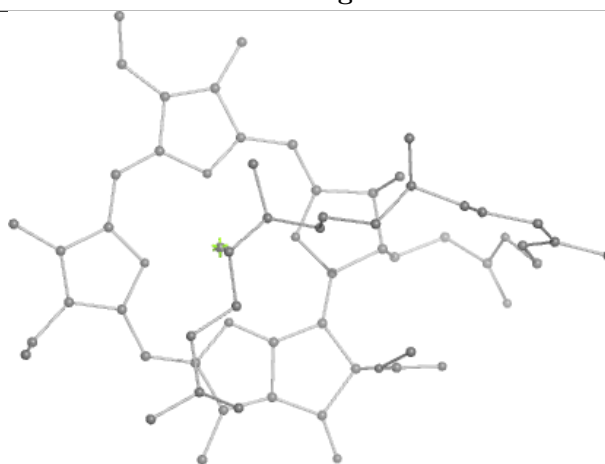
Bond lengths



Bond angles

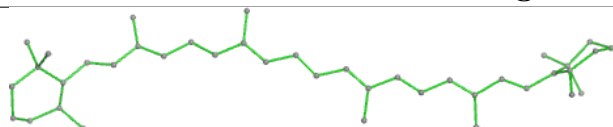


Torsions

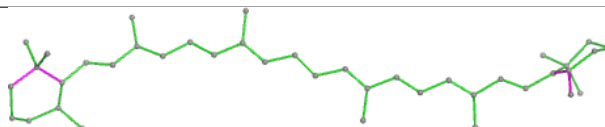


Rings

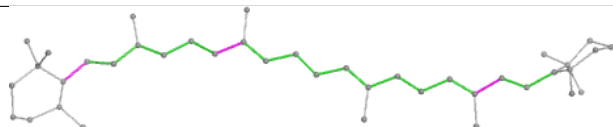
## Ligand BCR b 619



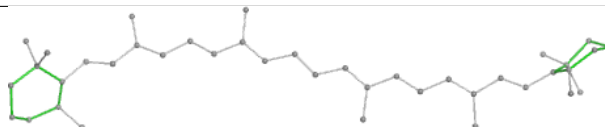
Bond lengths



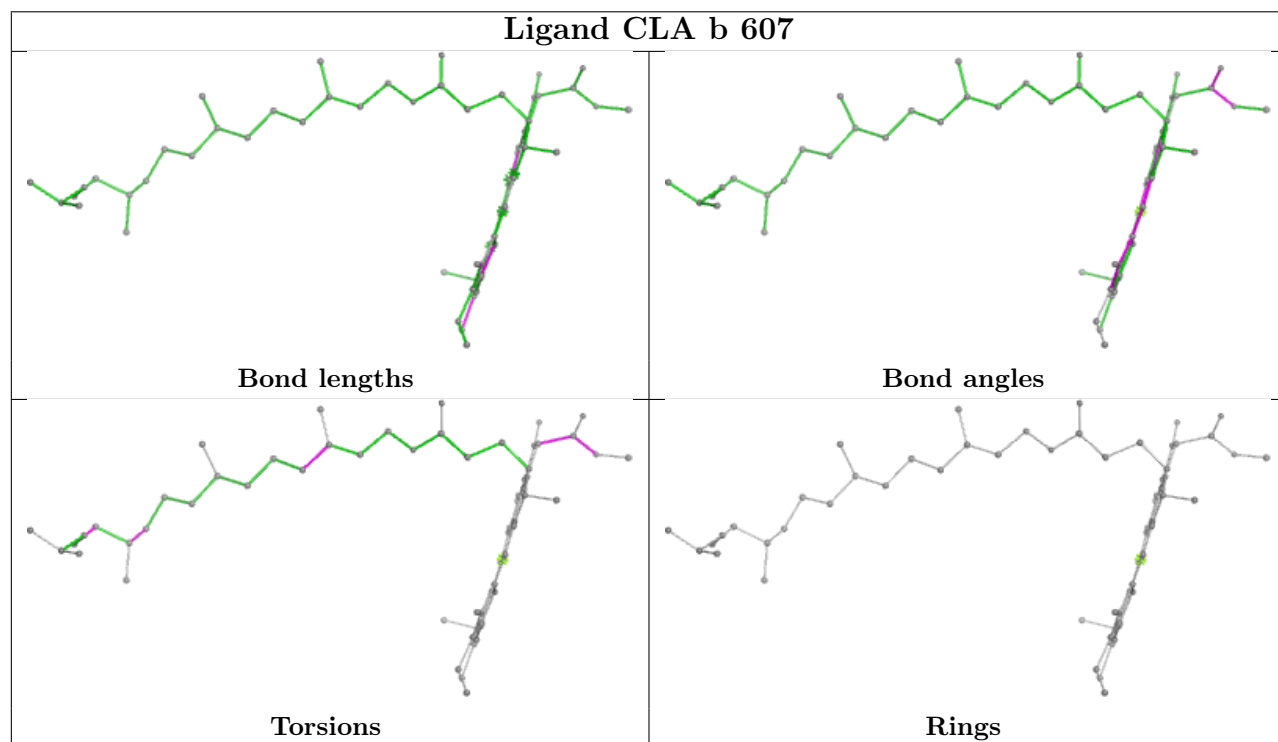
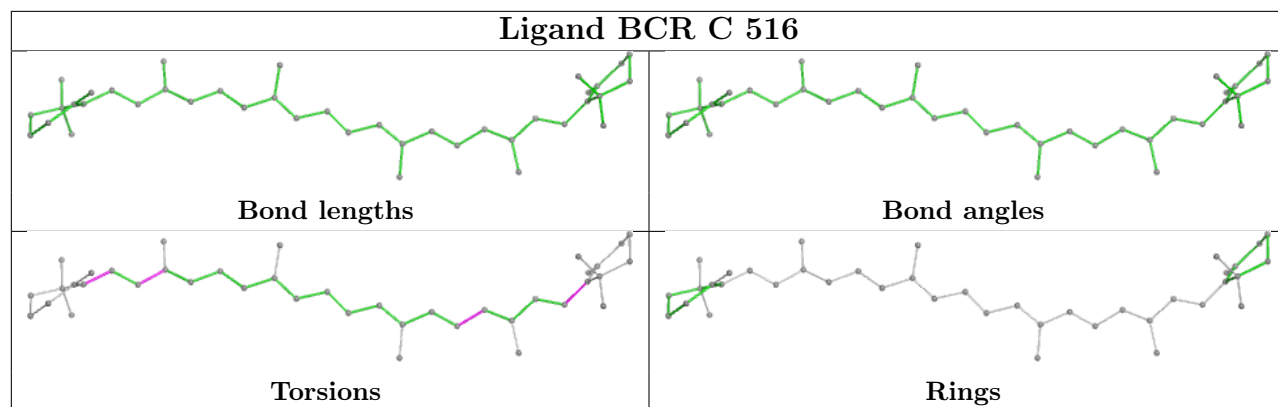
Bond angles



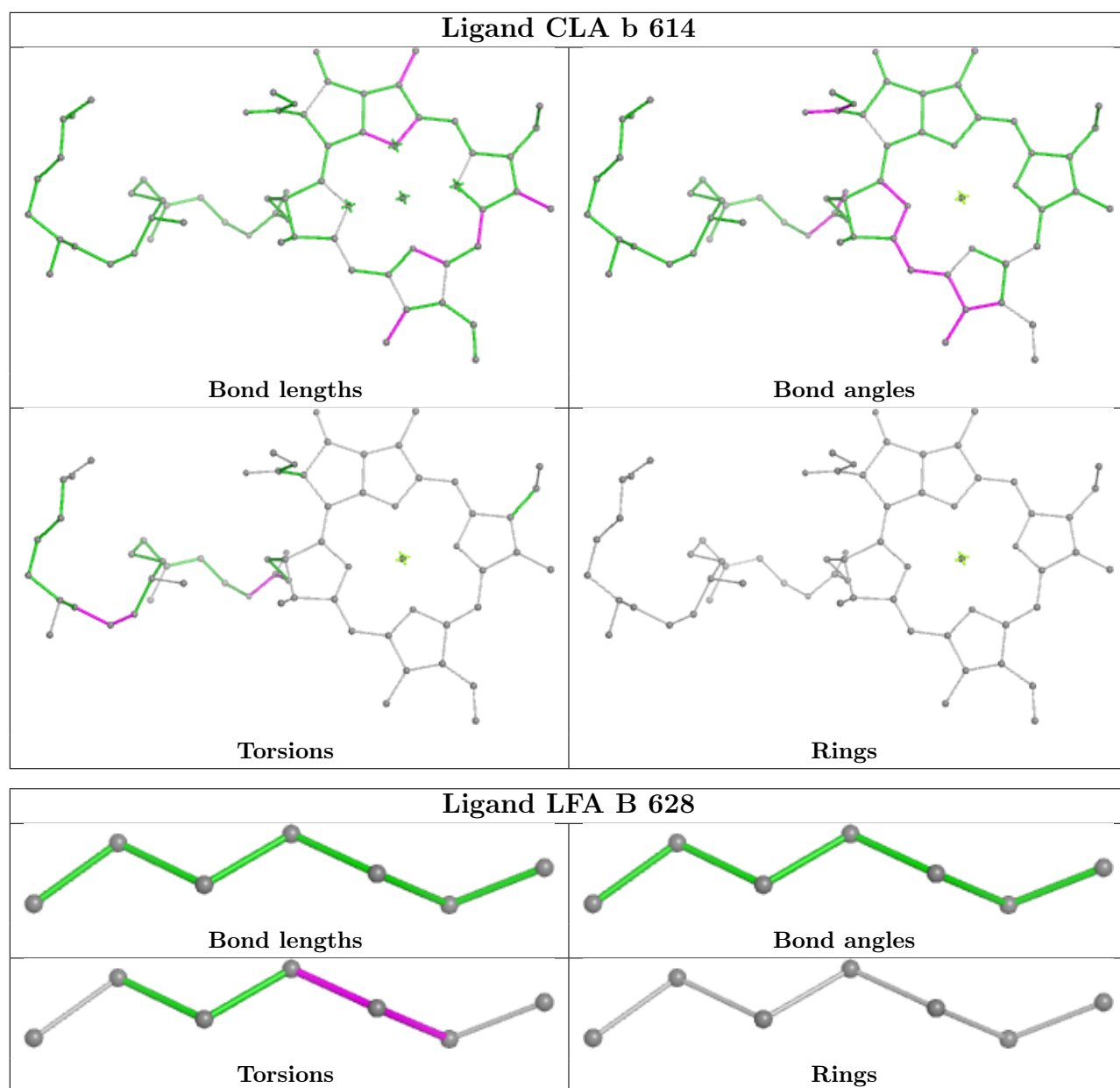
Torsions

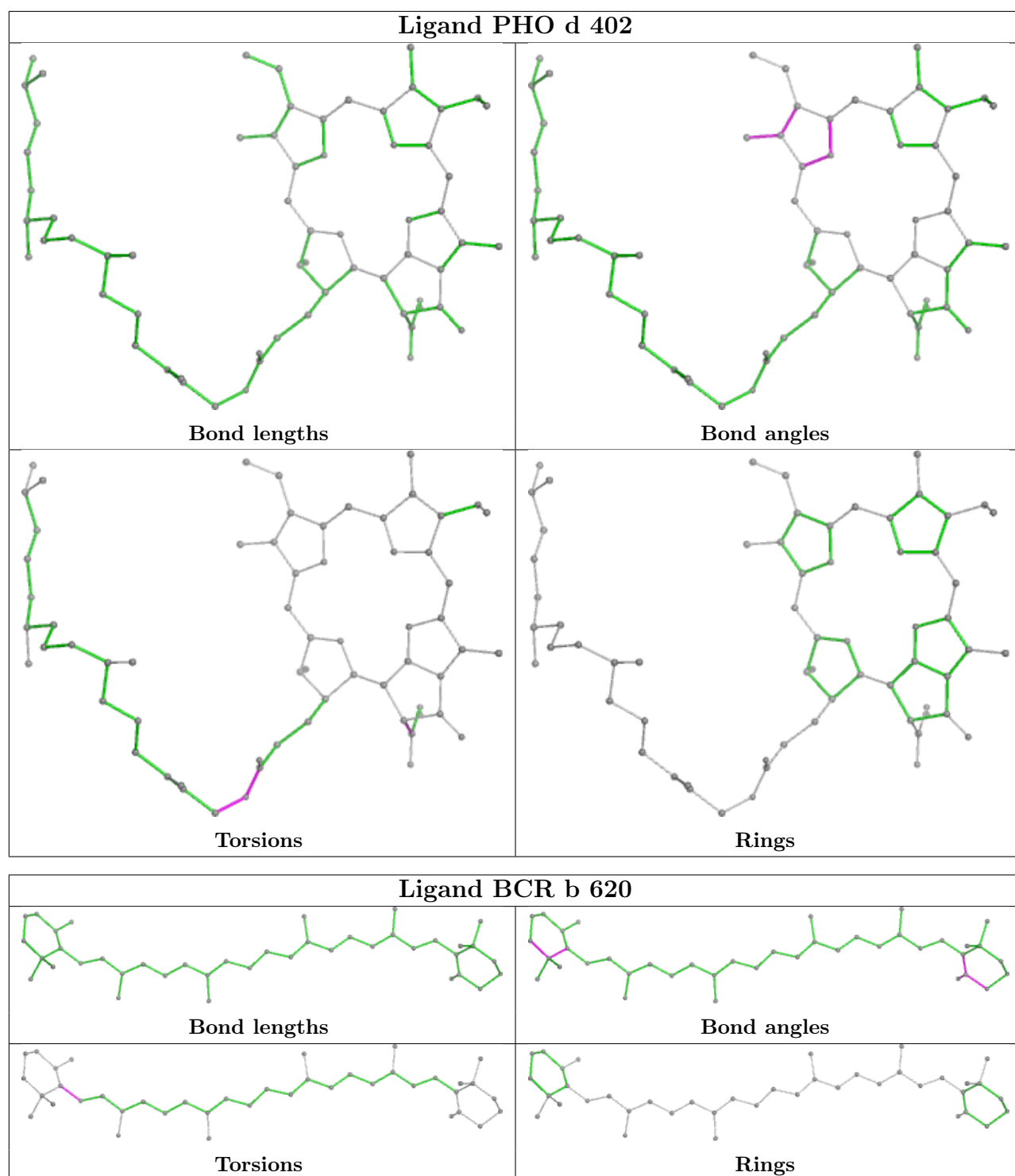


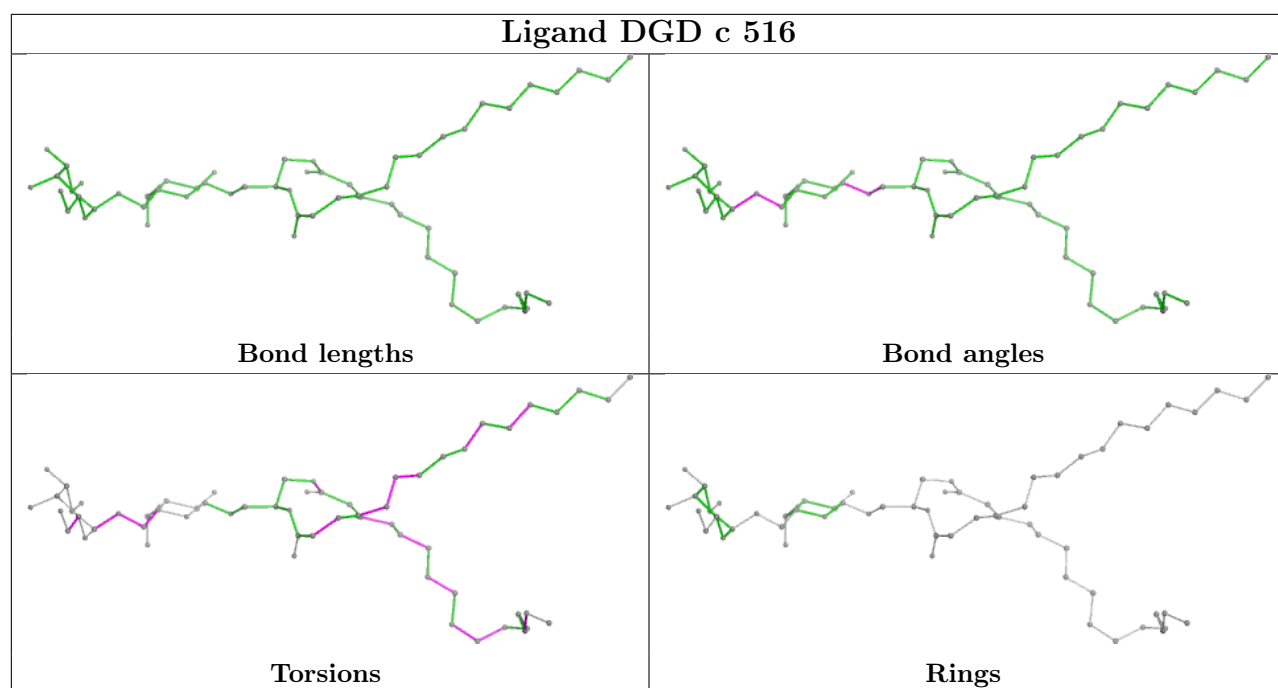
Rings

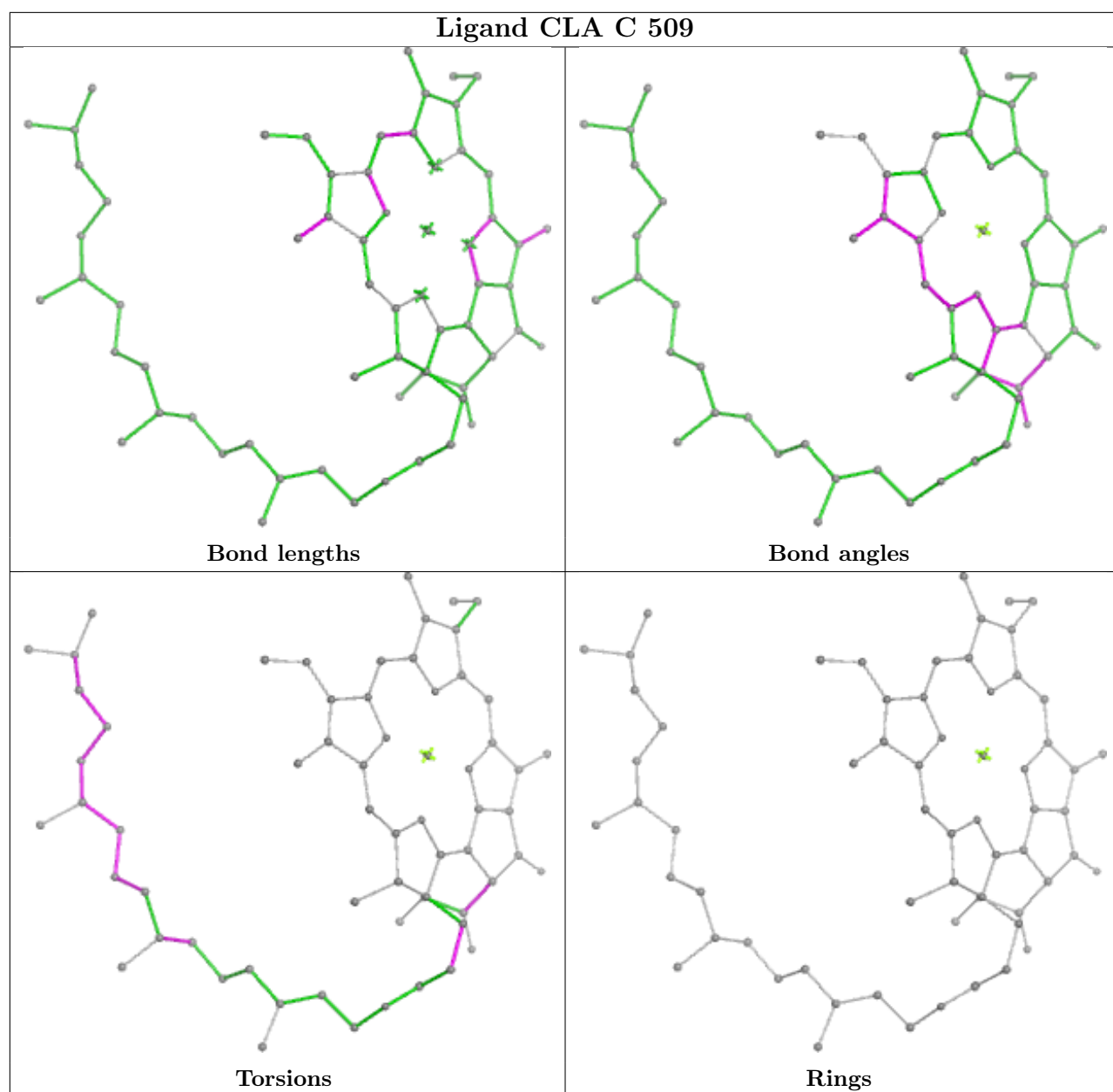


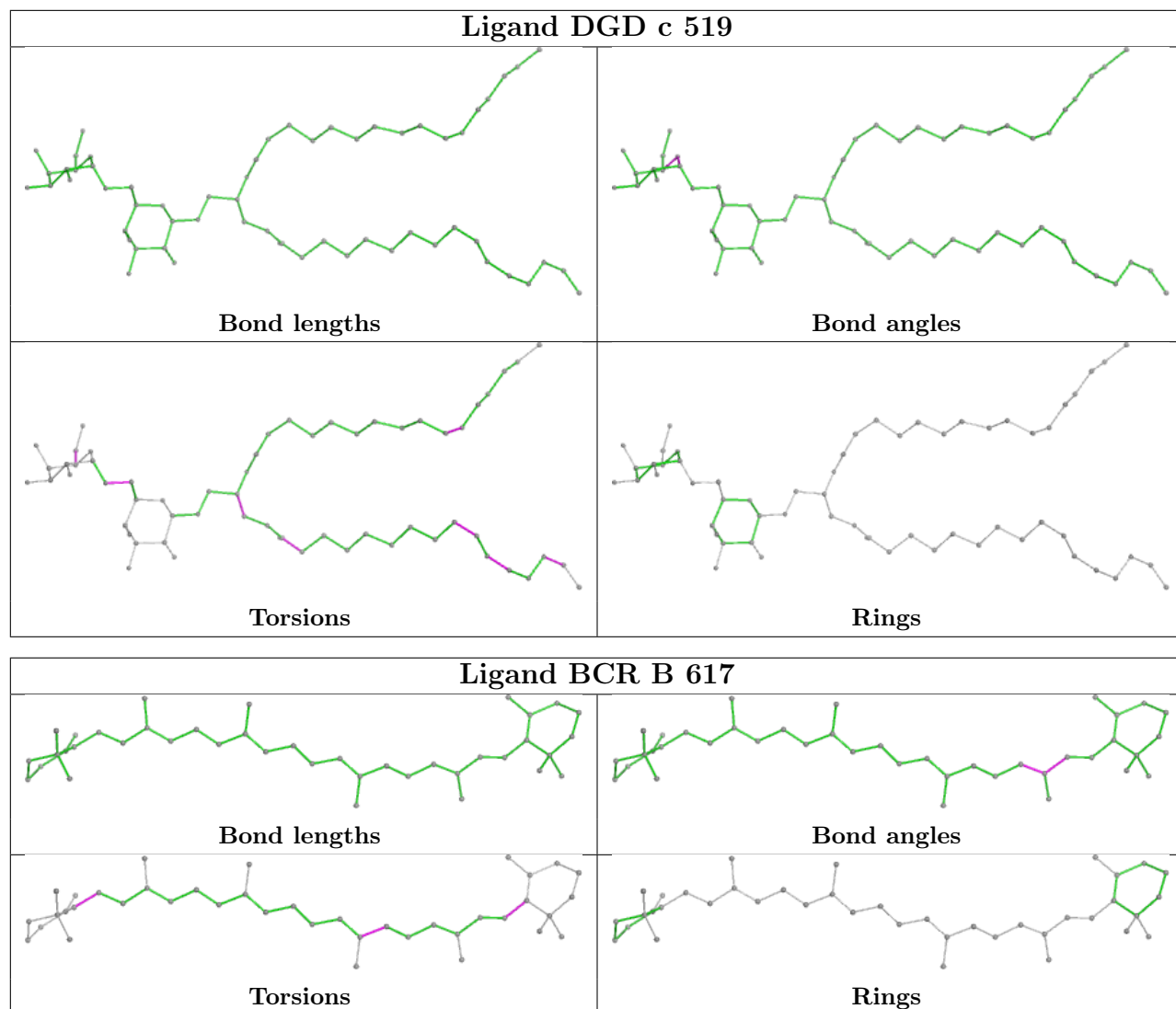


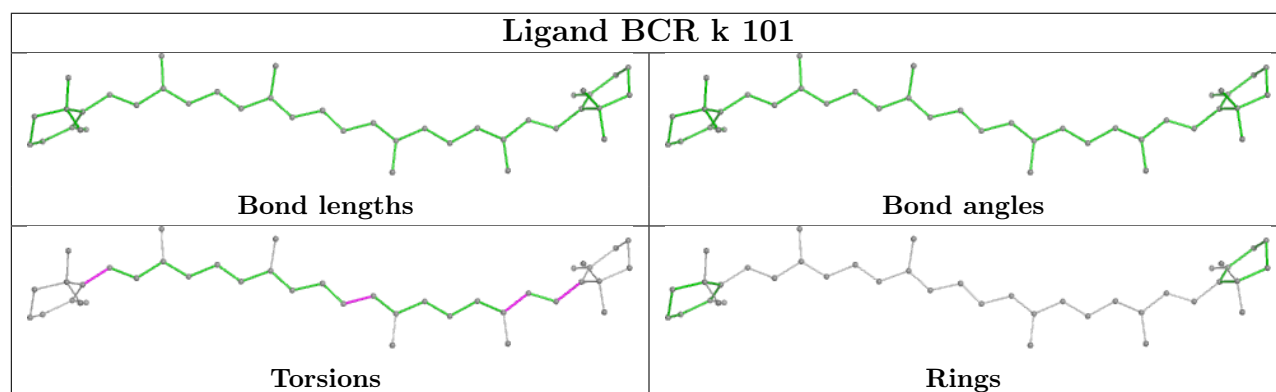
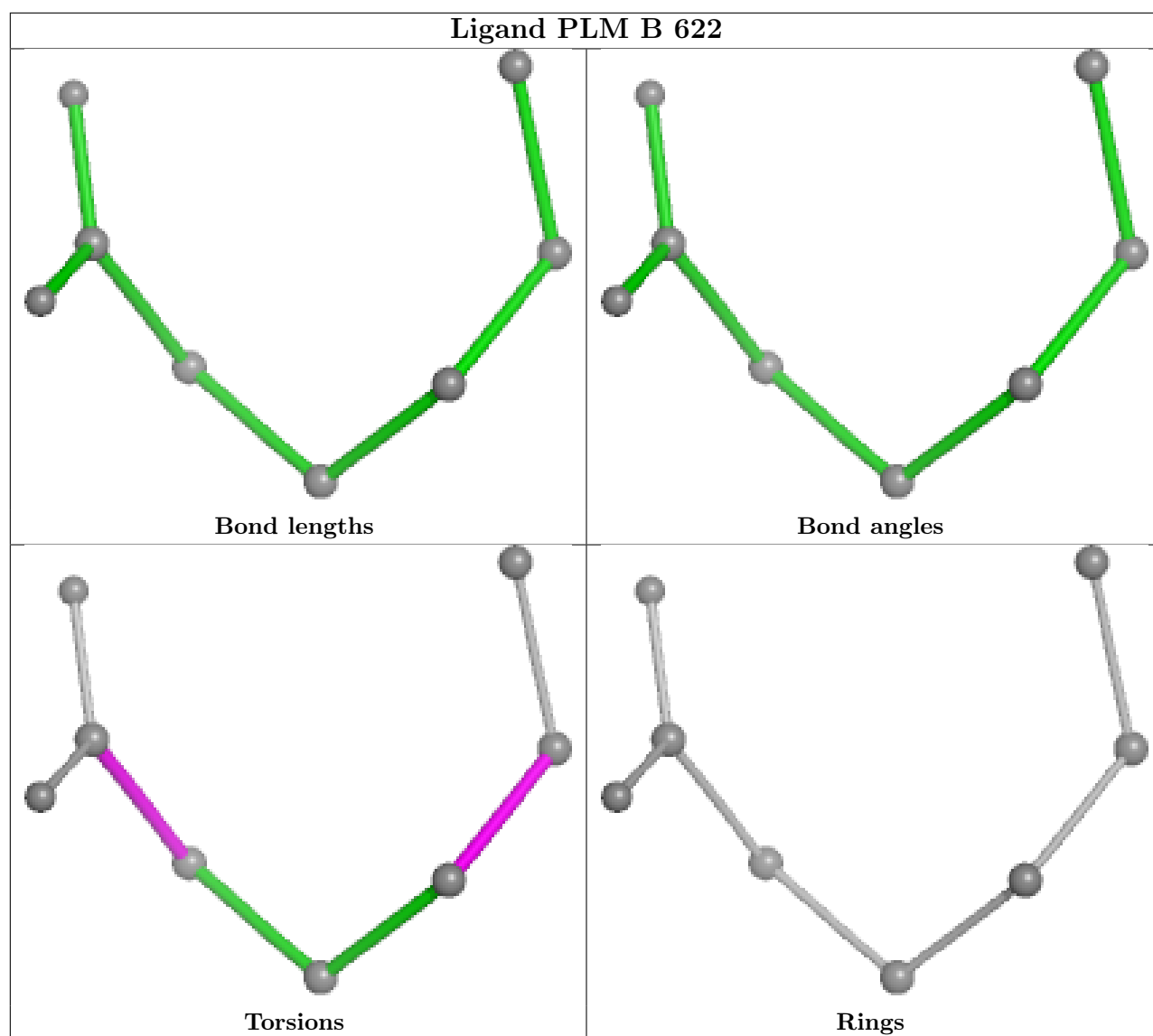




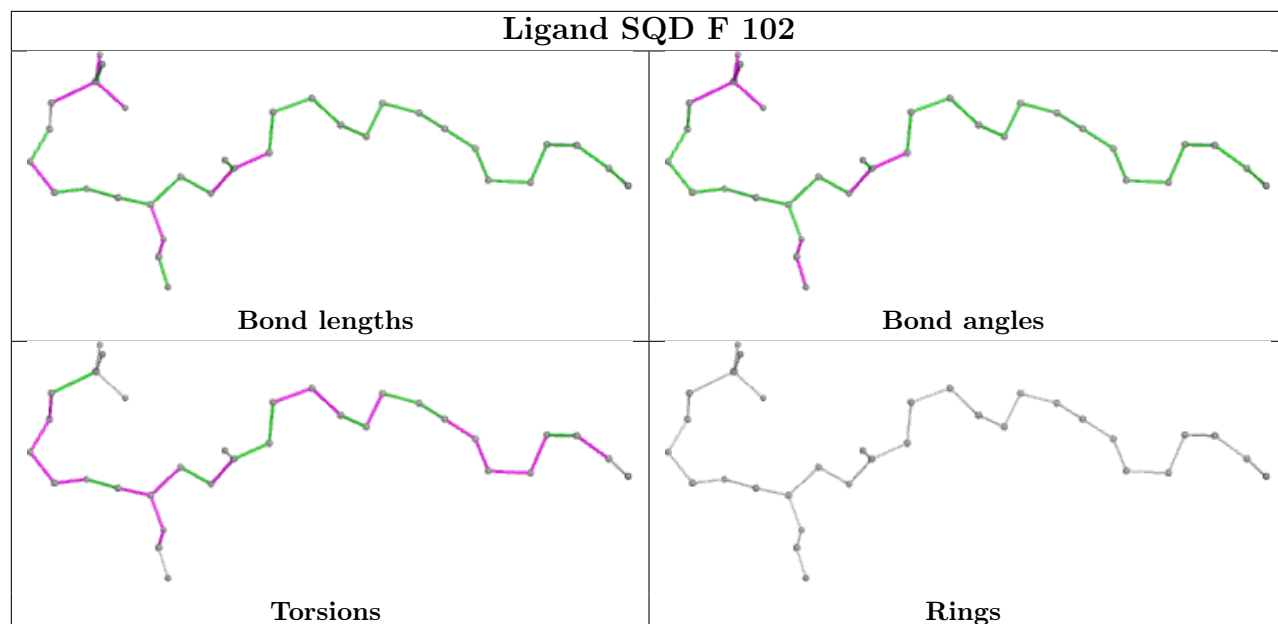




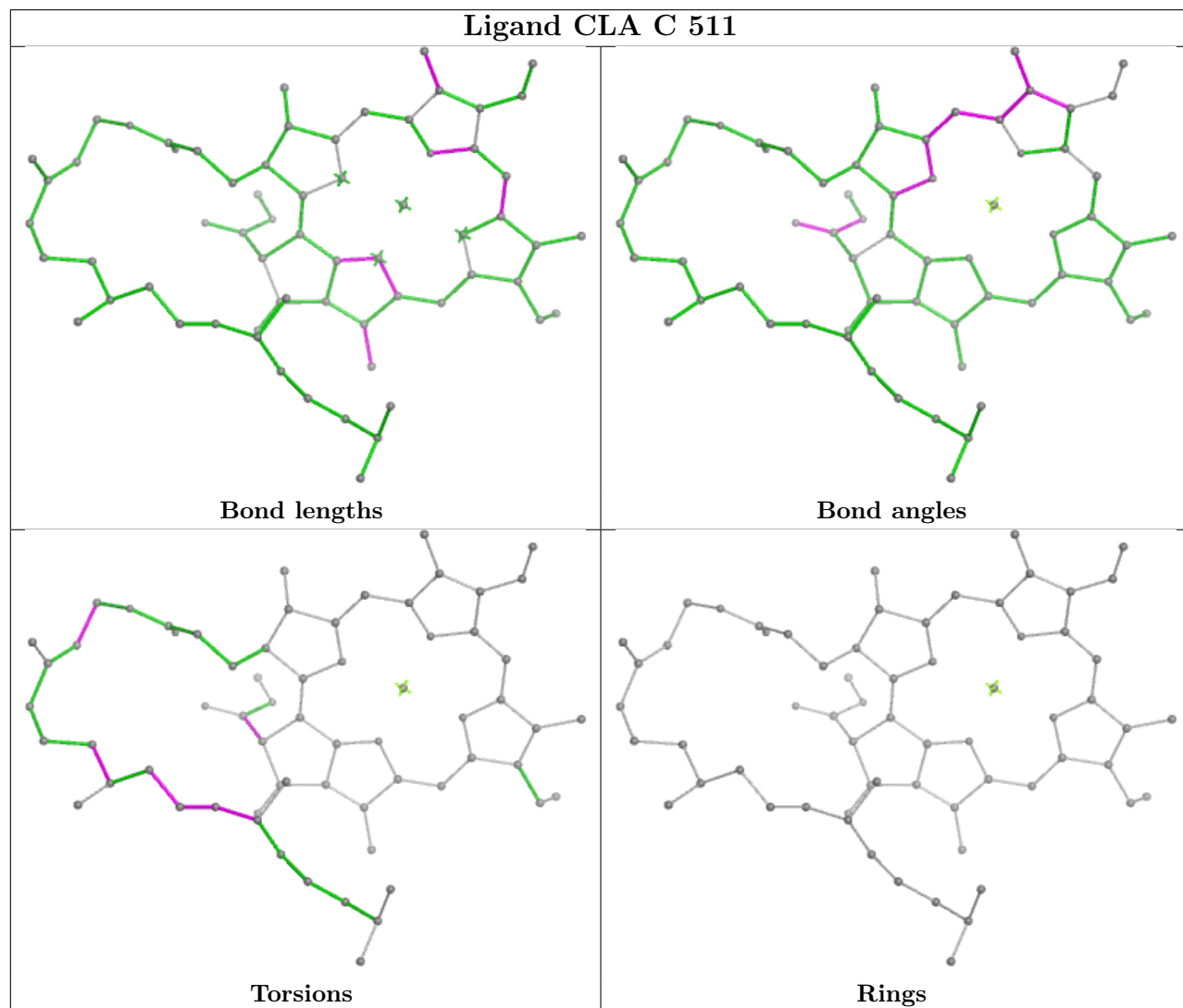


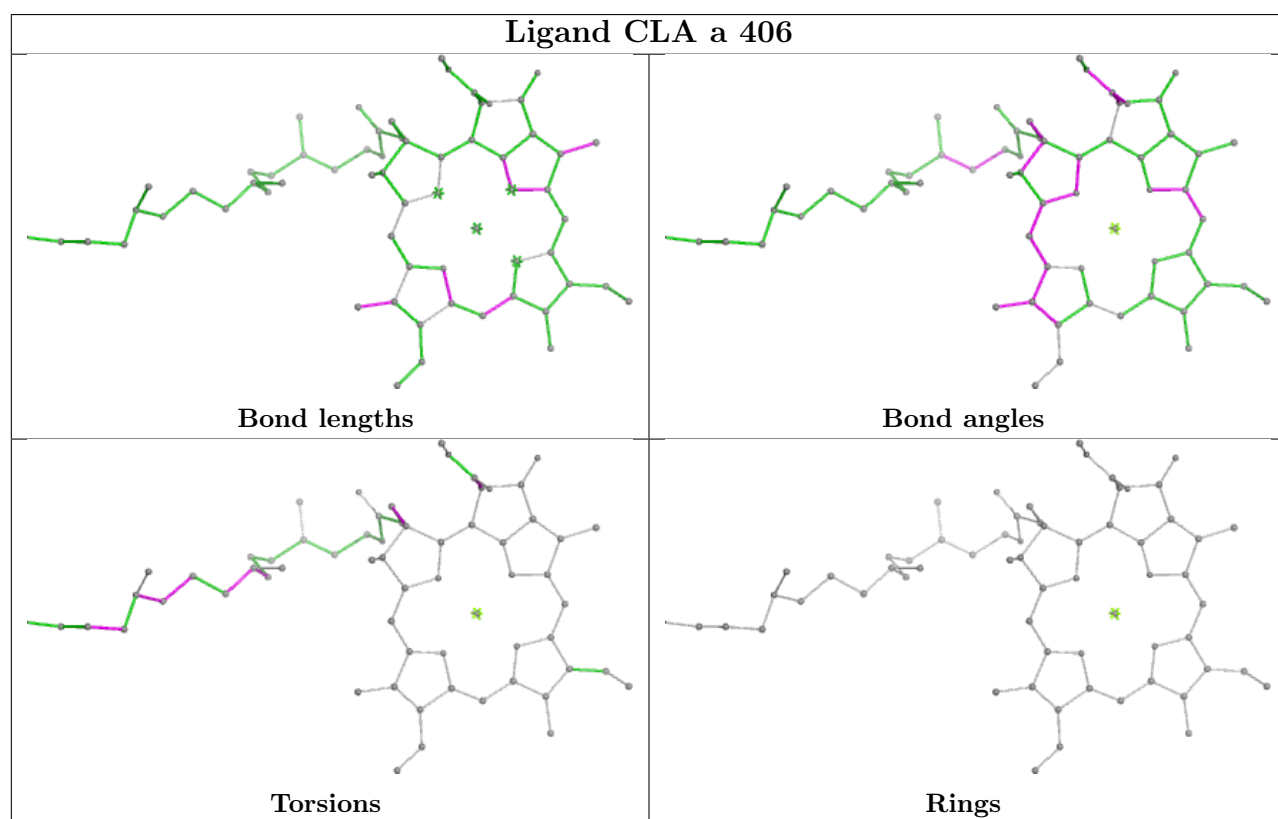
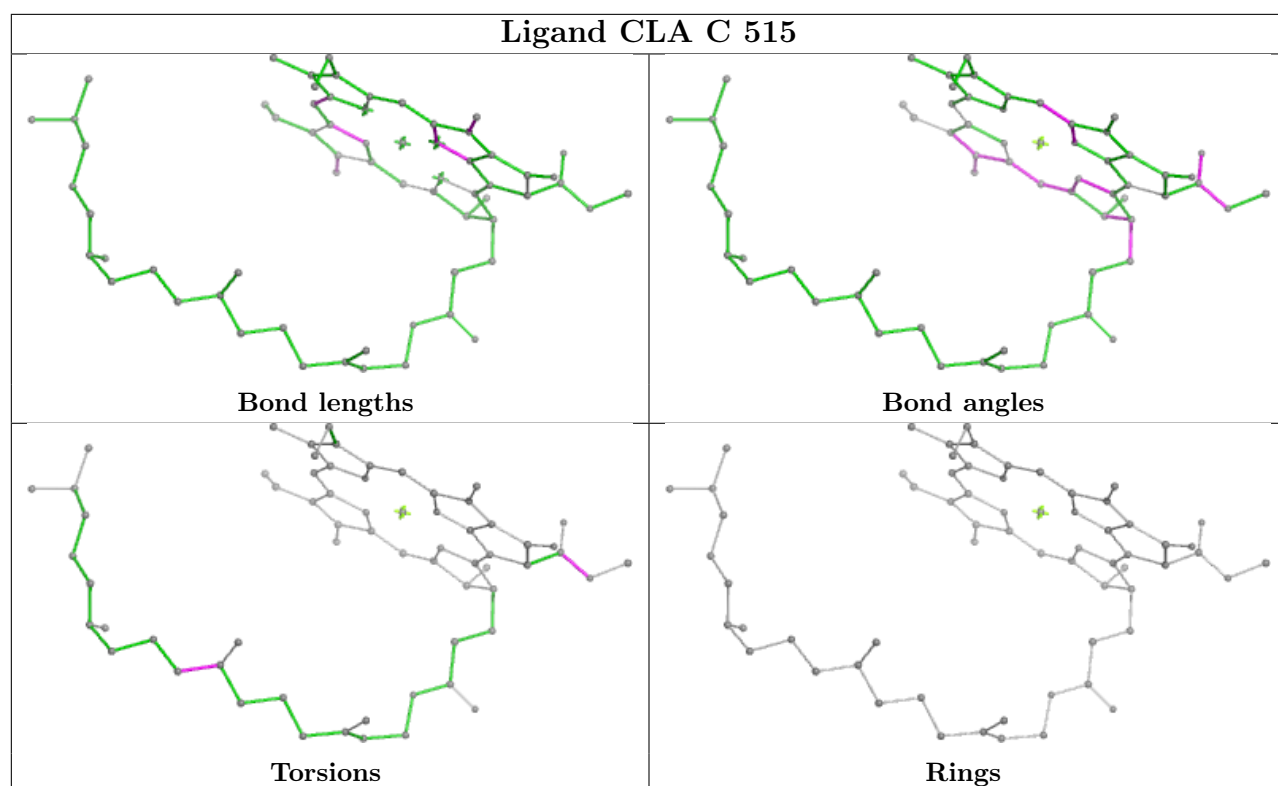


## Ligand SQD F 102

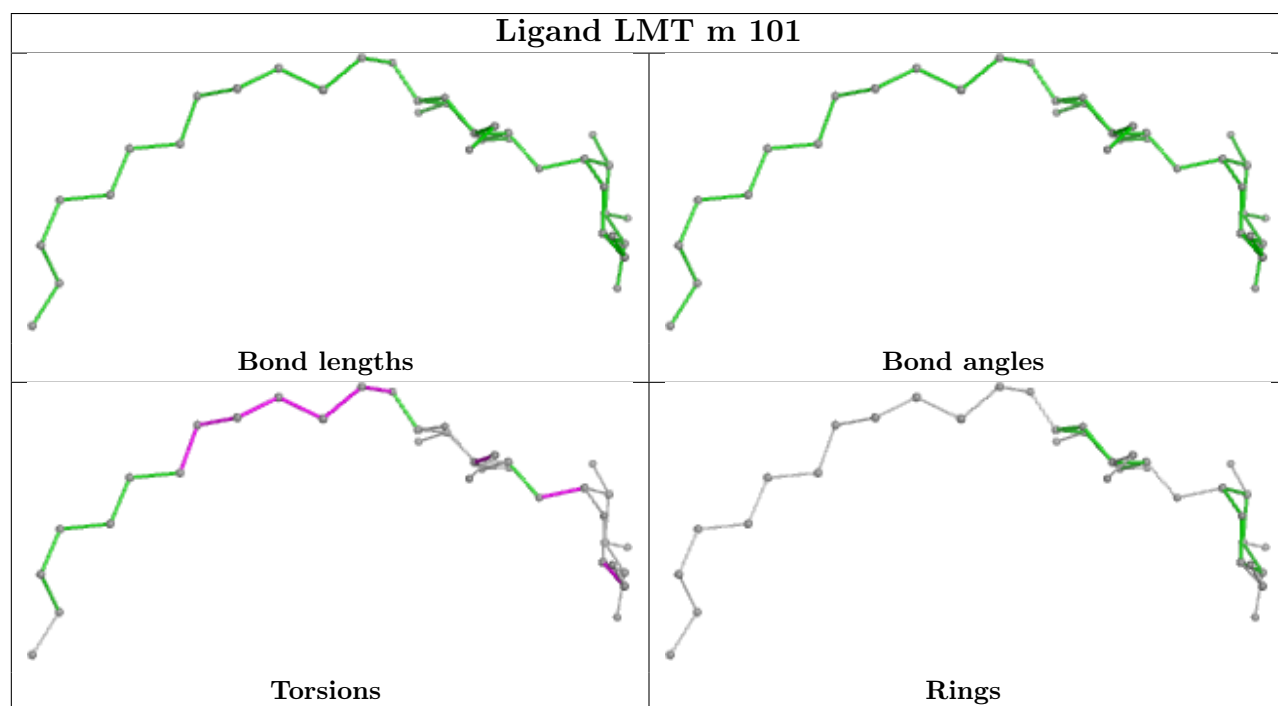
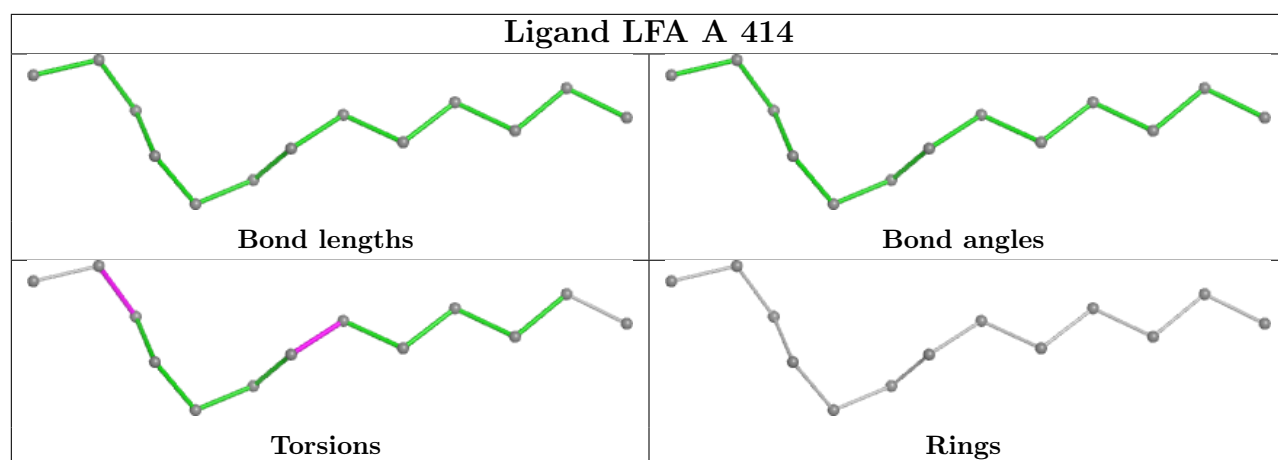


## Ligand CLA C 511

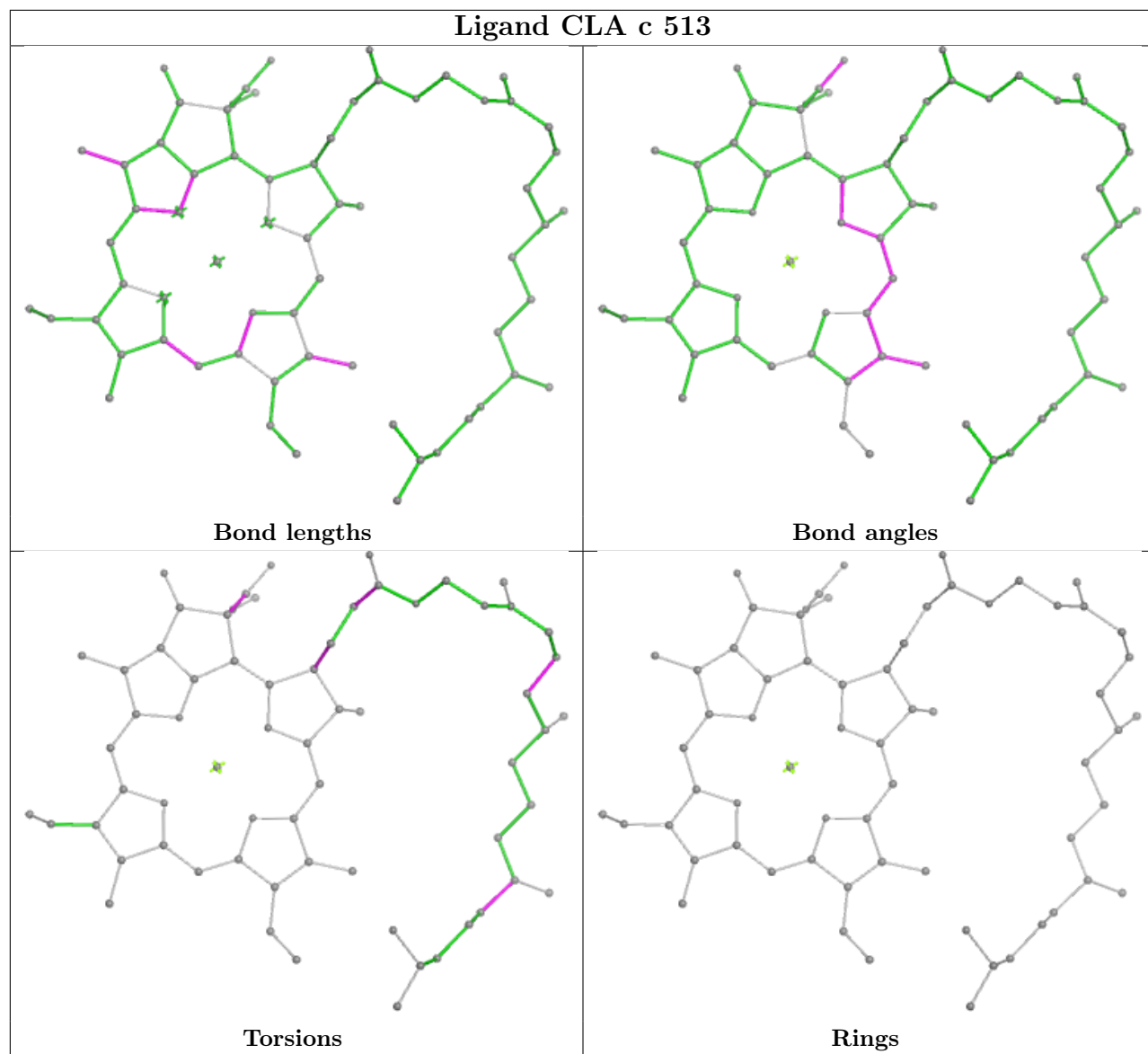


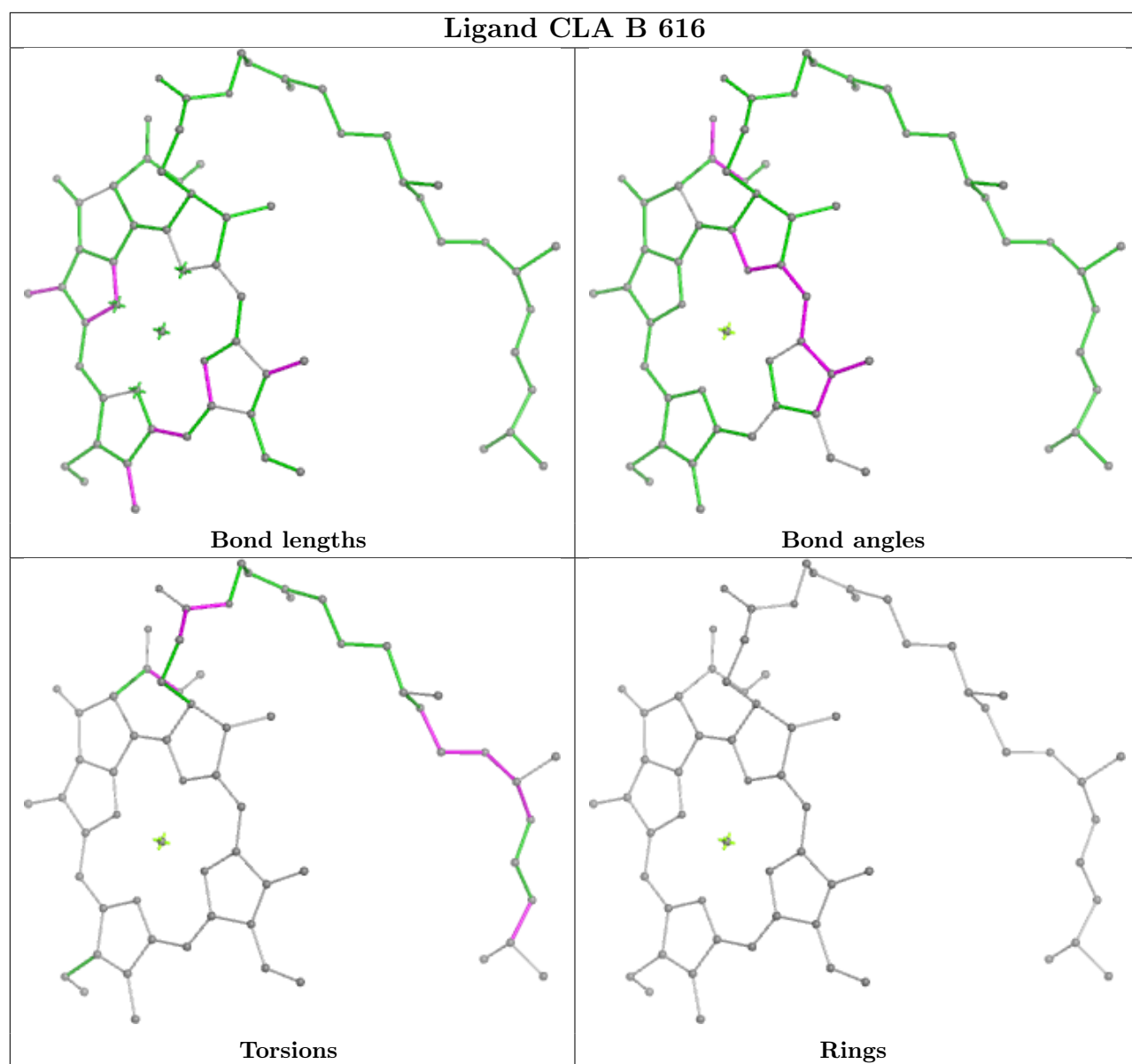


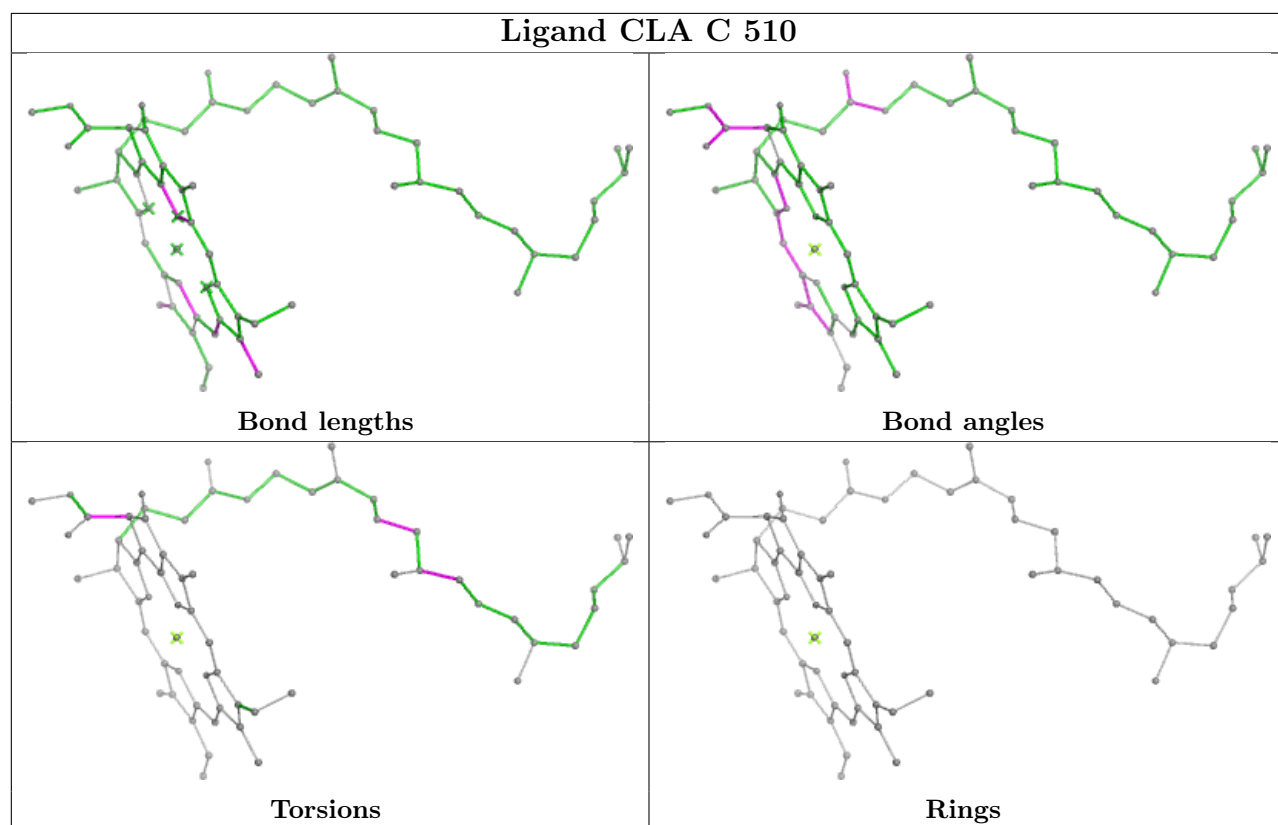
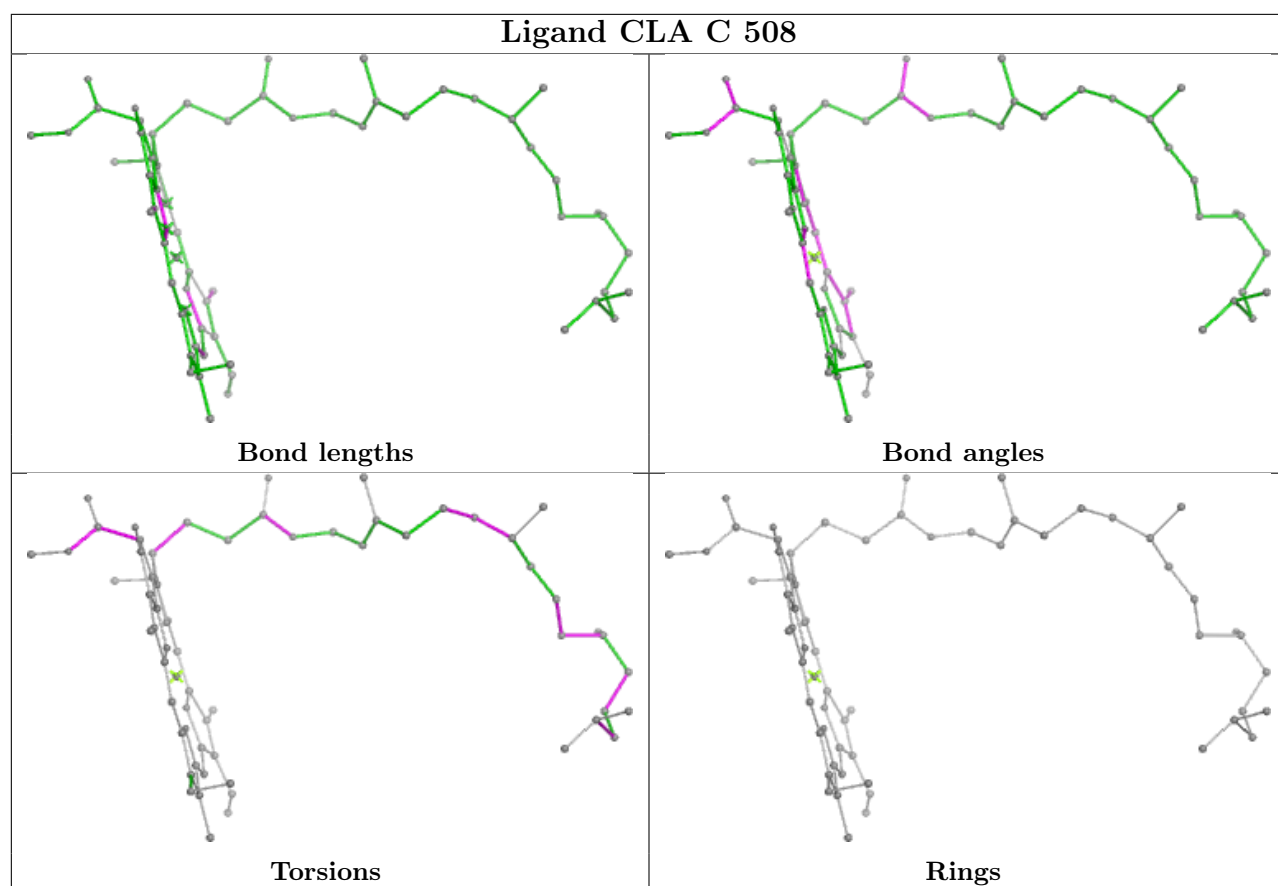


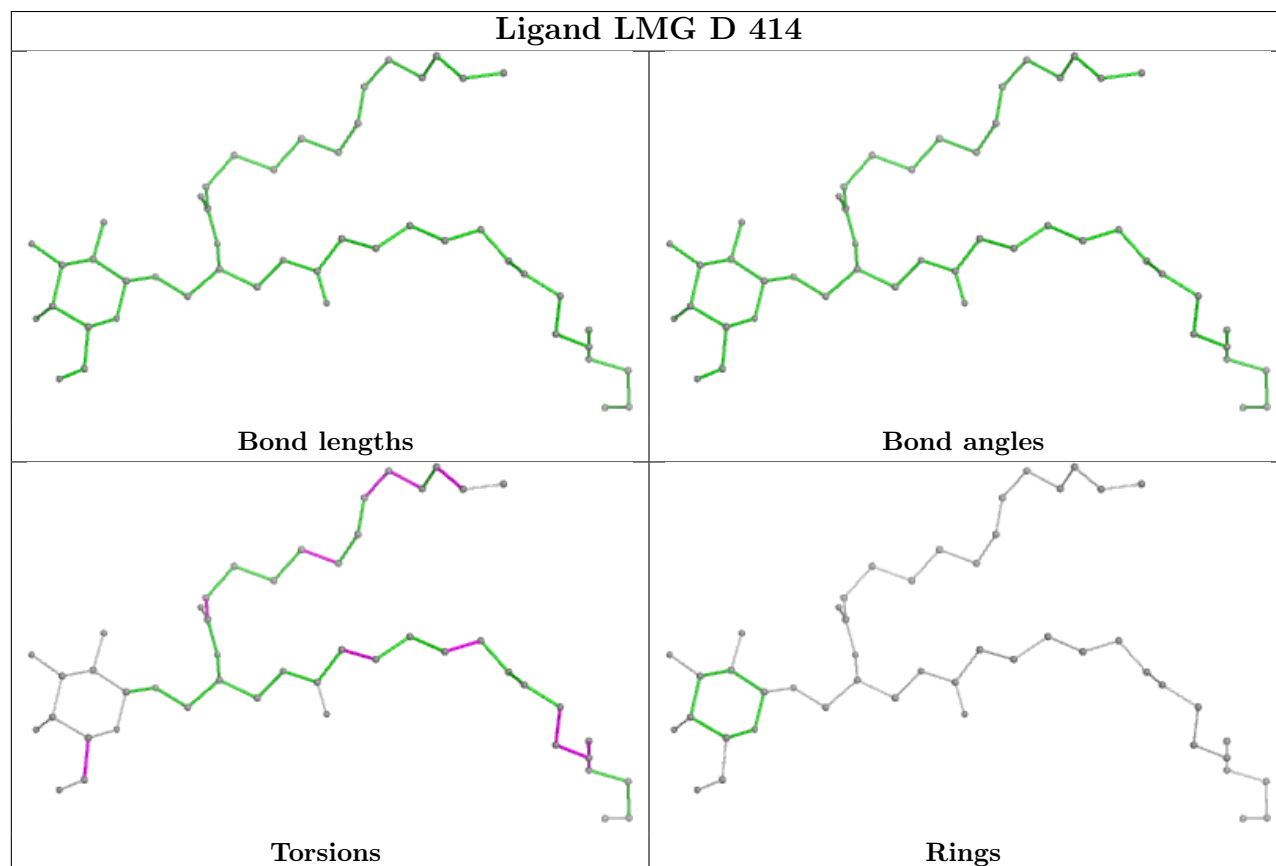
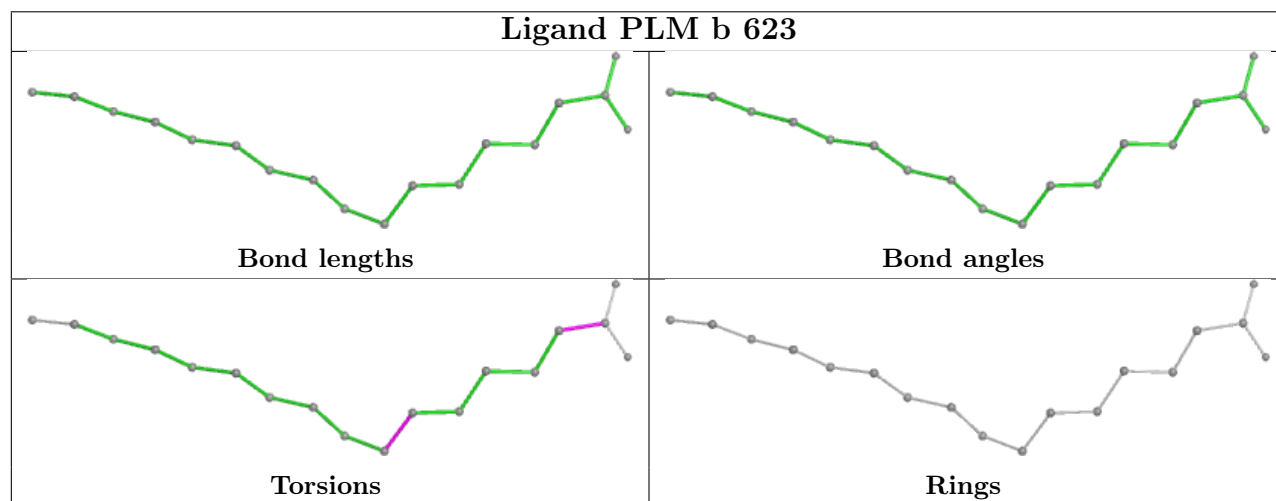
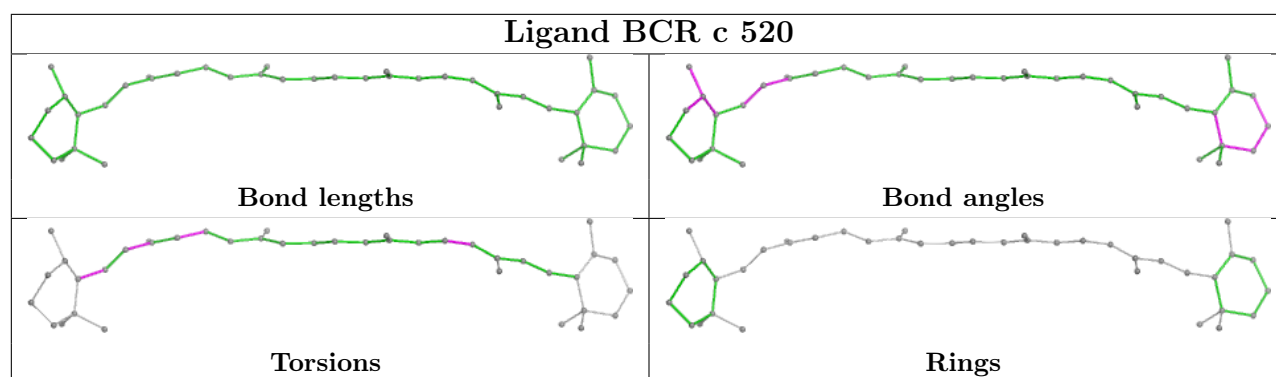


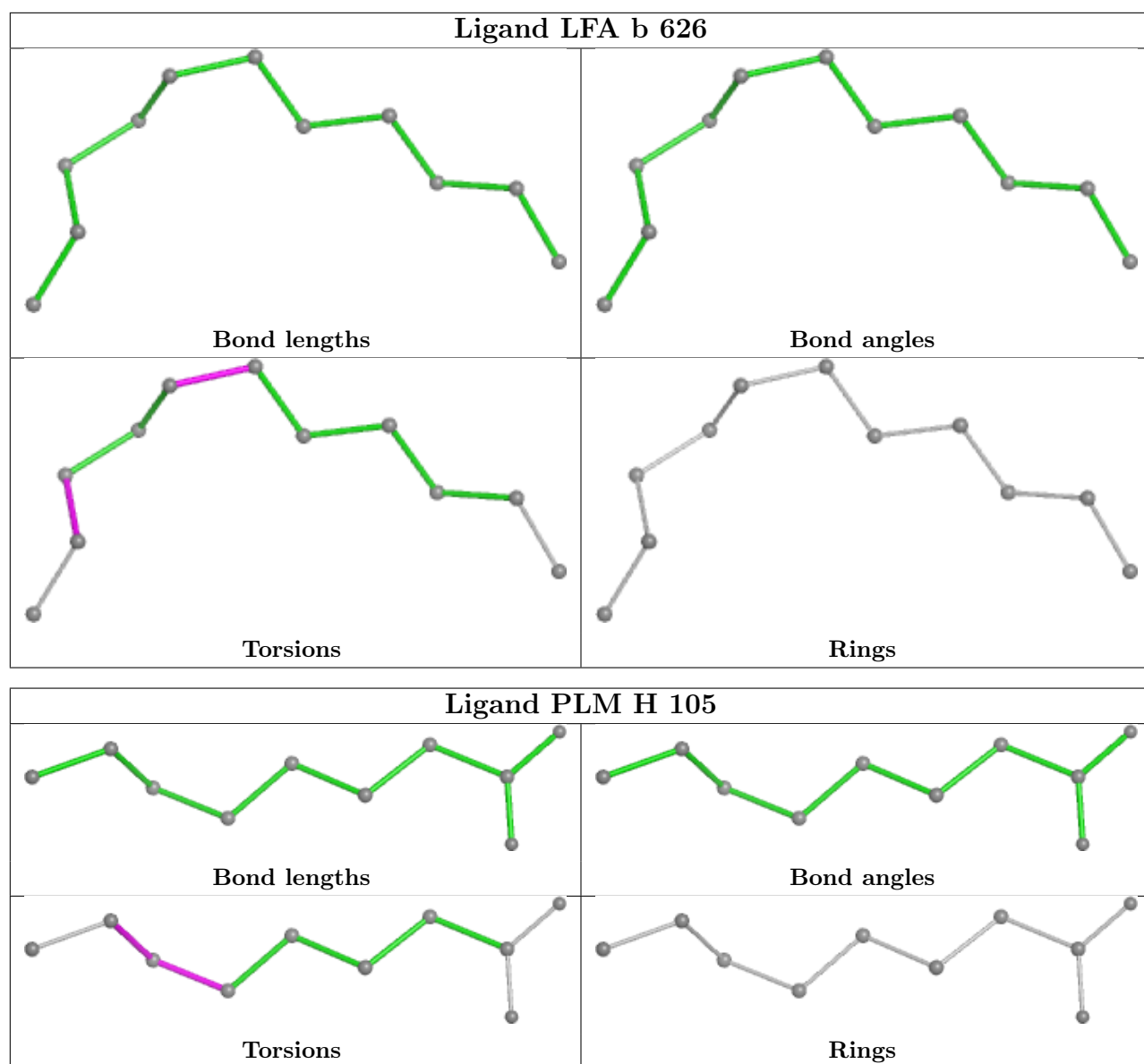
## Ligand CLA c 513

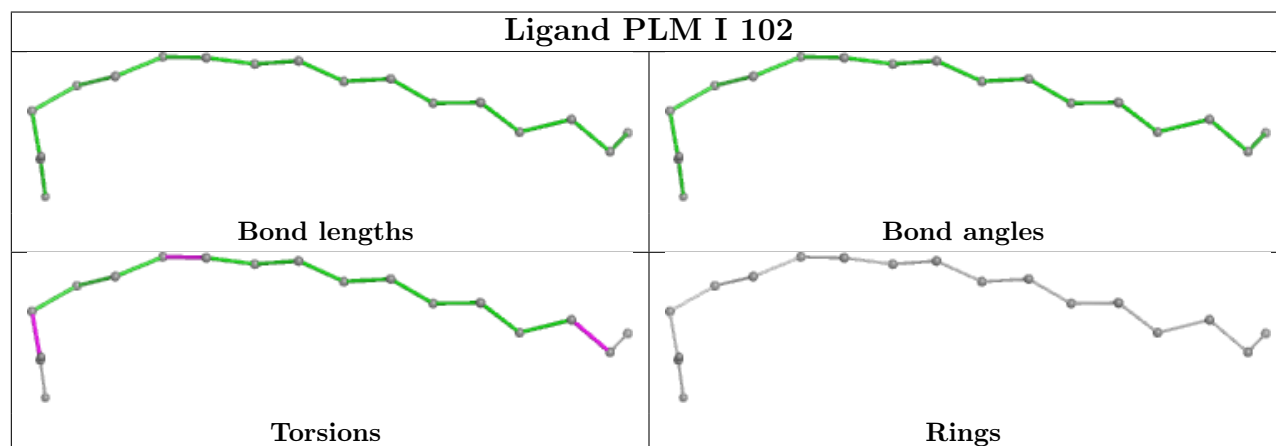
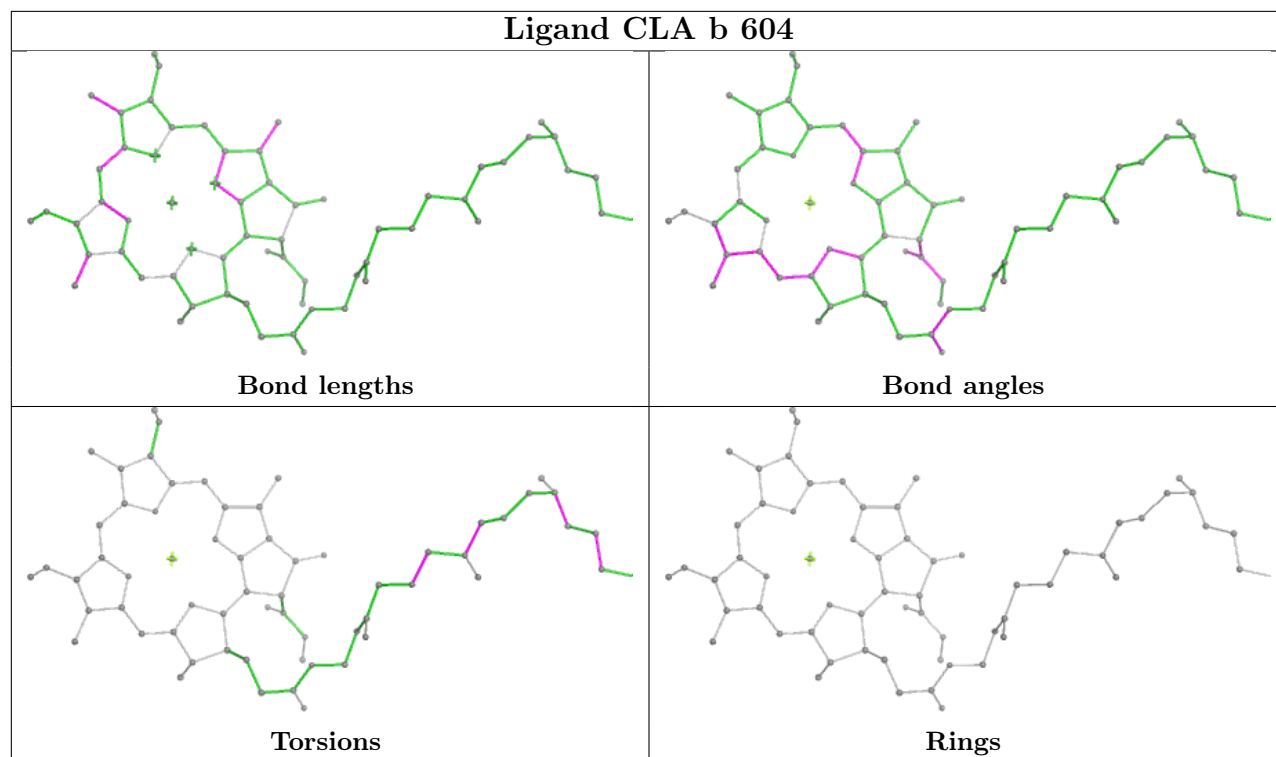


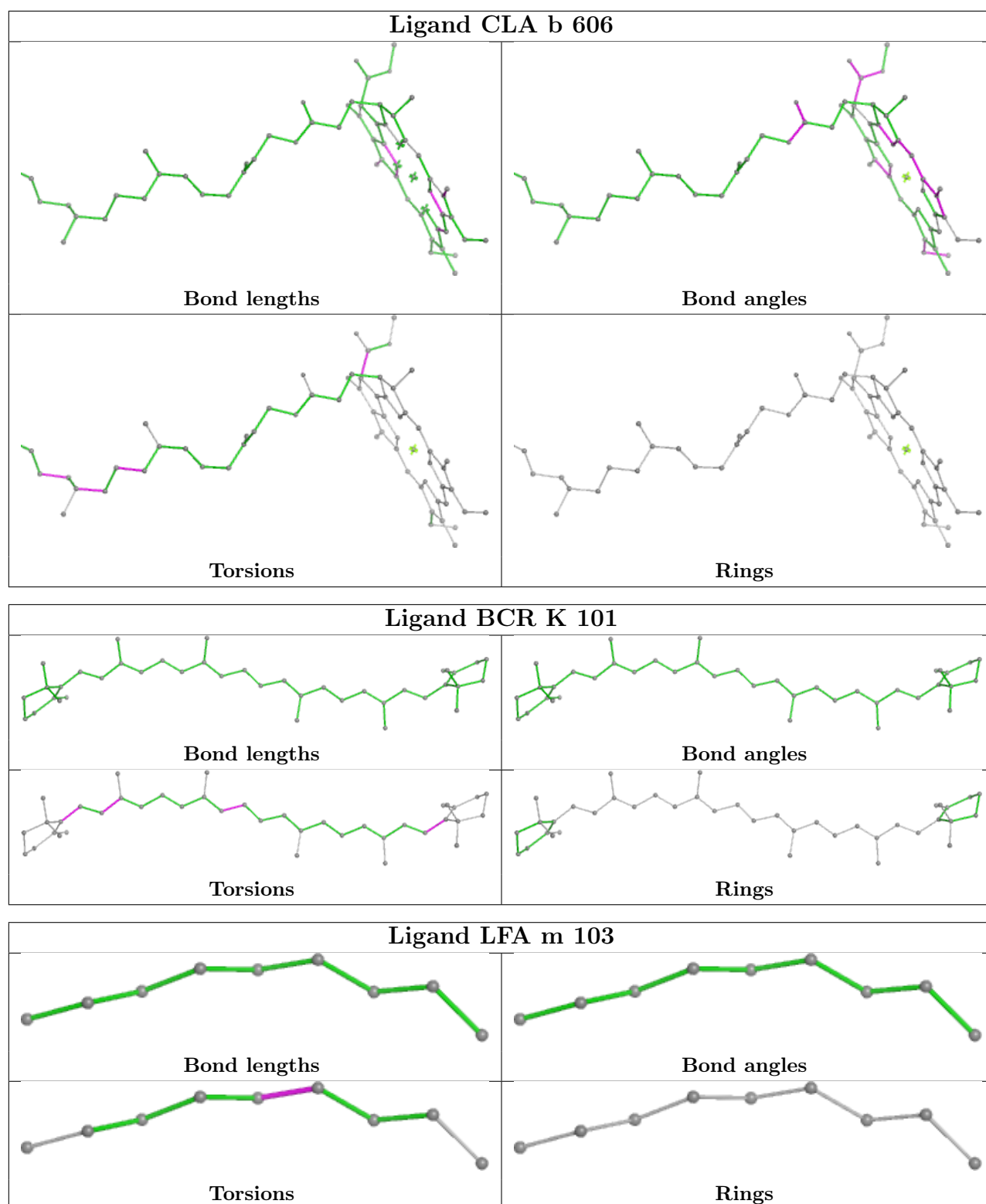




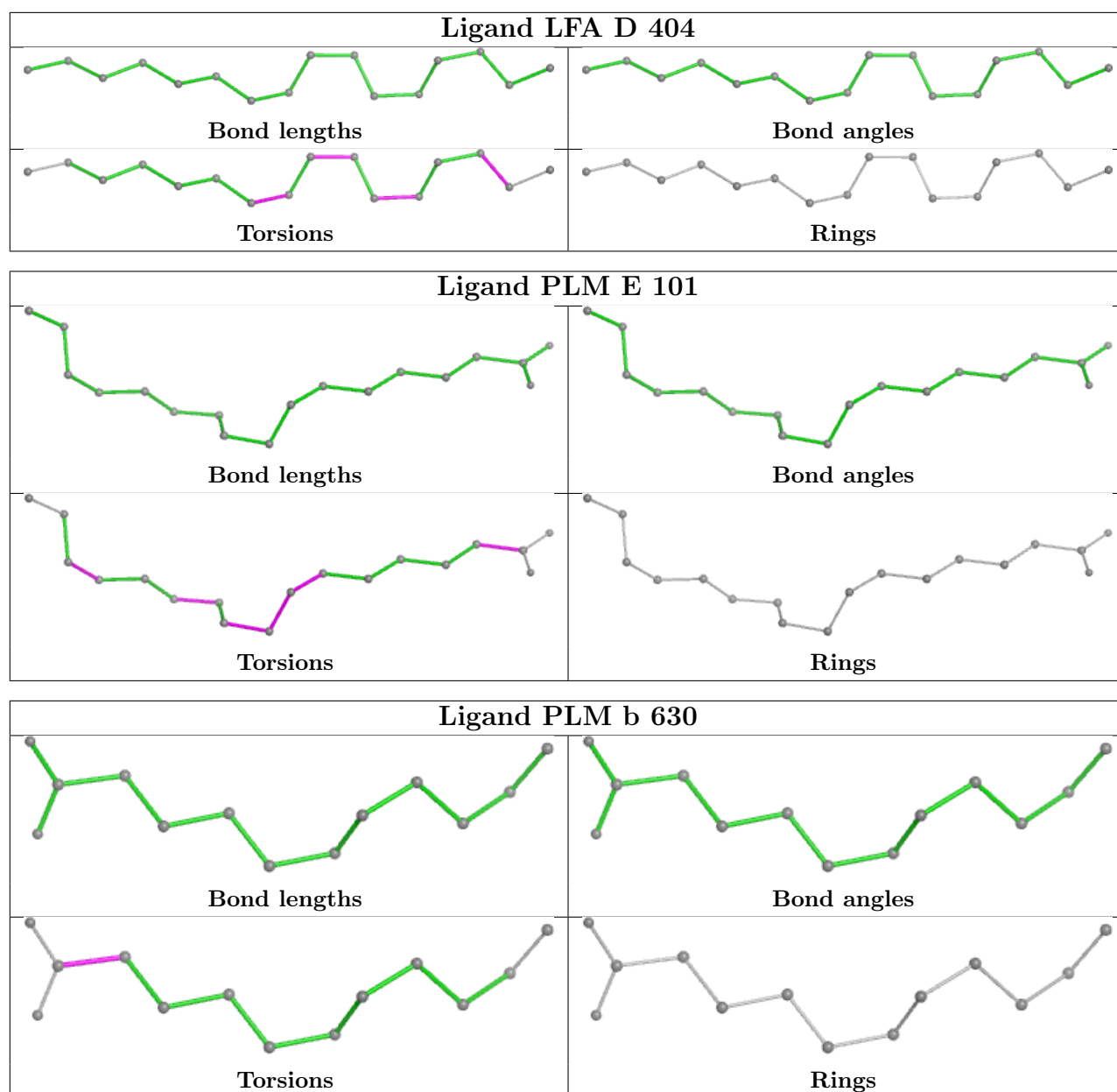


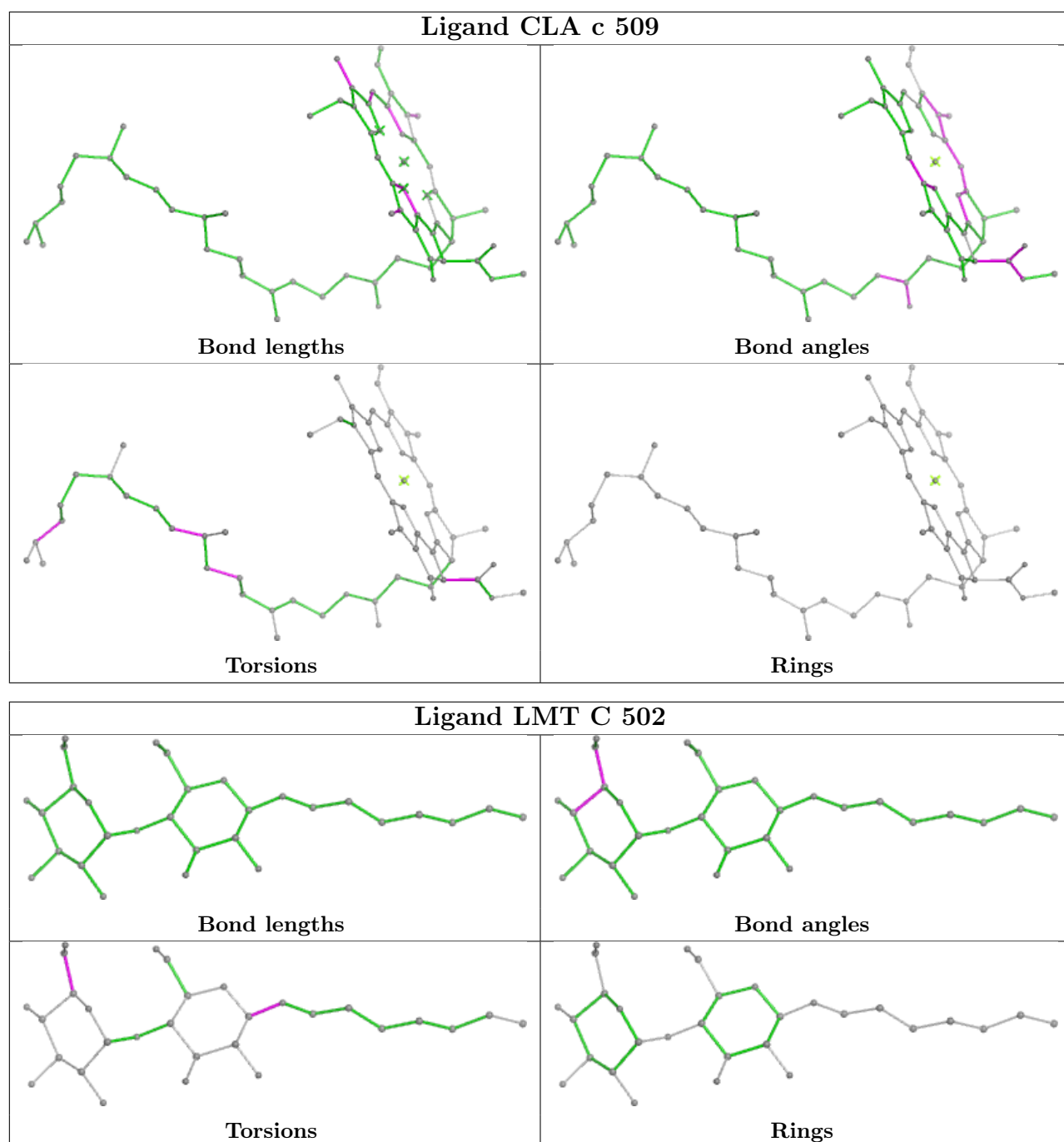


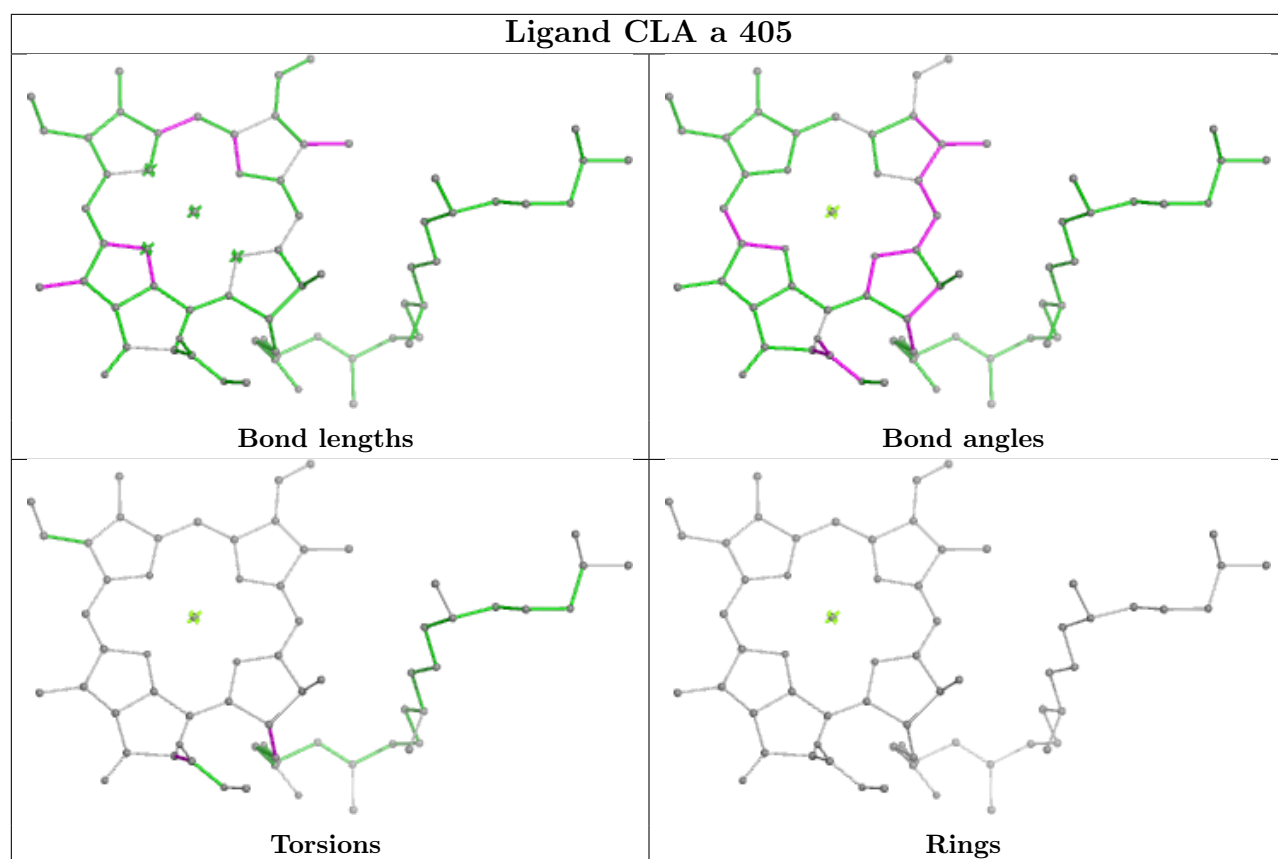




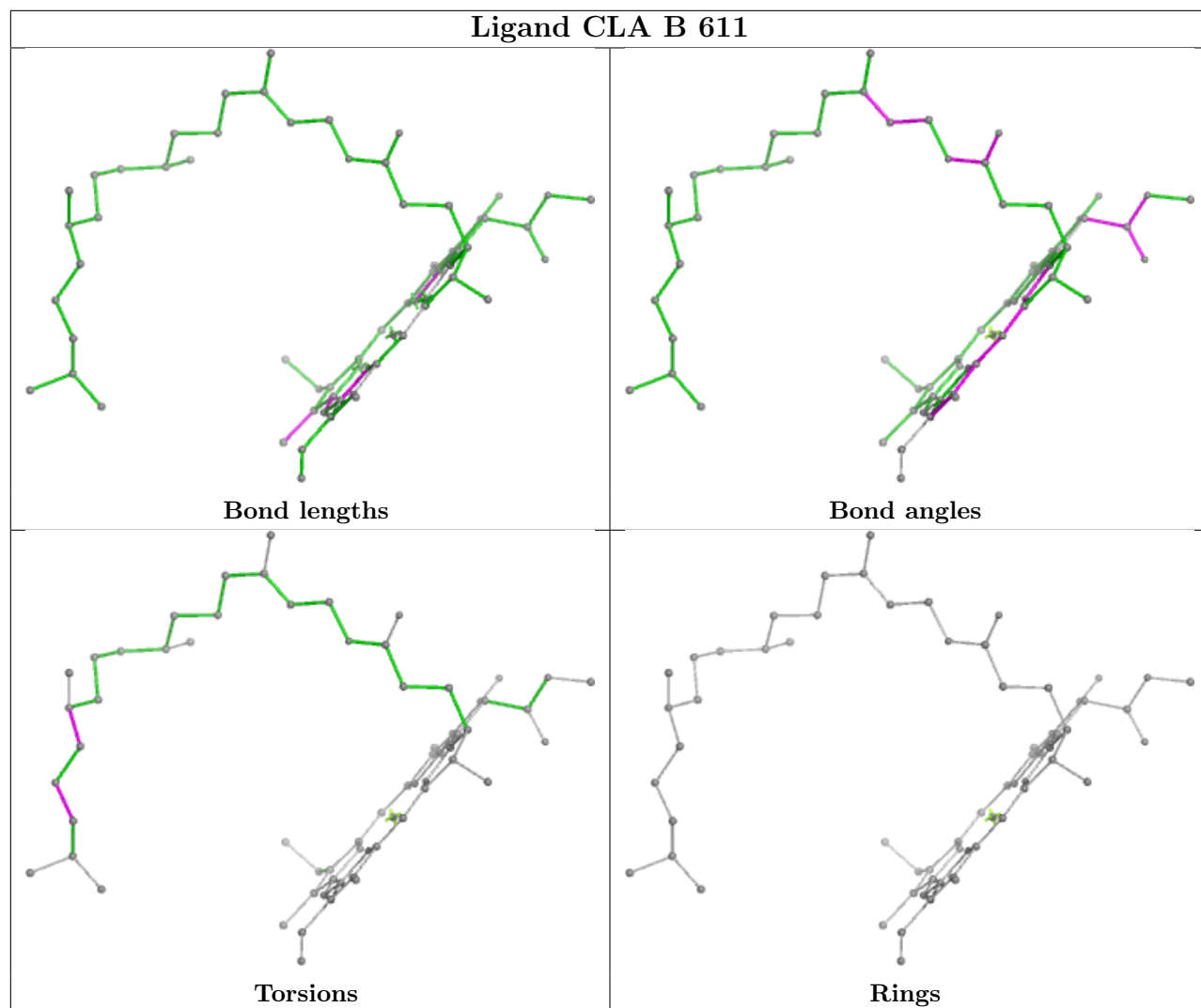




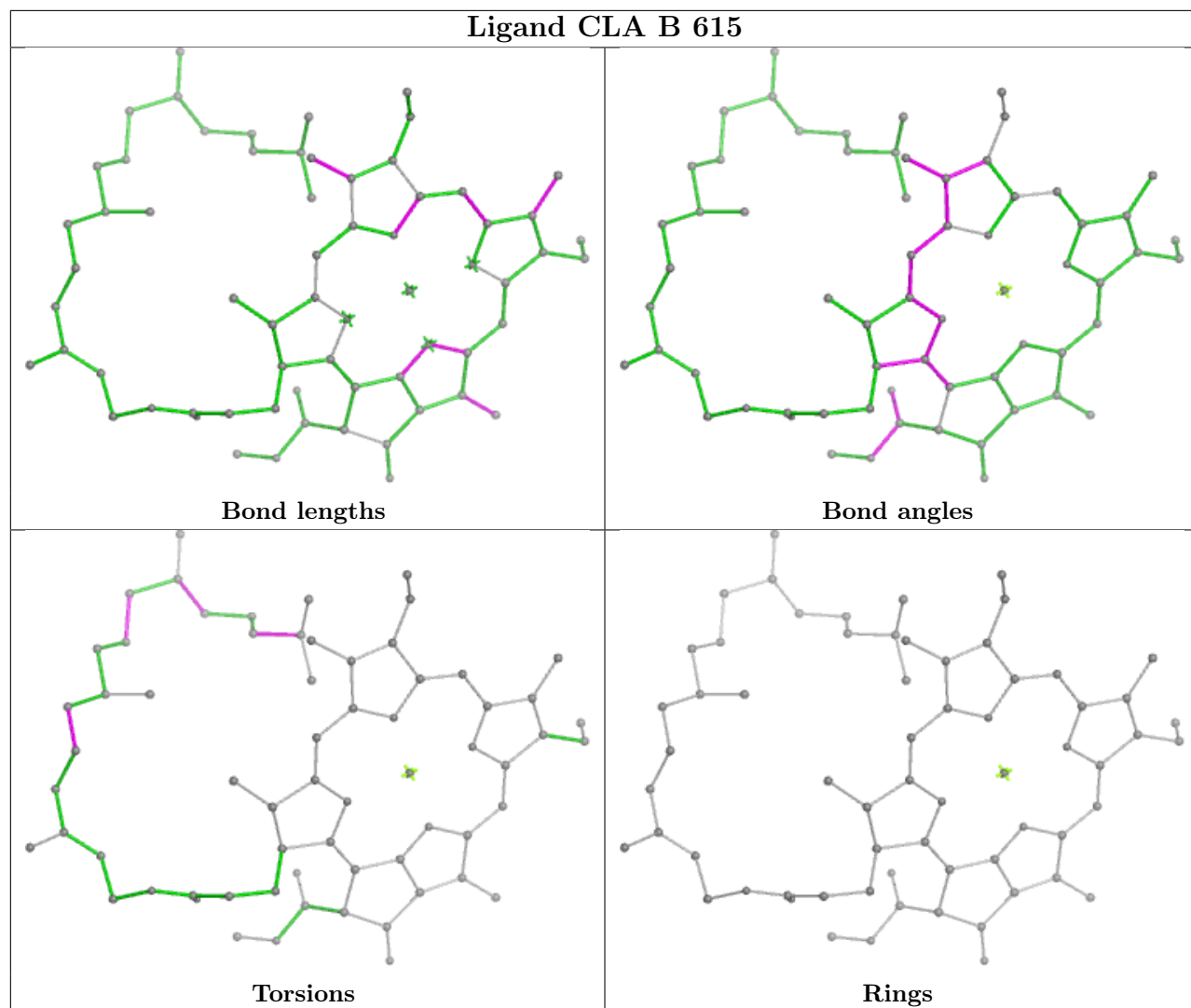


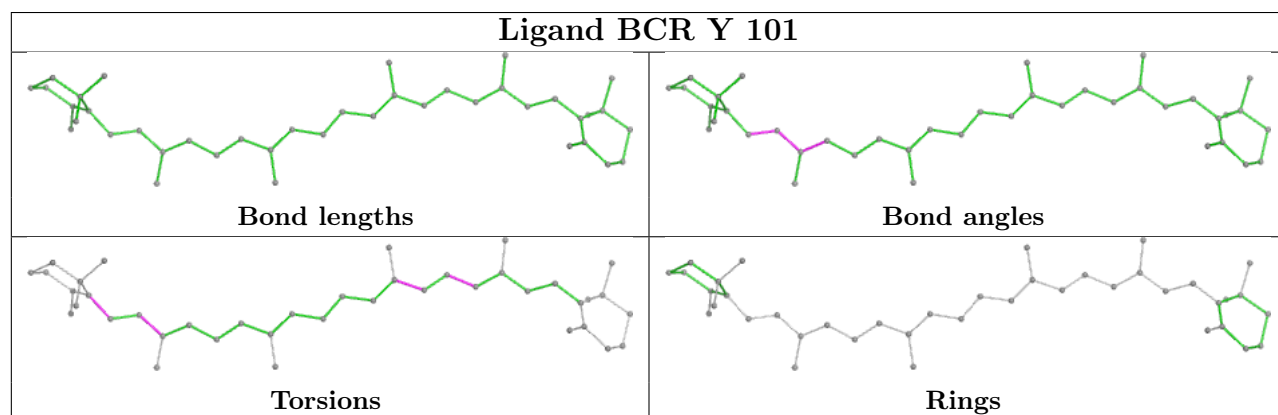
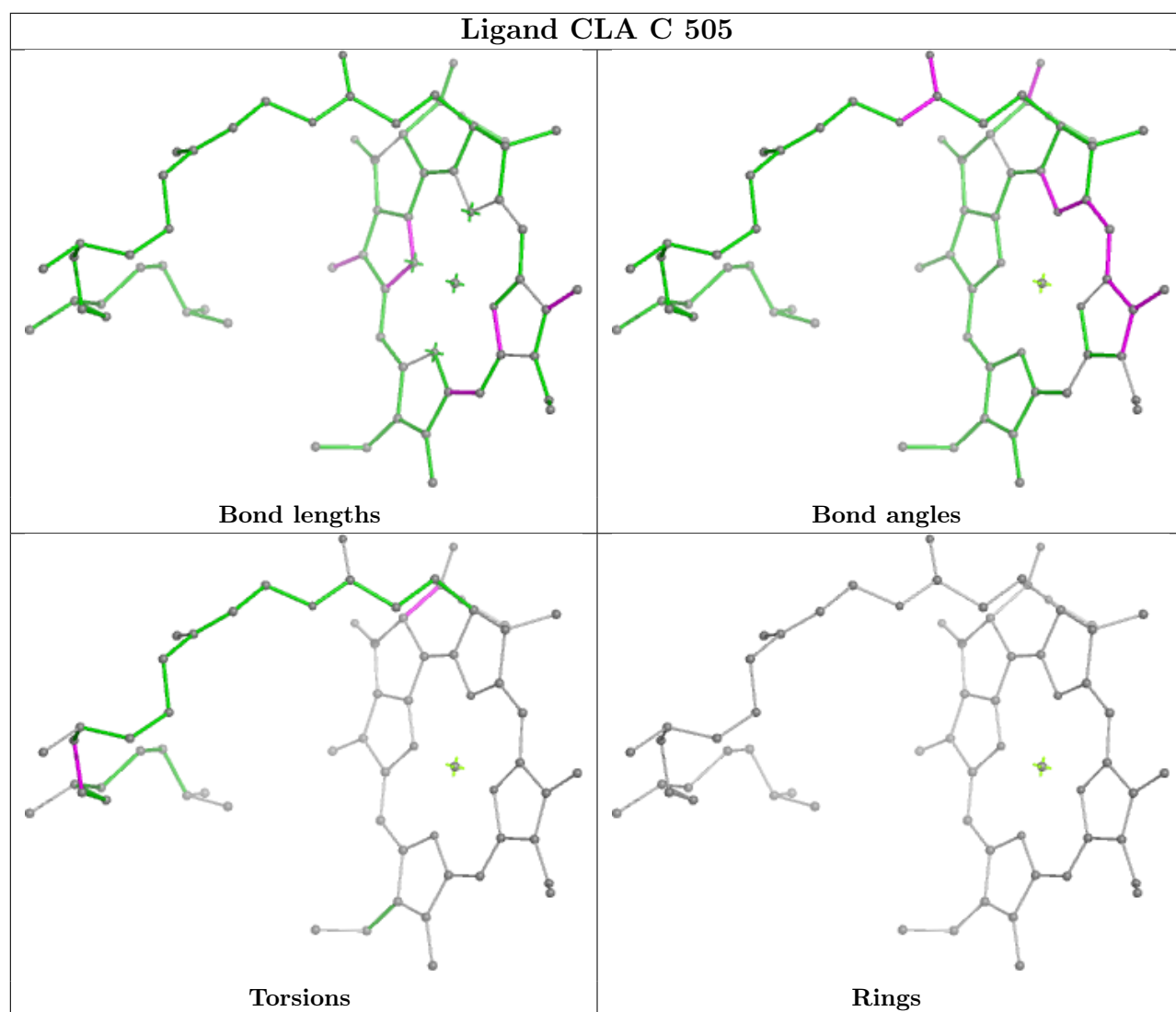


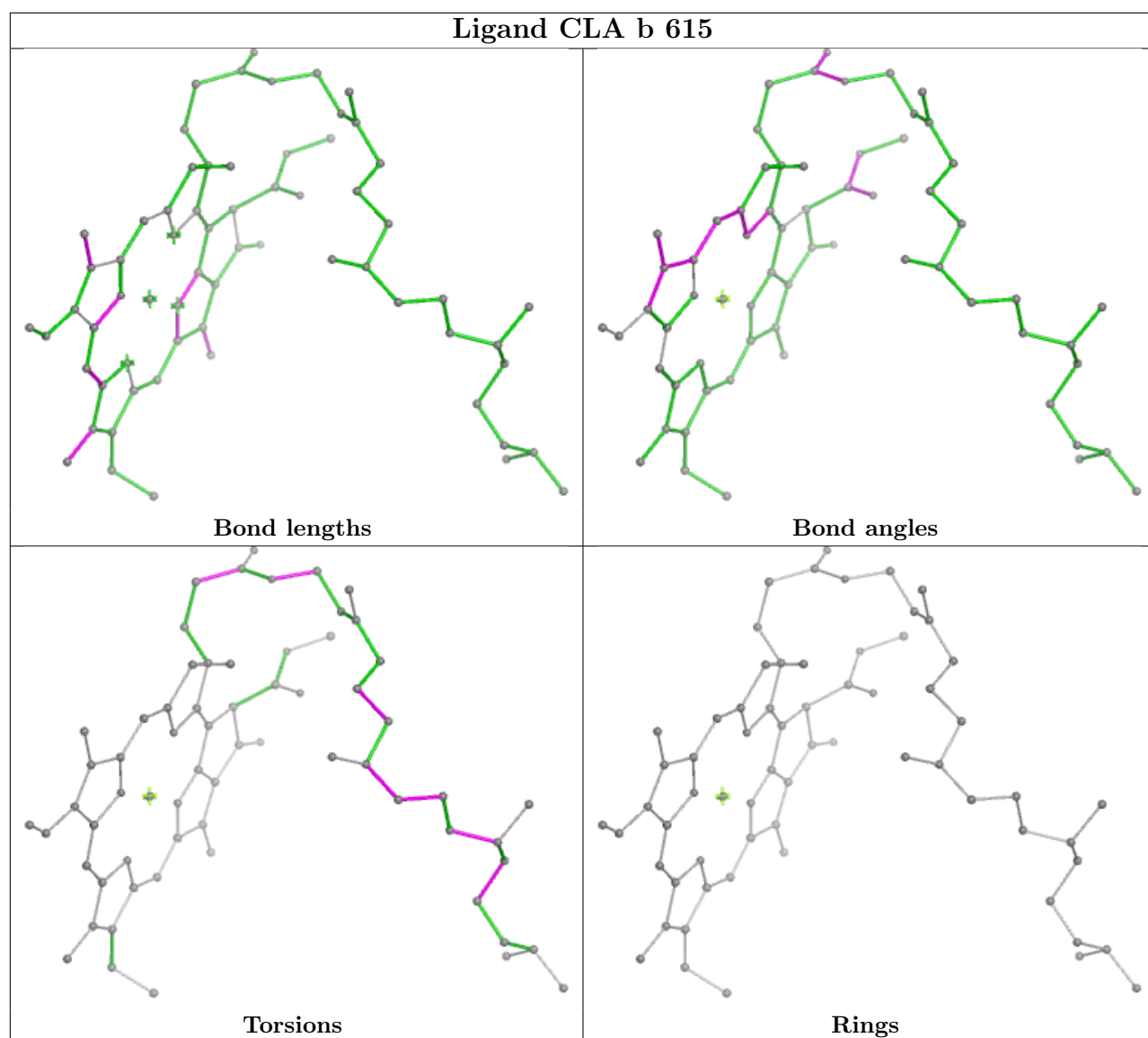
## Ligand CLA B 611

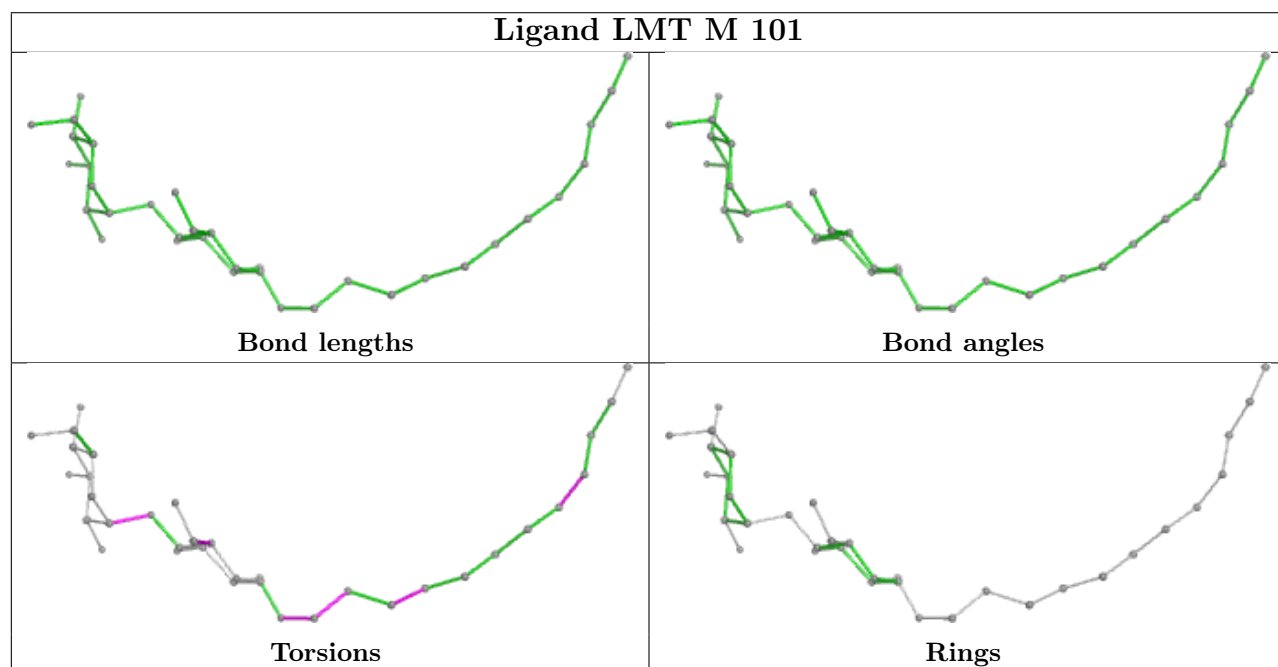
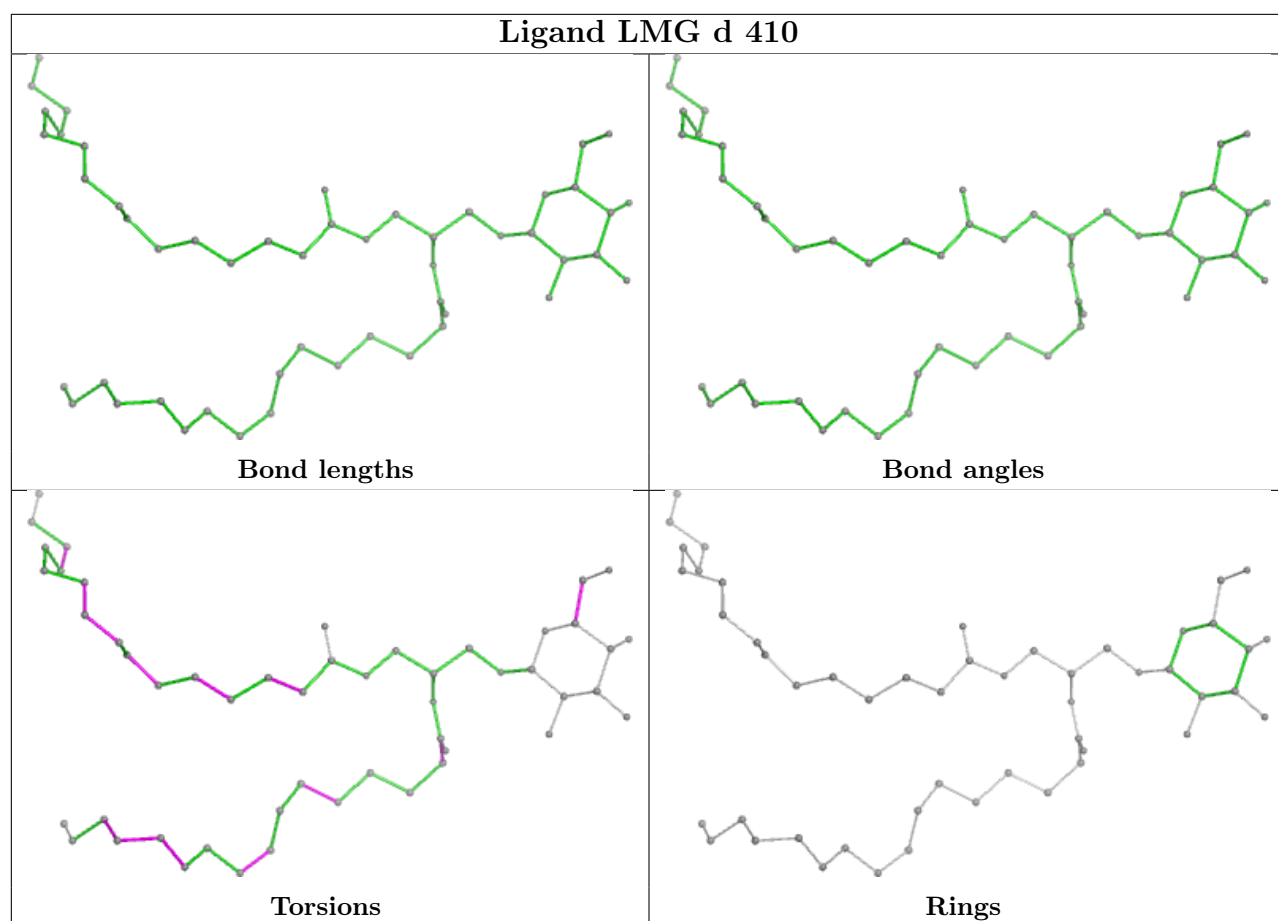


## Ligand CLA B 615

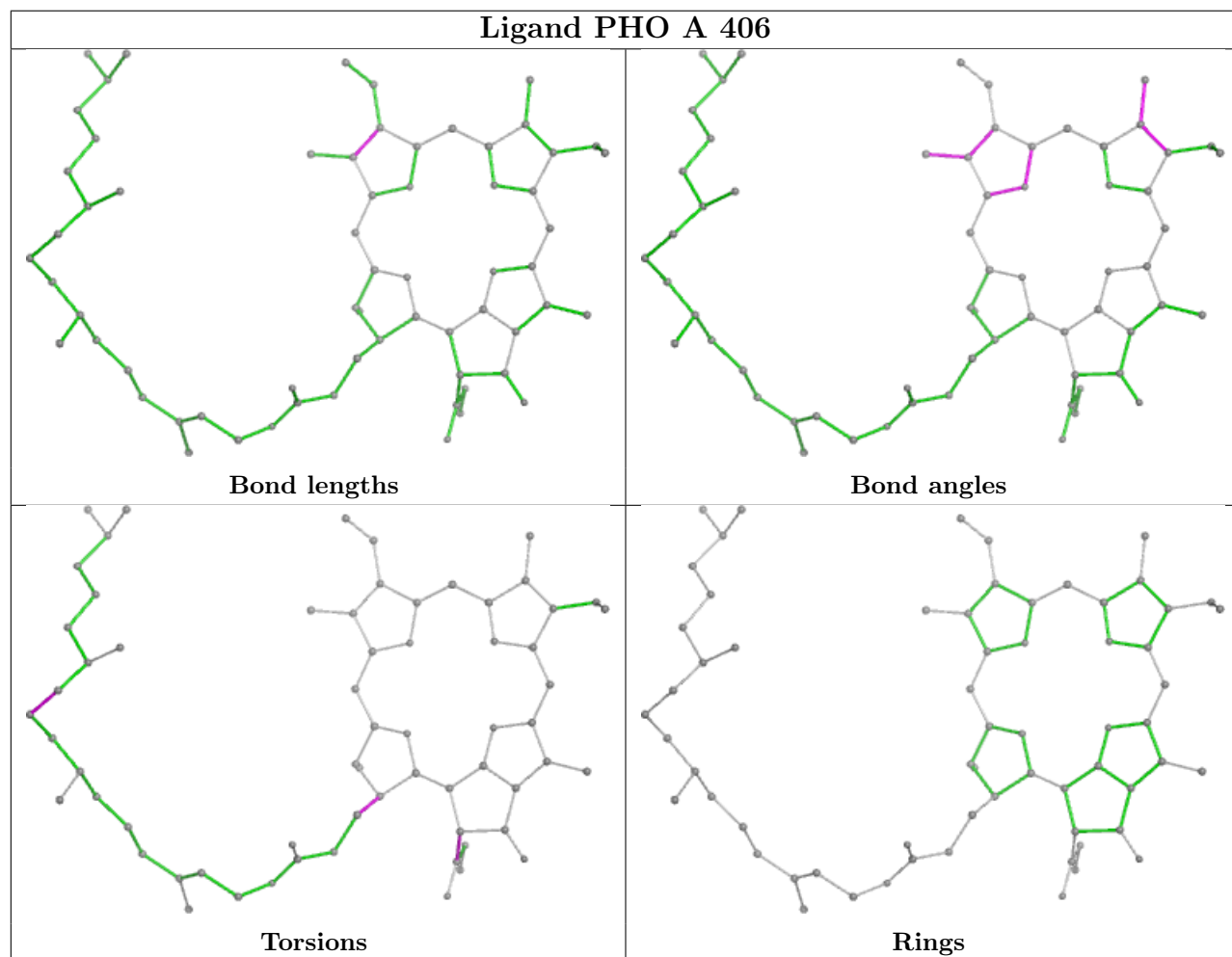
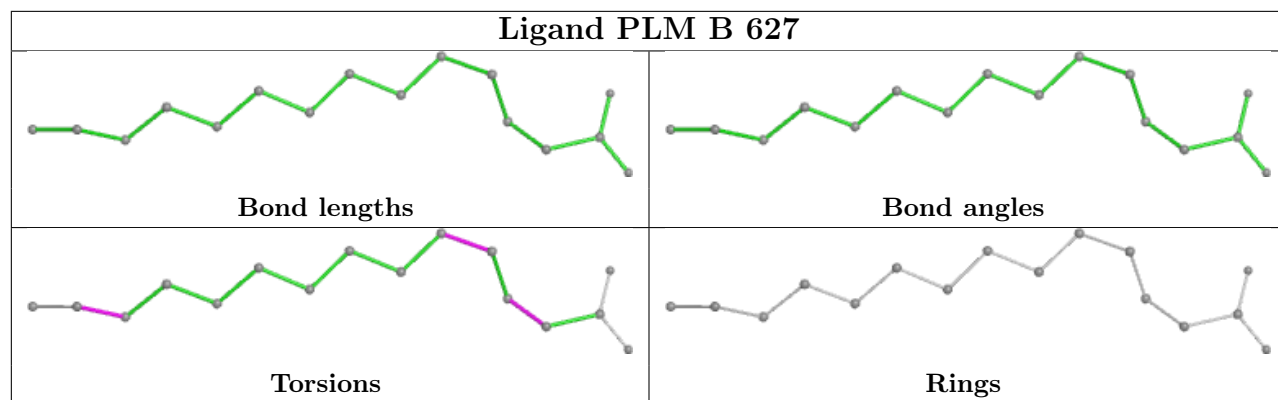


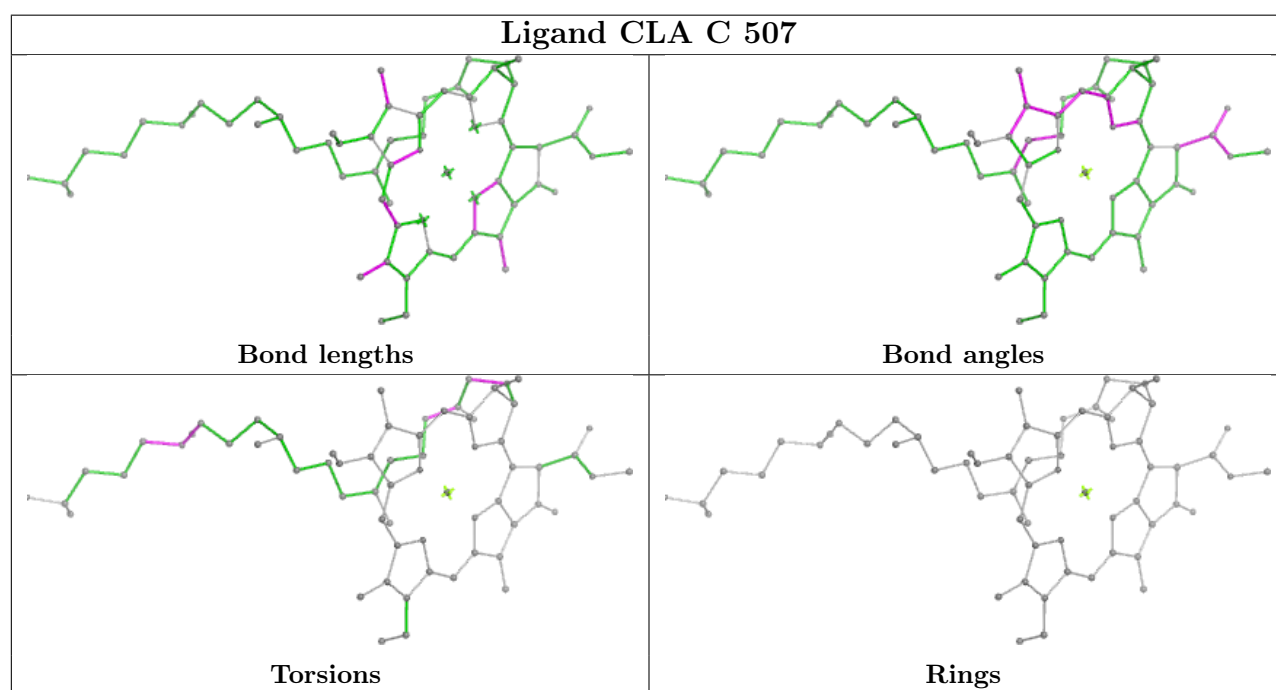
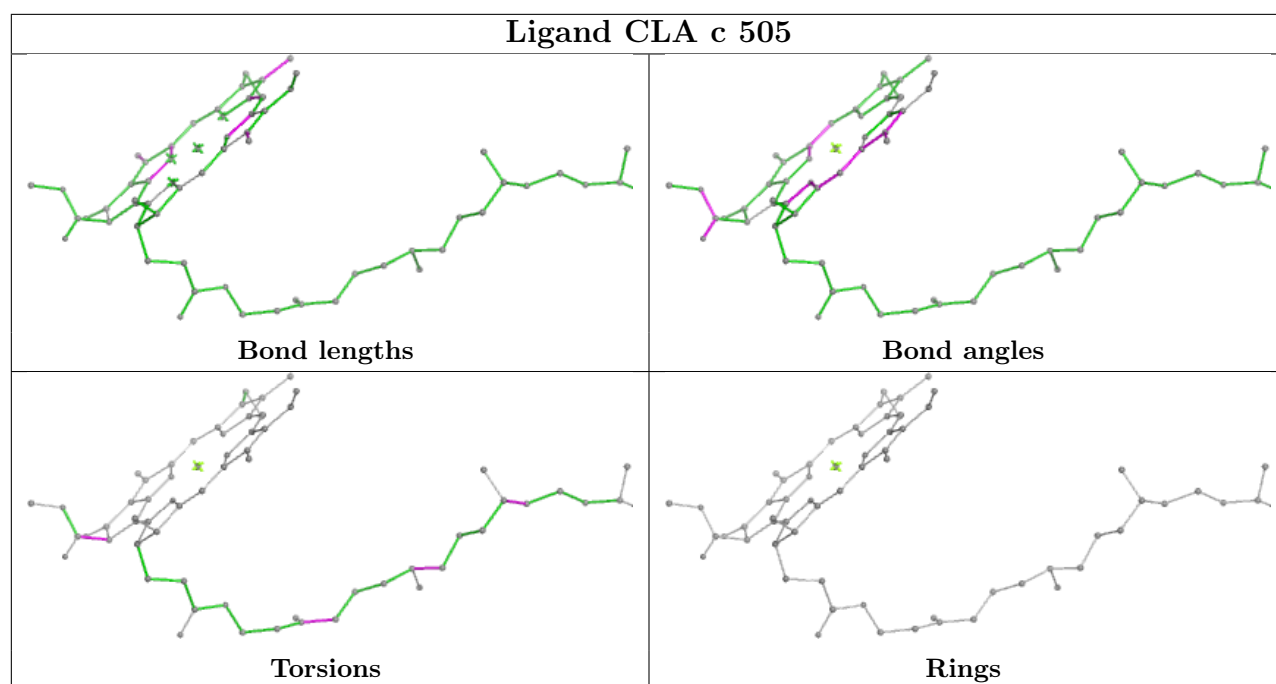


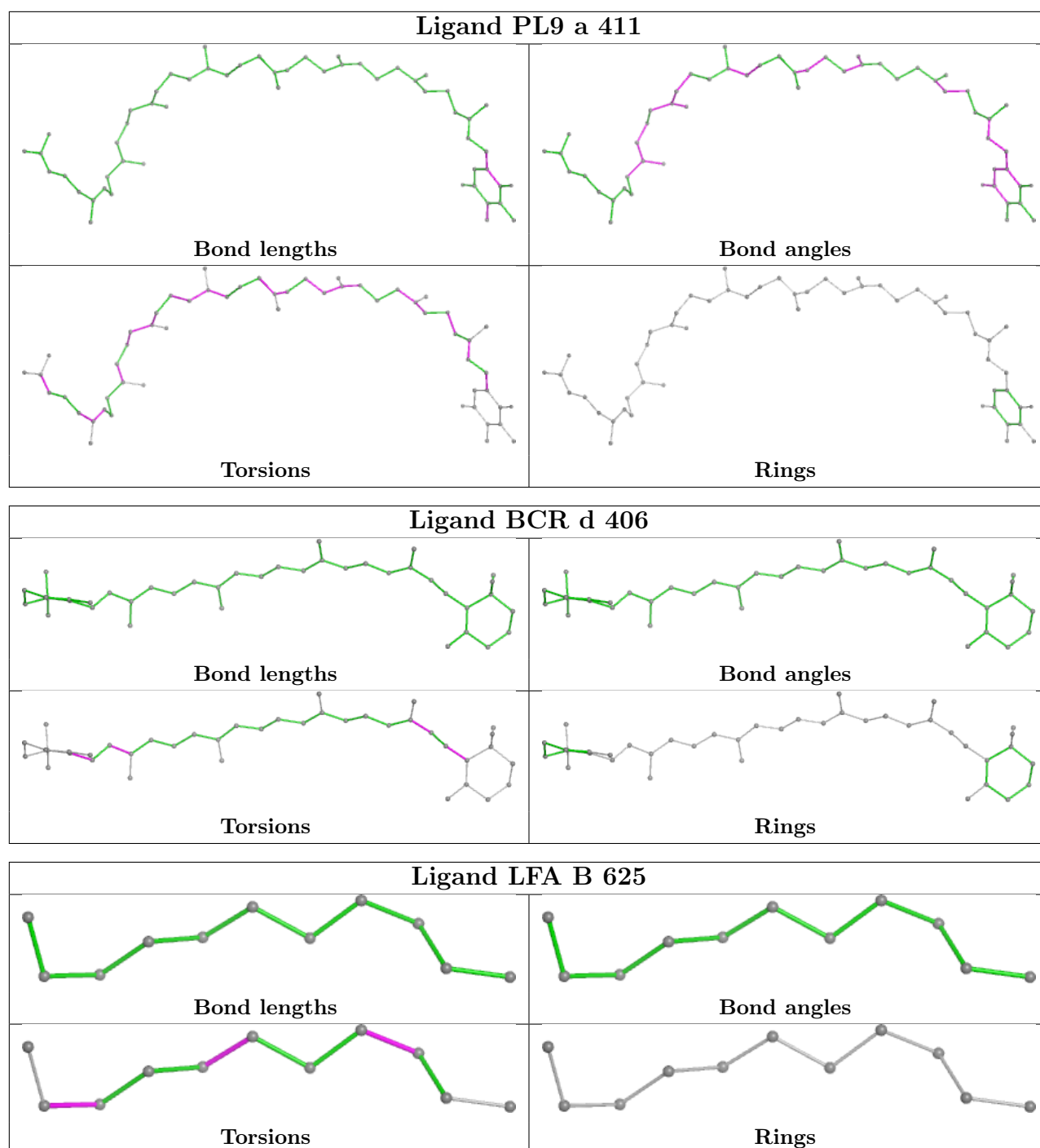


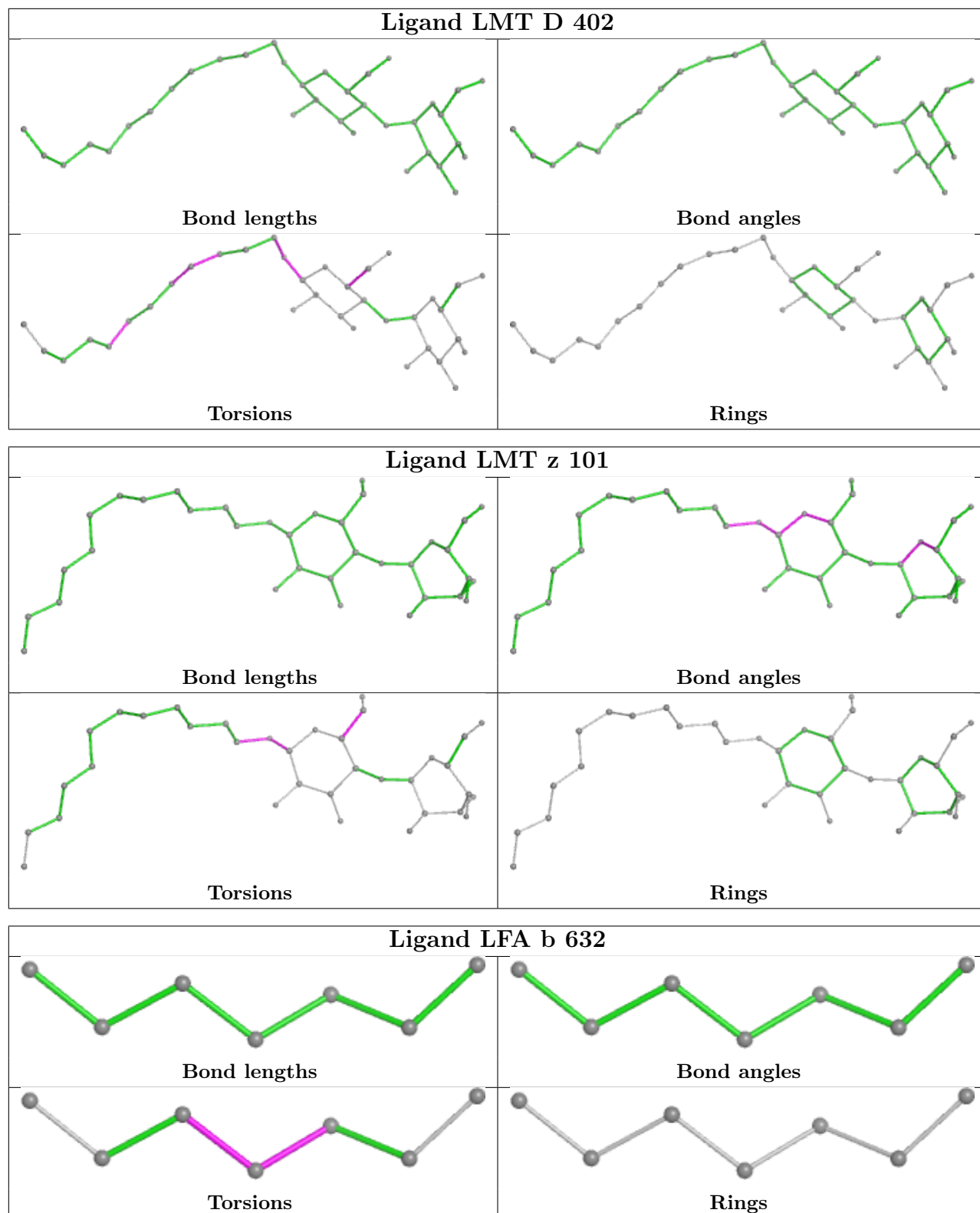


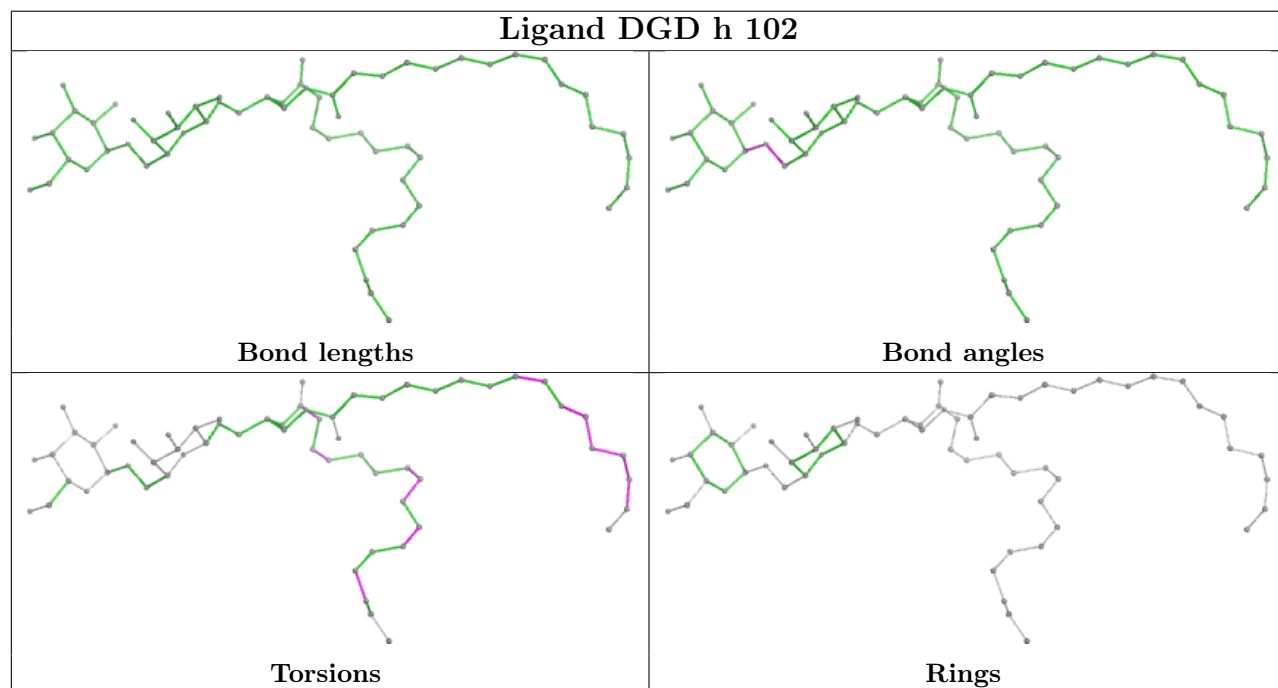
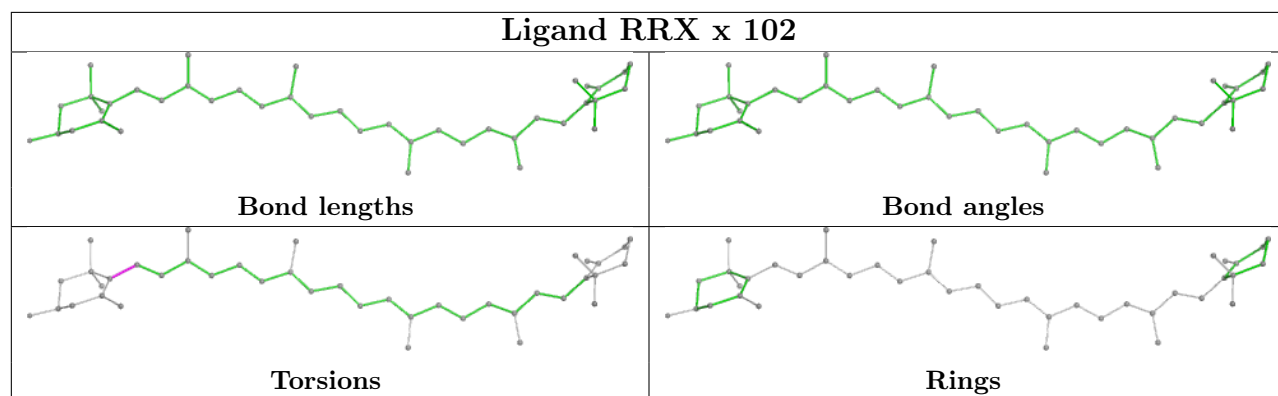
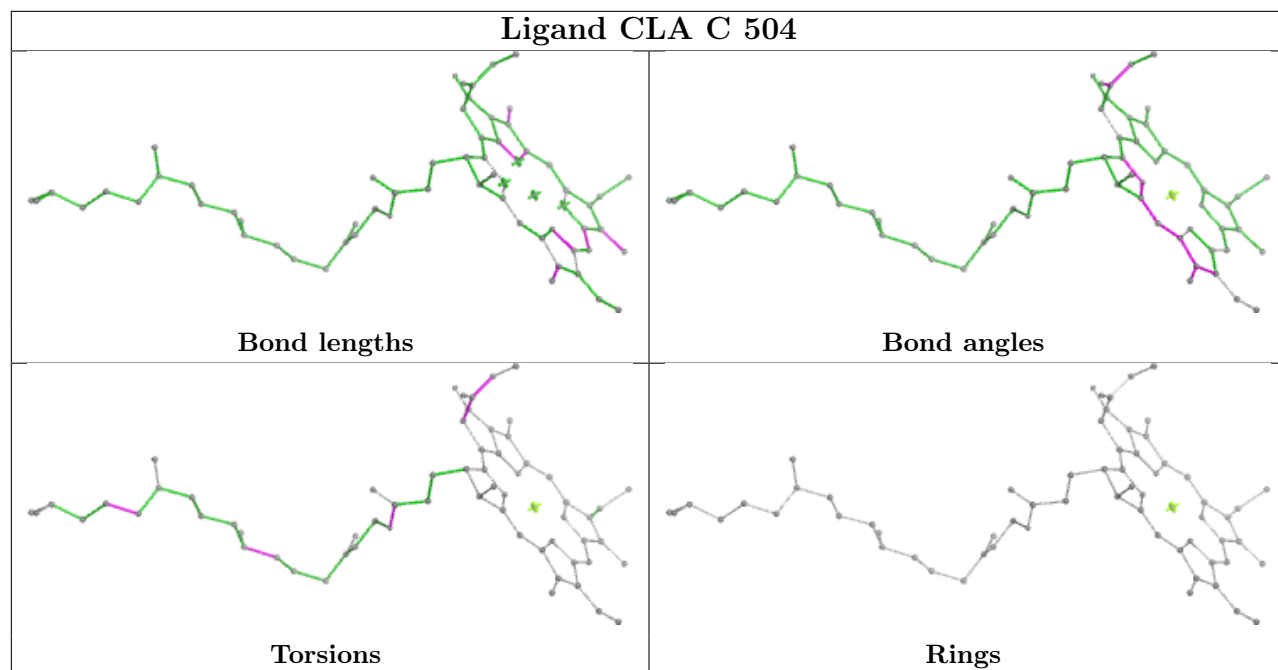




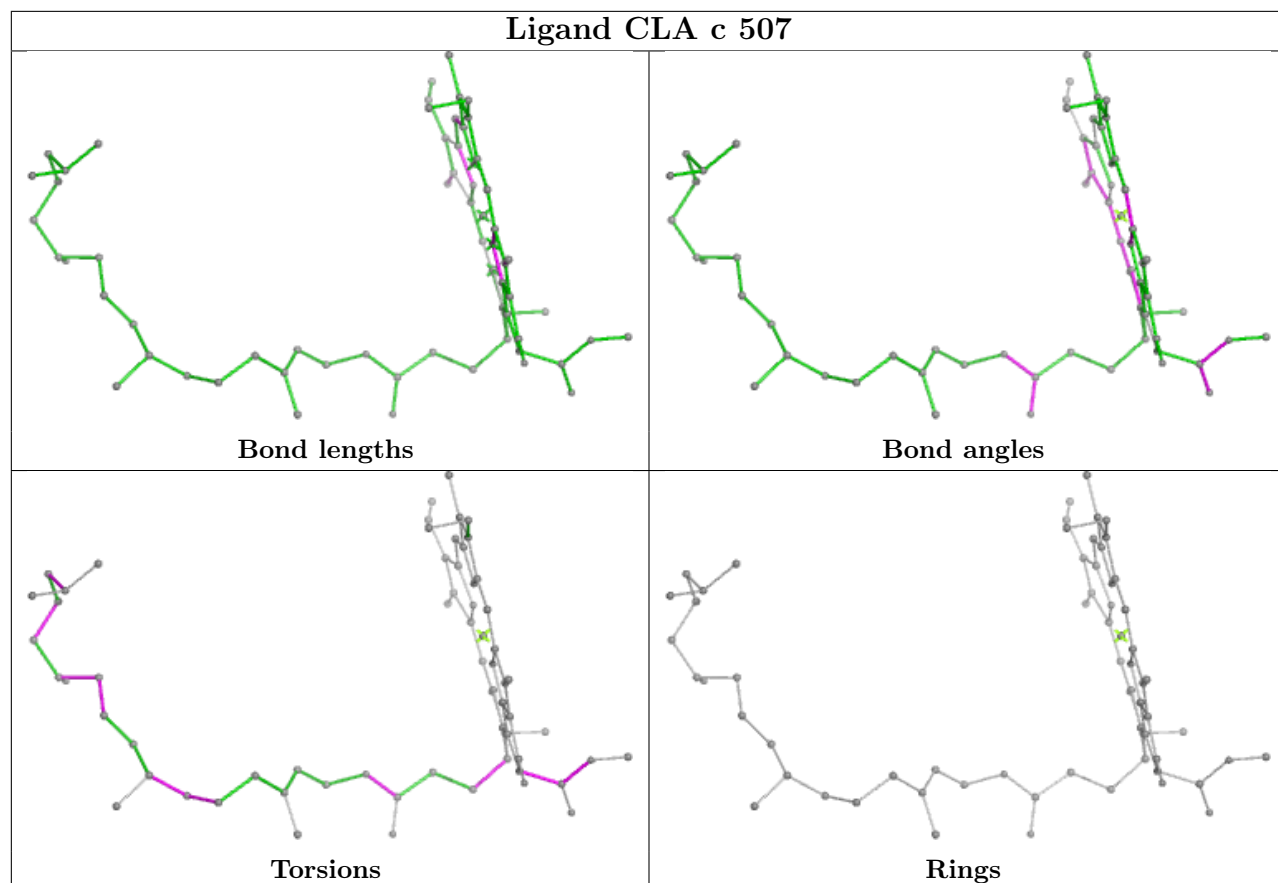




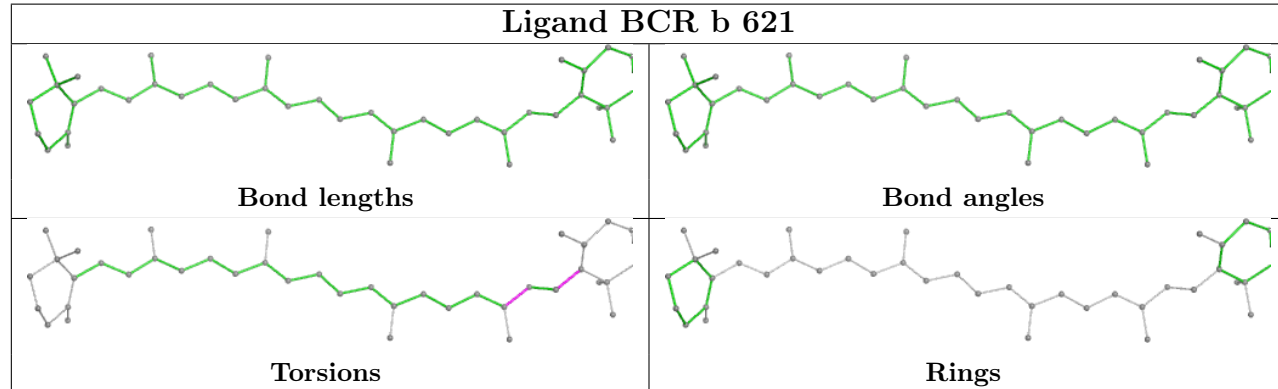


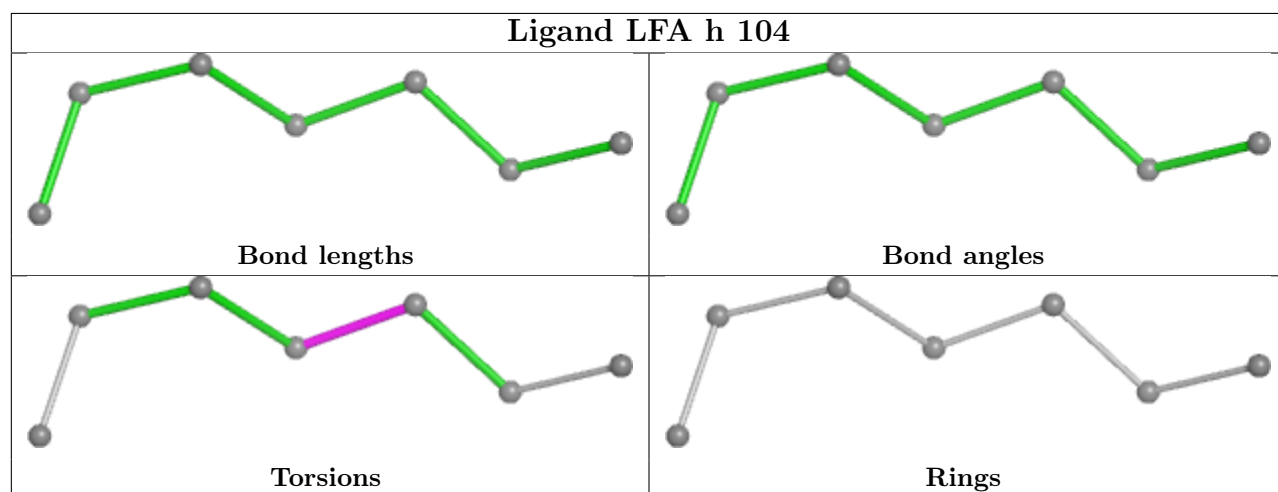
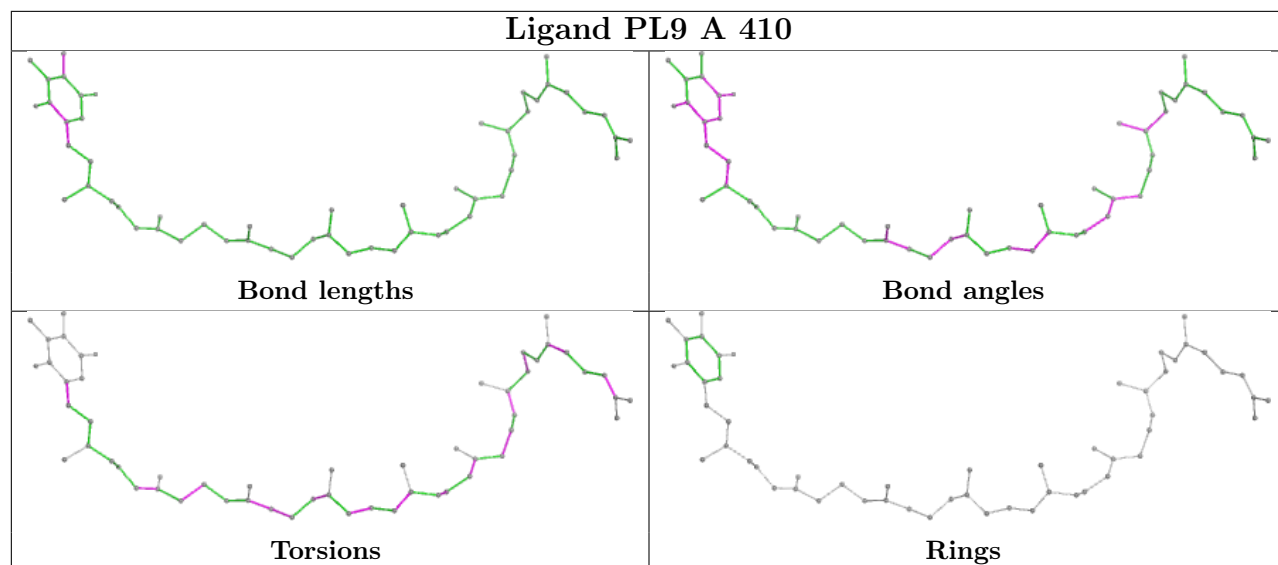


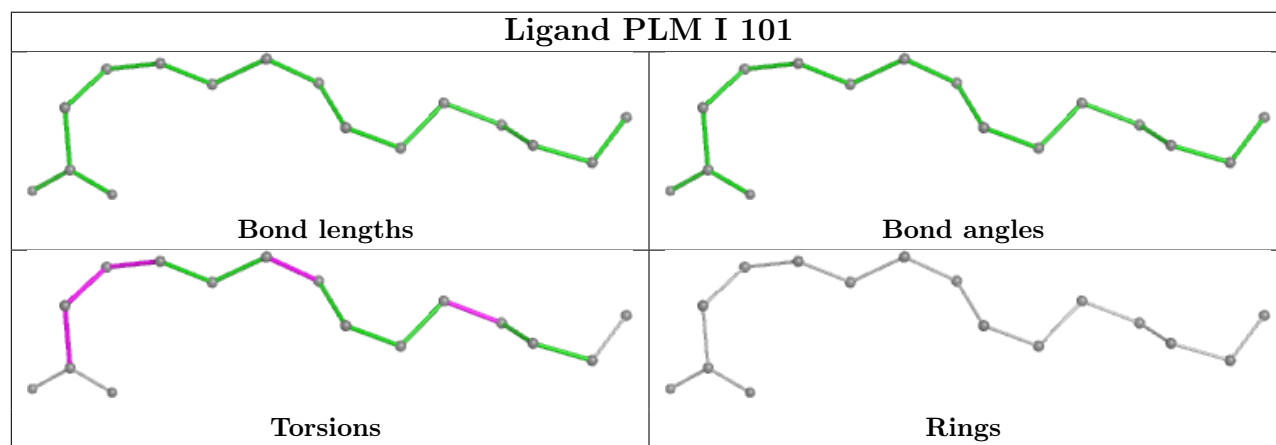
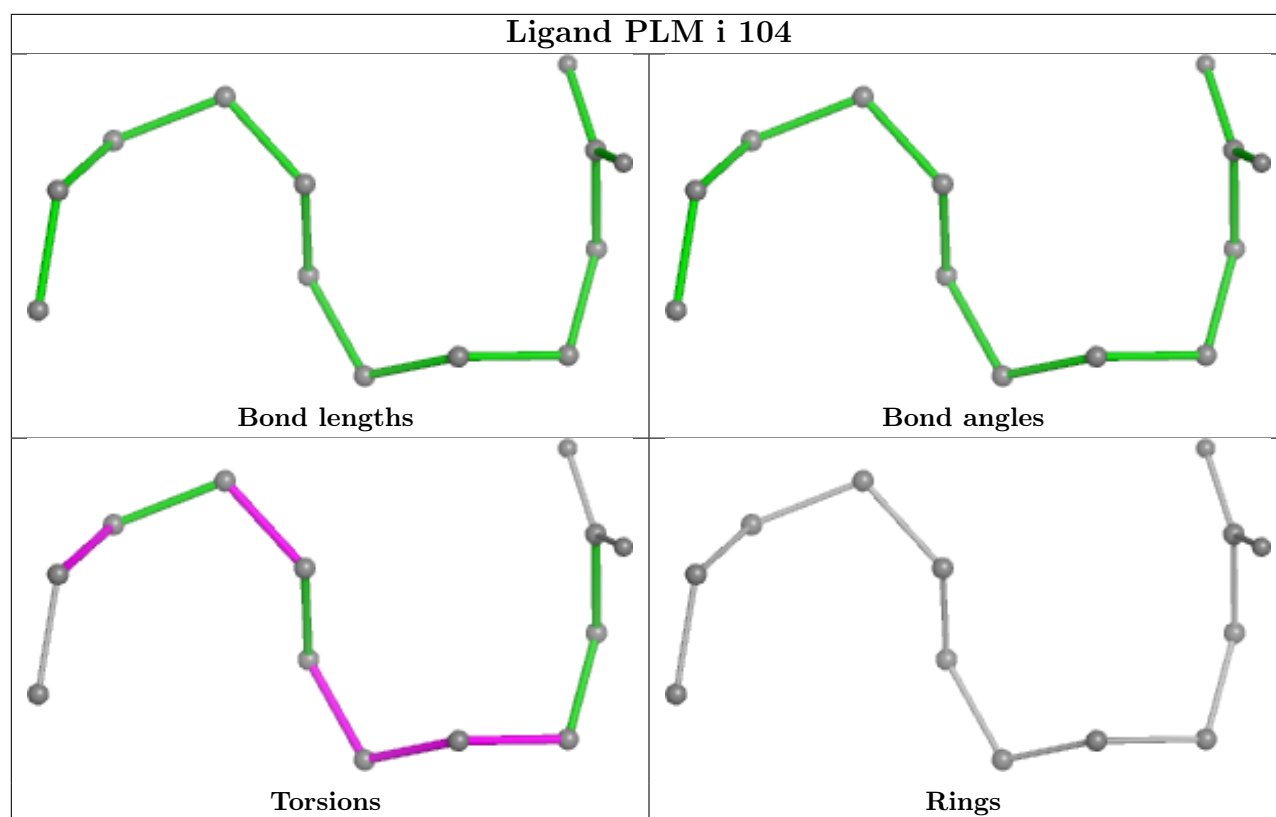
## Ligand CLA c 507



## Ligand BCR b 621

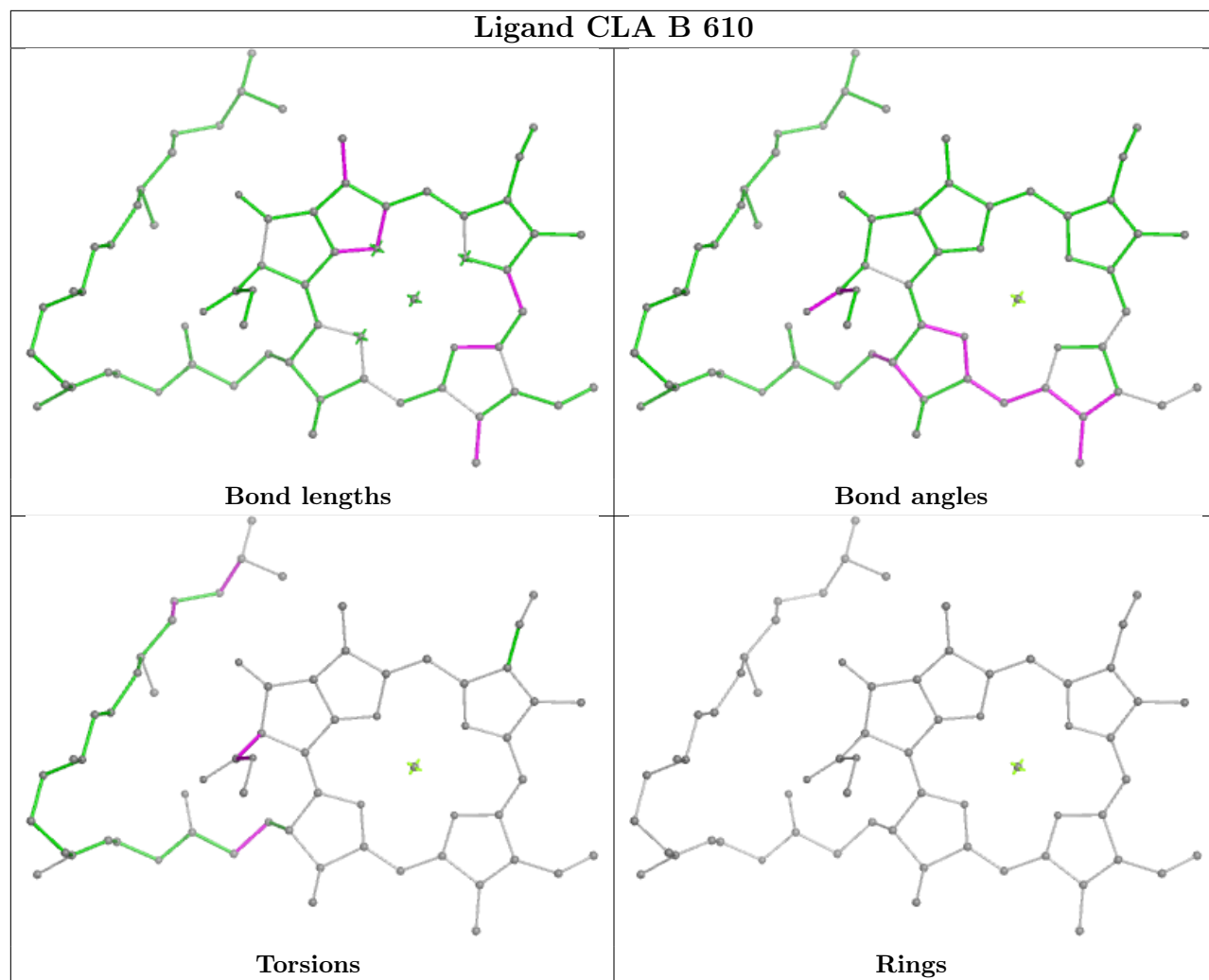


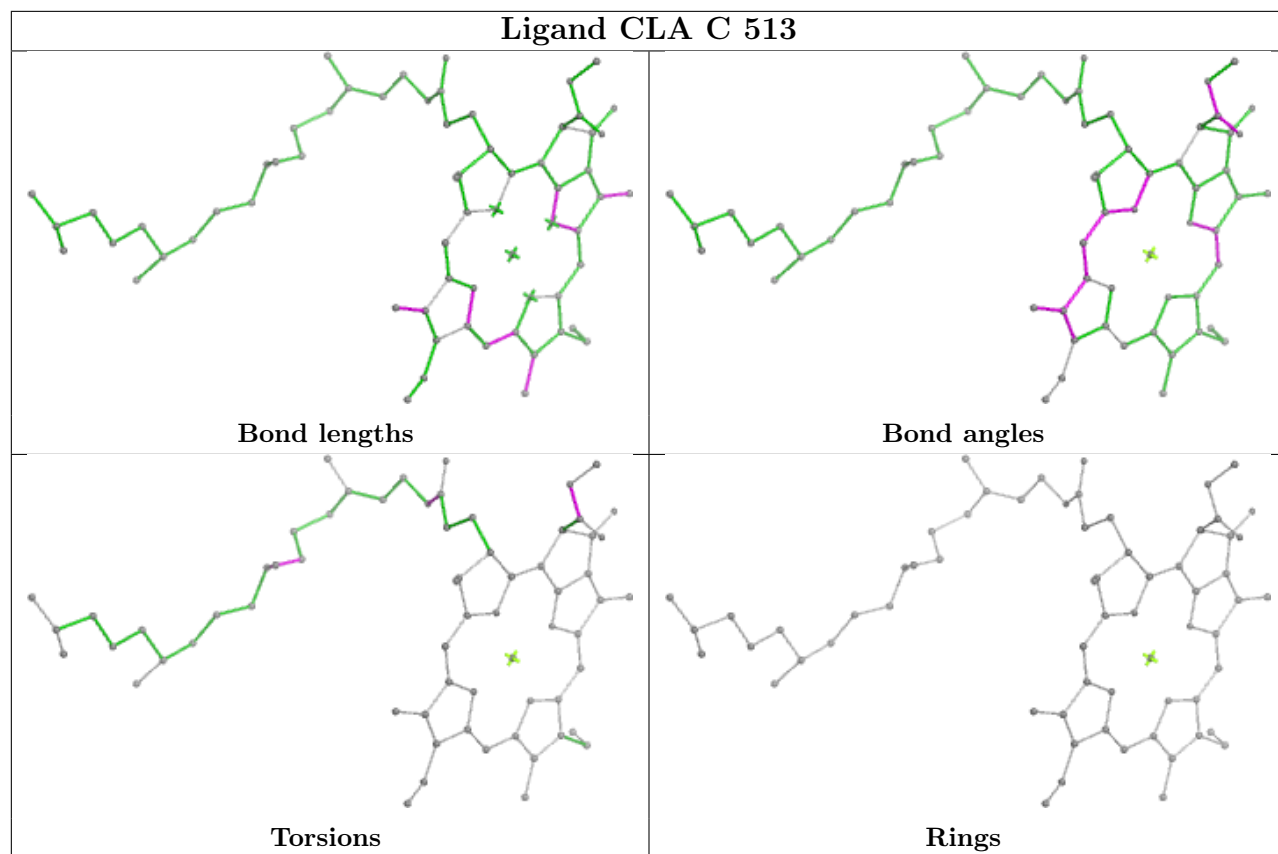


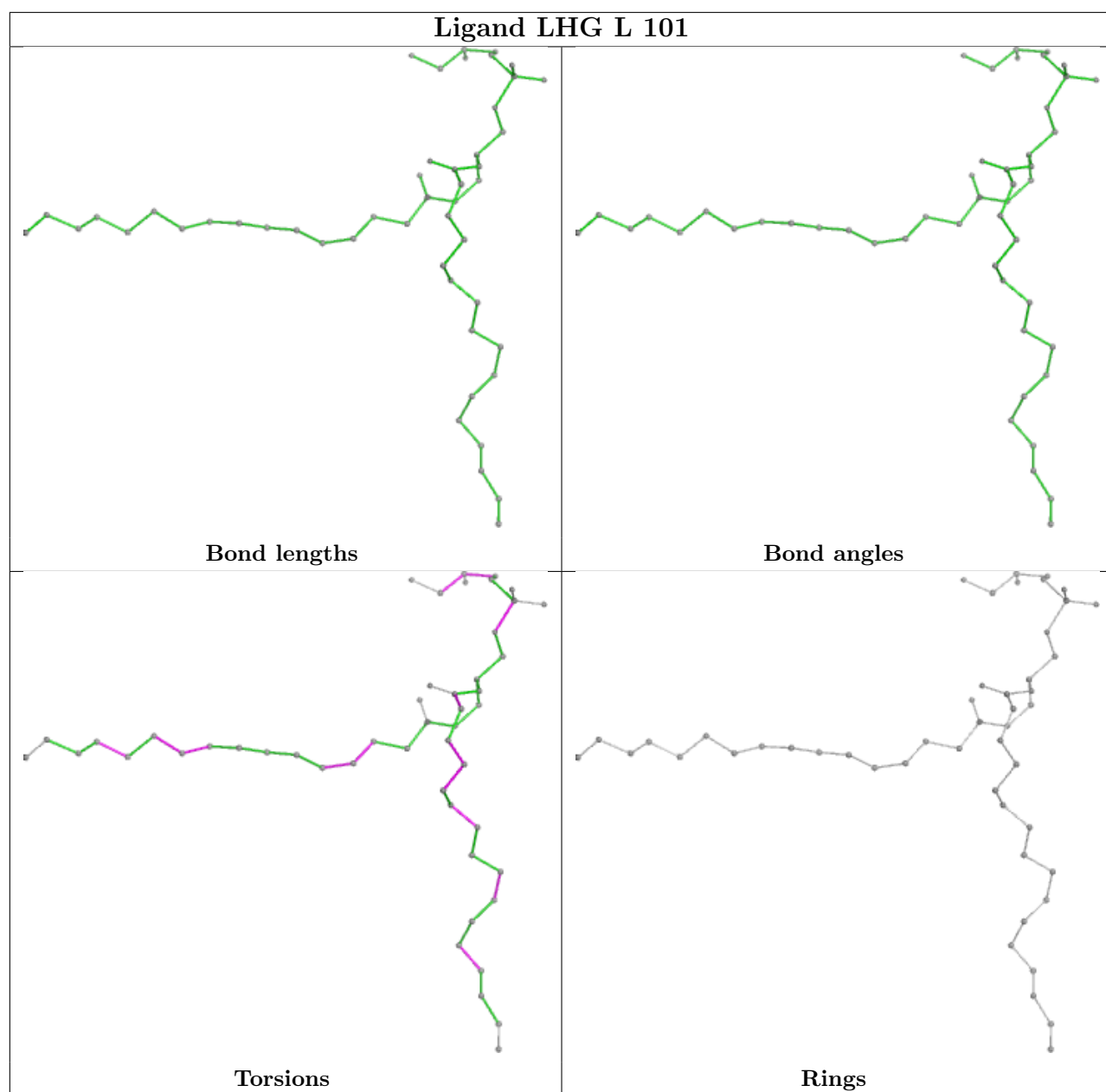


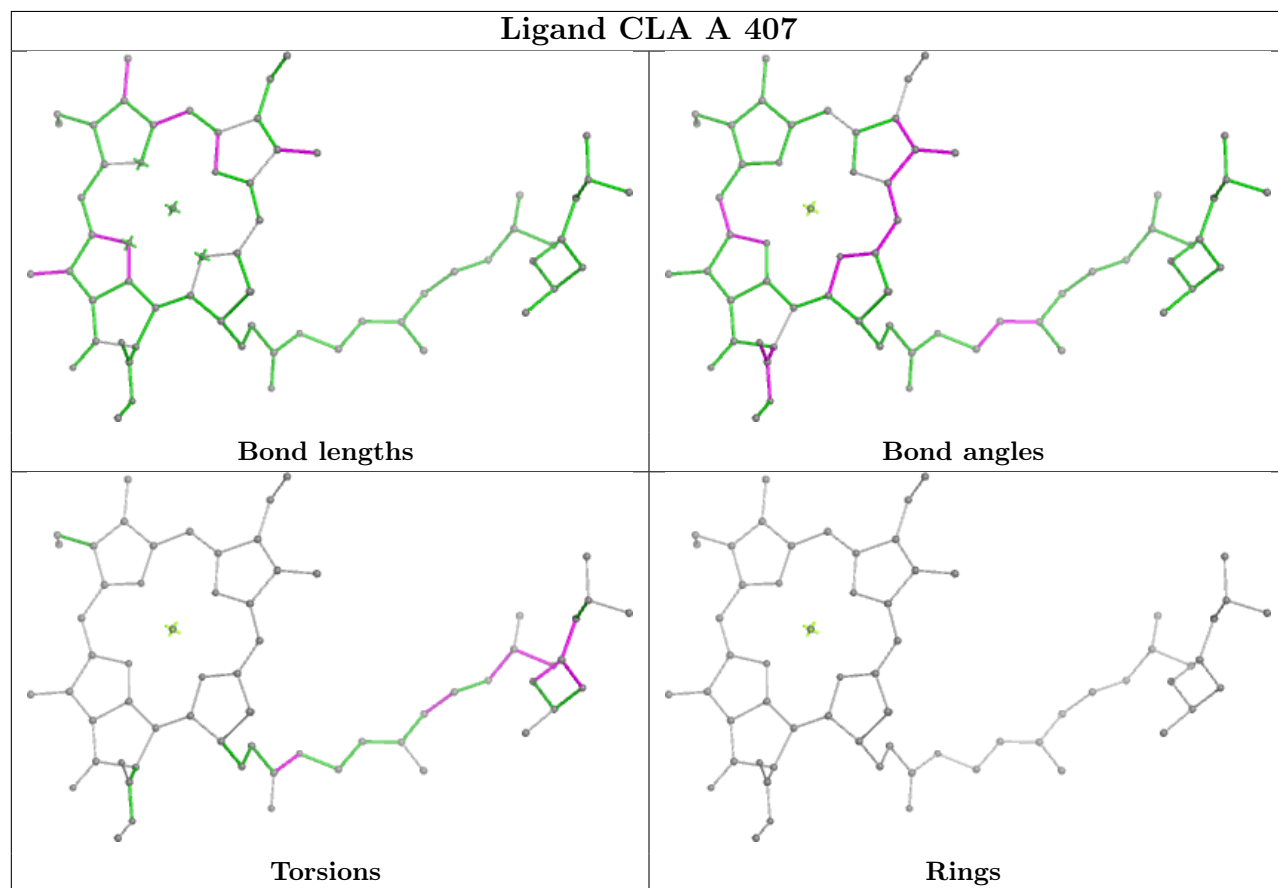
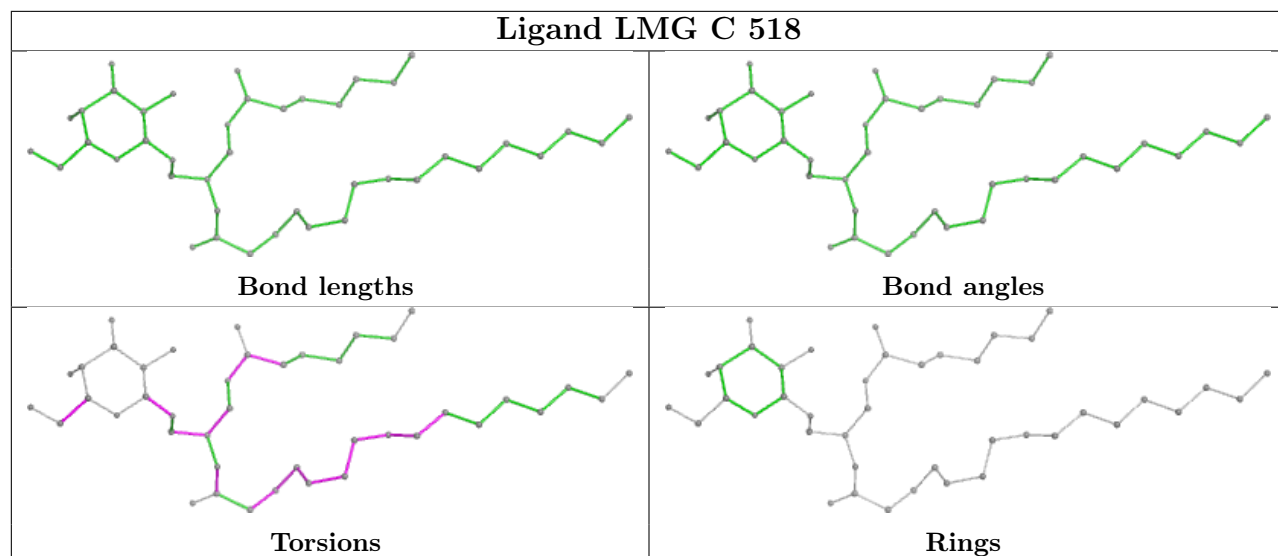


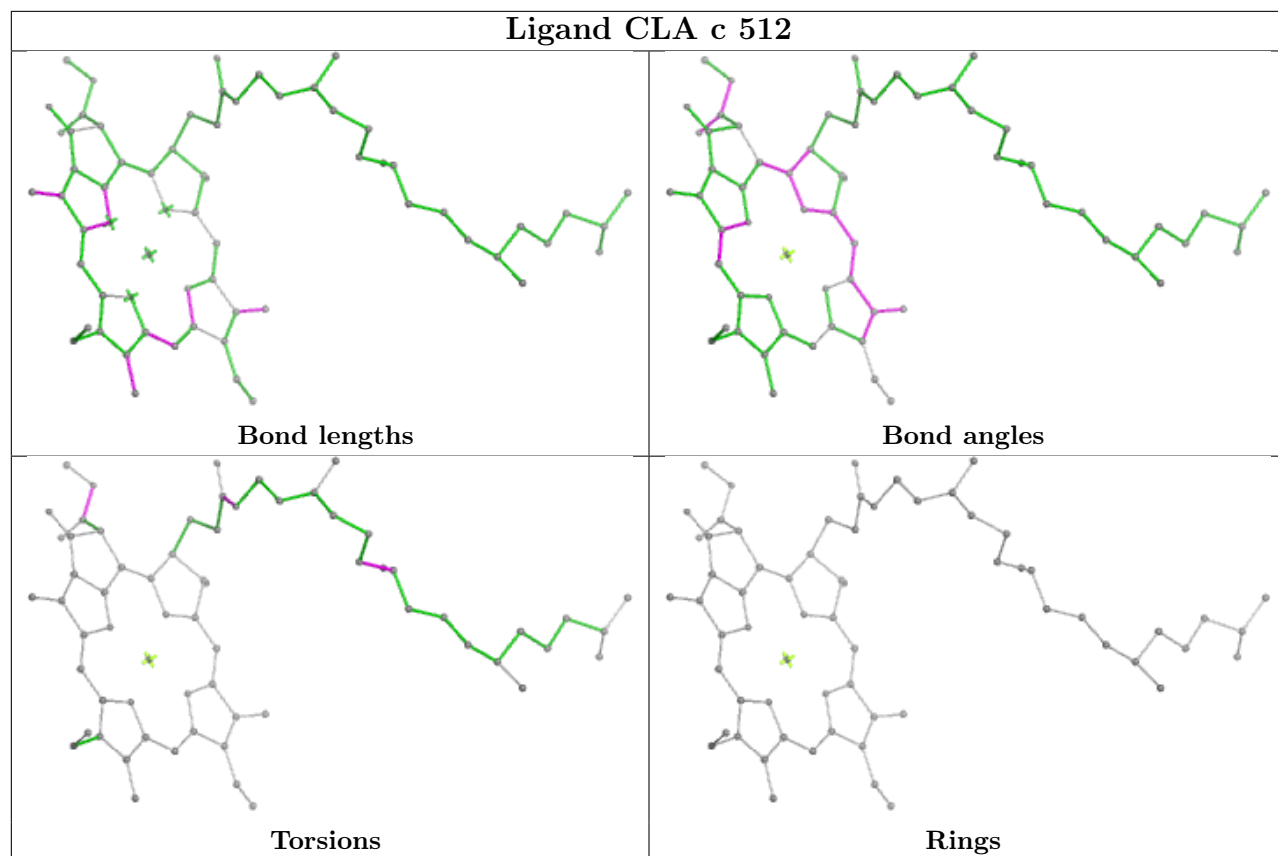
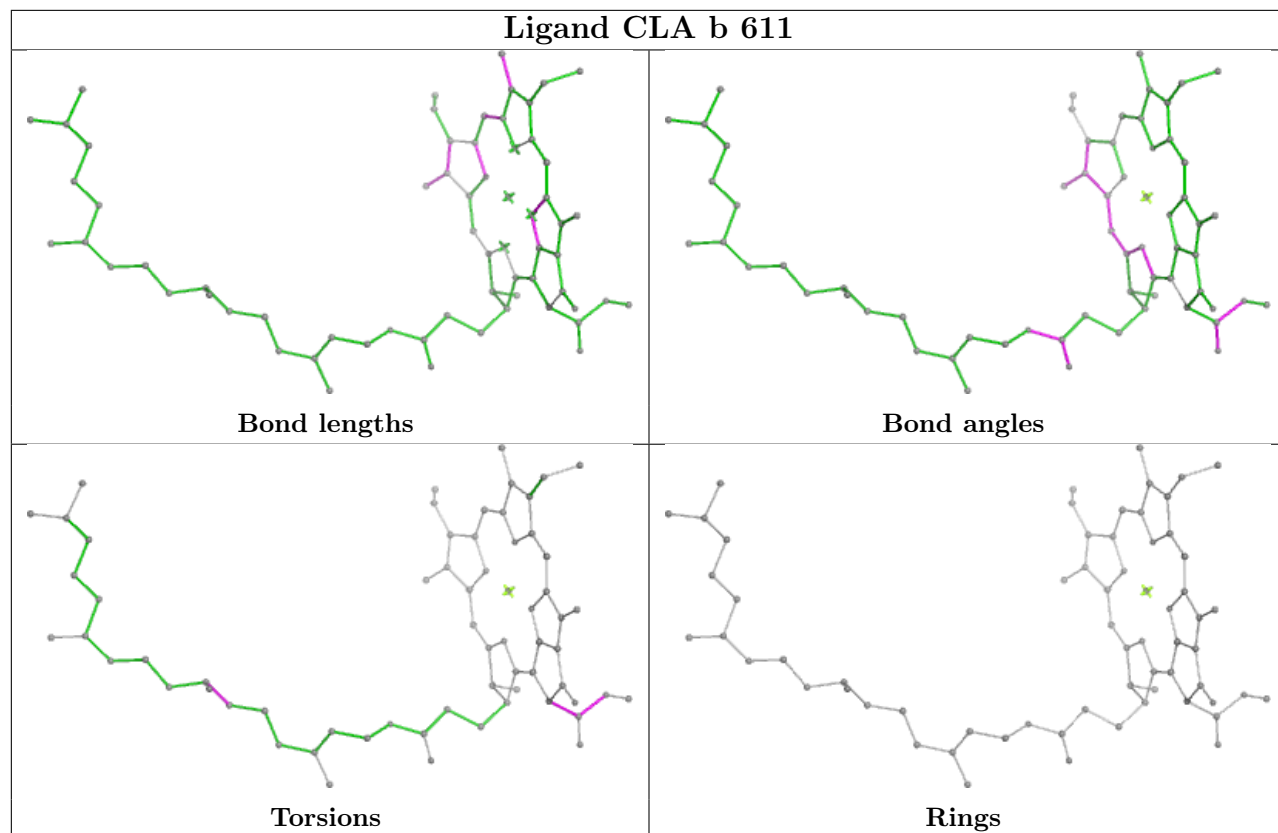
## Ligand CLA B 610

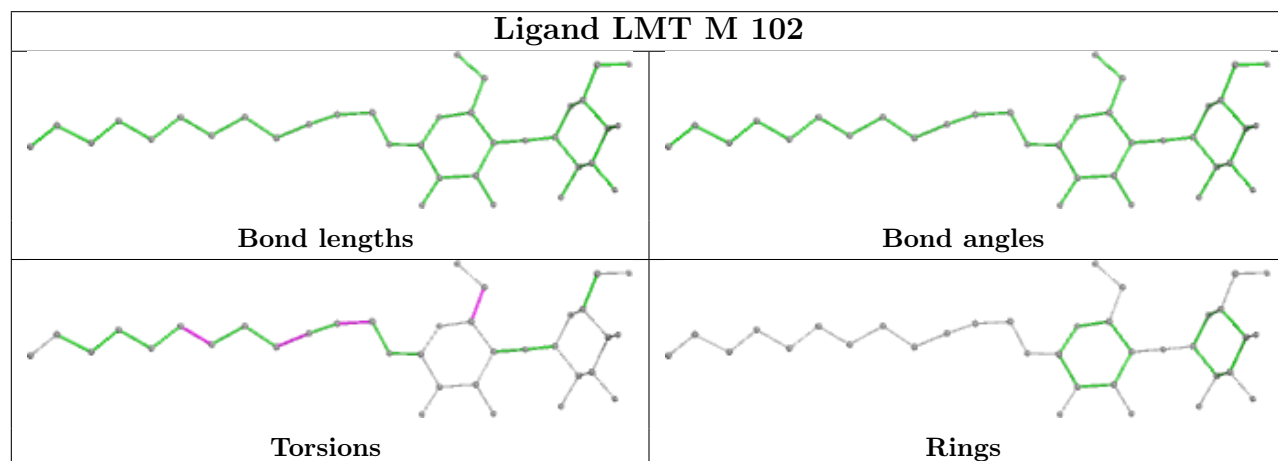
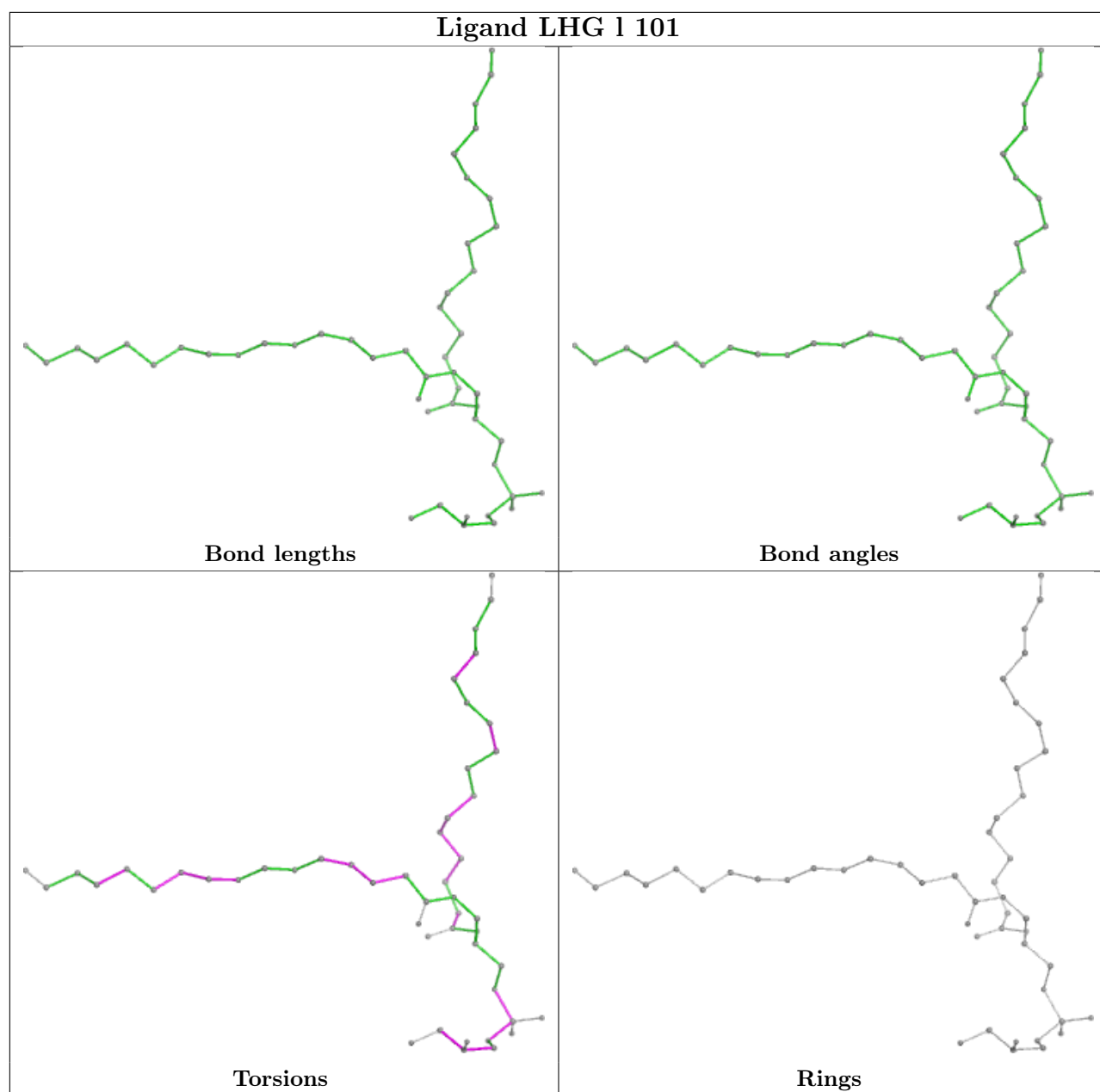


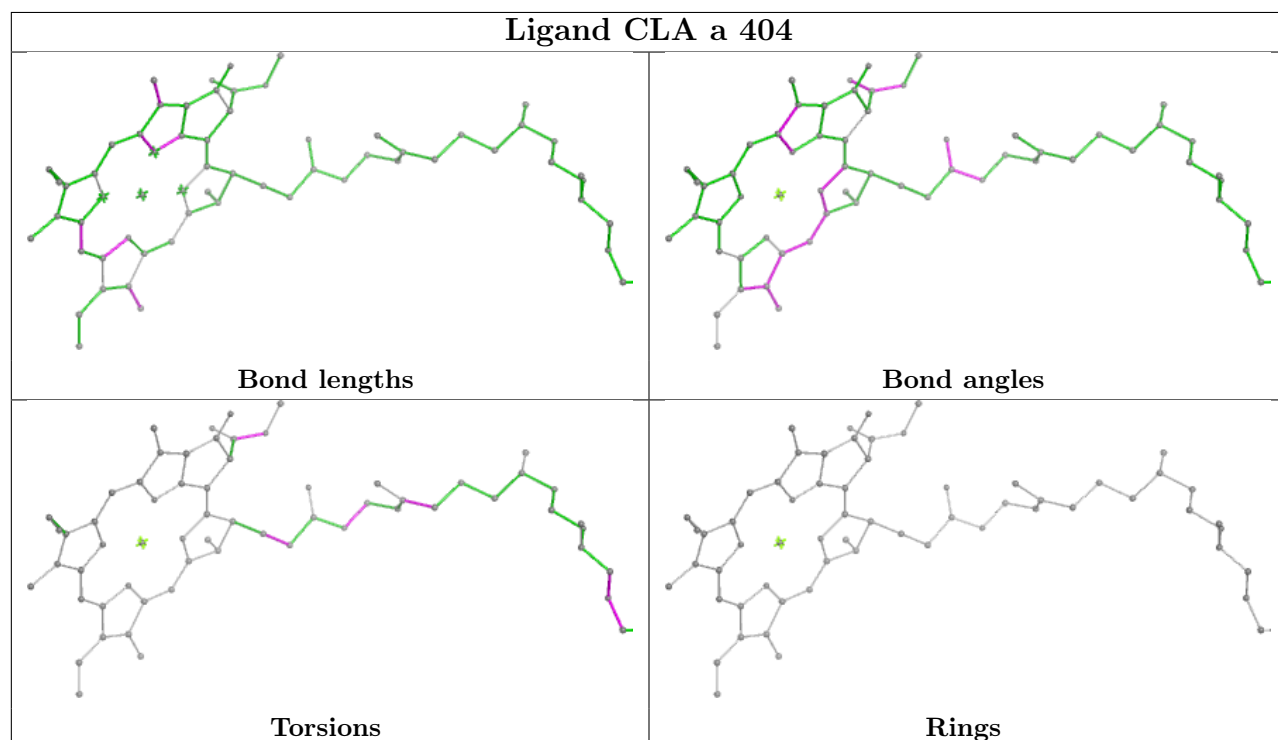
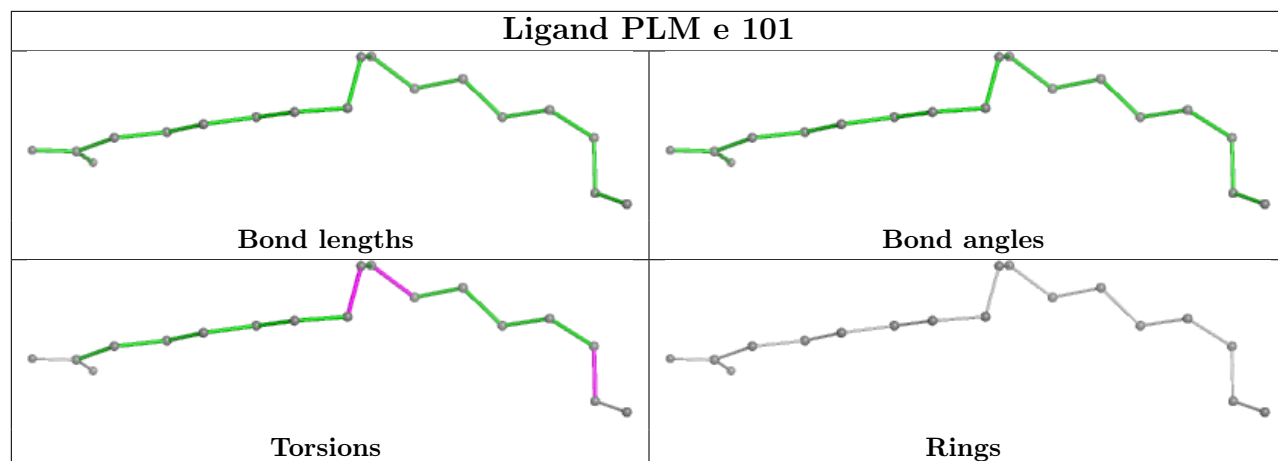


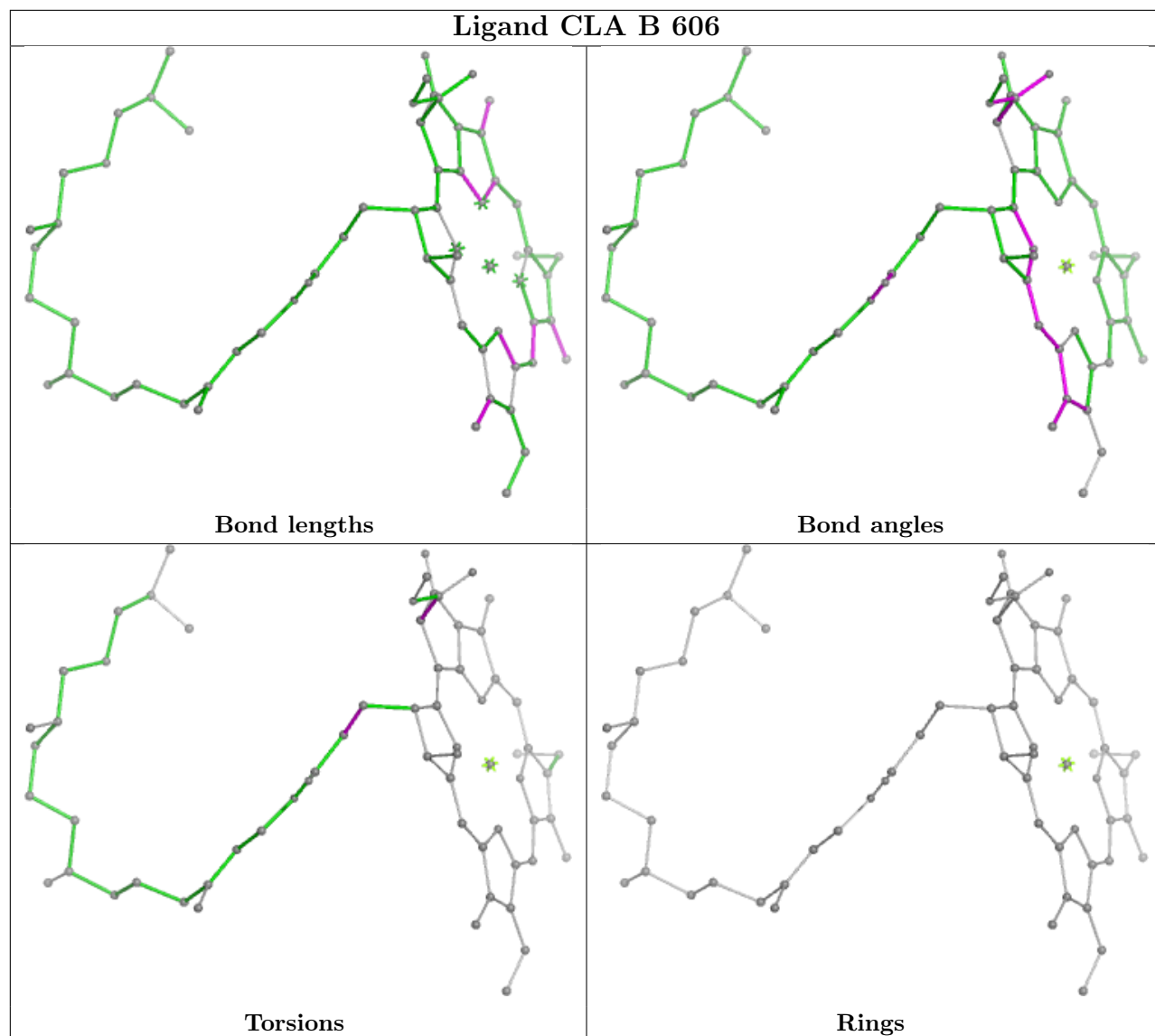




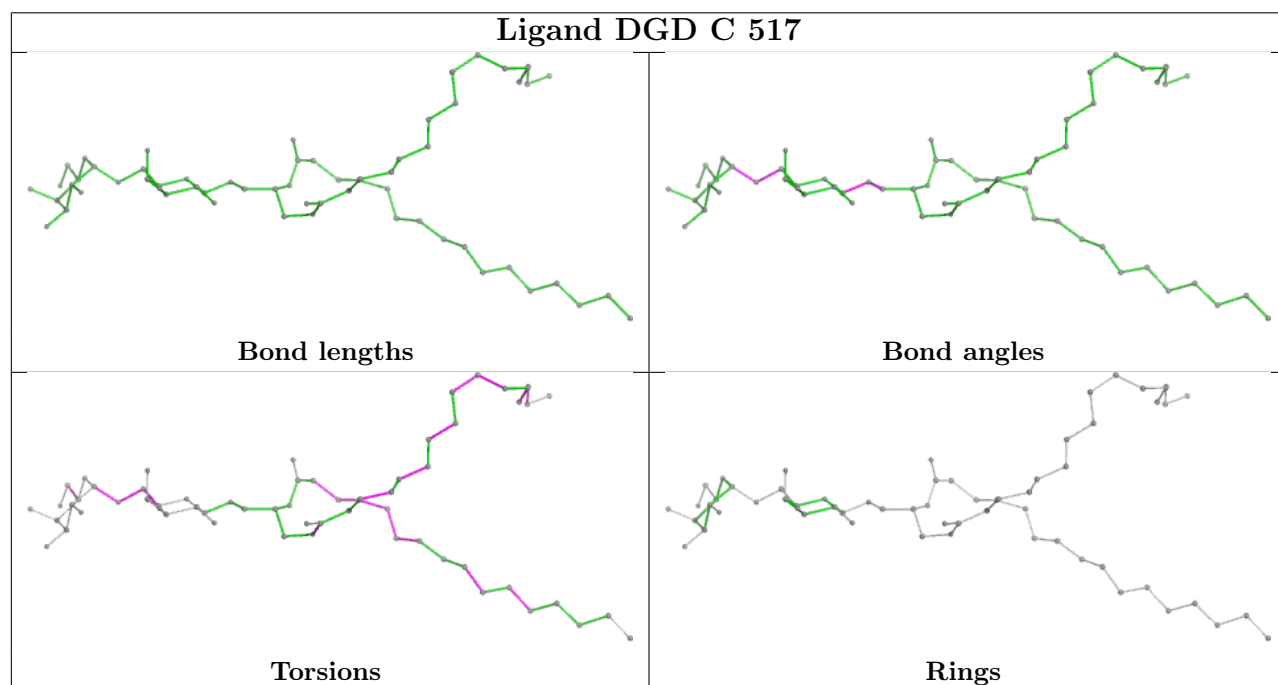
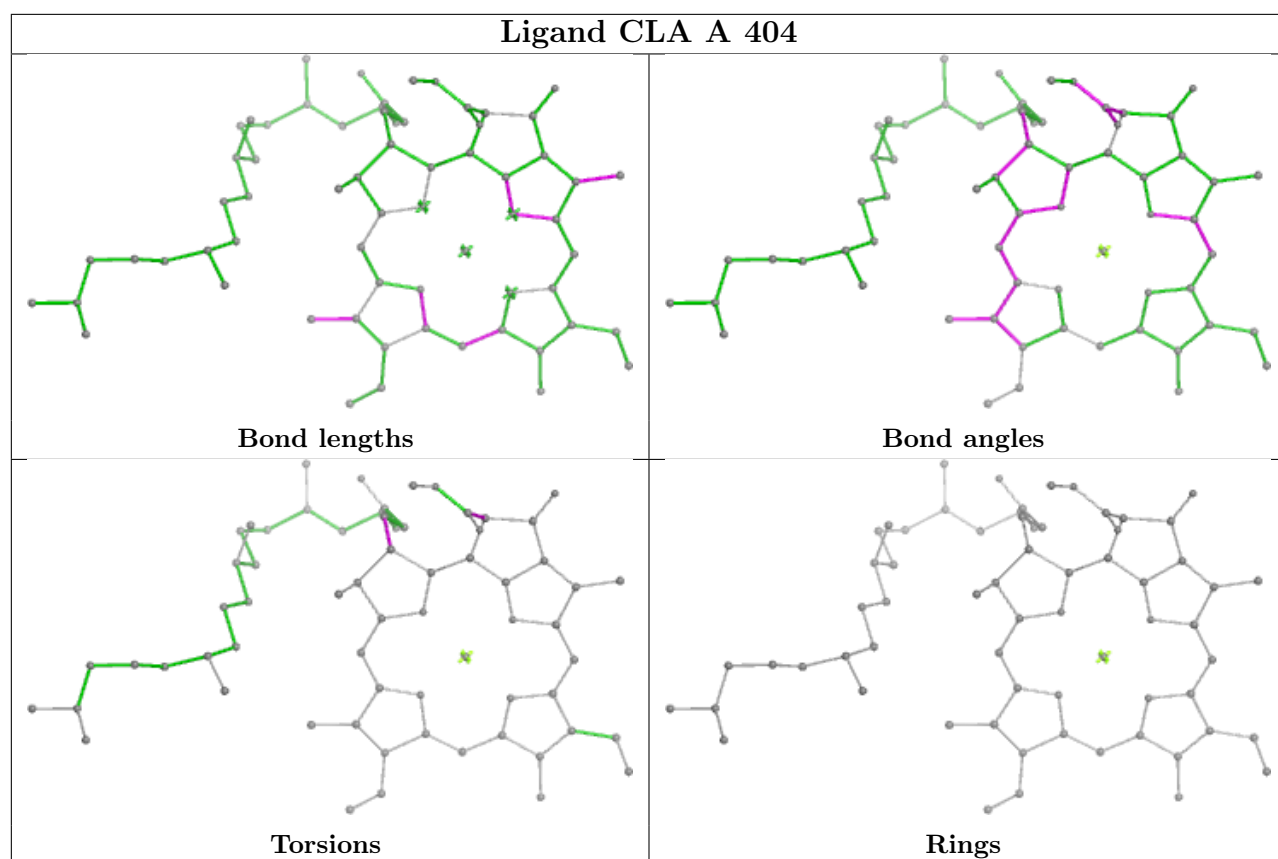
**Ligand CLA c 512****Ligand CLA b 611**

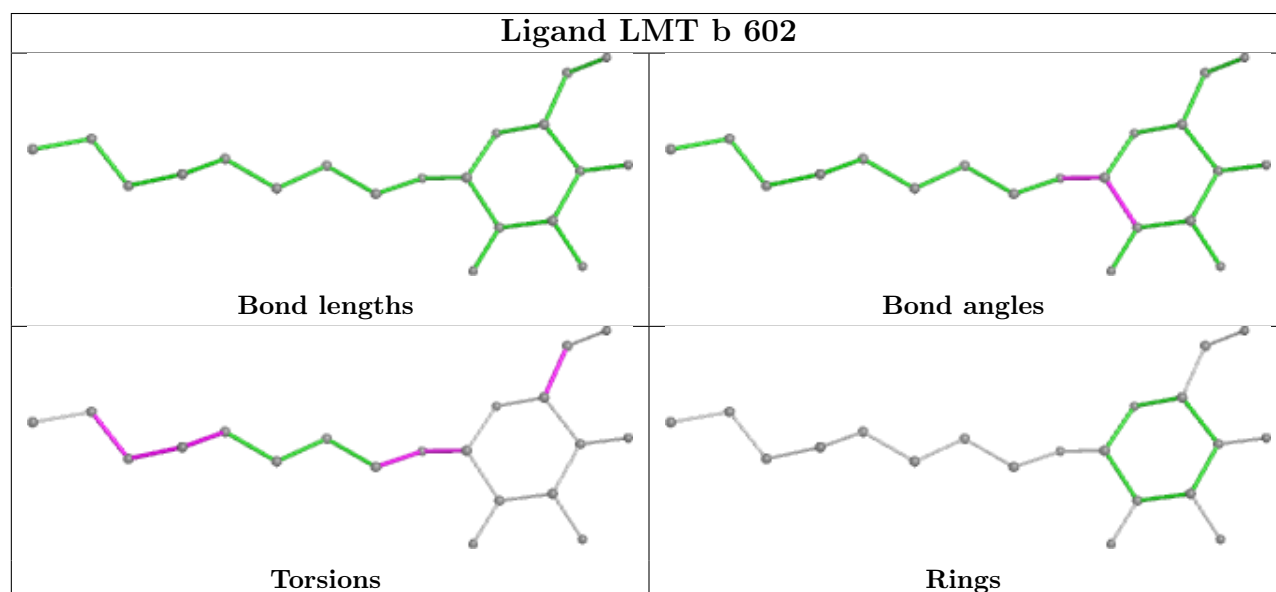
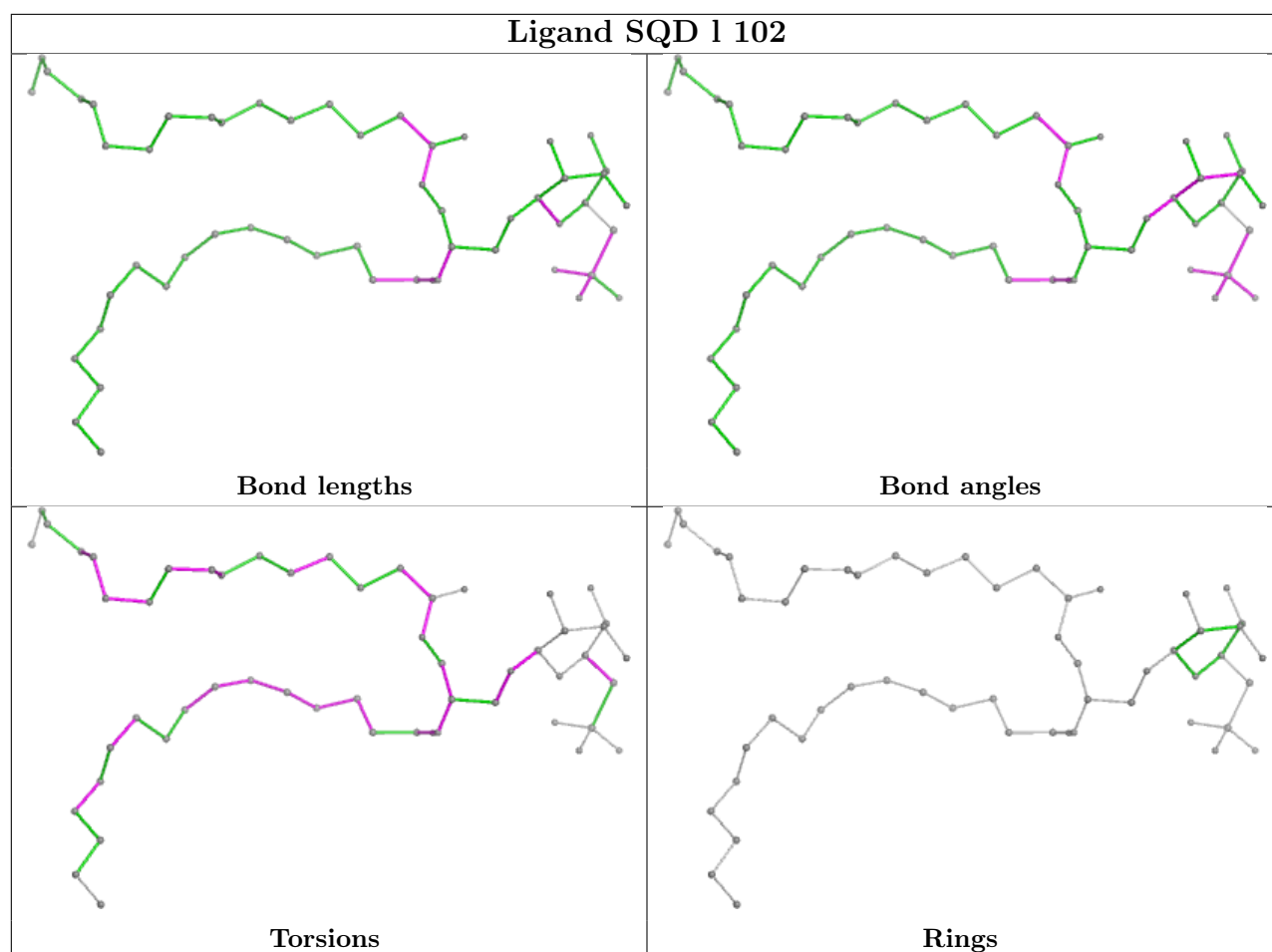


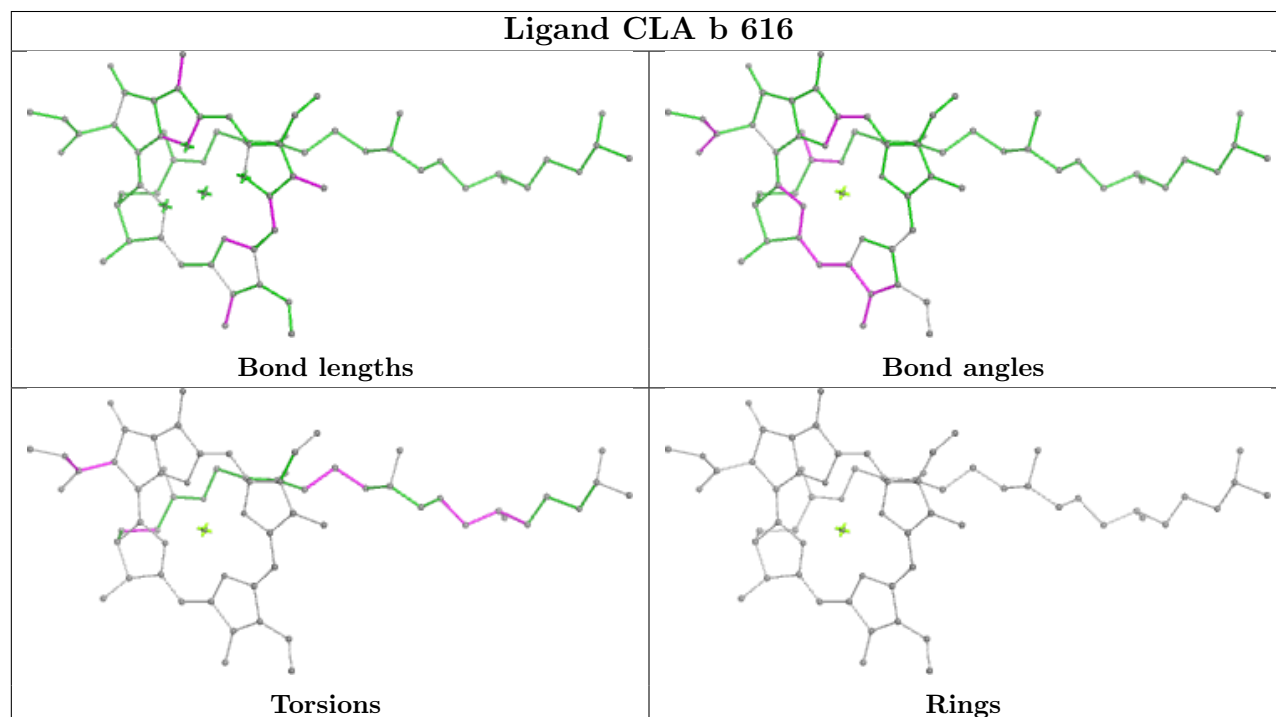
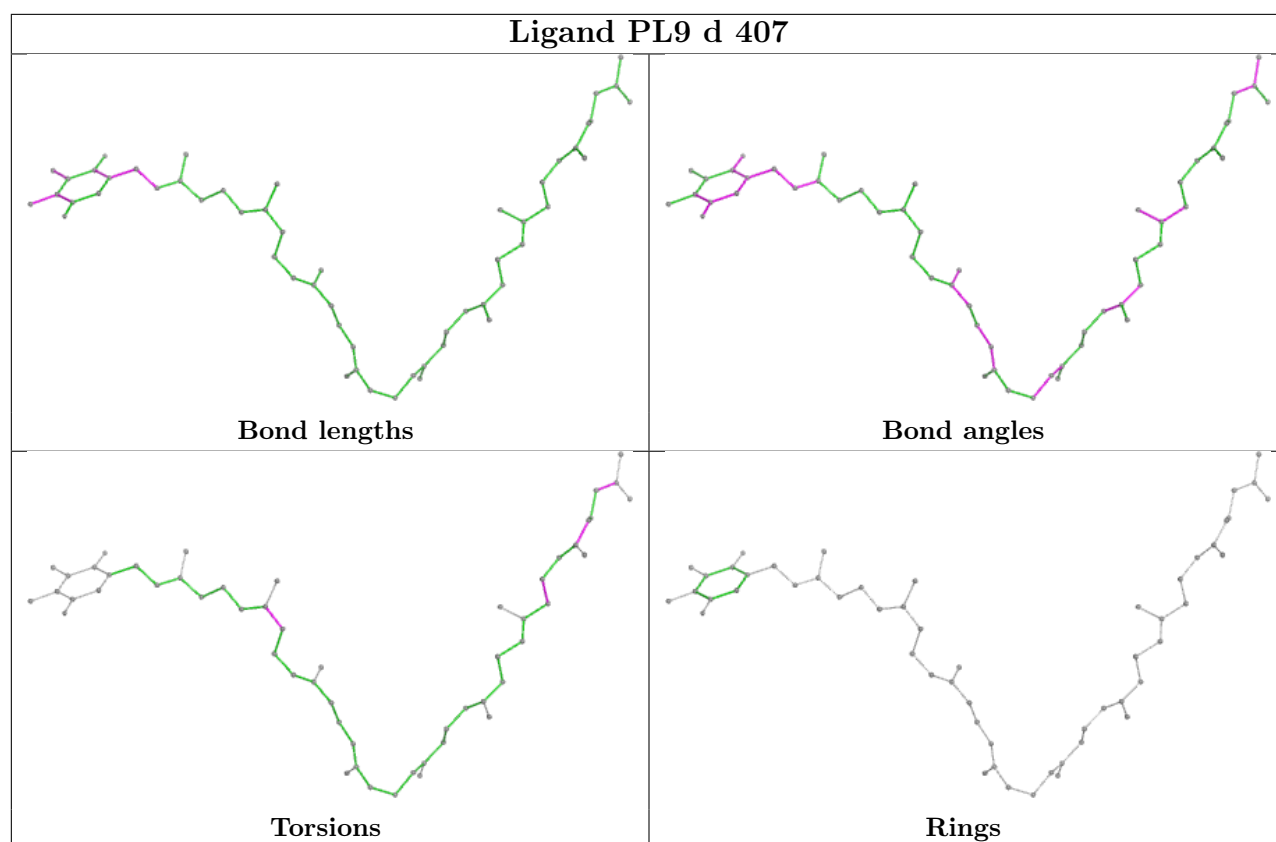


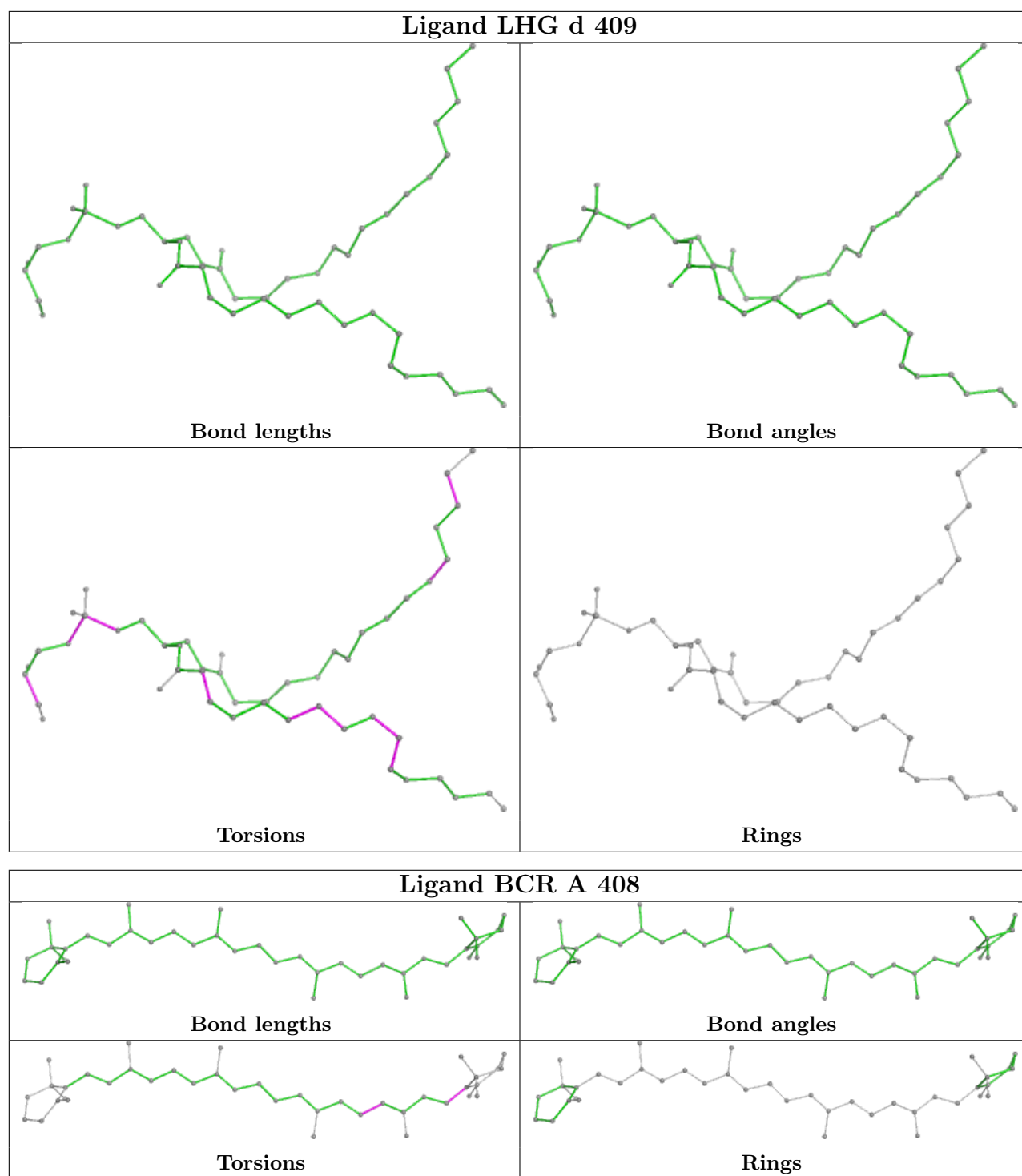












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

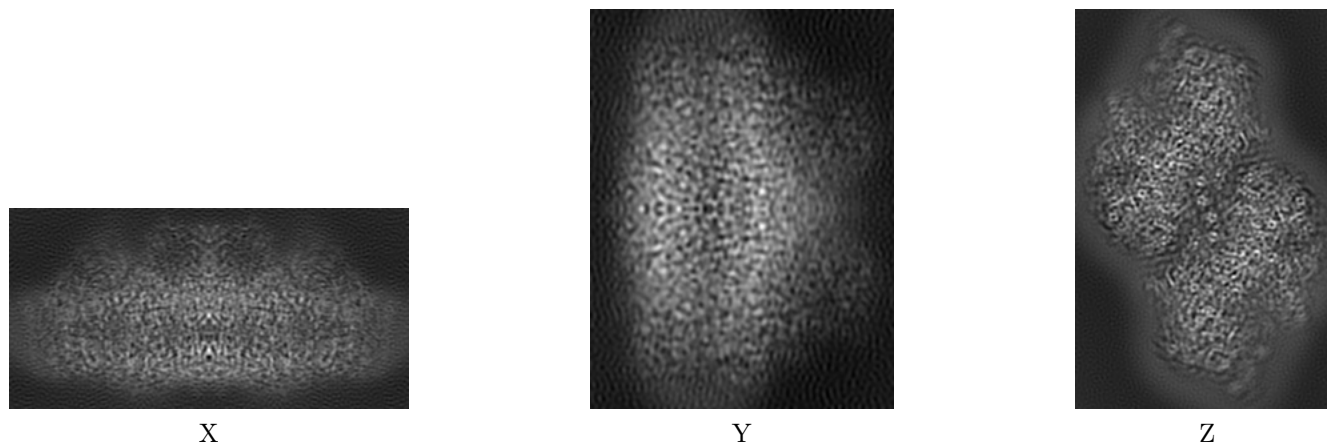
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51100. These allow visual inspection of the internal detail of the map and identification of artifacts.

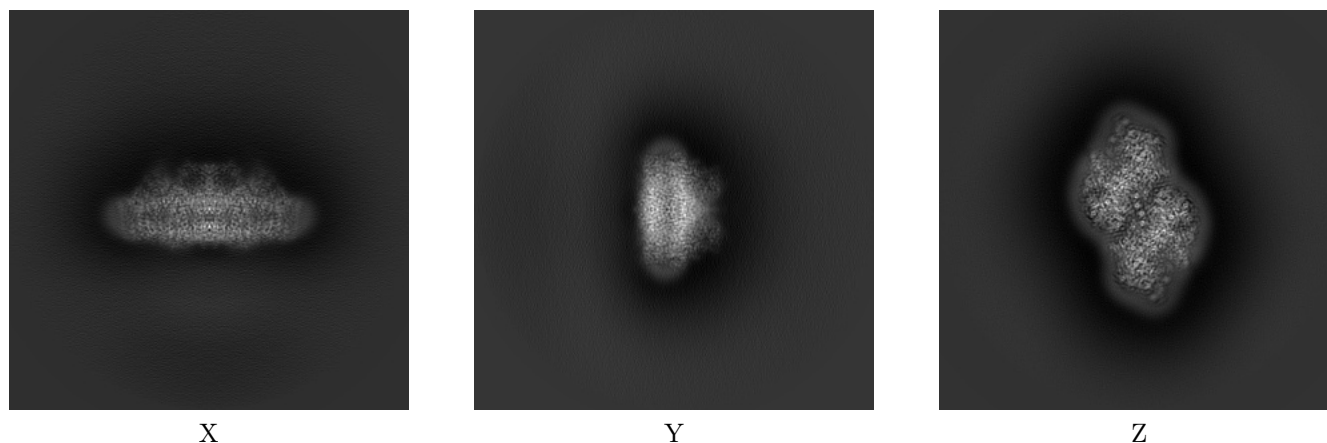
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



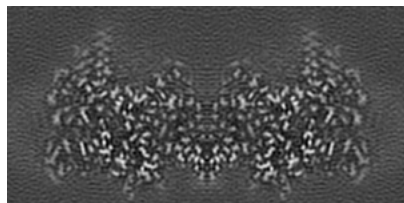
#### 6.1.2 Raw map



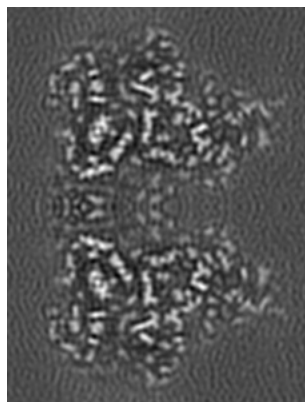
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

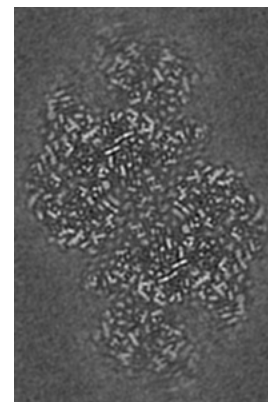
### 6.2.1 Primary map



X Index: 137

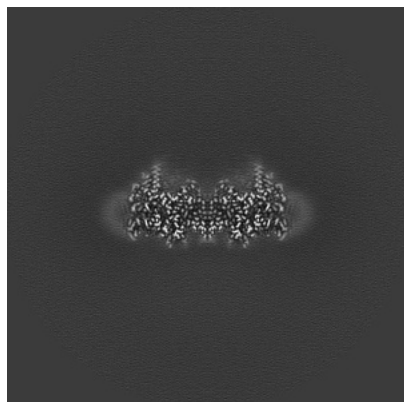


Y Index: 208

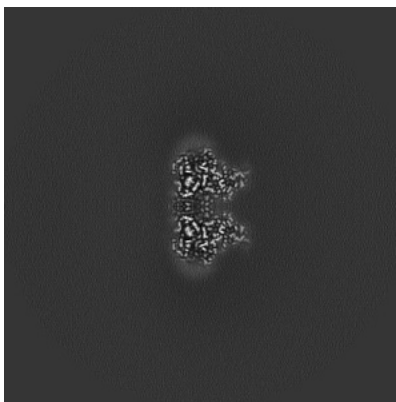


Z Index: 104

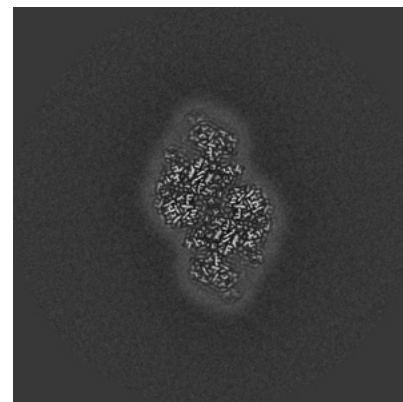
### 6.2.2 Raw map



X Index: 200



Y Index: 200

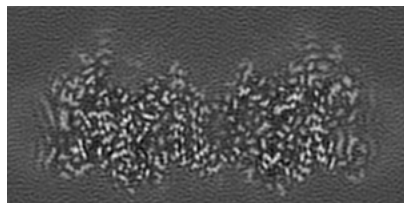


Z Index: 200

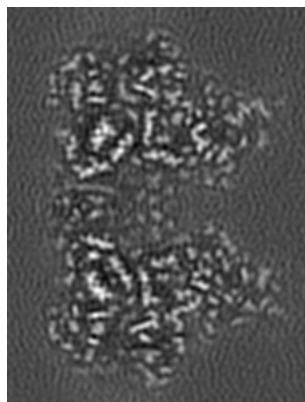
The images above show central slices of the map in three orthogonal directions.

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

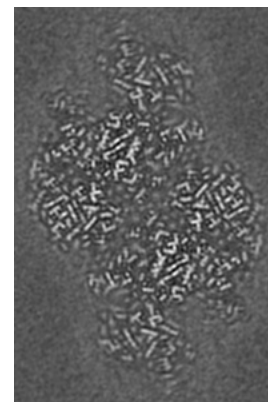
### 6.3.1 Primary map



X Index: 142

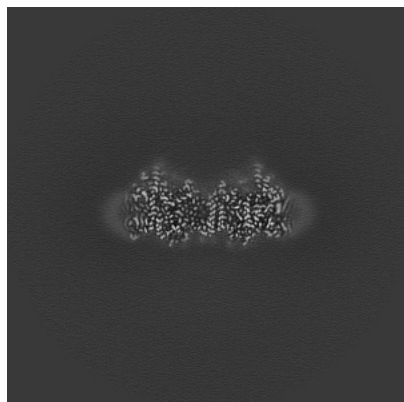


Y Index: 209

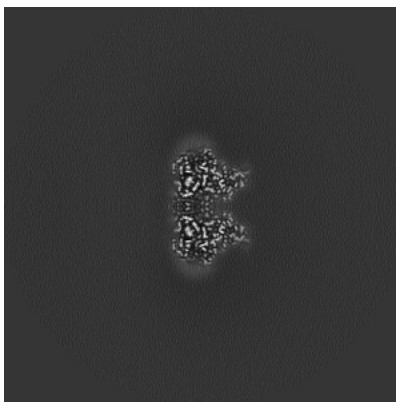


Z Index: 98

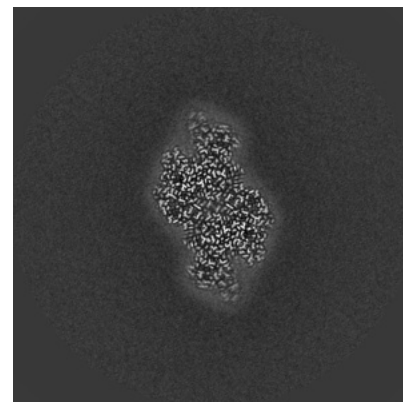
### 6.3.2 Raw map



X Index: 198



Y Index: 200



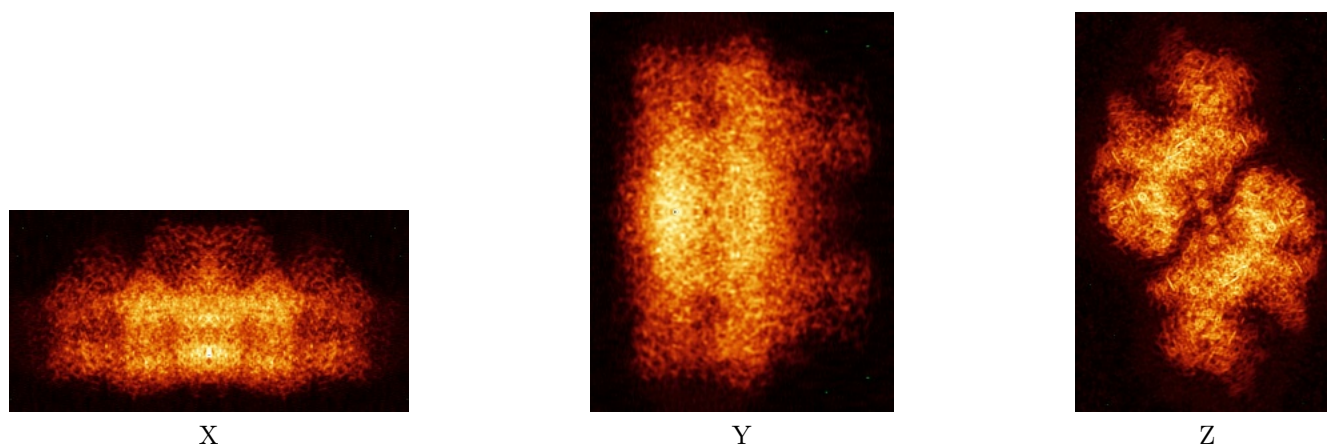
Z Index: 207

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

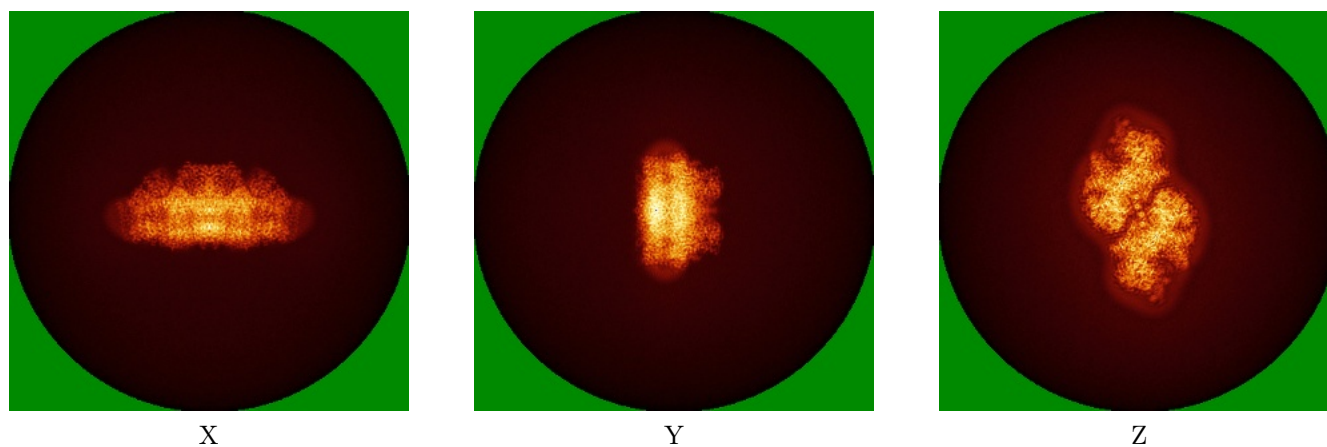


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



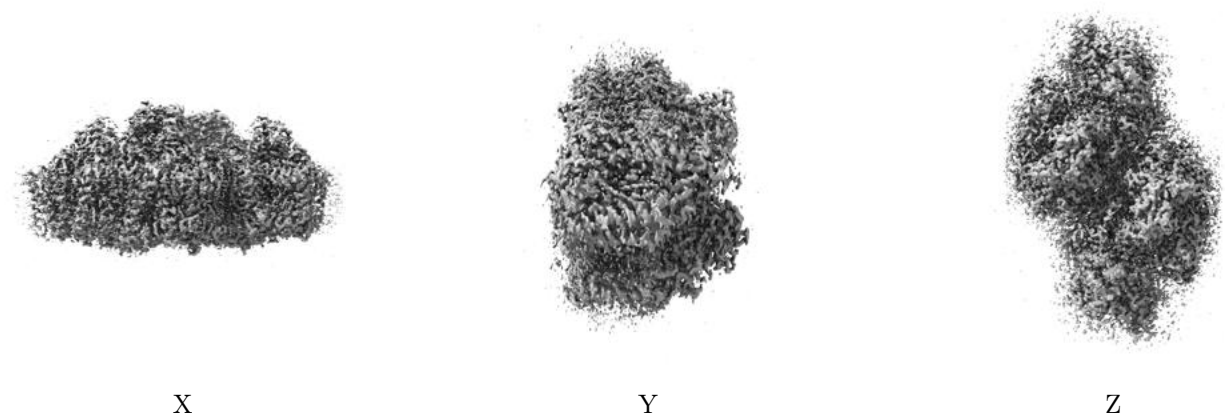
### 6.4.2 Raw map



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.

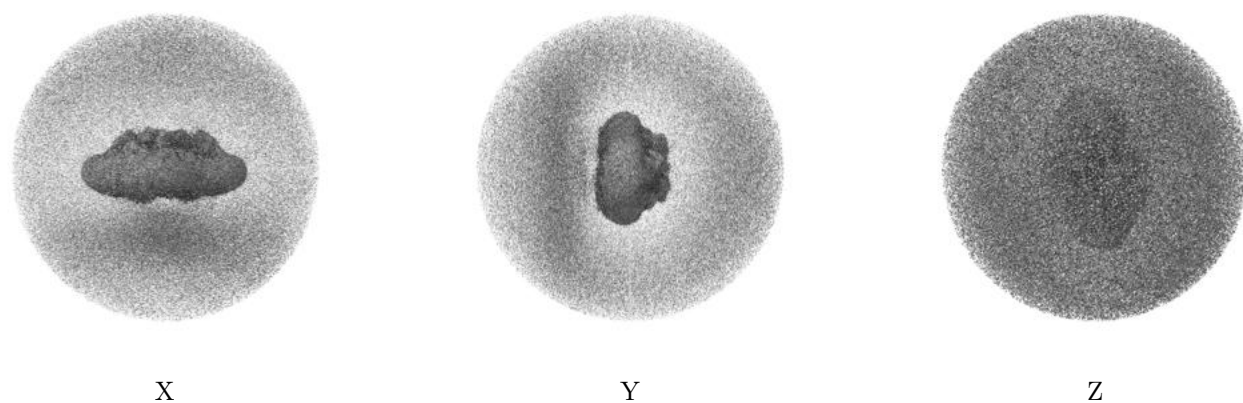
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.037. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

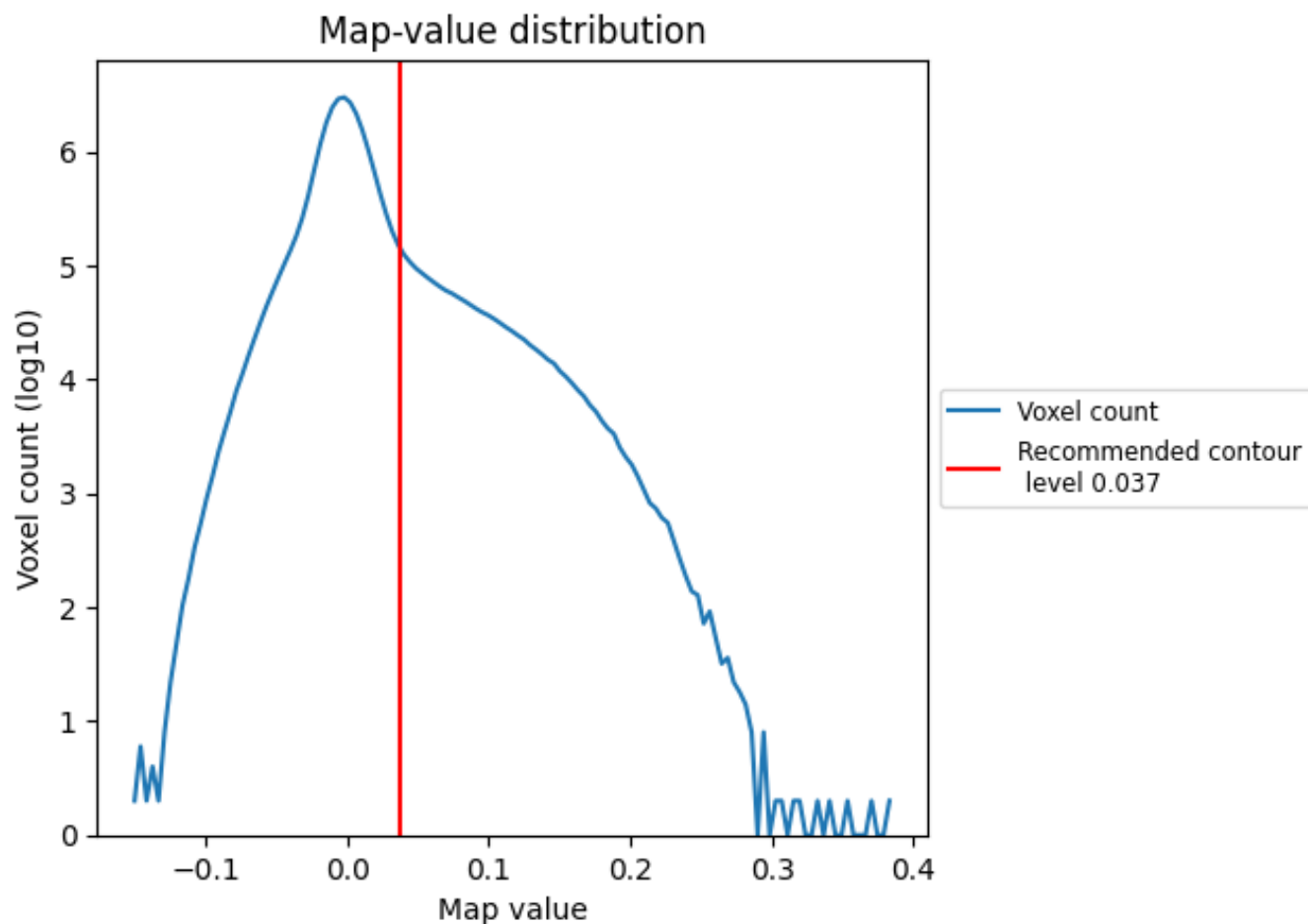
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

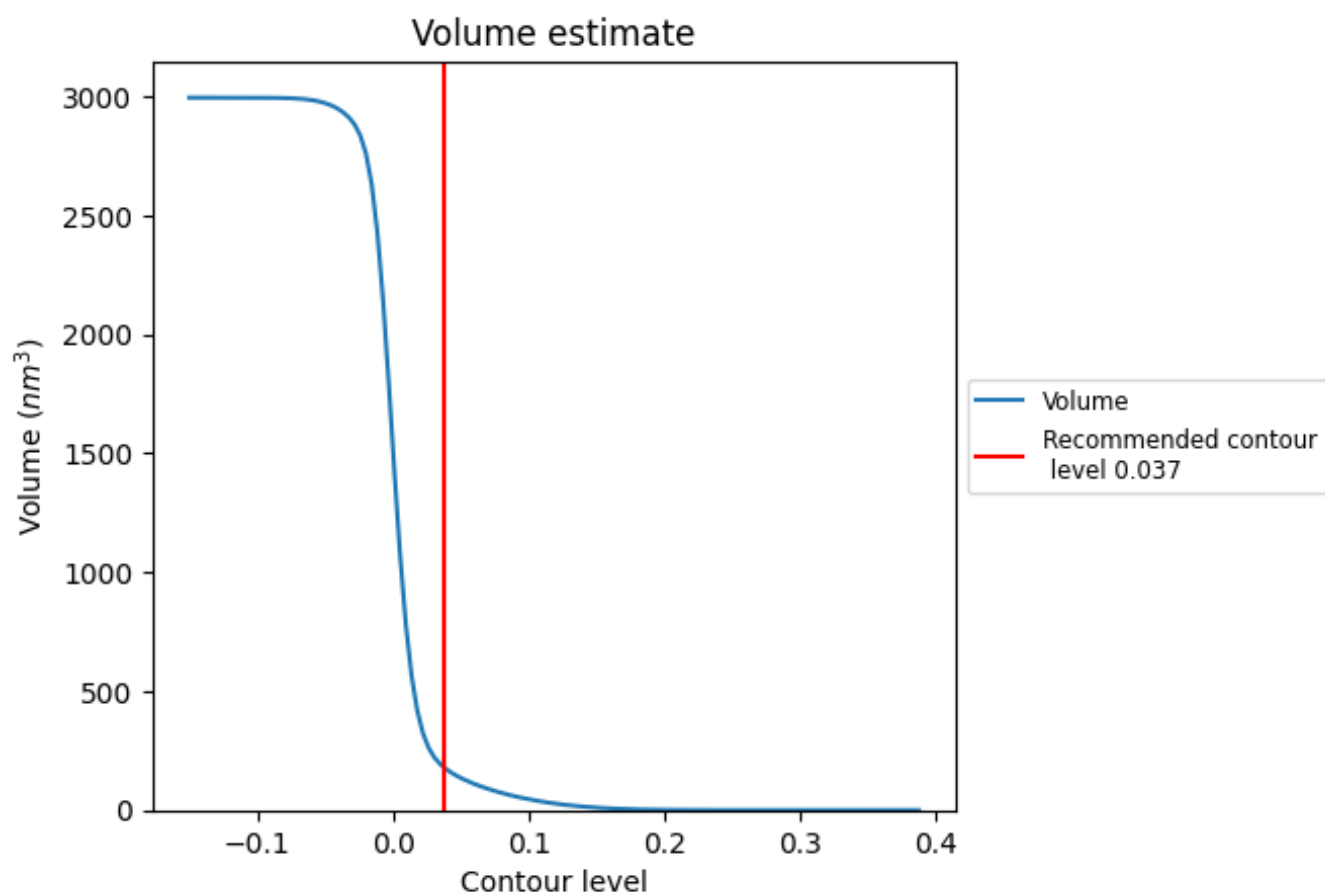
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm<sup>3</sup>; this corresponds to an approximate mass of 166 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.

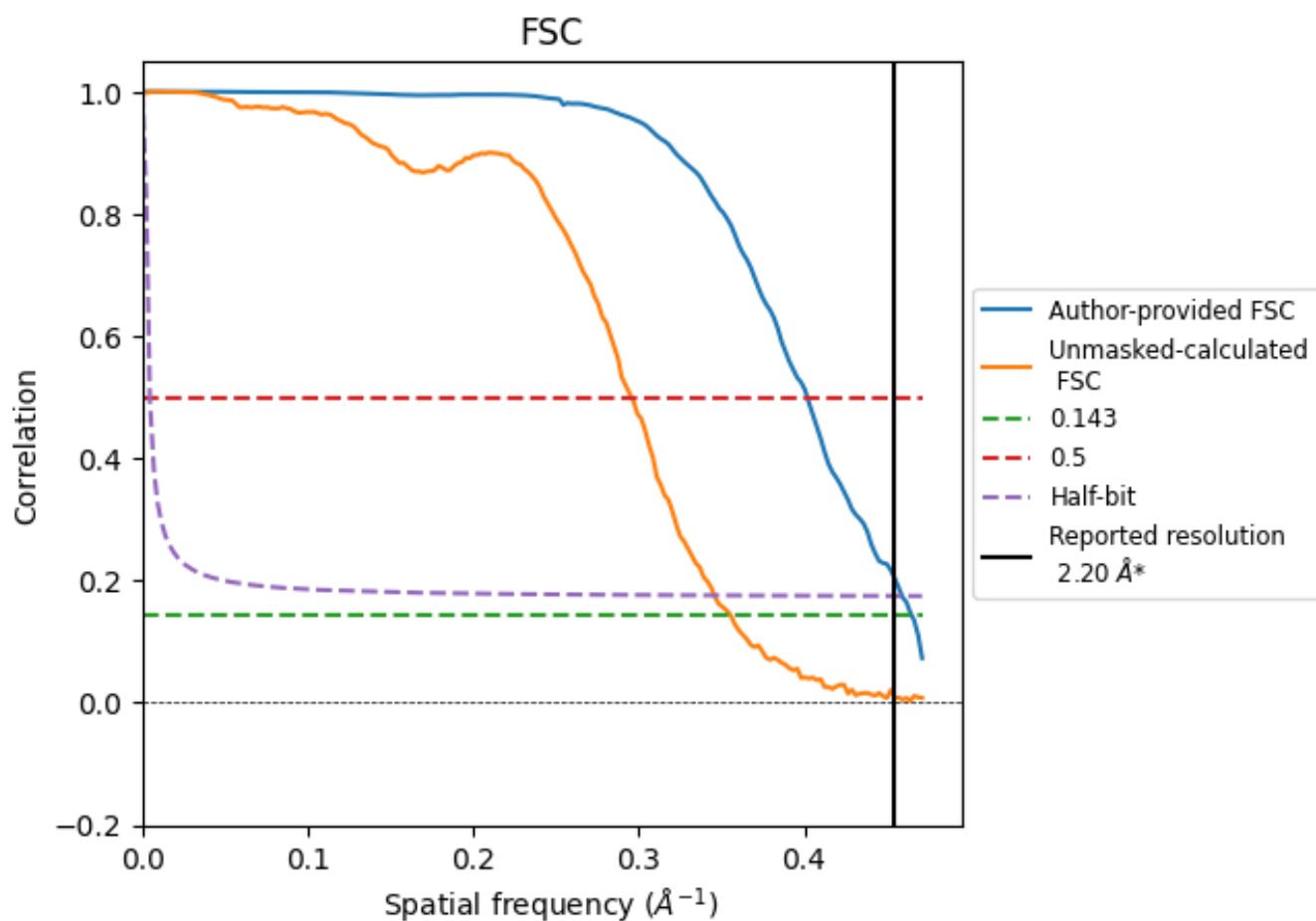
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 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 0.455  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

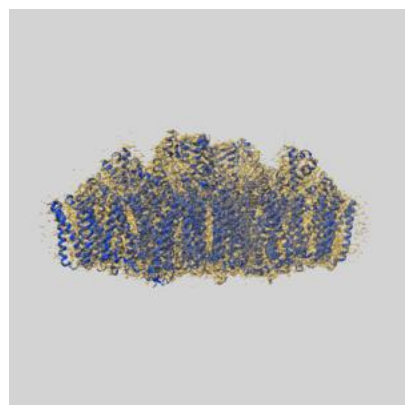
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.15	2.49	2.18
Unmasked-calculated*	2.81	3.38	2.89

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.81 differs from the reported value 2.2 by more than 10 %

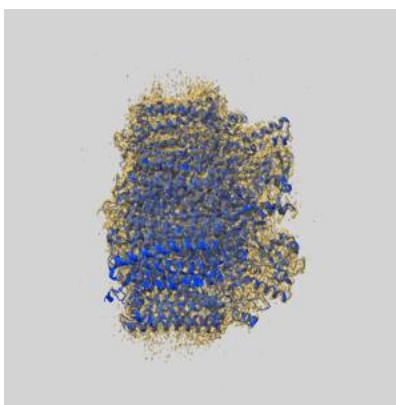
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51100 and PDB model 9G6F. Per-residue inclusion information can be found in section [3](#) on page [28](#).

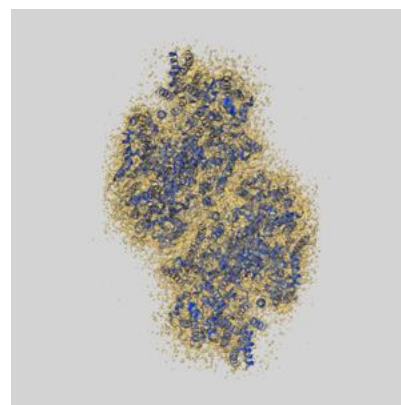
### 9.1 Map-model overlay [i](#)



X



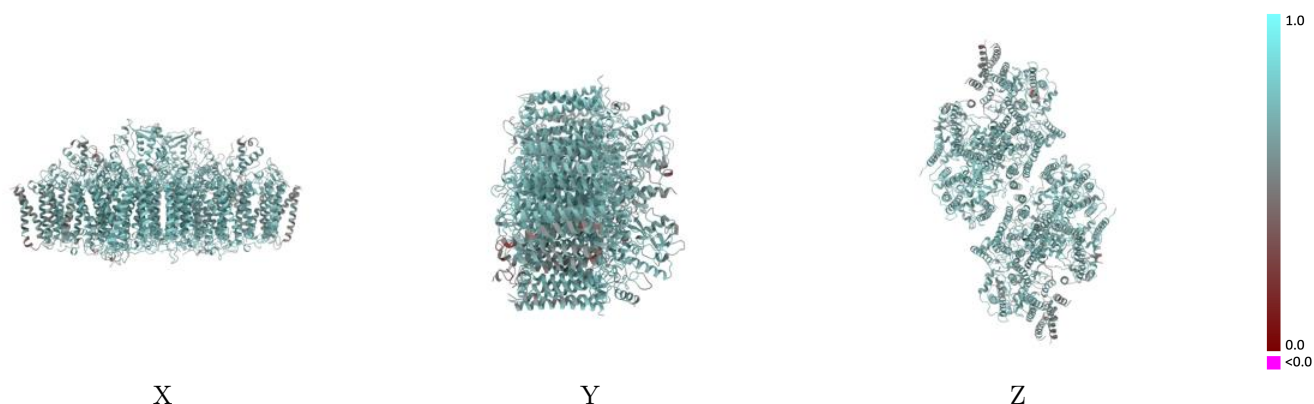
Y



Z

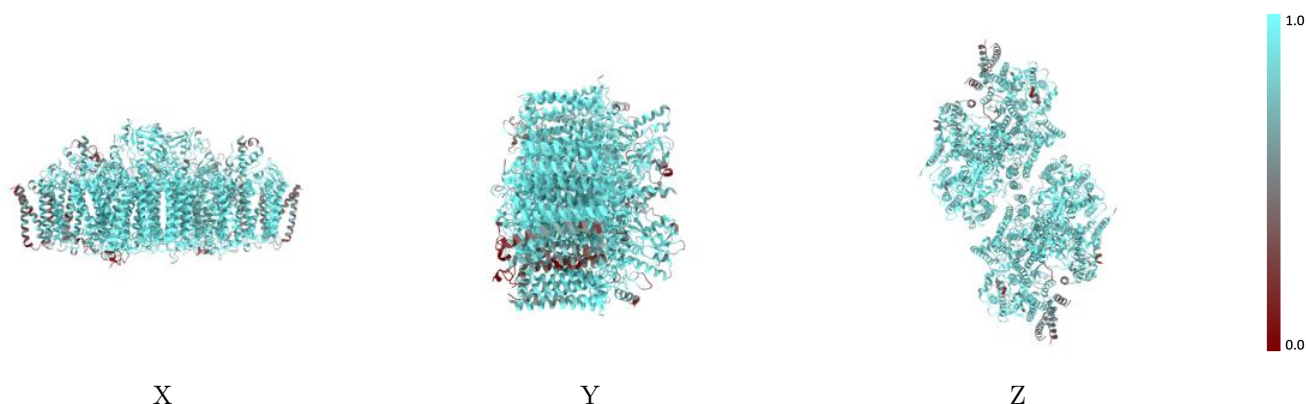
The images above show the 3D surface view of the map at the recommended contour level 0.037 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

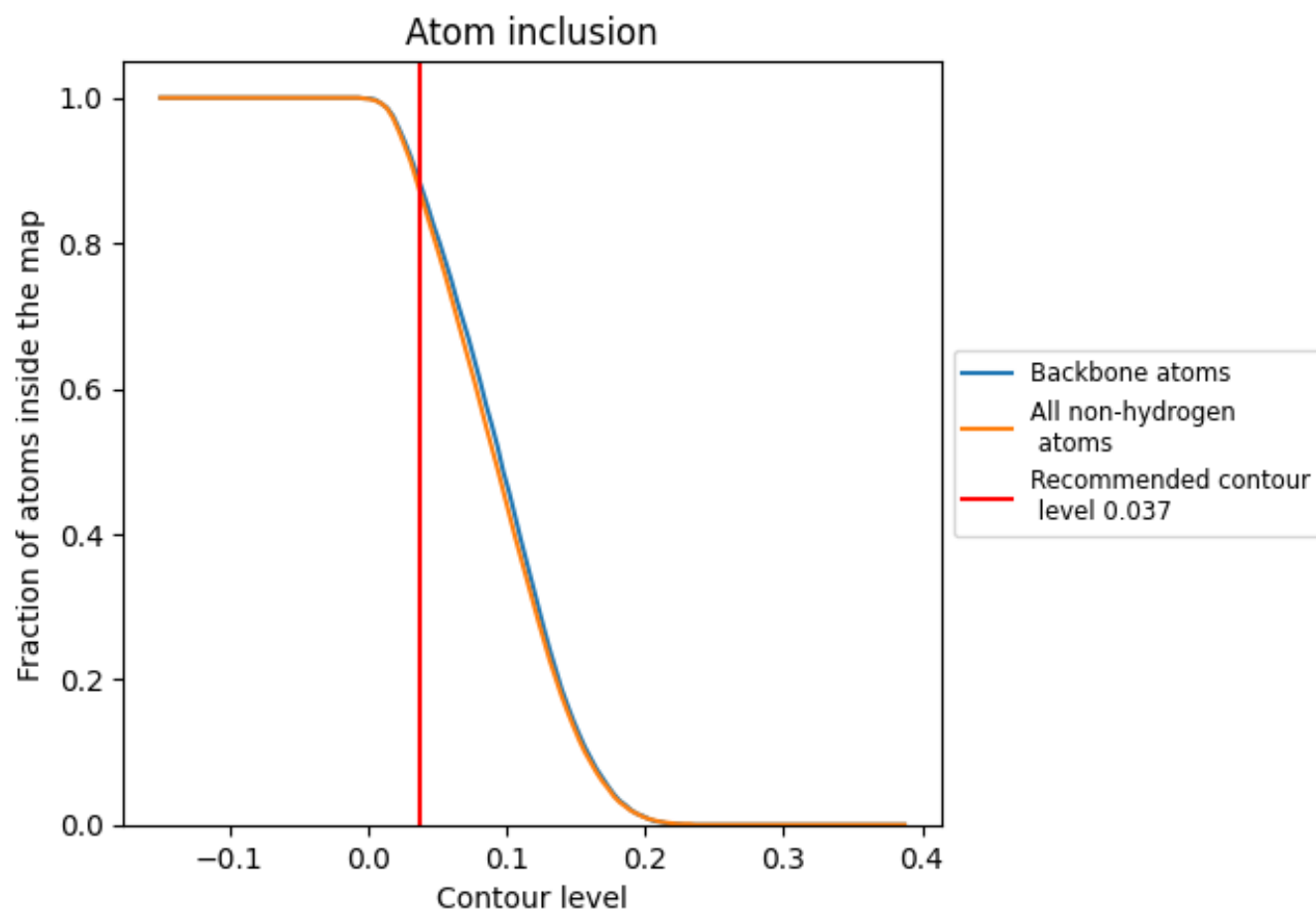
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.037).





































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.6690
A	 0.9290	 0.7000
B	 0.9110	 0.6820
C	 0.8770	 0.6630
D	 0.9410	 0.7010
E	 0.6890	 0.5760
F	 0.7370	 0.6100
H	 0.9250	 0.6760
I	 0.8870	 0.6710
J	 0.4120	 0.5200
K	 0.8350	 0.6350
L	 0.9010	 0.6850
M	 0.8520	 0.6610
T	 0.9250	 0.7070
X	 0.8610	 0.6600
Y	 0.5310	 0.5490
Z	 0.5040	 0.5240
a	 0.9150	 0.6910
b	 0.9120	 0.6900
c	 0.8530	 0.6460
d	 0.9430	 0.7060
e	 0.7130	 0.5940
f	 0.7000	 0.6030
h	 0.9460	 0.6910
i	 0.8380	 0.6470
j	 0.3790	 0.5080
k	 0.8510	 0.6250
l	 0.9040	 0.6820
m	 0.8600	 0.6680
t	 0.9020	 0.6800
x	 0.9120	 0.6730
y	 0.5590	 0.5650
z	 0.4920	 0.4990

