



## Full wwPDB EM Validation Report ⓘ

Jul 24, 2025 – 04:47 pm BST

PDB ID : 9G6H / pdb\_00009g6h  
EMDB ID : EMD-51102  
Title : active 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 model : 3KZI

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

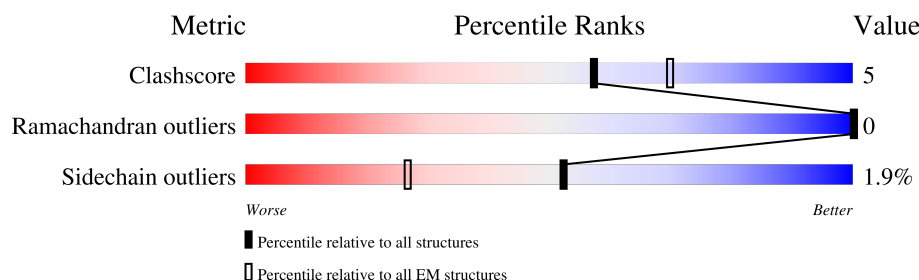
# 1 Overall quality at a glance

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	80% 12% 8%
1	a	360	81% 12% 8%
2	B	510	89% 10% .
2	b	510	89% 9% .
3	C	461	88% 9% ..
3	c	461	89% 9% .
4	D	352	87% 10% .
4	d	352	82% 14% .

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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	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	X	41	

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Mol	Chain	Length	Quality of chain
17	x	41	
18	Y	46	
18	y	46	
19	Z	62	
19	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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	407	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	514	X	-	-	-
22	CLA	C	515	X	-	-	-
22	CLA	C	516	X	-	-	-
22	CLA	C	517	X	-	-	-
22	CLA	D	401	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	D	406	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	408	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	c	515	X	-	-	-
22	CLA	c	516	X	-	-	-
22	CLA	c	517	X	-	-	-
22	CLA	c	518	X	-	-	-
22	CLA	d	401	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 51092 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	333	Total	C	N	O	S	0	0
			2597	1706	429	447	15		
1	a	333	Total	C	N	O	S	0	0
			2597	1706	429	447	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	505	Total	C	N	O	S	0	0
			3935	2586	660	676	13		
2	b	505	Total	C	N	O	S	0	0
			3929	2583	657	676	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	450	Total	C	N	O	S	0	0
			3458	2267	583	595	13		
3	c	450	Total	C	N	O	S	0	0
			3461	2268	583	597	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
			2710	1797	444	457	12		
4	d	341	Total	C	N	O	S	0	0
			2710	1797	444	457	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
			650	425	106	119		
5	e	81	Total	C	N	O	0	0
			650	425	106	119		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	34	Total	C	N	O	S	0	0
			275	187	45	42	1		
6	f	34	Total	C	N	O	S	0	0
			275	187	45	42	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	62	Total	C	N	O	S	0	0
			489	327	78	82	2		
7	h	62	Total	C	N	O	S	0	0
			489	327	78	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	36	Total	C	N	O	S	0	0
			293	199	46	47	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	36	Total	C	N	O	S	0	0
			257	174	40	42	1		
9	j	36	Total	C	N	O	S	0	0
			257	174	40	42	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			289	201	42	46		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total	C	N	O	0	0
			289	201	42	46		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	36	Total	C	N	O	0	0
			286	192	44	50		
11	l	36	Total	C	N	O	0	0
			286	192	44	50		

- 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
			254	170	38	45	1		
12	m	33	Total	C	N	O	S	0	0
			254	170	38	45	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	243	Total	C	N	O	S	0	0
			1799	1131	306	358	4		
13	o	243	Total	C	N	O	S	0	0
			1794	1128	303	359	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	30	Total	C	N	O	S	0	0
			256	180	36	38	2		
14	t	30	Total	C	N	O	S	0	0
			256	180	36	38	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	U	97	Total	C	N	O	0	0
			758	483	129	146		
15	u	97	Total	C	N	O	0	0
			758	483	129	146		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	137	Total	C	N	O	S	0	0
			1052	668	176	204	4		
16	v	137	Total	C	N	O	S	0	0
			1052	668	176	204	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	X	38	Total	C	N	O	0	0
			279	187	45	47		
17	x	38	Total	C	N	O	0	0
			275	185	44	46		

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	30	Total	C	N	O	S	0	0
			214	142	35	35	2		
18	y	30	Total	C	N	O	S	0	0
			214	142	35	35	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			458	317	67	72	2		
19	z	61	Total	C	N	O	S	0	0
			458	317	67	72	2		

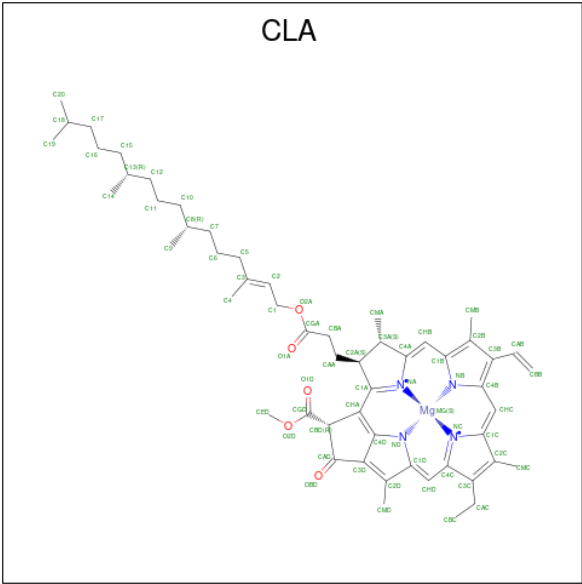
- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 21 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
21	A	2	Total	Cl	0
			2	2	
21	a	2	Total	Cl	0
			2	2	

- Molecule 22 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
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

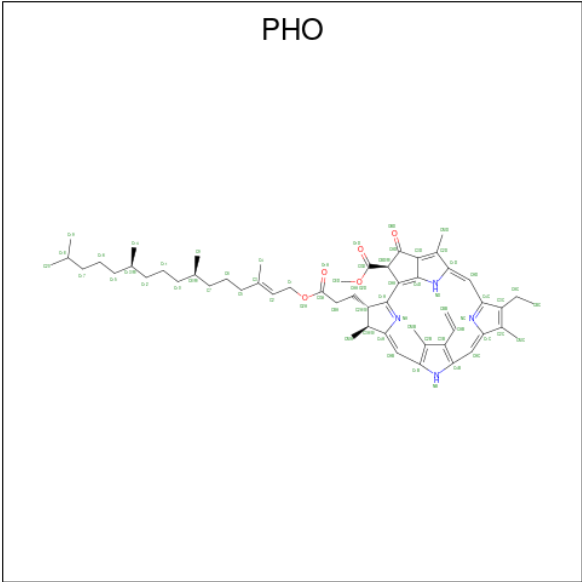
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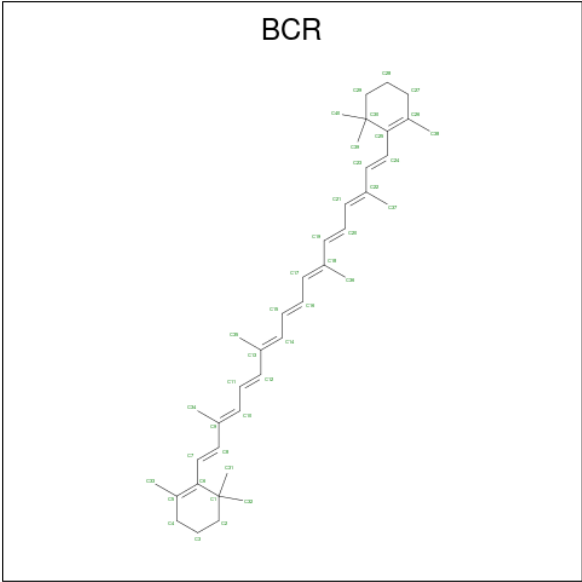
Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 23 is PHEOPHYTIN A (CCD ID: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



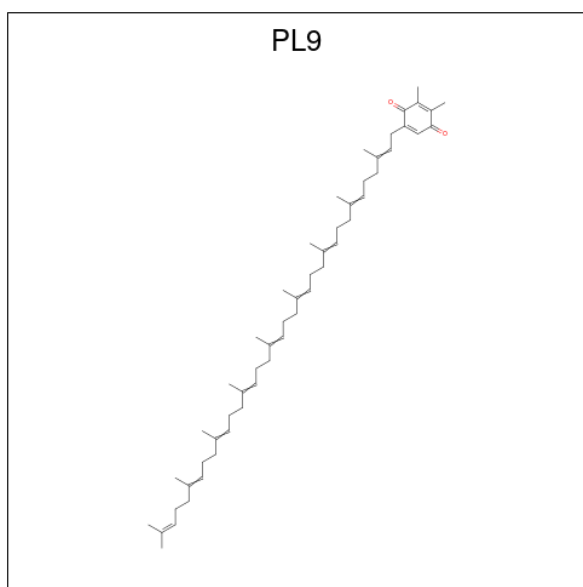
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	N	O	0
			64	55	4	5	
23	D	1	Total	C	N	O	0
			64	55	4	5	
23	a	1	Total	C	N	O	0
			64	55	4	5	
23	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



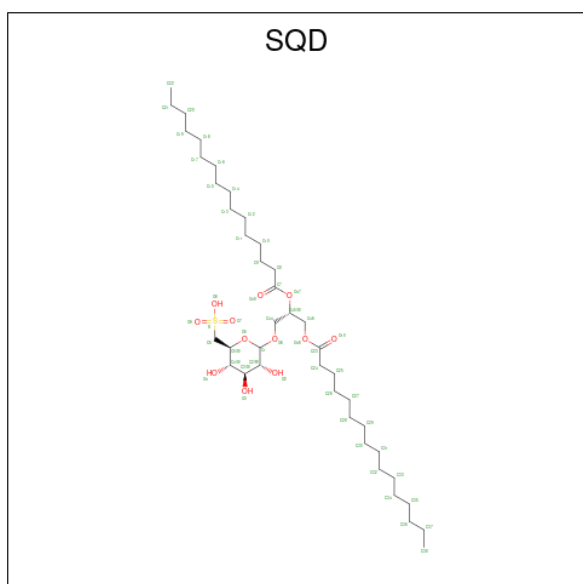
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	C	1	Total C 40 40	0
24	C	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	T	1	Total C 40 40	0
24	Y	1	Total C 40 40	0
24	a	1	Total C 40 40	0
24	b	1	Total C 40 40	0
24	b	1	Total C 40 40	0
24	b	1	Total C 40 40	0
24	c	1	Total C 40 40	0
24	c	1	Total C 40 40	0
24	f	1	Total C 40 40	0
24	k	1	Total C 40 40	0
24	y	1	Total C 40 40	0

- Molecule 25 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>).



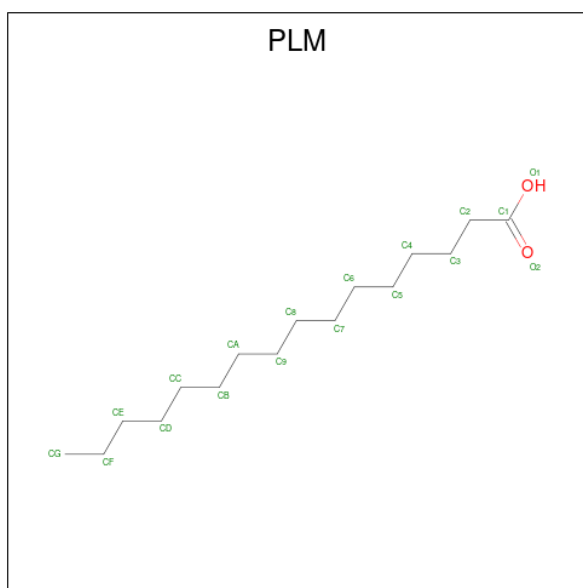
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			55	53	2	
25	D	1	Total	C	O	0
			55	53	2	
25	a	1	Total	C	O	0
			55	53	2	
25	d	1	Total	C	O	0
			55	53	2	

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



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			54	41	12	1	
26	A	1	Total	C	O	S	0
			51	38	12	1	
26	D	1	Total	C	O	S	0
			45	32	12	1	
26	a	1	Total	C	O	S	0
			54	41	12	1	
26	a	1	Total	C	O	S	0
			51	38	12	1	
26	b	1	Total	C	O	S	0
			54	41	12	1	
26	d	1	Total	C	O	S	0
			45	32	12	1	
26	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 27 is PALMITIC ACID (CCD ID: PLM) (formula:  $C_{16}H_{32}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			18	16	2	
27	A	1	Total	C	O	0
			12	10	2	
27	B	1	Total	C	O	0
			18	16	2	
27	B	1	Total	C	O	0
			14	12	2	

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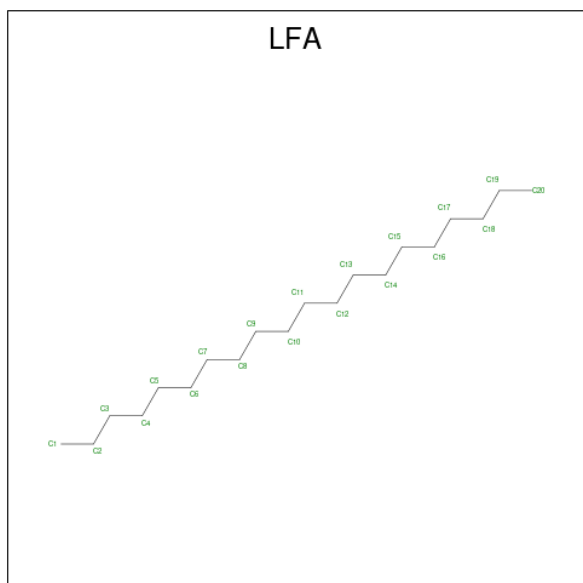
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			12	10	2	
27	B	1	Total	C	O	0
			17	15	2	
27	B	1	Total	C	O	0
			18	16	2	
27	C	1	Total	C	O	0
			15	13	2	
27	C	1	Total	C	O	0
			18	16	2	
27	C	1	Total	C	O	0
			16	14	2	
27	C	1	Total	C	O	0
			13	11	2	
27	D	1	Total	C	O	0
			13	11	2	
27	D	1	Total	C	O	0
			18	16	2	
27	E	1	Total	C	O	0
			18	16	2	
27	F	1	Total	C	O	0
			14	12	2	
27	H	1	Total	C	O	0
			12	10	2	
27	L	1	Total	C	O	0
			18	16	2	
27	M	1	Total	C	O	0
			16	14	2	
27	X	1	Total	C	O	0
			17	15	2	
27	a	1	Total	C	O	0
			18	16	2	
27	b	1	Total	C	O	0
			18	16	2	
27	b	1	Total	C	O	0
			13	11	2	
27	b	1	Total	C	O	0
			16	14	2	
27	b	1	Total	C	O	0
			18	16	2	
27	c	1	Total	C	O	0
			18	16	2	

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Mol	Chain	Residues	Atoms			AltConf
27	c	1	Total	C	O	0
			16	14	2	
27	c	1	Total	C	O	0
			18	16	2	
27	c	1	Total	C	O	0
			17	15	2	
27	d	1	Total	C	O	0
			12	10	2	
27	e	1	Total	C	O	0
			18	16	2	
27	e	1	Total	C	O	0
			18	16	2	
27	j	1	Total	C	O	0
			17	15	2	
27	j	1	Total	C	O	0
			18	16	2	
27	t	1	Total	C		0
			15	15		
27	x	1	Total	C	O	0
			18	16	2	

- Molecule 28 is EICOSANE (CCD ID: LFA) (formula:  $C_{20}H_{42}$ ).



Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	C	0
			12	12	

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Mol	Chain	Residues	Atoms	AltConf
28	B	1	Total C 8 8	0
28	B	1	Total C 7 7	0
28	B	1	Total C 8 8	0
28	B	1	Total C 5 5	0
28	C	1	Total C 9 9	0
28	E	1	Total C 20 20	0
28	H	1	Total C 10 10	0
28	I	1	Total C 20 20	0
28	I	1	Total C 11 11	0
28	I	1	Total C 8 8	0
28	J	1	Total C 20 20	0
28	J	1	Total C 11 11	0
28	T	1	Total C 17 17	0
28	a	1	Total C 7 7	0
28	a	1	Total C 11 11	0
28	a	1	Total C 7 7	0
28	b	1	Total C 8 8	0
28	b	1	Total C 4 4	0
28	d	1	Total C 13 13	0
28	d	1	Total C 14 14	0
28	i	1	Total C 20 20	0

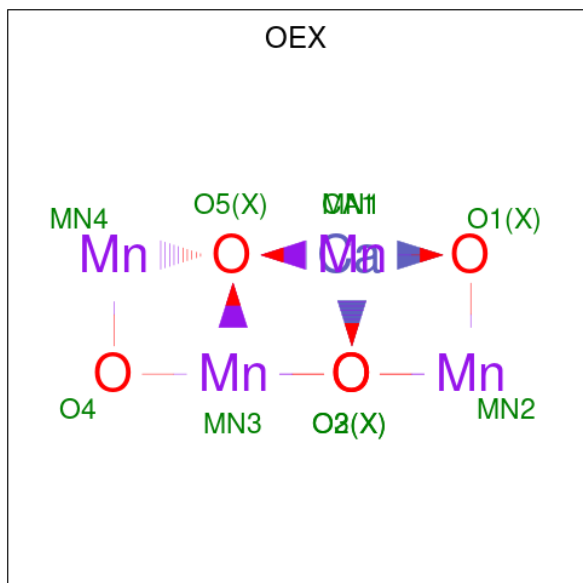
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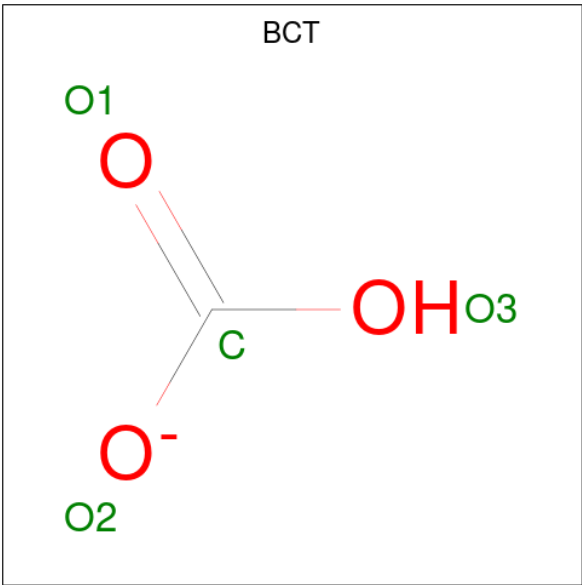
Mol	Chain	Residues	Atoms	AltConf
28	i	1	Total C 9 9	0
28	i	1	Total C 8 8	0

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



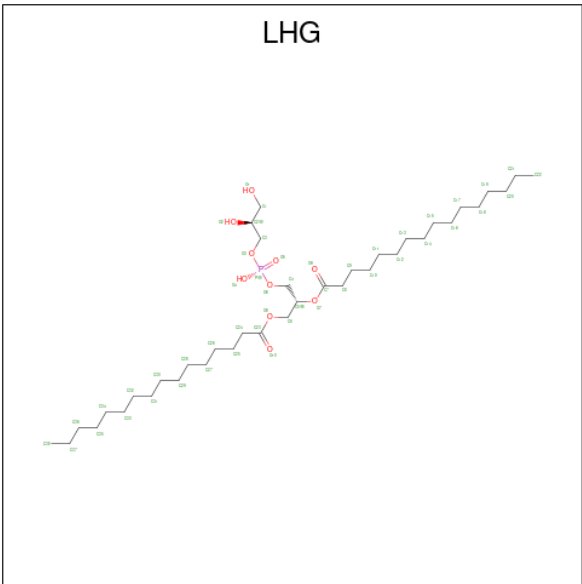
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total Ca Mn O 10 1 4 5	0
29	a	1	Total Ca Mn O 10 1 4 5	0

- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).



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

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



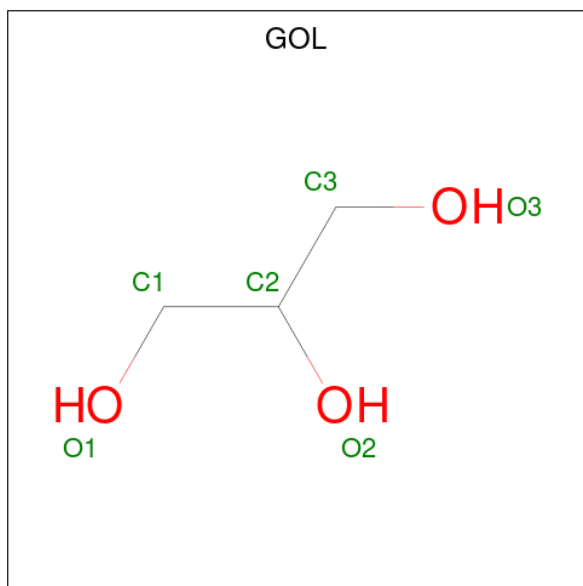
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	P	0
			46	35	10	1	

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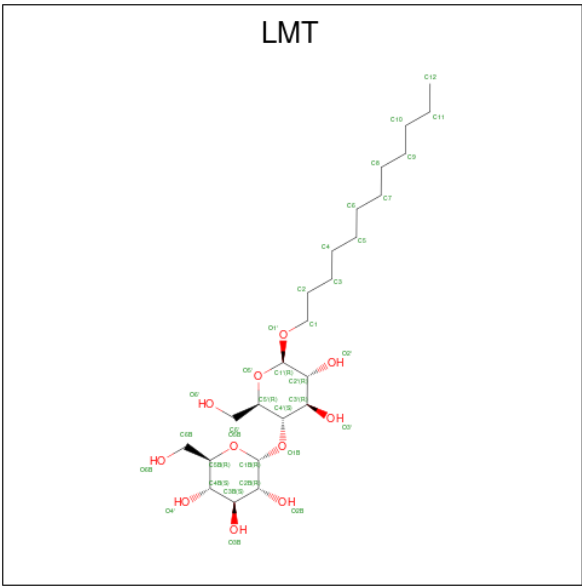
Mol	Chain	Residues	Atoms				AltConf
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	E	1	Total	C	O	P	0
			40	29	10	1	
31	L	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			49	38	10	1	
31	a	1	Total	C	O	P	0
			46	35	10	1	
31	d	1	Total	C	O	P	0
			49	38	10	1	
31	d	1	Total	C	O	P	0
			48	37	10	1	
31	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 32 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			6	3	3	
32	a	1	Total	C	O	0
			6	3	3	

- Molecule 33 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



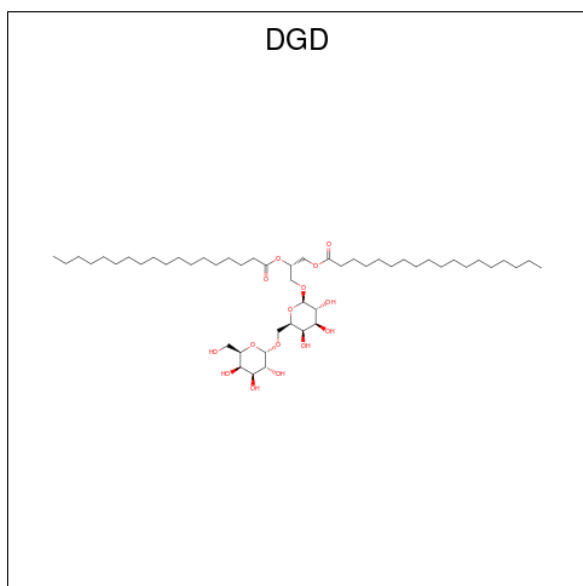
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			35	24	11	
33	B	1	Total	C	O	0
			35	24	11	
33	B	1	Total	C	O	0
			24	18	6	
33	B	1	Total	C	O	0
			35	24	11	
33	B	1	Total	C	O	0
			35	24	11	
33	C	1	Total	C	O	0
			35	24	11	
33	J	1	Total	C	O	0
			24	18	6	
33	M	1	Total	C	O	0
			35	24	11	
33	T	1	Total	C	O	0
			24	18	6	
33	T	1	Total	C	O	0
			35	24	11	
33	Z	1	Total	C	O	0
			35	24	11	
33	b	1	Total	C	O	0
			24	18	6	
33	f	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
33	i	1	Total	C	O	0
			35	24	11	
33	j	1	Total	C	O	0
			24	18	6	
33	m	1	Total	C	O	0
			35	24	11	
33	z	1	Total	C	O	0
			35	24	11	

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



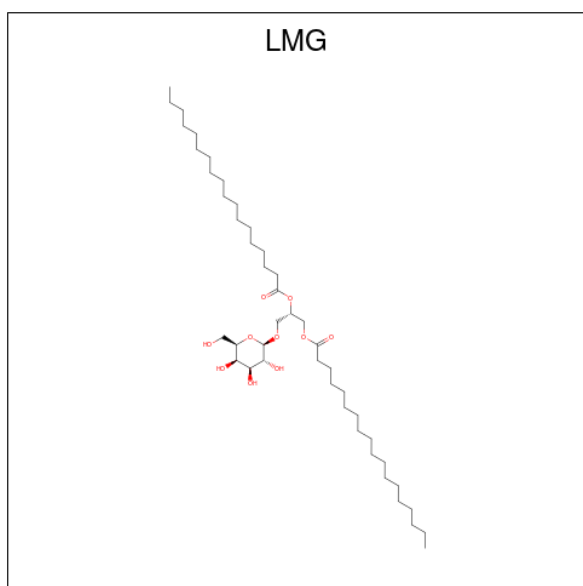
Mol	Chain	Residues	Atoms			AltConf
34	C	1	Total	C	O	0
			53	38	15	
34	C	1	Total	C	O	0
			54	39	15	
34	D	1	Total	C	O	0
			44	35	9	
34	H	1	Total	C	O	0
			58	43	15	
34	J	1	Total	C	O	0
			61	46	15	
34	c	1	Total	C	O	0
			53	38	15	
34	c	1	Total	C	O	0
			55	40	15	

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Mol	Chain	Residues	Atoms			AltConf
34	c	1	Total	C	O	0
			61	46	15	
34	d	1	Total	C	O	0
			47	36	11	
34	h	1	Total	C	O	0
			58	43	15	

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



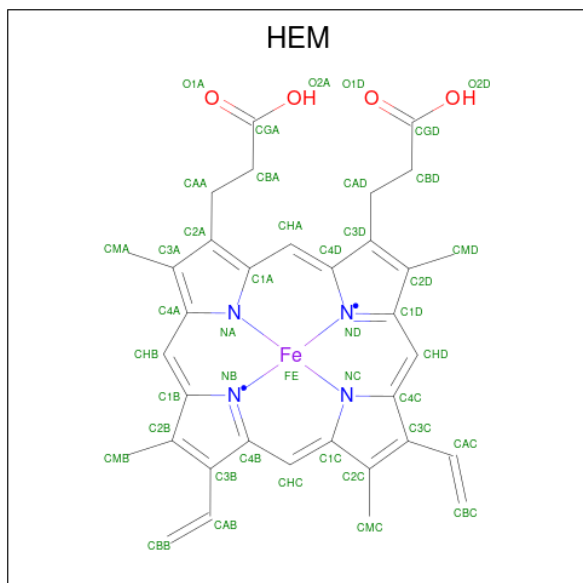
Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			51	41	10	
35	C	1	Total	C	O	0
			51	41	10	
35	D	1	Total	C	O	0
			47	37	10	
35	M	1	Total	C	O	0
			51	41	10	
35	Y	1	Total	C	O	0
			51	41	10	
35	c	1	Total	C	O	0
			51	41	10	
35	c	1	Total	C	O	0
			48	38	10	
35	d	1	Total	C	O	0
			47	37	10	

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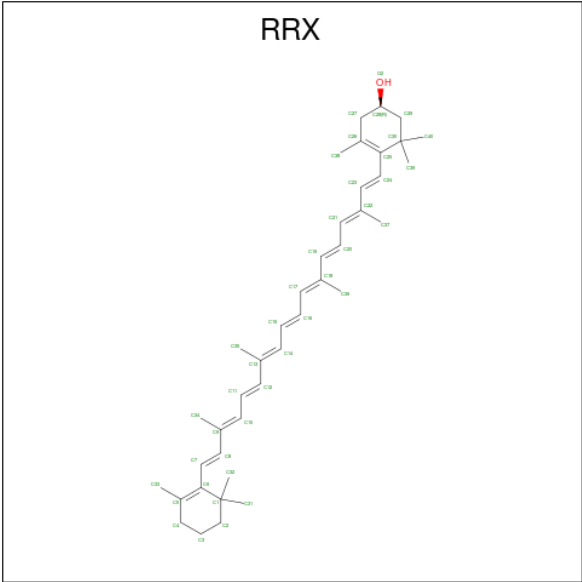
Mol	Chain	Residues	Atoms			AltConf
35	m	1	Total	C	O	0
			51	41	10	
35	y	1	Total	C	O	0
			51	41	10	

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					AltConf
36	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
36	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
36	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
36	v	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 37 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula:  $C_{40}H_{56}O$ ).



Mol	Chain	Residues	Atoms			AltConf
37	H	1	Total	C	O	0
			41	40	1	
37	h	1	Total	C	O	0
			41	40	1	

- Molecule 38 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
38	O	1	Total	Ca	0
			1	1	
38	o	1	Total	Ca	0
			1	1	

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	92	Total	O	0
			92	92	
39	B	133	Total	O	0
			133	133	
39	C	101	Total	O	1
			101	101	
39	D	91	Total	O	0
			91	91	
39	E	14	Total	O	0
			14	14	

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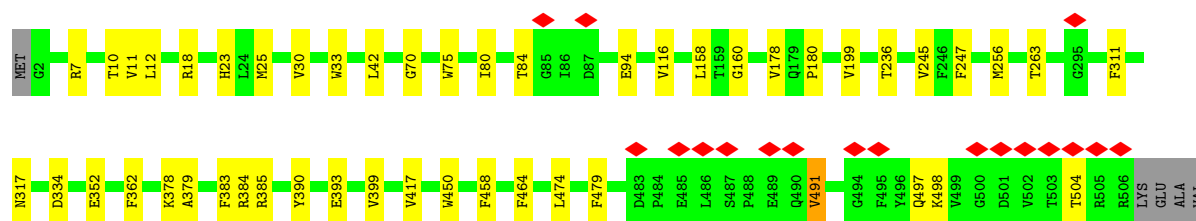
Mol	Chain	Residues	Atoms		AltConf
39	F	3	Total 3	O 3	0
39	H	11	Total 11	O 11	0
39	I	1	Total 1	O 1	0
39	J	4	Total 4	O 4	0
39	K	1	Total 1	O 1	0
39	L	8	Total 8	O 8	0
39	M	3	Total 3	O 3	0
39	O	37	Total 37	O 37	0
39	T	4	Total 4	O 4	0
39	U	14	Total 14	O 14	0
39	V	26	Total 26	O 26	0
39	X	3	Total 3	O 3	0
39	a	94	Total 94	O 94	0
39	b	137	Total 137	O 137	0
39	c	104	Total 104	O 104	0
39	d	91	Total 91	O 91	0
39	e	15	Total 15	O 15	0
39	f	4	Total 4	O 4	0
39	h	11	Total 11	O 11	0
39	i	3	Total 3	O 3	0
39	j	4	Total 4	O 4	0

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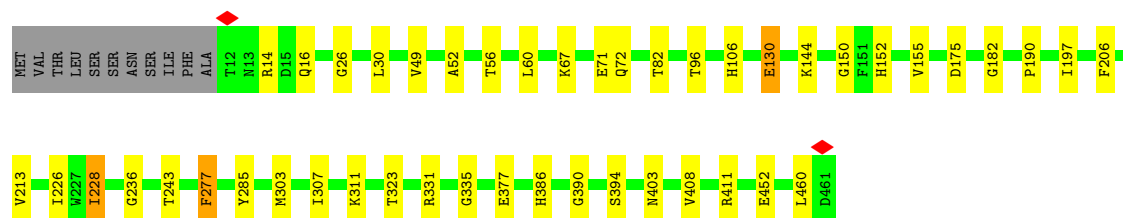
Mol	Chain	Residues	Atoms		AltConf
39	k	1	Total 1	O 1	0
39	l	10	Total 10	O 10	0
39	m	3	Total 3	O 3	0
39	o	39	Total 39	O 39	0
39	t	4	Total 4	O 4	0
39	u	13	Total 13	O 13	0
39	v	25	Total 25	O 25	0
39	x	2	Total 2	O 2	0





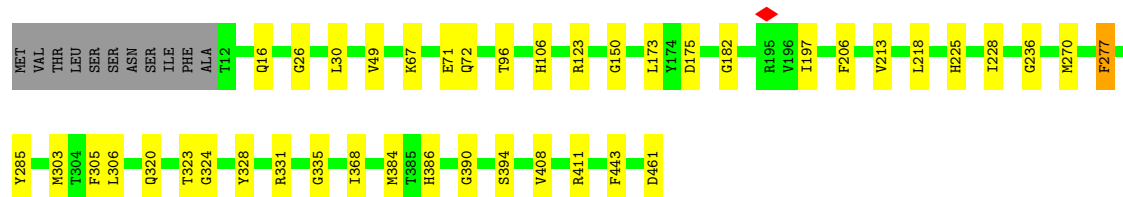
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 88% 9% ..



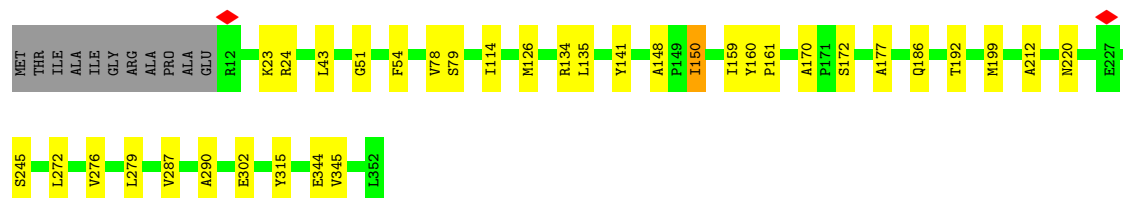
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 9% .



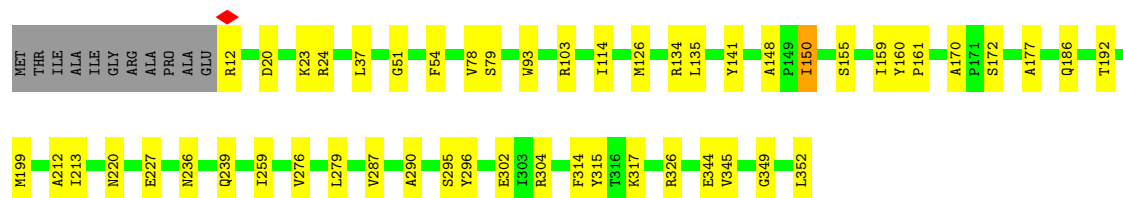
• Molecule 4: Photosystem II D2 protein

Chain D: 87% 10% .

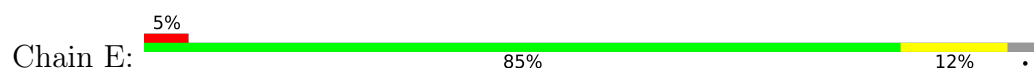


• Molecule 4: Photosystem II D2 protein

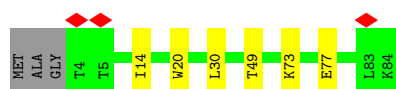
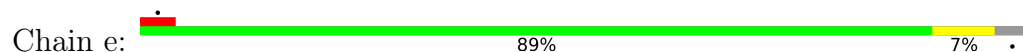
Chain d: 82% 14% .



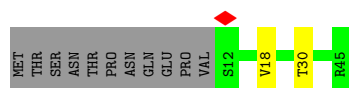
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



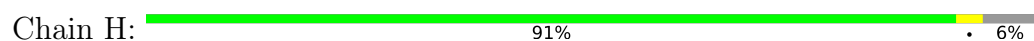
- Molecule 6: Cytochrome b559 subunit beta



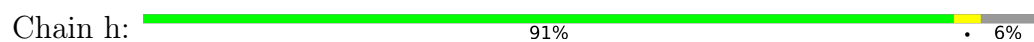
- Molecule 6: Cytochrome b559 subunit beta



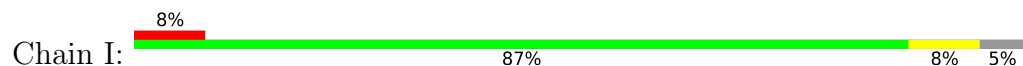
- Molecule 7: Photosystem II reaction center protein H

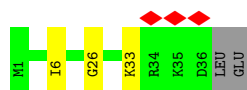


- Molecule 7: Photosystem II reaction center protein H

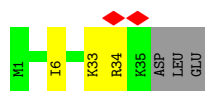
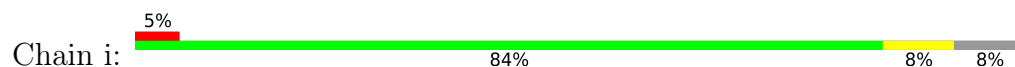


- Molecule 8: Photosystem II reaction center protein I

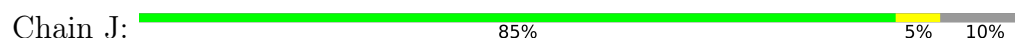




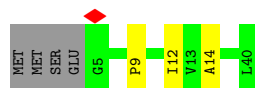
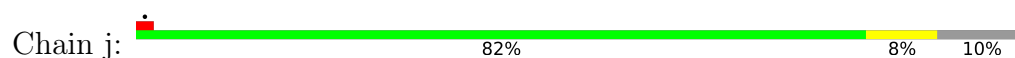
- Molecule 8: Photosystem II reaction center protein I



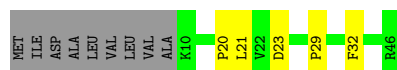
- Molecule 9: Photosystem II reaction center protein J



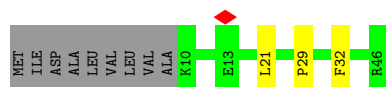
- Molecule 9: Photosystem II reaction center protein J



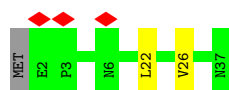
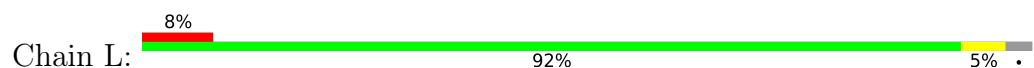
- Molecule 10: Photosystem II reaction center protein K



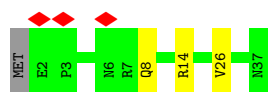
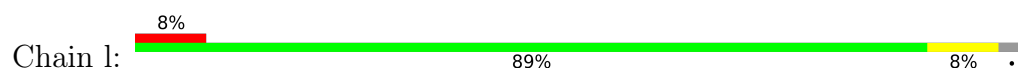
- Molecule 10: Photosystem II reaction center protein K



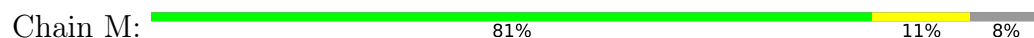
- Molecule 11: Photosystem II reaction center protein L



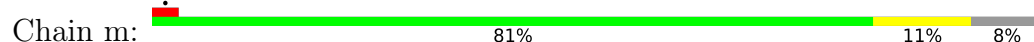
- Molecule 11: Photosystem II reaction center protein L



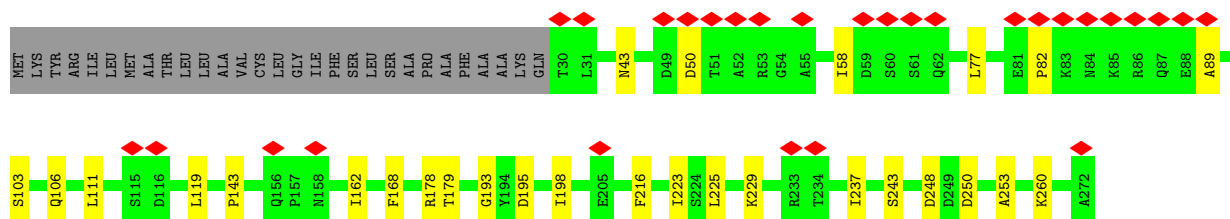
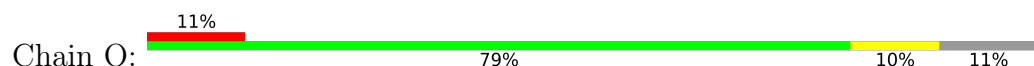
- Molecule 12: Photosystem II reaction center protein M



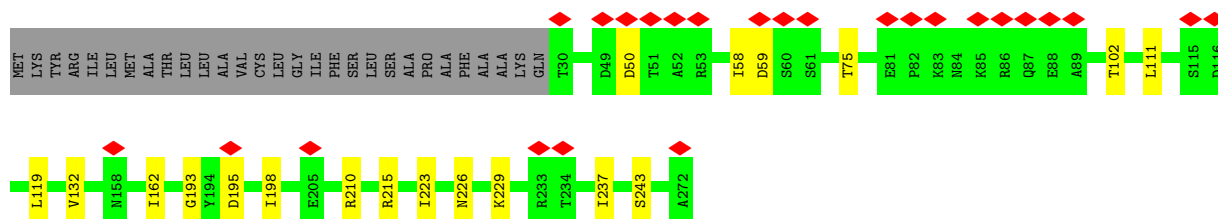
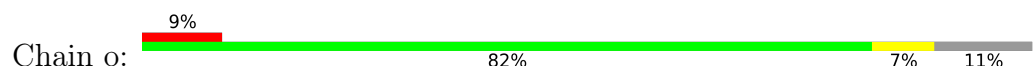
- Molecule 12: Photosystem II reaction center protein M



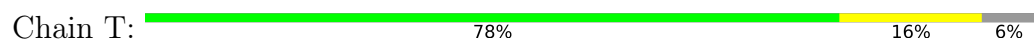
- Molecule 13: Photosystem II manganese-stabilizing polypeptide




- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T



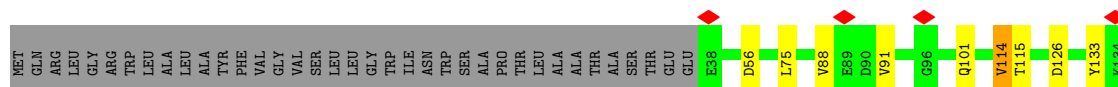
- Molecule 14: Photosystem II reaction center protein T

Chain t:  78% 16% 6%



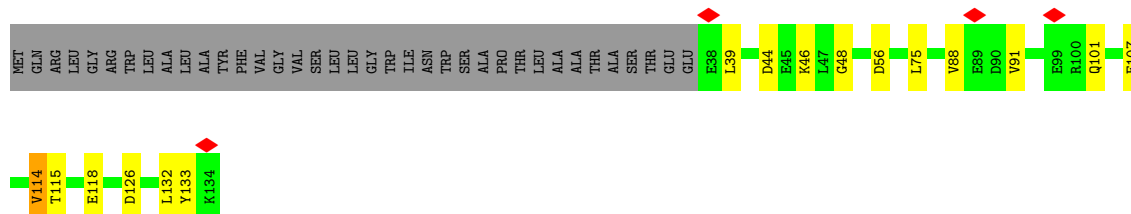
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  66% 6% 28%




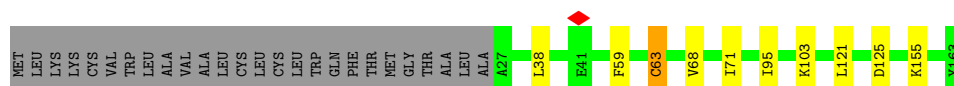
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  60% 11% 28%




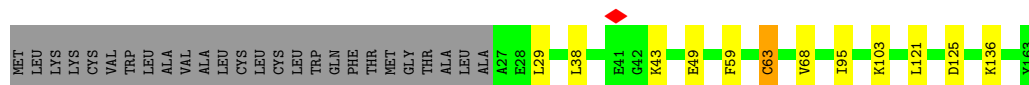
- Molecule 16: Cytochrome c-550

Chain V:  78% 6% 16%




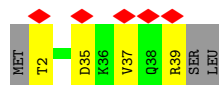
- Molecule 16: Cytochrome c-550

Chain v:  77% 7% 16%



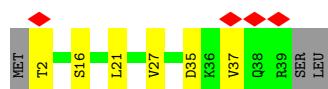
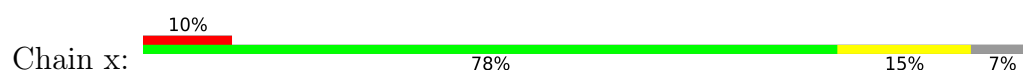
- Molecule 17: Photosystem II reaction center X protein

Chain X:  12% 83% 10% 7%

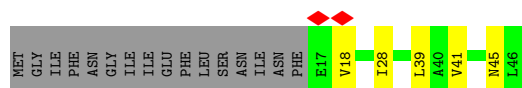


- Molecule 17: Photosystem II reaction center X protein

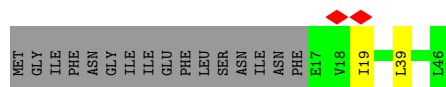




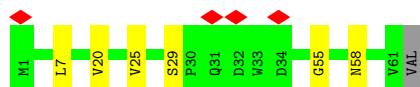
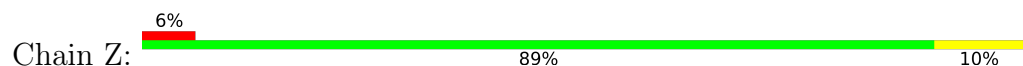
- Molecule 18: Photosystem II reaction center protein Ycf12



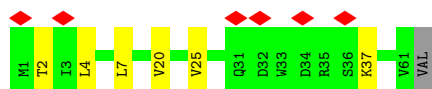
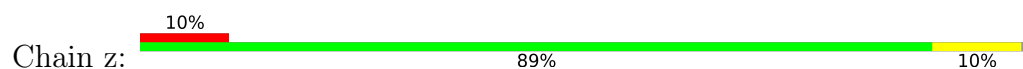
- Molecule 18: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	363811	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	0.369	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.043	Depositor
Map size (Å)	135.5, 210.0, 118.0	wwPDB
Map dimensions	236, 420, 271	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: GOL, OEX, FE2, CLA, PHO, CA, CL, LFA, BCR, LHG, FME, RRX, DGD, SQD, BCT, LMG, PLM, HEM, LMT, PL9

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	0.21	0/2682	0.42	0/3661
1	a	0.21	0/2682	0.43	0/3661
2	B	0.18	0/4075	0.37	0/5558
2	b	0.18	0/4069	0.37	0/5551
3	C	0.18	0/3571	0.38	0/4864
3	c	0.19	0/3574	0.39	0/4868
4	D	0.21	0/2805	0.41	0/3823
4	d	0.21	0/2805	0.42	0/3823
5	E	0.19	0/669	0.41	0/914
5	e	0.18	0/669	0.43	0/914
6	F	0.20	0/284	0.42	0/387
6	f	0.20	0/284	0.41	0/387
7	H	0.19	0/502	0.43	0/686
7	h	0.20	0/502	0.44	0/686
8	I	0.19	0/290	0.46	0/392
8	i	0.19	0/285	0.40	0/385
9	J	0.16	0/263	0.39	0/356
9	j	0.17	0/263	0.39	0/356
10	K	0.28	0/299	0.55	0/412
10	k	0.28	0/299	0.53	0/412
11	L	0.13	0/293	0.32	0/400
11	l	0.13	0/293	0.33	0/400
12	M	0.29	0/257	0.52	0/351
12	m	0.23	0/257	0.54	0/351
13	O	0.16	0/1830	0.40	0/2492
13	o	0.16	0/1825	0.39	0/2485
14	T	0.17	0/255	0.34	0/346
14	t	0.18	0/255	0.34	0/346
15	U	0.16	0/769	0.37	0/1044
15	u	0.16	0/769	0.38	0/1044
16	V	0.14	0/1073	0.33	0/1459

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.16	0/1073	0.35	0/1459
17	X	0.14	0/282	0.27	0/381
17	x	0.14	0/278	0.30	0/376
18	Y	0.29	0/215	0.59	0/291
18	y	0.28	0/215	0.45	0/291
19	Z	0.27	0/469	0.46	0/643
19	z	0.17	0/469	0.35	0/643
All	All	0.19	0/41749	0.40	0/56898

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2597	0	2493	31	0
1	a	2597	0	2493	30	0
2	B	3935	0	3773	37	0
2	b	3929	0	3762	37	0
3	C	3458	0	3380	31	0
3	c	3461	0	3382	26	0
4	D	2710	0	2615	26	0
4	d	2710	0	2615	38	0
5	E	650	0	629	6	0
5	e	650	0	629	5	0
6	F	275	0	282	2	0
6	f	275	0	282	2	0
7	H	489	0	502	1	0
7	h	489	0	502	1	0
8	I	293	0	309	1	0
8	i	288	0	307	1	0
9	J	257	0	268	1	0
9	j	257	0	268	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	K	289	0	294	3	0
10	k	289	0	294	2	0
11	L	286	0	289	3	0
11	l	286	0	289	3	0
12	M	254	0	272	4	0
12	m	254	0	272	4	0
13	O	1799	0	1745	16	0
13	o	1794	0	1736	11	0
14	T	256	0	256	5	0
14	t	256	0	256	5	0
15	U	758	0	757	4	0
15	u	758	0	757	7	0
16	V	1052	0	1053	5	0
16	v	1052	0	1053	6	0
17	X	279	0	307	3	0
17	x	275	0	301	4	0
18	Y	214	0	234	4	0
18	y	214	0	234	1	0
19	Z	458	0	488	2	0
19	z	458	0	488	1	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	2	0	0	1	0
21	a	2	0	0	1	0
22	A	195	0	216	5	0
22	B	1020	0	1113	23	0
22	C	845	0	936	23	0
22	D	195	0	216	3	0
22	a	195	0	216	5	0
22	b	1020	0	1113	27	0
22	c	845	0	936	23	0
22	d	195	0	216	5	0
23	A	64	0	74	1	0
23	D	64	0	74	1	0
23	a	128	0	148	3	0
24	A	40	0	56	1	0
24	B	160	0	224	10	0
24	C	80	0	112	6	0
24	F	40	0	56	1	0
24	K	40	0	56	1	0
24	T	40	0	56	2	0
24	Y	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	40	0	56	0	0
24	b	120	0	168	10	0
24	c	80	0	112	4	0
24	f	40	0	56	0	0
24	k	40	0	56	1	0
24	y	40	0	56	1	0
25	A	55	0	80	3	0
25	D	55	0	80	4	0
25	a	55	0	80	4	0
25	d	55	0	80	4	0
26	A	105	0	147	7	0
26	D	45	0	57	2	0
26	a	105	0	147	4	0
26	b	54	0	78	2	0
26	d	45	0	57	3	0
26	l	54	0	78	3	0
27	A	30	0	47	2	0
27	B	79	0	124	5	0
27	C	62	0	95	2	0
27	D	31	0	49	1	0
27	E	18	0	31	0	0
27	F	14	0	20	0	0
27	H	12	0	16	0	0
27	L	18	0	31	1	0
27	M	16	0	24	0	0
27	X	17	0	26	0	0
27	a	18	0	31	0	0
27	b	65	0	104	1	0
27	c	69	0	112	2	0
27	d	12	0	16	0	0
27	e	36	0	62	1	0
27	j	35	0	57	1	0
27	t	15	0	26	2	0
27	x	18	0	31	2	0
28	A	12	0	20	1	0
28	B	28	0	43	3	0
28	C	9	0	14	0	0
28	E	20	0	42	2	0
28	H	10	0	16	0	0
28	I	39	0	75	2	0
28	J	31	0	60	2	0
28	T	17	0	33	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	25	0	38	0	0
28	b	12	0	19	2	0
28	d	27	0	49	0	0
28	i	37	0	68	1	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	4	0	0	0	0
30	a	4	0	0	0	0
31	A	46	0	65	1	0
31	D	98	0	148	5	0
31	E	40	0	53	0	0
31	L	49	0	74	4	0
31	a	95	0	139	5	0
31	d	97	0	143	5	0
31	l	49	0	74	3	0
32	A	6	0	8	0	0
32	a	6	0	8	1	0
33	A	35	0	46	0	0
33	B	129	0	173	5	0
33	C	35	0	46	1	0
33	J	24	0	35	2	0
33	M	35	0	46	1	0
33	T	59	0	81	1	0
33	Z	35	0	46	0	0
33	b	24	0	35	0	0
33	f	35	0	46	0	0
33	i	35	0	46	0	0
33	j	24	0	35	0	0
33	m	35	0	46	1	0
33	z	35	0	46	1	0
34	C	107	0	130	2	0
34	D	44	0	57	2	0
34	H	58	0	74	1	0
34	J	61	0	83	3	0
34	c	169	0	215	4	0
34	d	47	0	59	1	0
34	h	58	0	74	0	0
35	C	102	0	144	1	0
35	D	47	0	64	2	0
35	M	51	0	72	5	0
35	Y	51	0	72	2	0
35	c	99	0	138	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	d	47	0	64	2	0
35	m	51	0	72	4	0
35	y	51	0	72	1	0
36	E	43	0	30	1	0
36	V	43	0	30	1	0
36	e	43	0	30	1	0
36	v	43	0	30	1	0
37	H	41	0	56	1	0
37	h	41	0	56	1	0
38	O	1	0	0	0	0
38	o	1	0	0	0	0
39	A	92	0	0	1	0
39	B	133	0	0	0	0
39	C	101	0	0	0	0
39	D	91	0	0	1	0
39	E	14	0	0	0	0
39	F	3	0	0	0	0
39	H	11	0	0	0	0
39	I	1	0	0	0	0
39	J	4	0	0	0	0
39	K	1	0	0	0	0
39	L	8	0	0	0	0
39	M	3	0	0	0	0
39	O	37	0	0	0	0
39	T	4	0	0	0	0
39	U	14	0	0	0	0
39	V	26	0	0	0	0
39	X	3	0	0	0	0
39	a	94	0	0	1	0
39	b	137	0	0	0	0
39	c	104	0	0	0	0
39	d	91	0	0	1	0
39	e	15	0	0	0	0
39	f	4	0	0	0	0
39	h	11	0	0	0	0
39	i	3	0	0	0	0
39	j	4	0	0	0	0
39	k	1	0	0	0	0
39	l	10	0	0	0	0
39	m	3	0	0	0	0
39	o	39	0	0	1	0
39	t	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	u	13	0	0	0	0
39	v	25	0	0	0	0
39	x	2	0	0	0	0
All	All	51092	0	51568	465	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 5.

All (465) 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	22:C:515:CLA:H2A	1.69	0.74
3:c:30:LEU:HD21	22:c:516:CLA:H2A	1.71	0.72
22:c:507:CLA:H61	22:c:517:CLA:H42	1.73	0.70
5:E:8:ARG:HE	5:E:13:ILE:HG12	1.60	0.66
3:C:303:MET:HE3	3:C:307:ILE:HD11	1.78	0.65
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.80	0.64
4:D:192:THR:HG23	22:D:405:CLA:HBC2	1.80	0.64
4:D:186:GLN:HB2	22:D:405:CLA:HBC1	1.79	0.64
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.79	0.64
4:d:186:GLN:HB2	22:d:403:CLA:HBC1	1.80	0.63
4:d:192:THR:HG23	22:d:403:CLA:HBC2	1.80	0.63
4:D:23:LYS:HG2	4:D:135:LEU:HD21	1.80	0.63
3:c:320:GLN:HE21	3:c:324:GLY:HA2	1.64	0.62
27:B:625:PLM:H21	1:a:102:LEU:HD12	1.83	0.61
21:A:402:CL:CL	39:D:584:HOH:O	2.53	0.61
14:t:14:ILE:HG21	27:t:101:PLM:H82	1.83	0.60
21:a:403:CL:CL	39:d:582:HOH:O	2.53	0.60
4:D:24:ARG:NH2	17:X:35:ASP:OD2	2.34	0.59
15:u:46:LYS:HE2	15:u:118:GLU:HB2	1.82	0.59
2:B:12:LEU:HB2	22:B:612:CLA:HMC2	1.84	0.58
4:d:54:PHE:O	5:e:49:THR:OG1	2.19	0.58
2:b:12:LEU:HB2	22:b:614:CLA:HMC2	1.84	0.58
3:C:14:ARG:NH2	18:Y:45:ASN:O	2.37	0.58
3:c:306:LEU:HD12	3:c:328:TYR:HB3	1.86	0.58
22:b:617:CLA:H161	7:h:7:LEU:HD21	1.86	0.58
35:D:409:LMG:H121	34:J:102:DGD:HB51	1.84	0.58
34:c:505:DGD:HB51	35:d:407:LMG:H121	1.85	0.57
26:d:412:SQD:H241	6:f:18:VAL:HG22	1.85	0.57
22:A:407:CLA:H152	22:C:510:CLA:H13	1.85	0.57
28:A:412:LFA:H142	27:A:413:PLM:H31	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:199:MET:HG2	25:d:402:PL9:H312	1.86	0.57
2:B:352:GLU:OE1	2:B:378:LYS:NZ	2.38	0.57
1:A:45:THR:HG21	26:A:410:SQD:H211	1.87	0.57
22:B:615:CLA:H161	7:H:7:LEU:HD21	1.86	0.57
31:a:415:LHG:H221	4:d:37:LEU:HD21	1.87	0.57
4:D:199:MET:HG2	25:D:404:PL9:H312	1.86	0.56
15:U:75:LEU:HD21	15:U:101:GLN:HB3	1.87	0.56
2:b:352:GLU:OE1	2:b:378:LYS:NZ	2.38	0.56
3:c:225:HIS:HA	3:c:228:ILE:HG22	1.87	0.56
13:O:77:LEU:HD12	13:O:260:LYS:HD2	1.87	0.56
1:a:215:HIS:ND1	25:a:410:PL9:O2	2.38	0.56
15:U:88:VAL:HG23	15:U:114:VAL:HG22	1.87	0.56
28:T:102:LFA:H51	24:b:602:BCR:H14C	1.86	0.56
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.87	0.56
28:B:626:LFA:H171	28:i:104:LFA:H141	1.87	0.56
4:D:126:MET:HE3	4:D:150:ILE:HD12	1.86	0.56
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.88	0.56
2:B:501:ASP:OD2	17:X:39:ARG:NH1	2.39	0.55
15:u:88:VAL:HG23	15:u:114:VAL:HG22	1.89	0.55
1:a:342:ASP:HB2	4:d:352:LEU:HD21	1.88	0.55
4:D:54:PHE:O	5:E:49:THR:OG1	2.19	0.55
23:a:420:PHO:HBC3	4:d:279:LEU:HD22	1.89	0.55
2:b:18:ARG:NH2	26:b:601:SQD:O9	2.36	0.55
4:d:126:MET:HE3	4:d:150:ILE:HD12	1.89	0.54
1:A:121:LEU:HD11	22:C:509:CLA:H152	1.89	0.54
3:C:311:LYS:NZ	3:C:377:GLU:OE1	2.40	0.54
34:c:504:DGD:HA21	22:c:509:CLA:H42	1.88	0.54
31:l:101:LHG:H322	12:m:18:PRO:HB3	1.88	0.54
3:C:52:ALA:O	3:C:56:THR:OG1	2.25	0.54
31:d:405:LHG:H351	31:d:405:LHG:H101	1.89	0.54
15:u:75:LEU:HD21	15:u:101:GLN:HB3	1.89	0.54
2:B:42:LEU:HD13	2:B:94:GLU:HG3	1.90	0.54
2:B:116:VAL:HG21	24:B:619:BCR:H271	1.90	0.54
4:D:279:LEU:HD22	23:D:403:PHO:HBC3	1.89	0.54
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.90	0.54
4:d:23:LYS:HE3	4:d:135:LEU:HD11	1.90	0.54
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.90	0.54
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.90	0.53
3:C:71:GLU:OE2	3:C:386:HIS:NE2	2.37	0.53
1:a:165:GLN:NE2	39:a:510:HOH:O	2.40	0.53
2:b:311:PHE:O	2:b:317:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:71:GLU:OE2	3:c:386:HIS:NE2	2.39	0.53
13:o:111:LEU:HG	13:o:119:LEU:HD12	1.90	0.53
1:A:267:ASN:HB3	1:A:270:SER:HB3	1.91	0.53
4:D:302:GLU:OE1	4:D:315:TYR:OH	2.22	0.53
1:A:215:HIS:ND1	25:A:409:PL9:O2	2.38	0.53
1:A:283:VAL:HA	1:A:286:THR:HG22	1.91	0.53
2:B:311:PHE:O	2:B:317:ASN:ND2	2.42	0.52
24:B:632:BCR:HC7	14:t:18:PHE:HD1	1.74	0.52
10:K:21:LEU:HD21	24:Y:102:BCR:HC31	1.90	0.52
3:C:331:ARG:NH1	3:C:335:GLY:O	2.42	0.52
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.90	0.52
3:c:331:ARG:NH1	3:c:335:GLY:O	2.42	0.52
24:B:617:BCR:H402	26:l:102:SQD:H82	1.92	0.52
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.24	0.52
3:c:285:TYR:O	3:c:411:ARG:NH2	2.42	0.52
25:a:410:PL9:H221	23:a:420:PHO:HMA2	1.92	0.52
15:u:56:ASP:OD2	15:u:115:THR:OG1	2.26	0.52
22:a:408:CLA:H152	22:c:511:CLA:H13	1.91	0.52
33:B:628:LMT:H102	27:B:629:PLM:HF1	1.91	0.51
4:D:23:LYS:HE2	4:D:135:LEU:HD11	1.92	0.51
13:O:195:ASP:OD1	13:O:195:ASP:N	2.43	0.51
22:c:513:CLA:HBC3	22:c:515:CLA:H71	1.92	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.51
1:A:85:SER:HA	1:A:109:GLY:HA3	1.93	0.51
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.93	0.51
1:A:46:ILE:HD13	26:A:410:SQD:H371	1.93	0.51
3:C:285:TYR:O	3:C:411:ARG:NH2	2.41	0.51
1:a:84:PRO:HA	1:a:112:TYR:CG	2.46	0.51
1:a:283:VAL:HA	1:a:286:THR:HG22	1.92	0.51
22:c:506:CLA:H203	22:c:512:CLA:H13	1.93	0.51
1:A:165:GLN:NE2	39:A:511:HOH:O	2.43	0.51
3:C:175:ASP:O	3:C:182:GLY:HA2	2.10	0.51
1:a:85:SER:HA	1:a:109:GLY:HA3	1.92	0.51
25:a:410:PL9:H422	26:d:412:SQD:H252	1.92	0.51
2:b:256:MET:HA	2:b:263:THR:HG21	1.93	0.51
22:C:512:CLA:HBC3	22:C:514:CLA:H71	1.91	0.50
34:D:411:DGD:HD4	5:E:45:ASP:HB3	1.93	0.50
14:T:18:PHE:HD1	24:b:602:BCR:HC7	1.76	0.50
3:c:26:GLY:HA3	22:c:516:CLA:HMD2	1.93	0.50
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.93	0.50
2:B:399:VAL:HG12	2:B:417:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:415:SQD:H262	31:A:417:LHG:H142	1.92	0.50
13:O:58:ILE:HG21	13:O:119:LEU:HD21	1.93	0.50
31:D:407:LHG:H101	31:D:407:LHG:H351	1.94	0.50
3:C:213:VAL:HG13	3:C:277:PHE:HA	1.93	0.50
10:k:21:LEU:HD21	24:y:102:BCR:HC31	1.92	0.50
2:B:39:LEU:HD13	33:B:630:LMT:H81	1.94	0.50
4:D:79:SER:HA	4:D:172:SER:HB3	1.94	0.49
13:o:195:ASP:OD1	13:o:195:ASP:N	2.43	0.49
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.95	0.49
22:b:609:CLA:H122	35:m:101:LMG:H241	1.93	0.49
1:a:201:GLY:HA3	1:a:286:THR:HB	1.94	0.49
18:y:39:LEU:HD21	19:z:25:VAL:HA	1.94	0.49
22:C:507:CLA:H18	22:C:514:CLA:HBB2	1.95	0.49
3:c:213:VAL:HG13	3:c:277:PHE:HA	1.94	0.49
13:o:223:ILE:HG13	13:o:243:SER:HB3	1.95	0.49
16:V:103:LYS:HG2	16:V:121:LEU:HD12	1.95	0.49
2:b:42:LEU:HD13	2:b:94:GLU:HG3	1.95	0.49
2:b:498:LYS:HE3	4:d:23:LYS:HE2	1.95	0.49
4:d:296:TYR:OH	4:d:326:ARG:NH1	2.40	0.49
31:a:415:LHG:HC42	27:e:102:PLM:H51	1.95	0.49
2:b:7:ARG:O	2:b:10:THR:OG1	2.25	0.49
12:m:14:PHE:HD2	35:m:101:LMG:H361	1.78	0.49
2:B:247:PHE:HB2	22:B:608:CLA:HBC1	1.96	0.48
13:O:111:LEU:HG	13:O:119:LEU:HD12	1.94	0.48
3:c:49:VAL:HG13	3:c:106:HIS:HD2	1.78	0.48
28:I:103:LFA:H121	28:b:623:LFA:H191	1.94	0.48
26:b:601:SQD:H112	22:b:616:CLA:H43	1.95	0.48
26:a:417:SQD:H302	22:c:513:CLA:H71	1.95	0.48
2:b:498:LYS:HA	4:d:24:ARG:HA	1.95	0.48
22:c:508:CLA:H18	22:c:515:CLA:HBB2	1.95	0.48
16:v:125:ASP:OD1	16:v:125:ASP:N	2.45	0.48
3:c:67:LYS:HE3	3:c:72:GLN:HG2	1.95	0.48
1:A:201:GLY:HA3	1:A:286:THR:HB	1.95	0.48
22:B:602:CLA:H101	22:B:609:CLA:H193	1.94	0.48
28:B:620:LFA:H81	33:B:630:LMT:H121	1.94	0.48
28:J:104:LFA:H62	18:Y:18:VAL:HG11	1.96	0.48
12:M:4:ASN:ND2	35:M:101:LMG:O10	2.44	0.48
11:l:26:VAL:HG21	31:l:101:LHG:H192	1.95	0.48
22:B:604:CLA:H172	22:B:604:CLA:H13	1.75	0.48
22:B:612:CLA:H171	22:B:613:CLA:HBB2	1.96	0.48
22:b:614:CLA:H171	22:b:615:CLA:HBB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:93:TRP:HB3	27:x:101:PLM:H41	1.95	0.48
31:d:406:LHG:H141	31:d:406:LHG:H292	1.95	0.48
2:B:256:MET:HA	2:B:263:THR:HG21	1.95	0.48
3:C:26:GLY:HA3	22:C:515:CLA:HMD2	1.95	0.48
26:D:412:SQD:H241	6:F:18:VAL:HG22	1.95	0.48
11:L:26:VAL:HG21	31:L:101:LHG:H192	1.95	0.48
2:b:23:HIS:ND1	22:b:617:CLA:OBD	2.30	0.48
1:A:38:ILE:HG23	26:A:410:SQD:H151	1.96	0.48
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.49	0.48
2:B:25:MET:HG2	24:B:617:BCR:H23C	1.96	0.48
22:b:604:CLA:H101	22:b:611:CLA:H193	1.95	0.48
3:c:306:LEU:HD21	3:c:368:ILE:HG23	1.96	0.48
34:C:504:DGD:HA21	22:C:508:CLA:H42	1.96	0.48
1:a:146:ALA:HB2	31:a:421:LHG:H261	1.95	0.48
2:b:474:LEU:HD11	22:b:610:CLA:HAA2	1.96	0.47
11:l:14:ARG:HH22	26:l:102:SQD:H3	1.79	0.47
2:b:399:VAL:HG12	2:b:417:VAL:HG22	1.96	0.47
2:B:498:LYS:HA	4:D:24:ARG:HA	1.96	0.47
4:d:79:SER:HA	4:d:172:SER:HB3	1.96	0.47
22:B:607:CLA:H2	35:M:101:LMG:H151	1.96	0.47
3:C:197:ILE:HG23	24:C:502:BCR:H382	1.96	0.47
1:a:77:ILE:HD11	14:t:6:TYR:HB3	1.97	0.47
2:b:385:ARG:NH2	13:o:193:GLY:O	2.44	0.47
22:c:507:CLA:HBB2	22:c:515:CLA:H151	1.96	0.47
2:B:497:GLN:HG3	2:B:506:ARG:HD2	1.97	0.47
33:B:630:LMT:H3O1	4:d:304:ARG:HH22	1.61	0.47
3:C:226:ILE:HD13	27:C:524:PLM:H61	1.96	0.47
22:C:506:CLA:HBB2	22:C:514:CLA:H151	1.97	0.47
33:J:103:LMT:H102	33:J:103:LMT:H71	1.69	0.47
14:T:7:VAL:HG12	33:T:101:LMT:H122	1.95	0.47
2:b:116:VAL:HG21	24:b:620:BCR:H292	1.97	0.47
2:b:247:PHE:HB2	22:b:610:CLA:HBC1	1.95	0.47
1:a:103:ASP:OD1	32:a:401:GOL:O2	2.28	0.47
2:B:109:LEU:HD13	26:a:411:SQD:H262	1.97	0.47
22:B:607:CLA:H122	35:M:101:LMG:H241	1.95	0.47
4:d:236:ASN:HB3	4:d:239:GLN:HB3	1.97	0.47
5:e:30:LEU:HD11	36:e:103:HEM:HAB	1.97	0.47
3:c:197:ILE:HG23	24:c:502:BCR:H382	1.97	0.47
16:v:103:LYS:HG2	16:v:121:LEU:HD12	1.96	0.46
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.96	0.46
1:A:131:TRP:CH2	22:C:509:CLA:HAA2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:VAL:HG11	22:C:516:CLA:HBA2	1.97	0.46
13:O:250:ASP:HB3	13:O:253:ALA:HB3	1.98	0.46
1:a:131:TRP:CH2	22:c:510:CLA:HAA2	2.50	0.46
3:C:49:VAL:HG13	3:C:106:HIS:HD2	1.79	0.46
27:D:402:PLM:H41	27:D:410:PLM:H82	1.98	0.46
2:b:158:LEU:HB3	2:b:199:VAL:HG22	1.96	0.46
3:c:206:PHE:HZ	35:c:519:LMG:H161	1.81	0.46
24:C:502:BCR:H16C	22:C:511:CLA:H142	1.96	0.46
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.97	0.46
1:a:214:MET:HB3	25:a:410:PL9:H103	1.97	0.46
3:c:123:ARG:NH1	33:z:101:LMT:O3B	2.48	0.46
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.97	0.46
22:b:609:CLA:H2	35:m:101:LMG:H151	1.98	0.46
24:B:617:BCR:H341	24:B:632:BCR:H24C	1.97	0.46
3:C:60:LEU:HD11	3:C:96:THR:HB	1.98	0.46
1:a:63:ILE:HB	3:c:323:THR:HG21	1.97	0.46
1:a:267:ASN:HB3	1:a:270:SER:HB3	1.96	0.46
1:a:340:PRO:HG3	15:u:133:TYR:CG	2.51	0.46
10:k:29:PRO:O	10:k:32:PHE:HB2	2.16	0.46
1:A:43:ALA:HB1	24:A:408:BCR:H362	1.97	0.46
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.97	0.46
3:C:190:PRO:HD2	27:C:524:PLM:H22	1.98	0.46
37:h:102:RRX:H3	17:x:2:THR:N	2.13	0.46
2:B:23:HIS:ND1	22:B:615:CLA:OBD	2.29	0.46
2:B:155:ALA:O	2:B:159:THR:OG1	2.28	0.46
22:b:615:CLA:H18	31:d:405:LHG:H202	1.98	0.46
22:A:404:CLA:H152	23:A:406:PHO:H52	1.98	0.46
24:B:632:BCR:H351	26:l:102:SQD:H201	1.98	0.46
5:E:30:LEU:HD11	36:E:104:HEM:HAB	1.97	0.46
33:J:103:LMT:H92	35:Y:101:LMG:H332	1.98	0.46
22:c:518:CLA:HBA2	27:c:520:PLM:H61	1.98	0.46
4:d:148:ALA:HB2	4:d:276:VAL:HG13	1.98	0.46
2:B:7:ARG:O	2:B:10:THR:OG1	2.26	0.45
2:B:33:TRP:CD1	24:B:632:BCR:H381	2.51	0.45
18:Y:39:LEU:HD21	19:Z:25:VAL:HA	1.98	0.45
22:a:406:CLA:HED1	34:c:505:DGD:HBW2	1.98	0.45
31:a:421:LHG:H151	31:a:421:LHG:H331	1.98	0.45
9:J:9:PRO:HD2	9:J:12:ILE:HD12	1.99	0.45
2:b:33:TRP:CD1	24:b:602:BCR:H381	2.51	0.45
22:b:615:CLA:H193	24:b:619:BCR:HC32	1.99	0.45
1:A:63:ILE:HB	3:C:323:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:390:GLY:HA3	3:c:408:VAL:HG22	1.97	0.45
15:u:44:ASP:OD1	15:u:44:ASP:N	2.49	0.45
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.99	0.45
17:x:16:SER:HB3	27:x:101:PLM:HA1	1.98	0.45
33:C:518:LMT:H6'2	8:I:26:GLY:HA3	1.99	0.45
12:M:14:PHE:HD2	35:M:101:LMG:H361	1.80	0.45
24:T:103:BCR:H23C	2:b:25:MET:HG2	1.98	0.45
26:A:415:SQD:O7	3:C:16:GLN:NE2	2.42	0.45
2:B:497:GLN:HB2	2:B:504:THR:HB	1.98	0.45
10:K:29:PRO:O	10:K:32:PHE:HB2	2.16	0.45
22:c:518:CLA:HBD	27:c:520:PLM:H32	1.98	0.45
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.98	0.45
12:M:31:SER:OG	12:m:31:SER:OG	2.34	0.45
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.52	0.45
3:C:452:GLU:OE2	4:D:245:SER:OG	2.32	0.45
24:T:103:BCR:H341	24:b:602:BCR:H24C	1.99	0.45
2:B:74:SER:OG	2:B:94:GLU:OE2	2.32	0.45
2:B:474:LEU:O	4:D:134:ARG:NH1	2.50	0.45
22:B:613:CLA:H193	24:B:618:BCR:HC32	1.99	0.45
27:B:622:PLM:H52	27:B:622:PLM:H82	1.77	0.45
34:C:504:DGD:HA42	35:Y:101:LMG:H391	1.98	0.45
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.99	0.45
13:o:58:ILE:HG21	13:o:119:LEU:HD21	1.98	0.45
25:A:409:PL9:H251	25:A:409:PL9:H271	1.59	0.44
22:C:505:CLA:C2D	22:C:507:CLA:H2	2.47	0.44
24:c:502:BCR:H16C	22:c:512:CLA:H142	1.99	0.44
22:B:615:CLA:H2	22:B:616:CLA:CBB	2.47	0.44
13:O:143:PRO:HG2	13:O:248:ASP:HB3	1.99	0.44
1:a:102:LEU:HD23	1:a:102:LEU:HA	1.84	0.44
4:d:12:ARG:NH1	4:d:20:ASP:OD2	2.51	0.44
28:I:103:LFA:H102	28:b:623:LFA:H171	1.99	0.44
31:a:415:LHG:H241	31:a:415:LHG:HC61	1.74	0.44
16:v:38:LEU:HD12	16:v:95:ILE:HB	1.99	0.44
2:B:91:TRP:HE1	27:B:621:PLM:H42	1.82	0.44
3:C:150:GLY:HA2	3:C:236:GLY:HA2	1.98	0.44
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.99	0.44
2:b:474:LEU:O	4:d:134:ARG:NH1	2.50	0.44
24:b:619:BCR:H24C	24:b:619:BCR:H371	1.87	0.44
9:j:9:PRO:HD2	9:j:12:ILE:HD12	1.99	0.44
13:o:210:ARG:HG3	13:o:215:ARG:HH12	1.81	0.44
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:498:LYS:HD2	4:d:20:ASP:HA	2.00	0.44
3:c:123:ARG:HD2	3:c:123:ARG:HA	1.80	0.44
22:d:401:CLA:H52	25:d:402:PL9:H151	2.00	0.44
14:t:11:ALA:HA	27:t:101:PLM:H52	2.00	0.44
5:E:10:PHE:HB3	28:E:102:LFA:H132	1.99	0.44
22:b:612:CLA:H192	22:b:617:CLA:HMD3	1.99	0.44
34:c:504:DGD:HBT2	22:c:513:CLA:H192	1.99	0.44
4:d:159:ILE:HG21	4:d:287:VAL:HG22	1.99	0.44
37:H:102:RRX:H3	17:X:2:THR:N	2.16	0.44
1:a:250:ALA:HA	2:b:491:VAL:HG11	2.00	0.44
22:c:506:CLA:C2D	22:c:508:CLA:H2	2.48	0.43
4:d:141:TYR:OH	31:d:405:LHG:O4	2.32	0.43
2:B:278:SER:HB3	2:B:281:GLN:HE21	1.82	0.43
2:B:383:PHE:N	4:D:344:GLU:O	2.44	0.43
22:B:610:CLA:H192	22:B:615:CLA:HMD3	2.00	0.43
22:C:514:CLA:HBC3	22:C:514:CLA:H192	2.00	0.43
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.00	0.43
4:d:103:ARG:HH21	5:e:77:GLU:HG2	1.83	0.43
22:B:611:CLA:H112	22:B:611:CLA:H72	1.81	0.43
33:M:102:LMT:H112	12:m:17:VAL:HG13	1.99	0.43
22:d:404:CLA:H202	22:d:404:CLA:H161	1.81	0.43
26:a:411:SQD:H161	26:a:411:SQD:H192	1.44	0.43
2:b:383:PHE:CZ	13:o:193:GLY:HA2	2.53	0.43
22:b:607:CLA:H41	22:b:607:CLA:H62	1.74	0.43
22:b:610:CLA:H3A	22:b:610:CLA:HBA2	1.84	0.43
22:b:617:CLA:H2	22:b:618:CLA:CBB	2.48	0.43
22:B:606:CLA:H61	22:B:606:CLA:H102	1.81	0.43
3:C:206:PHE:HZ	35:C:519:LMG:H161	1.82	0.43
1:a:93:PHE:HZ	22:a:408:CLA:HAA1	1.84	0.43
3:c:150:GLY:HA2	3:c:236:GLY:HA2	1.99	0.43
4:d:160:TYR:HA	4:d:290:ALA:HB2	2.01	0.43
2:B:464:PHE:HD2	22:B:611:CLA:HAC2	1.83	0.43
22:c:506:CLA:C3D	22:c:508:CLA:H2	2.49	0.43
4:d:51:GLY:HA3	4:d:78:VAL:HG22	2.01	0.43
35:m:101:LMG:H171	35:m:101:LMG:H142	1.90	0.43
16:v:59:PHE:HA	16:v:63:CYS:SG	2.59	0.43
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.01	0.43
2:b:384:ARG:NH2	4:d:349:GLY:O	2.48	0.43
9:j:14:ALA:HB2	27:j:103:PLM:H82	1.99	0.43
13:o:50:ASP:HA	13:o:229:LYS:HE2	2.00	0.43
3:C:403:ASN:OD1	34:J:102:DGD:O4D	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:17:VAL:HG13	33:m:102:LMT:H112	2.01	0.43
1:a:65:GLU:OE2	1:a:334:ARG:NH2	2.51	0.43
27:B:625:PLM:H52	28:B:626:LFA:H192	2.01	0.43
22:C:505:CLA:C3D	22:C:507:CLA:H2	2.48	0.43
4:D:159:ILE:HG21	4:D:287:VAL:HG22	2.01	0.43
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.01	0.43
25:A:409:PL9:H371	25:A:409:PL9:H351	1.75	0.43
22:B:604:CLA:H12	22:B:605:CLA:ND	2.34	0.43
3:C:394:SER:HA	3:C:408:VAL:HG23	2.00	0.43
4:D:141:TYR:OH	31:D:407:LHG:O4	2.31	0.43
13:O:50:ASP:HA	13:O:229:LYS:HE2	2.01	0.43
19:Z:55:GLY:O	19:Z:58:ASN:HB3	2.18	0.43
26:a:417:SQD:O7	3:c:16:GLN:NE2	2.41	0.42
2:b:464:PHE:HD2	22:b:613:CLA:HAC2	1.83	0.42
22:D:401:CLA:H52	25:D:404:PL9:H151	2.00	0.42
31:D:408:LHG:H182	14:T:17:PHE:HZ	1.85	0.42
24:c:502:BCR:H341	22:c:510:CLA:HBC2	2.01	0.42
34:d:410:DGD:HA51	34:d:410:DGD:HA22	1.81	0.42
26:d:412:SQD:H281	17:x:27:VAL:HG11	2.01	0.42
16:v:29:LEU:HD23	16:v:49:GLU:HG3	2.00	0.42
27:L:102:PLM:H41	27:L:102:PLM:H71	1.83	0.42
13:O:82:PRO:HG3	13:O:89:ALA:HB2	2.02	0.42
1:a:308:ASP:OD1	1:a:312:ASN:N	2.52	0.42
13:o:102:THR:HG22	13:o:132:VAL:HG22	2.01	0.42
22:C:505:CLA:H151	22:C:511:CLA:H52	2.00	0.42
36:V:201:HEM:HMB1	36:V:201:HEM:HBB2	2.02	0.42
22:b:606:CLA:H12	22:b:607:CLA:ND	2.34	0.42
3:c:270:MET:HG2	22:c:506:CLA:H61	2.02	0.42
22:c:515:CLA:H192	22:c:515:CLA:HBC3	2.00	0.42
4:d:24:ARG:NH2	17:x:35:ASP:OD2	2.50	0.42
4:d:302:GLU:OE2	4:d:315:TYR:OH	2.27	0.42
13:o:226:ASN:ND2	39:o:408:HOH:O	2.51	0.42
22:B:615:CLA:H2	22:B:616:CLA:HBB2	2.01	0.42
13:O:43:ASN:O	13:O:103:SER:OG	2.34	0.42
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.52	0.42
22:A:405:CLA:HED1	34:J:102:DGD:HBW2	2.00	0.42
26:A:415:SQD:H461	26:A:415:SQD:H241	1.78	0.42
22:C:516:CLA:H91	22:C:516:CLA:H111	1.80	0.42
35:D:409:LMG:H412	6:F:30:THR:HG21	2.01	0.42
24:F:101:BCR:H20C	24:F:101:BCR:H361	1.94	0.42
2:b:497:GLN:HB2	2:b:504:THR:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:d:402:PL9:H43	25:d:402:PL9:H472	1.88	0.42
2:B:450:TRP:NE1	22:B:607:CLA:HBA1	2.35	0.42
22:C:505:CLA:HBB2	22:C:511:CLA:H61	2.02	0.42
25:D:404:PL9:H201	31:L:101:LHG:H202	2.02	0.42
22:c:511:CLA:H18	22:c:511:CLA:H122	2.00	0.42
25:d:402:PL9:H201	31:l:101:LHG:H202	2.01	0.42
24:C:502:BCR:H352	22:C:510:CLA:H143	2.01	0.42
5:E:14:ILE:O	5:E:20:TRP:NE1	2.52	0.42
3:c:305:PHE:HE2	3:c:384:MET:HE1	1.85	0.42
35:d:407:LMG:H412	6:f:30:THR:HG21	2.01	0.42
27:A:413:PLM:H71	27:A:413:PLM:H42	1.73	0.42
35:M:101:LMG:H171	35:M:101:LMG:H142	1.89	0.42
22:a:405:CLA:H152	23:a:407:PHO:H52	2.01	0.42
1:A:183:MET:HB3	22:A:404:CLA:HBC2	2.02	0.42
1:A:277:ALA:HB1	26:A:415:SQD:H152	2.01	0.42
3:C:228:ILE:HD13	3:C:228:ILE:HA	1.91	0.42
28:E:102:LFA:H51	28:J:101:LFA:H42	2.01	0.42
10:K:20:PRO:O	10:K:23:ASP:HB2	2.19	0.42
11:L:22:LEU:HG	31:L:101:LHG:H181	2.02	0.42
35:c:524:LMG:HC8	35:c:524:LMG:HC1	1.83	0.42
2:B:422:ARG:NH1	13:O:195:ASP:OD2	2.53	0.41
26:D:412:SQD:H282	26:D:412:SQD:H311	1.84	0.41
2:b:393:GLU:HB3	15:u:48:GLY:HA2	2.01	0.41
13:o:162:ILE:HG21	13:o:237:ILE:HG21	2.02	0.41
1:A:308:ASP:OD1	1:A:312:ASN:N	2.53	0.41
2:B:33:TRP:HD1	24:B:632:BCR:H381	1.85	0.41
2:B:78:TRP:HZ3	2:B:80:ILE:HG23	1.85	0.41
3:C:67:LYS:HE3	3:C:72:GLN:HG2	2.01	0.41
16:V:125:ASP:OD1	16:V:125:ASP:N	2.49	0.41
35:c:524:LMG:H332	35:c:524:LMG:H361	1.83	0.41
4:d:161:PRO:HB3	4:d:170:ALA:HB2	2.02	0.41
31:d:406:LHG:H182	14:t:17:PHE:HZ	1.86	0.41
1:A:93:PHE:HZ	22:A:407:CLA:HAA1	1.85	0.41
3:C:82:THR:HG22	22:C:505:CLA:HED1	2.03	0.41
22:C:505:CLA:HBC1	22:C:516:CLA:H43	2.01	0.41
13:O:168:PHE:HB2	13:O:225:LEU:HB2	2.02	0.41
3:c:175:ASP:O	3:c:182:GLY:HA2	2.20	0.41
22:B:615:CLA:H91	22:B:615:CLA:H112	1.92	0.41
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.02	0.41
24:K:101:BCR:H20C	24:K:101:BCR:H361	1.87	0.41
13:O:162:ILE:HG21	13:O:237:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:450:TRP:NE1	22:b:609:CLA:HBA1	2.36	0.41
2:b:458:PHE:HB3	22:b:606:CLA:HBC2	2.03	0.41
22:b:605:CLA:H62	22:b:605:CLA:H41	1.92	0.41
2:B:30:VAL:HG12	22:B:605:CLA:HHD	2.02	0.41
2:B:458:PHE:HB3	22:B:604:CLA:HBC2	2.02	0.41
3:c:394:SER:HA	3:c:408:VAL:HG23	2.01	0.41
1:A:279:PRO:HG2	4:D:212:ALA:HB2	2.02	0.41
1:A:304:HIS:CE1	16:V:155:LYS:HD2	2.56	0.41
31:D:407:LHG:H201	31:L:101:LHG:H322	2.01	0.41
18:Y:28:ILE:HG23	24:Y:102:BCR:H10C	2.02	0.41
24:b:620:BCR:H20C	24:b:620:BCR:H361	1.94	0.41
4:d:155:SER:HA	4:d:159:ILE:HB	2.03	0.41
1:A:102:LEU:HD23	1:A:102:LEU:HA	1.87	0.41
1:a:183:MET:HB3	22:a:405:CLA:HBC2	2.03	0.41
1:a:279:PRO:HG2	4:d:212:ALA:HB2	2.02	0.41
2:b:160:GLY:HA3	2:b:180:PRO:HB3	2.02	0.41
22:b:606:CLA:H172	22:b:606:CLA:H13	1.76	0.41
22:b:617:CLA:H2	22:b:618:CLA:HBB2	2.03	0.41
24:b:619:BCR:H20C	24:b:619:BCR:H361	1.89	0.41
4:d:314:PHE:HA	4:d:317:LYS:HD3	2.03	0.41
33:B:633:LMT:H122	33:B:633:LMT:H91	1.82	0.41
16:V:38:LEU:HD12	16:V:95:ILE:HB	2.02	0.41
2:b:75:TRP:CE2	27:b:622:PLM:H41	2.55	0.41
22:b:608:CLA:H102	22:b:608:CLA:H61	1.77	0.41
36:v:201:HEM:HMB1	36:v:201:HEM:HBB2	2.01	0.41
1:A:217:SER:HA	4:D:272:LEU:HD12	2.03	0.41
2:B:112:CYS:HA	24:B:617:BCR:H282	2.03	0.41
2:B:201:HIS:HB2	22:B:602:CLA:CHB	2.51	0.41
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.03	0.41
3:C:130:GLU:H	3:C:130:GLU:HG2	1.62	0.41
24:C:501:BCR:H20C	24:C:501:BCR:H361	1.93	0.41
22:b:617:CLA:H61	22:b:617:CLA:H92	1.87	0.41
22:c:513:CLA:H151	35:y:101:LMG:H391	2.03	0.41
4:d:78:VAL:HG11	4:d:114:ILE:HD12	2.01	0.41
5:e:14:ILE:O	5:e:20:TRP:NE1	2.50	0.41
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.56	0.41
3:C:323:THR:O	13:O:178:ARG:NH1	2.52	0.41
3:C:390:GLY:HA3	3:C:408:VAL:HG22	2.03	0.41
31:D:408:LHG:H142	11:L:22:LEU:HD21	2.03	0.41
2:b:11:VAL:HG12	11:l:8:GLN:HG3	2.03	0.41
4:d:295:SER:O	4:d:295:SER:OG	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:443:PHE:HD2	8:i:33:LYS:HD3	1.86	0.40
24:c:501:BCR:H20C	24:c:501:BCR:H361	1.93	0.40
3:C:152:HIS:ND1	22:C:511:CLA:OBD	2.39	0.40
34:D:411:DGD:HA61	34:D:411:DGD:HB32	2.02	0.40
2:b:30:VAL:HG12	22:b:607:CLA:HHD	2.02	0.40
2:b:383:PHE:N	4:d:344:GLU:O	2.45	0.40
16:v:38:LEU:N	16:v:43:LYS:O	2.49	0.40
24:C:502:BCR:H343	22:C:509:CLA:HMD1	2.02	0.40
13:O:179:THR:HA	13:O:216:PHE:HE2	1.85	0.40
16:V:59:PHE:HA	16:V:63:CYS:SG	2.61	0.40
1:a:60:ILE:HD12	1:a:84:PRO:HD2	2.04	0.40
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.56	0.40
22:b:606:CLA:H93	22:b:607:CLA:HAB	2.03	0.40
25:D:404:PL9:H421	25:D:404:PL9:H401	1.89	0.40
34:H:101:DGD:HB32	34:H:101:DGD:HB61	1.66	0.40
14:T:14:ILE:HG21	28:T:102:LFA:H61	2.03	0.40
2:b:334:ASP:OD1	2:b:334:ASP:N	2.55	0.40
3:c:173:LEU:HB2	3:c:218:LEU:HD13	2.03	0.40
24:k:101:BCR:H20C	24:k:101:BCR:H361	1.95	0.40
22:B:604:CLA:H93	22:B:605:CLA:HAB	2.03	0.40
24:C:501:BCR:H24C	24:C:501:BCR:H371	1.71	0.40
22:C:513:CLA:H111	22:C:513:CLA:H91	1.92	0.40
2:b:33:TRP:HD1	24:b:602:BCR:H381	1.85	0.40
22:c:506:CLA:H111	22:c:506:CLA:H72	1.97	0.40
22:d:404:CLA:H121	22:d:404:CLA:H162	1.76	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	331/360 (92%)	326 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	331/360 (92%)	327 (99%)	4 (1%)	0	100	100
2	B	503/510 (99%)	499 (99%)	4 (1%)	0	100	100
2	b	503/510 (99%)	498 (99%)	5 (1%)	0	100	100
3	C	448/461 (97%)	442 (99%)	6 (1%)	0	100	100
3	c	448/461 (97%)	442 (99%)	6 (1%)	0	100	100
4	D	339/352 (96%)	332 (98%)	7 (2%)	0	100	100
4	d	339/352 (96%)	334 (98%)	5 (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	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	60/66 (91%)	58 (97%)	2 (3%)	0	100	100
7	h	60/66 (91%)	60 (100%)	0	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	34 (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	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
13	O	241/272 (89%)	234 (97%)	7 (3%)	0	100	100
13	o	241/272 (89%)	234 (97%)	7 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
15	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
16	V	135/163 (83%)	134 (99%)	1 (1%)	0	100	100
16	v	135/163 (83%)	133 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	X	36/41 (88%)	36 (100%)	0	0	100	100
17	x	36/41 (88%)	36 (100%)	0	0	100	100
18	Y	28/46 (61%)	28 (100%)	0	0	100	100
18	y	28/46 (61%)	28 (100%)	0	0	100	100
19	Z	59/62 (95%)	59 (100%)	0	0	100	100
19	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
All	All	5163/5650 (91%)	5090 (99%)	73 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	264/291 (91%)	262 (99%)	2 (1%)	79	88
1	a	264/291 (91%)	261 (99%)	3 (1%)	70	82
2	B	391/407 (96%)	385 (98%)	6 (2%)	60	75
2	b	390/407 (96%)	383 (98%)	7 (2%)	54	69
3	C	346/362 (96%)	340 (98%)	6 (2%)	56	71
3	c	347/362 (96%)	343 (99%)	4 (1%)	67	80
4	D	274/283 (97%)	271 (99%)	3 (1%)	70	82
4	d	274/283 (97%)	269 (98%)	5 (2%)	54	69
5	E	69/73 (94%)	67 (97%)	2 (3%)	37	50
5	e	69/73 (94%)	69 (100%)	0	100	100
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	52/55 (94%)	51 (98%)	1 (2%)	52	67
7	h	52/55 (94%)	51 (98%)	1 (2%)	52	67
8	I	31/34 (91%)	29 (94%)	2 (6%)	14	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	31/34 (91%)	29 (94%)	2 (6%)	14	16
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	29/37 (78%)	29 (100%)	0	100	100
10	k	29/37 (78%)	29 (100%)	0	100	100
11	L	32/35 (91%)	32 (100%)	0	100	100
11	l	32/35 (91%)	32 (100%)	0	100	100
12	M	29/33 (88%)	29 (100%)	0	100	100
12	m	29/33 (88%)	29 (100%)	0	100	100
13	O	190/228 (83%)	188 (99%)	2 (1%)	70	82
13	o	189/228 (83%)	186 (98%)	3 (2%)	58	73
14	T	25/28 (89%)	25 (100%)	0	100	100
14	t	25/28 (89%)	25 (100%)	0	100	100
15	U	80/112 (71%)	77 (96%)	3 (4%)	28	37
15	u	80/112 (71%)	74 (92%)	6 (8%)	11	12
16	V	114/138 (83%)	111 (97%)	3 (3%)	41	54
16	v	114/138 (83%)	111 (97%)	3 (3%)	41	54
17	X	30/34 (88%)	29 (97%)	1 (3%)	33	44
17	x	29/34 (85%)	27 (93%)	2 (7%)	13	14
18	Y	21/37 (57%)	20 (95%)	1 (5%)	21	28
18	y	21/37 (57%)	20 (95%)	1 (5%)	21	28
19	Z	48/52 (92%)	45 (94%)	3 (6%)	15	17
19	z	48/52 (92%)	43 (90%)	5 (10%)	5	5
All	All	4152/4612 (90%)	4075 (98%)	77 (2%)	52	67

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	244	GLU
2	B	80	ILE
2	B	84	THR
2	B	236	THR
2	B	245	VAL

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Mol	Chain	Res	Type
2	B	350	GLU
2	B	362	PHE
3	C	130	GLU
3	C	144	LYS
3	C	228	ILE
3	C	243	THR
3	C	277	PHE
3	C	460	LEU
4	D	43	LEU
4	D	150	ILE
4	D	345	VAL
5	E	5	THR
5	E	80	LEU
7	H	63	LYS
8	I	6	ILE
8	I	33	LYS
13	O	106	GLN
13	O	198	ILE
15	U	91	VAL
15	U	114	VAL
15	U	126	ASP
16	V	63	CYS
16	V	68	VAL
16	V	71	ILE
17	X	37	VAL
18	Y	41	VAL
19	Z	7	LEU
19	Z	20	VAL
19	Z	29	SER
1	a	35	VAL
1	a	230	THR
1	a	329	GLU
2	b	80	ILE
2	b	84	THR
2	b	236	THR
2	b	245	VAL
2	b	362	PHE
2	b	479	PHE
2	b	491	VAL
3	c	96	THR
3	c	277	PHE
3	c	303	MET

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Mol	Chain	Res	Type
3	c	461	ASP
4	d	150	ILE
4	d	213	ILE
4	d	227	GLU
4	d	259	ILE
4	d	345	VAL
7	h	63	LYS
8	i	6	ILE
8	i	34	ARG
13	o	59	ASP
13	o	75	THR
13	o	198	ILE
15	u	39	LEU
15	u	91	VAL
15	u	107	GLU
15	u	114	VAL
15	u	126	ASP
15	u	132	LEU
16	v	63	CYS
16	v	68	VAL
16	v	136	LYS
17	x	21	LEU
17	x	37	VAL
18	y	19	ILE
19	z	2	THR
19	z	4	LEU
19	z	7	LEU
19	z	20	VAL
19	z	37	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	19	ASN
1	A	165	GLN
1	A	303	ASN
2	B	281	GLN
2	B	282	GLN
2	B	394	GLN
2	B	438	ASN
3	C	16	GLN

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Mol	Chain	Res	Type
3	C	370	ASN
4	D	255	GLN
5	E	74	GLN
6	F	44	GLN
13	O	72	GLN
13	O	150	ASN
13	O	156	GLN
13	O	158	ASN
13	O	173	ASN
13	O	202	GLN
15	U	111	HIS
16	V	132	ASN
18	Y	21	GLN
19	Z	38	GLN
1	a	165	GLN
2	b	438	ASN
2	b	497	GLN
3	c	16	GLN
3	c	299	GLN
3	c	320	GLN
4	d	255	GLN
5	e	74	GLN
6	f	44	GLN
12	m	5	GLN
13	o	62	GLN
13	o	84	ASN
13	o	150	ASN
13	o	173	ASN
13	o	202	GLN
13	o	222	GLN
15	u	67	GLN
16	v	132	ASN
19	z	38	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	FME	I	1	8	8,9,10	0.36	0	7,9,11	0.84	0
14	FME	T	1	14	8,9,10	0.38	0	7,9,11	0.90	0
8	FME	i	1	8	8,9,10	0.38	0	7,9,11	0.85	0
14	FME	t	1	14	8,9,10	0.39	0	7,9,11	0.98	0

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
8	FME	I	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	4/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	C-CA-CB-CG
14	t	1	FME	C-CA-CB-CG
14	T	1	FME	N-CA-CB-CG
14	t	1	FME	N-CA-CB-CG
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
14	T	1	FME	CB-CA-N-CN

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 232 ligands modelled in this entry, 8 are monoatomic - leaving 224 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$
28	LFA	H	103	-	9,9,19	0.25	0	8,8,18	0.18	0
22	CLA	a	408	-	65,73,73	1.44	6 (9%)	76,113,113	1.42	9 (11%)
22	CLA	C	508	39	65,73,73	1.45	7 (10%)	76,113,113	1.49	7 (9%)
27	PLM	j	103	-	17,17,17	0.66	0	17,17,17	0.57	0
28	LFA	J	104	-	10,10,19	0.23	0	9,9,18	0.28	0
22	CLA	c	515	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	7 (9%)
22	CLA	D	401	39	65,73,73	1.42	6 (9%)	76,113,113	1.57	9 (11%)
36	HEM	v	201	16	41,50,50	1.46	3 (7%)	45,82,82	1.51	10 (22%)
24	BCR	B	617	-	41,41,41	0.34	0	56,56,56	0.73	0
36	HEM	e	103	6,5	41,50,50	1.47	4 (9%)	45,82,82	1.53	7 (15%)
27	PLM	b	622	-	12,12,17	0.79	0	12,12,17	0.69	0
27	PLM	M	103	-	15,15,17	0.67	0	15,15,17	0.68	0
35	LMG	C	519	-	51,51,55	0.51	0	59,59,63	0.65	0
24	BCR	f	101	-	41,41,41	0.35	0	56,56,56	0.93	3 (5%)
22	CLA	a	406	39	65,73,73	1.44	6 (9%)	76,113,113	1.51	9 (11%)
33	LMT	T	101	-	24,24,36	0.50	0	29,29,47	0.73	0
22	CLA	d	403	-	65,73,73	1.45	7 (10%)	76,113,113	1.37	6 (7%)
22	CLA	C	510	-	65,73,73	1.48	7 (10%)	76,113,113	1.52	10 (13%)
23	PHO	a	407	-	51,69,69	0.65	0	47,99,99	0.90	3 (6%)
22	CLA	C	509	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
24	BCR	C	502	-	41,41,41	0.35	0	56,56,56	0.82	2 (3%)
22	CLA	b	603	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	7 (9%)
22	CLA	c	510	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
33	LMT	b	626	-	24,24,36	0.48	0	29,29,47	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	c	509	39	65,73,73	1.46	7 (10%)	76,113,113	1.50	7 (9%)
22	CLA	b	606	-	65,73,73	1.48	6 (9%)	76,113,113	1.57	12 (15%)
33	LMT	C	518	-	36,36,36	0.49	0	47,47,47	1.19	4 (8%)
27	PLM	c	522	-	17,17,17	0.65	0	17,17,17	0.60	0
26	SQD	l	102	-	53,54,54	1.56	9 (16%)	62,65,65	1.47	7 (11%)
22	CLA	B	610	39	65,73,73	1.49	6 (9%)	76,113,113	1.43	8 (10%)
34	DGD	d	410	-	47,47,67	0.53	0	54,55,81	0.63	0
23	PHO	A	406	-	51,69,69	0.66	0	47,99,99	0.91	3 (6%)
22	CLA	b	618	-	45,53,73	1.72	7 (15%)	52,89,113	1.77	7 (13%)
24	BCR	A	408	-	41,41,41	0.30	0	56,56,56	0.63	0
22	CLA	c	511	-	65,73,73	1.48	7 (10%)	76,113,113	1.52	10 (13%)
22	CLA	B	602	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	7 (9%)
27	PLM	D	402	-	12,12,17	0.73	0	12,12,17	0.76	1 (8%)
22	CLA	D	406	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	10 (13%)
34	DGD	h	101	-	59,59,67	0.57	0	73,73,81	0.76	0
22	CLA	B	615	-	65,73,73	1.46	7 (10%)	76,113,113	1.36	8 (10%)
33	LMT	B	630	-	36,36,36	0.54	0	47,47,47	0.70	0
35	LMG	d	407	-	47,47,55	0.51	0	55,55,63	0.67	0
37	RRX	h	102	-	42,42,42	0.21	0	57,58,58	0.49	0
27	PLM	B	627	-	16,16,17	0.67	0	16,16,17	0.63	0
27	PLM	d	411	-	11,11,17	0.80	0	11,11,17	0.77	0
27	PLM	E	103	-	17,17,17	0.66	0	17,17,17	0.56	0
27	PLM	c	523	-	16,16,17	0.68	0	16,16,17	0.59	0
28	LFA	A	412	-	11,11,19	0.24	0	10,10,18	0.20	0
28	LFA	T	102	-	16,16,19	0.22	0	15,15,18	0.21	0
22	CLA	C	513	-	65,73,73	1.43	6 (9%)	76,113,113	1.53	7 (9%)
35	LMG	D	409	-	47,47,55	0.52	0	55,55,63	0.68	0
33	LMT	A	419	-	36,36,36	0.55	0	47,47,47	0.87	1 (2%)
27	PLM	B	629	-	17,17,17	0.66	0	17,17,17	0.64	0
28	LFA	b	623	-	7,7,19	0.25	0	6,6,18	0.22	0
33	LMT	f	102	-	36,36,36	0.48	0	47,47,47	0.87	2 (4%)
31	LHG	E	101	-	39,39,48	0.57	0	42,45,54	0.51	0
33	LMT	z	101	-	36,36,36	0.53	0	47,47,47	0.86	3 (6%)
24	BCR	y	102	-	41,41,41	0.35	0	56,56,56	0.93	1 (1%)
28	LFA	d	409	-	13,13,19	0.23	0	12,12,18	0.25	0
36	HEM	V	201	16	41,50,50	1.45	3 (7%)	45,82,82	1.51	9 (20%)
34	DGD	c	505	-	62,62,67	0.58	0	76,76,81	0.70	1 (1%)
31	LHG	d	405	-	48,48,48	0.50	0	51,54,54	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	PL9	a	410	-	55,55,55	1.10	4 (7%)	68,69,69	1.56	12 (17%)
22	CLA	c	508	-	65,73,73	1.46	6 (9%)	76,113,113	1.45	8 (10%)
27	PLM	C	523	-	15,15,17	0.69	0	15,15,17	0.64	0
24	BCR	Y	102	-	41,41,41	0.35	0	56,56,56	0.94	1 (1%)
27	PLM	e	102	-	17,17,17	0.62	0	17,17,17	0.63	0
22	CLA	B	616	-	45,53,73	1.72	7 (15%)	52,89,113	1.79	6 (11%)
22	CLA	b	609	39	65,73,73	1.46	7 (10%)	76,113,113	1.43	7 (9%)
27	PLM	B	621	-	17,17,17	0.63	0	17,17,17	0.64	0
22	CLA	b	617	-	65,73,73	1.44	6 (9%)	76,113,113	1.41	8 (10%)
33	LMT	T	104	-	36,36,36	0.51	0	47,47,47	0.72	0
28	LFA	B	620	-	7,7,19	0.23	0	6,6,18	0.22	0
24	BCR	B	619	-	41,41,41	0.32	0	56,56,56	1.04	2 (3%)
26	SQD	d	412	-	44,45,54	1.64	9 (20%)	53,56,65	1.59	10 (18%)
24	BCR	c	502	-	41,41,41	0.35	0	56,56,56	0.83	2 (3%)
22	CLA	B	606	-	65,73,73	1.47	6 (9%)	76,113,113	1.50	9 (11%)
22	CLA	b	605	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
28	LFA	C	521	-	8,8,19	0.22	0	7,7,18	0.29	0
26	SQD	a	411	-	53,54,54	1.57	8 (15%)	62,65,65	1.42	9 (14%)
28	LFA	d	408	-	12,12,19	0.23	0	11,11,18	0.20	0
35	LMG	M	101	-	51,51,55	0.49	0	59,59,63	0.59	0
22	CLA	C	517	-	65,73,73	1.41	6 (9%)	76,113,113	1.55	8 (10%)
27	PLM	B	622	-	13,13,17	0.73	0	13,13,17	0.68	0
26	SQD	A	415	-	50,51,54	1.55	7 (14%)	59,62,65	1.57	10 (16%)
28	LFA	b	624	-	3,3,19	0.38	0	2,2,18	0.51	0
33	LMT	J	103	-	24,24,36	0.50	0	29,29,47	0.91	1 (3%)
22	CLA	b	613	-	65,73,73	1.44	7 (10%)	76,113,113	1.50	8 (10%)
25	PL9	d	402	-	55,55,55	1.14	3 (5%)	68,69,69	1.51	13 (19%)
24	BCR	B	618	-	41,41,41	0.33	0	56,56,56	0.80	0
22	CLA	B	603	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
22	CLA	b	614	-	65,73,73	1.42	7 (10%)	76,113,113	1.51	8 (10%)
23	PHO	D	403	-	51,69,69	0.65	0	47,99,99	0.98	3 (6%)
27	PLM	A	411	-	17,17,17	0.68	0	17,17,17	0.60	0
32	GOL	a	401	-	5,5,5	0.34	0	5,5,5	0.39	0
27	PLM	C	522	-	17,17,17	0.65	0	17,17,17	0.73	1 (5%)
22	CLA	a	405	-	65,73,73	1.44	6 (9%)	76,113,113	1.47	7 (9%)
22	CLA	b	616	-	65,73,73	1.43	7 (10%)	76,113,113	1.45	7 (9%)
34	DGD	C	504	-	55,55,67	0.59	0	69,69,81	0.92	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	HEM	E	104	6,5	41,50,50	1.48	6 (14%)	45,82,82	1.54	7 (15%)
27	PLM	F	102	-	13,13,17	0.73	0	13,13,17	0.67	0
22	CLA	B	613	-	65,73,73	1.42	5 (7%)	76,113,113	1.44	8 (10%)
27	PLM	C	520	-	14,14,17	0.72	0	14,14,17	0.70	0
22	CLA	A	407	-	65,73,73	1.44	6 (9%)	76,113,113	1.42	9 (11%)
27	PLM	L	102	-	17,17,17	0.66	0	17,17,17	0.60	0
31	LHG	D	408	-	48,48,48	0.51	0	51,54,54	0.53	0
22	CLA	c	513	-	65,73,73	1.43	6 (9%)	76,113,113	1.55	9 (11%)
33	LMT	B	628	-	24,24,36	0.50	0	29,29,47	0.78	0
26	SQD	D	412	-	44,45,54	1.64	9 (20%)	53,56,65	1.58	10 (18%)
33	LMT	B	633	-	36,36,36	0.51	0	47,47,47	0.77	0
26	SQD	A	410	-	53,54,54	1.52	7 (13%)	62,65,65	1.35	6 (9%)
27	PLM	c	520	-	17,17,17	0.68	0	17,17,17	0.59	0
22	CLA	A	405	39	65,73,73	1.44	6 (9%)	76,113,113	1.51	9 (11%)
22	CLA	b	612	39	65,73,73	1.49	6 (9%)	76,113,113	1.43	8 (10%)
22	CLA	A	404	-	65,73,73	1.44	6 (9%)	76,113,113	1.48	7 (9%)
22	CLA	d	404	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	9 (11%)
24	BCR	C	501	-	41,41,41	0.35	0	56,56,56	1.04	1 (1%)
27	PLM	D	410	-	17,17,17	0.65	0	17,17,17	0.66	0
37	RRX	H	102	-	42,42,42	0.22	0	57,58,58	0.48	0
30	BCT	a	419	20	2,3,3	0.88	0	2,3,3	3.27	2 (100%)
29	OEX	a	416	3,39,1	0,15,15	-	-	-	-	-
34	DGD	H	101	-	59,59,67	0.56	0	73,73,81	0.78	0
28	LFA	J	101	-	19,19,19	0.24	0	18,18,18	0.22	0
24	BCR	c	501	-	41,41,41	0.36	0	56,56,56	1.08	2 (3%)
22	CLA	b	608	-	65,73,73	1.47	7 (10%)	76,113,113	1.47	8 (10%)
22	CLA	D	405	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	6 (7%)
22	CLA	B	609	-	65,73,73	1.47	5 (7%)	76,113,113	1.39	7 (9%)
27	PLM	a	412	-	17,17,17	0.67	0	17,17,17	0.67	0
35	LMG	C	525	-	51,51,55	0.50	0	59,59,63	0.87	3 (5%)
22	CLA	B	605	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	7 (9%)
22	CLA	B	612	-	65,73,73	1.41	7 (10%)	76,113,113	1.51	8 (10%)
28	LFA	E	102	-	19,19,19	0.24	0	18,18,18	0.20	0
24	BCR	a	409	-	41,41,41	0.30	0	56,56,56	0.65	0
31	LHG	a	415	-	48,48,48	0.51	0	51,54,54	0.52	0
27	PLM	b	621	-	17,17,17	0.65	0	17,17,17	0.58	0
31	LHG	d	406	-	47,47,48	0.51	0	50,53,54	0.53	0
26	SQD	a	417	-	50,51,54	1.54	6 (12%)	59,62,65	1.55	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
22	CLA	b	611	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	7 (9%)
28	LFA	i	104	-	7,7,19	0.24	0	6,6,18	0.20	0
35	LMG	m	101	-	51,51,55	0.50	0	59,59,63	0.57	0
31	LHG	D	407	-	48,48,48	0.51	0	51,54,54	0.57	0
27	PLM	b	625	-	15,15,17	0.68	0	15,15,17	0.64	0
31	LHG	l	101	-	48,48,48	0.51	0	51,54,54	0.52	0
22	CLA	C	516	-	65,73,73	1.45	6 (9%)	76,113,113	1.44	7 (9%)
28	LFA	a	413	-	6,6,19	0.25	0	5,5,18	0.18	0
34	DGD	D	411	-	44,44,67	0.54	0	52,52,81	0.74	1 (1%)
27	PLM	b	627	-	17,17,17	0.67	0	17,17,17	0.63	0
22	CLA	c	516	3	65,73,73	1.46	6 (9%)	76,113,113	1.50	8 (10%)
27	PLM	t	101	-	14,14,17	0.23	0	13,13,17	0.23	0
24	BCR	K	101	-	41,41,41	0.31	0	56,56,56	0.59	0
27	PLM	C	524	-	12,12,17	0.76	0	12,12,17	0.70	0
28	LFA	B	626	-	7,7,19	0.26	0	6,6,18	0.18	0
28	LFA	I	101	-	19,19,19	0.24	0	18,18,18	0.16	0
27	PLM	x	101	-	17,17,17	0.67	0	17,17,17	0.59	0
24	BCR	T	103	-	41,41,41	0.34	0	56,56,56	0.76	0
22	CLA	B	608	-	65,73,73	1.45	6 (9%)	76,113,113	1.50	9 (11%)
22	CLA	C	512	-	65,73,73	1.43	6 (9%)	76,113,113	1.53	9 (11%)
22	CLA	B	601	-	65,73,73	1.51	5 (7%)	76,113,113	1.35	7 (9%)
24	BCR	k	101	-	41,41,41	0.36	0	56,56,56	0.71	1 (1%)
35	LMG	c	519	-	51,51,55	0.52	0	59,59,63	0.64	0
27	PLM	X	101	-	16,16,17	0.71	0	16,16,17	0.59	0
35	LMG	c	524	-	48,48,55	0.49	0	56,56,63	0.69	0
22	CLA	b	607	-	65,73,73	1.46	6 (9%)	76,113,113	1.44	7 (9%)
28	LFA	I	103	-	7,7,19	0.25	0	6,6,18	0.21	0
22	CLA	B	607	39	65,73,73	1.46	6 (9%)	76,113,113	1.42	7 (9%)
22	CLA	B	611	-	65,73,73	1.44	7 (10%)	76,113,113	1.50	9 (11%)
27	PLM	B	625	-	11,11,17	0.82	0	11,11,17	0.79	0
31	LHG	L	101	-	48,48,48	0.50	0	51,54,54	0.56	0
33	LMT	j	101	-	24,24,36	0.52	0	29,29,47	0.83	0
33	LMT	i	102	-	36,36,36	0.49	0	47,47,47	1.17	5 (10%)
22	CLA	c	518	-	65,73,73	1.42	6 (9%)	76,113,113	1.55	7 (9%)
22	CLA	C	506	-	65,73,73	1.45	7 (10%)	76,113,113	1.43	6 (7%)
27	PLM	e	101	-	17,17,17	0.68	0	17,17,17	0.58	0
33	LMT	B	623	-	36,36,36	0.52	0	47,47,47	0.70	0
31	LHG	a	421	-	45,45,48	0.52	0	48,51,54	0.55	0
34	DGD	c	504	-	56,56,67	0.58	0	70,70,81	0.87	2 (2%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	604	-	65,73,73	1.48	6 (9%)	76,113,113	1.58	12 (15%)
30	BCT	A	416	20	2,3,3	0.87	0	2,3,3	3.26	2 (100%)
24	BCR	b	619	-	41,41,41	0.33	0	56,56,56	0.81	1 (1%)
27	PLM	H	104	-	11,11,17	0.80	0	11,11,17	0.73	0
22	CLA	C	511	39	65,73,73	1.46	6 (9%)	76,113,113	1.50	8 (10%)
24	BCR	B	632	-	41,41,41	0.36	0	56,56,56	1.52	7 (12%)
28	LFA	i	101	-	19,19,19	0.24	0	18,18,18	0.18	0
22	CLA	b	610	-	65,73,73	1.44	6 (9%)	76,113,113	1.49	9 (11%)
23	PHO	a	420	-	51,69,69	0.64	0	47,99,99	0.98	3 (6%)
24	BCR	F	101	-	41,41,41	0.36	0	56,56,56	0.85	2 (3%)
25	PL9	D	404	-	55,55,55	1.14	4 (7%)	68,69,69	1.50	13 (19%)
28	LFA	a	418	-	6,6,19	0.25	0	5,5,18	0.18	0
28	LFA	a	414	-	10,10,19	0.25	0	9,9,18	0.19	0
33	LMT	Z	101	-	36,36,36	0.54	0	47,47,47	0.94	3 (6%)
28	LFA	i	103	-	8,8,19	0.23	0	7,7,18	0.21	0
22	CLA	d	401	39	65,73,73	1.43	6 (9%)	76,113,113	1.57	7 (9%)
27	PLM	c	521	-	15,15,17	0.71	0	15,15,17	0.64	0
33	LMT	m	102	-	36,36,36	0.55	0	47,47,47	0.78	1 (2%)
28	LFA	I	102	-	10,10,19	0.23	0	9,9,18	0.24	0
22	CLA	C	514	-	65,73,73	1.45	6 (9%)	76,113,113	1.40	7 (9%)
22	CLA	c	514	-	65,73,73	1.43	6 (9%)	76,113,113	1.55	9 (11%)
28	LFA	B	624	-	6,6,19	0.25	0	5,5,18	0.19	0
35	LMG	Y	101	-	51,51,55	0.49	0	59,59,63	0.65	0
22	CLA	C	505	-	65,73,73	1.50	7 (10%)	76,113,113	1.34	5 (6%)
24	BCR	b	602	-	41,41,41	0.36	0	56,56,56	1.52	6 (10%)
22	CLA	c	506	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
27	PLM	j	102	-	16,16,17	0.69	0	16,16,17	0.69	0
35	LMG	y	101	-	51,51,55	0.51	0	59,59,63	0.97	4 (6%)
22	CLA	c	517	-	65,73,73	1.46	6 (9%)	76,113,113	1.45	8 (10%)
34	DGD	J	102	-	62,62,67	0.57	0	76,76,81	1.29	4 (5%)
22	CLA	c	512	39	65,73,73	1.44	6 (9%)	76,113,113	1.51	8 (10%)
22	CLA	b	604	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	7 (9%)
27	PLM	A	413	-	11,11,17	0.80	0	11,11,17	0.76	0
22	CLA	C	507	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	8 (10%)
22	CLA	b	615	-	65,73,73	1.42	6 (9%)	76,113,113	1.44	8 (10%)
22	CLA	c	507	-	65,73,73	1.44	6 (9%)	76,113,113	1.44	6 (7%)
28	LFA	B	631	-	4,4,19	0.29	0	3,3,18	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	PL9	A	409	-	55,55,55	1.09	4 (7%)	68,69,69	1.57	14 (20%)
26	SQD	b	601	-	53,54,54	1.52	9 (16%)	62,65,65	1.71	10 (16%)
33	LMT	M	102	-	36,36,36	0.54	0	47,47,47	0.77	0
22	CLA	C	515	3	65,73,73	1.45	6 (9%)	76,113,113	1.51	8 (10%)
34	DGD	C	503	-	54,54,67	0.65	0	68,68,81	0.72	1 (1%)
22	CLA	B	614	-	65,73,73	1.44	7 (10%)	76,113,113	1.45	7 (9%)
29	OEX	A	414	3,39,1	0,15,15	-	-	-	-	-
34	DGD	c	503	-	54,54,67	0.64	0	68,68,81	0.73	1 (1%)
32	GOL	A	418	-	5,5,5	0.34	0	5,5,5	0.38	0
24	BCR	b	620	-	41,41,41	0.33	0	56,56,56	0.91	2 (3%)
31	LHG	A	417	-	45,45,48	0.53	0	48,51,54	0.53	0

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
28	LFA	H	103	-	-	4/7/7/17	-
22	CLA	a	408	-	1/1/15/20	10/37/115/115	-
22	CLA	C	508	39	1/1/15/20	9/37/115/115	-
27	PLM	j	103	-	-	7/15/15/15	-
28	LFA	J	104	-	-	3/8/8/17	-
22	CLA	c	515	-	1/1/15/20	4/37/115/115	-
22	CLA	D	401	39	1/1/15/20	5/37/115/115	-
36	HEM	v	201	16	-	2/12/54/54	-
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
36	HEM	e	103	6,5	-	2/12/54/54	-
27	PLM	b	622	-	-	4/10/10/15	-
27	PLM	M	103	-	-	11/13/13/15	-
35	LMG	C	519	-	-	25/46/66/70	0/1/1/1
24	BCR	f	101	-	-	9/29/63/63	0/2/2/2
22	CLA	a	406	39	1/1/15/20	9/37/115/115	-
33	LMT	T	101	-	-	8/15/35/61	0/1/1/2
22	CLA	d	403	-	1/1/15/20	3/37/115/115	-
22	CLA	C	510	-	1/1/15/20	16/37/115/115	-
23	PHO	a	407	-	-	2/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	509	-	1/1/15/20	8/37/115/115	-
24	BCR	C	502	-	-	11/29/63/63	0/2/2/2
22	CLA	b	603	-	1/1/15/20	12/37/115/115	-
22	CLA	c	510	-	1/1/15/20	9/37/115/115	-
33	LMT	b	626	-	-	6/15/35/61	0/1/1/2
22	CLA	c	509	39	1/1/15/20	9/37/115/115	-
22	CLA	b	606	-	1/1/15/20	14/37/115/115	-
33	LMT	C	518	-	-	10/21/61/61	0/2/2/2
27	PLM	c	522	-	-	2/15/15/15	-
26	SQD	l	102	-	-	23/49/69/69	0/1/1/1
22	CLA	B	610	39	1/1/15/20	8/37/115/115	-
34	DGD	d	410	-	-	15/41/62/95	0/1/1/2
23	PHO	A	406	-	-	3/37/103/103	0/5/6/6
22	CLA	b	618	-	1/1/11/20	1/13/91/115	-
24	BCR	A	408	-	-	2/29/63/63	0/2/2/2
22	CLA	c	511	-	1/1/15/20	15/37/115/115	-
22	CLA	B	602	-	1/1/15/20	6/37/115/115	-
27	PLM	D	402	-	-	2/10/10/15	-
22	CLA	D	406	-	1/1/15/20	9/37/115/115	-
34	DGD	h	101	-	-	7/47/87/95	0/2/2/2
22	CLA	B	615	-	1/1/15/20	6/37/115/115	-
33	LMT	B	630	-	-	3/21/61/61	0/2/2/2
35	LMG	d	407	-	-	11/42/62/70	0/1/1/1
37	RRX	h	102	-	-	3/29/65/65	0/2/2/2
27	PLM	B	627	-	-	5/14/14/15	-
27	PLM	d	411	-	-	5/9/9/15	-
27	PLM	E	103	-	-	3/15/15/15	-
27	PLM	c	523	-	-	9/14/14/15	-
28	LFA	A	412	-	-	1/9/9/17	-
28	LFA	T	102	-	-	9/14/14/17	-
22	CLA	C	513	-	1/1/15/20	8/37/115/115	-
35	LMG	D	409	-	-	10/42/62/70	0/1/1/1
33	LMT	A	419	-	-	5/21/61/61	0/2/2/2
27	PLM	B	629	-	-	3/15/15/15	-
28	LFA	b	623	-	-	0/5/5/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMT	f	102	-	-	11/21/61/61	0/2/2/2
31	LHG	E	101	-	-	30/44/44/53	-
33	LMT	z	101	-	-	11/21/61/61	0/2/2/2
24	BCR	y	102	-	-	10/29/63/63	0/2/2/2
28	LFA	d	409	-	-	2/11/11/17	-
36	HEM	V	201	16	-	2/12/54/54	-
34	DGD	c	505	-	-	19/50/90/95	0/2/2/2
31	LHG	d	405	-	-	18/53/53/53	-
25	PL9	a	410	-	-	28/53/73/73	0/1/1/1
22	CLA	c	508	-	1/1/15/20	6/37/115/115	-
27	PLM	C	523	-	-	2/13/13/15	-
24	BCR	Y	102	-	-	10/29/63/63	0/2/2/2
27	PLM	e	102	-	-	8/15/15/15	-
22	CLA	B	616	-	1/1/11/20	1/13/91/115	-
22	CLA	b	609	39	1/1/15/20	6/37/115/115	-
27	PLM	B	621	-	-	8/15/15/15	-
22	CLA	b	617	-	1/1/15/20	6/37/115/115	-
33	LMT	T	104	-	-	8/21/61/61	0/2/2/2
28	LFA	B	620	-	-	5/5/5/17	-
24	BCR	B	619	-	-	2/29/63/63	0/2/2/2
26	SQD	d	412	-	-	11/40/60/69	0/1/1/1
24	BCR	c	502	-	-	10/29/63/63	0/2/2/2
22	CLA	B	606	-	1/1/15/20	6/37/115/115	-
22	CLA	b	605	-	1/1/15/20	12/37/115/115	-
28	LFA	C	521	-	-	5/6/6/17	-
26	SQD	a	411	-	-	25/49/69/69	0/1/1/1
28	LFA	d	408	-	-	7/10/10/17	-
35	LMG	M	101	-	-	20/46/66/70	0/1/1/1
22	CLA	C	517	-	1/1/15/20	5/37/115/115	-
27	PLM	B	622	-	-	4/11/11/15	-
26	SQD	A	415	-	-	15/46/66/69	0/1/1/1
28	LFA	b	624	-	-	0/1/1/17	-
33	LMT	J	103	-	-	12/15/35/61	0/1/1/2
22	CLA	b	613	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PL9	d	402	-	-	20/53/73/73	0/1/1/1
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
22	CLA	B	603	-	1/1/15/20	13/37/115/115	-
22	CLA	b	614	-	1/1/15/20	7/37/115/115	-
23	PHO	D	403	-	-	7/37/103/103	0/5/6/6
27	PLM	A	411	-	-	7/15/15/15	-
32	GOL	a	401	-	-	4/4/4/4	-
27	PLM	C	522	-	-	10/15/15/15	-
22	CLA	a	405	-	1/1/15/20	7/37/115/115	-
22	CLA	b	616	-	1/1/15/20	18/37/115/115	-
34	DGD	C	504	-	-	25/43/83/95	0/2/2/2
36	HEM	E	104	6,5	-	2/12/54/54	-
27	PLM	F	102	-	-	2/11/11/15	-
22	CLA	B	613	-	1/1/15/20	6/37/115/115	-
27	PLM	C	520	-	-	8/12/12/15	-
22	CLA	A	407	-	1/1/15/20	8/37/115/115	-
27	PLM	L	102	-	-	9/15/15/15	-
31	LHG	D	408	-	-	17/53/53/53	-
22	CLA	c	513	-	1/1/15/20	8/37/115/115	-
33	LMT	B	628	-	-	2/15/35/61	0/1/1/2
26	SQD	D	412	-	-	13/40/60/69	0/1/1/1
33	LMT	B	633	-	-	5/21/61/61	0/2/2/2
26	SQD	A	410	-	-	21/49/69/69	0/1/1/1
27	PLM	c	520	-	-	9/15/15/15	-
22	CLA	A	405	39	1/1/15/20	8/37/115/115	-
22	CLA	b	612	39	1/1/15/20	9/37/115/115	-
22	CLA	A	404	-	1/1/15/20	7/37/115/115	-
22	CLA	d	404	-	1/1/15/20	8/37/115/115	-
24	BCR	C	501	-	-	4/29/63/63	0/2/2/2
27	PLM	D	410	-	-	8/15/15/15	-
37	RRX	H	102	-	-	3/29/65/65	0/2/2/2
34	DGD	H	101	-	-	6/47/87/95	0/2/2/2
28	LFA	J	101	-	-	4/17/17/17	-
24	BCR	c	501	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	608	-	1/1/15/20	7/37/115/115	-
22	CLA	D	405	-	1/1/15/20	3/37/115/115	-
22	CLA	B	609	-	1/1/15/20	10/37/115/115	-
27	PLM	a	412	-	-	10/15/15/15	-
35	LMG	C	525	-	-	19/46/66/70	0/1/1/1
22	CLA	B	605	-	1/1/15/20	5/37/115/115	-
22	CLA	B	612	-	1/1/15/20	7/37/115/115	-
28	LFA	E	102	-	-	4/17/17/17	-
24	BCR	a	409	-	-	3/29/63/63	0/2/2/2
31	LHG	a	415	-	-	24/53/53/53	-
27	PLM	b	621	-	-	7/15/15/15	-
31	LHG	d	406	-	-	21/52/52/53	-
26	SQD	a	417	-	-	24/46/66/69	0/1/1/1
22	CLA	b	611	-	1/1/15/20	9/37/115/115	-
28	LFA	i	104	-	-	2/5/5/17	-
35	LMG	m	101	-	-	18/46/66/70	0/1/1/1
31	LHG	D	407	-	-	19/53/53/53	-
27	PLM	b	625	-	-	3/13/13/15	-
31	LHG	l	101	-	-	20/53/53/53	-
22	CLA	C	516	-	1/1/15/20	12/37/115/115	-
28	LFA	a	413	-	-	3/4/4/17	-
34	DGD	D	411	-	-	14/38/58/95	0/1/1/2
27	PLM	b	627	-	-	3/15/15/15	-
22	CLA	c	516	3	1/1/15/20	4/37/115/115	-
27	PLM	t	101	-	-	6/12/12/15	-
24	BCR	K	101	-	-	5/29/63/63	0/2/2/2
27	PLM	C	524	-	-	2/10/10/15	-
28	LFA	B	626	-	-	0/5/5/17	-
28	LFA	I	101	-	-	7/17/17/17	-
27	PLM	x	101	-	-	10/15/15/15	-
24	BCR	T	103	-	-	5/29/63/63	0/2/2/2
22	CLA	B	608	-	1/1/15/20	5/37/115/115	-
22	CLA	C	512	-	1/1/15/20	6/37/115/115	-
22	CLA	B	601	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	k	101	-	-	8/29/63/63	0/2/2/2
35	LMG	c	519	-	-	27/46/66/70	0/1/1/1
27	PLM	X	101	-	-	8/14/14/15	-
35	LMG	c	524	-	-	16/43/63/70	0/1/1/1
22	CLA	b	607	-	1/1/15/20	5/37/115/115	-
28	LFA	I	103	-	-	2/5/5/17	-
22	CLA	B	607	39	1/1/15/20	6/37/115/115	-
22	CLA	B	611	-	1/1/15/20	8/37/115/115	-
27	PLM	B	625	-	-	1/9/9/15	-
31	LHG	L	101	-	-	17/53/53/53	-
33	LMT	j	101	-	-	14/15/35/61	0/1/1/2
33	LMT	i	102	-	-	10/21/61/61	0/2/2/2
22	CLA	c	518	-	1/1/15/20	6/37/115/115	-
22	CLA	C	506	-	1/1/15/20	12/37/115/115	-
27	PLM	e	101	-	-	7/15/15/15	-
33	LMT	B	623	-	-	3/21/61/61	0/2/2/2
31	LHG	a	421	-	-	16/50/50/53	-
34	DGD	c	504	-	-	26/44/84/95	0/2/2/2
22	CLA	B	604	-	1/1/15/20	14/37/115/115	-
24	BCR	b	619	-	-	0/29/63/63	0/2/2/2
27	PLM	H	104	-	-	1/9/9/15	-
22	CLA	C	511	39	1/1/15/20	6/37/115/115	-
24	BCR	B	632	-	-	10/29/63/63	0/2/2/2
28	LFA	i	101	-	-	12/17/17/17	-
22	CLA	b	610	-	1/1/15/20	5/37/115/115	-
23	PHO	a	420	-	-	5/37/103/103	0/5/6/6
24	BCR	F	101	-	-	8/29/63/63	0/2/2/2
25	PL9	D	404	-	-	19/53/73/73	0/1/1/1
28	LFA	a	418	-	-	2/4/4/17	-
28	LFA	a	414	-	-	5/8/8/17	-
33	LMT	Z	101	-	-	11/21/61/61	0/2/2/2
28	LFA	i	103	-	-	4/6/6/17	-
22	CLA	d	401	39	1/1/15/20	5/37/115/115	-
27	PLM	c	521	-	-	4/13/13/15	-
33	LMT	m	102	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LFA	I	102	-	-	5/8/8/17	-
22	CLA	C	514	-	1/1/15/20	5/37/115/115	-
22	CLA	c	514	-	1/1/15/20	5/37/115/115	-
28	LFA	B	624	-	-	1/4/4/17	-
35	LMG	Y	101	-	-	10/46/66/70	0/1/1/1
22	CLA	C	505	-	1/1/15/20	8/37/115/115	-
24	BCR	b	602	-	-	9/29/63/63	0/2/2/2
22	CLA	c	506	-	1/1/15/20	4/37/115/115	-
27	PLM	j	102	-	-	6/14/14/15	-
35	LMG	y	101	-	-	14/46/66/70	0/1/1/1
22	CLA	c	517	-	1/1/15/20	16/37/115/115	-
34	DGD	J	102	-	-	17/50/90/95	0/2/2/2
22	CLA	c	512	39	1/1/15/20	6/37/115/115	-
22	CLA	b	604	-	1/1/15/20	5/37/115/115	-
27	PLM	A	413	-	-	7/9/9/15	-
22	CLA	C	507	-	1/1/15/20	3/37/115/115	-
22	CLA	b	615	-	1/1/15/20	6/37/115/115	-
22	CLA	c	507	-	1/1/15/20	10/37/115/115	-
28	LFA	B	631	-	-	0/2/2/17	-
25	PL9	A	409	-	-	28/53/73/73	0/1/1/1
26	SQD	b	601	-	-	28/49/69/69	0/1/1/1
33	LMT	M	102	-	-	4/21/61/61	0/2/2/2
22	CLA	C	515	3	1/1/15/20	6/37/115/115	-
34	DGD	C	503	-	-	21/42/82/95	0/2/2/2
22	CLA	B	614	-	1/1/15/20	17/37/115/115	-
34	DGD	c	503	-	-	22/42/82/95	0/2/2/2
32	GOL	A	418	-	-	0/4/4/4	-
24	BCR	b	620	-	-	3/29/63/63	0/2/2/2
31	LHG	A	417	-	-	15/50/50/53	-

All (534) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	601	CLA	C4B-NB	7.68	1.42	1.35
22	C	505	CLA	C4B-NB	7.53	1.41	1.35
22	b	603	CLA	C4B-NB	7.52	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	610	CLA	C4B-NB	7.42	1.41	1.35
22	C	507	CLA	C4B-NB	7.37	1.41	1.35
22	b	612	CLA	C4B-NB	7.35	1.41	1.35
22	C	510	CLA	C4B-NB	7.32	1.41	1.35
22	c	511	CLA	C4B-NB	7.32	1.41	1.35
22	c	506	CLA	C4B-NB	7.28	1.41	1.35
22	b	611	CLA	C4B-NB	7.27	1.41	1.35
22	c	517	CLA	C4B-NB	7.27	1.41	1.35
22	c	510	CLA	C4B-NB	7.26	1.41	1.35
22	B	604	CLA	C4B-NB	7.26	1.41	1.35
22	C	509	CLA	C4B-NB	7.25	1.41	1.35
22	B	615	CLA	C4B-NB	7.25	1.41	1.35
22	c	509	CLA	C4B-NB	7.23	1.41	1.35
22	b	606	CLA	C4B-NB	7.23	1.41	1.35
22	d	404	CLA	C4B-NB	7.22	1.41	1.35
22	b	608	CLA	C4B-NB	7.21	1.41	1.35
22	B	606	CLA	C4B-NB	7.20	1.41	1.35
22	B	602	CLA	C4B-NB	7.20	1.41	1.35
22	B	609	CLA	C4B-NB	7.19	1.41	1.35
22	b	605	CLA	C4B-NB	7.18	1.41	1.35
22	b	604	CLA	C4B-NB	7.16	1.41	1.35
22	c	515	CLA	C4B-NB	7.16	1.41	1.35
22	D	405	CLA	C4B-NB	7.16	1.41	1.35
22	b	609	CLA	C4B-NB	7.16	1.41	1.35
22	B	605	CLA	C4B-NB	7.16	1.41	1.35
22	B	608	CLA	C4B-NB	7.16	1.41	1.35
22	C	511	CLA	C4B-NB	7.15	1.41	1.35
22	B	611	CLA	C4B-NB	7.15	1.41	1.35
22	B	607	CLA	C4B-NB	7.15	1.41	1.35
22	C	516	CLA	C4B-NB	7.15	1.41	1.35
22	b	613	CLA	C4B-NB	7.14	1.41	1.35
22	d	403	CLA	C4B-NB	7.13	1.41	1.35
22	B	603	CLA	C4B-NB	7.13	1.41	1.35
22	C	515	CLA	C4B-NB	7.10	1.41	1.35
22	b	617	CLA	C4B-NB	7.10	1.41	1.35
22	c	516	CLA	C4B-NB	7.10	1.41	1.35
22	b	607	CLA	C4B-NB	7.09	1.41	1.35
22	b	610	CLA	C4B-NB	7.09	1.41	1.35
22	C	508	CLA	C4B-NB	7.07	1.41	1.35
22	c	508	CLA	C4B-NB	7.07	1.41	1.35
22	D	406	CLA	C4B-NB	7.05	1.41	1.35
22	c	512	CLA	C4B-NB	7.05	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	507	CLA	C4B-NB	7.03	1.41	1.35
22	C	506	CLA	C4B-NB	7.03	1.41	1.35
22	C	514	CLA	C4B-NB	7.02	1.41	1.35
22	B	614	CLA	C4B-NB	6.99	1.41	1.35
22	A	407	CLA	C4B-NB	6.97	1.41	1.35
22	a	408	CLA	C4B-NB	6.95	1.41	1.35
22	C	513	CLA	C4B-NB	6.94	1.41	1.35
22	d	401	CLA	C4B-NB	6.94	1.41	1.35
22	c	514	CLA	C4B-NB	6.92	1.41	1.35
22	c	518	CLA	C4B-NB	6.92	1.41	1.35
22	b	616	CLA	C4B-NB	6.91	1.41	1.35
22	b	615	CLA	C4B-NB	6.91	1.41	1.35
22	A	404	CLA	C4B-NB	6.90	1.41	1.35
22	c	513	CLA	C4B-NB	6.89	1.41	1.35
22	A	405	CLA	C4B-NB	6.88	1.41	1.35
22	C	512	CLA	C4B-NB	6.88	1.41	1.35
22	b	618	CLA	C4B-NB	6.88	1.41	1.35
22	D	401	CLA	C4B-NB	6.88	1.41	1.35
22	b	614	CLA	C4B-NB	6.88	1.41	1.35
22	a	406	CLA	C4B-NB	6.88	1.41	1.35
22	B	612	CLA	C4B-NB	6.86	1.41	1.35
22	B	613	CLA	C4B-NB	6.82	1.41	1.35
22	B	616	CLA	C4B-NB	6.80	1.41	1.35
22	a	405	CLA	C4B-NB	6.78	1.41	1.35
22	C	517	CLA	C4B-NB	6.72	1.41	1.35
26	A	410	SQD	O48-C23	4.66	1.47	1.33
26	a	417	SQD	O48-C23	4.66	1.47	1.33
26	b	601	SQD	O48-C23	4.66	1.46	1.33
26	a	411	SQD	O48-C23	4.65	1.46	1.33
26	D	412	SQD	O48-C23	4.64	1.46	1.33
26	A	415	SQD	O48-C23	4.62	1.46	1.33
26	l	102	SQD	O48-C23	4.58	1.46	1.33
26	d	412	SQD	O48-C23	4.57	1.46	1.33
25	a	410	PL9	C7-C3	-4.40	1.46	1.51
25	A	409	PL9	C7-C3	-4.12	1.47	1.51
36	E	104	HEM	C3C-CAC	4.03	1.56	1.47
36	e	103	HEM	C3C-CAC	3.99	1.56	1.47
36	v	201	HEM	C3C-CAC	3.95	1.55	1.47
22	d	404	CLA	C1D-ND	3.94	1.42	1.37
22	B	601	CLA	C1D-ND	3.92	1.42	1.37
36	V	201	HEM	C3C-CAC	3.92	1.55	1.47
22	c	508	CLA	C1D-ND	3.91	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	C1D-ND	3.90	1.42	1.37
22	b	606	CLA	C1D-ND	3.87	1.42	1.37
22	C	508	CLA	C1D-ND	3.85	1.42	1.37
22	D	406	CLA	C1D-ND	3.85	1.42	1.37
22	C	507	CLA	C1D-ND	3.85	1.42	1.37
22	b	608	CLA	C1D-ND	3.84	1.42	1.37
22	b	611	CLA	C1D-ND	3.84	1.42	1.37
22	B	606	CLA	C1D-ND	3.81	1.42	1.37
26	d	412	SQD	O5-C1	3.80	1.51	1.41
22	a	406	CLA	C1D-ND	3.79	1.42	1.37
26	D	412	SQD	O5-C1	3.78	1.51	1.41
22	c	506	CLA	C1D-ND	3.77	1.42	1.37
22	C	510	CLA	C1D-ND	3.77	1.42	1.37
22	c	511	CLA	C1D-ND	3.77	1.42	1.37
26	a	411	SQD	O5-C1	3.77	1.51	1.41
22	C	515	CLA	C1D-ND	3.76	1.42	1.37
22	A	405	CLA	C1D-ND	3.75	1.42	1.37
22	C	505	CLA	C1D-ND	3.75	1.42	1.37
22	B	616	CLA	C1D-ND	3.75	1.42	1.37
22	C	511	CLA	C1D-ND	3.75	1.42	1.37
22	C	512	CLA	C1D-ND	3.75	1.42	1.37
22	B	604	CLA	C1D-ND	3.74	1.42	1.37
22	B	614	CLA	C1D-ND	3.74	1.42	1.37
22	c	516	CLA	C1D-ND	3.74	1.42	1.37
22	B	609	CLA	C1D-ND	3.73	1.42	1.37
22	b	612	CLA	C1D-ND	3.73	1.42	1.37
22	B	610	CLA	C1D-ND	3.72	1.42	1.37
22	B	607	CLA	C1D-ND	3.71	1.42	1.37
22	c	513	CLA	C1D-ND	3.71	1.42	1.37
22	d	401	CLA	C1D-ND	3.71	1.42	1.37
22	b	618	CLA	C1D-ND	3.71	1.42	1.37
25	D	404	PL9	C7-C3	-3.70	1.47	1.51
22	c	509	CLA	C1D-ND	3.70	1.42	1.37
22	c	512	CLA	C1D-ND	3.69	1.42	1.37
25	d	402	PL9	C7-C3	-3.69	1.47	1.51
22	b	613	CLA	C1D-ND	3.69	1.42	1.37
22	a	405	CLA	C1D-ND	3.69	1.42	1.37
22	D	401	CLA	C1D-ND	3.68	1.42	1.37
22	b	609	CLA	C1D-ND	3.68	1.42	1.37
22	B	611	CLA	C1D-ND	3.67	1.42	1.37
22	A	404	CLA	C1D-ND	3.66	1.42	1.37
22	B	605	CLA	C1D-ND	3.66	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	607	CLA	C1D-ND	3.66	1.42	1.37
22	b	616	CLA	C1D-ND	3.66	1.42	1.37
22	c	518	CLA	C1D-ND	3.66	1.42	1.37
22	C	517	CLA	C1D-ND	3.65	1.42	1.37
22	A	407	CLA	C1D-ND	3.65	1.42	1.37
22	a	408	CLA	C1D-ND	3.63	1.42	1.37
22	B	615	CLA	C1D-ND	3.61	1.42	1.37
22	b	610	CLA	C1D-ND	3.60	1.42	1.37
22	B	613	CLA	C1D-ND	3.60	1.42	1.37
22	b	615	CLA	C1D-ND	3.59	1.42	1.37
22	B	602	CLA	C1D-ND	3.58	1.42	1.37
22	c	515	CLA	C1D-ND	3.57	1.42	1.37
22	b	604	CLA	C1D-ND	3.57	1.42	1.37
22	B	608	CLA	C1D-ND	3.56	1.42	1.37
22	C	506	CLA	C1D-ND	3.56	1.42	1.37
22	c	514	CLA	C1D-ND	3.55	1.42	1.37
22	b	617	CLA	C1D-ND	3.55	1.42	1.37
22	C	513	CLA	C1D-ND	3.54	1.42	1.37
22	C	514	CLA	C1D-ND	3.53	1.42	1.37
26	A	410	SQD	O47-C45	-3.49	1.37	1.46
26	a	417	SQD	O47-C45	-3.48	1.37	1.46
22	b	605	CLA	C1D-ND	3.48	1.42	1.37
22	c	507	CLA	C1D-ND	3.45	1.42	1.37
36	e	103	HEM	C3C-C2C	-3.45	1.35	1.40
26	a	411	SQD	O47-C45	-3.45	1.38	1.46
26	b	601	SQD	O47-C45	-3.45	1.38	1.46
36	E	104	HEM	C3C-C2C	-3.44	1.35	1.40
26	l	102	SQD	O47-C7	3.44	1.44	1.34
22	C	509	CLA	C1D-ND	3.44	1.42	1.37
26	D	412	SQD	O47-C45	-3.44	1.38	1.46
22	B	603	CLA	C1D-ND	3.43	1.42	1.37
22	d	401	CLA	C4D-ND	-3.41	1.33	1.37
36	V	201	HEM	C3C-C2C	-3.41	1.35	1.40
26	d	412	SQD	O47-C45	-3.41	1.38	1.46
22	D	401	CLA	C4D-ND	-3.40	1.33	1.37
22	c	510	CLA	C1D-ND	3.39	1.41	1.37
25	d	402	PL9	C3-C4	-3.38	1.44	1.49
36	v	201	HEM	C3C-C2C	-3.38	1.35	1.40
22	c	509	CLA	C4D-ND	-3.37	1.33	1.37
26	A	410	SQD	O5-C1	3.36	1.50	1.41
25	D	404	PL9	C3-C4	-3.36	1.44	1.49
26	l	102	SQD	O47-C45	-3.33	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	508	CLA	C4D-ND	-3.32	1.33	1.37
22	B	616	CLA	C4D-ND	-3.32	1.33	1.37
22	c	513	CLA	C4D-ND	-3.32	1.33	1.37
22	d	403	CLA	C4D-ND	-3.32	1.33	1.37
26	A	415	SQD	O47-C45	-3.31	1.38	1.46
26	a	417	SQD	O47-C7	3.31	1.43	1.34
26	l	102	SQD	O5-C1	3.30	1.50	1.41
26	a	411	SQD	O47-C7	3.30	1.43	1.34
26	b	601	SQD	O47-C7	3.30	1.43	1.34
26	D	412	SQD	O47-C7	3.29	1.43	1.34
22	C	512	CLA	C4D-ND	-3.29	1.33	1.37
26	A	415	SQD	O47-C7	3.28	1.43	1.34
26	d	412	SQD	O47-C7	3.27	1.43	1.34
22	c	514	CLA	CHC-C1C	3.27	1.43	1.35
22	b	618	CLA	C4D-ND	-3.26	1.33	1.37
26	A	410	SQD	O47-C7	3.26	1.43	1.34
22	D	405	CLA	C4D-ND	-3.25	1.33	1.37
22	C	513	CLA	CHC-C1C	3.24	1.43	1.35
22	a	406	CLA	C4D-ND	-3.24	1.33	1.37
22	c	511	CLA	C4D-ND	-3.23	1.33	1.37
22	A	405	CLA	C4D-ND	-3.23	1.33	1.37
22	d	403	CLA	C1D-ND	3.22	1.41	1.37
22	B	602	CLA	CHC-C1C	3.22	1.43	1.35
22	B	614	CLA	C4D-ND	-3.21	1.33	1.37
22	C	510	CLA	C4D-ND	-3.21	1.33	1.37
22	B	611	CLA	C4D-ND	-3.21	1.33	1.37
22	D	405	CLA	C1D-ND	3.20	1.41	1.37
22	B	607	CLA	C4D-ND	-3.20	1.33	1.37
22	c	517	CLA	C1D-ND	3.20	1.41	1.37
22	b	604	CLA	CHC-C1C	3.19	1.43	1.35
22	c	518	CLA	CHC-C1C	3.19	1.43	1.35
22	B	602	CLA	C4D-ND	-3.19	1.33	1.37
22	B	606	CLA	C4D-ND	-3.18	1.33	1.37
22	a	405	CLA	C4D-ND	-3.18	1.33	1.37
22	B	605	CLA	C4D-ND	-3.18	1.33	1.37
22	C	516	CLA	CHC-C1C	3.18	1.43	1.35
22	b	604	CLA	C4D-ND	-3.18	1.33	1.37
22	b	613	CLA	C4D-ND	-3.17	1.33	1.37
22	c	517	CLA	CHC-C1C	3.17	1.43	1.35
22	C	512	CLA	CHC-C1C	3.17	1.43	1.35
22	b	607	CLA	C4D-ND	-3.16	1.33	1.37
22	c	517	CLA	C4D-ND	-3.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	513	CLA	CHC-C1C	3.15	1.43	1.35
36	E	104	HEM	CAB-C3B	3.15	1.56	1.47
36	v	201	HEM	CAB-C3B	3.15	1.56	1.47
22	C	517	CLA	C4D-ND	-3.15	1.33	1.37
36	e	103	HEM	CAB-C3B	3.15	1.56	1.47
22	b	612	CLA	CHC-C1C	3.15	1.43	1.35
22	b	609	CLA	C4D-ND	-3.15	1.33	1.37
26	A	415	SQD	O5-C1	3.15	1.49	1.41
26	a	417	SQD	O5-C1	3.15	1.49	1.41
22	C	517	CLA	CHC-C1C	3.14	1.43	1.35
22	B	611	CLA	CHC-C1C	3.14	1.43	1.35
22	A	404	CLA	C4D-ND	-3.14	1.33	1.37
22	C	516	CLA	C1D-ND	3.14	1.41	1.37
22	D	406	CLA	C4D-ND	-3.13	1.33	1.37
22	a	408	CLA	CHC-C1C	3.13	1.43	1.35
22	c	518	CLA	C4D-ND	-3.13	1.33	1.37
22	B	610	CLA	CHC-C1C	3.13	1.43	1.35
22	b	613	CLA	CHC-C1C	3.13	1.43	1.35
22	C	516	CLA	C4D-ND	-3.12	1.33	1.37
22	B	612	CLA	C4D-ND	-3.12	1.33	1.37
36	V	201	HEM	CAB-C3B	3.12	1.55	1.47
22	c	510	CLA	CHC-C1C	3.12	1.43	1.35
22	c	516	CLA	CHC-C1C	3.11	1.43	1.35
22	b	616	CLA	CHC-C1C	3.11	1.42	1.35
22	b	616	CLA	C4D-ND	-3.11	1.33	1.37
22	B	608	CLA	CHC-C1C	3.11	1.42	1.35
22	D	406	CLA	CHC-C1C	3.11	1.42	1.35
22	b	614	CLA	C4D-ND	-3.11	1.33	1.37
22	C	509	CLA	CHC-C1C	3.11	1.42	1.35
22	B	614	CLA	CHC-C1C	3.11	1.42	1.35
22	B	601	CLA	CHC-C1C	3.10	1.42	1.35
22	A	407	CLA	CHC-C1C	3.10	1.42	1.35
22	C	514	CLA	C4D-ND	-3.10	1.33	1.37
26	l	102	SQD	C24-C23	3.10	1.59	1.50
22	a	405	CLA	CHC-C1C	3.10	1.42	1.35
22	b	612	CLA	C4D-ND	-3.09	1.33	1.37
22	d	404	CLA	CHC-C1C	3.09	1.42	1.35
22	d	403	CLA	CHC-C1C	3.09	1.42	1.35
22	D	405	CLA	CHC-C1C	3.09	1.42	1.35
22	b	607	CLA	CHC-C1C	3.09	1.42	1.35
26	a	411	SQD	C24-C23	3.08	1.59	1.50
22	c	510	CLA	C4D-ND	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	515	CLA	CHC-C1C	3.08	1.42	1.35
22	C	506	CLA	C4D-ND	-3.08	1.33	1.37
22	b	610	CLA	CHC-C1C	3.08	1.42	1.35
22	B	610	CLA	C4D-ND	-3.08	1.33	1.37
22	c	515	CLA	C4D-ND	-3.08	1.33	1.37
22	B	615	CLA	C4D-ND	-3.08	1.33	1.37
22	c	507	CLA	C4D-ND	-3.07	1.33	1.37
22	c	508	CLA	CHC-C1C	3.07	1.42	1.35
22	C	515	CLA	C4D-ND	-3.07	1.33	1.37
22	A	404	CLA	CHC-C1C	3.07	1.42	1.35
22	c	516	CLA	C4D-ND	-3.07	1.33	1.37
22	b	603	CLA	CHC-C1C	3.06	1.42	1.35
22	C	514	CLA	CHC-C1C	3.06	1.42	1.35
22	B	605	CLA	CHC-C1C	3.06	1.42	1.35
22	A	407	CLA	C4D-ND	-3.05	1.33	1.37
22	b	614	CLA	C1D-ND	3.05	1.41	1.37
22	c	514	CLA	C4D-ND	-3.05	1.33	1.37
22	C	507	CLA	C4D-ND	-3.04	1.33	1.37
22	c	515	CLA	CHC-C1C	3.04	1.42	1.35
22	C	513	CLA	C4D-ND	-3.04	1.33	1.37
22	d	404	CLA	C4D-ND	-3.04	1.33	1.37
22	b	614	CLA	CHC-C1C	3.04	1.42	1.35
22	b	605	CLA	C4D-ND	-3.04	1.33	1.37
22	b	608	CLA	C4D-ND	-3.04	1.33	1.37
22	c	506	CLA	C4D-ND	-3.04	1.33	1.37
26	A	410	SQD	C24-C23	3.03	1.59	1.50
22	a	408	CLA	C4D-ND	-3.03	1.33	1.37
22	b	608	CLA	CHC-C1C	3.03	1.42	1.35
22	C	510	CLA	CHC-C1C	3.03	1.42	1.35
22	c	508	CLA	C4D-ND	-3.03	1.33	1.37
22	B	609	CLA	CHC-C1C	3.03	1.42	1.35
22	B	606	CLA	CHC-C1C	3.02	1.42	1.35
22	c	512	CLA	CHC-C1C	3.02	1.42	1.35
22	C	511	CLA	CHC-C1C	3.02	1.42	1.35
22	B	607	CLA	CHC-C1C	3.02	1.42	1.35
22	C	507	CLA	CHC-C1C	3.01	1.42	1.35
22	b	615	CLA	CHC-C1C	3.01	1.42	1.35
22	b	611	CLA	CHC-C1C	3.01	1.42	1.35
22	B	603	CLA	C4D-ND	-3.01	1.33	1.37
22	C	511	CLA	C4D-ND	-3.01	1.33	1.37
22	c	511	CLA	CHC-C1C	3.01	1.42	1.35
22	C	505	CLA	C4D-ND	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	C4D-ND	-3.01	1.33	1.37
22	c	506	CLA	CHC-C1C	3.01	1.42	1.35
22	b	609	CLA	CHC-C1C	3.00	1.42	1.35
22	C	508	CLA	CHC-C1C	3.00	1.42	1.35
22	B	612	CLA	CHC-C1C	3.00	1.42	1.35
22	b	605	CLA	CHC-C1C	3.00	1.42	1.35
26	a	417	SQD	C24-C23	3.00	1.59	1.50
26	d	412	SQD	C24-C23	3.00	1.59	1.50
22	B	613	CLA	CHC-C1C	3.00	1.42	1.35
22	b	617	CLA	C4D-ND	-3.00	1.33	1.37
26	A	415	SQD	C24-C23	3.00	1.59	1.50
26	D	412	SQD	C24-C23	2.99	1.59	1.50
22	b	603	CLA	C4D-ND	-2.99	1.33	1.37
22	c	512	CLA	C4D-ND	-2.98	1.33	1.37
22	b	617	CLA	CHC-C1C	2.98	1.42	1.35
22	C	509	CLA	C4D-ND	-2.98	1.33	1.37
22	B	603	CLA	CHC-C1C	2.98	1.42	1.35
22	B	612	CLA	C1D-ND	2.97	1.41	1.37
22	c	509	CLA	CHC-C1C	2.97	1.42	1.35
22	b	615	CLA	C4D-ND	-2.97	1.33	1.37
22	b	611	CLA	C4D-ND	-2.97	1.33	1.37
22	B	609	CLA	C4D-ND	-2.96	1.33	1.37
22	B	615	CLA	CHC-C1C	2.96	1.42	1.35
22	D	401	CLA	CHC-C1C	2.95	1.42	1.35
22	d	401	CLA	CHC-C1C	2.95	1.42	1.35
22	C	506	CLA	CHC-C1C	2.95	1.42	1.35
22	B	608	CLA	C4D-ND	-2.94	1.33	1.37
22	C	505	CLA	CHC-C1C	2.94	1.42	1.35
26	b	601	SQD	C24-C23	2.94	1.59	1.50
22	b	606	CLA	C4D-ND	-2.93	1.33	1.37
26	b	601	SQD	O5-C1	2.93	1.49	1.41
22	b	610	CLA	C4D-ND	-2.92	1.33	1.37
22	c	507	CLA	CHC-C1C	2.92	1.42	1.35
22	A	405	CLA	CHC-C1C	2.91	1.42	1.35
22	B	601	CLA	C4D-ND	-2.91	1.33	1.37
22	B	604	CLA	C4D-ND	-2.91	1.33	1.37
22	a	406	CLA	CHC-C1C	2.90	1.42	1.35
22	b	618	CLA	CHC-C1C	2.90	1.42	1.35
22	b	605	CLA	CMB-C2B	-2.88	1.45	1.51
25	a	410	PL9	C3-C4	-2.87	1.44	1.49
25	A	409	PL9	C3-C4	-2.87	1.44	1.49
22	B	603	CLA	CMB-C2B	-2.86	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	616	CLA	CHC-C1C	2.85	1.42	1.35
22	B	604	CLA	CHC-C1C	2.83	1.42	1.35
22	b	606	CLA	CHC-C1C	2.79	1.42	1.35
22	c	511	CLA	CMB-C2B	-2.75	1.45	1.51
22	B	604	CLA	CMB-C2B	-2.74	1.45	1.51
22	b	606	CLA	CMB-C2B	-2.73	1.46	1.51
22	C	510	CLA	CMB-C2B	-2.72	1.46	1.51
25	A	409	PL9	C6-C1	-2.63	1.43	1.48
22	B	609	CLA	CMB-C2B	-2.60	1.46	1.51
22	B	612	CLA	CMD-C2D	-2.58	1.45	1.50
22	b	614	CLA	CMD-C2D	-2.58	1.45	1.50
22	B	606	CLA	CMB-C2B	-2.57	1.46	1.51
25	D	404	PL9	C6-C1	-2.57	1.44	1.48
22	b	610	CLA	CMB-C2B	-2.56	1.46	1.51
22	B	608	CLA	CMB-C2B	-2.56	1.46	1.51
22	b	611	CLA	CMB-C2B	-2.56	1.46	1.51
22	B	612	CLA	CMB-C2B	-2.55	1.46	1.51
22	c	510	CLA	CMD-C2D	-2.54	1.45	1.50
22	b	608	CLA	CMB-C2B	-2.54	1.46	1.51
22	a	406	CLA	CMB-C2B	-2.54	1.46	1.51
22	C	509	CLA	CMD-C2D	-2.53	1.45	1.50
25	d	402	PL9	C6-C1	-2.52	1.44	1.48
22	A	405	CLA	CMB-C2B	-2.52	1.46	1.51
22	B	616	CLA	CMC-C2C	-2.51	1.45	1.50
22	b	618	CLA	CMC-C2C	-2.51	1.45	1.50
22	b	603	CLA	CMB-C2B	-2.51	1.46	1.51
25	a	410	PL9	C6-C1	-2.50	1.44	1.48
22	a	408	CLA	CMB-C2B	-2.50	1.46	1.51
22	b	614	CLA	CMB-C2B	-2.50	1.46	1.51
22	D	401	CLA	CMB-C2B	-2.49	1.46	1.51
22	c	515	CLA	CMB-C2B	-2.49	1.46	1.51
22	c	509	CLA	CMB-C2B	-2.48	1.46	1.51
22	c	507	CLA	CMB-C2B	-2.48	1.46	1.51
22	B	607	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	609	CLA	CMB-C2B	-2.48	1.46	1.51
22	A	407	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	514	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	508	CLA	CMB-C2B	-2.46	1.46	1.51
22	b	615	CLA	CMB-C2B	-2.46	1.46	1.51
22	b	612	CLA	CMB-C2B	-2.46	1.46	1.51
22	d	401	CLA	CMB-C2B	-2.45	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	CMB-C2B	-2.45	1.46	1.51
22	c	510	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	601	CLA	CMB-C2B	-2.45	1.46	1.51
22	c	513	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	516	CLA	CMB-C2B	-2.44	1.46	1.51
22	C	505	CLA	CMB-C2B	-2.43	1.46	1.51
22	D	406	CLA	CMB-C2B	-2.43	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	610	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	603	CLA	CMD-C2D	-2.42	1.45	1.50
22	c	506	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	616	CLA	CMB-C2B	-2.42	1.46	1.51
22	C	507	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.42	1.46	1.51
22	C	509	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	602	CLA	CMB-C2B	-2.41	1.46	1.51
22	A	404	CLA	CMD-C2D	-2.41	1.45	1.50
22	C	512	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	516	CLA	CMB-C2B	-2.41	1.46	1.51
22	d	404	CLA	CMB-C2B	-2.40	1.46	1.51
22	b	618	CLA	CMB-C2B	-2.40	1.46	1.51
22	c	515	CLA	CMD-C2D	-2.39	1.45	1.50
22	b	617	CLA	CMB-C2B	-2.39	1.46	1.51
22	b	605	CLA	CMD-C2D	-2.39	1.45	1.50
22	c	517	CLA	CMB-C2B	-2.38	1.46	1.51
22	C	515	CLA	CMB-C2B	-2.38	1.46	1.51
22	b	616	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	607	CLA	CMB-C2B	-2.37	1.46	1.51
22	C	514	CLA	CMD-C2D	-2.37	1.45	1.50
22	d	403	CLA	CMD-C2D	-2.37	1.45	1.50
22	a	405	CLA	CMD-C2D	-2.37	1.45	1.50
22	a	405	CLA	CMB-C2B	-2.36	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.36	1.46	1.51
22	D	405	CLA	CMB-C2B	-2.35	1.46	1.51
22	C	511	CLA	CMB-C2B	-2.35	1.46	1.51
22	D	405	CLA	CMD-C2D	-2.35	1.45	1.50
22	B	605	CLA	CMB-C2B	-2.35	1.46	1.51
22	b	613	CLA	CMB-C2B	-2.35	1.46	1.51
22	d	403	CLA	CMB-C2B	-2.35	1.46	1.51
22	B	604	CLA	CMD-C2D	-2.34	1.45	1.50
22	A	404	CLA	CMB-C2B	-2.34	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	CMB-C2B	-2.33	1.46	1.51
22	b	604	CLA	CMB-C2B	-2.33	1.46	1.51
22	b	606	CLA	CMD-C2D	-2.30	1.45	1.50
22	b	614	CLA	CMC-C2C	-2.30	1.45	1.50
22	c	514	CLA	CMB-C2B	-2.29	1.46	1.51
22	c	518	CLA	CMB-C2B	-2.27	1.46	1.51
22	C	513	CLA	CMB-C2B	-2.27	1.46	1.51
22	C	517	CLA	CMB-C2B	-2.26	1.46	1.51
26	D	412	SQD	O5-C5	2.26	1.49	1.44
26	a	411	SQD	O5-C5	2.24	1.49	1.44
22	B	605	CLA	CMD-C2D	-2.22	1.46	1.50
22	B	612	CLA	CMC-C2C	-2.22	1.46	1.50
22	B	606	CLA	CMC-C2C	-2.21	1.46	1.50
26	d	412	SQD	O5-C5	2.21	1.49	1.44
22	C	516	CLA	CMD-C2D	-2.20	1.46	1.50
25	a	410	PL9	C53-C6	-2.20	1.46	1.50
22	B	608	CLA	CMD-C2D	-2.18	1.46	1.50
22	b	607	CLA	CMD-C2D	-2.18	1.46	1.50
22	b	613	CLA	CMC-C2C	-2.18	1.46	1.50
22	b	610	CLA	CMD-C2D	-2.18	1.46	1.50
26	D	412	SQD	O7-S	2.16	1.51	1.45
26	l	102	SQD	O7-S	2.16	1.51	1.45
22	c	513	CLA	CMC-C2C	-2.16	1.46	1.50
26	l	102	SQD	O9-S	2.15	1.51	1.45
25	A	409	PL9	C53-C6	-2.15	1.46	1.50
22	C	512	CLA	CMC-C2C	-2.15	1.46	1.50
26	b	601	SQD	C46-C45	2.15	1.57	1.50
26	d	412	SQD	O9-S	2.15	1.51	1.45
26	b	601	SQD	O7-S	2.15	1.51	1.45
26	a	411	SQD	O9-S	2.15	1.51	1.45
22	c	517	CLA	CMD-C2D	-2.14	1.46	1.50
26	l	102	SQD	C8-C7	2.13	1.56	1.50
26	d	412	SQD	O7-S	2.13	1.51	1.45
26	b	601	SQD	O9-S	2.13	1.51	1.45
22	B	611	CLA	CMC-C2C	-2.13	1.46	1.50
22	C	506	CLA	CMC-C2C	-2.12	1.46	1.50
26	A	415	SQD	O9-S	2.12	1.51	1.45
26	D	412	SQD	O9-S	2.12	1.51	1.45
22	b	604	CLA	CMD-C2D	-2.12	1.46	1.50
22	a	408	CLA	CMD-C2D	-2.12	1.46	1.50
22	c	507	CLA	CMC-C2C	-2.12	1.46	1.50
22	C	508	CLA	CMC-C2C	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	406	CLA	CMD-C2D	-2.12	1.46	1.50
26	A	410	SQD	O9-S	2.11	1.51	1.45
22	B	602	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	615	CLA	CMD-C2D	-2.11	1.46	1.50
22	c	514	CLA	CMD-C2D	-2.10	1.46	1.50
22	C	505	CLA	CMD-C2D	-2.10	1.46	1.50
22	c	509	CLA	CMC-C2C	-2.10	1.46	1.50
22	A	407	CLA	CMD-C2D	-2.10	1.46	1.50
22	b	617	CLA	CMD-C2D	-2.09	1.46	1.50
22	B	610	CLA	CMD-C2D	-2.09	1.46	1.50
22	C	513	CLA	CMD-C2D	-2.09	1.46	1.50
36	E	104	HEM	CMB-C2B	2.09	1.55	1.50
22	c	511	CLA	CMC-C2C	-2.08	1.46	1.50
22	c	516	CLA	CMC-C2C	-2.08	1.46	1.50
22	D	401	CLA	CMD-C2D	-2.08	1.46	1.50
22	A	405	CLA	CMD-C2D	-2.07	1.46	1.50
22	b	608	CLA	CMC-C2C	-2.07	1.46	1.50
26	a	417	SQD	O9-S	2.07	1.51	1.45
22	b	612	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	614	CLA	CMC-C2C	-2.07	1.46	1.50
26	d	412	SQD	C8-C7	2.07	1.56	1.50
26	A	410	SQD	O7-S	2.07	1.51	1.45
22	C	510	CLA	CMC-C2C	-2.06	1.46	1.50
26	l	102	SQD	C46-C45	2.06	1.57	1.50
22	B	616	CLA	CMD-C2D	-2.06	1.46	1.50
22	c	508	CLA	CMC-C2C	-2.05	1.46	1.50
22	c	506	CLA	CMD-C2D	-2.05	1.46	1.50
22	C	515	CLA	CMC-C2C	-2.05	1.46	1.50
36	e	103	HEM	CMB-C2B	2.05	1.55	1.50
22	b	609	CLA	CMD-C2D	-2.04	1.46	1.50
22	b	616	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	607	CLA	CMD-C2D	-2.04	1.46	1.50
22	b	613	CLA	CMD-C2D	-2.04	1.46	1.50
22	D	406	CLA	CMC-C2C	-2.04	1.46	1.50
22	C	508	CLA	CMD-C2D	-2.04	1.46	1.50
36	E	104	HEM	FE-NB	2.03	2.06	1.96
22	C	507	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	615	CLA	CMC-C2C	-2.03	1.46	1.50
26	A	415	SQD	C8-C7	2.03	1.56	1.50
22	C	507	CLA	CMC-C2C	-2.03	1.46	1.50
22	C	511	CLA	CMD-C2D	-2.03	1.46	1.50
22	c	511	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	505	CLA	C3B-C2B	-2.03	1.37	1.40
22	d	404	CLA	CMC-C2C	-2.03	1.46	1.50
22	d	401	CLA	CMD-C2D	-2.03	1.46	1.50
22	b	604	CLA	CMC-C2C	-2.03	1.46	1.50
26	a	411	SQD	O7-S	2.03	1.51	1.45
22	C	506	CLA	CMD-C2D	-2.03	1.46	1.50
22	C	517	CLA	CMC-C2C	-2.03	1.46	1.50
22	b	608	CLA	CMD-C2D	-2.03	1.46	1.50
22	b	609	CLA	CMC-C2C	-2.03	1.46	1.50
22	B	602	CLA	CMC-C2C	-2.02	1.46	1.50
26	b	601	SQD	C44-C45	2.02	1.56	1.50
36	E	104	HEM	FE-ND	2.02	2.06	1.96
22	c	510	CLA	CMC-C2C	-2.02	1.46	1.50
22	c	512	CLA	CMD-C2D	-2.02	1.46	1.50
25	D	404	PL9	C53-C6	-2.02	1.46	1.50
22	B	614	CLA	CMD-C2D	-2.02	1.46	1.50
22	d	403	CLA	CMC-C2C	-2.02	1.46	1.50
22	d	404	CLA	CMD-C2D	-2.02	1.46	1.50
22	c	509	CLA	CMD-C2D	-2.02	1.46	1.50
22	C	510	CLA	CMD-C2D	-2.01	1.46	1.50
22	b	615	CLA	CMD-C2D	-2.01	1.46	1.50
22	b	616	CLA	CMC-C2C	-2.01	1.46	1.50
26	D	412	SQD	C8-C7	2.01	1.56	1.50
22	B	611	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	605	CLA	CMC-C2C	-2.01	1.46	1.50
22	b	618	CLA	CMD-C2D	-2.01	1.46	1.50
22	c	518	CLA	CMC-C2C	-2.01	1.46	1.50

All (795) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	606	CLA	C4A-NA-C1A	7.94	110.28	106.71
22	C	516	CLA	C4A-NA-C1A	7.92	110.27	106.71
22	B	604	CLA	C4A-NA-C1A	7.80	110.21	106.71
22	C	511	CLA	C4A-NA-C1A	7.58	110.11	106.71
22	c	517	CLA	C4A-NA-C1A	7.51	110.08	106.71
22	c	509	CLA	C4A-NA-C1A	7.51	110.08	106.71
22	b	608	CLA	C4A-NA-C1A	7.39	110.03	106.71
22	c	512	CLA	C4A-NA-C1A	7.37	110.02	106.71
22	b	609	CLA	C4A-NA-C1A	7.36	110.01	106.71
22	B	606	CLA	C4A-NA-C1A	7.34	110.01	106.71
22	b	614	CLA	C4A-NA-C1A	7.34	110.01	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	508	CLA	C4A-NA-C1A	7.32	110.00	106.71
22	c	507	CLA	C4A-NA-C1A	7.32	110.00	106.71
22	B	612	CLA	C4A-NA-C1A	7.30	109.99	106.71
22	B	607	CLA	C4A-NA-C1A	7.28	109.98	106.71
22	B	616	CLA	C4A-NA-C1A	7.26	109.97	106.71
22	c	511	CLA	C4A-NA-C1A	7.26	109.97	106.71
22	C	506	CLA	C4A-NA-C1A	7.25	109.96	106.71
22	C	515	CLA	C4A-NA-C1A	7.21	109.95	106.71
22	d	401	CLA	C4A-NA-C1A	7.16	109.92	106.71
22	b	618	CLA	C4A-NA-C1A	7.15	109.92	106.71
22	C	509	CLA	C4A-NA-C1A	7.15	109.92	106.71
22	c	510	CLA	C4A-NA-C1A	7.14	109.92	106.71
22	D	401	CLA	C4A-NA-C1A	7.12	109.91	106.71
22	b	616	CLA	C4A-NA-C1A	7.10	109.90	106.71
22	C	510	CLA	C4A-NA-C1A	7.10	109.90	106.71
22	C	513	CLA	C4A-NA-C1A	7.08	109.89	106.71
22	B	614	CLA	C4A-NA-C1A	7.05	109.87	106.71
22	c	514	CLA	C4A-NA-C1A	7.05	109.87	106.71
22	B	605	CLA	C4A-NA-C1A	7.04	109.87	106.71
22	c	513	CLA	C4A-NA-C1A	7.04	109.87	106.71
22	b	607	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	a	406	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	c	516	CLA	C4A-NA-C1A	7.00	109.86	106.71
22	b	613	CLA	C4A-NA-C1A	6.99	109.85	106.71
22	A	405	CLA	C4A-NA-C1A	6.98	109.84	106.71
22	D	406	CLA	C4A-NA-C1A	6.95	109.83	106.71
22	b	615	CLA	C4A-NA-C1A	6.94	109.83	106.71
22	B	611	CLA	C4A-NA-C1A	6.93	109.82	106.71
22	B	613	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	b	603	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	C	512	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	c	515	CLA	C4A-NA-C1A	6.87	109.80	106.71
22	B	601	CLA	C4A-NA-C1A	6.82	109.77	106.71
22	D	405	CLA	C4A-NA-C1A	6.81	109.77	106.71
22	c	518	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	B	609	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	C	517	CLA	C4A-NA-C1A	6.79	109.76	106.71
22	b	617	CLA	C4A-NA-C1A	6.79	109.76	106.71
22	C	505	CLA	C4A-NA-C1A	6.78	109.76	106.71
22	C	514	CLA	C4A-NA-C1A	6.78	109.75	106.71
22	d	403	CLA	C4A-NA-C1A	6.78	109.75	106.71
22	C	507	CLA	C4A-NA-C1A	6.74	109.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	605	CLA	C4A-NA-C1A	6.74	109.73	106.71
22	B	608	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	b	611	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	b	610	CLA	C4A-NA-C1A	6.67	109.71	106.71
22	d	404	CLA	C4A-NA-C1A	6.67	109.71	106.71
22	c	506	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	B	615	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	B	603	CLA	C4A-NA-C1A	6.54	109.64	106.71
22	a	408	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	A	407	CLA	C4A-NA-C1A	6.47	109.61	106.71
22	a	405	CLA	C4A-NA-C1A	6.43	109.60	106.71
22	A	404	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	c	508	CLA	C4A-NA-C1A	6.33	109.55	106.71
22	b	612	CLA	C4A-NA-C1A	6.28	109.53	106.71
24	b	602	BCR	C15-C14-C13	6.28	136.27	127.31
22	B	610	CLA	C4A-NA-C1A	6.19	109.49	106.71
22	B	602	CLA	C4A-NA-C1A	6.14	109.47	106.71
22	b	604	CLA	C4A-NA-C1A	6.09	109.44	106.71
24	B	632	BCR	C15-C14-C13	6.08	135.98	127.31
34	J	102	DGD	O5D-C1E-C2E	5.99	117.65	108.30
34	J	102	DGD	C6D-O5D-C1E	5.60	124.68	113.74
22	C	512	CLA	CMB-C2B-C1B	-5.22	120.44	128.46
22	c	518	CLA	CMB-C2B-C1B	-5.20	120.47	128.46
22	C	517	CLA	CMB-C2B-C1B	-5.20	120.47	128.46
22	c	513	CLA	CMB-C2B-C1B	-5.20	120.48	128.46
25	a	410	PL9	C7-C3-C4	5.18	121.09	116.88
22	c	511	CLA	CMB-C2B-C1B	-5.11	120.62	128.46
25	A	409	PL9	C7-C3-C4	5.10	121.03	116.88
26	b	601	SQD	O6-C1-C2	5.10	116.26	108.30
22	D	401	CLA	CMB-C2B-C1B	-5.06	120.69	128.46
22	d	401	CLA	CMB-C2B-C1B	-5.06	120.69	128.46
22	C	510	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
26	l	102	SQD	O7-S-C6	4.99	112.88	106.94
22	b	614	CLA	CMB-C2B-C1B	-4.96	120.84	128.46
22	A	404	CLA	CMB-C2B-C1B	-4.94	120.86	128.46
26	b	601	SQD	O7-S-C6	4.91	112.78	106.94
22	a	405	CLA	CMB-C2B-C1B	-4.90	120.93	128.46
22	C	513	CLA	CMB-C2B-C1B	-4.90	120.93	128.46
22	B	612	CLA	CMB-C2B-C1B	-4.90	120.94	128.46
22	b	613	CLA	CMB-C2B-C1B	-4.89	120.95	128.46
22	c	514	CLA	CMB-C2B-C1B	-4.89	120.95	128.46
22	B	611	CLA	CMB-C2B-C1B	-4.88	120.96	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	508	CLA	CMB-C2B-C1B	-4.82	121.06	128.46
25	d	402	PL9	C7-C3-C4	4.72	120.72	116.88
25	D	404	PL9	C7-C3-C4	4.72	120.71	116.88
22	B	616	CLA	CMB-C2B-C1B	-4.69	121.25	128.46
22	b	618	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
26	l	102	SQD	O47-C7-C8	4.66	121.56	111.50
22	c	518	CLA	CMB-C2B-C3B	4.57	133.22	124.68
22	C	517	CLA	CMB-C2B-C3B	4.57	133.22	124.68
22	b	610	CLA	CMB-C2B-C1B	-4.53	121.51	128.46
22	B	613	CLA	CMB-C2B-C1B	-4.52	121.51	128.46
22	b	604	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
22	b	615	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
22	C	508	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
22	c	509	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
22	A	405	CLA	CMB-C2B-C1B	-4.49	121.56	128.46
22	a	406	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
22	B	608	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
22	B	602	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
22	c	516	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
22	C	515	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
22	C	507	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
22	C	512	CLA	CMB-C2B-C3B	4.33	132.78	124.68
22	c	513	CLA	CMB-C2B-C3B	4.33	132.77	124.68
26	d	412	SQD	O47-C7-C8	4.32	120.81	111.50
22	c	512	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
22	C	511	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
34	J	102	DGD	O5D-C6D-C5D	4.17	116.76	109.05
22	d	401	CLA	CMB-C2B-C3B	4.17	132.47	124.68
22	D	401	CLA	CMB-C2B-C3B	4.16	132.47	124.68
22	C	513	CLA	CMB-C2B-C3B	4.16	132.46	124.68
22	c	514	CLA	CMB-C2B-C3B	4.16	132.46	124.68
22	B	614	CLA	CMB-C2B-C1B	-4.16	122.08	128.46
24	B	632	BCR	C16-C15-C14	4.16	131.99	123.47
22	A	404	CLA	CMB-C2B-C3B	4.15	132.44	124.68
22	C	514	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
22	a	405	CLA	CMB-C2B-C3B	4.13	132.41	124.68
22	c	515	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
22	B	606	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
22	b	616	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
26	b	601	SQD	C1-O5-C5	-4.07	105.69	113.69
26	a	411	SQD	O9-S-C6	4.05	111.75	106.94
22	B	611	CLA	CMB-C2B-C3B	4.04	132.24	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	412	SQD	O47-C7-C8	4.04	120.21	111.50
22	c	508	CLA	CMB-C2B-C3B	4.04	132.23	124.68
22	b	614	CLA	CMB-C2B-C3B	4.03	132.22	124.68
22	B	605	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
26	b	601	SQD	O47-C7-C8	4.01	120.15	111.50
22	b	613	CLA	CMB-C2B-C3B	4.00	132.17	124.68
30	a	419	BCT	O2-C-O1	3.98	129.86	119.55
30	A	416	BCT	O2-C-O1	3.97	129.85	119.55
22	B	612	CLA	CMB-C2B-C3B	3.97	132.10	124.68
26	A	415	SQD	O47-C7-C8	3.96	120.04	111.50
26	d	412	SQD	O9-S-C6	3.96	111.65	106.94
33	i	102	LMT	C1B-O5B-C5B	3.95	121.44	113.69
26	a	417	SQD	O9-S-C6	3.95	111.63	106.94
22	b	607	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
22	B	610	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
22	b	612	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
22	B	607	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
26	A	415	SQD	O9-S-C6	3.91	111.58	106.94
22	b	617	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
22	a	408	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
22	c	511	CLA	CMB-C2B-C3B	3.90	131.98	124.68
22	b	609	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
22	b	618	CLA	CMB-C2B-C3B	3.89	131.95	124.68
26	A	410	SQD	O47-C7-C8	3.89	119.88	111.50
22	b	605	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
22	B	616	CLA	CMB-C2B-C3B	3.87	131.92	124.68
22	B	603	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
22	b	608	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
22	b	604	CLA	CMB-C2B-C3B	3.85	131.89	124.68
22	C	510	CLA	CMB-C2B-C3B	3.85	131.87	124.68
22	A	407	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
22	B	602	CLA	CMB-C2B-C3B	3.82	131.82	124.68
26	A	415	SQD	O6-C1-C2	3.80	114.24	108.30
22	d	403	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
22	D	405	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
22	c	512	CLA	CMB-C2B-C3B	3.78	131.75	124.68
26	a	411	SQD	O47-C7-C8	3.77	119.62	111.50
22	b	610	CLA	CMB-C2B-C3B	3.75	131.69	124.68
26	D	412	SQD	O5-C5-C4	3.74	116.48	109.69
22	C	515	CLA	CMB-C2B-C3B	3.74	131.67	124.68
22	c	516	CLA	CMB-C2B-C3B	3.73	131.66	124.68
22	B	608	CLA	CMB-C2B-C3B	3.72	131.64	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	417	SQD	O47-C7-C8	3.72	119.51	111.50
22	a	406	CLA	CMB-C2B-C3B	3.71	131.61	124.68
22	b	615	CLA	CMB-C2B-C3B	3.70	131.61	124.68
24	B	632	BCR	C15-C16-C17	-3.70	115.90	123.47
22	A	405	CLA	CMB-C2B-C3B	3.69	131.59	124.68
26	b	601	SQD	O9-S-O7	-3.68	101.20	113.95
22	B	613	CLA	CMB-C2B-C3B	3.68	131.56	124.68
22	C	507	CLA	CMB-C2B-C3B	3.68	131.56	124.68
34	C	504	DGD	C6D-O5D-C1E	3.67	120.91	113.74
22	C	511	CLA	CMB-C2B-C3B	3.66	131.52	124.68
26	a	417	SQD	O6-C1-C2	3.65	114.01	108.30
26	a	417	SQD	O9-S-O7	-3.65	101.31	113.95
26	a	411	SQD	O9-S-O7	-3.65	101.33	113.95
22	C	508	CLA	CMB-C2B-C3B	3.64	131.50	124.68
26	d	412	SQD	O7-S-C6	3.63	111.25	106.94
24	b	602	BCR	C16-C15-C14	3.63	130.91	123.47
26	A	415	SQD	O7-S-C6	3.62	111.25	106.94
22	c	509	CLA	CMB-C2B-C3B	3.62	131.44	124.68
33	C	518	LMT	C1B-O5B-C5B	3.59	120.73	113.69
34	c	504	DGD	C6D-O5D-C1E	3.58	120.73	113.74
25	a	410	PL9	C7-C3-C2	-3.57	118.60	123.30
26	a	417	SQD	O7-S-C6	3.57	111.18	106.94
22	c	510	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
24	b	602	BCR	C15-C16-C17	-3.56	116.17	123.47
26	A	410	SQD	O9-S-O7	-3.55	101.68	113.95
26	A	410	SQD	O9-S-C6	3.54	111.15	106.94
26	A	415	SQD	O9-S-O7	-3.54	101.70	113.95
22	B	601	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
22	B	614	CLA	CMB-C2B-C3B	3.53	131.28	124.68
22	b	611	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
22	b	616	CLA	CMB-C2B-C3B	3.53	131.28	124.68
25	A	409	PL9	C7-C3-C2	-3.49	118.70	123.30
36	e	103	HEM	CMC-C2C-C3C	3.49	131.22	124.68
36	E	104	HEM	CMC-C2C-C3C	3.49	131.21	124.68
26	D	412	SQD	O9-S-O7	-3.49	101.88	113.95
22	C	506	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
26	D	412	SQD	O7-S-C6	3.47	111.07	106.94
22	b	603	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
26	d	412	SQD	O9-S-O7	-3.47	101.96	113.95
22	C	509	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
22	B	609	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
22	B	606	CLA	CMB-C2B-C3B	3.44	131.12	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	l	102	SQD	O9-S-O7	-3.43	102.08	113.95
22	c	507	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	c	515	CLA	CMB-C2B-C3B	3.41	131.06	124.68
22	b	604	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
36	E	104	HEM	CBA-CAA-C2A	-3.41	106.80	112.62
22	C	514	CLA	CMB-C2B-C3B	3.40	131.04	124.68
35	C	525	LMG	C4-C3-C2	3.40	116.75	110.82
22	B	602	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
22	B	605	CLA	CMB-C2B-C3B	3.38	131.00	124.68
22	c	512	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
26	l	102	SQD	O9-S-C6	3.36	110.93	106.94
26	d	412	SQD	O5-C5-C4	3.36	115.80	109.69
22	b	617	CLA	CMB-C2B-C3B	3.35	130.94	124.68
22	b	607	CLA	CMB-C2B-C3B	3.32	130.89	124.68
22	C	511	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
22	a	408	CLA	CMB-C2B-C3B	3.29	130.83	124.68
22	c	517	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
22	C	516	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
22	B	610	CLA	CMB-C2B-C3B	3.28	130.81	124.68
23	a	420	PHO	CMB-C2B-C3B	3.27	130.80	124.68
22	b	612	CLA	CMB-C2B-C3B	3.27	130.79	124.68
22	A	407	CLA	CMB-C2B-C3B	3.26	130.78	124.68
23	D	403	PHO	CMB-C2B-C3B	3.25	130.76	124.68
22	A	407	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
22	d	404	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
22	a	408	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
22	B	614	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
22	d	403	CLA	CMB-C2B-C3B	3.21	130.69	124.68
22	B	612	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
22	B	615	CLA	CMB-C2B-C1B	-3.21	123.54	128.46
36	E	104	HEM	C4B-CHC-C1C	3.19	126.77	122.56
25	a	410	PL9	C40-C39-C41	3.18	120.62	115.27
36	e	103	HEM	CBA-CAA-C2A	-3.18	107.19	112.62
36	v	201	HEM	C4B-CHC-C1C	3.18	126.75	122.56
22	b	614	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
22	D	406	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
22	D	405	CLA	CMB-C2B-C3B	3.17	130.62	124.68
36	e	103	HEM	C4B-CHC-C1C	3.17	126.75	122.56
26	A	410	SQD	O7-S-C6	3.17	110.70	106.94
22	B	607	CLA	CMB-C2B-C3B	3.17	130.60	124.68
25	d	402	PL9	C7-C3-C2	-3.16	119.14	123.30
22	c	517	CLA	CMB-C2B-C1B	-3.16	123.61	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	616	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
22	C	512	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
22	b	608	CLA	CMB-C2B-C3B	3.15	130.56	124.68
22	b	609	CLA	CMB-C2B-C3B	3.15	130.56	124.68
22	C	516	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
25	D	404	PL9	C7-C3-C2	-3.14	119.17	123.30
22	B	604	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
22	B	606	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
22	c	513	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
22	D	406	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
22	b	618	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
22	B	616	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
22	c	518	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
36	V	201	HEM	C4B-CHC-C1C	3.10	126.65	122.56
24	b	602	BCR	C12-C13-C14	-3.09	114.20	118.94
33	A	419	LMT	C2'-C3'-C4'	3.09	116.73	109.68
22	b	606	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
22	C	517	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	d	404	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
35	C	525	LMG	O6-C5-C4	3.04	115.22	109.69
35	y	101	LMG	O6-C5-C4	3.04	115.21	109.69
22	C	513	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	B	611	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
24	c	501	BCR	C7-C8-C9	-3.02	121.67	126.23
22	c	510	CLA	CMB-C2B-C3B	3.02	130.32	124.68
22	b	608	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
22	c	514	CLA	CHB-C4A-NA	3.00	128.66	124.51
26	b	601	SQD	O9-S-C6	3.00	110.50	106.94
36	v	201	HEM	C1B-NB-C4B	2.99	108.16	105.07
36	e	103	HEM	C4D-ND-C1D	2.97	108.14	105.07
26	a	411	SQD	O5-C5-C4	2.97	115.08	109.69
22	c	514	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
22	a	406	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
22	D	401	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
34	D	411	DGD	C3G-O3G-C1D	2.95	119.50	113.74
36	E	104	HEM	C4D-ND-C1D	2.95	108.12	105.07
22	A	405	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
22	C	513	CLA	CHB-C4A-NA	2.94	128.58	124.51
36	E	104	HEM	CBD-CAD-C3D	-2.94	104.46	112.63
36	e	103	HEM	CBD-CAD-C3D	-2.93	104.50	112.63
22	b	611	CLA	CMB-C2B-C3B	2.92	130.14	124.68
22	b	603	CLA	O2D-CGD-O1D	-2.92	118.14	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	409	PL9	C40-C39-C41	2.91	120.17	115.27
24	B	632	BCR	C12-C13-C14	-2.91	114.47	118.94
22	B	603	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	C	509	CLA	CMB-C2B-C3B	2.91	130.12	124.68
24	C	501	BCR	C7-C8-C9	-2.90	121.85	126.23
25	d	402	PL9	C40-C39-C41	2.90	120.16	115.27
22	b	612	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
36	V	201	HEM	C1B-NB-C4B	2.90	108.07	105.07
22	c	507	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	B	601	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
22	d	401	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	C	506	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
26	A	415	SQD	O48-C23-C24	2.89	120.98	111.91
22	c	508	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	b	605	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	B	608	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	C	506	CLA	CMB-C2B-C3B	2.87	130.06	124.68
22	b	613	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	C	515	CLA	CHB-C4A-NA	2.87	128.48	124.51
22	C	505	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	B	609	CLA	CMB-C2B-C3B	2.86	130.04	124.68
26	D	412	SQD	O8-S-C6	2.86	110.30	105.74
22	B	610	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	C	511	CLA	CHB-C4A-NA	2.86	128.47	124.51
26	a	411	SQD	O8-S-C6	2.86	110.30	105.74
22	b	608	CLA	CHB-C4A-NA	2.86	128.46	124.51
22	C	516	CLA	CHB-C4A-NA	2.86	128.46	124.51
26	D	412	SQD	O9-S-C6	2.85	110.33	106.94
24	B	619	BCR	C23-C22-C21	-2.85	114.56	118.94
22	c	516	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	D	404	PL9	C40-C39-C41	2.85	120.06	115.27
22	b	610	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
26	D	412	SQD	O48-C23-C24	2.85	120.84	111.91
26	a	417	SQD	O8-S-C6	2.84	110.27	105.74
22	c	510	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	c	516	CLA	CHB-C4A-NA	2.84	128.43	124.51
22	C	509	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	c	507	CLA	CMB-C2B-C3B	2.82	129.96	124.68
24	b	620	BCR	C23-C22-C21	-2.82	114.61	118.94
25	d	402	PL9	C7-C8-C9	-2.82	122.11	126.79
25	D	404	PL9	C7-C8-C9	-2.81	122.11	126.79
22	c	506	CLA	O2D-CGD-O1D	-2.81	118.35	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	512	CLA	CHB-C4A-NA	2.81	128.39	124.51
22	B	603	CLA	CMB-C2B-C3B	2.80	129.93	124.68
25	A	409	PL9	C36-C34-C33	-2.80	115.44	121.12
35	y	101	LMG	C9-C8-C7	2.80	118.42	111.79
22	b	609	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	A	410	SQD	O8-S-C6	2.79	110.19	105.74
22	C	515	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	B	615	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
22	b	605	CLA	CMB-C2B-C3B	2.78	129.89	124.68
26	d	412	SQD	O48-C23-C24	2.77	120.61	111.91
22	c	515	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	D	406	CLA	CMB-C2B-C3B	2.76	129.84	124.68
22	B	604	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	b	606	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	C	514	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
22	B	615	CLA	CMB-C2B-C3B	2.75	129.82	124.68
22	C	517	CLA	CHB-C4A-NA	2.75	128.31	124.51
22	c	518	CLA	CHB-C4A-NA	2.75	128.31	124.51
22	b	617	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	B	607	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	A	407	CLA	CHB-C4A-NA	2.74	128.29	124.51
22	B	613	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
22	B	604	CLA	C4-C3-C5	2.74	119.87	115.27
22	c	506	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
26	a	411	SQD	O48-C23-C24	2.72	120.45	111.91
22	C	507	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
22	B	606	CLA	CHB-C4A-NA	2.72	128.27	124.51
36	v	201	HEM	CBD-CAD-C3D	-2.72	105.08	112.63
22	B	604	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	C	510	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
25	a	410	PL9	C36-C34-C33	-2.71	115.63	121.12
22	c	509	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
22	B	610	CLA	CAA-CBA-CGA	-2.70	105.36	113.25
22	b	612	CLA	CAA-CBA-CGA	-2.70	105.36	113.25
22	c	517	CLA	CHB-C4A-NA	2.70	128.24	124.51
22	b	616	CLA	CHB-C4A-NA	2.70	128.24	124.51
22	B	601	CLA	CMB-C2B-C3B	2.69	129.72	124.68
22	D	401	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	C	516	CLA	CMB-C2B-C3B	2.69	129.71	124.68
22	B	615	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	c	511	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
22	b	615	CLA	O2D-CGD-O1D	-2.69	118.58	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	401	CLA	CHB-C4A-NA	2.69	128.23	124.51
36	V	201	HEM	CBD-CAD-C3D	-2.69	105.17	112.63
22	b	617	CLA	CHB-C4A-NA	2.68	128.22	124.51
33	f	102	LMT	C1B-O5B-C5B	2.68	118.96	113.69
22	b	612	CLA	CAA-C2A-C3A	-2.68	105.43	112.78
22	C	508	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
22	c	517	CLA	CMB-C2B-C3B	2.68	129.69	124.68
22	B	610	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
22	b	606	CLA	C4-C3-C5	2.68	119.78	115.27
22	D	405	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
22	B	614	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	a	408	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	b	614	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	c	518	CLA	CHD-C1D-ND	-2.67	122.00	124.45
22	B	608	CLA	CHB-C4A-NA	2.67	128.20	124.51
36	V	201	HEM	C4D-ND-C1D	2.67	107.83	105.07
22	B	612	CLA	CHB-C4A-NA	2.67	128.20	124.51
22	d	404	CLA	CMB-C2B-C3B	2.66	129.66	124.68
26	A	415	SQD	O8-S-C6	2.66	109.98	105.74
26	a	411	SQD	O7-S-C6	2.66	110.10	106.94
25	d	402	PL9	C27-C28-C29	-2.66	121.26	127.66
26	b	601	SQD	O8-S-C6	2.66	109.97	105.74
22	b	606	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
24	b	620	BCR	C2-C1-C6	2.65	114.56	110.48
26	A	410	SQD	O48-C23-C24	2.65	120.22	111.91
22	D	406	CLA	CHB-C4A-NA	2.65	128.17	124.51
22	c	507	CLA	CHB-C4A-NA	2.64	128.17	124.51
22	b	610	CLA	CHB-C4A-NA	2.64	128.17	124.51
25	D	404	PL9	C27-C28-C29	-2.64	121.30	127.66
22	b	603	CLA	CMB-C2B-C3B	2.64	129.61	124.68
22	c	511	CLA	CHB-C4A-NA	2.63	128.15	124.51
33	C	518	LMT	C1'-O5'-C5'	2.63	118.84	113.69
26	a	417	SQD	O48-C23-C24	2.62	120.14	111.91
22	d	404	CLA	CHB-C4A-NA	2.62	128.14	124.51
22	C	517	CLA	CHD-C1D-ND	-2.62	122.04	124.45
22	C	508	CLA	CHB-C4A-NA	2.62	128.13	124.51
36	V	201	HEM	CMC-C2C-C3C	2.61	129.57	124.68
22	c	509	CLA	CHB-C4A-NA	2.61	128.12	124.51
24	B	619	BCR	C2-C1-C6	2.61	114.50	110.48
26	A	415	SQD	O5-C5-C4	2.61	114.43	109.69
22	d	403	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
22	C	506	CLA	CHB-C4A-NA	2.60	128.11	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	510	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	B	607	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	B	605	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	b	603	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	A	409	PL9	C7-C8-C9	-2.59	122.49	126.79
22	b	609	CLA	CHB-C4A-NA	2.58	128.09	124.51
22	b	607	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	C	510	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
22	b	611	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
22	B	601	CLA	CHB-C4A-NA	2.58	128.07	124.51
22	B	605	CLA	CHD-C1D-ND	-2.57	122.09	124.45
36	v	201	HEM	C4D-ND-C1D	2.57	107.73	105.07
22	b	612	CLA	CHB-C4A-NA	2.57	128.07	124.51
36	v	201	HEM	CMC-C2C-C3C	2.57	129.49	124.68
25	a	410	PL9	C7-C8-C9	-2.57	122.52	126.79
22	B	603	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
22	B	609	CLA	CHB-C4A-NA	2.56	128.05	124.51
35	y	101	LMG	C7-O1-C1	2.56	118.74	113.74
22	a	406	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	C	505	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	A	404	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
22	a	408	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
33	Z	101	LMT	C1'-O5'-C5'	2.55	118.70	113.69
22	a	405	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
22	b	611	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	A	407	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
22	B	602	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	B	610	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	b	605	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
22	B	605	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
22	b	607	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
26	D	412	SQD	C1-O5-C5	2.54	118.67	113.69
22	b	604	CLA	CHB-C4A-NA	2.53	128.02	124.51
22	A	405	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	d	401	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
22	b	613	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	B	609	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	D	401	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
22	B	607	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
22	b	609	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
25	D	404	PL9	C22-C23-C24	-2.52	121.58	127.66
22	B	616	CLA	CHB-C4A-NA	2.52	128.00	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	513	CLA	CHB-C4A-NA	2.52	128.00	124.51
25	d	402	PL9	C22-C23-C24	-2.51	121.61	127.66
26	a	417	SQD	O5-C5-C4	2.51	114.26	109.69
22	b	607	CLA	CHD-C1D-ND	-2.51	122.14	124.45
22	B	610	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
23	a	407	PHO	C1B-NB-C4B	2.51	112.24	107.09
22	C	517	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
26	b	601	SQD	O48-C23-C24	2.50	119.76	111.91
26	d	412	SQD	O8-S-C6	2.50	109.72	105.74
22	b	612	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
22	B	606	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
36	V	201	HEM	CMB-C2B-C1B	-2.50	121.24	125.04
22	c	518	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
22	B	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	c	512	CLA	O2D-CGD-CBD	2.49	115.70	111.27
22	c	511	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
25	A	409	PL9	C22-C23-C24	-2.49	121.67	127.66
24	b	602	BCR	C19-C18-C17	-2.49	115.12	118.94
26	b	601	SQD	C4-C3-C2	2.49	115.17	110.82
26	l	102	SQD	O48-C23-C24	2.49	119.71	111.91
23	A	406	PHO	C1B-NB-C4B	2.48	112.19	107.09
22	c	508	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	C	507	CLA	CHB-C4A-NA	2.48	127.94	124.51
24	b	602	BCR	C16-C17-C18	2.48	130.85	127.31
22	C	508	CLA	CHD-C1D-ND	-2.48	122.18	124.45
22	C	508	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
33	f	102	LMT	C1-O1'-C1'	2.48	117.94	113.84
22	c	513	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
34	c	503	DGD	C6D-O5D-C1E	2.47	118.56	113.74
22	a	408	CLA	O2D-CGD-CBD	2.46	115.65	111.27
22	b	618	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	A	404	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	A	409	PL9	C27-C28-C29	-2.46	121.73	127.66
26	D	412	SQD	O5-C1-C2	2.46	115.56	110.35
33	Z	101	LMT	C1'-C2'-C3'	-2.46	104.87	110.00
22	d	404	CLA	O2D-CGD-CBD	2.46	115.64	111.27
22	b	604	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
23	a	420	PHO	C1B-NB-C4B	2.45	112.13	107.09
22	c	509	CLA	C1B-CHB-C4A	-2.45	125.25	130.12
22	C	512	CLA	CHB-C4A-NA	2.45	127.91	124.51
22	A	405	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
22	A	407	CLA	O2D-CGD-CBD	2.45	115.62	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
35	y	101	LMG	C4-C3-C2	2.45	115.09	110.82
22	a	406	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
26	a	411	SQD	C1-O5-C5	2.44	118.47	113.69
22	B	611	CLA	CHD-C1D-ND	-2.44	122.21	124.45
25	a	410	PL9	C22-C23-C24	-2.44	121.79	127.66
22	b	613	CLA	CHD-C1D-ND	-2.43	122.22	124.45
22	C	516	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	D	403	PHO	C4A-C3A-C2A	-2.43	100.53	102.84
26	d	412	SQD	C1-O5-C5	2.43	118.46	113.69
22	B	614	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	C	512	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	c	510	CLA	CHB-C4A-NA	2.43	127.87	124.51
34	c	504	DGD	C3G-O3G-C1D	2.43	118.48	113.74
22	a	405	CLA	CHB-C4A-NA	2.42	127.86	124.51
33	z	101	LMT	C1'-O5'-C5'	2.42	118.44	113.69
22	c	506	CLA	CHB-C4A-NA	2.42	127.86	124.51
24	f	101	BCR	C23-C22-C21	-2.42	115.23	118.94
22	B	613	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	b	615	CLA	CHB-C4A-NA	2.42	127.86	124.51
34	C	503	DGD	C6D-O5D-C1E	2.41	118.46	113.74
25	D	404	PL9	O1-C4-C3	-2.41	118.06	120.72
22	C	512	CLA	O2D-CGD-CBD	2.41	115.56	111.27
25	d	402	PL9	O1-C4-C3	-2.41	118.06	120.72
26	D	412	SQD	C3-C4-C5	2.41	114.54	110.24
22	C	511	CLA	O2D-CGD-CBD	2.41	115.55	111.27
22	c	517	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
22	B	614	CLA	CHD-C1D-ND	-2.40	122.25	124.45
22	c	510	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
26	b	601	SQD	C3-C4-C5	2.40	114.51	110.24
22	D	401	CLA	CHD-C1D-ND	-2.40	122.25	124.45
24	B	632	BCR	C19-C18-C17	-2.39	115.27	118.94
22	C	509	CLA	CHB-C4A-NA	2.39	127.82	124.51
22	b	616	CLA	CHD-C1D-ND	-2.39	122.26	124.45
22	c	509	CLA	CHD-C1D-ND	-2.38	122.26	124.45
22	c	514	CLA	C16-C15-C13	-2.38	108.22	115.92
36	v	201	HEM	CMB-C2B-C1B	-2.38	121.41	125.04
22	A	405	CLA	O2D-CGD-CBD	2.38	115.50	111.27
23	D	403	PHO	C1B-NB-C4B	2.38	111.98	107.09
22	B	604	CLA	C1-C2-C3	-2.38	121.93	126.04
22	C	509	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
22	c	513	CLA	O2D-CGD-CBD	2.37	115.49	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	BCR	C7-C8-C9	-2.37	122.65	126.23
36	E	104	HEM	C1B-NB-C4B	2.37	107.52	105.07
22	b	608	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	a	406	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
22	d	404	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
22	b	616	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
24	c	502	BCR	C7-C8-C9	-2.36	122.67	126.23
22	b	614	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
36	e	103	HEM	C1B-NB-C4B	2.36	107.51	105.07
30	a	419	BCT	O3-C-O1	-2.35	113.44	119.55
24	k	101	BCR	C11-C10-C9	2.35	130.67	127.31
23	a	420	PHO	C4A-C3A-C2A	-2.35	100.60	102.84
36	V	201	HEM	C3B-C2B-C1B	2.35	108.23	106.49
22	c	506	CLA	CMB-C2B-C3B	2.35	129.07	124.68
22	a	406	CLA	O2D-CGD-CBD	2.35	115.44	111.27
22	c	512	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
25	A	409	PL9	C37-C38-C39	-2.35	122.01	127.66
30	A	416	BCT	O3-C-O1	-2.34	113.47	119.55
22	B	612	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	C	511	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	B	613	CLA	O1D-CGD-CBD	2.34	129.26	124.48
26	l	102	SQD	C3-C4-C5	2.34	114.41	110.24
22	d	401	CLA	CHD-C1D-ND	-2.33	122.31	124.45
22	B	608	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	c	515	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	B	604	CLA	CMB-C2B-C3B	2.33	129.04	124.68
22	A	405	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
22	b	610	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
25	d	402	PL9	C20-C19-C21	2.33	119.18	115.27
36	V	201	HEM	C3D-C4D-ND	-2.32	107.58	110.17
22	d	404	CLA	CHD-C1D-ND	-2.32	122.32	124.45
33	C	518	LMT	C1-O1'-C1'	2.32	117.68	113.84
22	C	514	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	C	513	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
25	a	410	PL9	C27-C28-C29	-2.31	122.09	127.66
22	c	514	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
22	B	608	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
36	v	201	HEM	C3D-C4D-ND	-2.31	107.60	110.17
22	c	506	CLA	CHD-C1D-ND	-2.31	122.33	124.45
22	b	615	CLA	O1D-CGD-CBD	2.31	129.20	124.48
24	F	101	BCR	C24-C23-C22	-2.30	122.75	126.23
22	B	606	CLA	O2D-CGD-CBD	2.30	115.36	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	412	SQD	O5-C1-C2	2.30	115.21	110.35
22	b	611	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
22	B	609	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
22	b	609	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	B	607	CLA	CHD-C1D-ND	-2.29	122.35	124.45
25	D	404	PL9	C20-C19-C21	2.29	119.12	115.27
22	D	406	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
26	l	102	SQD	C1-O5-C5	-2.28	109.21	113.69
22	A	404	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
24	c	501	BCR	C24-C23-C22	-2.28	122.79	126.23
22	D	406	CLA	O2D-CGD-CBD	2.28	115.32	111.27
33	i	102	LMT	C1'-O5'-C5'	2.28	118.16	113.69
22	d	403	CLA	CHB-C4A-NA	2.28	127.66	124.51
22	a	405	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	b	604	CLA	O2D-CGD-CBD	2.27	115.31	111.27
22	C	514	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
33	Z	101	LMT	C3'-C4'-C5'	-2.27	105.72	110.93
22	D	405	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	C	505	CLA	CHD-C1D-ND	-2.27	122.37	124.45
22	c	508	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
22	B	601	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
22	B	602	CLA	O2D-CGD-CBD	2.26	115.29	111.27
22	c	515	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
22	b	606	CLA	CMB-C2B-C3B	2.26	128.91	124.68
22	b	610	CLA	CHD-C1D-ND	-2.26	122.38	124.45
22	d	403	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
22	b	603	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
22	C	507	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
22	B	611	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
33	J	103	LMT	C1'-O5'-C5'	2.25	118.11	113.69
22	b	605	CLA	CHB-C4A-NA	2.25	127.62	124.51
22	B	603	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
22	c	513	CLA	CHD-C1D-ND	-2.25	122.39	124.45
22	D	405	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
22	B	603	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	b	613	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
22	D	406	CLA	C1-C2-C3	-2.24	122.17	126.04
22	b	605	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
22	C	512	CLA	CHD-C1D-ND	-2.23	122.40	124.45
35	C	525	LMG	C1-O6-C5	2.23	118.07	113.69
34	C	504	DGD	C3G-O3G-C1D	2.23	118.10	113.74
22	b	610	CLA	O2A-CGA-O1A	-2.23	117.96	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	512	CLA	C2A-C1A-CHA	2.23	127.76	123.86
22	B	615	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
22	B	616	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
26	a	417	SQD	C3-C4-C5	2.23	114.21	110.24
22	D	406	CLA	CHD-C1D-ND	-2.23	122.41	124.45
22	C	507	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
22	B	608	CLA	CHD-C1D-ND	-2.22	122.41	124.45
22	b	607	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	c	508	CLA	CHD-C1D-ND	-2.22	122.42	124.45
22	C	507	CLA	CHD-C1D-ND	-2.22	122.42	124.45
26	A	415	SQD	C3-C4-C5	2.22	114.19	110.24
34	J	102	DGD	O2E-C2E-C1E	2.22	115.43	110.05
25	a	410	PL9	C37-C38-C39	-2.21	122.33	127.66
22	b	618	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
22	B	606	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
27	C	522	PLM	O2-C1-C2	-2.20	116.02	123.08
22	C	517	CLA	CAA-C2A-C3A	-2.20	106.77	112.78
36	v	201	HEM	C4C-CHD-C1D	2.20	125.45	122.56
26	d	412	SQD	C3-C4-C5	2.19	114.15	110.24
22	B	605	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
22	B	604	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
24	f	101	BCR	C29-C30-C25	2.18	113.84	110.48
23	A	406	PHO	CMB-C2B-C3B	2.18	128.76	124.68
22	b	617	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
22	B	611	CLA	O2D-CGD-CBD	2.17	115.13	111.27
23	a	407	PHO	CMB-C2B-C3B	2.17	128.74	124.68
34	c	505	DGD	C6D-O5D-C1E	2.17	117.98	113.74
22	c	507	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
22	C	506	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
26	a	411	SQD	O5-C1-C2	2.17	114.94	110.35
24	b	619	BCR	C29-C30-C25	2.17	113.82	110.48
22	b	606	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
22	A	404	CLA	C2D-C1D-ND	-2.16	108.51	110.10
25	d	402	PL9	C32-C33-C34	-2.16	122.45	127.66
25	A	409	PL9	C32-C33-C34	-2.16	122.45	127.66
22	C	511	CLA	C2A-C1A-CHA	2.16	127.64	123.86
22	c	514	CLA	C11-C12-C13	-2.16	108.93	115.92
33	i	102	LMT	O1B-C4'-C3'	2.16	113.02	107.28
36	v	201	HEM	C3B-C2B-C1B	2.16	108.08	106.49
22	C	515	CLA	C2A-C1A-CHA	2.15	127.63	123.86
25	D	404	PL9	C32-C33-C34	-2.15	122.48	127.66
33	i	102	LMT	C1B-C2B-C3B	2.15	114.47	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	608	CLA	O2D-CGD-CBD	2.15	115.09	111.27
22	B	613	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
22	d	404	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
22	c	510	CLA	O2D-CGD-CBD	2.14	115.08	111.27
24	f	101	BCR	C20-C21-C22	2.14	130.37	127.31
22	a	405	CLA	C2D-C1D-ND	-2.14	108.53	110.10
22	b	615	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
22	C	510	CLA	C1-C2-C3	-2.14	122.34	126.04
22	A	407	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
22	A	407	CLA	CHD-C1D-ND	-2.14	122.49	124.45
22	c	517	CLA	C11-C12-C13	-2.14	109.02	115.92
22	c	508	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
24	c	502	BCR	C38-C26-C27	-2.13	109.52	113.62
22	C	510	CLA	CHD-C1D-ND	-2.13	122.50	124.45
24	C	502	BCR	C38-C26-C27	-2.13	109.53	113.62
36	V	201	HEM	C4C-CHD-C1D	2.12	125.36	122.56
22	C	514	CLA	CHD-C1D-ND	-2.12	122.51	124.45
24	Y	102	BCR	C20-C21-C22	2.12	130.34	127.31
22	B	606	CLA	CHD-C1D-ND	-2.12	122.51	124.45
22	a	408	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
25	D	404	PL9	O2-C1-C2	-2.12	116.93	121.78
25	A	409	PL9	C25-C24-C26	2.11	118.83	115.27
22	B	613	CLA	CHD-C1D-ND	-2.11	122.51	124.45
22	A	405	CLA	CHD-C1D-ND	-2.11	122.51	124.45
22	b	606	CLA	C1-C2-C3	-2.11	122.39	126.04
22	D	406	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	C	509	CLA	O2D-CGD-CBD	2.11	115.02	111.27
22	C	505	CLA	CMB-C2B-C1B	-2.11	125.22	128.46
22	C	515	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
22	b	606	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
22	a	406	CLA	CHD-C1D-ND	-2.11	122.52	124.45
22	c	511	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
25	A	409	PL9	O1-C4-C3	-2.10	118.40	120.72
22	a	408	CLA	CHD-C1D-ND	-2.10	122.52	124.45
22	B	611	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
33	m	102	LMT	C1-O1'-C1'	2.10	117.32	113.84
25	d	402	PL9	O2-C1-C2	-2.10	116.97	121.78
22	c	516	CLA	CHD-C1D-ND	-2.10	122.53	124.45
22	c	517	CLA	O2D-CGD-CBD	2.09	114.99	111.27
22	b	608	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	b	615	CLA	CHD-C1D-ND	-2.09	122.53	124.45
22	b	613	CLA	O2A-CGA-O1A	-2.09	118.32	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	516	CLA	O2D-CGD-CBD	2.09	114.98	111.27
22	B	609	CLA	CHD-C1D-ND	-2.08	122.54	124.45
25	a	410	PL9	C26-C24-C23	-2.08	116.90	121.12
25	d	402	PL9	C36-C34-C33	-2.08	116.90	121.12
22	b	611	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	D	401	CLA	O2D-CGD-CBD	2.08	114.96	111.27
22	B	604	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
22	b	606	CLA	C16-C15-C13	-2.07	109.21	115.92
33	C	518	LMT	O1B-C4'-C3'	2.07	112.80	107.28
25	D	404	PL9	C37-C38-C39	-2.07	122.67	127.66
25	D	404	PL9	O2-C1-C6	2.07	124.17	120.59
22	B	612	CLA	O2D-CGD-CBD	2.07	114.94	111.27
36	v	201	HEM	C4A-C3A-C2A	2.07	108.43	107.00
22	c	516	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
25	d	402	PL9	O2-C1-C6	2.07	124.17	120.59
22	C	512	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
24	B	632	BCR	C16-C17-C18	2.06	130.25	127.31
22	b	614	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
22	C	515	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	c	506	CLA	C1-C2-C3	-2.06	122.48	126.04
24	y	102	BCR	C20-C21-C22	2.06	130.25	127.31
25	d	402	PL9	C37-C38-C39	-2.06	122.70	127.66
22	c	515	CLA	CHD-C1D-ND	-2.06	122.56	124.45
36	E	104	HEM	CMB-C2B-C1B	-2.06	121.90	125.04
25	A	409	PL9	C26-C24-C23	-2.06	116.95	121.12
25	a	410	PL9	O1-C4-C3	-2.06	118.45	120.72
36	e	103	HEM	CMB-C2B-C1B	-2.06	121.91	125.04
22	c	516	CLA	C2A-C1A-CHA	2.06	127.46	123.86
33	i	102	LMT	O5B-C5B-C4B	2.06	113.43	109.69
22	B	604	CLA	C16-C15-C13	-2.05	109.28	115.92
22	C	510	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	a	410	PL9	O2-C1-C2	-2.05	117.08	121.78
22	c	511	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	B	612	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
33	z	101	LMT	C1'-C2'-C3'	-2.04	105.74	110.00
22	B	603	CLA	C2D-C1D-ND	-2.04	108.60	110.10
34	C	504	DGD	C4D-C3D-C2D	2.04	114.38	110.82
25	a	410	PL9	C20-C19-C21	2.04	118.70	115.27
22	b	606	CLA	C11-C12-C13	-2.04	109.33	115.92
22	B	615	CLA	C2A-C1A-CHA	2.03	127.42	123.86
25	A	409	PL9	C31-C32-C33	-2.03	105.20	111.88
22	B	615	CLA	O2A-CGA-O1A	-2.03	118.46	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	604	CLA	C2A-C1A-CHA	2.03	127.41	123.86
22	c	514	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	B	608	CLA	O2D-CGD-CBD	2.03	114.88	111.27
26	A	415	SQD	C44-O6-C1	-2.03	109.77	113.74
22	c	513	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
34	C	504	DGD	O6E-C1E-O5D	2.03	114.77	109.97
23	A	406	PHO	CMC-C2C-C3C	2.02	128.76	124.94
24	B	632	BCR	C2-C3-C4	2.02	115.90	111.38
22	C	510	CLA	O1D-CGD-CBD	2.02	128.62	124.48
33	z	101	LMT	C3'-C4'-C5'	-2.02	106.29	110.93
24	F	101	BCR	C23-C22-C21	-2.02	115.84	118.94
22	c	511	CLA	C1-C2-C3	-2.02	122.55	126.04
22	b	614	CLA	O2D-CGD-CBD	2.02	114.86	111.27
22	b	603	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	b	617	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	c	511	CLA	O1D-CGD-CBD	2.02	128.61	124.48
22	b	617	CLA	C2A-C1A-CHA	2.01	127.38	123.86
22	b	606	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
22	B	601	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
27	D	402	PLM	O2-C1-C2	-2.01	116.62	123.08
25	D	404	PL9	C36-C34-C33	-2.01	117.05	121.12
22	D	401	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
22	b	610	CLA	O2D-CGD-CBD	2.01	114.84	111.27
23	a	407	PHO	CMC-C2C-C3C	2.01	128.73	124.94
22	b	618	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
22	B	604	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
22	C	513	CLA	CHD-C1D-ND	-2.00	122.61	124.45
25	A	409	PL9	O2-C1-C2	-2.00	117.20	121.78

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	404	CLA	ND
22	A	405	CLA	ND
22	A	407	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	608	CLA	ND
22	B	609	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	508	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	C	513	CLA	ND
22	C	514	CLA	ND
22	C	515	CLA	ND
22	C	516	CLA	ND
22	C	517	CLA	ND
22	D	401	CLA	ND
22	D	405	CLA	ND
22	D	406	CLA	ND
22	a	405	CLA	ND
22	a	406	CLA	ND
22	a	408	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	607	CLA	ND
22	b	608	CLA	ND
22	b	609	CLA	ND
22	b	610	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	617	CLA	ND
22	b	618	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	508	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND
22	c	514	CLA	ND
22	c	515	CLA	ND
22	c	516	CLA	ND
22	c	517	CLA	ND
22	c	518	CLA	ND
22	d	401	CLA	ND
22	d	403	CLA	ND
22	d	404	CLA	ND

All (1911) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	404	CLA	CBD-CGD-O2D-CED
22	A	405	CLA	CHA-CBD-CGD-O1D
22	B	601	CLA	CHA-CBD-CGD-O1D
22	B	601	CLA	CHA-CBD-CGD-O2D
22	B	602	CLA	CHA-CBD-CGD-O1D
22	B	602	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	C2-C3-C5-C6
22	B	603	CLA	C4-C3-C5-C6
22	B	604	CLA	C4-C3-C5-C6
22	B	614	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	C	512	CLA	CHA-CBD-CGD-O1D
22	C	512	CLA	CHA-CBD-CGD-O2D
22	D	401	CLA	CHA-CBD-CGD-O1D
22	D	401	CLA	CHA-CBD-CGD-O2D
22	a	405	CLA	CBD-CGD-O2D-CED
22	a	406	CLA	CHA-CBD-CGD-O1D
22	a	406	CLA	CHA-CBD-CGD-O2D
22	b	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	b	603	CLA	CHA-CBD-CGD-O2D
22	b	604	CLA	CHA-CBD-CGD-O1D
22	b	604	CLA	CHA-CBD-CGD-O2D
22	b	605	CLA	C2-C3-C5-C6
22	b	605	CLA	C4-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6
22	b	607	CLA	C2-C3-C5-C6
22	b	607	CLA	C4-C3-C5-C6
22	b	616	CLA	CHA-CBD-CGD-O1D
22	b	616	CLA	CHA-CBD-CGD-O2D
22	b	616	CLA	CAD-CBD-CGD-O1D
22	b	616	CLA	CAD-CBD-CGD-O2D
22	c	508	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	CHA-CBD-CGD-O1D
22	c	513	CLA	CHA-CBD-CGD-O2D
22	d	401	CLA	CHA-CBD-CGD-O1D
22	d	401	CLA	CHA-CBD-CGD-O2D
24	B	617	BCR	C1-C6-C7-C8
24	B	619	BCR	C37-C22-C23-C24
24	C	501	BCR	C7-C8-C9-C10
24	C	501	BCR	C7-C8-C9-C34
24	C	502	BCR	C7-C8-C9-C10
24	C	502	BCR	C7-C8-C9-C34
24	C	502	BCR	C23-C24-C25-C26
24	F	101	BCR	C1-C6-C7-C8
24	F	101	BCR	C7-C8-C9-C10
24	F	101	BCR	C7-C8-C9-C34
24	F	101	BCR	C23-C24-C25-C26
24	T	103	BCR	C1-C6-C7-C8
24	Y	102	BCR	C5-C6-C7-C8
24	Y	102	BCR	C17-C18-C19-C20
24	Y	102	BCR	C36-C18-C19-C20
24	Y	102	BCR	C21-C22-C23-C24
24	Y	102	BCR	C37-C22-C23-C24
24	b	602	BCR	C13-C14-C15-C16
24	b	620	BCR	C21-C22-C23-C24
24	b	620	BCR	C37-C22-C23-C24
24	c	501	BCR	C7-C8-C9-C10
24	c	501	BCR	C7-C8-C9-C34
24	c	502	BCR	C7-C8-C9-C10
24	c	502	BCR	C7-C8-C9-C34
24	c	502	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	f	101	BCR	C1-C6-C7-C8
24	f	101	BCR	C7-C8-C9-C10
24	f	101	BCR	C7-C8-C9-C34
24	f	101	BCR	C23-C24-C25-C26
24	k	101	BCR	C9-C10-C11-C12
24	k	101	BCR	C11-C12-C13-C14
24	k	101	BCR	C11-C12-C13-C35
24	k	101	BCR	C21-C22-C23-C24
24	k	101	BCR	C37-C22-C23-C24
24	y	102	BCR	C5-C6-C7-C8
24	y	102	BCR	C17-C18-C19-C20
24	y	102	BCR	C36-C18-C19-C20
24	y	102	BCR	C21-C22-C23-C24
24	y	102	BCR	C37-C22-C23-C24
25	A	409	PL9	C7-C8-C9-C10
25	A	409	PL9	C7-C8-C9-C11
25	A	409	PL9	C17-C18-C19-C20
25	A	409	PL9	C32-C33-C34-C35
25	A	409	PL9	C33-C34-C36-C37
25	A	409	PL9	C34-C36-C37-C38
25	A	409	PL9	C37-C38-C39-C41
25	D	404	PL9	C24-C26-C27-C28
25	D	404	PL9	C27-C28-C29-C30
25	D	404	PL9	C27-C28-C29-C31
25	D	404	PL9	C32-C33-C34-C35
25	D	404	PL9	C44-C46-C47-C48
25	a	410	PL9	C7-C8-C9-C10
25	a	410	PL9	C7-C8-C9-C11
25	a	410	PL9	C12-C13-C14-C15
25	a	410	PL9	C12-C13-C14-C16
25	a	410	PL9	C17-C18-C19-C20
25	a	410	PL9	C25-C24-C26-C27
25	a	410	PL9	C24-C26-C27-C28
25	a	410	PL9	C32-C33-C34-C35
25	a	410	PL9	C37-C38-C39-C41
25	d	402	PL9	C24-C26-C27-C28
25	d	402	PL9	C27-C28-C29-C30
25	d	402	PL9	C27-C28-C29-C31
25	d	402	PL9	C32-C33-C34-C35
25	d	402	PL9	C44-C46-C47-C48
26	A	410	SQD	C5-C6-S-O7
26	A	410	SQD	C5-C6-S-O8

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Mol	Chain	Res	Type	Atoms
26	A	415	SQD	O6-C44-C45-O47
26	A	415	SQD	O10-C23-O48-C46
26	A	415	SQD	C24-C23-O48-C46
26	D	412	SQD	O6-C44-C45-O47
26	a	417	SQD	O10-C23-O48-C46
26	a	417	SQD	C24-C23-O48-C46
26	b	601	SQD	O49-C7-O47-C45
26	b	601	SQD	C5-C6-S-O7
26	b	601	SQD	C5-C6-S-O8
26	d	412	SQD	O6-C44-C45-O47
26	l	102	SQD	O49-C7-O47-C45
26	l	102	SQD	C8-C7-O47-C45
26	l	102	SQD	O5-C5-C6-S
31	D	407	LHG	C1-C2-C3-O3
31	D	407	LHG	O2-C2-C3-O3
31	D	407	LHG	C8-C7-O7-C5
31	D	408	LHG	O1-C1-C2-C3
31	D	408	LHG	C4-O6-P-O4
31	E	101	LHG	C3-O3-P-O4
31	E	101	LHG	C4-O6-P-O4
31	E	101	LHG	C4-O6-P-O5
31	L	101	LHG	C3-O3-P-O4
31	L	101	LHG	C4-O6-P-O4
31	a	415	LHG	C3-O3-P-O4
31	a	415	LHG	C3-O3-P-O5
31	a	415	LHG	C4-O6-P-O3
31	d	405	LHG	C1-C2-C3-O3
31	d	405	LHG	O2-C2-C3-O3
31	d	405	LHG	C8-C7-O7-C5
31	d	406	LHG	O1-C1-C2-C3
31	d	406	LHG	C4-O6-P-O4
31	l	101	LHG	C3-O3-P-O4
31	l	101	LHG	C4-O6-P-O4
32	a	401	GOL	O1-C1-C2-C3
33	B	633	LMT	C2'-C1'-O1'-C1
33	B	633	LMT	O5'-C1'-O1'-C1
33	J	103	LMT	C2'-C1'-O1'-C1
33	J	103	LMT	O5'-C1'-O1'-C1
33	J	103	LMT	C2-C1-O1'-C1'
33	M	102	LMT	C2-C1-O1'-C1'
33	T	101	LMT	O5'-C1'-O1'-C1
33	T	104	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
33	Z	101	LMT	C2'-C1'-O1'-C1
33	Z	101	LMT	O5'-C1'-O1'-C1
33	Z	101	LMT	C2-C1-O1'-C1'
33	b	626	LMT	O5'-C1'-O1'-C1
33	b	626	LMT	C2-C1-O1'-C1'
33	j	101	LMT	C2'-C1'-O1'-C1
33	j	101	LMT	O5'-C1'-O1'-C1
33	z	101	LMT	C2'-C1'-O1'-C1
33	z	101	LMT	O5'-C1'-O1'-C1
33	z	101	LMT	C2-C1-O1'-C1'
34	C	503	DGD	O2G-C2G-C3G-O3G
34	C	504	DGD	C2D-C1D-O3G-C3G
34	C	504	DGD	O6D-C1D-O3G-C3G
34	C	504	DGD	C2E-C1E-O5D-C6D
34	C	504	DGD	O6E-C1E-O5D-C6D
34	D	411	DGD	C2B-C1B-O2G-C2G
34	D	411	DGD	O1G-C1G-C2G-O2G
34	D	411	DGD	O6D-C1D-O3G-C3G
34	J	102	DGD	O2G-C2G-C3G-O3G
34	c	503	DGD	O2G-C2G-C3G-O3G
34	c	504	DGD	O1G-C1G-C2G-O2G
34	c	504	DGD	O6D-C1D-O3G-C3G
34	c	504	DGD	C2E-C1E-O5D-C6D
34	c	504	DGD	O6E-C1E-O5D-C6D
34	d	410	DGD	C2B-C1B-O2G-C2G
35	Y	101	LMG	O6-C1-O1-C7
35	c	524	LMG	O6-C1-O1-C7
22	c	508	CLA	O1D-CGD-O2D-CED
31	a	415	LHG	O10-C23-O8-C6
22	C	515	CLA	CBD-CGD-O2D-CED
22	b	612	CLA	CBD-CGD-O2D-CED
22	c	516	CLA	CBD-CGD-O2D-CED
26	b	601	SQD	O10-C23-O48-C46
34	J	102	DGD	O1A-C1A-O1G-C1G
35	C	525	LMG	O10-C28-O8-C9
35	c	519	LMG	O10-C28-O8-C9
22	A	404	CLA	O1D-CGD-O2D-CED
22	a	405	CLA	O1D-CGD-O2D-CED
34	C	504	DGD	O6D-C5D-C6D-O5D
22	B	610	CLA	CBD-CGD-O2D-CED
22	B	614	CLA	CBD-CGD-O2D-CED
22	b	616	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	D	407	LHG	O9-C7-O7-C5
31	d	405	LHG	O9-C7-O7-C5
34	D	411	DGD	O1B-C1B-O2G-C2G
34	d	410	DGD	O1B-C1B-O2G-C2G
22	B	614	CLA	C3-C5-C6-C7
22	b	616	CLA	C3-C5-C6-C7
31	a	415	LHG	C24-C23-O8-C6
34	J	102	DGD	C2A-C1A-O1G-C1G
35	C	519	LMG	C29-C28-O8-C9
35	C	525	LMG	C29-C28-O8-C9
33	i	102	LMT	O5B-C5B-C6B-O6B
26	b	601	SQD	C8-C7-O47-C45
25	a	410	PL9	C47-C48-C49-C50
22	b	611	CLA	CBD-CGD-O2D-CED
34	c	504	DGD	O6D-C5D-C6D-O5D
33	C	518	LMT	O5B-C5B-C6B-O6B
34	C	504	DGD	O6E-C5E-C6E-O5E
34	C	504	DGD	C4D-C5D-C6D-O5D
34	c	504	DGD	C4D-C5D-C6D-O5D
22	B	605	CLA	C4-C3-C5-C6
22	B	604	CLA	C2-C3-C5-C6
22	B	605	CLA	C2-C3-C5-C6
22	b	606	CLA	C2-C3-C5-C6
22	c	517	CLA	O1A-CGA-O2A-C1
22	b	603	CLA	C3-C5-C6-C7
22	c	517	CLA	CBA-CGA-O2A-C1
26	b	601	SQD	C24-C23-O48-C46
35	c	519	LMG	C29-C28-O8-C9
34	c	504	DGD	O6E-C5E-C6E-O5E
25	A	409	PL9	C37-C38-C39-C40
25	a	410	PL9	C37-C38-C39-C40
22	B	609	CLA	CBD-CGD-O2D-CED
33	T	101	LMT	C7-C8-C9-C10
33	j	101	LMT	C3-C4-C5-C6
26	d	412	SQD	O49-C7-O47-C45
25	A	409	PL9	C12-C13-C14-C16
25	A	409	PL9	C17-C18-C19-C21
25	A	409	PL9	C32-C33-C34-C36
25	D	404	PL9	C32-C33-C34-C36
25	a	410	PL9	C17-C18-C19-C21
25	a	410	PL9	C27-C28-C29-C31
25	a	410	PL9	C32-C33-C34-C36

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Mol	Chain	Res	Type	Atoms
25	d	402	PL9	C32-C33-C34-C36
35	C	519	LMG	O10-C28-O8-C9
24	B	632	BCR	C13-C14-C15-C16
35	Y	101	LMG	O6-C5-C6-O5
22	B	603	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	CBD-CGD-O2D-CED
22	B	601	CLA	C3-C5-C6-C7
33	i	102	LMT	C4B-C5B-C6B-O6B
26	d	412	SQD	C8-C7-O47-C45
22	B	607	CLA	CBD-CGD-O2D-CED
22	C	506	CLA	CBD-CGD-O2D-CED
22	b	605	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED
33	M	102	LMT	O5'-C5'-C6'-O6'
27	a	412	PLM	C8-C9-CA-CB
26	A	410	SQD	C16-C17-C18-C19
26	a	411	SQD	C16-C17-C18-C19
33	b	626	LMT	C5-C6-C7-C8
33	i	102	LMT	C3'-C4'-O1B-C1B
34	C	503	DGD	C4A-C5A-C6A-C7A
33	C	518	LMT	C3'-C4'-O1B-C1B
22	B	604	CLA	C3-C5-C6-C7
22	b	606	CLA	C3-C5-C6-C7
33	B	628	LMT	O5'-C5'-C6'-O6'
33	m	102	LMT	O5'-C5'-C6'-O6'
35	y	101	LMG	O6-C5-C6-O5
33	C	518	LMT	C4B-C5B-C6B-O6B
27	L	102	PLM	C4-C5-C6-C7
28	a	414	LFA	C9-C10-C11-C12
25	A	409	PL9	C47-C48-C49-C50
33	f	102	LMT	O5'-C5'-C6'-O6'
33	j	101	LMT	O5'-C5'-C6'-O6'
25	A	409	PL9	C15-C14-C16-C17
25	A	409	PL9	C25-C24-C26-C27
34	C	504	DGD	C4E-C5E-C6E-O5E
25	A	409	PL9	C13-C14-C16-C17
25	A	409	PL9	C23-C24-C26-C27
25	a	410	PL9	C23-C24-C26-C27
22	B	606	CLA	C2A-CAA-CBA-CGA
22	C	511	CLA	C2A-CAA-CBA-CGA
22	b	608	CLA	C2A-CAA-CBA-CGA
22	c	512	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	D	412	SQD	O5-C1-O6-C44
26	l	102	SQD	O5-C1-O6-C44
25	A	409	PL9	C44-C46-C47-C48
25	a	410	PL9	C9-C11-C12-C13
25	a	410	PL9	C19-C21-C22-C23
25	a	410	PL9	C44-C46-C47-C48
31	E	101	LHG	C13-C14-C15-C16
33	T	104	LMT	O5B-C5B-C6B-O6B
33	M	102	LMT	C4'-C5'-C6'-O6'
34	C	504	DGD	C2B-C1B-O2G-C2G
34	c	504	DGD	C2B-C1B-O2G-C2G
33	m	102	LMT	C4'-C5'-C6'-O6'
25	A	409	PL9	C12-C13-C14-C15
22	c	516	CLA	O1D-CGD-O2D-CED
34	d	410	DGD	C4A-C5A-C6A-C7A
25	A	409	PL9	C27-C28-C29-C31
33	C	518	LMT	C4'-C5'-C6'-O6'
33	f	102	LMT	C4'-C5'-C6'-O6'
34	c	504	DGD	C4E-C5E-C6E-O5E
22	C	516	CLA	CBA-CGA-O2A-C1
22	D	406	CLA	CBA-CGA-O2A-C1
22	c	510	CLA	CBA-CGA-O2A-C1
22	d	404	CLA	CBA-CGA-O2A-C1
26	l	102	SQD	C24-C23-O48-C46
35	y	101	LMG	C29-C28-O8-C9
33	J	103	LMT	C7-C8-C9-C10
35	y	101	LMG	O10-C28-O8-C9
33	j	101	LMT	C4'-C5'-C6'-O6'
31	E	101	LHG	O6-C4-C5-O7
34	D	411	DGD	C9B-CAB-CBB-CCB
34	J	102	DGD	O6D-C5D-C6D-O5D
22	B	613	CLA	C15-C16-C17-C18
31	E	101	LHG	C23-C24-C25-C26
35	c	524	LMG	C2-C1-O1-C7
35	y	101	LMG	C2-C1-O1-C7
26	a	417	SQD	O6-C44-C45-O47
26	l	102	SQD	O47-C45-C46-O48
22	B	601	CLA	C11-C10-C8-C9
22	B	601	CLA	C14-C13-C15-C16
22	C	506	CLA	C14-C13-C15-C16
22	C	513	CLA	C6-C7-C8-C9
22	b	603	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	603	CLA	C14-C13-C15-C16
22	c	514	CLA	C6-C7-C8-C9
22	c	517	CLA	C6-C7-C8-C9
22	A	407	CLA	C15-C16-C17-C18
24	B	617	BCR	C36-C18-C19-C20
24	B	632	BCR	C7-C8-C9-C34
24	B	632	BCR	C37-C22-C23-C24
24	C	502	BCR	C11-C12-C13-C35
24	C	502	BCR	C36-C18-C19-C20
24	T	103	BCR	C36-C18-C19-C20
24	b	602	BCR	C7-C8-C9-C34
24	c	502	BCR	C36-C18-C19-C20
24	B	619	BCR	C21-C22-C23-C24
24	B	632	BCR	C7-C8-C9-C10
24	b	602	BCR	C7-C8-C9-C10
33	Z	101	LMT	O5B-C5B-C6B-O6B
33	Z	101	LMT	O5'-C5'-C6'-O6'
33	z	101	LMT	O5'-C5'-C6'-O6'
34	C	503	DGD	C2B-C1B-O2G-C2G
34	c	503	DGD	C2B-C1B-O2G-C2G
34	H	101	DGD	C3B-C4B-C5B-C6B
22	C	516	CLA	O1A-CGA-O2A-C1
22	a	405	CLA	C15-C16-C17-C18
22	C	516	CLA	CBD-CGD-O2D-CED
22	C	515	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	C3-C5-C6-C7
22	C	509	CLA	CBA-CGA-O2A-C1
22	A	404	CLA	C15-C16-C17-C18
22	B	602	CLA	C13-C15-C16-C17
22	d	404	CLA	C15-C16-C17-C18
22	b	612	CLA	O1D-CGD-O2D-CED
33	b	626	LMT	C7-C8-C9-C10
22	C	517	CLA	C10-C11-C12-C13
22	b	615	CLA	C15-C16-C17-C18
22	c	517	CLA	C10-C11-C12-C13
22	c	517	CLA	C15-C16-C17-C18
22	D	406	CLA	O1A-CGA-O2A-C1
26	D	412	SQD	C23-C24-C25-C26
26	a	417	SQD	C7-C8-C9-C10
27	b	621	PLM	C1-C2-C3-C4
31	E	101	LHG	C7-C8-C9-C10
34	D	411	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
35	C	519	LMG	C28-C29-C30-C31
35	Y	101	LMG	C10-C11-C12-C13
22	B	614	CLA	C5-C6-C7-C8
34	C	504	DGD	O1B-C1B-O2G-C2G
34	c	504	DGD	O1B-C1B-O2G-C2G
22	B	611	CLA	C15-C16-C17-C18
22	C	513	CLA	C13-C15-C16-C17
22	b	604	CLA	C13-C15-C16-C17
26	A	415	SQD	C7-C8-C9-C10
27	L	102	PLM	C1-C2-C3-C4
34	c	505	DGD	C1A-C2A-C3A-C4A
22	b	616	CLA	C5-C6-C7-C8
22	B	610	CLA	O1D-CGD-O2D-CED
22	C	515	CLA	C6-C7-C8-C10
22	C	516	CLA	C6-C7-C8-C10
22	c	515	CLA	C6-C7-C8-C10
22	d	404	CLA	O1A-CGA-O2A-C1
26	l	102	SQD	O10-C23-O48-C46
34	J	102	DGD	C4D-C5D-C6D-O5D
22	A	404	CLA	C13-C15-C16-C17
22	C	516	CLA	C8-C10-C11-C12
22	b	613	CLA	C15-C16-C17-C18
33	z	101	LMT	O5B-C5B-C6B-O6B
22	c	510	CLA	O1A-CGA-O2A-C1
35	Y	101	LMG	C4-C5-C6-O5
35	y	101	LMG	C4-C5-C6-O5
22	B	614	CLA	O1D-CGD-O2D-CED
22	b	616	CLA	O1D-CGD-O2D-CED
25	A	409	PL9	C24-C26-C27-C28
27	B	621	PLM	C1-C2-C3-C4
33	f	102	LMT	O5B-C5B-C6B-O6B
22	B	601	CLA	C8-C10-C11-C12
22	B	603	CLA	C5-C6-C7-C8
22	C	510	CLA	C5-C6-C7-C8
22	b	603	CLA	C8-C10-C11-C12
33	J	103	LMT	O1'-C1-C2-C3
33	f	102	LMT	C4B-C5B-C6B-O6B
22	B	610	CLA	C15-C16-C17-C18
22	b	612	CLA	C15-C16-C17-C18
31	A	417	LHG	C29-C30-C31-C32
22	b	611	CLA	O1D-CGD-O2D-CED
22	C	509	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	c	521	PLM	C5-C6-C7-C8
22	a	405	CLA	C13-C15-C16-C17
22	c	511	CLA	C5-C6-C7-C8
31	E	101	LHG	C3-O3-P-O6
31	E	101	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O3
31	a	415	LHG	C3-O3-P-O6
31	l	101	LHG	C4-O6-P-O3
34	c	505	DGD	C9B-CAB-CBB-CCB
22	A	407	CLA	CBA-CGA-O2A-C1
22	c	511	CLA	CBA-CGA-O2A-C1
35	c	524	LMG	C29-C28-O8-C9
22	C	507	CLA	CBD-CGD-O2D-CED
33	T	104	LMT	C4B-C5B-C6B-O6B
33	z	101	LMT	C4'-C5'-C6'-O6'
27	C	522	PLM	C1-C2-C3-C4
34	c	503	DGD	C1B-C2B-C3B-C4B
35	c	519	LMG	C28-C29-C30-C31
34	C	503	DGD	O1B-C1B-O2G-C2G
34	c	503	DGD	O1B-C1B-O2G-C2G
25	a	410	PL9	C28-C29-C31-C32
33	i	102	LMT	O1'-C1-C2-C3
22	c	517	CLA	C2A-CAA-CBA-CGA
33	T	101	LMT	C4'-C5'-C6'-O6'
22	C	510	CLA	CBA-CGA-O2A-C1
31	E	101	LHG	C24-C23-O8-C6
22	b	605	CLA	C5-C6-C7-C8
27	e	102	PLM	CC-CD-CE-CF
31	d	406	LHG	C11-C10-C9-C8
31	l	101	LHG	C13-C14-C15-C16
33	B	630	LMT	C7-C8-C9-C10
35	M	101	LMG	C36-C37-C38-C39
22	C	510	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
26	D	412	SQD	C8-C7-O47-C45
26	A	410	SQD	C29-C30-C31-C32
26	a	411	SQD	C14-C15-C16-C17
27	L	102	PLM	C6-C7-C8-C9
27	M	103	PLM	C7-C8-C9-CA
27	c	520	PLM	C5-C6-C7-C8
27	c	523	PLM	C5-C6-C7-C8
27	x	101	PLM	CB-CC-CD-CE

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Mol	Chain	Res	Type	Atoms
28	I	101	LFA	C3-C4-C5-C6
28	T	102	LFA	C10-C11-C12-C13
28	T	102	LFA	C13-C14-C15-C16
31	A	417	LHG	C16-C17-C18-C19
31	D	408	LHG	C11-C10-C9-C8
31	l	101	LHG	C10-C11-C12-C13
33	i	102	LMT	C4-C5-C6-C7
34	C	503	DGD	C5B-C6B-C7B-C8B
34	D	411	DGD	C5B-C6B-C7B-C8B
35	C	525	LMG	C20-C21-C22-C23
35	M	101	LMG	C31-C32-C33-C34
22	C	508	CLA	CBA-CGA-O2A-C1
25	a	410	PL9	C47-C48-C49-C51
26	a	411	SQD	C33-C34-C35-C36
26	b	601	SQD	C30-C31-C32-C33
27	C	522	PLM	C3-C4-C5-C6
28	J	104	LFA	C11-C12-C13-C14
28	a	414	LFA	C10-C11-C12-C13
28	d	408	LFA	C15-C16-C17-C18
28	i	103	LFA	C9-C10-C11-C12
31	L	101	LHG	C10-C11-C12-C13
31	a	421	LHG	C11-C12-C13-C14
33	B	630	LMT	C6-C7-C8-C9
33	J	103	LMT	C11-C10-C9-C8
35	C	519	LMG	C12-C13-C14-C15
35	d	407	LMG	C15-C16-C17-C18
22	B	609	CLA	O1D-CGD-O2D-CED
26	D	412	SQD	O49-C7-O47-C45
35	M	101	LMG	C28-C29-C30-C31
22	d	404	CLA	CBD-CGD-O2D-CED
26	a	411	SQD	C15-C16-C17-C18
26	b	601	SQD	C9-C10-C11-C12
26	b	601	SQD	C12-C13-C14-C15
26	b	601	SQD	C14-C15-C16-C17
27	M	103	PLM	C3-C4-C5-C6
31	E	101	LHG	C11-C10-C9-C8
31	E	101	LHG	C14-C15-C16-C17
31	L	101	LHG	C32-C33-C34-C35
31	d	405	LHG	C25-C26-C27-C28
34	c	504	DGD	C7B-C8B-C9B-CAB
35	c	519	LMG	C17-C18-C19-C20
35	c	519	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
35	d	407	LMG	C12-C13-C14-C15
27	e	102	PLM	C3-C4-C5-C6
27	x	101	PLM	C2-C3-C4-C5
27	x	101	PLM	C4-C5-C6-C7
28	T	102	LFA	C11-C10-C9-C8
28	a	414	LFA	C12-C13-C14-C15
31	L	101	LHG	C34-C35-C36-C37
34	C	504	DGD	C6B-C7B-C8B-C9B
34	J	102	DGD	C9B-CAB-CBB-CCB
34	c	504	DGD	C6B-C7B-C8B-C9B
34	h	101	DGD	C7B-C8B-C9B-CAB
35	c	519	LMG	C34-C35-C36-C37
35	m	101	LMG	C31-C32-C33-C34
31	D	408	LHG	O2-C2-C3-O3
27	a	412	PLM	C7-C8-C9-CA
28	E	102	LFA	C14-C15-C16-C17
31	D	407	LHG	C25-C26-C27-C28
33	f	102	LMT	C4-C5-C6-C7
34	C	504	DGD	C9A-CAA-CBA-CCA
35	M	101	LMG	C33-C34-C35-C36
35	Y	101	LMG	C11-C12-C13-C14
22	b	604	CLA	C3-C5-C6-C7
26	b	601	SQD	C7-C8-C9-C10
33	A	419	LMT	C2'-C1'-O1'-C1
33	i	102	LMT	C2'-C1'-O1'-C1
34	D	411	DGD	C2D-C1D-O3G-C3G
34	c	504	DGD	C2D-C1D-O3G-C3G
35	Y	101	LMG	C2-C1-O1-C7
26	a	411	SQD	C9-C10-C11-C12
27	L	102	PLM	CC-CD-CE-CF
27	b	621	PLM	CC-CD-CE-CF
27	c	520	PLM	C3-C4-C5-C6
28	T	102	LFA	C3-C4-C5-C6
28	T	102	LFA	C5-C6-C7-C8
31	L	101	LHG	C13-C14-C15-C16
35	m	101	LMG	C19-C20-C21-C22
25	d	402	PL9	C15-C14-C16-C17
28	H	103	LFA	C11-C10-C9-C8
31	a	421	LHG	C24-C25-C26-C27
33	Z	101	LMT	C7-C8-C9-C10
35	M	101	LMG	C19-C20-C21-C22
25	D	404	PL9	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C14-C13-C15-C16
22	c	510	CLA	C11-C12-C13-C14
22	c	516	CLA	C6-C7-C8-C9
22	b	609	CLA	O1D-CGD-O2D-CED
26	b	601	SQD	C17-C18-C19-C20
27	e	101	PLM	CC-CD-CE-CF
28	I	101	LFA	C7-C8-C9-C10
31	A	417	LHG	C24-C25-C26-C27
31	d	405	LHG	C11-C12-C13-C14
33	J	103	LMT	C5-C6-C7-C8
34	C	504	DGD	C4B-C5B-C6B-C7B
34	c	504	DGD	C2B-C3B-C4B-C5B
34	c	504	DGD	C4B-C5B-C6B-C7B
35	m	101	LMG	C30-C31-C32-C33
22	B	607	CLA	C2A-CAA-CBA-CGA
22	b	609	CLA	C2A-CAA-CBA-CGA
24	B	617	BCR	C37-C22-C23-C24
24	F	101	BCR	C37-C22-C23-C24
24	K	101	BCR	C37-C22-C23-C24
24	f	101	BCR	C37-C22-C23-C24
27	C	522	PLM	C7-C8-C9-CA
27	x	101	PLM	CC-CD-CE-CF
28	I	101	LFA	C4-C5-C6-C7
31	a	415	LHG	C24-C25-C26-C27
34	c	504	DGD	C2A-C3A-C4A-C5A
35	c	519	LMG	C31-C32-C33-C34
35	m	101	LMG	C12-C13-C14-C15
35	m	101	LMG	C33-C34-C35-C36
31	A	417	LHG	O1-C1-C2-C3
31	D	407	LHG	O1-C1-C2-C3
31	a	421	LHG	O1-C1-C2-C3
31	d	405	LHG	O1-C1-C2-C3
24	F	101	BCR	C21-C22-C23-C24
24	f	101	BCR	C21-C22-C23-C24
22	d	404	CLA	C3-C5-C6-C7
34	J	102	DGD	C2B-C1B-O2G-C2G
26	b	601	SQD	C29-C30-C31-C32
27	X	101	PLM	C4-C5-C6-C7
27	c	520	PLM	C4-C5-C6-C7
27	x	101	PLM	C3-C4-C5-C6
28	H	103	LFA	C11-C12-C13-C14
34	c	503	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
35	M	101	LMG	C12-C13-C14-C15
35	m	101	LMG	C28-C29-C30-C31
26	a	411	SQD	C17-C18-C19-C20
26	a	417	SQD	C25-C26-C27-C28
26	b	601	SQD	C16-C17-C18-C19
27	a	412	PLM	CA-CB-CC-CD
27	j	103	PLM	C9-CA-CB-CC
28	a	418	LFA	C7-C8-C9-C10
31	a	415	LHG	C26-C27-C28-C29
31	l	101	LHG	C29-C30-C31-C32
34	h	101	DGD	C2B-C3B-C4B-C5B
35	C	519	LMG	C29-C30-C31-C32
35	D	409	LMG	C12-C13-C14-C15
35	D	409	LMG	C35-C36-C37-C38
35	m	101	LMG	C39-C40-C41-C42
22	B	615	CLA	C16-C17-C18-C19
22	b	617	CLA	C16-C17-C18-C19
22	b	617	CLA	C16-C17-C18-C20
33	A	419	LMT	O5'-C1'-O1'-C1
23	D	403	PHO	C8-C10-C11-C12
26	A	415	SQD	C12-C13-C14-C15
26	a	417	SQD	C9-C10-C11-C12
26	a	417	SQD	C30-C31-C32-C33
27	a	412	PLM	C6-C7-C8-C9
27	b	621	PLM	C3-C4-C5-C6
27	c	523	PLM	C3-C4-C5-C6
28	i	103	LFA	C11-C12-C13-C14
31	D	408	LHG	C32-C33-C34-C35
31	E	101	LHG	C15-C16-C17-C18
31	E	101	LHG	C17-C18-C19-C20
31	E	101	LHG	C25-C26-C27-C28
33	B	633	LMT	C11-C10-C9-C8
33	J	103	LMT	C6-C7-C8-C9
33	j	101	LMT	C11-C10-C9-C8
33	z	101	LMT	C7-C8-C9-C10
34	d	410	DGD	C6B-C7B-C8B-C9B
35	c	519	LMG	C12-C13-C14-C15
22	B	611	CLA	CBD-CGD-O2D-CED
26	A	410	SQD	C17-C18-C19-C20
26	a	417	SQD	C27-C28-C29-C30
27	c	520	PLM	C7-C8-C9-CA
27	e	102	PLM	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	B	620	LFA	C11-C10-C9-C8
28	T	102	LFA	C11-C12-C13-C14
33	z	101	LMT	O1'-C1-C2-C3
34	C	504	DGD	C3B-C4B-C5B-C6B
35	d	407	LMG	C35-C36-C37-C38
26	A	415	SQD	C23-C24-C25-C26
34	C	503	DGD	C1B-C2B-C3B-C4B
22	A	407	CLA	O1A-CGA-O2A-C1
31	E	101	LHG	O10-C23-O8-C6
26	A	410	SQD	C11-C12-C13-C14
27	B	621	PLM	C5-C6-C7-C8
27	D	410	PLM	CB-CC-CD-CE
35	M	101	LMG	C39-C40-C41-C42
35	c	519	LMG	C19-C20-C21-C22
22	a	405	CLA	C3-C5-C6-C7
22	a	408	CLA	CBA-CGA-O2A-C1
33	f	102	LMT	C6-C7-C8-C9
35	c	519	LMG	C18-C19-C20-C21
35	m	101	LMG	C18-C19-C20-C21
33	T	104	LMT	C2-C1-O1'-C1'
33	j	101	LMT	C2-C1-O1'-C1'
26	a	417	SQD	C14-C15-C16-C17
27	A	413	PLM	C4-C5-C6-C7
27	D	410	PLM	C3-C4-C5-C6
27	M	103	PLM	CA-CB-CC-CD
31	d	406	LHG	C14-C15-C16-C17
34	J	102	DGD	CCB-CDB-CEB-CFB
34	c	505	DGD	C4B-C5B-C6B-C7B
34	d	410	DGD	C4B-C5B-C6B-C7B
35	M	101	LMG	C18-C19-C20-C21
35	c	519	LMG	C38-C39-C40-C41
22	c	511	CLA	O1A-CGA-O2A-C1
22	B	615	CLA	C16-C17-C18-C20
27	B	622	PLM	C3-C4-C5-C6
28	J	101	LFA	C5-C6-C7-C8
31	D	407	LHG	C11-C12-C13-C14
34	h	101	DGD	C4B-C5B-C6B-C7B
35	C	519	LMG	C18-C19-C20-C21
35	C	525	LMG	C19-C20-C21-C22
22	B	603	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	O1D-CGD-O2D-CED
34	c	503	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
22	A	404	CLA	C3-C5-C6-C7
34	C	504	DGD	C1B-C2B-C3B-C4B
34	c	504	DGD	C1B-C2B-C3B-C4B
27	C	520	PLM	C9-CA-CB-CC
31	a	421	LHG	C12-C13-C14-C15
23	a	407	PHO	C4-C3-C5-C6
25	a	410	PL9	C45-C44-C46-C47
22	c	509	CLA	CBA-CGA-O2A-C1
34	c	503	DGD	C2A-C1A-O1G-C1G
23	A	406	PHO	C2-C3-C5-C6
23	a	407	PHO	C2-C3-C5-C6
25	d	402	PL9	C23-C24-C26-C27
22	c	507	CLA	O1D-CGD-O2D-CED
22	C	516	CLA	C2A-CAA-CBA-CGA
32	a	401	GOL	O1-C1-C2-O2
26	b	601	SQD	C24-C25-C26-C27
31	D	407	LHG	C11-C10-C9-C8
31	L	101	LHG	C33-C34-C35-C36
31	a	415	LHG	C14-C15-C16-C17
34	C	504	DGD	C2B-C3B-C4B-C5B
34	c	503	DGD	C4A-C5A-C6A-C7A
35	C	519	LMG	C38-C39-C40-C41
35	c	524	LMG	O10-C28-O8-C9
31	d	406	LHG	O2-C2-C3-O3
23	a	420	PHO	C8-C10-C11-C12
33	j	101	LMT	C4-C5-C6-C7
33	B	628	LMT	C4'-C5'-C6'-O6'
27	c	520	PLM	C6-C7-C8-C9
27	j	102	PLM	CB-CC-CD-CE
31	a	421	LHG	C14-C15-C16-C17
31	l	101	LHG	C30-C31-C32-C33
33	J	103	LMT	C4-C5-C6-C7
35	M	101	LMG	C30-C31-C32-C33
35	c	519	LMG	C30-C31-C32-C33
22	C	510	CLA	O1A-CGA-O2A-C1
27	t	101	PLM	C8-C9-CA-CB
34	C	504	DGD	C5B-C6B-C7B-C8B
34	J	102	DGD	O1B-C1B-O2G-C2G
34	C	503	DGD	O6D-C5D-C6D-O5D
34	c	503	DGD	O6D-C5D-C6D-O5D
27	A	411	PLM	C3-C4-C5-C6
27	c	523	PLM	CB-CC-CD-CE

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Mol	Chain	Res	Type	Atoms
35	D	409	LMG	C15-C16-C17-C18
35	y	101	LMG	C29-C30-C31-C32
22	C	508	CLA	C13-C15-C16-C17
22	a	408	CLA	C15-C16-C17-C18
22	C	508	CLA	O1A-CGA-O2A-C1
33	T	101	LMT	C1-C2-C3-C4
33	j	101	LMT	C1-C2-C3-C4
26	A	410	SQD	C27-C28-C29-C30
26	a	417	SQD	C31-C32-C33-C34
26	b	601	SQD	C25-C26-C27-C28
28	I	101	LFA	C13-C14-C15-C16
31	l	101	LHG	C31-C32-C33-C34
34	c	505	DGD	CCB-CDB-CEB-CFB
26	d	412	SQD	C23-C24-C25-C26
24	A	408	BCR	C23-C24-C25-C26
24	B	617	BCR	C5-C6-C7-C8
24	B	632	BCR	C1-C6-C7-C8
24	B	632	BCR	C5-C6-C7-C8
24	C	502	BCR	C5-C6-C7-C8
24	C	502	BCR	C23-C24-C25-C30
24	F	101	BCR	C5-C6-C7-C8
24	F	101	BCR	C23-C24-C25-C30
24	T	103	BCR	C5-C6-C7-C8
24	Y	102	BCR	C1-C6-C7-C8
24	a	409	BCR	C23-C24-C25-C26
24	b	602	BCR	C1-C6-C7-C8
24	b	602	BCR	C5-C6-C7-C8
24	c	502	BCR	C5-C6-C7-C8
24	c	502	BCR	C23-C24-C25-C30
24	f	101	BCR	C5-C6-C7-C8
24	f	101	BCR	C23-C24-C25-C30
24	k	101	BCR	C23-C24-C25-C26
24	k	101	BCR	C23-C24-C25-C30
24	y	102	BCR	C1-C6-C7-C8
34	J	102	DGD	C4B-C5B-C6B-C7B
35	C	519	LMG	C16-C17-C18-C19
35	C	525	LMG	C21-C22-C23-C24
34	C	503	DGD	C2A-C1A-O1G-C1G
28	i	101	LFA	C9-C10-C11-C12
31	D	407	LHG	C24-C25-C26-C27
22	a	408	CLA	O1A-CGA-O2A-C1
26	l	102	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
31	a	415	LHG	C23-C24-C25-C26
33	Z	101	LMT	C4'-C5'-C6'-O6'
28	i	101	LFA	C14-C15-C16-C17
25	D	404	PL9	C47-C48-C49-C51
25	d	402	PL9	C47-C48-C49-C51
26	A	410	SQD	C11-C10-C9-C8
26	D	412	SQD	C32-C33-C34-C35
22	b	616	CLA	C4-C3-C5-C6
23	A	406	PHO	C4-C3-C5-C6
25	D	404	PL9	C15-C14-C16-C17
25	D	404	PL9	C35-C34-C36-C37
25	D	404	PL9	C45-C44-C46-C47
25	d	402	PL9	C35-C34-C36-C37
25	d	402	PL9	C45-C44-C46-C47
22	C	514	CLA	C6-C7-C8-C10
22	c	510	CLA	C11-C12-C13-C15
22	c	516	CLA	C6-C7-C8-C10
22	c	517	CLA	C6-C7-C8-C10
22	D	406	CLA	C3-C5-C6-C7
22	c	509	CLA	O1A-CGA-O2A-C1
34	c	503	DGD	O1A-C1A-O1G-C1G
34	c	504	DGD	C5B-C6B-C7B-C8B
24	B	632	BCR	C15-C16-C17-C18
34	d	410	DGD	C2A-C1A-O1G-C1G
26	A	410	SQD	C9-C10-C11-C12
27	E	103	PLM	CB-CC-CD-CE
31	L	101	LHG	C31-C32-C33-C34
33	b	626	LMT	O1'-C1-C2-C3
34	H	101	DGD	C2B-C3B-C4B-C5B
22	B	607	CLA	O1D-CGD-O2D-CED
22	b	617	CLA	C5-C6-C7-C8
27	b	621	PLM	C7-C8-C9-CA
35	m	101	LMG	C36-C37-C38-C39
25	D	404	PL9	C47-C48-C49-C50
33	f	102	LMT	C5-C6-C7-C8
26	a	417	SQD	C23-C24-C25-C26
35	C	519	LMG	C10-C11-C12-C13
27	B	621	PLM	CC-CD-CE-CF
28	B	620	LFA	C9-C10-C11-C12
28	i	104	LFA	C11-C12-C13-C14
33	T	104	LMT	C7-C8-C9-C10
28	i	101	LFA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
31	d	405	LHG	C24-C25-C26-C27
35	d	407	LMG	O6-C5-C6-O5
34	c	505	DGD	C2A-C1A-O1G-C1G
33	i	102	LMT	O5'-C1'-O1'-C1
25	A	409	PL9	C39-C41-C42-C43
27	C	522	PLM	C2-C3-C4-C5
27	L	102	PLM	CB-CC-CD-CE
27	c	520	PLM	CB-CC-CD-CE
31	L	101	LHG	C11-C10-C9-C8
31	l	101	LHG	C16-C17-C18-C19
35	C	519	LMG	C11-C12-C13-C14
26	A	410	SQD	C8-C7-O47-C45
31	E	101	LHG	C8-C7-O7-C5
34	c	505	DGD	C2B-C1B-O2G-C2G
35	c	524	LMG	C11-C10-O7-C8
27	c	520	PLM	C2-C3-C4-C5
35	c	524	LMG	C18-C19-C20-C21
22	D	406	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
22	c	517	CLA	CBD-CGD-O2D-CED
28	H	103	LFA	C9-C10-C11-C12
31	E	101	LHG	O9-C7-O7-C5
33	Z	101	LMT	C4B-C5B-C6B-O6B
34	J	102	DGD	C1B-C2B-C3B-C4B
33	T	101	LMT	C2'-C1'-O1'-C1
34	J	102	DGD	C2E-C1E-O5D-C6D
34	C	504	DGD	O1G-C1G-C2G-O2G
34	d	410	DGD	O2G-C2G-C3G-O3G
35	y	101	LMG	O1-C7-C8-O7
35	D	409	LMG	O6-C5-C6-O5
27	B	621	PLM	C6-C7-C8-C9
33	j	101	LMT	O1'-C1-C2-C3
35	Y	101	LMG	C30-C31-C32-C33
27	X	101	PLM	C3-C4-C5-C6
31	D	407	LHG	C15-C16-C17-C18
31	a	421	LHG	C30-C31-C32-C33
22	B	604	CLA	C8-C10-C11-C12
27	B	622	PLM	C1-C2-C3-C4
27	c	523	PLM	C1-C2-C3-C4
33	z	101	LMT	C1-C2-C3-C4
22	B	603	CLA	C6-C7-C8-C9
22	B	614	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	C	512	CLA	C11-C10-C8-C9
22	C	514	CLA	C6-C7-C8-C9
22	C	515	CLA	C6-C7-C8-C9
22	b	605	CLA	C6-C7-C8-C9
22	b	616	CLA	C11-C12-C13-C14
22	c	515	CLA	C6-C7-C8-C9
22	b	605	CLA	O1D-CGD-O2D-CED
26	D	412	SQD	C24-C25-C26-C27
27	A	413	PLM	C3-C4-C5-C6
27	L	102	PLM	C5-C6-C7-C8
28	B	624	LFA	C6-C7-C8-C9
31	d	406	LHG	C33-C34-C35-C36
31	l	101	LHG	C33-C34-C35-C36
33	B	633	LMT	C9-C10-C11-C12
22	A	404	CLA	C2A-CAA-CBA-CGA
22	B	601	CLA	C2A-CAA-CBA-CGA
22	B	610	CLA	C2A-CAA-CBA-CGA
22	a	405	CLA	C2A-CAA-CBA-CGA
22	b	603	CLA	C2A-CAA-CBA-CGA
22	b	612	CLA	C2A-CAA-CBA-CGA
26	A	415	SQD	C9-C10-C11-C12
26	a	411	SQD	C26-C27-C28-C29
28	I	101	LFA	C14-C15-C16-C17
35	C	519	LMG	C17-C18-C19-C20
27	b	622	PLM	C3-C4-C5-C6
31	D	408	LHG	C17-C18-C19-C20
33	T	104	LMT	C2-C3-C4-C5
34	C	503	DGD	O1A-C1A-O1G-C1G
22	A	405	CLA	C1A-C2A-CAA-CBA
22	A	407	CLA	C1A-C2A-CAA-CBA
22	C	517	CLA	C1A-C2A-CAA-CBA
22	D	401	CLA	C1A-C2A-CAA-CBA
22	a	406	CLA	C1A-C2A-CAA-CBA
22	a	408	CLA	C1A-C2A-CAA-CBA
22	d	401	CLA	C1A-C2A-CAA-CBA
33	C	518	LMT	O5'-C5'-C6'-O6'
26	A	410	SQD	O49-C7-O47-C45
27	C	522	PLM	C9-CA-CB-CC
31	d	405	LHG	C11-C10-C9-C8
34	C	504	DGD	C5A-C6A-C7A-C8A
22	B	615	CLA	C5-C6-C7-C8
22	c	511	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	b	601	SQD	C28-C29-C30-C31
28	a	413	LFA	C9-C10-C11-C12
31	A	417	LHG	C10-C11-C12-C13
26	a	417	SQD	C10-C11-C12-C13
28	i	101	LFA	C15-C16-C17-C18
35	c	524	LMG	C17-C18-C19-C20
22	c	509	CLA	C13-C15-C16-C17
33	f	102	LMT	C11-C10-C9-C8
26	b	601	SQD	C23-C24-C25-C26
22	B	611	CLA	C16-C17-C18-C20
27	M	103	PLM	C2-C3-C4-C5
28	I	102	LFA	C11-C12-C13-C14
31	A	417	LHG	C25-C26-C27-C28
22	b	606	CLA	C8-C10-C11-C12
26	l	102	SQD	C11-C12-C13-C14
31	D	408	LHG	C1-C2-C3-O3
31	E	101	LHG	C1-C2-C3-O3
25	D	404	PL9	C25-C24-C26-C27
25	d	402	PL9	C25-C24-C26-C27
27	B	627	PLM	C4-C5-C6-C7
27	L	102	PLM	C7-C8-C9-CA
31	a	421	LHG	C17-C18-C19-C20
35	M	101	LMG	C17-C18-C19-C20
22	C	513	CLA	C10-C11-C12-C13
26	A	410	SQD	C12-C13-C14-C15
27	c	523	PLM	CA-CB-CC-CD
27	e	101	PLM	C5-C6-C7-C8
28	i	104	LFA	C13-C14-C15-C16
35	c	519	LMG	C33-C34-C35-C36
35	m	101	LMG	C17-C18-C19-C20
28	H	103	LFA	C7-C8-C9-C10
22	b	613	CLA	C16-C17-C18-C20
26	a	417	SQD	C44-C45-C46-O48
26	d	412	SQD	O6-C44-C45-C46
26	l	102	SQD	C44-C45-C46-O48
31	E	101	LHG	C4-C5-C6-O8
31	E	101	LHG	C19-C20-C21-C22
31	a	415	LHG	C4-C5-C6-O8
33	z	101	LMT	C4-C5-C6-C7
34	C	503	DGD	C1G-C2G-C3G-O3G
34	J	102	DGD	C1G-C2G-C3G-O3G
34	c	503	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
35	C	519	LMG	C7-C8-C9-O8
35	D	409	LMG	C16-C17-C18-C19
35	Y	101	LMG	C7-C8-C9-O8
35	c	519	LMG	C7-C8-C9-O8
35	c	519	LMG	C11-C12-C13-C14
22	c	508	CLA	C8-C10-C11-C12
27	A	413	PLM	C5-C6-C7-C8
28	B	620	LFA	C10-C11-C12-C13
28	C	521	LFA	C10-C11-C12-C13
31	l	101	LHG	C11-C10-C9-C8
31	D	407	LHG	C23-C24-C25-C26
26	a	411	SQD	C45-C44-O6-C1
34	C	504	DGD	C5D-C6D-O5D-C1E
34	J	102	DGD	C5D-C6D-O5D-C1E
34	c	504	DGD	C5D-C6D-O5D-C1E
35	c	524	LMG	C8-C7-O1-C1
35	M	101	LMG	O6-C5-C6-O5
22	C	516	CLA	O1D-CGD-O2D-CED
26	a	417	SQD	C32-C33-C34-C35
28	a	413	LFA	C11-C12-C13-C14
33	b	626	LMT	C11-C10-C9-C8
27	D	402	PLM	C1-C2-C3-C4
26	a	411	SQD	C19-C20-C21-C22
35	y	101	LMG	O6-C1-O1-C7
31	d	406	LHG	C17-C18-C19-C20
31	D	408	LHG	O1-C1-C2-O2
31	E	101	LHG	O1-C1-C2-O2
31	d	406	LHG	O1-C1-C2-O2
26	D	412	SQD	C10-C11-C12-C13
27	M	103	PLM	CB-CC-CD-CE
33	C	518	LMT	C5'-C4'-O1B-C1B
34	d	410	DGD	O1A-C1A-O1G-C1G
34	C	503	DGD	C4D-C5D-C6D-O5D
34	c	503	DGD	C4D-C5D-C6D-O5D
35	c	524	LMG	C29-C30-C31-C32
35	c	519	LMG	C11-C10-O7-C8
34	C	503	DGD	O6E-C5E-C6E-O5E
34	c	503	DGD	O6E-C5E-C6E-O5E
35	C	525	LMG	O6-C5-C6-O5
26	a	417	SQD	C29-C30-C31-C32
28	I	101	LFA	C11-C10-C9-C8
31	a	415	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
31	d	405	LHG	C23-C24-C25-C26
34	c	504	DGD	C1A-C2A-C3A-C4A
27	c	520	PLM	CD-CE-CF-CG
33	i	102	LMT	C5'-C4'-O1B-C1B
26	d	412	SQD	C10-C11-C12-C13
33	j	101	LMT	C9-C10-C11-C12
28	a	414	LFA	C13-C14-C15-C16
31	d	406	LHG	C32-C33-C34-C35
22	C	507	CLA	C8-C10-C11-C12
22	C	510	CLA	C13-C15-C16-C17
31	d	405	LHG	C14-C15-C16-C17
34	c	504	DGD	C3B-C4B-C5B-C6B
34	c	505	DGD	O1A-C1A-O1G-C1G
22	B	611	CLA	C16-C17-C18-C19
31	d	406	LHG	C34-C35-C36-C37
34	C	503	DGD	C2B-C3B-C4B-C5B
34	h	101	DGD	C7A-C8A-C9A-CAA
34	d	410	DGD	O6D-C5D-C6D-O5D
35	c	519	LMG	O6-C5-C6-O5
27	A	413	PLM	C7-C8-C9-CA
33	i	102	LMT	C4'-C5'-C6'-O6'
22	C	507	CLA	O1D-CGD-O2D-CED
22	C	510	CLA	O1D-CGD-O2D-CED
28	I	103	LFA	C10-C11-C12-C13
34	H	101	DGD	C7A-C8A-C9A-CAA
34	c	504	DGD	C7A-C8A-C9A-CAA
22	C	516	CLA	C10-C11-C12-C13
28	C	521	LFA	C6-C7-C8-C9
26	A	415	SQD	O47-C7-C8-C9
34	c	505	DGD	O2G-C2G-C3G-O3G
35	c	519	LMG	O1-C7-C8-O7
31	a	415	LHG	C13-C14-C15-C16
31	a	421	LHG	C32-C33-C34-C35
35	C	525	LMG	C11-C12-C13-C14
34	c	505	DGD	O1B-C1B-O2G-C2G
22	C	510	CLA	C10-C11-C12-C13
26	b	601	SQD	C19-C20-C21-C22
27	L	102	PLM	CD-CE-CF-CG
28	d	408	LFA	C13-C14-C15-C16
31	a	415	LHG	C25-C26-C27-C28
35	d	407	LMG	C16-C17-C18-C19
35	C	519	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
27	c	521	PLM	C4-C5-C6-C7
27	t	101	PLM	CC-CD-CE-CF
28	d	408	LFA	C11-C10-C9-C8
34	C	504	DGD	C7B-C8B-C9B-CAB
22	B	603	CLA	C6-C7-C8-C10
22	B	606	CLA	C12-C13-C15-C16
22	B	614	CLA	C11-C12-C13-C15
22	B	614	CLA	C12-C13-C15-C16
22	B	615	CLA	C12-C13-C15-C16
22	C	508	CLA	C12-C13-C15-C16
22	C	509	CLA	C11-C12-C13-C15
22	C	510	CLA	C11-C12-C13-C15
22	C	512	CLA	C11-C10-C8-C7
22	a	408	CLA	C11-C10-C8-C7
22	b	605	CLA	C6-C7-C8-C10
22	b	616	CLA	C11-C12-C13-C15
22	b	616	CLA	C12-C13-C15-C16
22	b	617	CLA	C12-C13-C15-C16
22	c	509	CLA	C12-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C15
22	c	513	CLA	C11-C10-C8-C7
22	c	514	CLA	C6-C7-C8-C10
22	a	408	CLA	C3-C5-C6-C7
26	a	411	SQD	C25-C26-C27-C28
22	B	614	CLA	C11-C12-C13-C14
22	C	509	CLA	C11-C12-C13-C14
22	C	516	CLA	C6-C7-C8-C9
22	C	517	CLA	C14-C13-C15-C16
22	b	616	CLA	C14-C13-C15-C16
22	c	507	CLA	C14-C13-C15-C16
22	c	513	CLA	C11-C10-C8-C9
26	A	415	SQD	C17-C18-C19-C20
35	m	101	LMG	C32-C33-C34-C35
35	m	101	LMG	C34-C35-C36-C37
22	C	506	CLA	CBA-CGA-O2A-C1
22	c	507	CLA	CBA-CGA-O2A-C1
22	c	510	CLA	C2A-CAA-CBA-CGA
34	D	411	DGD	CBB-CCB-CDB-CEB
33	Z	101	LMT	C1-C2-C3-C4
33	i	102	LMT	C1-C2-C3-C4
24	B	632	BCR	C21-C22-C23-C24
34	c	503	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
35	c	519	LMG	C32-C33-C34-C35
27	a	412	PLM	C3-C4-C5-C6
26	A	410	SQD	C14-C15-C16-C17
31	d	405	LHG	C15-C16-C17-C18
31	a	421	LHG	C7-C8-C9-C10
22	c	511	CLA	C10-C11-C12-C13
25	d	402	PL9	C47-C48-C49-C50
27	A	411	PLM	C2-C3-C4-C5
33	B	630	LMT	C11-C10-C9-C8
22	b	613	CLA	C16-C17-C18-C19
31	E	101	LHG	O6-C4-C5-C6
26	A	410	SQD	C13-C14-C15-C16
28	I	102	LFA	C12-C13-C14-C15
26	d	412	SQD	C7-C8-C9-C10
27	c	521	PLM	C7-C8-C9-CA
22	B	614	CLA	C4-C3-C5-C6
25	A	409	PL9	C12-C11-C9-C10
22	b	616	CLA	C2-C3-C5-C6
27	j	102	PLM	C1-C2-C3-C4
35	c	524	LMG	O9-C10-O7-C8
26	a	417	SQD	C11-C12-C13-C14
28	i	101	LFA	C13-C14-C15-C16
31	D	407	LHG	C14-C15-C16-C17
27	e	102	PLM	C1-C2-C3-C4
27	A	413	PLM	C2-C3-C4-C5
27	X	101	PLM	C6-C7-C8-C9
33	f	102	LMT	O1'-C1-C2-C3
35	C	519	LMG	C19-C20-C21-C22
26	a	411	SQD	C31-C32-C33-C34
28	B	620	LFA	C6-C7-C8-C9
31	L	101	LHG	C16-C17-C18-C19
33	j	101	LMT	C2-C3-C4-C5
33	j	101	LMT	C6-C7-C8-C9
34	d	410	DGD	C3B-C4B-C5B-C6B
35	C	525	LMG	C32-C33-C34-C35
25	A	409	PL9	C47-C48-C49-C51
33	f	102	LMT	C2-C1-O1'-C1'
33	m	102	LMT	C2-C1-O1'-C1'
26	a	417	SQD	C12-C13-C14-C15
27	F	102	PLM	C4-C5-C6-C7
27	j	103	PLM	C3-C4-C5-C6
28	I	102	LFA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
35	M	101	LMG	C20-C21-C22-C23
22	c	517	CLA	C3-C5-C6-C7
35	m	101	LMG	C20-C21-C22-C23
22	B	614	CLA	C10-C11-C12-C13
26	A	415	SQD	O6-C44-C45-C46
26	D	412	SQD	O6-C44-C45-C46
26	a	411	SQD	O6-C44-C45-C46
26	a	417	SQD	O6-C44-C45-C46
34	C	504	DGD	O1G-C1G-C2G-C3G
34	D	411	DGD	O1G-C1G-C2G-C3G
34	d	410	DGD	C1G-C2G-C3G-O3G
35	y	101	LMG	O1-C7-C8-C9
27	D	410	PLM	CD-CE-CF-CG
27	X	101	PLM	C7-C8-C9-CA
28	I	102	LFA	C13-C14-C15-C16
26	l	102	SQD	C32-C33-C34-C35
27	H	104	PLM	C7-C8-C9-CA
33	T	104	LMT	C5-C6-C7-C8
22	B	613	CLA	C10-C11-C12-C13
27	D	410	PLM	C5-C6-C7-C8
31	a	415	LHG	C17-C18-C19-C20
22	d	404	CLA	O1D-CGD-O2D-CED
35	y	101	LMG	C10-C11-C12-C13
22	c	507	CLA	O1A-CGA-O2A-C1
33	f	102	LMT	C1-C2-C3-C4
22	B	611	CLA	O1D-CGD-O2D-CED
31	A	417	LHG	O1-C1-C2-O2
22	b	614	CLA	C10-C11-C12-C13
27	C	520	PLM	CA-CB-CC-CD
27	d	411	PLM	C5-C6-C7-C8
28	J	104	LFA	C12-C13-C14-C15
33	Z	101	LMT	O1'-C1-C2-C3
22	C	506	CLA	O1A-CGA-O2A-C1
27	A	411	PLM	CD-CE-CF-CG
28	i	101	LFA	C3-C4-C5-C6
31	a	415	LHG	O2-C2-C3-O3
26	a	411	SQD	C13-C14-C15-C16
33	J	103	LMT	C3-C4-C5-C6
33	C	518	LMT	C4-C5-C6-C7
26	a	411	SQD	O6-C44-C45-O47
31	E	101	LHG	O7-C5-C6-O8
31	a	415	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
35	c	519	LMG	O7-C8-C9-O8
22	B	612	CLA	C10-C11-C12-C13
26	a	417	SQD	C17-C18-C19-C20
31	D	408	LHG	C14-C15-C16-C17
34	c	504	DGD	C8B-C9B-CAB-CBB
27	b	622	PLM	C7-C8-C9-CA
28	I	102	LFA	C14-C15-C16-C17
25	A	409	PL9	C19-C21-C22-C23
31	d	406	LHG	C1-C2-C3-O3
27	A	411	PLM	C9-CA-CB-CC
27	C	520	PLM	C6-C7-C8-C9
28	T	102	LFA	C12-C13-C14-C15
22	B	608	CLA	C2-C1-O2A-CGA
22	B	613	CLA	C2-C1-O2A-CGA
22	b	610	CLA	C2-C1-O2A-CGA
22	b	615	CLA	C2-C1-O2A-CGA
22	C	509	CLA	C6-C7-C8-C9
22	C	510	CLA	C11-C12-C13-C14
22	c	507	CLA	C6-C7-C8-C9
22	c	511	CLA	C11-C12-C13-C14
27	x	101	PLM	CA-CB-CC-CD
31	A	417	LHG	C17-C18-C19-C20
22	C	513	CLA	C8-C10-C11-C12
31	A	417	LHG	C2-C3-O3-P
31	E	101	LHG	C2-C3-O3-P
26	D	412	SQD	C25-C26-C27-C28
27	C	523	PLM	C5-C6-C7-C8
22	C	509	CLA	C2A-CAA-CBA-CGA
24	B	617	BCR	C23-C24-C25-C26
24	K	101	BCR	C23-C24-C25-C26
24	Y	102	BCR	C23-C24-C25-C26
24	b	620	BCR	C23-C24-C25-C26
24	c	502	BCR	C1-C6-C7-C8
24	y	102	BCR	C23-C24-C25-C26
22	B	613	CLA	C5-C6-C7-C8
22	b	615	CLA	C5-C6-C7-C8
24	C	502	BCR	C11-C12-C13-C14
22	D	406	CLA	C13-C15-C16-C17
22	b	616	CLA	C10-C11-C12-C13
34	C	504	DGD	C2A-C3A-C4A-C5A
35	c	519	LMG	O9-C10-O7-C8
27	M	103	PLM	C9-CA-CB-CC

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Mol	Chain	Res	Type	Atoms
28	T	102	LFA	C7-C8-C9-C10
22	c	513	CLA	C16-C17-C18-C19
26	a	417	SQD	C24-C25-C26-C27
22	c	517	CLA	O1D-CGD-O2D-CED
26	A	415	SQD	C13-C14-C15-C16
34	C	503	DGD	C6A-C7A-C8A-C9A
22	A	405	CLA	C12-C13-C15-C16
22	B	601	CLA	C11-C12-C13-C15
22	B	604	CLA	C6-C7-C8-C10
22	C	509	CLA	C6-C7-C8-C10
22	C	513	CLA	C6-C7-C8-C10
22	C	517	CLA	C12-C13-C15-C16
22	D	405	CLA	C11-C12-C13-C15
22	a	406	CLA	C12-C13-C15-C16
22	b	603	CLA	C11-C12-C13-C15
22	b	606	CLA	C6-C7-C8-C10
22	d	403	CLA	C11-C12-C13-C15
22	C	511	CLA	O1D-CGD-O2D-CED
33	B	623	LMT	C11-C10-C9-C8
35	M	101	LMG	C13-C14-C15-C16
24	C	501	BCR	C19-C20-C21-C22
24	c	501	BCR	C19-C20-C21-C22
28	i	101	LFA	C16-C17-C18-C19
34	J	102	DGD	C6B-C7B-C8B-C9B
35	m	101	LMG	C13-C14-C15-C16
22	b	614	CLA	CBA-CGA-O2A-C1
22	c	514	CLA	C10-C11-C12-C13
35	c	519	LMG	C16-C17-C18-C19
34	h	101	DGD	CCA-CDA-CEA-CFA
35	c	524	LMG	C12-C13-C14-C15
27	B	627	PLM	C5-C6-C7-C8
27	c	523	PLM	CC-CD-CE-CF
22	B	612	CLA	CBA-CGA-O2A-C1
31	d	406	LHG	C12-C13-C14-C15
34	H	101	DGD	CCA-CDA-CEA-CFA
34	c	505	DGD	C6B-C7B-C8B-C9B
27	B	622	PLM	C5-C6-C7-C8
22	B	603	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	C	513	CLA	CAD-CBD-CGD-O2D
22	C	514	CLA	CAD-CBD-CGD-O2D
22	b	605	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	CAD-CBD-CGD-O2D
22	c	514	CLA	CAD-CBD-CGD-O2D
22	c	518	CLA	CAD-CBD-CGD-O2D
27	e	102	PLM	C8-C9-CA-CB
31	l	101	LHG	C34-C35-C36-C37
35	c	524	LMG	C15-C16-C17-C18
33	T	101	LMT	O5'-C5'-C6'-O6'
26	l	102	SQD	C14-C15-C16-C17
33	C	518	LMT	O5'-C1'-O1'-C1
34	C	503	DGD	O6E-C1E-O5D-C6D
34	c	503	DGD	O6E-C1E-O5D-C6D
35	c	519	LMG	C10-C11-C12-C13
31	a	421	LHG	C2-C3-O3-P
34	c	505	DGD	O1G-C1G-C2G-C3G
34	d	410	DGD	O1G-C1G-C2G-C3G
27	j	103	PLM	CA-CB-CC-CD
28	a	414	LFA	C6-C7-C8-C9
22	b	615	CLA	C10-C11-C12-C13
23	D	403	PHO	C10-C11-C12-C13
27	j	103	PLM	C6-C7-C8-C9
22	c	506	CLA	C2A-CAA-CBA-CGA
23	a	420	PHO	C10-C11-C12-C13
31	D	408	LHG	C9-C10-C11-C12
27	F	102	PLM	C2-C3-C4-C5
31	d	406	LHG	C9-C10-C11-C12
22	A	405	CLA	CHA-CBD-CGD-O2D
22	B	604	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D
22	B	609	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O2D
22	C	506	CLA	CHA-CBD-CGD-O1D
22	C	506	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	CHA-CBD-CGD-O1D
22	b	606	CLA	CHA-CBD-CGD-O1D
22	b	608	CLA	CHA-CBD-CGD-O1D
22	b	608	CLA	CHA-CBD-CGD-O2D
22	b	611	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	512	CLA	CHA-CBD-CGD-O1D
33	C	518	LMT	C2'-C1'-O1'-C1
27	C	522	PLM	C6-C7-C8-C9
26	A	410	SQD	O47-C45-C46-O48
26	a	417	SQD	O47-C45-C46-O48
34	c	505	DGD	O6E-C5E-C6E-O5E
22	B	612	CLA	O1A-CGA-O2A-C1
33	j	101	LMT	C7-C8-C9-C10
31	D	407	LHG	O1-C1-C2-O2
31	a	421	LHG	O1-C1-C2-O2
31	d	405	LHG	O1-C1-C2-O2
34	C	503	DGD	C5A-C6A-C7A-C8A
35	C	525	LMG	C16-C17-C18-C19
25	A	409	PL9	C4-C3-C7-C8
25	a	410	PL9	C4-C3-C7-C8
22	B	601	CLA	C11-C12-C13-C14
22	B	604	CLA	C6-C7-C8-C9
22	B	611	CLA	C14-C13-C15-C16
22	b	603	CLA	C11-C12-C13-C14
27	D	410	PLM	CA-CB-CC-CD
34	D	411	DGD	C4B-C5B-C6B-C7B
22	b	614	CLA	O1A-CGA-O2A-C1
27	d	411	PLM	C4-C5-C6-C7
22	C	505	CLA	C2A-CAA-CBA-CGA
27	b	625	PLM	C9-CA-CB-CC
31	D	407	LHG	C29-C30-C31-C32
27	B	625	PLM	C4-C5-C6-C7
27	e	102	PLM	C7-C8-C9-CA
24	B	617	BCR	C17-C18-C19-C20
24	C	502	BCR	C17-C18-C19-C20
24	c	502	BCR	C17-C18-C19-C20
27	x	101	PLM	C5-C6-C7-C8
22	C	505	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C1A-C2A-CAA-CBA
22	c	509	CLA	C1A-C2A-CAA-CBA
22	b	608	CLA	C16-C17-C18-C19
22	c	513	CLA	C16-C17-C18-C20
22	A	404	CLA	C2-C1-O2A-CGA
22	a	405	CLA	C2-C1-O2A-CGA
24	Y	102	BCR	C19-C20-C21-C22
31	L	101	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
31	d	406	LHG	C4-O6-P-O3
28	d	408	LFA	C11-C12-C13-C14
22	D	406	CLA	O1D-CGD-O2D-CED
28	i	101	LFA	C4-C5-C6-C7
31	L	101	LHG	C4-O6-P-O5
31	a	415	LHG	C4-O6-P-O4
31	l	101	LHG	C4-O6-P-O5
22	B	609	CLA	C16-C17-C18-C20
22	a	408	CLA	C16-C17-C18-C19
22	c	511	CLA	C16-C17-C18-C19
22	c	510	CLA	C13-C15-C16-C17
27	A	411	PLM	CC-CD-CE-CF
28	i	103	LFA	C10-C11-C12-C13
33	z	101	LMT	C4B-C5B-C6B-O6B
26	A	415	SQD	C14-C15-C16-C17
27	j	102	PLM	CA-CB-CC-CD
28	J	101	LFA	C10-C11-C12-C13
34	h	101	DGD	C3B-C4B-C5B-C6B
22	B	601	CLA	CAD-CBD-CGD-O1D
22	B	609	CLA	CAD-CBD-CGD-O1D
22	C	506	CLA	CAD-CBD-CGD-O1D
22	C	510	CLA	CAD-CBD-CGD-O1D
22	b	603	CLA	CAD-CBD-CGD-O1D
22	b	611	CLA	CAD-CBD-CGD-O1D
22	c	507	CLA	CAD-CBD-CGD-O1D
22	c	508	CLA	CAD-CBD-CGD-O1D
22	c	511	CLA	CAD-CBD-CGD-O1D
26	A	410	SQD	C5-C6-S-O9
26	b	601	SQD	C5-C6-S-O9
26	l	102	SQD	C5-C6-S-O7
22	c	513	CLA	C5-C6-C7-C8
26	a	411	SQD	C27-C28-C29-C30
33	Z	101	LMT	C11-C10-C9-C8
34	c	505	DGD	C1B-C2B-C3B-C4B
26	a	411	SQD	C32-C33-C34-C35
28	I	103	LFA	C11-C10-C9-C8
34	H	101	DGD	C6B-C7B-C8B-C9B
26	a	411	SQD	C11-C12-C13-C14
31	d	405	LHG	C29-C30-C31-C32
35	C	525	LMG	C12-C13-C14-C15
35	M	101	LMG	C16-C17-C18-C19
22	C	512	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	a	410	PL9	C15-C14-C16-C17
22	A	407	CLA	C11-C10-C8-C7
22	B	601	CLA	C11-C10-C8-C7
22	B	604	CLA	C11-C12-C13-C15
22	B	609	CLA	C12-C13-C15-C16
22	C	505	CLA	C11-C12-C13-C15
22	b	603	CLA	C11-C10-C8-C7
22	b	606	CLA	C11-C12-C13-C15
22	b	611	CLA	C12-C13-C15-C16
22	c	511	CLA	C6-C7-C8-C10
22	c	518	CLA	C11-C10-C8-C7
22	c	518	CLA	C12-C13-C15-C16
25	D	404	PL9	C13-C14-C16-C17
25	D	404	PL9	C33-C34-C36-C37
25	d	402	PL9	C13-C14-C16-C17
31	d	405	LHG	C19-C20-C21-C22
24	y	102	BCR	C19-C20-C21-C22
27	B	629	PLM	C6-C7-C8-C9
27	b	627	PLM	C1-C2-C3-C4
22	c	512	CLA	O1D-CGD-O2D-CED
35	C	525	LMG	C14-C15-C16-C17
35	m	101	LMG	C16-C17-C18-C19
26	D	412	SQD	C9-C10-C11-C12
27	C	522	PLM	C4-C5-C6-C7
28	d	408	LFA	C16-C17-C18-C19
26	A	410	SQD	C44-C45-C46-O48
26	l	102	SQD	O6-C44-C45-C46
28	i	101	LFA	C10-C11-C12-C13
34	c	504	DGD	O1G-C1G-C2G-C3G
34	c	505	DGD	C1G-C2G-C3G-O3G
35	C	519	LMG	O1-C7-C8-C9
35	c	519	LMG	O1-C7-C8-C9
35	c	519	LMG	C39-C40-C41-C42
26	l	102	SQD	O6-C44-C45-O47
34	c	505	DGD	O1G-C1G-C2G-O2G
35	C	519	LMG	O1-C7-C8-O7
35	C	519	LMG	O7-C8-C9-O8
35	Y	101	LMG	O7-C8-C9-O8
26	b	601	SQD	C11-C12-C13-C14
33	C	518	LMT	O1'-C1-C2-C3
35	C	525	LMG	C15-C16-C17-C18
26	a	417	SQD	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
27	X	101	PLM	C5-C6-C7-C8
31	l	101	LHG	C18-C19-C20-C21
35	M	101	LMG	C34-C35-C36-C37
35	C	525	LMG	C8-C7-O1-C1
26	d	412	SQD	O47-C7-C8-C9
26	b	601	SQD	C33-C34-C35-C36
26	l	102	SQD	C13-C14-C15-C16
28	d	408	LFA	C10-C11-C12-C13
22	A	405	CLA	C14-C13-C15-C16
22	B	610	CLA	C11-C12-C13-C14
22	a	406	CLA	C14-C13-C15-C16
22	b	606	CLA	C6-C7-C8-C9
22	b	608	CLA	C14-C13-C15-C16
22	b	612	CLA	C11-C12-C13-C14
22	b	613	CLA	C14-C13-C15-C16
23	D	403	PHO	C11-C10-C8-C9
23	a	420	PHO	C11-C10-C8-C9
26	a	417	SQD	C11-C10-C9-C8
27	B	621	PLM	C8-C9-CA-CB
22	B	608	CLA	C13-C15-C16-C17
27	t	101	PLM	C1-C2-C3-C4
35	C	519	LMG	C32-C33-C34-C35
28	d	409	LFA	C12-C13-C14-C15
31	a	421	LHG	C26-C27-C28-C29
28	C	521	LFA	C11-C10-C9-C8
24	B	617	BCR	C21-C22-C23-C24
24	T	103	BCR	C17-C18-C19-C20
28	E	102	LFA	C5-C6-C7-C8
35	C	525	LMG	C17-C18-C19-C20
27	C	522	PLM	C5-C6-C7-C8
31	E	101	LHG	C10-C11-C12-C13
25	D	404	PL9	C38-C39-C41-C42
34	c	504	DGD	C3A-C4A-C5A-C6A
22	B	601	CLA	C10-C11-C12-C13
22	B	602	CLA	C8-C10-C11-C12
22	b	610	CLA	C13-C15-C16-C17
26	l	102	SQD	C12-C13-C14-C15
33	B	633	LMT	C5-C6-C7-C8
26	l	102	SQD	O48-C23-C24-C25
31	a	421	LHG	C9-C10-C11-C12
26	b	601	SQD	C46-C45-O47-C7
33	J	103	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
28	a	418	LFA	C6-C7-C8-C9
22	D	405	CLA	C2-C1-O2A-CGA
22	d	403	CLA	C2-C1-O2A-CGA
27	j	103	PLM	C2-C3-C4-C5
31	L	101	LHG	C9-C10-C11-C12
35	y	101	LMG	C16-C17-C18-C19
27	C	523	PLM	C8-C9-CA-CB
35	C	525	LMG	C13-C14-C15-C16
22	C	505	CLA	C16-C17-C18-C20
22	b	603	CLA	C10-C11-C12-C13
31	D	407	LHG	C12-C13-C14-C15
24	B	632	BCR	C23-C24-C25-C30
24	C	502	BCR	C1-C6-C7-C8
24	K	101	BCR	C1-C6-C7-C8
37	h	102	RRX	C23-C24-C25-C30
37	h	102	RRX	C23-C24-C25-C26
25	d	402	PL9	C33-C34-C36-C37
25	d	402	PL9	C38-C39-C41-C42
33	m	102	LMT	C4-C5-C6-C7
35	c	519	LMG	C20-C21-C22-C23
22	a	408	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C20
28	i	101	LFA	C2-C3-C4-C5
22	a	406	CLA	C2A-CAA-CBA-CGA
25	a	410	PL9	C39-C41-C42-C43
34	C	503	DGD	C2E-C1E-O5D-C6D
34	c	503	DGD	C2E-C1E-O5D-C6D
34	d	410	DGD	O1G-C1G-C2G-O2G
27	C	520	PLM	C7-C8-C9-CA
22	b	613	CLA	CBD-CGD-O2D-CED
31	D	408	LHG	C3-O3-P-O6
31	D	408	LHG	C4-O6-P-O3
31	d	406	LHG	C3-O3-P-O6
31	l	101	LHG	C3-O3-P-O6
22	B	606	CLA	C16-C17-C18-C19
28	d	409	LFA	C9-C10-C11-C12
35	D	409	LMG	C14-C15-C16-C17
31	A	417	LHG	C4-C5-C6-O8
34	D	411	DGD	C6B-C7B-C8B-C9B
22	B	611	CLA	C12-C13-C15-C16
22	B	614	CLA	C2-C3-C5-C6
22	c	510	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	a	410	PL9	C43-C44-C46-C47
22	B	604	CLA	C11-C12-C13-C14
22	B	609	CLA	C14-C13-C15-C16
22	B	615	CLA	C14-C13-C15-C16
22	C	508	CLA	C14-C13-C15-C16
22	D	405	CLA	C11-C12-C13-C14
22	a	408	CLA	C11-C10-C8-C9
22	b	606	CLA	C11-C12-C13-C14
22	b	617	CLA	C14-C13-C15-C16
22	c	509	CLA	C14-C13-C15-C16
22	d	403	CLA	C11-C12-C13-C14
24	c	502	BCR	C13-C14-C15-C16
22	C	513	CLA	C16-C17-C18-C19
27	c	523	PLM	C6-C7-C8-C9
28	i	101	LFA	C5-C6-C7-C8
35	D	409	LMG	C32-C33-C34-C35
22	A	405	CLA	C2A-CAA-CBA-CGA
35	d	407	LMG	C10-C11-C12-C13
27	M	103	PLM	C6-C7-C8-C9
31	d	406	LHG	C25-C26-C27-C28
28	B	620	LFA	C7-C8-C9-C10
31	E	101	LHG	O1-C1-C2-C3
27	t	101	PLM	CA-CB-CC-CD
35	d	407	LMG	C34-C35-C36-C37
31	E	101	LHG	C18-C19-C20-C21
25	D	404	PL9	C37-C38-C39-C41
22	B	609	CLA	C16-C17-C18-C19
28	J	101	LFA	C6-C7-C8-C9
31	L	101	LHG	C35-C36-C37-C38
31	l	101	LHG	C9-C10-C11-C12
33	M	102	LMT	C4-C5-C6-C7
34	C	504	DGD	C7A-C8A-C9A-CAA
34	d	410	DGD	C2A-C3A-C4A-C5A
24	C	502	BCR	C19-C20-C21-C22
24	b	602	BCR	C15-C16-C17-C18
24	c	502	BCR	C19-C20-C21-C22
26	d	412	SQD	C32-C33-C34-C35
25	a	410	PL9	C14-C16-C17-C18
31	D	407	LHG	C19-C20-C21-C22
27	a	412	PLM	O2-C1-C2-C3
31	D	408	LHG	C15-C16-C17-C18
22	b	611	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	a	410	PL9	C40-C39-C41-C42
31	A	417	LHG	C11-C12-C13-C14
33	B	623	LMT	C1-C2-C3-C4
27	b	625	PLM	O2-C1-C2-C3
36	e	103	HEM	CAD-CBD-CGD-O1D
22	B	614	CLA	C2A-CAA-CBA-CGA
35	C	519	LMG	C20-C21-C22-C23
35	C	525	LMG	C22-C23-C24-C25
22	b	613	CLA	O1D-CGD-O2D-CED
26	b	601	SQD	C31-C32-C33-C34
22	B	607	CLA	C3A-C2A-CAA-CBA
22	B	608	CLA	C3A-C2A-CAA-CBA
22	b	609	CLA	C3A-C2A-CAA-CBA
22	b	610	CLA	C3A-C2A-CAA-CBA
27	c	522	PLM	O2-C1-C2-C3
35	D	409	LMG	C34-C35-C36-C37
26	d	412	SQD	C24-C25-C26-C27
31	d	405	LHG	C12-C13-C14-C15
33	T	101	LMT	C6-C7-C8-C9
34	D	411	DGD	CCB-CDB-CEB-CFB
36	e	103	HEM	CAD-CBD-CGD-O2D
35	D	409	LMG	C10-C11-C12-C13
35	d	407	LMG	C32-C33-C34-C35
22	A	407	CLA	C11-C10-C8-C9
22	B	604	CLA	C11-C10-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	D	401	CLA	C11-C12-C13-C14
22	b	606	CLA	C11-C10-C8-C9
22	c	510	CLA	C6-C7-C8-C9
22	c	518	CLA	C11-C10-C8-C9
22	c	518	CLA	C14-C13-C15-C16
22	d	401	CLA	C11-C12-C13-C14
22	d	404	CLA	C11-C12-C13-C14
31	A	417	LHG	C26-C27-C28-C29
35	c	519	LMG	C40-C41-C42-C43
26	a	411	SQD	C11-C10-C9-C8
28	C	521	LFA	C7-C8-C9-C10
28	J	104	LFA	C9-C10-C11-C12
26	b	601	SQD	C35-C36-C37-C38
35	y	101	LMG	C40-C41-C42-C43
36	E	104	HEM	CAD-CBD-CGD-O2D
27	B	627	PLM	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
31	A	417	LHG	C30-C31-C32-C33
22	D	406	CLA	C16-C17-C18-C19
22	C	515	CLA	CBA-CGA-O2A-C1
26	l	102	SQD	C28-C29-C30-C31
27	j	102	PLM	CC-CD-CE-CF
27	j	102	PLM	O2-C1-C2-C3
27	d	411	PLM	O2-C1-C2-C3
22	C	508	CLA	C1A-C2A-CAA-CBA
22	c	518	CLA	C1A-C2A-CAA-CBA
22	B	603	CLA	C11-C10-C8-C7
22	B	604	CLA	C12-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C7
22	C	506	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C7
22	b	606	CLA	C12-C13-C15-C16
22	b	608	CLA	C12-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C7
22	c	517	CLA	C11-C12-C13-C15
31	D	408	LHG	C25-C26-C27-C28
27	C	522	PLM	O2-C1-C2-C3
27	d	411	PLM	O1-C1-C2-C3
27	t	101	PLM	CB-CC-CD-CE
24	y	102	BCR	C9-C10-C11-C12
26	d	412	SQD	C28-C29-C30-C31
27	b	625	PLM	O1-C1-C2-C3
36	E	104	HEM	CAD-CBD-CGD-O1D
28	i	101	LFA	C17-C18-C19-C20
22	A	407	CLA	C3-C5-C6-C7
22	B	605	CLA	C2A-CAA-CBA-CGA
22	b	607	CLA	C2A-CAA-CBA-CGA
28	I	101	LFA	C12-C13-C14-C15
34	h	101	DGD	O2G-C1B-C2B-C3B
26	a	411	SQD	C30-C31-C32-C33
27	e	101	PLM	C3-C4-C5-C6
27	C	524	PLM	O2-C1-C2-C3
27	j	102	PLM	O1-C1-C2-C3
22	b	617	CLA	C10-C11-C12-C13
31	a	421	LHG	C28-C29-C30-C31
35	C	519	LMG	C33-C34-C35-C36
28	J	101	LFA	C2-C3-C4-C5
26	a	411	SQD	O47-C45-C46-O48
31	A	417	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
24	Y	102	BCR	C9-C10-C11-C12
22	B	610	CLA	C16-C17-C18-C19
27	B	621	PLM	C7-C8-C9-CA
27	D	410	PLM	O1-C1-C2-C3
27	a	412	PLM	O1-C1-C2-C3
36	V	201	HEM	CAD-CBD-CGD-O2D
28	T	102	LFA	C6-C7-C8-C9
22	C	506	CLA	C2-C1-O2A-CGA
22	c	507	CLA	C2-C1-O2A-CGA
28	E	102	LFA	C13-C14-C15-C16
22	D	406	CLA	C11-C12-C13-C14
22	b	611	CLA	C14-C13-C15-C16
22	C	515	CLA	O1A-CGA-O2A-C1
35	C	519	LMG	C30-C31-C32-C33
31	E	101	LHG	O2-C2-C3-O3
26	D	412	SQD	C27-C28-C29-C30
22	B	603	CLA	C2A-CAA-CBA-CGA
22	b	605	CLA	C2A-CAA-CBA-CGA
22	b	616	CLA	C2A-CAA-CBA-CGA
27	c	522	PLM	O1-C1-C2-C3
26	A	415	SQD	O49-C7-C8-C9
24	A	408	BCR	C23-C24-C25-C30
24	Y	102	BCR	C23-C24-C25-C30
24	a	409	BCR	C23-C24-C25-C30
24	b	602	BCR	C23-C24-C25-C30
24	k	101	BCR	C1-C6-C7-C8
24	y	102	BCR	C23-C24-C25-C30
37	H	102	RRX	C23-C24-C25-C30
37	H	102	RRX	C23-C24-C25-C26
37	H	102	RRX	C1-C6-C7-C8
37	h	102	RRX	C1-C6-C7-C8
26	D	412	SQD	O47-C7-C8-C9
26	a	417	SQD	O47-C7-C8-C9
34	H	101	DGD	O2G-C1B-C2B-C3B
27	D	410	PLM	C6-C7-C8-C9
33	B	623	LMT	O1'-C1-C2-C3
34	c	503	DGD	C9A-CAA-CBA-CCA
27	C	524	PLM	O1-C1-C2-C3
22	C	512	CLA	C5-C6-C7-C8
32	a	401	GOL	C1-C2-C3-O3
34	C	504	DGD	C3A-C4A-C5A-C6A
24	b	602	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	K	101	BCR	C21-C22-C23-C24
22	b	612	CLA	C16-C17-C18-C19
27	M	103	PLM	O1-C1-C2-C3
34	c	505	DGD	C7A-C8A-C9A-CAA
34	C	503	DGD	C5D-C6D-O5D-C1E
34	c	503	DGD	C5D-C6D-O5D-C1E
27	b	621	PLM	C2-C3-C4-C5
33	J	103	LMT	C2-C3-C4-C5
27	B	629	PLM	O1-C1-C2-C3
27	C	522	PLM	O1-C1-C2-C3
27	D	410	PLM	O2-C1-C2-C3
22	C	506	CLA	C15-C16-C17-C18
22	b	604	CLA	C8-C10-C11-C12
22	b	608	CLA	C10-C11-C12-C13
22	d	404	CLA	C16-C17-C18-C20
34	c	503	DGD	C8A-C9A-CAA-CBA
22	C	511	CLA	C5-C6-C7-C8
22	C	510	CLA	C6-C7-C8-C10
22	D	401	CLA	C11-C12-C13-C15
22	b	613	CLA	C12-C13-C15-C16
22	d	401	CLA	C11-C12-C13-C15
23	D	403	PHO	C11-C10-C8-C7
23	a	420	PHO	C11-C10-C8-C7
27	e	101	PLM	O2-C1-C2-C3
32	a	401	GOL	O2-C2-C3-O3
24	C	501	BCR	C9-C10-C11-C12
27	A	411	PLM	C5-C6-C7-C8
31	a	421	LHG	C29-C30-C31-C32
27	e	101	PLM	O1-C1-C2-C3
36	V	201	HEM	CAD-CBD-CGD-O1D
22	B	612	CLA	CAA-CBA-CGA-O2A
22	b	615	CLA	CAA-CBA-CGA-O2A
22	B	609	CLA	C15-C16-C17-C18
27	B	629	PLM	O2-C1-C2-C3
26	b	601	SQD	C26-C27-C28-C29
22	B	613	CLA	CAA-CBA-CGA-O2A
22	b	614	CLA	CAA-CBA-CGA-O2A
26	a	411	SQD	O48-C23-C24-C25
22	C	508	CLA	C4-C3-C5-C6
25	D	404	PL9	C30-C29-C31-C32
25	a	410	PL9	C12-C11-C9-C10
25	d	402	PL9	C30-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
28	A	412	LFA	C11-C10-C9-C8
25	A	409	PL9	C28-C29-C31-C32
31	d	406	LHG	C26-C27-C28-C29
22	B	610	CLA	C16-C17-C18-C20
22	C	510	CLA	C16-C17-C18-C19
22	B	612	CLA	C11-C10-C8-C9
22	C	505	CLA	C11-C12-C13-C14
22	b	614	CLA	C11-C10-C8-C9
22	c	511	CLA	C6-C7-C8-C9
22	c	517	CLA	C11-C12-C13-C14
27	c	521	PLM	C3-C4-C5-C6
26	A	415	SQD	C29-C30-C31-C32
33	T	104	LMT	C6-C7-C8-C9
23	D	403	PHO	C3A-C2A-CAA-CBA
27	a	412	PLM	C2-C3-C4-C5
31	a	415	LHG	O8-C23-C24-C25
35	c	524	LMG	C34-C35-C36-C37
27	C	520	PLM	O2-C1-C2-C3
22	B	607	CLA	CAD-CBD-CGD-O2D
22	B	610	CLA	CAD-CBD-CGD-O2D
22	B	616	CLA	CAD-CBD-CGD-O2D
22	C	509	CLA	CAD-CBD-CGD-O2D
22	C	517	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	b	612	CLA	CAD-CBD-CGD-O2D
22	b	618	CLA	CAD-CBD-CGD-O2D
22	c	510	CLA	CAD-CBD-CGD-O2D
22	D	406	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C19
22	b	612	CLA	C16-C17-C18-C20
31	D	407	LHG	C26-C27-C28-C29
35	C	525	LMG	O9-C10-O7-C8
25	d	402	PL9	C37-C38-C39-C41
31	d	405	LHG	C26-C27-C28-C29
34	c	504	DGD	C5A-C6A-C7A-C8A
22	c	517	CLA	C4-C3-C5-C6
25	A	409	PL9	C35-C34-C36-C37
26	b	601	SQD	O5-C1-O6-C44
25	A	409	PL9	C12-C11-C9-C8
22	C	514	CLA	CAA-CBA-CGA-O2A
22	c	515	CLA	CAA-CBA-CGA-O2A
34	C	503	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
34	c	503	DGD	O2G-C1B-C2B-C3B
27	B	621	PLM	C4-C5-C6-C7
27	D	402	PLM	C4-C5-C6-C7
31	a	415	LHG	C10-C11-C12-C13
26	a	411	SQD	C44-C45-C46-O48
27	e	102	PLM	O2-C1-C2-C3
27	x	101	PLM	O2-C1-C2-C3
34	c	505	DGD	O1G-C1A-C2A-C3A
26	b	601	SQD	C13-C14-C15-C16
35	Y	101	LMG	C12-C13-C14-C15
35	m	101	LMG	C10-C11-C12-C13
27	M	103	PLM	O2-C1-C2-C3
27	b	622	PLM	O1-C1-C2-C3
27	b	627	PLM	O1-C1-C2-C3
27	x	101	PLM	O1-C1-C2-C3
36	v	201	HEM	CAD-CBD-CGD-O1D
36	v	201	HEM	CAD-CBD-CGD-O2D
22	C	513	CLA	O2A-C1-C2-C3
22	C	516	CLA	O2A-C1-C2-C3
22	c	514	CLA	O2A-C1-C2-C3
22	c	517	CLA	O2A-C1-C2-C3
23	A	406	PHO	O2A-C1-C2-C3
22	A	407	CLA	C8-C10-C11-C12
22	c	511	CLA	C15-C16-C17-C18
27	C	520	PLM	C8-C9-CA-CB
35	d	407	LMG	C33-C34-C35-C36
26	A	410	SQD	C10-C11-C12-C13
35	m	101	LMG	O9-C10-O7-C8
22	B	603	CLA	CHA-CBD-CGD-O2D
22	B	604	CLA	CHA-CBD-CGD-O2D
22	B	609	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O2D
22	C	511	CLA	CHA-CBD-CGD-O1D
22	C	511	CLA	CHA-CBD-CGD-O2D
22	b	605	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	CHA-CBD-CGD-O2D
22	b	611	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CHA-CBD-CGD-O2D
22	c	511	CLA	CHA-CBD-CGD-O1D
22	c	511	CLA	CHA-CBD-CGD-O2D
22	c	512	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	f	101	BCR	C13-C14-C15-C16
27	b	622	PLM	O2-C1-C2-C3
27	b	627	PLM	O2-C1-C2-C3
26	l	102	SQD	O47-C7-C8-C9
31	d	406	LHG	C15-C16-C17-C18
35	C	519	LMG	C34-C35-C36-C37
35	C	525	LMG	C29-C30-C31-C32
22	c	517	CLA	C13-C15-C16-C17
35	m	101	LMG	O8-C28-C29-C30
27	b	621	PLM	CB-CC-CD-CE
22	C	516	CLA	C13-C15-C16-C17
23	D	403	PHO	CHA-CBD-CGD-O1D
23	D	403	PHO	CHA-CBD-CGD-O2D
23	a	420	PHO	CHA-CBD-CGD-O1D
27	a	412	PLM	C4-C5-C6-C7
27	j	103	PLM	CD-CE-CF-CG
33	A	419	LMT	C4-C5-C6-C7
27	e	102	PLM	O1-C1-C2-C3
35	C	519	LMG	C40-C41-C42-C43
35	c	524	LMG	C28-C29-C30-C31
27	C	520	PLM	C2-C3-C4-C5
27	L	102	PLM	C8-C9-CA-CB
35	M	101	LMG	O9-C10-O7-C8
35	y	101	LMG	O9-C10-O7-C8
35	C	519	LMG	O6-C1-O1-C7
22	B	603	CLA	C11-C10-C8-C9
22	B	604	CLA	C14-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C9
22	b	605	CLA	C11-C10-C8-C9
22	b	606	CLA	C14-C13-C15-C16
27	t	101	PLM	C5-C6-C7-C8
35	d	407	LMG	C14-C15-C16-C17
31	a	415	LHG	O7-C7-C8-C9
26	a	411	SQD	C5-C6-S-O8
28	i	103	LFA	C7-C8-C9-C10
27	C	520	PLM	O1-C1-C2-C3
28	d	408	LFA	C17-C18-C19-C20
31	d	406	LHG	C28-C29-C30-C31
22	B	608	CLA	CBA-CGA-O2A-C1
26	l	102	SQD	C11-C10-C9-C8
27	d	411	PLM	C1-C2-C3-C4
22	B	613	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	b	615	CLA	CAA-CBA-CGA-O1A
34	c	503	DGD	O1B-C1B-C2B-C3B
31	l	101	LHG	O1-C1-C2-C3
31	D	407	LHG	C33-C34-C35-C36
35	D	409	LMG	C37-C38-C39-C40
27	X	101	PLM	O2-C1-C2-C3
22	b	610	CLA	CBA-CGA-O2A-C1
27	M	103	PLM	C8-C9-CA-CB
22	B	607	CLA	C1A-C2A-CAA-CBA
22	B	608	CLA	C1A-C2A-CAA-CBA
22	b	609	CLA	C1A-C2A-CAA-CBA
22	b	610	CLA	C1A-C2A-CAA-CBA
31	a	421	LHG	C27-C28-C29-C30
22	C	510	CLA	C16-C17-C18-C20
26	l	102	SQD	O49-C7-C8-C9
22	a	408	CLA	C8-C10-C11-C12
27	x	101	PLM	C8-C9-CA-CB
27	a	412	PLM	CB-CC-CD-CE
28	a	413	LFA	C10-C11-C12-C13
22	C	514	CLA	CAA-CBA-CGA-O1A
22	b	614	CLA	CAA-CBA-CGA-O1A
22	c	515	CLA	CAA-CBA-CGA-O1A
26	a	411	SQD	O10-C23-C24-C25
34	C	503	DGD	O1B-C1B-C2B-C3B
26	a	411	SQD	C10-C11-C12-C13
34	C	503	DGD	C8A-C9A-CAA-CBA
26	A	410	SQD	O48-C23-C24-C25
27	B	622	PLM	C6-C7-C8-C9
28	E	102	LFA	C6-C7-C8-C9
31	D	408	LHG	C11-C12-C13-C14
27	X	101	PLM	C1-C2-C3-C4
22	B	612	CLA	CAA-CBA-CGA-O1A
34	d	410	DGD	C8B-C9B-CAB-CBB
27	c	523	PLM	O1-C1-C2-C3
22	B	602	CLA	C15-C16-C17-C18
31	a	415	LHG	O10-C23-C24-C25
31	E	101	LHG	C16-C17-C18-C19
35	c	524	LMG	C14-C15-C16-C17
22	a	406	CLA	C13-C15-C16-C17
31	A	417	LHG	C15-C16-C17-C18
31	D	408	LHG	C3-O3-P-O5
31	D	408	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
31	L	101	LHG	C3-O3-P-O5
31	d	406	LHG	C3-O3-P-O5
31	d	406	LHG	C4-O6-P-O5
26	A	415	SQD	C30-C31-C32-C33
27	b	621	PLM	C5-C6-C7-C8
33	A	419	LMT	C6-C7-C8-C9
34	c	503	DGD	C2B-C3B-C4B-C5B
35	c	524	LMG	C16-C17-C18-C19
24	B	632	BCR	C23-C24-C25-C26
24	K	101	BCR	C5-C6-C7-C8
24	T	103	BCR	C23-C24-C25-C26
26	A	410	SQD	C26-C27-C28-C29
27	e	101	PLM	C9-CA-CB-CC
27	B	627	PLM	O1-C1-C2-C3
26	l	102	SQD	C27-C28-C29-C30
25	D	404	PL9	C42-C43-C44-C46
31	d	405	LHG	C33-C34-C35-C36
22	B	604	CLA	CAD-CBD-CGD-O1D
22	B	605	CLA	CAD-CBD-CGD-O1D
22	C	508	CLA	CAD-CBD-CGD-O1D
22	b	606	CLA	CAD-CBD-CGD-O1D
22	b	607	CLA	CAD-CBD-CGD-O1D
22	c	509	CLA	CAD-CBD-CGD-O1D
34	c	505	DGD	O1A-C1A-C2A-C3A
27	j	103	PLM	C8-C9-CA-CB
35	C	519	LMG	C31-C32-C33-C34
35	y	101	LMG	C39-C40-C41-C42
34	D	411	DGD	O2G-C1B-C2B-C3B
22	A	405	CLA	C6-C7-C8-C9
22	a	406	CLA	C6-C7-C8-C9
27	M	103	PLM	C5-C6-C7-C8
22	c	513	CLA	C13-C15-C16-C17
22	c	506	CLA	CAA-CBA-CGA-O2A
22	B	605	CLA	C13-C15-C16-C17
22	b	607	CLA	C13-C15-C16-C17
22	c	517	CLA	C8-C10-C11-C12
27	X	101	PLM	O1-C1-C2-C3
35	M	101	LMG	C10-C11-C12-C13
27	A	411	PLM	C8-C9-CA-CB
28	C	521	LFA	C11-C12-C13-C14
31	l	101	LHG	C26-C27-C28-C29
34	c	505	DGD	C8A-C9A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	614	CLA	CAA-CBA-CGA-O2A
22	b	616	CLA	CAA-CBA-CGA-O2A
31	D	407	LHG	O7-C7-C8-C9
31	l	101	LHG	O7-C7-C8-C9
22	b	613	CLA	C8-C10-C11-C12
35	M	101	LMG	C29-C30-C31-C32
35	d	407	LMG	C37-C38-C39-C40
26	A	410	SQD	O10-C23-C24-C25
22	b	612	CLA	C13-C15-C16-C17
25	d	402	PL9	C42-C43-C44-C46
22	C	516	CLA	C11-C12-C13-C15
22	a	406	CLA	C6-C7-C8-C10
25	d	402	PL9	C43-C44-C46-C47
27	A	413	PLM	O2-C1-C2-C3
27	c	523	PLM	O2-C1-C2-C3
22	C	505	CLA	CAA-CBA-CGA-O2A
31	L	101	LHG	O7-C7-C8-C9
35	C	525	LMG	O8-C28-C29-C30
27	B	621	PLM	C2-C3-C4-C5
34	J	102	DGD	C7A-C8A-C9A-CAA
24	b	602	BCR	C21-C22-C23-C24
27	E	103	PLM	O1-C1-C2-C3
27	c	520	PLM	O2-C1-C2-C3
24	a	409	BCR	C19-C20-C21-C22
27	e	101	PLM	CA-CB-CC-CD
33	A	419	LMT	C2-C1-O1'-C1'
33	T	101	LMT	C2-C1-O1'-C1'
31	l	101	LHG	O9-C7-C8-C9
27	A	413	PLM	O1-C1-C2-C3
27	E	103	PLM	C7-C8-C9-CA
22	B	611	CLA	C8-C10-C11-C12
22	c	512	CLA	C5-C6-C7-C8
34	J	102	DGD	O6E-C5E-C6E-O5E
22	A	405	CLA	C13-C15-C16-C17
22	B	615	CLA	C10-C11-C12-C13
31	a	415	LHG	O9-C7-C8-C9
22	B	603	CLA	C13-C15-C16-C17
22	C	505	CLA	C13-C15-C16-C17
22	b	616	CLA	C8-C10-C11-C12
31	a	415	LHG	C16-C17-C18-C19
35	M	101	LMG	C14-C15-C16-C17
35	M	101	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
27	B	627	PLM	O2-C1-C2-C3

There are no ring outliers.

163 monomers are involved in 253 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	408	CLA	2	0
22	C	508	CLA	1	0
27	j	103	PLM	1	0
28	J	104	LFA	1	0
22	c	515	CLA	4	0
22	D	401	CLA	1	0
36	v	201	HEM	1	0
24	B	617	BCR	4	0
36	e	103	HEM	1	0
27	b	622	PLM	1	0
35	C	519	LMG	1	0
22	a	406	CLA	1	0
33	T	101	LMT	1	0
22	d	403	CLA	2	0
22	C	510	CLA	2	0
23	a	407	PHO	1	0
22	C	509	CLA	3	0
24	C	502	BCR	4	0
22	c	510	CLA	2	0
22	c	509	CLA	1	0
22	b	606	CLA	4	0
33	C	518	LMT	1	0
26	l	102	SQD	3	0
22	B	610	CLA	1	0
34	d	410	DGD	1	0
23	A	406	PHO	1	0
22	b	618	CLA	2	0
24	A	408	BCR	1	0
22	c	511	CLA	2	0
22	B	602	CLA	2	0
27	D	402	PLM	1	0
22	B	615	CLA	6	0
33	B	630	LMT	3	0
35	d	407	LMG	2	0
37	h	102	RRX	1	0
28	A	412	LFA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	T	102	LFA	2	0
22	C	513	CLA	1	0
35	D	409	LMG	2	0
27	B	629	PLM	1	0
28	b	623	LFA	2	0
33	z	101	LMT	1	0
24	y	102	BCR	1	0
36	V	201	HEM	1	0
34	c	505	DGD	2	0
31	d	405	LHG	3	0
25	a	410	PL9	4	0
22	c	508	CLA	3	0
24	Y	102	BCR	2	0
27	e	102	PLM	1	0
22	B	616	CLA	2	0
22	b	609	CLA	3	0
27	B	621	PLM	1	0
22	b	617	CLA	6	0
28	B	620	LFA	1	0
24	B	619	BCR	1	0
26	d	412	SQD	3	0
24	c	502	BCR	3	0
22	B	606	CLA	1	0
22	b	605	CLA	1	0
26	a	411	SQD	2	0
35	M	101	LMG	5	0
27	B	622	PLM	1	0
26	A	415	SQD	4	0
33	J	103	LMT	2	0
22	b	613	CLA	1	0
25	d	402	PL9	4	0
24	B	618	BCR	1	0
22	b	614	CLA	2	0
23	D	403	PHO	1	0
32	a	401	GOL	1	0
22	a	405	CLA	2	0
22	b	616	CLA	1	0
34	C	504	DGD	2	0
36	E	104	HEM	1	0
22	B	613	CLA	2	0
22	A	407	CLA	2	0
27	L	102	PLM	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	D	408	LHG	2	0
22	c	513	CLA	4	0
33	B	628	LMT	1	0
26	D	412	SQD	2	0
33	B	633	LMT	1	0
26	A	410	SQD	3	0
27	c	520	PLM	2	0
22	A	405	CLA	1	0
22	b	612	CLA	1	0
22	A	404	CLA	2	0
22	d	404	CLA	2	0
24	C	501	BCR	2	0
27	D	410	PLM	1	0
37	H	102	RRX	1	0
34	H	101	DGD	1	0
28	J	101	LFA	1	0
24	c	501	BCR	1	0
22	b	608	CLA	1	0
22	D	405	CLA	2	0
22	B	609	CLA	1	0
22	B	605	CLA	3	0
22	B	612	CLA	2	0
28	E	102	LFA	2	0
31	a	415	LHG	3	0
31	d	406	LHG	2	0
26	a	417	SQD	2	0
22	b	611	CLA	1	0
28	i	104	LFA	1	0
35	m	101	LMG	4	0
31	D	407	LHG	3	0
31	l	101	LHG	3	0
22	C	516	CLA	3	0
34	D	411	DGD	2	0
22	c	516	CLA	2	0
27	t	101	PLM	2	0
24	K	101	BCR	1	0
27	C	524	PLM	2	0
28	B	626	LFA	2	0
27	x	101	PLM	2	0
24	T	103	BCR	2	0
22	B	608	CLA	1	0
22	C	512	CLA	1	0

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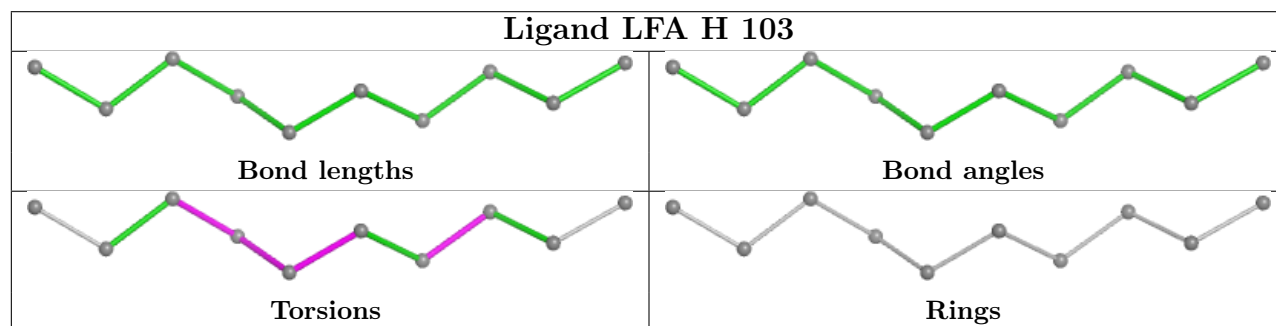
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	k	101	BCR	1	0
35	c	519	LMG	1	0
35	c	524	LMG	2	0
22	b	607	CLA	4	0
28	I	103	LFA	2	0
22	B	607	CLA	3	0
22	B	611	CLA	2	0
27	B	625	PLM	2	0
31	L	101	LHG	4	0
22	c	518	CLA	2	0
22	C	506	CLA	1	0
31	a	421	LHG	2	0
34	c	504	DGD	2	0
22	B	604	CLA	4	0
24	b	619	BCR	3	0
22	C	511	CLA	4	0
24	B	632	BCR	5	0
22	b	610	CLA	3	0
23	a	420	PHO	2	0
24	F	101	BCR	1	0
25	D	404	PL9	4	0
22	d	401	CLA	1	0
33	m	102	LMT	1	0
22	C	514	CLA	4	0
35	Y	101	LMG	2	0
22	C	505	CLA	6	0
24	b	602	BCR	5	0
22	c	506	CLA	5	0
35	y	101	LMG	1	0
22	c	517	CLA	1	0
34	J	102	DGD	3	0
22	c	512	CLA	2	0
22	b	604	CLA	1	0
27	A	413	PLM	2	0
22	C	507	CLA	3	0
22	b	615	CLA	3	0
22	c	507	CLA	2	0
25	A	409	PL9	3	0
26	b	601	SQD	2	0
33	M	102	LMT	1	0
22	C	515	CLA	2	0
24	b	620	BCR	2	0

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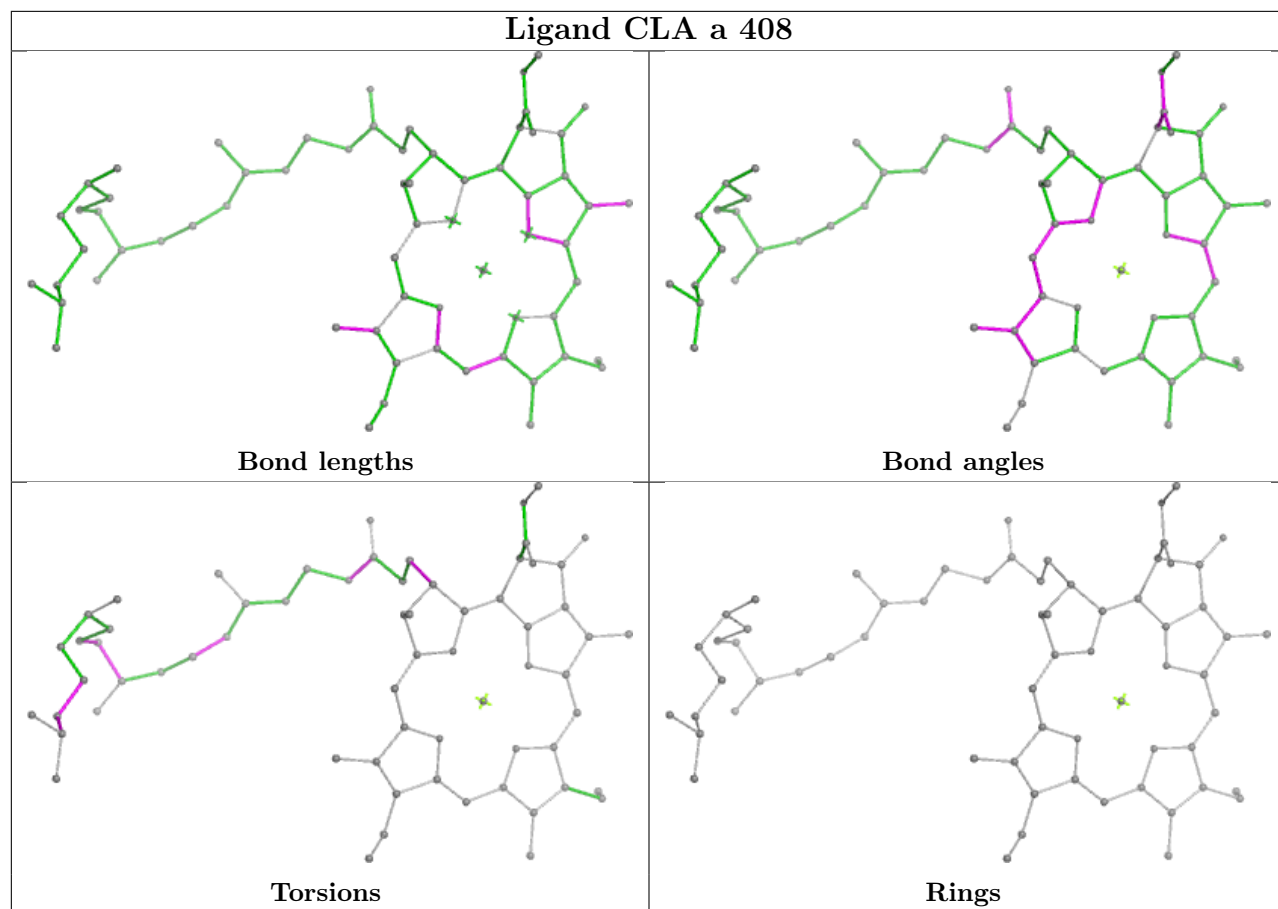
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	417	LHG	1	0

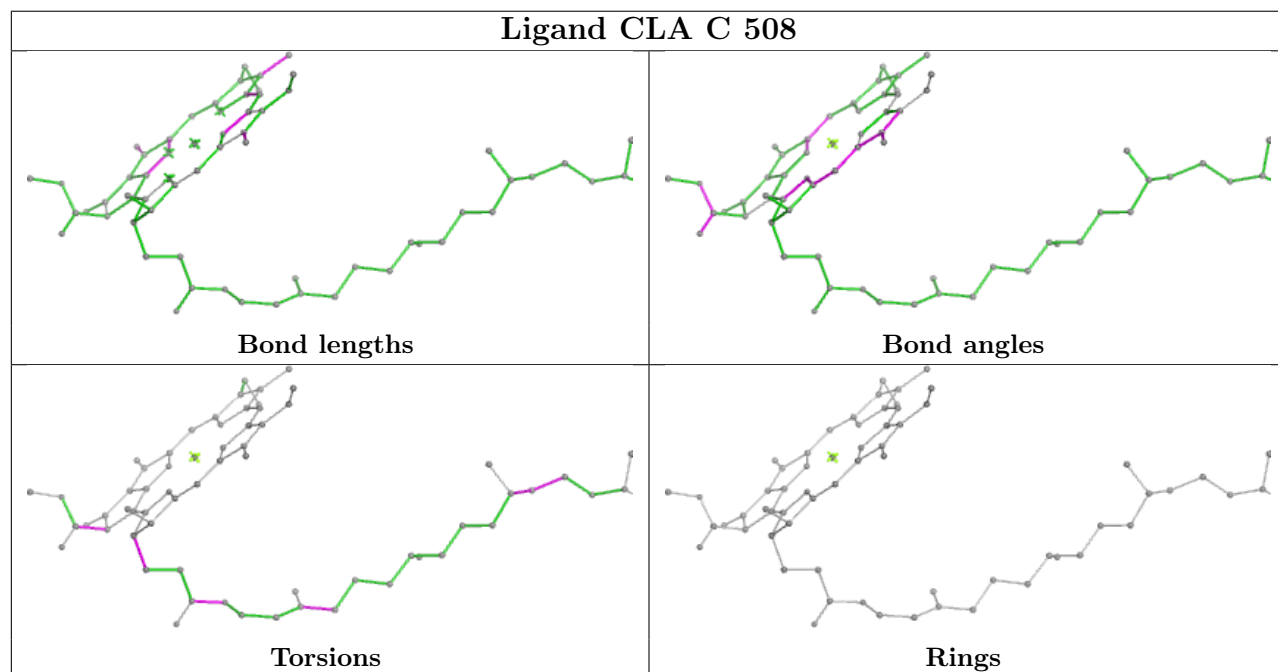
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

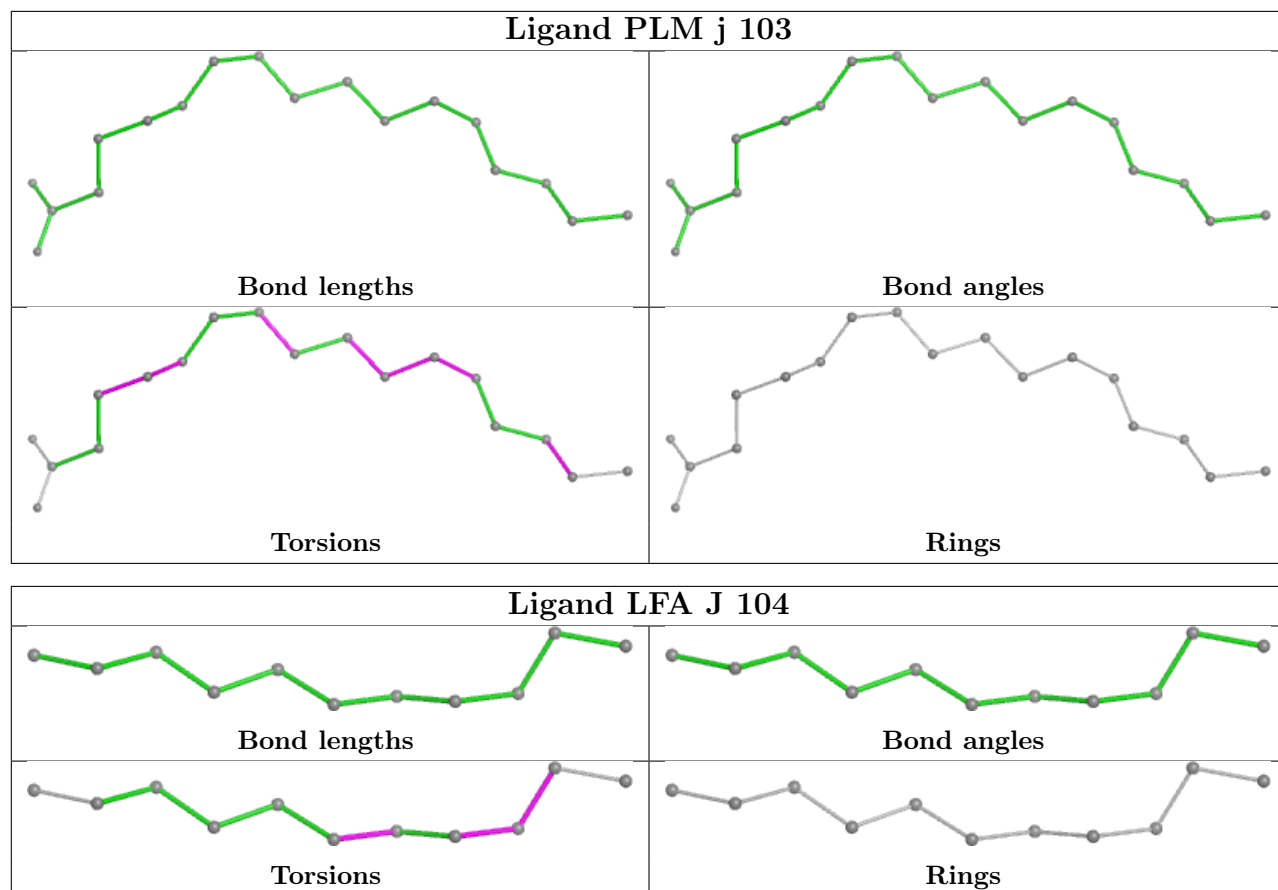


## Ligand CLA a 408

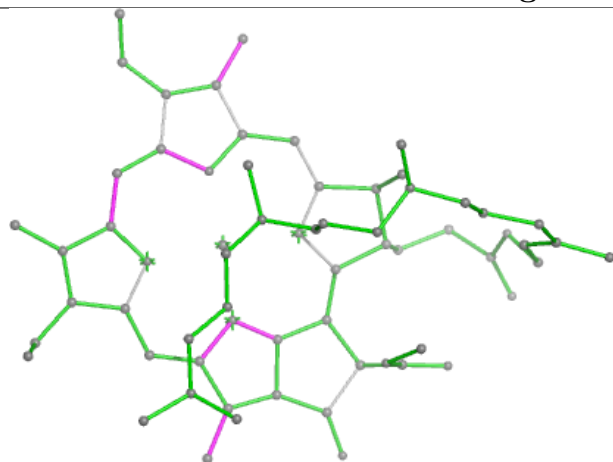


## Ligand CLA C 508

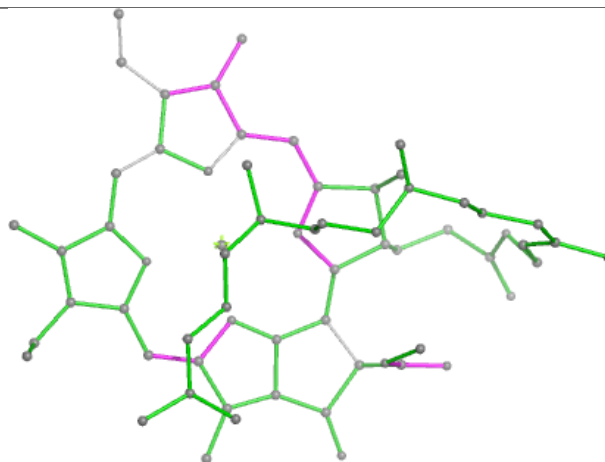




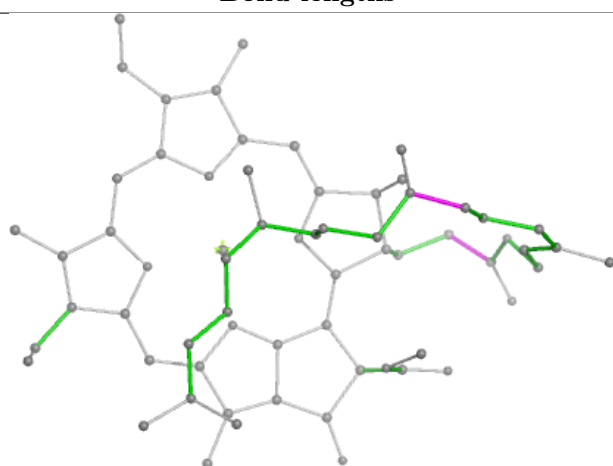
## Ligand CLA c 515



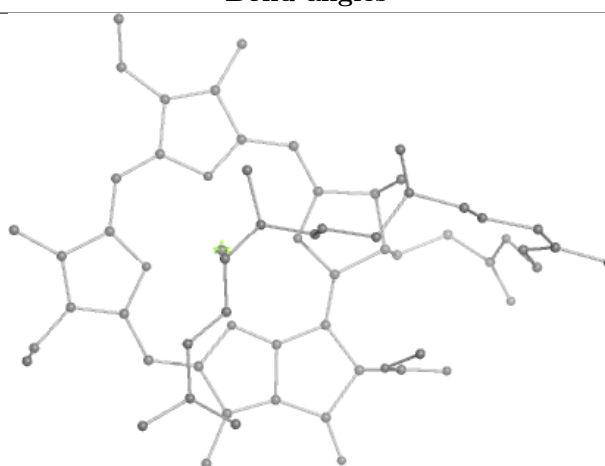
Bond lengths



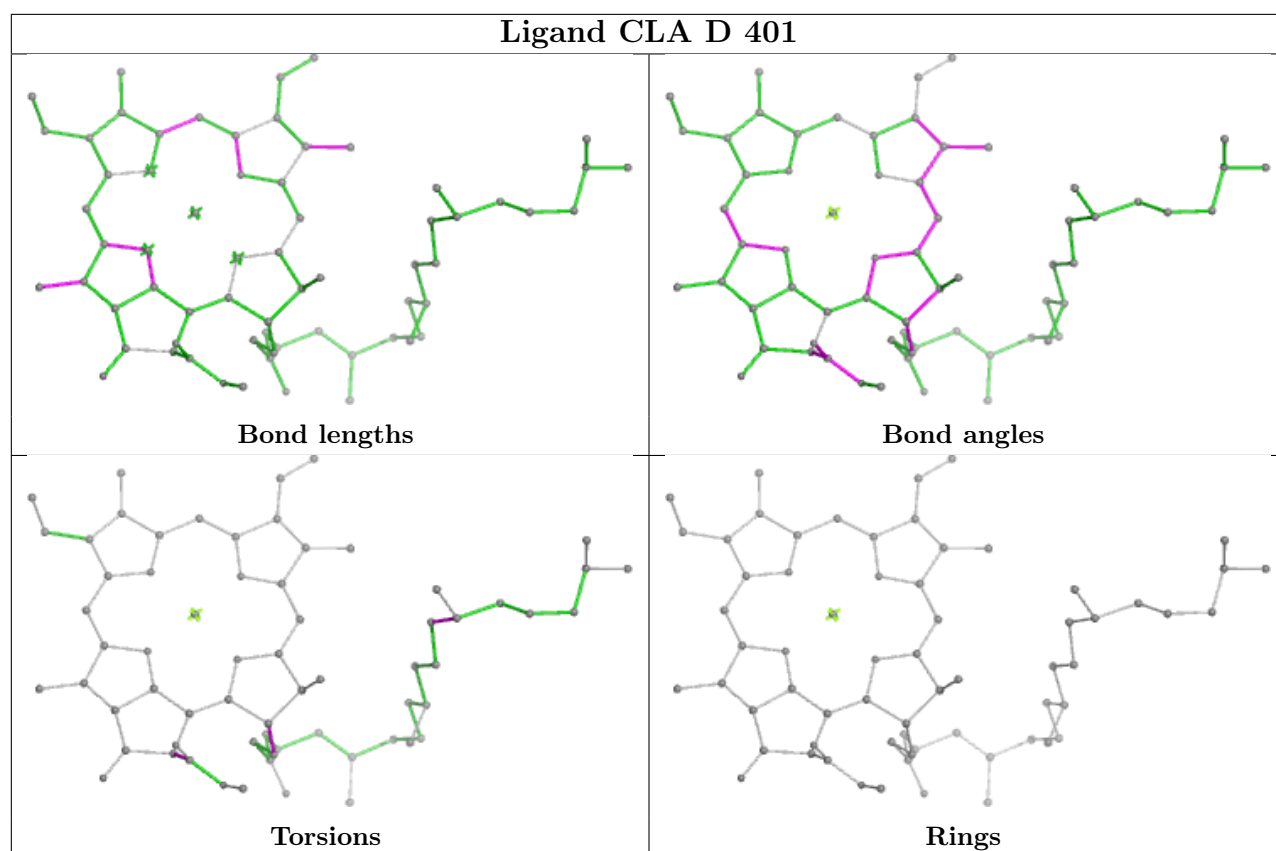
Bond angles



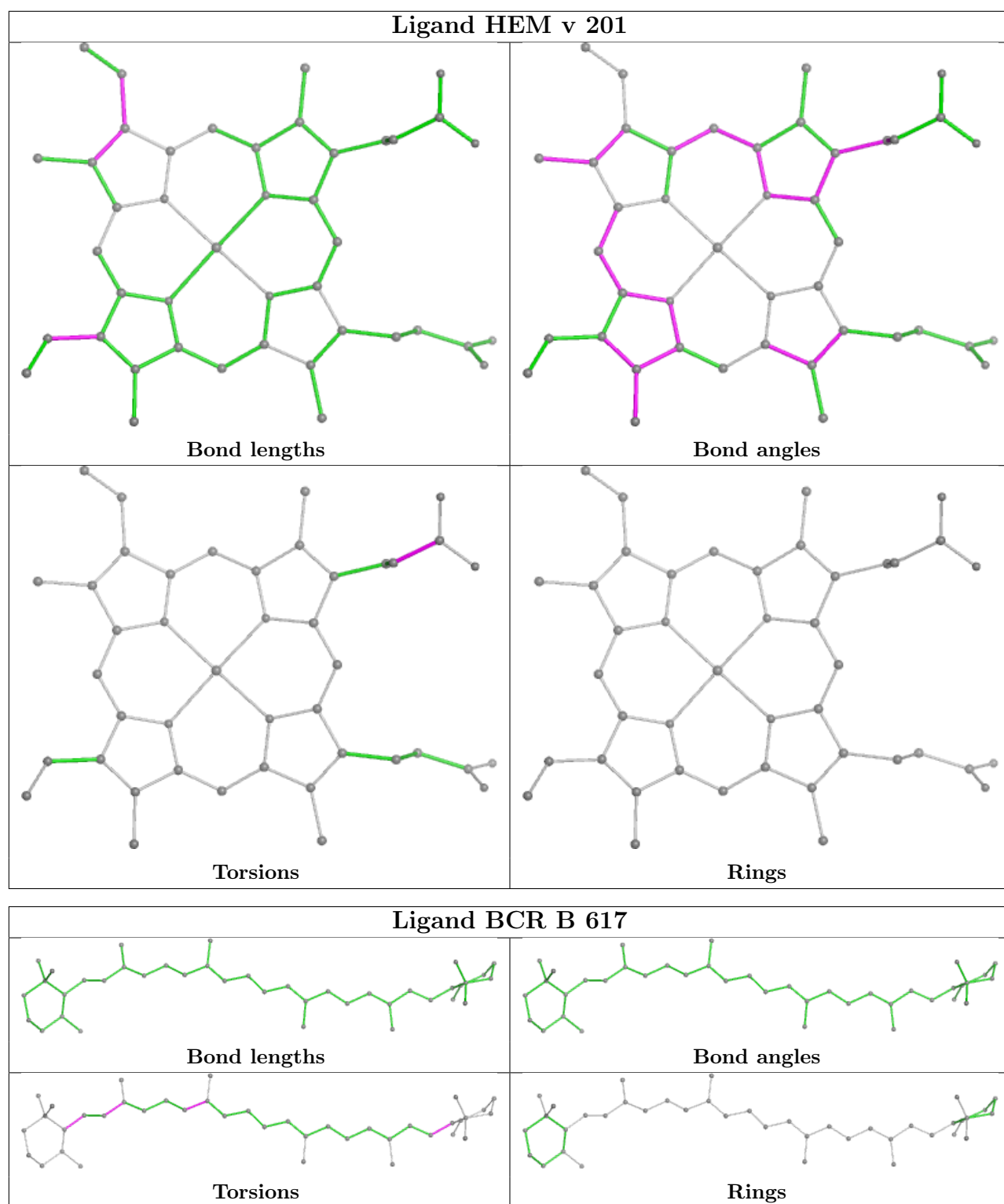
Torsions

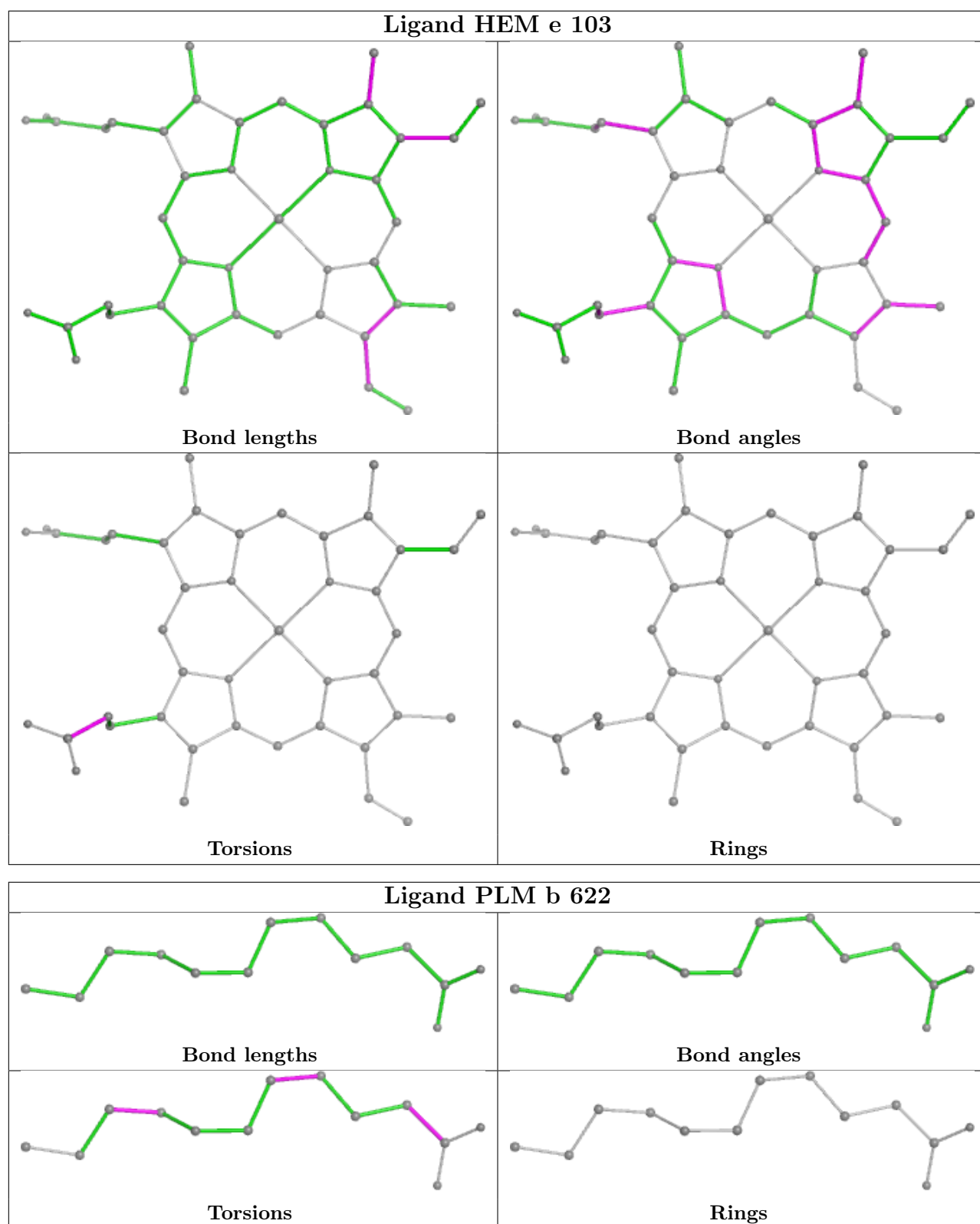


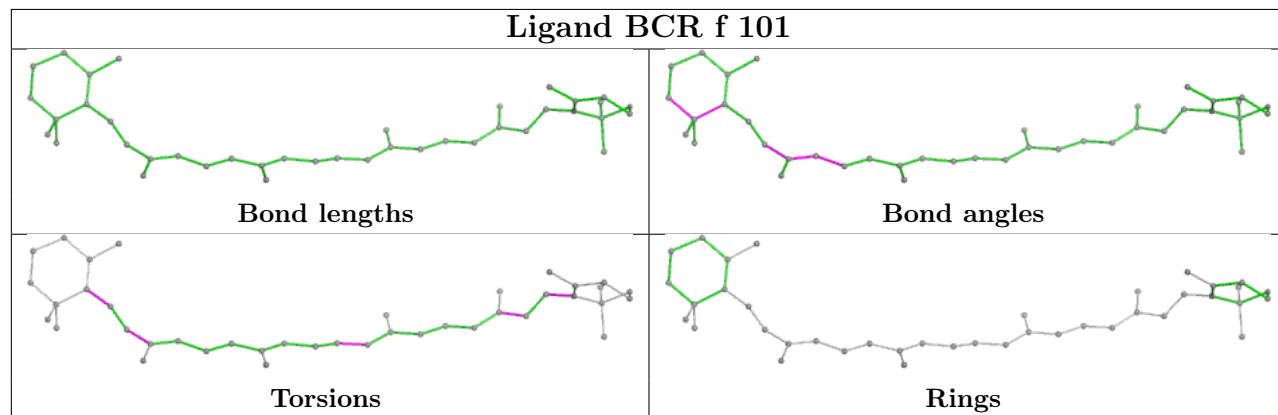
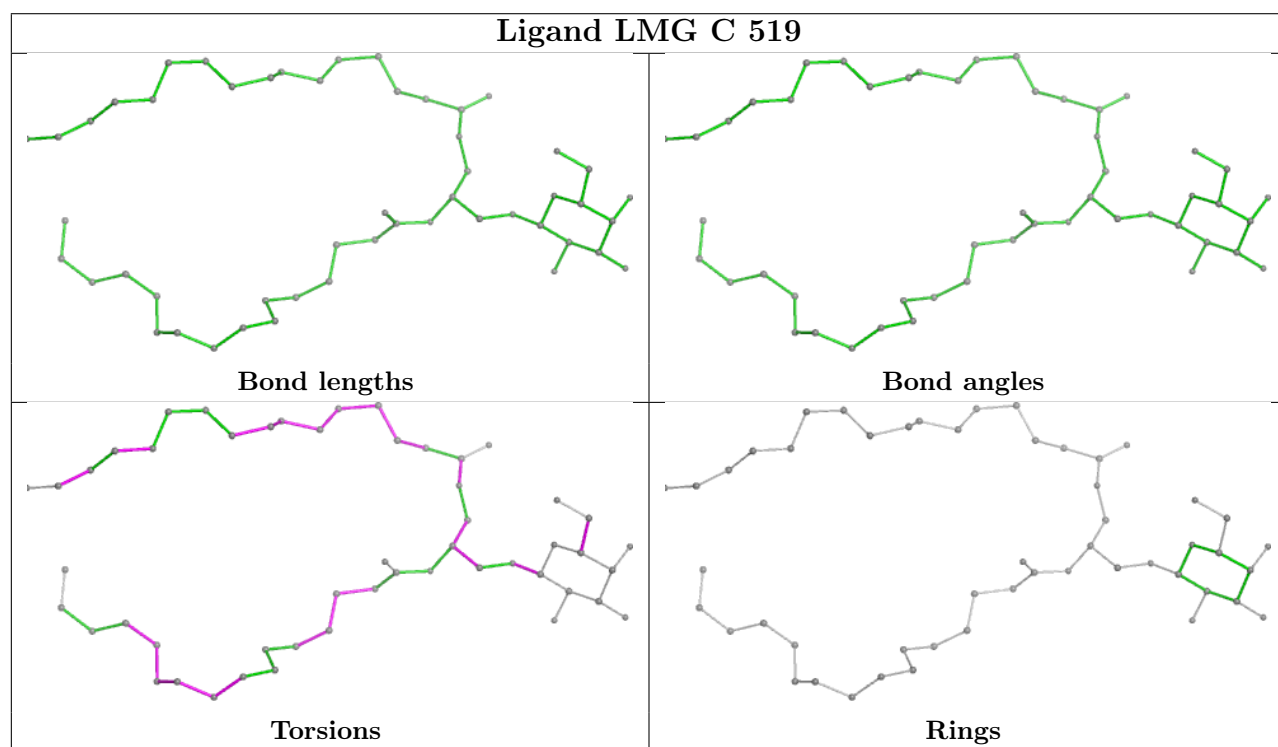
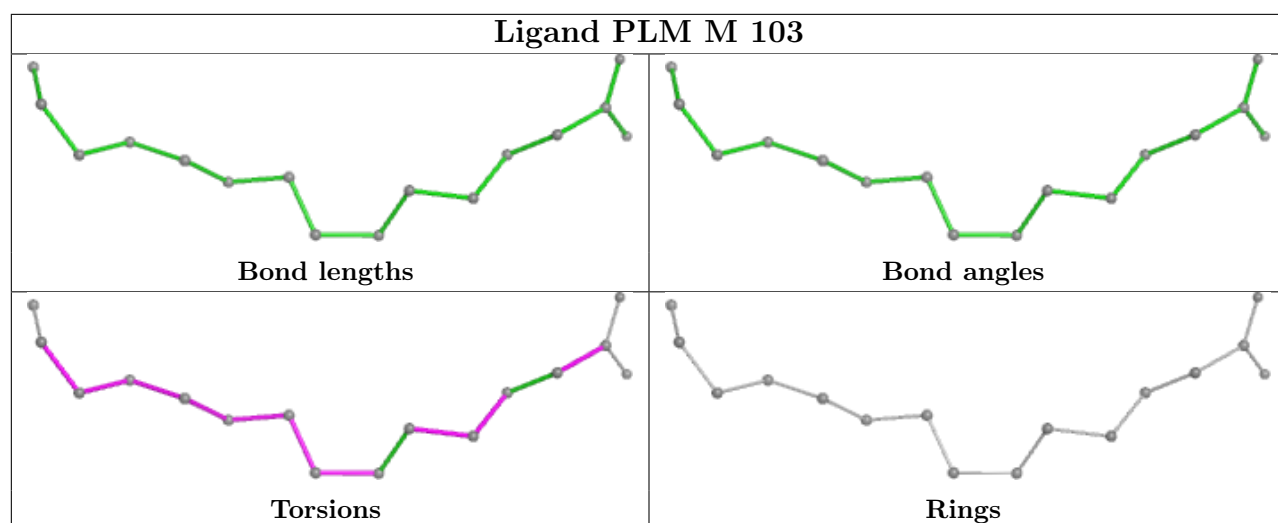
Rings

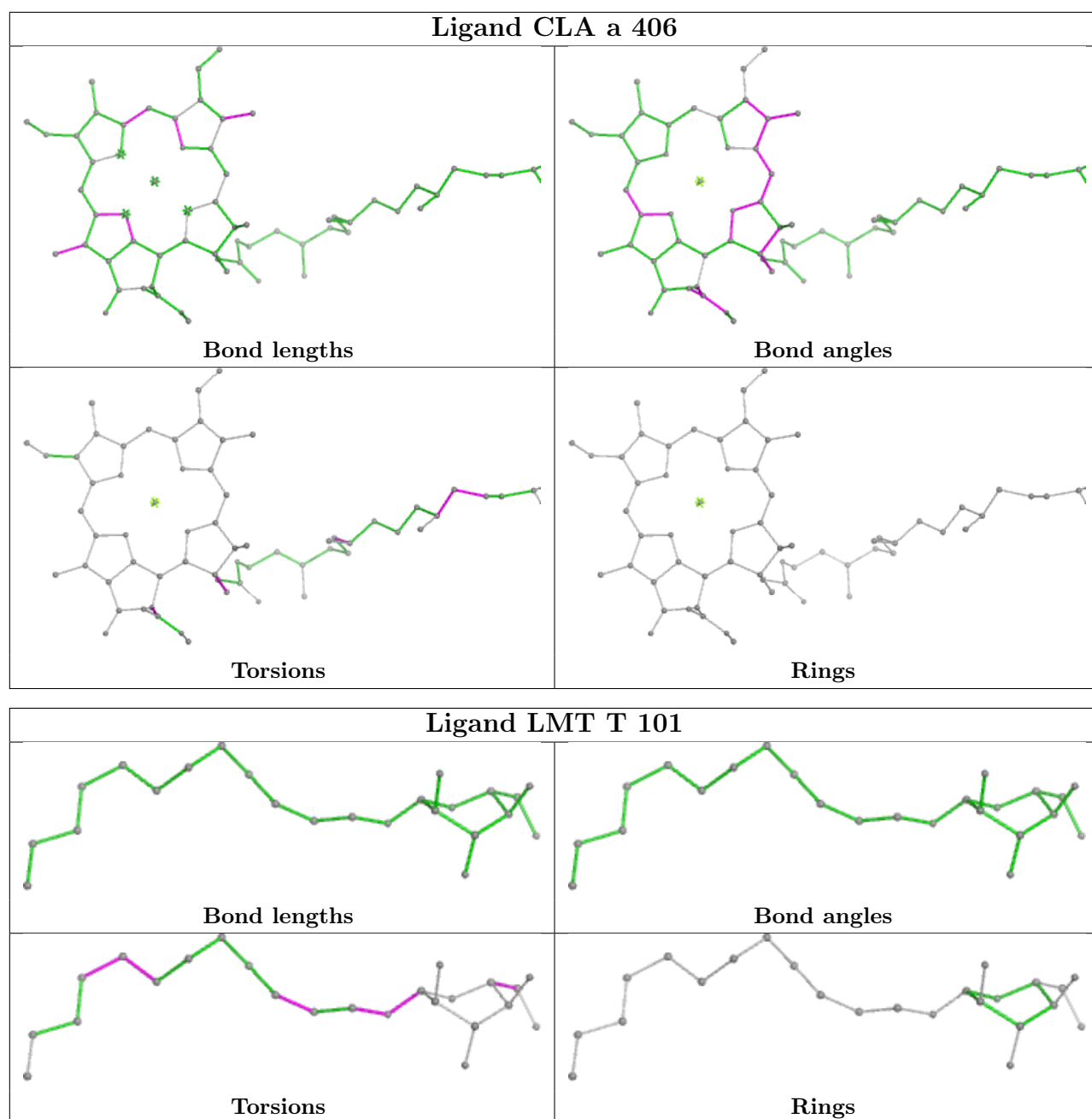


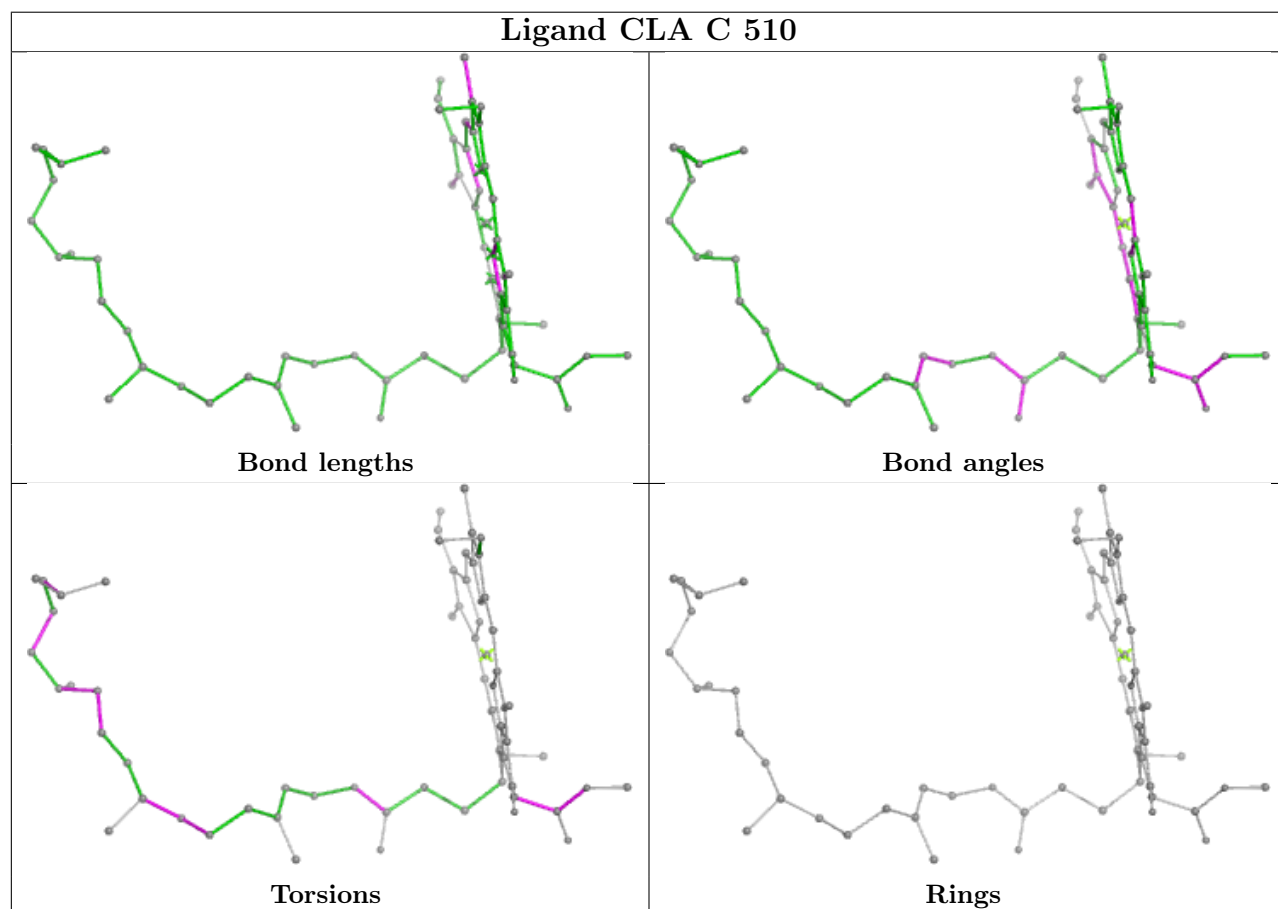
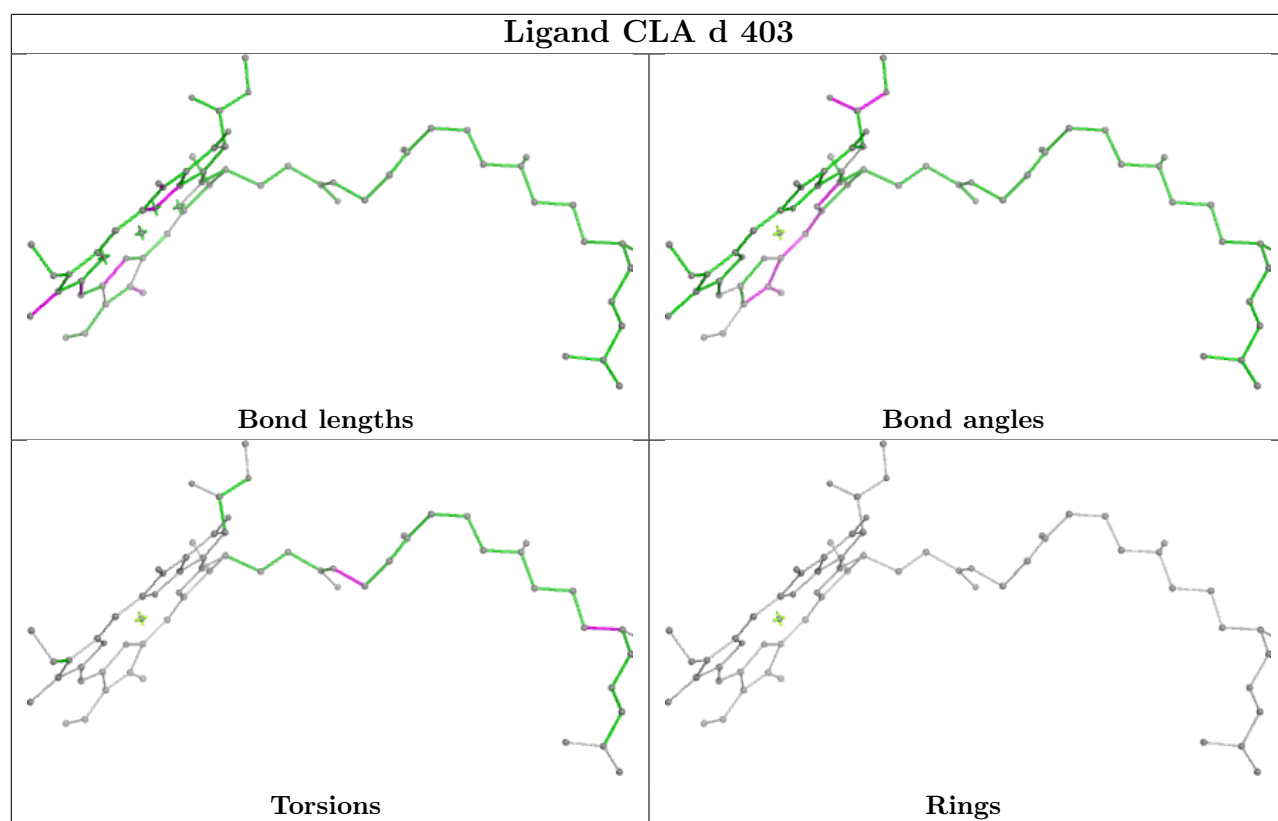


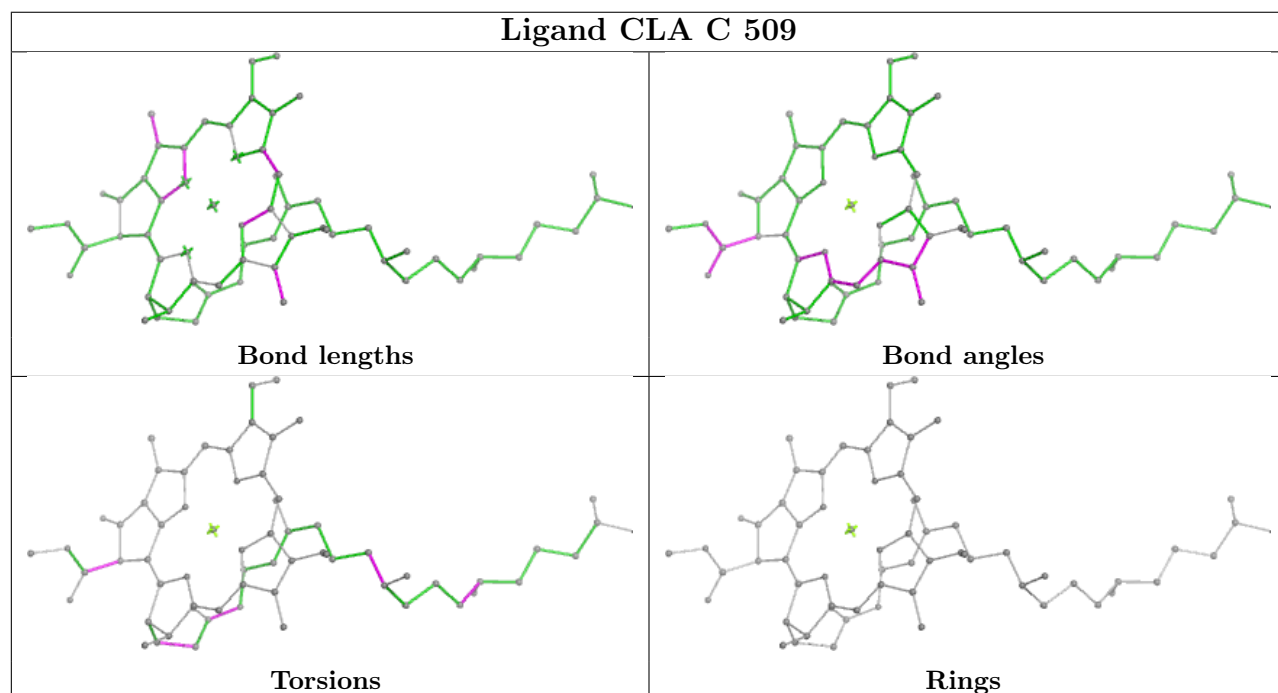
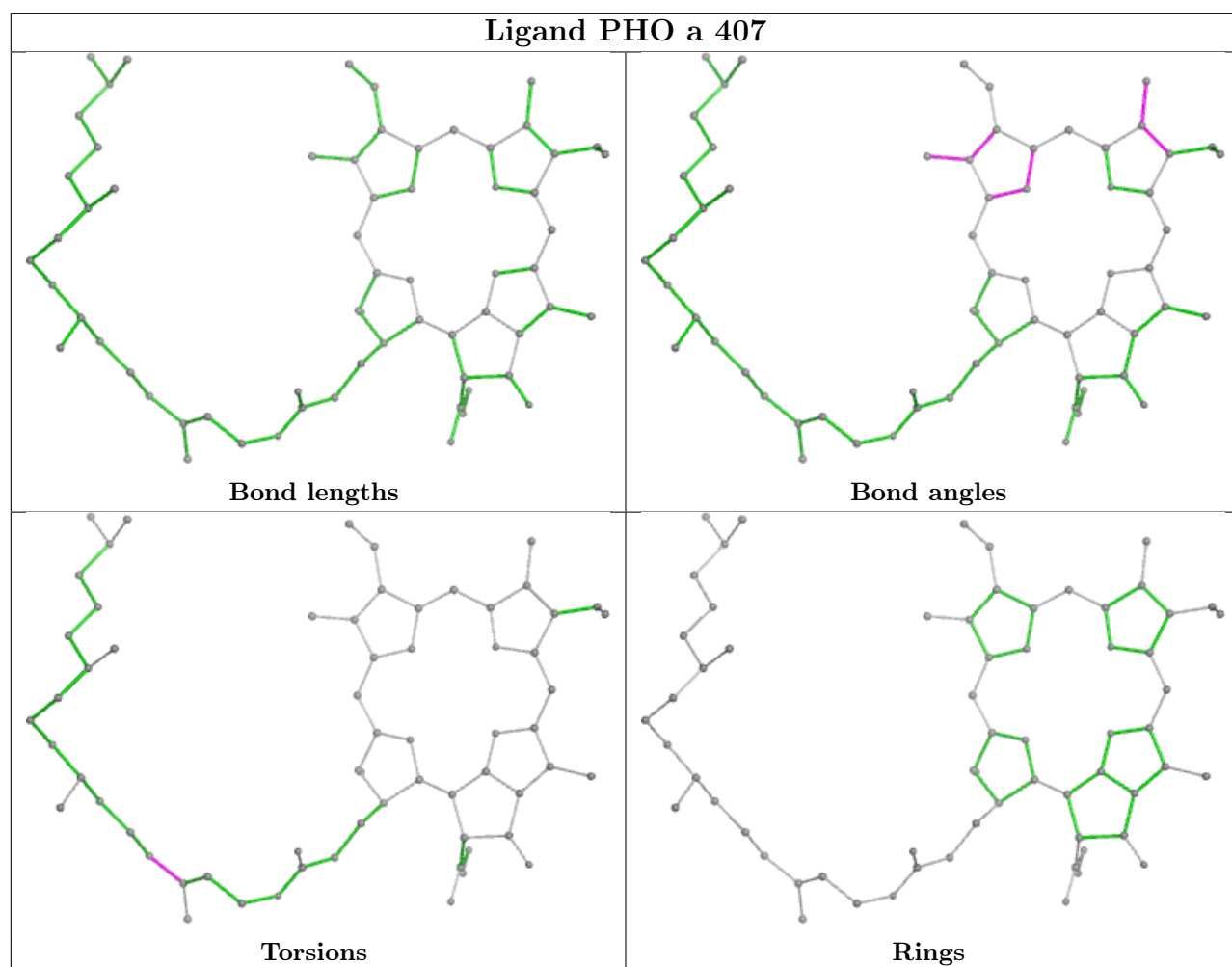


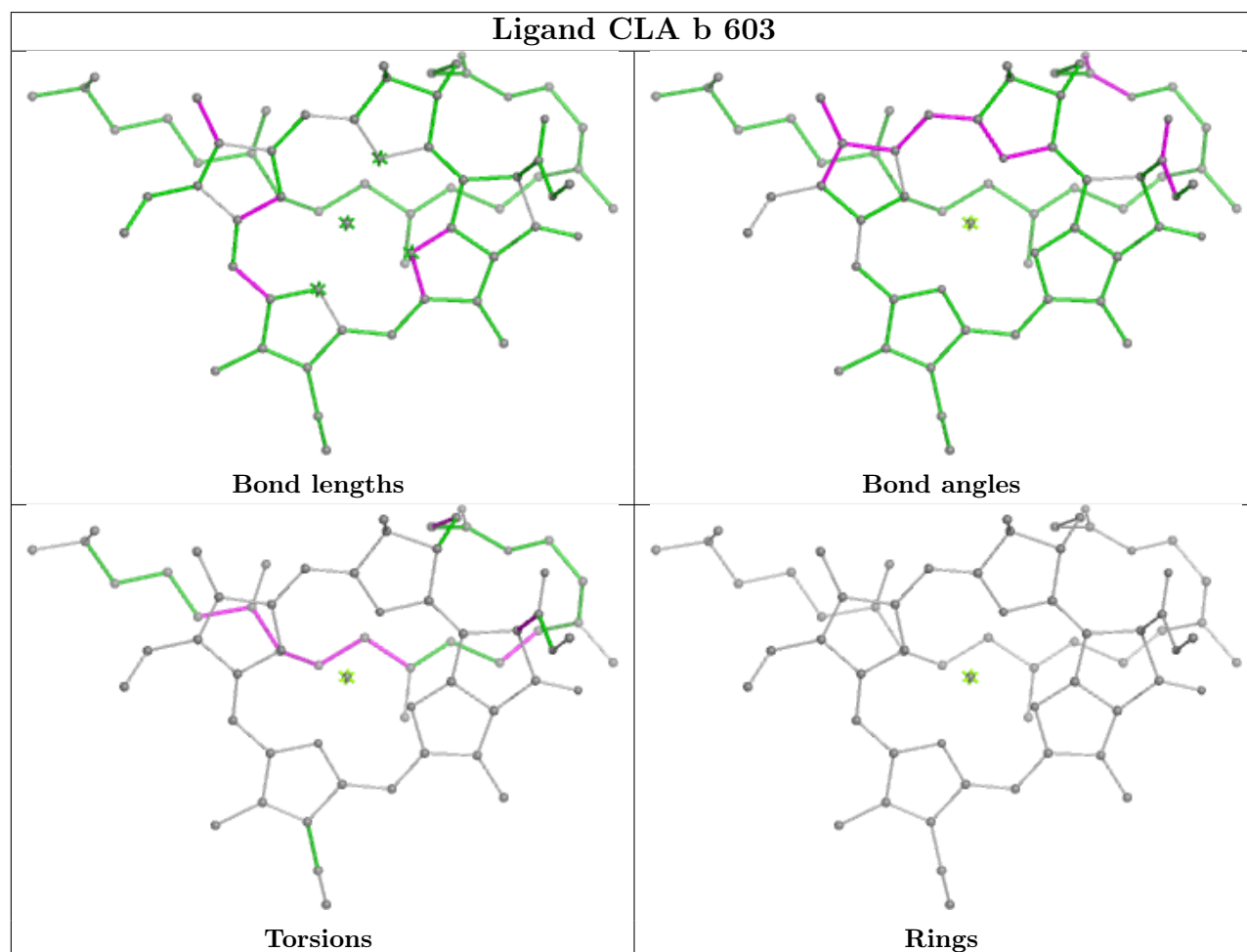
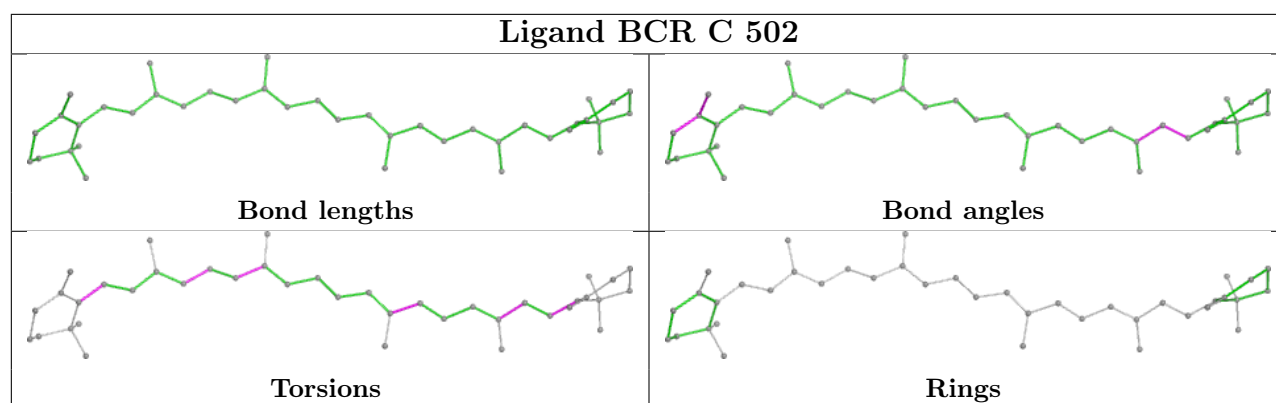


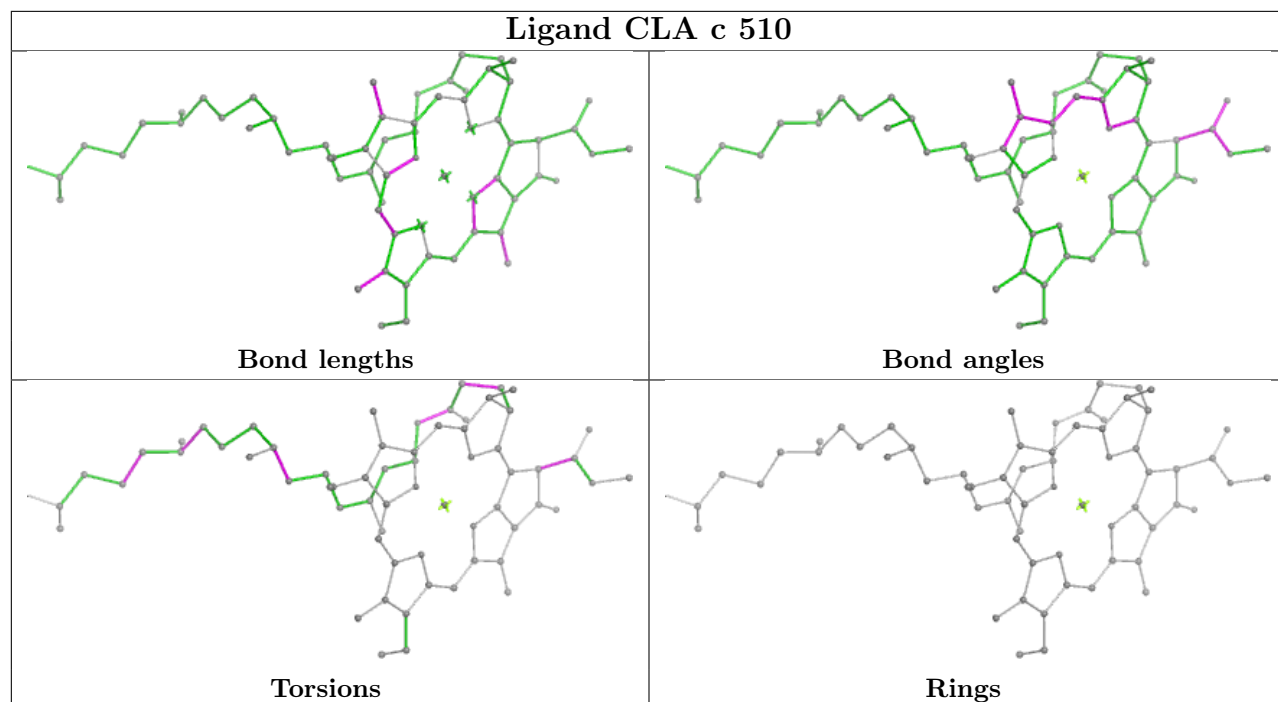
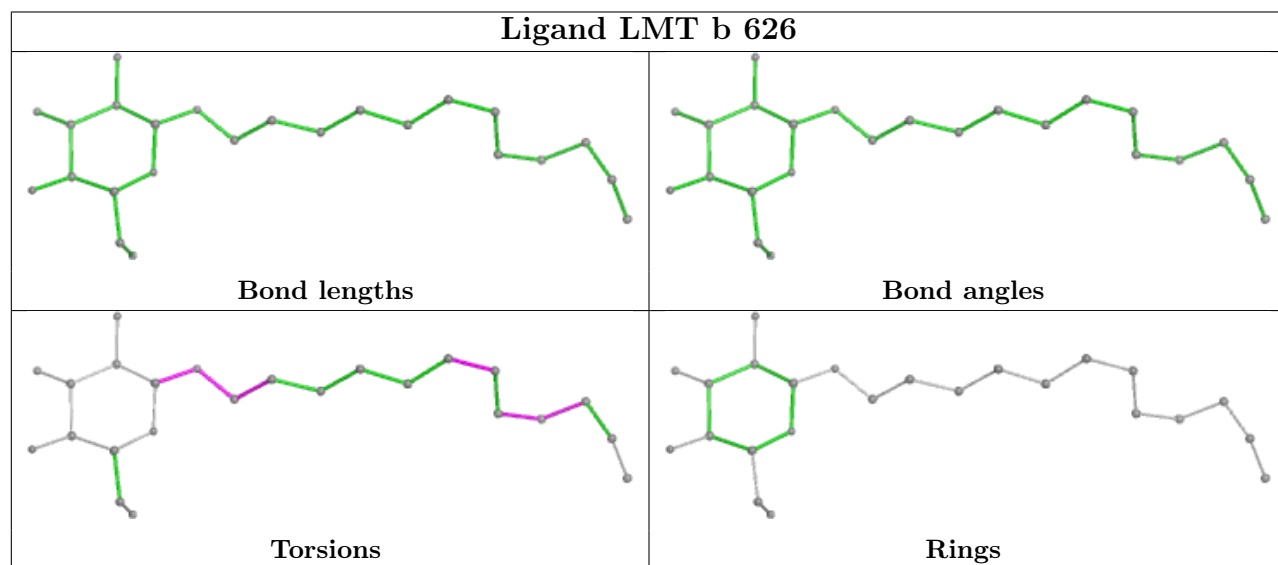




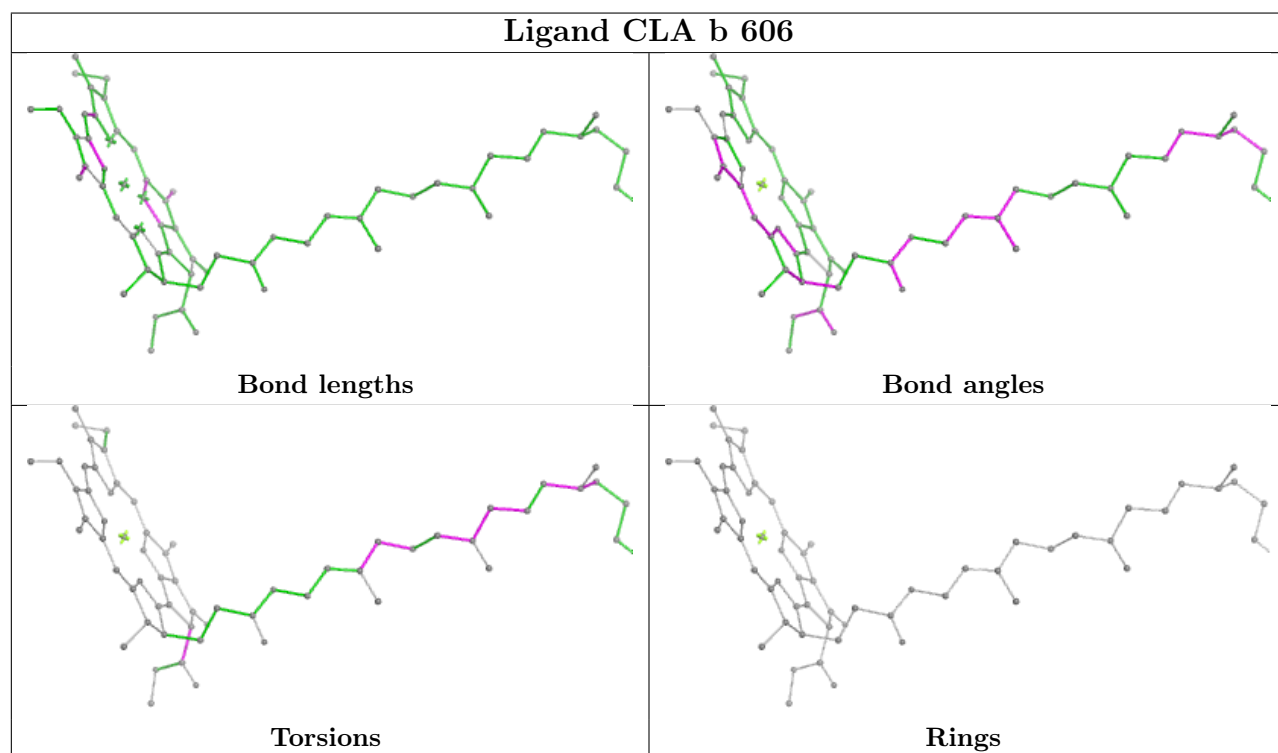
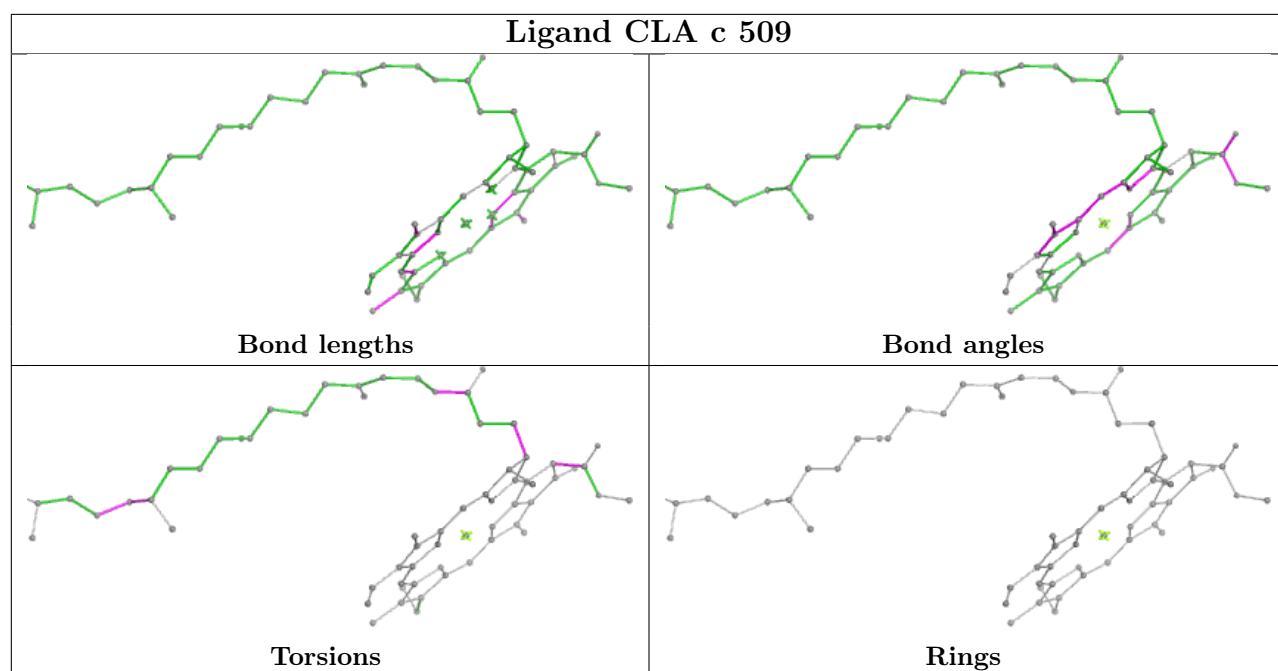


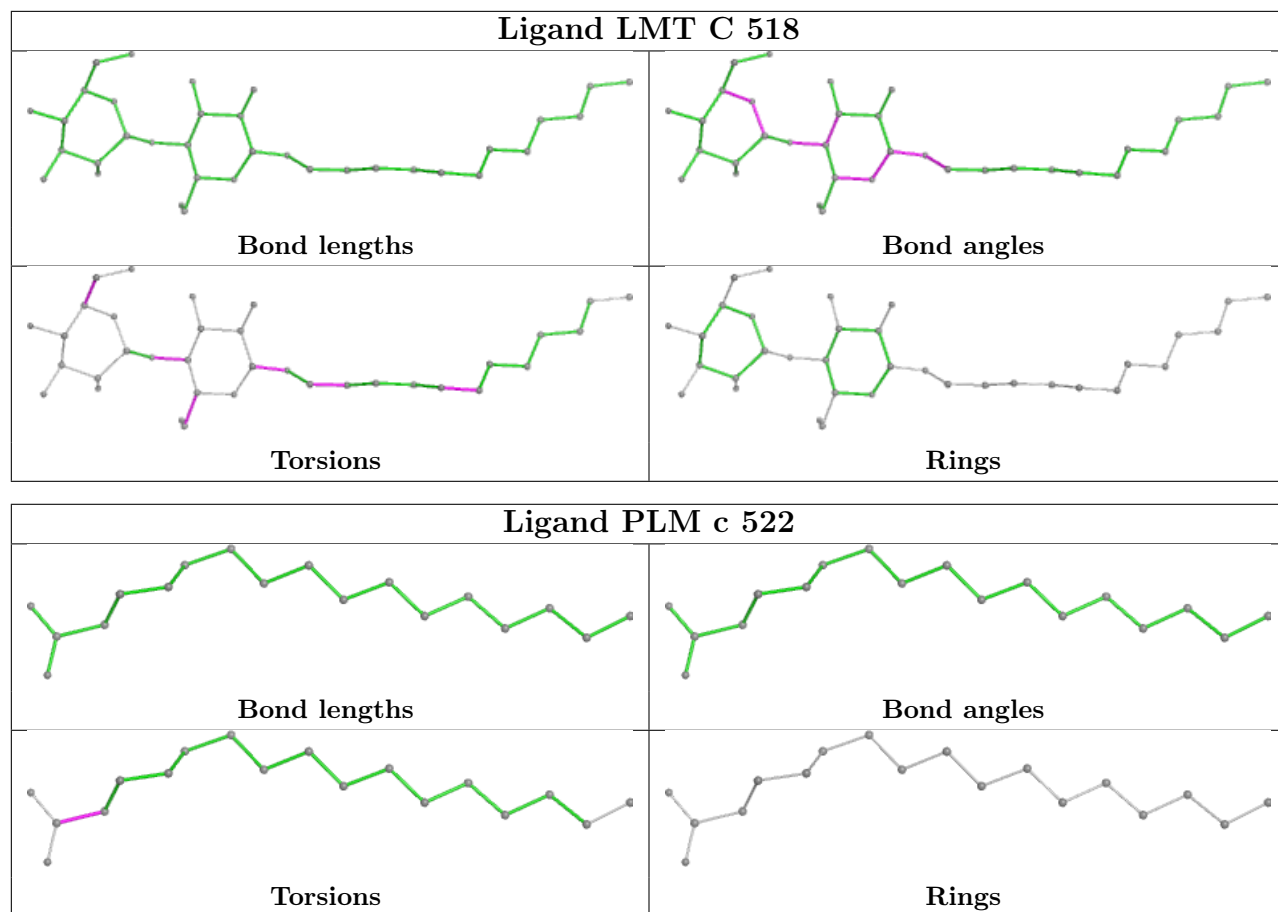


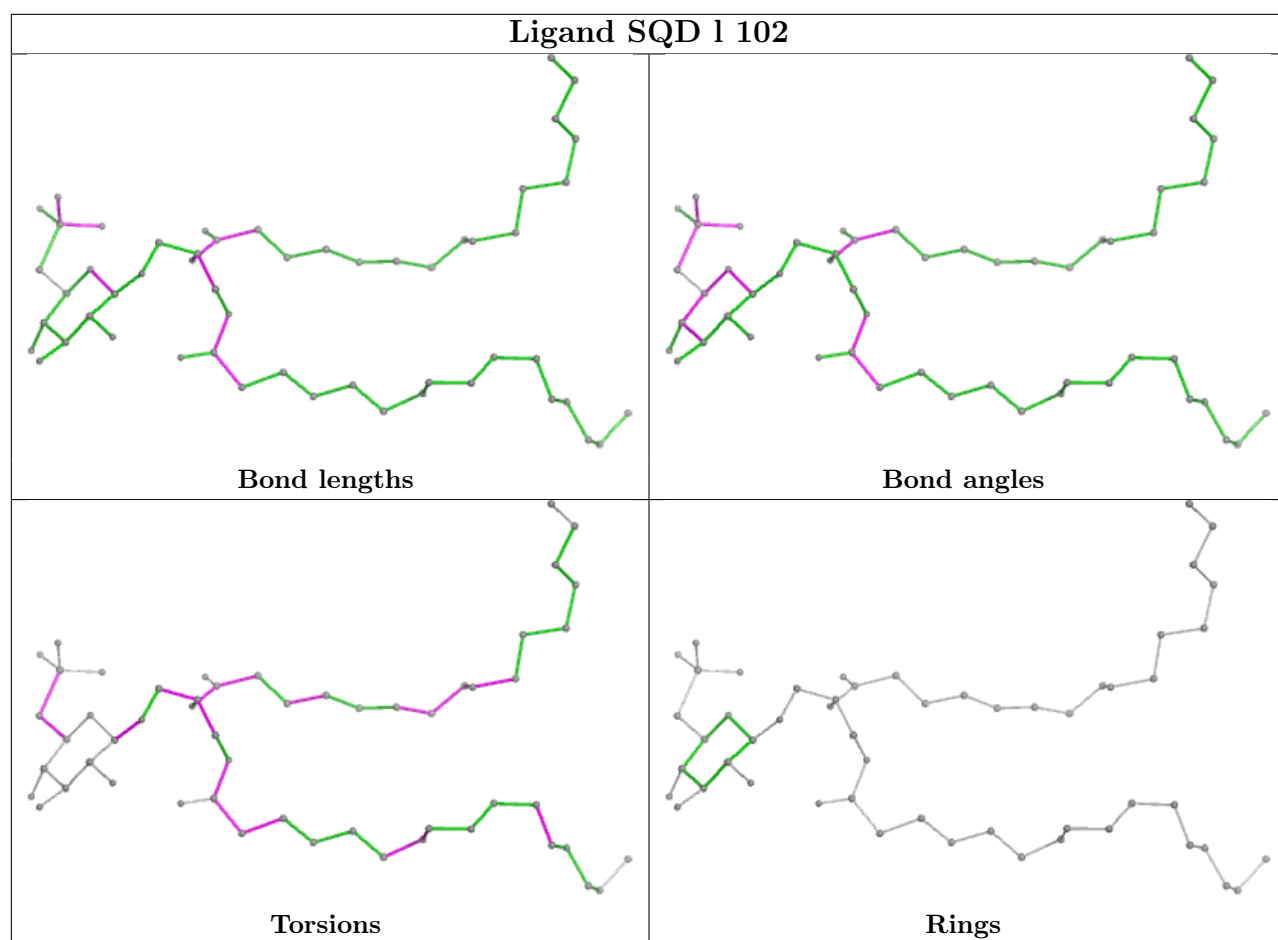


**Ligand CLA c 510****Ligand LMT b 626**

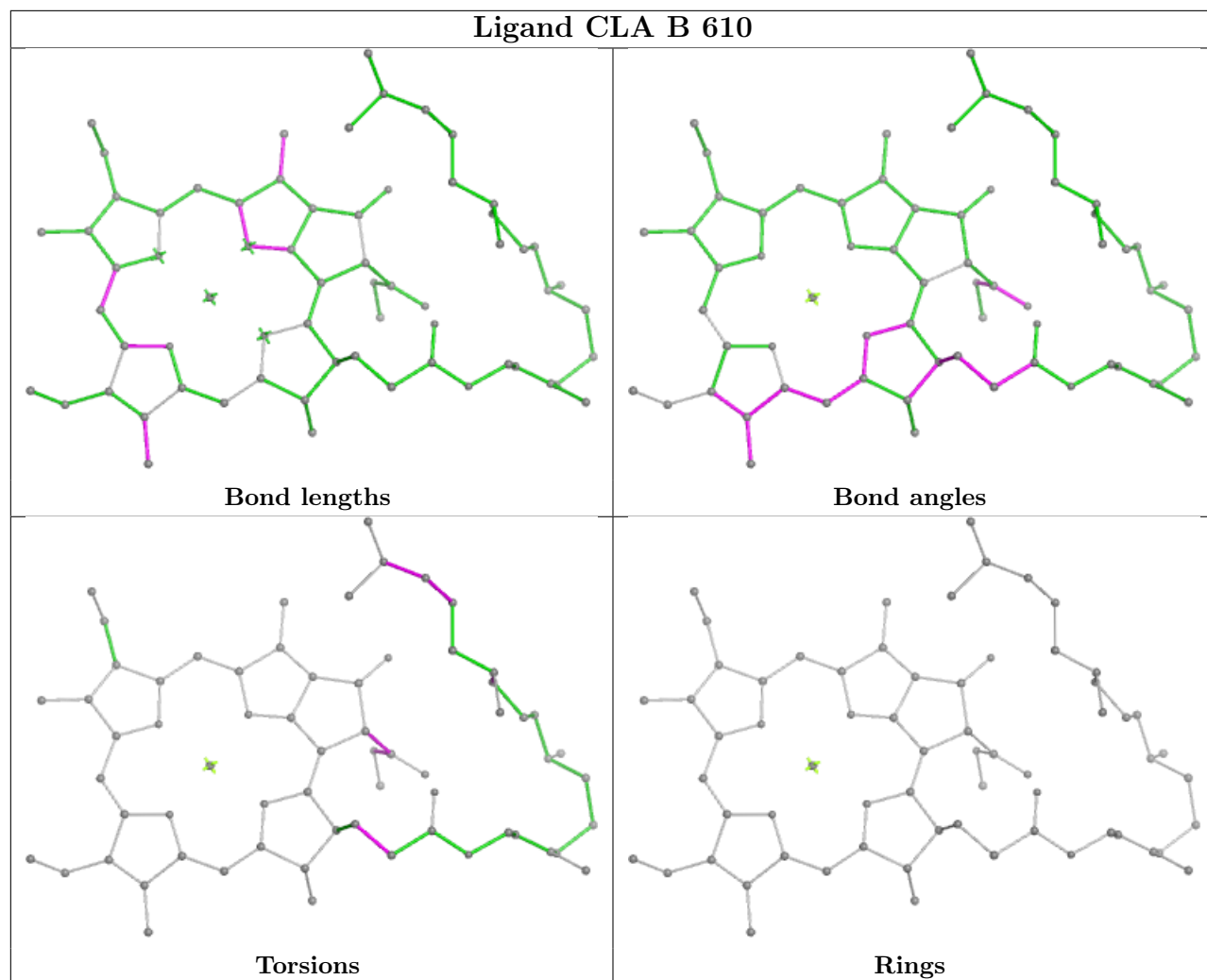


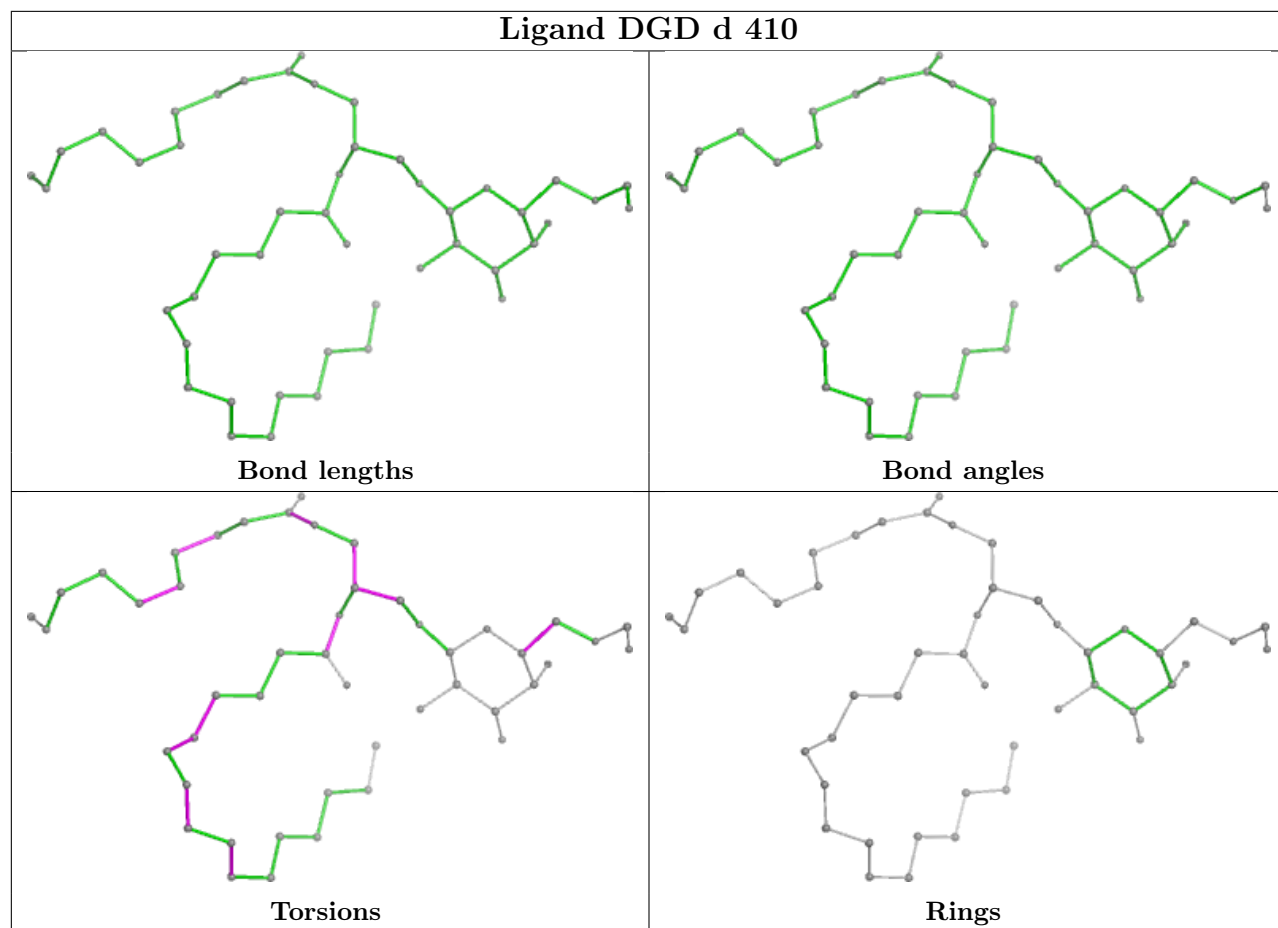


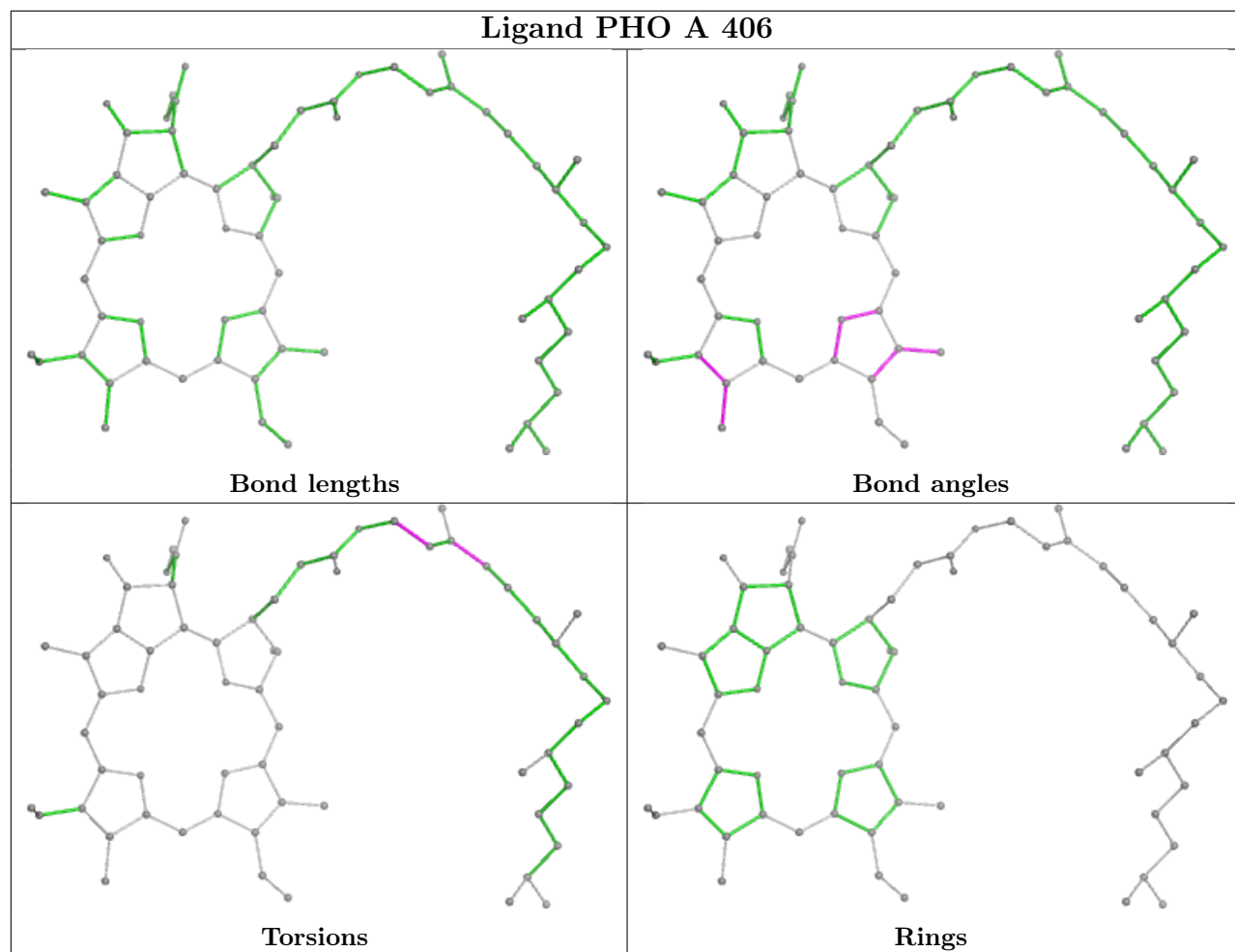




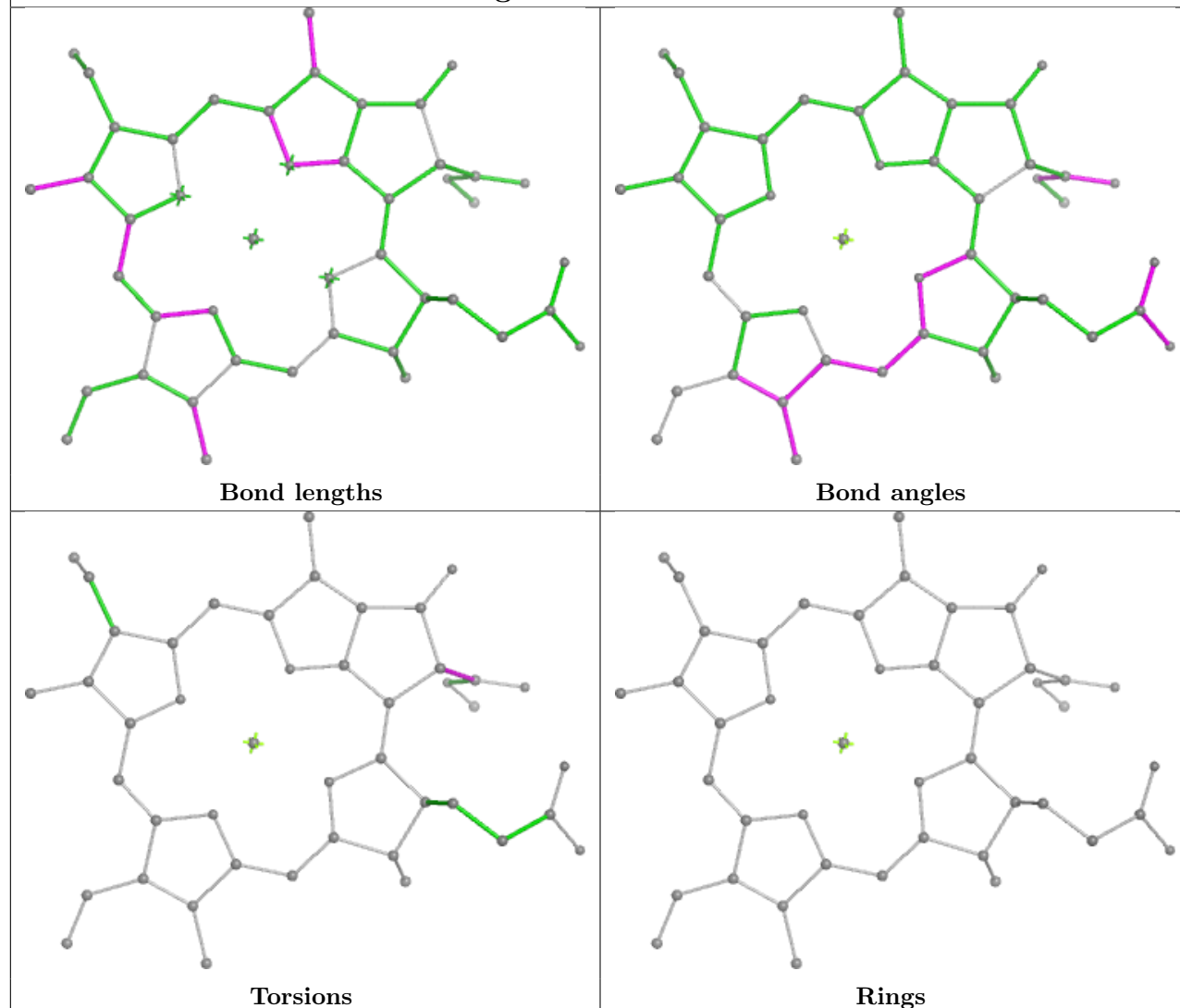
## Ligand CLA B 610



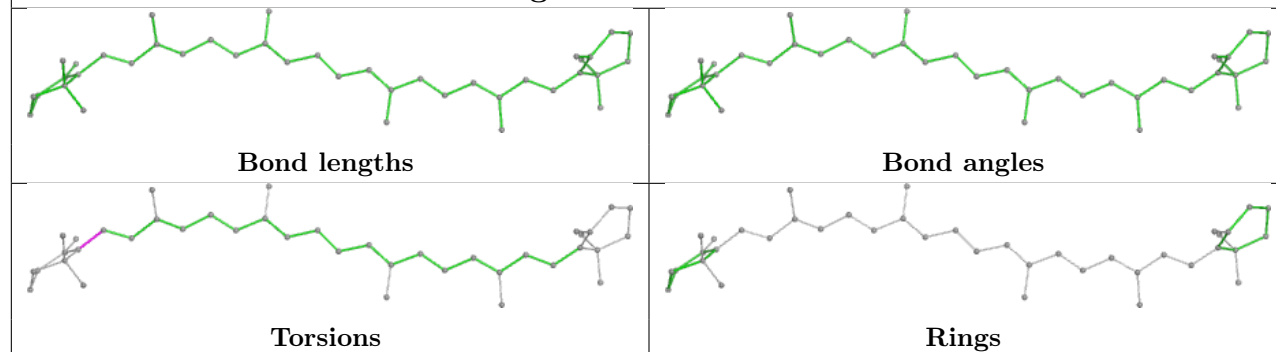


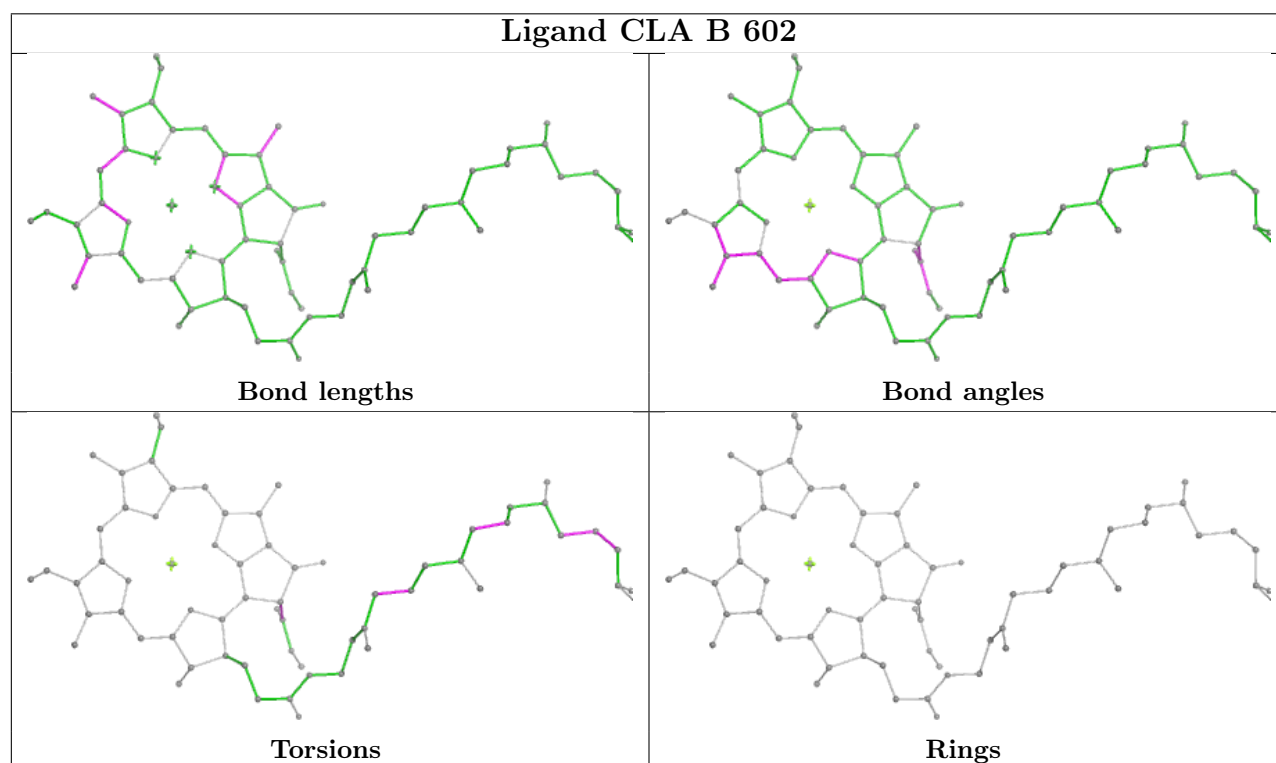
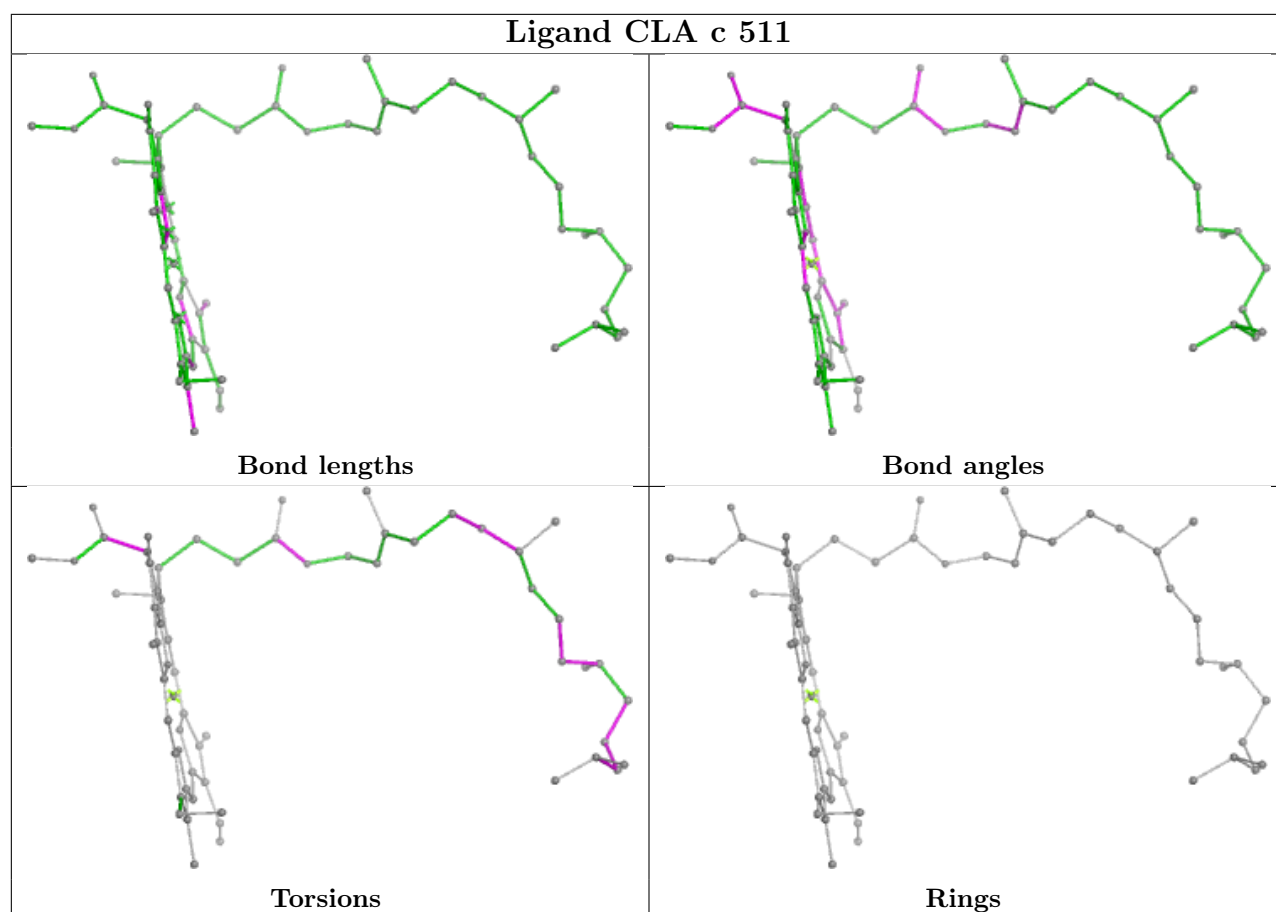


## Ligand CLA b 618

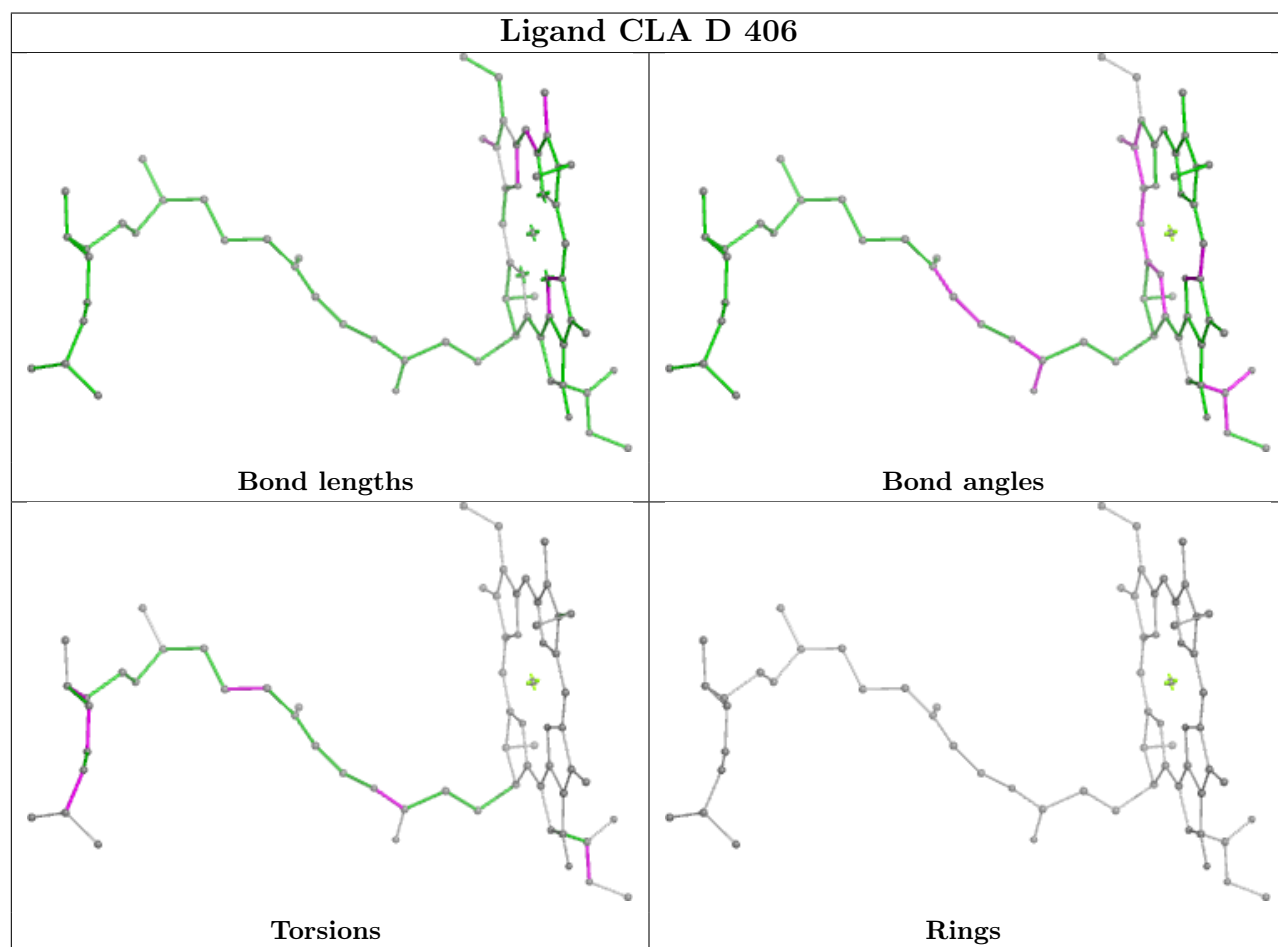
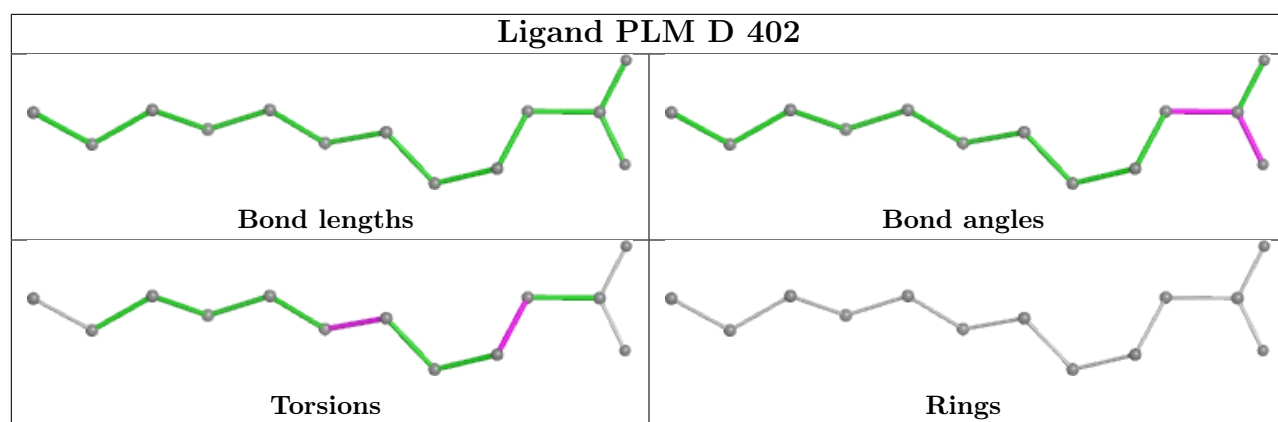


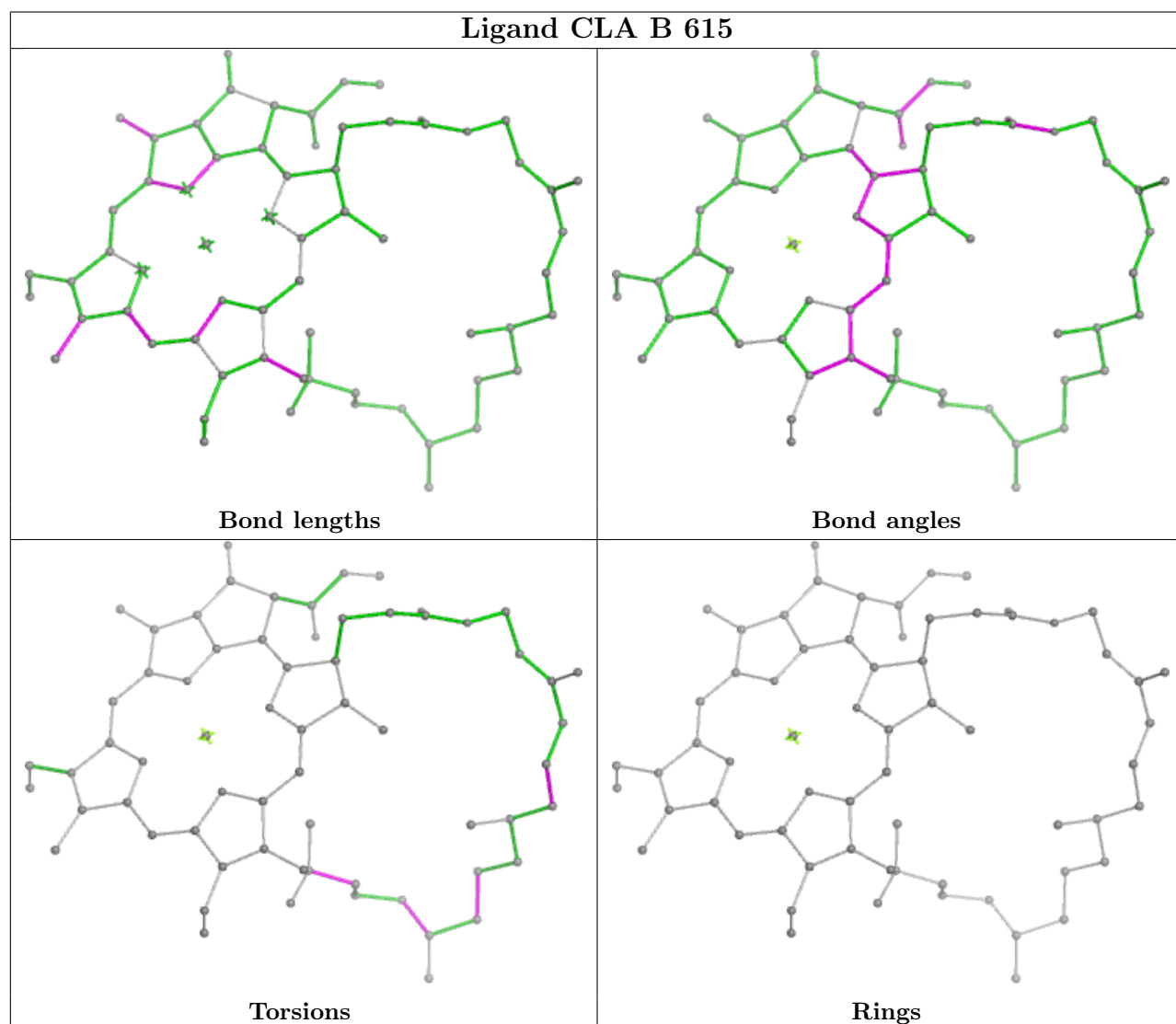
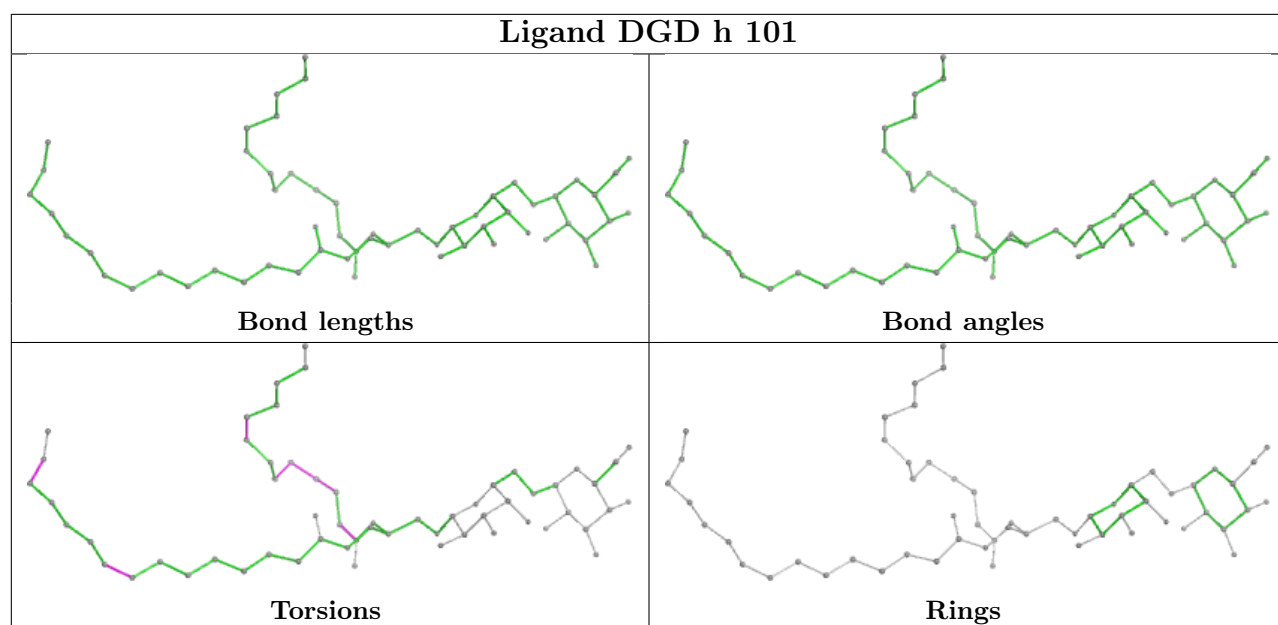
## Ligand BCR A 408

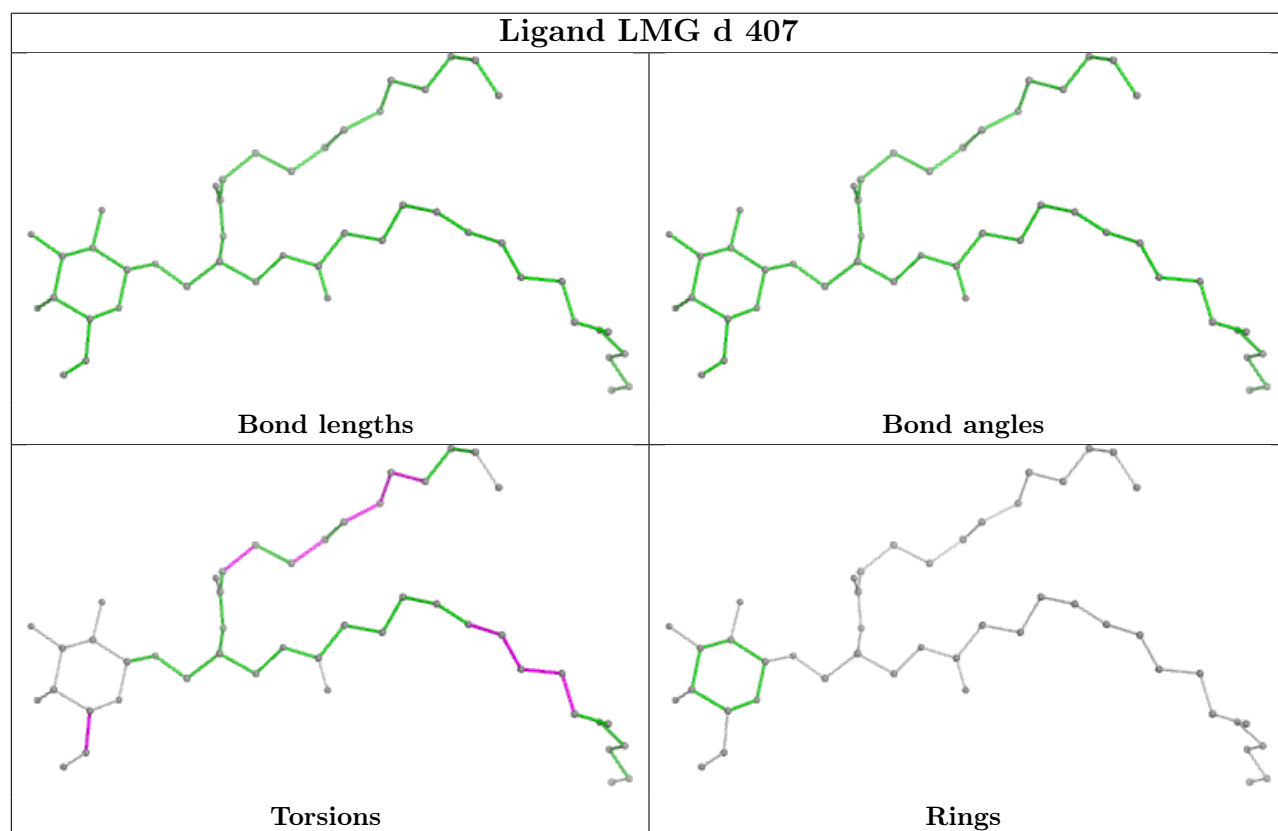
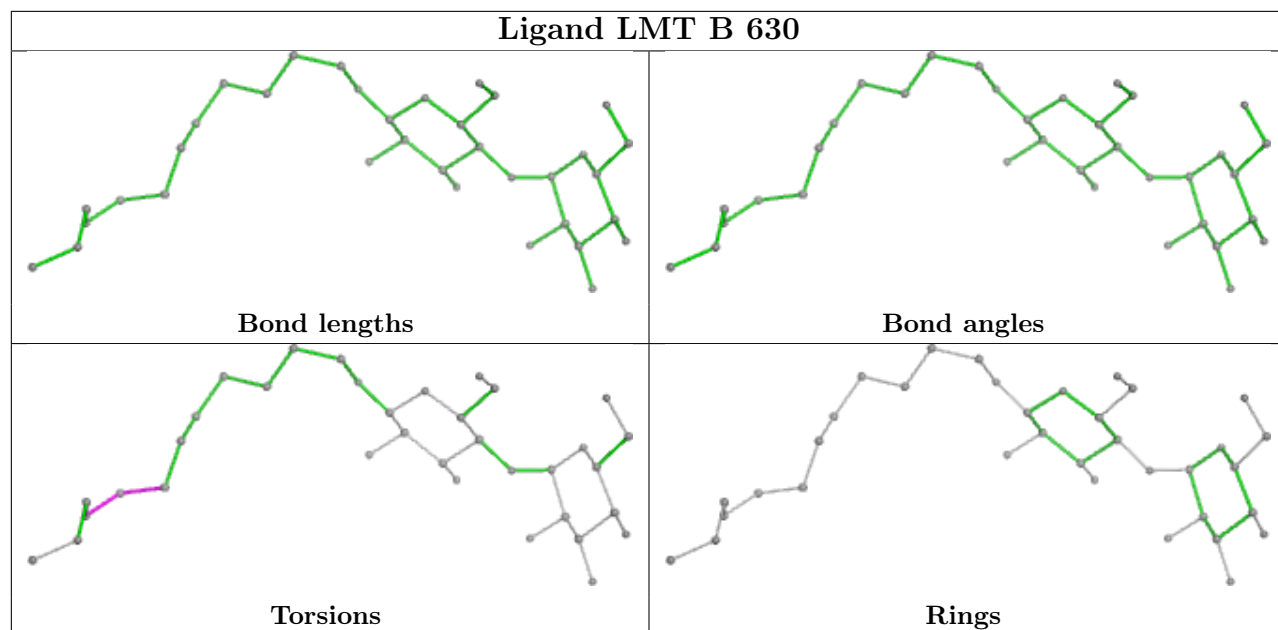


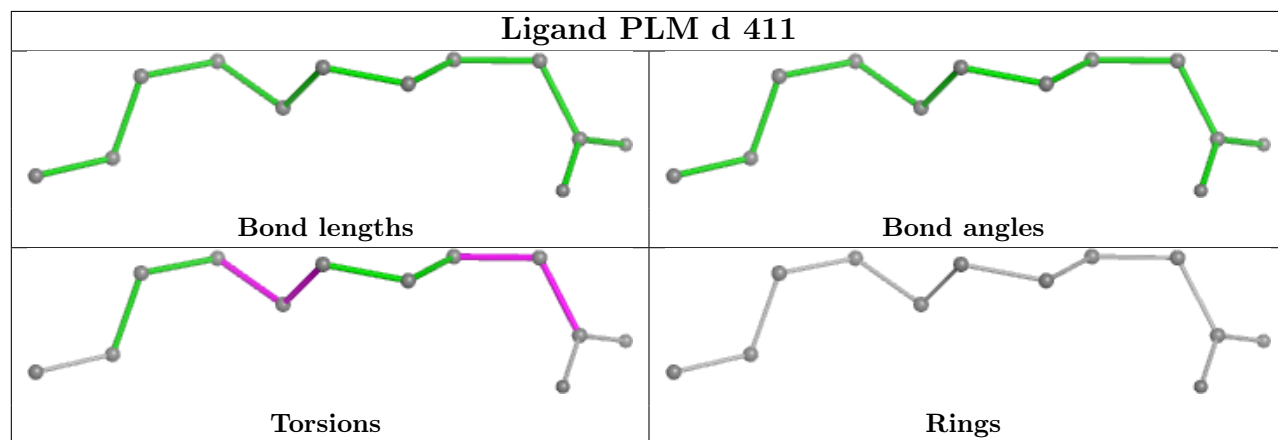
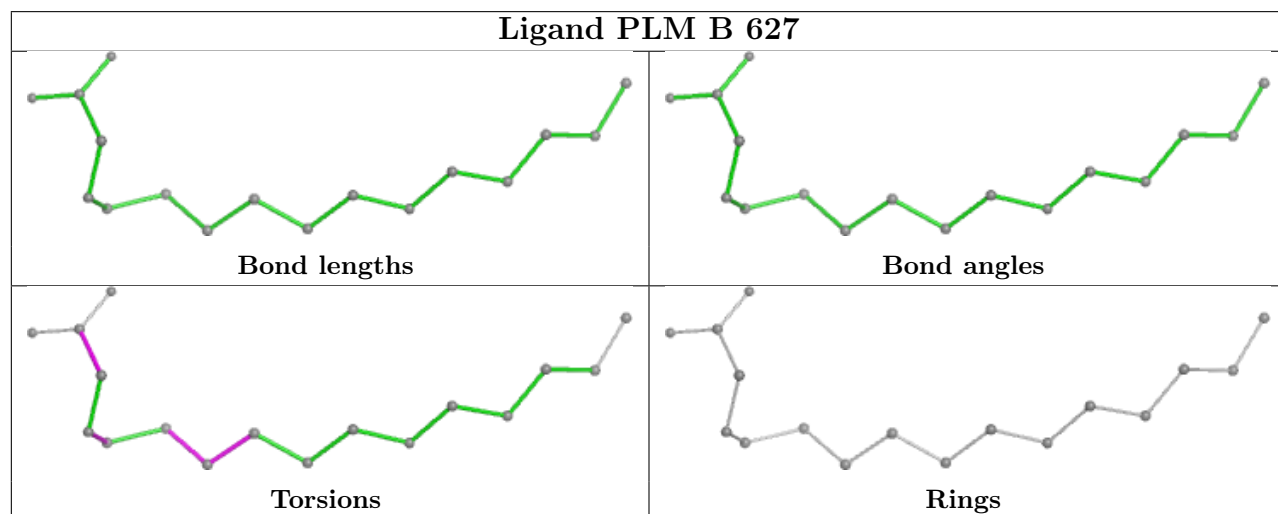
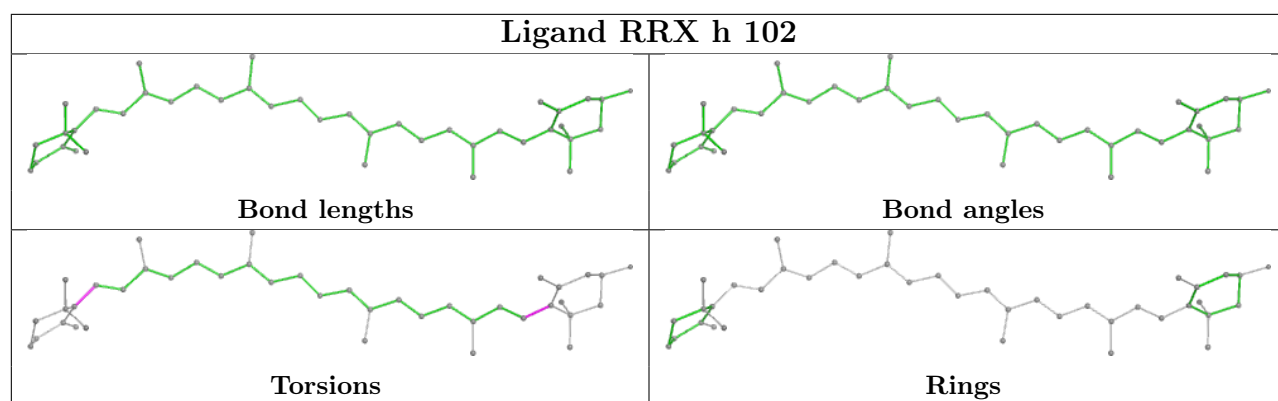


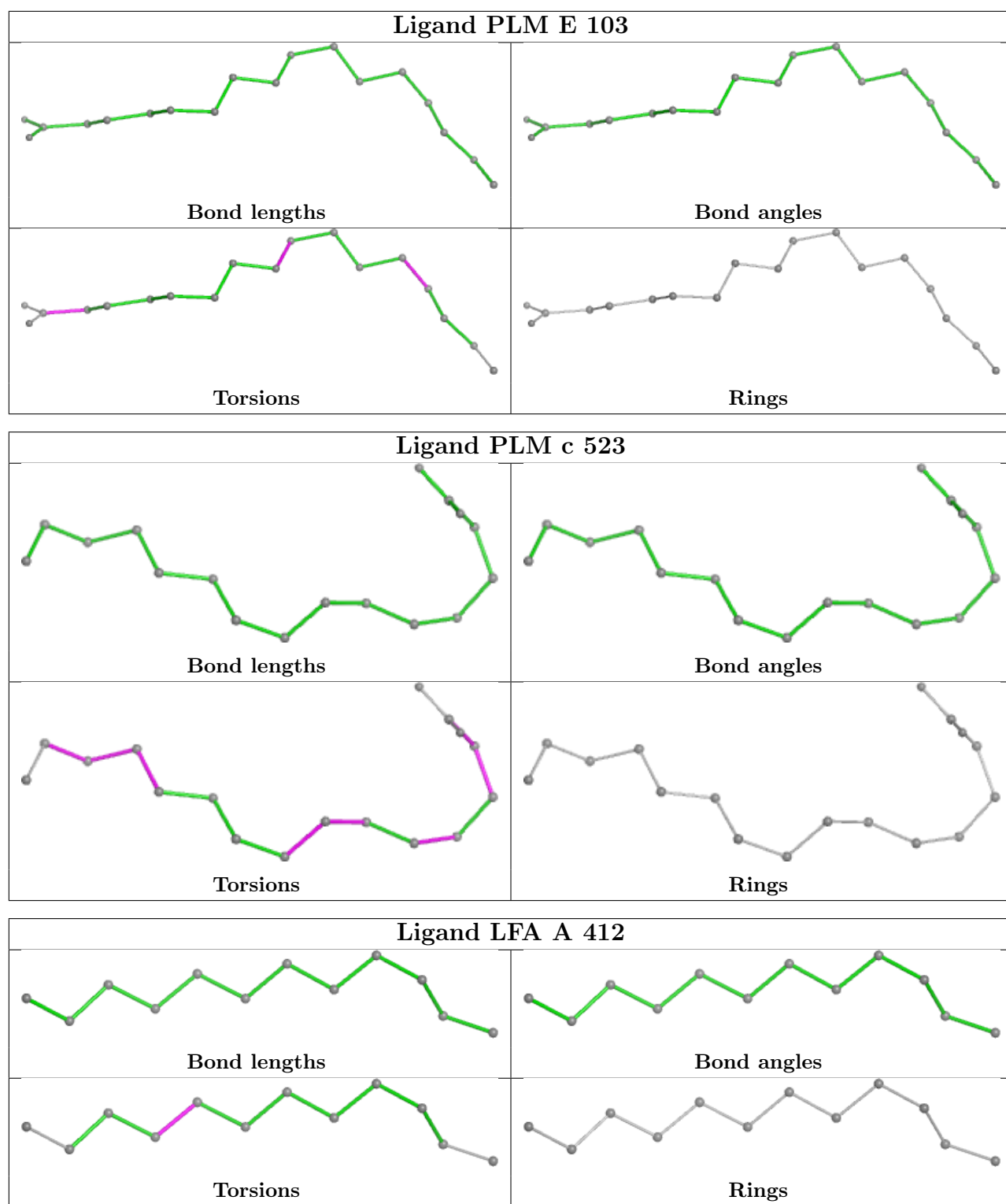


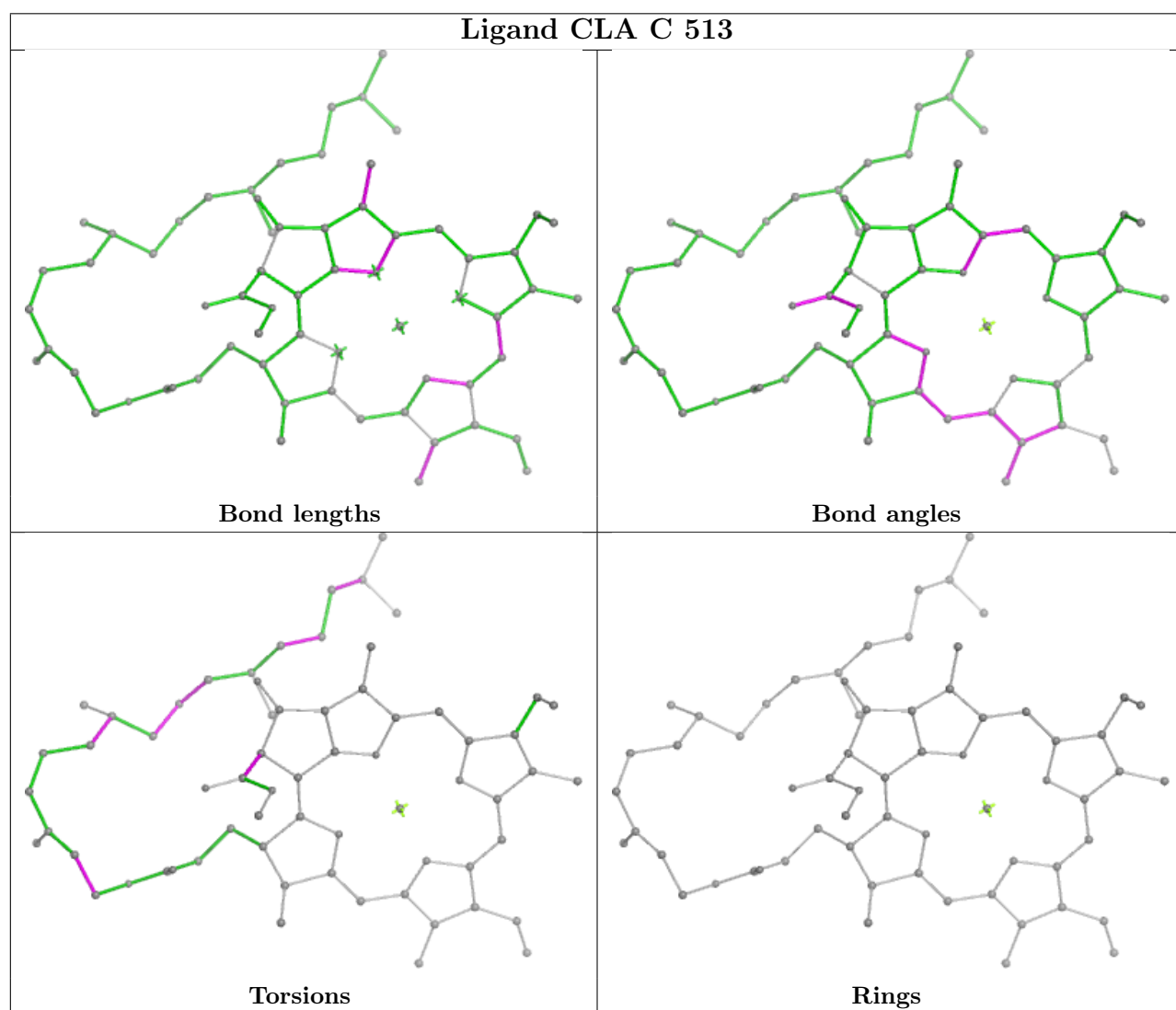
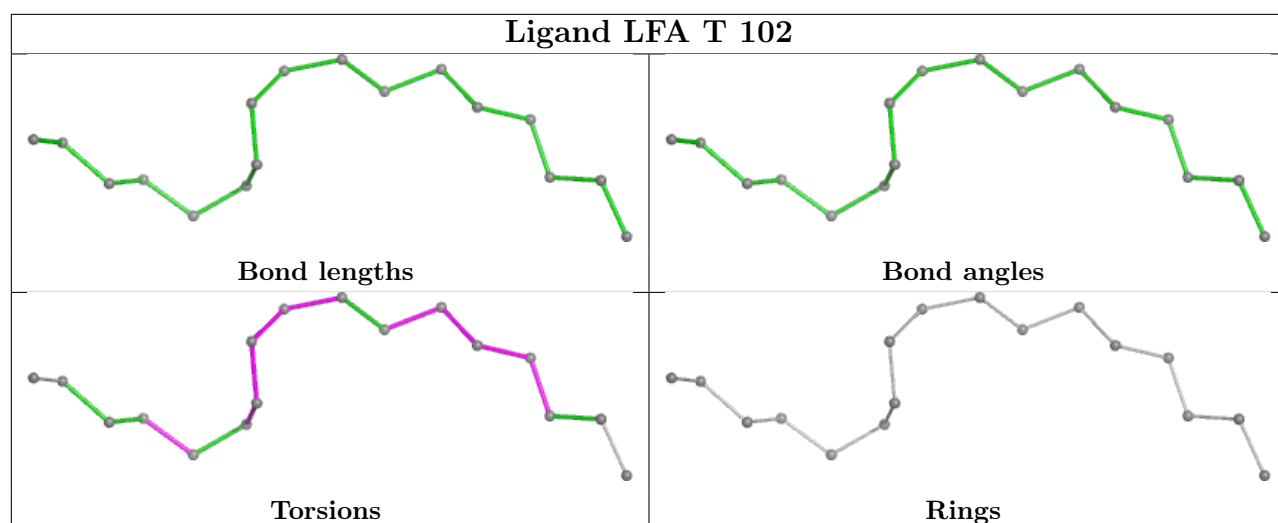


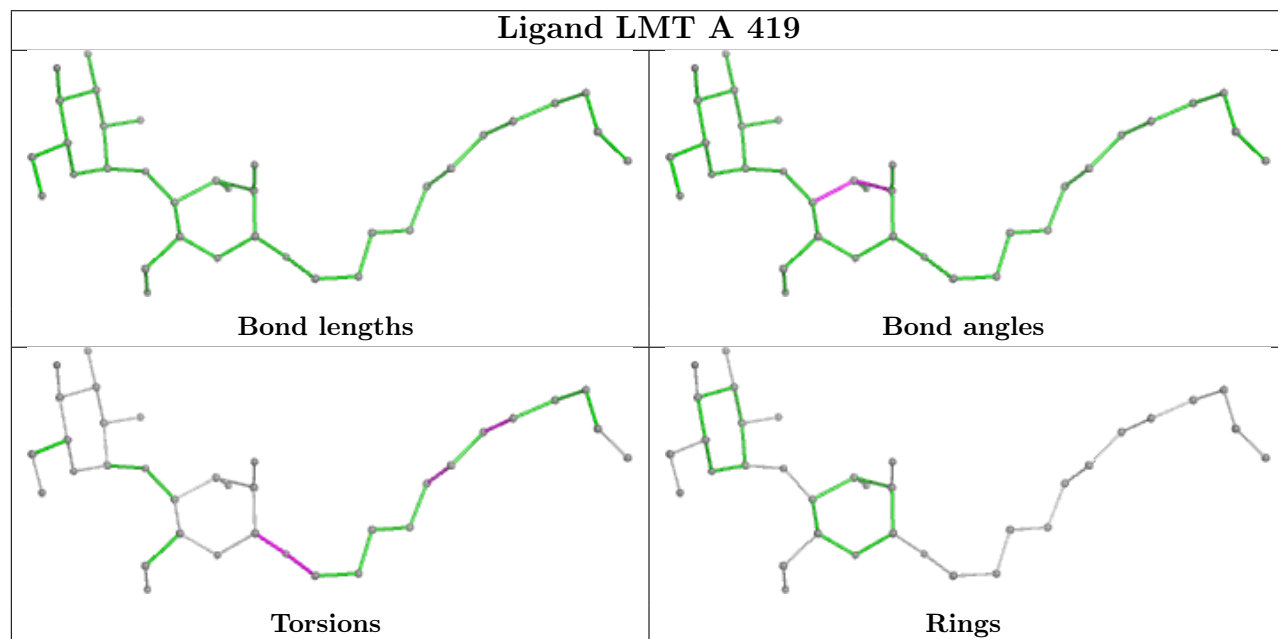
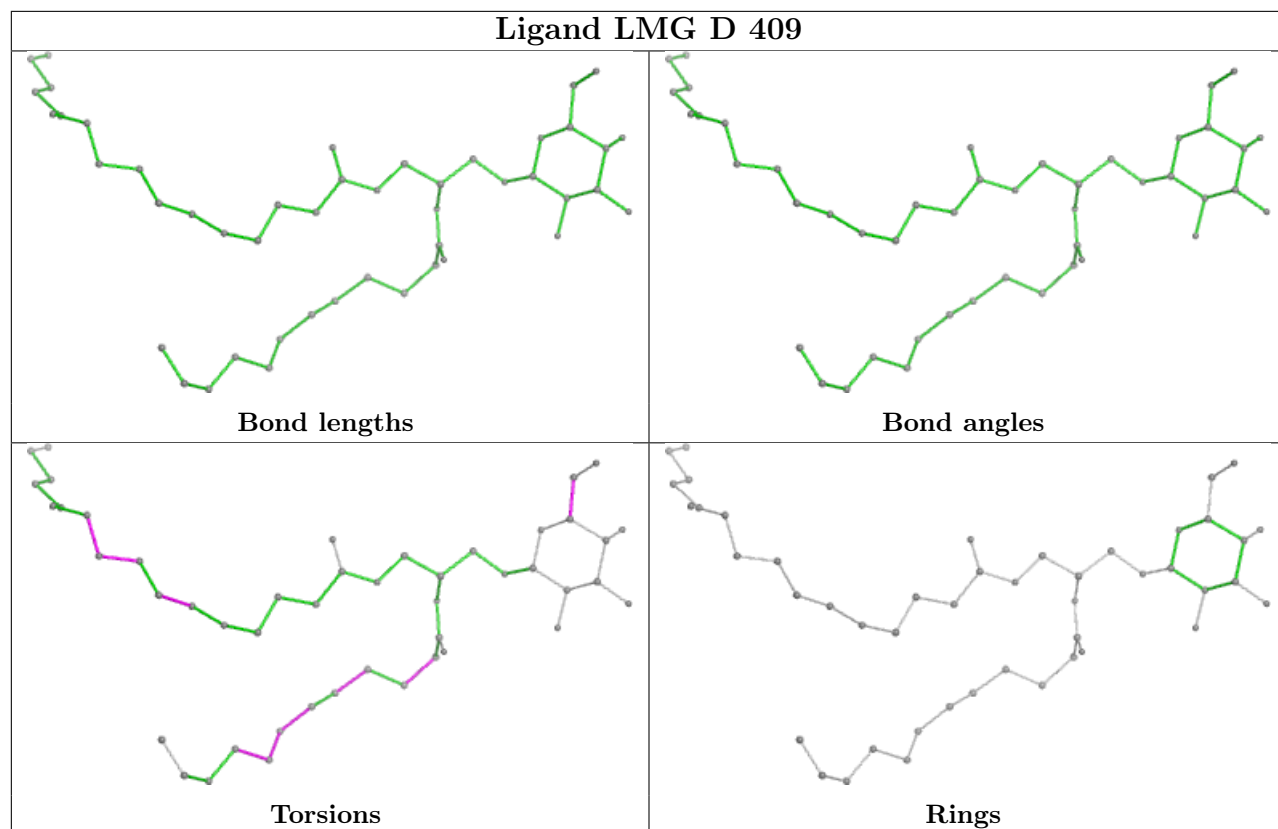


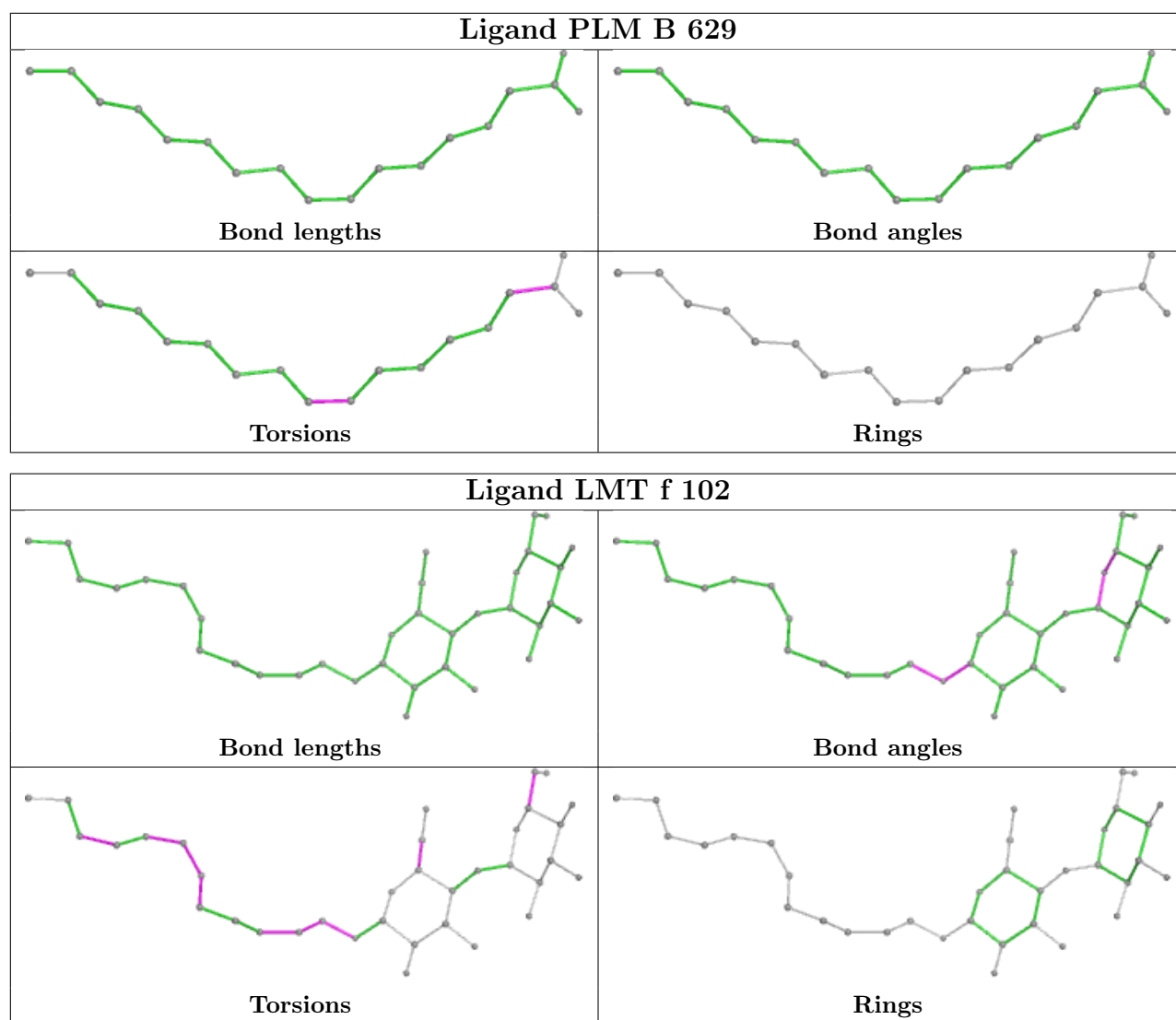




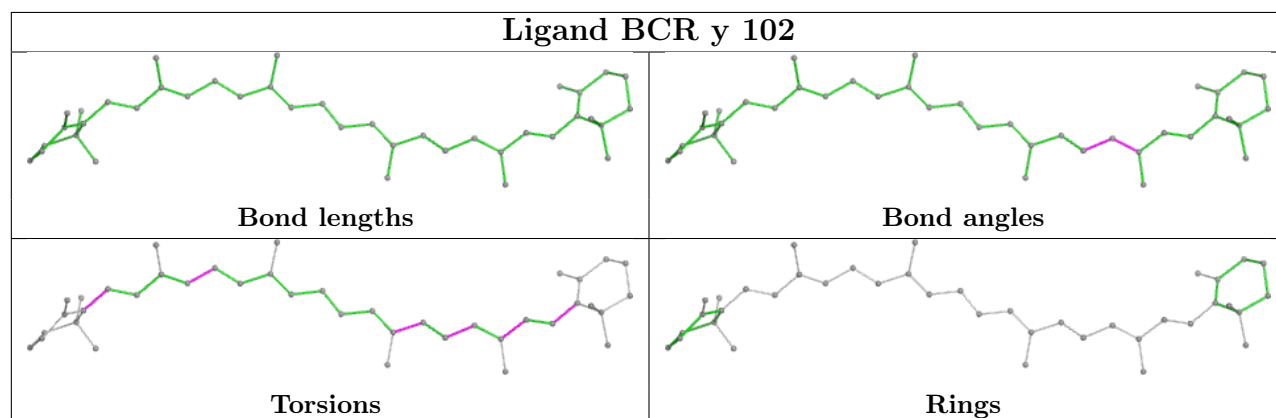
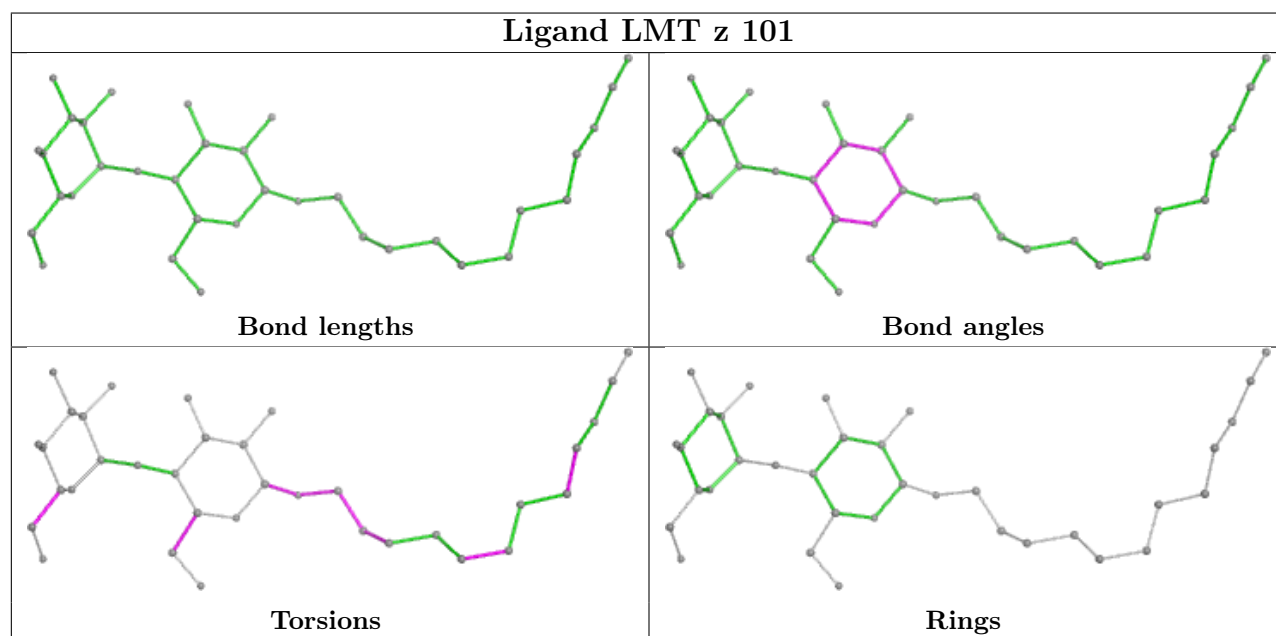
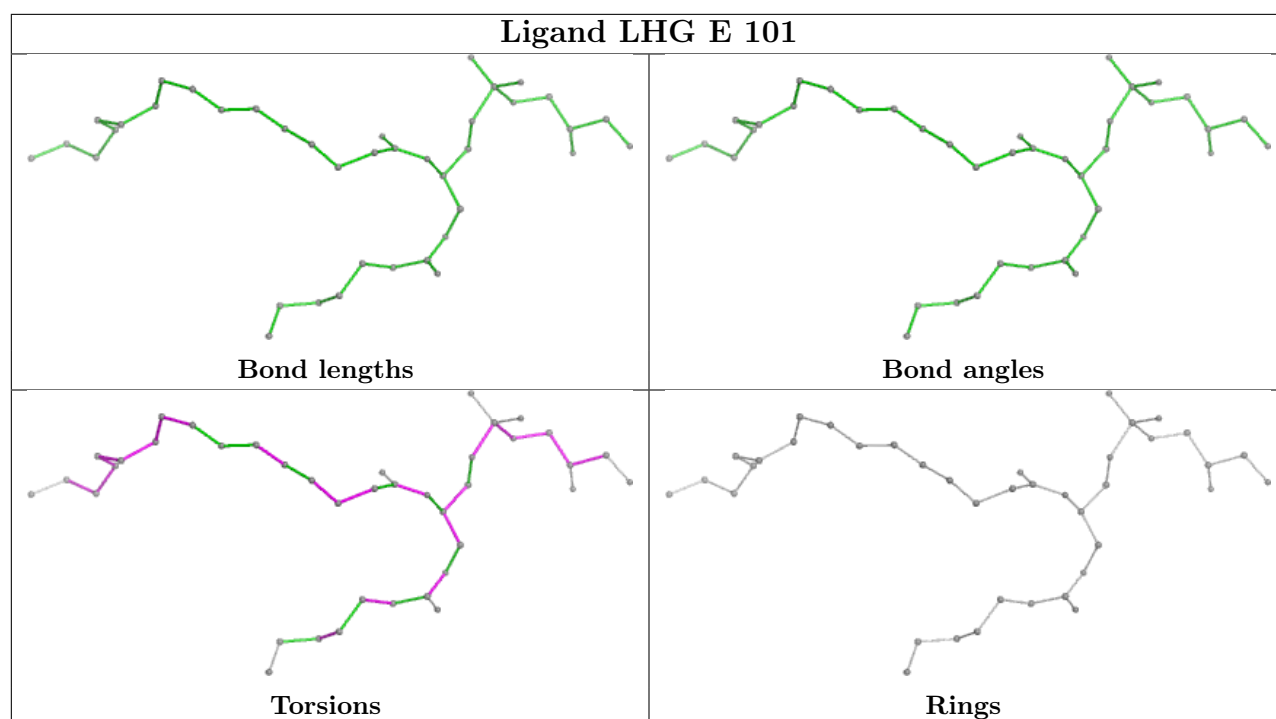


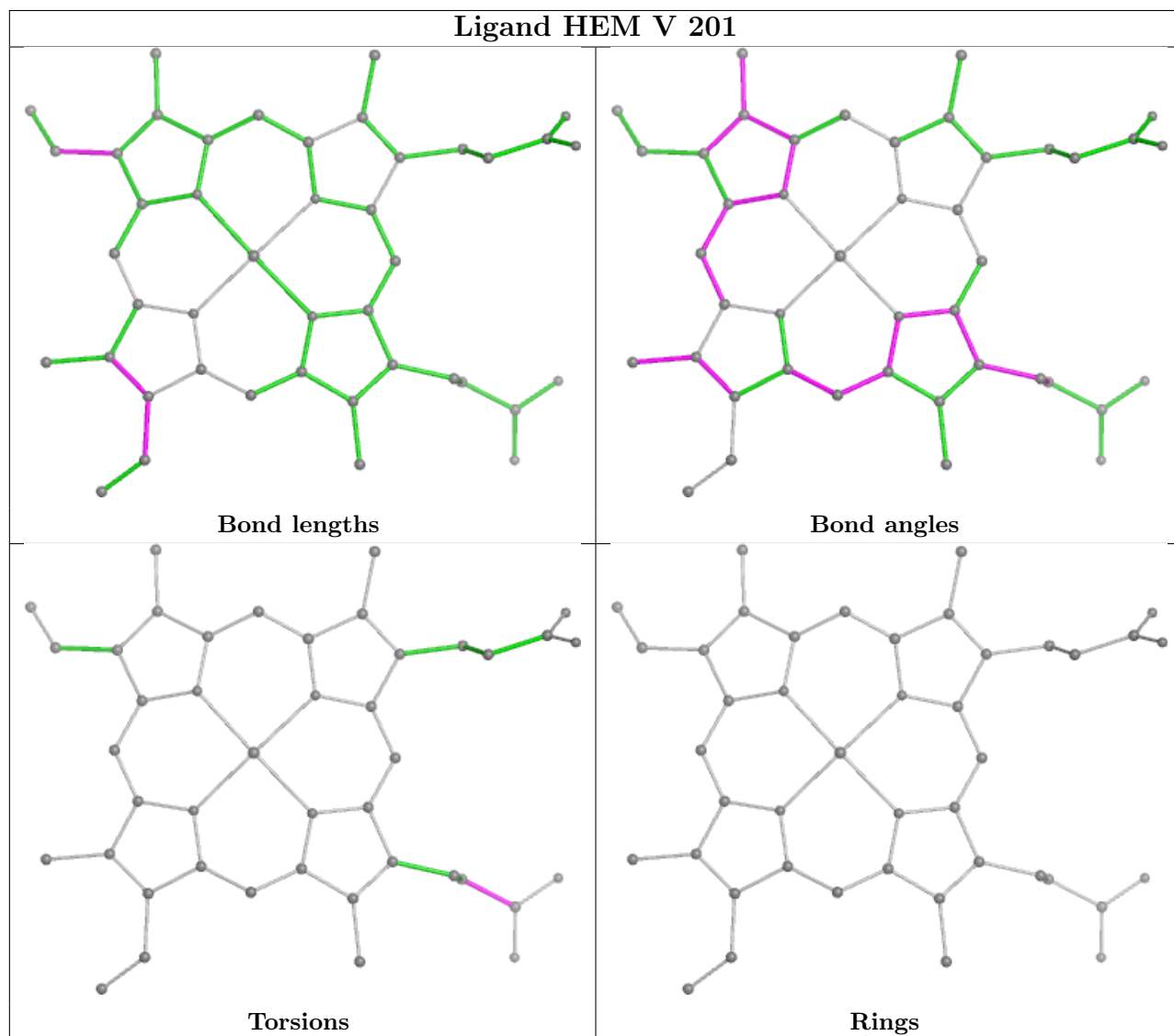
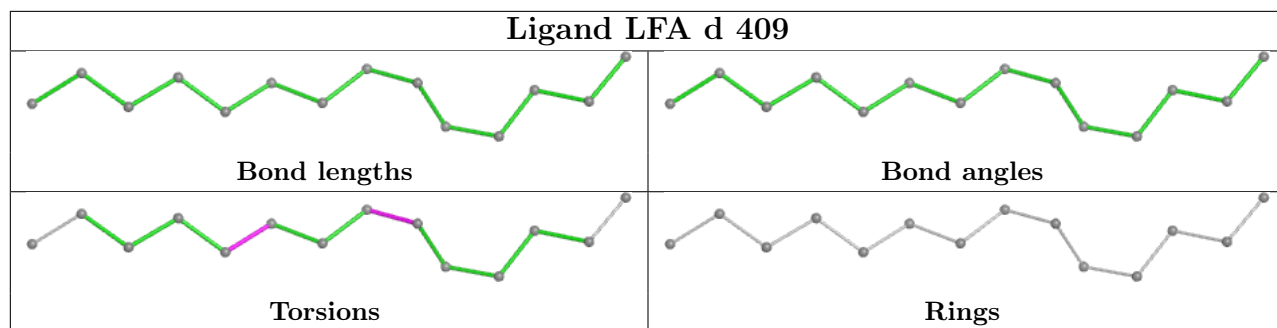


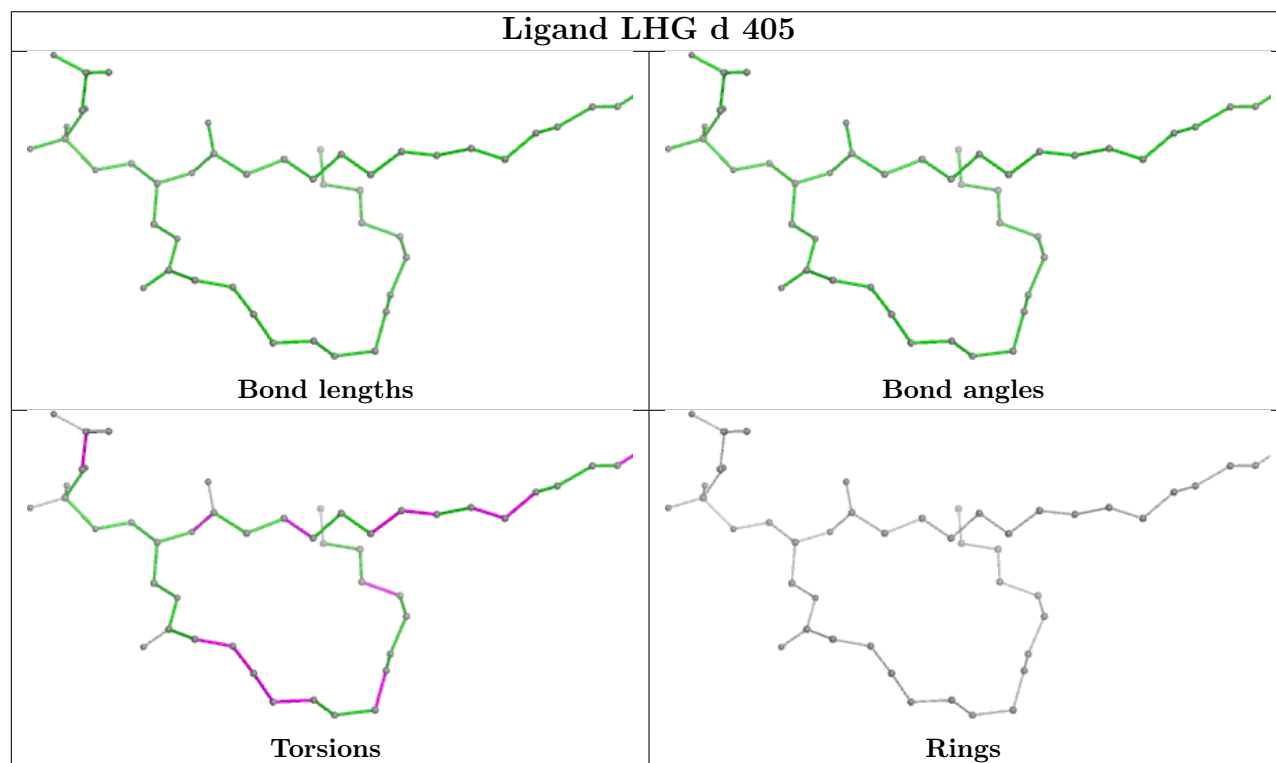
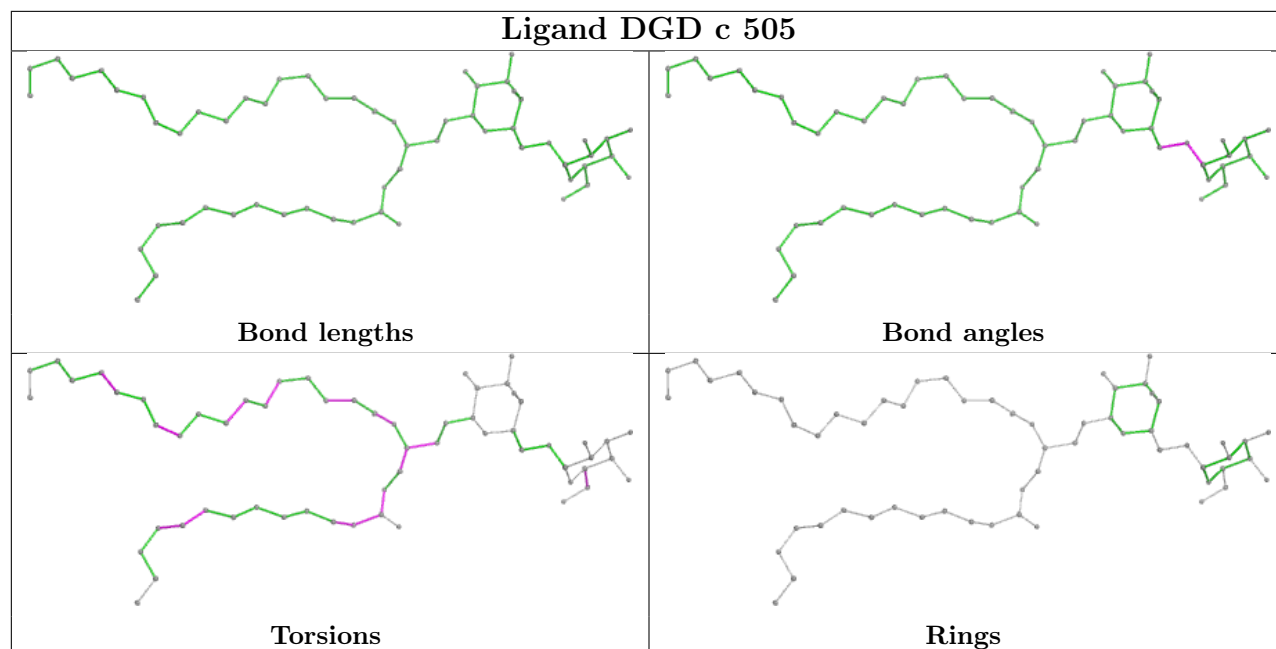


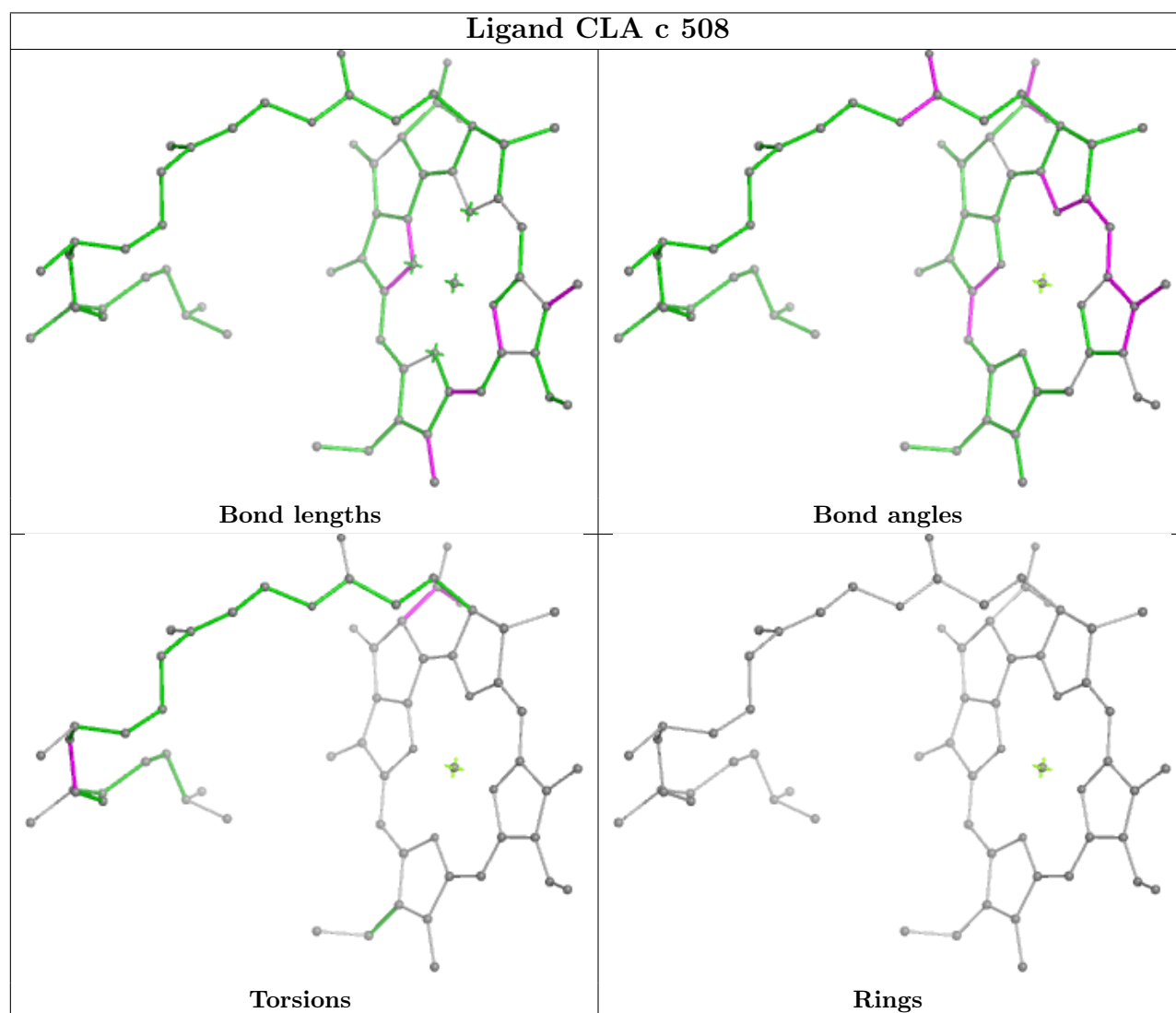
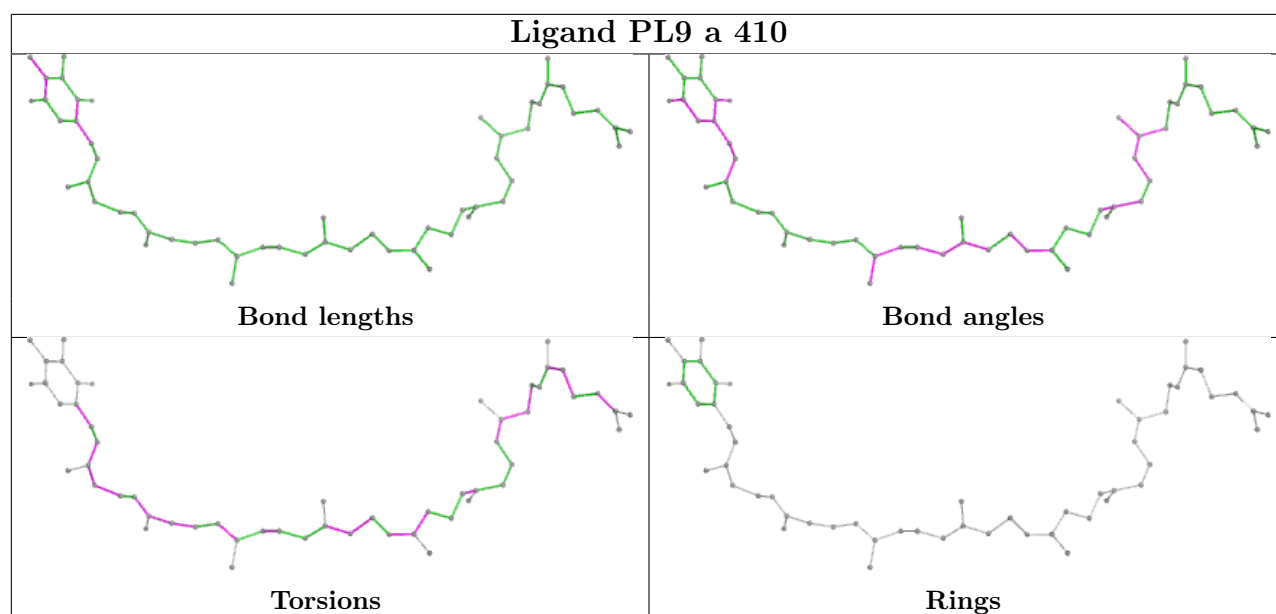


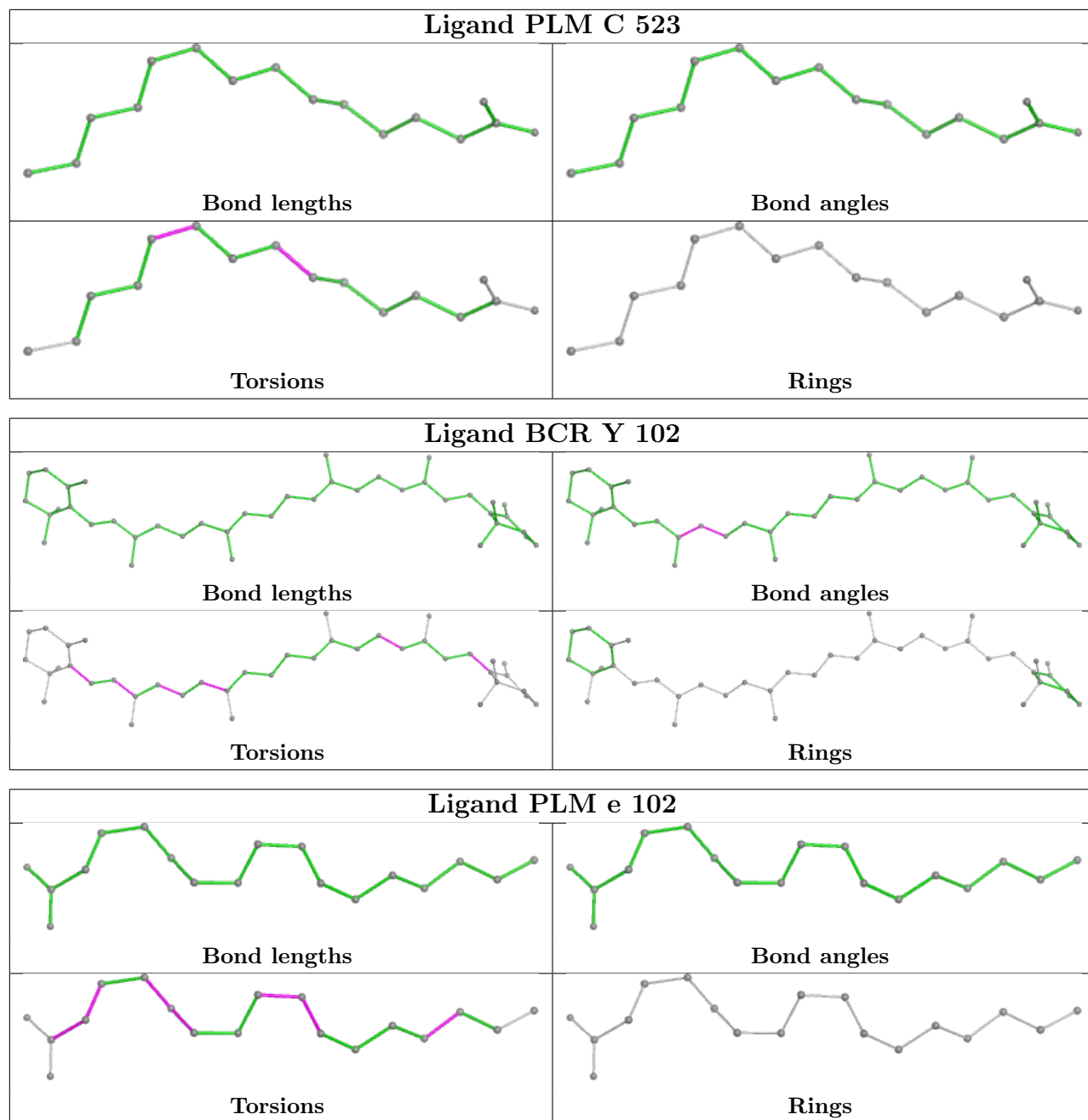




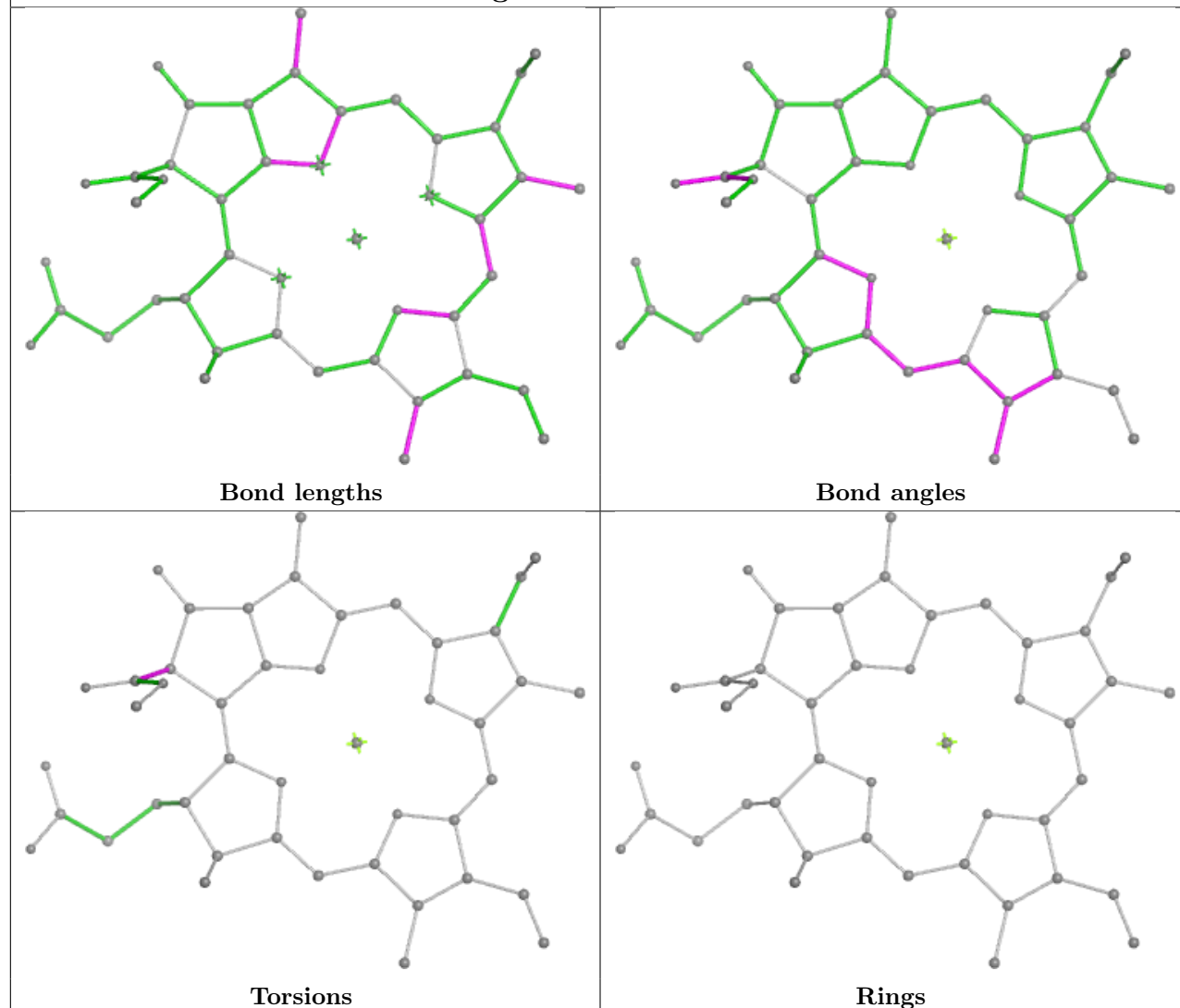


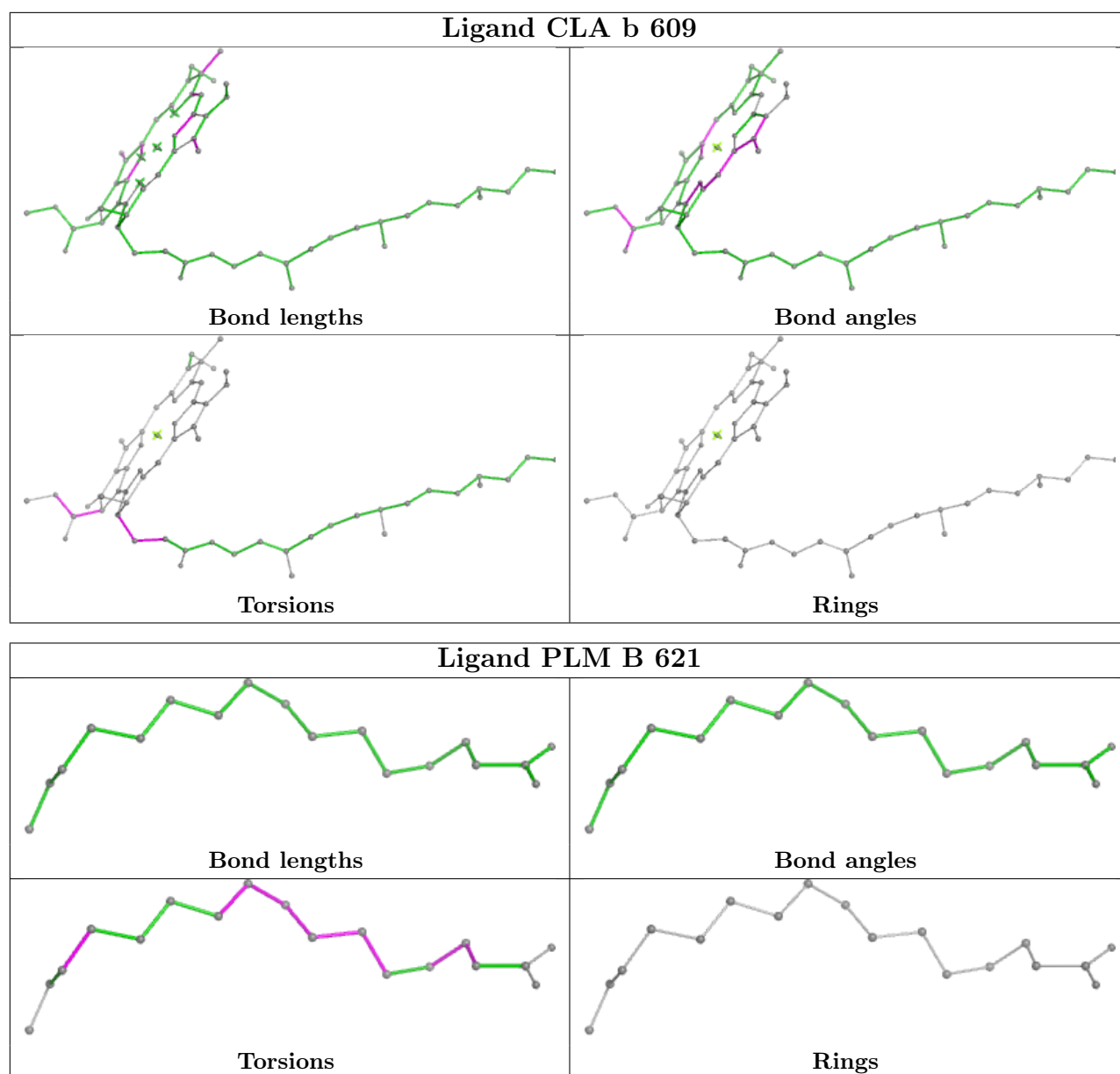




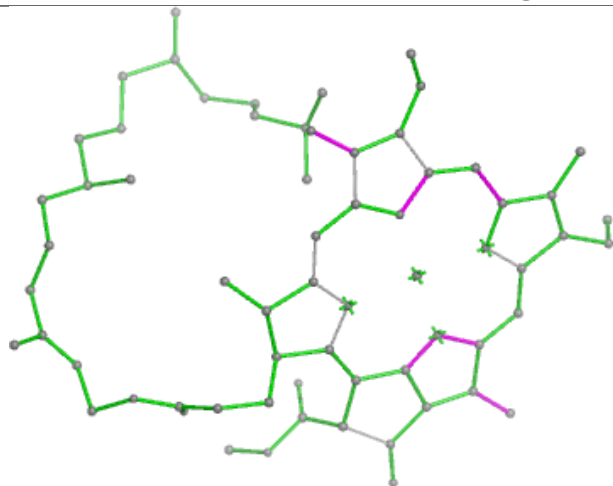


## Ligand CLA B 616

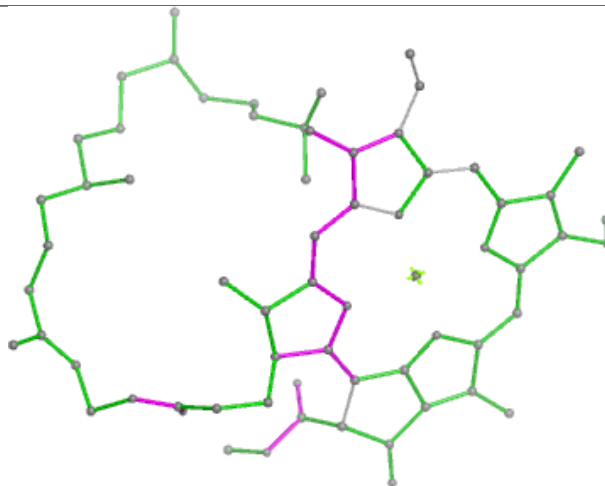




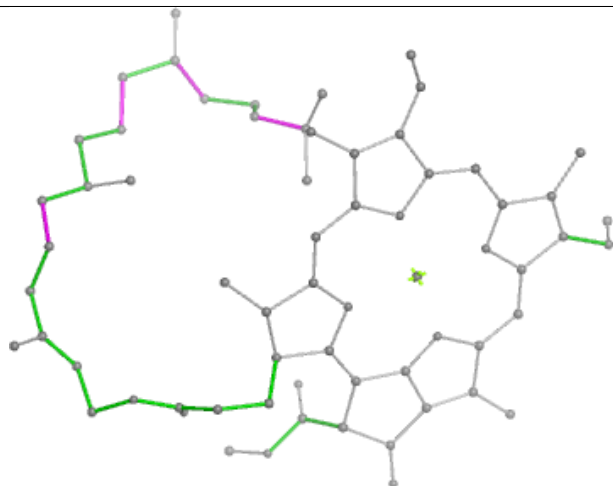
## Ligand CLA b 617



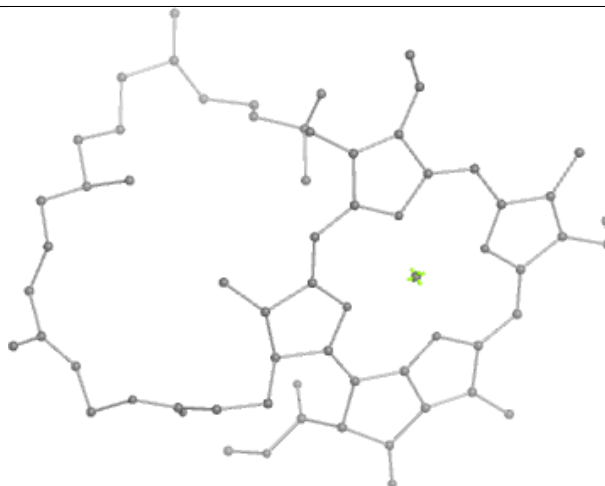
Bond lengths



Bond angles

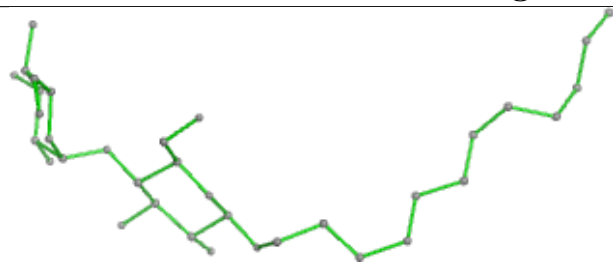


Torsions

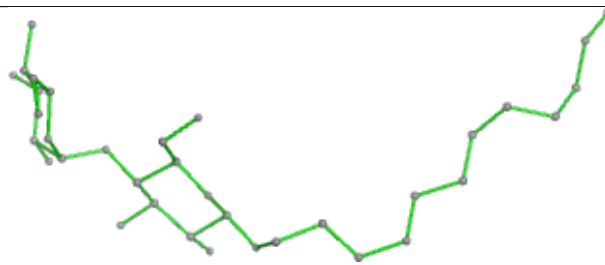


Rings

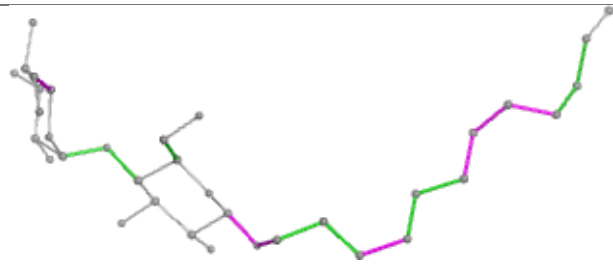
## Ligand LMT T 104



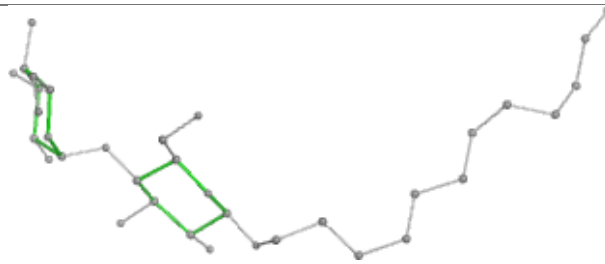
Bond lengths



Bond angles

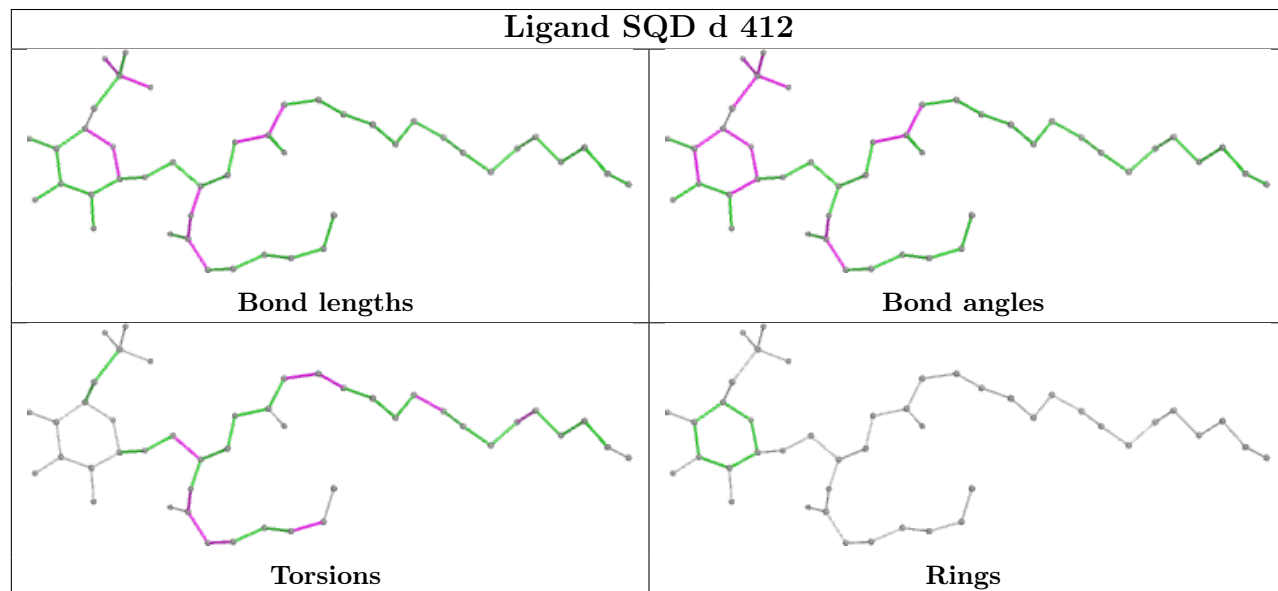
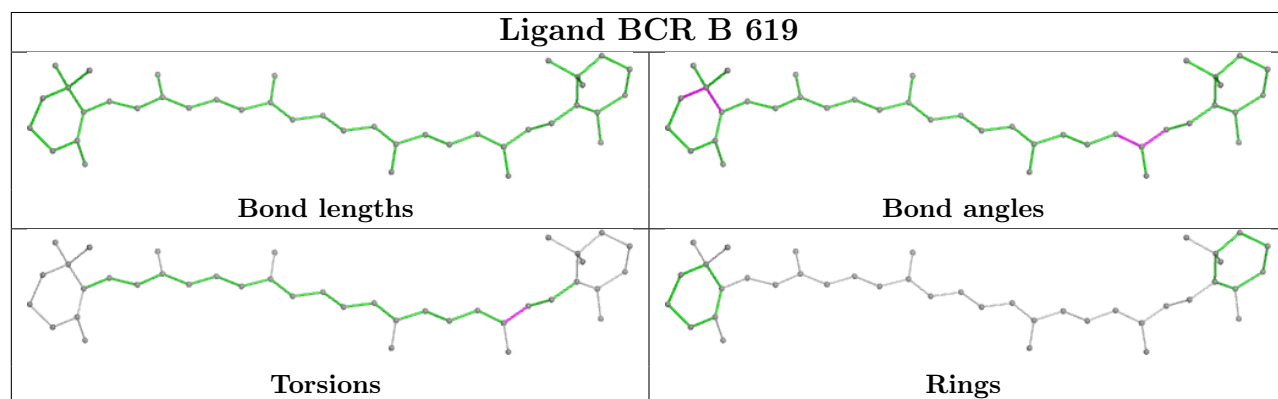
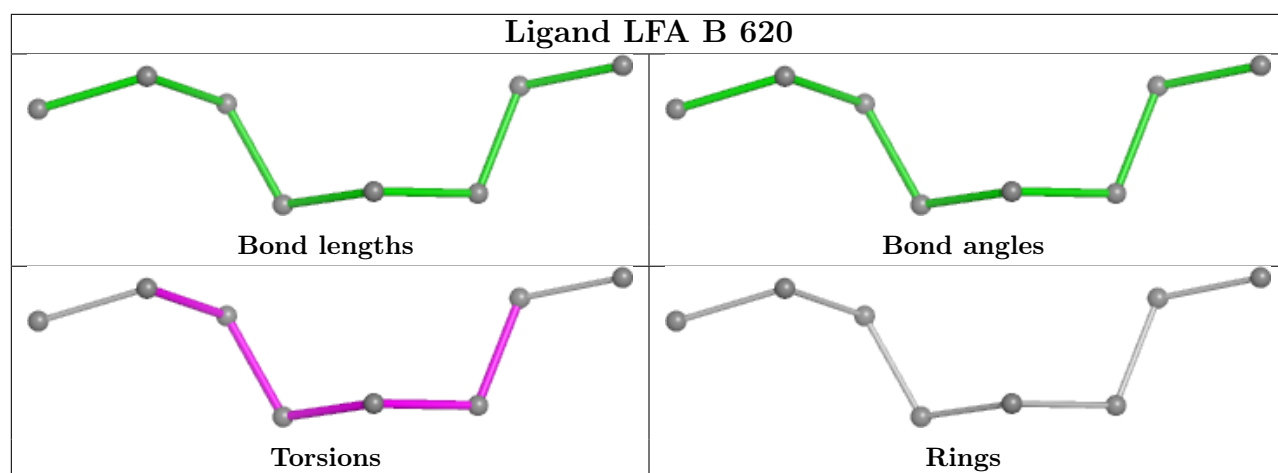


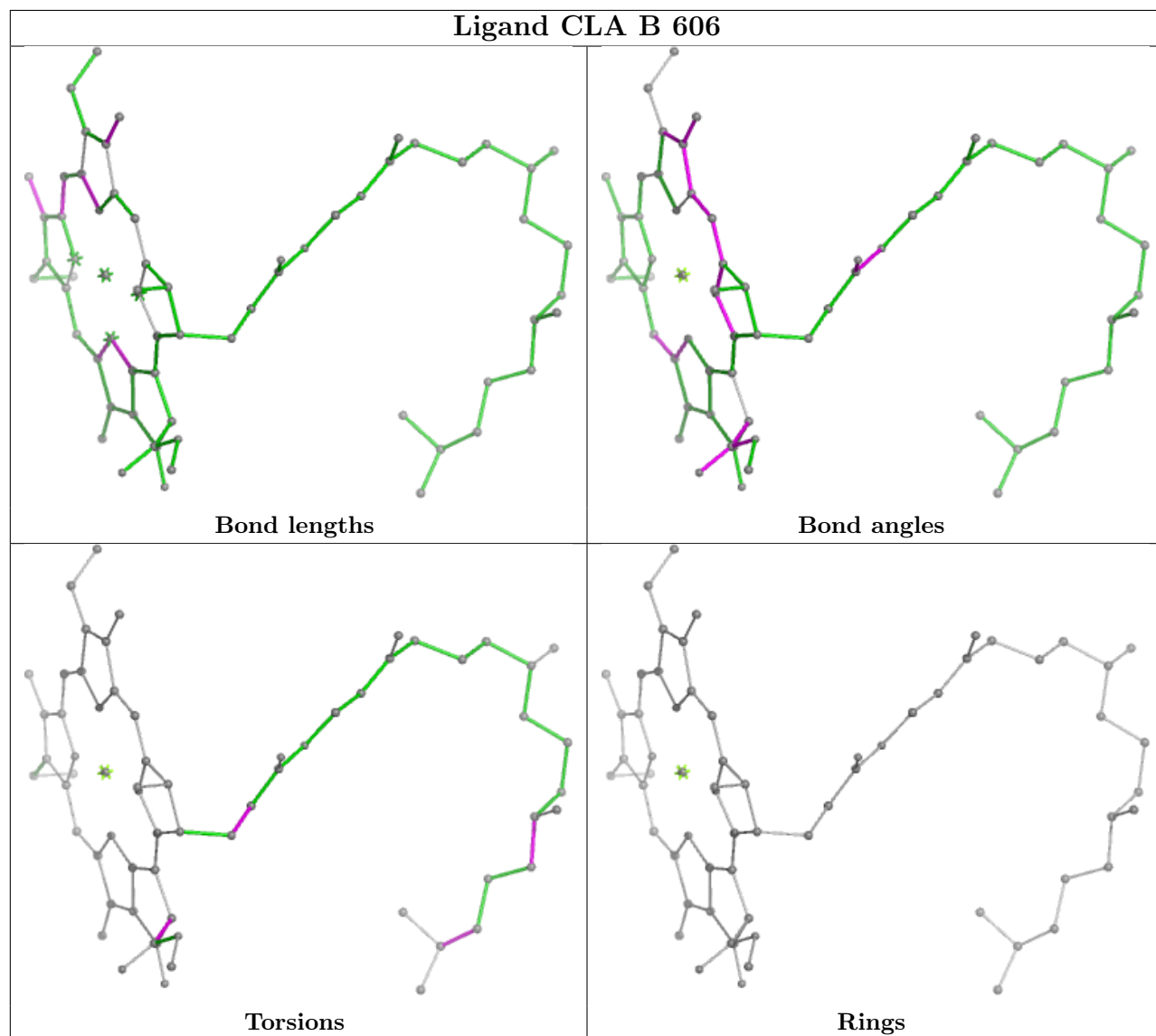
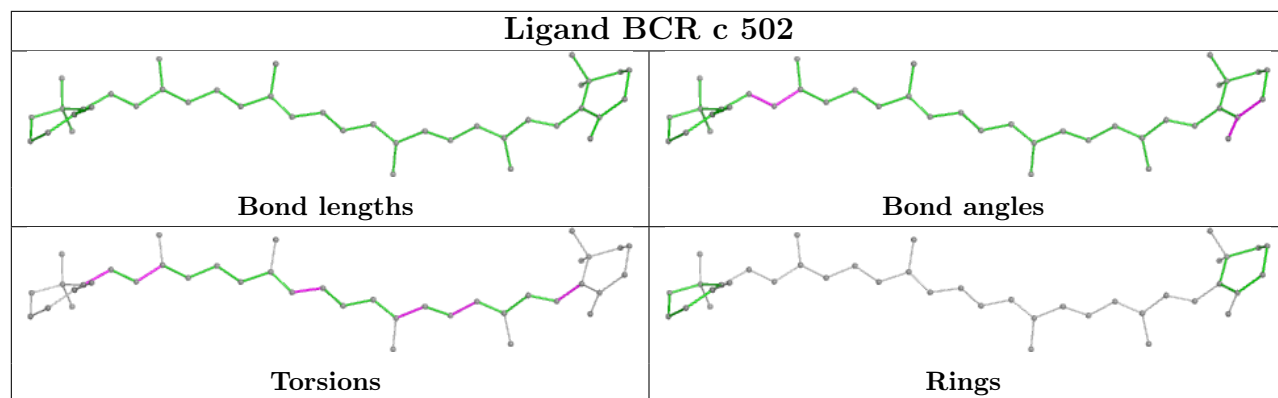
Torsions

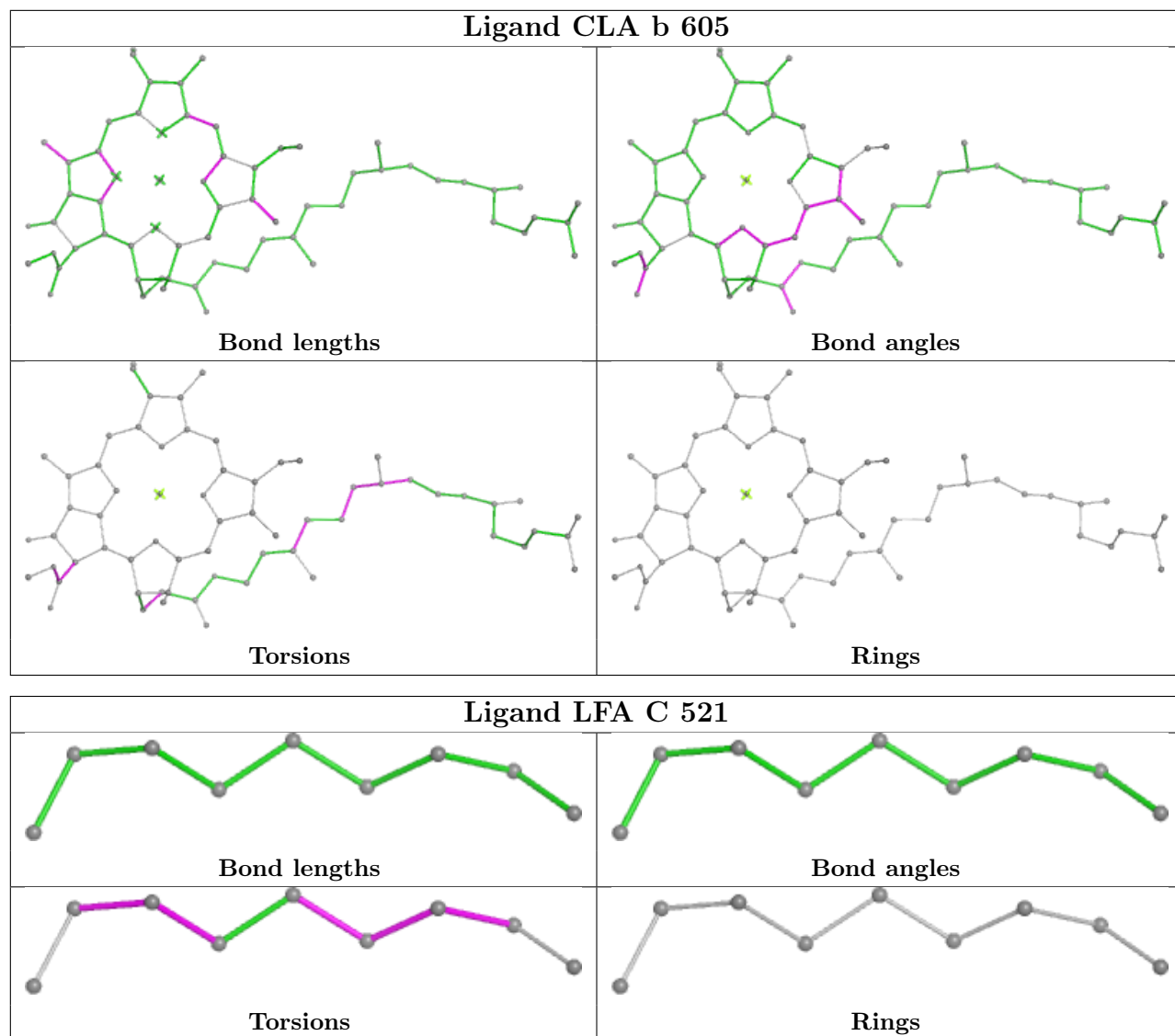


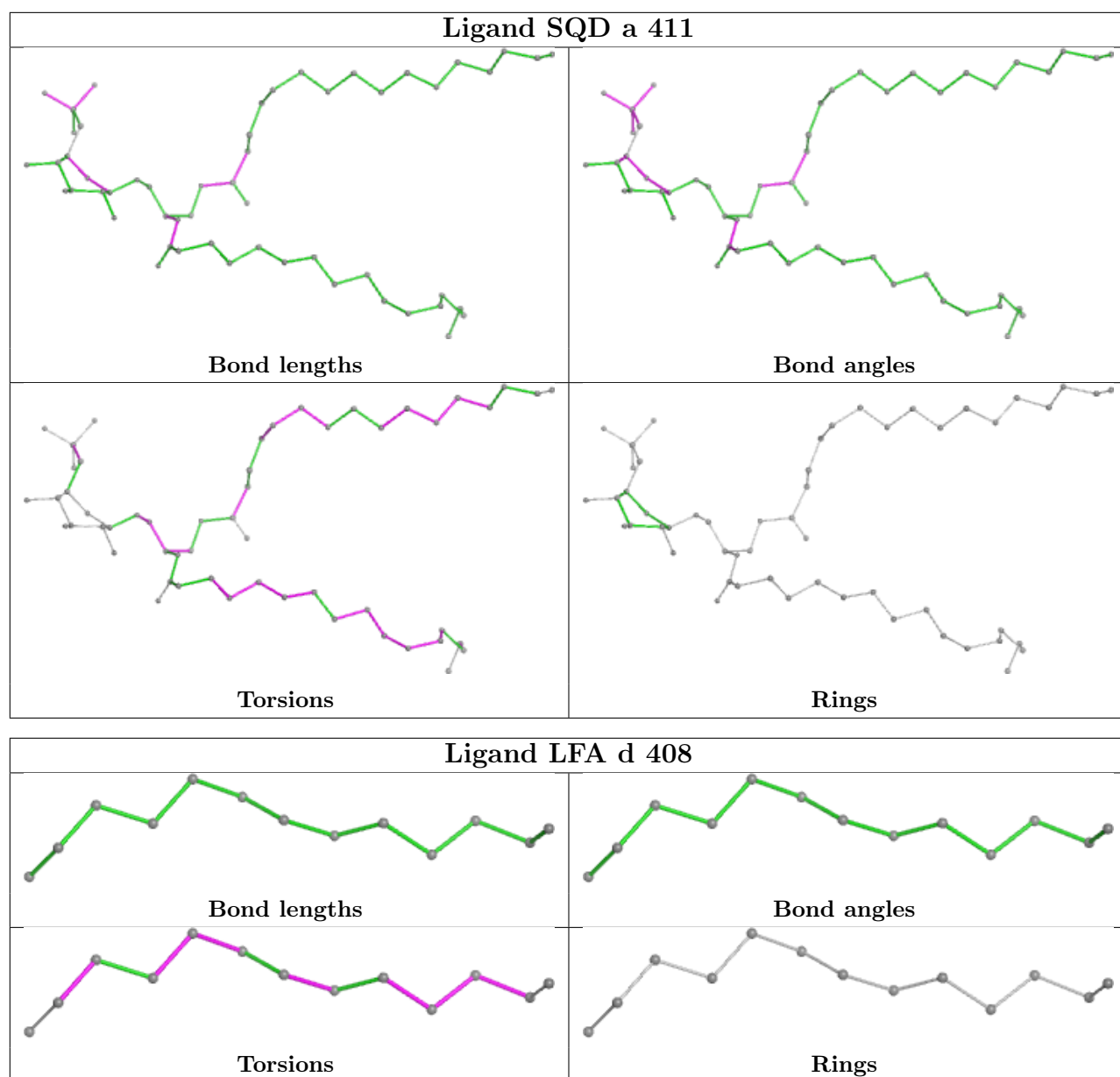
Rings

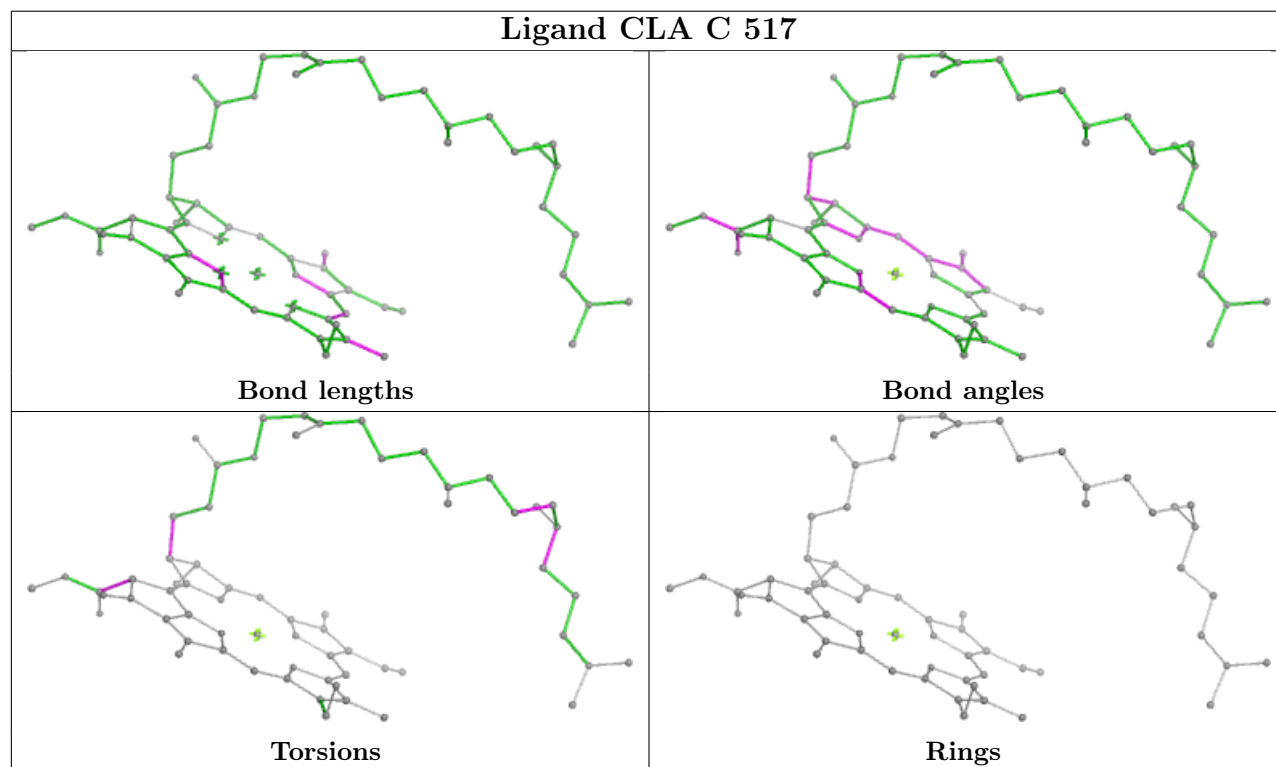
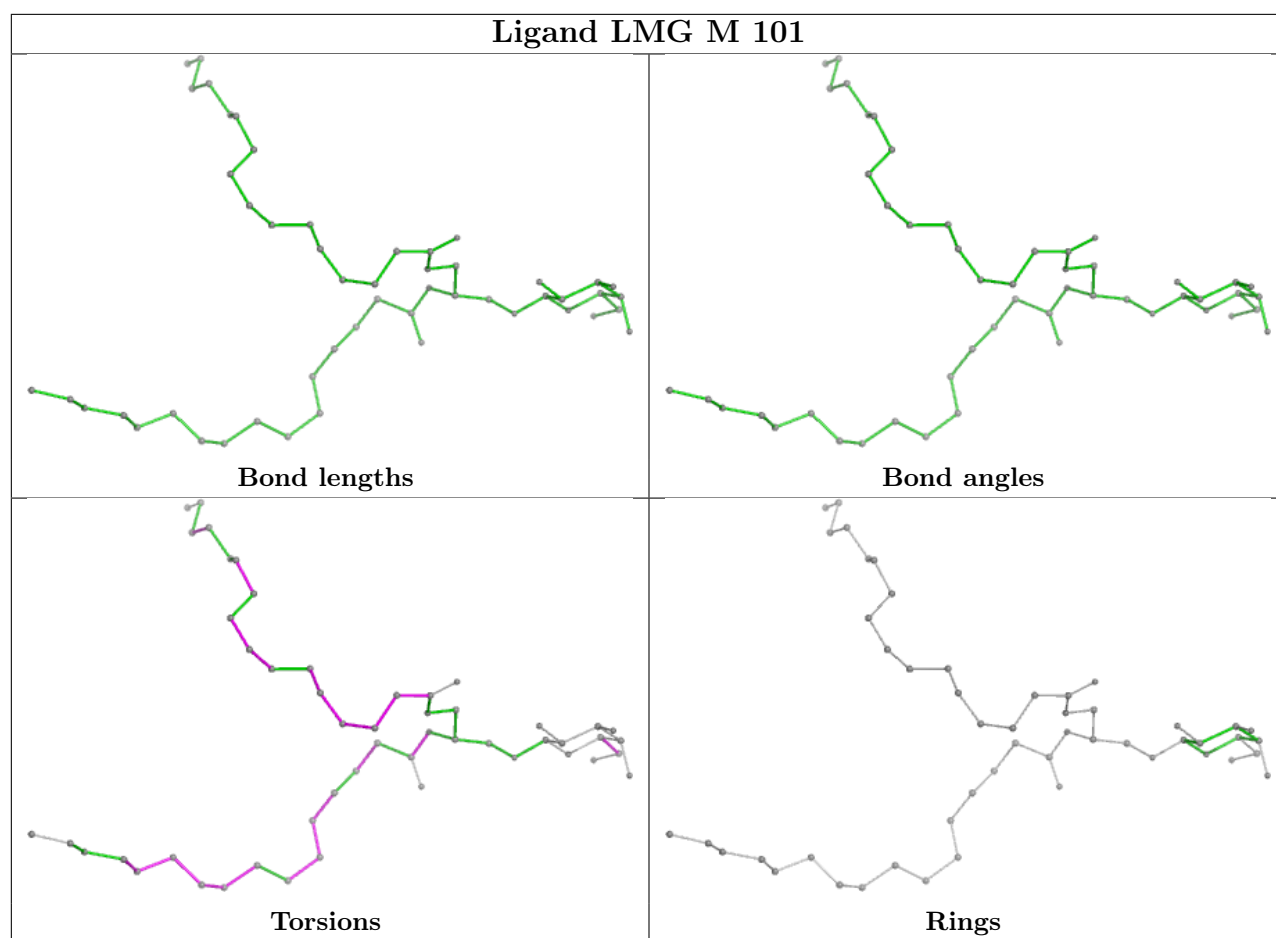


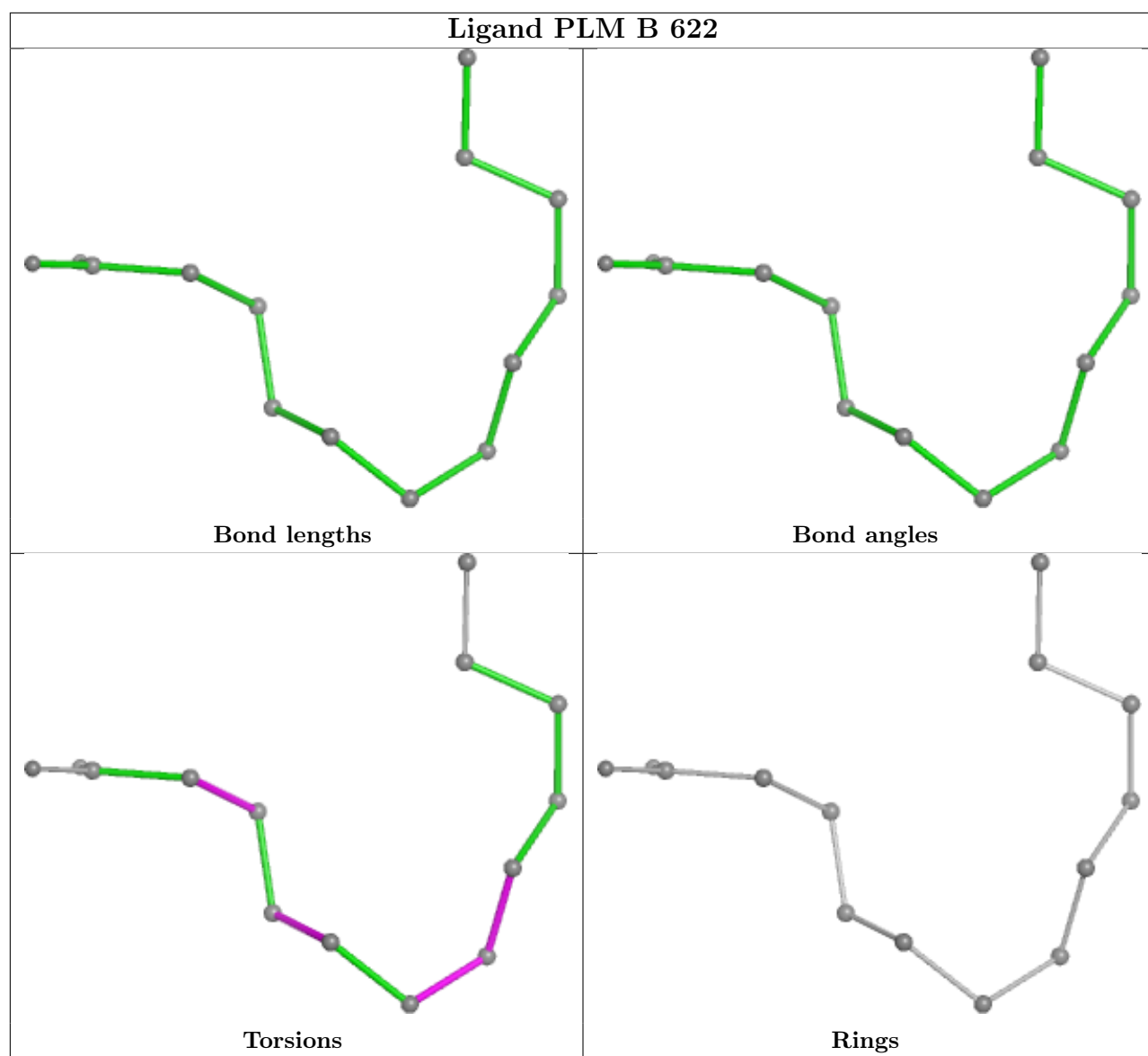


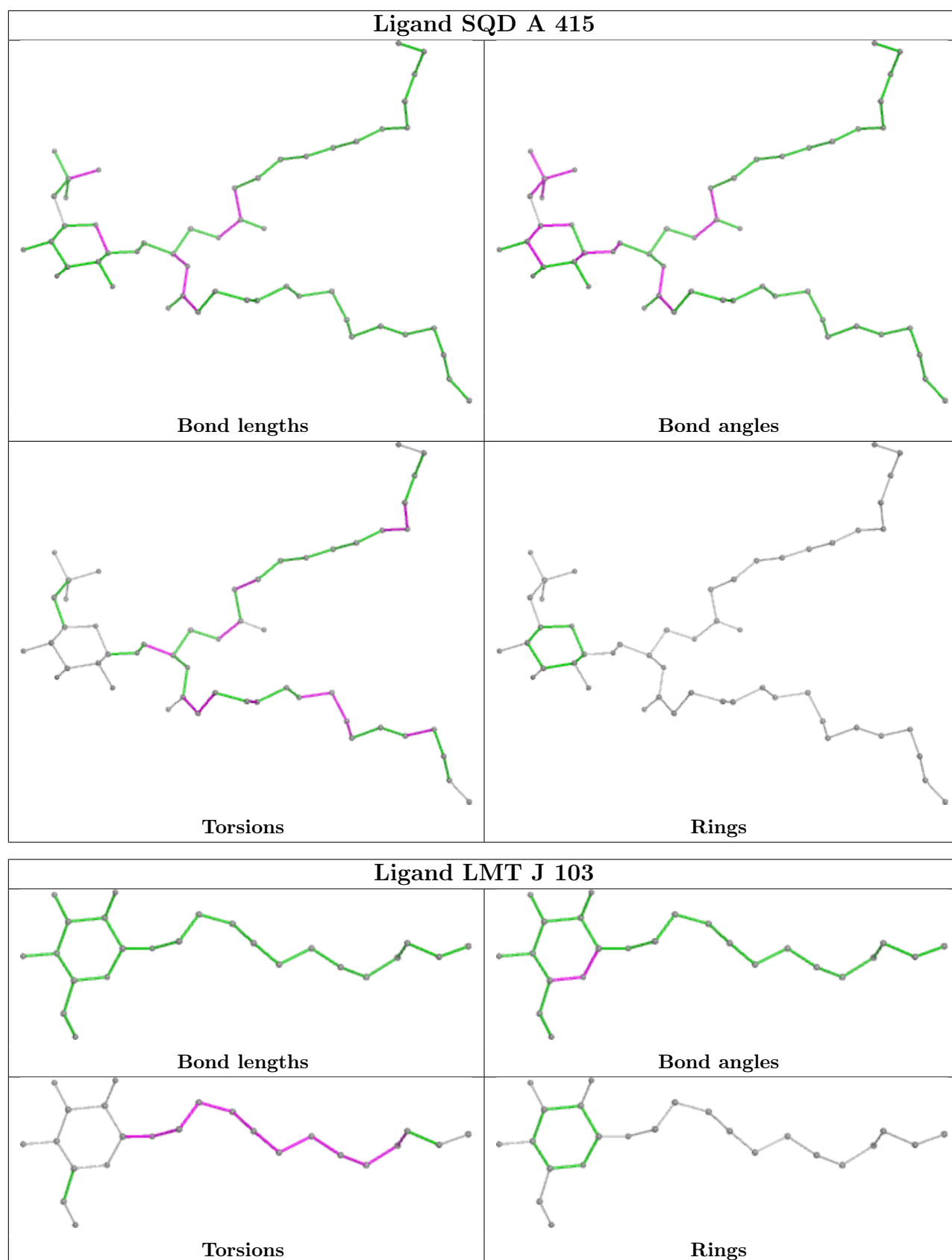


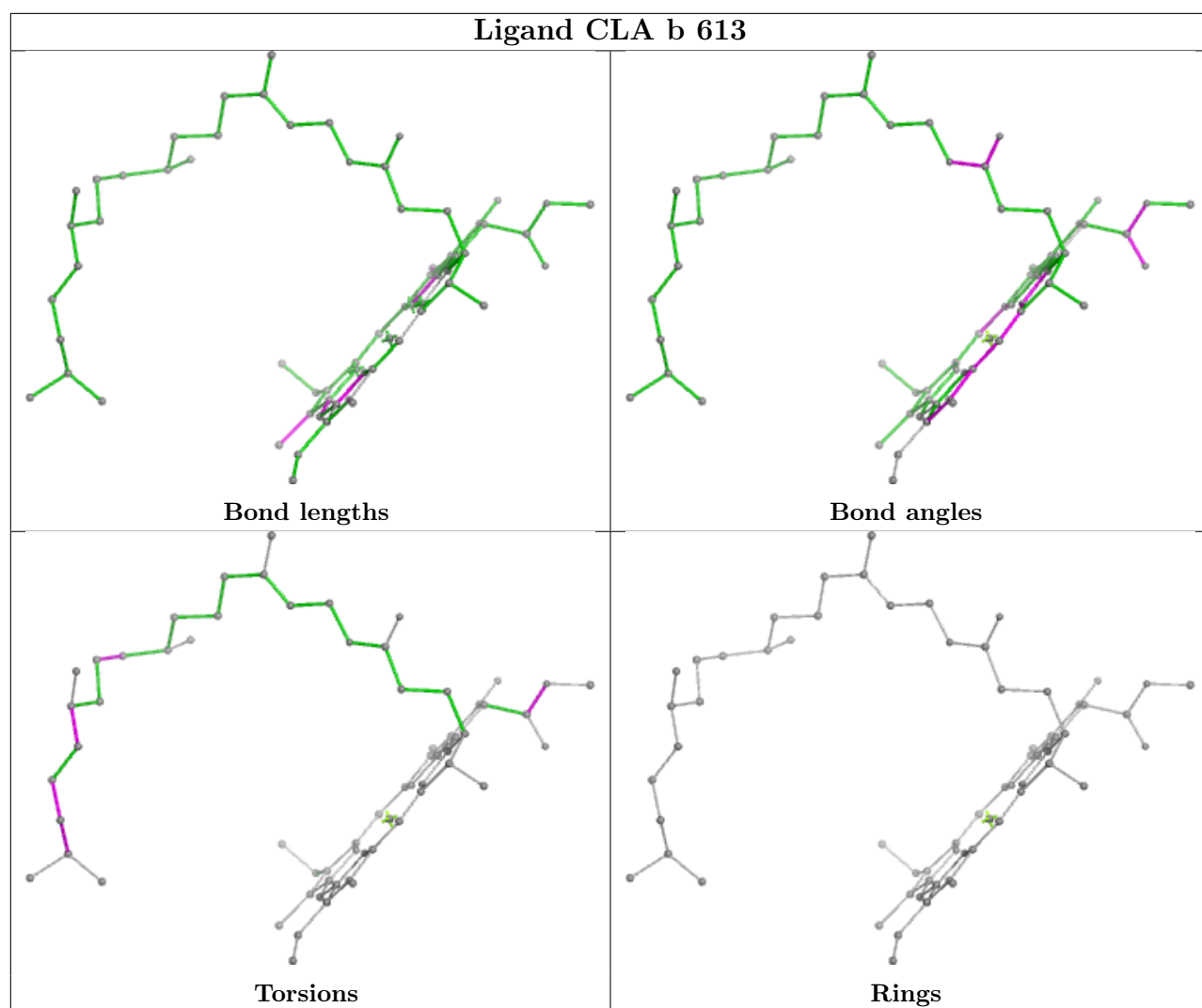




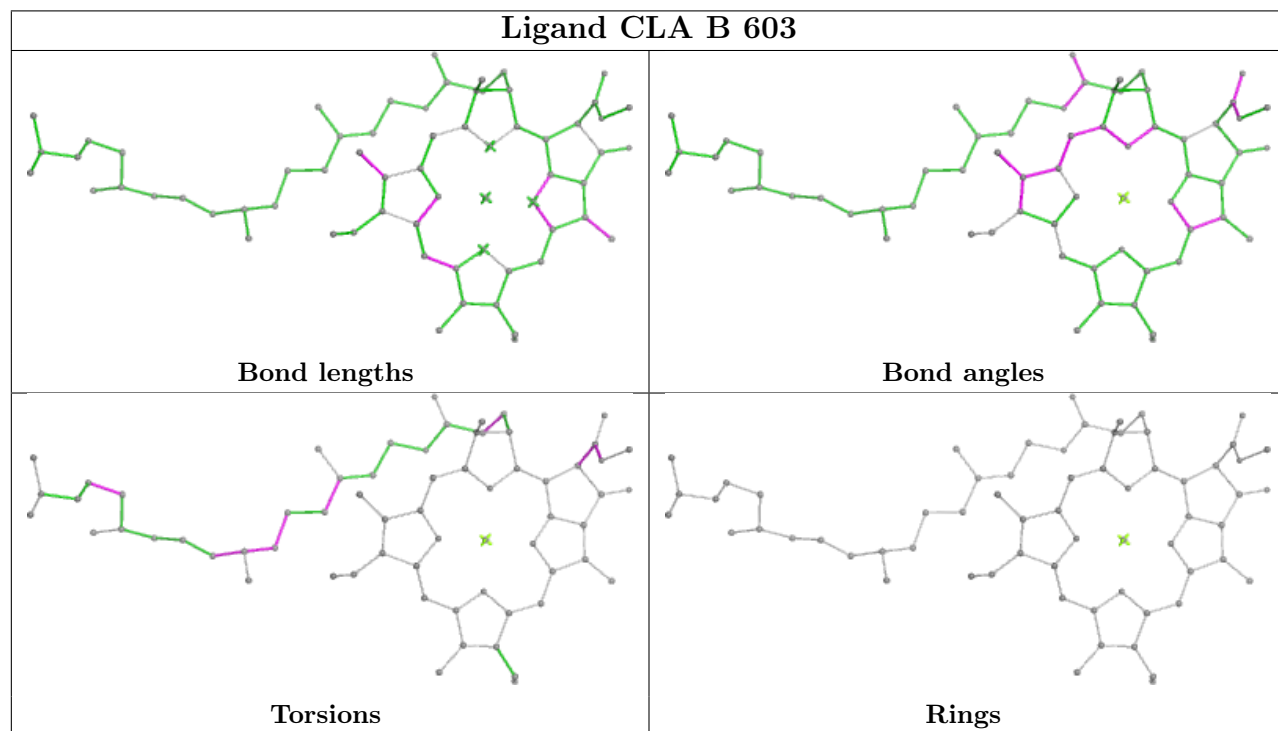
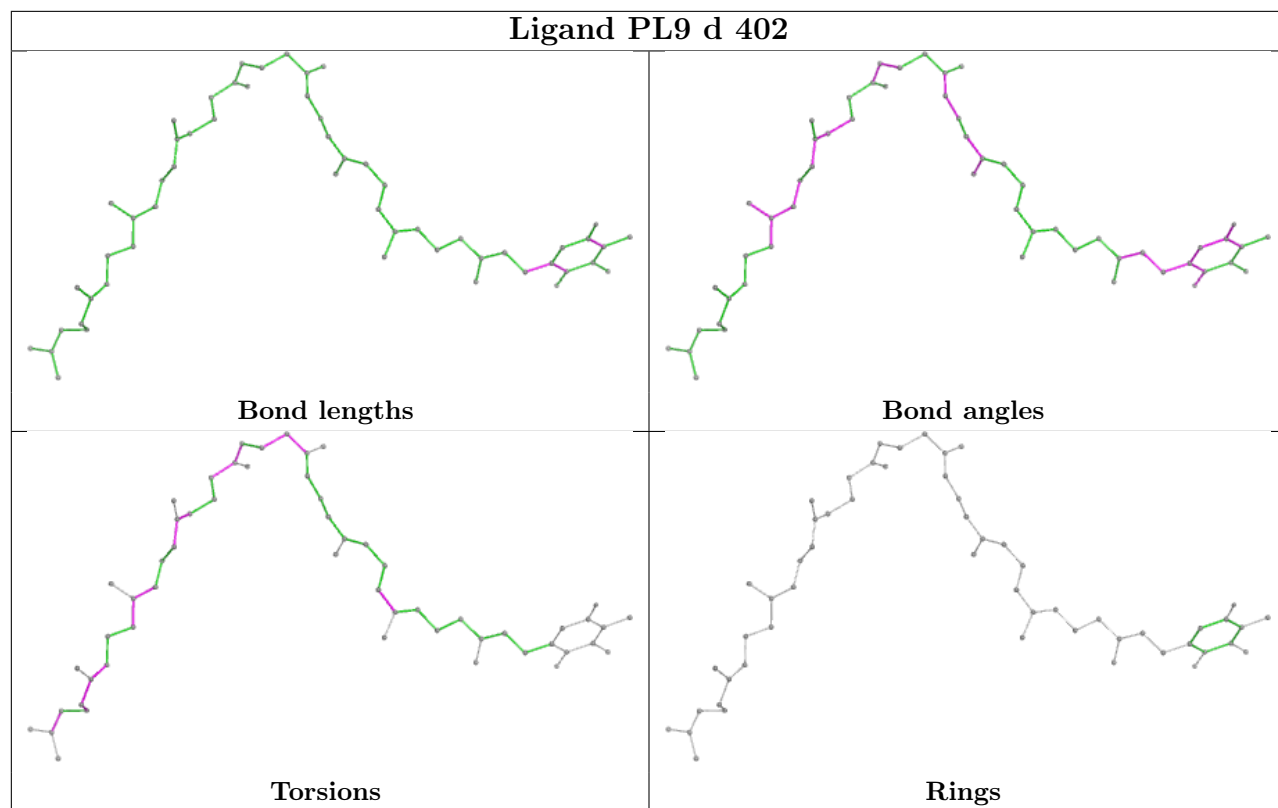


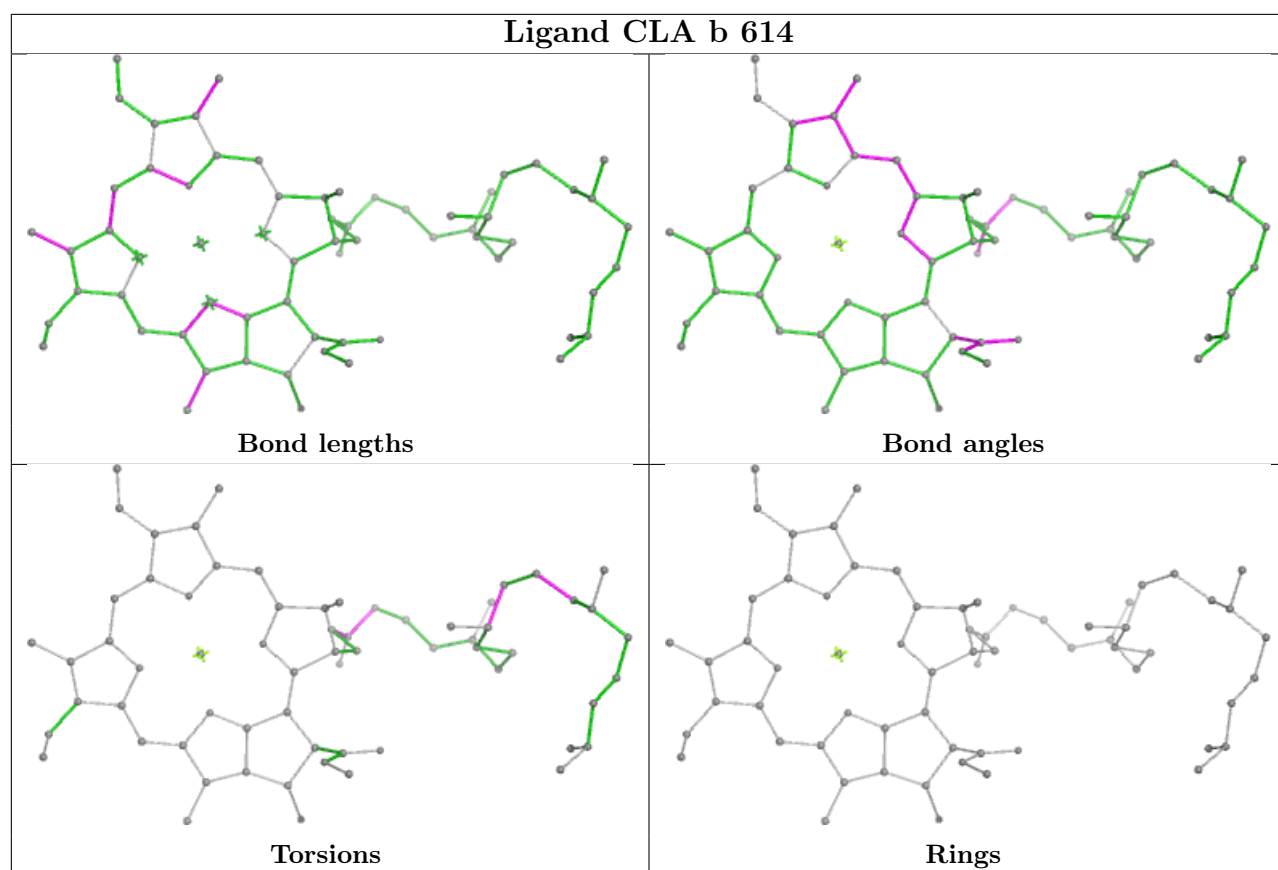


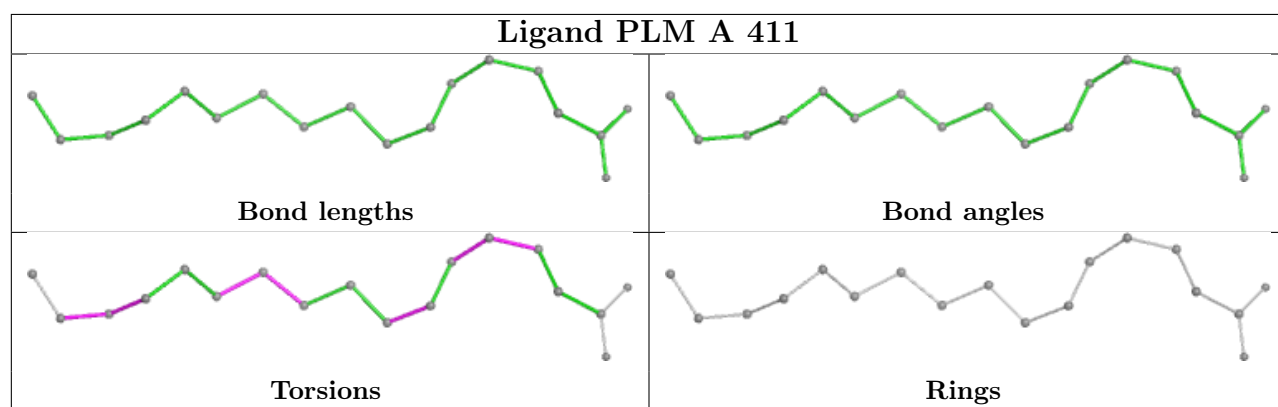
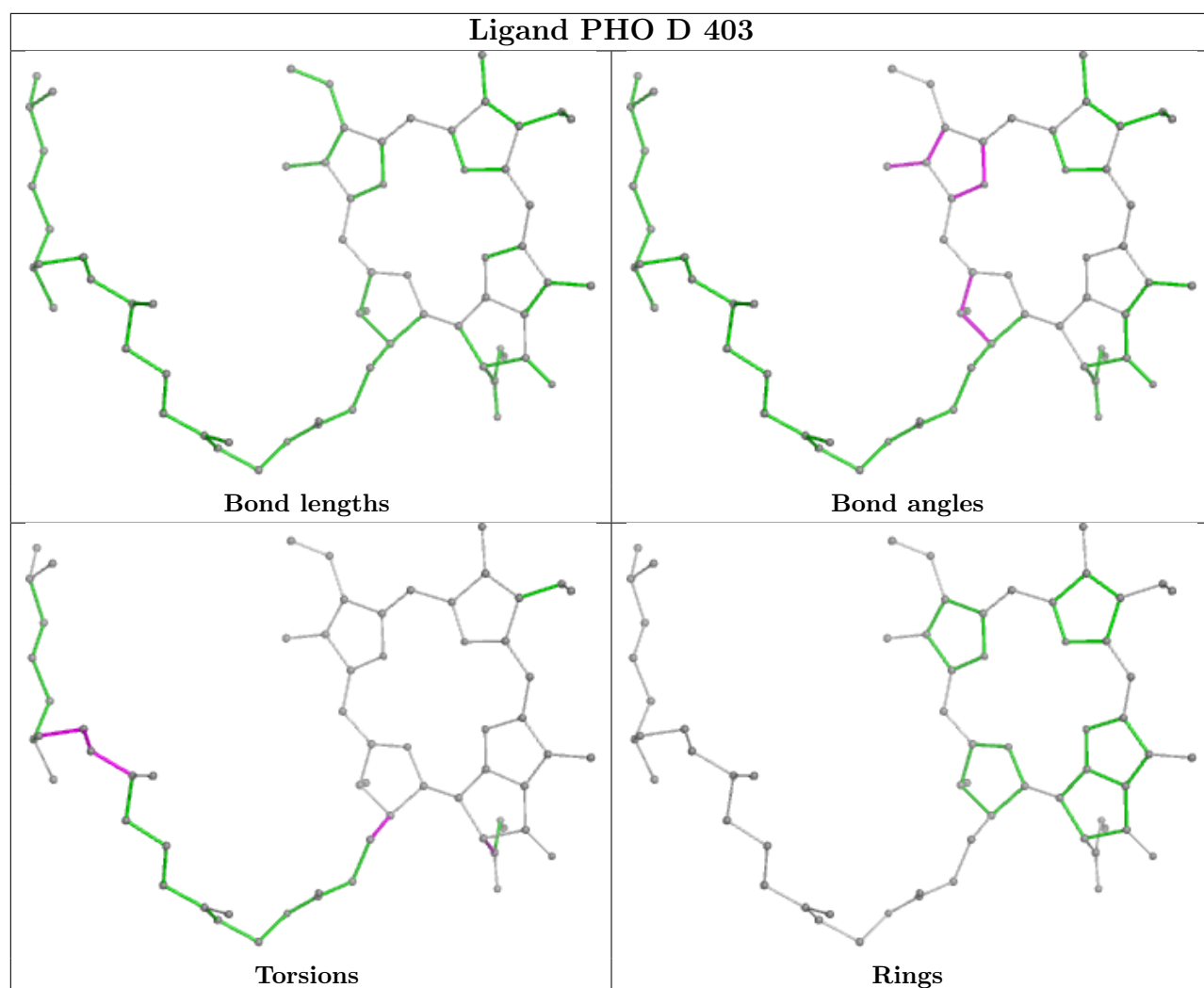


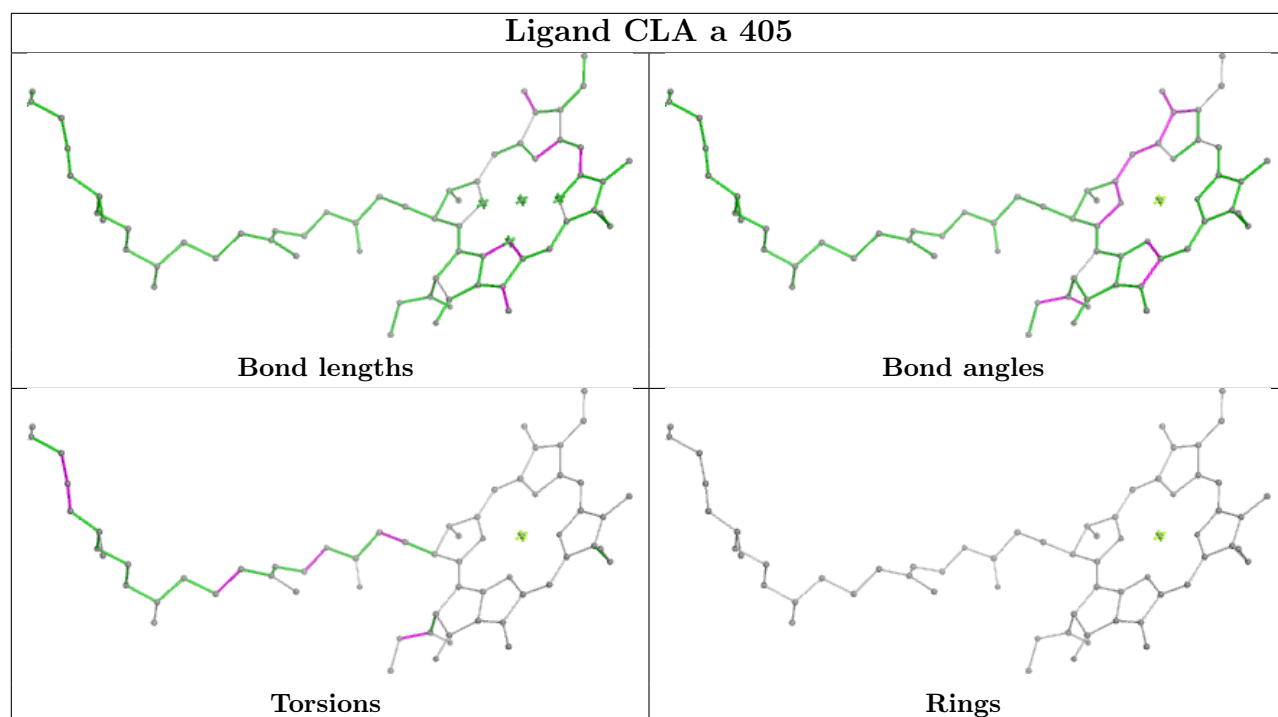
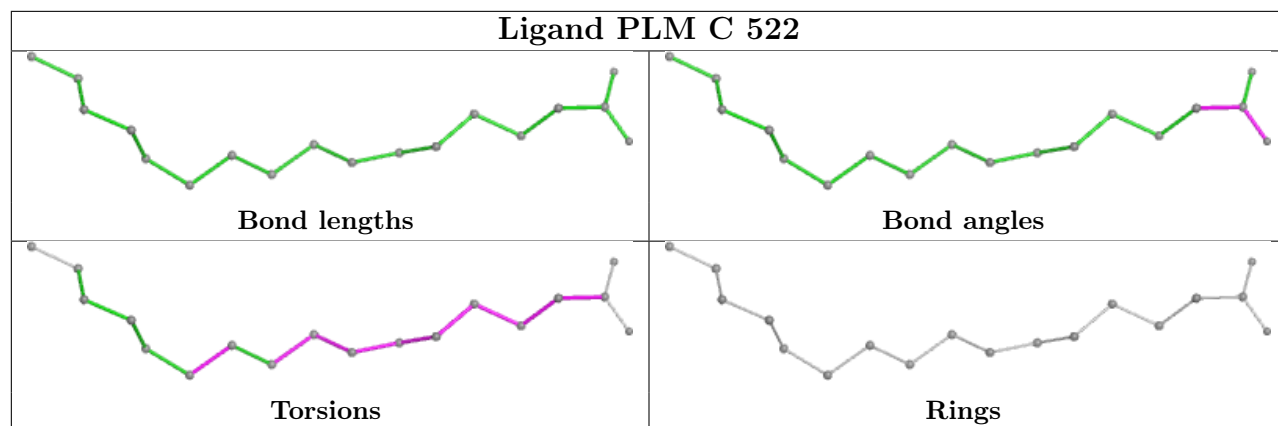


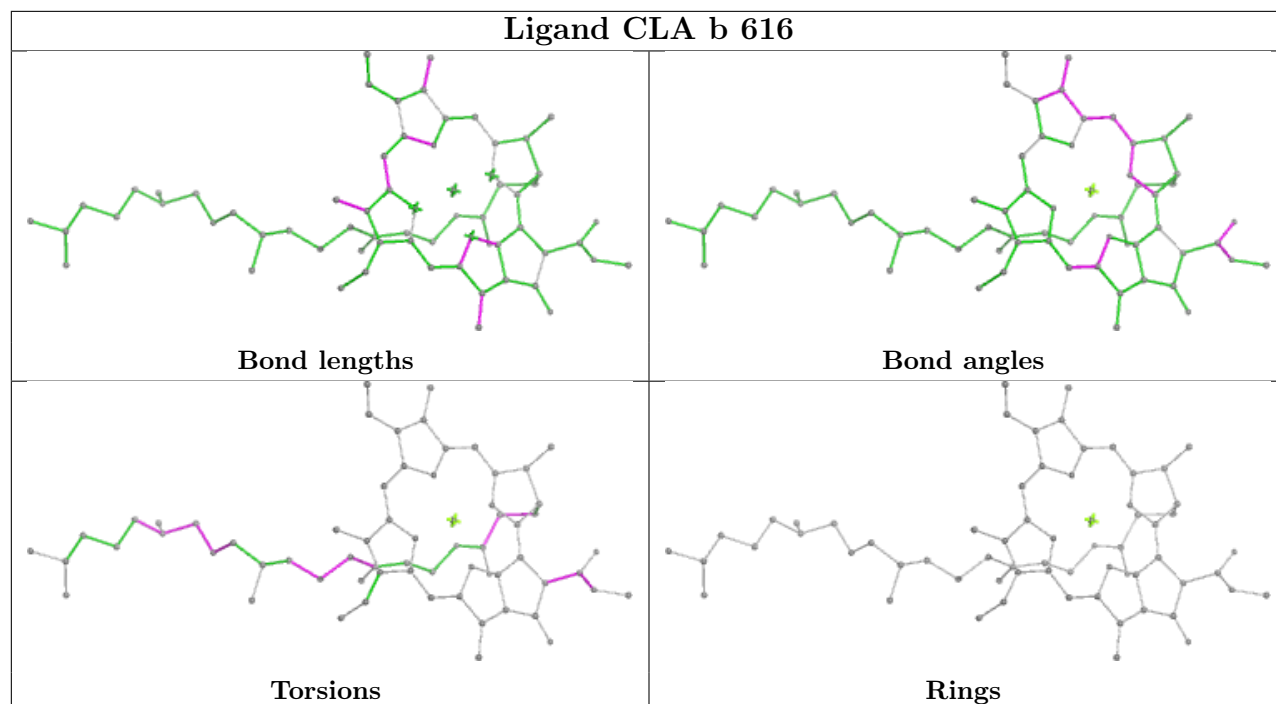
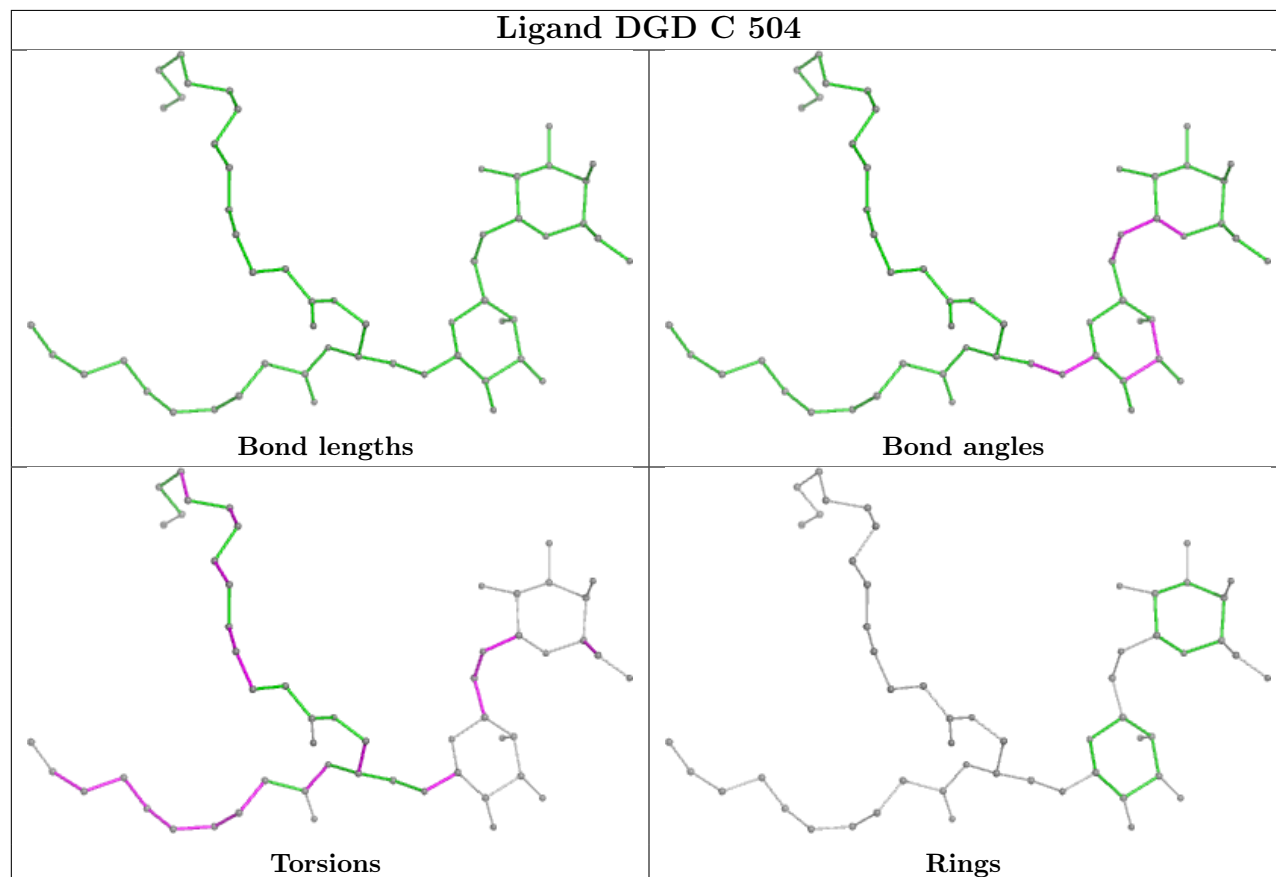


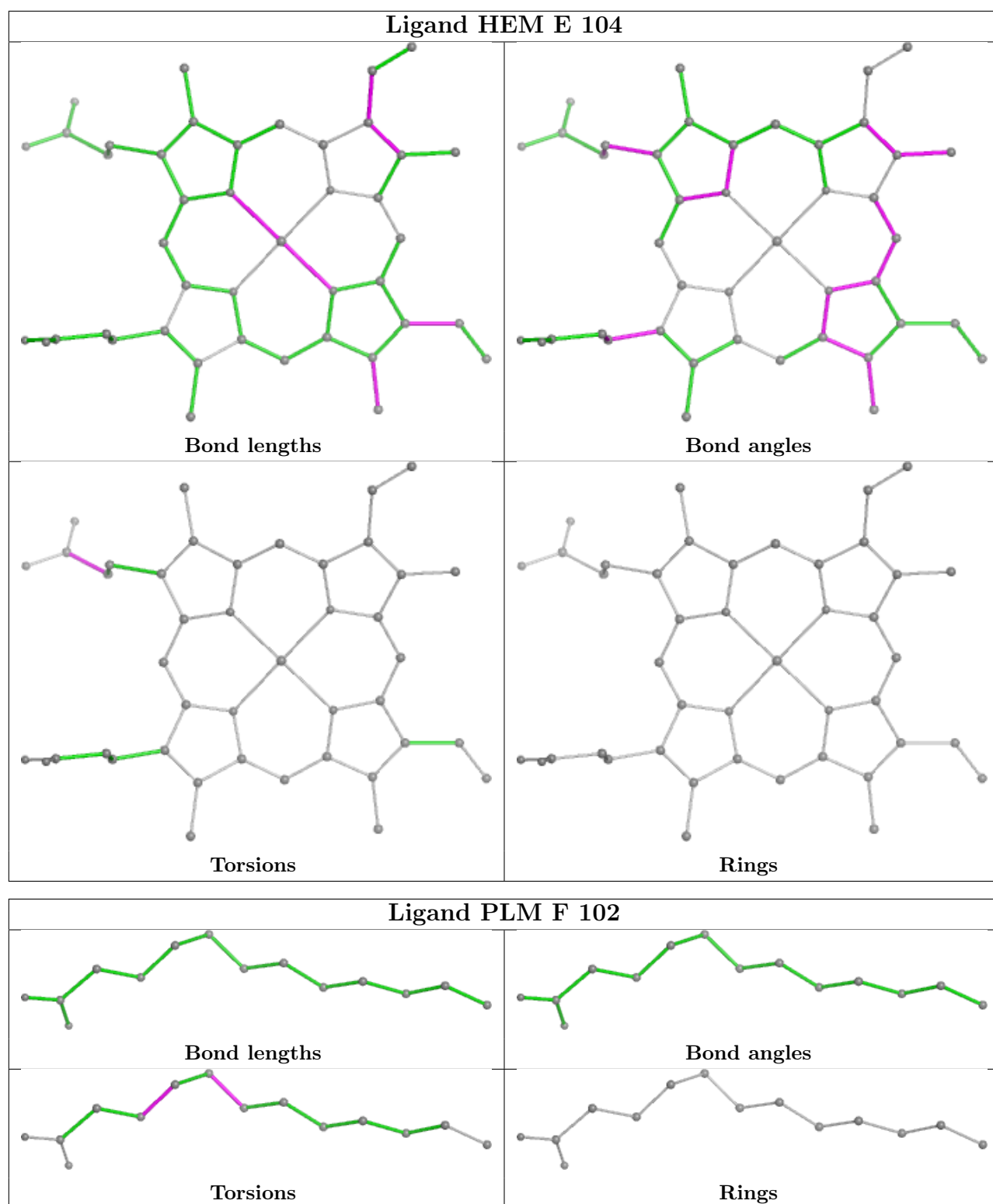




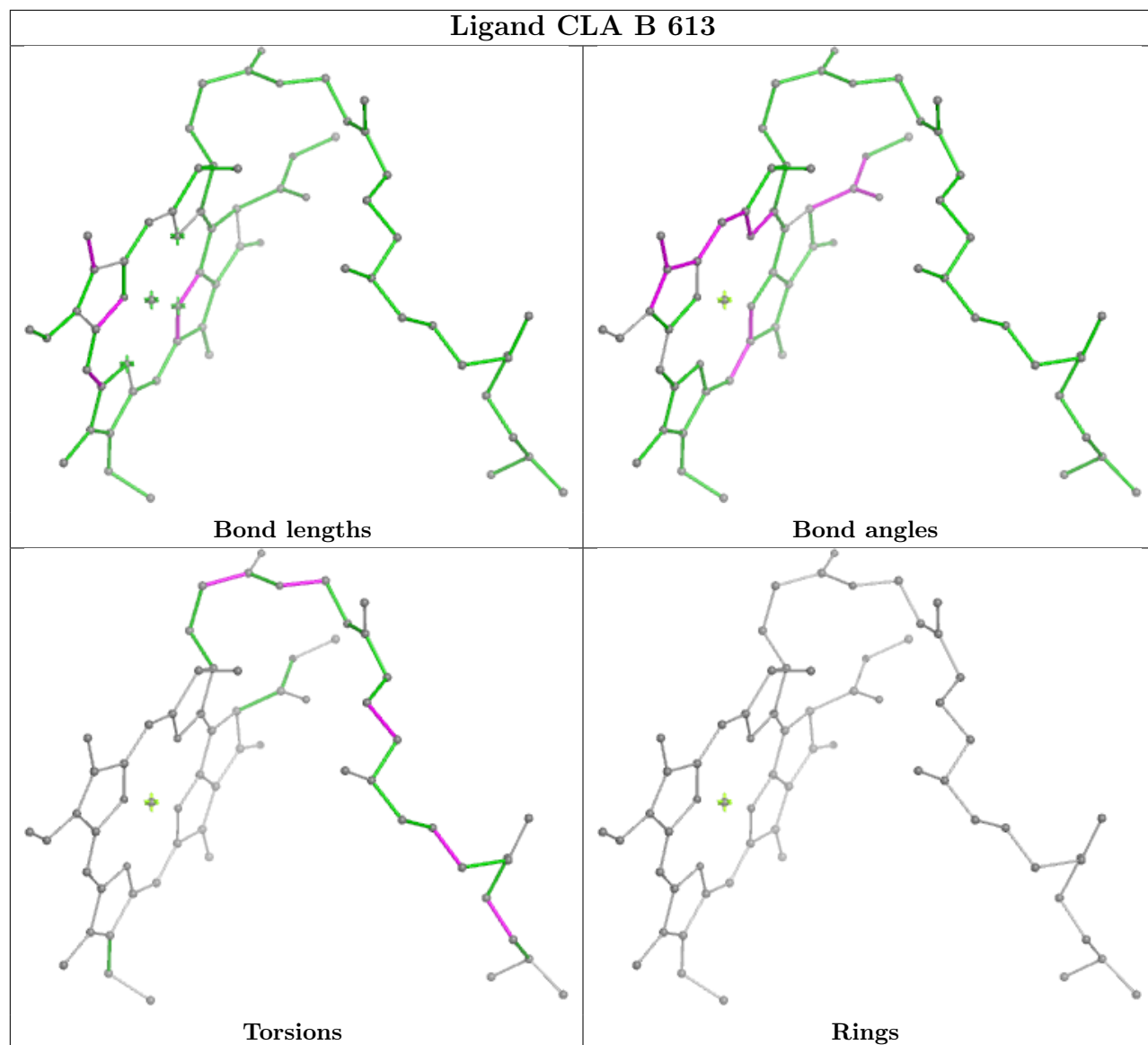




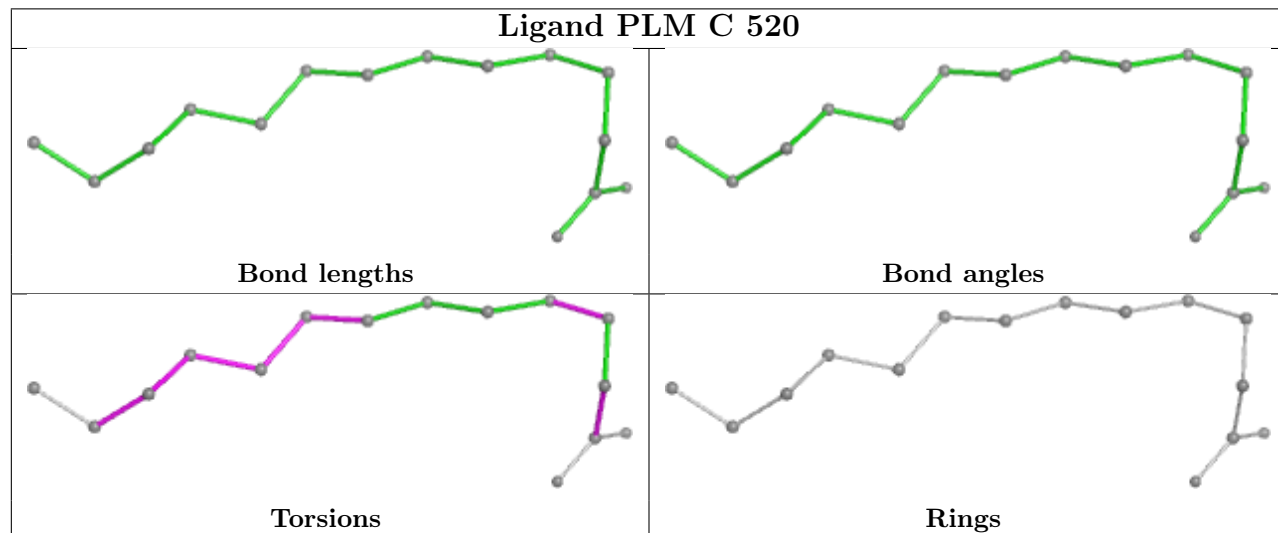
**Ligand CLA b 616****Ligand DGD C 504**

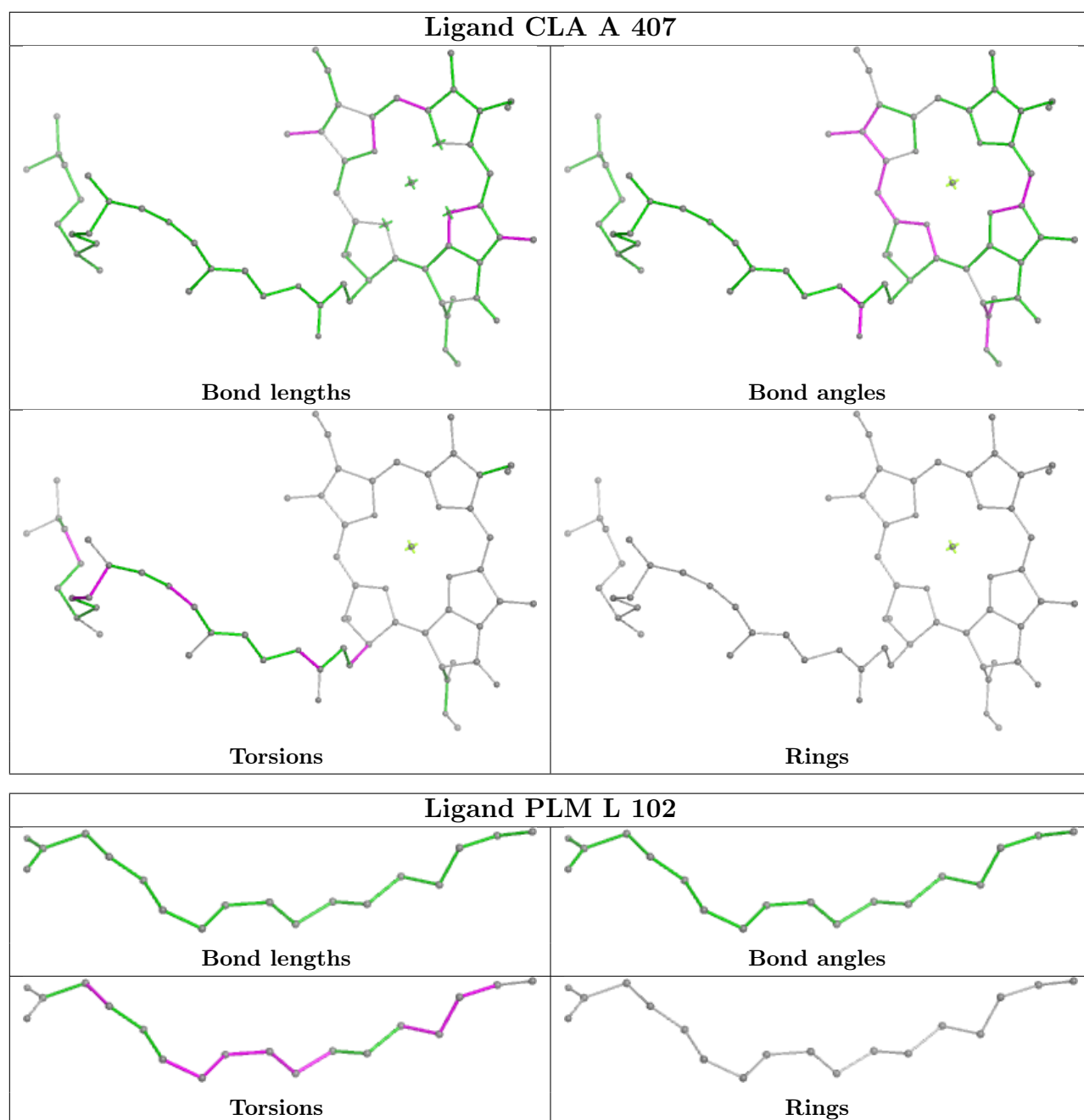


## Ligand CLA B 613

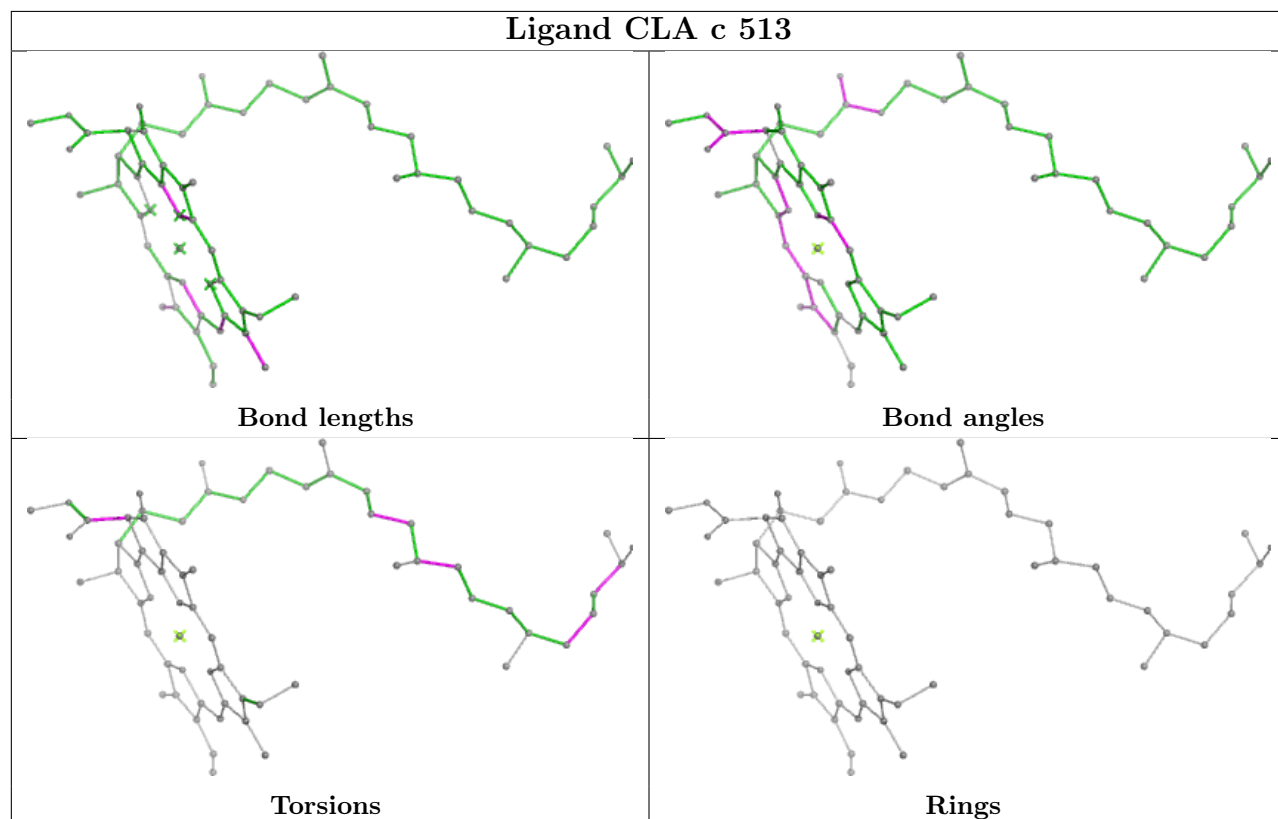
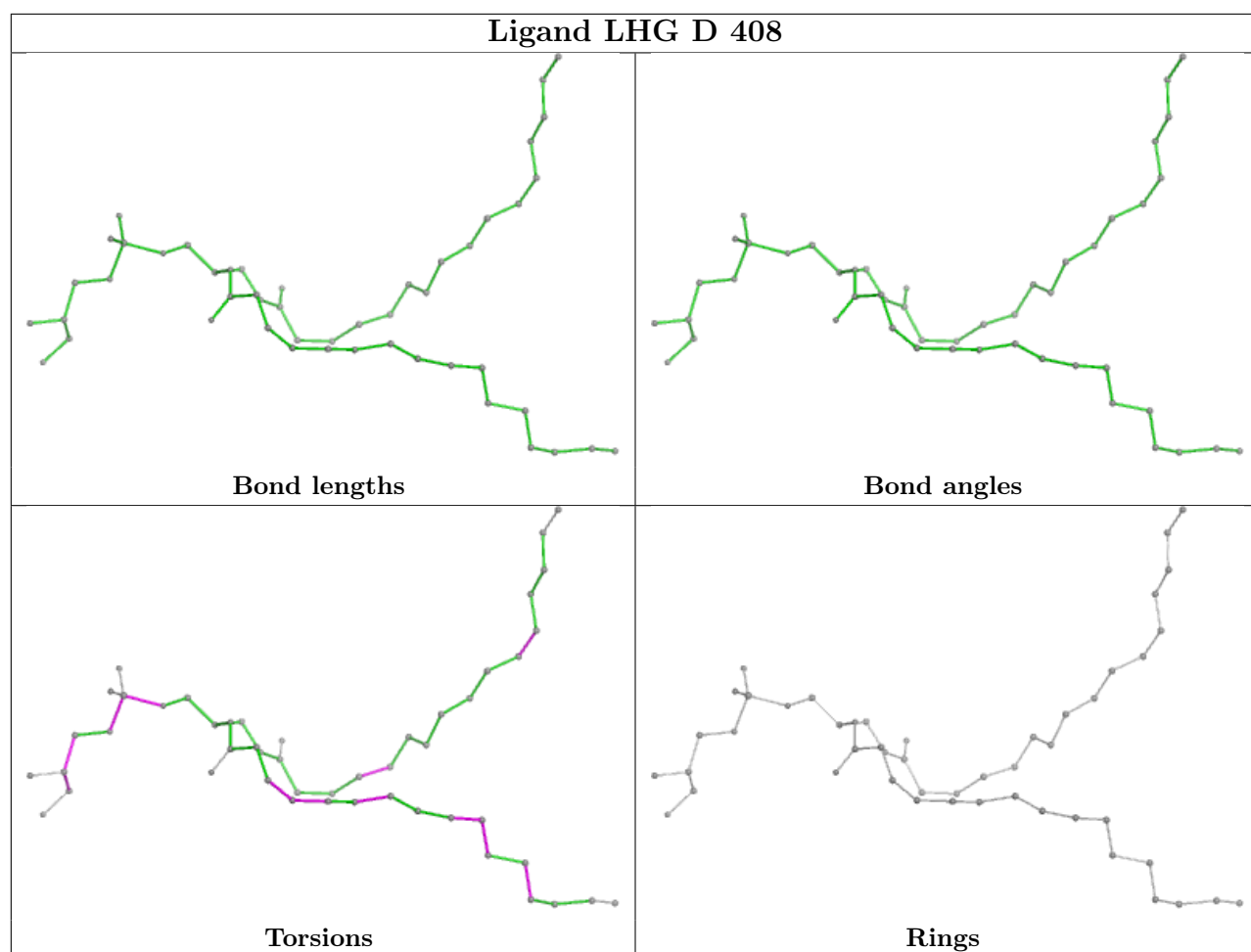


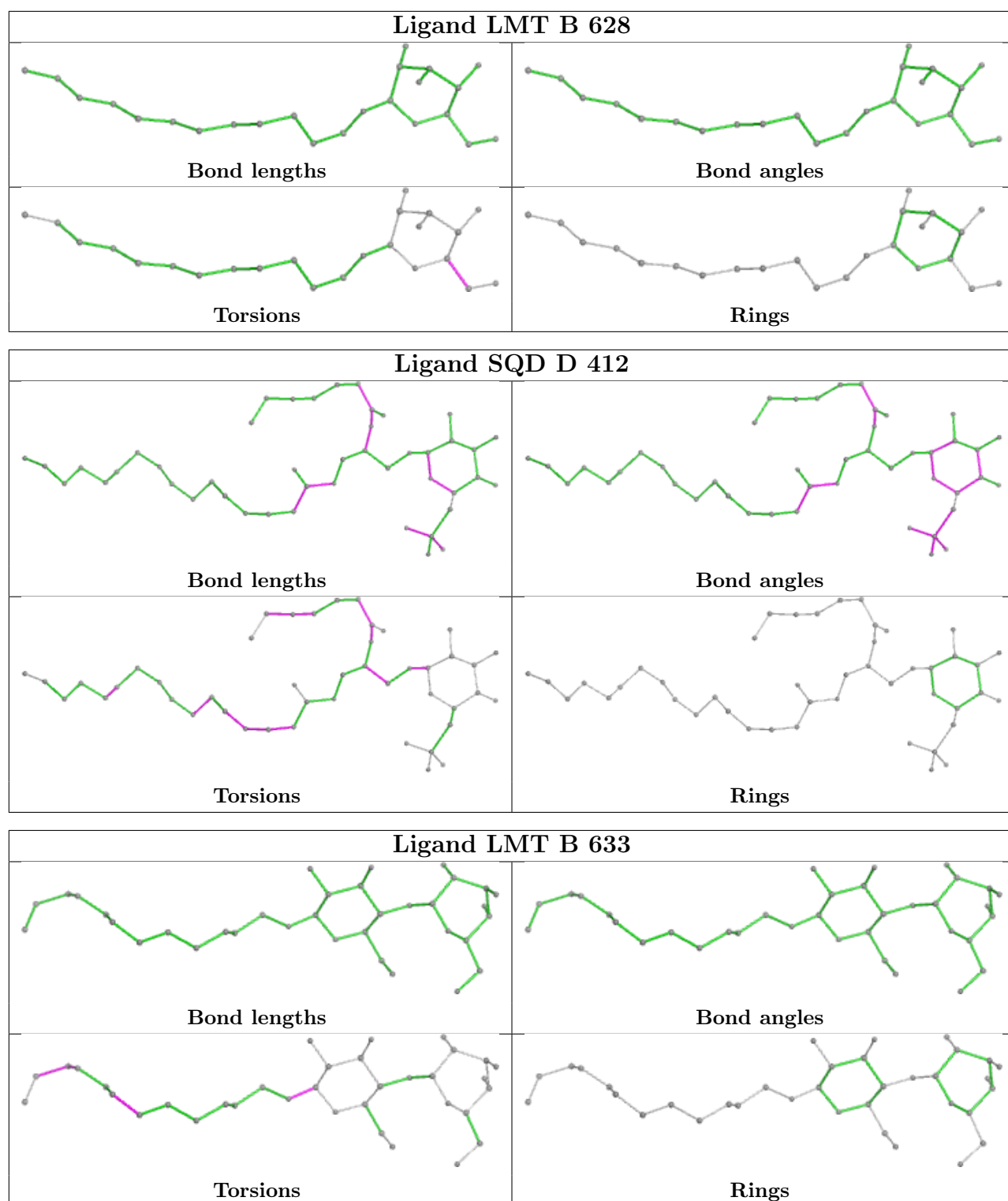
## Ligand PLM C 520

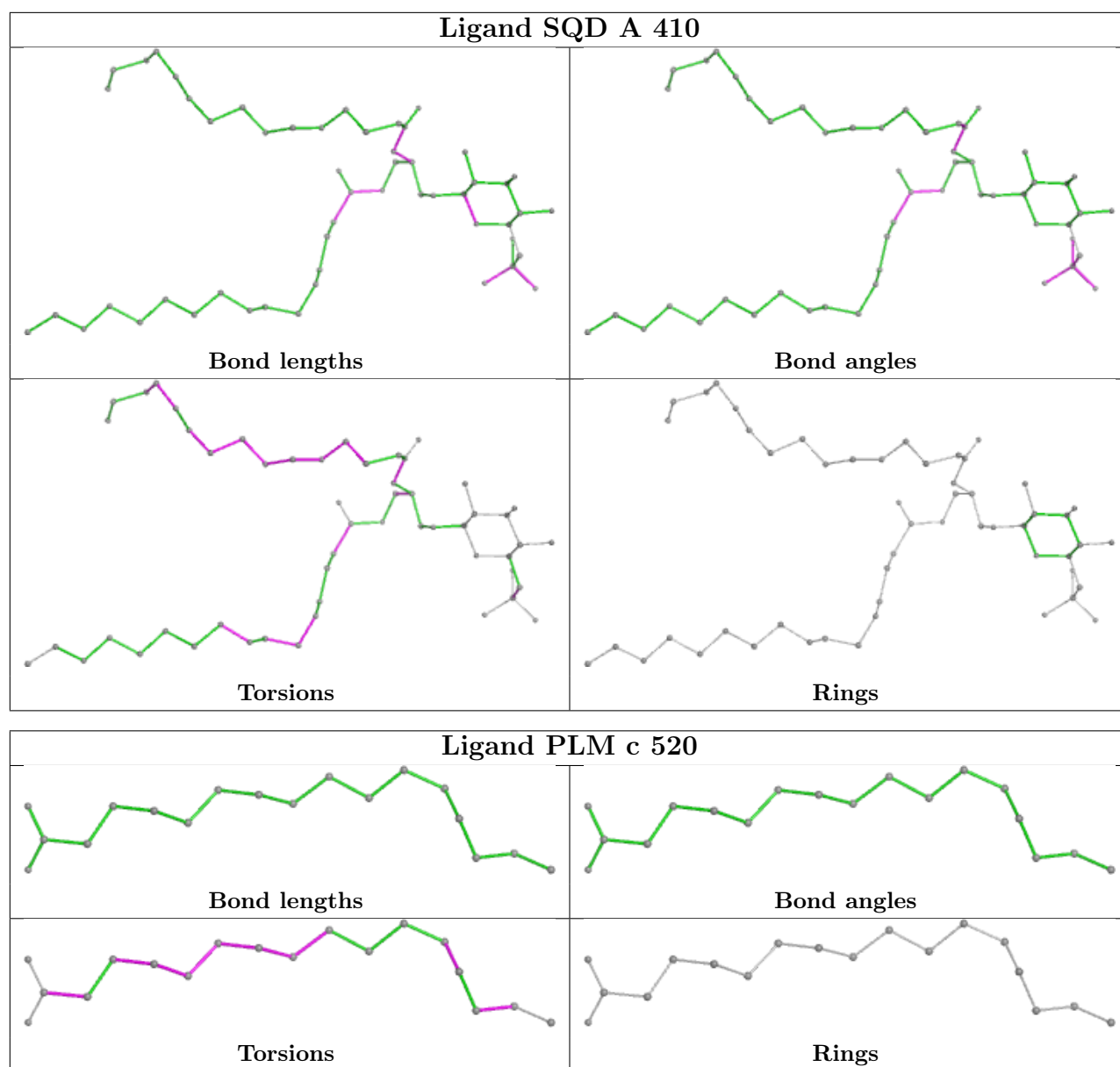


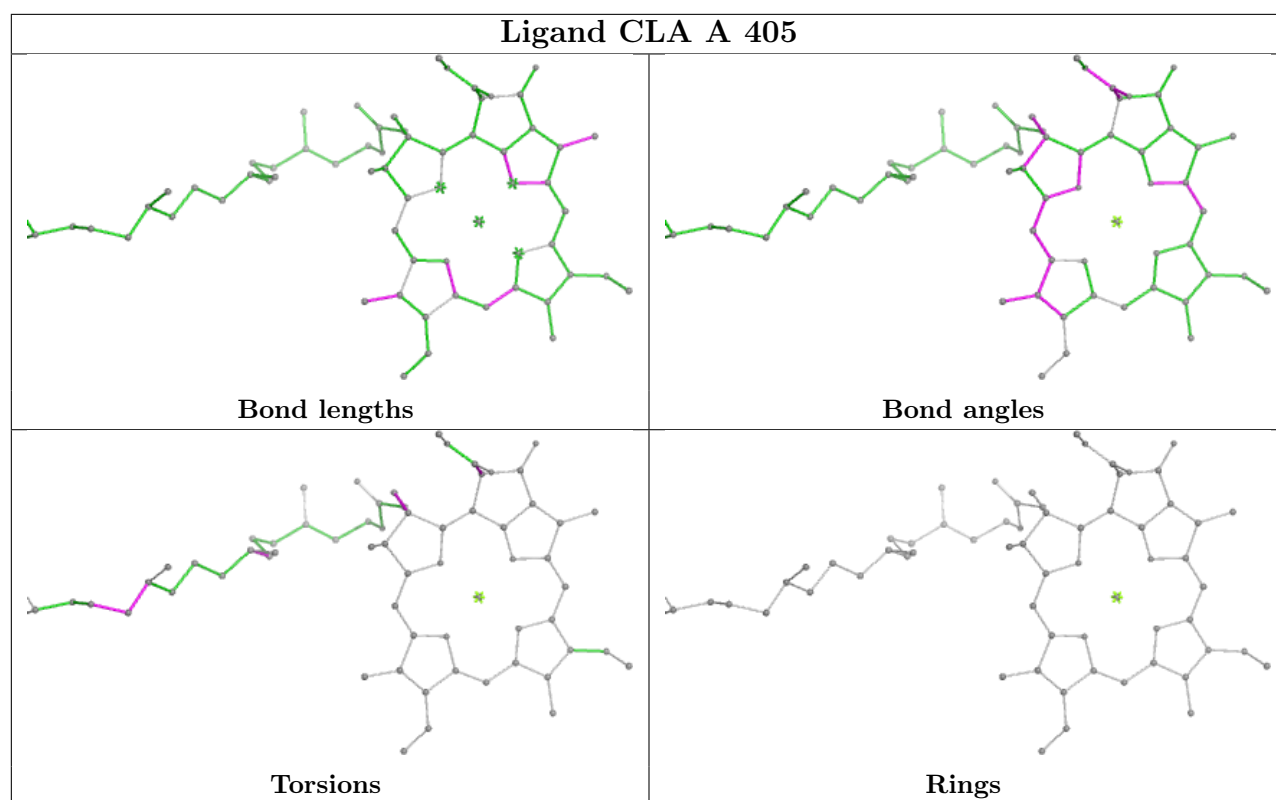




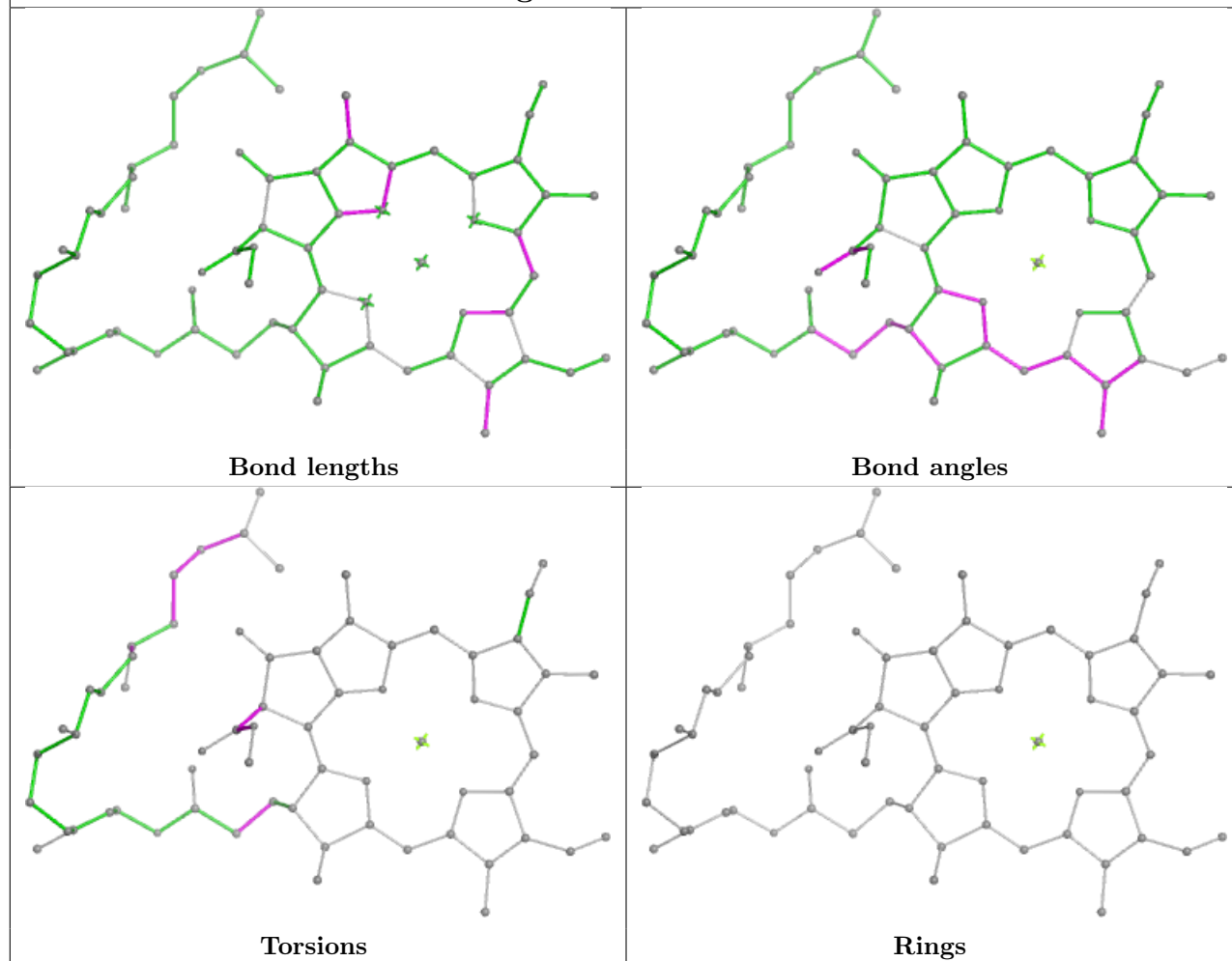




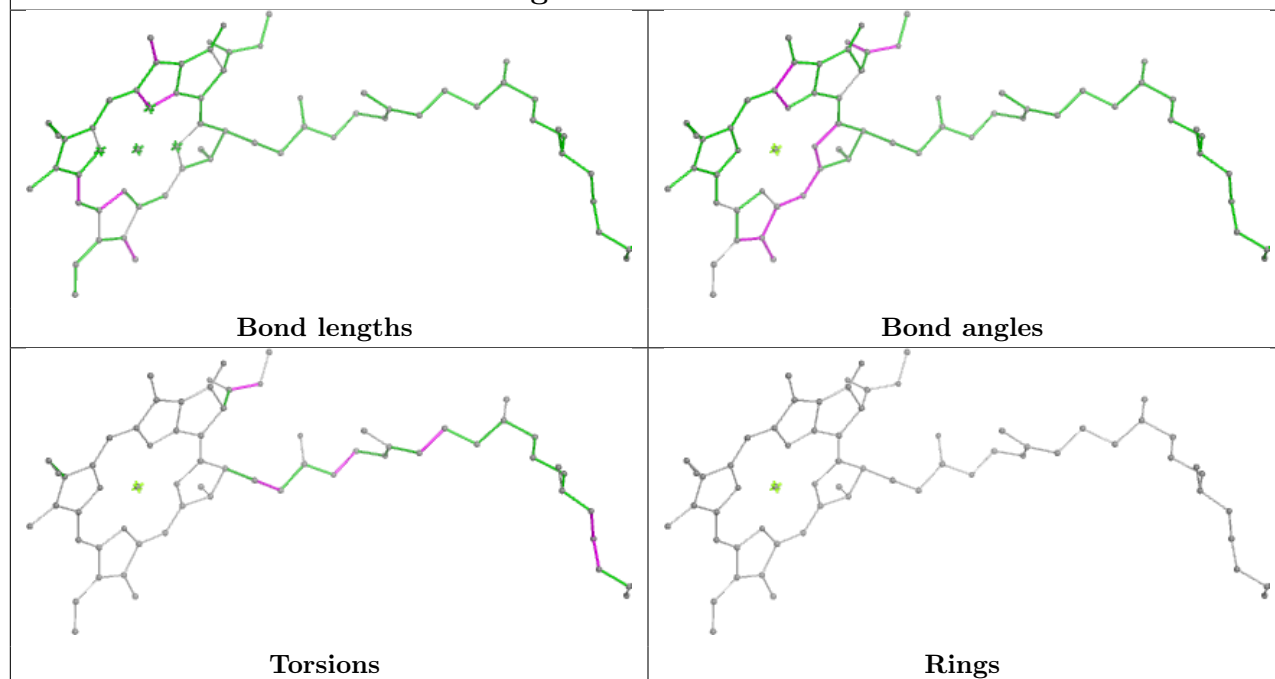


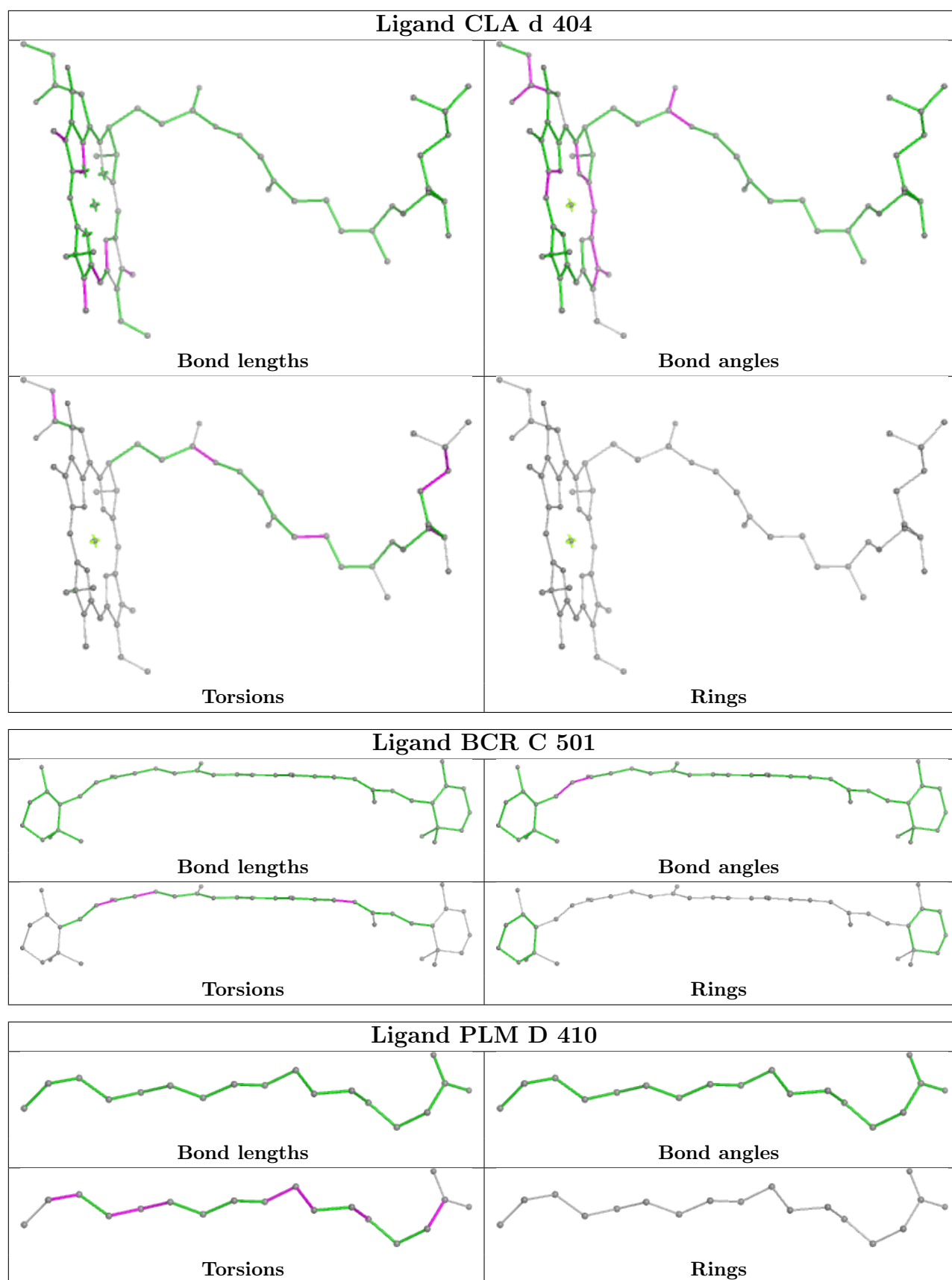


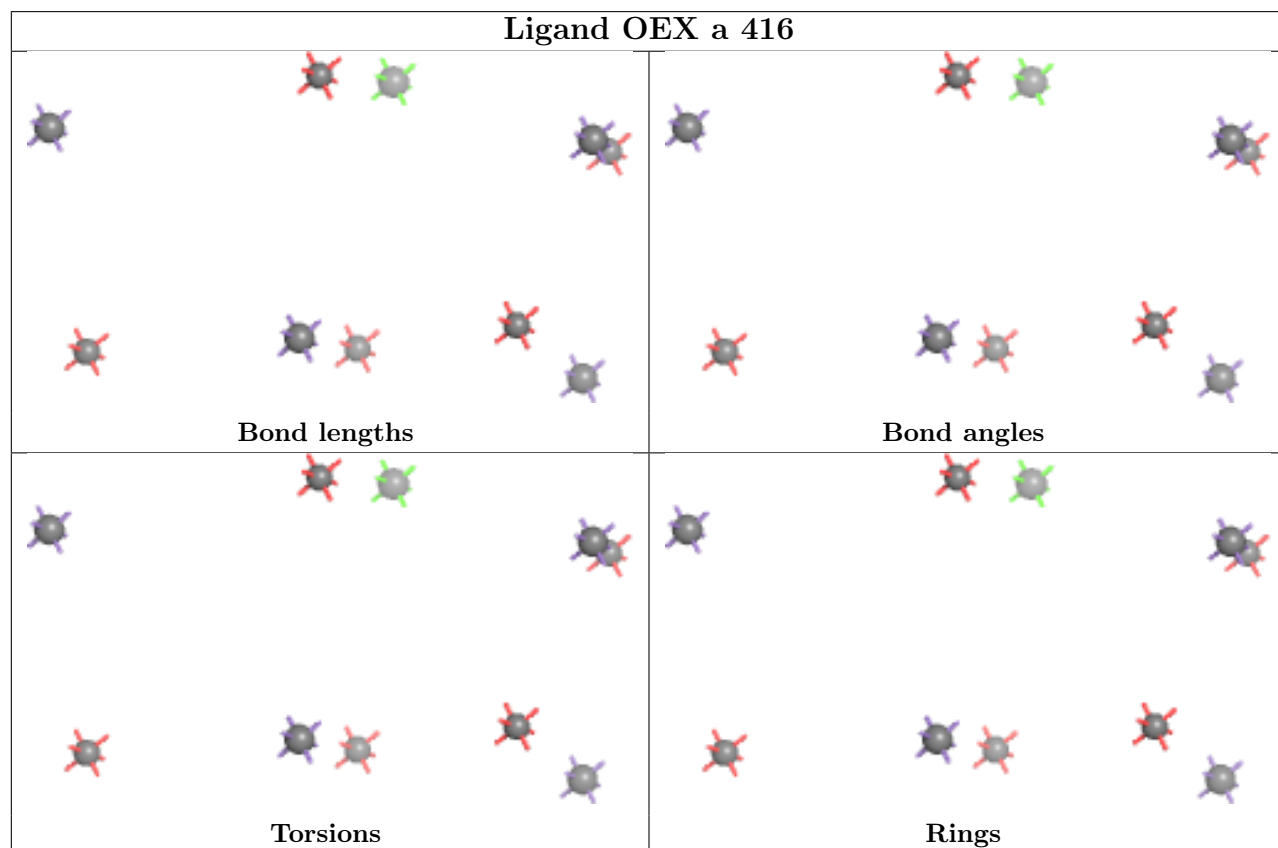
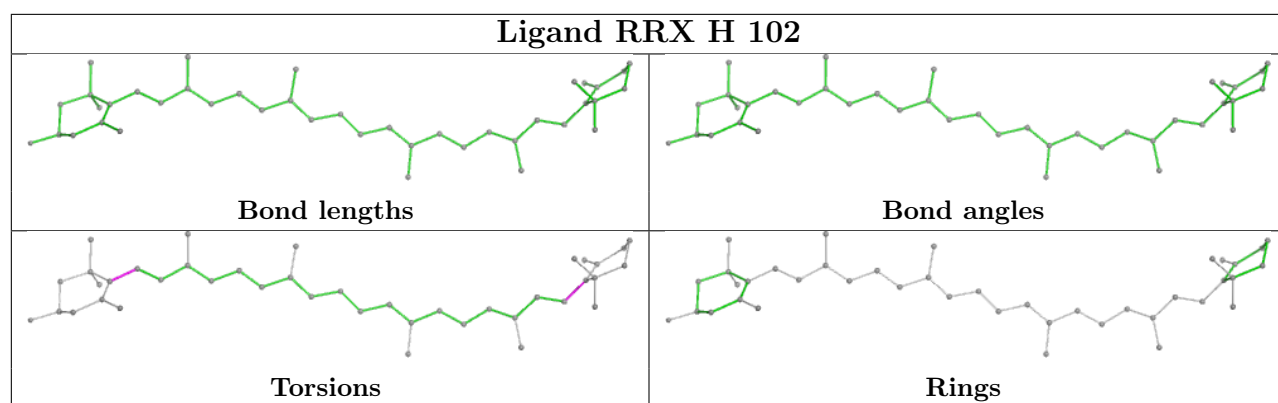
## Ligand CLA b 612

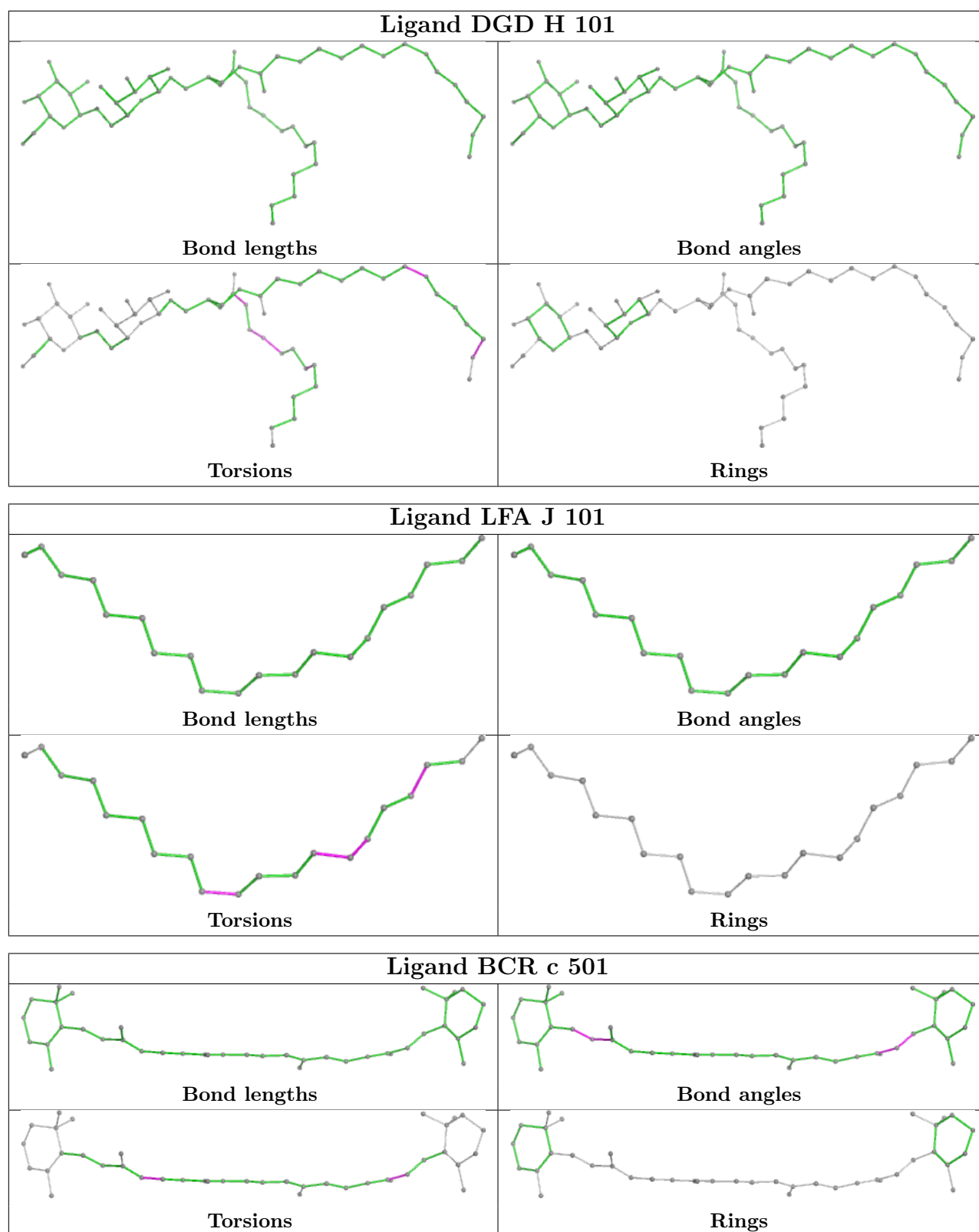


## Ligand CLA A 404

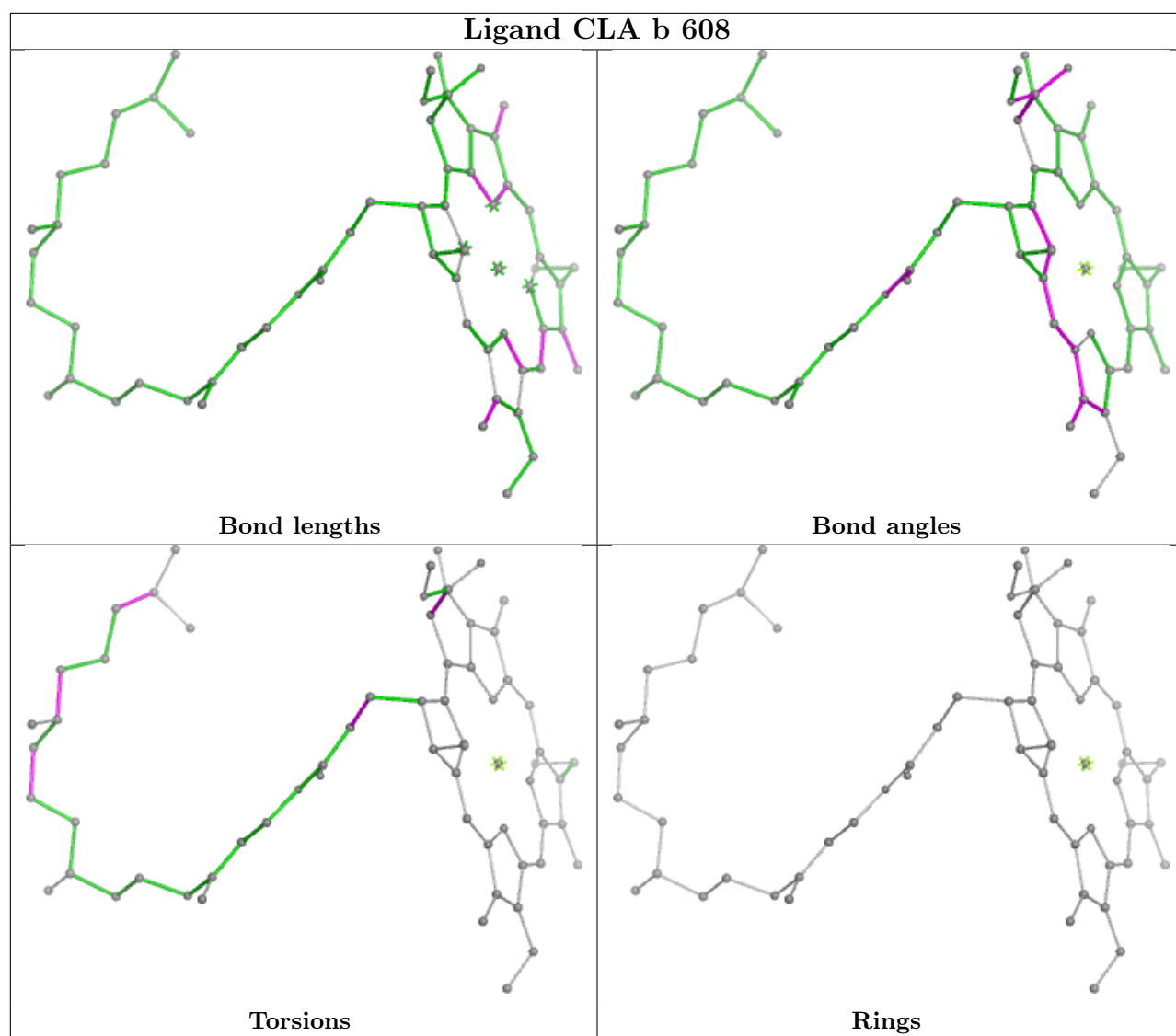


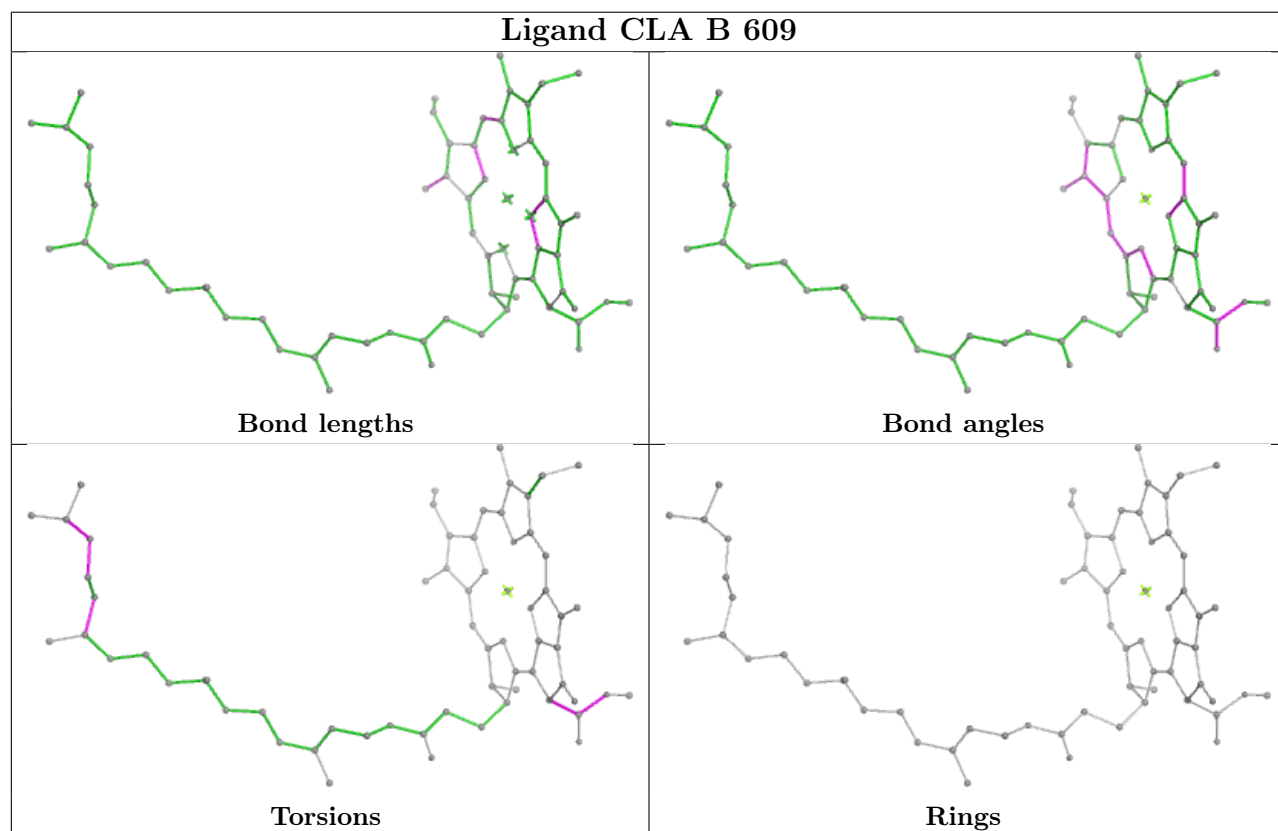
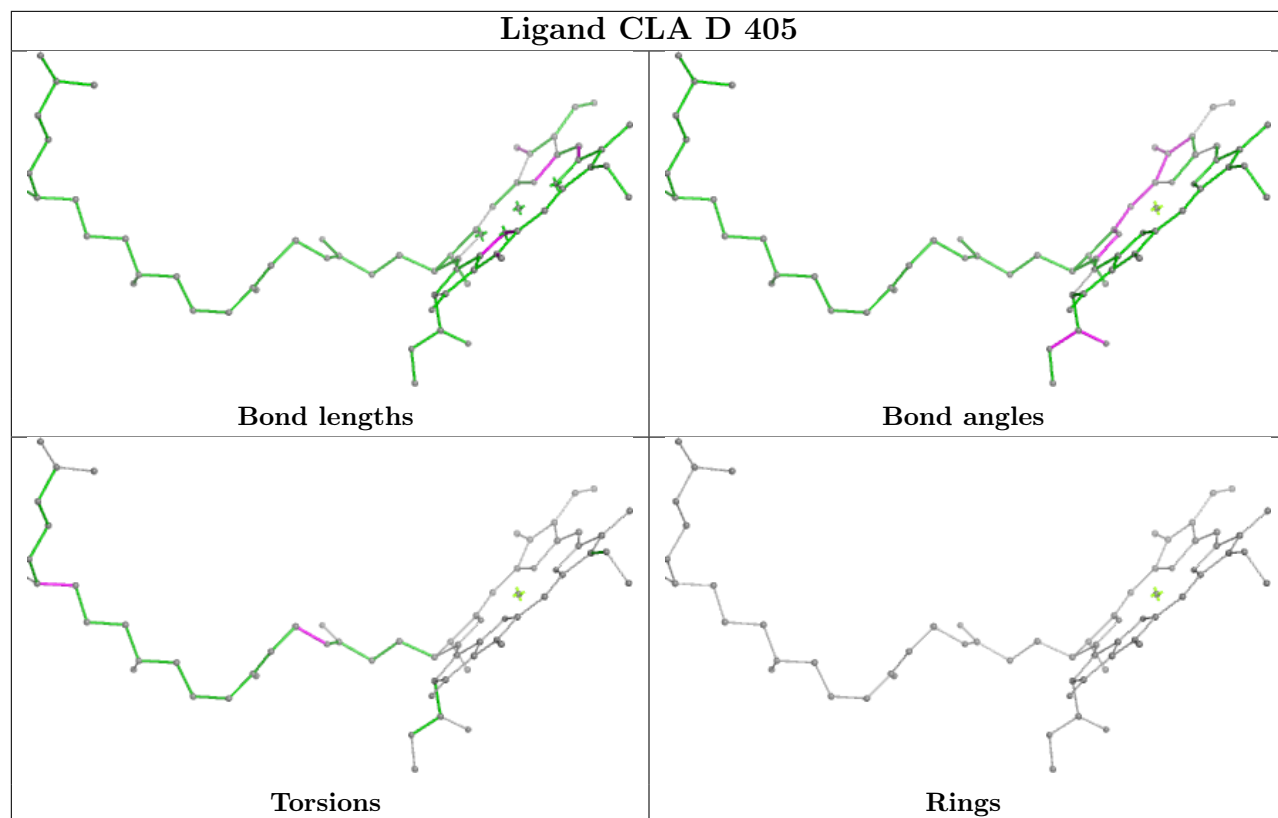


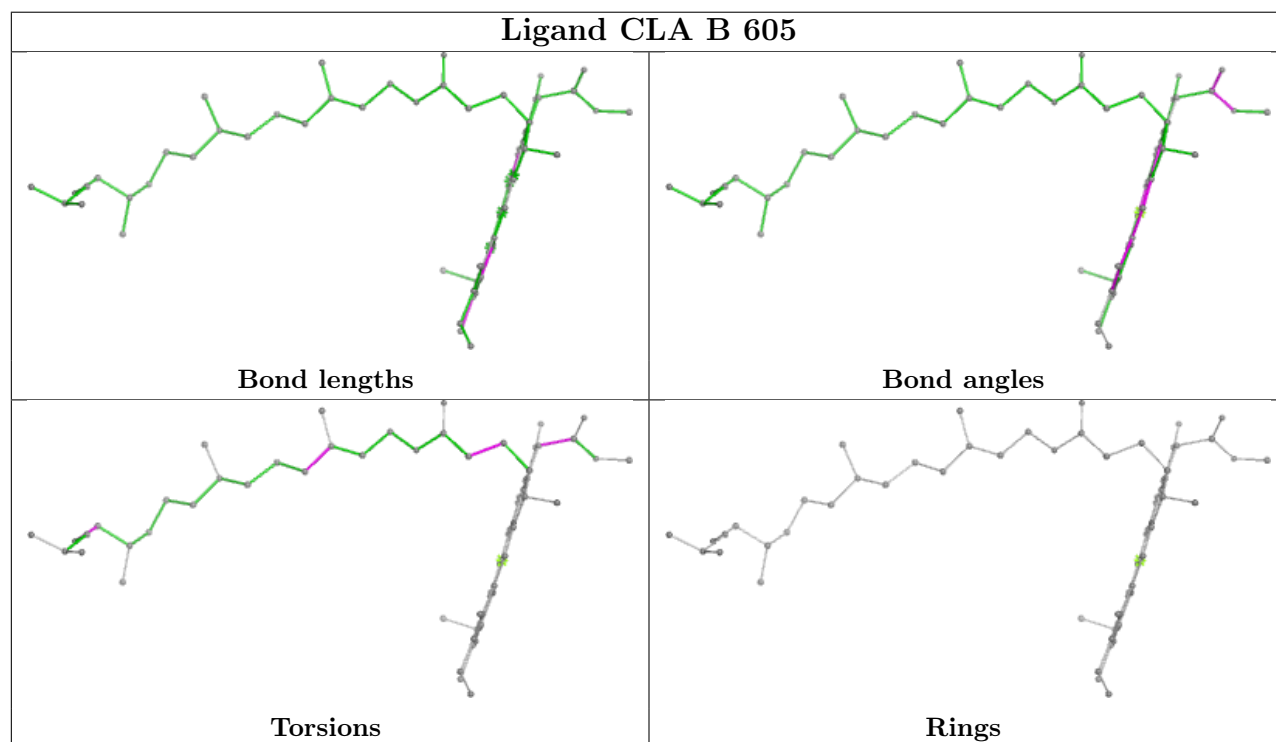
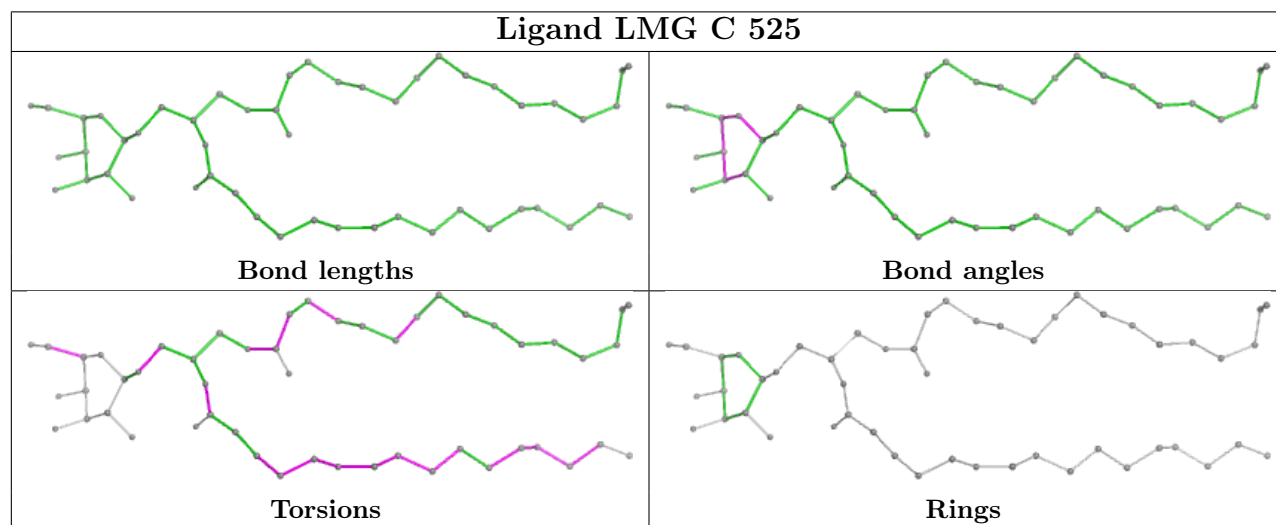
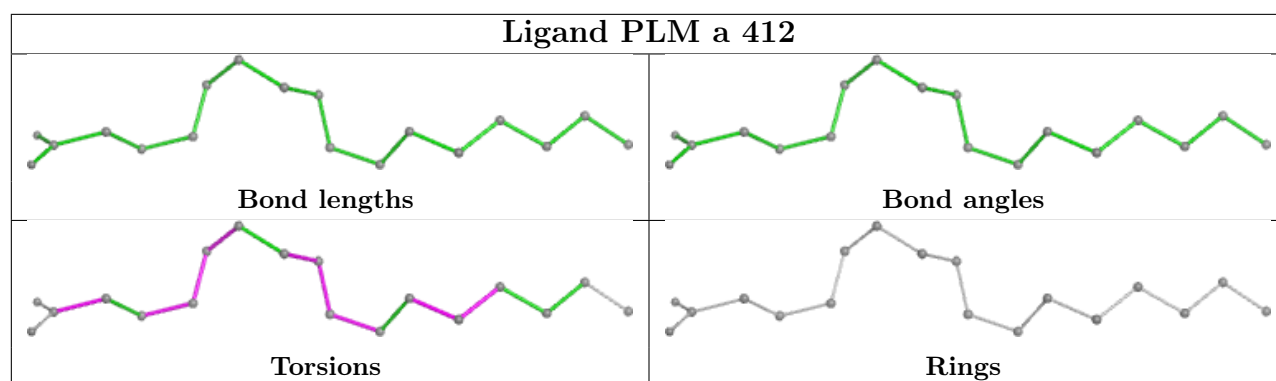


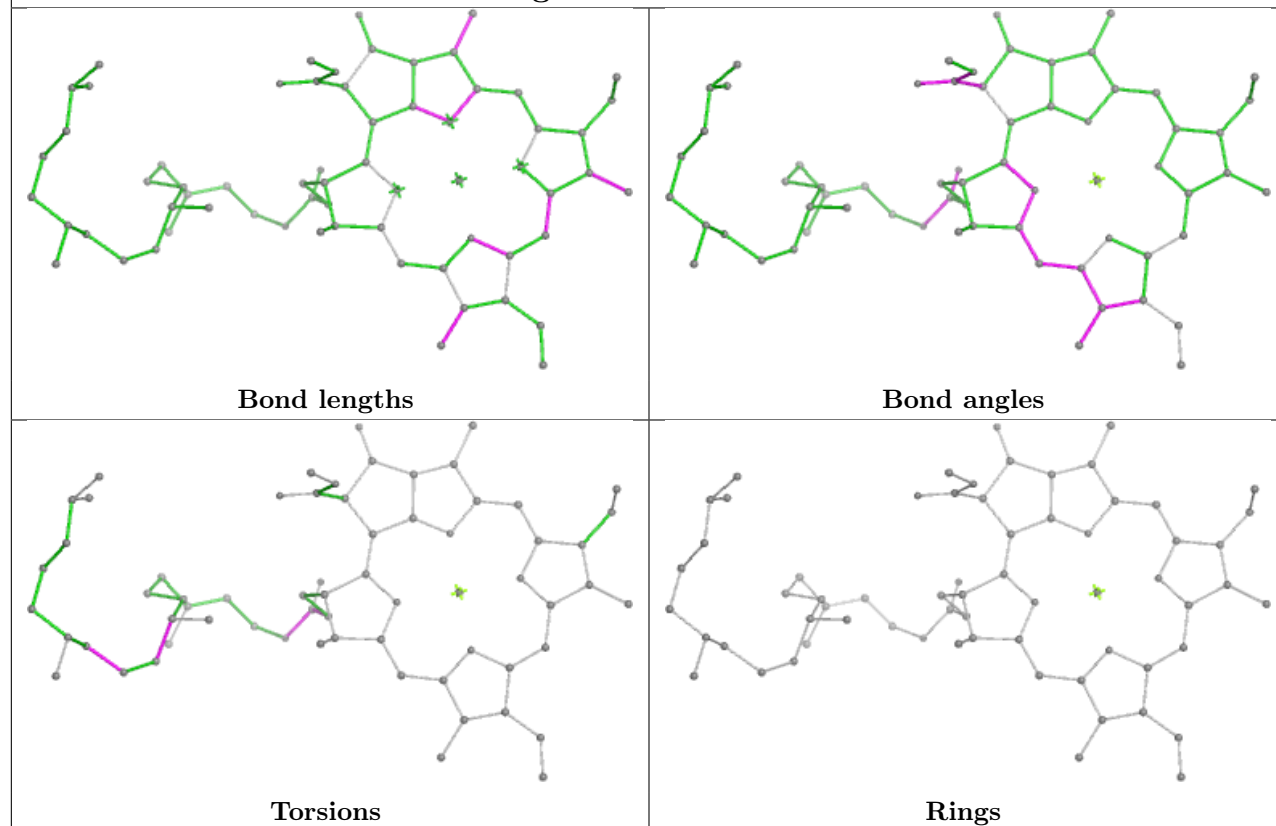
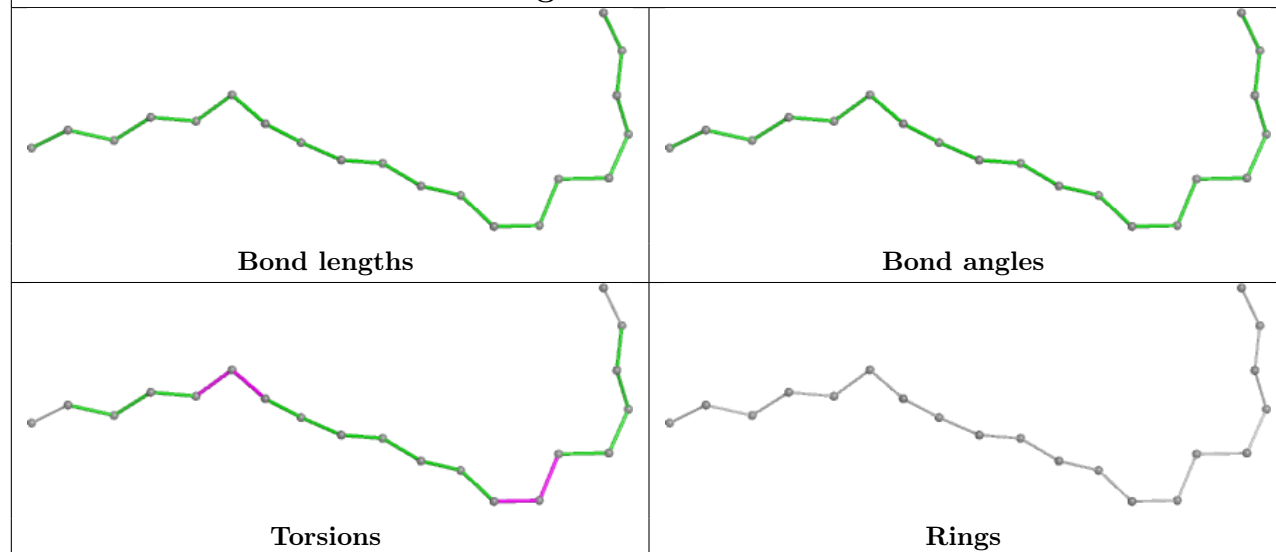


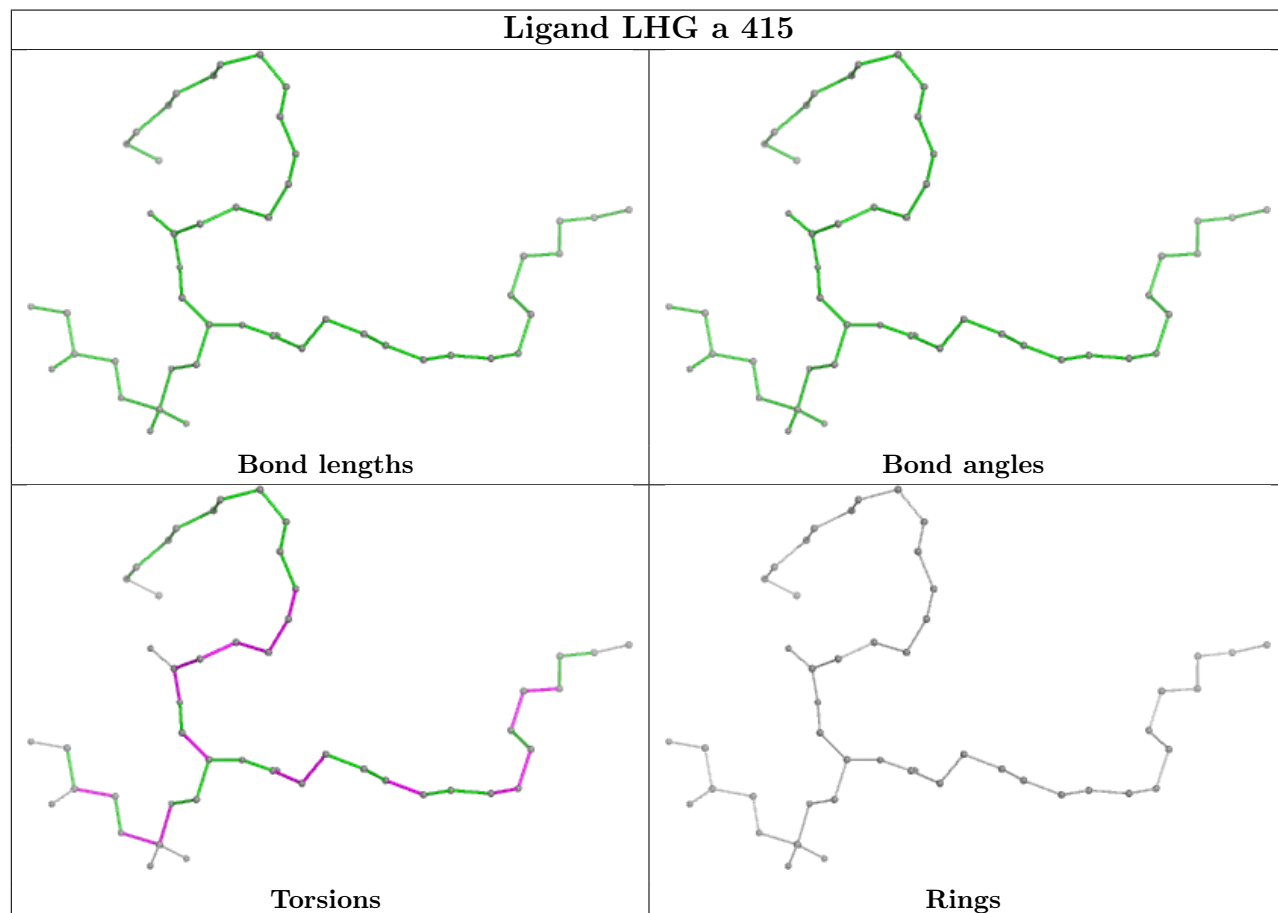
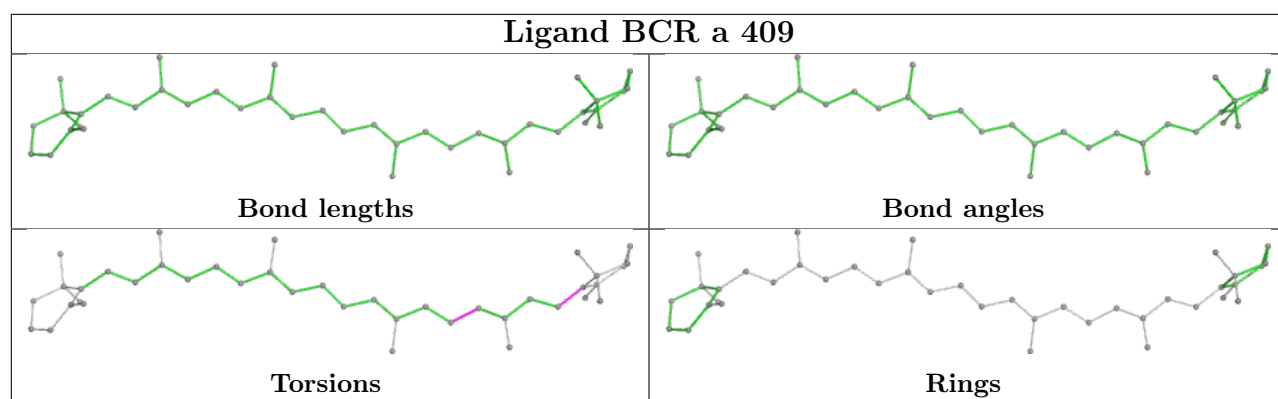


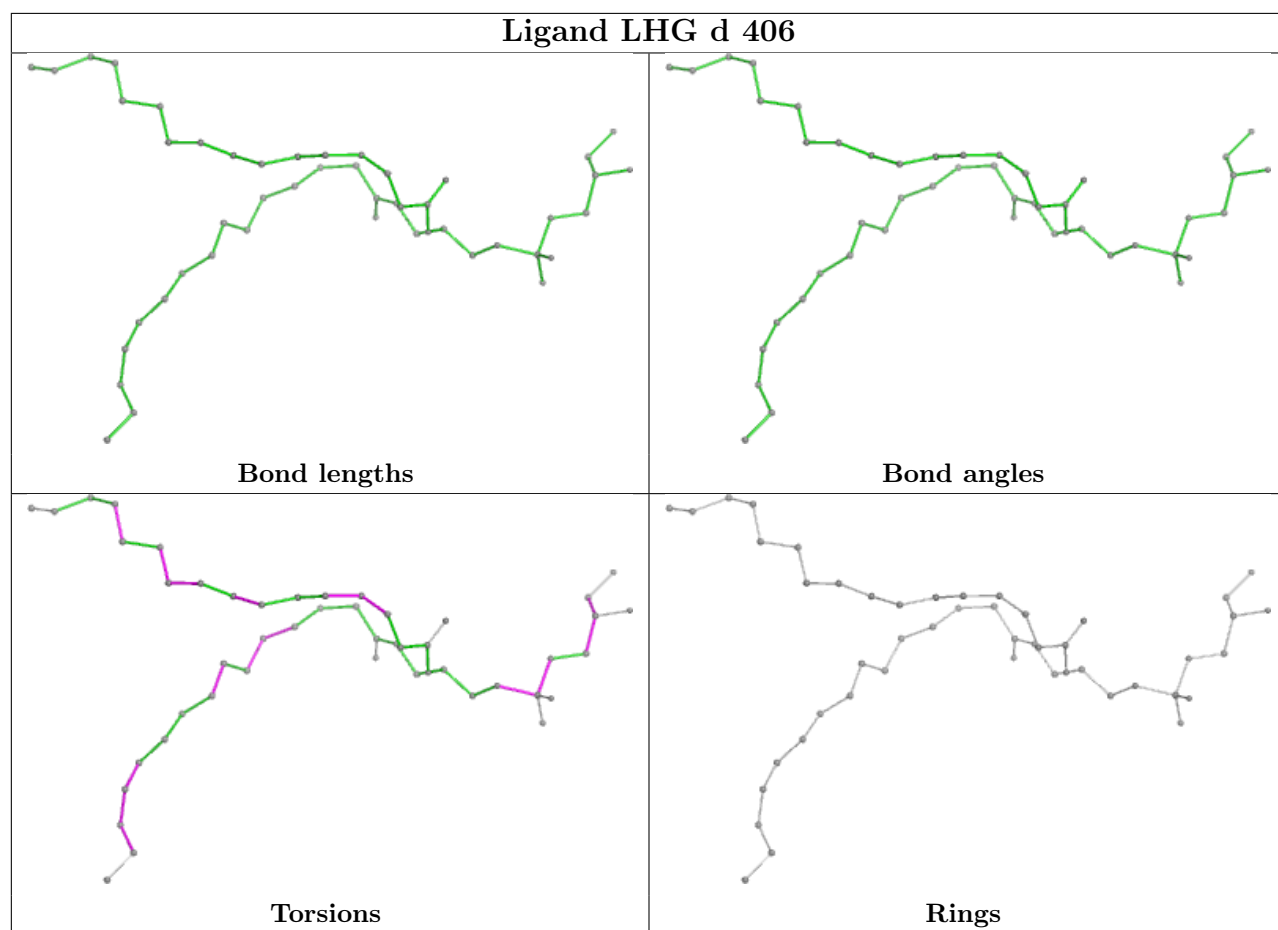
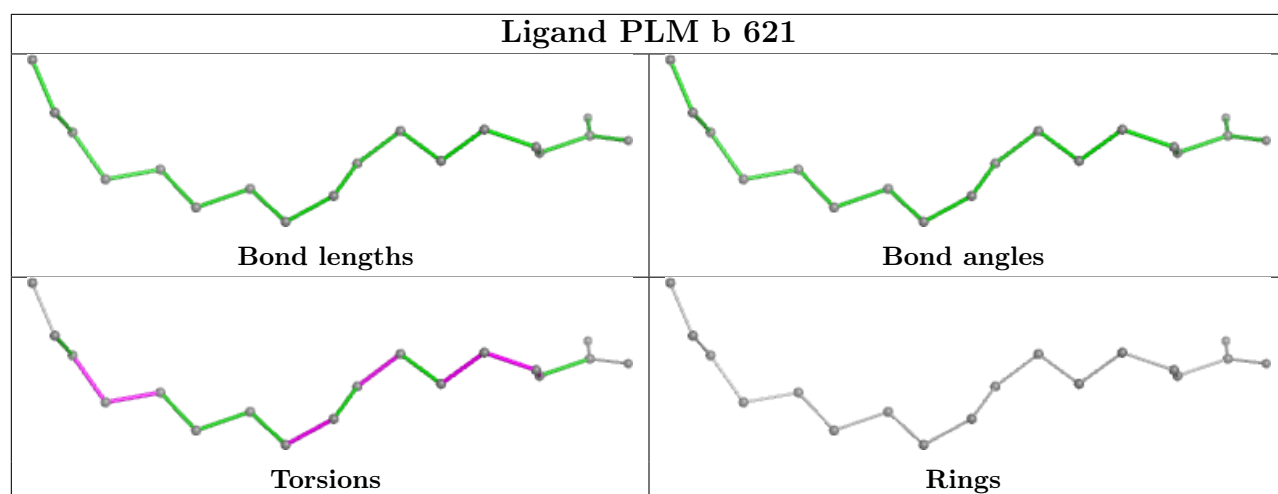


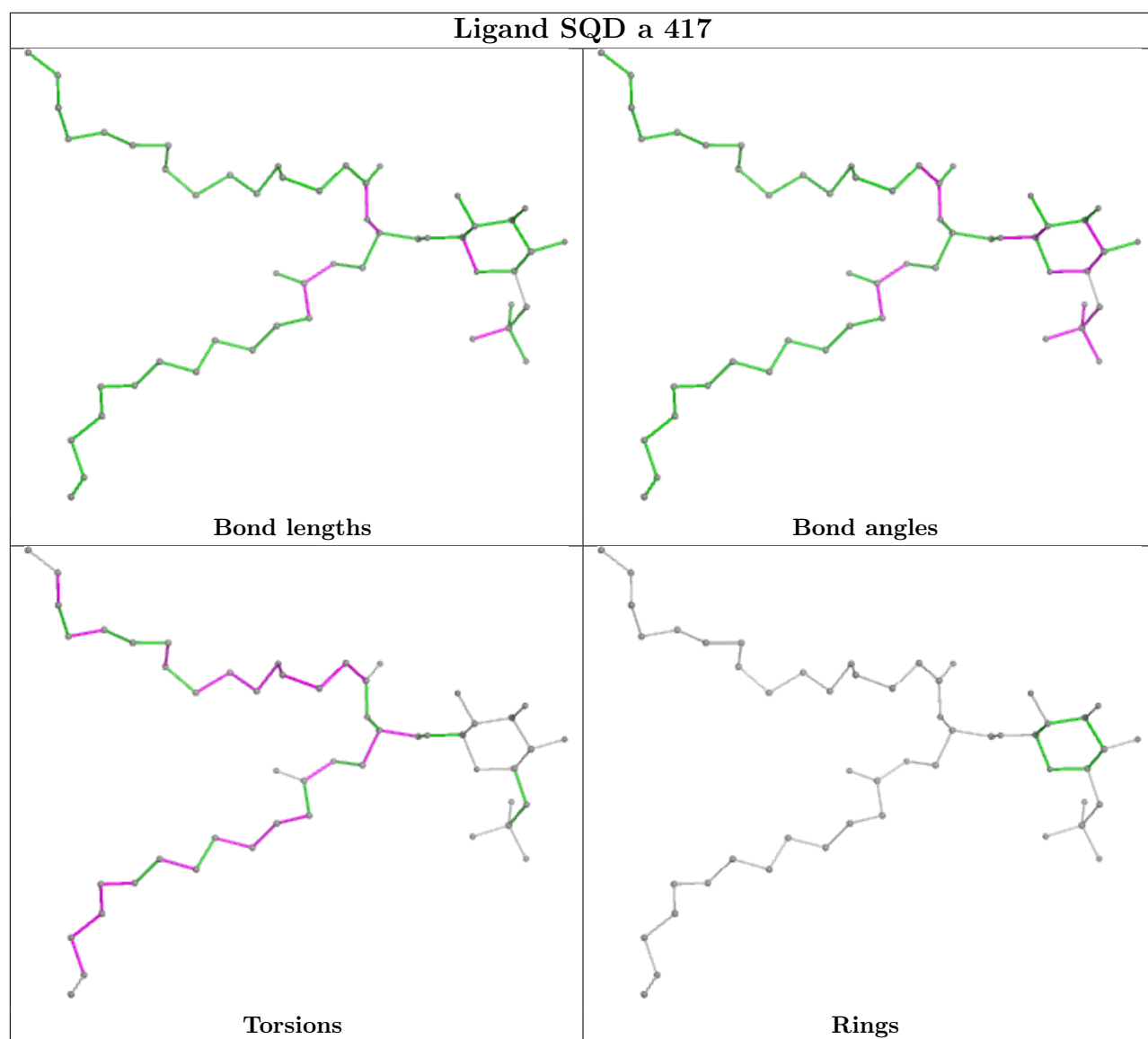


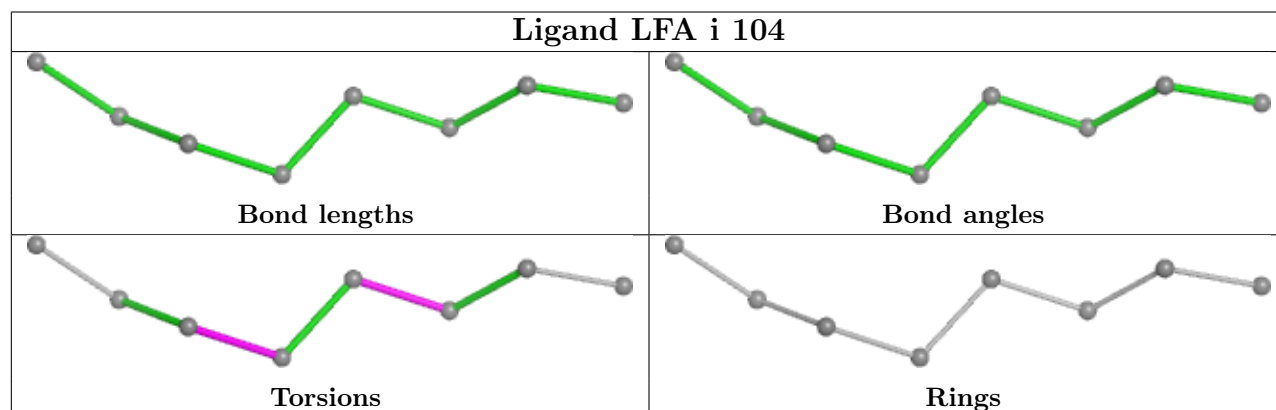
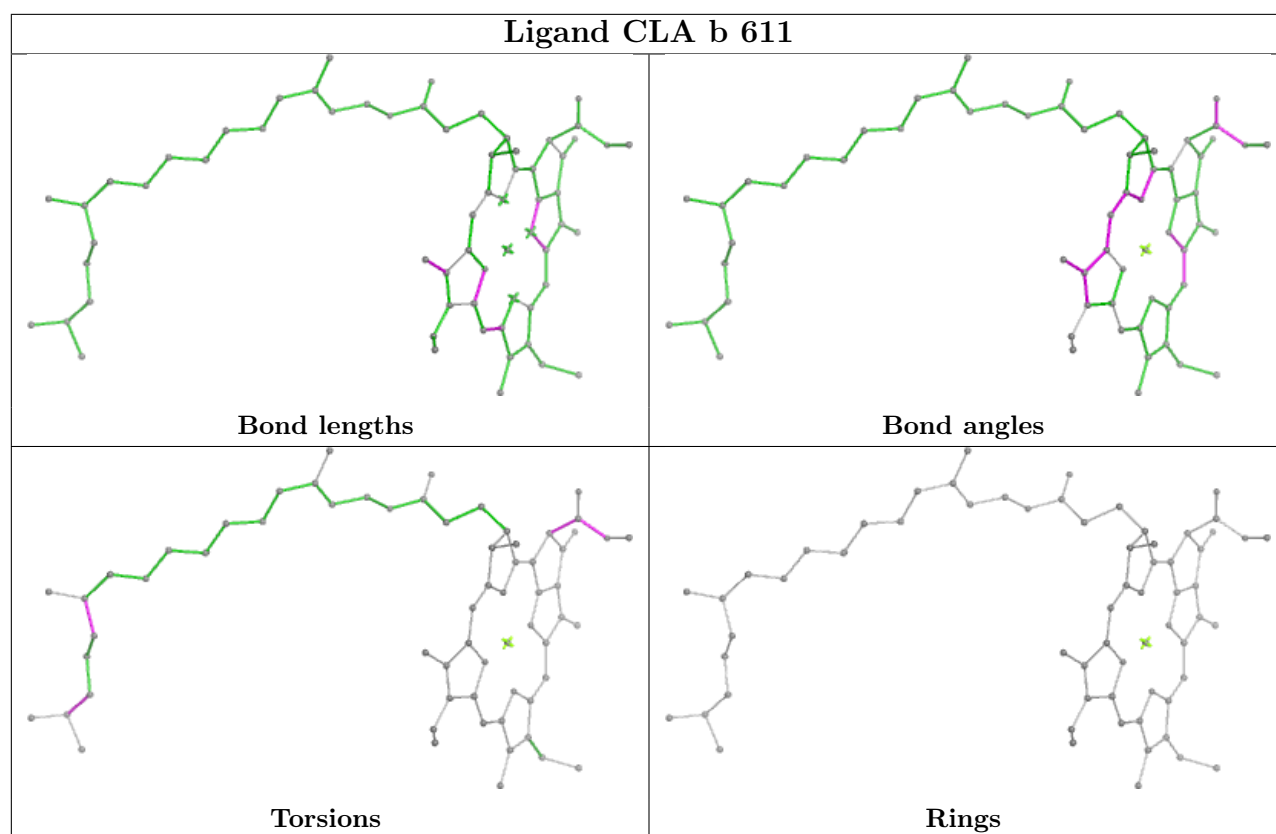


**Ligand CLA B 612****Ligand LFA E 102**

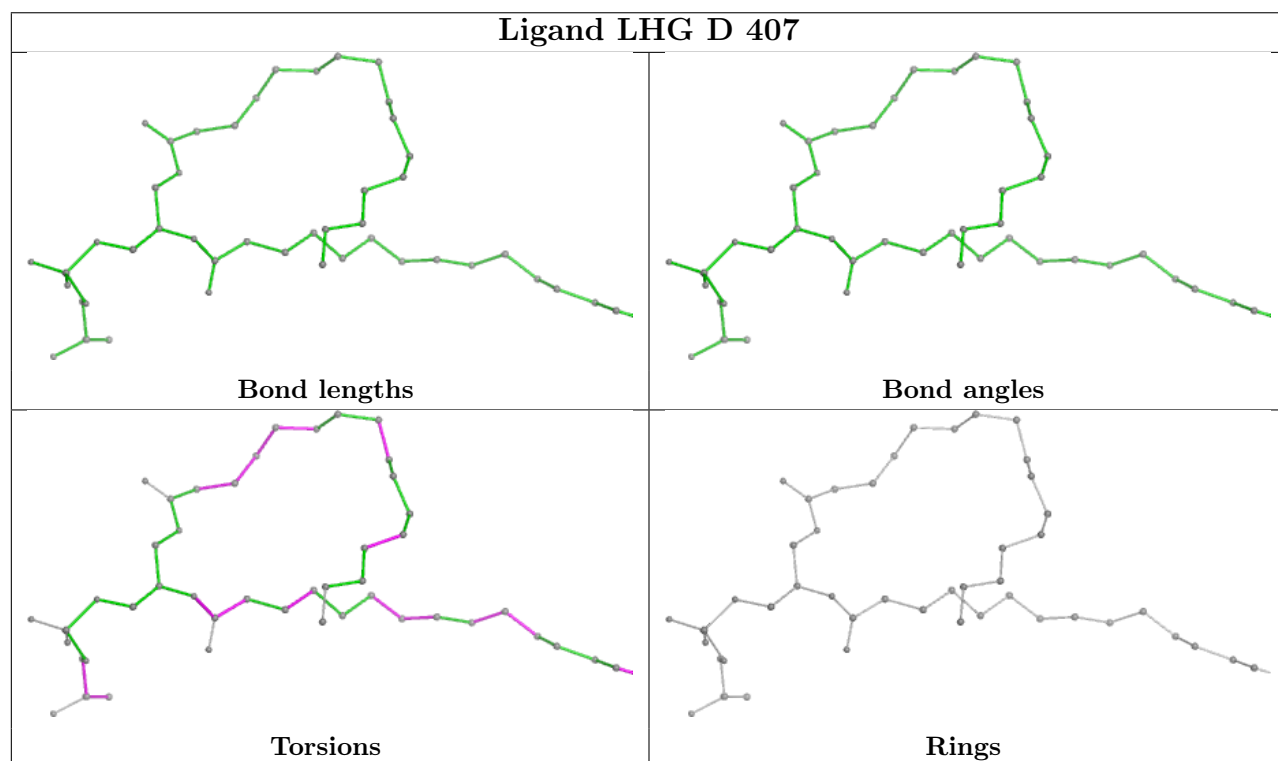
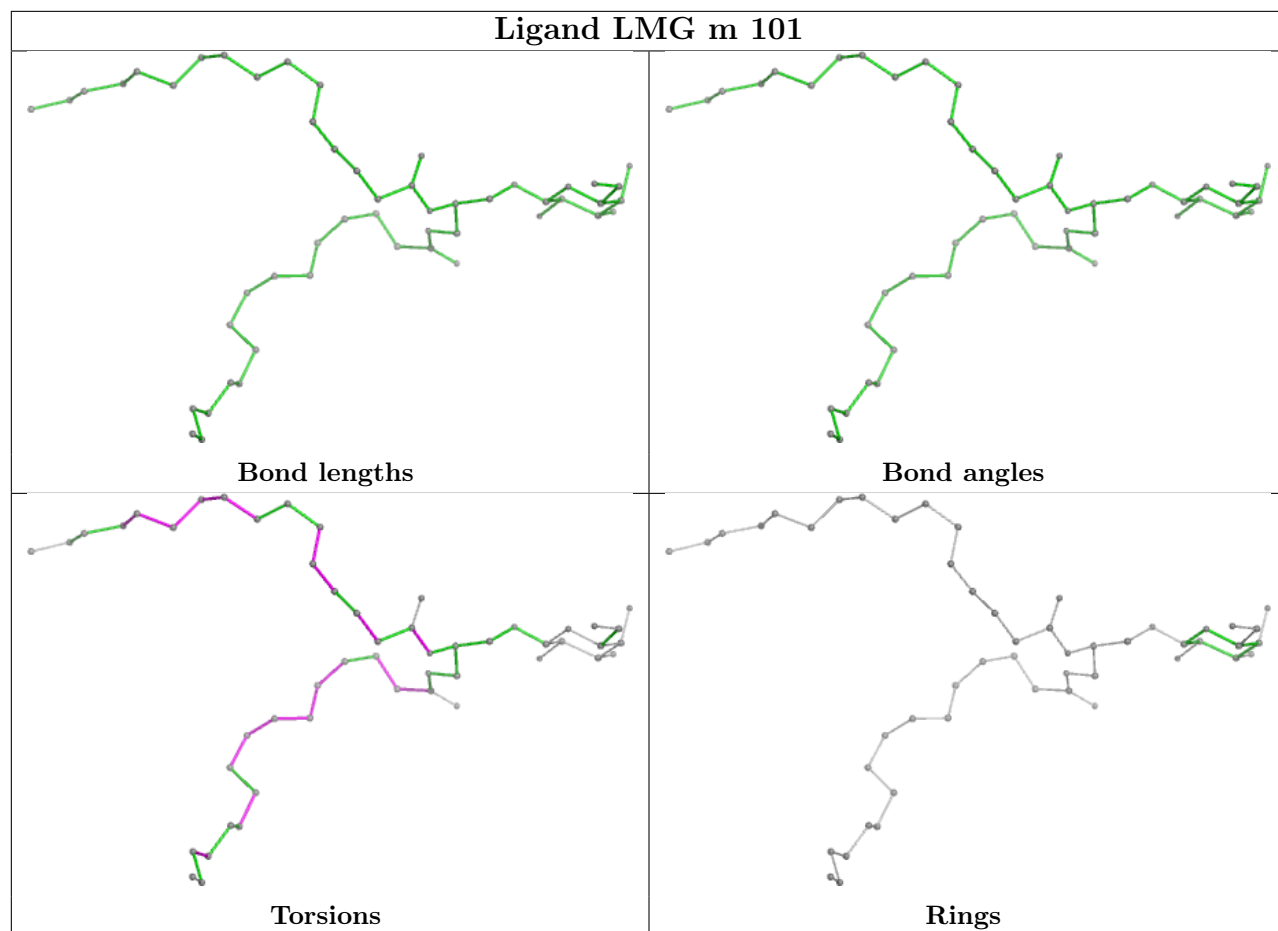


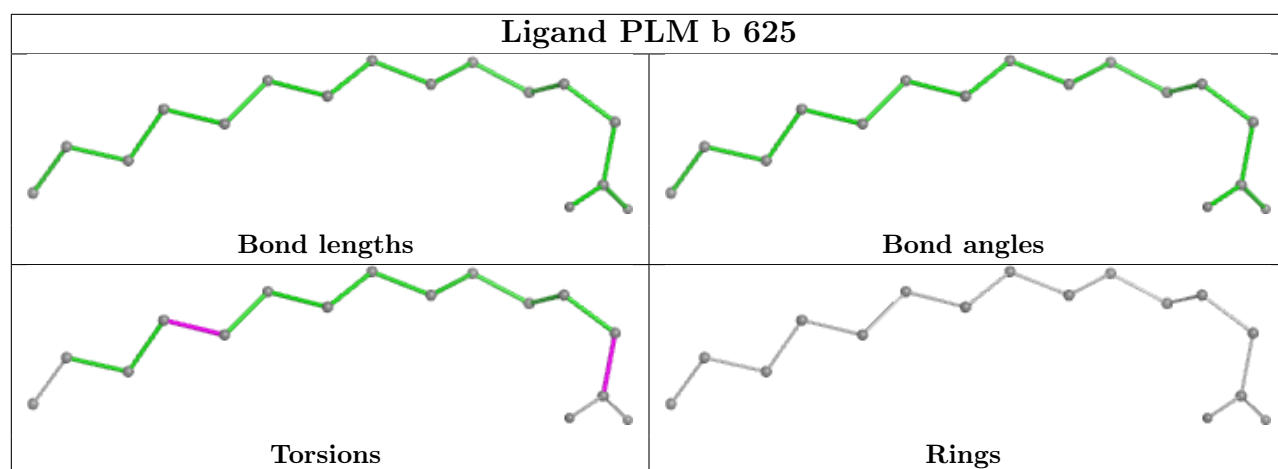


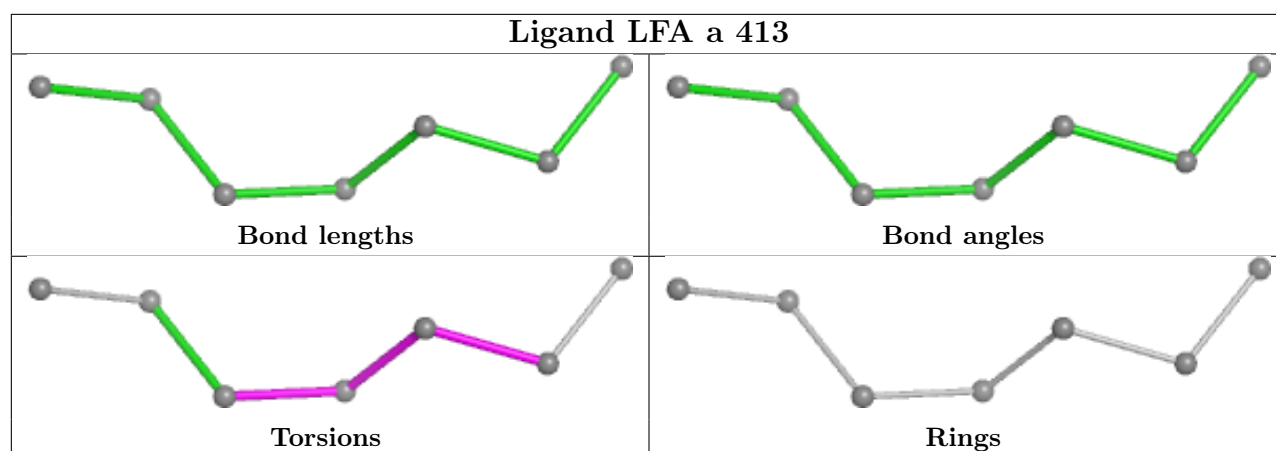
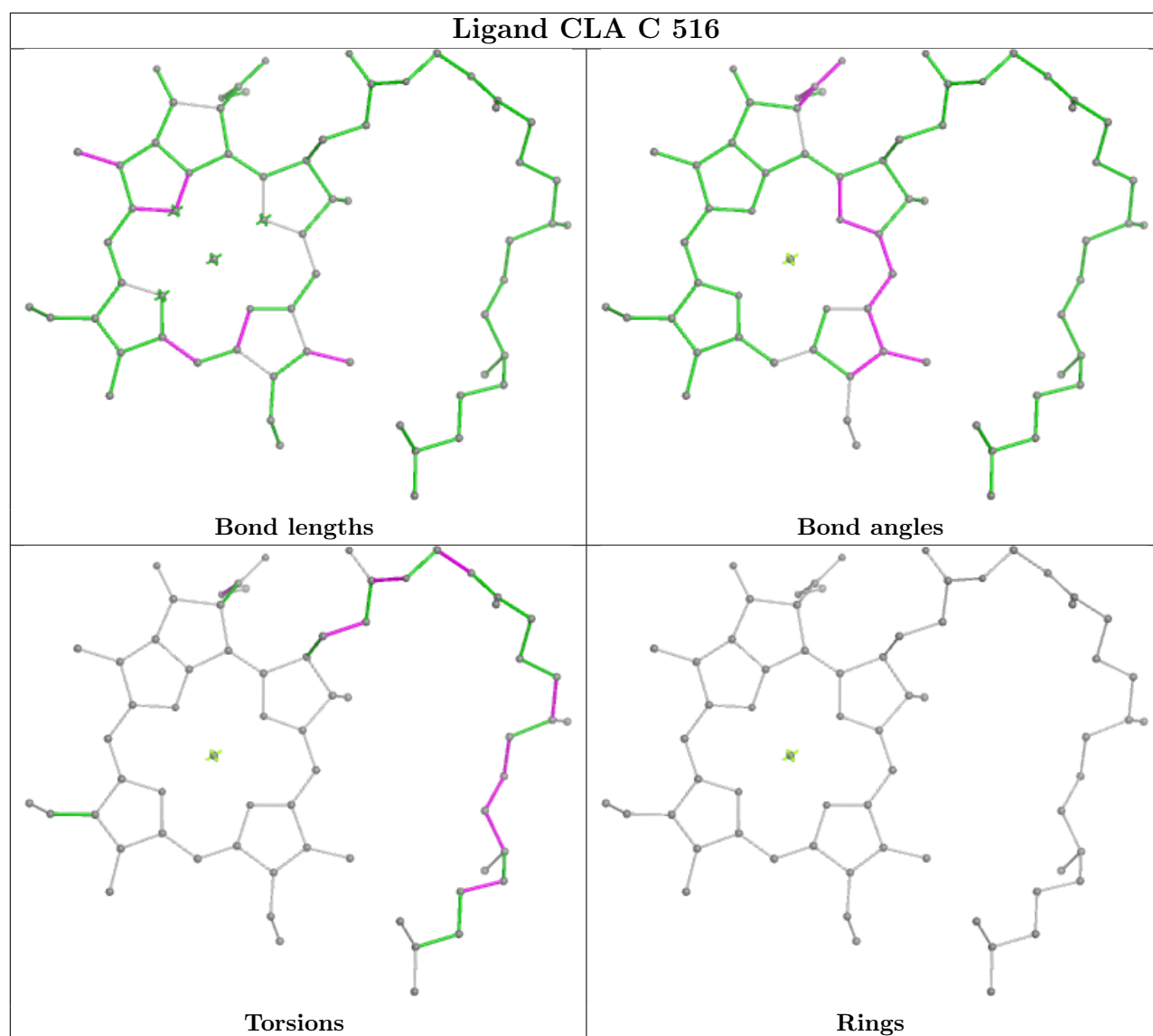


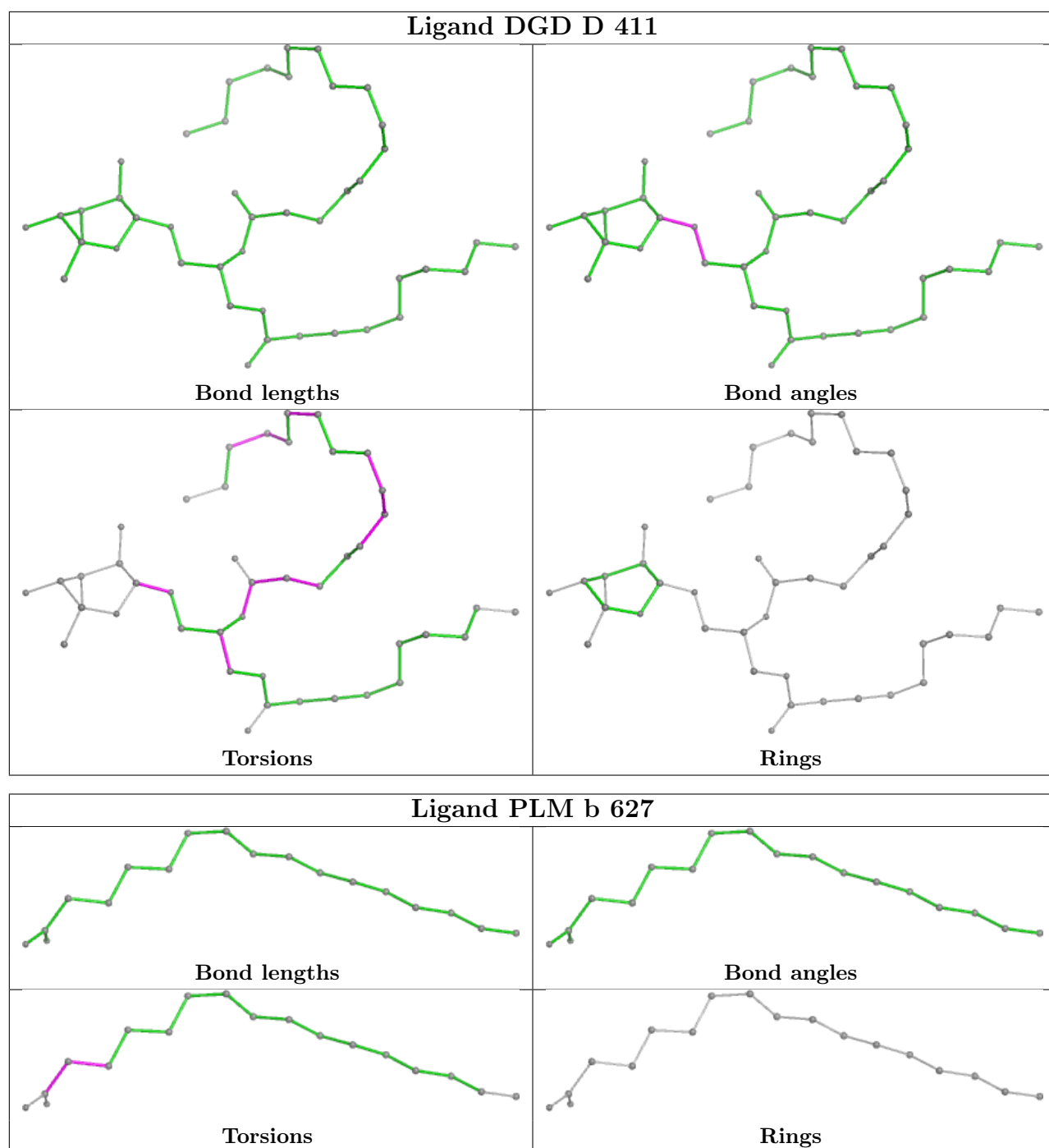


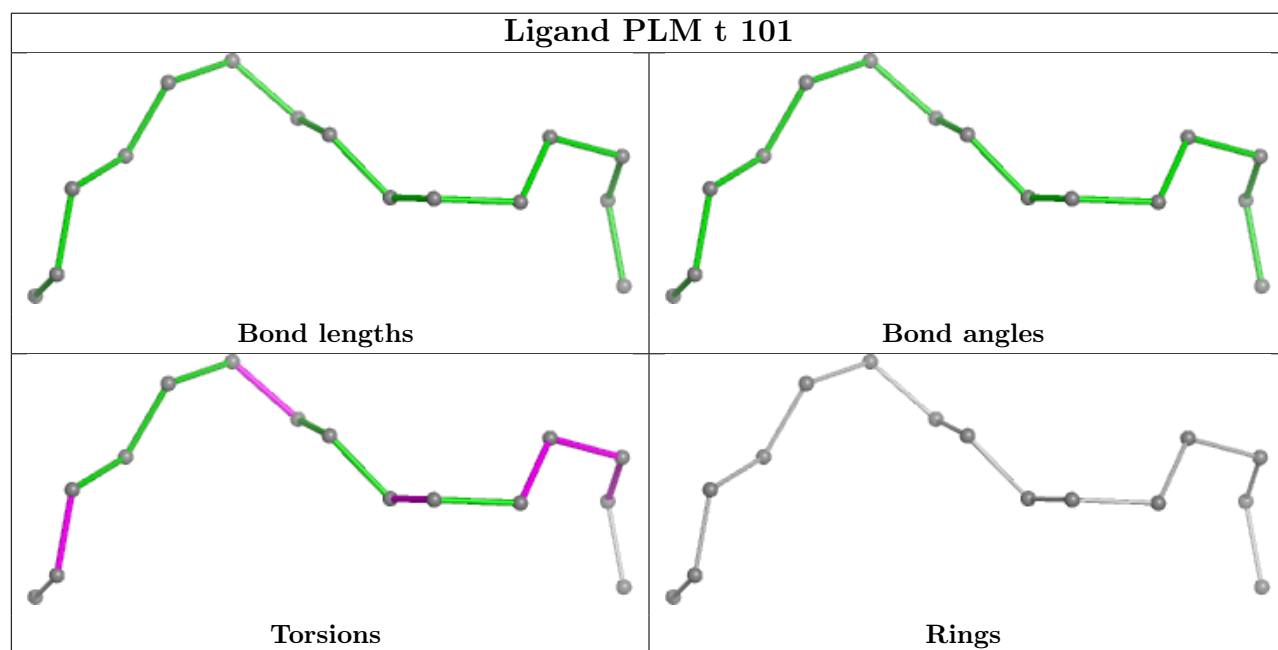
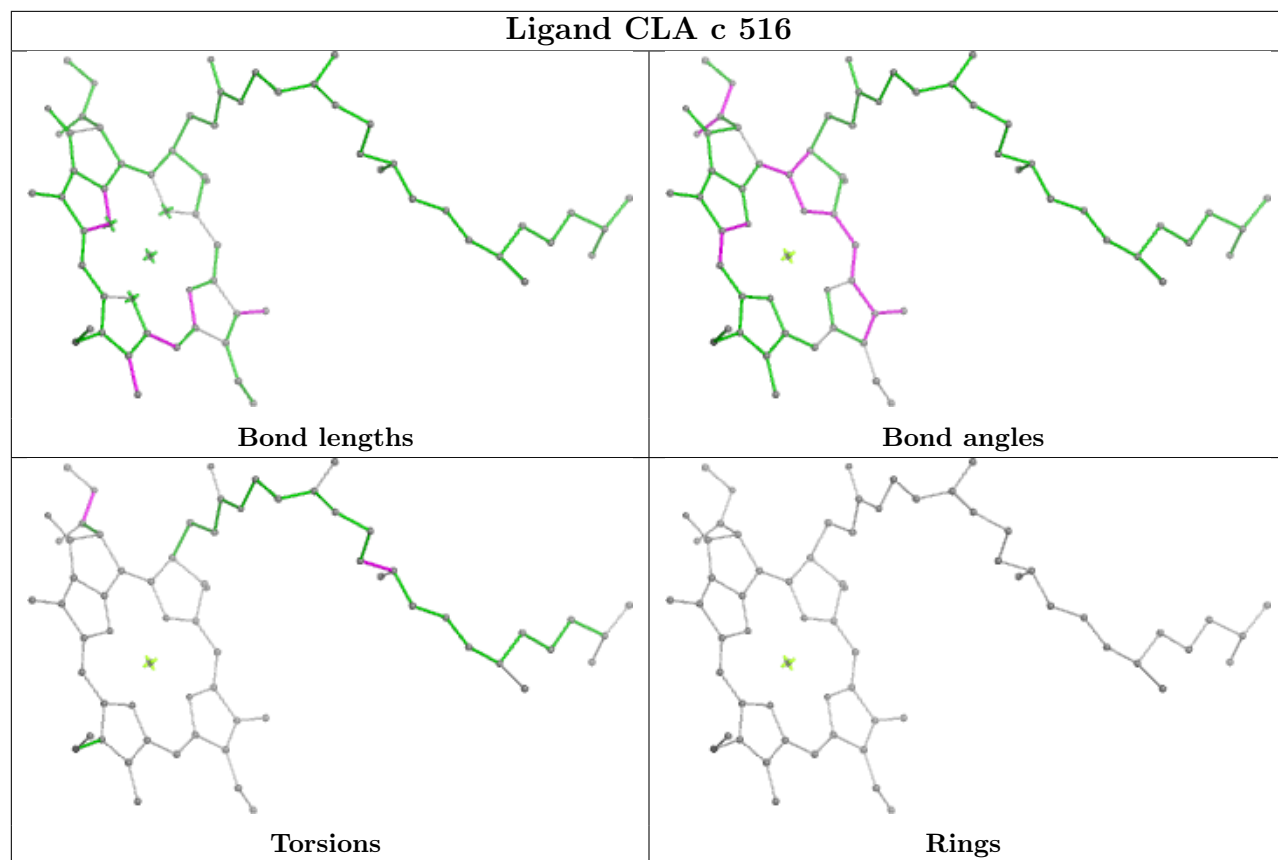


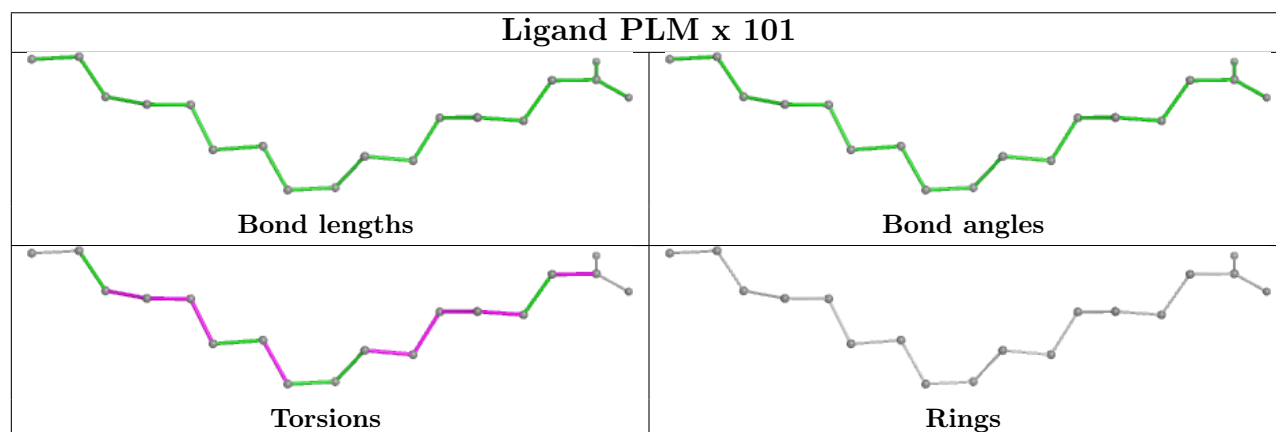
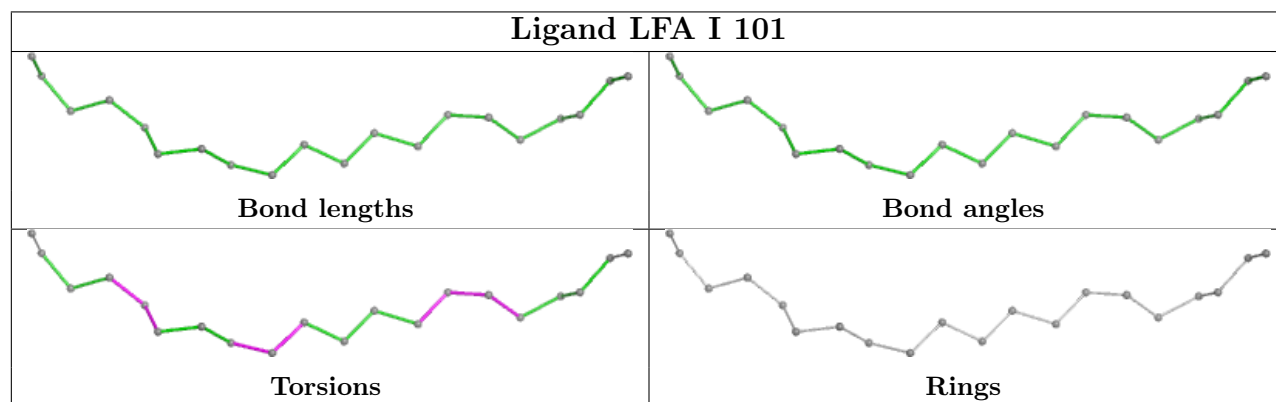
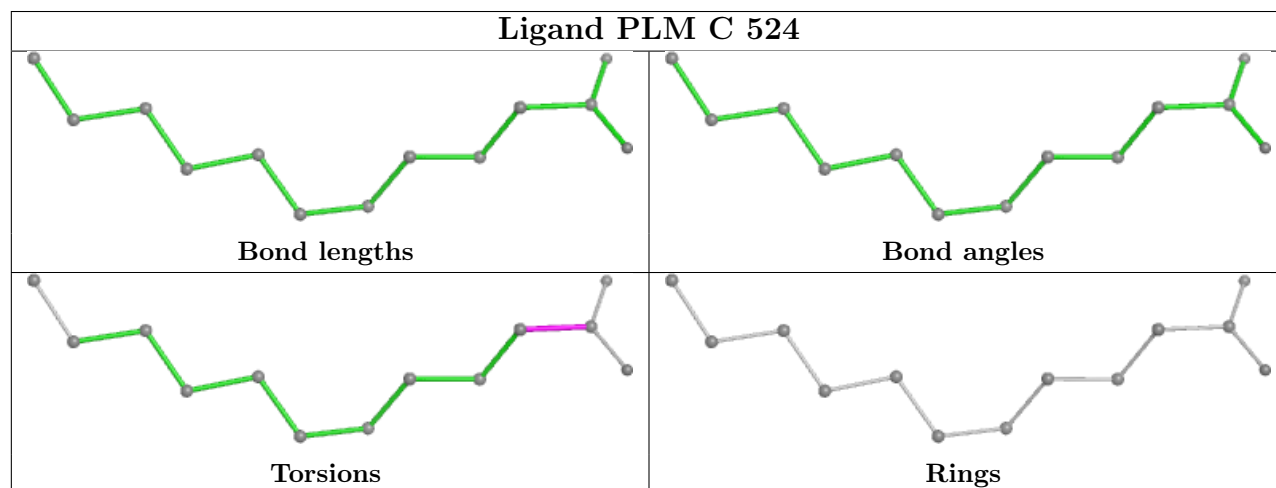
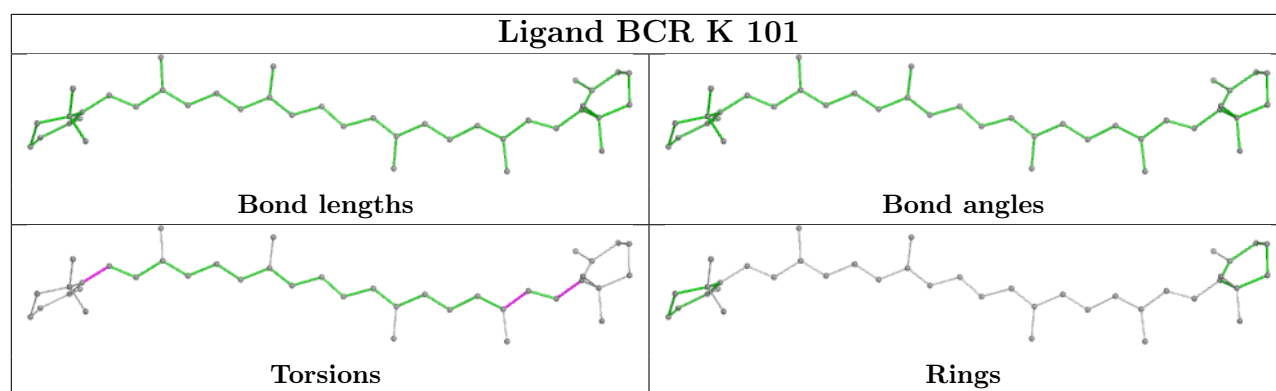


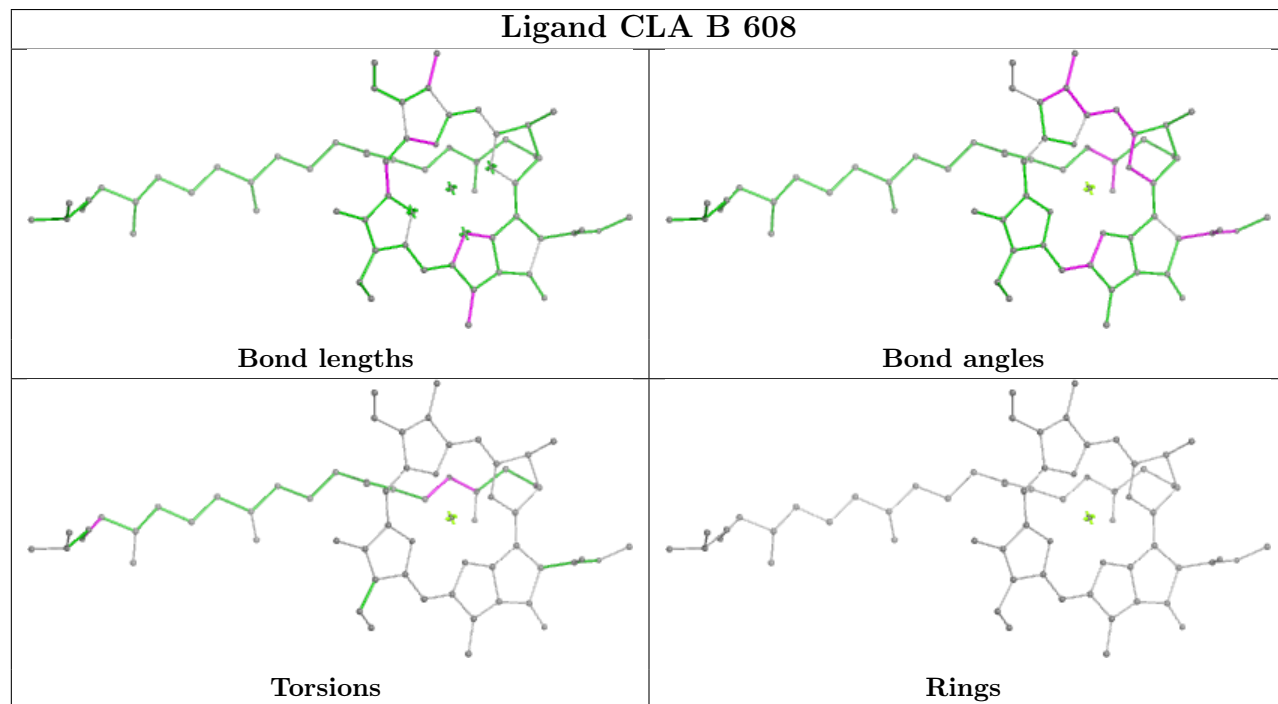
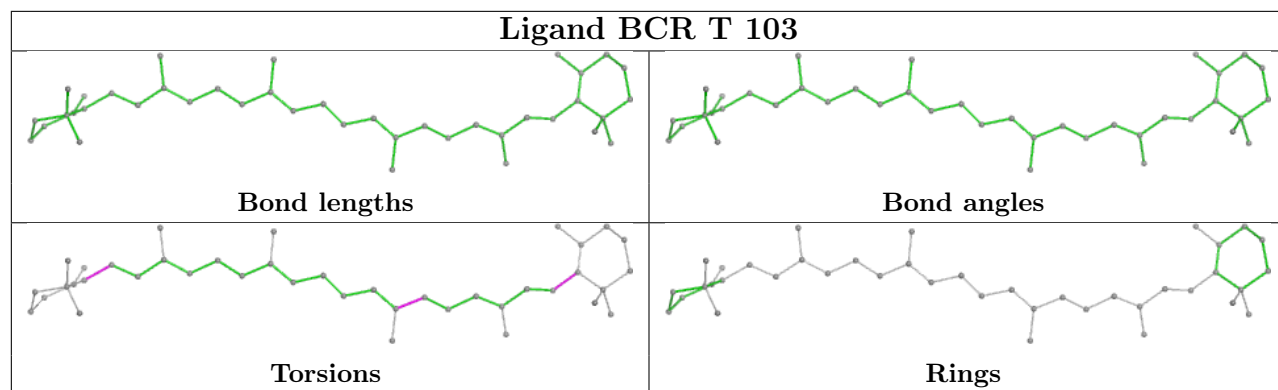




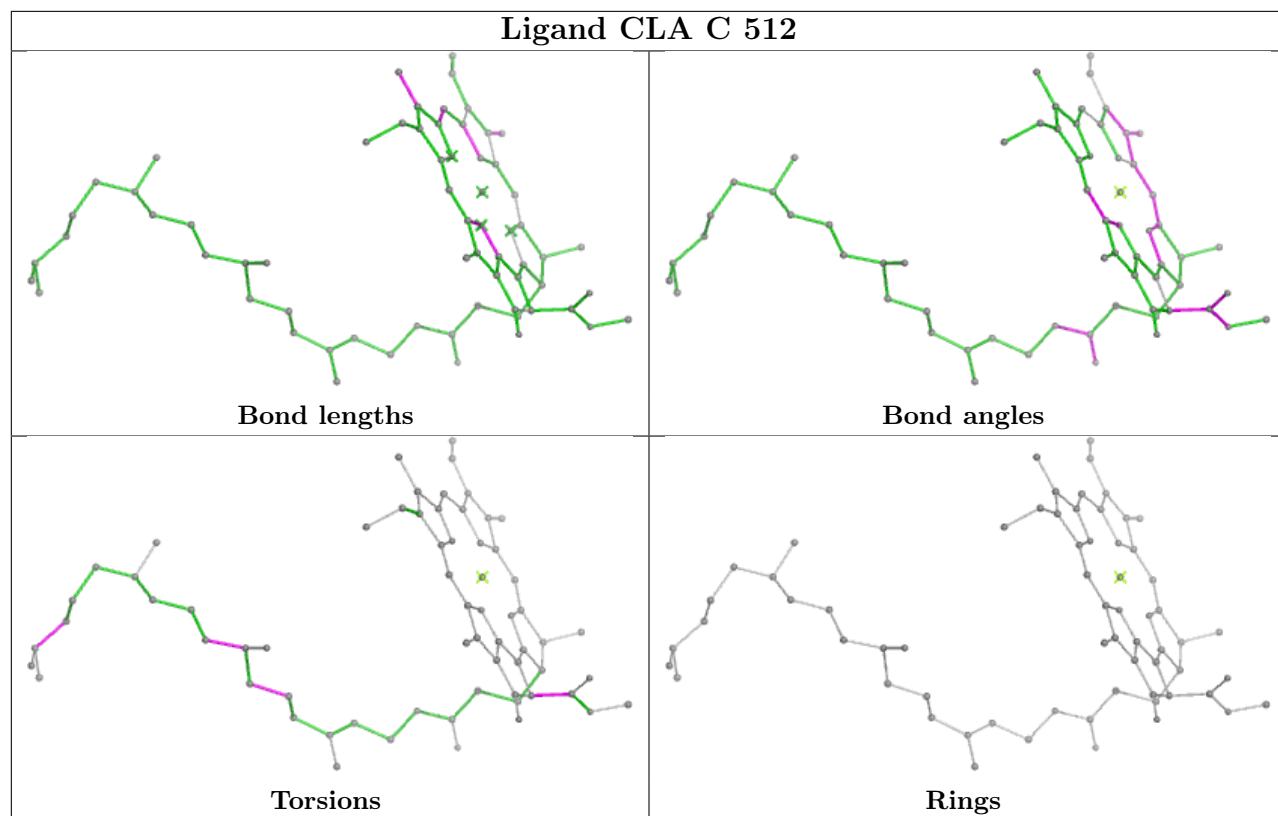




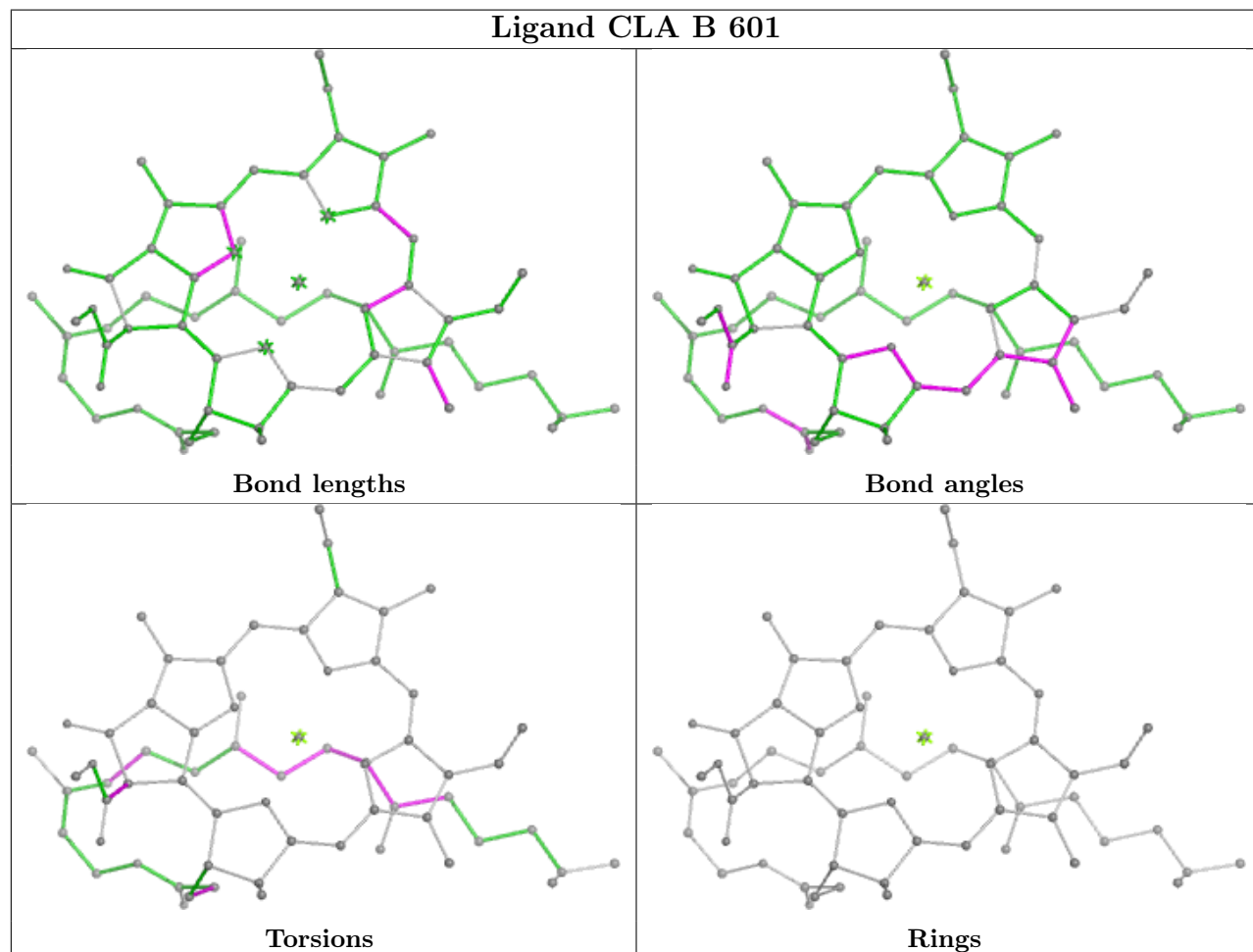




## Ligand CLA C 512

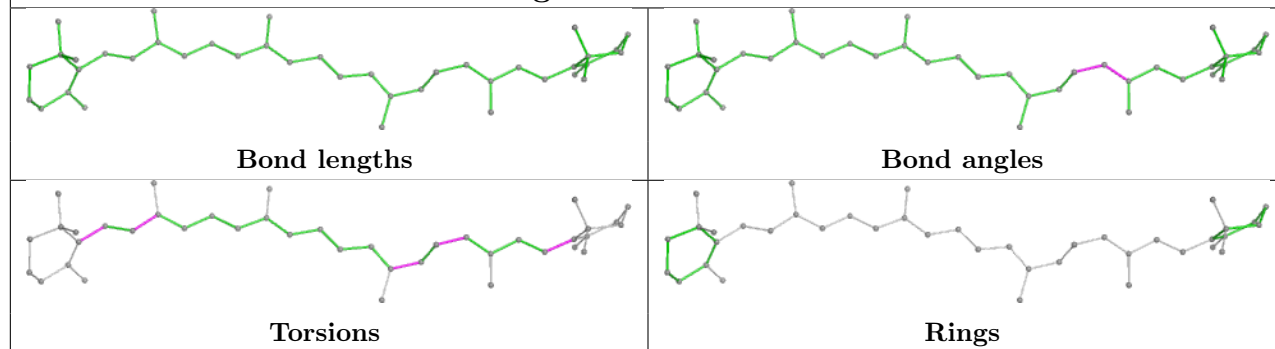


## Ligand CLA B 601

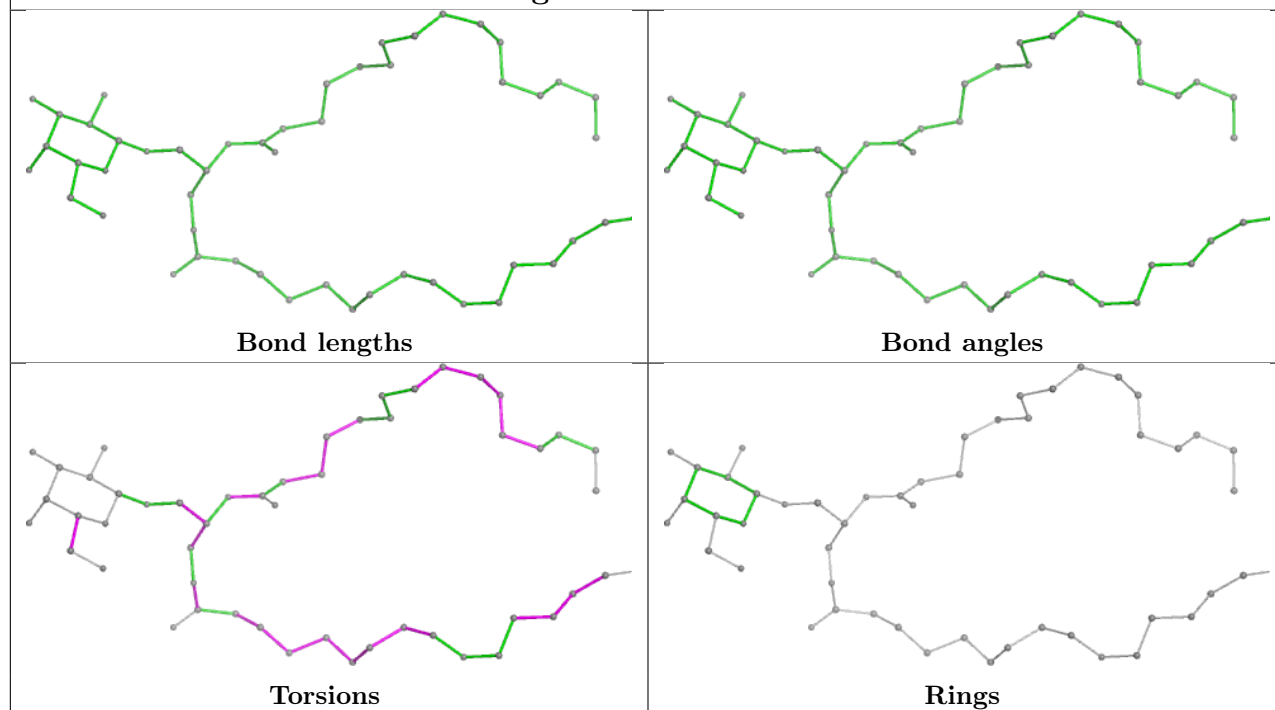




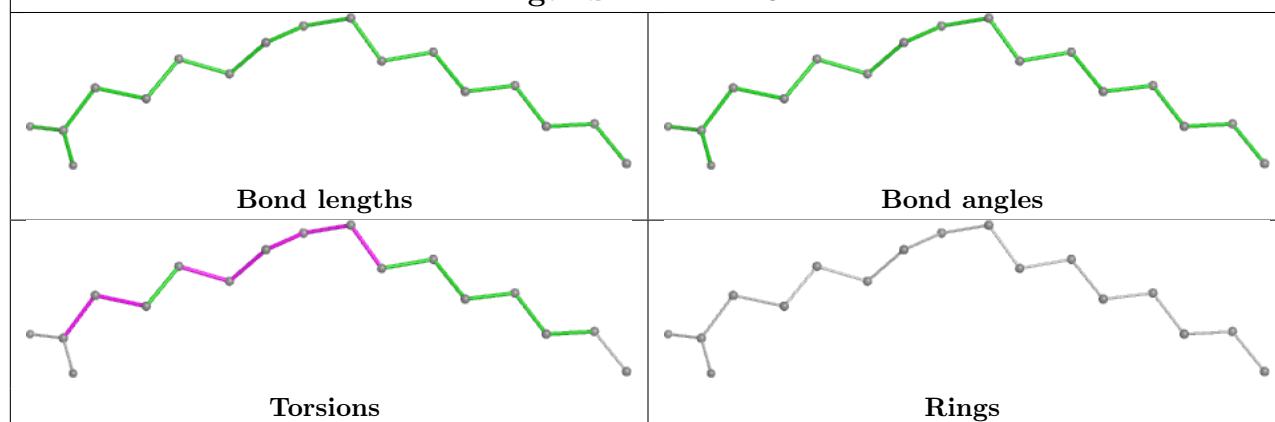
## Ligand BCR k 101

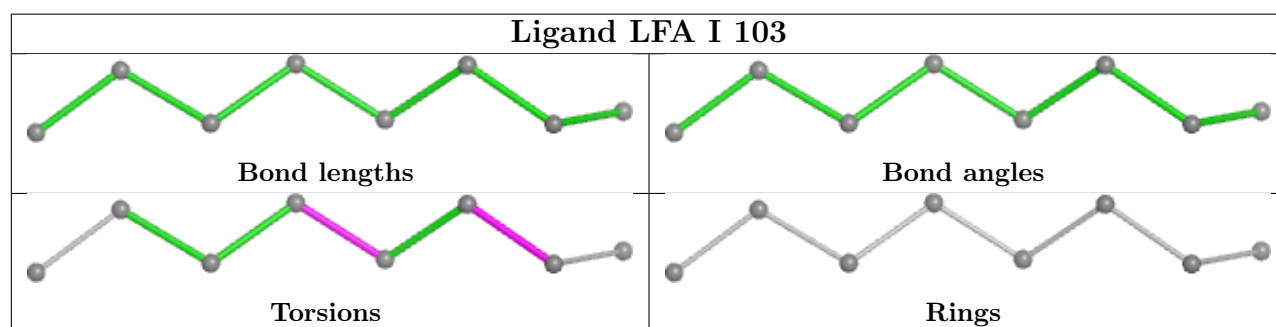
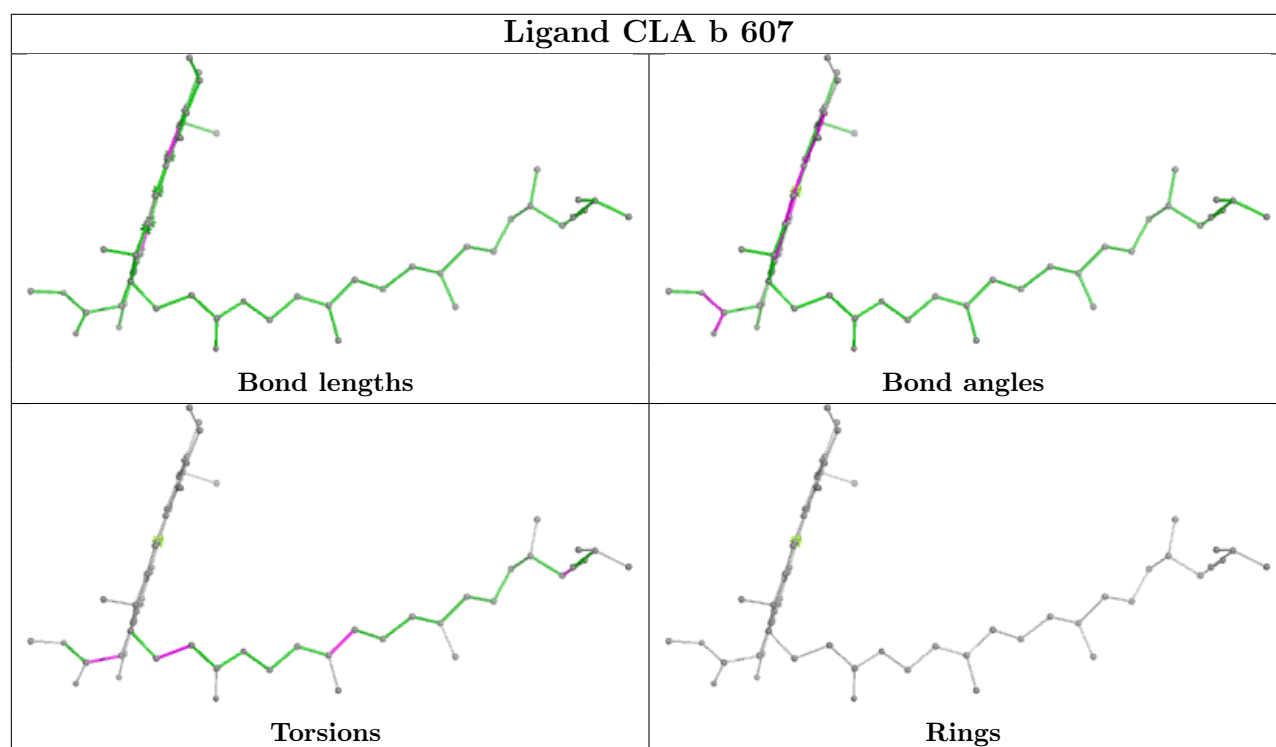
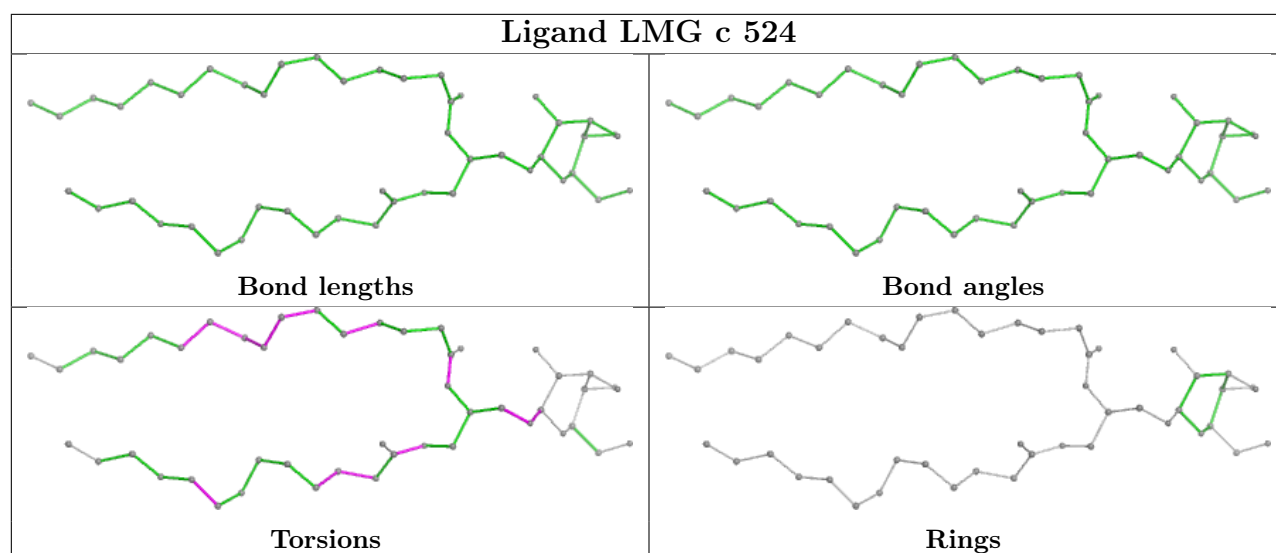


## Ligand LMG c 519

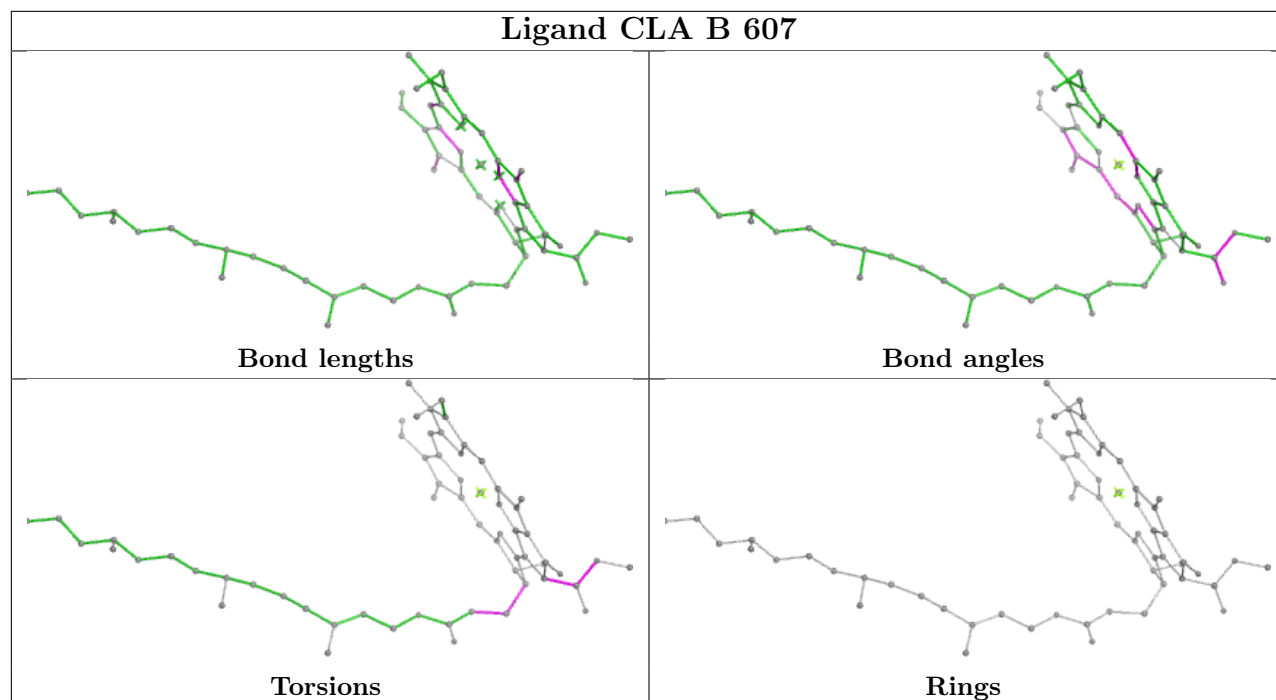


## Ligand PLM X 101

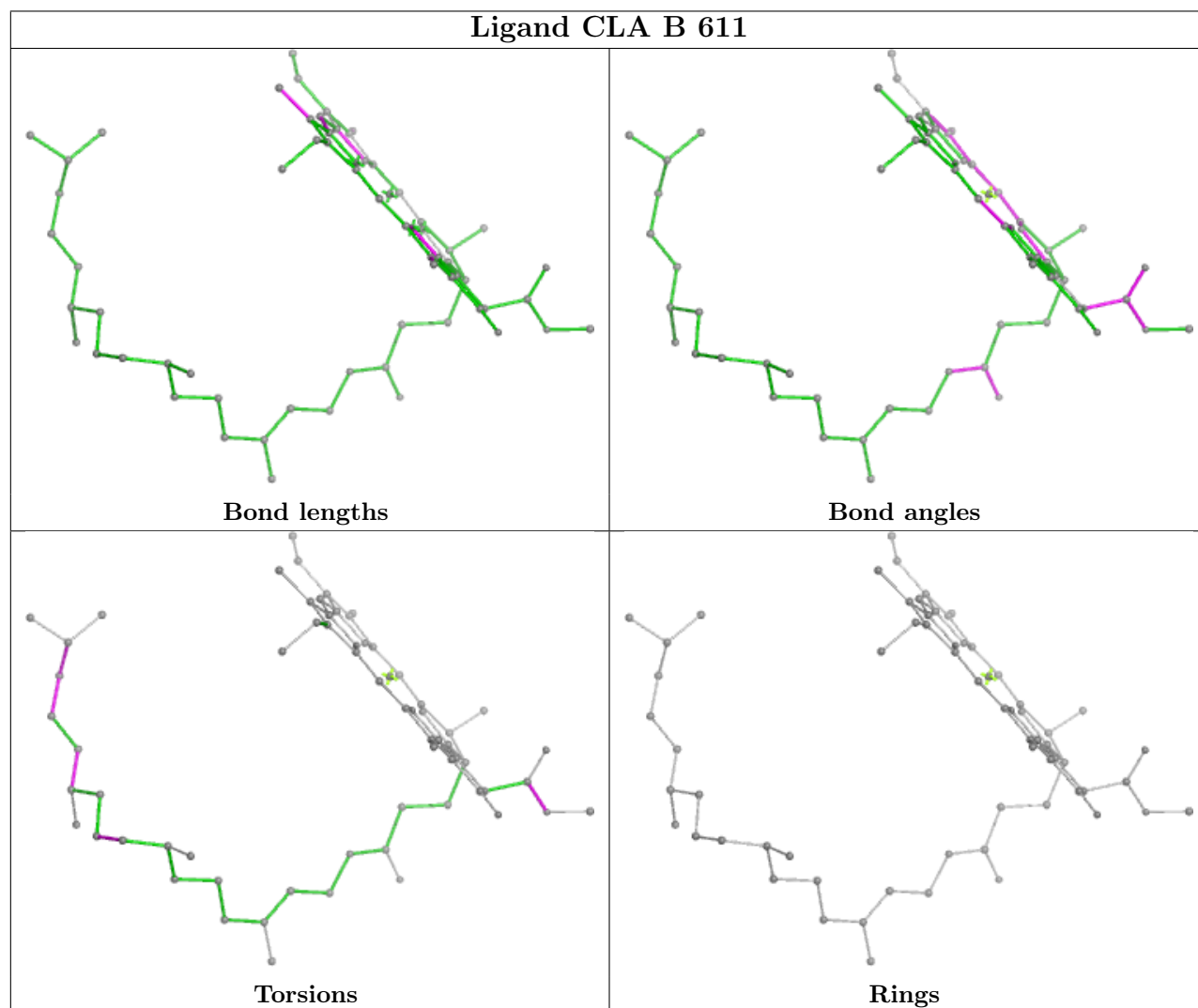


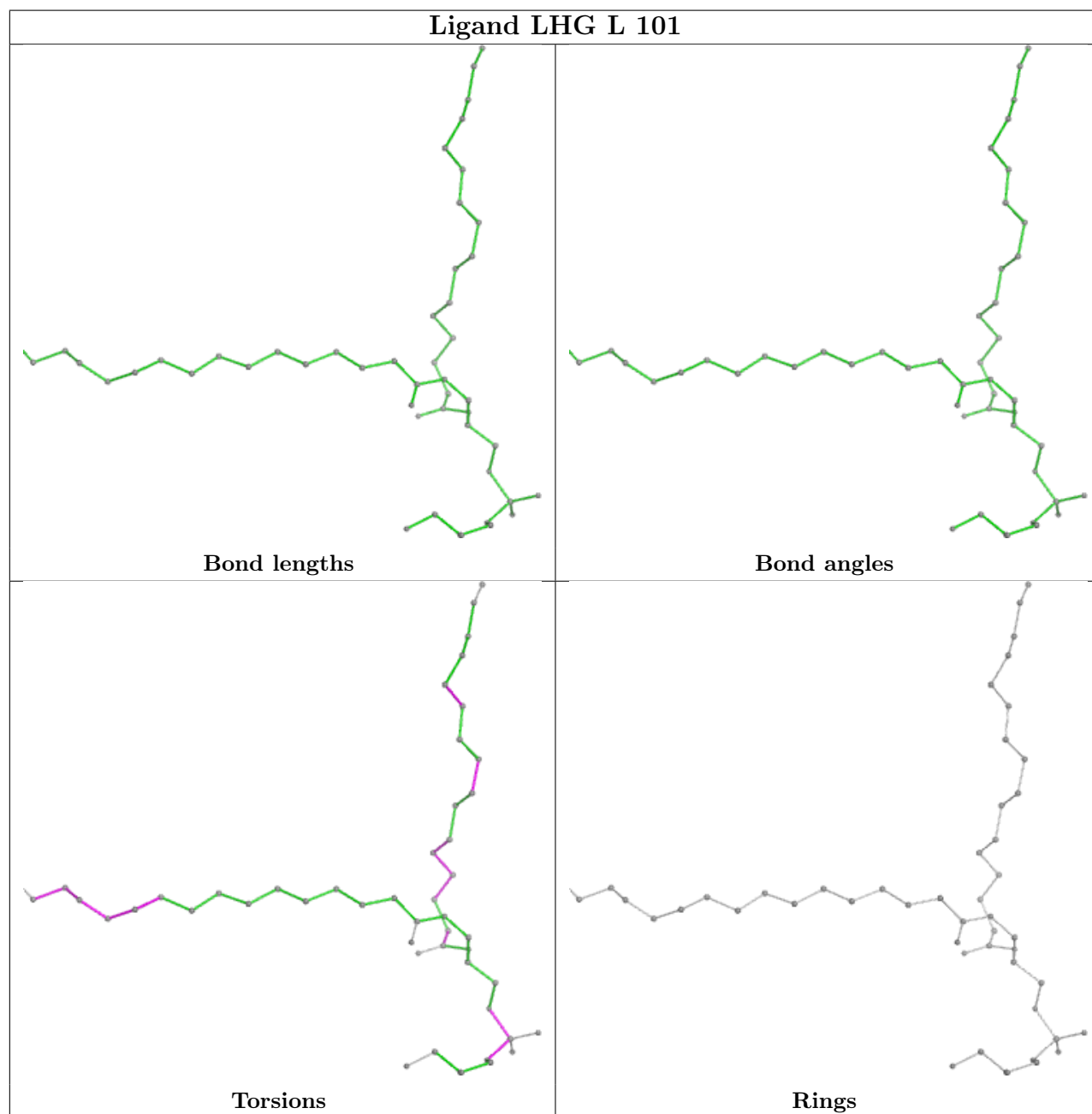
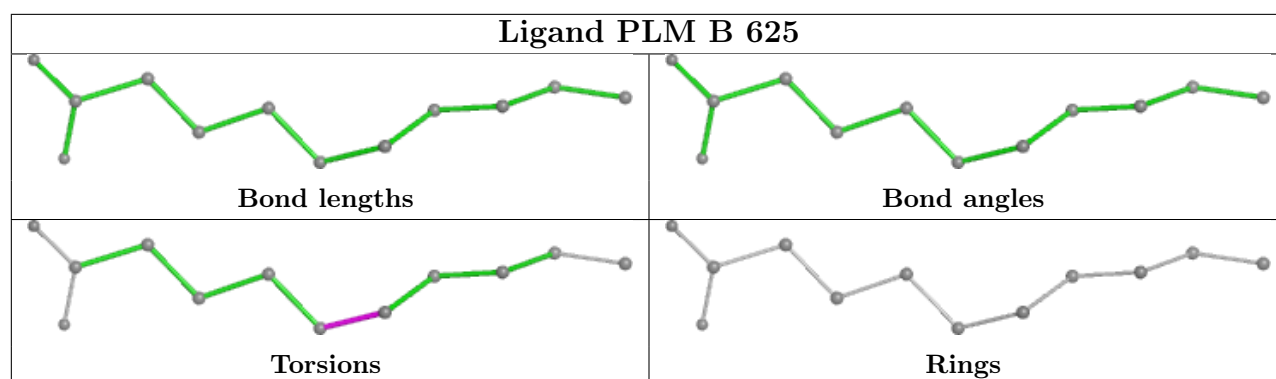


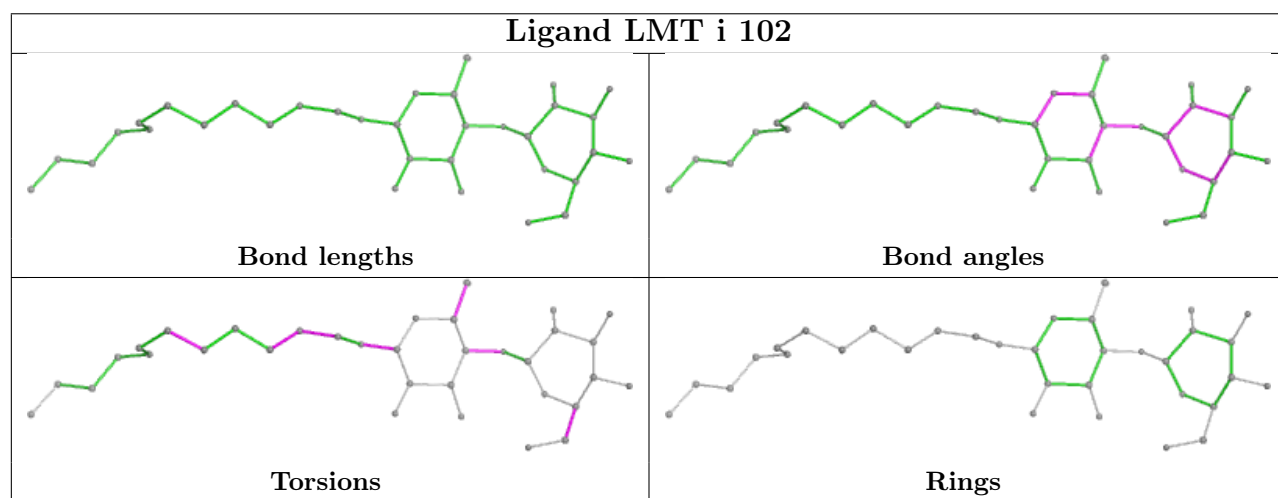
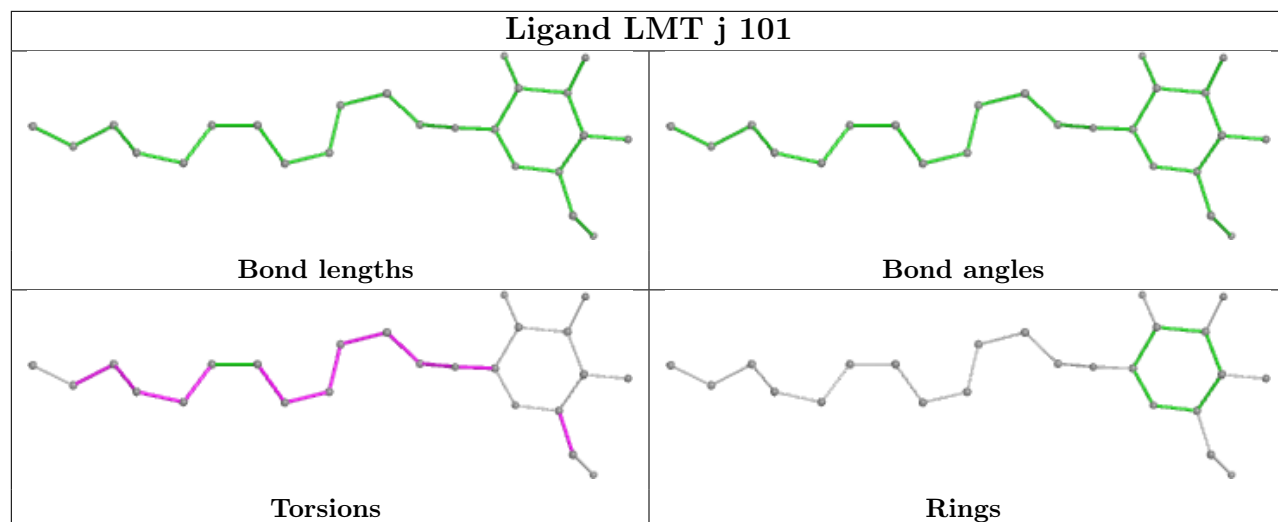
## Ligand CLA B 607

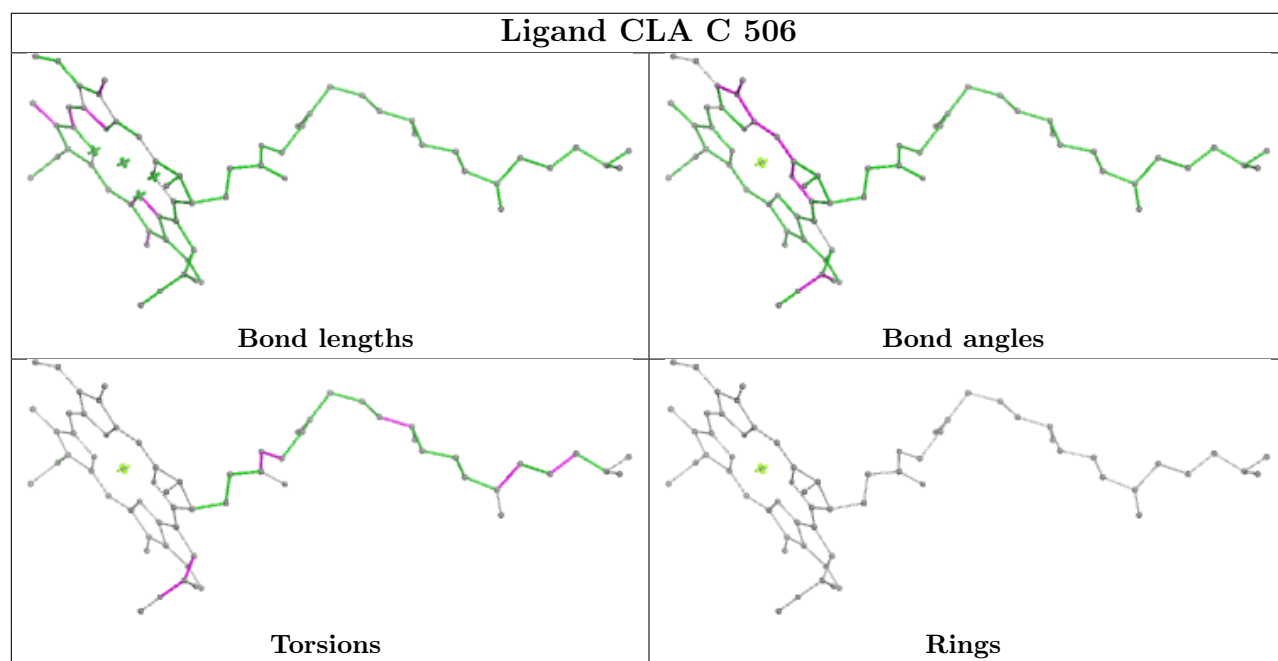
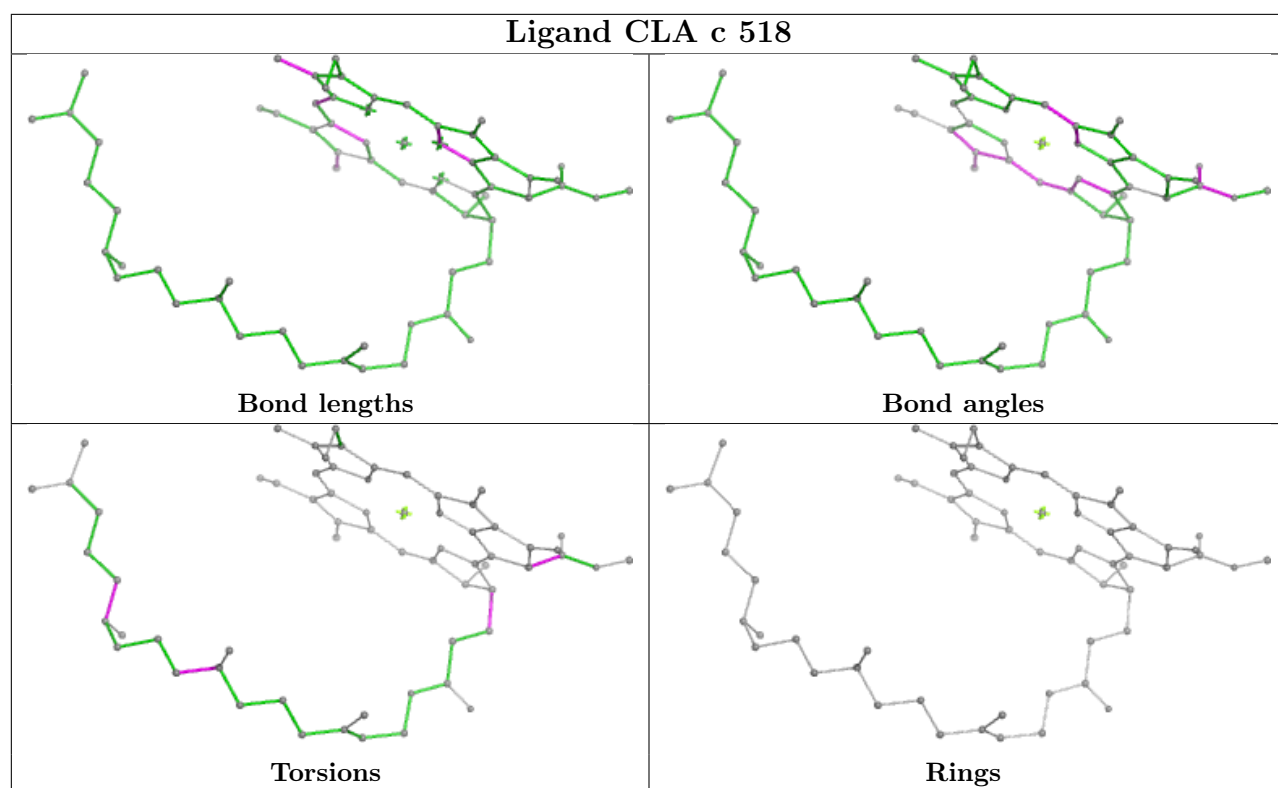


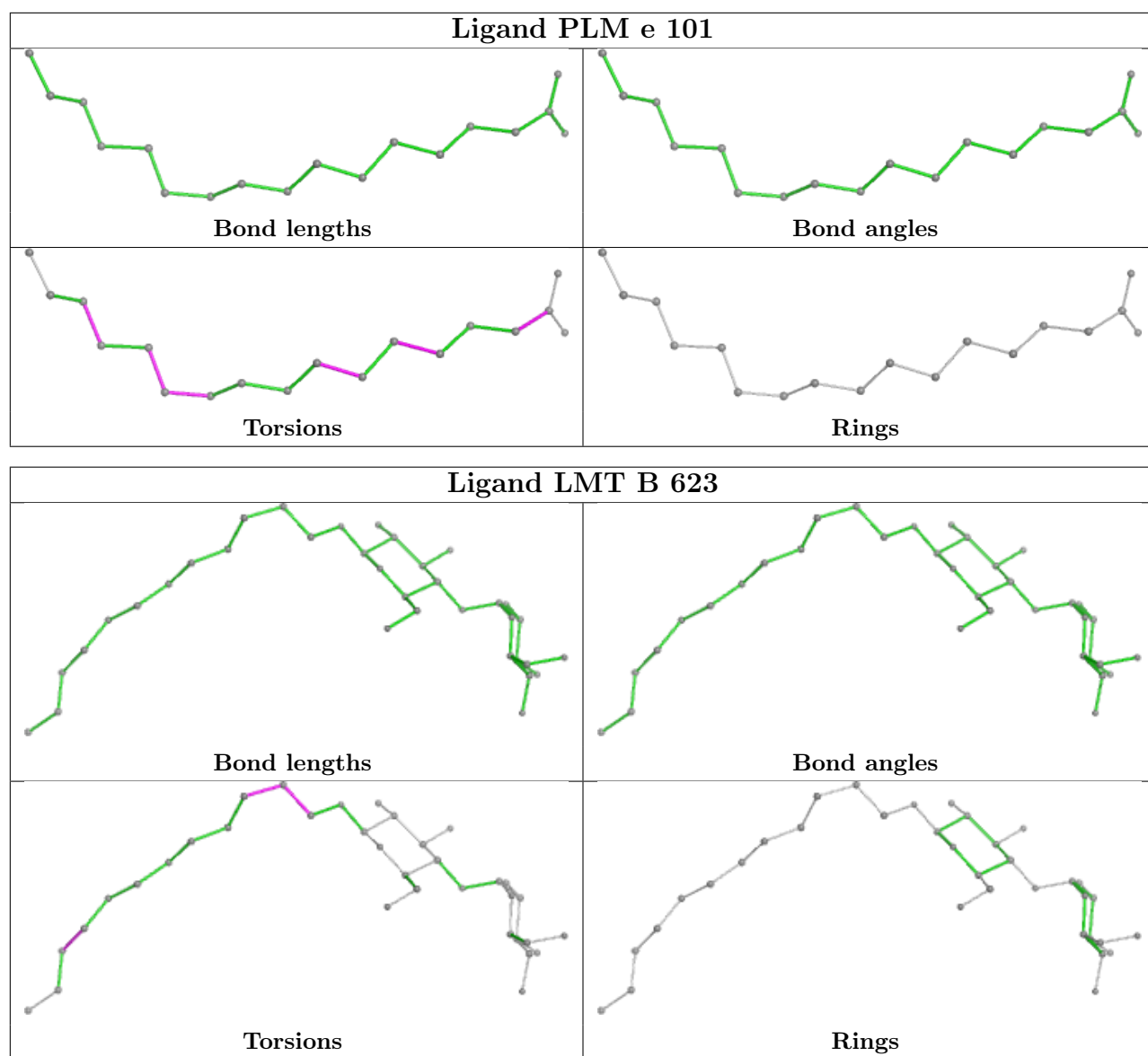
## Ligand CLA B 611



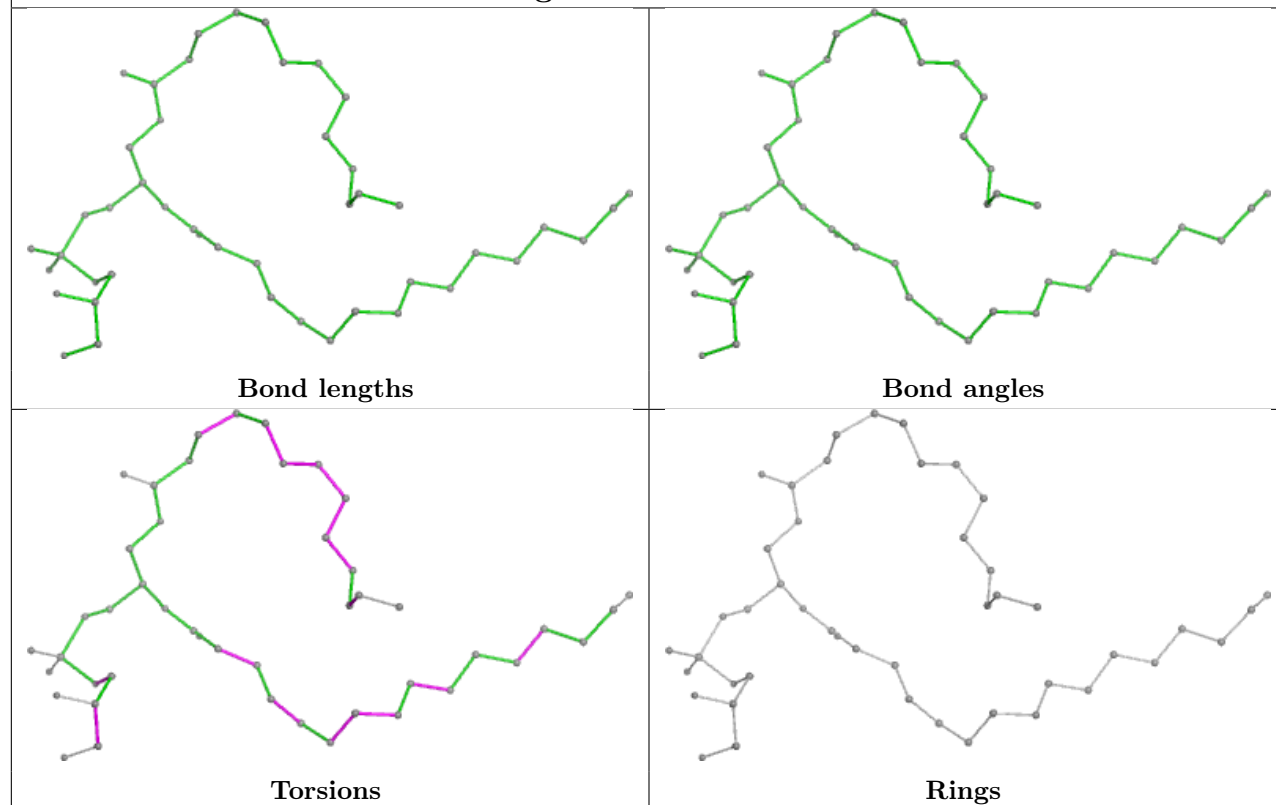




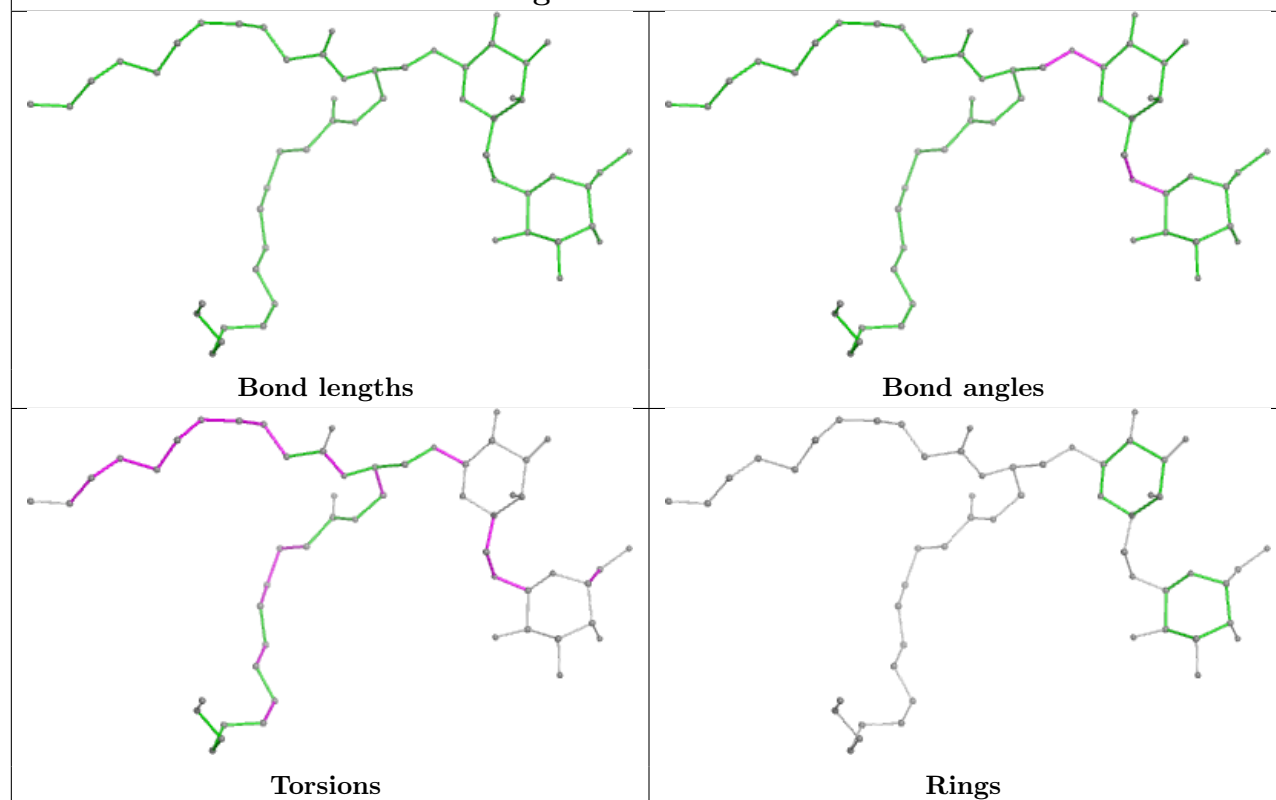




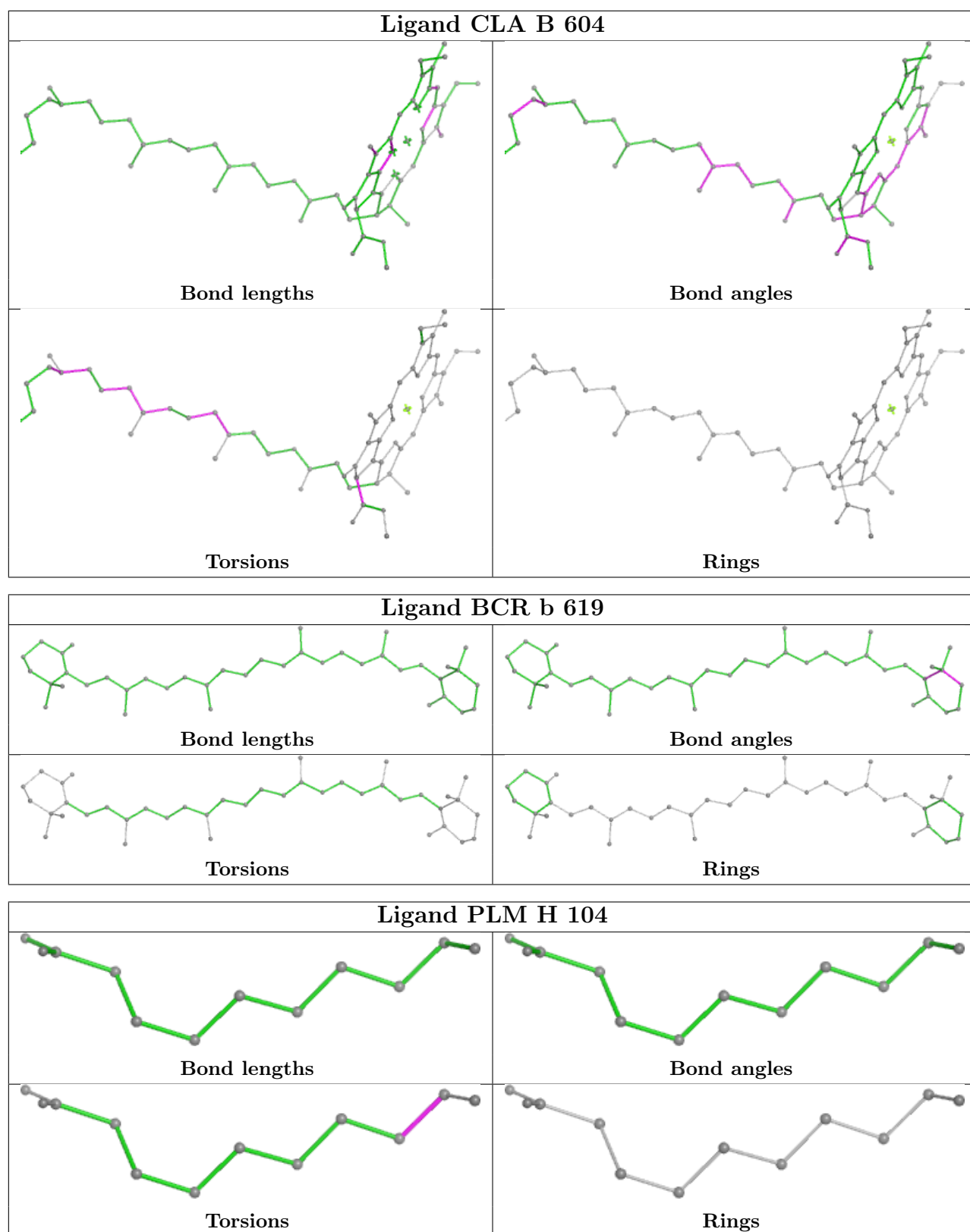
## Ligand LHG a 421



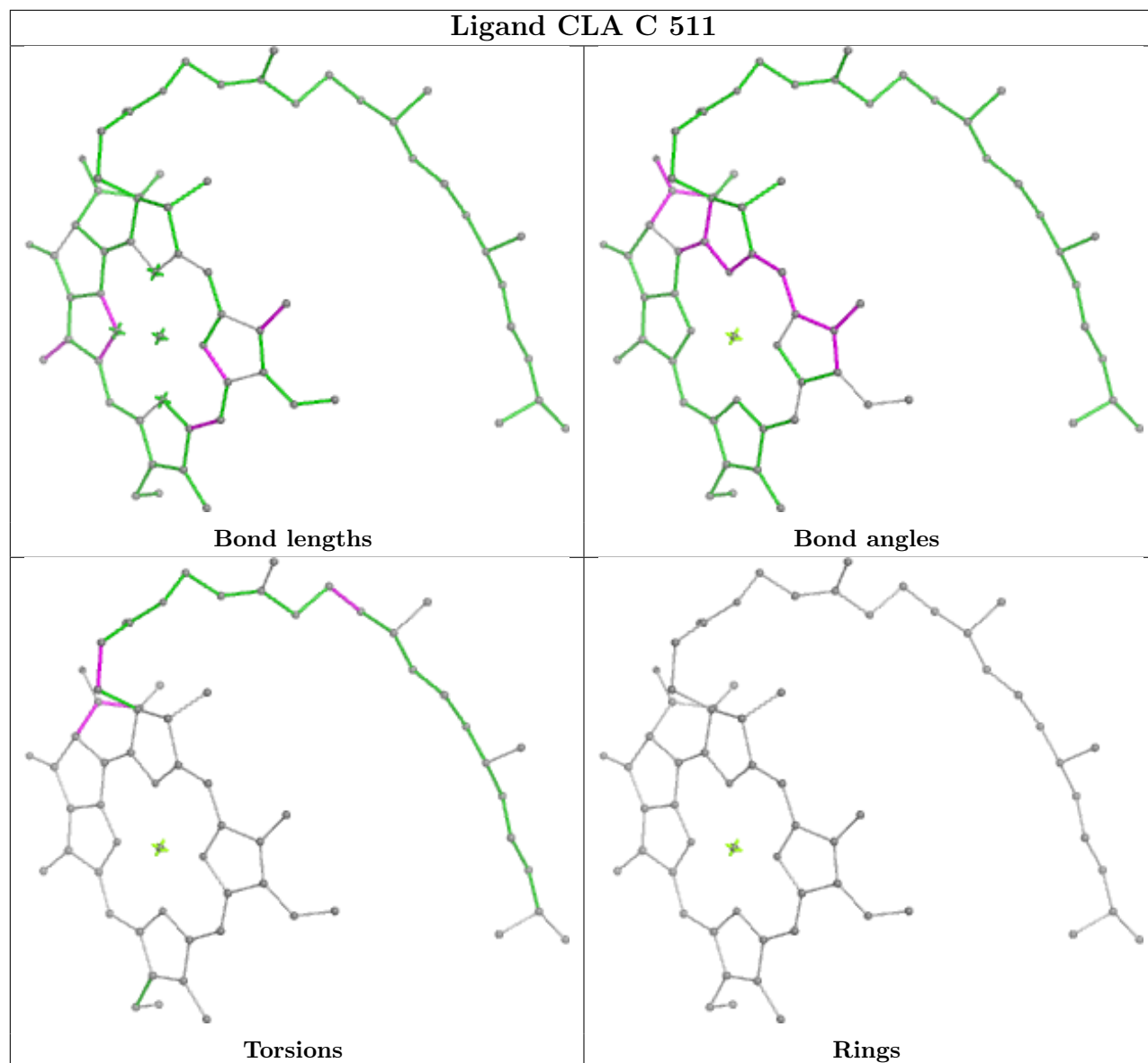
## Ligand DGD c 504



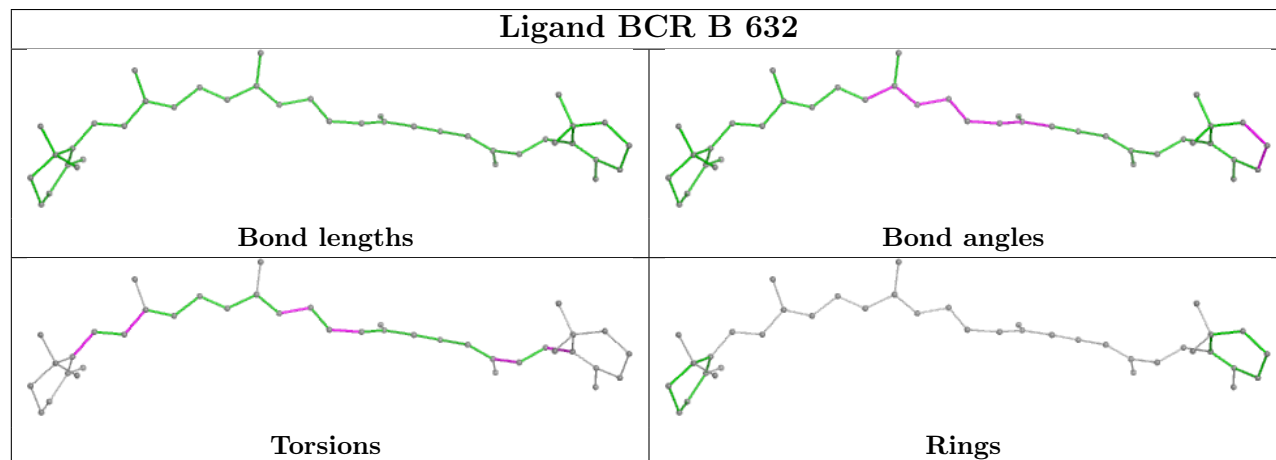


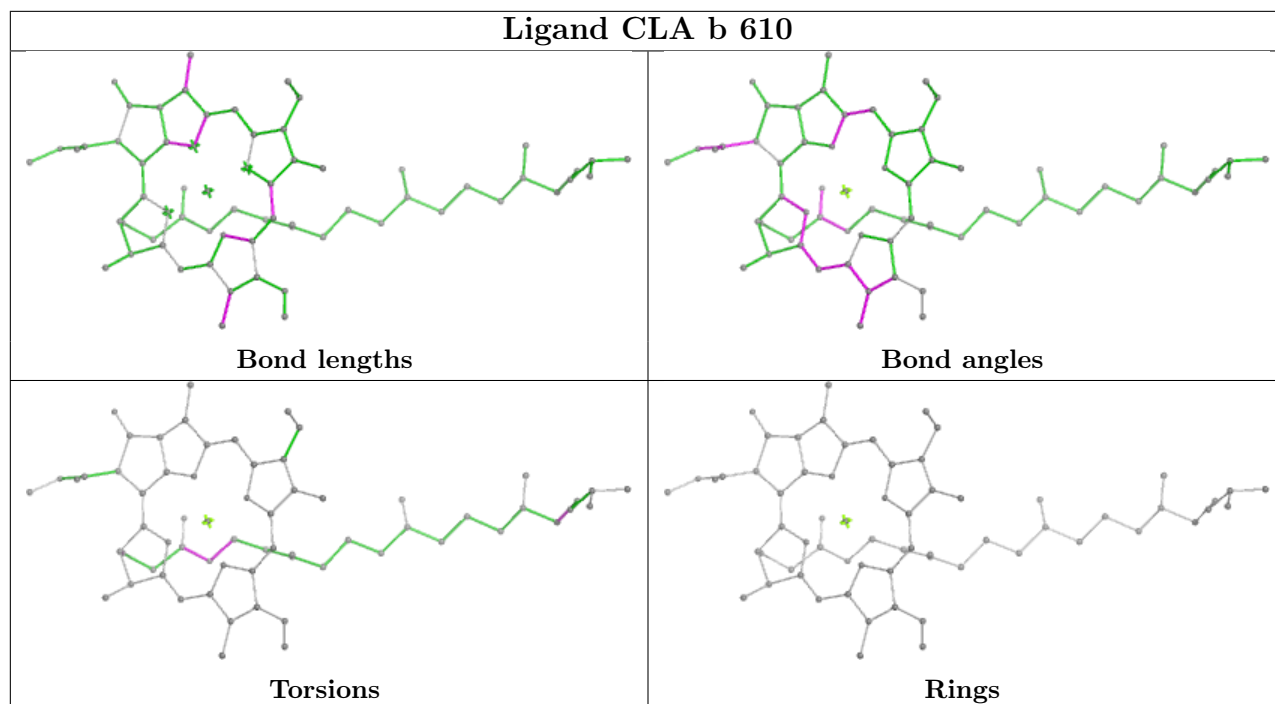
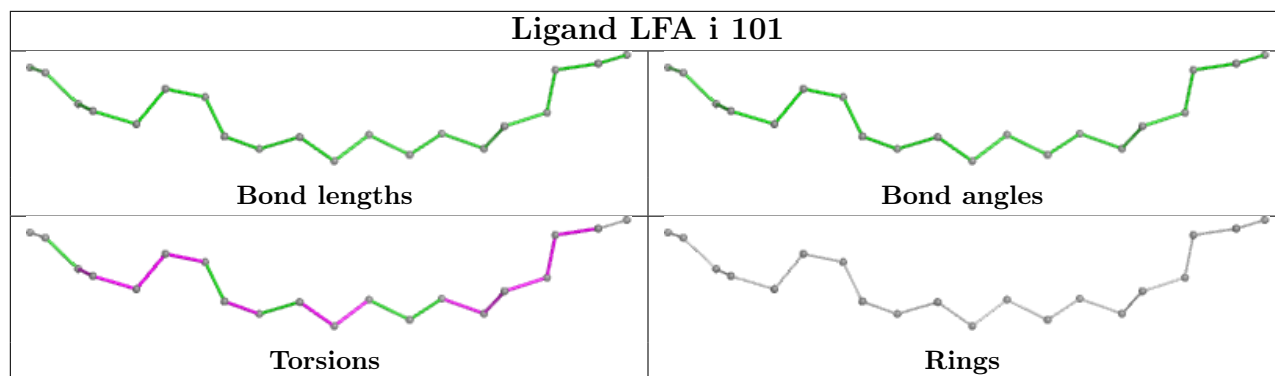


## Ligand CLA C 511

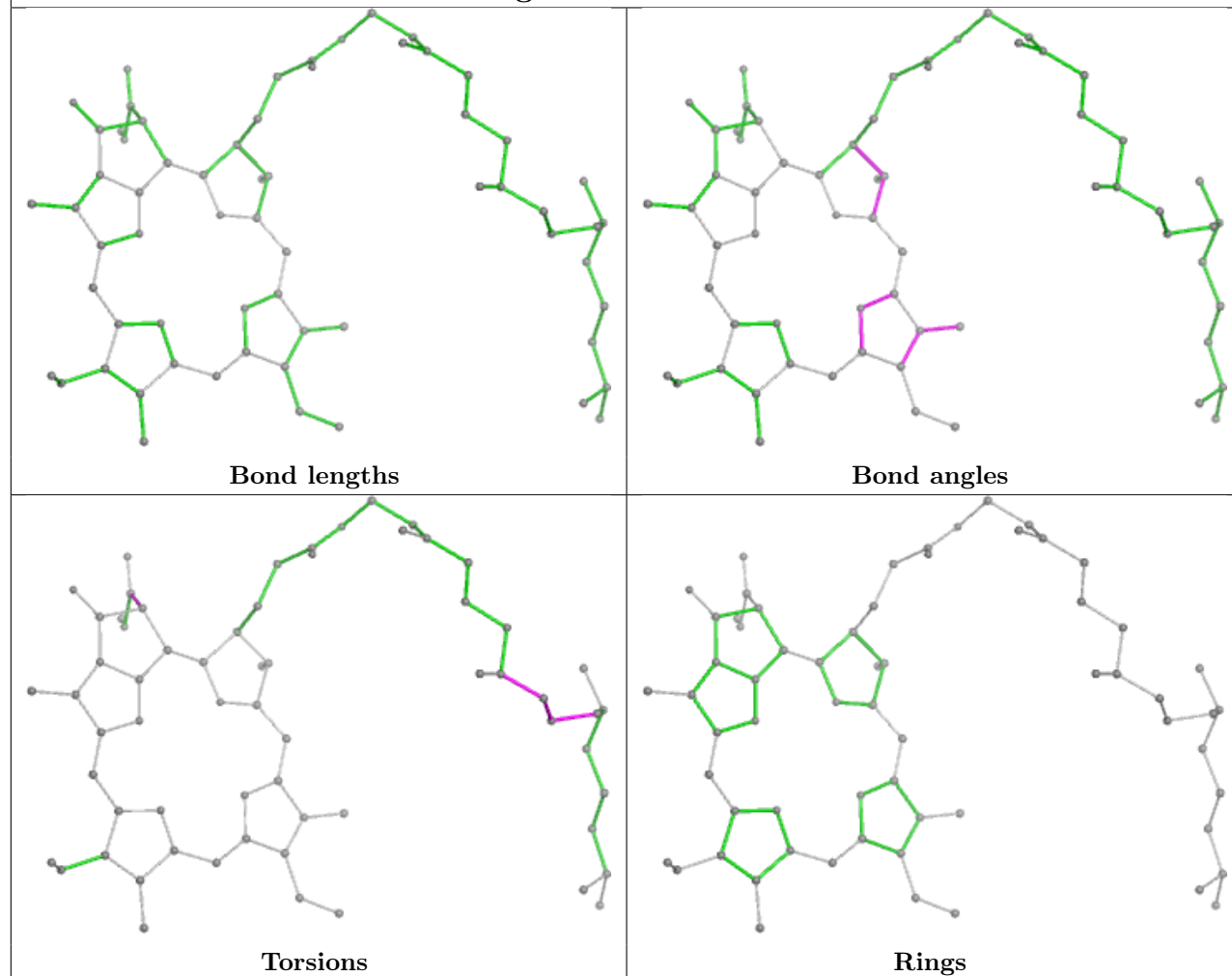


## Ligand BCR B 632

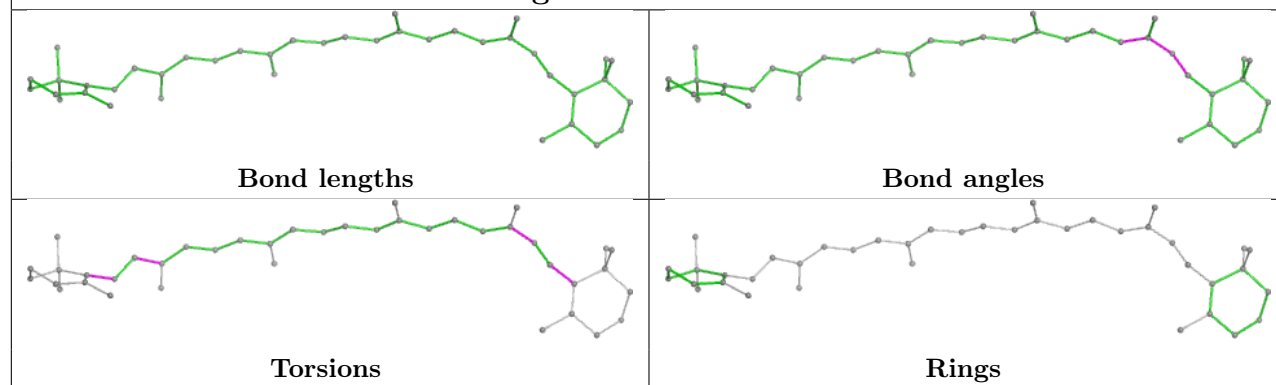


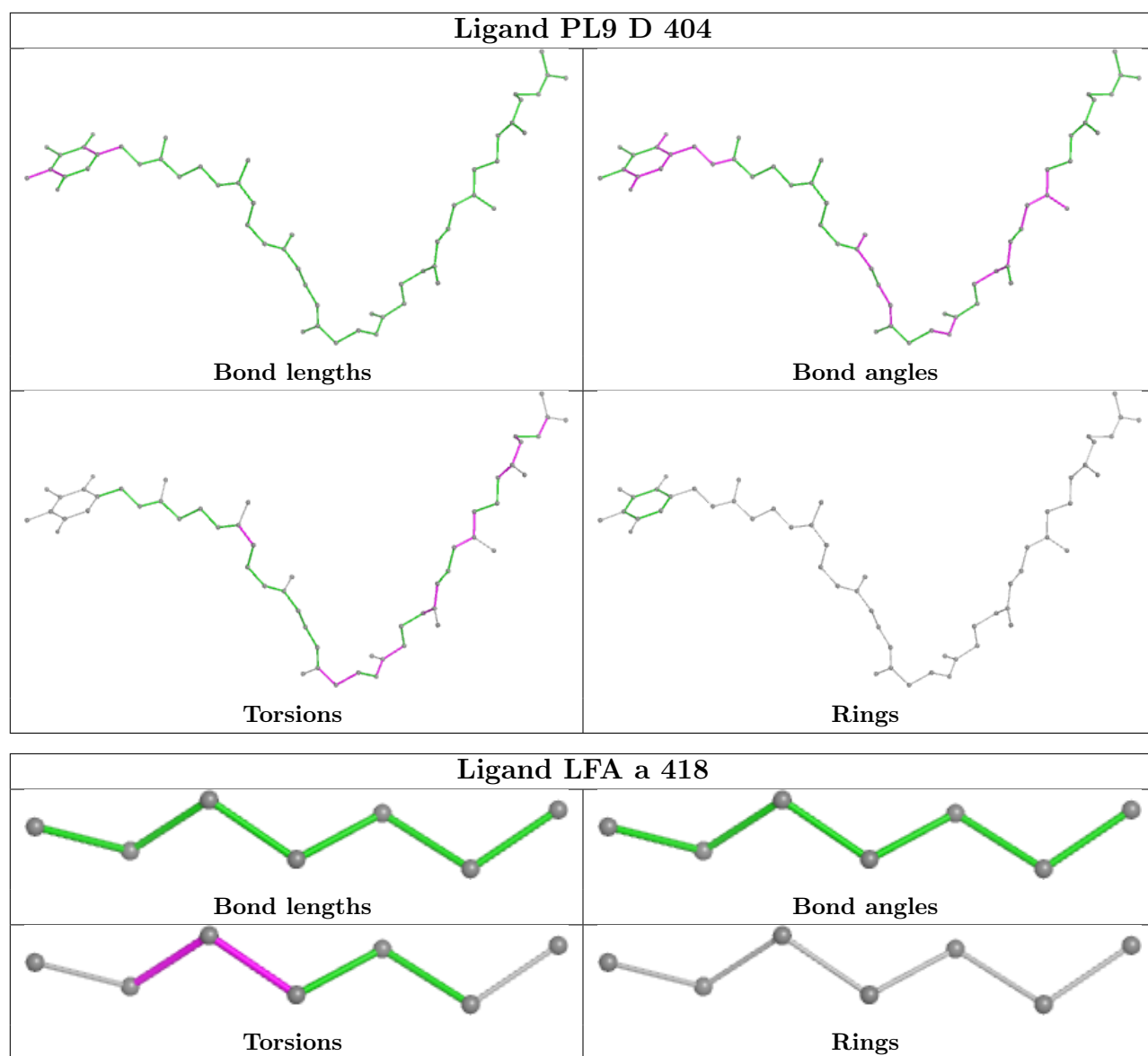


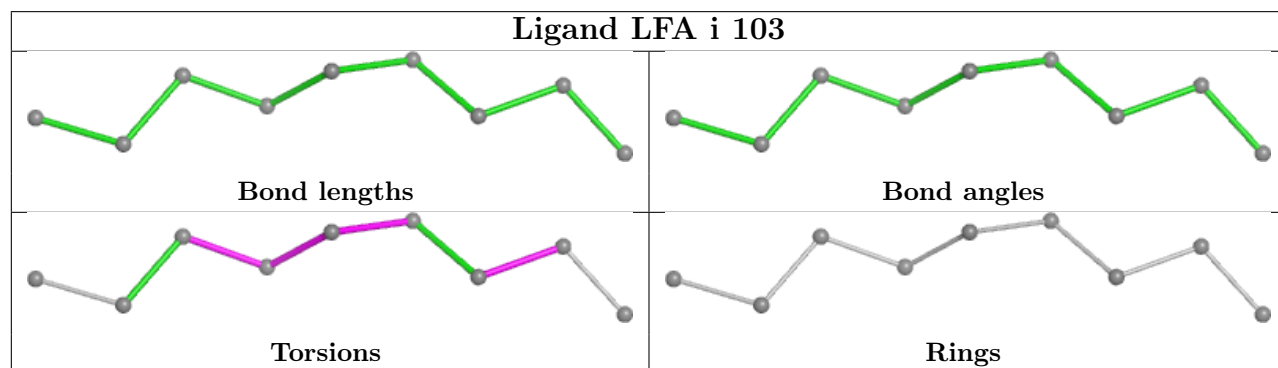
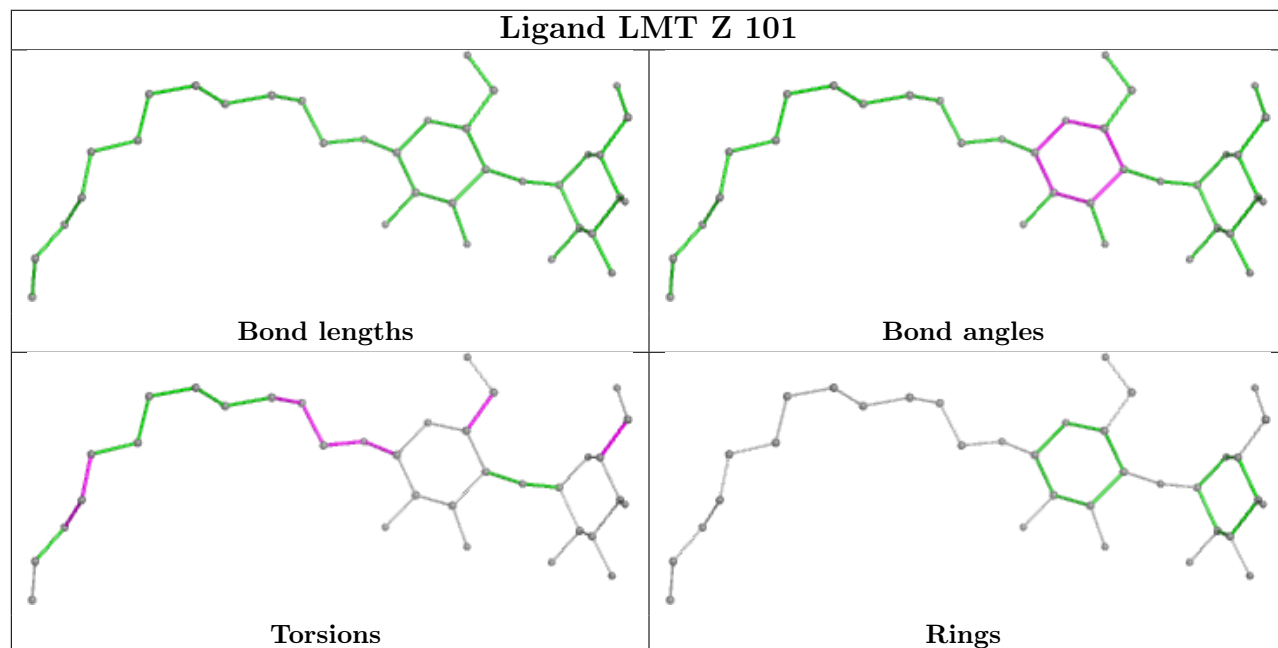
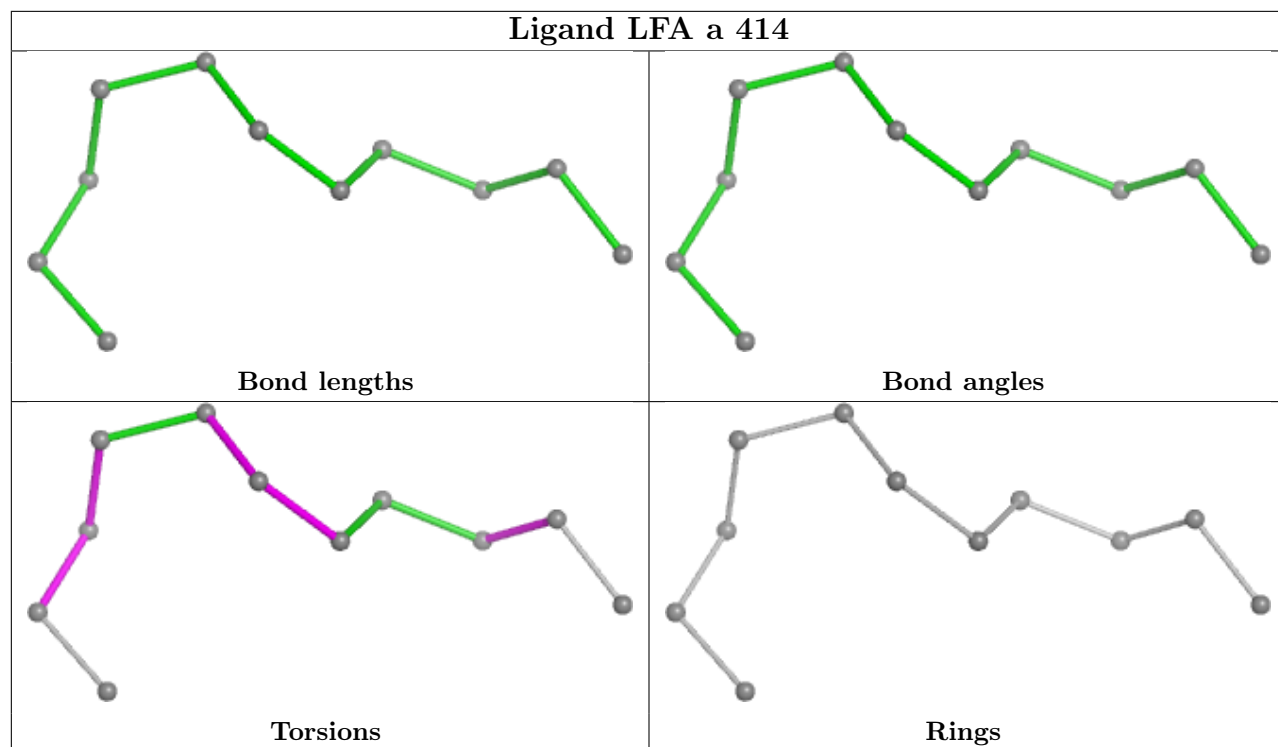
## Ligand PHO a 420

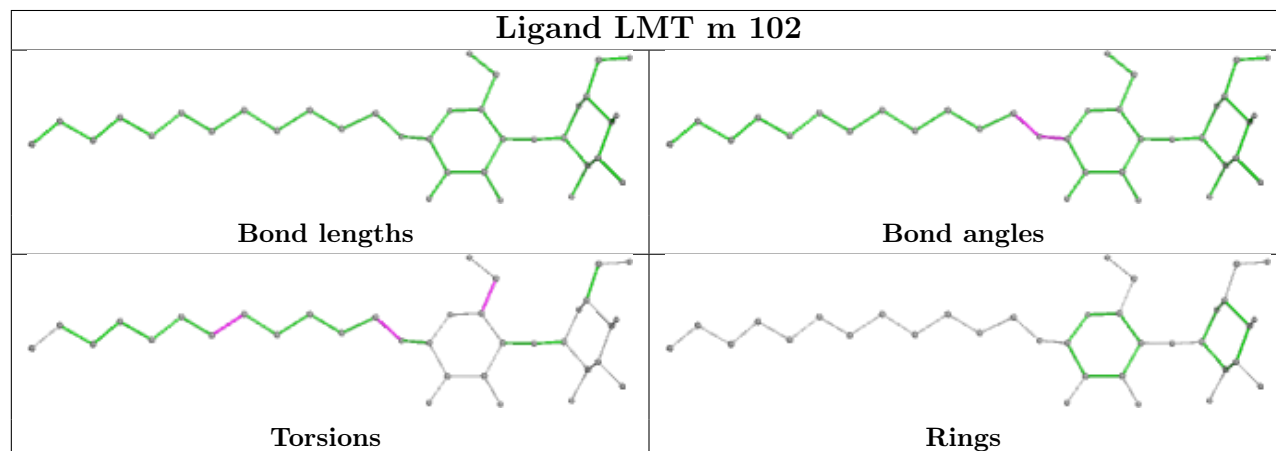
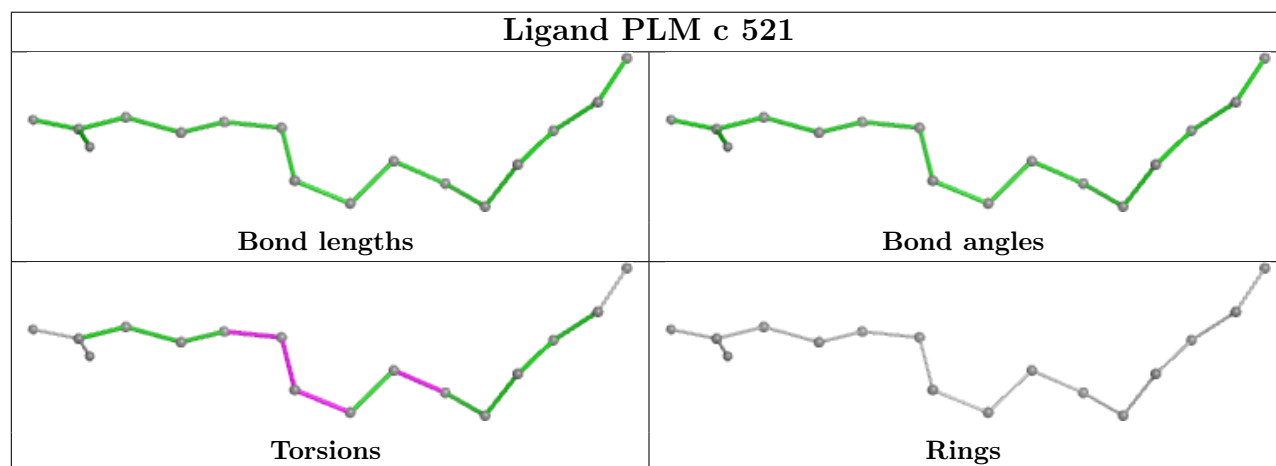
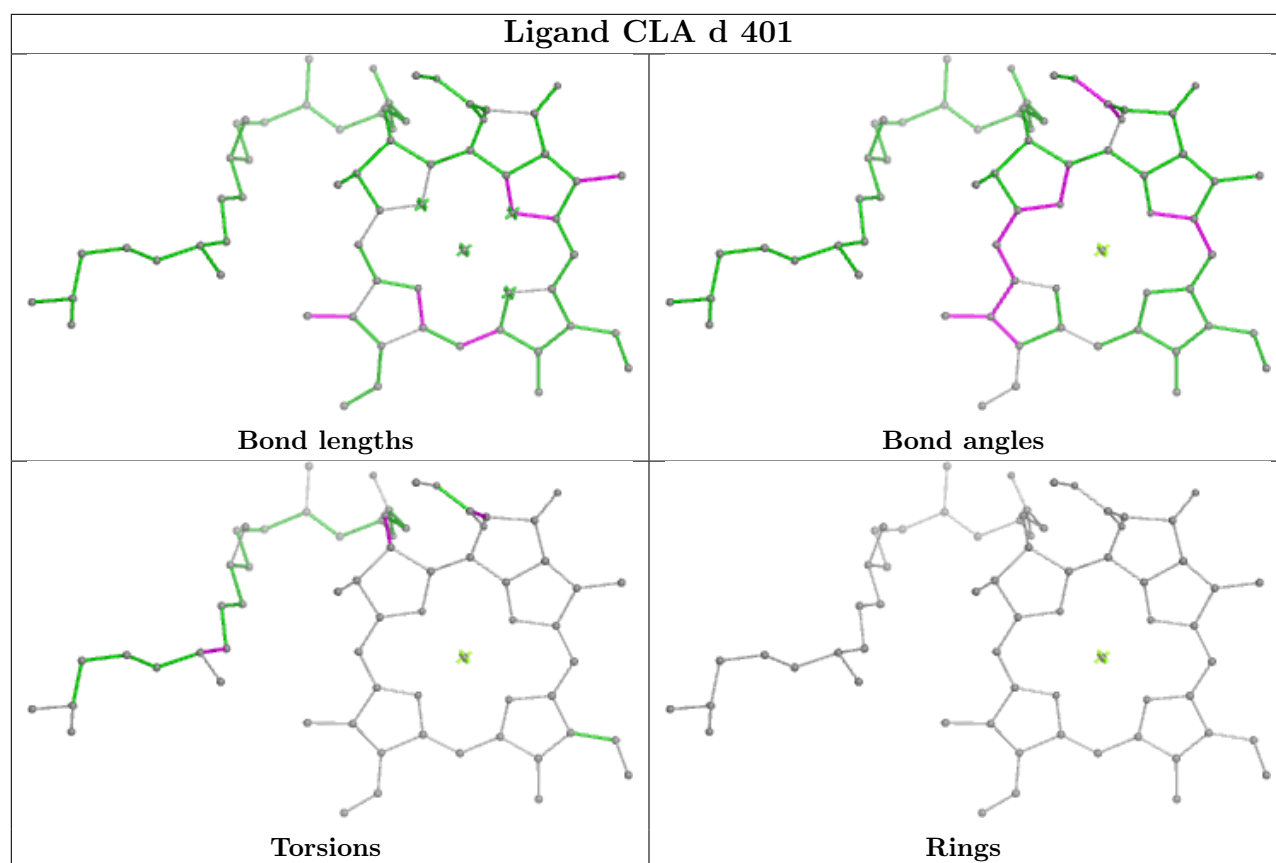


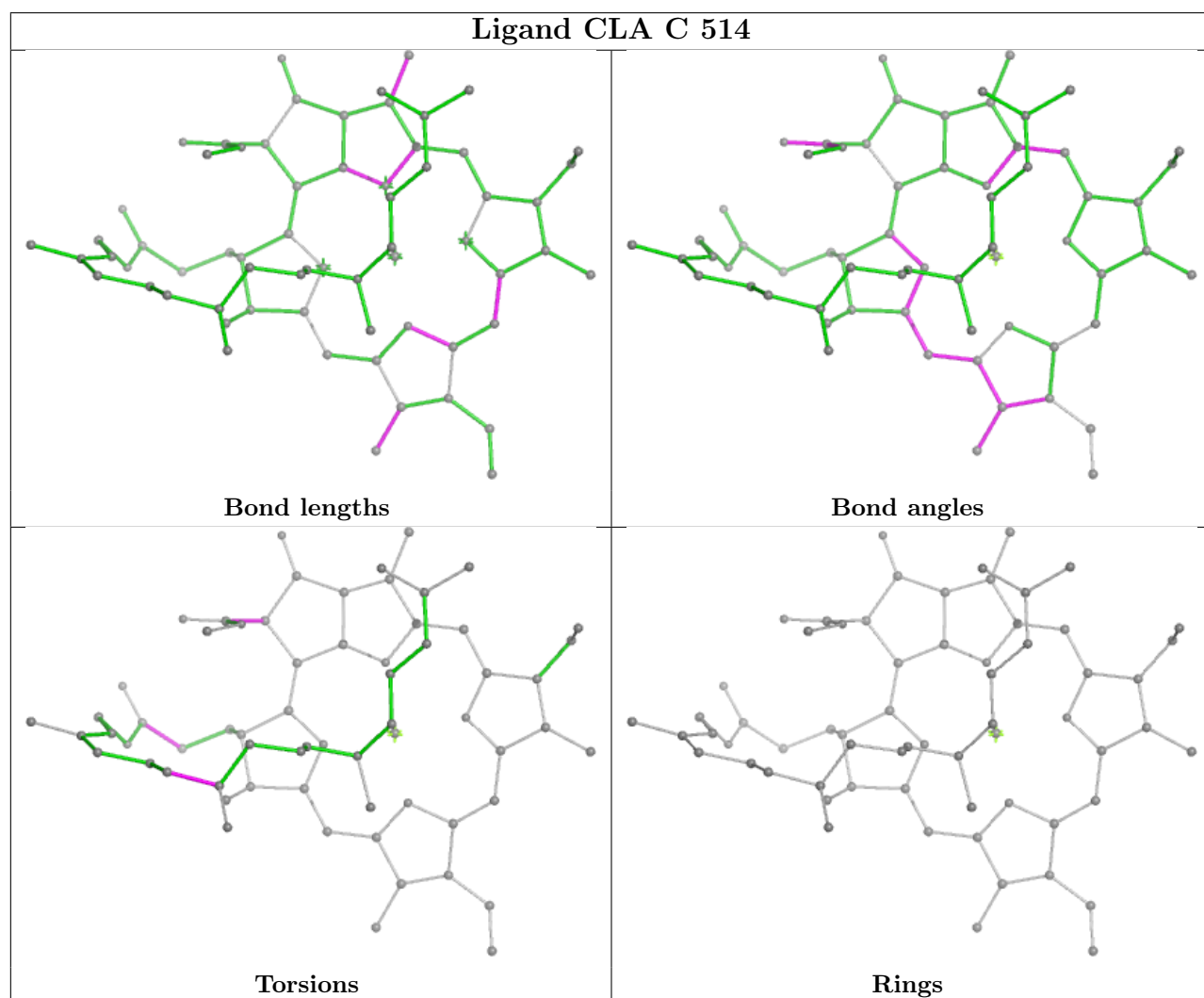
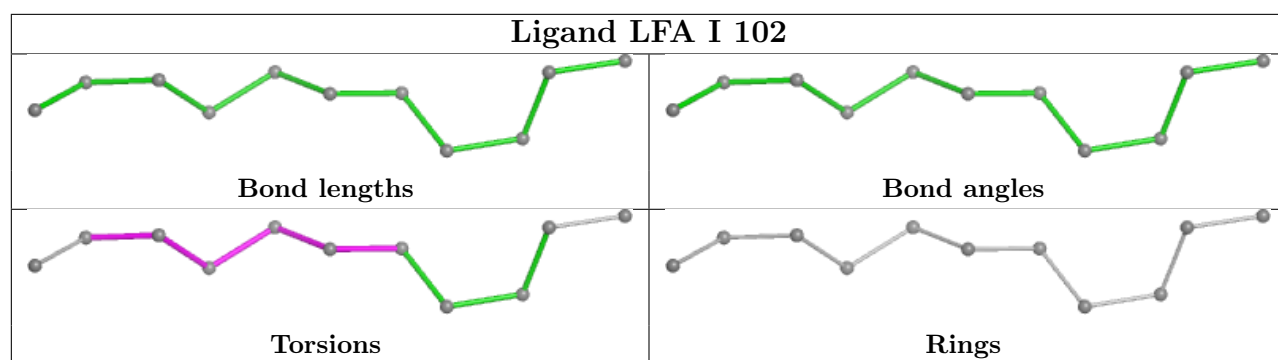
## Ligand BCR F 101





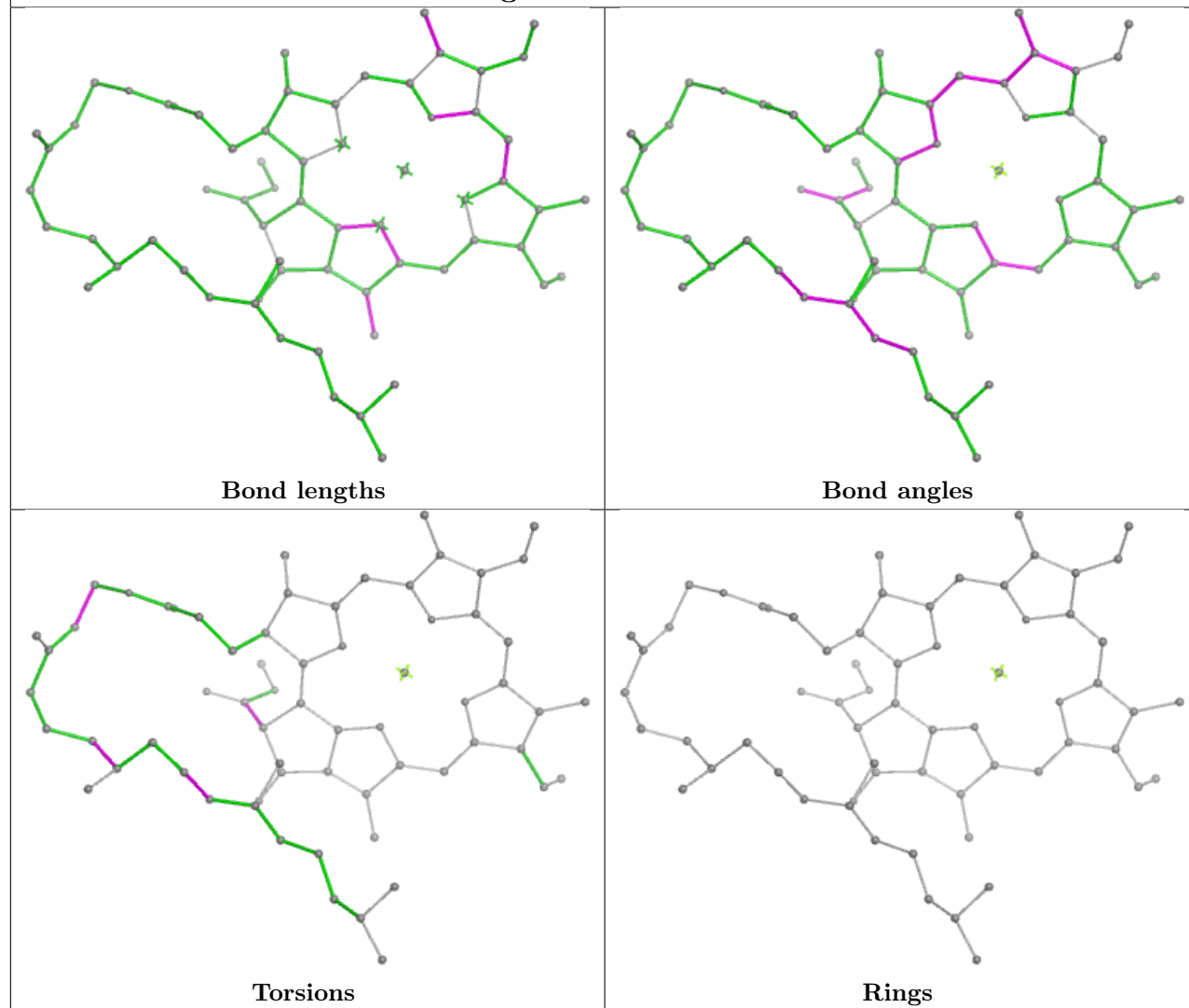




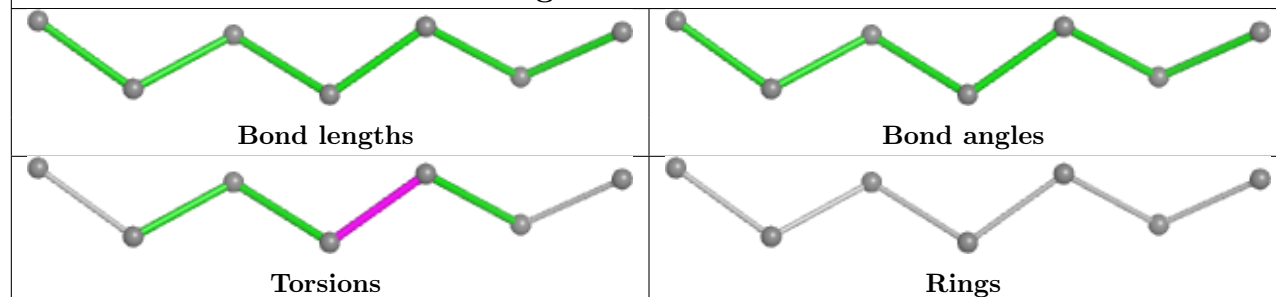


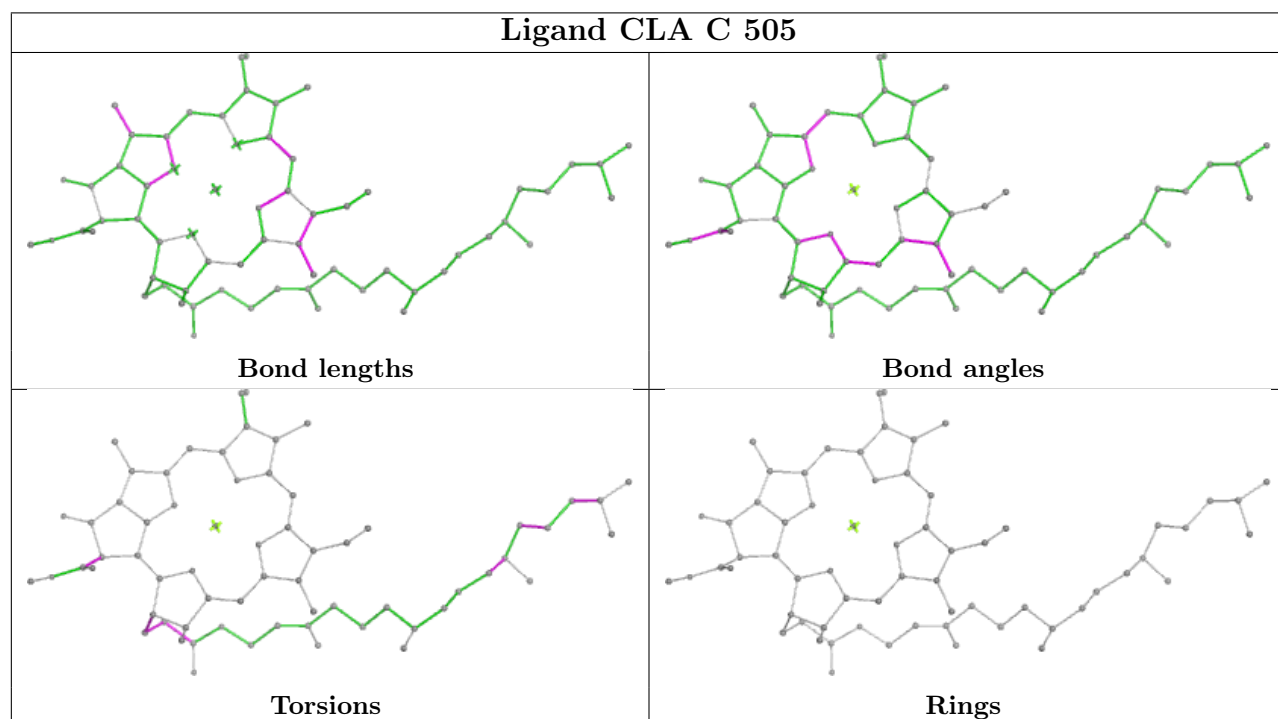
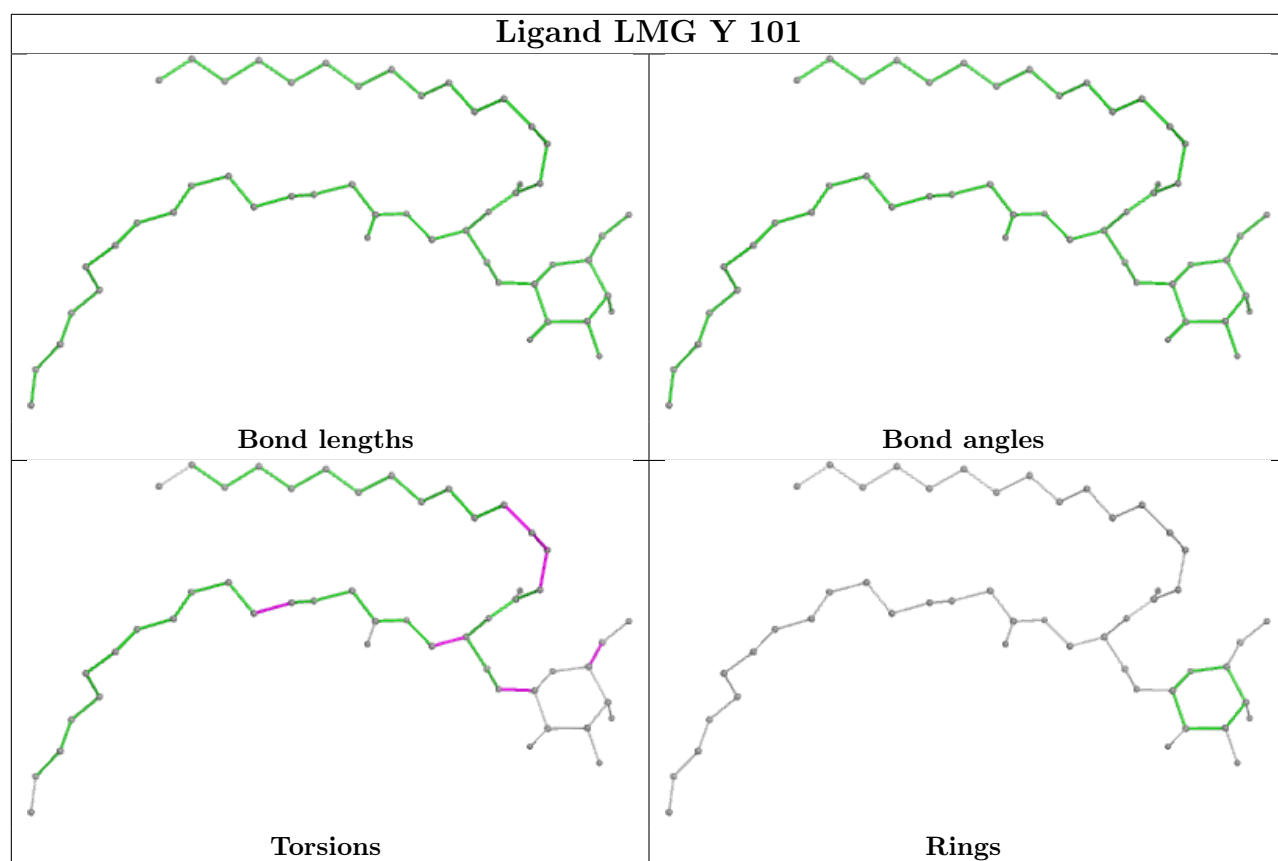


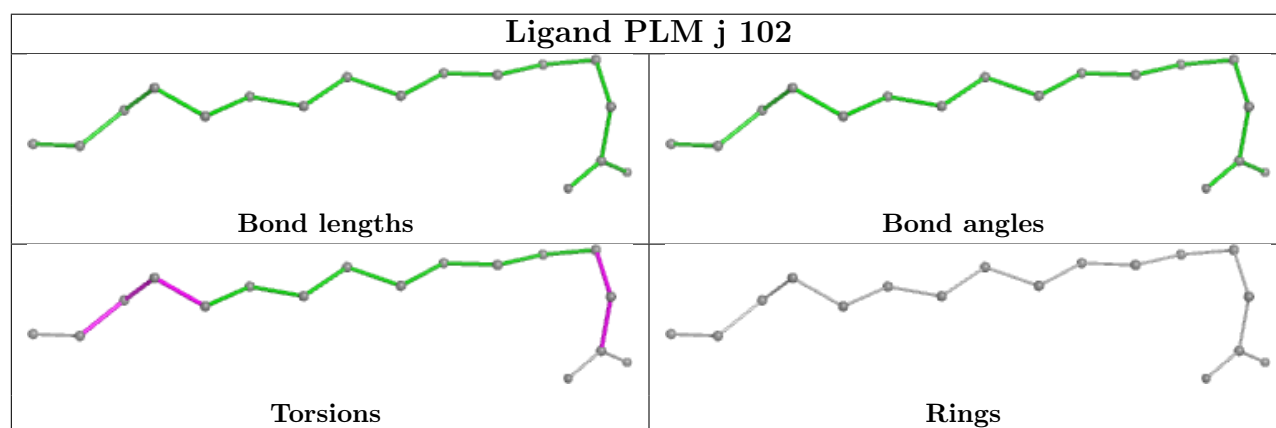
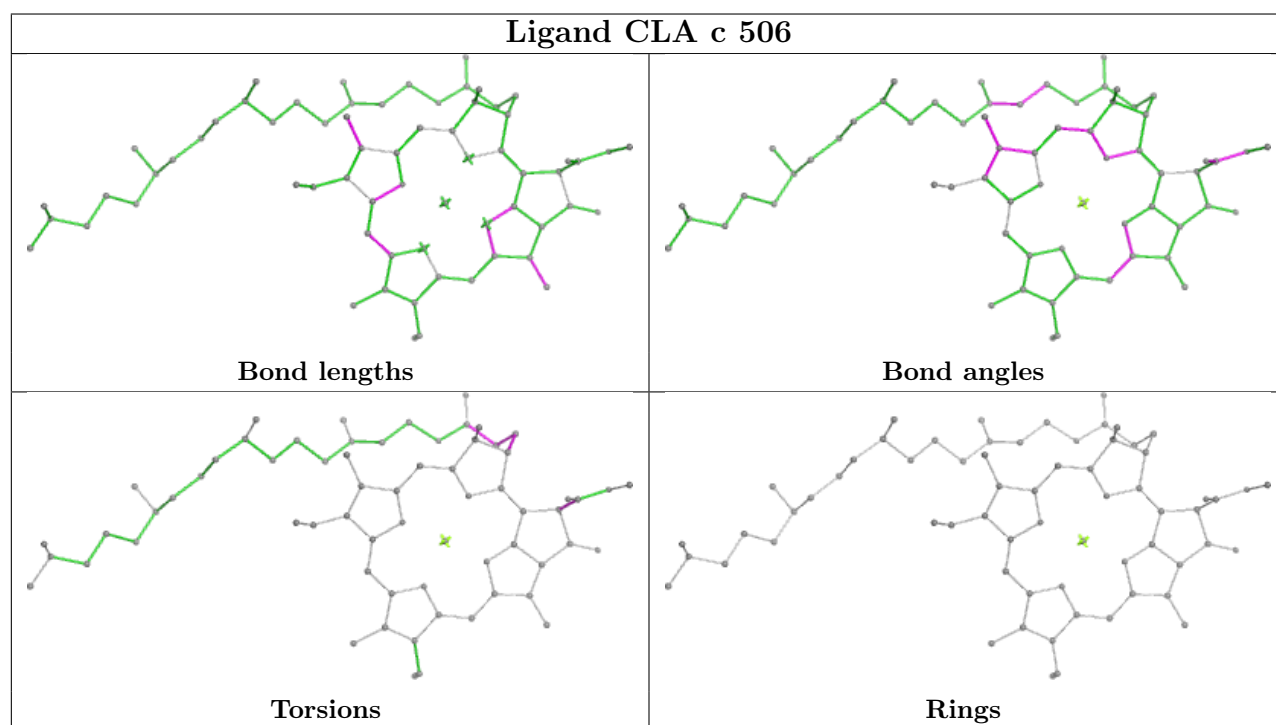
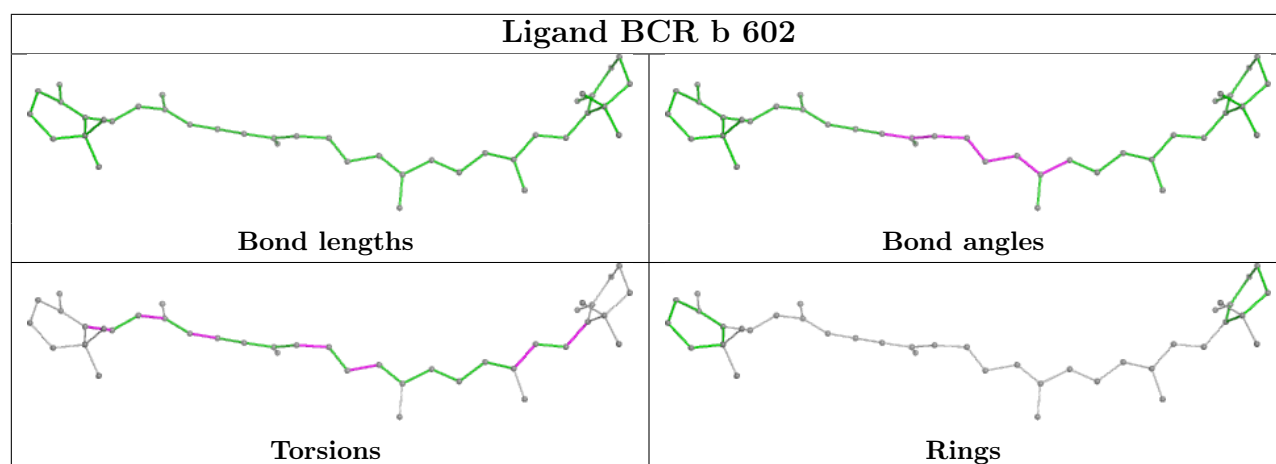
## Ligand CLA c 514

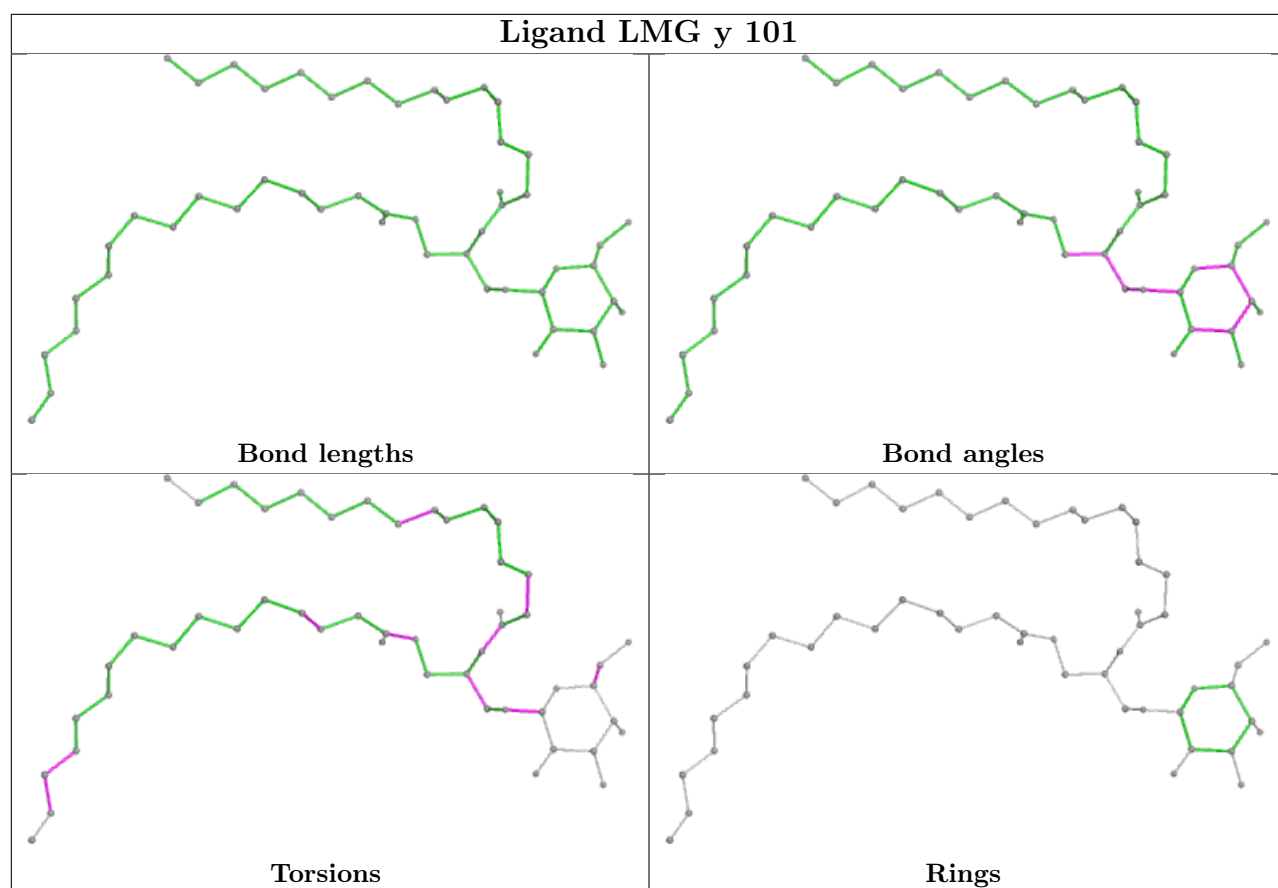


## Ligand LFA B 624

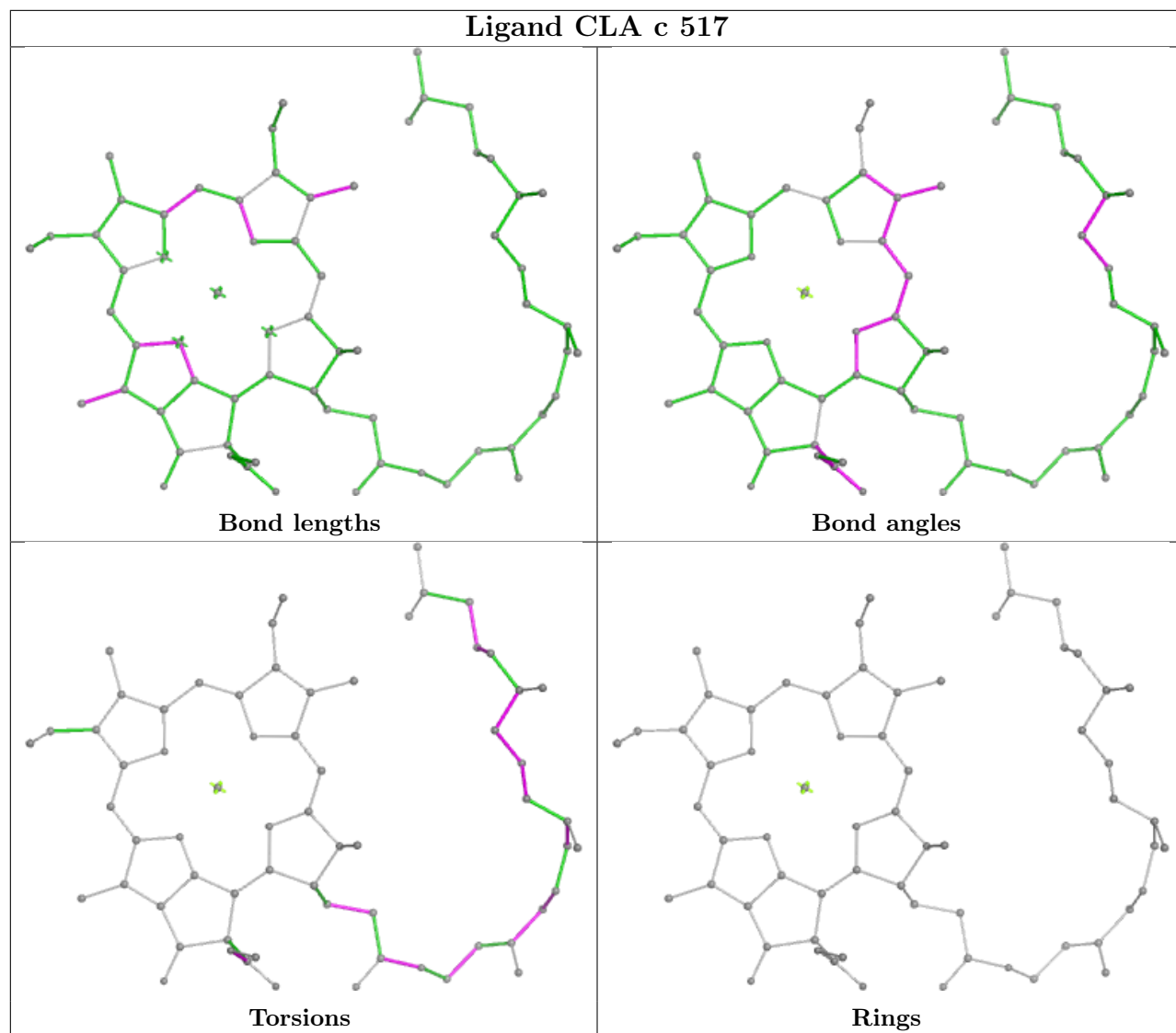




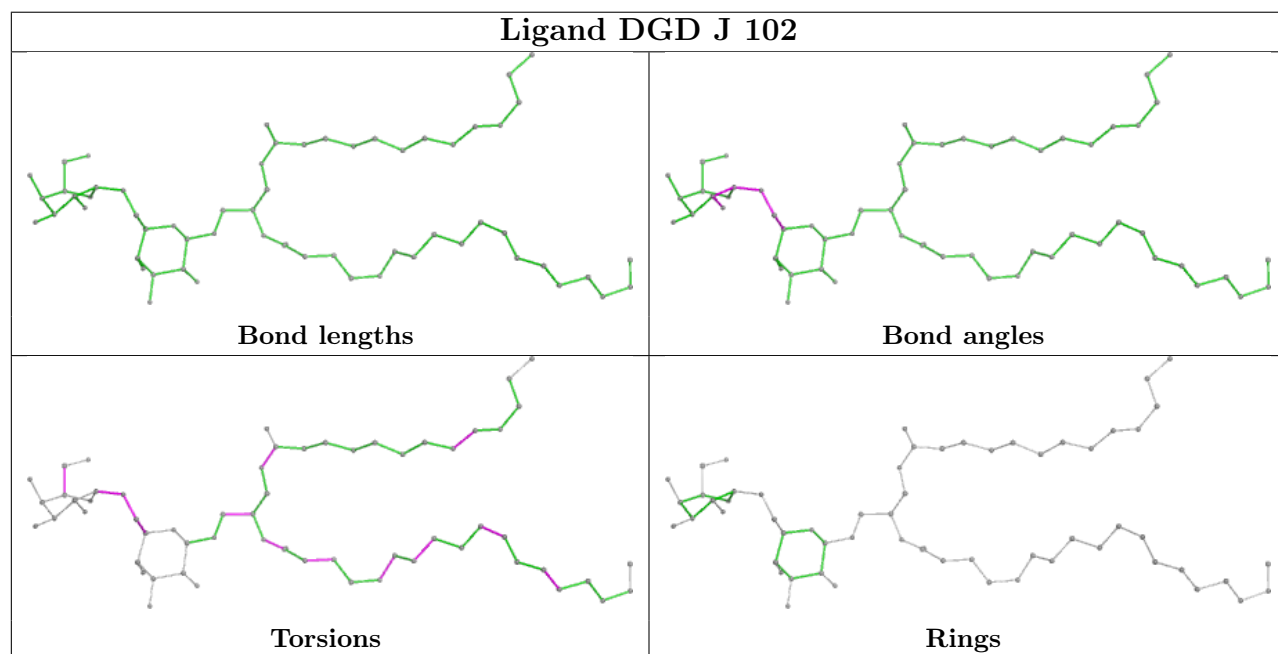




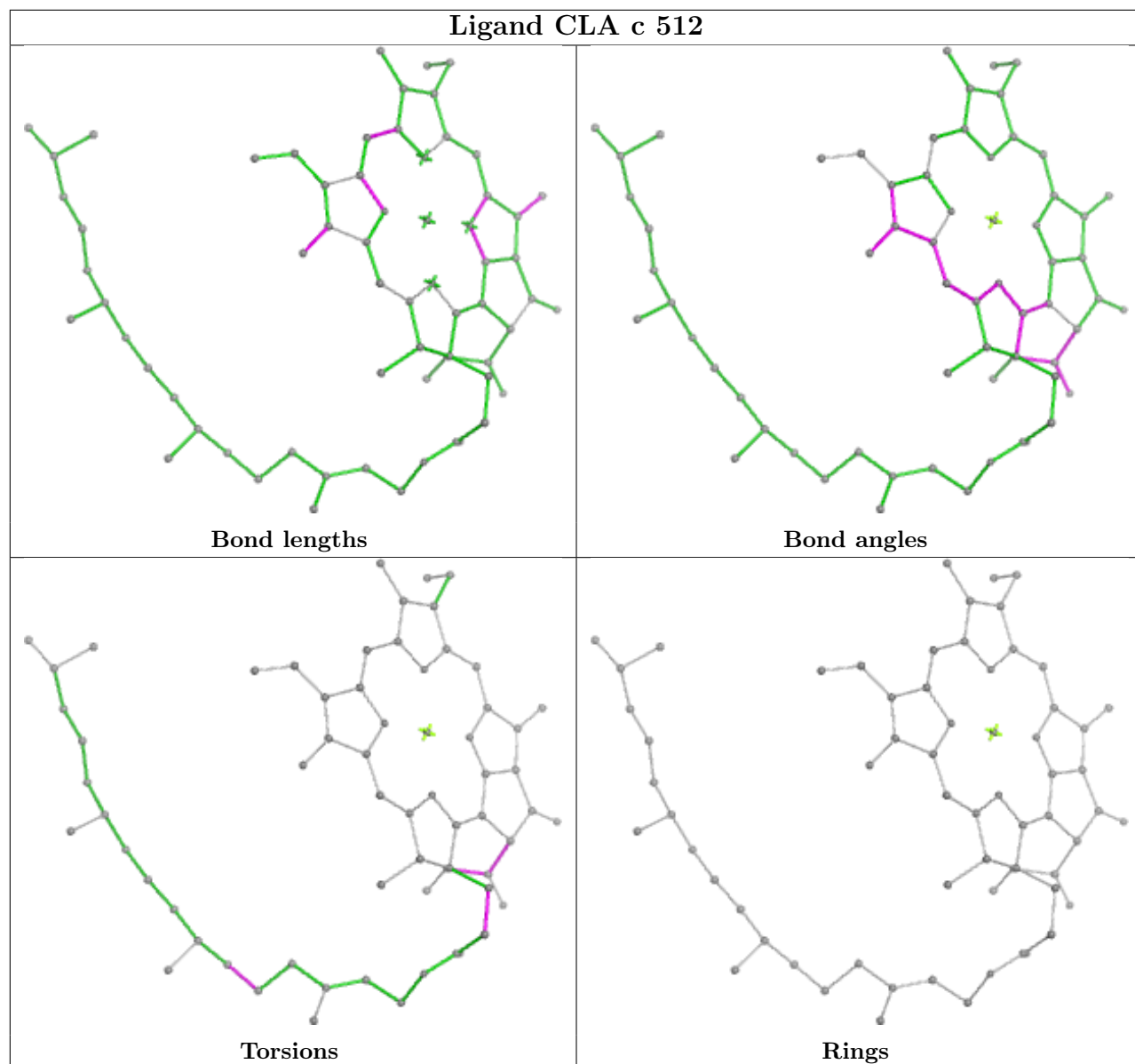
## Ligand CLA c 517

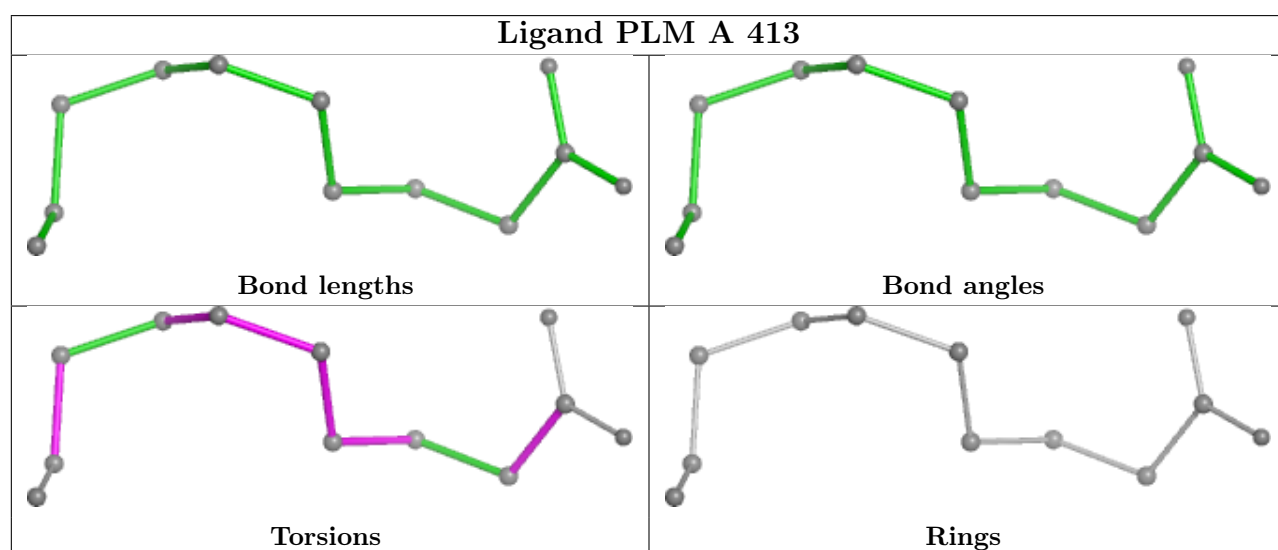
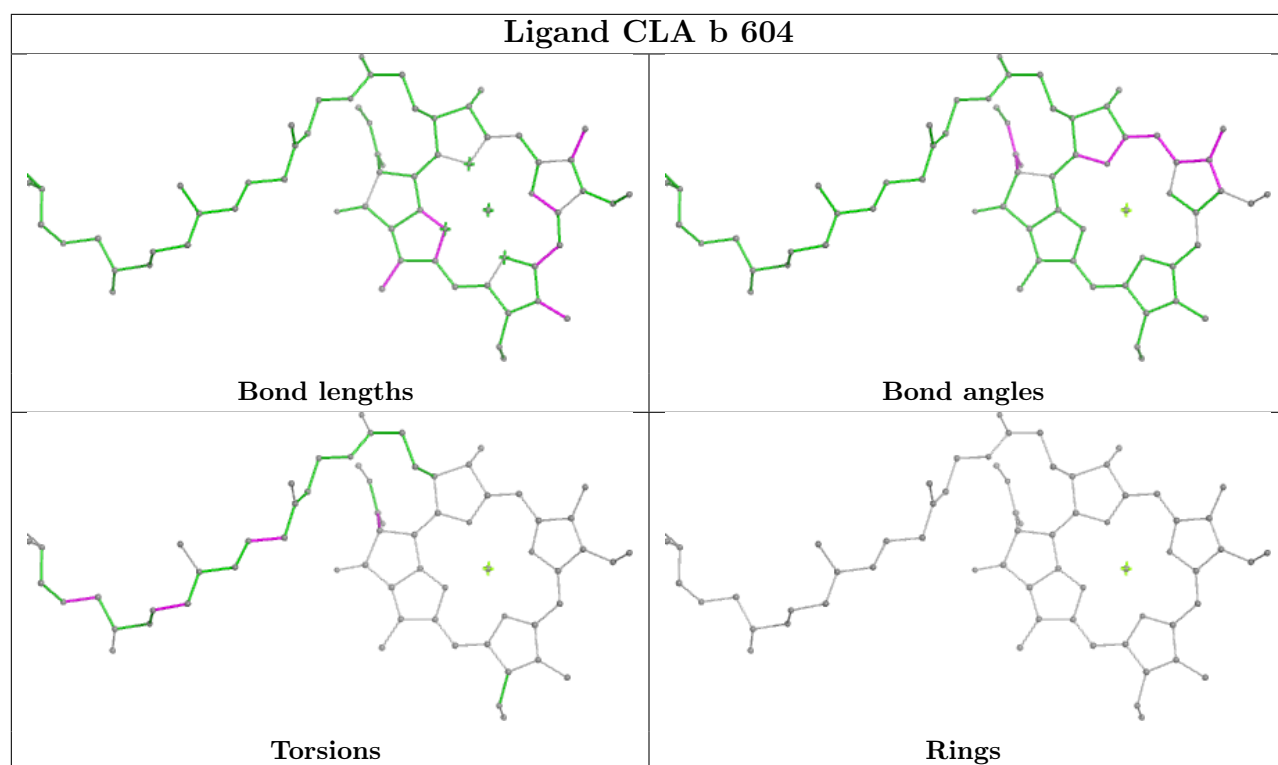


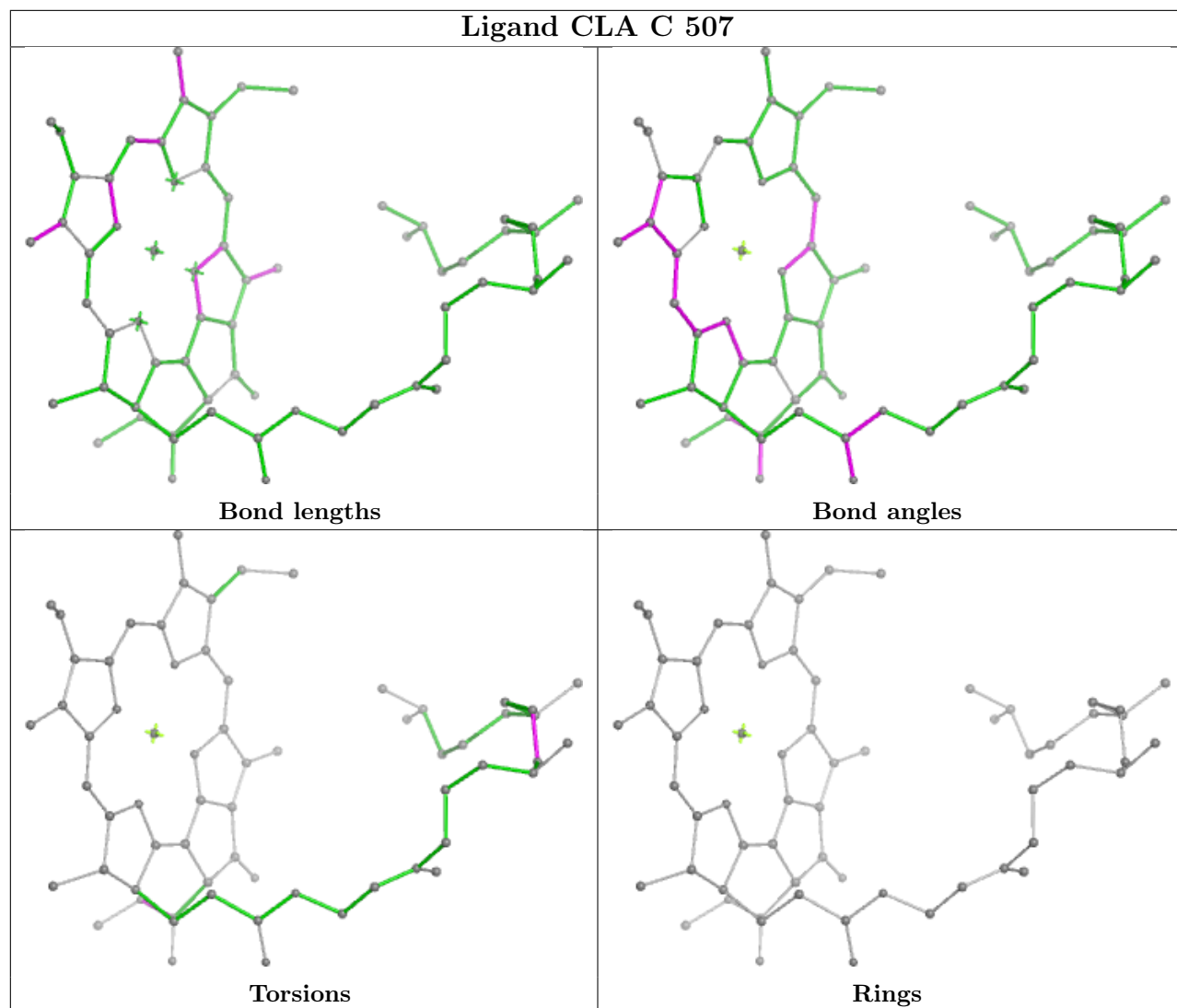
## Ligand DGD J 102



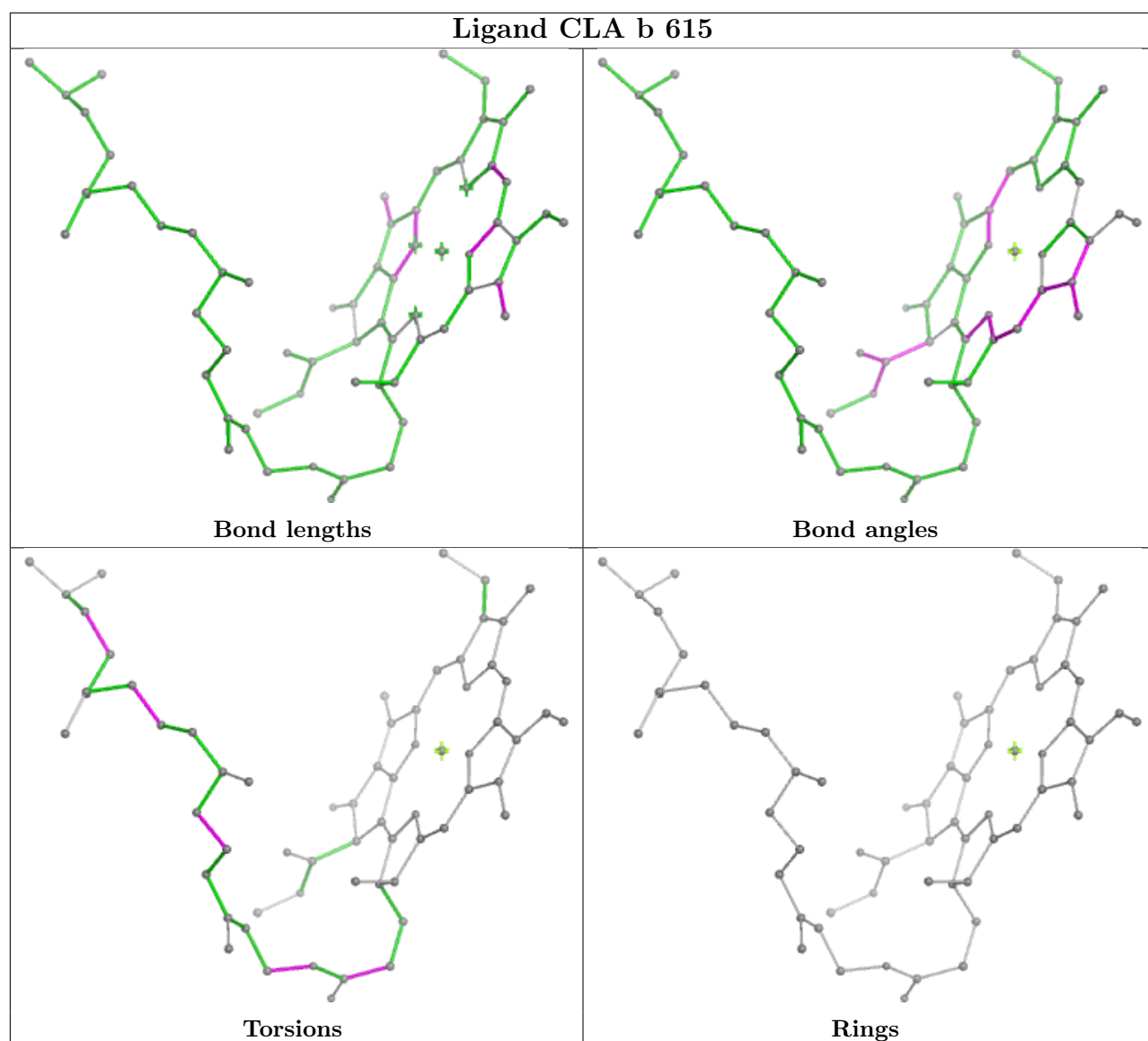
## Ligand CLA c 512

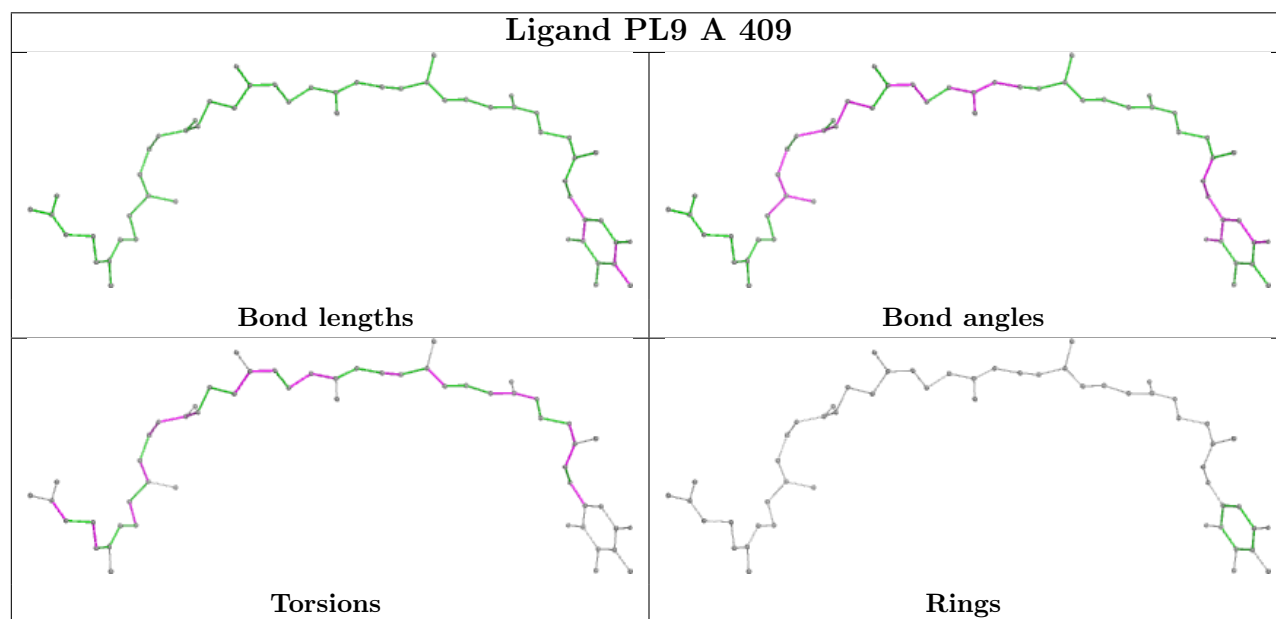
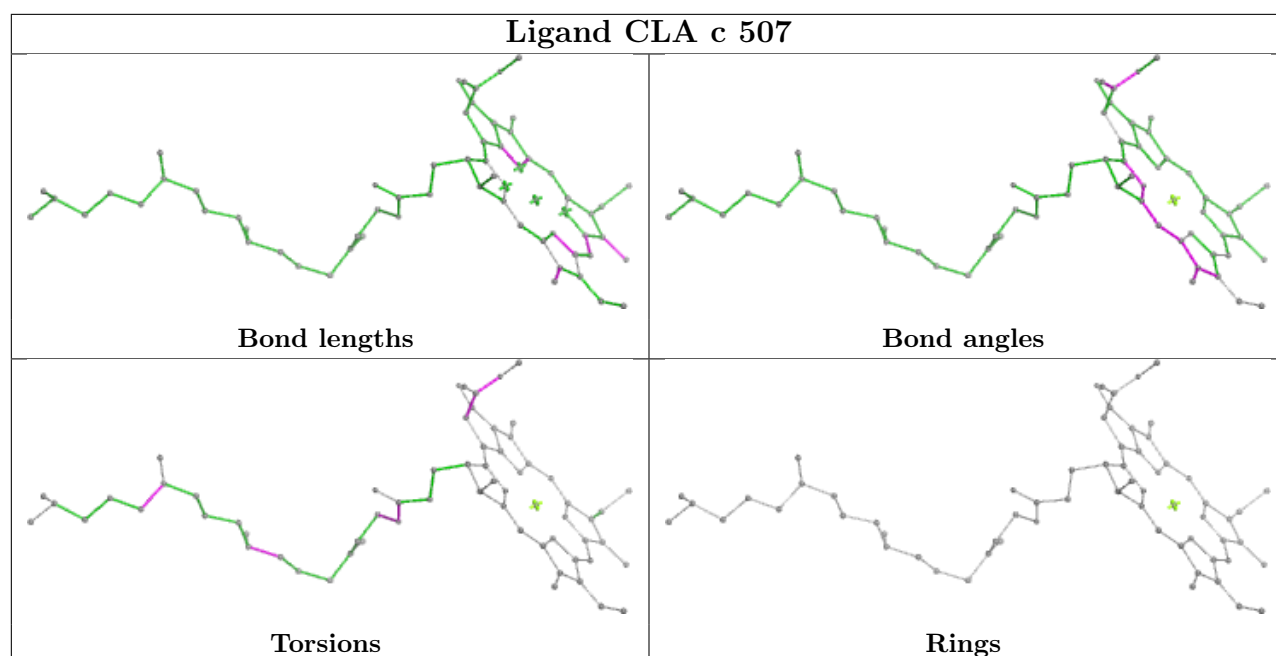


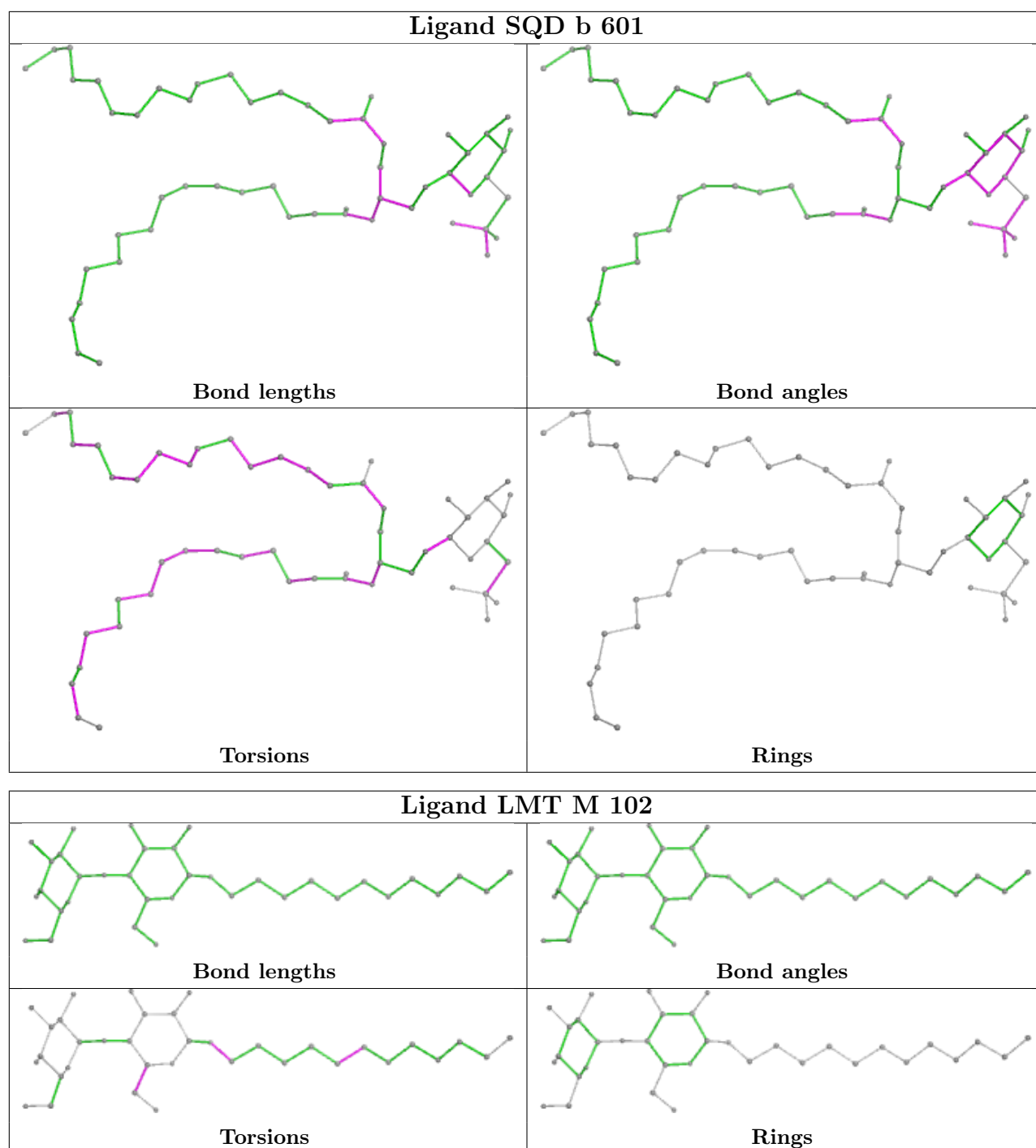


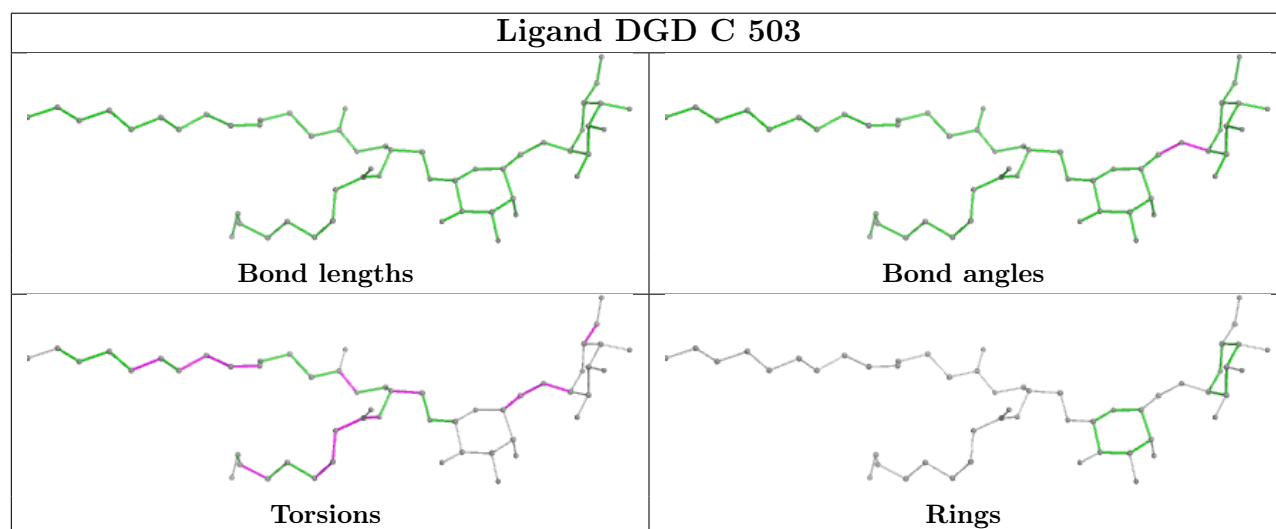
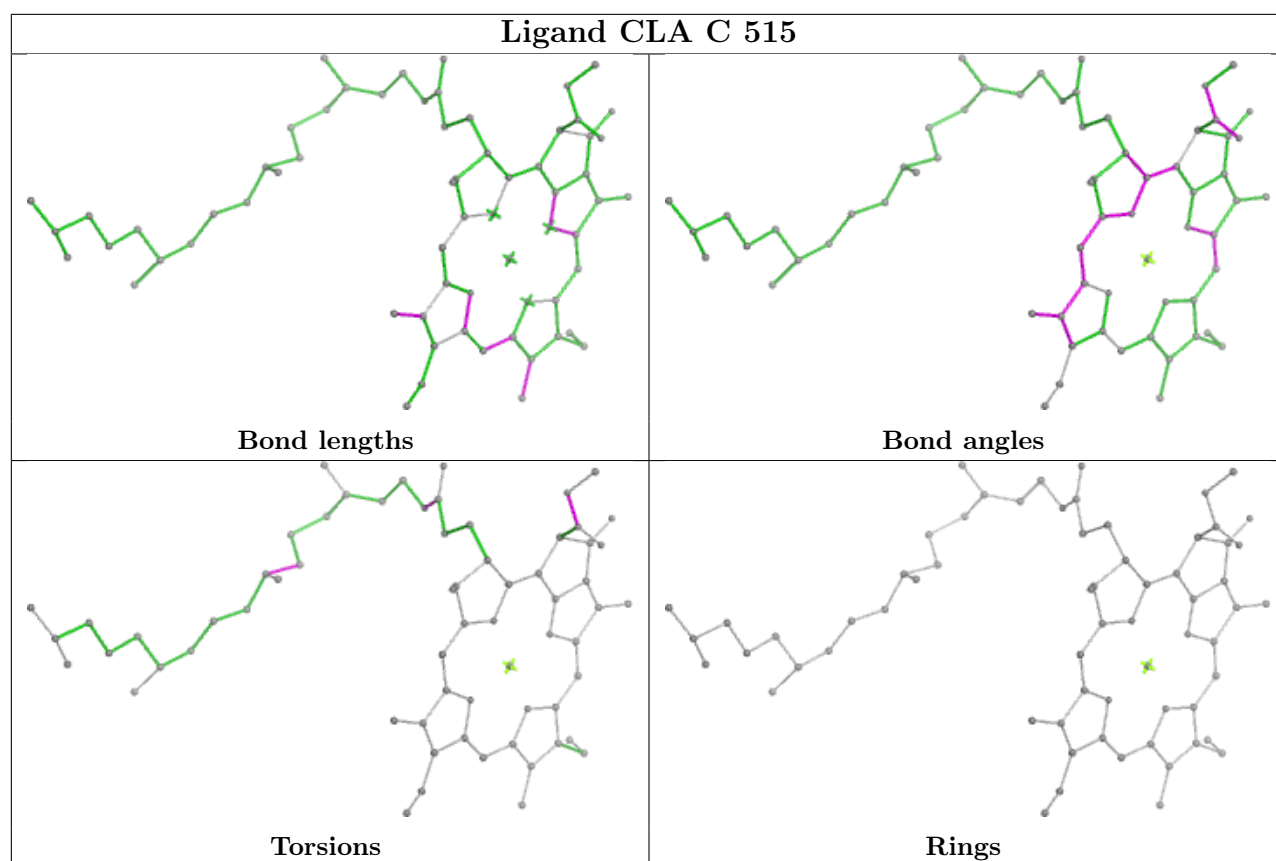


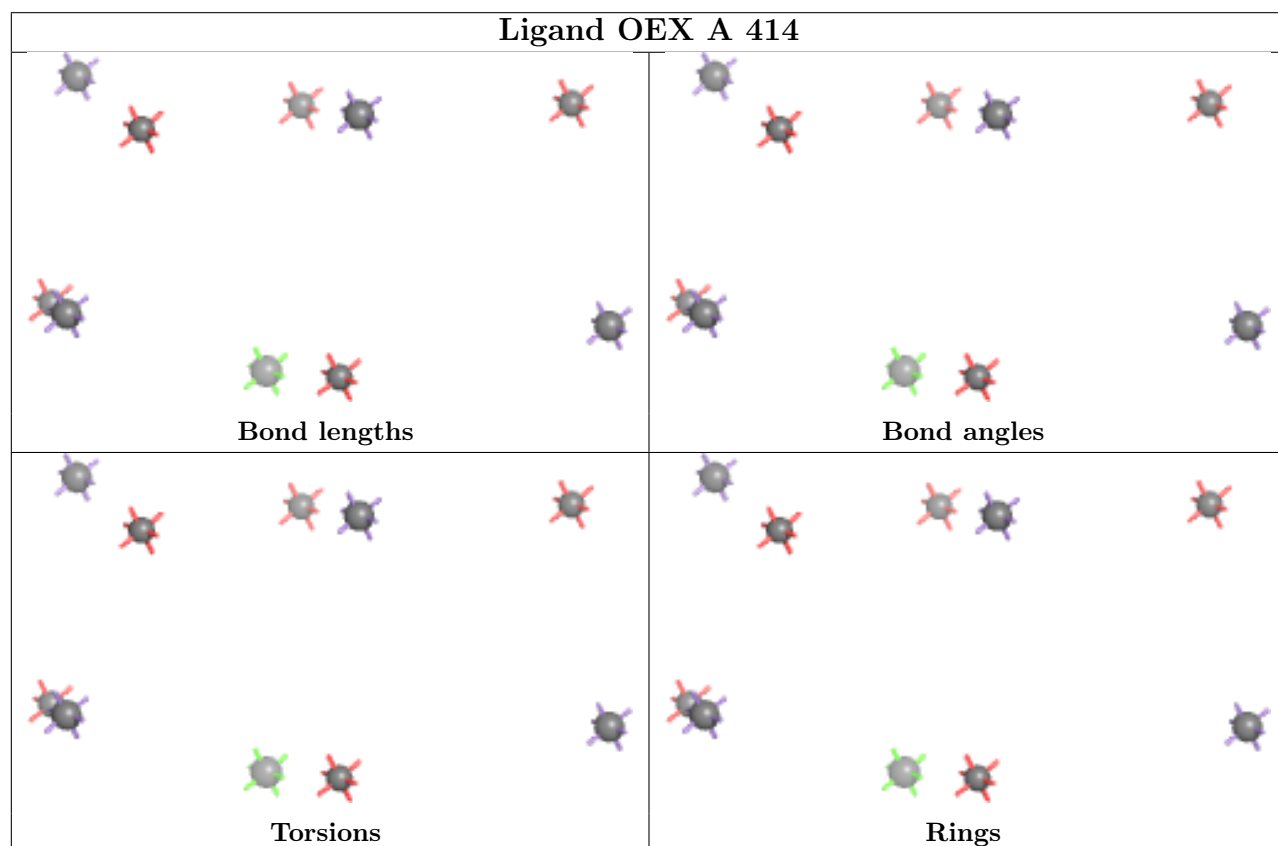
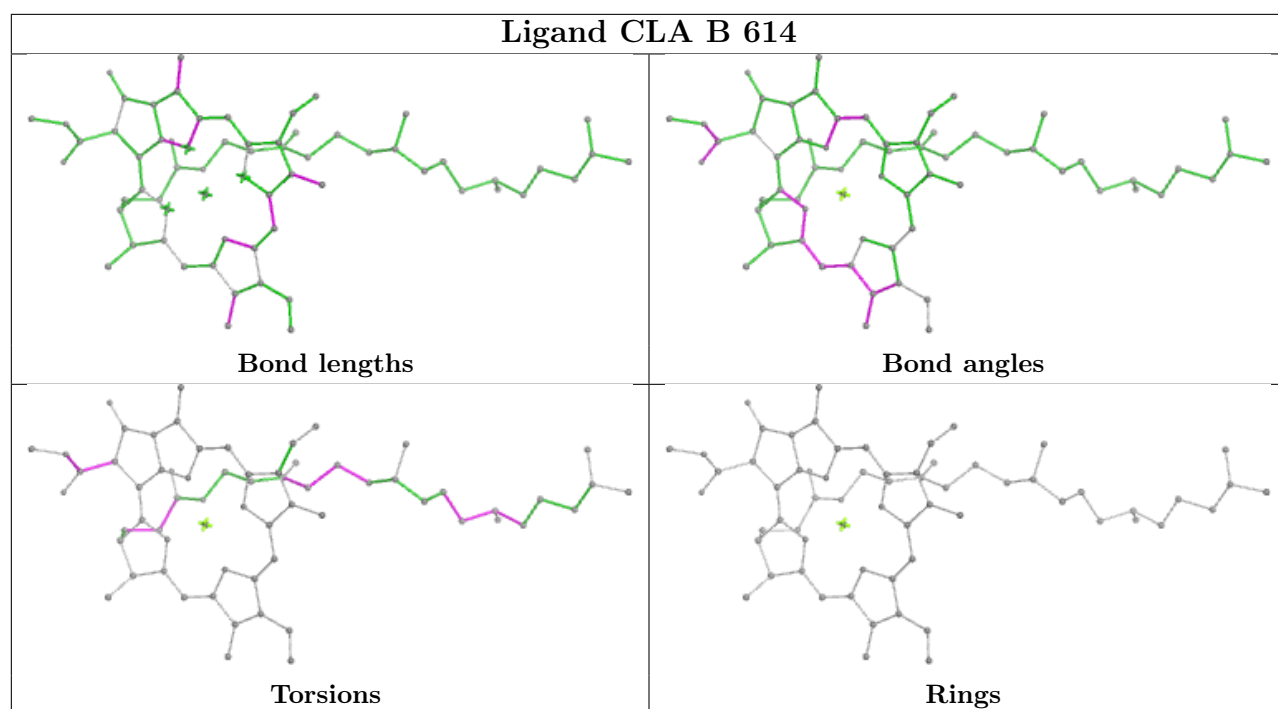


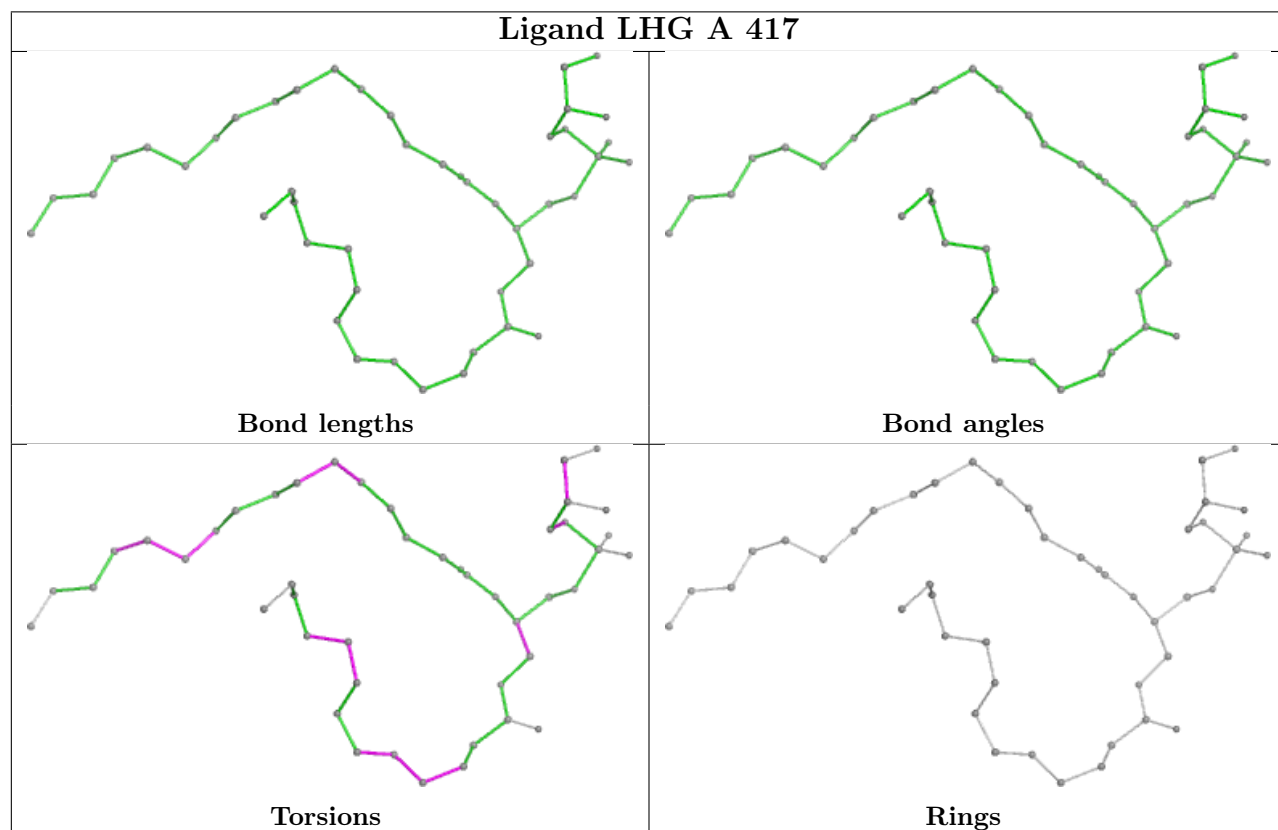
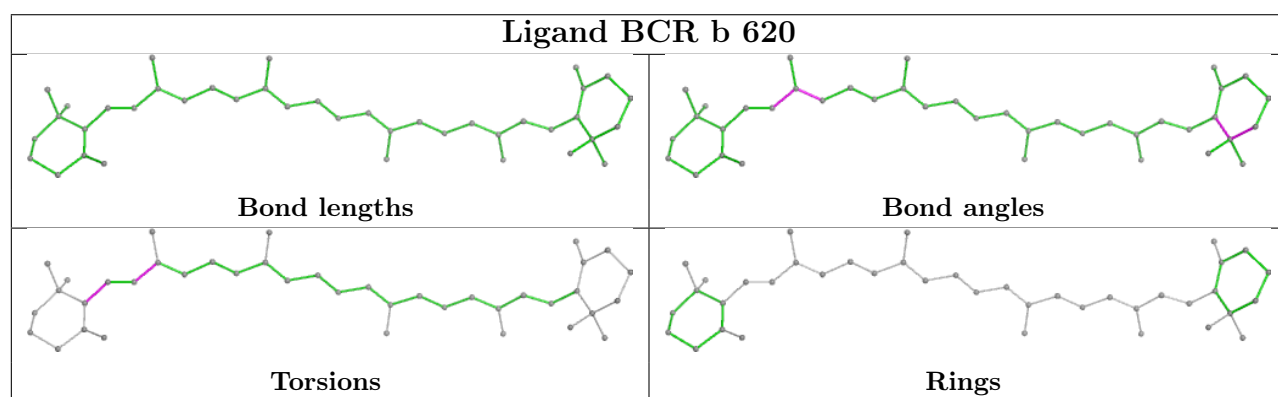
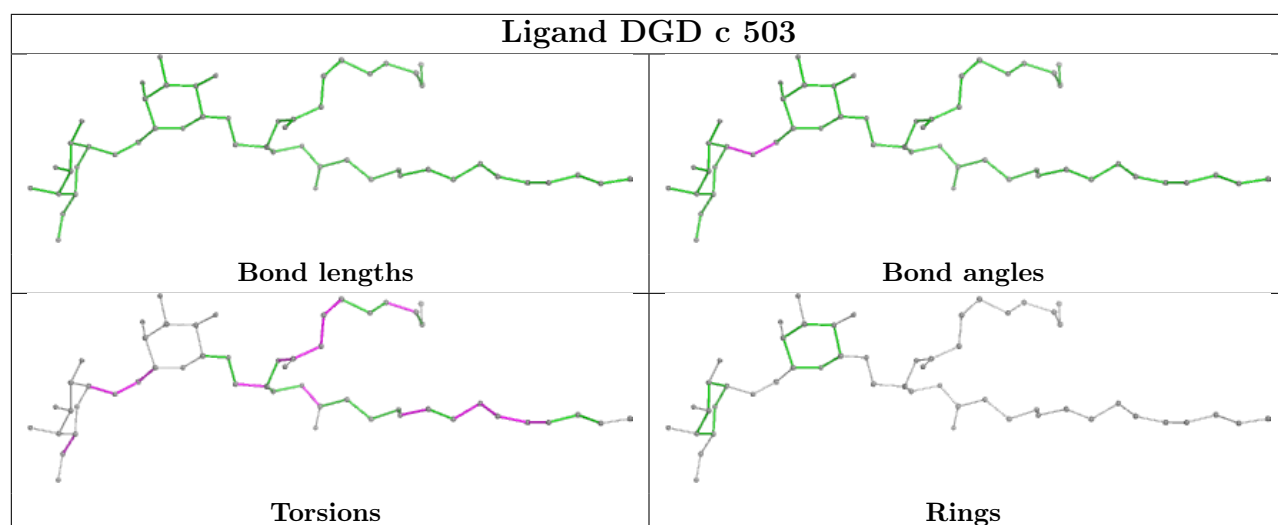












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

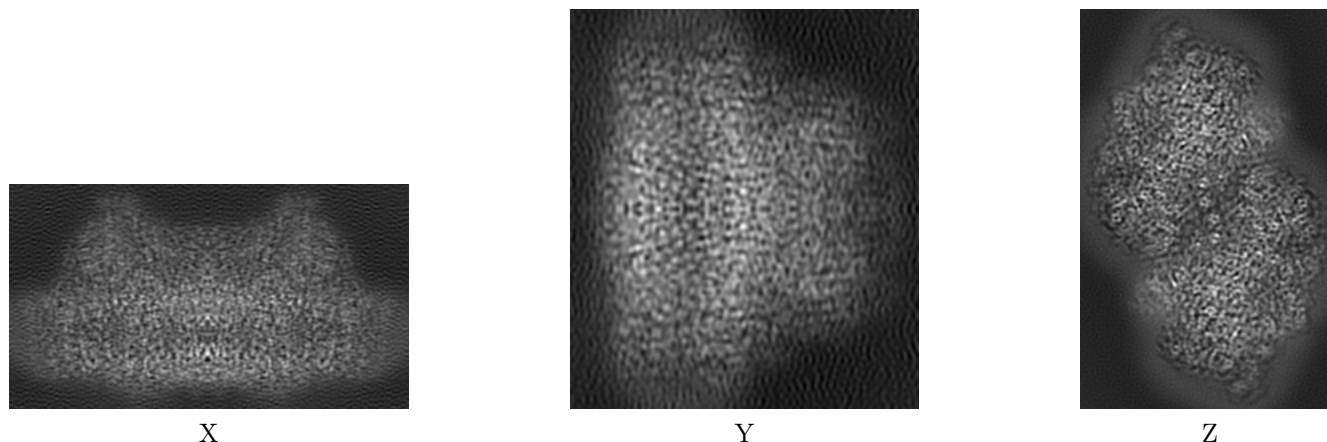
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51102. These allow visual inspection of the internal detail of the map and identification of artifacts.

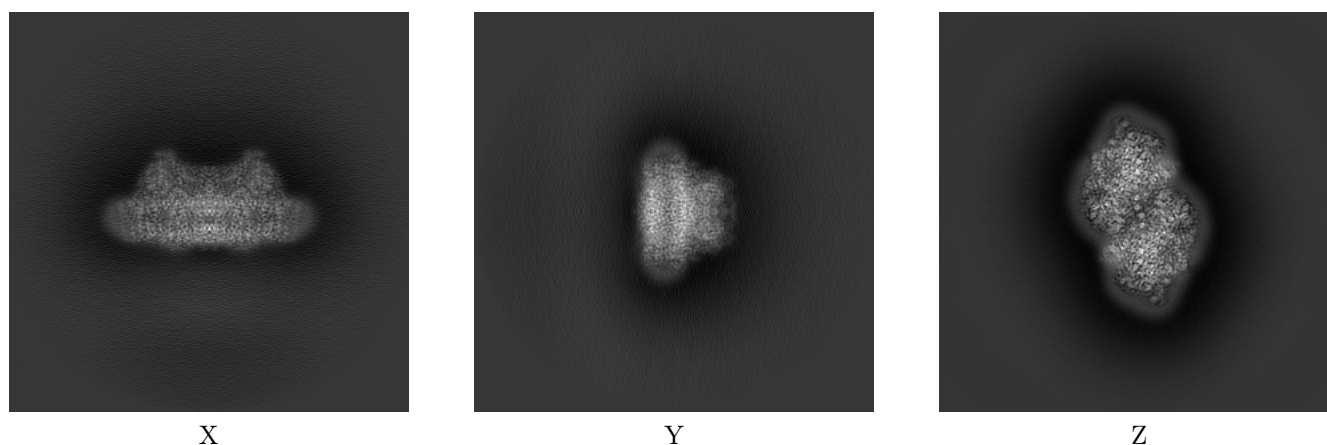
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



#### 6.1.2 Raw map

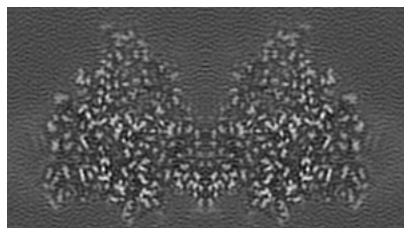


The images above show the map projected in three orthogonal directions.

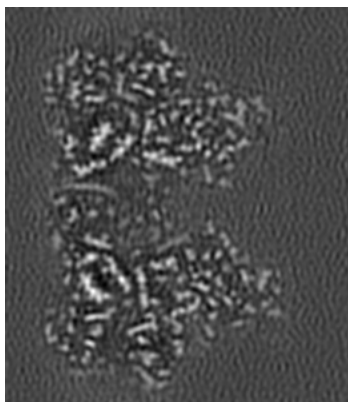


## 6.2 Central slices [i](#)

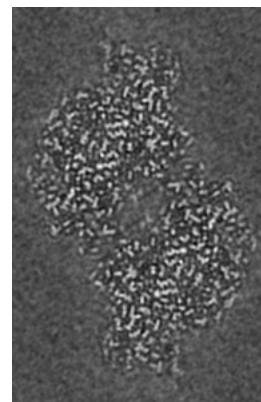
### 6.2.1 Primary map



X Index: 135

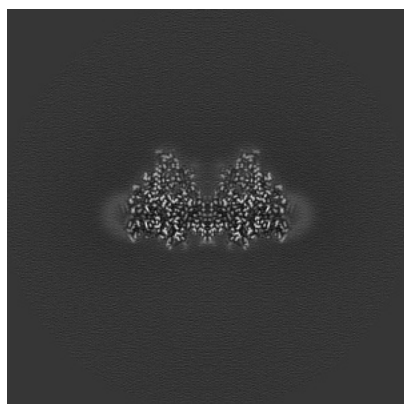


Y Index: 210

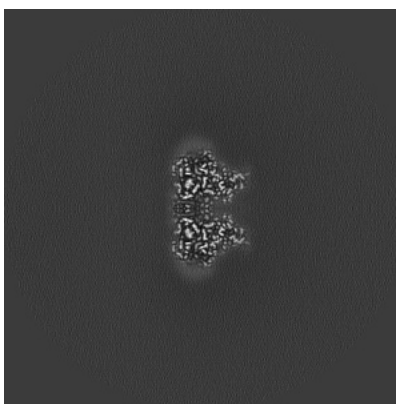


Z Index: 118

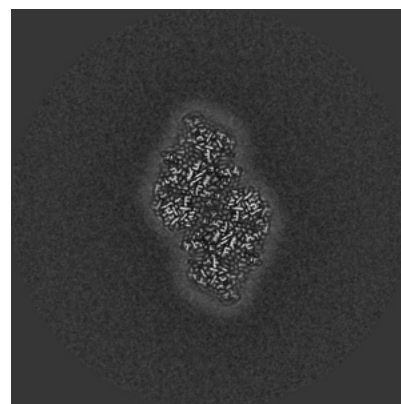
### 6.2.2 Raw map



X Index: 200



Y Index: 200

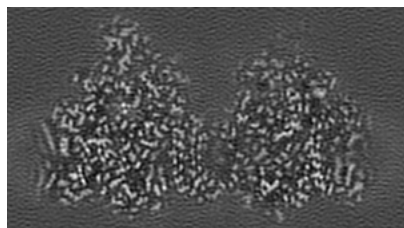


Z Index: 200

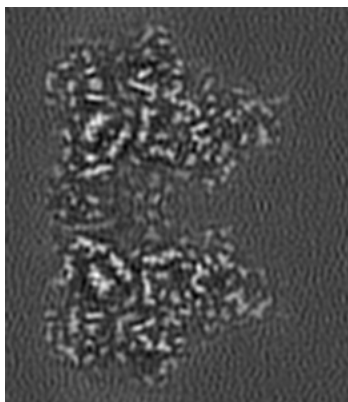
The images above show central slices of the map in three orthogonal directions.

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

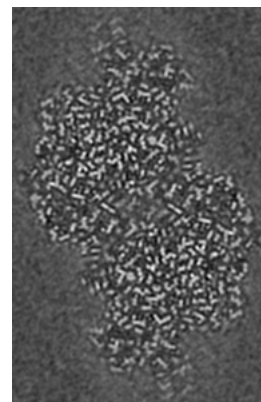
### 6.3.1 Primary map



X Index: 141

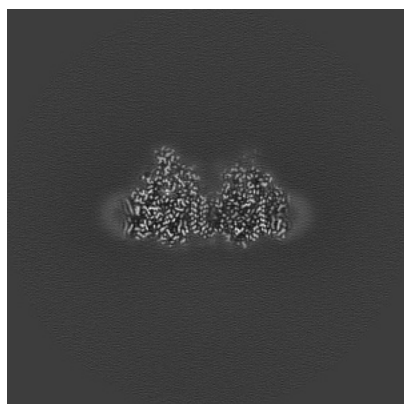


Y Index: 207

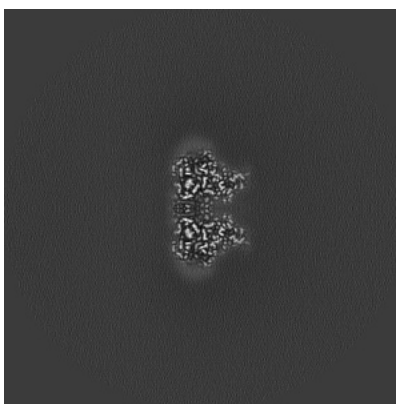


Z Index: 110

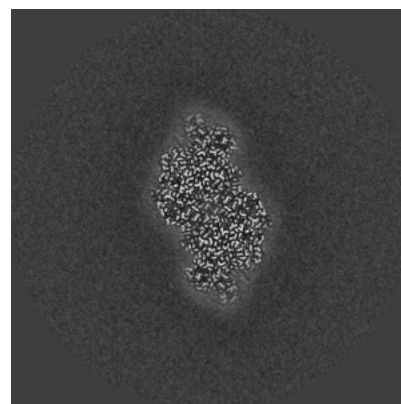
### 6.3.2 Raw map



X Index: 203



Y Index: 200

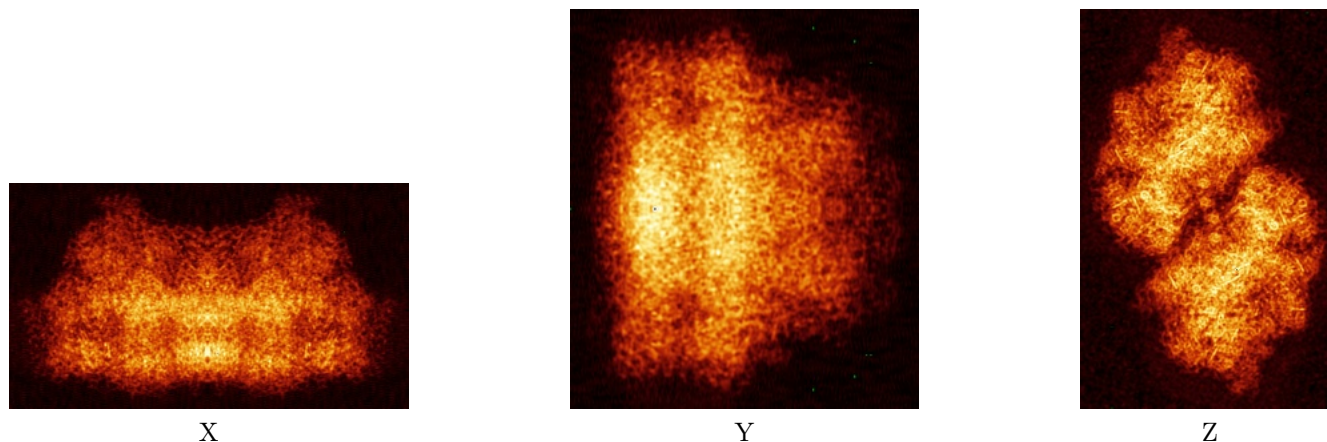


Z Index: 207

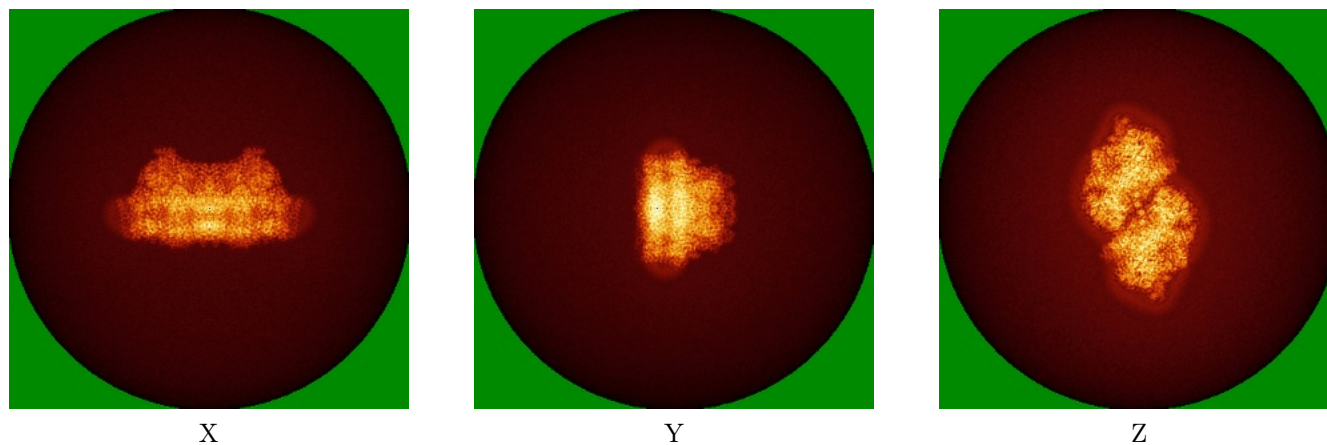
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



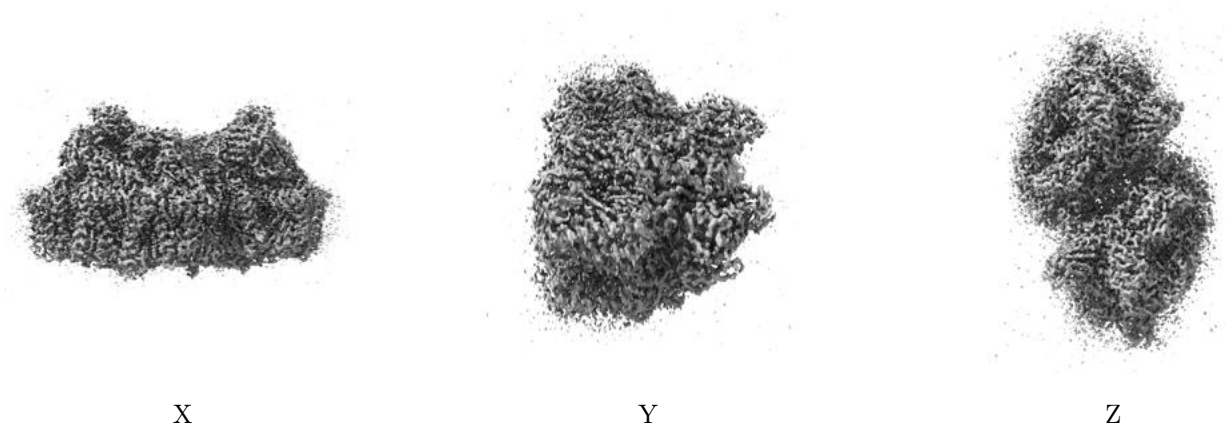
### 6.4.2 Raw map



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.

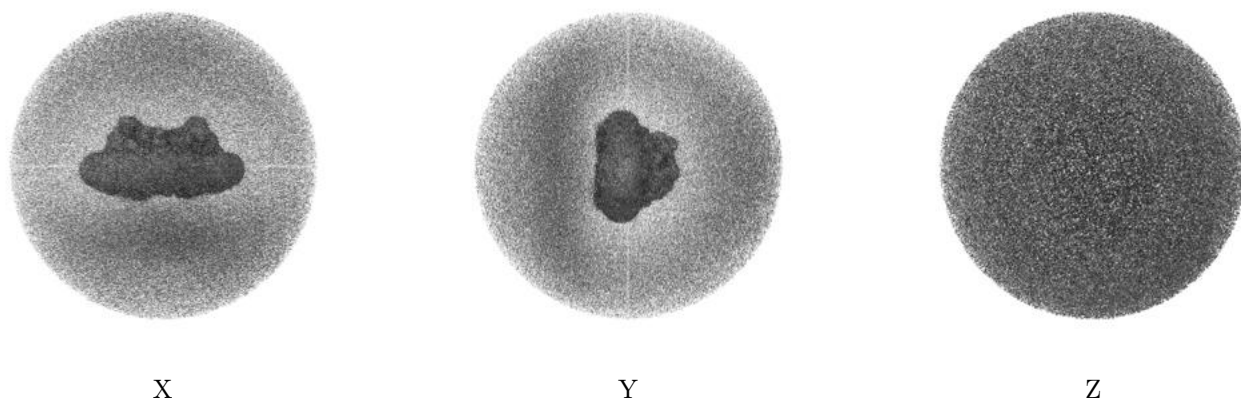
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.043. 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.

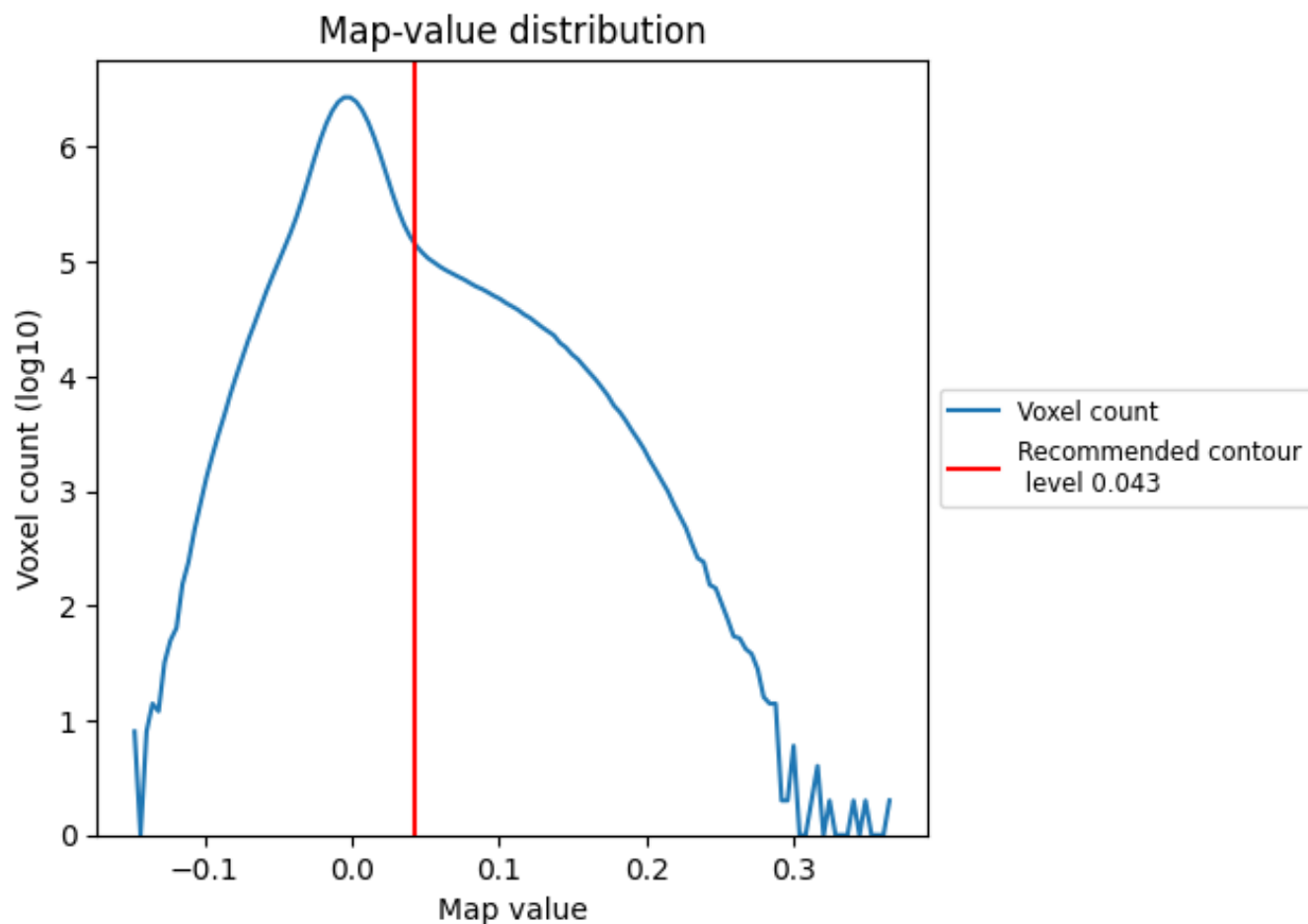
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

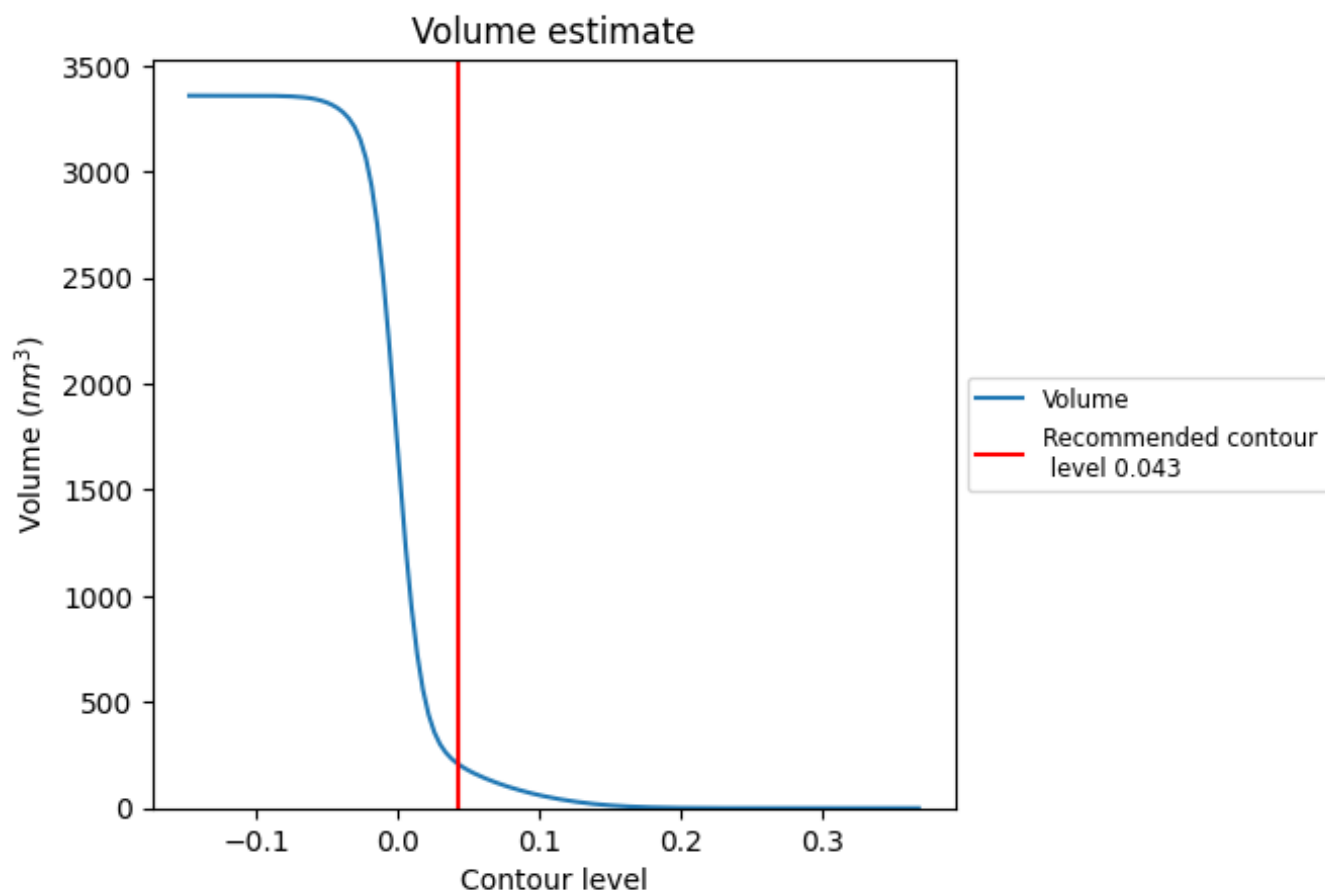
This section contains the results of statistical analysis of the map.

### 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 208 nm<sup>3</sup>; this corresponds to an approximate mass of 188 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](#)

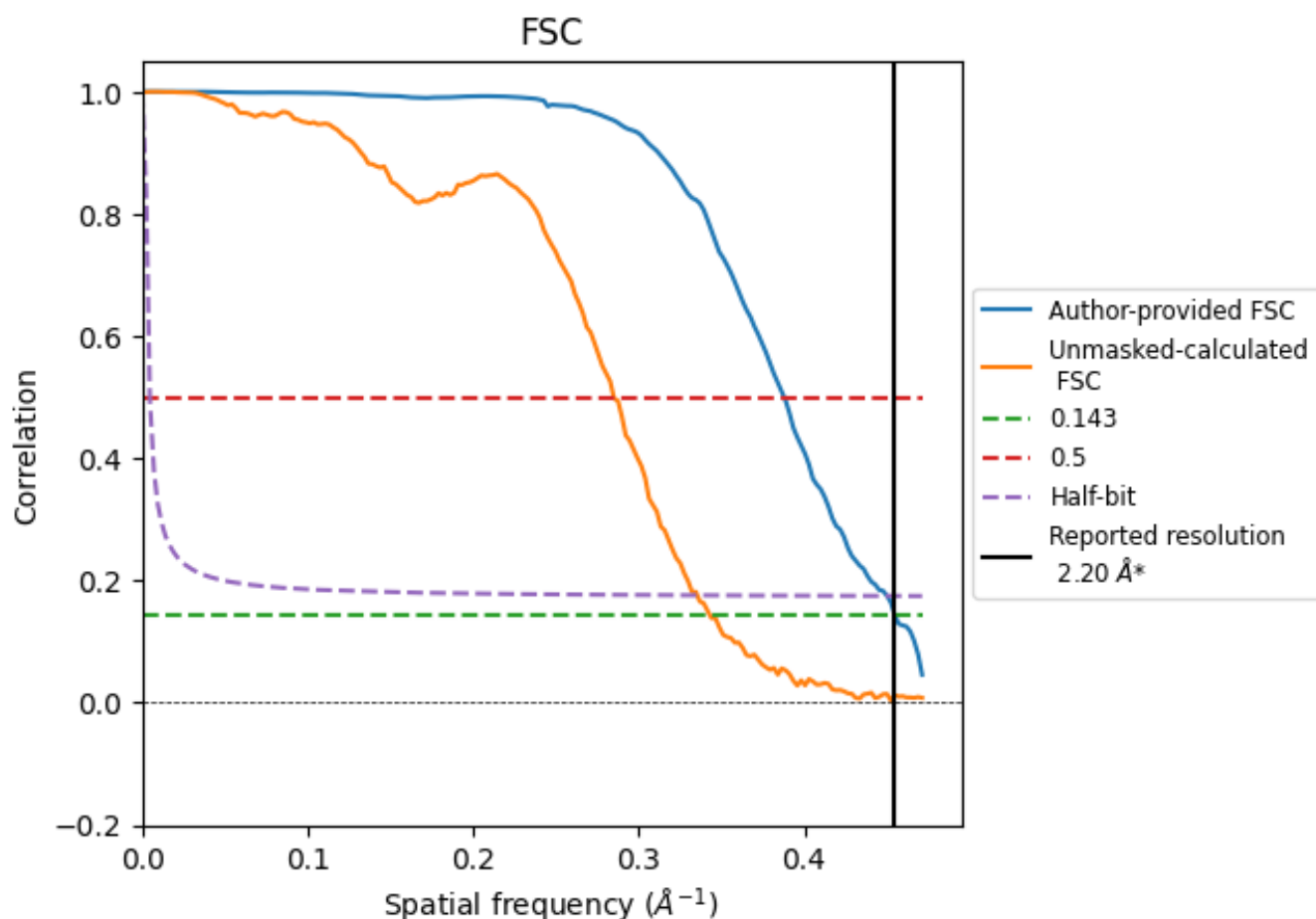
This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.



## 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 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.20	2.58	2.22
Unmasked-calculated*	2.91	3.51	2.98

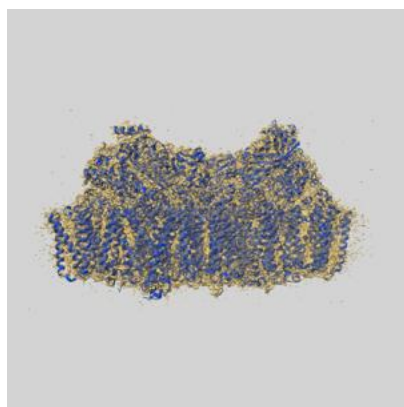
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.91 differs from the reported value 2.2 by more than 10 %



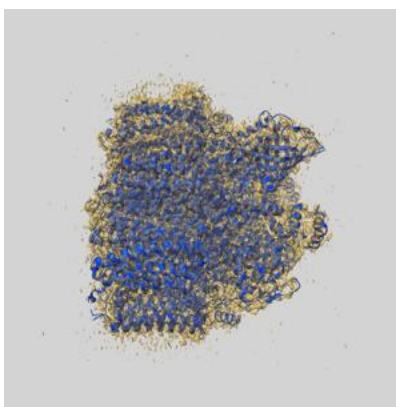
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51102 and PDB model 9G6H. Per-residue inclusion information can be found in section 3 on page 31.

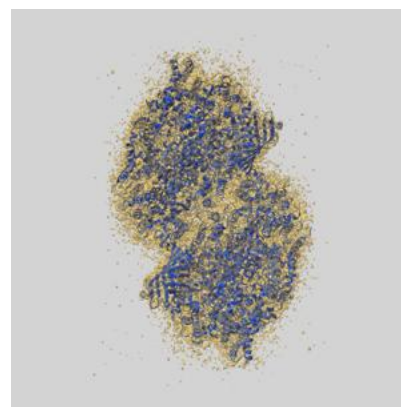
### 9.1 Map-model overlay [i](#)



X



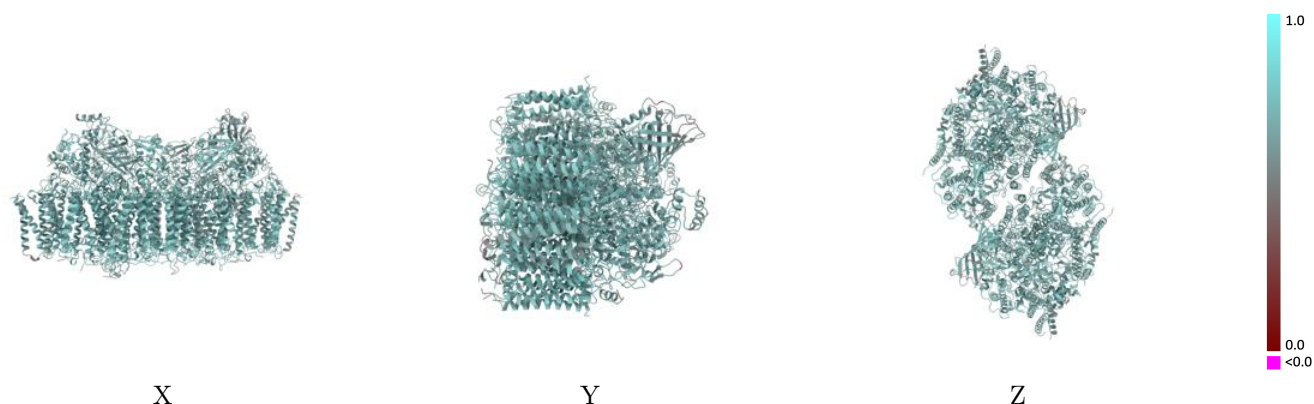
Y



Z

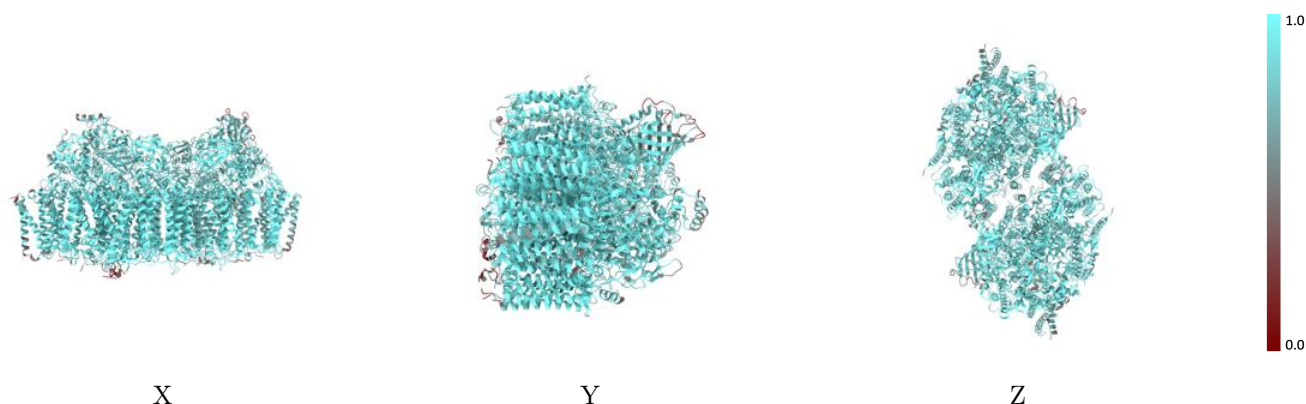
The images above show the 3D surface view of the map at the recommended contour level 0.043 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



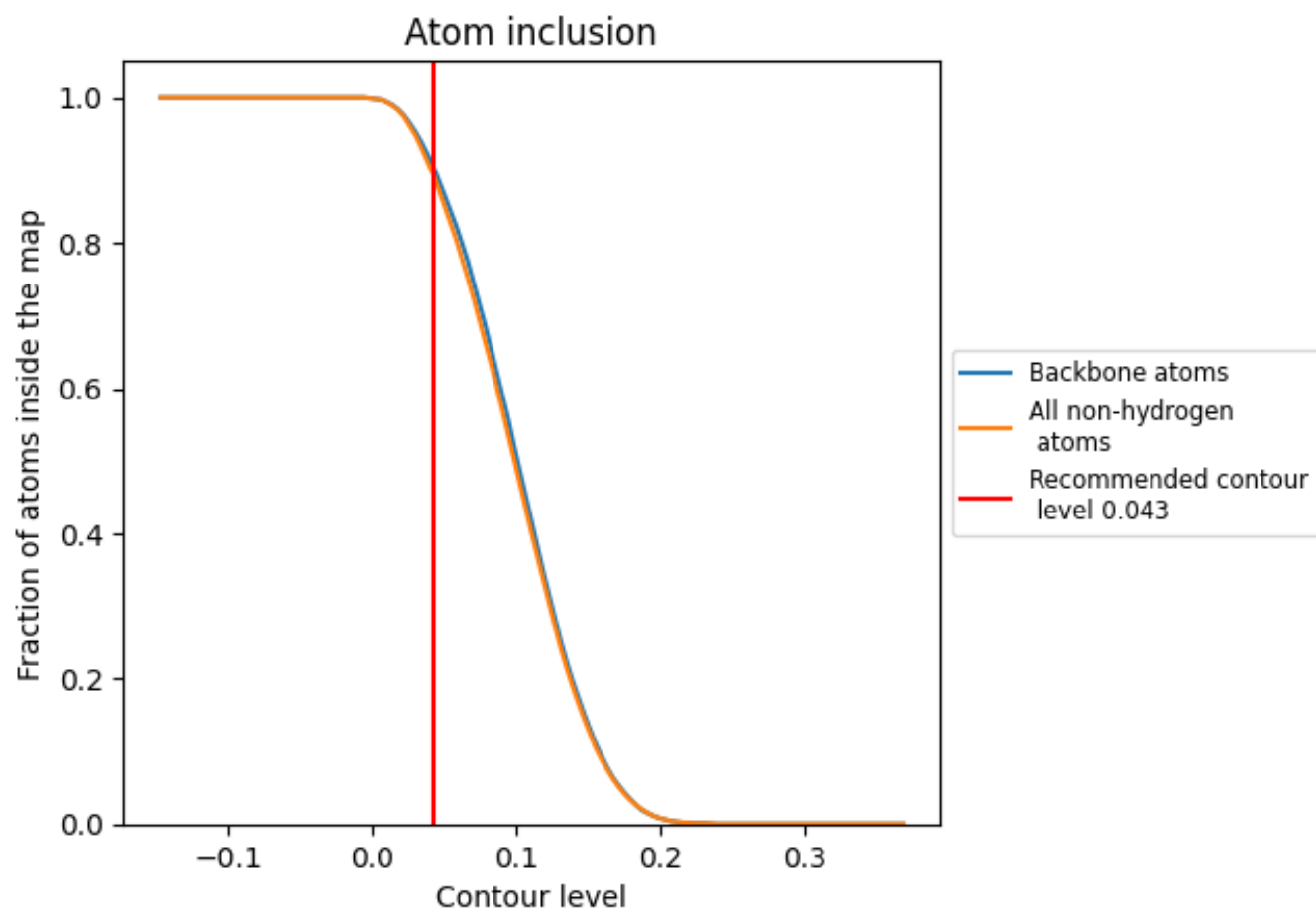
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.043).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ







The table lists the average atom inclusion at the recommended contour level (0.043) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.6750
A	 0.9290	 0.6920
B	 0.9020	 0.6840
C	 0.9120	 0.6720
D	 0.9410	 0.7010
E	 0.8180	 0.6390
F	 0.8700	 0.6710
H	 0.9370	 0.6870
I	 0.8590	 0.6510
J	 0.8580	 0.6480
K	 0.9170	 0.6600
L	 0.8850	 0.6850
M	 0.8820	 0.6790
O	 0.7840	 0.6190
T	 0.8090	 0.6570
U	 0.8060	 0.6350
V	 0.8710	 0.6520
X	 0.8060	 0.6460
Y	 0.7430	 0.6010
Z	 0.7220	 0.6020
a	 0.9340	 0.7020
b	 0.9100	 0.6800
c	 0.9250	 0.6900
d	 0.9370	 0.6980
e	 0.8460	 0.6510
f	 0.8490	 0.6620
h	 0.9360	 0.6790
i	 0.8280	 0.6660
j	 0.8490	 0.6640
k	 0.9080	 0.6710
l	 0.8550	 0.6720
m	 0.8730	 0.6780
o	 0.7940	 0.6320
t	 0.9100	 0.6970
u	 0.8210	 0.6440



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
v	 0.8840	 0.6620
x	 0.8110	 0.6410
y	 0.7430	 0.6080
z	 0.7650	 0.6220