



Full wwPDB EM Validation Report ⓘ

Jun 7, 2026 – 08:20 am BST

PDB ID : 9T5T / pdb_00009t5t
EMDB ID : EMD-55593
Title : Chlorophyll f-containing dimeric far-red Photosystem II from *Chroococcidiopsis thermalis* PCC 7203
Authors : Leong, H.F.; Consoli, G.; Murray, J.W.; Fantuzzi, A.; Rutherford, A.W.
Deposited on : 2025-11-05
Resolution : 2.17 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

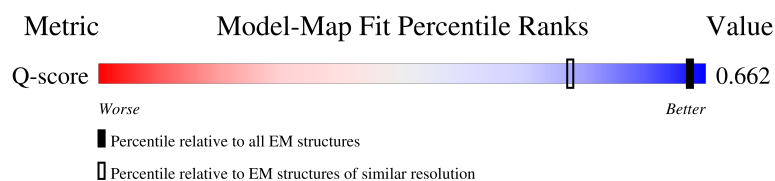
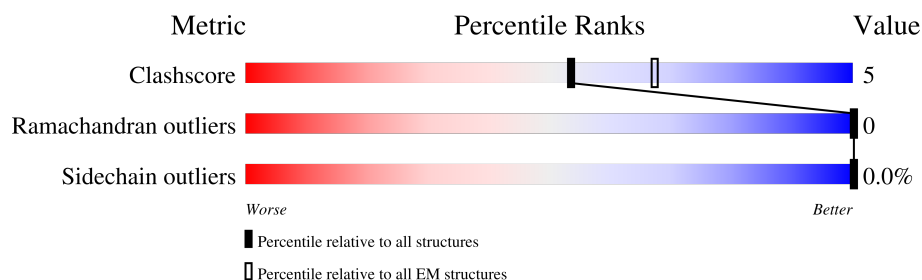
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.













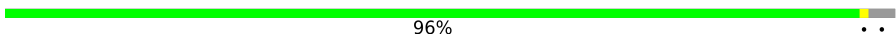
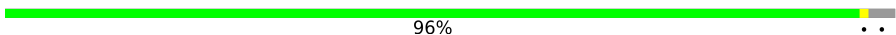













Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2651 (1.67 - 2.67)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	369	 79% 11% 9%
1	a	369	 78% 12% 9%
2	B	520	 89% 8% .
2	b	520	 88% 9% .

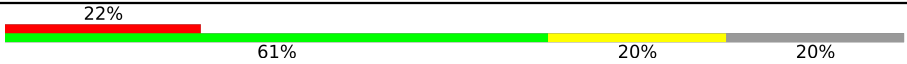


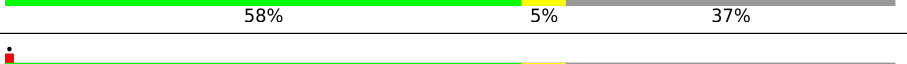
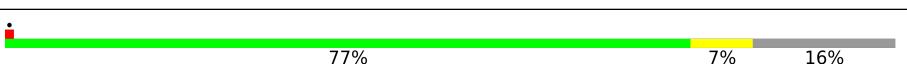
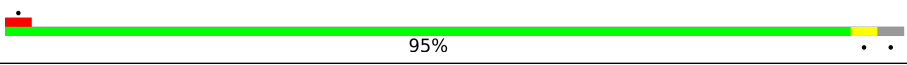
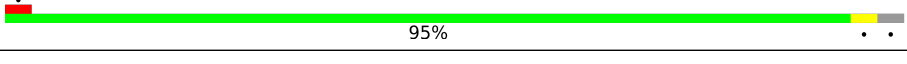

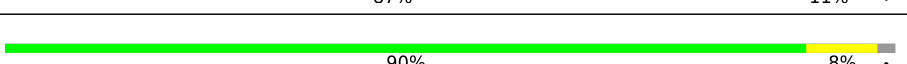

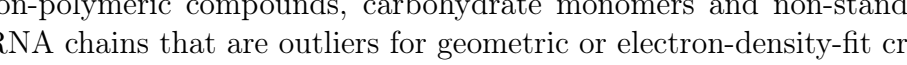
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Mol	Chain	Length	Quality of chain
3	C	466	
3	c	466	
4	D	352	
4	d	352	
5	E	82	
5	e	82	
6	F	44	
6	f	44	
7	G	48	
7	g	48	
8	H	69	
8	h	69	
9	I	38	
9	i	38	
10	J	39	
10	j	39	
11	K	60	
11	k	60	
12	L	41	
12	l	41	
13	M	37	
13	m	37	
14	O	274	
14	o	274	
15	R	41	

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Mol	Chain	Length	Quality of chain
15	r	41	
16	T	32	
16	t	32	
17	U	153	
17	u	153	
18	V	163	
18	v	163	
19	X	39	
19	x	39	
20	Y	43	
20	y	43	
21	Z	63	
21	z	63	

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
26	CL7	A	406	X	-	-	-
26	CL7	a	406	X	-	-	-
34	F6C	B	608	X	-	-	-
34	F6C	B	614	X	-	-	-
34	F6C	B	617	X	-	-	-
34	F6C	C	507	X	-	-	-
34	F6C	b	608	X	-	-	-
34	F6C	b	614	X	-	-	-
34	F6C	b	617	X	-	-	-
34	F6C	c	507	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 52226 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2616	1708	430	460	18		
1	a	334	Total	C	N	O	S	0	0
			2616	1708	430	460	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	504	Total	C	N	O	S	0	0
			3970	2597	669	688	16		
2	b	504	Total	C	N	O	S	0	0
			3970	2597	669	688	16		

- 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
			3475	2267	591	606	11		
3	c	450	Total	C	N	O	S	0	0
			3475	2267	591	606	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	340	Total	C	N	O	S	0	0
			2733	1812	443	465	13		
4	d	340	Total	C	N	O	S	0	0
			2733	1812	443	465	13		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	78	Total	C	N	O	0	0
			639	418	104	117		
5	e	78	Total	C	N	O	0	0
			639	418	104	117		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	36	Total	C	N	O	S	0	0
			293	200	48	44	1		
6	f	36	Total	C	N	O	S	0	0
			293	200	48	44	1		

- Molecule 7 is a protein called PsbH2'.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	40	Total	C	N	O	S	0	0
			301	198	47	55	1		
7	g	40	Total	C	N	O	S	0	0
			301	198	47	55	1		

- Molecule 8 is a protein called Photosystem II phosphoprotein PsbH.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			535	361	87	84	3		
8	h	67	Total	C	N	O	S	0	0
			535	361	87	84	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			274	187	43	43	1		
9	i	34	Total	C	N	O	S	0	0
			274	187	43	43	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			266	178	42	46		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	36	Total	C	N	O	0	0
			266	178	42	46		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			299	209	43	47		
11	k	37	Total	C	N	O	0	0
			299	209	43	47		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	36	Total	C	N	O	0	0
			294	196	46	52		
12	l	36	Total	C	N	O	0	0
			294	196	46	52		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	34	Total	C	N	O	S	0	0
			266	178	40	47	1		
13	m	34	Total	C	N	O	S	0	0
			266	178	40	47	1		

- Molecule 14 is a protein called Photosystem II extrinsic protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	243	Total	C	N	O	S	0	0
			1832	1151	308	369	4		
14	o	243	Total	C	N	O	S	0	0
			1832	1151	308	369	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	R	33	Total	C	N	O	0	0
			252	170	43	39		
15	r	33	Total	C	N	O	0	0
			252	170	43	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			239	162	36	40	1		
16	t	30	Total	C	N	O	S	0	0
			239	162	36	40	1		

- Molecule 17 is a protein called Photosystem II extrinsic protein U.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	97	Total	C	N	O	S	0	0
			765	474	136	153	2		
17	u	97	Total	C	N	O	S	0	0
			765	474	136	153	2		

- Molecule 18 is a protein called Photosystem II extrinsic protein V.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	137	Total	C	N	O	S	0	0
			1048	652	180	211	5		
18	v	137	Total	C	N	O	S	0	0
			1048	652	180	211	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	38	Total	C	N	O	S	0	0
			297	199	46	50	2		
19	x	38	Total	C	N	O	S	0	0
			297	199	46	50	2		

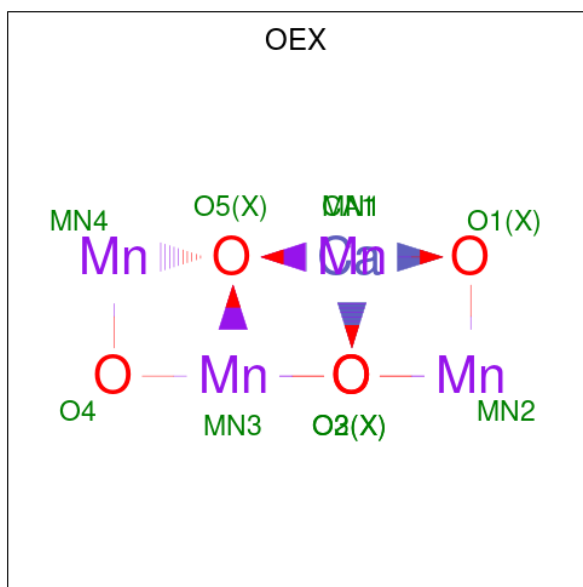
- Molecule 20 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	32	Total	C	N	O	S	0	0
			250	168	39	42	1		
20	y	32	Total	C	N	O	S	0	0
			250	168	39	42	1		

- Molecule 21 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	62	Total	C	N	O	S	0	0
			482	334	73	74	1		
21	z	62	Total	C	N	O	S	0	0
			482	334	73	74	1		

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



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

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

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

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

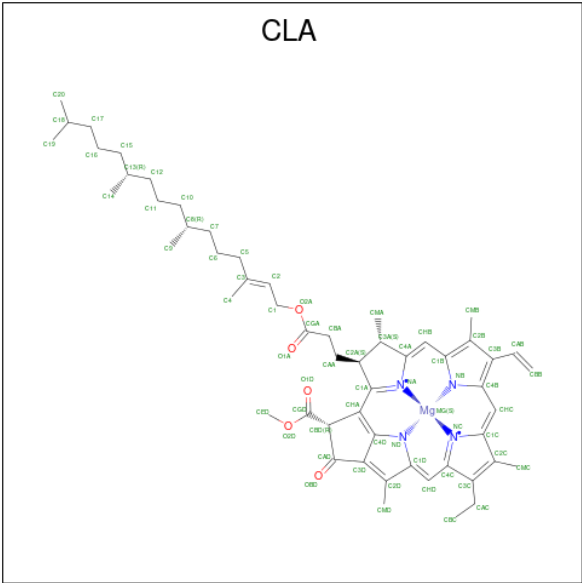
Mol	Chain	Residues	Atoms		AltConf
24	A	2	Total	Cl	0
			2	2	

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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	C	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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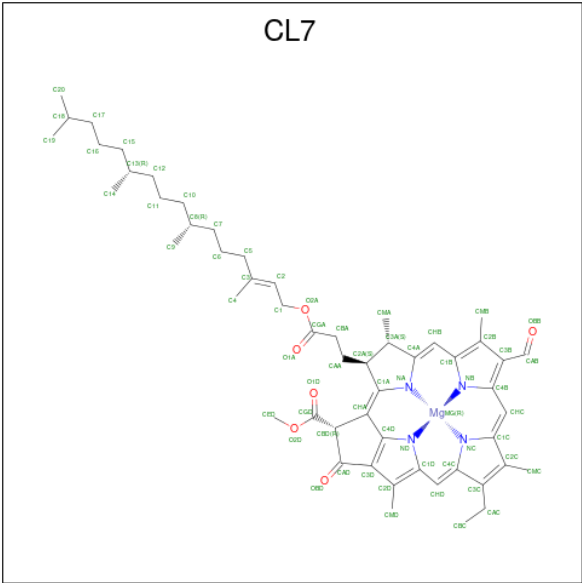
Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total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

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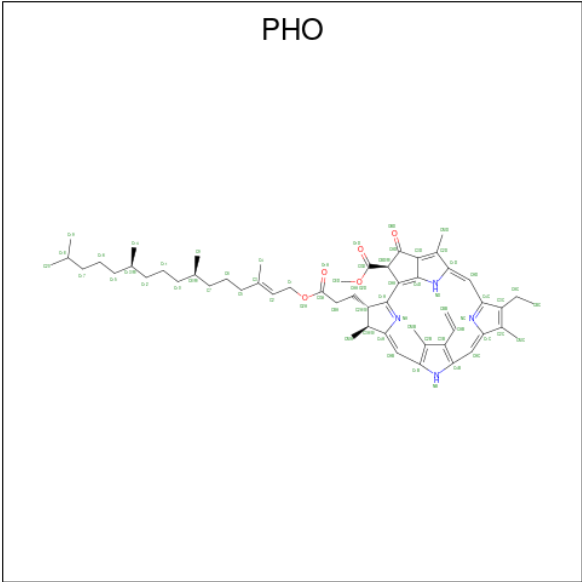
Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 26 is CHLOROPHYLL D (CCD ID: CL7) (formula: C₅₄H₇₀MgN₄O₆).



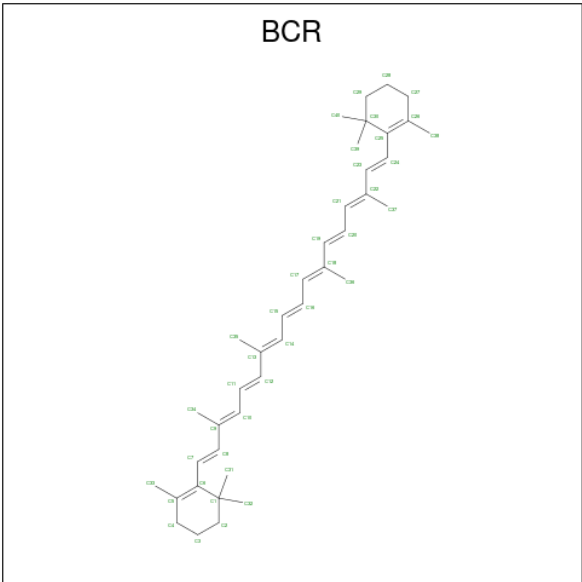
Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
26	a	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



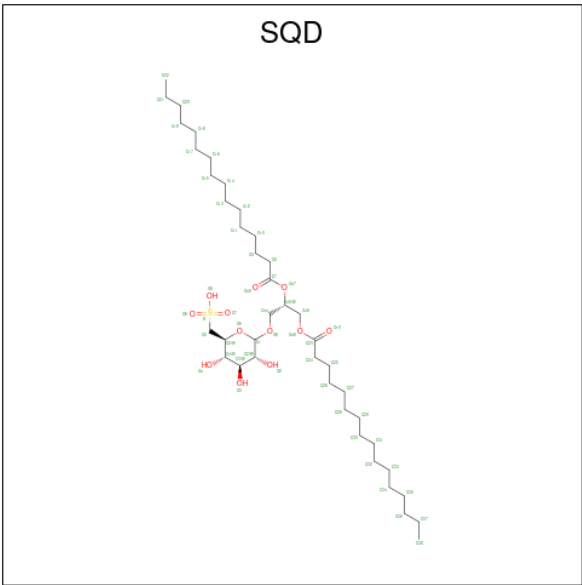
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	N	O	0
			64	55	4	5	
27	A	1	Total	C	N	O	0
			64	55	4	5	
27	a	1	Total	C	N	O	0
			64	55	4	5	
27	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 28 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



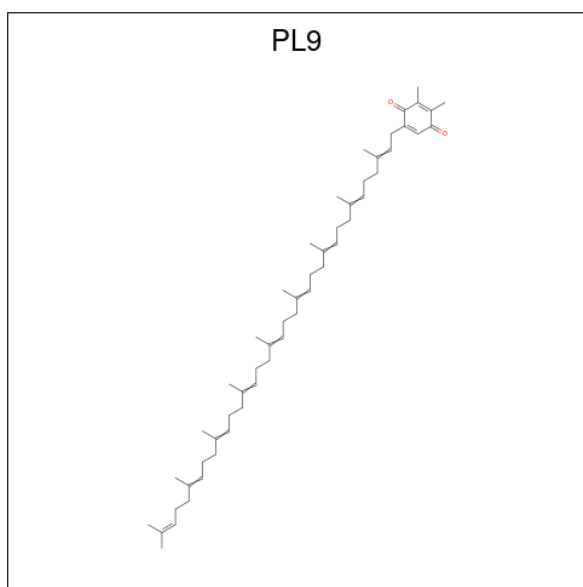
Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	C	1	Total C 40 40	0
28	C	1	Total C 40 40	0
28	D	1	Total C 40 40	0
28	K	1	Total C 40 40	0
28	K	1	Total C 40 40	0
28	a	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	d	1	Total C 40 40	0
28	k	1	Total C 40 40	0
28	k	1	Total C 40 40	0

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



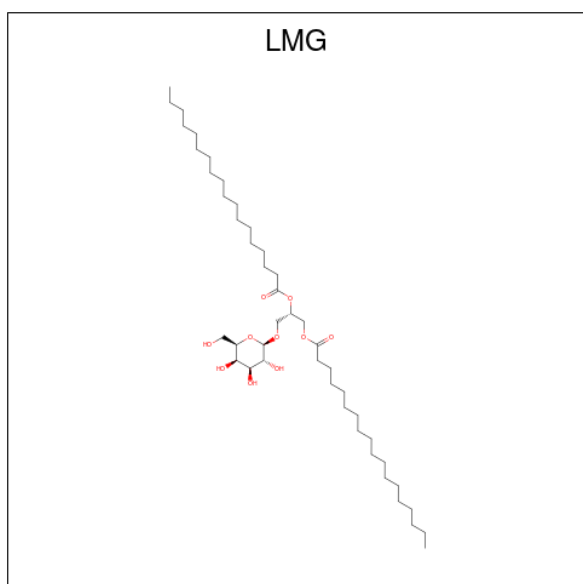
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O	S	0
			54	41	12	1	
29	A	1	Total	C	O	S	0
			54	41	12	1	
29	B	1	Total	C	O	S	0
			54	41	12	1	
29	C	1	Total	C	O	S	0
			38	25	12	1	
29	D	1	Total	C	O	S	0
			45	32	12	1	
29	H	1	Total	C	O	S	0
			54	41	12	1	
29	a	1	Total	C	O	S	0
			54	41	12	1	
29	a	1	Total	C	O	S	0
			54	41	12	1	
29	b	1	Total	C	O	S	0
			54	41	12	1	
29	c	1	Total	C	O	S	0
			38	25	12	1	
29	d	1	Total	C	O	S	0
			45	32	12	1	
29	h	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 30 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: C₅₃H₈₀O₂).



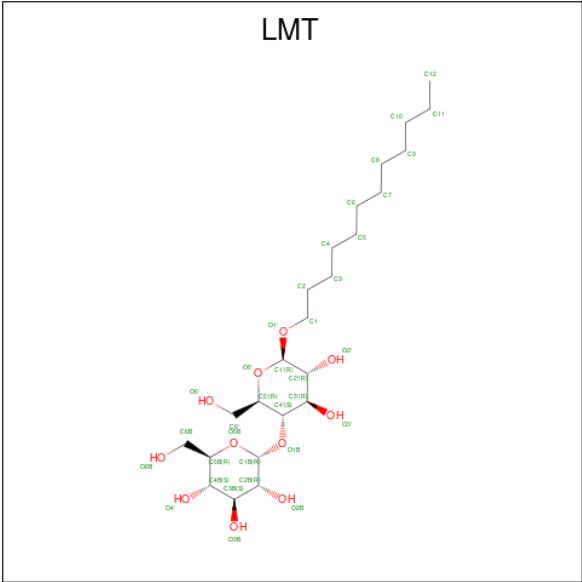
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			55	53	2	
30	D	1	Total	C	O	0
			55	53	2	
30	a	1	Total	C	O	0
			55	53	2	
30	d	1	Total	C	O	0
			55	53	2	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			48	38	10	
31	B	1	Total	C	O	0
			55	45	10	
31	C	1	Total	C	O	0
			51	41	10	
31	C	1	Total	C	O	0
			53	43	10	
31	D	1	Total	C	O	0
			51	41	10	
31	L	1	Total	C	O	0
			55	45	10	
31	a	1	Total	C	O	0
			48	38	10	
31	b	1	Total	C	O	0
			55	45	10	
31	c	1	Total	C	O	0
			51	41	10	
31	c	1	Total	C	O	0
			53	43	10	
31	d	1	Total	C	O	0
			51	41	10	
31	l	1	Total	C	O	0
			55	45	10	
31	P	1	Total	C	O	0
			47	37	10	
31	p	1	Total	C	O	0
			47	37	10	

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



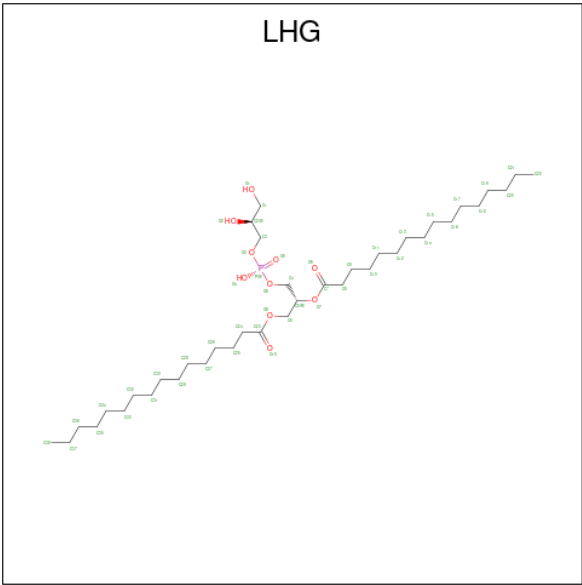
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			32	21	11	
32	A	1	Total	C	O	0
			35	24	11	
32	B	1	Total	C	O	0
			25	19	6	
32	C	1	Total	C	O	0
			32	21	11	
32	F	1	Total	C	O	0
			35	24	11	
32	G	1	Total	C	O	0
			35	24	11	
32	L	1	Total	C	O	0
			35	24	11	
32	L	1	Total	C	O	0
			35	24	11	
32	M	1	Total	C	O	0
			35	24	11	
32	Z	1	Total	C	O	0
			35	24	11	
32	a	1	Total	C	O	0
			32	21	11	
32	a	1	Total	C	O	0
			35	24	11	
32	b	1	Total	C	O	0
			25	19	6	
32	c	1	Total	C	O	0
			32	21	11	

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Mol	Chain	Residues	Atoms			AltConf
32	f	1	Total	C	O	0
			35	24	11	
32	g	1	Total	C	O	0
			35	24	11	
32	l	1	Total	C	O	0
			35	24	11	
32	l	1	Total	C	O	0
			35	24	11	
32	m	1	Total	C	O	0
			35	24	11	
32	z	1	Total	C	O	0
			35	24	11	

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	P	0
			49	38	10	1	
33	A	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			49	38	10	1	
33	D	1	Total	C	O	P	0
			41	30	10	1	

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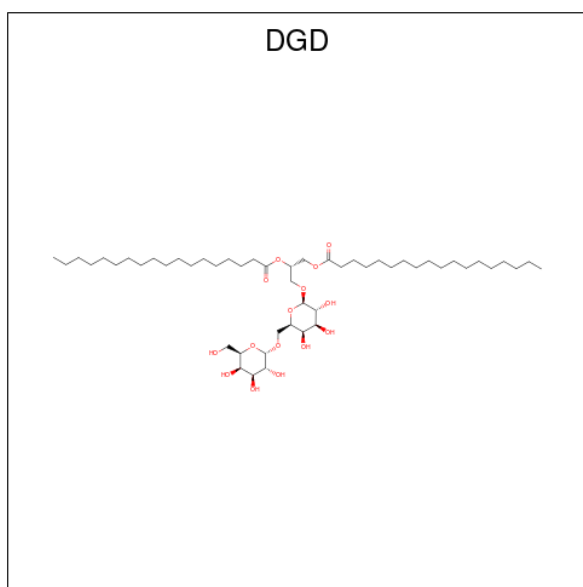
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Mol	Chain	Residues	Atoms				AltConf
33	E	1	Total	C	O	P	0
			49	38	10	1	
33	E	1	Total	C	O	P	0
			49	38	10	1	
33	J	1	Total	C	O	P	0
			49	38	10	1	
33	L	1	Total	C	O	P	0
			49	38	10	1	
33	a	1	Total	C	O	P	0
			49	38	10	1	
33	a	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			49	38	10	1	
33	d	1	Total	C	O	P	0
			41	30	10	1	
33	e	1	Total	C	O	P	0
			49	38	10	1	
33	e	1	Total	C	O	P	0
			49	38	10	1	
33	j	1	Total	C	O	P	0
			49	38	10	1	
33	l	1	Total	C	O	P	0
			49	38	10	1	
33	P	1	Total	C	O	P	0
			49	38	10	1	
33	p	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 34 is Chlorophyll F (CCD ID: F6C) (formula: $C_{55}H_{68}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).

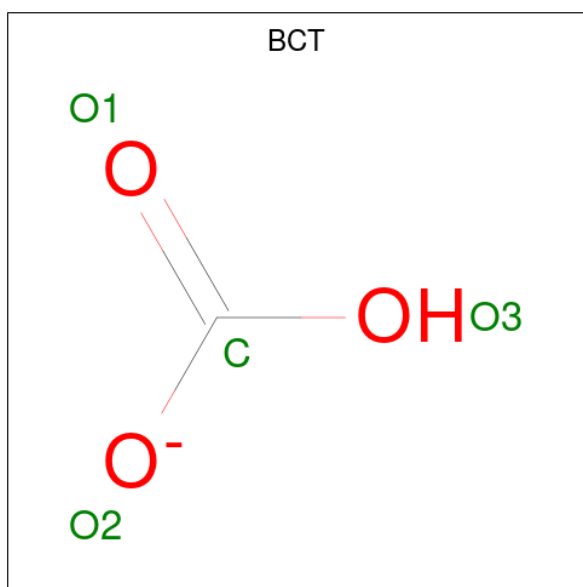


- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



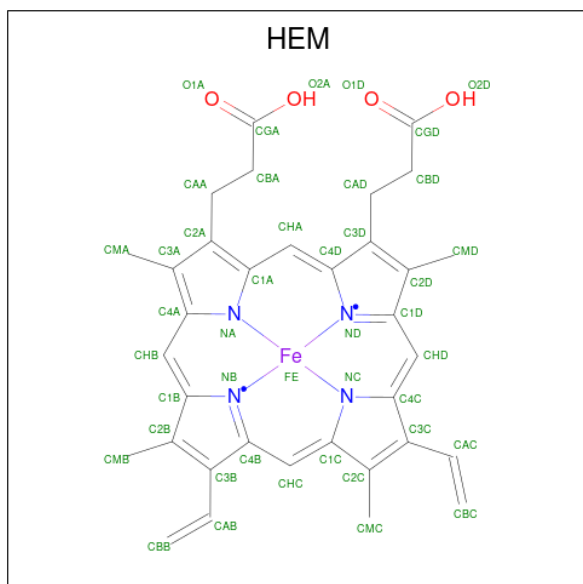
Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			62	47	15	
35	C	1	Total	C	O	0
			62	47	15	
35	C	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			62	47	15	

- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



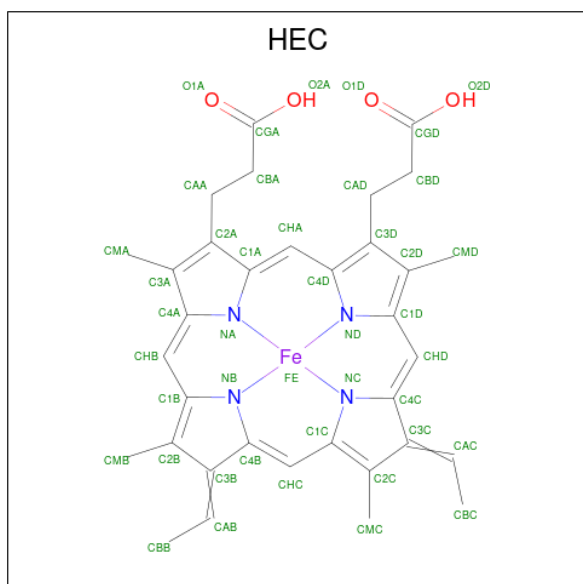
Mol	Chain	Residues	Atoms					AltConf
37	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

- Molecule 38 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	27	Total	O	0
			27	27	
39	A	24	Total	O	0
			24	24	
39	A	5	Total	O	0
			5	5	
39	A	1	Total	O	0
			1	1	
39	A	1	Total	O	0
			1	1	
39	A	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
39	A	1	Total 1	O 1	0
39	A	1	Total 1	O 1	0
39	A	1	Total 1	O 1	0
39	A	1	Total 1	O 1	0
39	A	1	Total 1	O 1	0
39	B	18	Total 18	O 18	0
39	B	3	Total 3	O 3	0
39	B	16	Total 16	O 16	0
39	B	1	Total 1	O 1	0
39	B	38	Total 38	O 38	0
39	B	1	Total 1	O 1	0
39	B	1	Total 1	O 1	0
39	B	1	Total 1	O 1	0
39	B	1	Total 1	O 1	0
39	B	1	Total 1	O 1	0
39	C	16	Total 16	O 16	0
39	C	8	Total 8	O 8	0
39	C	12	Total 12	O 12	0
39	C	2	Total 2	O 2	0
39	C	5	Total 5	O 5	0
39	C	3	Total 3	O 3	0

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Mol	Chain	Residues	Atoms	AltConf
39	C	11	Total O 11 11	0
39	C	5	Total O 5 5	0
39	C	1	Total O 1 1	0
39	C	1	Total O 1 1	0
39	C	1	Total O 1 1	0
39	C	1	Total O 1 1	0
39	C	1	Total O 1 1	0
39	C	1	Total O 1 1	0
39	D	1	Total O 1 1	0
39	D	1	Total O 1 1	0
39	D	1	Total O 1 1	0
39	D	1	Total O 1 1	0
39	D	1	Total O 1 1	0
39	D	15	Total O 15 15	0
39	D	1	Total O 1 1	0
39	D	3	Total O 3 3	0
39	D	5	Total O 5 5	0
39	D	4	Total O 4 4	0
39	D	17	Total O 17 17	0
39	D	5	Total O 5 5	0
39	E	4	Total O 4 4	0

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Mol	Chain	Residues	Atoms	AltConf
39	F	1	Total O 1 1	0
39	G	1	Total O 1 1	0
39	G	1	Total O 1 1	0
39	H	1	Total O 1 1	0
39	H	1	Total O 1 1	0
39	H	1	Total O 1 1	0
39	H	1	Total O 1 1	0
39	H	3	Total O 3 3	0
39	H	1	Total O 1 1	0
39	L	3	Total O 3 3	0
39	O	1	Total O 1 1	0
39	O	1	Total O 1 1	0
39	O	1	Total O 1 1	0
39	O	6	Total O 6 6	0
39	O	11	Total O 11 11	0
39	T	1	Total O 1 1	0
39	U	5	Total O 5 5	0
39	U	1	Total O 1 1	0
39	U	1	Total O 1 1	0
39	U	1	Total O 1 1	0
39	V	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
39	V	1	Total O 1 1	0
39	V	1	Total O 1 1	0
39	V	1	Total O 1 1	0
39	V	2	Total O 2 2	0
39	V	3	Total O 3 3	0
39	V	5	Total O 5 5	0
39	X	1	Total O 1 1	0
39	a	27	Total O 27 27	0
39	a	24	Total O 24 24	0
39	a	5	Total O 5 5	0
39	a	1	Total O 1 1	0
39	a	1	Total O 1 1	0
39	a	1	Total O 1 1	0
39	a	1	Total O 1 1	0
39	a	1	Total O 1 1	0
39	a	1	Total O 1 1	0
39	a	1	Total O 1 1	0
39	a	1	Total O 1 1	0
39	b	18	Total O 18 18	0
39	b	2	Total O 2 2	0
39	b	17	Total O 17 17	0

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Mol	Chain	Residues	Atoms	AltConf
39	b	1	Total O 1 1	0
39	b	38	Total O 38 38	0
39	b	1	Total O 1 1	0
39	b	1	Total O 1 1	0
39	b	1	Total O 1 1	0
39	b	1	Total O 1 1	0
39	b	1	Total O 1 1	0
39	c	16	Total O 16 16	0
39	c	8	Total O 8 8	0
39	c	12	Total O 12 12	0
39	c	2	Total O 2 2	0
39	c	5	Total O 5 5	0
39	c	3	Total O 3 3	0
39	c	11	Total O 11 11	0
39	c	5	Total O 5 5	0
39	c	1	Total O 1 1	0
39	c	1	Total O 1 1	0
39	c	1	Total O 1 1	0
39	c	1	Total O 1 1	0
39	c	1	Total O 1 1	0
39	c	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
39	d	1	Total O 1 1	0
39	d	1	Total O 1 1	0
39	d	1	Total O 1 1	0
39	d	1	Total O 1 1	0
39	d	1	Total O 1 1	0
39	d	15	Total O 15 15	0
39	d	1	Total O 1 1	0
39	d	3	Total O 3 3	0
39	d	5	Total O 5 5	0
39	d	4	Total O 4 4	0
39	d	17	Total O 17 17	0
39	d	5	Total O 5 5	0
39	e	4	Total O 4 4	0
39	f	1	Total O 1 1	0
39	g	1	Total O 1 1	0
39	g	1	Total O 1 1	0
39	h	1	Total O 1 1	0
39	h	1	Total O 1 1	0
39	h	1	Total O 1 1	0
39	h	1	Total O 1 1	0
39	h	3	Total O 3 3	0

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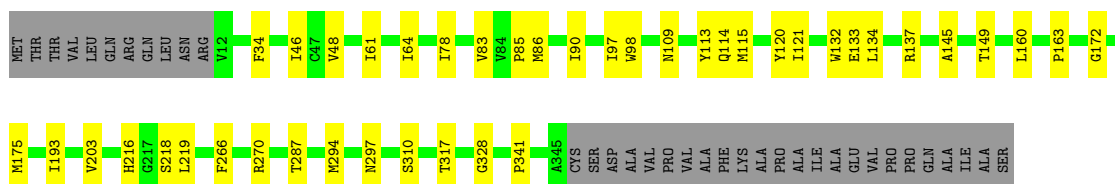
Mol	Chain	Residues	Atoms	AltConf
39	h	1	Total O 1 1	0
39	l	3	Total O 3 3	0
39	o	1	Total O 1 1	0
39	o	1	Total O 1 1	0
39	o	1	Total O 1 1	0
39	o	6	Total O 6 6	0
39	o	11	Total O 11 11	0
39	t	1	Total O 1 1	0
39	u	5	Total O 5 5	0
39	u	1	Total O 1 1	0
39	u	1	Total O 1 1	0
39	u	1	Total O 1 1	0
39	v	1	Total O 1 1	0
39	v	1	Total O 1 1	0
39	v	1	Total O 1 1	0
39	v	1	Total O 1 1	0
39	v	2	Total O 2 2	0
39	v	3	Total O 3 3	0
39	v	5	Total O 5 5	0
39	x	1	Total O 1 1	0

3 Residue-property plots [i](#)


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

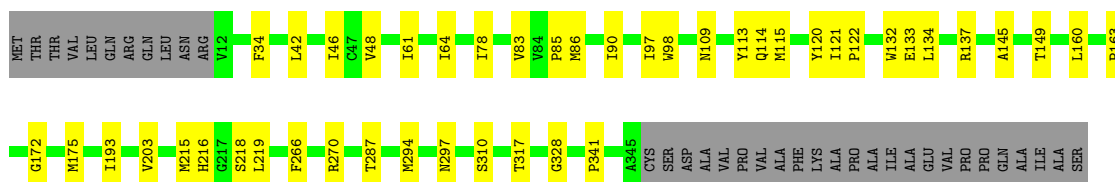
- Molecule 1: Photosystem II protein D1

Chain A: 



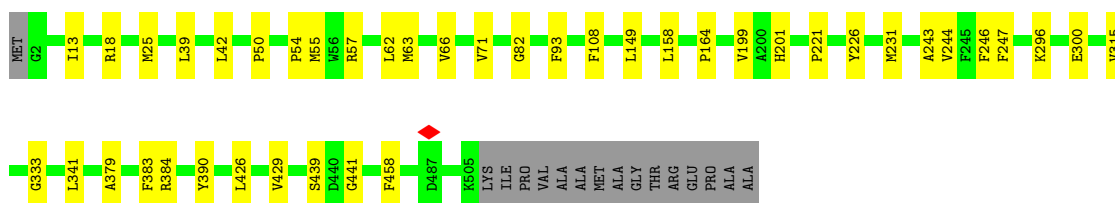
- Molecule 1: Photosystem II protein D1

Chain a: 




- Molecule 2: Photosystem II CP47 reaction center protein

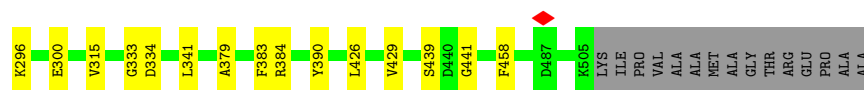
Chain B: 



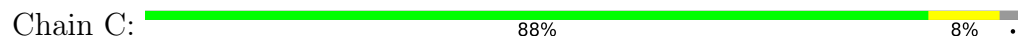
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b: 

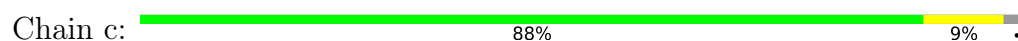




- Molecule 3: Photosystem II CP43 reaction center protein



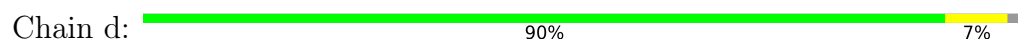
- Molecule 3: Photosystem II CP43 reaction center protein



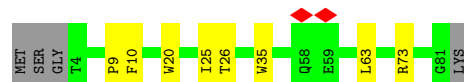
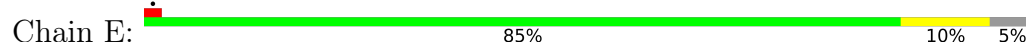
- Molecule 4: Photosystem II D2 protein




- Molecule 4: Photosystem II D2 protein

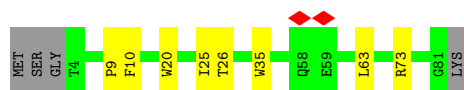


- Molecule 5: Cytochrome b559 subunit alpha




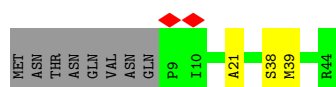
- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  85% 10% 5%




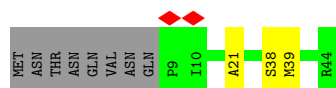
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  5% 75% 7% 18%




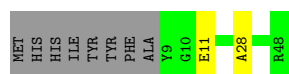
- Molecule 6: Cytochrome b559 subunit beta

Chain f:  5% 75% 7% 18%




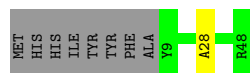
- Molecule 7: PsbH2'

Chain G:  79% 17%



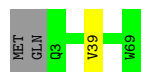
- Molecule 7: PsbH2'

Chain g:  81% 17%



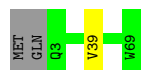
- Molecule 8: Photosystem II phosphoprotein PsbH

Chain H:  96% 4% 2%




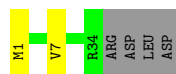
- Molecule 8: Photosystem II phosphoprotein PsbH

Chain h:  96% 4% 2%




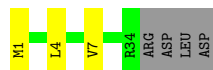
- Molecule 9: Photosystem II reaction center protein I

Chain I:  84% 5% 11%



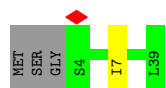
- Molecule 9: Photosystem II reaction center protein I

Chain i:  82% 8% 11%



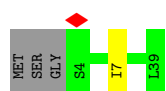
- Molecule 10: Photosystem II reaction center protein J

Chain J:  90% 8%



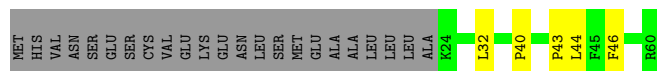
- Molecule 10: Photosystem II reaction center protein J

Chain j:  90% 8%



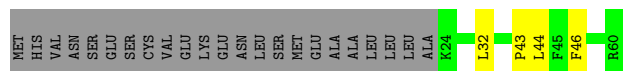
- Molecule 11: Photosystem II reaction center protein K

Chain K:  53% 8% 38%




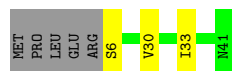
- Molecule 11: Photosystem II reaction center protein K

Chain k:  55% 7% 38%




- Molecule 12: Photosystem II reaction center protein L

Chain L:  80% 7% 12%




- Molecule 12: Photosystem II reaction center protein L

Chain L:  80% 7% 12%




- Molecule 13: Photosystem II reaction center protein M

Chain M:  78% 14% 8%




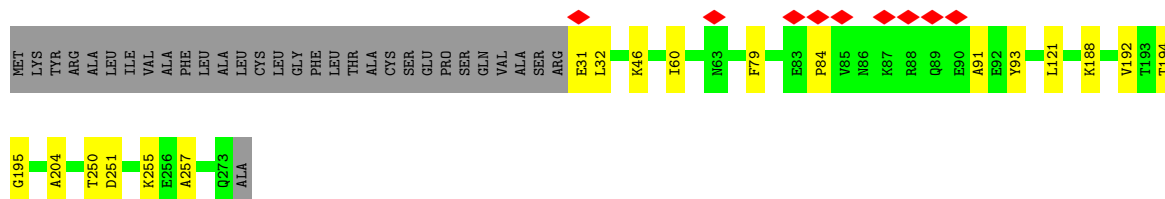
- Molecule 13: Photosystem II reaction center protein M

Chain m:  78% 14% 8%




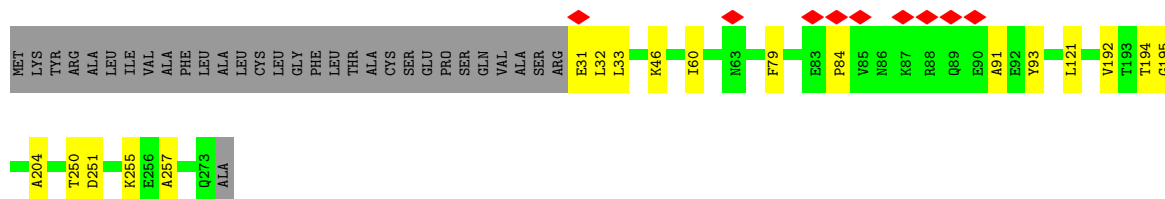
- Molecule 14: Photosystem II extrinsic protein O

Chain O:  82% 7% 11%



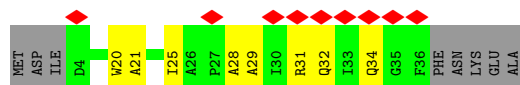
- Molecule 14: Photosystem II extrinsic protein O

Chain o:  82% 7% 11%

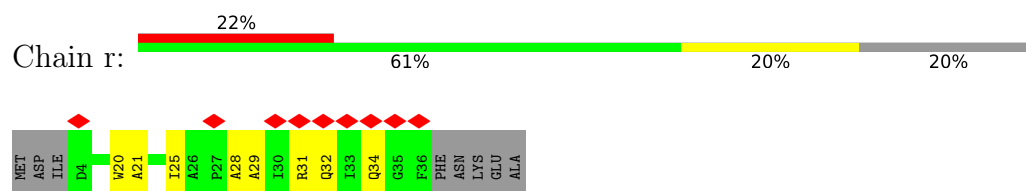


- Molecule 15: Photosystem II reaction center protein Y

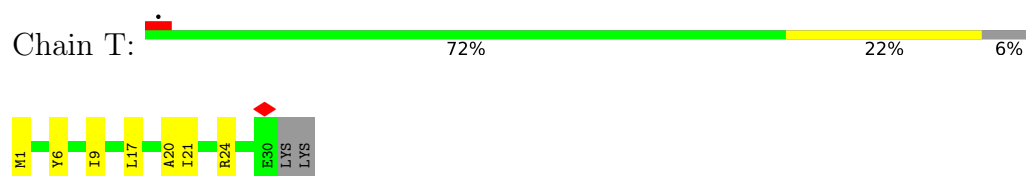
Chain R:  22% 61% 20% 20%



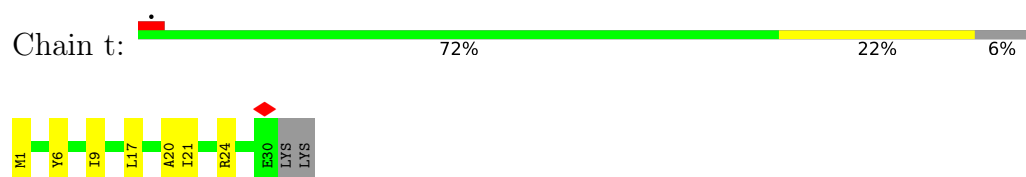
- Molecule 15: Photosystem II reaction center protein Y



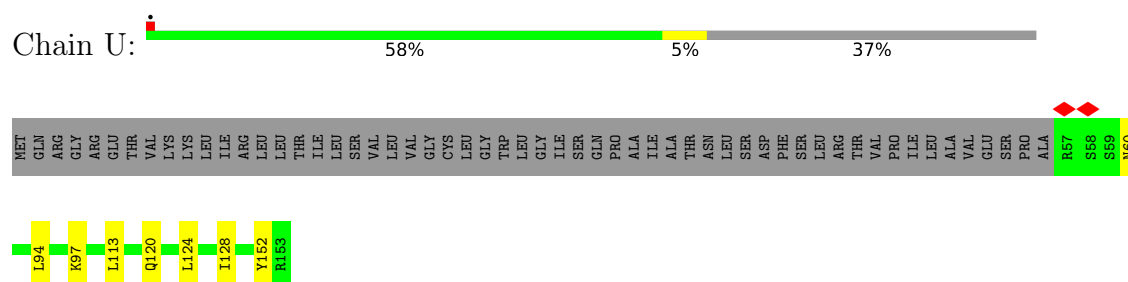
- Molecule 16: Photosystem II reaction center protein T



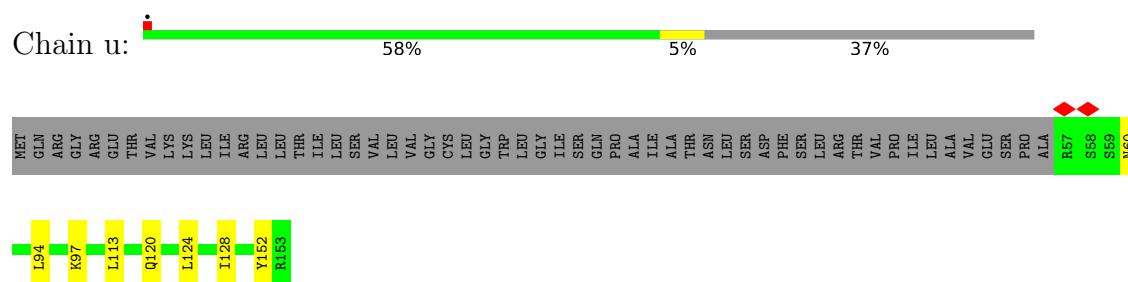
- Molecule 16: Photosystem II reaction center protein T



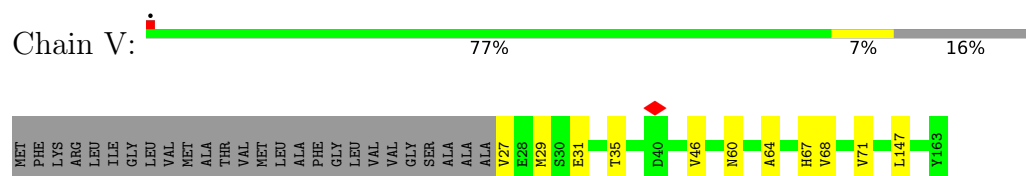
- Molecule 17: Photosystem II extrinsic protein U




- Molecule 17: Photosystem II extrinsic protein U



- Molecule 18: Photosystem II extrinsic protein V



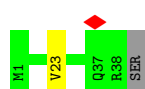
- Molecule 18: Photosystem II extrinsic protein V

Chain v:  77% 7% 16%



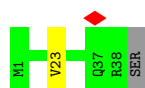
- Molecule 19: Photosystem II reaction center protein X

Chain X:  95% . .



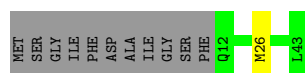
- Molecule 19: Photosystem II reaction center protein X

Chain x:  95% . .



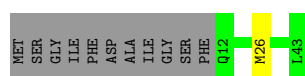
- Molecule 20: Photosystem II reaction center protein Psb30

Chain Y:  72% . 26%



- Molecule 20: Photosystem II reaction center protein Psb30

Chain y:  72% . 26%




- Molecule 21: Photosystem II reaction center protein Z

Chain Z:  87% 11% .



- Molecule 21: Photosystem II reaction center protein Z

Chain z:  90% 8% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	49763	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.357	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	469.94998, 469.94998, 469.94998	wwPDB
Map dimensions	650, 650, 650	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.723, 0.723, 0.723	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, PHO, LHG, HEC, LMT, DGD, F6C, FE2, CL7, CL, HEM, BCT, SQD, OEX, FME, LMG, BCR, 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	0.25	0/2702	0.33	0/3688
1	a	0.25	0/2702	0.33	0/3688
2	B	0.24	0/4103	0.30	0/5580
2	b	0.24	0/4103	0.30	0/5580
3	C	0.22	0/3586	0.29	0/4882
3	c	0.23	0/3586	0.29	0/4882
4	D	0.25	0/2832	0.32	0/3857
4	d	0.25	0/2832	0.32	0/3857
5	E	0.21	0/659	0.28	0/899
5	e	0.21	0/659	0.28	0/899
6	F	0.22	0/303	0.31	0/414
6	f	0.22	0/303	0.31	0/414
7	G	0.17	0/307	0.18	0/416
7	g	0.17	0/307	0.18	0/416
8	H	0.21	0/552	0.27	0/749
8	h	0.21	0/552	0.27	0/749
9	I	0.20	0/271	0.27	0/368
9	i	0.20	0/271	0.27	0/368
10	J	0.17	0/273	0.27	0/372
10	j	0.17	0/273	0.27	0/372
11	K	0.22	0/309	0.34	0/423
11	k	0.22	0/309	0.34	0/423
12	L	0.21	0/301	0.26	0/407
12	l	0.22	0/301	0.26	0/407
13	M	0.22	0/260	0.37	0/354
13	m	0.22	0/260	0.37	0/354
14	O	0.19	0/1863	0.31	0/2529
14	o	0.19	0/1863	0.31	0/2529
15	R	0.16	0/258	0.30	0/353
15	r	0.16	0/258	0.30	0/353
16	T	0.20	0/234	0.26	0/318

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.20	0/234	0.27	0/318
17	U	0.17	0/777	0.26	0/1051
17	u	0.17	0/777	0.26	0/1051
18	V	0.20	0/1066	0.26	0/1444
18	v	0.20	0/1066	0.26	0/1444
19	X	0.18	0/292	0.25	0/396
19	x	0.18	0/292	0.25	0/396
20	Y	0.14	0/255	0.28	0/346
20	y	0.14	0/255	0.28	0/346
21	Z	0.16	0/495	0.23	0/679
21	z	0.16	0/495	0.23	0/679
All	All	0.22	0/43396	0.30	0/59050

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	2616	0	2508	34	0
1	a	2616	0	2508	37	0
2	B	3970	0	3820	32	0
2	b	3970	0	3820	34	0
3	C	3475	0	3382	28	0
3	c	3475	0	3382	30	0
4	D	2733	0	2617	20	0
4	d	2733	0	2617	19	0
5	E	639	0	617	10	0
5	e	639	0	617	10	0
6	F	293	0	304	3	0
6	f	293	0	304	3	0
7	G	301	0	302	2	0
7	g	301	0	302	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	535	0	554	2	0
8	h	535	0	554	2	0
9	I	274	0	288	2	0
9	i	274	0	288	3	0
10	J	266	0	272	1	0
10	j	266	0	272	1	0
11	K	299	0	315	4	0
11	k	299	0	315	3	0
12	L	294	0	298	3	0
12	l	294	0	298	3	0
13	M	266	0	280	6	0
13	m	266	0	280	6	0
14	O	1832	0	1791	12	0
14	o	1832	0	1791	13	0
15	R	252	0	265	6	0
15	r	252	0	265	6	0
16	T	239	0	252	7	0
16	t	239	0	252	7	0
17	U	765	0	739	5	0
17	u	765	0	739	5	0
18	V	1048	0	1027	8	0
18	v	1048	0	1027	9	0
19	X	297	0	320	1	0
19	x	297	0	320	1	0
20	Y	250	0	259	1	0
20	y	250	0	259	1	0
21	Z	482	0	520	5	0
21	z	482	0	520	3	0
22	A	10	0	0	0	0
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	195	0	216	7	0
25	B	845	0	936	34	0
25	C	771	0	843	40	0
25	D	130	0	144	5	0
25	a	195	0	216	8	0
25	b	845	0	936	34	0
25	c	771	0	843	38	0
25	d	130	0	144	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	65	0	70	1	0
26	a	65	0	70	1	0
27	A	128	0	148	6	0
27	a	128	0	148	6	0
28	A	40	0	56	2	0
28	B	160	0	224	9	0
28	C	80	0	112	1	0
28	D	40	0	56	3	0
28	K	80	0	112	6	0
28	a	40	0	56	0	0
28	b	160	0	224	7	0
28	c	80	0	112	2	0
28	d	40	0	56	2	0
28	k	80	0	112	5	0
29	A	108	0	156	8	0
29	B	54	0	78	3	0
29	C	38	0	40	1	0
29	D	45	0	57	1	0
29	H	54	0	78	1	0
29	a	108	0	156	7	0
29	b	54	0	78	3	0
29	c	38	0	40	1	0
29	d	45	0	57	1	0
29	h	54	0	78	2	0
30	A	55	0	80	6	0
30	D	55	0	80	0	0
30	a	55	0	80	6	0
30	d	55	0	80	0	0
31	A	48	0	69	2	0
31	B	55	0	86	3	0
31	C	104	0	151	8	0
31	D	51	0	72	1	0
31	L	55	0	86	2	0
31	P	47	0	67	1	0
31	a	48	0	69	2	0
31	b	55	0	86	2	0
31	c	104	0	151	8	0
31	d	51	0	72	2	0
31	l	55	0	86	2	0
31	p	47	0	67	1	0
32	A	67	0	83	3	0
32	B	25	0	35	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	C	32	0	37	0	0
32	F	35	0	46	0	0
32	G	35	0	46	0	0
32	L	70	0	92	2	0
32	M	35	0	46	3	0
32	Z	35	0	46	1	0
32	a	67	0	83	3	0
32	b	25	0	35	0	0
32	c	32	0	37	0	0
32	f	35	0	46	0	0
32	g	35	0	46	0	0
32	l	70	0	92	1	0
32	m	35	0	46	3	0
32	z	35	0	46	1	0
33	A	98	0	148	6	0
33	D	139	0	203	2	0
33	E	98	0	148	4	0
33	J	49	0	74	4	0
33	L	49	0	74	1	0
33	P	49	0	74	3	0
33	a	98	0	148	7	0
33	d	139	0	203	2	0
33	e	98	0	148	4	0
33	j	49	0	74	3	0
33	l	49	0	74	1	0
33	p	49	0	74	3	0
34	B	183	0	0	1	0
34	C	66	0	0	0	0
34	b	183	0	0	1	0
34	c	66	0	0	0	0
35	C	186	0	246	7	0
35	c	186	0	246	6	0
36	D	4	0	0	0	0
36	d	4	0	0	0	0
37	F	43	0	30	5	0
37	f	43	0	30	5	0
38	V	43	0	30	0	0
38	v	43	0	30	0	0
39	A	64	0	0	0	0
39	B	81	0	0	0	0
39	C	68	0	0	0	0
39	D	55	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	E	4	0	0	0	0
39	F	1	0	0	0	0
39	G	2	0	0	0	0
39	H	8	0	0	0	0
39	L	3	0	0	0	0
39	O	20	0	0	0	0
39	T	1	0	0	0	0
39	U	8	0	0	0	0
39	V	14	0	0	0	0
39	X	1	0	0	0	0
39	a	64	0	0	0	0
39	b	81	0	0	0	0
39	c	68	0	0	0	0
39	d	55	0	0	0	0
39	e	4	0	0	0	0
39	f	1	0	0	0	0
39	g	2	0	0	0	0
39	h	8	0	0	0	0
39	l	3	0	0	0	0
39	o	20	0	0	0	0
39	t	1	0	0	0	0
39	u	8	0	0	0	0
39	v	14	0	0	0	0
39	x	1	0	0	0	0
All	All	52226	0	52410	540	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 (540) 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)
11:k:32:LEU:HD13	28:k:102:BCR:H312	1.70	0.73
2:b:50:PRO:HG2	2:b:82:GLY:HA2	1.71	0.73
11:K:32:LEU:HD13	28:K:102:BCR:H312	1.70	0.73
2:B:50:PRO:HG2	2:B:82:GLY:HA2	1.71	0.72
2:B:149:LEU:HD11	25:B:606:CLA:H151	1.73	0.71
2:b:149:LEU:HD11	25:b:606:CLA:H151	1.73	0.70
18:v:35:THR:HG22	18:v:46:VAL:HG22	1.73	0.70
18:V:35:THR:HG22	18:V:46:VAL:HG22	1.73	0.69
1:a:97:ILE:HG21	33:a:416:LHG:HC92	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:616:CLA:HHC	25:B:616:CLA:HBB1	1.78	0.66
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.76	0.66
25:C:512:CLA:HHC	25:C:512:CLA:HBB1	1.78	0.66
25:b:610:CLA:HHC	25:b:610:CLA:HBB1	1.77	0.66
1:A:97:ILE:HG21	33:A:416:LHG:HC92	1.76	0.66
2:b:54:PRO:HD2	2:b:57:ARG:HG3	1.76	0.66
25:c:512:CLA:HHC	25:c:512:CLA:HBB1	1.78	0.66
25:B:610:CLA:HHC	25:B:610:CLA:HBB1	1.77	0.65
1:a:193:ILE:HG13	1:a:294:MET:HE1	1.78	0.65
25:b:616:CLA:HHC	25:b:616:CLA:HBB1	1.77	0.65
25:B:602:CLA:HHC	25:B:602:CLA:HBB1	1.78	0.65
25:B:606:CLA:H142	25:B:616:CLA:HBA1	1.78	0.65
25:b:606:CLA:H142	25:b:616:CLA:HBA1	1.78	0.65
4:d:192:THR:HG23	25:d:402:CLA:HBC2	1.80	0.64
4:D:192:THR:HG23	25:D:402:CLA:HBC2	1.80	0.64
25:b:606:CLA:HHC	25:b:606:CLA:HBB1	1.79	0.64
4:d:186:GLN:HB2	25:d:402:CLA:HBC1	1.80	0.64
1:A:193:ILE:HG13	1:A:294:MET:HE1	1.78	0.64
25:B:611:CLA:HHC	25:B:611:CLA:HBB1	1.79	0.64
2:b:243:ALA:HA	2:b:246:PHE:CE1	2.33	0.64
25:b:611:CLA:HHC	25:b:611:CLA:HBB1	1.79	0.64
25:A:407:CLA:HHC	25:A:407:CLA:HBB1	1.81	0.63
25:b:602:CLA:HHC	25:b:602:CLA:HBB1	1.78	0.63
25:a:407:CLA:HHC	25:a:407:CLA:HBB1	1.81	0.63
2:B:243:ALA:HA	2:B:246:PHE:CE1	2.33	0.63
25:B:606:CLA:HHC	25:B:606:CLA:HBB1	1.79	0.62
25:C:501:CLA:H152	25:C:506:CLA:H143	1.82	0.62
4:D:186:GLN:HB2	25:D:402:CLA:HBC1	1.80	0.62
33:P:629:LHG:HC31	33:P:629:LHG:HC5	1.82	0.61
3:C:41:LEU:HD22	3:C:134:GLU:HG2	1.82	0.61
25:c:501:CLA:H152	25:c:506:CLA:H143	1.81	0.60
25:c:508:CLA:H203	11:k:44:LEU:HD11	1.83	0.60
25:C:508:CLA:H203	11:K:44:LEU:HD11	1.83	0.60
3:c:41:LEU:HD22	3:c:134:GLU:HG2	1.82	0.59
33:p:629:LHG:HC31	33:p:629:LHG:HC5	1.82	0.59
25:C:512:CLA:H121	31:C:902:LMG:H222	1.85	0.59
28:D:404:BCR:H383	31:D:411:LMG:H171	1.85	0.58
29:a:412:SQD:H302	25:c:508:CLA:H93	1.85	0.58
25:c:512:CLA:H121	31:c:902:LMG:H222	1.85	0.58
28:d:404:BCR:H383	31:d:411:LMG:H171	1.85	0.58
29:A:412:SQD:H302	25:C:508:CLA:H93	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HD11	1:A:109:ASN:HB3	1.87	0.57
2:B:458:PHE:HB3	25:B:605:CLA:HBC2	1.88	0.56
21:Z:10:LEU:HD23	21:Z:55:ILE:HD13	1.87	0.56
5:e:10:PHE:H	33:e:101:LHG:HC32	1.71	0.56
2:b:458:PHE:HB3	25:b:605:CLA:HBC2	1.88	0.56
12:L:33:ILE:HG13	16:T:9:ILE:HG22	1.87	0.56
27:A:409:PHO:HBC3	4:D:279:LEU:HD22	1.87	0.56
14:O:250:THR:HG22	14:O:257:ALA:HB2	1.86	0.56
14:o:250:THR:HG22	14:o:257:ALA:HB2	1.86	0.56
1:A:134:LEU:HD23	4:D:256:ILE:HG12	1.88	0.56
12:l:33:ILE:HG13	16:t:9:ILE:HG22	1.87	0.56
28:B:620:BCR:H281	32:a:674:LMT:H11	1.89	0.55
2:B:42:LEU:HD11	2:B:93:PHE:HB3	1.89	0.55
27:a:409:PHO:HBC3	4:d:279:LEU:HD22	1.87	0.55
2:b:42:LEU:HD11	2:b:93:PHE:HB3	1.89	0.55
37:F:101:HEM:HBC2	37:F:101:HEM:HMC2	1.89	0.55
1:a:90:ILE:HD11	1:a:109:ASN:HB3	1.87	0.55
3:c:311:LEU:HD12	3:c:333:TYR:HB3	1.89	0.55
21:z:10:LEU:HD23	21:z:55:ILE:HD13	1.87	0.55
1:a:134:LEU:HD23	4:d:256:ILE:HG12	1.88	0.55
30:a:414:PL9:H502	4:d:39:PRO:HB3	1.89	0.55
37:f:101:HEM:HBC2	37:f:101:HEM:HMC2	1.88	0.55
5:E:10:PHE:H	33:E:101:LHG:HC32	1.71	0.55
28:B:618:BCR:H383	31:L:212:LMG:H331	1.89	0.54
3:C:209:GLY:HA2	29:C:903:SQD:H461	1.90	0.54
30:A:414:PL9:H502	4:D:39:PRO:HB3	1.89	0.54
3:C:276:ALA:HB2	25:C:502:CLA:HBC3	1.89	0.54
3:C:368:LEU:HB3	3:C:373:ILE:HD11	1.89	0.54
3:c:368:LEU:HB3	3:c:373:ILE:HD11	1.89	0.54
3:C:65:MET:HE3	28:K:102:BCR:HC21	1.90	0.54
33:D:409:LHG:H291	16:T:17:LEU:HD22	1.90	0.54
3:c:276:ALA:HB2	25:c:502:CLA:HBC3	1.89	0.54
1:a:46:ILE:HD11	27:a:408:PHO:H51	1.90	0.54
32:A:674:LMT:H11	28:b:620:BCR:H281	1.89	0.54
25:A:407:CLA:H152	30:A:414:PL9:H261	1.90	0.54
25:c:502:CLA:H101	31:c:902:LMG:H431	1.90	0.54
25:B:615:CLA:HBB1	25:B:615:CLA:HMB1	1.90	0.54
3:C:311:LEU:HD12	3:C:333:TYR:HB3	1.89	0.53
14:O:79:PHE:HB3	14:O:93:TYR:HB3	1.90	0.53
25:b:605:CLA:H193	25:b:610:CLA:HBB2	1.90	0.53
31:A:415:LMG:HC92	33:A:416:LHG:H102	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:605:CLA:H193	25:B:610:CLA:HBB2	1.90	0.53
25:C:502:CLA:H101	31:C:902:LMG:H431	1.90	0.53
28:b:618:BCR:H383	31:l:212:LMG:H331	1.89	0.53
3:c:65:MET:HE3	28:k:102:BCR:HC21	1.90	0.53
3:c:209:GLY:HA2	29:c:903:SQD:H461	1.90	0.53
1:A:218:SER:HA	4:D:272:LEU:HD12	1.89	0.53
35:c:517:DGD:HB22	31:c:519:LMG:H321	1.89	0.53
1:A:46:ILE:HD11	27:A:408:PHO:H51	1.90	0.53
25:B:609:CLA:HBB1	25:B:609:CLA:HMB1	1.90	0.53
25:a:410:CLA:HBB1	25:a:410:CLA:HMB1	1.91	0.53
25:c:502:CLA:HBB1	25:c:502:CLA:HMB1	1.91	0.53
25:c:502:CLA:H51	25:c:509:CLA:H42	1.91	0.53
1:a:218:SER:HA	4:d:272:LEU:HD12	1.89	0.53
25:a:407:CLA:H152	30:a:414:PL9:H261	1.90	0.53
25:B:613:CLA:HBB1	25:B:613:CLA:HMB3	1.91	0.53
35:C:517:DGD:HB22	31:C:519:LMG:H321	1.89	0.53
33:d:409:LHG:H291	16:t:17:LEU:HD22	1.90	0.52
25:A:410:CLA:HMB1	25:A:410:CLA:HBB1	1.91	0.52
25:C:509:CLA:HBB1	25:C:509:CLA:HMB1	1.92	0.52
12:L:6:SER:N	32:a:674:LMT:H4O1	2.07	0.52
25:b:609:CLA:HMB1	25:b:609:CLA:HBB1	1.90	0.52
14:o:79:PHE:HB3	14:o:93:TYR:HB3	1.90	0.52
33:a:416:LHG:H102	31:a:415:LMG:HC92	1.91	0.52
3:c:267:GLN:HG2	25:c:505:CLA:HMD1	1.92	0.52
31:A:415:LMG:H241	29:A:417:SQD:H221	1.91	0.52
32:A:674:LMT:H4O1	12:l:6:SER:N	2.07	0.52
25:C:510:CLA:HMB3	25:C:510:CLA:HBB1	1.91	0.52
25:B:604:CLA:HBB1	25:B:604:CLA:HMB1	1.92	0.52
25:c:508:CLA:HBB1	25:c:508:CLA:HMB1	1.91	0.52
25:d:403:CLA:HMB1	25:d:403:CLA:HBB1	1.92	0.52
3:C:167:LEU:HD23	31:C:902:LMG:H411	1.92	0.52
25:D:403:CLA:HMB1	25:D:403:CLA:HBB1	1.92	0.52
3:c:167:LEU:HD23	31:c:902:LMG:H411	1.92	0.52
25:c:513:CLA:HBB1	25:c:513:CLA:HMB1	1.92	0.52
25:C:502:CLA:H51	25:C:509:CLA:H42	1.91	0.51
29:a:417:SQD:H221	31:a:415:LMG:H241	1.91	0.51
5:e:26:THR:HG21	37:f:101:HEM:C4B	2.45	0.51
15:r:28:ALA:HA	15:r:31:ARG:HE	1.75	0.51
4:d:62:GLY:HA3	5:e:63:LEU:HD13	1.93	0.51
1:A:98:TRP:HA	9:I:1:FME:HG2	1.93	0.51
5:E:26:THR:HG21	37:F:101:HEM:C4B	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:ARG:HG3	5:E:73:ARG:HE	1.76	0.51
1:a:83:VAL:HB	1:a:175:MET:HB2	1.93	0.51
4:d:53:THR:HG22	6:f:39:MET:HE1	1.93	0.51
25:B:605:CLA:HMB3	25:B:605:CLA:HBB1	1.91	0.51
13:M:34:GLY:HA3	32:l:210:LMT:H2B	1.92	0.51
1:a:98:TRP:HA	9:i:1:FME:HG2	1.92	0.51
25:c:509:CLA:HMB1	25:c:509:CLA:HBB1	1.92	0.51
1:A:83:VAL:HB	1:A:175:MET:HB2	1.93	0.51
3:C:465:LEU:HD11	4:D:255:GLN:HG3	1.93	0.51
4:D:62:GLY:HA3	5:E:63:LEU:HD13	1.92	0.51
35:c:517:DGD:HA32	33:j:101:LHG:H292	1.93	0.51
2:B:18:ARG:HH22	31:L:212:LMG:HC5	1.76	0.51
3:C:158:LEU:HD21	25:C:506:CLA:HAB	1.93	0.51
3:C:267:GLN:HG2	25:C:505:CLA:HMD1	1.92	0.51
4:D:53:THR:HG22	6:F:39:MET:HE1	1.93	0.51
30:a:414:PL9:H403	6:f:21:ALA:HB2	1.92	0.51
25:b:604:CLA:HMB1	25:b:604:CLA:HBB1	1.92	0.51
30:A:414:PL9:H403	6:F:21:ALA:HB2	1.92	0.51
25:C:502:CLA:HMB1	25:C:502:CLA:HBB1	1.91	0.51
2:b:18:ARG:HH22	31:l:212:LMG:HC5	1.76	0.51
25:c:510:CLA:HBB1	25:c:510:CLA:HMB3	1.91	0.51
3:C:119:ALA:HB1	32:Z:102:LMT:H111	1.93	0.50
25:C:510:CLA:HED2	25:C:510:CLA:H43	1.93	0.50
15:R:28:ALA:HA	15:R:31:ARG:HE	1.75	0.50
25:b:613:CLA:HBB1	25:b:613:CLA:HMB1	1.92	0.50
21:z:13:LEU:HD22	21:z:55:ILE:HD12	1.93	0.50
2:B:221:PRO:HA	25:B:610:CLA:HED3	1.93	0.50
3:C:115:LEU:HD13	28:K:102:BCR:H323	1.93	0.50
35:C:517:DGD:HA32	33:J:101:LHG:H292	1.93	0.50
25:b:605:CLA:HMB3	25:b:605:CLA:HBB1	1.92	0.50
4:d:55:VAL:HG21	4:d:110:LEU:HD12	1.94	0.50
3:c:115:LEU:HD13	28:k:102:BCR:H323	1.93	0.50
25:c:510:CLA:HED2	25:c:510:CLA:H43	1.93	0.50
4:d:103:ARG:HG3	5:e:73:ARG:HE	1.76	0.50
2:B:39:LEU:HD13	33:a:419:LHG:H241	1.92	0.50
25:C:513:CLA:HBB1	25:C:513:CLA:HMB3	1.94	0.50
2:b:221:PRO:HA	25:b:610:CLA:HED3	1.93	0.50
2:B:384:ARG:HG2	14:O:194:THR:HG22	1.94	0.50
33:A:419:LHG:H241	2:b:39:LEU:HD13	1.92	0.50
4:D:51:GLY:HA3	4:D:78:VAL:HG22	1.94	0.50
25:c:503:CLA:HBB1	25:c:503:CLA:HMB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:179:PHE:HA	4:D:182:LEU:HD12	1.94	0.50
3:c:158:LEU:HD21	25:c:506:CLA:HAB	1.93	0.50
33:A:416:LHG:H302	9:I:7:VAL:HG11	1.93	0.50
25:B:616:CLA:H2	34:B:617:F6C:CBB	2.42	0.50
25:C:506:CLA:HMB3	25:C:506:CLA:HBB1	1.93	0.50
25:C:508:CLA:HMB3	25:C:508:CLA:HBB1	1.92	0.50
4:D:55:VAL:HG21	4:D:110:LEU:HD12	1.94	0.49
5:E:9:PRO:HA	33:E:101:LHG:HC11	1.94	0.49
33:a:416:LHG:H302	9:i:7:VAL:HG11	1.93	0.49
32:L:210:LMT:H2B	13:m:34:GLY:HA3	1.92	0.49
25:b:616:CLA:H2	34:b:617:F6C:CBB	2.42	0.49
2:B:244:VAL:HG21	25:B:611:CLA:HBB	1.94	0.49
25:C:503:CLA:HBB1	25:C:503:CLA:HMB1	1.93	0.49
1:a:85:PRO:HA	1:a:113:TYR:CG	2.47	0.49
3:c:119:ALA:HB1	32:z:102:LMT:H111	1.93	0.49
3:C:399:SER:HA	3:C:413:VAL:HG23	1.95	0.49
25:C:501:CLA:HBB1	25:C:501:CLA:HMB3	1.94	0.49
21:Z:13:LEU:HD22	21:Z:55:ILE:HD12	1.93	0.49
1:A:85:PRO:HA	1:A:113:TYR:CG	2.47	0.49
14:O:192:VAL:HA	17:U:60:ASN:HD21	1.77	0.49
2:b:384:ARG:HG2	14:o:194:THR:HG22	1.94	0.49
25:c:501:CLA:HMB3	25:c:501:CLA:HBB1	1.94	0.49
4:d:314:PHE:HA	4:d:317:LYS:HD3	1.94	0.49
5:e:10:PHE:HE1	37:f:101:HEM:HBD2	1.77	0.49
18:v:29:MET:HE1	18:v:147:LEU:HD21	1.95	0.49
1:A:145:ALA:O	1:A:149:THR:HG23	2.13	0.49
31:c:519:LMG:H211	33:j:101:LHG:H311	1.95	0.49
25:C:511:CLA:HBB1	25:C:511:CLA:HMB3	1.95	0.49
5:E:10:PHE:HE1	37:F:101:HEM:HBD2	1.77	0.49
5:E:35:TRP:CD2	6:F:38:SER:HB3	2.48	0.49
3:c:399:SER:HA	3:c:413:VAL:HG23	1.95	0.49
3:c:465:LEU:HD11	4:d:255:GLN:HG3	1.93	0.49
4:D:314:PHE:HA	4:D:317:LYS:HD3	1.94	0.49
17:U:124:LEU:O	17:U:128:ILE:HG12	2.13	0.49
18:V:60:ASN:HA	18:V:64:ALA:HB2	1.94	0.49
4:d:51:GLY:HA3	4:d:78:VAL:HG22	1.94	0.49
18:v:60:ASN:HA	18:v:64:ALA:HB2	1.94	0.49
25:b:612:CLA:HBB1	25:b:612:CLA:HMB3	1.94	0.48
25:c:511:CLA:HBB1	25:c:511:CLA:HMB3	1.95	0.48
4:d:179:PHE:HA	4:d:182:LEU:HD12	1.94	0.48
5:e:35:TRP:CD2	6:f:38:SER:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:o:192:VAL:HA	17:u:60:ASN:HD21	1.77	0.48
25:C:503:CLA:H18	25:C:510:CLA:HBB2	1.95	0.48
25:c:505:CLA:HBB1	25:c:505:CLA:HMB3	1.95	0.48
5:e:9:PRO:HA	33:e:101:LHG:HC11	1.94	0.48
25:C:505:CLA:HBB1	25:C:505:CLA:HMB3	1.95	0.48
25:c:503:CLA:H18	25:c:510:CLA:HBB2	1.95	0.48
25:c:506:CLA:HMB3	25:c:506:CLA:HBB1	1.93	0.48
29:a:412:SQD:H301	29:a:412:SQD:H331	1.51	0.48
25:b:603:CLA:HBB1	25:b:603:CLA:HMB1	1.95	0.48
1:A:328:GLY:HA3	4:D:325:ALA:HA	1.96	0.48
18:V:67:HIS:HA	18:V:71:VAL:O	2.13	0.48
1:a:145:ALA:O	1:a:149:THR:HG23	2.13	0.48
18:v:67:HIS:HA	18:v:71:VAL:O	2.13	0.48
31:C:519:LMG:H211	33:J:101:LHG:H311	1.95	0.48
2:b:333:GLY:O	2:b:439:SER:HB3	2.14	0.48
25:B:603:CLA:HBB1	25:B:603:CLA:HMB1	1.95	0.48
3:c:409:SER:HB2	18:v:68:VAL:HG23	1.96	0.48
17:u:124:LEU:O	17:u:128:ILE:HG12	2.13	0.48
3:C:77:MET:HE1	3:C:89:ALA:HB2	1.94	0.48
1:a:266:PHE:HE1	29:a:412:SQD:H81	1.79	0.48
28:b:619:BCR:HC8	28:b:619:BCR:H311	1.96	0.48
3:c:77:MET:HE1	3:c:89:ALA:HB2	1.94	0.48
3:C:88:ILE:HG22	3:C:93:PHE:HB2	1.95	0.48
15:R:29:ALA:O	15:R:32:GLN:HG3	2.14	0.48
33:D:409:LHG:H311	16:T:21:ILE:HD11	1.96	0.48
18:V:29:MET:HE1	18:V:147:LEU:HD21	1.95	0.48
2:b:66:VAL:HG12	2:b:71:VAL:HB	1.96	0.48
25:c:508:CLA:HBC3	25:c:510:CLA:H62	1.96	0.48
2:b:244:VAL:HG21	25:b:611:CLA:HHB	1.94	0.47
25:B:612:CLA:HBB1	25:B:612:CLA:HMB3	1.94	0.47
28:D:404:BCR:H10C	33:E:244:LHG:H192	1.96	0.47
28:d:404:BCR:H10C	33:e:244:LHG:H192	1.96	0.47
29:A:417:SQD:H152	29:A:417:SQD:H182	1.51	0.47
28:B:619:BCR:HC8	28:B:619:BCR:H311	1.96	0.47
25:b:602:CLA:CGA	25:b:602:CLA:H52	2.44	0.47
25:c:512:CLA:H62	25:c:512:CLA:H41	1.64	0.47
33:d:409:LHG:H311	16:t:21:ILE:HD11	1.96	0.47
2:B:66:VAL:HG12	2:B:71:VAL:HB	1.96	0.47
29:a:417:SQD:H111	29:a:417:SQD:H142	1.60	0.47
25:c:508:CLA:H162	35:c:518:DGD:HBN2	1.96	0.47
1:a:48:VAL:HG21	1:a:115:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:26:THR:HG21	37:f:101:HEM:C3B	2.50	0.47
1:A:132:TRP:CH2	25:C:505:CLA:HAA2	2.50	0.47
2:B:333:GLY:O	2:B:439:SER:HB3	2.14	0.47
5:E:26:THR:HG21	37:F:101:HEM:C3B	2.50	0.47
1:a:328:GLY:HA3	4:d:325:ALA:HA	1.96	0.47
32:a:674:LMT:H3'	32:a:674:LMT:H1B	1.56	0.47
25:b:607:CLA:HMB3	25:b:607:CLA:HBB1	1.95	0.47
28:b:627:BCR:H20C	28:b:627:BCR:H361	1.71	0.47
1:A:64:ILE:HB	3:C:328:THR:HG21	1.97	0.47
1:A:266:PHE:HE1	29:A:412:SQD:H81	1.79	0.47
29:A:417:SQD:H111	29:A:417:SQD:H142	1.59	0.47
26:A:406:CL7:H142	27:A:408:PHO:H172	1.97	0.47
25:A:405:CLA:HBB1	25:A:405:CLA:HMB1	1.96	0.47
3:C:409:SER:HB2	18:V:68:VAL:HG23	1.96	0.47
1:a:64:ILE:HB	3:c:328:THR:HG21	1.97	0.47
25:a:405:CLA:HBB1	25:a:405:CLA:HMB1	1.96	0.47
29:b:622:SQD:H301	29:b:622:SQD:H332	1.45	0.47
3:c:88:ILE:HG22	3:c:93:PHE:HB2	1.95	0.47
15:r:29:ALA:O	15:r:32:GLN:HG3	2.14	0.47
25:C:508:CLA:HBC3	25:C:510:CLA:H62	1.96	0.46
33:a:416:LHG:H272	33:a:416:LHG:H301	1.67	0.46
32:A:674:LMT:H1B	32:A:674:LMT:H3'	1.56	0.46
28:B:627:BCR:H20C	28:B:627:BCR:H361	1.71	0.46
33:a:416:LHG:H302	33:a:416:LHG:H332	1.80	0.46
2:B:247:PHE:CE2	25:B:603:CLA:H102	2.50	0.46
2:B:441:GLY:HA2	14:O:204:ALA:HB3	1.97	0.46
25:B:602:CLA:H52	25:B:602:CLA:CGA	2.44	0.46
1:A:34:PHE:HE1	25:C:505:CLA:H92	1.80	0.46
3:c:144:TRP:CH2	25:c:509:CLA:H171	2.51	0.46
1:a:132:TRP:CH2	25:c:505:CLA:HAA2	2.50	0.46
1:A:48:VAL:HG21	1:A:115:MET:HE2	1.96	0.46
29:A:412:SQD:H152	29:A:412:SQD:H121	1.72	0.46
2:b:441:GLY:HA2	14:o:204:ALA:HB3	1.97	0.46
25:b:604:CLA:HMC3	25:b:605:CLA:H202	1.98	0.46
1:a:270:ARG:HG3	4:d:235:PHE:HB2	1.97	0.46
18:v:31:GLU:O	18:v:35:THR:HG23	2.16	0.46
1:A:86:MET:HG2	1:A:90:ILE:HD12	1.98	0.46
31:B:628:LMG:H442	7:G:28:ALA:HB1	1.98	0.46
29:h:102:SQD:H321	29:h:102:SQD:H291	1.73	0.46
1:A:270:ARG:HG3	4:D:235:PHE:HB2	1.97	0.46
2:b:247:PHE:CE2	25:b:603:CLA:H102	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:508:CLA:H162	35:C:518:DGD:HBN2	1.96	0.45
16:T:1:FME:SD	13:m:6:LEU:HD21	2.57	0.45
26:a:406:CL7:H142	27:a:408:PHO:H172	1.97	0.45
31:b:628:LMG:H442	7:g:28:ALA:HB1	1.98	0.45
32:M:101:LMT:H42	16:t:1:FME:HE1	1.99	0.45
16:T:1:FME:HE1	32:m:101:LMT:H42	1.99	0.45
25:b:615:CLA:H61	25:b:615:CLA:H41	1.78	0.45
25:B:604:CLA:HMC3	25:B:605:CLA:H202	1.98	0.45
25:B:607:CLA:HMB1	25:B:607:CLA:HBB1	1.97	0.45
3:C:144:TRP:CH2	25:C:509:CLA:H171	2.51	0.45
25:C:512:CLA:H41	25:C:512:CLA:H62	1.64	0.45
1:a:86:MET:HG2	1:a:90:ILE:HD12	1.98	0.45
14:O:60:ILE:HG21	14:O:121:LEU:HD21	1.99	0.45
1:a:34:PHE:HE1	25:c:505:CLA:H92	1.80	0.45
1:a:133:GLU:O	1:a:137:ARG:HG2	2.17	0.45
25:b:611:CLA:H122	25:b:616:CLA:HAA1	1.98	0.45
28:b:619:BCR:HC21	29:b:622:SQD:H172	1.99	0.45
14:o:84:PRO:HB3	14:o:91:ALA:HB2	1.99	0.45
33:A:416:LHG:H272	33:A:416:LHG:H301	1.67	0.45
28:B:619:BCR:HC21	29:B:622:SQD:H172	1.99	0.45
29:B:622:SQD:H301	29:B:622:SQD:H332	1.45	0.45
4:D:134:ARG:HD2	4:D:134:ARG:HA	1.71	0.45
1:a:216:HIS:HA	30:a:414:PL9:O1	2.16	0.45
2:b:149:LEU:HD21	31:b:628:LMG:H371	1.99	0.45
3:c:452:ILE:HG21	3:c:457:GLU:HG3	1.98	0.45
27:A:408:PHO:H2	27:A:408:PHO:H61	1.73	0.45
13:M:27:ILE:HG22	13:m:28:GLN:HB3	1.99	0.45
2:B:243:ALA:HA	2:B:246:PHE:CD1	2.52	0.45
25:B:611:CLA:H122	25:B:616:CLA:HAA1	1.98	0.45
14:O:84:PRO:HB3	14:O:91:ALA:HB2	1.98	0.45
3:c:84:LEU:HD13	25:c:503:CLA:HED3	1.99	0.45
1:A:216:HIS:HA	30:A:414:PL9:O1	2.16	0.45
2:b:201:HIS:HB2	25:b:603:CLA:CHB	2.47	0.45
1:a:120:TYR:CZ	27:a:408:PHO:H142	2.52	0.45
29:d:407:SQD:H342	29:d:407:SQD:H372	1.65	0.45
2:B:341:LEU:HD12	2:B:429:VAL:HG12	1.98	0.45
25:a:410:CLA:H61	25:a:410:CLA:H41	1.87	0.45
25:c:504:CLA:HBB1	25:c:504:CLA:HMB3	1.99	0.45
1:A:120:TYR:CZ	27:A:408:PHO:H142	2.52	0.44
1:A:133:GLU:O	1:A:137:ARG:HG2	2.17	0.44
2:B:149:LEU:HD21	31:B:628:LMG:H371	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:452:ILE:HG21	3:C:457:GLU:HG3	1.98	0.44
25:C:504:CLA:HMB3	25:C:504:CLA:HBB1	1.99	0.44
5:E:20:TRP:CD1	10:J:7:ILE:HD12	2.52	0.44
18:V:31:GLU:O	18:V:35:THR:HG23	2.16	0.44
2:b:315:VAL:HG12	2:b:426:LEU:HB3	1.99	0.44
3:C:84:LEU:HD13	25:C:503:CLA:HED3	1.99	0.44
2:b:341:LEU:HD12	2:b:429:VAL:HG12	1.98	0.44
14:o:60:ILE:HG21	14:o:121:LEU:HD21	1.99	0.44
17:u:97:LYS:HG2	17:u:113:LEU:HD13	1.99	0.44
2:B:201:HIS:HB2	25:B:603:CLA:CHB	2.47	0.44
8:H:39:VAL:HG22	33:P:629:LHG:H312	1.98	0.44
27:a:409:PHO:HBA2	25:d:402:CLA:H142	2.00	0.44
25:c:501:CLA:C4D	25:c:503:CLA:H2	2.48	0.44
8:h:39:VAL:HG22	33:p:629:LHG:H312	1.98	0.44
1:A:78:ILE:HD11	16:T:6:TYR:HB3	1.99	0.44
2:b:243:ALA:HA	2:b:246:PHE:CD1	2.52	0.44
31:d:411:LMG:H392	31:d:411:LMG:H421	1.79	0.44
14:o:46:LYS:HA	14:o:46:LYS:HD3	1.66	0.44
31:C:902:LMG:H421	31:C:902:LMG:H452	1.73	0.44
1:a:297:ASN:HB2	3:c:393:PRO:O	2.18	0.44
2:b:201:HIS:HB2	25:b:603:CLA:C1B	2.48	0.44
8:h:39:VAL:HG13	33:p:629:LHG:H331	2.00	0.44
25:C:501:CLA:C4D	25:C:503:CLA:H2	2.48	0.44
13:M:28:GLN:HB3	13:m:27:ILE:HG22	1.99	0.44
8:H:39:VAL:HG13	33:P:629:LHG:H331	2.00	0.44
12:L:30:VAL:HG11	33:L:101:LHG:H201	2.00	0.44
5:e:20:TRP:CD1	10:j:7:ILE:HD12	2.52	0.44
30:A:414:PL9:H503	19:X:23:VAL:HG21	1.99	0.43
27:A:409:PHO:HBA2	25:D:402:CLA:H142	2.00	0.43
13:M:6:LEU:HD21	16:t:1:FME:SD	2.57	0.43
21:Z:20:LEU:HD23	21:Z:20:LEU:HA	1.85	0.43
16:t:20:ALA:O	16:t:24:ARG:HB3	2.18	0.43
3:c:64:LEU:HD22	25:c:503:CLA:HED2	2.00	0.43
5:e:25:ILE:HD12	15:r:20:TRP:CE2	2.53	0.43
12:l:30:VAL:HG11	33:l:101:LHG:H201	2.00	0.43
2:B:315:VAL:HG12	2:B:426:LEU:HB3	1.99	0.43
28:K:102:BCR:H20C	28:K:102:BCR:H361	1.90	0.43
15:R:28:ALA:HB2	15:R:31:ARG:HH21	1.84	0.43
2:b:55:MET:HE2	2:b:63:MET:HE2	2.00	0.43
17:U:97:LYS:HG2	17:U:113:LEU:HD13	1.99	0.43
25:b:615:CLA:HBB1	25:b:615:CLA:HMB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:110:LEU:HD23	4:d:110:LEU:HA	1.85	0.43
1:a:78:ILE:HD11	16:t:6:TYR:HB3	1.99	0.43
1:a:341:PRO:HD3	17:u:152:TYR:CZ	2.54	0.43
15:r:28:ALA:HB2	15:r:31:ARG:HH21	1.84	0.43
5:E:25:ILE:HD12	15:R:20:TRP:CE2	2.53	0.43
2:b:62:LEU:HD13	25:b:606:CLA:HED3	2.01	0.43
1:A:341:PRO:HD3	17:U:152:TYR:CZ	2.54	0.43
25:B:605:CLA:H52	25:B:605:CLA:H8	1.94	0.43
3:C:306:GLN:HB2	3:C:389:MET:HG3	2.01	0.43
1:a:203:VAL:HG11	25:a:407:CLA:C3D	2.49	0.43
30:a:414:PL9:H503	19:x:23:VAL:HG21	1.99	0.43
33:e:101:LHG:H352	33:e:101:LHG:H322	1.86	0.43
17:u:94:LEU:HD21	17:u:120:GLN:HB3	2.00	0.43
2:B:164:PRO:HG3	25:B:607:CLA:O1D	2.19	0.43
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.01	0.43
4:D:81:PRO:HA	4:D:108:GLY:HA3	2.01	0.43
25:b:616:CLA:H112	25:b:616:CLA:H161	2.01	0.43
14:o:31:GLU:HG2	14:o:32:LEU:H	1.84	0.43
1:A:287:THR:HG23	25:A:405:CLA:HED3	2.00	0.43
2:B:55:MET:HE2	2:B:63:MET:HE2	2.00	0.43
28:B:618:BCR:H341	28:B:618:BCR:H11C	1.86	0.43
3:C:64:LEU:HD22	25:C:503:CLA:HED2	2.00	0.43
13:M:25:LEU:O	13:M:28:GLN:HG3	2.18	0.43
4:d:81:PRO:HA	4:d:108:GLY:HA3	2.01	0.43
1:A:121:ILE:HG21	1:A:160:LEU:HD12	2.01	0.42
21:Z:51:LEU:HD23	21:Z:51:LEU:HA	1.88	0.42
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.01	0.42
1:A:297:ASN:HB2	3:C:393:PRO:O	2.18	0.42
2:B:62:LEU:HD13	25:B:606:CLA:HED3	2.01	0.42
14:O:31:GLU:HG2	14:O:32:LEU:H	1.84	0.42
3:c:397:LEU:HD12	3:c:397:LEU:HA	1.89	0.42
1:A:61:ILE:HD12	1:A:85:PRO:HD2	2.01	0.42
28:A:411:BCR:H20C	28:A:411:BCR:H361	1.86	0.42
16:T:20:ALA:O	16:T:24:ARG:HB3	2.18	0.42
29:A:412:SQD:H301	29:A:412:SQD:H331	1.51	0.42
2:B:383:PHE:CZ	14:O:195:GLY:HA2	2.55	0.42
17:U:94:LEU:HD21	17:U:120:GLN:HB3	2.00	0.42
2:b:383:PHE:CZ	14:o:195:GLY:HA2	2.55	0.42
35:c:517:DGD:HA31	31:c:519:LMG:H331	2.02	0.42
21:z:24:VAL:HG22	21:z:41:LEU:HD22	2.01	0.42
2:B:201:HIS:HB2	25:B:603:CLA:C1B	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C:517:DGD:HA81	35:C:517:DGD:HAE2	1.82	0.42
2:b:164:PRO:HG3	25:b:607:CLA:O1D	2.19	0.42
2:b:296:LYS:HE3	2:b:300:GLU:HB3	2.02	0.42
25:d:402:CLA:HMB3	25:d:402:CLA:HBB1	2.00	0.42
37:f:101:HEM:HMB1	37:f:101:HEM:HBB2	2.02	0.42
13:m:25:LEU:O	13:m:28:GLN:HG3	2.18	0.42
37:F:101:HEM:HBB2	37:F:101:HEM:HMB1	2.02	0.42
29:b:622:SQD:H441	32:m:101:LMT:H22	2.02	0.42
25:c:502:CLA:H71	31:c:902:LMG:H431	2.02	0.42
31:p:628:LMG:H201	31:p:628:LMG:H232	1.87	0.42
2:B:296:LYS:HE3	2:B:300:GLU:HB3	2.01	0.42
29:D:407:SQD:H342	29:D:407:SQD:H372	1.65	0.42
1:a:86:MET:HE1	1:a:114:GLN:NE2	2.35	0.42
2:b:25:MET:HE1	2:b:108:PHE:CD1	2.55	0.42
15:r:31:ARG:O	15:r:34:GLN:HG3	2.20	0.42
28:A:411:BCR:H24C	28:A:411:BCR:H371	1.91	0.42
2:B:13:ILE:HG13	25:B:613:CLA:HAC2	2.02	0.42
25:B:603:CLA:H141	29:H:102:SQD:H192	2.02	0.42
28:B:619:BCR:H15C	28:B:619:BCR:H351	1.92	0.42
7:G:11:GLU:H	7:G:11:GLU:HG2	1.69	0.42
32:M:101:LMT:H2'	32:M:101:LMT:H12	1.85	0.42
14:O:46:LYS:HD3	14:O:46:LYS:HA	1.66	0.42
3:c:108:PHE:HE2	28:c:514:BCR:HC31	1.84	0.42
3:c:306:GLN:HB2	3:c:389:MET:HG3	2.01	0.42
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.55	0.42
15:R:31:ARG:O	15:R:34:GLN:HG3	2.20	0.42
21:Z:24:VAL:HG22	21:Z:41:LEU:HD22	2.01	0.42
1:a:287:THR:HG23	25:a:405:CLA:HED3	2.00	0.42
29:A:417:SQD:H302	29:A:417:SQD:H271	1.70	0.42
25:D:402:CLA:HBB1	25:D:402:CLA:HMB3	2.01	0.42
11:K:43:PRO:O	11:K:46:PHE:HB2	2.20	0.42
14:o:251:ASP:HB2	14:o:255:LYS:HD2	2.02	0.42
1:A:163:PRO:HG3	1:A:172:GLY:HA2	2.02	0.41
1:A:203:VAL:HG11	25:A:407:CLA:C3D	2.49	0.41
25:C:501:CLA:H172	35:C:516:DGD:HB72	2.02	0.41
25:C:502:CLA:H71	31:C:902:LMG:H431	2.02	0.41
28:K:101:BCR:H321	28:K:101:BCR:HC8	2.02	0.41
1:a:61:ILE:HD12	1:a:85:PRO:HD2	2.01	0.41
1:A:86:MET:HE1	1:A:114:GLN:NE2	2.35	0.41
3:C:108:PHE:HE2	28:C:514:BCR:HC31	1.85	0.41
14:O:188:LYS:HD2	14:O:188:LYS:HA	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:251:ASP:HB2	14:O:255:LYS:HD2	2.02	0.41
15:R:21:ALA:O	15:R:25:ILE:HG12	2.21	0.41
29:a:412:SQD:H121	29:a:412:SQD:H152	1.72	0.41
33:E:101:LHG:H352	33:E:101:LHG:H322	1.86	0.41
1:a:163:PRO:HG3	1:a:172:GLY:HA2	2.02	0.41
18:v:130:MET:HE3	18:v:130:MET:HB3	1.94	0.41
1:A:310:SER:HB3	18:V:27:VAL:O	2.21	0.41
35:C:517:DGD:HA31	31:C:519:LMG:H331	2.02	0.41
1:a:122:PRO:HD3	35:c:516:DGD:HAT2	2.03	0.41
28:c:514:BCR:H20C	28:c:514:BCR:H361	1.86	0.41
2:B:158:LEU:HB3	2:B:199:VAL:HG22	2.01	0.41
33:J:101:LHG:H182	20:Y:26:MET:HE1	2.02	0.41
18:V:27:VAL:HG23	18:V:29:MET:HG3	2.03	0.41
1:a:121:ILE:HG21	1:a:160:LEU:HD12	2.01	0.41
2:b:158:LEU:HB3	2:b:199:VAL:HG22	2.01	0.41
18:v:27:VAL:HG23	18:v:29:MET:HG3	2.03	0.41
25:B:616:CLA:H161	25:B:616:CLA:H112	2.01	0.41
29:B:622:SQD:H441	32:M:101:LMT:H22	2.02	0.41
3:C:182:TRP:CH2	3:C:355:LYS:HG2	2.56	0.41
2:b:3:LEU:HD13	2:b:8:VAL:HA	2.03	0.41
3:c:379:PRO:HA	3:c:382:ILE:HD12	2.02	0.41
25:c:501:CLA:HBC1	25:c:502:CLA:H93	2.02	0.41
15:r:21:ALA:O	15:r:25:ILE:HG12	2.21	0.41
1:A:219:LEU:HD12	30:A:414:PL9:C4	2.50	0.41
25:A:410:CLA:H61	25:A:410:CLA:H41	1.87	0.41
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.56	0.41
25:B:606:CLA:H112	25:B:616:CLA:H42	2.03	0.41
13:M:6:LEU:HD23	13:M:6:LEU:HA	1.86	0.41
28:b:619:BCR:H15C	28:b:619:BCR:H351	1.92	0.41
3:c:182:TRP:CH2	3:c:355:LYS:HG2	2.56	0.41
1:A:317:THR:HA	4:D:63:VAL:HG13	2.03	0.41
2:b:13:ILE:HG13	25:b:613:CLA:HAC2	2.02	0.41
25:c:501:CLA:H172	35:c:516:DGD:HB72	2.02	0.41
11:k:43:PRO:O	11:k:46:PHE:HB2	2.20	0.41
31:P:628:LMG:H231	31:P:628:LMG:H262	1.94	0.41
33:A:416:LHG:H302	33:A:416:LHG:H332	1.80	0.41
28:B:620:BCR:H331	31:B:628:LMG:H402	2.03	0.41
3:C:395:GLY:HA3	3:C:413:VAL:HG22	2.02	0.41
25:C:511:CLA:HBA1	28:K:102:BCR:H271	2.03	0.41
32:L:213:LMT:H1B	32:L:213:LMT:H3'	1.62	0.41
1:a:219:LEU:HD12	30:a:414:PL9:C4	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:409:PHO:H72	27:a:409:PHO:H112	1.89	0.41
2:b:226:TYR:CD2	2:b:231:MET:HB2	2.56	0.41
25:b:603:CLA:H141	29:h:102:SQD:H192	2.02	0.41
25:b:606:CLA:H112	25:b:616:CLA:H42	2.03	0.41
1:a:42:LEU:HD23	1:a:42:LEU:HA	1.90	0.41
25:a:407:CLA:H102	25:a:407:CLA:H61	1.91	0.41
28:k:101:BCR:H321	28:k:101:BCR:HC8	2.02	0.41
25:C:504:CLA:H161	25:C:504:CLA:H121	1.90	0.40
35:C:517:DGD:HA52	33:J:101:LHG:H332	2.03	0.40
29:a:417:SQD:H152	29:a:417:SQD:H182	1.51	0.40
3:c:395:GLY:HA3	3:c:413:VAL:HG22	2.02	0.40
25:c:504:CLA:H121	25:c:504:CLA:H161	1.90	0.40
31:c:902:LMG:H381	31:c:902:LMG:H412	1.96	0.40
1:A:163:PRO:HG3	1:A:172:GLY:CA	2.52	0.40
2:B:149:LEU:HD13	25:B:606:CLA:H91	2.04	0.40
28:D:404:BCR:H20C	28:D:404:BCR:H361	1.88	0.40
1:a:317:THR:HA	4:d:63:VAL:HG13	2.03	0.40
2:b:112:CYS:HA	28:b:618:BCR:H282	2.03	0.40
33:j:101:LHG:H182	20:y:26:MET:HE1	2.02	0.40
14:o:31:GLU:HB3	14:o:33:LEU:HG	2.04	0.40
3:C:379:PRO:HA	3:C:382:ILE:HD12	2.02	0.40
25:C:505:CLA:H151	25:C:505:CLA:H112	1.92	0.40
25:C:508:CLA:HBA2	25:C:510:CLA:H11	2.03	0.40
25:b:605:CLA:HBA1	25:b:606:CLA:O1A	2.21	0.40
3:c:269:LEU:HD21	25:c:508:CLA:CAB	2.51	0.40
25:c:511:CLA:HBA1	28:k:102:BCR:H271	2.03	0.40
28:B:619:BCR:H24C	28:B:619:BCR:H371	1.87	0.40
25:C:501:CLA:HBC1	25:C:502:CLA:H93	2.02	0.40
1:a:163:PRO:HG3	1:a:172:GLY:CA	2.52	0.40
33:a:416:LHG:HC91	9:i:4:LEU:HD22	2.04	0.40
32:m:101:LMT:H2'	32:m:101:LMT:H12	1.85	0.40
3:C:269:LEU:HD21	25:C:508:CLA:CAB	2.51	0.40
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.04	0.40
11:K:40:PRO:O	11:K:43:PRO:HD2	2.21	0.40
1:a:215:MET:HE3	1:a:215:MET:HB3	1.91	0.40
1:a:310:SER:HB3	18:v:27:VAL:O	2.21	0.40
2:b:334:ASP:HA	14:o:204:ALA:HB1	2.03	0.40
3:c:180:ASP:O	3:c:187:GLY:HA2	2.21	0.40
13:m:6:LEU:HD23	13:m:6:LEU:HA	1.86	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	332/369 (90%)	326 (98%)	6 (2%)	0	100	100
1	a	332/369 (90%)	326 (98%)	6 (2%)	0	100	100
2	B	502/520 (96%)	499 (99%)	3 (1%)	0	100	100
2	b	502/520 (96%)	499 (99%)	3 (1%)	0	100	100
3	C	448/466 (96%)	443 (99%)	5 (1%)	0	100	100
3	c	448/466 (96%)	443 (99%)	5 (1%)	0	100	100
4	D	338/352 (96%)	332 (98%)	6 (2%)	0	100	100
4	d	338/352 (96%)	332 (98%)	6 (2%)	0	100	100
5	E	76/82 (93%)	75 (99%)	1 (1%)	0	100	100
5	e	76/82 (93%)	75 (99%)	1 (1%)	0	100	100
6	F	34/44 (77%)	34 (100%)	0	0	100	100
6	f	34/44 (77%)	34 (100%)	0	0	100	100
7	G	38/48 (79%)	38 (100%)	0	0	100	100
7	g	38/48 (79%)	38 (100%)	0	0	100	100
8	H	65/69 (94%)	64 (98%)	1 (2%)	0	100	100
8	h	65/69 (94%)	64 (98%)	1 (2%)	0	100	100
9	I	32/38 (84%)	30 (94%)	2 (6%)	0	100	100
9	i	32/38 (84%)	30 (94%)	2 (6%)	0	100	100
10	J	34/39 (87%)	32 (94%)	2 (6%)	0	100	100
10	j	34/39 (87%)	32 (94%)	2 (6%)	0	100	100
11	K	35/60 (58%)	35 (100%)	0	0	100	100
11	k	35/60 (58%)	35 (100%)	0	0	100	100
12	L	34/41 (83%)	34 (100%)	0	0	100	100
12	l	34/41 (83%)	34 (100%)	0	0	100	100
13	M	32/37 (86%)	31 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	32/37 (86%)	31 (97%)	1 (3%)	0	100	100
14	O	241/274 (88%)	234 (97%)	7 (3%)	0	100	100
14	o	241/274 (88%)	234 (97%)	7 (3%)	0	100	100
15	R	31/41 (76%)	31 (100%)	0	0	100	100
15	r	31/41 (76%)	31 (100%)	0	0	100	100
16	T	28/32 (88%)	28 (100%)	0	0	100	100
16	t	28/32 (88%)	28 (100%)	0	0	100	100
17	U	95/153 (62%)	92 (97%)	3 (3%)	0	100	100
17	u	95/153 (62%)	92 (97%)	3 (3%)	0	100	100
18	V	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
18	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
19	X	36/39 (92%)	36 (100%)	0	0	100	100
19	x	36/39 (92%)	36 (100%)	0	0	100	100
20	Y	30/43 (70%)	30 (100%)	0	0	100	100
20	y	30/43 (70%)	30 (100%)	0	0	100	100
21	Z	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
21	z	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
All	All	5312/5946 (89%)	5224 (98%)	88 (2%)	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	273/301 (91%)	273 (100%)	0	100	100
1	a	273/301 (91%)	273 (100%)	0	100	100
2	B	402/412 (98%)	402 (100%)	0	100	100
2	b	402/412 (98%)	402 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	341/357 (96%)	340 (100%)	1 (0%)	86	92
3	c	341/357 (96%)	340 (100%)	1 (0%)	86	92
4	D	281/291 (97%)	281 (100%)	0	100	100
4	d	281/291 (97%)	281 (100%)	0	100	100
5	E	69/73 (94%)	69 (100%)	0	100	100
5	e	69/73 (94%)	69 (100%)	0	100	100
6	F	31/39 (80%)	31 (100%)	0	100	100
6	f	31/39 (80%)	31 (100%)	0	100	100
7	G	30/37 (81%)	30 (100%)	0	100	100
7	g	30/37 (81%)	30 (100%)	0	100	100
8	H	56/58 (97%)	56 (100%)	0	100	100
8	h	56/58 (97%)	56 (100%)	0	100	100
9	I	29/33 (88%)	29 (100%)	0	100	100
9	i	29/33 (88%)	29 (100%)	0	100	100
10	J	28/30 (93%)	28 (100%)	0	100	100
10	j	28/30 (93%)	28 (100%)	0	100	100
11	K	32/52 (62%)	32 (100%)	0	100	100
11	k	32/52 (62%)	32 (100%)	0	100	100
12	L	34/39 (87%)	34 (100%)	0	100	100
12	l	34/39 (87%)	34 (100%)	0	100	100
13	M	29/32 (91%)	29 (100%)	0	100	100
13	m	29/32 (91%)	29 (100%)	0	100	100
14	O	196/228 (86%)	196 (100%)	0	100	100
14	o	196/228 (86%)	196 (100%)	0	100	100
15	R	24/31 (77%)	24 (100%)	0	100	100
15	r	24/31 (77%)	24 (100%)	0	100	100
16	T	23/25 (92%)	23 (100%)	0	100	100
16	t	23/25 (92%)	23 (100%)	0	100	100
17	U	80/129 (62%)	80 (100%)	0	100	100
17	u	80/129 (62%)	80 (100%)	0	100	100
18	V	114/132 (86%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	v	114/132 (86%)	114 (100%)	0	100	100
19	X	33/34 (97%)	33 (100%)	0	100	100
19	x	33/34 (97%)	33 (100%)	0	100	100
20	Y	26/34 (76%)	26 (100%)	0	100	100
20	y	26/34 (76%)	26 (100%)	0	100	100
21	Z	51/52 (98%)	51 (100%)	0	100	100
21	z	51/52 (98%)	51 (100%)	0	100	100
All	All	4364/4838 (90%)	4362 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	320	ASN
3	c	320	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	HIS
2	B	129	ASN
2	B	489	GLN
3	C	40	ASN
3	C	222	ASN
3	C	309	ASN
4	D	350	ASN
14	O	183	ASN
14	O	221	ASN
1	a	338	HIS
2	b	129	ASN
2	b	489	GLN
3	c	40	ASN
3	c	222	ASN
3	c	309	ASN
3	c	411	ASN
4	d	186	GLN
4	d	350	ASN
14	o	183	ASN
14	o	221	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	$\# Z > 2$
19	FME	X	1	19	8,9,10	0.35	0	7,9,11	0.90	0
13	FME	m	1	13	8,9,10	0.35	0	7,9,11	0.91	0
9	FME	i	1	9	8,9,10	0.34	0	7,9,11	0.99	0
19	FME	x	1	19	8,9,10	0.35	0	7,9,11	0.90	0
16	FME	T	1	16	8,9,10	0.35	0	7,9,11	0.95	0
9	FME	I	1	9	8,9,10	0.34	0	7,9,11	0.99	0
16	FME	t	1	16	8,9,10	0.35	0	7,9,11	0.95	0
13	FME	M	1	13	8,9,10	0.35	0	7,9,11	0.91	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
19	FME	X	1	19	-	0/7/9/11	-
13	FME	m	1	13	-	2/7/9/11	-
9	FME	i	1	9	-	4/7/9/11	-
19	FME	x	1	19	-	0/7/9/11	-
16	FME	T	1	16	-	2/7/9/11	-
9	FME	I	1	9	-	4/7/9/11	-
16	FME	t	1	16	-	2/7/9/11	-
13	FME	M	1	13	-	2/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	1	FME	N-CA-CB-CG
9	I	1	FME	C-CA-CB-CG
9	i	1	FME	N-CA-CB-CG
9	i	1	FME	C-CA-CB-CG
9	I	1	FME	CA-CB-CG-SD
9	i	1	FME	CA-CB-CG-SD
16	T	1	FME	N-CA-CB-CG
16	t	1	FME	N-CA-CB-CG
16	T	1	FME	CB-CG-SD-CE
16	t	1	FME	CB-CG-SD-CE
13	M	1	FME	CB-CG-SD-CE
13	m	1	FME	CB-CG-SD-CE
13	M	1	FME	CA-CB-CG-SD
13	m	1	FME	CA-CB-CG-SD
9	I	1	FME	CB-CG-SD-CE
9	i	1	FME	CB-CG-SD-CE

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	i	1	FME	1	0
16	T	1	FME	2	0
9	I	1	FME	1	0
16	t	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 184 ligands modelled in this entry, 6 are monoatomic - leaving 178 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
38	HEC	V	201	18	46,50,50	3.53	5 (10%)	60,82,82	1.49	8 (13%)
28	BCR	B	627	-	41,41,41	0.32	0	56,56,56	0.92	2 (3%)
31	LMG	D	411	-	51,51,55	0.59	0	59,59,63	0.65	1 (1%)
32	LMT	z	102	-	36,36,36	0.54	0	47,47,47	1.00	2 (4%)
31	LMG	A	415	-	48,48,55	0.59	0	56,56,63	0.69	0
28	BCR	a	411	-	41,41,41	0.34	0	56,56,56	0.49	0
32	LMT	C	904	-	33,33,36	0.61	0	44,44,47	0.63	0
29	SQD	D	407	-	44,45,54	1.57	5 (11%)	53,56,65	1.61	8 (15%)
35	DGD	C	516	-	63,63,67	0.66	0	77,77,81	0.69	1 (1%)
33	LHG	D	410	-	40,40,48	0.58	0	43,46,54	0.54	0
25	CLA	B	607	2	69,73,73	1.23	8 (11%)	83,113,113	0.93	4 (4%)
34	F6C	B	614	2	72,74,74	1.67	10 (13%)	81,114,114	2.02	15 (18%)
30	PL9	D	405	-	55,55,55	1.46	7 (12%)	68,69,69	1.52	12 (17%)
25	CLA	c	502	3	69,73,73	1.19	8 (11%)	83,113,113	0.99	5 (6%)
33	LHG	E	101	-	48,48,48	0.52	0	51,54,54	0.49	0
25	CLA	A	410	1	69,73,73	1.18	8 (11%)	83,113,113	0.97	4 (4%)
25	CLA	B	616	2	69,73,73	1.23	8 (11%)	83,113,113	1.00	4 (4%)
28	BCR	A	411	-	41,41,41	0.33	0	56,56,56	0.49	0
25	CLA	c	505	3	69,73,73	1.21	8 (11%)	83,113,113	0.92	4 (4%)
25	CLA	a	407	39	69,73,73	1.17	6 (8%)	83,113,113	1.00	4 (4%)
25	CLA	A	405	1	69,73,73	1.18	7 (10%)	83,113,113	0.96	4 (4%)
25	CLA	D	403	4	69,73,73	1.19	7 (10%)	83,113,113	0.94	4 (4%)
34	F6C	B	608	39	72,74,74	1.67	11 (15%)	81,114,114	2.02	14 (17%)
25	CLA	b	607	2	69,73,73	1.23	8 (11%)	83,113,113	0.93	4 (4%)
25	CLA	b	609	2	69,73,73	1.18	7 (10%)	83,113,113	0.94	4 (4%)
25	CLA	c	508	3	69,73,73	1.20	8 (11%)	83,113,113	0.93	4 (4%)
29	SQD	c	903	-	37,38,54	1.67	7 (18%)	46,49,65	1.54	8 (17%)
28	BCR	B	620	-	41,41,41	0.35	0	56,56,56	0.70	0
28	BCR	b	619	-	41,41,41	0.35	0	56,56,56	0.69	1 (1%)
25	CLA	d	402	4	69,73,73	1.21	8 (11%)	83,113,113	0.94	4 (4%)
25	CLA	c	511	3	69,73,73	1.22	8 (11%)	83,113,113	0.94	4 (4%)
32	LMT	b	675	-	25,25,36	0.53	0	30,30,47	0.68	0
33	LHG	a	419	-	48,48,48	0.51	0	51,54,54	0.50	0
25	CLA	C	504	39	69,73,73	1.20	7 (10%)	83,113,113	0.93	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	503	3	69,73,73	1.21	8 (11%)	83,113,113	0.99	5 (6%)
36	BCT	d	401	23	2,3,3	0.89	0	2,3,3	3.27	2 (100%)
28	BCR	k	102	-	41,41,41	0.34	0	56,56,56	0.84	1 (1%)
30	PL9	a	414	-	55,55,55	1.11	4 (7%)	68,69,69	1.50	13 (19%)
35	DGD	C	517	-	63,63,67	0.64	0	77,77,81	0.71	0
31	LMG	b	628	-	55,55,55	0.52	0	63,63,63	0.60	0
25	CLA	C	502	3	69,73,73	1.19	8 (11%)	83,113,113	0.99	5 (6%)
32	LMT	L	213	-	36,36,36	0.54	0	47,47,47	0.78	1 (2%)
37	HEM	f	101	5,6	50,50,50	1.38	7 (14%)	66,82,82	1.08	4 (6%)
28	BCR	c	514	-	41,41,41	0.31	0	56,56,56	0.59	0
25	CLA	B	613	2	69,73,73	1.18	7 (10%)	83,113,113	1.01	4 (4%)
32	LMT	l	210	-	36,36,36	0.53	0	47,47,47	1.01	1 (2%)
25	CLA	B	609	2	69,73,73	1.19	7 (10%)	83,113,113	0.94	4 (4%)
25	CLA	b	603	2	69,73,73	1.18	6 (8%)	83,113,113	0.94	4 (4%)
31	LMG	C	519	-	51,51,55	0.55	0	59,59,63	0.68	1 (1%)
37	HEM	F	101	5,6	50,50,50	1.38	7 (14%)	66,82,82	1.08	4 (6%)
25	CLA	d	403	4	69,73,73	1.19	7 (10%)	83,113,113	0.94	5 (6%)
35	DGD	C	518	-	63,63,67	0.65	0	77,77,81	0.69	1 (1%)
32	LMT	a	674	-	36,36,36	0.56	0	47,47,47	0.76	0
33	LHG	P	629	-	48,48,48	0.49	0	51,54,54	0.63	1 (1%)
27	PHO	A	409	-	58,69,69	1.97	9 (15%)	56,99,99	1.58	7 (12%)
26	CL7	a	406	39	71,73,73	1.16	5 (7%)	80,113,113	0.87	3 (3%)
31	LMG	C	902	-	53,53,55	0.46	0	61,61,63	0.61	0
22	OEX	a	401	1,3	0,15,15	-	-	-	-	-
25	CLA	a	410	1	69,73,73	1.18	8 (11%)	83,113,113	0.97	4 (4%)
32	LMT	m	101	-	36,36,36	0.57	0	47,47,47	0.64	0
33	LHG	L	101	-	48,48,48	0.53	0	51,54,54	0.52	0
25	CLA	b	611	39	69,73,73	1.18	7 (10%)	83,113,113	1.01	4 (4%)
31	LMG	c	902	-	53,53,55	0.46	0	61,61,63	0.61	0
22	OEX	A	401	1,3	0,15,15	-	-	-	-	-
29	SQD	a	412	-	53,54,54	1.52	9 (16%)	62,65,65	1.42	7 (11%)
25	CLA	C	509	3	69,73,73	1.20	8 (11%)	83,113,113	0.96	5 (6%)
25	CLA	D	402	4	69,73,73	1.20	8 (11%)	83,113,113	0.94	4 (4%)
25	CLA	B	602	39	69,73,73	1.18	7 (10%)	83,113,113	0.98	4 (4%)
25	CLA	b	610	2	69,73,73	1.19	8 (11%)	83,113,113	1.03	5 (6%)
25	CLA	b	612	2	69,73,73	1.21	7 (10%)	83,113,113	1.00	4 (4%)
28	BCR	d	404	-	41,41,41	0.32	0	56,56,56	0.67	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	504	39	69,73,73	1.20	7 (10%)	83,113,113	0.93	5 (6%)
25	CLA	c	506	3	69,73,73	1.19	7 (10%)	83,113,113	0.95	4 (4%)
30	PL9	A	414	-	55,55,55	1.11	4 (7%)	68,69,69	1.50	13 (19%)
25	CLA	c	513	3	60,64,73	1.26	7 (11%)	72,102,113	0.97	4 (5%)
25	CLA	A	407	39	69,73,73	1.18	6 (8%)	83,113,113	1.00	4 (4%)
29	SQD	h	102	-	53,54,54	1.46	5 (9%)	62,65,65	1.60	8 (12%)
33	LHG	e	244	-	48,48,48	0.51	0	51,54,54	0.50	0
25	CLA	b	615	2	69,73,73	1.19	7 (10%)	83,113,113	0.99	4 (4%)
33	LHG	d	409	-	48,48,48	0.52	0	51,54,54	0.49	0
25	CLA	B	610	2	69,73,73	1.20	8 (11%)	83,113,113	1.03	5 (6%)
28	BCR	D	404	-	41,41,41	0.32	0	56,56,56	0.67	1 (1%)
34	F6C	b	614	2	72,74,74	1.67	10 (13%)	81,114,114	2.02	15 (18%)
27	PHO	A	408	-	58,69,69	1.95	10 (17%)	56,99,99	1.54	7 (12%)
25	CLA	C	506	3	69,73,73	1.19	7 (10%)	83,113,113	0.95	4 (4%)
29	SQD	b	622	-	53,54,54	1.49	6 (11%)	62,65,65	1.57	9 (14%)
31	LMG	l	212	-	55,55,55	0.51	0	63,63,63	0.66	0
25	CLA	B	603	2	69,73,73	1.18	6 (8%)	83,113,113	0.94	4 (4%)
28	BCR	B	618	-	41,41,41	0.32	0	56,56,56	0.79	1 (1%)
35	DGD	c	517	-	63,63,67	0.64	0	77,77,81	0.71	0
30	PL9	d	405	-	55,55,55	1.46	7 (12%)	68,69,69	1.52	12 (17%)
25	CLA	B	615	2	69,73,73	1.19	7 (10%)	83,113,113	0.99	4 (4%)
33	LHG	a	416	-	48,48,48	0.51	0	51,54,54	0.51	0
31	LMG	a	415	-	48,48,55	0.59	0	56,56,63	0.69	0
32	LMT	F	102	-	36,36,36	0.55	0	47,47,47	0.65	0
25	CLA	C	512	3	69,73,73	1.19	6 (8%)	83,113,113	0.97	4 (4%)
32	LMT	f	102	-	36,36,36	0.55	0	47,47,47	0.65	0
25	CLA	c	509	3	69,73,73	1.20	8 (11%)	83,113,113	0.96	5 (6%)
28	BCR	c	515	-	41,41,41	0.37	0	56,56,56	0.69	1 (1%)
25	CLA	B	611	39	69,73,73	1.18	7 (10%)	83,113,113	1.01	4 (4%)
28	BCR	k	101	-	41,41,41	0.33	0	56,56,56	0.83	0
25	CLA	B	606	2	69,73,73	1.20	6 (8%)	83,113,113	1.13	5 (6%)
25	CLA	b	605	2	69,73,73	1.25	8 (11%)	83,113,113	0.88	4 (4%)
25	CLA	B	612	2	69,73,73	1.21	7 (10%)	83,113,113	1.00	4 (4%)
29	SQD	A	412	-	53,54,54	1.52	9 (16%)	62,65,65	1.42	7 (11%)
34	F6C	b	617	2	57,59,74	1.85	11 (19%)	63,96,114	2.31	16 (25%)
25	CLA	c	501	3	69,73,73	1.19	7 (10%)	83,113,113	1.00	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
28	BCR	b	627	-	41,41,41	0.32	0	56,56,56	0.92	2 (3%)
32	LMT	g	104	-	36,36,36	0.57	0	47,47,47	0.64	0
25	CLA	C	505	3	69,73,73	1.21	8 (11%)	83,113,113	0.92	4 (4%)
29	SQD	a	417	-	53,54,54	1.47	7 (13%)	62,65,65	1.49	8 (12%)
33	LHG	A	416	-	48,48,48	0.51	0	51,54,54	0.51	0
28	BCR	K	101	-	41,41,41	0.33	0	56,56,56	0.83	0
31	LMG	d	411	-	51,51,55	0.59	0	59,59,63	0.65	1 (1%)
25	CLA	C	513	3	60,64,73	1.26	7 (11%)	72,102,113	0.97	4 (5%)
28	BCR	B	619	-	41,41,41	0.35	0	56,56,56	0.69	1 (1%)
25	CLA	b	616	2	69,73,73	1.23	8 (11%)	83,113,113	1.00	4 (4%)
29	SQD	B	622	-	53,54,54	1.49	6 (11%)	62,65,65	1.57	9 (14%)
34	F6C	c	507	39	72,74,74	1.67	11 (15%)	81,114,114	2.08	16 (19%)
25	CLA	c	512	3	69,73,73	1.19	6 (8%)	83,113,113	0.97	4 (4%)
32	LMT	B	675	-	25,25,36	0.53	0	30,30,47	0.68	0
32	LMT	c	904	-	33,33,36	0.61	0	44,44,47	0.63	0
28	BCR	K	102	-	41,41,41	0.34	0	56,56,56	0.84	1 (1%)
33	LHG	E	244	-	48,48,48	0.50	0	51,54,54	0.50	0
34	F6C	b	608	39	72,74,74	1.67	11 (15%)	81,114,114	2.02	14 (17%)
25	CLA	C	501	3	69,73,73	1.19	7 (10%)	83,113,113	1.00	5 (6%)
32	LMT	A	675	-	33,33,36	0.59	0	44,44,47	0.80	1 (2%)
31	LMG	L	212	-	55,55,55	0.51	0	63,63,63	0.66	0
32	LMT	L	210	-	36,36,36	0.53	0	47,47,47	1.01	1 (2%)
25	CLA	b	604	2	69,73,73	1.20	8 (11%)	83,113,113	0.90	3 (3%)
25	CLA	C	510	3	69,73,73	1.18	7 (10%)	83,113,113	0.95	4 (4%)
31	LMG	c	519	-	51,51,55	0.55	0	59,59,63	0.68	1 (1%)
31	LMG	B	628	-	55,55,55	0.52	0	63,63,63	0.59	0
33	LHG	D	409	-	48,48,48	0.52	0	51,54,54	0.49	0
34	F6C	B	617	2	57,59,74	1.85	11 (19%)	63,96,114	2.31	16 (25%)
28	BCR	C	515	-	41,41,41	0.37	0	56,56,56	0.69	1 (1%)
25	CLA	b	606	2	69,73,73	1.20	6 (8%)	83,113,113	1.13	5 (6%)
27	PHO	a	409	-	58,69,69	1.97	9 (15%)	56,99,99	1.58	7 (12%)
32	LMT	A	674	-	36,36,36	0.56	0	47,47,47	0.76	0
33	LHG	D	408	-	48,48,48	0.53	0	51,54,54	0.53	0
29	SQD	H	102	-	53,54,54	1.46	5 (9%)	62,65,65	1.60	8 (12%)
26	CL7	A	406	39	71,73,73	1.16	5 (7%)	80,113,113	0.87	3 (3%)
33	LHG	d	410	-	40,40,48	0.58	0	43,46,54	0.54	0
28	BCR	b	618	-	41,41,41	0.32	0	56,56,56	0.79	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	613	2	69,73,73	1.18	7 (10%)	83,113,113	1.01	4 (4%)
32	LMT	G	104	-	36,36,36	0.57	0	47,47,47	0.64	0
29	SQD	d	407	-	44,45,54	1.57	5 (11%)	53,56,65	1.61	8 (15%)
33	LHG	d	408	-	48,48,48	0.53	0	51,54,54	0.53	0
25	CLA	C	503	3	69,73,73	1.21	8 (11%)	83,113,113	0.99	5 (6%)
33	LHG	A	419	-	48,48,48	0.51	0	51,54,54	0.50	0
33	LHG	J	101	-	48,48,48	0.50	0	51,54,54	0.49	0
34	F6C	C	507	39	72,74,74	1.67	11 (15%)	81,114,114	2.08	16 (19%)
25	CLA	c	510	3	69,73,73	1.18	7 (10%)	83,113,113	0.95	4 (4%)
33	LHG	e	101	-	48,48,48	0.52	0	51,54,54	0.49	0
25	CLA	B	604	2	69,73,73	1.20	8 (11%)	83,113,113	0.90	3 (3%)
28	BCR	C	514	-	41,41,41	0.31	0	56,56,56	0.59	0
32	LMT	a	675	-	33,33,36	0.59	0	44,44,47	0.80	1 (2%)
32	LMT	M	101	-	36,36,36	0.57	0	47,47,47	0.64	0
31	LMG	p	628	-	47,47,55	0.50	0	55,55,63	0.61	0
32	LMT	l	213	-	36,36,36	0.54	0	47,47,47	0.78	1 (2%)
25	CLA	b	602	39	69,73,73	1.18	7 (10%)	83,113,113	0.98	4 (4%)
29	SQD	A	417	-	53,54,54	1.47	7 (13%)	62,65,65	1.49	8 (12%)
33	LHG	j	101	-	48,48,48	0.50	0	51,54,54	0.49	0
38	HEC	v	201	18	46,50,50	3.53	5 (10%)	60,82,82	1.49	8 (13%)
33	LHG	l	101	-	48,48,48	0.52	0	51,54,54	0.52	0
33	LHG	p	629	-	48,48,48	0.49	0	51,54,54	0.63	1 (1%)
25	CLA	C	508	3	69,73,73	1.20	8 (11%)	83,113,113	0.93	4 (4%)
32	LMT	Z	102	-	36,36,36	0.54	0	47,47,47	1.00	2 (4%)
35	DGD	c	518	-	63,63,67	0.65	0	77,77,81	0.69	1 (1%)
35	DGD	c	516	-	63,63,67	0.66	0	77,77,81	0.69	1 (1%)
25	CLA	a	405	1	69,73,73	1.18	7 (10%)	83,113,113	0.96	4 (4%)
25	CLA	C	511	3	69,73,73	1.22	8 (11%)	83,113,113	0.94	4 (4%)
28	BCR	b	620	-	41,41,41	0.35	0	56,56,56	0.70	0
27	PHO	a	408	-	58,69,69	1.95	10 (17%)	56,99,99	1.54	7 (12%)
25	CLA	B	605	2	69,73,73	1.25	8 (11%)	83,113,113	0.88	4 (4%)
29	SQD	C	903	-	37,38,54	1.67	7 (18%)	46,49,65	1.54	8 (17%)
31	LMG	P	628	-	47,47,55	0.50	0	55,55,63	0.61	0
36	BCT	D	401	23	2,3,3	0.88	0	2,3,3	3.27	2 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	HEC	V	201	18	-	4/14/54/54	-
28	BCR	B	627	-	-	7/29/63/63	0/2/2/2
31	LMG	D	411	-	-	6/46/66/70	0/1/1/1
32	LMT	z	102	-	-	10/21/61/61	0/2/2/2
31	LMG	A	415	-	-	12/43/63/70	0/1/1/1
28	BCR	a	411	-	-	2/29/63/63	0/2/2/2
32	LMT	C	904	-	-	3/18/58/61	0/2/2/2
29	SQD	D	407	-	-	17/40/60/69	0/1/1/1
35	DGD	C	516	-	-	20/51/91/95	0/2/2/2
33	LHG	D	410	-	-	26/45/45/53	-
25	CLA	B	607	2	-	5/39/115/115	-
34	F6C	B	614	2	1/1/10/16	21/41/97/97	-
30	PL9	D	405	-	-	15/53/73/73	0/1/1/1
25	CLA	c	502	3	-	10/39/115/115	-
33	LHG	E	101	-	-	27/53/53/53	-
25	CLA	A	410	1	-	5/39/115/115	-
25	CLA	B	616	2	-	6/39/115/115	-
28	BCR	A	411	-	-	2/29/63/63	0/2/2/2
25	CLA	c	505	3	-	1/39/115/115	-
25	CLA	a	407	39	-	2/39/115/115	-
25	CLA	A	405	1	-	4/39/115/115	-
34	F6C	B	608	39	1/1/10/16	10/41/97/97	-
25	CLA	D	403	4	-	2/39/115/115	-
25	CLA	b	607	2	-	5/39/115/115	-
25	CLA	b	609	2	-	1/39/115/115	-
25	CLA	c	508	3	-	3/39/115/115	-
29	SQD	c	903	-	-	21/33/53/69	0/1/1/1
28	BCR	B	620	-	-	4/29/63/63	0/2/2/2
28	BCR	b	619	-	-	7/29/63/63	0/2/2/2
25	CLA	d	402	4	-	3/39/115/115	-
25	CLA	c	511	3	-	0/39/115/115	-
32	LMT	b	675	-	-	10/17/37/61	0/1/1/2
33	LHG	a	419	-	-	15/53/53/53	-
25	CLA	C	504	39	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	503	3	-	2/39/115/115	-
28	BCR	k	102	-	-	3/29/63/63	0/2/2/2
30	PL9	a	414	-	-	18/53/73/73	0/1/1/1
35	DGD	C	517	-	-	17/51/91/95	0/2/2/2
31	LMG	b	628	-	-	18/50/70/70	0/1/1/1
25	CLA	C	502	3	-	10/39/115/115	-
32	LMT	L	213	-	-	6/21/61/61	0/2/2/2
37	HEM	f	101	5,6	-	1/14/54/54	-
28	BCR	c	514	-	-	0/29/63/63	0/2/2/2
25	CLA	B	613	2	-	4/39/115/115	-
32	LMT	l	210	-	-	10/21/61/61	0/2/2/2
25	CLA	B	609	2	-	1/39/115/115	-
25	CLA	b	603	2	-	3/39/115/115	-
31	LMG	C	519	-	-	12/46/66/70	0/1/1/1
37	HEM	F	101	5,6	-	1/14/54/54	-
25	CLA	d	403	4	-	2/39/115/115	-
35	DGD	C	518	-	-	16/51/91/95	0/2/2/2
32	LMT	a	674	-	-	6/21/61/61	0/2/2/2
33	LHG	P	629	-	-	21/53/53/53	-
27	PHO	A	409	-	-	3/37/103/103	0/5/6/6
26	CL7	a	406	39	2/2/15/20	2/39/115/115	-
31	LMG	C	902	-	-	18/48/68/70	0/1/1/1
25	CLA	a	410	1	-	5/39/115/115	-
32	LMT	m	101	-	-	7/21/61/61	0/2/2/2
33	LHG	L	101	-	-	11/53/53/53	-
25	CLA	b	611	39	-	1/39/115/115	-
31	LMG	c	902	-	-	18/48/68/70	0/1/1/1
29	SQD	a	412	-	-	25/49/69/69	0/1/1/1
25	CLA	C	509	3	-	5/39/115/115	-
25	CLA	D	402	4	-	3/39/115/115	-
25	CLA	B	602	39	-	9/39/115/115	-
25	CLA	b	610	2	-	3/39/115/115	-
25	CLA	b	612	2	-	0/39/115/115	-
28	BCR	d	404	-	-	8/29/63/63	0/2/2/2
25	CLA	c	504	39	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	506	3	-	1/39/115/115	-
30	PL9	A	414	-	-	18/53/73/73	0/1/1/1
25	CLA	c	513	3	-	3/29/105/115	-
25	CLA	A	407	39	-	2/39/115/115	-
29	SQD	h	102	-	-	19/49/69/69	0/1/1/1
33	LHG	e	244	-	-	24/53/53/53	-
25	CLA	b	615	2	-	6/39/115/115	-
34	F6C	b	614	2	1/1/10/16	21/41/97/97	-
25	CLA	B	610	2	-	3/39/115/115	-
28	BCR	D	404	-	-	8/29/63/63	0/2/2/2
33	LHG	d	409	-	-	12/53/53/53	-
27	PHO	A	408	-	-	4/37/103/103	0/5/6/6
25	CLA	C	506	3	-	1/39/115/115	-
29	SQD	b	622	-	-	18/49/69/69	0/1/1/1
31	LMG	l	212	-	-	21/50/70/70	0/1/1/1
25	CLA	B	603	2	-	3/39/115/115	-
28	BCR	B	618	-	-	4/29/63/63	0/2/2/2
35	DGD	c	517	-	-	17/51/91/95	0/2/2/2
30	PL9	d	405	-	-	15/53/73/73	0/1/1/1
25	CLA	B	615	2	-	6/39/115/115	-
33	LHG	a	416	-	-	24/53/53/53	-
31	LMG	a	415	-	-	12/43/63/70	0/1/1/1
32	LMT	F	102	-	-	5/21/61/61	0/2/2/2
25	CLA	C	512	3	-	6/39/115/115	-
32	LMT	f	102	-	-	5/21/61/61	0/2/2/2
25	CLA	c	509	3	-	5/39/115/115	-
28	BCR	c	515	-	-	4/29/63/63	0/2/2/2
25	CLA	B	611	39	-	1/39/115/115	-
28	BCR	k	101	-	-	6/29/63/63	0/2/2/2
25	CLA	B	606	2	-	6/39/115/115	-
25	CLA	b	605	2	-	2/39/115/115	-
25	CLA	B	612	2	-	0/39/115/115	-
34	F6C	b	617	2	1/1/7/16	6/23/79/97	-
29	SQD	A	412	-	-	25/49/69/69	0/1/1/1
25	CLA	c	501	3	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	b	627	-	-	7/29/63/63	0/2/2/2
32	LMT	g	104	-	-	8/21/61/61	0/2/2/2
25	CLA	C	505	3	-	1/39/115/115	-
29	SQD	a	417	-	-	31/49/69/69	0/1/1/1
33	LHG	A	416	-	-	24/53/53/53	-
28	BCR	K	101	-	-	6/29/63/63	0/2/2/2
31	LMG	d	411	-	-	6/46/66/70	0/1/1/1
25	CLA	C	513	3	-	3/29/105/115	-
28	BCR	B	619	-	-	7/29/63/63	0/2/2/2
34	F6C	c	507	39	1/1/10/16	17/41/97/97	-
25	CLA	b	616	2	-	6/39/115/115	-
29	SQD	B	622	-	-	18/49/69/69	0/1/1/1
25	CLA	c	512	3	-	6/39/115/115	-
32	LMT	B	675	-	-	10/17/37/61	0/1/1/2
32	LMT	c	904	-	-	3/18/58/61	0/2/2/2
28	BCR	K	102	-	-	3/29/63/63	0/2/2/2
34	F6C	b	608	39	1/1/10/16	10/41/97/97	-
33	LHG	E	244	-	-	24/53/53/53	-
25	CLA	C	501	3	-	3/39/115/115	-
32	LMT	A	675	-	-	1/18/58/61	0/2/2/2
31	LMG	L	212	-	-	21/50/70/70	0/1/1/1
32	LMT	L	210	-	-	10/21/61/61	0/2/2/2
25	CLA	b	604	2	-	3/39/115/115	-
25	CLA	C	510	3	-	3/39/115/115	-
31	LMG	c	519	-	-	12/46/66/70	0/1/1/1
31	LMG	B	628	-	-	18/50/70/70	0/1/1/1
33	LHG	D	409	-	-	12/53/53/53	-
34	F6C	B	617	2	1/1/7/16	6/23/79/97	-
28	BCR	C	515	-	-	4/29/63/63	0/2/2/2
25	CLA	b	606	2	-	6/39/115/115	-
27	PHO	a	409	-	-	3/37/103/103	0/5/6/6
32	LMT	A	674	-	-	6/21/61/61	0/2/2/2
33	LHG	D	408	-	-	15/53/53/53	-
29	SQD	H	102	-	-	19/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CL7	A	406	39	2/2/15/20	2/39/115/115	-
33	LHG	d	410	-	-	26/45/45/53	-
28	BCR	b	618	-	-	4/29/63/63	0/2/2/2
25	CLA	b	613	2	-	4/39/115/115	-
32	LMT	G	104	-	-	8/21/61/61	0/2/2/2
29	SQD	d	407	-	-	17/40/60/69	0/1/1/1
33	LHG	d	408	-	-	15/53/53/53	-
25	CLA	C	503	3	-	2/39/115/115	-
33	LHG	A	419	-	-	15/53/53/53	-
33	LHG	J	101	-	-	29/53/53/53	-
34	F6C	C	507	39	1/1/10/16	17/41/97/97	-
25	CLA	c	510	3	-	3/39/115/115	-
33	LHG	e	101	-	-	27/53/53/53	-
25	CLA	B	604	2	-	3/39/115/115	-
28	BCR	C	514	-	-	0/29/63/63	0/2/2/2
32	LMT	a	675	-	-	1/18/58/61	0/2/2/2
32	LMT	M	101	-	-	7/21/61/61	0/2/2/2
31	LMG	p	628	-	-	19/42/62/70	0/1/1/1
32	LMT	l	213	-	-	6/21/61/61	0/2/2/2
25	CLA	b	602	39	-	9/39/115/115	-
29	SQD	A	417	-	-	31/49/69/69	0/1/1/1
33	LHG	j	101	-	-	29/53/53/53	-
38	HEC	v	201	18	-	4/14/54/54	-
33	LHG	l	101	-	-	11/53/53/53	-
33	LHG	p	629	-	-	21/53/53/53	-
25	CLA	C	508	3	-	3/39/115/115	-
32	LMT	Z	102	-	-	10/21/61/61	0/2/2/2
35	DGD	c	518	-	-	16/51/91/95	0/2/2/2
35	DGD	c	516	-	-	20/51/91/95	0/2/2/2
25	CLA	a	405	1	-	4/39/115/115	-
25	CLA	C	511	3	-	0/39/115/115	-
28	BCR	b	620	-	-	4/29/63/63	0/2/2/2
27	PHO	a	408	-	-	4/37/103/103	0/5/6/6
25	CLA	B	605	2	-	2/39/115/115	-
29	SQD	C	903	-	-	21/33/53/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	P	628	-	-	19/42/62/70	0/1/1/1

All (696) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	v	201	HEC	CAC-C3C	15.70	1.55	1.34
38	V	201	HEC	CAC-C3C	15.70	1.55	1.34
38	v	201	HEC	CAB-C3B	15.69	1.55	1.34
38	V	201	HEC	CAB-C3B	15.68	1.54	1.34
27	a	409	PHO	C1B-C2B	9.01	1.49	1.39
27	A	409	PHO	C1B-C2B	9.01	1.49	1.39
27	A	408	PHO	C1B-C2B	8.77	1.49	1.39
27	a	408	PHO	C1B-C2B	8.77	1.49	1.39
34	c	507	F6C	C2A-C3A	8.60	1.55	1.36
34	C	507	F6C	C2A-C3A	8.60	1.55	1.36
34	B	608	F6C	C2A-C3A	8.59	1.55	1.36
34	b	608	F6C	C2A-C3A	8.59	1.55	1.36
34	b	614	F6C	C2A-C3A	8.56	1.55	1.36
34	B	614	F6C	C2A-C3A	8.56	1.54	1.36
34	B	617	F6C	C2A-C3A	8.47	1.54	1.36
34	b	617	F6C	C2A-C3A	8.46	1.54	1.36
27	A	409	PHO	C3B-C4B	7.35	1.49	1.41
27	a	409	PHO	C3B-C4B	7.34	1.49	1.41
27	A	408	PHO	C3B-C4B	7.16	1.49	1.41
27	a	408	PHO	C3B-C4B	7.16	1.49	1.41
30	d	405	PL9	C7-C3	-4.94	1.46	1.51
30	D	405	PL9	C7-C3	-4.93	1.46	1.51
26	A	406	CL7	C1C-C2C	-4.77	1.35	1.45
26	a	406	CL7	C1C-C2C	-4.77	1.35	1.45
25	b	612	CLA	C4C-C3C	-4.64	1.37	1.45
25	B	612	CLA	C4C-C3C	-4.64	1.37	1.45
25	a	405	CLA	C4C-C3C	-4.61	1.37	1.45
29	D	407	SQD	O48-C23	4.60	1.46	1.33
29	d	407	SQD	O48-C23	4.60	1.46	1.33
25	A	405	CLA	C4C-C3C	-4.60	1.37	1.45
25	B	604	CLA	C4C-C3C	-4.59	1.37	1.45
25	b	604	CLA	C4C-C3C	-4.59	1.37	1.45
25	b	613	CLA	C4C-C3C	-4.58	1.37	1.45
29	a	412	SQD	O48-C23	4.58	1.46	1.33
29	A	412	SQD	O48-C23	4.57	1.46	1.33
25	B	613	CLA	C4C-C3C	-4.57	1.37	1.45
25	C	501	CLA	C4C-C3C	-4.56	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	501	CLA	C4C-C3C	-4.56	1.37	1.45
25	B	606	CLA	C4C-C3C	-4.56	1.37	1.45
25	c	509	CLA	C4C-C3C	-4.55	1.37	1.45
25	b	606	CLA	C4C-C3C	-4.55	1.37	1.45
25	B	612	CLA	C1C-C2C	-4.55	1.35	1.44
25	C	509	CLA	C4C-C3C	-4.55	1.37	1.45
25	C	511	CLA	C4C-C3C	-4.55	1.37	1.45
25	B	616	CLA	C4C-C3C	-4.54	1.37	1.45
25	D	403	CLA	C4C-C3C	-4.54	1.37	1.45
25	b	616	CLA	C4C-C3C	-4.54	1.37	1.45
25	c	511	CLA	C4C-C3C	-4.54	1.37	1.45
25	d	403	CLA	C4C-C3C	-4.54	1.37	1.45
25	B	611	CLA	C4C-C3C	-4.54	1.37	1.45
25	b	611	CLA	C4C-C3C	-4.54	1.37	1.45
25	B	615	CLA	C4C-C3C	-4.54	1.37	1.45
25	b	612	CLA	C1C-C2C	-4.54	1.35	1.44
34	B	614	F6C	OMB-CMB	-4.54	1.11	1.22
25	b	605	CLA	C1C-C2C	-4.54	1.35	1.44
25	B	605	CLA	C1C-C2C	-4.53	1.35	1.44
25	d	402	CLA	C4C-C3C	-4.53	1.37	1.45
34	b	614	F6C	OMB-CMB	-4.53	1.11	1.22
25	D	402	CLA	C4C-C3C	-4.52	1.37	1.45
25	C	510	CLA	C4C-C3C	-4.52	1.37	1.45
25	c	510	CLA	C4C-C3C	-4.52	1.37	1.45
25	B	609	CLA	C4C-C3C	-4.52	1.37	1.45
25	a	410	CLA	C4C-C3C	-4.52	1.37	1.45
29	B	622	SQD	O48-C23	4.52	1.46	1.33
25	A	410	CLA	C4C-C3C	-4.52	1.37	1.45
25	B	603	CLA	C4C-C3C	-4.52	1.37	1.45
29	b	622	SQD	O48-C23	4.52	1.46	1.33
25	b	615	CLA	C4C-C3C	-4.52	1.37	1.45
25	c	512	CLA	C4C-C3C	-4.52	1.37	1.45
25	b	603	CLA	C4C-C3C	-4.52	1.37	1.45
25	c	508	CLA	C4C-C3C	-4.52	1.37	1.45
25	B	605	CLA	C4C-C3C	-4.51	1.37	1.45
26	A	406	CL7	C4C-C3C	-4.51	1.37	1.45
25	C	512	CLA	C4C-C3C	-4.51	1.37	1.45
25	b	605	CLA	C4C-C3C	-4.51	1.37	1.45
25	C	508	CLA	C4C-C3C	-4.51	1.37	1.45
25	C	513	CLA	C4C-C3C	-4.51	1.37	1.45
25	A	407	CLA	C4C-C3C	-4.51	1.37	1.45
25	c	513	CLA	C4C-C3C	-4.51	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	406	CL7	C4C-C3C	-4.51	1.37	1.45
25	b	609	CLA	C4C-C3C	-4.51	1.37	1.45
25	C	504	CLA	C4C-C3C	-4.50	1.37	1.45
25	c	504	CLA	C4C-C3C	-4.50	1.37	1.45
34	b	617	F6C	OMB-CMB	-4.50	1.11	1.22
25	b	607	CLA	C4C-C3C	-4.50	1.37	1.45
25	b	610	CLA	C4C-C3C	-4.50	1.37	1.45
25	B	607	CLA	C4C-C3C	-4.50	1.37	1.45
25	B	610	CLA	C4C-C3C	-4.50	1.37	1.45
25	a	407	CLA	C4C-C3C	-4.50	1.37	1.45
25	b	602	CLA	C4C-C3C	-4.50	1.37	1.45
25	B	602	CLA	C4C-C3C	-4.49	1.37	1.45
34	B	608	F6C	OMB-CMB	-4.49	1.11	1.22
34	b	608	F6C	OMB-CMB	-4.49	1.11	1.22
25	C	503	CLA	C4C-C3C	-4.49	1.37	1.45
25	c	503	CLA	C4C-C3C	-4.49	1.37	1.45
34	B	617	F6C	OMB-CMB	-4.49	1.11	1.22
25	C	501	CLA	C1C-C2C	-4.48	1.35	1.44
25	c	501	CLA	C1C-C2C	-4.48	1.35	1.44
25	C	505	CLA	C4C-C3C	-4.48	1.37	1.45
25	A	405	CLA	C1C-C2C	-4.48	1.35	1.44
25	c	504	CLA	C1C-C2C	-4.48	1.35	1.44
25	c	505	CLA	C4C-C3C	-4.48	1.37	1.45
25	C	504	CLA	C1C-C2C	-4.47	1.35	1.44
25	C	506	CLA	C4C-C3C	-4.47	1.37	1.45
25	c	506	CLA	C4C-C3C	-4.47	1.37	1.45
25	B	609	CLA	C1C-C2C	-4.47	1.35	1.44
25	a	405	CLA	C1C-C2C	-4.46	1.35	1.44
25	b	609	CLA	C1C-C2C	-4.46	1.35	1.44
25	B	607	CLA	C1C-C2C	-4.45	1.35	1.44
25	b	607	CLA	C1C-C2C	-4.45	1.36	1.44
29	C	903	SQD	O48-C23	4.45	1.46	1.33
29	c	903	SQD	O48-C23	4.45	1.46	1.33
25	D	402	CLA	C1C-C2C	-4.44	1.36	1.44
25	B	606	CLA	C1C-C2C	-4.43	1.36	1.44
25	d	402	CLA	C1C-C2C	-4.43	1.36	1.44
25	C	502	CLA	C1C-C2C	-4.43	1.36	1.44
25	b	606	CLA	C1C-C2C	-4.43	1.36	1.44
25	b	616	CLA	C1C-C2C	-4.43	1.36	1.44
25	B	616	CLA	C1C-C2C	-4.43	1.36	1.44
29	a	417	SQD	O48-C23	4.42	1.46	1.33
25	b	610	CLA	C1C-C2C	-4.42	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	502	CLA	C1C-C2C	-4.42	1.36	1.44
29	A	417	SQD	O48-C23	4.42	1.46	1.33
25	B	610	CLA	C1C-C2C	-4.42	1.36	1.44
25	C	510	CLA	C1C-C2C	-4.42	1.36	1.44
25	B	604	CLA	C1C-C2C	-4.42	1.36	1.44
25	b	604	CLA	C1C-C2C	-4.42	1.36	1.44
25	c	510	CLA	C1C-C2C	-4.42	1.36	1.44
25	C	505	CLA	C1C-C2C	-4.39	1.36	1.44
25	c	505	CLA	C1C-C2C	-4.39	1.36	1.44
25	b	613	CLA	C1C-C2C	-4.39	1.36	1.44
34	c	507	F6C	OMB-CMB	-4.39	1.11	1.22
25	B	613	CLA	C1C-C2C	-4.39	1.36	1.44
34	C	507	F6C	OMB-CMB	-4.39	1.11	1.22
25	C	509	CLA	C1C-C2C	-4.39	1.36	1.44
25	c	509	CLA	C1C-C2C	-4.38	1.36	1.44
25	c	502	CLA	C4C-C3C	-4.38	1.37	1.45
25	C	503	CLA	C1C-C2C	-4.38	1.36	1.44
25	c	503	CLA	C1C-C2C	-4.38	1.36	1.44
25	C	502	CLA	C4C-C3C	-4.38	1.37	1.45
25	b	615	CLA	C1C-C2C	-4.38	1.36	1.44
29	h	102	SQD	O48-C23	4.37	1.46	1.33
25	B	615	CLA	C1C-C2C	-4.37	1.36	1.44
29	H	102	SQD	O48-C23	4.37	1.46	1.33
25	D	403	CLA	C1C-C2C	-4.37	1.36	1.44
25	c	506	CLA	C1C-C2C	-4.37	1.36	1.44
25	C	511	CLA	C1C-C2C	-4.36	1.36	1.44
25	c	511	CLA	C1C-C2C	-4.36	1.36	1.44
25	C	506	CLA	C1C-C2C	-4.36	1.36	1.44
25	d	403	CLA	C1C-C2C	-4.36	1.36	1.44
25	A	410	CLA	C1C-C2C	-4.35	1.36	1.44
25	a	410	CLA	C1C-C2C	-4.35	1.36	1.44
25	b	603	CLA	C1C-C2C	-4.35	1.36	1.44
25	B	603	CLA	C1C-C2C	-4.35	1.36	1.44
25	C	508	CLA	C1C-C2C	-4.35	1.36	1.44
25	c	508	CLA	C1C-C2C	-4.34	1.36	1.44
25	B	611	CLA	C1C-C2C	-4.33	1.36	1.44
25	b	611	CLA	C1C-C2C	-4.33	1.36	1.44
25	A	407	CLA	C1C-C2C	-4.32	1.36	1.44
25	b	602	CLA	C1C-C2C	-4.32	1.36	1.44
25	a	407	CLA	C1C-C2C	-4.32	1.36	1.44
25	C	512	CLA	C1C-C2C	-4.31	1.36	1.44
25	c	512	CLA	C1C-C2C	-4.31	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	602	CLA	C1C-C2C	-4.31	1.36	1.44
25	C	513	CLA	C1C-C2C	-4.30	1.36	1.44
25	c	513	CLA	C1C-C2C	-4.30	1.36	1.44
38	v	201	HEC	CBC-CAC	-4.18	1.33	1.49
38	V	201	HEC	CBC-CAC	-4.18	1.33	1.49
25	c	511	CLA	MG-NA	4.14	2.16	2.06
25	C	511	CLA	MG-NA	4.14	2.16	2.06
38	V	201	HEC	CBB-CAB	-4.11	1.34	1.49
38	v	201	HEC	CBB-CAB	-4.11	1.34	1.49
34	B	608	F6C	C4A-C3A	4.11	1.53	1.45
34	b	608	F6C	C4A-C3A	4.10	1.53	1.45
26	a	406	CL7	MG-NA	4.09	2.13	2.05
26	A	406	CL7	MG-NA	4.08	2.13	2.05
30	D	405	PL9	C3-C4	-4.07	1.42	1.49
30	d	405	PL9	C3-C4	-4.07	1.42	1.49
25	B	605	CLA	MG-NA	4.04	2.15	2.06
25	b	605	CLA	MG-NA	4.04	2.15	2.06
25	b	607	CLA	MG-NA	4.00	2.15	2.06
25	B	607	CLA	MG-NA	4.00	2.15	2.06
25	B	616	CLA	MG-NA	3.97	2.15	2.06
25	b	616	CLA	MG-NA	3.97	2.15	2.06
25	C	503	CLA	MG-NA	3.96	2.15	2.06
25	c	503	CLA	MG-NA	3.96	2.15	2.06
34	b	614	F6C	C4A-C3A	3.95	1.53	1.45
34	B	614	F6C	C4A-C3A	3.95	1.53	1.45
34	c	507	F6C	C4A-C3A	3.91	1.53	1.45
34	C	507	F6C	C4A-C3A	3.91	1.53	1.45
34	b	617	F6C	C4A-C3A	3.91	1.53	1.45
34	B	617	F6C	C4A-C3A	3.90	1.53	1.45
25	C	508	CLA	MG-NA	3.77	2.15	2.06
25	C	505	CLA	MG-NA	3.77	2.15	2.06
25	c	505	CLA	MG-NA	3.77	2.15	2.06
25	c	508	CLA	MG-NA	3.76	2.15	2.06
25	C	509	CLA	MG-NA	3.72	2.15	2.06
25	c	502	CLA	MG-NA	3.71	2.15	2.06
25	C	502	CLA	MG-NA	3.71	2.15	2.06
25	c	509	CLA	MG-NA	3.70	2.15	2.06
25	B	602	CLA	MG-NA	3.69	2.15	2.06
25	b	602	CLA	MG-NA	3.69	2.15	2.06
25	C	501	CLA	MG-NA	3.68	2.15	2.06
25	c	501	CLA	MG-NA	3.68	2.15	2.06
27	A	408	PHO	C1D-C2D	3.67	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	408	PHO	C1D-C2D	3.67	1.43	1.39
25	b	612	CLA	MG-NA	3.66	2.15	2.06
25	B	612	CLA	MG-NA	3.65	2.15	2.06
29	A	412	SQD	O47-C45	-3.65	1.37	1.46
29	a	412	SQD	O47-C45	-3.65	1.37	1.46
25	b	606	CLA	MG-NA	3.64	2.14	2.06
29	h	102	SQD	O47-C45	-3.64	1.37	1.46
29	H	102	SQD	O47-C45	-3.64	1.37	1.46
25	C	504	CLA	MG-NA	3.63	2.14	2.06
25	B	606	CLA	MG-NA	3.63	2.14	2.06
25	c	504	CLA	MG-NA	3.63	2.14	2.06
25	c	512	CLA	MG-NA	3.62	2.14	2.06
25	C	512	CLA	MG-NA	3.61	2.14	2.06
25	C	506	CLA	MG-NA	3.61	2.14	2.06
25	c	506	CLA	MG-NA	3.61	2.14	2.06
25	B	610	CLA	MG-NA	3.60	2.14	2.06
25	b	610	CLA	MG-NA	3.60	2.14	2.06
27	A	409	PHO	C1D-C2D	3.59	1.43	1.39
27	a	409	PHO	C1D-C2D	3.59	1.43	1.39
29	B	622	SQD	O47-C45	-3.57	1.37	1.46
29	b	622	SQD	O47-C45	-3.57	1.37	1.46
25	D	403	CLA	MG-NA	3.57	2.14	2.06
25	b	609	CLA	MG-NA	3.57	2.14	2.06
25	d	403	CLA	MG-NA	3.56	2.14	2.06
25	B	609	CLA	MG-NA	3.56	2.14	2.06
25	b	615	CLA	MG-NA	3.53	2.14	2.06
25	B	615	CLA	MG-NA	3.53	2.14	2.06
25	b	604	CLA	MG-NA	3.53	2.14	2.06
25	d	402	CLA	MG-NA	3.53	2.14	2.06
25	C	513	CLA	MG-NA	3.53	2.14	2.06
25	c	513	CLA	MG-NA	3.53	2.14	2.06
25	B	604	CLA	MG-NA	3.52	2.14	2.06
25	D	402	CLA	MG-NA	3.52	2.14	2.06
29	d	407	SQD	O47-C45	-3.50	1.37	1.46
29	D	407	SQD	O47-C45	-3.50	1.37	1.46
25	b	603	CLA	MG-NA	3.47	2.14	2.06
25	C	510	CLA	MG-NA	3.47	2.14	2.06
25	c	510	CLA	MG-NA	3.47	2.14	2.06
25	B	603	CLA	MG-NA	3.47	2.14	2.06
25	a	410	CLA	MG-NA	3.45	2.14	2.06
25	A	410	CLA	MG-NA	3.44	2.14	2.06
29	C	903	SQD	O47-C7	3.42	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	903	SQD	O47-C7	3.42	1.43	1.34
37	F	101	HEM	FE-NB	3.38	2.05	1.94
37	f	101	HEM	FE-NB	3.38	2.05	1.94
34	C	507	F6C	C1A-C2A	3.36	1.52	1.45
34	c	507	F6C	C1A-C2A	3.35	1.52	1.45
25	B	611	CLA	MG-NA	3.35	2.14	2.06
25	b	611	CLA	MG-NA	3.35	2.14	2.06
25	B	613	CLA	MG-NA	3.35	2.14	2.06
25	b	613	CLA	MG-NA	3.34	2.14	2.06
25	A	405	CLA	MG-NA	3.34	2.14	2.06
25	a	405	CLA	MG-NA	3.34	2.14	2.06
25	a	407	CLA	MG-NA	3.30	2.14	2.06
25	A	407	CLA	MG-NA	3.30	2.14	2.06
34	b	614	F6C	C1A-C2A	3.29	1.52	1.45
34	B	614	F6C	C1A-C2A	3.28	1.52	1.45
29	A	417	SQD	O47-C7	3.28	1.43	1.34
29	a	417	SQD	O47-C7	3.28	1.43	1.34
37	F	101	HEM	FE-NA	3.28	2.06	1.95
37	f	101	HEM	FE-NA	3.28	2.06	1.95
29	A	417	SQD	O47-C45	-3.27	1.38	1.46
29	a	417	SQD	O47-C45	-3.26	1.38	1.46
34	b	608	F6C	C1A-C2A	3.25	1.52	1.45
34	B	608	F6C	C1A-C2A	3.25	1.52	1.45
34	B	617	F6C	C1A-C2A	3.24	1.52	1.45
29	d	407	SQD	O47-C7	3.24	1.43	1.34
34	b	617	F6C	C1A-C2A	3.24	1.52	1.45
29	D	407	SQD	O47-C7	3.23	1.43	1.34
30	a	414	PL9	C7-C3	-3.23	1.48	1.51
30	D	405	PL9	C6-C1	-3.22	1.42	1.48
30	A	414	PL9	C7-C3	-3.22	1.48	1.51
30	d	405	PL9	C6-C1	-3.22	1.42	1.48
29	C	903	SQD	O47-C45	-3.20	1.38	1.46
29	c	903	SQD	O47-C45	-3.20	1.38	1.46
29	A	412	SQD	O47-C7	3.18	1.43	1.34
29	a	412	SQD	O47-C7	3.18	1.43	1.34
30	A	414	PL9	C3-C4	-3.16	1.44	1.49
27	A	409	PHO	C4D-CHA	3.16	1.44	1.39
30	a	414	PL9	C3-C4	-3.15	1.44	1.49
27	a	409	PHO	C4D-CHA	3.15	1.44	1.39
29	a	412	SQD	O5-C1	3.15	1.49	1.41
29	A	412	SQD	O5-C1	3.15	1.49	1.41
29	C	903	SQD	O5-C1	3.11	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	903	SQD	O5-C1	3.10	1.49	1.41
29	B	622	SQD	O47-C7	3.08	1.43	1.34
29	b	622	SQD	O47-C7	3.07	1.43	1.34
29	H	102	SQD	O47-C7	3.06	1.42	1.34
29	h	102	SQD	O47-C7	3.06	1.42	1.34
29	D	407	SQD	O5-C1	3.06	1.49	1.41
29	d	407	SQD	O5-C1	3.06	1.49	1.41
29	b	622	SQD	O5-C1	3.01	1.49	1.41
27	a	408	PHO	C4D-CHA	3.01	1.44	1.39
29	B	622	SQD	O5-C1	3.01	1.49	1.41
27	A	408	PHO	C4D-CHA	3.01	1.44	1.39
29	A	412	SQD	C24-C23	3.00	1.59	1.50
29	a	412	SQD	C24-C23	3.00	1.59	1.50
37	F	101	HEM	CAB-C3B	3.00	1.55	1.47
37	f	101	HEM	CAB-C3B	3.00	1.55	1.47
29	A	417	SQD	O5-C1	2.97	1.49	1.41
29	a	417	SQD	O5-C1	2.97	1.49	1.41
37	f	101	HEM	CAC-C3C	2.96	1.55	1.47
37	F	101	HEM	CAC-C3C	2.96	1.55	1.47
29	b	622	SQD	C24-C23	2.95	1.59	1.50
29	B	622	SQD	C24-C23	2.94	1.59	1.50
29	D	407	SQD	C24-C23	2.93	1.59	1.50
29	d	407	SQD	C24-C23	2.93	1.59	1.50
25	B	605	CLA	C1D-C2D	-2.93	1.39	1.45
25	b	605	CLA	C1D-C2D	-2.93	1.39	1.45
29	C	903	SQD	C24-C23	2.93	1.59	1.50
29	c	903	SQD	C24-C23	2.93	1.59	1.50
29	H	102	SQD	C24-C23	2.90	1.59	1.50
29	h	102	SQD	C24-C23	2.90	1.59	1.50
29	A	417	SQD	C24-C23	2.88	1.59	1.50
29	a	417	SQD	C24-C23	2.88	1.59	1.50
27	A	409	PHO	CMC-C2C	-2.85	1.46	1.50
29	h	102	SQD	O5-C1	2.85	1.49	1.41
29	H	102	SQD	O5-C1	2.85	1.49	1.41
27	a	409	PHO	CMC-C2C	-2.85	1.46	1.50
34	b	608	F6C	C1D-ND	2.84	1.42	1.37
34	B	608	F6C	C1D-ND	2.83	1.42	1.37
37	F	101	HEM	FE-ND	2.82	2.03	1.94
37	f	101	HEM	FE-ND	2.82	2.03	1.94
34	C	507	F6C	C1D-ND	2.77	1.41	1.37
34	c	507	F6C	C1D-ND	2.76	1.41	1.37
30	D	405	PL9	C53-C6	-2.75	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	405	PL9	C53-C6	-2.75	1.45	1.50
34	b	614	F6C	C1D-ND	2.75	1.41	1.37
34	B	614	F6C	C1D-ND	2.74	1.41	1.37
25	B	616	CLA	C3D-C4D	-2.72	1.38	1.44
27	A	409	PHO	C4D-ND	-2.72	1.34	1.38
27	a	409	PHO	C4D-ND	-2.72	1.34	1.38
25	b	616	CLA	C3D-C4D	-2.72	1.38	1.44
25	a	407	CLA	C3D-C4D	-2.71	1.38	1.44
25	A	407	CLA	C3D-C4D	-2.71	1.38	1.44
27	A	408	PHO	C4D-ND	-2.71	1.34	1.38
27	a	408	PHO	C4D-ND	-2.71	1.34	1.38
25	B	615	CLA	C3D-C4D	-2.70	1.38	1.44
25	b	615	CLA	C3D-C4D	-2.69	1.38	1.44
25	d	402	CLA	C3D-C4D	-2.69	1.38	1.44
25	D	402	CLA	C3D-C4D	-2.68	1.38	1.44
25	C	510	CLA	C3D-C4D	-2.68	1.38	1.44
25	c	510	CLA	C3D-C4D	-2.68	1.38	1.44
25	B	606	CLA	C3D-C4D	-2.68	1.38	1.44
25	B	603	CLA	C3D-C4D	-2.68	1.38	1.44
25	B	609	CLA	C3D-C4D	-2.67	1.38	1.44
25	b	603	CLA	C3D-C4D	-2.67	1.38	1.44
25	b	606	CLA	C3D-C4D	-2.67	1.38	1.44
25	b	609	CLA	C3D-C4D	-2.67	1.38	1.44
25	B	605	CLA	C3D-C4D	-2.66	1.38	1.44
25	b	605	CLA	C3D-C4D	-2.66	1.38	1.44
25	A	410	CLA	C3D-C4D	-2.66	1.38	1.44
25	a	410	CLA	C3D-C4D	-2.66	1.38	1.44
25	B	611	CLA	C3D-C4D	-2.65	1.38	1.44
25	b	611	CLA	C3D-C4D	-2.65	1.38	1.44
25	A	405	CLA	C3D-C4D	-2.65	1.38	1.44
25	C	508	CLA	C3D-C4D	-2.65	1.38	1.44
25	a	405	CLA	C3D-C4D	-2.65	1.38	1.44
34	B	617	F6C	C1D-ND	2.65	1.41	1.37
25	B	604	CLA	C3D-C4D	-2.65	1.38	1.44
25	c	508	CLA	C3D-C4D	-2.65	1.38	1.44
25	b	604	CLA	C3D-C4D	-2.64	1.38	1.44
34	b	617	F6C	C1D-ND	2.64	1.41	1.37
25	B	613	CLA	C3D-C4D	-2.64	1.38	1.44
25	b	613	CLA	C3D-C4D	-2.64	1.38	1.44
25	b	612	CLA	C3D-C4D	-2.64	1.38	1.44
25	B	612	CLA	C3D-C4D	-2.64	1.38	1.44
25	c	504	CLA	C3D-C4D	-2.63	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	504	CLA	C3D-C4D	-2.62	1.38	1.44
27	A	408	PHO	CMC-C2C	-2.62	1.46	1.50
27	a	408	PHO	CMC-C2C	-2.62	1.46	1.50
25	d	403	CLA	C3D-C4D	-2.61	1.38	1.44
25	D	403	CLA	C3D-C4D	-2.61	1.38	1.44
25	C	505	CLA	C3D-C4D	-2.61	1.38	1.44
25	c	505	CLA	C3D-C4D	-2.61	1.38	1.44
25	c	509	CLA	C3D-C4D	-2.60	1.38	1.44
25	C	509	CLA	C3D-C4D	-2.60	1.38	1.44
25	C	502	CLA	C3D-C4D	-2.59	1.38	1.44
25	c	502	CLA	C3D-C4D	-2.59	1.38	1.44
27	a	408	PHO	CMD-C2D	-2.59	1.46	1.51
25	B	610	CLA	C3D-C4D	-2.59	1.38	1.44
25	b	607	CLA	C3D-C4D	-2.59	1.38	1.44
25	b	610	CLA	C3D-C4D	-2.59	1.38	1.44
25	B	607	CLA	C3D-C4D	-2.59	1.38	1.44
27	A	408	PHO	CMD-C2D	-2.59	1.46	1.51
25	c	506	CLA	C3D-C4D	-2.58	1.38	1.44
25	C	506	CLA	C3D-C4D	-2.58	1.38	1.44
25	c	505	CLA	C1D-C2D	-2.57	1.40	1.45
25	C	505	CLA	C1D-C2D	-2.57	1.40	1.45
25	C	512	CLA	C3D-C4D	-2.56	1.38	1.44
25	c	512	CLA	C3D-C4D	-2.56	1.38	1.44
25	b	604	CLA	C1D-C2D	-2.55	1.40	1.45
25	C	501	CLA	C3D-C4D	-2.55	1.38	1.44
25	c	501	CLA	C3D-C4D	-2.55	1.38	1.44
25	B	604	CLA	C1D-C2D	-2.55	1.40	1.45
25	C	503	CLA	C3D-C4D	-2.54	1.38	1.44
25	c	503	CLA	C3D-C4D	-2.54	1.38	1.44
27	A	409	PHO	CMD-C2D	-2.54	1.46	1.51
27	a	409	PHO	CMD-C2D	-2.54	1.46	1.51
25	b	616	CLA	C1D-C2D	-2.53	1.40	1.45
25	c	511	CLA	C3D-C4D	-2.53	1.38	1.44
25	B	616	CLA	C1D-C2D	-2.53	1.40	1.45
25	C	511	CLA	C3D-C4D	-2.53	1.38	1.44
25	c	513	CLA	C3D-C4D	-2.53	1.38	1.44
25	C	513	CLA	C3D-C4D	-2.52	1.38	1.44
25	b	607	CLA	C1D-C2D	-2.50	1.40	1.45
25	B	607	CLA	C1D-C2D	-2.50	1.40	1.45
34	B	617	F6C	C4D-ND	-2.50	1.32	1.37
34	b	617	F6C	C4D-ND	-2.49	1.32	1.37
25	b	605	CLA	C1B-NB	-2.45	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	605	CLA	C1B-NB	-2.45	1.34	1.37
25	b	612	CLA	C1D-C2D	-2.45	1.40	1.45
25	B	602	CLA	C3D-C4D	-2.45	1.38	1.44
25	b	602	CLA	C3D-C4D	-2.45	1.38	1.44
25	B	612	CLA	C1D-C2D	-2.45	1.40	1.45
25	C	511	CLA	C1D-C2D	-2.44	1.40	1.45
25	c	511	CLA	C1D-C2D	-2.44	1.40	1.45
34	B	614	F6C	C4D-ND	-2.44	1.33	1.37
34	b	614	F6C	C4D-ND	-2.44	1.33	1.37
34	C	507	F6C	C4B-NB	2.42	1.41	1.37
27	a	408	PHO	CMB-C2B	-2.42	1.46	1.51
27	A	408	PHO	CMB-C2B	-2.41	1.46	1.51
34	c	507	F6C	C4B-NB	2.41	1.41	1.37
25	A	407	CLA	C1B-C2B	-2.41	1.37	1.43
25	a	407	CLA	C1B-C2B	-2.41	1.37	1.43
25	B	611	CLA	C1B-C2B	-2.40	1.37	1.43
25	b	611	CLA	C1B-C2B	-2.40	1.37	1.43
25	b	606	CLA	C1B-C2B	-2.40	1.37	1.43
27	A	408	PHO	CAC-C3C	-2.40	1.47	1.51
25	B	606	CLA	C1B-C2B	-2.39	1.37	1.43
27	a	408	PHO	CAC-C3C	-2.39	1.47	1.51
25	b	606	CLA	C1D-C2D	-2.39	1.40	1.45
25	B	606	CLA	C1D-C2D	-2.39	1.40	1.45
25	c	509	CLA	C1D-C2D	-2.39	1.40	1.45
25	C	509	CLA	C1D-C2D	-2.39	1.40	1.45
25	C	504	CLA	C1D-C2D	-2.38	1.40	1.45
25	C	512	CLA	C1B-C2B	-2.38	1.37	1.43
25	b	616	CLA	C1B-C2B	-2.38	1.37	1.43
25	c	504	CLA	C1D-C2D	-2.38	1.40	1.45
25	c	512	CLA	C1B-C2B	-2.38	1.37	1.43
25	B	616	CLA	C1B-C2B	-2.38	1.37	1.43
25	B	603	CLA	C1D-C2D	-2.37	1.40	1.45
30	A	414	PL9	C6-C1	-2.37	1.44	1.48
30	a	414	PL9	C6-C1	-2.37	1.44	1.48
25	d	402	CLA	C1D-C2D	-2.37	1.40	1.45
25	b	603	CLA	C1D-C2D	-2.37	1.40	1.45
25	D	402	CLA	C1D-C2D	-2.36	1.40	1.45
25	B	610	CLA	C1B-C2B	-2.36	1.37	1.43
25	b	610	CLA	C1B-C2B	-2.36	1.37	1.43
25	b	602	CLA	C1D-C2D	-2.36	1.40	1.45
25	B	602	CLA	C1D-C2D	-2.36	1.40	1.45
34	C	507	F6C	C4D-ND	-2.36	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	c	507	F6C	C4D-ND	-2.36	1.33	1.37
25	c	505	CLA	MG-NC	2.35	2.11	2.06
25	d	402	CLA	MG-NC	2.35	2.11	2.06
25	D	402	CLA	MG-NC	2.35	2.11	2.06
25	C	508	CLA	C1D-C2D	-2.35	1.40	1.45
25	c	508	CLA	C1D-C2D	-2.35	1.40	1.45
25	C	505	CLA	MG-NC	2.35	2.11	2.06
25	B	607	CLA	MG-NC	2.34	2.11	2.06
26	A	406	CL7	C1B-C2B	-2.34	1.37	1.43
27	A	409	PHO	CMB-C2B	-2.34	1.46	1.51
26	a	406	CL7	C1B-C2B	-2.34	1.37	1.43
25	b	607	CLA	MG-NC	2.34	2.11	2.06
27	a	409	PHO	CMB-C2B	-2.34	1.46	1.51
34	B	608	F6C	C4B-NB	2.34	1.41	1.37
25	C	506	CLA	C1D-C2D	-2.34	1.40	1.45
25	C	513	CLA	C1D-C2D	-2.33	1.40	1.45
25	c	513	CLA	C1D-C2D	-2.33	1.40	1.45
25	c	506	CLA	C1D-C2D	-2.33	1.40	1.45
25	A	410	CLA	C1D-C2D	-2.33	1.40	1.45
25	a	410	CLA	C1D-C2D	-2.33	1.40	1.45
25	B	609	CLA	C1D-C2D	-2.33	1.40	1.45
25	b	609	CLA	C1D-C2D	-2.33	1.40	1.45
34	b	608	F6C	C4B-NB	2.33	1.41	1.37
25	C	503	CLA	MG-NC	2.33	2.11	2.06
25	c	503	CLA	MG-NC	2.33	2.11	2.06
30	a	414	PL9	C53-C6	-2.32	1.45	1.50
25	B	615	CLA	C1D-C2D	-2.32	1.40	1.45
25	b	615	CLA	C1D-C2D	-2.32	1.40	1.45
30	A	414	PL9	C53-C6	-2.32	1.45	1.50
25	C	502	CLA	C1D-C2D	-2.32	1.40	1.45
25	c	502	CLA	C1D-C2D	-2.32	1.40	1.45
25	C	503	CLA	C1D-C2D	-2.31	1.40	1.45
25	c	503	CLA	C1D-C2D	-2.31	1.40	1.45
25	b	609	CLA	C1B-C2B	-2.31	1.37	1.43
25	b	610	CLA	C1D-C2D	-2.31	1.40	1.45
25	B	609	CLA	C1B-C2B	-2.31	1.37	1.43
25	B	610	CLA	C1D-C2D	-2.31	1.40	1.45
25	B	613	CLA	C1D-C2D	-2.31	1.40	1.45
25	b	602	CLA	C1B-C2B	-2.31	1.37	1.43
25	B	605	CLA	C1B-C2B	-2.31	1.37	1.43
25	B	602	CLA	C1B-C2B	-2.31	1.37	1.43
25	C	510	CLA	C1D-C2D	-2.30	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	510	CLA	C1D-C2D	-2.30	1.40	1.45
25	b	605	CLA	C1B-C2B	-2.30	1.37	1.43
34	B	617	F6C	CMC-C2C	-2.30	1.45	1.50
34	b	617	F6C	CMC-C2C	-2.30	1.45	1.50
34	B	614	F6C	C4B-NB	2.30	1.41	1.37
30	d	405	PL9	C7-C8	-2.30	1.47	1.50
30	D	405	PL9	C52-C5	-2.29	1.45	1.50
34	b	614	F6C	C4B-NB	2.29	1.41	1.37
25	d	403	CLA	C1B-C2B	-2.29	1.37	1.43
25	D	403	CLA	C1B-C2B	-2.29	1.37	1.43
25	b	613	CLA	C1D-C2D	-2.29	1.40	1.45
34	B	608	F6C	C4D-ND	-2.29	1.33	1.37
34	b	608	F6C	C4D-ND	-2.28	1.33	1.37
30	D	405	PL9	C7-C8	-2.28	1.47	1.50
25	C	512	CLA	C1D-C2D	-2.28	1.40	1.45
25	c	512	CLA	C1D-C2D	-2.28	1.40	1.45
34	B	617	F6C	CMD-C2D	-2.28	1.46	1.50
30	d	405	PL9	C52-C5	-2.28	1.46	1.50
25	d	403	CLA	C1D-C2D	-2.27	1.40	1.45
25	D	403	CLA	C1D-C2D	-2.27	1.40	1.45
34	b	617	F6C	CMD-C2D	-2.27	1.46	1.50
26	A	406	CL7	MG-NC	2.26	2.10	2.05
25	C	503	CLA	C1B-C2B	-2.26	1.37	1.43
25	c	503	CLA	C1B-C2B	-2.26	1.37	1.43
26	a	406	CL7	MG-NC	2.25	2.10	2.05
25	C	506	CLA	MG-NC	2.25	2.11	2.06
25	B	611	CLA	C1D-C2D	-2.25	1.40	1.45
25	b	611	CLA	C1D-C2D	-2.25	1.40	1.45
25	B	603	CLA	C1B-C2B	-2.25	1.38	1.43
25	c	506	CLA	MG-NC	2.25	2.11	2.06
25	a	407	CLA	C1D-C2D	-2.24	1.40	1.45
25	b	603	CLA	C1B-C2B	-2.24	1.38	1.43
25	A	407	CLA	C1D-C2D	-2.24	1.40	1.45
25	C	511	CLA	MG-NC	2.24	2.11	2.06
25	B	612	CLA	C1B-C2B	-2.24	1.38	1.43
25	C	506	CLA	C1B-C2B	-2.24	1.38	1.43
25	c	506	CLA	C1B-C2B	-2.24	1.38	1.43
25	c	511	CLA	MG-NC	2.24	2.11	2.06
25	c	508	CLA	C1B-C2B	-2.24	1.38	1.43
25	C	509	CLA	C1B-C2B	-2.23	1.38	1.43
25	C	508	CLA	C1B-C2B	-2.23	1.38	1.43
25	b	612	CLA	C1B-C2B	-2.23	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	509	CLA	C1B-C2B	-2.23	1.38	1.43
25	A	410	CLA	C1B-C2B	-2.23	1.38	1.43
25	C	510	CLA	C1B-C2B	-2.23	1.38	1.43
25	c	510	CLA	C1B-C2B	-2.23	1.38	1.43
25	C	513	CLA	C1B-C2B	-2.23	1.38	1.43
25	a	410	CLA	C1B-C2B	-2.22	1.38	1.43
25	c	513	CLA	C1B-C2B	-2.22	1.38	1.43
25	B	604	CLA	C1B-C2B	-2.22	1.38	1.43
25	b	604	CLA	C1B-C2B	-2.22	1.38	1.43
25	C	502	CLA	C1B-C2B	-2.22	1.38	1.43
25	c	502	CLA	C1B-C2B	-2.22	1.38	1.43
25	b	613	CLA	C1B-NB	-2.21	1.35	1.37
25	c	505	CLA	C1B-NB	-2.21	1.35	1.37
25	C	505	CLA	C1B-NB	-2.21	1.35	1.37
34	c	507	F6C	C2B-C1B	2.21	1.49	1.44
34	C	507	F6C	C2B-C1B	2.21	1.49	1.44
25	b	615	CLA	C1B-C2B	-2.20	1.38	1.43
25	B	613	CLA	C1B-NB	-2.20	1.35	1.37
25	b	613	CLA	C1B-C2B	-2.20	1.38	1.43
25	B	615	CLA	C1B-C2B	-2.20	1.38	1.43
25	B	609	CLA	C1B-NB	-2.20	1.35	1.37
25	B	613	CLA	C1B-C2B	-2.20	1.38	1.43
25	b	609	CLA	C1B-NB	-2.19	1.35	1.37
25	B	607	CLA	C1B-C2B	-2.19	1.38	1.43
25	b	607	CLA	C1B-C2B	-2.19	1.38	1.43
34	B	608	F6C	C2B-C1B	2.19	1.49	1.44
25	C	505	CLA	C1B-C2B	-2.19	1.38	1.43
25	C	502	CLA	MG-NC	2.18	2.11	2.06
25	c	502	CLA	MG-NC	2.18	2.11	2.06
29	A	412	SQD	O9-S	2.18	1.51	1.45
25	c	505	CLA	C1B-C2B	-2.18	1.38	1.43
25	B	615	CLA	C1B-NB	-2.18	1.35	1.37
25	b	615	CLA	C1B-NB	-2.18	1.35	1.37
29	a	412	SQD	O9-S	2.18	1.51	1.45
25	C	501	CLA	C1D-C2D	-2.18	1.41	1.45
25	c	501	CLA	C1D-C2D	-2.18	1.41	1.45
34	b	608	F6C	C2B-C1B	2.17	1.49	1.44
25	c	508	CLA	MG-NC	2.17	2.11	2.06
25	C	504	CLA	C1B-C2B	-2.17	1.38	1.43
25	C	508	CLA	MG-NC	2.17	2.11	2.06
25	A	405	CLA	C1D-C2D	-2.17	1.41	1.45
25	c	504	CLA	C1B-C2B	-2.17	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	402	CLA	C1B-C2B	-2.17	1.38	1.43
29	A	417	SQD	O9-S	2.17	1.51	1.45
25	a	405	CLA	C1D-C2D	-2.16	1.41	1.45
34	B	617	F6C	C4B-NB	2.16	1.41	1.37
34	b	617	F6C	MG-NB	-2.16	2.01	2.06
29	a	417	SQD	O9-S	2.16	1.51	1.45
25	c	511	CLA	C1B-C2B	-2.16	1.38	1.43
34	B	617	F6C	MG-NB	-2.16	2.01	2.06
25	d	402	CLA	C1B-C2B	-2.16	1.38	1.43
25	C	511	CLA	C1B-C2B	-2.16	1.38	1.43
34	b	617	F6C	C4B-NB	2.16	1.41	1.37
34	B	614	F6C	C2B-C1B	2.16	1.49	1.44
34	b	614	F6C	C2B-C1B	2.15	1.49	1.44
25	b	607	CLA	C1B-NB	-2.15	1.35	1.37
25	b	612	CLA	C1B-NB	-2.15	1.35	1.37
34	B	614	F6C	CMD-C2D	-2.15	1.46	1.50
29	C	903	SQD	O9-S	2.15	1.51	1.45
29	c	903	SQD	O9-S	2.15	1.51	1.45
25	C	510	CLA	C1B-NB	-2.14	1.35	1.37
25	c	510	CLA	C1B-NB	-2.14	1.35	1.37
25	B	607	CLA	C1B-NB	-2.14	1.35	1.37
25	B	612	CLA	C1B-NB	-2.14	1.35	1.37
25	C	501	CLA	C1B-C2B	-2.13	1.38	1.43
25	c	501	CLA	C1B-C2B	-2.13	1.38	1.43
25	B	604	CLA	MG-NC	2.13	2.11	2.06
25	c	509	CLA	C1B-NB	-2.13	1.35	1.37
27	A	408	PHO	C3B-C2B	-2.13	1.37	1.40
27	a	408	PHO	C3B-C2B	-2.13	1.37	1.40
25	C	509	CLA	C1B-NB	-2.13	1.35	1.37
29	A	412	SQD	O7-S	2.13	1.51	1.45
34	b	614	F6C	CMD-C2D	-2.13	1.46	1.50
29	a	412	SQD	O7-S	2.13	1.51	1.45
25	b	604	CLA	C1B-NB	-2.12	1.35	1.37
25	B	604	CLA	C1B-NB	-2.12	1.35	1.37
25	b	604	CLA	MG-NC	2.12	2.11	2.06
25	C	511	CLA	C1B-NB	-2.12	1.35	1.37
25	c	511	CLA	C1B-NB	-2.11	1.35	1.37
27	a	409	PHO	CAC-C3C	-2.11	1.47	1.51
25	b	616	CLA	MG-NC	2.11	2.11	2.06
27	A	409	PHO	CAC-C3C	-2.11	1.47	1.51
34	B	614	F6C	CMC-C2C	-2.11	1.46	1.50
25	B	616	CLA	MG-NC	2.11	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	502	CLA	C1B-NB	-2.11	1.35	1.37
34	b	614	F6C	CMC-C2C	-2.11	1.46	1.50
34	c	507	F6C	CMD-C2D	-2.10	1.46	1.50
25	c	502	CLA	C1B-NB	-2.10	1.35	1.37
34	C	507	F6C	CMD-C2D	-2.10	1.46	1.50
25	b	610	CLA	MG-NC	2.10	2.11	2.06
25	B	610	CLA	MG-NC	2.10	2.11	2.06
25	D	403	CLA	C1B-NB	-2.09	1.35	1.37
25	d	403	CLA	C1B-NB	-2.09	1.35	1.37
25	C	501	CLA	C1B-NB	-2.09	1.35	1.37
25	c	501	CLA	C1B-NB	-2.09	1.35	1.37
37	f	101	HEM	C2A-C3A	-2.08	1.33	1.38
37	F	101	HEM	C2A-C3A	-2.08	1.33	1.38
25	c	504	CLA	C1B-NB	-2.07	1.35	1.37
25	C	509	CLA	MG-NC	2.07	2.11	2.06
25	C	504	CLA	C1B-NB	-2.07	1.35	1.37
25	b	602	CLA	C1B-NB	-2.07	1.35	1.37
34	C	507	F6C	C1A-NA	2.07	1.40	1.37
29	a	417	SQD	O7-S	2.07	1.51	1.45
25	c	509	CLA	MG-NC	2.07	2.11	2.06
25	B	602	CLA	C1B-NB	-2.07	1.35	1.37
29	A	417	SQD	O7-S	2.07	1.51	1.45
34	b	608	F6C	CMD-C2D	-2.07	1.46	1.50
25	C	503	CLA	C1B-NB	-2.07	1.35	1.37
25	c	503	CLA	C1B-NB	-2.07	1.35	1.37
34	c	507	F6C	C1A-NA	2.06	1.40	1.37
34	B	608	F6C	CMD-C2D	-2.06	1.46	1.50
38	V	201	HEC	C3C-C2C	-2.06	1.34	1.41
38	v	201	HEC	C3C-C2C	-2.06	1.34	1.41
37	f	101	HEM	FE-NC	2.06	2.02	1.95
25	d	402	CLA	C1B-NB	-2.06	1.35	1.37
37	F	101	HEM	FE-NC	2.06	2.02	1.95
25	a	410	CLA	MG-NC	2.05	2.11	2.06
25	A	410	CLA	MG-NC	2.05	2.11	2.06
34	b	608	F6C	CMC-C2C	-2.05	1.46	1.50
34	B	608	F6C	CMC-C2C	-2.04	1.46	1.50
25	A	410	CLA	C1B-NB	-2.04	1.35	1.37
25	D	402	CLA	C1B-NB	-2.04	1.35	1.37
25	a	405	CLA	C1B-NB	-2.04	1.35	1.37
25	B	605	CLA	MG-NC	2.04	2.11	2.06
25	C	508	CLA	C1B-NB	-2.04	1.35	1.37
25	B	616	CLA	C1B-NB	-2.04	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	508	CLA	C1B-NB	-2.04	1.35	1.37
25	a	405	CLA	C1B-C2B	-2.04	1.38	1.43
30	d	405	PL9	C31-C29	-2.04	1.47	1.51
25	a	410	CLA	C1B-NB	-2.04	1.35	1.37
25	b	605	CLA	MG-NC	2.04	2.11	2.06
25	b	616	CLA	C1B-NB	-2.04	1.35	1.37
30	D	405	PL9	C31-C29	-2.04	1.47	1.51
34	B	608	F6C	C3B-C4B	2.03	1.48	1.44
25	A	405	CLA	C1B-NB	-2.03	1.35	1.37
25	A	405	CLA	C1B-C2B	-2.03	1.38	1.43
34	C	507	F6C	CMC-C2C	-2.03	1.46	1.50
29	a	412	SQD	C8-C7	2.03	1.56	1.50
29	A	412	SQD	C8-C7	2.03	1.56	1.50
34	b	608	F6C	C3B-C4B	2.03	1.48	1.44
25	B	610	CLA	C1B-NB	-2.03	1.35	1.37
25	b	610	CLA	C1B-NB	-2.03	1.35	1.37
29	C	903	SQD	O7-S	2.02	1.51	1.45
29	c	903	SQD	O7-S	2.02	1.51	1.45
29	a	412	SQD	C6-S	2.02	1.84	1.77
29	A	412	SQD	C6-S	2.02	1.84	1.77
34	b	617	F6C	C2B-C1B	2.02	1.48	1.44
34	c	507	F6C	CMC-C2C	-2.02	1.46	1.50
25	C	513	CLA	MG-NC	2.01	2.11	2.06
34	B	617	F6C	C2B-C1B	2.01	1.48	1.44
25	c	513	CLA	MG-NC	2.01	2.11	2.06
29	B	622	SQD	O9-S	2.01	1.50	1.45
29	b	622	SQD	O9-S	2.01	1.50	1.45
25	b	611	CLA	C1B-NB	-2.00	1.35	1.37
25	B	611	CLA	C1B-NB	-2.00	1.35	1.37

All (617) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	507	F6C	CAA-C2A-C3A	-9.25	110.65	127.88
34	c	507	F6C	CAA-C2A-C3A	-9.24	110.66	127.88
34	B	617	F6C	CAA-C2A-C3A	-8.81	111.48	127.88
34	b	617	F6C	CAA-C2A-C3A	-8.81	111.48	127.88
34	b	614	F6C	CAA-C2A-C3A	-8.52	112.02	127.88
34	B	614	F6C	CAA-C2A-C3A	-8.51	112.03	127.88
34	B	608	F6C	CAA-C2A-C3A	-8.26	112.49	127.88
34	b	608	F6C	CAA-C2A-C3A	-8.26	112.50	127.88
34	C	507	F6C	CMA-C3A-C4A	-7.12	112.17	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	614	F6C	CMA-C3A-C4A	-7.11	112.19	124.71
34	B	614	F6C	CMA-C3A-C4A	-7.11	112.19	124.71
34	B	617	F6C	CMA-C3A-C4A	-7.10	112.20	124.71
34	c	507	F6C	CMA-C3A-C4A	-7.10	112.20	124.71
34	b	617	F6C	CMA-C3A-C4A	-7.09	112.21	124.71
34	b	608	F6C	CMA-C3A-C4A	-6.95	112.47	124.71
34	B	608	F6C	CMA-C3A-C4A	-6.94	112.48	124.71
27	A	409	PHO	C4D-CHA-CBD	-6.91	105.39	108.52
27	a	409	PHO	C4D-CHA-CBD	-6.91	105.39	108.52
27	a	408	PHO	C4D-CHA-CBD	-6.75	105.46	108.52
27	A	408	PHO	C4D-CHA-CBD	-6.74	105.47	108.52
34	B	617	F6C	CAA-C2A-C1A	-6.67	109.75	128.11
34	b	617	F6C	CAA-C2A-C1A	-6.67	109.75	128.11
34	B	608	F6C	CAA-C2A-C1A	-6.63	109.86	128.11
34	b	608	F6C	CAA-C2A-C1A	-6.63	109.86	128.11
34	B	614	F6C	CAA-C2A-C1A	-6.43	110.41	128.11
34	b	614	F6C	CAA-C2A-C1A	-6.42	110.42	128.11
34	c	507	F6C	CAA-C2A-C1A	-6.40	110.49	128.11
34	C	507	F6C	CAA-C2A-C1A	-6.40	110.50	128.11
38	V	201	HEC	CBB-CAB-C3B	-5.55	117.66	127.86
38	v	201	HEC	CBB-CAB-C3B	-5.55	117.66	127.86
34	b	608	F6C	CMA-C3A-C2A	-5.30	111.74	126.12
34	B	608	F6C	CMA-C3A-C2A	-5.29	111.75	126.12
34	b	614	F6C	CMA-C3A-C2A	-5.25	111.85	126.12
34	B	614	F6C	CMA-C3A-C2A	-5.25	111.86	126.12
34	B	617	F6C	CMA-C3A-C2A	-5.21	111.98	126.12
34	b	617	F6C	CMA-C3A-C2A	-5.21	111.98	126.12
34	c	507	F6C	C4A-NA-C1A	5.10	109.96	106.33
34	C	507	F6C	C4A-NA-C1A	5.10	109.96	106.33
30	a	414	PL9	C7-C3-C4	4.98	120.93	116.88
34	c	507	F6C	CMA-C3A-C2A	-4.98	112.60	126.12
34	C	507	F6C	CMA-C3A-C2A	-4.98	112.60	126.12
30	A	414	PL9	C7-C3-C4	4.97	120.92	116.88
30	D	405	PL9	C7-C3-C4	4.70	120.70	116.88
30	d	405	PL9	C7-C3-C4	4.69	120.69	116.88
29	b	622	SQD	O7-S-C6	4.55	112.35	106.94
29	B	622	SQD	O7-S-C6	4.55	112.35	106.94
29	H	102	SQD	O9-S-C6	4.54	112.34	106.94
29	h	102	SQD	O9-S-C6	4.54	112.33	106.94
34	b	614	F6C	C4A-NA-C1A	4.50	109.53	106.33
34	B	614	F6C	C4A-NA-C1A	4.48	109.52	106.33
29	d	407	SQD	O7-S-C6	4.44	112.22	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	407	SQD	O7-S-C6	4.44	112.22	106.94
29	a	412	SQD	O9-S-C6	4.43	112.20	106.94
29	A	412	SQD	O9-S-C6	4.42	112.20	106.94
29	D	407	SQD	O9-S-C6	4.38	112.14	106.94
29	d	407	SQD	O9-S-C6	4.38	112.14	106.94
29	D	407	SQD	O47-C7-C8	4.37	120.92	111.50
29	d	407	SQD	O47-C7-C8	4.37	120.92	111.50
34	b	617	F6C	C4A-NA-C1A	4.29	109.39	106.33
34	B	617	F6C	C4A-NA-C1A	4.28	109.38	106.33
29	H	102	SQD	O47-C7-C8	4.28	120.72	111.50
29	h	102	SQD	O47-C7-C8	4.27	120.71	111.50
34	B	608	F6C	C4A-NA-C1A	4.18	109.30	106.33
34	b	608	F6C	C4A-NA-C1A	4.18	109.30	106.33
25	b	613	CLA	CHD-C1D-ND	-4.17	120.62	124.45
25	B	613	CLA	CHD-C1D-ND	-4.16	120.63	124.45
29	A	417	SQD	O47-C7-C8	4.13	120.40	111.50
29	a	417	SQD	O47-C7-C8	4.13	120.40	111.50
36	d	401	BCT	O2-C-O1	4.11	130.20	119.55
36	D	401	BCT	O2-C-O1	4.11	130.20	119.55
25	A	405	CLA	CHD-C1D-ND	-4.09	120.69	124.45
38	v	201	HEC	CBC-CAC-C3C	-4.09	120.34	127.86
38	V	201	HEC	CBC-CAC-C3C	-4.09	120.34	127.86
25	a	407	CLA	CHD-C1D-ND	-4.09	120.69	124.45
25	a	405	CLA	CHD-C1D-ND	-4.09	120.70	124.45
25	A	407	CLA	CHD-C1D-ND	-4.08	120.70	124.45
29	C	903	SQD	O9-S-C6	4.08	111.78	106.94
29	c	903	SQD	O9-S-C6	4.08	111.78	106.94
29	H	102	SQD	O9-S-O7	-4.02	100.04	113.95
25	B	611	CLA	CHD-C1D-ND	-4.02	120.76	124.45
25	b	611	CLA	CHD-C1D-ND	-4.02	120.76	124.45
29	h	102	SQD	O9-S-O7	-4.02	100.05	113.95
25	B	610	CLA	C4D-CHA-C1A	4.01	126.13	121.25
25	b	610	CLA	C4D-CHA-C1A	4.01	126.13	121.25
34	b	608	F6C	C1A-C2A-C3A	-4.01	102.75	106.97
29	b	622	SQD	O9-S-C6	4.01	111.70	106.94
29	B	622	SQD	O9-S-C6	4.01	111.70	106.94
34	B	608	F6C	C1A-C2A-C3A	-4.00	102.75	106.97
25	B	615	CLA	CHD-C1D-ND	-4.00	120.78	124.45
25	b	615	CLA	CHD-C1D-ND	-3.99	120.78	124.45
29	b	622	SQD	O9-S-O7	-3.97	100.21	113.95
29	B	622	SQD	O9-S-O7	-3.97	100.22	113.95
29	B	622	SQD	O47-C7-C8	3.96	120.04	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	622	SQD	O47-C7-C8	3.96	120.04	111.50
29	C	903	SQD	O47-C7-C8	3.92	119.96	111.50
29	c	903	SQD	O47-C7-C8	3.92	119.96	111.50
25	c	501	CLA	CHD-C1D-ND	-3.90	120.87	124.45
25	C	501	CLA	CHD-C1D-ND	-3.90	120.87	124.45
29	a	417	SQD	O9-S-C6	3.89	111.57	106.94
29	A	417	SQD	O9-S-C6	3.89	111.56	106.94
25	C	502	CLA	C4D-CHA-C1A	3.88	125.97	121.25
25	c	502	CLA	C4D-CHA-C1A	3.88	125.97	121.25
25	b	613	CLA	C4D-CHA-C1A	3.86	125.95	121.25
25	B	613	CLA	C4D-CHA-C1A	3.85	125.94	121.25
25	B	610	CLA	CHD-C1D-ND	-3.83	120.93	124.45
25	b	610	CLA	CHD-C1D-ND	-3.83	120.93	124.45
29	D	407	SQD	O9-S-O7	-3.83	100.71	113.95
29	d	407	SQD	O9-S-O7	-3.83	100.71	113.95
25	C	512	CLA	CHD-C1D-ND	-3.81	120.95	124.45
25	c	512	CLA	CHD-C1D-ND	-3.81	120.96	124.45
25	d	402	CLA	CHD-C1D-ND	-3.80	120.96	124.45
25	B	612	CLA	C4D-CHA-C1A	3.80	125.87	121.25
25	b	612	CLA	C4D-CHA-C1A	3.80	125.87	121.25
25	a	410	CLA	CHD-C1D-ND	-3.80	120.96	124.45
25	D	402	CLA	CHD-C1D-ND	-3.80	120.97	124.45
25	A	410	CLA	CHD-C1D-ND	-3.79	120.97	124.45
25	b	606	CLA	C4D-CHA-C1A	3.79	125.86	121.25
25	B	606	CLA	C4D-CHA-C1A	3.78	125.85	121.25
25	C	501	CLA	C4D-CHA-C1A	3.78	125.85	121.25
25	c	501	CLA	C4D-CHA-C1A	3.78	125.85	121.25
25	A	407	CLA	C4D-CHA-C1A	3.77	125.83	121.25
25	a	407	CLA	C4D-CHA-C1A	3.76	125.82	121.25
29	a	417	SQD	O9-S-O7	-3.76	100.94	113.95
29	A	417	SQD	O9-S-O7	-3.76	100.94	113.95
29	A	412	SQD	O9-S-O7	-3.75	100.96	113.95
29	a	412	SQD	O9-S-O7	-3.75	100.97	113.95
25	c	506	CLA	C4D-CHA-C1A	3.75	125.81	121.25
25	C	506	CLA	C4D-CHA-C1A	3.75	125.81	121.25
25	b	611	CLA	C4D-CHA-C1A	3.75	125.81	121.25
25	B	611	CLA	C4D-CHA-C1A	3.74	125.81	121.25
25	D	403	CLA	CHD-C1D-ND	-3.74	121.01	124.45
25	a	410	CLA	C4D-CHA-C1A	3.74	125.80	121.25
25	d	403	CLA	CHD-C1D-ND	-3.74	121.02	124.45
25	A	410	CLA	C4D-CHA-C1A	3.74	125.80	121.25
25	C	504	CLA	C4D-CHA-C1A	3.73	125.79	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	504	CLA	C4D-CHA-C1A	3.73	125.79	121.25
29	C	903	SQD	O9-S-O7	-3.72	101.08	113.95
29	c	903	SQD	O9-S-O7	-3.72	101.08	113.95
29	H	102	SQD	O6-C1-C2	3.72	114.11	108.30
29	h	102	SQD	O6-C1-C2	3.72	114.11	108.30
25	B	609	CLA	CHD-C1D-ND	-3.71	121.04	124.45
25	B	607	CLA	C4D-CHA-C1A	3.71	125.77	121.25
25	b	607	CLA	C4D-CHA-C1A	3.71	125.77	121.25
25	b	609	CLA	CHD-C1D-ND	-3.71	121.04	124.45
25	c	508	CLA	C4D-CHA-C1A	3.71	125.76	121.25
25	C	508	CLA	C4D-CHA-C1A	3.71	125.76	121.25
25	b	603	CLA	CHD-C1D-ND	-3.70	121.06	124.45
25	B	603	CLA	CHD-C1D-ND	-3.69	121.06	124.45
25	c	510	CLA	CHD-C1D-ND	-3.67	121.08	124.45
25	C	510	CLA	CHD-C1D-ND	-3.67	121.08	124.45
25	c	513	CLA	CHD-C1D-ND	-3.67	121.08	124.45
25	C	510	CLA	C4D-CHA-C1A	3.67	125.71	121.25
25	C	513	CLA	CHD-C1D-ND	-3.66	121.09	124.45
25	c	510	CLA	C4D-CHA-C1A	3.66	125.71	121.25
25	C	503	CLA	C4D-CHA-C1A	3.65	125.69	121.25
25	c	503	CLA	C4D-CHA-C1A	3.65	125.69	121.25
25	C	508	CLA	CHD-C1D-ND	-3.65	121.10	124.45
25	D	403	CLA	C4D-CHA-C1A	3.65	125.69	121.25
25	d	403	CLA	C4D-CHA-C1A	3.65	125.69	121.25
25	c	508	CLA	CHD-C1D-ND	-3.65	121.10	124.45
34	B	617	F6C	C1A-C2A-C3A	-3.65	103.13	106.97
28	B	627	BCR	C20-C21-C22	-3.64	122.11	127.31
25	d	402	CLA	C4D-CHA-C1A	3.64	125.68	121.25
28	b	627	BCR	C20-C21-C22	-3.64	122.12	127.31
34	b	617	F6C	C1A-C2A-C3A	-3.63	103.14	106.97
25	D	402	CLA	C4D-CHA-C1A	3.63	125.67	121.25
25	B	615	CLA	C4D-CHA-C1A	3.63	125.66	121.25
25	b	615	CLA	C4D-CHA-C1A	3.63	125.66	121.25
34	B	608	F6C	CHB-C4A-NA	3.62	127.78	124.45
34	b	608	F6C	CHB-C4A-NA	3.62	127.78	124.45
25	B	616	CLA	C4D-CHA-C1A	3.61	125.64	121.25
29	a	412	SQD	O47-C7-C8	3.61	119.28	111.50
25	b	616	CLA	C4D-CHA-C1A	3.61	125.64	121.25
29	A	412	SQD	O47-C7-C8	3.61	119.28	111.50
25	c	513	CLA	C4D-CHA-C1A	3.60	125.63	121.25
25	C	513	CLA	C4D-CHA-C1A	3.60	125.63	121.25
25	b	612	CLA	CHD-C1D-ND	-3.58	121.16	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H	102	SQD	O7-S-C6	3.58	111.19	106.94
25	B	612	CLA	CHD-C1D-ND	-3.58	121.16	124.45
29	h	102	SQD	O7-S-C6	3.58	111.19	106.94
25	c	509	CLA	CHD-C1D-ND	-3.57	121.17	124.45
25	C	512	CLA	C4D-CHA-C1A	3.57	125.59	121.25
25	c	512	CLA	C4D-CHA-C1A	3.57	125.59	121.25
34	B	614	F6C	CHB-C4A-NA	3.56	127.73	124.45
34	b	614	F6C	C1A-C2A-C3A	-3.56	103.22	106.97
34	b	614	F6C	CHB-C4A-NA	3.56	127.72	124.45
25	C	502	CLA	CHD-C1D-ND	-3.55	121.19	124.45
25	c	502	CLA	CHD-C1D-ND	-3.55	121.19	124.45
25	C	509	CLA	C4D-CHA-C1A	3.55	125.56	121.25
25	C	509	CLA	CHD-C1D-ND	-3.54	121.20	124.45
34	B	614	F6C	C1A-C2A-C3A	-3.54	103.25	106.97
25	c	509	CLA	C4D-CHA-C1A	3.53	125.55	121.25
25	C	503	CLA	CHD-C1D-ND	-3.53	121.21	124.45
25	c	503	CLA	CHD-C1D-ND	-3.53	121.21	124.45
25	C	506	CLA	CHD-C1D-ND	-3.51	121.23	124.45
29	a	412	SQD	O7-S-C6	3.50	111.10	106.94
29	A	412	SQD	O7-S-C6	3.50	111.10	106.94
25	B	606	CLA	O2A-C1-C2	3.50	117.83	108.64
25	b	606	CLA	O2A-C1-C2	3.50	117.83	108.64
25	c	506	CLA	CHD-C1D-ND	-3.50	121.24	124.45
25	C	504	CLA	CHD-C1D-ND	-3.48	121.26	124.45
25	c	504	CLA	CHD-C1D-ND	-3.48	121.26	124.45
25	c	511	CLA	C4D-CHA-C1A	3.47	125.47	121.25
25	C	511	CLA	C4D-CHA-C1A	3.47	125.47	121.25
25	A	405	CLA	C4D-CHA-C1A	3.47	125.47	121.25
25	a	405	CLA	C4D-CHA-C1A	3.47	125.47	121.25
25	B	609	CLA	C4D-CHA-C1A	3.45	125.45	121.25
25	b	606	CLA	CHD-C1D-ND	-3.45	121.28	124.45
25	b	609	CLA	C4D-CHA-C1A	3.45	125.44	121.25
25	B	606	CLA	CHD-C1D-ND	-3.44	121.29	124.45
25	B	604	CLA	C4D-CHA-C1A	3.44	125.44	121.25
25	b	604	CLA	C4D-CHA-C1A	3.44	125.43	121.25
27	a	409	PHO	CMB-C2B-C3B	3.43	131.10	124.68
27	A	409	PHO	CMB-C2B-C3B	3.43	131.10	124.68
27	A	408	PHO	C2B-C1B-NB	-3.42	107.17	109.53
27	a	408	PHO	C2B-C1B-NB	-3.42	107.17	109.53
26	A	406	CL7	CHD-C1D-ND	-3.41	120.64	124.26
25	B	603	CLA	C4D-CHA-C1A	3.41	125.39	121.25
25	b	603	CLA	C4D-CHA-C1A	3.40	125.39	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	406	CL7	CHD-C1D-ND	-3.38	120.67	124.26
34	b	617	F6C	CHB-C4A-NA	3.38	127.56	124.45
34	c	507	F6C	CHB-C4A-NA	3.38	127.56	124.45
34	B	617	F6C	CHB-C4A-NA	3.37	127.55	124.45
34	C	507	F6C	CHB-C4A-NA	3.37	127.55	124.45
25	b	602	CLA	C4D-CHA-C1A	3.36	125.34	121.25
25	B	602	CLA	C4D-CHA-C1A	3.35	125.33	121.25
34	C	507	F6C	O2D-CGD-O1D	-3.35	117.28	123.84
34	c	507	F6C	O2D-CGD-O1D	-3.35	117.29	123.84
27	a	409	PHO	O1D-CGD-CBD	3.31	130.25	124.74
25	c	505	CLA	C4D-CHA-C1A	3.31	125.27	121.25
25	C	505	CLA	C4D-CHA-C1A	3.30	125.27	121.25
27	A	409	PHO	O1D-CGD-CBD	3.30	130.24	124.74
25	b	602	CLA	CHD-C1D-ND	-3.30	121.42	124.45
25	B	602	CLA	CHD-C1D-ND	-3.30	121.42	124.45
25	b	607	CLA	CHD-C1D-ND	-3.28	121.44	124.45
25	B	607	CLA	CHD-C1D-ND	-3.28	121.44	124.45
27	a	409	PHO	C2B-C1B-NB	-3.27	107.27	109.53
27	A	409	PHO	C2B-C1B-NB	-3.27	107.27	109.53
25	b	616	CLA	CHD-C1D-ND	-3.25	121.47	124.45
25	B	616	CLA	CHD-C1D-ND	-3.25	121.47	124.45
29	B	622	SQD	O5-C5-C4	3.23	115.56	109.69
29	b	622	SQD	O5-C5-C4	3.23	115.56	109.69
30	D	405	PL9	C7-C8-C9	-3.22	121.43	126.79
30	D	405	PL9	C7-C3-C2	-3.22	119.07	123.30
30	d	405	PL9	C7-C3-C2	-3.21	119.08	123.30
30	d	405	PL9	C7-C8-C9	-3.21	121.45	126.79
25	C	511	CLA	CHD-C1D-ND	-3.19	121.52	124.45
25	c	511	CLA	CHD-C1D-ND	-3.19	121.52	124.45
29	A	417	SQD	O7-S-C6	3.15	110.68	106.94
30	A	414	PL9	C7-C3-C2	-3.15	119.16	123.30
30	a	414	PL9	C7-C3-C2	-3.15	119.16	123.30
29	a	417	SQD	O7-S-C6	3.14	110.68	106.94
34	b	617	F6C	O2D-CGD-O1D	-3.09	117.80	123.84
34	B	617	F6C	O2D-CGD-O1D	-3.09	117.80	123.84
29	A	412	SQD	O8-S-C6	3.08	110.65	105.74
27	A	408	PHO	O2D-CGD-O1D	-3.08	117.81	123.84
27	a	408	PHO	O2D-CGD-O1D	-3.08	117.81	123.84
29	a	412	SQD	O8-S-C6	3.08	110.65	105.74
29	b	622	SQD	C1-C2-C3	-3.05	103.64	110.00
29	B	622	SQD	C1-C2-C3	-3.05	103.65	110.00
25	b	604	CLA	CHD-C1D-ND	-3.05	121.65	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	604	CLA	CHD-C1D-ND	-3.04	121.66	124.45
34	b	608	F6C	O2D-CGD-O1D	-3.03	117.92	123.84
34	B	608	F6C	O2D-CGD-O1D	-3.03	117.92	123.84
34	B	614	F6C	O2D-CGD-O1D	-2.99	118.00	123.84
34	b	614	F6C	O2D-CGD-O1D	-2.98	118.01	123.84
28	b	618	BCR	C11-C10-C9	-2.96	123.08	127.31
29	C	903	SQD	O7-S-C6	2.96	110.46	106.94
29	c	903	SQD	O7-S-C6	2.96	110.46	106.94
28	B	618	BCR	C11-C10-C9	-2.96	123.09	127.31
29	A	417	SQD	C1-O5-C5	-2.92	107.97	113.69
27	a	408	PHO	CMB-C2B-C3B	2.92	130.13	124.68
25	B	605	CLA	CHA-C1A-NA	-2.92	119.72	126.40
25	b	605	CLA	CHA-C1A-NA	-2.92	119.72	126.40
27	A	408	PHO	CMB-C2B-C3B	2.91	130.13	124.68
29	a	417	SQD	C1-O5-C5	-2.91	107.97	113.69
34	c	507	F6C	C1A-C2A-C3A	-2.91	103.91	106.97
34	C	507	F6C	C1A-C2A-C3A	-2.90	103.92	106.97
29	A	417	SQD	O8-S-C6	2.88	110.34	105.74
29	a	417	SQD	O8-S-C6	2.88	110.34	105.74
27	A	409	PHO	O2D-CGD-O1D	-2.87	118.22	123.84
27	a	409	PHO	O2D-CGD-O1D	-2.87	118.22	123.84
33	P	629	LHG	C5-O7-C7	2.86	124.84	117.79
33	p	629	LHG	C5-O7-C7	2.86	124.84	117.79
29	H	102	SQD	O48-C23-C24	2.86	120.88	111.91
29	h	102	SQD	O48-C23-C24	2.86	120.87	111.91
25	C	505	CLA	CHD-C1D-ND	-2.85	121.84	124.45
25	c	505	CLA	CHD-C1D-ND	-2.85	121.84	124.45
30	A	414	PL9	C40-C39-C41	2.84	120.05	115.27
30	a	414	PL9	C40-C39-C41	2.84	120.05	115.27
29	B	622	SQD	O6-C1-C2	2.79	112.66	108.30
29	b	622	SQD	O6-C1-C2	2.79	112.66	108.30
25	C	505	CLA	CHA-C1A-NA	-2.79	120.01	126.40
25	c	505	CLA	CHA-C1A-NA	-2.79	120.01	126.40
25	c	511	CLA	CHA-C1A-NA	-2.77	120.04	126.40
29	D	407	SQD	C3-C4-C5	2.77	115.19	110.24
29	d	407	SQD	C3-C4-C5	2.77	115.19	110.24
25	C	511	CLA	CHA-C1A-NA	-2.77	120.05	126.40
25	C	503	CLA	CHA-C1A-NA	-2.77	120.06	126.40
25	c	503	CLA	CHA-C1A-NA	-2.77	120.06	126.40
25	b	602	CLA	CHA-C1A-NA	-2.76	120.08	126.40
25	B	602	CLA	CHA-C1A-NA	-2.76	120.09	126.40
25	B	610	CLA	CHA-C1A-NA	-2.75	120.09	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	414	PL9	C22-C23-C24	-2.75	121.03	127.66
25	b	610	CLA	CHA-C1A-NA	-2.75	120.09	126.40
30	a	414	PL9	C22-C23-C24	-2.75	121.03	127.66
38	V	201	HEC	C4C-NC-C1C	2.75	108.04	105.35
38	v	201	HEC	C4C-NC-C1C	2.75	108.04	105.35
25	C	511	CLA	C4A-NA-C1A	2.72	107.93	106.71
25	c	511	CLA	C4A-NA-C1A	2.72	107.93	106.71
38	v	201	HEC	C4D-ND-C1D	2.72	108.01	105.35
38	V	201	HEC	C4D-ND-C1D	2.72	108.01	105.35
25	B	616	CLA	CHA-C1A-NA	-2.71	120.19	126.40
25	b	616	CLA	CHA-C1A-NA	-2.71	120.19	126.40
29	C	903	SQD	O8-S-C6	2.71	110.06	105.74
29	c	903	SQD	O8-S-C6	2.71	110.06	105.74
29	H	102	SQD	O8-S-C6	2.71	110.06	105.74
29	h	102	SQD	O8-S-C6	2.71	110.05	105.74
25	B	602	CLA	C4A-NA-C1A	2.70	107.92	106.71
25	C	502	CLA	CHA-C1A-NA	-2.70	120.21	126.40
25	c	502	CLA	CHA-C1A-NA	-2.70	120.21	126.40
29	a	412	SQD	O48-C23-C24	2.70	120.38	111.91
29	A	412	SQD	O48-C23-C24	2.70	120.37	111.91
25	B	607	CLA	CHA-C1A-NA	-2.69	120.23	126.40
25	b	607	CLA	CHA-C1A-NA	-2.69	120.24	126.40
25	b	602	CLA	C4A-NA-C1A	2.69	107.91	106.71
25	b	613	CLA	CHA-C1A-NA	-2.69	120.25	126.40
25	B	613	CLA	CHA-C1A-NA	-2.68	120.25	126.40
34	c	507	F6C	CBD-CHA-C4D	-2.67	105.53	108.54
34	C	507	F6C	CBD-CHA-C4D	-2.67	105.53	108.54
34	b	617	F6C	OMB-CMB-C2B	-2.67	119.66	125.69
30	d	405	PL9	C40-C39-C41	2.66	119.75	115.27
25	B	604	CLA	CHA-C1A-NA	-2.66	120.30	126.40
25	C	509	CLA	CHA-C1A-NA	-2.66	120.30	126.40
25	b	604	CLA	CHA-C1A-NA	-2.66	120.31	126.40
30	D	405	PL9	C40-C39-C41	2.66	119.74	115.27
34	B	608	F6C	C4A-C3A-C2A	-2.66	103.06	106.94
34	b	608	F6C	C4A-C3A-C2A	-2.66	103.06	106.94
25	c	509	CLA	CHA-C1A-NA	-2.66	120.32	126.40
25	d	403	CLA	CHA-C1A-NA	-2.65	120.32	126.40
25	c	506	CLA	CHA-C1A-NA	-2.65	120.32	126.40
25	C	506	CLA	CHA-C1A-NA	-2.65	120.32	126.40
25	D	403	CLA	CHA-C1A-NA	-2.65	120.32	126.40
29	h	102	SQD	C1-O5-C5	-2.65	108.48	113.69
29	H	102	SQD	C1-O5-C5	-2.65	108.48	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	617	F6C	OMB-CMB-C2B	-2.65	119.69	125.69
25	c	508	CLA	CHA-C1A-NA	-2.65	120.33	126.40
25	C	508	CLA	CHA-C1A-NA	-2.65	120.33	126.40
25	C	504	CLA	CHA-C1A-NA	-2.64	120.35	126.40
25	c	501	CLA	CHA-C1A-NA	-2.64	120.35	126.40
25	c	504	CLA	CHA-C1A-NA	-2.64	120.35	126.40
25	C	501	CLA	CHA-C1A-NA	-2.64	120.36	126.40
29	A	417	SQD	O6-C1-C2	2.63	112.41	108.30
29	a	417	SQD	O6-C1-C2	2.63	112.41	108.30
25	b	606	CLA	CHA-C1A-NA	-2.63	120.38	126.40
25	B	606	CLA	CHA-C1A-NA	-2.63	120.38	126.40
25	B	609	CLA	CHA-C1A-NA	-2.62	120.39	126.40
25	A	410	CLA	CHA-C1A-NA	-2.62	120.39	126.40
25	a	410	CLA	CHA-C1A-NA	-2.62	120.39	126.40
25	C	513	CLA	CHA-C1A-NA	-2.62	120.39	126.40
25	b	609	CLA	CHA-C1A-NA	-2.62	120.39	126.40
25	c	513	CLA	CHA-C1A-NA	-2.62	120.39	126.40
25	B	612	CLA	CHA-C1A-NA	-2.62	120.41	126.40
25	b	612	CLA	CHA-C1A-NA	-2.62	120.41	126.40
25	C	510	CLA	CHA-C1A-NA	-2.61	120.42	126.40
25	c	510	CLA	CHA-C1A-NA	-2.61	120.42	126.40
34	C	507	F6C	OMB-CMB-C2B	-2.61	119.79	125.69
34	c	507	F6C	OMB-CMB-C2B	-2.61	119.80	125.69
25	c	503	CLA	C4A-NA-C1A	2.60	107.88	106.71
34	b	617	F6C	C4A-C3A-C2A	-2.60	103.15	106.94
25	b	611	CLA	CHA-C1A-NA	-2.60	120.45	126.40
25	C	503	CLA	C4A-NA-C1A	2.60	107.87	106.71
25	C	512	CLA	CHA-C1A-NA	-2.60	120.45	126.40
25	D	402	CLA	CHA-C1A-NA	-2.60	120.45	126.40
25	B	611	CLA	CHA-C1A-NA	-2.60	120.45	126.40
25	c	512	CLA	CHA-C1A-NA	-2.60	120.45	126.40
25	d	402	CLA	CHA-C1A-NA	-2.60	120.45	126.40
34	B	617	F6C	C4A-C3A-C2A	-2.59	103.15	106.94
30	D	405	PL9	C27-C28-C29	-2.59	121.42	127.66
30	d	405	PL9	C27-C28-C29	-2.59	121.42	127.66
25	b	615	CLA	CHA-C1A-NA	-2.59	120.47	126.40
25	A	407	CLA	CHA-C1A-NA	-2.59	120.48	126.40
25	a	407	CLA	CHA-C1A-NA	-2.58	120.48	126.40
25	B	615	CLA	CHA-C1A-NA	-2.58	120.48	126.40
30	d	405	PL9	C22-C23-C24	-2.57	121.46	127.66
25	b	603	CLA	CHA-C1A-NA	-2.57	120.51	126.40
30	D	405	PL9	C22-C23-C24	-2.57	121.47	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	603	CLA	CHA-C1A-NA	-2.57	120.51	126.40
30	a	414	PL9	C27-C28-C29	-2.56	121.49	127.66
27	a	408	PHO	C1C-C2C-C3C	-2.56	106.48	108.61
30	A	414	PL9	C27-C28-C29	-2.56	121.49	127.66
27	A	408	PHO	C1C-C2C-C3C	-2.56	106.48	108.61
38	v	201	HEC	C4A-NA-C1A	2.54	107.84	105.35
38	V	201	HEC	C4A-NA-C1A	2.54	107.84	105.35
34	b	617	F6C	CMB-C2B-C1B	-2.54	121.75	128.26
34	B	614	F6C	C4A-C3A-C2A	-2.54	103.23	106.94
25	A	405	CLA	CHA-C1A-NA	-2.53	120.59	126.40
25	a	405	CLA	CHA-C1A-NA	-2.53	120.59	126.40
29	d	407	SQD	O5-C5-C4	2.53	114.28	109.69
25	c	502	CLA	C4A-NA-C1A	2.53	107.84	106.71
32	L	210	LMT	C1B-O1B-C4'	2.53	124.22	117.96
29	D	407	SQD	O5-C5-C4	2.53	114.28	109.69
32	l	210	LMT	C1B-O1B-C4'	2.53	124.21	117.96
34	b	614	F6C	C4A-C3A-C2A	-2.52	103.25	106.94
25	c	509	CLA	C4A-NA-C1A	2.52	107.84	106.71
25	C	502	CLA	C4A-NA-C1A	2.52	107.84	106.71
34	B	617	F6C	CMB-C2B-C1B	-2.52	121.80	128.26
25	C	509	CLA	C4A-NA-C1A	2.51	107.84	106.71
25	C	501	CLA	C4A-NA-C1A	2.51	107.83	106.71
34	b	608	F6C	OMB-CMB-C2B	-2.51	120.02	125.69
29	B	622	SQD	O48-C23-C24	2.50	119.77	111.91
25	c	501	CLA	C4A-NA-C1A	2.50	107.83	106.71
29	b	622	SQD	O48-C23-C24	2.50	119.76	111.91
34	B	608	F6C	OMB-CMB-C2B	-2.50	120.03	125.69
34	C	507	F6C	C3A-C4A-NA	2.50	111.94	110.10
34	c	507	F6C	C3A-C4A-NA	2.49	111.94	110.10
29	D	407	SQD	O48-C23-C24	2.49	119.71	111.91
29	d	407	SQD	O48-C23-C24	2.49	119.71	111.91
34	B	617	F6C	C3A-C4A-NA	2.48	111.93	110.10
34	C	507	F6C	C4A-C3A-C2A	-2.47	103.34	106.94
34	c	507	F6C	C4A-C3A-C2A	-2.47	103.34	106.94
34	B	614	F6C	C3A-C4A-NA	2.47	111.92	110.10
34	b	617	F6C	C3A-C4A-NA	2.46	111.92	110.10
25	B	606	CLA	C1-O2A-CGA	-2.45	110.00	116.44
25	b	606	CLA	C1-O2A-CGA	-2.45	110.00	116.44
34	b	614	F6C	C3A-C4A-NA	2.45	111.91	110.10
29	C	903	SQD	O48-C23-C24	2.45	119.58	111.91
29	c	903	SQD	O48-C23-C24	2.45	119.58	111.91
34	B	614	F6C	CHB-C4A-C3A	-2.45	120.35	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	408	PHO	O1D-CGD-CBD	2.44	128.81	124.74
25	c	505	CLA	C4A-NA-C1A	2.44	107.80	106.71
27	a	408	PHO	O1D-CGD-CBD	2.44	128.80	124.74
34	b	614	F6C	CHB-C4A-C3A	-2.44	120.37	125.48
25	C	505	CLA	C4A-NA-C1A	2.43	107.80	106.71
34	B	617	F6C	C1-C2-C3	-2.43	122.82	126.75
34	b	617	F6C	C1-C2-C3	-2.42	122.83	126.75
25	b	607	CLA	C4A-NA-C1A	2.42	107.79	106.71
25	B	616	CLA	C4A-NA-C1A	2.42	107.79	106.71
25	B	607	CLA	C4A-NA-C1A	2.41	107.79	106.71
25	b	616	CLA	C4A-NA-C1A	2.41	107.79	106.71
29	A	417	SQD	O48-C23-C24	2.41	119.46	111.91
29	a	417	SQD	O48-C23-C24	2.41	119.46	111.91
34	b	614	F6C	CBD-CHA-C4D	-2.40	105.83	108.54
34	B	614	F6C	CBD-CHA-C4D	-2.40	105.84	108.54
34	B	614	F6C	OMB-CMB-C2B	-2.40	120.26	125.69
27	A	409	PHO	C1-C2-C3	-2.39	121.90	126.04
27	a	409	PHO	C1-C2-C3	-2.39	121.91	126.04
34	b	614	F6C	OMB-CMB-C2B	-2.39	120.29	125.69
30	d	405	PL9	O1-C4-C3	-2.39	118.09	120.72
28	k	102	BCR	C7-C8-C9	-2.38	122.64	126.23
28	K	102	BCR	C7-C8-C9	-2.38	122.65	126.23
34	C	507	F6C	CHB-C4A-C3A	-2.37	120.50	125.48
34	c	507	F6C	CHB-C4A-C3A	-2.37	120.50	125.48
38	V	201	HEC	C4B-NB-C1B	2.37	107.67	105.35
30	D	405	PL9	O1-C4-C3	-2.37	118.11	120.72
38	v	201	HEC	C4B-NB-C1B	2.37	107.67	105.35
34	B	617	F6C	CHB-C4A-C3A	-2.37	120.52	125.48
34	b	617	F6C	CHB-C4A-C3A	-2.36	120.52	125.48
29	b	622	SQD	C3-C4-C5	2.35	114.42	110.24
25	B	605	CLA	C2A-C1A-CHA	2.35	127.96	123.86
29	B	622	SQD	C3-C4-C5	2.34	114.42	110.24
30	D	405	PL9	C20-C19-C21	2.34	119.21	115.27
25	b	605	CLA	C2A-C1A-CHA	2.34	127.95	123.86
30	d	405	PL9	C20-C19-C21	2.34	119.21	115.27
37	f	101	HEM	C1B-NB-C4B	2.33	107.48	105.07
37	F	101	HEM	C1B-NB-C4B	2.33	107.47	105.07
34	b	608	F6C	CHB-C4A-C3A	-2.32	120.62	125.48
26	A	406	CL7	CHA-C1A-NA	-2.32	120.50	125.98
34	B	608	F6C	CHB-C4A-C3A	-2.32	120.62	125.48
35	C	516	DGD	C6D-O5D-C1E	2.31	118.26	113.74
30	A	414	PL9	C7-C8-C9	-2.31	122.94	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	516	DGD	C6D-O5D-C1E	2.31	118.26	113.74
26	a	406	CL7	CHA-C1A-NA	-2.31	120.51	125.98
25	b	612	CLA	C4A-NA-C1A	2.31	107.75	106.71
30	a	414	PL9	C7-C8-C9	-2.31	122.94	126.79
25	a	407	CLA	CHD-C1D-C2D	2.31	130.33	125.48
25	A	407	CLA	CHD-C1D-C2D	2.31	130.32	125.48
25	B	612	CLA	C4A-NA-C1A	2.30	107.74	106.71
25	B	613	CLA	CHD-C1D-C2D	2.30	130.31	125.48
25	b	613	CLA	CHD-C1D-C2D	2.30	130.31	125.48
37	f	101	HEM	C4C-NC-C1C	2.29	107.59	105.35
25	A	405	CLA	CHD-C1D-C2D	2.28	130.26	125.48
37	F	101	HEM	C4C-NC-C1C	2.28	107.58	105.35
25	a	405	CLA	CHD-C1D-C2D	2.28	130.26	125.48
26	a	406	CL7	C3C-C4C-NC	-2.28	108.53	110.18
26	A	406	CL7	C3C-C4C-NC	-2.27	108.53	110.18
37	F	101	HEM	C4A-NA-C1A	2.26	107.56	105.35
29	D	407	SQD	O8-S-C6	2.26	109.34	105.74
29	d	407	SQD	O8-S-C6	2.26	109.33	105.74
37	f	101	HEM	C4A-NA-C1A	2.25	107.56	105.35
29	A	412	SQD	O5-C5-C4	2.25	113.78	109.69
29	a	412	SQD	O5-C5-C4	2.25	113.78	109.69
25	B	615	CLA	CHD-C1D-C2D	2.25	130.20	125.48
25	b	615	CLA	CHD-C1D-C2D	2.25	130.19	125.48
25	c	501	CLA	CHD-C1D-C2D	2.24	130.18	125.48
25	C	501	CLA	CHD-C1D-C2D	2.24	130.18	125.48
25	B	611	CLA	CHD-C1D-C2D	2.24	130.18	125.48
25	b	611	CLA	CHD-C1D-C2D	2.24	130.18	125.48
34	C	507	F6C	O2D-CGD-CBD	2.23	115.24	111.27
30	A	414	PL9	C20-C19-C21	2.23	119.03	115.27
30	a	414	PL9	C20-C19-C21	2.23	119.03	115.27
34	c	507	F6C	O2D-CGD-CBD	2.23	115.23	111.27
38	v	201	HEC	C2A-C1A-NA	-2.23	108.16	110.32
32	z	102	LMT	C1B-O5B-C5B	2.22	118.05	113.69
32	Z	102	LMT	C1B-O5B-C5B	2.22	118.05	113.69
38	V	201	HEC	C2A-C1A-NA	-2.22	108.16	110.32
34	B	608	F6C	CMB-C2B-C1B	-2.21	122.59	128.26
31	c	519	LMG	O1-C7-C8	-2.21	105.58	110.90
31	C	519	LMG	O1-C7-C8	-2.21	105.58	110.90
30	a	414	PL9	O1-C4-C3	-2.20	118.30	120.72
34	b	608	F6C	CMB-C2B-C1B	-2.20	122.61	128.26
30	a	414	PL9	C37-C38-C39	-2.20	122.37	127.66
30	A	414	PL9	O1-C4-C3	-2.20	118.30	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	414	PL9	C37-C38-C39	-2.19	122.38	127.66
25	c	510	CLA	CHD-C1D-C2D	2.19	130.08	125.48
25	C	510	CLA	CHD-C1D-C2D	2.19	130.08	125.48
32	Z	102	LMT	O1B-C1B-C2B	2.19	113.77	108.10
32	z	102	LMT	O1B-C1B-C2B	2.19	113.77	108.10
25	b	610	CLA	CHD-C1D-C2D	2.18	130.06	125.48
25	B	610	CLA	CHD-C1D-C2D	2.18	130.06	125.48
25	A	410	CLA	CHD-C1D-C2D	2.17	130.04	125.48
29	C	903	SQD	C46-C45-C44	-2.17	106.64	111.79
25	a	410	CLA	CHD-C1D-C2D	2.17	130.04	125.48
29	c	903	SQD	C46-C45-C44	-2.17	106.65	111.79
29	c	903	SQD	O6-C1-C2	2.17	111.69	108.30
29	C	903	SQD	O6-C1-C2	2.17	111.69	108.30
30	A	414	PL9	C32-C33-C34	-2.17	122.44	127.66
30	a	414	PL9	C32-C33-C34	-2.17	122.44	127.66
34	B	617	F6C	CBD-CHA-C4D	-2.17	106.10	108.54
37	F	101	HEM	C4D-ND-C1D	2.16	107.31	105.07
34	b	617	F6C	CBD-CHA-C4D	-2.16	106.10	108.54
37	f	101	HEM	C4D-ND-C1D	2.16	107.31	105.07
25	b	603	CLA	CHD-C1D-C2D	2.16	130.01	125.48
25	B	603	CLA	CHD-C1D-C2D	2.16	130.00	125.48
30	A	414	PL9	O2-C1-C2	-2.15	116.86	121.78
30	a	414	PL9	O2-C1-C2	-2.15	116.86	121.78
25	B	609	CLA	CHD-C1D-C2D	2.14	129.97	125.48
25	b	609	CLA	CHD-C1D-C2D	2.14	129.97	125.48
28	b	627	BCR	C24-C23-C22	2.14	129.47	126.23
28	B	627	BCR	C24-C23-C22	2.14	129.46	126.23
30	A	414	PL9	O2-C1-C6	2.14	124.29	120.59
30	a	414	PL9	O2-C1-C6	2.14	124.29	120.59
34	B	608	F6C	C1-C2-C3	-2.13	122.35	126.04
34	b	608	F6C	C1-C2-C3	-2.13	122.36	126.04
28	d	404	BCR	C7-C8-C9	-2.13	123.02	126.23
27	A	409	PHO	CMA-C3A-C4A	-2.13	109.71	114.38
27	a	409	PHO	CMA-C3A-C4A	-2.13	109.72	114.38
28	D	404	BCR	C7-C8-C9	-2.13	123.02	126.23
36	D	401	BCT	O3-C-O1	-2.12	114.04	119.55
25	D	403	CLA	CHD-C1D-C2D	2.12	129.92	125.48
25	d	403	CLA	CHD-C1D-C2D	2.12	129.92	125.48
36	d	401	BCT	O3-C-O1	-2.12	114.06	119.55
34	c	507	F6C	CMB-C2B-C1B	-2.11	122.84	128.26
25	C	512	CLA	CHD-C1D-C2D	2.11	129.91	125.48
25	c	512	CLA	CHD-C1D-C2D	2.11	129.91	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	405	PL9	O2-C1-C2	-2.11	116.95	121.78
34	C	507	F6C	CMB-C2B-C1B	-2.11	122.85	128.26
30	D	405	PL9	O2-C1-C2	-2.11	116.95	121.78
32	L	213	LMT	O3B-C3B-C2B	-2.11	105.48	110.35
32	l	213	LMT	O3B-C3B-C2B	-2.11	105.48	110.35
30	D	405	PL9	C31-C32-C33	-2.10	104.97	111.88
30	d	405	PL9	C31-C32-C33	-2.10	104.97	111.88
25	C	502	CLA	CHD-C1D-C2D	2.10	129.89	125.48
25	c	502	CLA	CHD-C1D-C2D	2.10	129.89	125.48
34	b	614	F6C	CMB-C2B-C1B	-2.10	122.87	128.26
25	d	402	CLA	CHD-C1D-C2D	2.10	129.89	125.48
30	a	414	PL9	C12-C13-C14	-2.09	122.62	127.66
34	B	614	F6C	CMB-C2B-C1B	-2.09	122.89	128.26
25	D	402	CLA	CHD-C1D-C2D	2.09	129.87	125.48
30	A	414	PL9	C12-C13-C14	-2.09	122.62	127.66
28	C	515	BCR	C19-C18-C17	-2.08	115.74	118.94
28	c	515	BCR	C19-C18-C17	-2.08	115.74	118.94
25	b	610	CLA	C4A-NA-C1A	2.08	107.64	106.71
25	B	610	CLA	C4A-NA-C1A	2.08	107.64	106.71
25	C	503	CLA	CHD-C1D-C2D	2.07	129.83	125.48
25	c	503	CLA	CHD-C1D-C2D	2.07	129.83	125.48
34	B	617	F6C	O2A-CGA-O1A	-2.07	118.36	123.59
25	c	509	CLA	CHD-C1D-C2D	2.07	129.83	125.48
34	b	617	F6C	O2A-CGA-O1A	-2.07	118.36	123.59
34	c	507	F6C	O2A-CGA-O1A	-2.07	118.38	123.59
34	C	507	F6C	O2A-CGA-O1A	-2.06	118.38	123.59
30	d	405	PL9	O2-C1-C6	2.06	124.16	120.59
30	D	405	PL9	O2-C1-C6	2.06	124.16	120.59
25	C	509	CLA	CHD-C1D-C2D	2.06	129.80	125.48
25	C	508	CLA	CHD-C1D-C2D	2.06	129.79	125.48
25	c	508	CLA	CHD-C1D-C2D	2.06	129.79	125.48
38	v	201	HEC	C3D-C4D-ND	-2.05	107.85	110.15
25	C	506	CLA	CHD-C1D-C2D	2.05	129.78	125.48
25	c	513	CLA	CHD-C1D-C2D	2.05	129.78	125.48
38	V	201	HEC	C3D-C4D-ND	-2.05	107.86	110.15
25	C	513	CLA	CHD-C1D-C2D	2.05	129.78	125.48
25	c	506	CLA	CHD-C1D-C2D	2.05	129.78	125.48
31	d	411	LMG	C1-C2-C3	-2.05	105.73	110.00
34	b	614	F6C	C1-C2-C3	-2.04	122.51	126.04
31	D	411	LMG	C1-C2-C3	-2.04	105.74	110.00
27	A	408	PHO	CMA-C3A-C4A	-2.04	109.91	114.38
27	a	408	PHO	CMA-C3A-C4A	-2.04	109.91	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	614	F6C	C1-C2-C3	-2.03	122.53	126.04
32	a	675	LMT	C2'-C3'-C4'	2.03	114.33	109.68
25	c	504	CLA	CHD-C1D-C2D	2.03	129.75	125.48
32	A	675	LMT	C2'-C3'-C4'	2.03	114.32	109.68
25	C	504	CLA	CHD-C1D-C2D	2.03	129.74	125.48
25	c	504	CLA	C4A-NA-C1A	2.02	107.61	106.71
25	C	504	CLA	C4A-NA-C1A	2.02	107.61	106.71
30	D	405	PL9	C46-C47-C48	-2.02	105.26	111.88
30	d	405	PL9	C46-C47-C48	-2.01	105.26	111.88
25	B	605	CLA	C4D-CHA-C1A	2.01	123.70	121.25
25	b	605	CLA	C4D-CHA-C1A	2.01	123.70	121.25
35	C	518	DGD	C6D-O5D-C1E	2.01	117.67	113.74
35	c	518	DGD	C6D-O5D-C1E	2.01	117.67	113.74
34	b	608	F6C	C3A-C4A-NA	2.01	111.58	110.10
25	B	605	CLA	C4A-NA-C1A	2.01	107.61	106.71
28	b	619	BCR	C11-C10-C9	-2.00	124.45	127.31
34	B	608	F6C	C3A-C4A-NA	2.00	111.58	110.10
28	B	619	BCR	C11-C10-C9	-2.00	124.45	127.31
25	b	605	CLA	C4A-NA-C1A	2.00	107.61	106.71
25	d	403	CLA	C4A-NA-C1A	2.00	107.61	106.71

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	A	406	CL7	NC
26	A	406	CL7	NA
26	a	406	CL7	NC
26	a	406	CL7	NA
34	B	608	F6C	NA
34	B	614	F6C	NA
34	B	617	F6C	NA
34	C	507	F6C	NA
34	b	608	F6C	NA
34	b	614	F6C	NA
34	b	617	F6C	NA
34	c	507	F6C	NA

All (1620) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	407	CLA	CHA-CBD-CGD-O1D
25	A	407	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	A	410	CLA	C2-C3-C5-C6
25	A	410	CLA	C4-C3-C5-C6
25	B	602	CLA	CHA-CBD-CGD-O1D
25	B	602	CLA	CHA-CBD-CGD-O2D
25	B	602	CLA	CAD-CBD-CGD-O1D
25	B	602	CLA	CAD-CBD-CGD-O2D
25	B	604	CLA	C4-C3-C5-C6
25	B	606	CLA	O2A-C1-C2-C3
25	B	606	CLA	C4-C3-C5-C6
25	C	508	CLA	CHA-CBD-CGD-O1D
25	C	508	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	C4-C3-C5-C6
25	a	407	CLA	CHA-CBD-CGD-O1D
25	a	407	CLA	CHA-CBD-CGD-O2D
25	a	410	CLA	C2-C3-C5-C6
25	a	410	CLA	C4-C3-C5-C6
25	b	602	CLA	CHA-CBD-CGD-O1D
25	b	602	CLA	CHA-CBD-CGD-O2D
25	b	602	CLA	CAD-CBD-CGD-O1D
25	b	602	CLA	CAD-CBD-CGD-O2D
25	b	604	CLA	C4-C3-C5-C6
25	b	606	CLA	O2A-C1-C2-C3
25	b	606	CLA	C4-C3-C5-C6
25	c	508	CLA	CHA-CBD-CGD-O1D
25	c	508	CLA	CHA-CBD-CGD-O2D
25	c	512	CLA	C4-C3-C5-C6
28	B	619	BCR	C1-C6-C7-C8
28	B	620	BCR	C5-C6-C7-C8
28	B	620	BCR	C7-C8-C9-C10
28	B	620	BCR	C7-C8-C9-C34
28	B	627	BCR	C23-C24-C25-C26
28	D	404	BCR	C1-C6-C7-C8
28	D	404	BCR	C5-C6-C7-C8
28	D	404	BCR	C7-C8-C9-C10
28	D	404	BCR	C7-C8-C9-C34
28	D	404	BCR	C23-C24-C25-C26
28	K	102	BCR	C7-C8-C9-C10
28	K	102	BCR	C7-C8-C9-C34
28	K	101	BCR	C1-C6-C7-C8
28	K	101	BCR	C5-C6-C7-C8
28	K	101	BCR	C17-C18-C19-C20
28	K	101	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
28	K	101	BCR	C21-C22-C23-C24
28	K	101	BCR	C37-C22-C23-C24
28	b	619	BCR	C1-C6-C7-C8
28	b	620	BCR	C5-C6-C7-C8
28	b	620	BCR	C7-C8-C9-C10
28	b	620	BCR	C7-C8-C9-C34
28	b	627	BCR	C23-C24-C25-C26
28	d	404	BCR	C1-C6-C7-C8
28	d	404	BCR	C5-C6-C7-C8
28	d	404	BCR	C7-C8-C9-C10
28	d	404	BCR	C7-C8-C9-C34
28	d	404	BCR	C23-C24-C25-C26
28	k	102	BCR	C7-C8-C9-C10
28	k	102	BCR	C7-C8-C9-C34
28	k	101	BCR	C1-C6-C7-C8
28	k	101	BCR	C5-C6-C7-C8
28	k	101	BCR	C17-C18-C19-C20
28	k	101	BCR	C36-C18-C19-C20
28	k	101	BCR	C21-C22-C23-C24
28	k	101	BCR	C37-C22-C23-C24
29	A	412	SQD	O5-C5-C6-S
29	A	417	SQD	C8-C7-O47-C45
29	B	622	SQD	C5-C6-S-O7
29	C	903	SQD	C2-C1-O6-C44
29	C	903	SQD	O5-C1-O6-C44
29	C	903	SQD	C8-C7-O47-C45
29	C	903	SQD	C5-C6-S-O7
29	C	903	SQD	C5-C6-S-O8
29	C	903	SQD	C5-C6-S-O9
29	D	407	SQD	O10-C23-O48-C46
29	H	102	SQD	O5-C1-O6-C44
29	H	102	SQD	O49-C7-O47-C45
29	H	102	SQD	C8-C7-O47-C45
29	a	417	SQD	C8-C7-O47-C45
29	a	412	SQD	O5-C5-C6-S
29	b	622	SQD	C5-C6-S-O7
29	c	903	SQD	C2-C1-O6-C44
29	c	903	SQD	O5-C1-O6-C44
29	c	903	SQD	C8-C7-O47-C45
29	c	903	SQD	C5-C6-S-O7
29	c	903	SQD	C5-C6-S-O8
29	c	903	SQD	C5-C6-S-O9

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Mol	Chain	Res	Type	Atoms
29	d	407	SQD	O10-C23-O48-C46
29	h	102	SQD	O5-C1-O6-C44
29	h	102	SQD	O49-C7-O47-C45
29	h	102	SQD	C8-C7-O47-C45
30	A	414	PL9	C9-C11-C12-C13
30	A	414	PL9	C12-C13-C14-C16
30	A	414	PL9	C33-C34-C36-C37
30	A	414	PL9	C35-C34-C36-C37
30	D	405	PL9	C7-C8-C9-C11
30	D	405	PL9	C12-C11-C9-C8
30	D	405	PL9	C47-C48-C49-C51
30	a	414	PL9	C9-C11-C12-C13
30	a	414	PL9	C12-C13-C14-C16
30	a	414	PL9	C33-C34-C36-C37
30	a	414	PL9	C35-C34-C36-C37
30	d	405	PL9	C7-C8-C9-C11
30	d	405	PL9	C12-C11-C9-C8
30	d	405	PL9	C47-C48-C49-C51
31	B	628	LMG	O1-C7-C8-O7
31	B	628	LMG	C11-C10-O7-C8
31	C	902	LMG	C2-C1-O1-C7
31	C	902	LMG	O6-C1-O1-C7
31	L	212	LMG	C2-C1-O1-C7
31	L	212	LMG	O6-C1-O1-C7
31	b	628	LMG	O1-C7-C8-O7
31	b	628	LMG	C11-C10-O7-C8
31	c	902	LMG	C2-C1-O1-C7
31	c	902	LMG	O6-C1-O1-C7
31	l	212	LMG	C2-C1-O1-C7
31	l	212	LMG	O6-C1-O1-C7
31	P	628	LMG	O9-C10-O7-C8
31	p	628	LMG	O9-C10-O7-C8
32	C	904	LMT	C2-C1-O1'-C1'
32	c	904	LMT	C2-C1-O1'-C1'
33	A	419	LHG	C3-O3-P-O6
33	A	419	LHG	C4-O6-P-O4
33	A	416	LHG	C3-O3-P-O4
33	A	416	LHG	C3-O3-P-O5
33	A	416	LHG	C8-C7-O7-C5
33	D	408	LHG	C1-C2-C3-O3
33	D	408	LHG	C3-O3-P-O4
33	D	409	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
33	D	410	LHG	C1-C2-C3-O3
33	D	410	LHG	C3-O3-P-O4
33	D	410	LHG	C3-O3-P-O5
33	D	410	LHG	C3-O3-P-O6
33	D	410	LHG	C4-O6-P-O3
33	D	410	LHG	C4-O6-P-O4
33	D	410	LHG	C4-O6-P-O5
33	E	101	LHG	C4-O6-P-O5
33	E	244	LHG	C1-C2-C3-O3
33	E	244	LHG	C3-O3-P-O5
33	E	244	LHG	C4-O6-P-O4
33	E	244	LHG	C4-O6-P-O5
33	E	244	LHG	C5-C4-O6-P
33	J	101	LHG	C4-O6-P-O5
33	a	419	LHG	C3-O3-P-O6
33	a	419	LHG	C4-O6-P-O4
33	a	416	LHG	C3-O3-P-O4
33	a	416	LHG	C3-O3-P-O5
33	a	416	LHG	C8-C7-O7-C5
33	d	408	LHG	C1-C2-C3-O3
33	d	408	LHG	C3-O3-P-O4
33	d	409	LHG	C4-O6-P-O4
33	d	410	LHG	C1-C2-C3-O3
33	d	410	LHG	C3-O3-P-O4
33	d	410	LHG	C3-O3-P-O5
33	d	410	LHG	C3-O3-P-O6
33	d	410	LHG	C4-O6-P-O3
33	d	410	LHG	C4-O6-P-O4
33	d	410	LHG	C4-O6-P-O5
33	e	101	LHG	C4-O6-P-O5
33	e	244	LHG	C1-C2-C3-O3
33	e	244	LHG	C3-O3-P-O5
33	e	244	LHG	C4-O6-P-O4
33	e	244	LHG	C4-O6-P-O5
33	e	244	LHG	C5-C4-O6-P
33	j	101	LHG	C4-O6-P-O5
33	P	629	LHG	C4-O6-P-O4
33	P	629	LHG	C8-C7-O7-C5
33	p	629	LHG	C4-O6-P-O4
33	p	629	LHG	C8-C7-O7-C5
34	B	608	F6C	C1-C2-C3-C4
34	B	608	F6C	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
34	B	614	F6C	C1A-C2A-CAA-CBA
34	B	614	F6C	C1B-C2B-CMB-OMB
34	B	614	F6C	C3B-C2B-CMB-OMB
34	B	617	F6C	C1A-C2A-CAA-CBA
34	C	507	F6C	C3B-C2B-CMB-OMB
34	C	507	F6C	C1-C2-C3-C4
34	C	507	F6C	C2-C3-C5-C6
34	C	507	F6C	C4-C3-C5-C6
34	b	608	F6C	C1-C2-C3-C4
34	b	608	F6C	C1-C2-C3-C5
34	b	614	F6C	C1A-C2A-CAA-CBA
34	b	614	F6C	C1B-C2B-CMB-OMB
34	b	614	F6C	C3B-C2B-CMB-OMB
34	b	617	F6C	C1A-C2A-CAA-CBA
34	c	507	F6C	C3B-C2B-CMB-OMB
34	c	507	F6C	C1-C2-C3-C4
34	c	507	F6C	C2-C3-C5-C6
34	c	507	F6C	C4-C3-C5-C6
38	V	201	HEC	C2B-C3B-CAB-CBB
38	V	201	HEC	C4B-C3B-CAB-CBB
38	V	201	HEC	C2C-C3C-CAC-CBC
38	V	201	HEC	C4C-C3C-CAC-CBC
38	v	201	HEC	C2B-C3B-CAB-CBB
38	v	201	HEC	C4B-C3B-CAB-CBB
38	v	201	HEC	C2C-C3C-CAC-CBC
38	v	201	HEC	C4C-C3C-CAC-CBC
32	L	213	LMT	C3'-C4'-O1B-C1B
32	l	213	LMT	C3'-C4'-O1B-C1B
32	A	674	LMT	C3'-C4'-O1B-C1B
32	a	674	LMT	C3'-C4'-O1B-C1B
33	A	416	LHG	O10-C23-O8-C6
33	a	416	LHG	O10-C23-O8-C6
29	D	407	SQD	C24-C23-O48-C46
29	d	407	SQD	C24-C23-O48-C46
33	A	416	LHG	C24-C23-O8-C6
33	a	416	LHG	C24-C23-O8-C6
29	A	417	SQD	O10-C23-O48-C46
29	a	417	SQD	O10-C23-O48-C46
31	L	212	LMG	O10-C28-O8-C9
31	l	212	LMG	O10-C28-O8-C9
29	A	417	SQD	O49-C7-O47-C45
29	a	417	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
31	B	628	LMG	O9-C10-O7-C8
31	b	628	LMG	O9-C10-O7-C8
33	A	416	LHG	O9-C7-O7-C5
33	a	416	LHG	O9-C7-O7-C5
31	L	212	LMG	C29-C28-O8-C9
31	l	212	LMG	C29-C28-O8-C9
31	P	628	LMG	C11-C10-O7-C8
31	p	628	LMG	C11-C10-O7-C8
30	D	405	PL9	C47-C48-C49-C50
30	d	405	PL9	C47-C48-C49-C50
25	B	604	CLA	C2-C3-C5-C6
25	B	606	CLA	C2-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
25	b	606	CLA	C2-C3-C5-C6
29	C	903	SQD	O10-C23-O48-C46
29	c	903	SQD	O10-C23-O48-C46
34	C	507	F6C	C3-C5-C6-C7
34	c	507	F6C	C3-C5-C6-C7
29	A	417	SQD	C24-C23-O48-C46
29	a	417	SQD	C24-C23-O48-C46
33	E	101	LHG	C24-C23-O8-C6
33	e	101	LHG	C24-C23-O8-C6
34	C	507	F6C	C1-C2-C3-C5
34	c	507	F6C	C1-C2-C3-C5
30	A	414	PL9	C27-C28-C29-C30
30	a	414	PL9	C27-C28-C29-C30
29	C	903	SQD	O49-C7-O47-C45
29	c	903	SQD	O49-C7-O47-C45
33	P	629	LHG	O9-C7-O7-C5
33	p	629	LHG	O9-C7-O7-C5
30	A	414	PL9	C27-C28-C29-C31
30	a	414	PL9	C27-C28-C29-C31
33	A	416	LHG	O2-C2-C3-O3
33	D	408	LHG	O2-C2-C3-O3
33	D	410	LHG	O2-C2-C3-O3
33	E	244	LHG	O2-C2-C3-O3
33	a	416	LHG	O2-C2-C3-O3
33	d	408	LHG	O2-C2-C3-O3
33	d	410	LHG	O2-C2-C3-O3
33	e	244	LHG	O2-C2-C3-O3
29	C	903	SQD	C24-C23-O48-C46
29	c	903	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
31	B	628	LMG	C29-C28-O8-C9
31	b	628	LMG	C29-C28-O8-C9
31	B	628	LMG	O10-C28-O8-C9
31	b	628	LMG	O10-C28-O8-C9
33	E	101	LHG	O10-C23-O8-C6
33	e	101	LHG	O10-C23-O8-C6
25	B	615	CLA	C4-C3-C5-C6
25	b	615	CLA	C4-C3-C5-C6
25	B	615	CLA	C2-C3-C5-C6
25	C	512	CLA	C2-C3-C5-C6
25	b	615	CLA	C2-C3-C5-C6
25	c	512	CLA	C2-C3-C5-C6
25	B	607	CLA	C2A-CAA-CBA-CGA
25	b	607	CLA	C2A-CAA-CBA-CGA
29	D	407	SQD	O5-C1-O6-C44
29	d	407	SQD	O5-C1-O6-C44
30	A	414	PL9	C34-C36-C37-C38
30	D	405	PL9	C39-C41-C42-C43
30	a	414	PL9	C34-C36-C37-C38
30	d	405	PL9	C39-C41-C42-C43
31	B	628	LMG	C30-C31-C32-C33
31	b	628	LMG	C30-C31-C32-C33
33	P	629	LHG	C1-C2-C3-O3
33	p	629	LHG	C1-C2-C3-O3
33	D	410	LHG	C24-C23-O8-C6
33	d	410	LHG	C24-C23-O8-C6
34	B	617	F6C	CBA-CGA-O2A-C1
34	b	617	F6C	CBA-CGA-O2A-C1
32	B	675	LMT	O5'-C5'-C6'-O6'
32	G	104	LMT	O5'-C5'-C6'-O6'
32	b	675	LMT	O5'-C5'-C6'-O6'
32	g	104	LMT	O5'-C5'-C6'-O6'
29	A	412	SQD	C7-C8-C9-C10
29	a	412	SQD	C7-C8-C9-C10
33	E	101	LHG	C23-C24-C25-C26
33	e	101	LHG	C23-C24-C25-C26
33	A	416	LHG	C11-C12-C13-C14
33	a	416	LHG	C11-C12-C13-C14
33	A	419	LHG	C32-C33-C34-C35
33	a	419	LHG	C32-C33-C34-C35
31	C	902	LMG	C38-C39-C40-C41
31	c	902	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
33	P	629	LHG	O2-C2-C3-O3
33	p	629	LHG	O2-C2-C3-O3
32	B	675	LMT	C2'-C1'-O1'-C1
32	b	675	LMT	C2'-C1'-O1'-C1
25	B	615	CLA	C11-C10-C8-C9
25	b	615	CLA	C11-C10-C8-C9
34	B	608	F6C	C6-C7-C8-C9
34	B	614	F6C	C6-C7-C8-C9
34	b	608	F6C	C6-C7-C8-C9
34	b	614	F6C	C6-C7-C8-C9
29	B	622	SQD	C30-C31-C32-C33
29	b	622	SQD	C30-C31-C32-C33
28	B	618	BCR	C7-C8-C9-C34
28	B	619	BCR	C11-C12-C13-C35
28	B	627	BCR	C37-C22-C23-C24
28	D	404	BCR	C37-C22-C23-C24
28	b	618	BCR	C7-C8-C9-C34
28	b	619	BCR	C11-C12-C13-C35
28	b	627	BCR	C37-C22-C23-C24
28	d	404	BCR	C37-C22-C23-C24
28	B	618	BCR	C7-C8-C9-C10
28	B	627	BCR	C21-C22-C23-C24
28	D	404	BCR	C21-C22-C23-C24
28	b	618	BCR	C7-C8-C9-C10
28	b	627	BCR	C21-C22-C23-C24
28	d	404	BCR	C21-C22-C23-C24
33	A	419	LHG	C23-C24-C25-C26
33	a	419	LHG	C23-C24-C25-C26
33	D	410	LHG	O10-C23-O8-C6
25	C	502	CLA	C5-C6-C7-C8
25	c	502	CLA	C5-C6-C7-C8
32	F	102	LMT	O5'-C5'-C6'-O6'
32	f	102	LMT	O5'-C5'-C6'-O6'
31	P	628	LMG	C29-C28-O8-C9
31	p	628	LMG	C29-C28-O8-C9
32	L	210	LMT	O5'-C5'-C6'-O6'
32	l	210	LMT	O5'-C5'-C6'-O6'
35	C	518	DGD	C8A-C9A-CAA-CBA
35	c	518	DGD	C8A-C9A-CAA-CBA
29	H	102	SQD	C23-C24-C25-C26
29	h	102	SQD	C23-C24-C25-C26
33	d	410	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
25	B	607	CLA	C13-C15-C16-C17
25	b	607	CLA	C13-C15-C16-C17
29	A	417	SQD	C23-C24-C25-C26
29	a	417	SQD	C23-C24-C25-C26
31	C	519	LMG	C10-C11-C12-C13
31	c	519	LMG	C10-C11-C12-C13
31	A	415	LMG	C29-C28-O8-C9
31	a	415	LMG	C29-C28-O8-C9
32	L	210	LMT	C3'-C4'-O1B-C1B
32	l	210	LMT	C3'-C4'-O1B-C1B
33	A	416	LHG	C27-C28-C29-C30
33	a	416	LHG	C27-C28-C29-C30
33	E	244	LHG	C2-C3-O3-P
33	e	244	LHG	C2-C3-O3-P
29	H	102	SQD	C7-C8-C9-C10
29	h	102	SQD	C7-C8-C9-C10
29	A	412	SQD	C30-C31-C32-C33
29	a	412	SQD	C30-C31-C32-C33
34	B	617	F6C	O1A-CGA-O2A-C1
34	b	617	F6C	O1A-CGA-O2A-C1
32	B	675	LMT	C4'-C5'-C6'-O6'
32	b	675	LMT	C4'-C5'-C6'-O6'
30	D	405	PL9	C9-C11-C12-C13
30	D	405	PL9	C34-C36-C37-C38
30	d	405	PL9	C9-C11-C12-C13
30	d	405	PL9	C34-C36-C37-C38
32	M	101	LMT	O1'-C1-C2-C3
32	m	101	LMT	O1'-C1-C2-C3
32	A	674	LMT	O1'-C1-C2-C3
32	a	674	LMT	O1'-C1-C2-C3
29	A	417	SQD	C15-C16-C17-C18
29	a	417	SQD	C15-C16-C17-C18
34	C	507	F6C	C1A-C2A-CAA-CBA
34	c	507	F6C	C1A-C2A-CAA-CBA
25	B	615	CLA	C10-C11-C12-C13
25	b	615	CLA	C10-C11-C12-C13
33	A	419	LHG	C4-O6-P-O3
33	A	416	LHG	C3-O3-P-O6
33	D	408	LHG	C3-O3-P-O6
33	E	101	LHG	C3-O3-P-O6
33	E	244	LHG	C3-O3-P-O6
33	E	244	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
33	a	419	LHG	C4-O6-P-O3
33	a	416	LHG	C3-O3-P-O6
33	d	408	LHG	C3-O3-P-O6
33	e	101	LHG	C3-O3-P-O6
33	e	244	LHG	C3-O3-P-O6
33	e	244	LHG	C4-O6-P-O3
33	P	629	LHG	C4-O6-P-O3
33	p	629	LHG	C4-O6-P-O3
31	C	519	LMG	C29-C28-O8-C9
31	c	519	LMG	C29-C28-O8-C9
33	E	244	LHG	C24-C23-O8-C6
33	e	244	LHG	C24-C23-O8-C6
32	Z	102	LMT	O1'-C1-C2-C3
32	z	102	LMT	O1'-C1-C2-C3
34	B	614	F6C	C5-C6-C7-C8
34	b	614	F6C	C5-C6-C7-C8
33	P	629	LHG	C7-C8-C9-C10
33	p	629	LHG	C7-C8-C9-C10
34	B	614	F6C	C15-C16-C17-C18
34	b	614	F6C	C15-C16-C17-C18
34	C	507	F6C	C16-C17-C18-C20
34	c	507	F6C	C16-C17-C18-C20
29	H	102	SQD	C24-C23-O48-C46
29	h	102	SQD	C24-C23-O48-C46
33	A	419	LHG	C15-C16-C17-C18
33	a	419	LHG	C15-C16-C17-C18
28	B	627	BCR	C9-C10-C11-C12
28	b	627	BCR	C9-C10-C11-C12
33	E	244	LHG	C11-C12-C13-C14
33	e	244	LHG	C11-C12-C13-C14
33	D	410	LHG	C8-C7-O7-C5
33	d	410	LHG	C8-C7-O7-C5
29	A	412	SQD	C11-C10-C9-C8
29	A	412	SQD	C29-C30-C31-C32
29	A	417	SQD	C11-C12-C13-C14
29	A	417	SQD	C24-C25-C26-C27
29	D	407	SQD	C33-C34-C35-C36
29	a	417	SQD	C11-C12-C13-C14
29	a	417	SQD	C24-C25-C26-C27
29	a	412	SQD	C11-C10-C9-C8
29	a	412	SQD	C29-C30-C31-C32
29	d	407	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
31	A	415	LMG	C33-C34-C35-C36
31	C	902	LMG	C12-C13-C14-C15
31	a	415	LMG	C33-C34-C35-C36
31	c	902	LMG	C12-C13-C14-C15
33	E	101	LHG	C14-C15-C16-C17
33	J	101	LHG	C11-C12-C13-C14
33	e	101	LHG	C14-C15-C16-C17
33	j	101	LHG	C11-C12-C13-C14
29	B	622	SQD	C24-C23-O48-C46
29	A	417	SQD	C11-C10-C9-C8
29	a	417	SQD	C11-C10-C9-C8
31	C	519	LMG	C30-C31-C32-C33
31	c	519	LMG	C30-C31-C32-C33
33	D	408	LHG	C25-C26-C27-C28
33	E	101	LHG	C24-C25-C26-C27
33	E	101	LHG	C34-C35-C36-C37
33	E	244	LHG	C9-C10-C11-C12
33	d	408	LHG	C25-C26-C27-C28
33	e	101	LHG	C24-C25-C26-C27
33	e	101	LHG	C34-C35-C36-C37
33	e	244	LHG	C9-C10-C11-C12
35	C	517	DGD	C9A-CAA-CBA-CCA
35	c	517	DGD	C9A-CAA-CBA-CCA
29	C	903	SQD	C46-C45-O47-C7
29	c	903	SQD	C46-C45-O47-C7
33	D	410	LHG	O9-C7-O7-C5
33	d	410	LHG	O9-C7-O7-C5
34	B	617	F6C	C1-C2-C3-C5
34	b	617	F6C	C1-C2-C3-C5
33	J	101	LHG	C23-C24-C25-C26
33	j	101	LHG	C23-C24-C25-C26
33	A	416	LHG	C11-C10-C9-C8
33	D	410	LHG	C27-C28-C29-C30
33	L	101	LHG	C27-C28-C29-C30
33	a	416	LHG	C11-C10-C9-C8
33	d	410	LHG	C27-C28-C29-C30
33	l	101	LHG	C27-C28-C29-C30
31	A	415	LMG	O10-C28-O8-C9
31	a	415	LMG	O10-C28-O8-C9
31	P	628	LMG	O10-C28-O8-C9
31	p	628	LMG	O10-C28-O8-C9
33	A	419	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
33	a	419	LHG	C27-C28-C29-C30
29	A	417	SQD	C10-C11-C12-C13
29	B	622	SQD	C33-C34-C35-C36
29	a	417	SQD	C10-C11-C12-C13
29	b	622	SQD	C33-C34-C35-C36
31	L	212	LMG	C30-C31-C32-C33
35	C	518	DGD	CAA-CBA-CCA-CDA
35	C	518	DGD	C6B-C7B-C8B-C9B
35	c	518	DGD	CAA-CBA-CCA-CDA
35	c	518	DGD	C6B-C7B-C8B-C9B
29	b	622	SQD	C24-C23-O48-C46
29	A	412	SQD	C16-C17-C18-C19
29	a	412	SQD	C16-C17-C18-C19
31	L	212	LMG	C20-C21-C22-C23
31	l	212	LMG	C20-C21-C22-C23
31	l	212	LMG	C30-C31-C32-C33
33	J	101	LHG	C32-C33-C34-C35
33	j	101	LHG	C32-C33-C34-C35
35	C	516	DGD	C4A-C5A-C6A-C7A
35	c	516	DGD	C4A-C5A-C6A-C7A
31	C	519	LMG	O10-C28-O8-C9
31	c	519	LMG	O10-C28-O8-C9
33	E	244	LHG	O10-C23-O8-C6
33	e	244	LHG	O10-C23-O8-C6
30	A	414	PL9	C12-C13-C14-C15
30	A	414	PL9	C32-C33-C34-C35
30	a	414	PL9	C12-C13-C14-C15
30	a	414	PL9	C32-C33-C34-C35
29	A	417	SQD	C9-C10-C11-C12
29	a	417	SQD	C9-C10-C11-C12
35	C	517	DGD	C9B-CAB-CBB-CCB
35	c	517	DGD	C9B-CAB-CBB-CCB
25	A	410	CLA	C14-C13-C15-C16
25	a	410	CLA	C14-C13-C15-C16
29	D	407	SQD	C26-C27-C28-C29
29	d	407	SQD	C26-C27-C28-C29
33	E	101	LHG	C12-C13-C14-C15
33	J	101	LHG	C9-C10-C11-C12
33	e	101	LHG	C12-C13-C14-C15
33	j	101	LHG	C9-C10-C11-C12
28	B	619	BCR	C7-C8-C9-C34
28	b	619	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
33	A	416	LHG	C17-C18-C19-C20
33	A	416	LHG	C25-C26-C27-C28
33	L	101	LHG	C10-C11-C12-C13
33	a	416	LHG	C17-C18-C19-C20
33	a	416	LHG	C25-C26-C27-C28
33	l	101	LHG	C10-C11-C12-C13
33	J	101	LHG	O1-C1-C2-C3
33	j	101	LHG	O1-C1-C2-C3
33	P	629	LHG	O1-C1-C2-C3
33	p	629	LHG	O1-C1-C2-C3
28	B	619	BCR	C7-C8-C9-C10
28	b	619	BCR	C7-C8-C9-C10
31	D	411	LMG	C16-C17-C18-C19
31	a	415	LMG	C16-C17-C18-C19
31	d	411	LMG	C16-C17-C18-C19
29	A	417	SQD	C34-C35-C36-C37
29	H	102	SQD	C13-C14-C15-C16
29	a	417	SQD	C34-C35-C36-C37
29	h	102	SQD	C13-C14-C15-C16
31	A	415	LMG	C16-C17-C18-C19
31	C	902	LMG	C41-C42-C43-C44
31	D	411	LMG	C17-C18-C19-C20
31	L	212	LMG	C39-C40-C41-C42
31	L	212	LMG	C40-C41-C42-C43
31	c	902	LMG	C41-C42-C43-C44
31	d	411	LMG	C17-C18-C19-C20
31	l	212	LMG	C39-C40-C41-C42
31	l	212	LMG	C40-C41-C42-C43
32	L	210	LMT	C6-C7-C8-C9
32	M	101	LMT	C6-C7-C8-C9
32	Z	102	LMT	C6-C7-C8-C9
32	l	210	LMT	C6-C7-C8-C9
32	m	101	LMT	C6-C7-C8-C9
32	z	102	LMT	C6-C7-C8-C9
33	A	416	LHG	C10-C11-C12-C13
33	A	416	LHG	C29-C30-C31-C32
33	E	101	LHG	C27-C28-C29-C30
33	a	416	LHG	C29-C30-C31-C32
33	e	101	LHG	C27-C28-C29-C30
35	C	516	DGD	C7A-C8A-C9A-CAA
35	C	517	DGD	C8A-C9A-CAA-CBA
35	C	517	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
35	c	516	DGD	C7A-C8A-C9A-CAA
35	c	517	DGD	C8A-C9A-CAA-CBA
35	c	517	DGD	CBA-CCA-CDA-CEA
32	Z	102	LMT	O5'-C5'-C6'-O6'
32	z	102	LMT	O5'-C5'-C6'-O6'
29	A	417	SQD	C33-C34-C35-C36
29	B	622	SQD	C17-C18-C19-C20
29	D	407	SQD	C25-C26-C27-C28
29	a	417	SQD	C33-C34-C35-C36
29	b	622	SQD	C17-C18-C19-C20
29	d	407	SQD	C25-C26-C27-C28
31	C	902	LMG	C40-C41-C42-C43
31	c	902	LMG	C40-C41-C42-C43
32	Z	102	LMT	C7-C8-C9-C10
32	z	102	LMT	C7-C8-C9-C10
33	a	416	LHG	C10-C11-C12-C13
33	e	244	LHG	C30-C31-C32-C33
29	B	622	SQD	C29-C30-C31-C32
29	b	622	SQD	C29-C30-C31-C32
33	E	244	LHG	C30-C31-C32-C33
31	P	628	LMG	C16-C17-C18-C19
31	p	628	LMG	C16-C17-C18-C19
29	B	622	SQD	C13-C14-C15-C16
29	B	622	SQD	C32-C33-C34-C35
29	b	622	SQD	C13-C14-C15-C16
33	E	101	LHG	C11-C10-C9-C8
33	e	101	LHG	C11-C10-C9-C8
35	C	518	DGD	CBA-CCA-CDA-CEA
35	c	518	DGD	CBA-CCA-CDA-CEA
29	b	622	SQD	C32-C33-C34-C35
32	G	104	LMT	C5-C6-C7-C8
32	Z	102	LMT	C5-C6-C7-C8
32	g	104	LMT	C5-C6-C7-C8
32	z	102	LMT	C5-C6-C7-C8
29	A	412	SQD	C24-C25-C26-C27
29	a	412	SQD	C24-C25-C26-C27
33	J	101	LHG	C15-C16-C17-C18
33	j	101	LHG	C15-C16-C17-C18
33	P	629	LHG	C18-C19-C20-C21
33	p	629	LHG	C18-C19-C20-C21
29	D	407	SQD	O6-C44-C45-C46
29	d	407	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
29	A	412	SQD	C10-C11-C12-C13
29	a	412	SQD	C10-C11-C12-C13
35	C	517	DGD	CCA-CDA-CEA-CFA
35	c	517	DGD	CCA-CDA-CEA-CFA
25	B	602	CLA	O2A-C1-C2-C3
25	b	602	CLA	O2A-C1-C2-C3
30	D	405	PL9	C15-C14-C16-C17
30	d	405	PL9	C15-C14-C16-C17
30	D	405	PL9	C43-C44-C46-C47
30	d	405	PL9	C43-C44-C46-C47
33	J	101	LHG	C8-C7-O7-C5
33	j	101	LHG	C8-C7-O7-C5
32	C	904	LMT	C1-C2-C3-C4
32	c	904	LMT	C1-C2-C3-C4
29	A	417	SQD	C13-C14-C15-C16
29	A	417	SQD	C29-C30-C31-C32
29	D	407	SQD	C27-C28-C29-C30
29	H	102	SQD	C30-C31-C32-C33
29	a	417	SQD	C13-C14-C15-C16
29	d	407	SQD	C27-C28-C29-C30
29	h	102	SQD	C30-C31-C32-C33
33	A	416	LHG	C9-C10-C11-C12
33	a	416	LHG	C9-C10-C11-C12
35	C	516	DGD	CBB-CCB-CDB-CEB
35	c	516	DGD	CBB-CCB-CDB-CEB
29	a	417	SQD	C29-C30-C31-C32
32	F	102	LMT	C1-C2-C3-C4
32	f	102	LMT	C1-C2-C3-C4
32	L	210	LMT	C4'-C5'-C6'-O6'
32	l	210	LMT	C4'-C5'-C6'-O6'
31	C	902	LMG	C10-C11-C12-C13
31	c	902	LMG	C10-C11-C12-C13
33	A	416	LHG	C1-C2-C3-O3
33	a	416	LHG	C1-C2-C3-O3
29	H	102	SQD	C24-C25-C26-C27
29	h	102	SQD	C24-C25-C26-C27
33	E	101	LHG	C15-C16-C17-C18
33	e	101	LHG	C15-C16-C17-C18
29	B	622	SQD	O10-C23-O48-C46
29	H	102	SQD	O10-C23-O48-C46
29	b	622	SQD	O10-C23-O48-C46
29	h	102	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
29	C	903	SQD	C26-C27-C28-C29
29	c	903	SQD	C26-C27-C28-C29
31	C	519	LMG	C39-C40-C41-C42
31	c	519	LMG	C39-C40-C41-C42
32	L	210	LMT	C5'-C4'-O1B-C1B
32	l	210	LMT	C5'-C4'-O1B-C1B
33	E	244	LHG	C23-C24-C25-C26
33	e	244	LHG	C23-C24-C25-C26
28	A	411	BCR	C23-C24-C25-C26
28	B	618	BCR	C1-C6-C7-C8
28	B	618	BCR	C5-C6-C7-C8
28	B	619	BCR	C5-C6-C7-C8
28	B	620	BCR	C1-C6-C7-C8
28	B	627	BCR	C23-C24-C25-C30
28	D	404	BCR	C23-C24-C25-C30
28	a	411	BCR	C23-C24-C25-C26
28	b	618	BCR	C1-C6-C7-C8
28	b	618	BCR	C5-C6-C7-C8
28	b	619	BCR	C5-C6-C7-C8
28	b	620	BCR	C1-C6-C7-C8
28	b	627	BCR	C23-C24-C25-C30
28	d	404	BCR	C23-C24-C25-C30
32	B	675	LMT	C2-C3-C4-C5
32	b	675	LMT	C2-C3-C4-C5
31	C	902	LMG	C29-C28-O8-C9
31	c	902	LMG	C29-C28-O8-C9
29	A	412	SQD	C8-C7-O47-C45
29	a	412	SQD	C8-C7-O47-C45
32	G	104	LMT	C2-C3-C4-C5
32	g	104	LMT	C2-C3-C4-C5
33	E	244	LHG	C10-C11-C12-C13
33	e	244	LHG	C10-C11-C12-C13
29	D	407	SQD	C9-C10-C11-C12
31	P	628	LMG	C18-C19-C20-C21
32	L	210	LMT	C4-C5-C6-C7
32	l	210	LMT	C4-C5-C6-C7
29	d	407	SQD	C9-C10-C11-C12
31	p	628	LMG	C18-C19-C20-C21
25	B	616	CLA	C12-C13-C15-C16
25	b	616	CLA	C12-C13-C15-C16
34	B	608	F6C	C6-C7-C8-C10
34	b	608	F6C	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
33	J	101	LHG	O9-C7-O7-C5
33	j	101	LHG	O9-C7-O7-C5
29	A	412	SQD	C9-C10-C11-C12
29	a	412	SQD	C9-C10-C11-C12
33	D	410	LHG	C26-C27-C28-C29
33	d	410	LHG	C26-C27-C28-C29
32	G	104	LMT	C4'-C5'-C6'-O6'
32	g	104	LMT	C4'-C5'-C6'-O6'
33	A	416	LHG	C28-C29-C30-C31
33	a	416	LHG	C28-C29-C30-C31
31	C	519	LMG	C21-C22-C23-C24
31	C	902	LMG	C33-C34-C35-C36
31	c	519	LMG	C21-C22-C23-C24
31	c	902	LMG	C33-C34-C35-C36
32	B	675	LMT	C5-C6-C7-C8
32	b	675	LMT	C5-C6-C7-C8
29	A	417	SQD	C16-C17-C18-C19
29	a	417	SQD	C16-C17-C18-C19
32	B	675	LMT	C7-C8-C9-C10
32	b	675	LMT	C7-C8-C9-C10
32	m	101	LMT	C7-C8-C9-C10
33	A	416	LHG	C30-C31-C32-C33
33	E	101	LHG	C31-C32-C33-C34
33	a	416	LHG	C30-C31-C32-C33
33	e	101	LHG	C31-C32-C33-C34
35	C	516	DGD	C8A-C9A-CAA-CBA
35	C	516	DGD	CBA-CCA-CDA-CEA
35	c	516	DGD	C8A-C9A-CAA-CBA
35	c	516	DGD	CBA-CCA-CDA-CEA
34	B	614	F6C	C16-C17-C18-C20
34	b	614	F6C	C16-C17-C18-C20
32	Z	102	LMT	O5'-C1'-O1'-C1
32	z	102	LMT	O5'-C1'-O1'-C1
25	C	504	CLA	C15-C16-C17-C18
25	c	504	CLA	C15-C16-C17-C18
31	L	212	LMG	C15-C16-C17-C18
31	l	212	LMG	C15-C16-C17-C18
32	M	101	LMT	C7-C8-C9-C10
33	E	244	LHG	C7-C8-C9-C10
33	e	244	LHG	C7-C8-C9-C10
33	D	410	LHG	C29-C30-C31-C32
33	d	410	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	C11-C12-C13-C14
33	l	101	LHG	C11-C12-C13-C14
29	C	903	SQD	C9-C10-C11-C12
29	c	903	SQD	C9-C10-C11-C12
32	A	674	LMT	C2'-C1'-O1'-C1
32	M	101	LMT	C2'-C1'-O1'-C1
32	a	674	LMT	C2'-C1'-O1'-C1
32	m	101	LMT	C2'-C1'-O1'-C1
31	L	212	LMG	O7-C8-C9-O8
31	l	212	LMG	O7-C8-C9-O8
29	a	417	SQD	C25-C26-C27-C28
31	C	519	LMG	C32-C33-C34-C35
29	A	417	SQD	C25-C26-C27-C28
31	A	415	LMG	C23-C24-C25-C26
31	a	415	LMG	C23-C24-C25-C26
31	c	519	LMG	C32-C33-C34-C35
33	J	101	LHG	C17-C18-C19-C20
33	j	101	LHG	C17-C18-C19-C20
32	Z	102	LMT	O5B-C5B-C6B-O6B
32	z	102	LMT	O5B-C5B-C6B-O6B
30	A	414	PL9	C4-C3-C7-C8
30	D	405	PL9	C4-C3-C7-C8
30	a	414	PL9	C4-C3-C7-C8
30	d	405	PL9	C4-C3-C7-C8
33	D	409	LHG	C28-C29-C30-C31
33	d	409	LHG	C28-C29-C30-C31
25	B	616	CLA	C14-C13-C15-C16
25	b	616	CLA	C14-C13-C15-C16
31	A	415	LMG	O6-C5-C6-O5
31	a	415	LMG	O6-C5-C6-O5
29	H	102	SQD	C27-C28-C29-C30
29	h	102	SQD	C27-C28-C29-C30
31	A	415	LMG	C17-C18-C19-C20
31	a	415	LMG	C17-C18-C19-C20
31	C	902	LMG	C15-C16-C17-C18
31	c	902	LMG	C15-C16-C17-C18
33	D	408	LHG	C16-C17-C18-C19
31	C	902	LMG	O10-C28-O8-C9
31	c	902	LMG	O10-C28-O8-C9
29	A	412	SQD	O49-C7-O47-C45
29	a	412	SQD	O49-C7-O47-C45
33	D	409	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
33	d	409	LHG	C8-C7-O7-C5
33	d	408	LHG	C16-C17-C18-C19
32	B	675	LMT	C1-C2-C3-C4
32	b	675	LMT	C1-C2-C3-C4
33	L	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O3
25	a	405	CLA	C2C-C3C-CAC-CBC
31	B	628	LMG	C37-C38-C39-C40
25	A	405	CLA	C2C-C3C-CAC-CBC
31	b	628	LMG	C37-C38-C39-C40
29	B	622	SQD	C14-C15-C16-C17
29	b	622	SQD	C14-C15-C16-C17
29	C	903	SQD	C27-C28-C29-C30
29	c	903	SQD	C27-C28-C29-C30
35	C	518	DGD	CDA-CEA-CFA-CGA
35	c	518	DGD	CDA-CEA-CFA-CGA
37	F	101	HEM	C3D-CAD-CBD-CGD
37	f	101	HEM	C3D-CAD-CBD-CGD
34	B	614	F6C	C16-C17-C18-C19
34	C	507	F6C	C16-C17-C18-C19
34	b	614	F6C	C16-C17-C18-C19
34	c	507	F6C	C16-C17-C18-C19
35	C	517	DGD	C8B-C9B-CAB-CBB
35	c	517	DGD	C8B-C9B-CAB-CBB
31	C	902	LMG	C16-C17-C18-C19
31	c	902	LMG	C16-C17-C18-C19
29	B	622	SQD	C11-C10-C9-C8
31	A	415	LMG	C34-C35-C36-C37
31	a	415	LMG	C34-C35-C36-C37
32	A	674	LMT	O5B-C5B-C6B-O6B
32	a	674	LMT	O5B-C5B-C6B-O6B
32	L	213	LMT	C4'-C5'-C6'-O6'
32	l	213	LMT	C4'-C5'-C6'-O6'
29	H	102	SQD	C26-C27-C28-C29
29	b	622	SQD	C11-C10-C9-C8
29	h	102	SQD	C26-C27-C28-C29
33	E	244	LHG	C26-C27-C28-C29
33	e	244	LHG	C26-C27-C28-C29
35	C	518	DGD	O6D-C5D-C6D-O5D
33	A	419	LHG	C24-C25-C26-C27
33	a	419	LHG	C24-C25-C26-C27
31	A	415	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
31	B	628	LMG	O1-C7-C8-C9
31	b	628	LMG	O1-C7-C8-C9
31	a	415	LMG	C30-C31-C32-C33
35	c	518	DGD	O6D-C5D-C6D-O5D
29	C	903	SQD	C45-C44-O6-C1
29	c	903	SQD	C45-C44-O6-C1
35	C	517	DGD	C2G-C3G-O3G-C1D
35	C	517	DGD	C5D-C6D-O5D-C1E
35	c	517	DGD	C2G-C3G-O3G-C1D
35	c	517	DGD	C5D-C6D-O5D-C1E
29	D	407	SQD	C10-C11-C12-C13
29	d	407	SQD	C10-C11-C12-C13
33	E	101	LHG	C29-C30-C31-C32
33	e	101	LHG	C29-C30-C31-C32
35	C	517	DGD	C4A-C5A-C6A-C7A
35	c	517	DGD	C4A-C5A-C6A-C7A
33	D	408	LHG	C23-C24-C25-C26
33	d	408	LHG	C23-C24-C25-C26
31	D	411	LMG	O6-C5-C6-O5
31	d	411	LMG	O6-C5-C6-O5
35	C	518	DGD	CDB-CEB-CFB-CGB
35	c	518	DGD	CDB-CEB-CFB-CGB
31	D	411	LMG	C19-C20-C21-C22
31	d	411	LMG	C19-C20-C21-C22
31	C	902	LMG	C42-C43-C44-C45
31	c	902	LMG	C42-C43-C44-C45
25	C	509	CLA	C10-C11-C12-C13
25	c	509	CLA	C10-C11-C12-C13
33	P	629	LHG	C4-C5-O7-C7
33	p	629	LHG	C4-C5-O7-C7
32	F	102	LMT	O5B-C5B-C6B-O6B
32	f	102	LMT	O5B-C5B-C6B-O6B
34	B	617	F6C	C1-C2-C3-C4
34	b	617	F6C	C1-C2-C3-C4
29	A	412	SQD	C25-C26-C27-C28
29	a	412	SQD	C25-C26-C27-C28
31	C	902	LMG	O6-C5-C6-O5
31	c	902	LMG	O6-C5-C6-O5
35	C	516	DGD	O6E-C5E-C6E-O5E
35	c	516	DGD	O6E-C5E-C6E-O5E
33	A	419	LHG	C2-C3-O3-P
33	a	419	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
35	C	517	DGD	C6A-C7A-C8A-C9A
35	c	517	DGD	C6A-C7A-C8A-C9A
29	A	417	SQD	C27-C28-C29-C30
29	a	417	SQD	C27-C28-C29-C30
29	B	622	SQD	C25-C26-C27-C28
29	b	622	SQD	C25-C26-C27-C28
25	D	402	CLA	C13-C15-C16-C17
25	d	402	CLA	C13-C15-C16-C17
32	Z	102	LMT	C2'-C1'-O1'-C1
32	z	102	LMT	C2'-C1'-O1'-C1
35	C	517	DGD	C2E-C1E-O5D-C6D
35	c	517	DGD	C2E-C1E-O5D-C6D
33	a	416	LHG	C32-C33-C34-C35
29	A	412	SQD	C13-C14-C15-C16
29	a	412	SQD	C13-C14-C15-C16
33	A	416	LHG	C32-C33-C34-C35
29	A	417	SQD	C31-C32-C33-C34
29	a	417	SQD	C31-C32-C33-C34
31	C	519	LMG	C16-C17-C18-C19
31	c	519	LMG	C16-C17-C18-C19
33	A	416	LHG	C12-C13-C14-C15
33	a	416	LHG	C12-C13-C14-C15
30	D	405	PL9	C45-C44-C46-C47
30	d	405	PL9	C45-C44-C46-C47
25	B	615	CLA	C11-C10-C8-C7
25	B	616	CLA	C11-C12-C13-C15
25	b	615	CLA	C11-C10-C8-C7
25	b	616	CLA	C11-C12-C13-C15
34	C	507	F6C	C11-C10-C8-C7
34	c	507	F6C	C11-C10-C8-C7
34	C	507	F6C	C11-C10-C8-C9
34	c	507	F6C	C11-C10-C8-C9
32	F	102	LMT	C4'-C5'-C6'-O6'
32	f	102	LMT	C4'-C5'-C6'-O6'
35	C	518	DGD	C2A-C3A-C4A-C5A
35	c	518	DGD	C2A-C3A-C4A-C5A
28	C	515	BCR	C36-C18-C19-C20
28	c	515	BCR	C36-C18-C19-C20
33	D	410	LHG	C25-C26-C27-C28
33	E	101	LHG	C30-C31-C32-C33
33	d	410	LHG	C25-C26-C27-C28
33	e	101	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
29	A	412	SQD	C15-C16-C17-C18
29	a	412	SQD	C15-C16-C17-C18
33	D	408	LHG	C18-C19-C20-C21
33	d	408	LHG	C18-C19-C20-C21
33	D	410	LHG	O6-C4-C5-C6
33	E	101	LHG	O6-C4-C5-C6
33	d	410	LHG	O6-C4-C5-C6
33	e	101	LHG	O6-C4-C5-C6
33	P	629	LHG	O6-C4-C5-C6
33	p	629	LHG	O6-C4-C5-C6
34	B	614	F6C	C8-C10-C11-C12
34	b	614	F6C	C8-C10-C11-C12
25	C	502	CLA	C4-C3-C5-C6
25	c	502	CLA	C4-C3-C5-C6
33	D	409	LHG	O9-C7-O7-C5
33	d	409	LHG	O9-C7-O7-C5
29	C	903	SQD	C25-C26-C27-C28
29	c	903	SQD	C25-C26-C27-C28
32	G	104	LMT	C7-C8-C9-C10
32	g	104	LMT	C7-C8-C9-C10
29	A	412	SQD	C24-C23-O48-C46
29	a	412	SQD	C24-C23-O48-C46
32	F	102	LMT	O1'-C1-C2-C3
32	f	102	LMT	O1'-C1-C2-C3
33	J	101	LHG	C5-C4-O6-P
33	j	101	LHG	C5-C4-O6-P
32	G	104	LMT	O1'-C1-C2-C3
32	M	101	LMT	C2-C1-O1'-C1'
32	Z	102	LMT	C2-C1-O1'-C1'
32	m	101	LMT	C2-C1-O1'-C1'
32	z	102	LMT	C2-C1-O1'-C1'
31	B	628	LMG	C11-C12-C13-C14
32	g	104	LMT	O1'-C1-C2-C3
33	D	410	LHG	C11-C12-C13-C14
33	E	244	LHG	C35-C36-C37-C38
33	e	244	LHG	C35-C36-C37-C38
29	D	407	SQD	C24-C25-C26-C27
29	d	407	SQD	C24-C25-C26-C27
31	b	628	LMG	C11-C12-C13-C14
33	d	410	LHG	C11-C12-C13-C14
29	C	903	SQD	O6-C44-C45-C46
29	c	903	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
33	E	101	LHG	C13-C14-C15-C16
33	e	101	LHG	C13-C14-C15-C16
35	c	516	DGD	O6D-C5D-C6D-O5D
33	J	101	LHG	C11-C10-C9-C8
33	j	101	LHG	C11-C10-C9-C8
35	C	517	DGD	CAA-CBA-CCA-CDA
35	c	517	DGD	CAA-CBA-CCA-CDA
35	C	516	DGD	O6D-C5D-C6D-O5D
29	A	417	SQD	C7-C8-C9-C10
29	a	417	SQD	C7-C8-C9-C10
30	A	414	PL9	C47-C48-C49-C50
30	a	414	PL9	C47-C48-C49-C50
33	J	101	LHG	O1-C1-C2-O2
33	j	101	LHG	O1-C1-C2-O2
33	D	410	LHG	O6-C4-C5-O7
33	E	101	LHG	O6-C4-C5-O7
33	d	410	LHG	O6-C4-C5-O7
33	e	101	LHG	O6-C4-C5-O7
35	C	516	DGD	CDB-CEB-CFB-CGB
35	c	516	DGD	CDB-CEB-CFB-CGB
33	A	419	LHG	C12-C13-C14-C15
33	a	419	LHG	C12-C13-C14-C15
31	P	628	LMG	C20-C21-C22-C23
31	p	628	LMG	C20-C21-C22-C23
35	C	516	DGD	C5A-C6A-C7A-C8A
35	c	516	DGD	C5A-C6A-C7A-C8A
29	A	417	SQD	O47-C45-C46-O48
29	a	417	SQD	O47-C45-C46-O48
33	E	101	LHG	C11-C12-C13-C14
33	e	101	LHG	C11-C12-C13-C14
34	B	608	F6C	C3A-C2A-CAA-CBA
34	b	608	F6C	C3A-C2A-CAA-CBA
29	A	412	SQD	C33-C34-C35-C36
29	a	412	SQD	C33-C34-C35-C36
30	A	414	PL9	C14-C16-C17-C18
30	a	414	PL9	C14-C16-C17-C18
29	B	622	SQD	C26-C27-C28-C29
29	D	407	SQD	C32-C33-C34-C35
29	b	622	SQD	C26-C27-C28-C29
29	d	407	SQD	C32-C33-C34-C35
32	b	675	LMT	C4-C5-C6-C7
25	B	602	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
25	b	602	CLA	C2-C1-O2A-CGA
32	B	675	LMT	C4-C5-C6-C7
25	C	502	CLA	C11-C10-C8-C9
25	c	502	CLA	C11-C10-C8-C9
32	M	101	LMT	C2-C3-C4-C5
32	m	101	LMT	C2-C3-C4-C5
31	B	628	LMG	C31-C32-C33-C34
31	b	628	LMG	C31-C32-C33-C34
34	C	507	F6C	C8-C10-C11-C12
34	c	507	F6C	C8-C10-C11-C12
31	A	415	LMG	C18-C19-C20-C21
31	L	212	LMG	C42-C43-C44-C45
31	a	415	LMG	C18-C19-C20-C21
31	l	212	LMG	C42-C43-C44-C45
28	A	411	BCR	C23-C24-C25-C30
28	C	515	BCR	C5-C6-C7-C8
28	a	411	BCR	C23-C24-C25-C30
28	c	515	BCR	C5-C6-C7-C8
28	B	619	BCR	C11-C12-C13-C14
28	b	619	BCR	C11-C12-C13-C14
29	A	412	SQD	C27-C28-C29-C30
29	A	417	SQD	C17-C18-C19-C20
29	a	417	SQD	C17-C18-C19-C20
29	a	412	SQD	C27-C28-C29-C30
25	A	410	CLA	C12-C13-C15-C16
25	a	410	CLA	C12-C13-C15-C16
29	A	417	SQD	C19-C20-C21-C22
29	a	417	SQD	C19-C20-C21-C22
29	D	407	SQD	C29-C30-C31-C32
29	d	407	SQD	C29-C30-C31-C32
33	D	409	LHG	C31-C32-C33-C34
33	d	409	LHG	C31-C32-C33-C34
29	A	417	SQD	C18-C19-C20-C21
29	a	417	SQD	C18-C19-C20-C21
31	C	902	LMG	C39-C40-C41-C42
31	c	902	LMG	C39-C40-C41-C42
33	P	629	LHG	C14-C15-C16-C17
25	B	607	CLA	C10-C11-C12-C13
25	b	607	CLA	C10-C11-C12-C13
34	B	614	F6C	CBD-CGD-O2D-CED
31	C	902	LMG	C34-C35-C36-C37
31	c	902	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
33	p	629	LHG	C14-C15-C16-C17
25	B	606	CLA	CAD-CBD-CGD-O2D
25	B	611	CLA	CAD-CBD-CGD-O2D
25	b	606	CLA	CAD-CBD-CGD-O2D
25	b	611	CLA	CAD-CBD-CGD-O2D
29	A	417	SQD	C46-C45-O47-C7
29	a	417	SQD	C46-C45-O47-C7
33	A	416	LHG	C6-C5-O7-C7
33	a	416	LHG	C6-C5-O7-C7
34	C	507	F6C	CAD-CBD-CGD-O2D
34	c	507	F6C	CAD-CBD-CGD-O2D
34	B	614	F6C	C10-C11-C12-C13
34	b	614	F6C	C10-C11-C12-C13
35	C	517	DGD	O6E-C1E-O5D-C6D
35	c	517	DGD	O6E-C1E-O5D-C6D
30	D	405	PL9	C44-C46-C47-C48
30	d	405	PL9	C44-C46-C47-C48
34	b	614	F6C	CBD-CGD-O2D-CED
33	P	629	LHG	O6-C4-C5-O7
33	p	629	LHG	O6-C4-C5-O7
34	B	608	F6C	C1A-C2A-CAA-CBA
34	b	608	F6C	C1A-C2A-CAA-CBA
29	D	407	SQD	C30-C31-C32-C33
29	d	407	SQD	C30-C31-C32-C33
33	J	101	LHG	C10-C11-C12-C13
33	j	101	LHG	C10-C11-C12-C13
33	l	101	LHG	C26-C27-C28-C29
32	B	675	LMT	C3-C4-C5-C6
33	L	101	LHG	C26-C27-C28-C29
25	B	613	CLA	CHA-CBD-CGD-O1D
25	B	613	CLA	CHA-CBD-CGD-O2D
25	C	502	CLA	CHA-CBD-CGD-O1D
25	b	613	CLA	CHA-CBD-CGD-O1D
25	b	613	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CHA-CBD-CGD-O1D
26	A	406	CL7	CHA-CBD-CGD-O2D
26	A	406	CL7	CHA-CBD-CGD-O1D
26	a	406	CL7	CHA-CBD-CGD-O2D
26	a	406	CL7	CHA-CBD-CGD-O1D
32	b	675	LMT	C3-C4-C5-C6
29	A	412	SQD	O10-C23-O48-C46
29	a	412	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
31	P	628	LMG	C23-C24-C25-C26
31	p	628	LMG	C23-C24-C25-C26
31	B	628	LMG	C41-C42-C43-C44
29	D	407	SQD	C34-C35-C36-C37
29	d	407	SQD	C34-C35-C36-C37
31	b	628	LMG	C41-C42-C43-C44
29	B	622	SQD	C31-C32-C33-C34
29	b	622	SQD	C31-C32-C33-C34
33	E	101	LHG	O1-C1-C2-O2
33	e	101	LHG	O1-C1-C2-O2
35	C	516	DGD	CDA-CEA-CFA-CGA
35	c	516	DGD	CDA-CEA-CFA-CGA
29	A	417	SQD	C12-C13-C14-C15
29	a	417	SQD	C12-C13-C14-C15
33	J	101	LHG	C34-C35-C36-C37
33	j	101	LHG	C34-C35-C36-C37
35	C	516	DGD	C4D-C5D-C6D-O5D
35	c	516	DGD	C4D-C5D-C6D-O5D
33	A	416	LHG	C19-C20-C21-C22
33	J	101	LHG	C25-C26-C27-C28
33	a	416	LHG	C19-C20-C21-C22
33	j	101	LHG	C25-C26-C27-C28
29	B	622	SQD	C5-C6-S-O8
29	b	622	SQD	C5-C6-S-O8
31	C	519	LMG	C31-C32-C33-C34
31	c	519	LMG	C31-C32-C33-C34
29	C	903	SQD	C24-C25-C26-C27
29	c	903	SQD	C24-C25-C26-C27
32	G	104	LMT	C6-C7-C8-C9
32	g	104	LMT	C6-C7-C8-C9
28	C	515	BCR	C17-C18-C19-C20
28	c	515	BCR	C17-C18-C19-C20
31	B	628	LMG	C40-C41-C42-C43
31	b	628	LMG	C40-C41-C42-C43
33	E	101	LHG	C4-O6-P-O3
33	J	101	LHG	C4-O6-P-O3
33	e	101	LHG	C4-O6-P-O3
33	j	101	LHG	C4-O6-P-O3
33	D	410	LHG	C24-C25-C26-C27
33	d	410	LHG	C24-C25-C26-C27
30	A	414	PL9	C47-C48-C49-C51
30	a	414	PL9	C47-C48-C49-C51

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Mol	Chain	Res	Type	Atoms
33	J	101	LHG	C2-C3-O3-P
33	j	101	LHG	C2-C3-O3-P
33	P	629	LHG	C2-C3-O3-P
33	P	629	LHG	C5-C4-O6-P
33	p	629	LHG	C2-C3-O3-P
33	p	629	LHG	C5-C4-O6-P
33	A	419	LHG	C3-O3-P-O4
33	D	408	LHG	C3-O3-P-O5
33	E	101	LHG	C3-O3-P-O4
33	E	101	LHG	C3-O3-P-O5
33	E	244	LHG	C3-O3-P-O4
33	a	419	LHG	C3-O3-P-O4
33	d	408	LHG	C3-O3-P-O5
33	e	101	LHG	C3-O3-P-O4
33	e	101	LHG	C3-O3-P-O5
33	e	244	LHG	C3-O3-P-O4
33	P	629	LHG	C4-O6-P-O5
33	p	629	LHG	C4-O6-P-O5
31	B	628	LMG	C32-C33-C34-C35
31	b	628	LMG	C32-C33-C34-C35
29	A	412	SQD	O5-C1-O6-C44
29	a	412	SQD	O5-C1-O6-C44
32	C	904	LMT	O5'-C1'-O1'-C1
32	c	904	LMT	O5'-C1'-O1'-C1
25	A	410	CLA	C15-C16-C17-C18
25	a	410	CLA	C15-C16-C17-C18
29	C	903	SQD	C10-C11-C12-C13
29	c	903	SQD	C10-C11-C12-C13
29	C	903	SQD	C11-C12-C13-C14
29	b	622	SQD	C10-C11-C12-C13
29	c	903	SQD	C11-C12-C13-C14
33	D	409	LHG	C33-C34-C35-C36
33	d	409	LHG	C33-C34-C35-C36
25	B	613	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	505	CLA	CAD-CBD-CGD-O1D
25	b	613	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	505	CLA	CAD-CBD-CGD-O1D
29	A	417	SQD	C5-C6-S-O7
29	D	407	SQD	C5-C6-S-O7
29	a	417	SQD	C5-C6-S-O7

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Mol	Chain	Res	Type	Atoms
29	d	407	SQD	C5-C6-S-O7
29	B	622	SQD	C10-C11-C12-C13
33	A	416	LHG	C24-C25-C26-C27
31	L	212	LMG	C14-C15-C16-C17
33	a	416	LHG	C24-C25-C26-C27
33	J	101	LHG	C7-C8-C9-C10
33	j	101	LHG	C7-C8-C9-C10
31	l	212	LMG	C14-C15-C16-C17
31	A	415	LMG	C22-C23-C24-C25
31	a	415	LMG	C22-C23-C24-C25
29	H	102	SQD	C35-C36-C37-C38
29	h	102	SQD	C35-C36-C37-C38
33	J	101	LHG	C35-C36-C37-C38
33	j	101	LHG	C35-C36-C37-C38
31	C	519	LMG	C15-C16-C17-C18
31	l	212	LMG	C16-C17-C18-C19
33	L	101	LHG	C12-C13-C14-C15
31	L	212	LMG	C16-C17-C18-C19
31	c	519	LMG	C15-C16-C17-C18
33	l	101	LHG	C12-C13-C14-C15
34	C	507	F6C	C1B-C2B-CMB-OMB
34	c	507	F6C	C1B-C2B-CMB-OMB
35	C	518	DGD	O6E-C5E-C6E-O5E
35	c	518	DGD	O6E-C5E-C6E-O5E
29	D	407	SQD	O6-C44-C45-O47
29	d	407	SQD	O6-C44-C45-O47
25	A	405	CLA	C4C-C3C-CAC-CBC
31	L	212	LMG	C35-C36-C37-C38
25	a	405	CLA	C4C-C3C-CAC-CBC
31	l	212	LMG	C35-C36-C37-C38
29	B	622	SQD	C45-C44-O6-C1
29	b	622	SQD	C45-C44-O6-C1
33	J	101	LHG	O7-C7-C8-C9
33	j	101	LHG	O7-C7-C8-C9
33	D	408	LHG	C28-C29-C30-C31
33	d	408	LHG	C28-C29-C30-C31
25	B	606	CLA	C3-C5-C6-C7
25	b	606	CLA	C3-C5-C6-C7
33	P	629	LHG	O1-C1-C2-O2
33	p	629	LHG	O1-C1-C2-O2
29	H	102	SQD	C33-C34-C35-C36
29	h	102	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
33	P	629	LHG	C31-C32-C33-C34
33	p	629	LHG	C31-C32-C33-C34
35	c	516	DGD	C6B-C7B-C8B-C9B
31	C	519	LMG	C12-C13-C14-C15
31	c	519	LMG	C12-C13-C14-C15
35	C	516	DGD	C6B-C7B-C8B-C9B
33	L	101	LHG	C25-C26-C27-C28
33	l	101	LHG	C25-C26-C27-C28
35	c	516	DGD	C9A-CAA-CBA-CCA
29	h	102	SQD	C11-C12-C13-C14
35	C	516	DGD	C9A-CAA-CBA-CCA
31	C	519	LMG	C28-C29-C30-C31
31	c	519	LMG	C28-C29-C30-C31
29	H	102	SQD	C11-C12-C13-C14
34	B	614	F6C	O1D-CGD-O2D-CED
25	A	405	CLA	C2-C1-O2A-CGA
25	a	405	CLA	C2-C1-O2A-CGA
27	A	408	PHO	C2-C1-O2A-CGA
27	a	408	PHO	C2-C1-O2A-CGA
34	b	614	F6C	O1D-CGD-O2D-CED
33	D	410	LHG	C2-C3-O3-P
33	d	410	LHG	C2-C3-O3-P
31	B	628	LMG	C22-C23-C24-C25
31	P	628	LMG	C32-C33-C34-C35
31	p	628	LMG	C32-C33-C34-C35
31	b	628	LMG	C22-C23-C24-C25
25	B	602	CLA	C4-C3-C5-C6
25	b	602	CLA	C4-C3-C5-C6
34	B	614	F6C	C4-C3-C5-C6
34	b	614	F6C	C4-C3-C5-C6
32	L	213	LMT	C7-C8-C9-C10
32	l	213	LMT	C7-C8-C9-C10
33	D	410	LHG	C23-C24-C25-C26
30	A	414	PL9	C29-C31-C32-C33
30	a	414	PL9	C29-C31-C32-C33
33	A	419	LHG	C16-C17-C18-C19
33	a	419	LHG	C16-C17-C18-C19
29	C	903	SQD	O6-C44-C45-O47
29	c	903	SQD	O6-C44-C45-O47
33	A	419	LHG	C31-C32-C33-C34
33	a	419	LHG	C31-C32-C33-C34
33	D	409	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
33	D	409	LHG	C4-O6-P-O3
33	J	101	LHG	C3-O3-P-O6
33	d	409	LHG	C3-O3-P-O6
33	d	409	LHG	C4-O6-P-O3
33	j	101	LHG	C3-O3-P-O6
31	B	628	LMG	C10-C11-C12-C13
33	d	410	LHG	C23-C24-C25-C26
33	E	244	LHG	C5-C6-O8-C23
33	e	244	LHG	C5-C6-O8-C23
31	b	628	LMG	C10-C11-C12-C13
29	A	417	SQD	C44-C45-C46-O48
29	a	417	SQD	C44-C45-C46-O48
31	L	212	LMG	C7-C8-C9-O8
31	l	212	LMG	C7-C8-C9-O8
33	a	419	LHG	C26-C27-C28-C29
35	C	518	DGD	C4A-C5A-C6A-C7A
35	c	518	DGD	C4A-C5A-C6A-C7A
25	C	502	CLA	C12-C13-C15-C16
25	c	502	CLA	C12-C13-C15-C16
34	B	608	F6C	C11-C10-C8-C7
34	B	614	F6C	C11-C12-C13-C15
34	b	608	F6C	C11-C10-C8-C7
34	b	614	F6C	C11-C12-C13-C15
33	A	419	LHG	C26-C27-C28-C29
27	A	409	PHO	C2C-C3C-CAC-CBC
27	a	409	PHO	C2C-C3C-CAC-CBC
28	B	627	BCR	C11-C12-C13-C35
35	C	516	DGD	CAB-CBB-CCB-CDB
35	c	516	DGD	CAB-CBB-CCB-CDB
33	D	408	LHG	C24-C25-C26-C27
33	d	408	LHG	C24-C25-C26-C27
30	A	414	PL9	C2-C3-C7-C8
30	a	414	PL9	C2-C3-C7-C8
28	B	619	BCR	C9-C10-C11-C12
28	K	102	BCR	C19-C20-C21-C22
28	b	619	BCR	C9-C10-C11-C12
28	k	102	BCR	C19-C20-C21-C22
31	L	212	LMG	O9-C10-O7-C8
33	D	409	LHG	C26-C27-C28-C29
29	a	412	SQD	C19-C20-C21-C22
33	d	409	LHG	C26-C27-C28-C29
25	D	403	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	d	403	CLA	C4-C3-C5-C6
29	A	412	SQD	C19-C20-C21-C22
31	l	212	LMG	O9-C10-O7-C8
25	B	609	CLA	C2-C1-O2A-CGA
25	C	512	CLA	C2-C1-O2A-CGA
25	b	609	CLA	C2-C1-O2A-CGA
25	c	512	CLA	C2-C1-O2A-CGA
33	D	410	LHG	O7-C5-C6-O8
33	d	410	LHG	O7-C5-C6-O8
35	C	517	DGD	C6B-C7B-C8B-C9B
35	c	517	DGD	C6B-C7B-C8B-C9B
33	a	419	LHG	C18-C19-C20-C21
32	A	674	LMT	C7-C8-C9-C10
32	a	674	LMT	C7-C8-C9-C10
33	A	419	LHG	C18-C19-C20-C21
33	E	244	LHG	C31-C32-C33-C34
33	e	244	LHG	C31-C32-C33-C34
25	C	509	CLA	C6-C7-C8-C9
25	c	509	CLA	C6-C7-C8-C9
34	C	507	F6C	C6-C7-C8-C9
34	c	507	F6C	C6-C7-C8-C9
33	J	101	LHG	C1-C2-C3-O3
33	j	101	LHG	C1-C2-C3-O3
35	C	518	DGD	O1G-C1G-C2G-C3G
35	c	518	DGD	O1G-C1G-C2G-C3G
32	L	210	LMT	C5-C6-C7-C8
32	l	210	LMT	C5-C6-C7-C8
25	D	403	CLA	O2A-C1-C2-C3
25	d	403	CLA	O2A-C1-C2-C3
32	L	210	LMT	O5'-C1'-O1'-C1
32	l	210	LMT	O5'-C1'-O1'-C1
35	C	516	DGD	O6E-C1E-O5D-C6D
35	c	516	DGD	O6E-C1E-O5D-C6D
28	b	627	BCR	C11-C12-C13-C35
33	D	408	LHG	C32-C33-C34-C35
33	d	408	LHG	C32-C33-C34-C35
31	P	628	LMG	C9-C8-O7-C10
31	p	628	LMG	C9-C8-O7-C10
33	J	101	LHG	C4-C5-O7-C7
33	j	101	LHG	C4-C5-O7-C7
25	B	615	CLA	C8-C10-C11-C12
25	b	615	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	B	606	CLA	C11-C12-C13-C15
25	B	616	CLA	C6-C7-C8-C10
25	b	606	CLA	C11-C12-C13-C15
25	b	616	CLA	C6-C7-C8-C10
32	L	213	LMT	O5'-C5'-C6'-O6'
33	E	244	LHG	C33-C34-C35-C36
33	e	244	LHG	C33-C34-C35-C36
32	l	213	LMT	O5'-C5'-C6'-O6'
30	A	414	PL9	C13-C14-C16-C17
30	a	414	PL9	C13-C14-C16-C17
33	J	101	LHG	O2-C2-C3-O3
33	j	101	LHG	O2-C2-C3-O3
31	b	628	LMG	C15-C16-C17-C18
31	b	628	LMG	C17-C18-C19-C20
33	d	408	LHG	C15-C16-C17-C18
31	B	628	LMG	C15-C16-C17-C18
31	B	628	LMG	C17-C18-C19-C20
33	D	408	LHG	C15-C16-C17-C18
33	d	408	LHG	C17-C18-C19-C20
33	D	408	LHG	C17-C18-C19-C20
35	C	516	DGD	C5B-C6B-C7B-C8B
35	c	516	DGD	C5B-C6B-C7B-C8B
33	E	101	LHG	C1-C2-C3-O3
33	e	101	LHG	C1-C2-C3-O3
25	D	402	CLA	C2-C1-O2A-CGA
25	d	402	CLA	C2-C1-O2A-CGA
31	L	212	LMG	O6-C5-C6-O5
31	l	212	LMG	O6-C5-C6-O5
29	A	417	SQD	C32-C33-C34-C35
29	a	417	SQD	C32-C33-C34-C35
32	M	101	LMT	C5-C6-C7-C8
32	m	101	LMT	C5-C6-C7-C8
28	C	515	BCR	C1-C6-C7-C8
28	c	515	BCR	C1-C6-C7-C8
33	e	244	LHG	C24-C25-C26-C27
33	D	408	LHG	O1-C1-C2-C3
33	d	408	LHG	O1-C1-C2-C3
33	E	244	LHG	C24-C25-C26-C27
31	a	415	LMG	C31-C32-C33-C34
32	L	213	LMT	C5-C6-C7-C8
32	l	213	LMT	C5-C6-C7-C8
31	A	415	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
35	C	516	DGD	C5D-C6D-O5D-C1E
35	c	516	DGD	C5D-C6D-O5D-C1E
31	L	212	LMG	C11-C10-O7-C8
31	l	212	LMG	C11-C10-O7-C8
31	D	411	LMG	C40-C41-C42-C43
31	d	411	LMG	C40-C41-C42-C43
35	C	517	DGD	CAB-CBB-CCB-CDB
35	c	517	DGD	CAB-CBB-CCB-CDB
34	B	614	F6C	C3A-C2A-CAA-CBA
34	b	614	F6C	C3A-C2A-CAA-CBA
27	A	408	PHO	C2A-CAA-CBA-CGA
27	a	408	PHO	C2A-CAA-CBA-CGA
32	L	213	LMT	C9-C10-C11-C12
32	l	213	LMT	C9-C10-C11-C12
31	L	212	LMG	C4-C5-C6-O5
31	l	212	LMG	C4-C5-C6-O5
29	H	102	SQD	C18-C19-C20-C21
29	h	102	SQD	C18-C19-C20-C21
31	C	902	LMG	C35-C36-C37-C38
25	B	610	CLA	C4-C3-C5-C6
25	b	610	CLA	C4-C3-C5-C6
34	B	608	F6C	C4-C3-C5-C6
34	b	608	F6C	C4-C3-C5-C6
31	c	902	LMG	C35-C36-C37-C38
25	B	610	CLA	C2-C3-C5-C6
25	b	610	CLA	C2-C3-C5-C6
30	A	414	PL9	C28-C29-C31-C32
30	a	414	PL9	C28-C29-C31-C32
25	C	502	CLA	C13-C15-C16-C17
25	c	502	CLA	C13-C15-C16-C17
34	B	614	F6C	C1-C2-C3-C4
34	b	614	F6C	C1-C2-C3-C4
34	B	614	F6C	CAA-CBA-CGA-O2A
34	b	614	F6C	CAA-CBA-CGA-O2A
29	A	417	SQD	C2-C1-O6-C44
29	a	417	SQD	C2-C1-O6-C44
32	L	210	LMT	C2'-C1'-O1'-C1
32	l	210	LMT	C2'-C1'-O1'-C1
35	C	516	DGD	C2E-C1E-O5D-C6D
35	c	516	DGD	C2E-C1E-O5D-C6D
29	A	412	SQD	C12-C13-C14-C15
29	a	412	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
29	H	102	SQD	O6-C44-C45-O47
29	h	102	SQD	O6-C44-C45-O47
31	P	628	LMG	O1-C7-C8-O7
31	p	628	LMG	O1-C7-C8-O7
35	C	518	DGD	C6A-C7A-C8A-C9A
35	c	518	DGD	C6A-C7A-C8A-C9A
33	J	101	LHG	C14-C15-C16-C17
33	j	101	LHG	C14-C15-C16-C17
29	A	412	SQD	C31-C32-C33-C34
29	a	412	SQD	C31-C32-C33-C34
30	D	405	PL9	C30-C29-C31-C32
30	d	405	PL9	C30-C29-C31-C32
25	C	502	CLA	C2-C3-C5-C6
25	c	502	CLA	C2-C3-C5-C6
34	B	608	F6C	C11-C10-C8-C9
34	B	614	F6C	C14-C13-C15-C16
34	b	608	F6C	C11-C10-C8-C9
34	b	614	F6C	C14-C13-C15-C16
33	L	101	LHG	C32-C33-C34-C35
33	l	101	LHG	C32-C33-C34-C35
25	C	510	CLA	CAA-CBA-CGA-O2A
25	B	605	CLA	CAD-CBD-CGD-O2D
25	B	607	CLA	CAD-CBD-CGD-O2D
25	B	610	CLA	CAD-CBD-CGD-O2D
25	C	501	CLA	CAD-CBD-CGD-O2D
25	C	510	CLA	CAD-CBD-CGD-O2D
25	b	605	CLA	CAD-CBD-CGD-O2D
25	b	607	CLA	CAD-CBD-CGD-O2D
25	b	610	CLA	CAD-CBD-CGD-O2D
25	c	501	CLA	CAD-CBD-CGD-O2D
25	c	510	CLA	CAD-CBD-CGD-O2D
31	P	628	LMG	C7-C8-O7-C10
31	p	628	LMG	C7-C8-O7-C10
33	J	101	LHG	C6-C5-O7-C7
33	j	101	LHG	C6-C5-O7-C7
34	B	608	F6C	CAD-CBD-CGD-O2D
34	b	608	F6C	CAD-CBD-CGD-O2D
25	B	603	CLA	C2-C1-O2A-CGA
25	b	603	CLA	C2-C1-O2A-CGA
25	c	510	CLA	CAA-CBA-CGA-O2A
25	B	616	CLA	C4-C3-C5-C6
25	b	616	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	D	405	PL9	C12-C11-C9-C10
30	d	405	PL9	C12-C11-C9-C10
33	j	101	LHG	C13-C14-C15-C16
33	P	629	LHG	C32-C33-C34-C35
32	Z	102	LMT	C4'-C5'-C6'-O6'
32	z	102	LMT	C4'-C5'-C6'-O6'
32	B	675	LMT	O5'-C1'-O1'-C1
32	b	675	LMT	O5'-C1'-O1'-C1
33	J	101	LHG	C13-C14-C15-C16
33	p	629	LHG	C32-C33-C34-C35
31	P	628	LMG	C24-C25-C26-C27
31	p	628	LMG	C24-C25-C26-C27
25	B	603	CLA	O2A-C1-C2-C3
25	C	509	CLA	O2A-C1-C2-C3
25	C	513	CLA	O2A-C1-C2-C3
25	D	402	CLA	O2A-C1-C2-C3
25	b	603	CLA	O2A-C1-C2-C3
25	c	509	CLA	O2A-C1-C2-C3
25	c	513	CLA	O2A-C1-C2-C3
25	d	402	CLA	O2A-C1-C2-C3
34	C	507	F6C	O1A-CGA-O2A-C1
34	c	507	F6C	O1A-CGA-O2A-C1
25	C	502	CLA	CHA-CBD-CGD-O2D
25	C	503	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CHA-CBD-CGD-O2D
25	c	503	CLA	CHA-CBD-CGD-O2D
30	D	405	PL9	C12-C13-C14-C16
30	d	405	PL9	C12-C13-C14-C16
25	C	512	CLA	CAA-CBA-CGA-O2A
25	c	512	CLA	CAA-CBA-CGA-O2A
35	C	518	DGD	O1G-C1A-C2A-C3A
35	c	518	DGD	O1G-C1A-C2A-C3A
31	P	628	LMG	O7-C8-C9-O8
31	p	628	LMG	O7-C8-C9-O8
35	C	517	DGD	C5A-C6A-C7A-C8A
35	c	517	DGD	C5A-C6A-C7A-C8A
33	L	101	LHG	O7-C7-C8-C9
33	l	101	LHG	O7-C7-C8-C9
35	C	518	DGD	C4D-C5D-C6D-O5D
35	c	518	DGD	C4D-C5D-C6D-O5D
27	A	409	PHO	CHA-CBD-CGD-O1D
27	A	409	PHO	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	a	409	PHO	CHA-CBD-CGD-O1D
27	a	409	PHO	CHA-CBD-CGD-O2D
32	a	675	LMT	O5'-C5'-C6'-O6'
35	C	518	DGD	C7B-C8B-C9B-CAB
35	c	518	DGD	C7B-C8B-C9B-CAB
32	A	675	LMT	O5'-C5'-C6'-O6'
27	A	408	PHO	C2-C3-C5-C6
27	a	408	PHO	C2-C3-C5-C6
34	B	614	F6C	C2-C3-C5-C6
34	b	614	F6C	C2-C3-C5-C6
32	G	104	LMT	C9-C10-C11-C12
33	e	101	LHG	C18-C19-C20-C21
25	C	509	CLA	C3-C5-C6-C7
25	c	509	CLA	C3-C5-C6-C7
32	g	104	LMT	C9-C10-C11-C12
33	E	101	LHG	C18-C19-C20-C21
25	A	405	CLA	C2B-C3B-CAB-CBB
25	B	603	CLA	C2B-C3B-CAB-CBB
25	B	604	CLA	C2B-C3B-CAB-CBB
25	B	605	CLA	C2B-C3B-CAB-CBB
25	B	613	CLA	C2B-C3B-CAB-CBB
25	C	501	CLA	C2B-C3B-CAB-CBB
25	C	508	CLA	C2B-C3B-CAB-CBB
25	C	509	CLA	C2B-C3B-CAB-CBB
25	C	513	CLA	C2B-C3B-CAB-CBB
25	a	405	CLA	C2B-C3B-CAB-CBB
25	b	603	CLA	C2B-C3B-CAB-CBB
25	b	604	CLA	C2B-C3B-CAB-CBB
25	b	605	CLA	C2B-C3B-CAB-CBB
25	b	613	CLA	C2B-C3B-CAB-CBB
25	c	501	CLA	C2B-C3B-CAB-CBB
25	c	508	CLA	C2B-C3B-CAB-CBB
25	c	509	CLA	C2B-C3B-CAB-CBB
25	c	513	CLA	C2B-C3B-CAB-CBB
29	A	412	SQD	C23-C24-C25-C26
29	a	412	SQD	C23-C24-C25-C26
29	A	412	SQD	C4-C5-C6-S
29	a	412	SQD	C4-C5-C6-S
29	H	102	SQD	C15-C16-C17-C18
29	h	102	SQD	C15-C16-C17-C18
25	C	503	CLA	C10-C11-C12-C13
25	c	503	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	B	628	LMG	C24-C25-C26-C27
31	C	902	LMG	C30-C31-C32-C33
31	b	628	LMG	C24-C25-C26-C27
31	c	902	LMG	C30-C31-C32-C33
25	B	607	CLA	C4-C3-C5-C6
25	C	513	CLA	C4-C3-C5-C6
25	b	607	CLA	C4-C3-C5-C6
25	c	513	CLA	C4-C3-C5-C6
29	B	622	SQD	C15-C16-C17-C18
29	b	622	SQD	C15-C16-C17-C18
29	C	903	SQD	O48-C23-C24-C25
29	c	903	SQD	O48-C23-C24-C25
31	P	628	LMG	C11-C12-C13-C14
31	P	628	LMG	C12-C13-C14-C15
31	p	628	LMG	C11-C12-C13-C14
31	p	628	LMG	C12-C13-C14-C15
32	L	210	LMT	C7-C8-C9-C10
32	l	210	LMT	C7-C8-C9-C10
34	C	507	F6C	CBA-CGA-O2A-C1
34	c	507	F6C	CBA-CGA-O2A-C1
31	P	628	LMG	O1-C7-C8-C9
31	P	628	LMG	C7-C8-C9-O8
31	p	628	LMG	O1-C7-C8-C9
31	p	628	LMG	C7-C8-C9-O8
35	C	516	DGD	C1G-C2G-C3G-O3G
35	c	516	DGD	C1G-C2G-C3G-O3G
34	B	614	F6C	CAA-CBA-CGA-O1A
34	b	614	F6C	CAA-CBA-CGA-O1A
25	C	510	CLA	CAA-CBA-CGA-O1A
25	c	510	CLA	CAA-CBA-CGA-O1A
25	B	602	CLA	C2-C3-C5-C6
25	b	602	CLA	C2-C3-C5-C6
29	H	102	SQD	C32-C33-C34-C35
29	h	102	SQD	C32-C33-C34-C35
31	L	212	LMG	C19-C20-C21-C22
31	l	212	LMG	C19-C20-C21-C22
33	D	409	LHG	C3-O3-P-O5
33	D	409	LHG	C4-O6-P-O5
33	L	101	LHG	C4-O6-P-O4
33	d	409	LHG	C3-O3-P-O5
33	d	409	LHG	C4-O6-P-O5
33	l	101	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
33	P	629	LHG	C3-O3-P-O5
33	p	629	LHG	C3-O3-P-O5
35	C	517	DGD	O2G-C1B-C2B-C3B
35	c	517	DGD	O2G-C1B-C2B-C3B
29	A	412	SQD	O47-C7-C8-C9
29	a	412	SQD	O47-C7-C8-C9
31	P	628	LMG	C4-C5-C6-O5
31	p	628	LMG	C4-C5-C6-O5
35	C	516	DGD	C8B-C9B-CAB-CBB
35	c	516	DGD	C8B-C9B-CAB-CBB
33	D	410	LHG	C30-C31-C32-C33
33	d	410	LHG	C30-C31-C32-C33
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	506	CLA	CAD-CBD-CGD-O1D
25	C	512	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O1D
25	c	512	CLA	CAD-CBD-CGD-O1D
33	D	409	LHG	C7-C8-C9-C10
33	d	409	LHG	C7-C8-C9-C10
25	C	512	CLA	CAA-CBA-CGA-O1A
25	c	512	CLA	CAA-CBA-CGA-O1A
25	C	502	CLA	C14-C13-C15-C16
25	c	502	CLA	C14-C13-C15-C16
25	C	501	CLA	CAA-CBA-CGA-O2A
25	c	501	CLA	CAA-CBA-CGA-O2A
33	d	410	LHG	O7-C7-C8-C9
33	L	101	LHG	O9-C7-C8-C9
33	l	101	LHG	O9-C7-C8-C9
35	C	518	DGD	O1A-C1A-C2A-C3A
35	c	518	DGD	O1A-C1A-C2A-C3A
33	E	101	LHG	C32-C33-C34-C35
33	e	101	LHG	C32-C33-C34-C35
33	D	410	LHG	O7-C7-C8-C9
33	E	101	LHG	O7-C7-C8-C9
33	e	101	LHG	O7-C7-C8-C9
34	B	617	F6C	C3A-C2A-CAA-CBA
34	b	617	F6C	C3A-C2A-CAA-CBA
31	l	212	LMG	C12-C13-C14-C15
31	L	212	LMG	C12-C13-C14-C15
27	A	408	PHO	C4-C3-C5-C6
27	a	408	PHO	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	B	616	CLA	C2-C3-C5-C6
25	b	616	CLA	C2-C3-C5-C6
33	J	101	LHG	C28-C29-C30-C31
33	j	101	LHG	C28-C29-C30-C31
32	a	674	LMT	C6-C7-C8-C9
32	A	674	LMT	C6-C7-C8-C9
28	B	627	BCR	C11-C12-C13-C14
28	b	627	BCR	C11-C12-C13-C14
25	b	602	CLA	CAA-CBA-CGA-O2A
31	D	411	LMG	C39-C40-C41-C42
31	d	411	LMG	C39-C40-C41-C42
29	A	417	SQD	O5-C1-O6-C44
29	a	417	SQD	O5-C1-O6-C44
34	B	614	F6C	O1A-CGA-O2A-C1
34	b	614	F6C	O1A-CGA-O2A-C1
33	D	410	LHG	O9-C7-C8-C9
33	d	410	LHG	O9-C7-C8-C9
30	A	414	PL9	C44-C46-C47-C48
30	a	414	PL9	C44-C46-C47-C48
33	P	629	LHG	C13-C14-C15-C16
33	p	629	LHG	C13-C14-C15-C16
25	B	602	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

146 monomers are involved in 328 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	627	BCR	1	0
31	D	411	LMG	1	0
32	z	102	LMT	1	0
31	A	415	LMG	2	0
29	D	407	SQD	1	0
35	C	516	DGD	1	0
25	B	607	CLA	2	0
25	c	502	CLA	6	0
33	E	101	LHG	3	0
25	A	410	CLA	2	0
25	B	616	CLA	6	0
28	A	411	BCR	2	0
25	c	505	CLA	4	0
25	a	407	CLA	4	0
25	A	405	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	D	403	CLA	1	0
25	b	607	CLA	2	0
25	b	609	CLA	1	0
25	c	508	CLA	6	0
29	c	903	SQD	1	0
28	B	620	BCR	2	0
28	b	619	BCR	3	0
25	d	402	CLA	4	0
25	c	511	CLA	2	0
33	a	419	LHG	1	0
25	C	504	CLA	2	0
25	c	503	CLA	5	0
28	k	102	BCR	4	0
30	a	414	PL9	6	0
35	C	517	DGD	5	0
31	b	628	LMG	2	0
25	C	502	CLA	6	0
32	L	213	LMT	1	0
37	f	101	HEM	5	0
28	c	514	BCR	2	0
25	B	613	CLA	2	0
32	l	210	LMT	1	0
25	B	609	CLA	1	0
25	b	603	CLA	5	0
31	C	519	LMG	3	0
37	F	101	HEM	5	0
25	d	403	CLA	1	0
35	C	518	DGD	1	0
32	a	674	LMT	3	0
33	P	629	LHG	3	0
27	A	409	PHO	2	0
26	a	406	CL7	1	0
31	C	902	LMG	5	0
25	a	410	CLA	2	0
32	m	101	LMT	3	0
33	L	101	LHG	1	0
25	b	611	CLA	3	0
31	c	902	LMG	5	0
29	a	412	SQD	4	0
25	C	509	CLA	3	0
25	D	402	CLA	4	0
25	B	602	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	610	CLA	3	0
25	b	612	CLA	1	0
28	d	404	BCR	2	0
25	c	504	CLA	2	0
25	c	506	CLA	3	0
30	A	414	PL9	6	0
25	c	513	CLA	1	0
25	A	407	CLA	3	0
29	h	102	SQD	2	0
33	e	244	LHG	1	0
25	b	615	CLA	2	0
33	d	409	LHG	2	0
25	B	610	CLA	3	0
28	D	404	BCR	3	0
27	A	408	PHO	4	0
25	C	506	CLA	3	0
29	b	622	SQD	3	0
31	l	212	LMG	2	0
25	B	603	CLA	5	0
28	B	618	BCR	2	0
35	c	517	DGD	3	0
25	B	615	CLA	1	0
33	a	416	LHG	6	0
31	a	415	LMG	2	0
25	C	512	CLA	3	0
25	c	509	CLA	3	0
25	B	611	CLA	3	0
28	k	101	BCR	1	0
25	B	606	CLA	6	0
25	b	605	CLA	5	0
25	B	612	CLA	1	0
29	A	412	SQD	4	0
34	b	617	F6C	1	0
25	c	501	CLA	5	0
28	b	627	BCR	1	0
25	C	505	CLA	5	0
29	a	417	SQD	3	0
33	A	416	LHG	5	0
28	K	101	BCR	1	0
31	d	411	LMG	2	0
25	C	513	CLA	1	0
28	B	619	BCR	4	0

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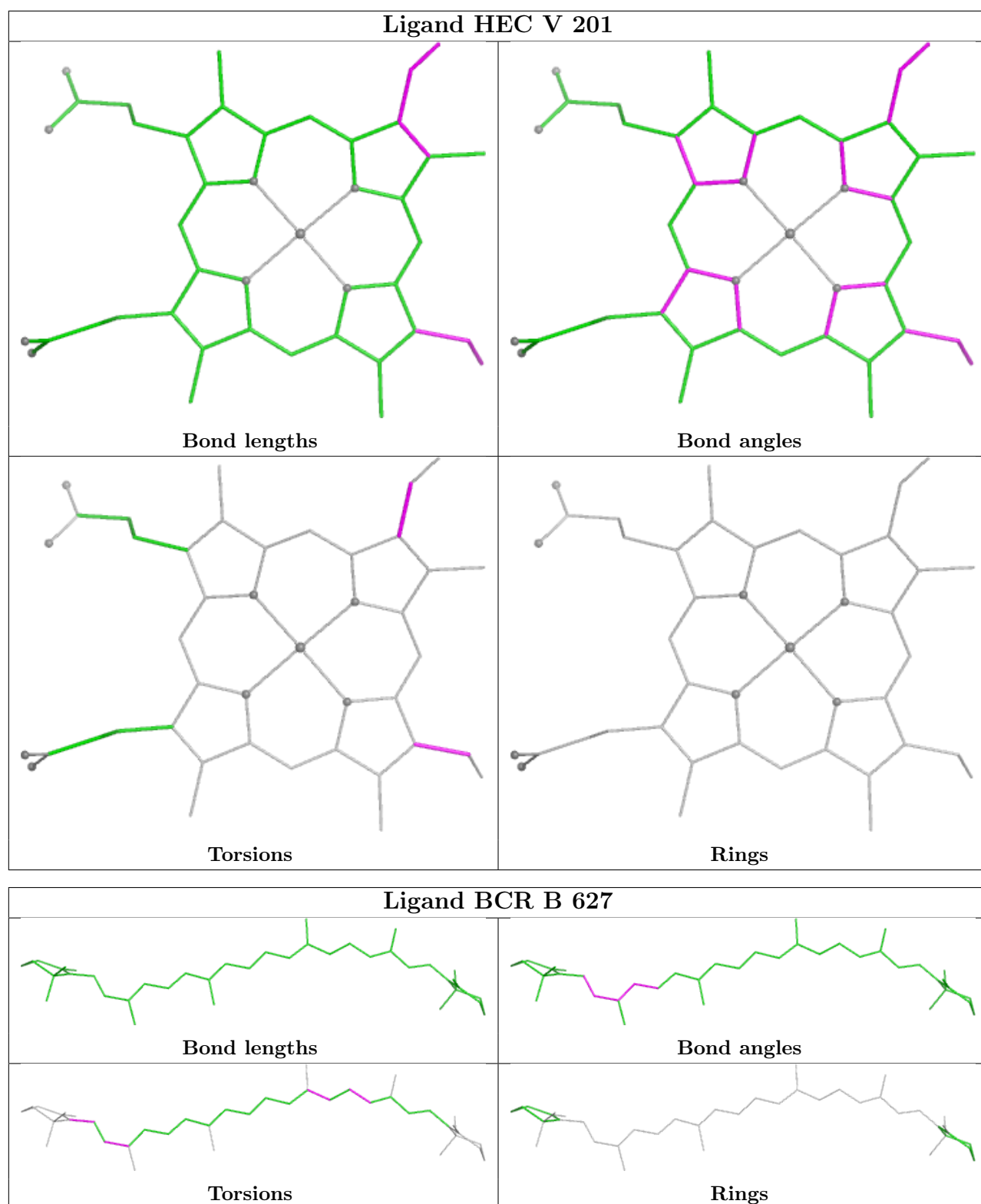
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	616	CLA	6	0
29	B	622	SQD	3	0
25	c	512	CLA	3	0
28	K	102	BCR	5	0
33	E	244	LHG	1	0
25	C	501	CLA	5	0
31	L	212	LMG	2	0
32	L	210	LMT	1	0
25	b	604	CLA	2	0
25	C	510	CLA	5	0
31	c	519	LMG	3	0
31	B	628	LMG	3	0
33	D	409	LHG	2	0
34	B	617	F6C	1	0
25	b	606	CLA	6	0
27	a	409	PHO	3	0
32	A	674	LMT	3	0
29	H	102	SQD	1	0
26	A	406	CL7	1	0
28	b	618	BCR	2	0
25	b	613	CLA	2	0
29	d	407	SQD	1	0
25	C	503	CLA	5	0
33	A	419	LHG	1	0
33	J	101	LHG	4	0
25	c	510	CLA	4	0
33	e	101	LHG	3	0
25	B	604	CLA	2	0
28	C	514	BCR	1	0
32	M	101	LMT	3	0
31	p	628	LMG	1	0
25	b	602	CLA	2	0
29	A	417	SQD	4	0
33	j	101	LHG	3	0
33	l	101	LHG	1	0
33	p	629	LHG	3	0
25	C	508	CLA	7	0
32	Z	102	LMT	1	0
35	c	518	DGD	1	0
35	c	516	DGD	2	0
25	a	405	CLA	2	0
25	C	511	CLA	2	0

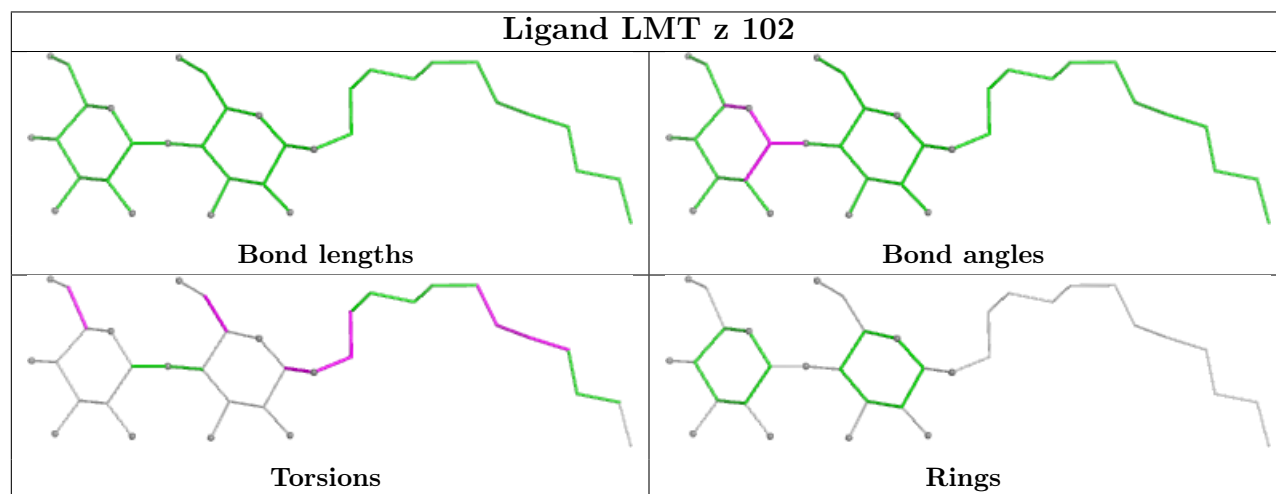
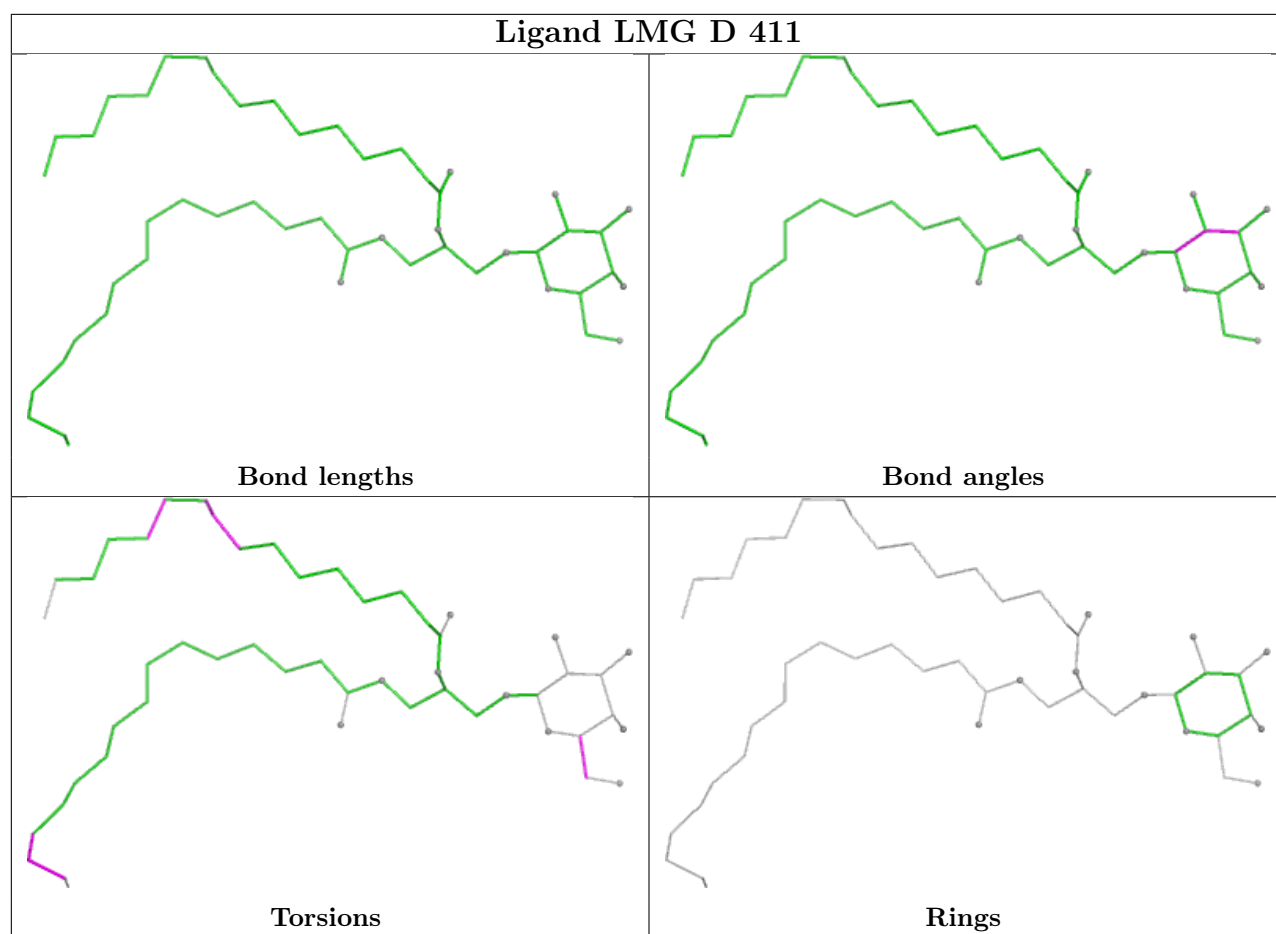
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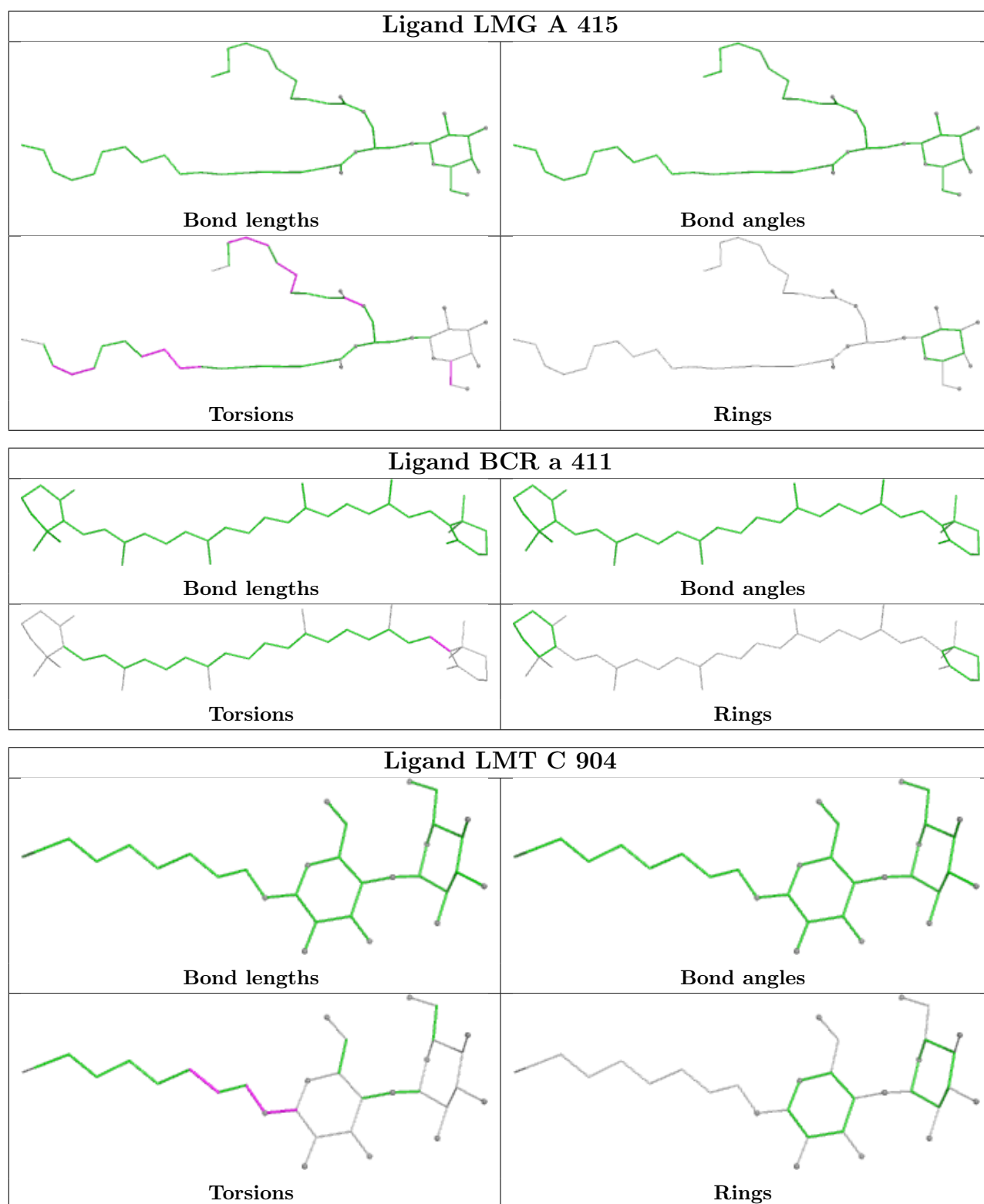
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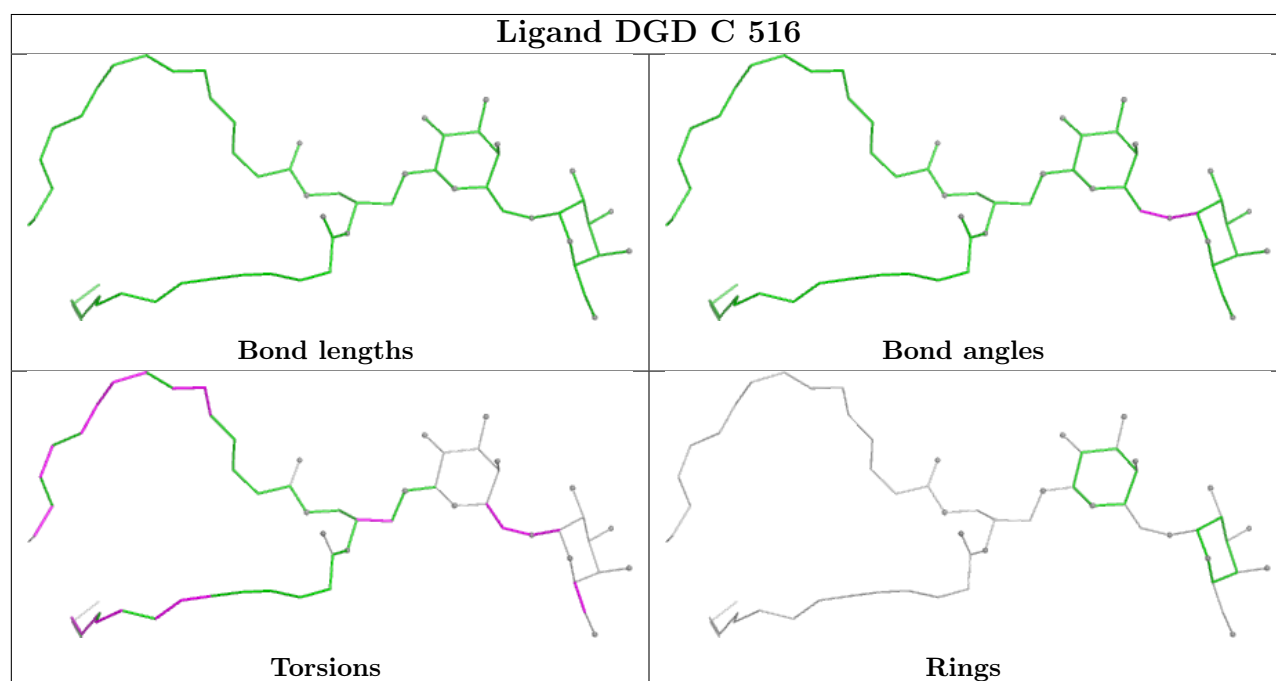
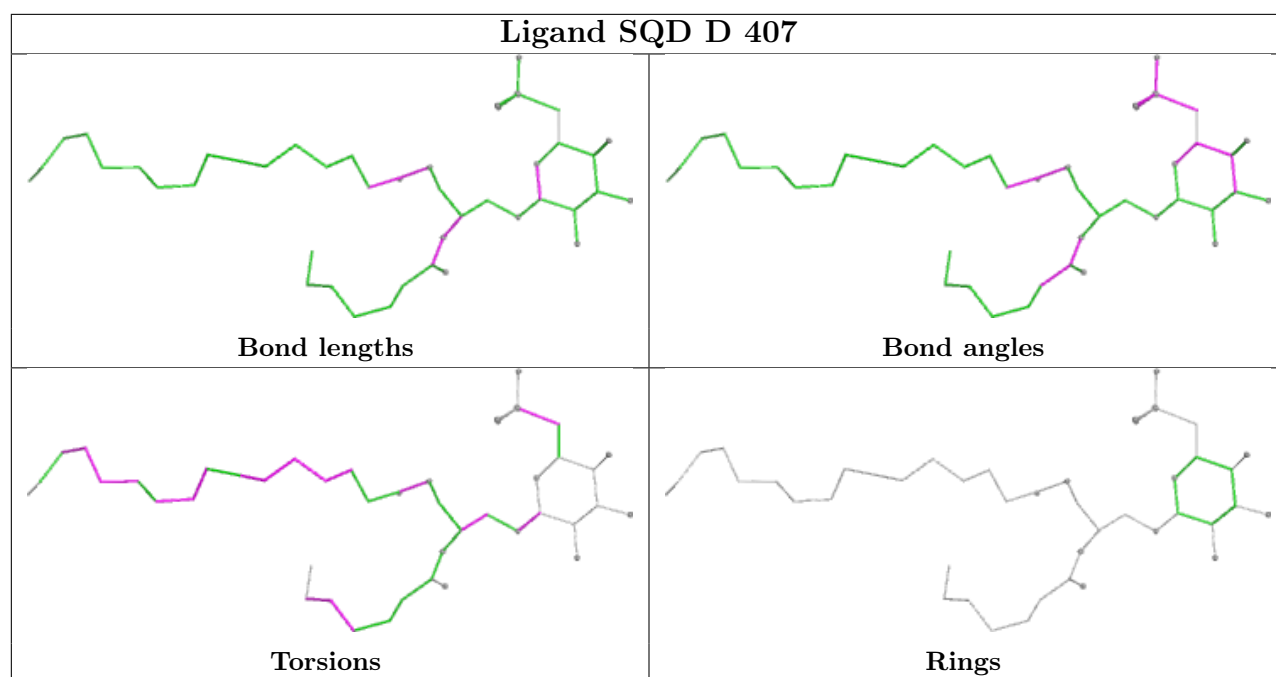
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	b	620	BCR	1	0
27	a	408	PHO	3	0
25	B	605	CLA	5	0
29	C	903	SQD	1	0
31	P	628	LMG	1	0

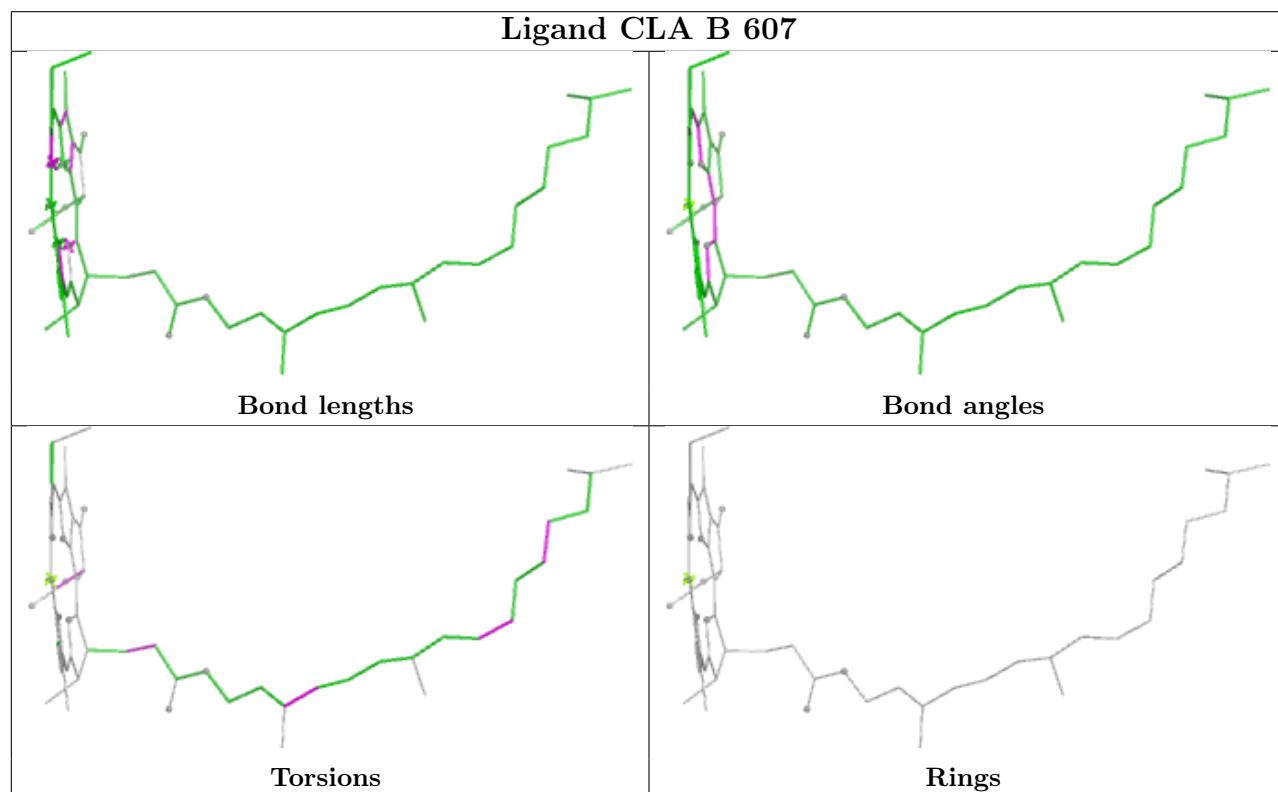
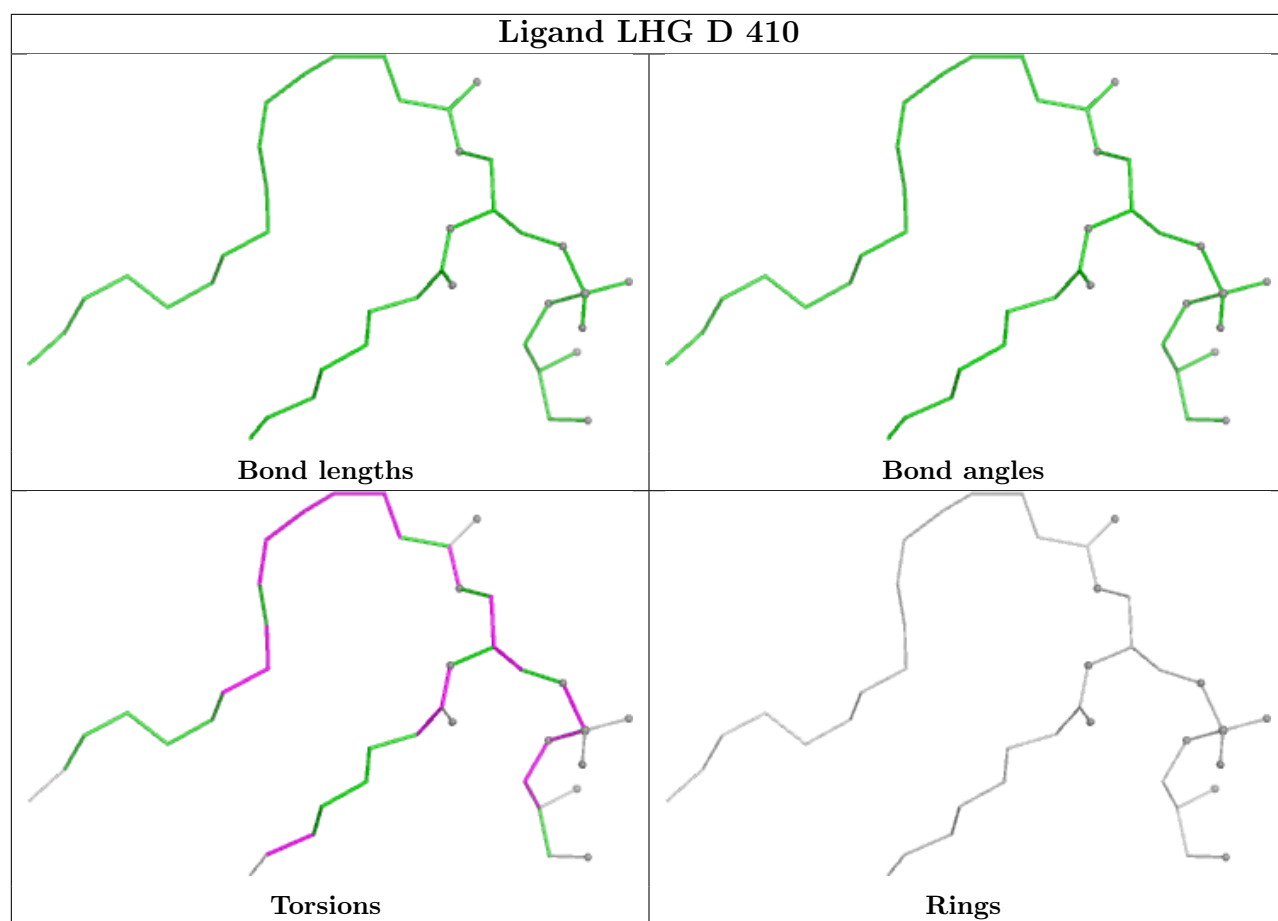
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

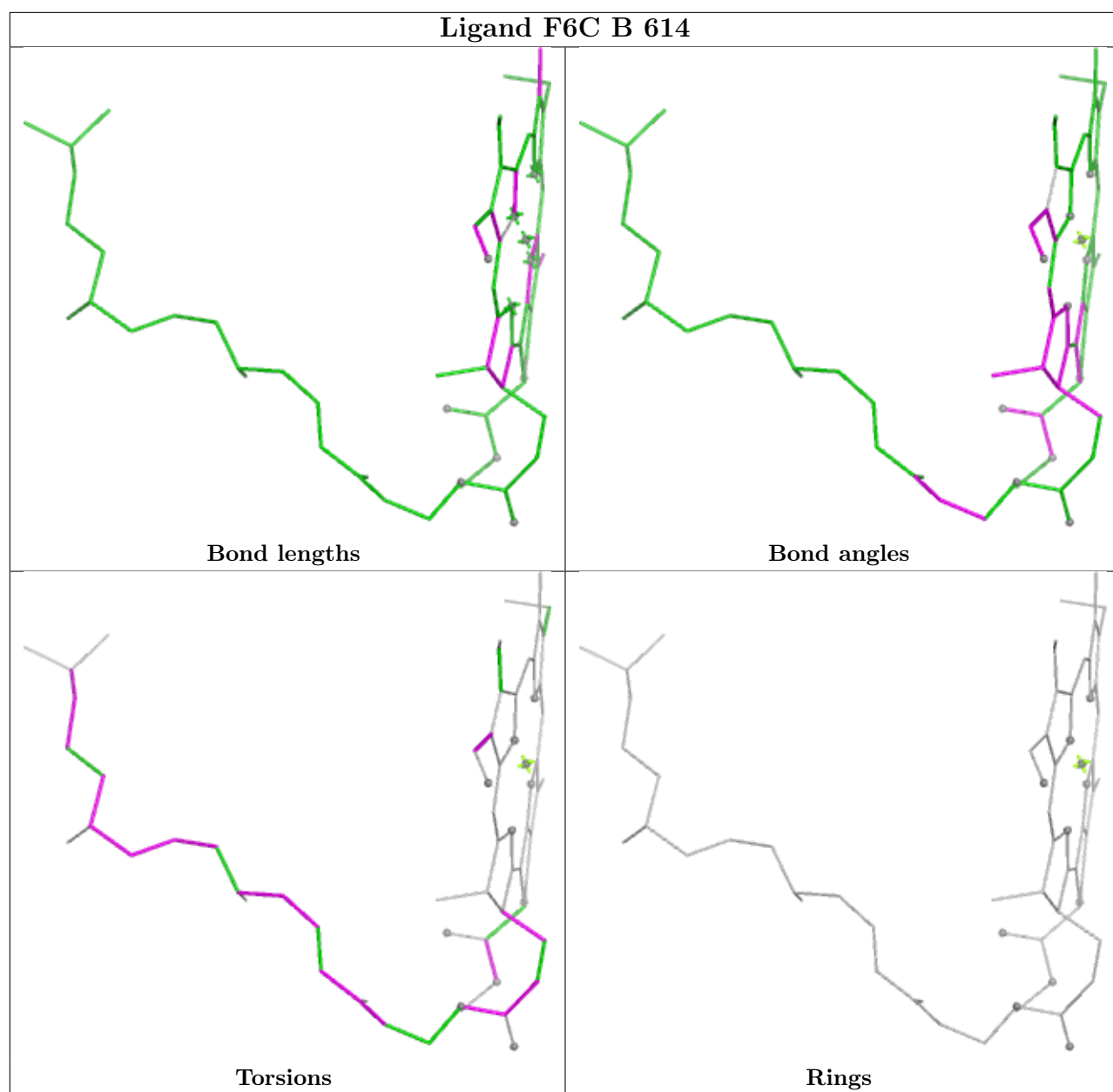


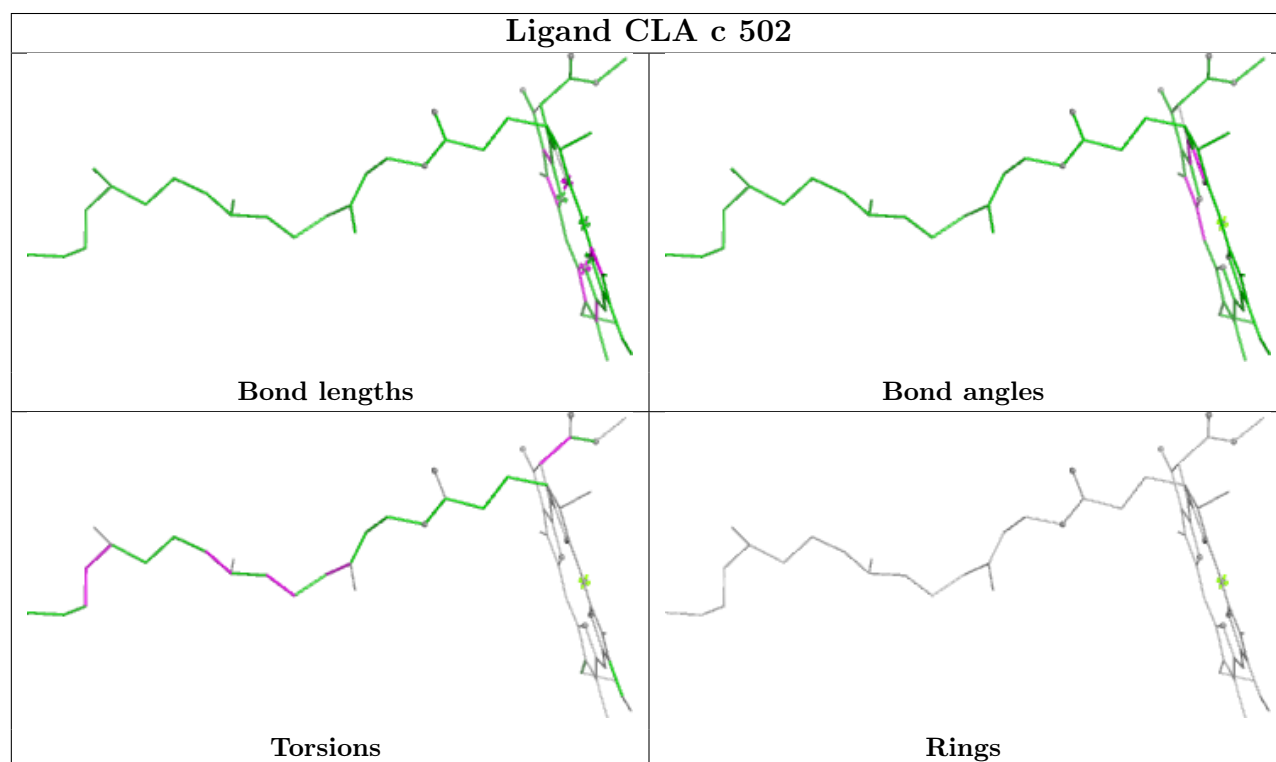
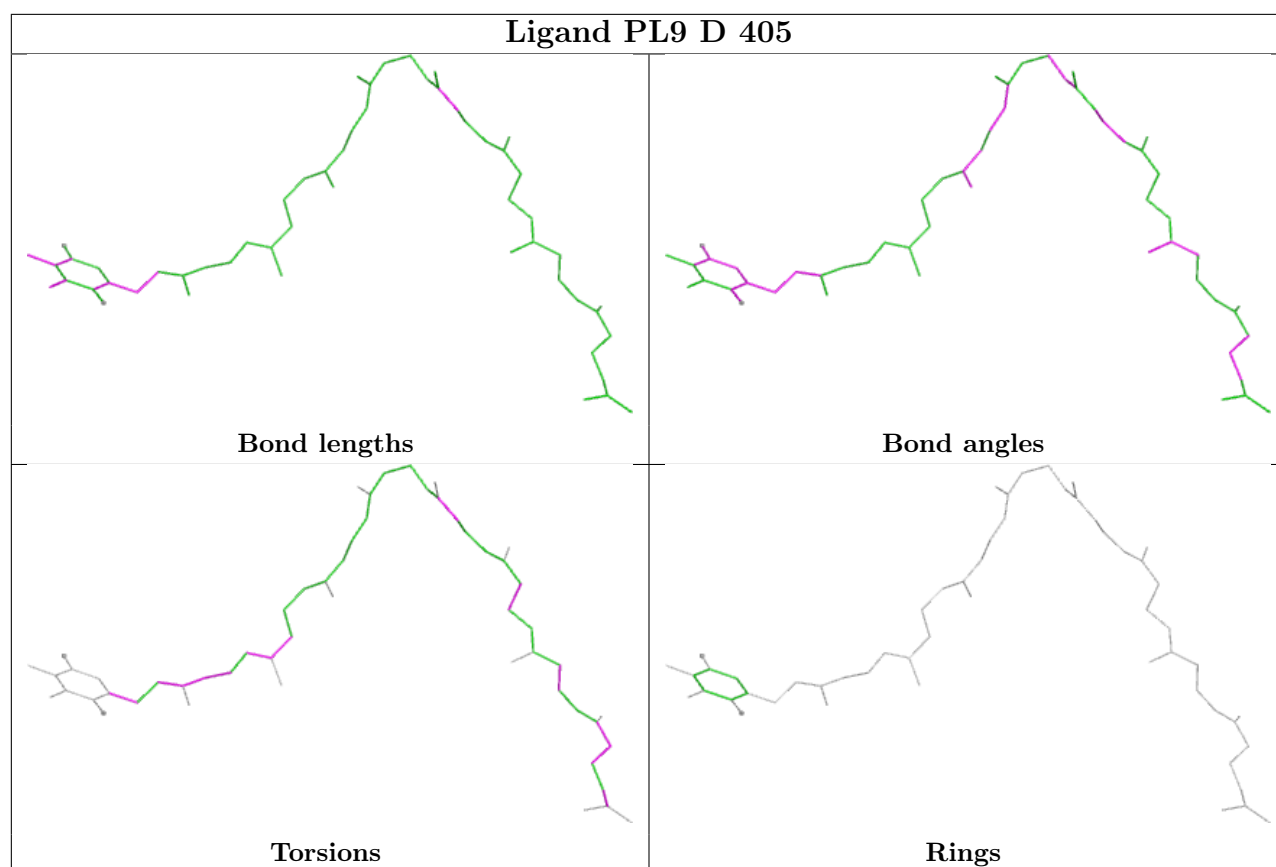




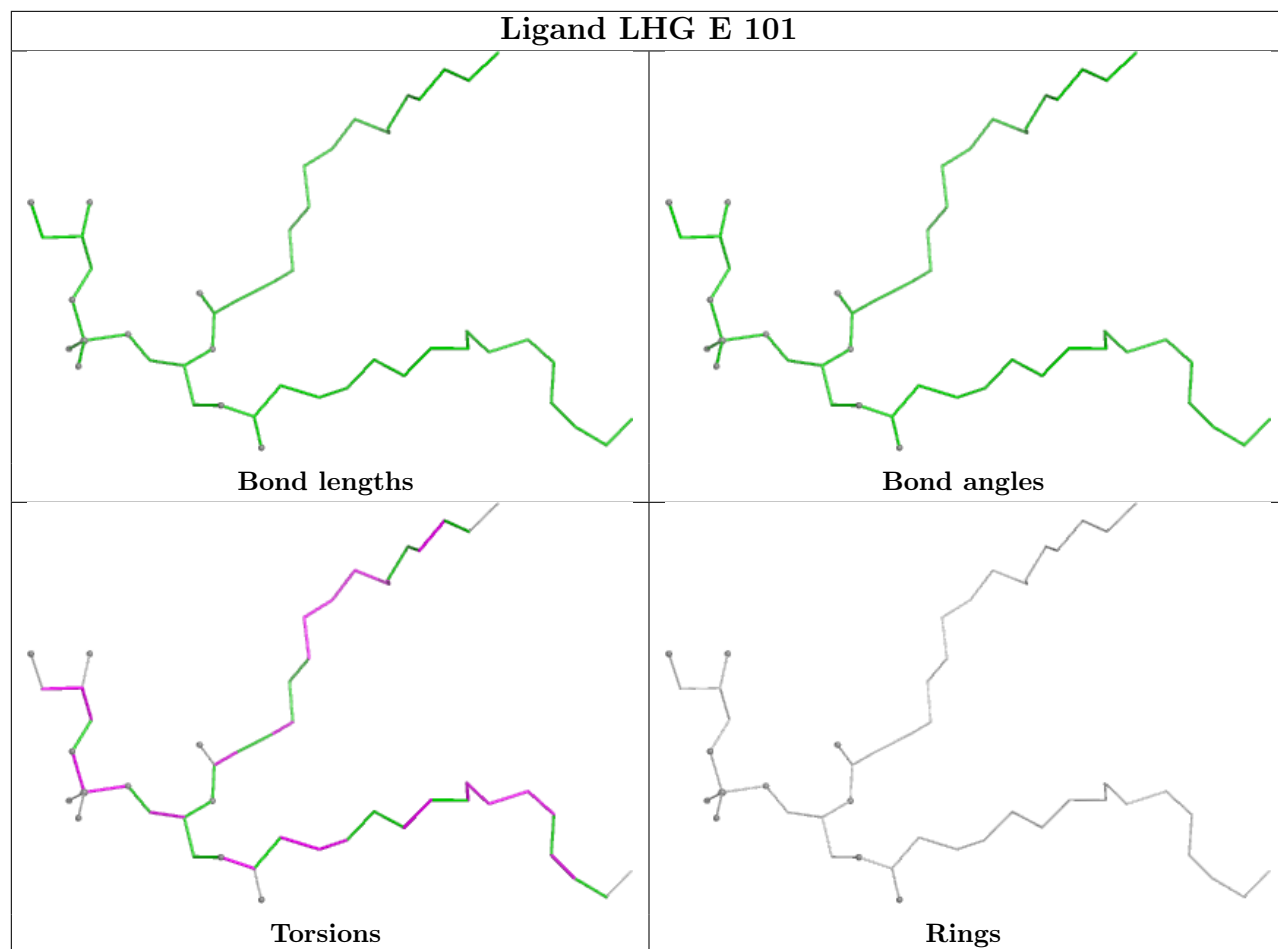




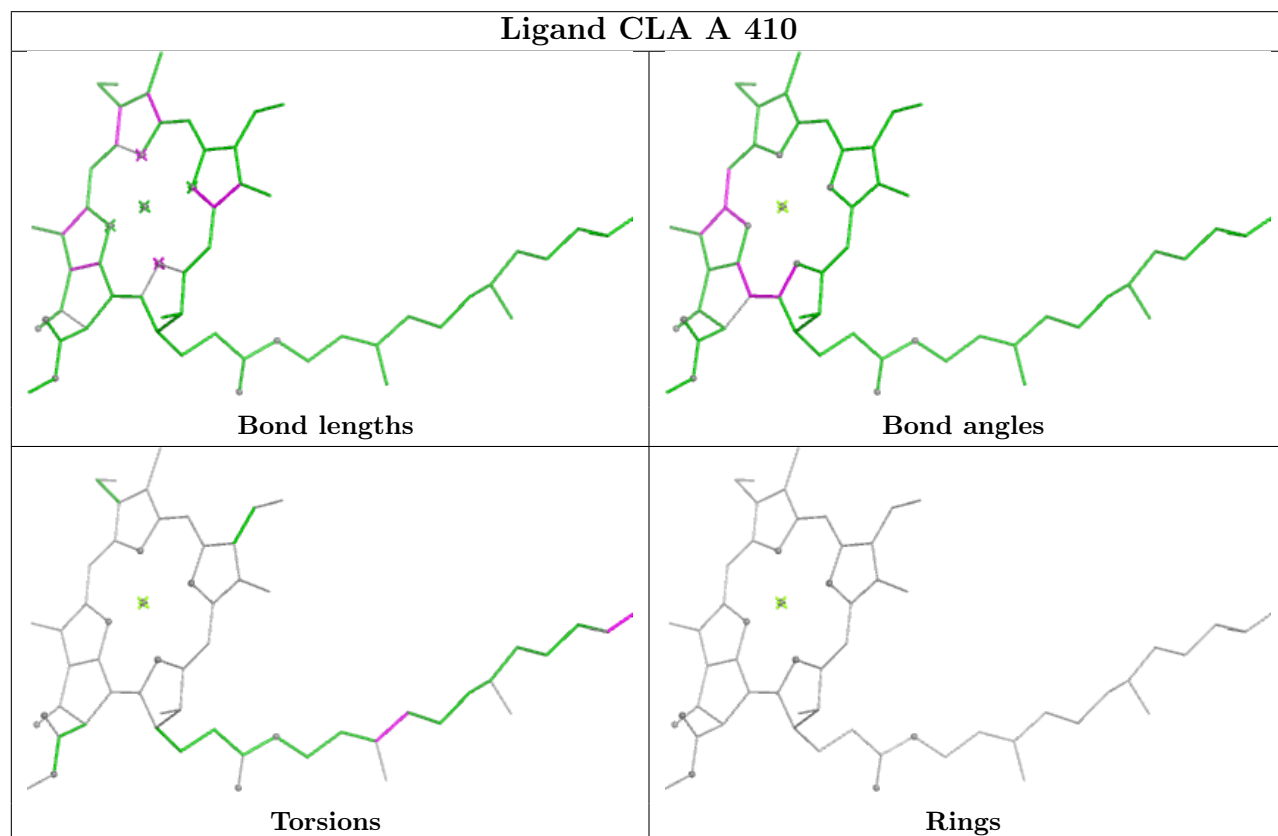




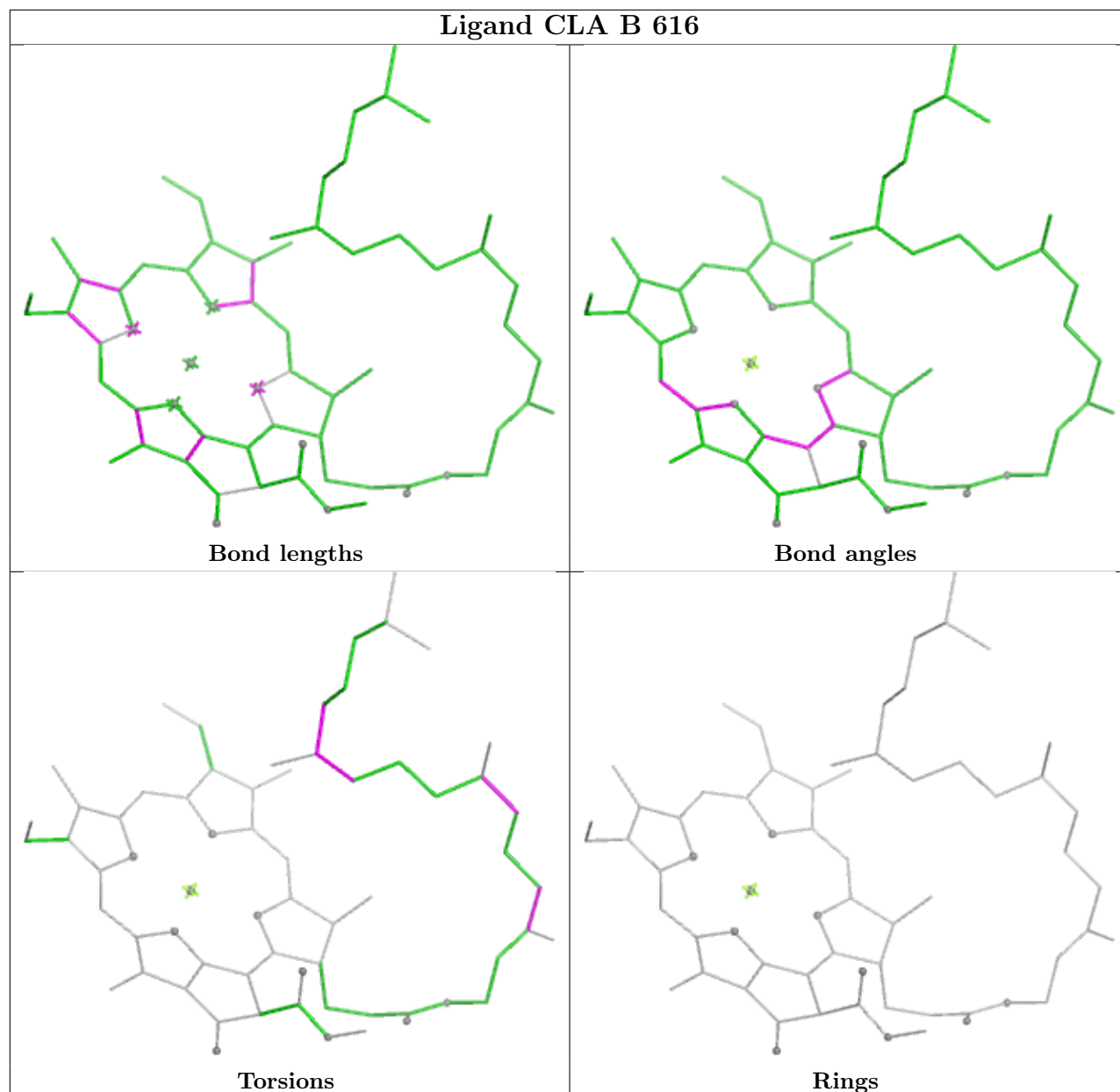
Ligand LHG E 101



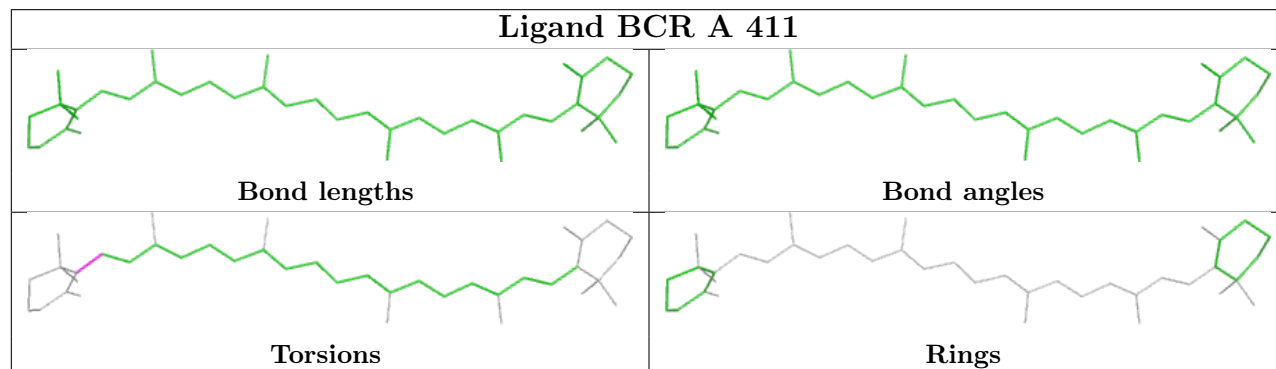
Ligand CLA A 410

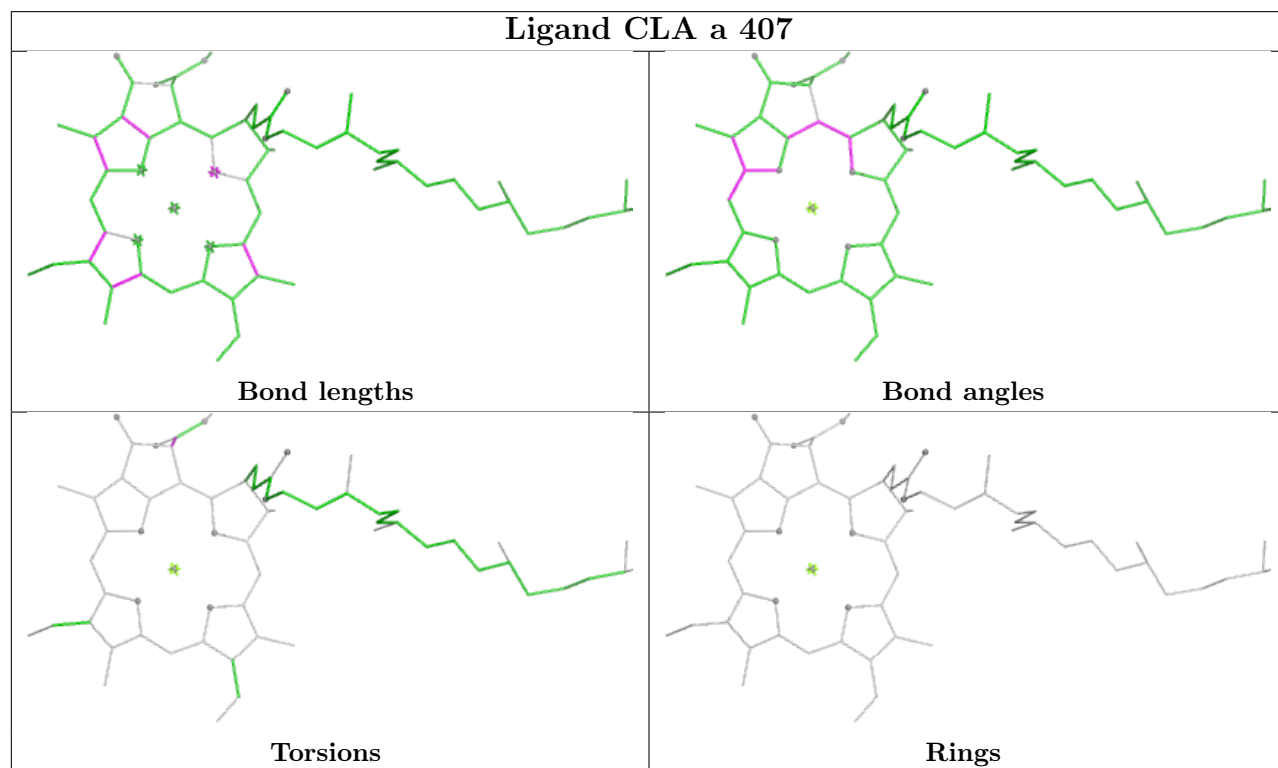
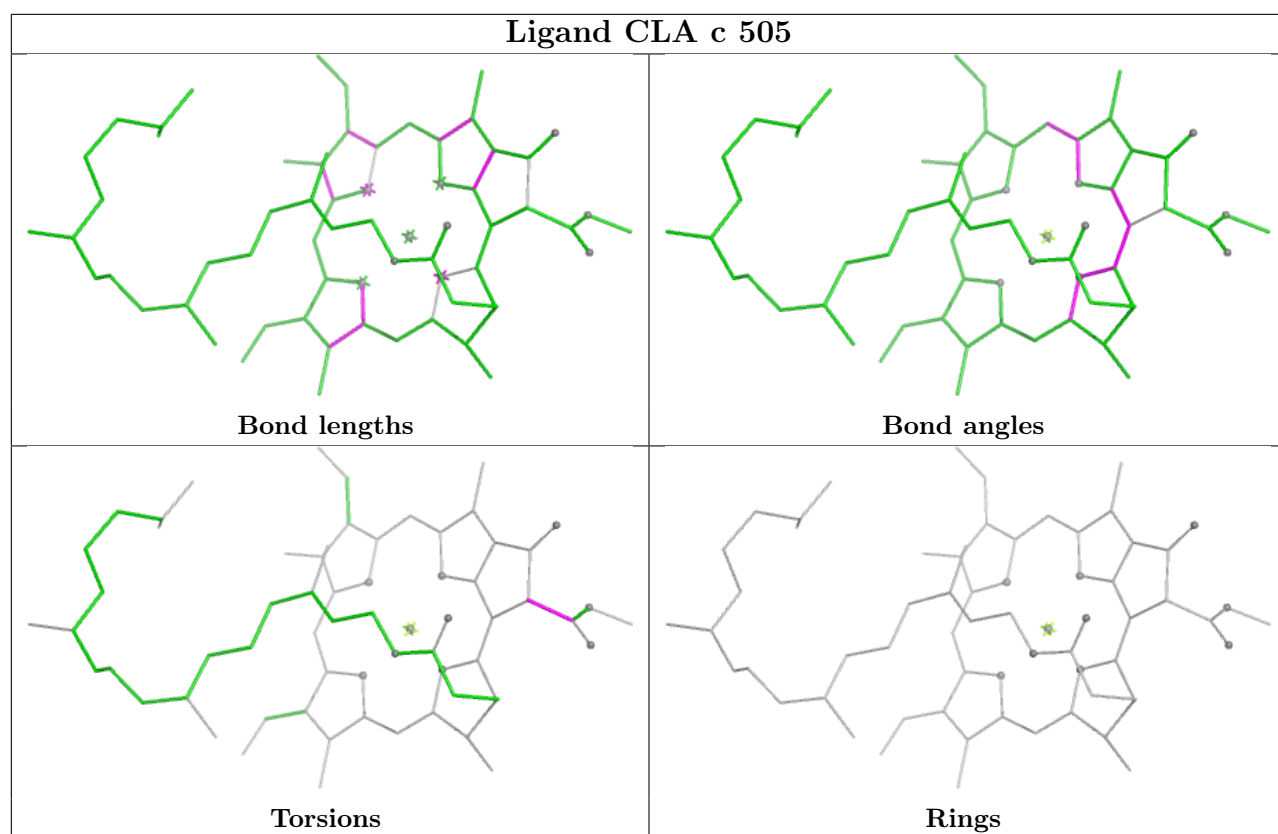


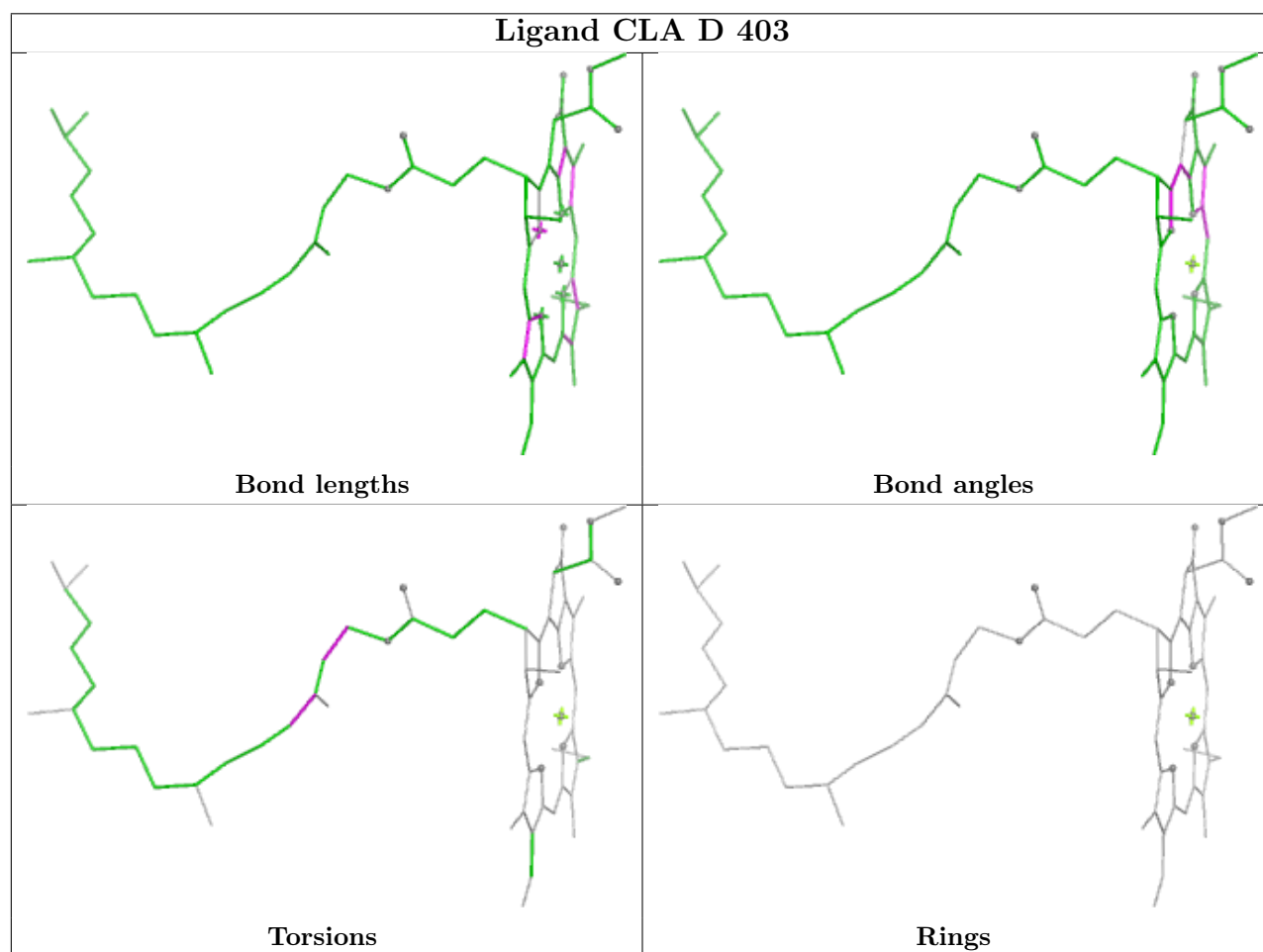
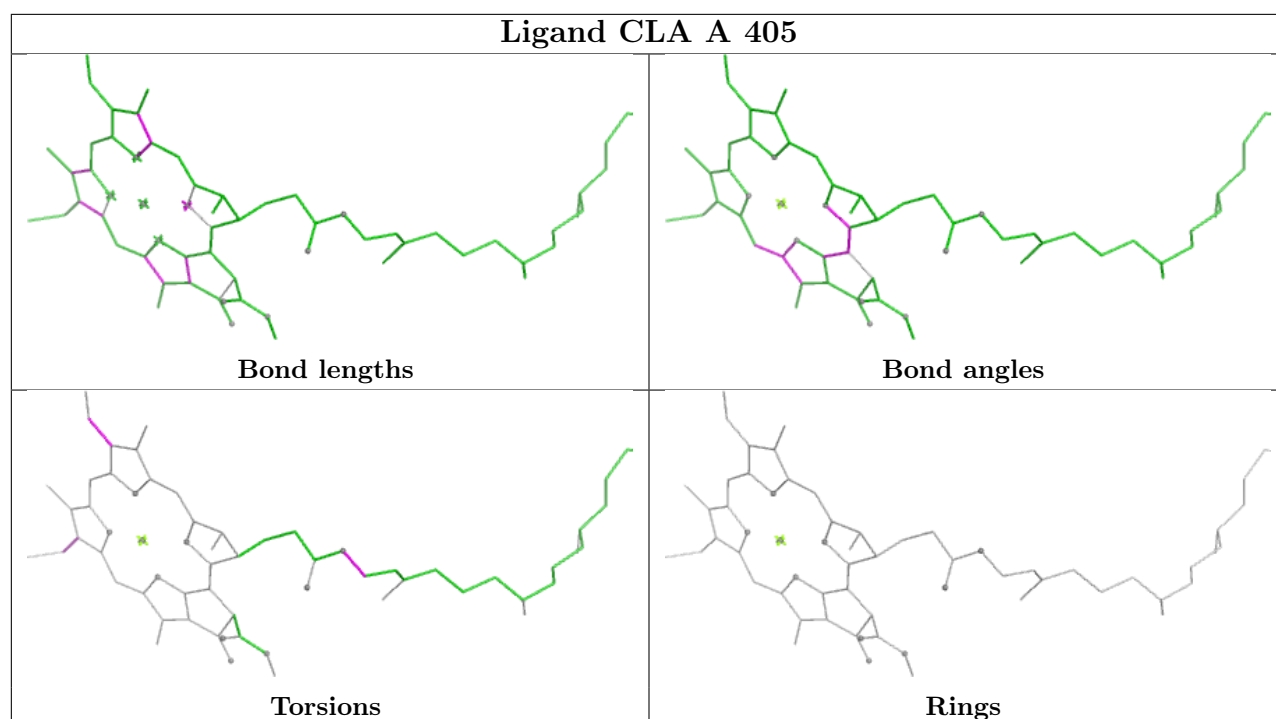
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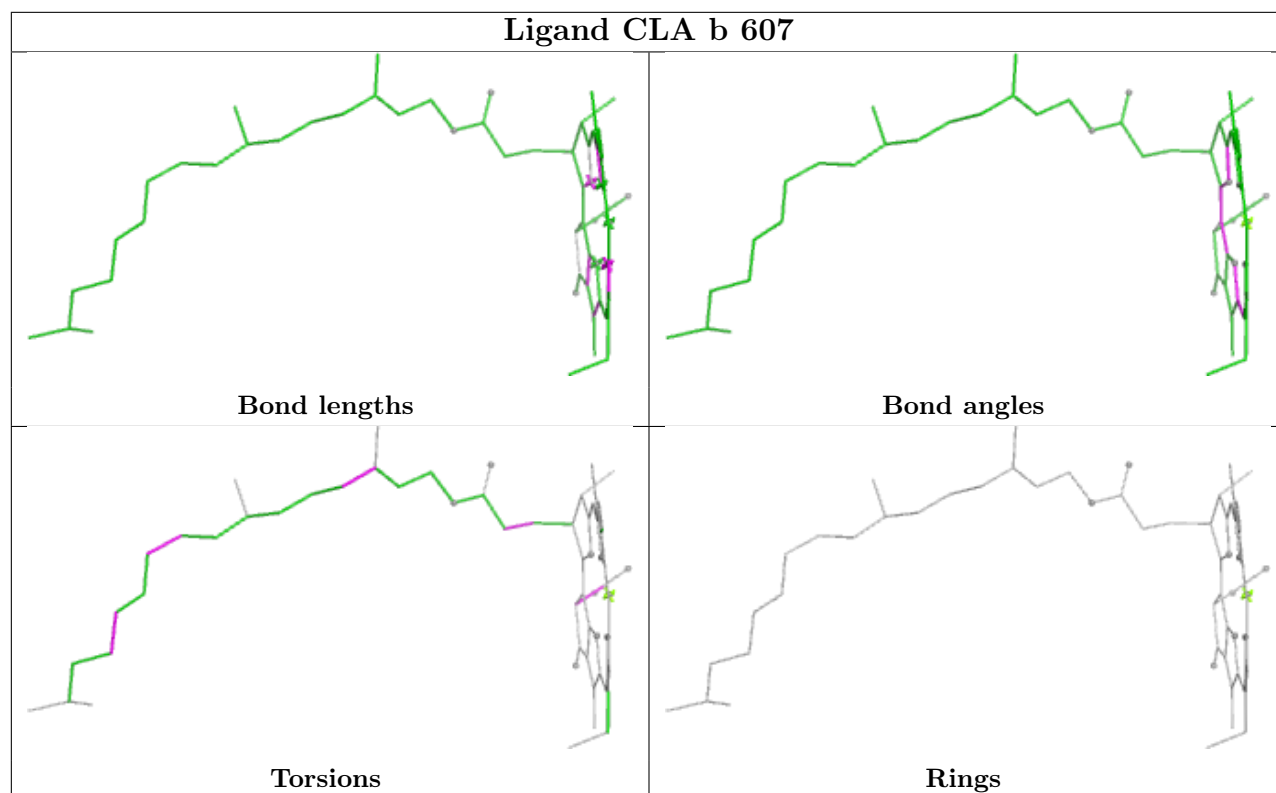
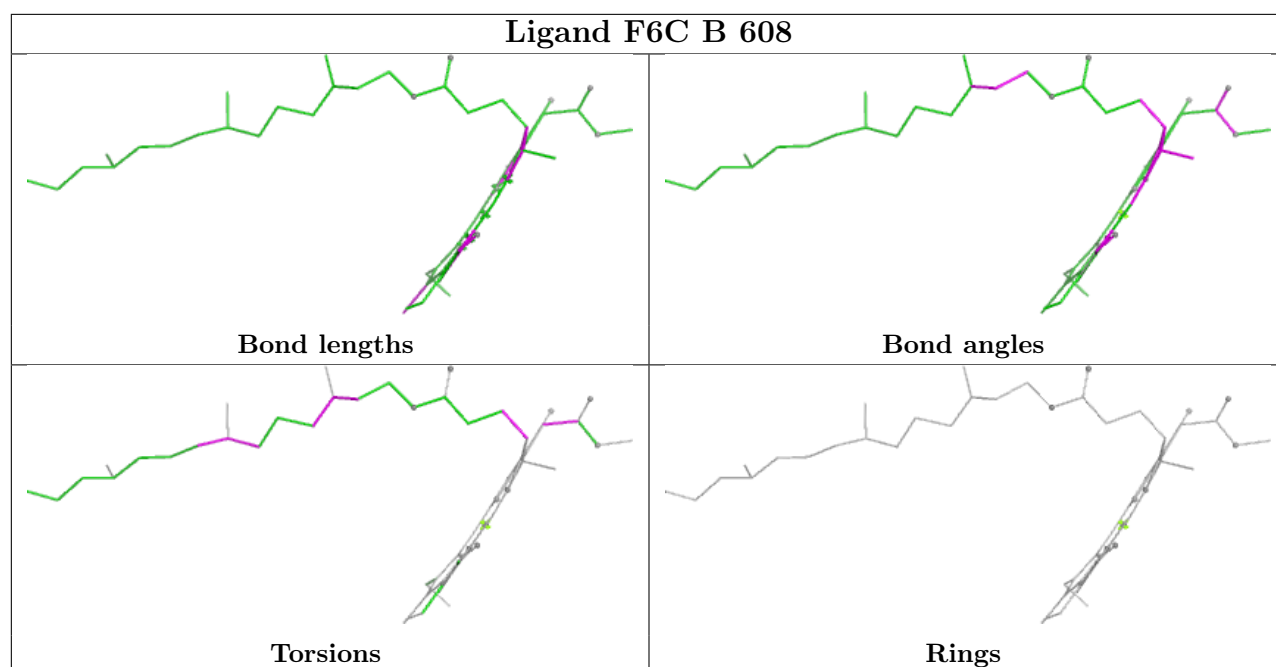


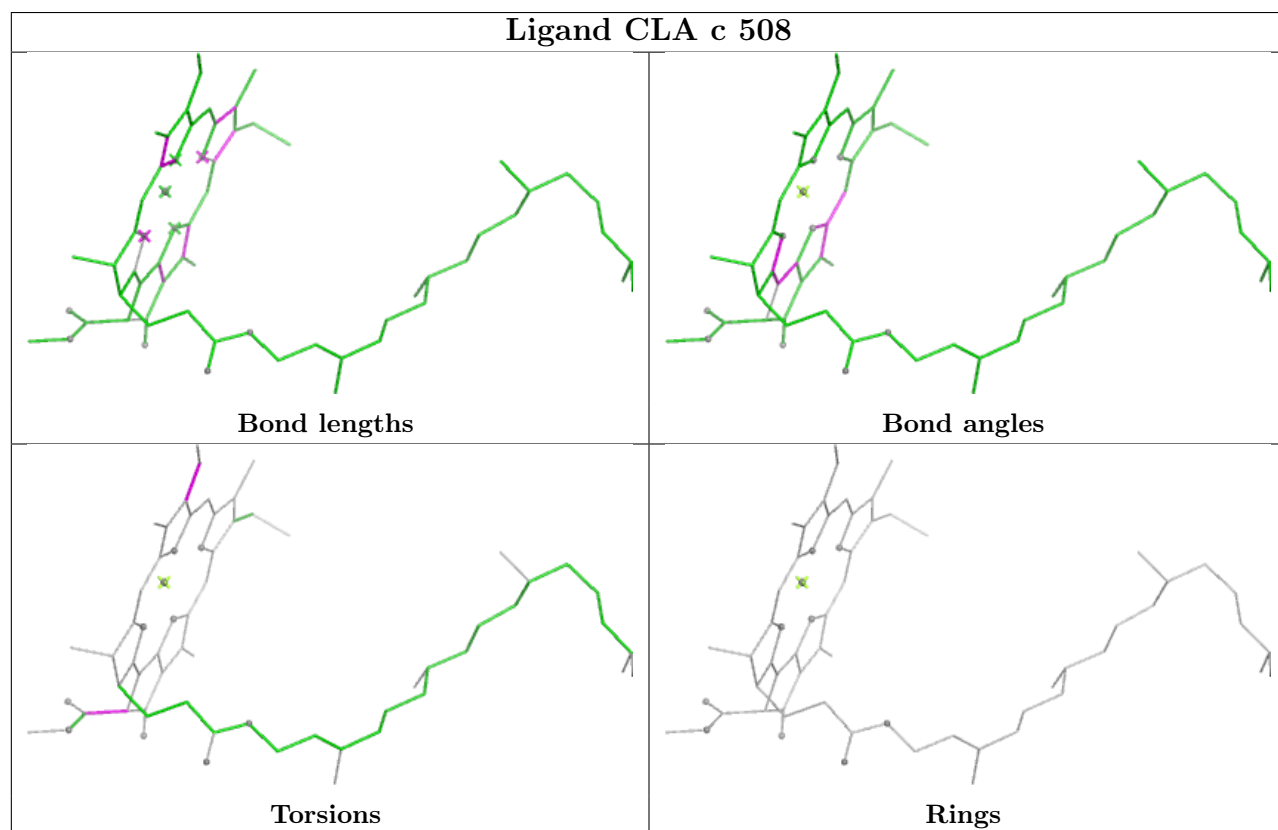
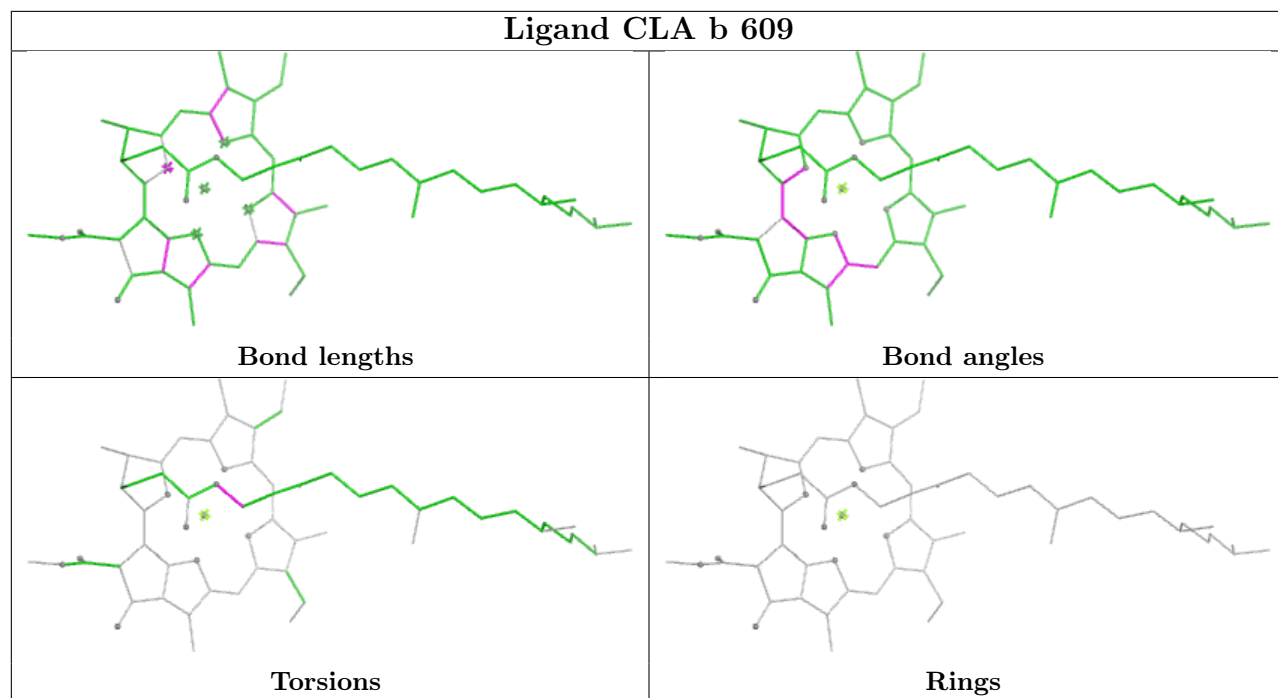
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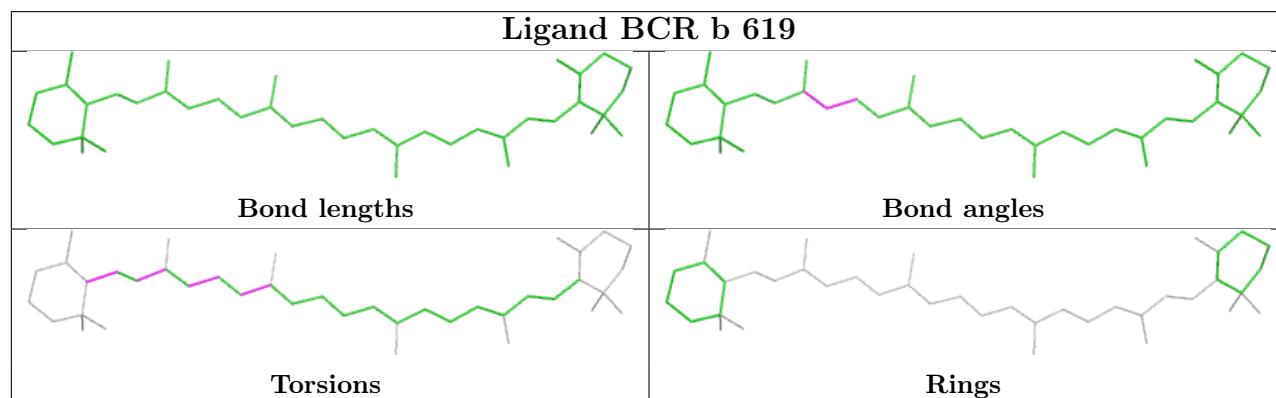
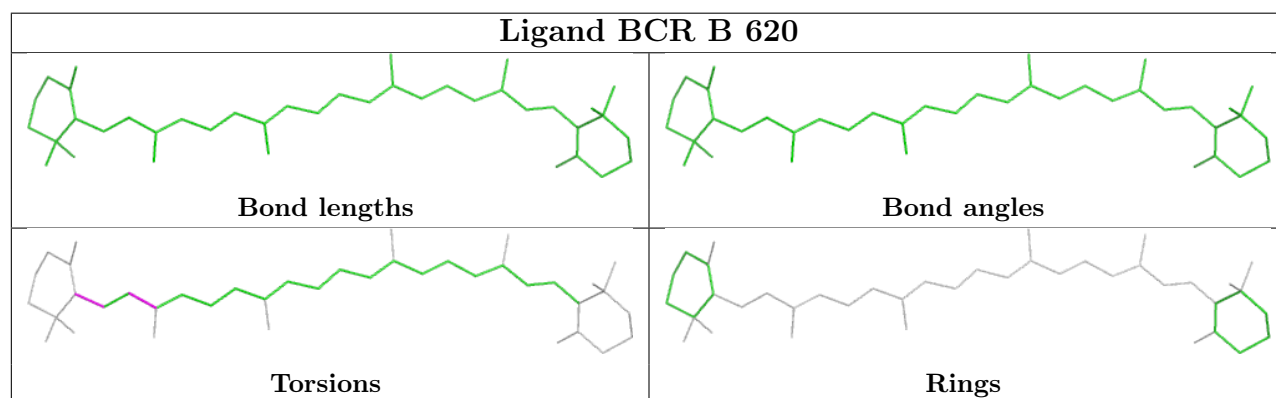
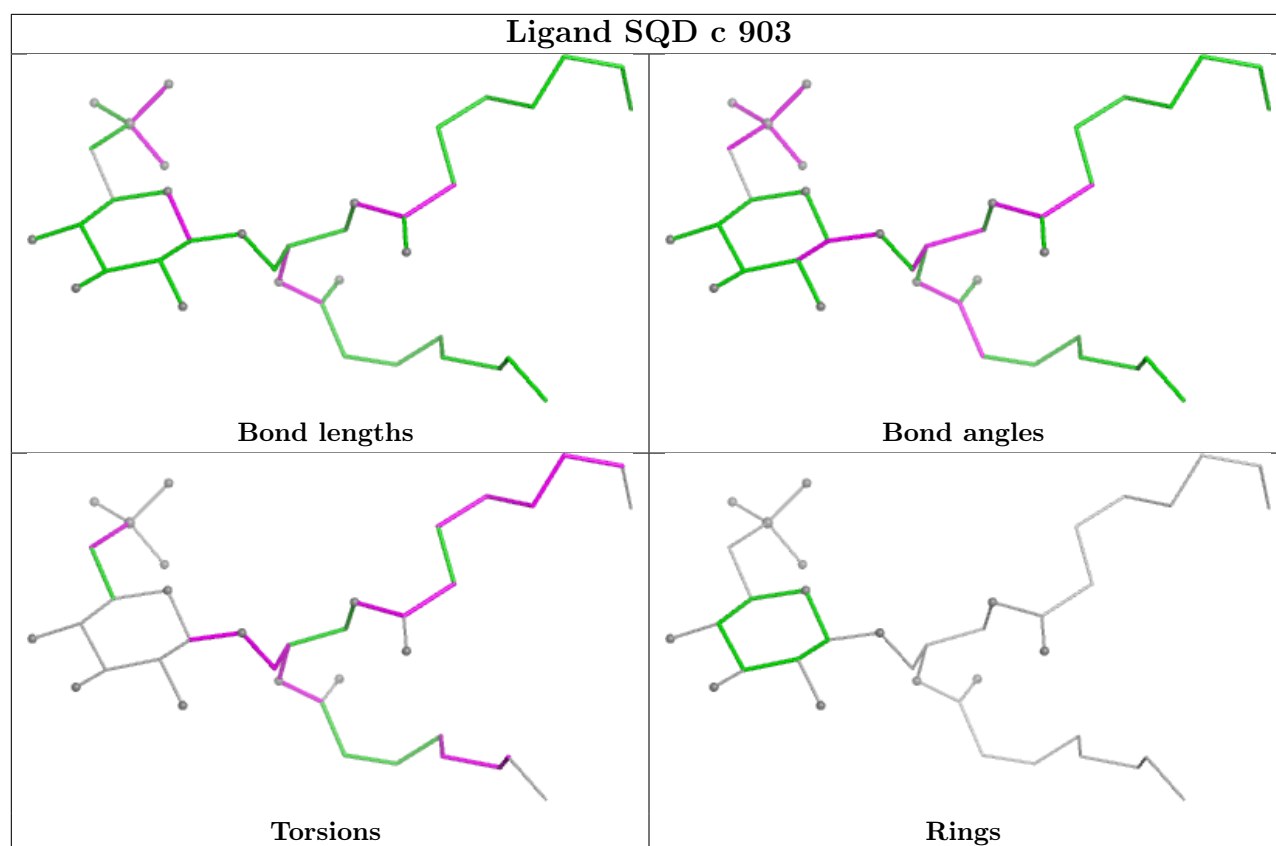


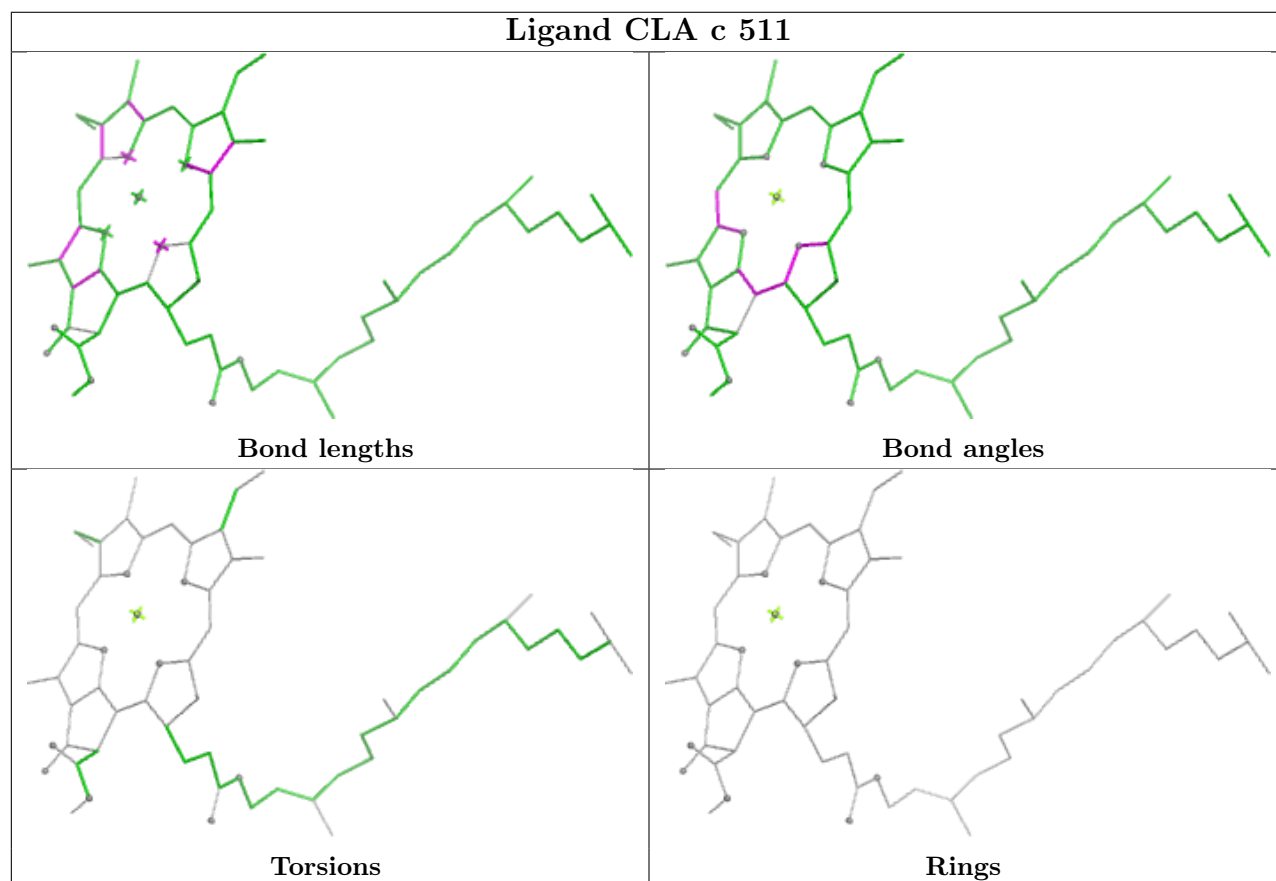
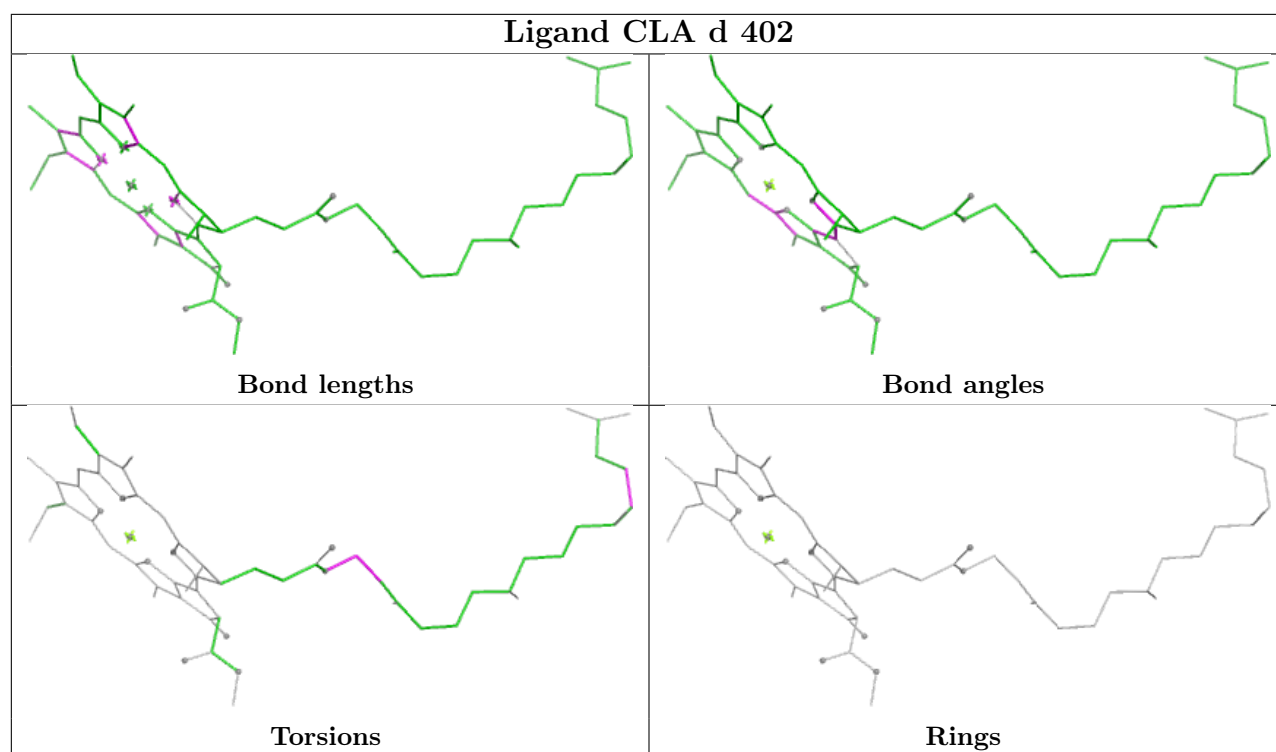


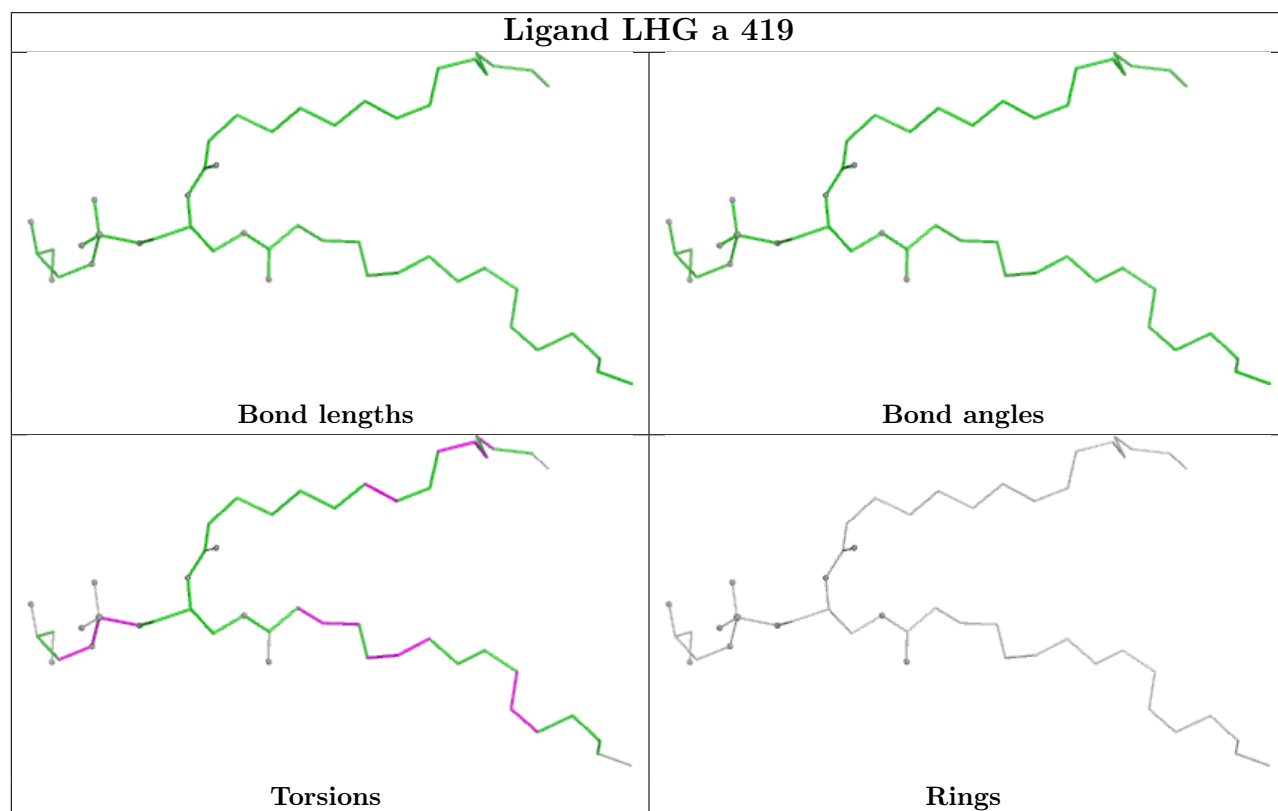
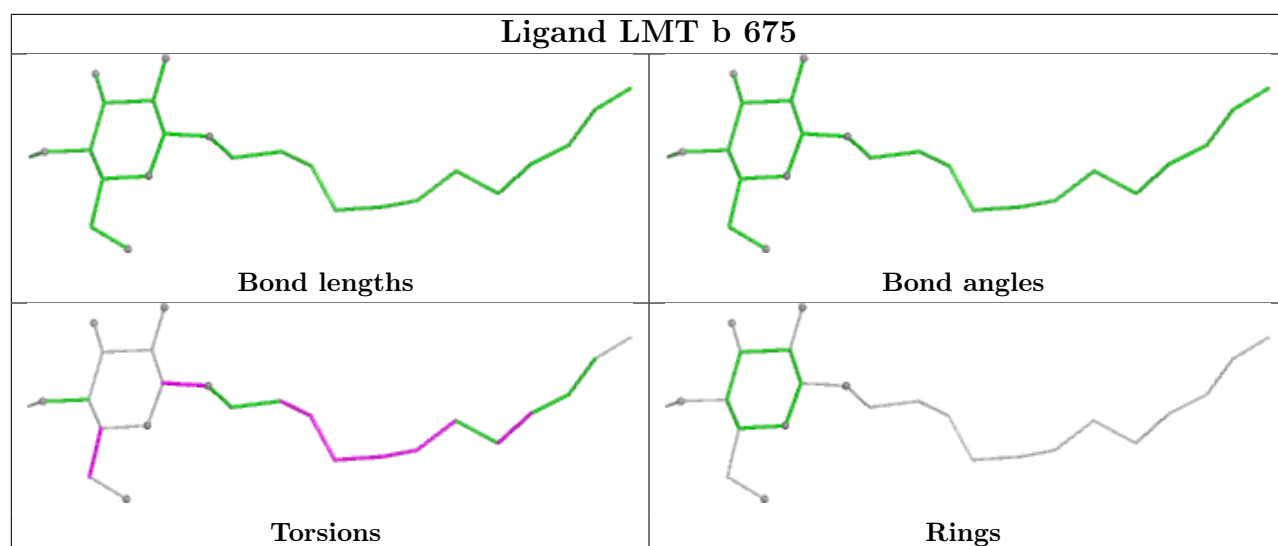


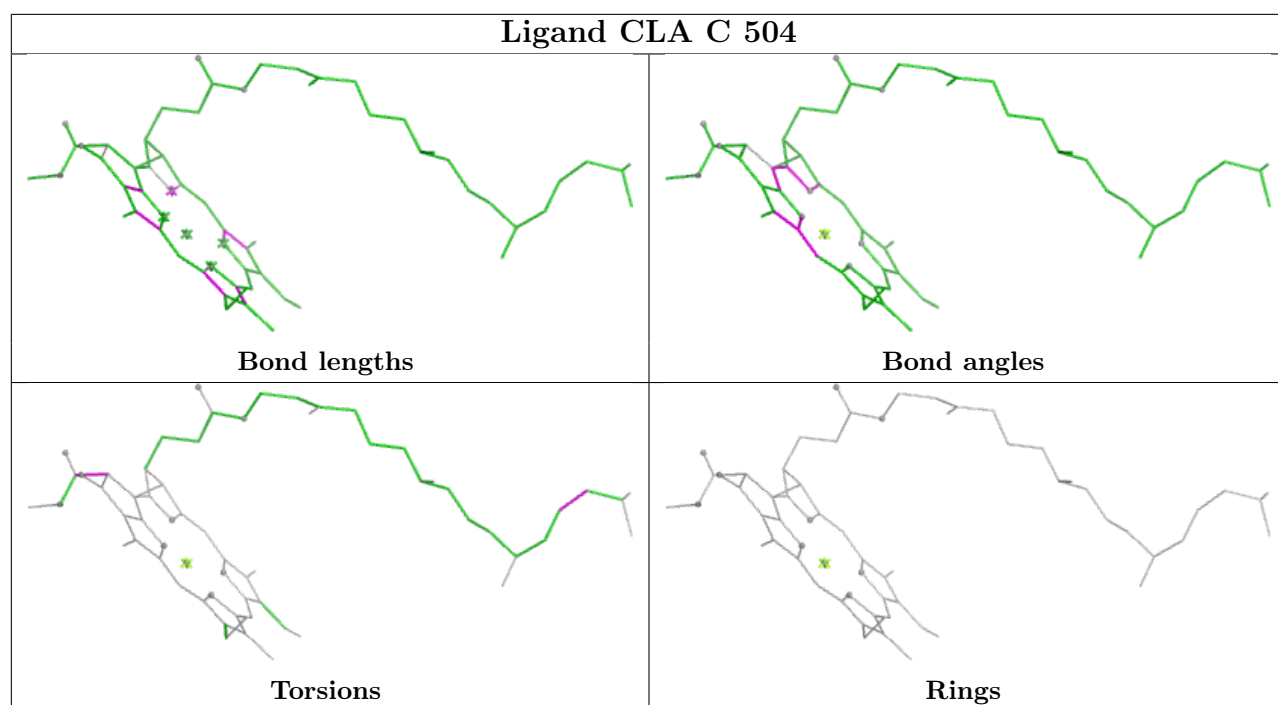




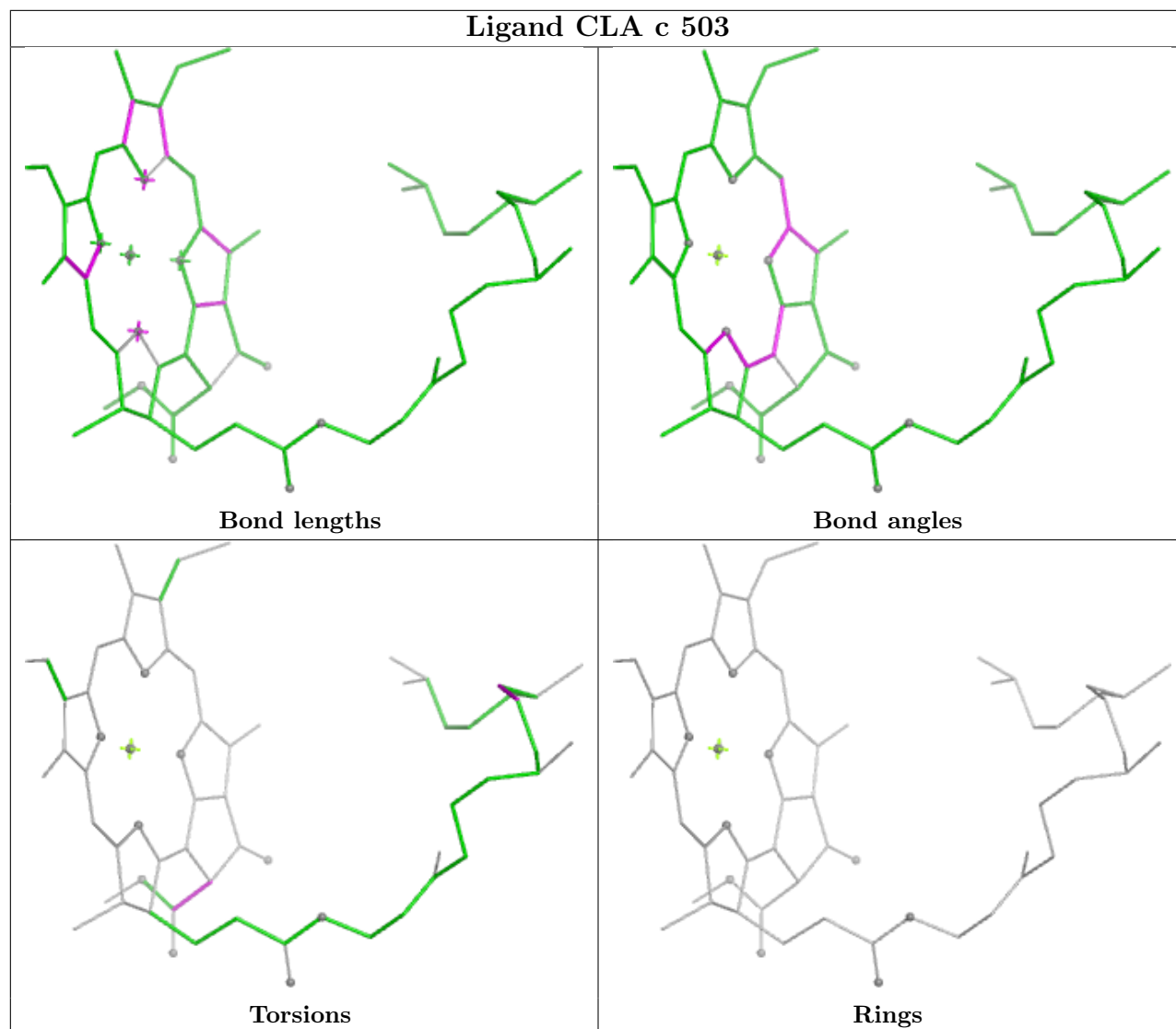




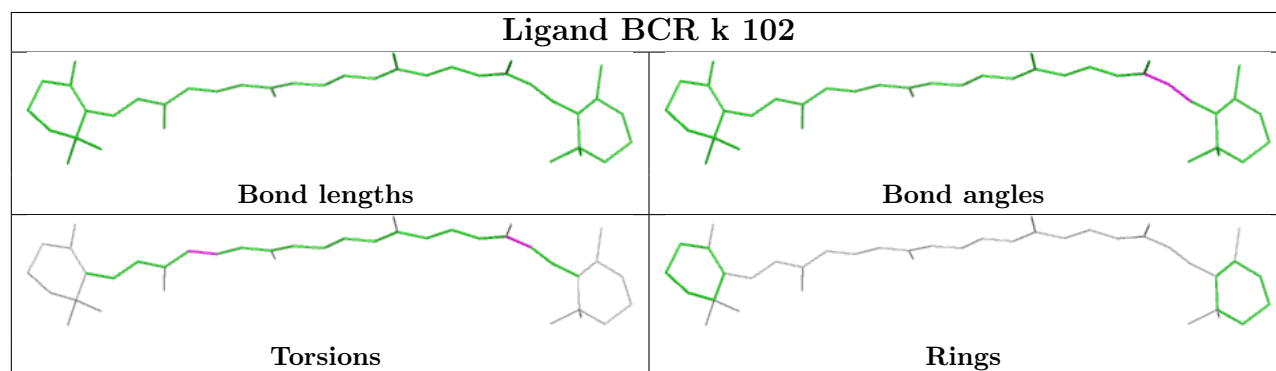


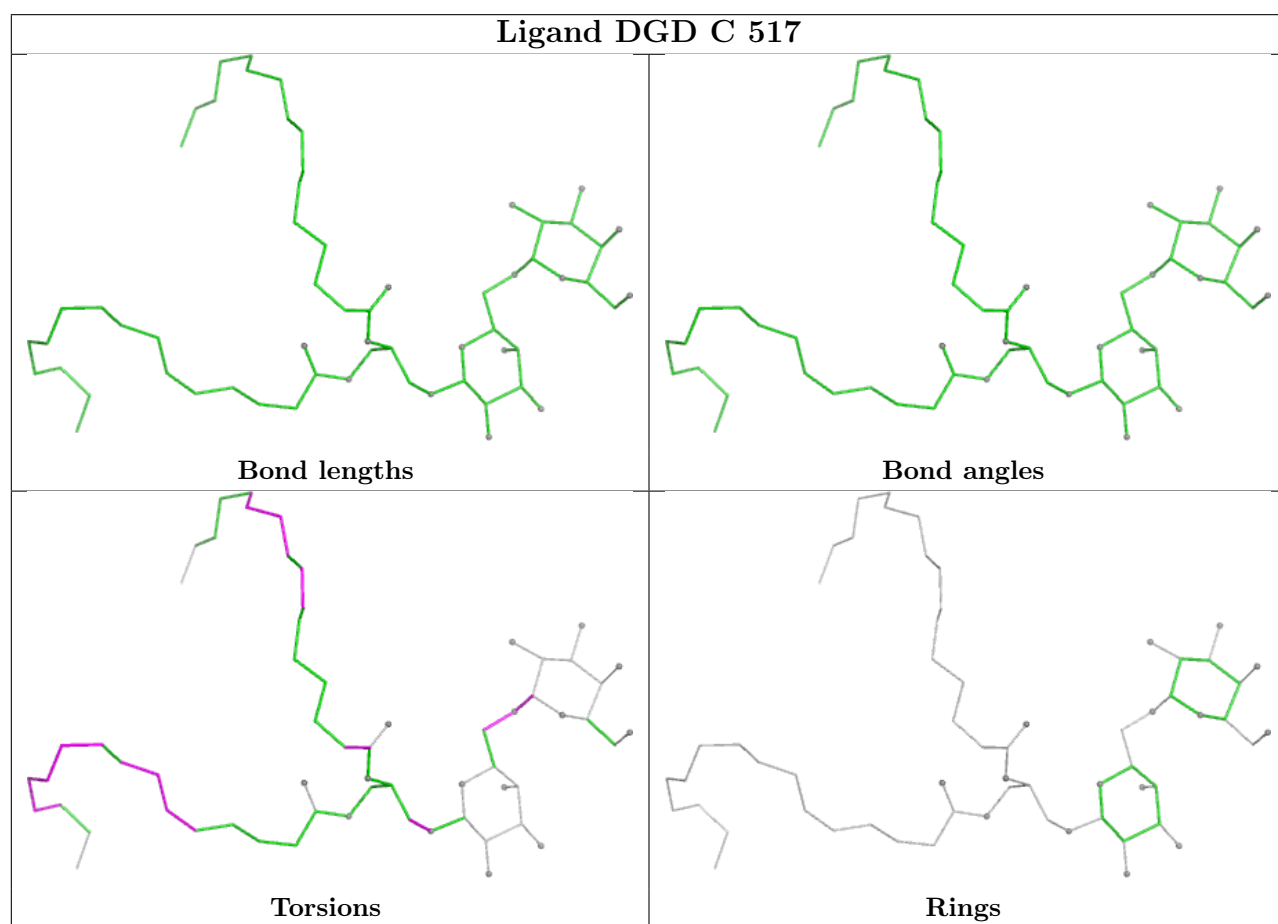
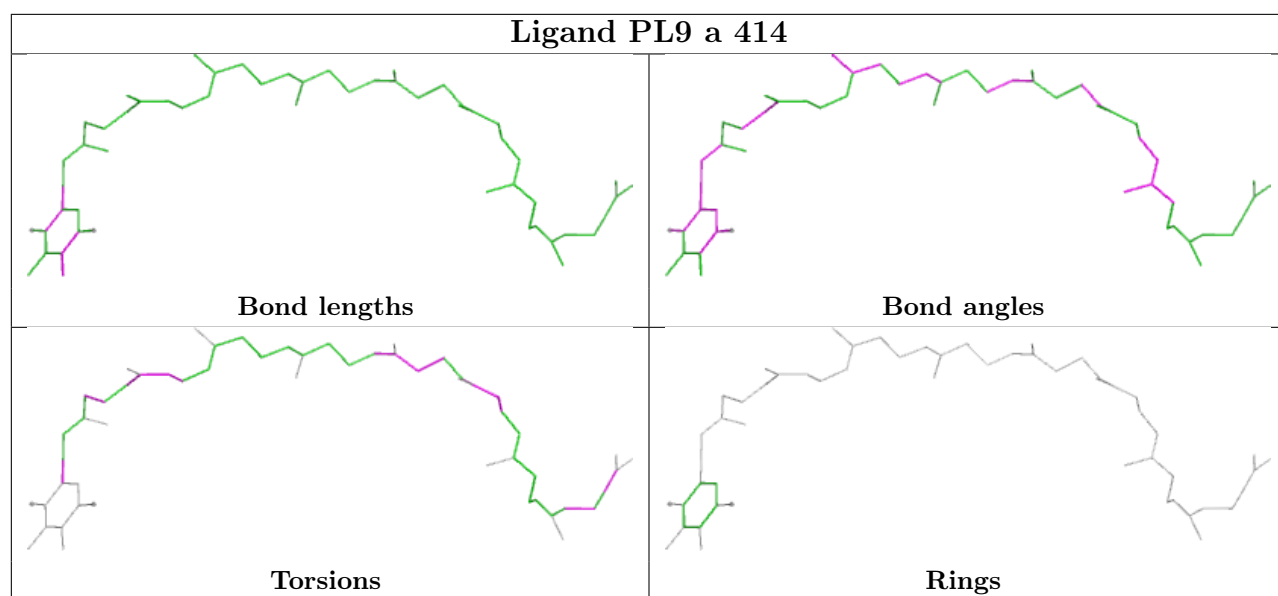


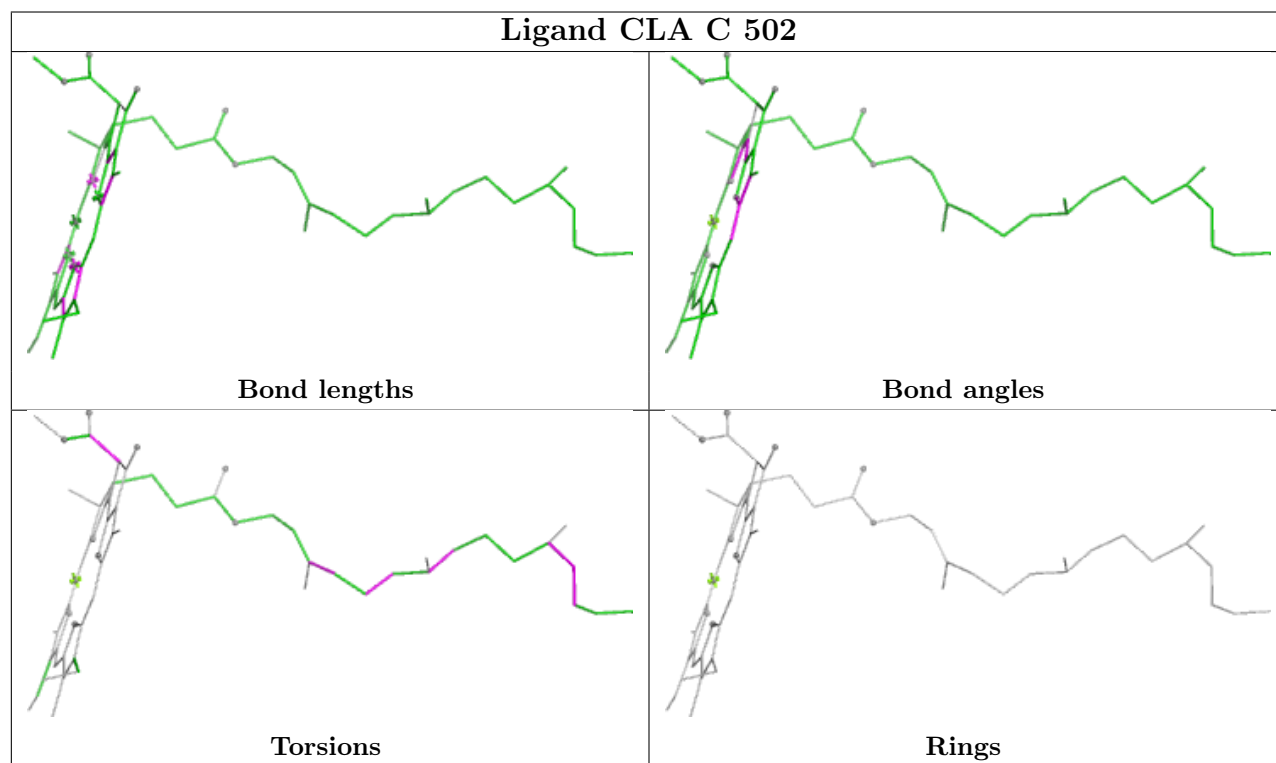
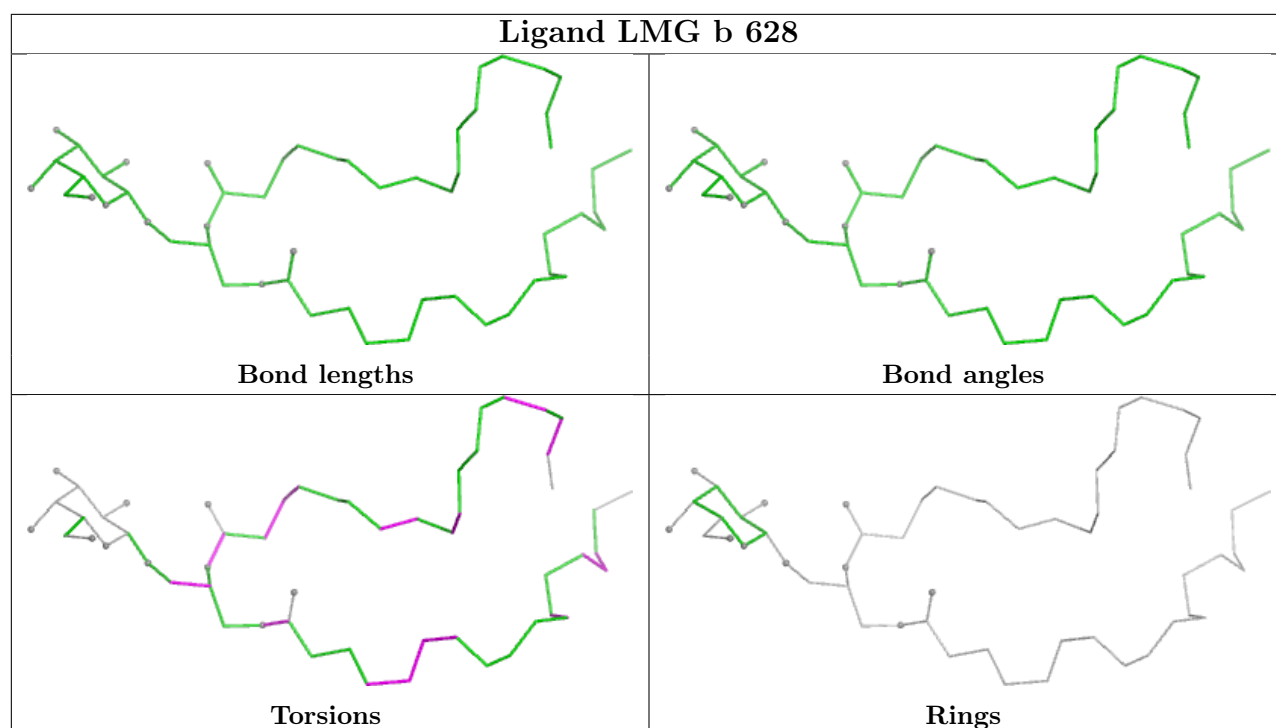
Ligand CLA c 503

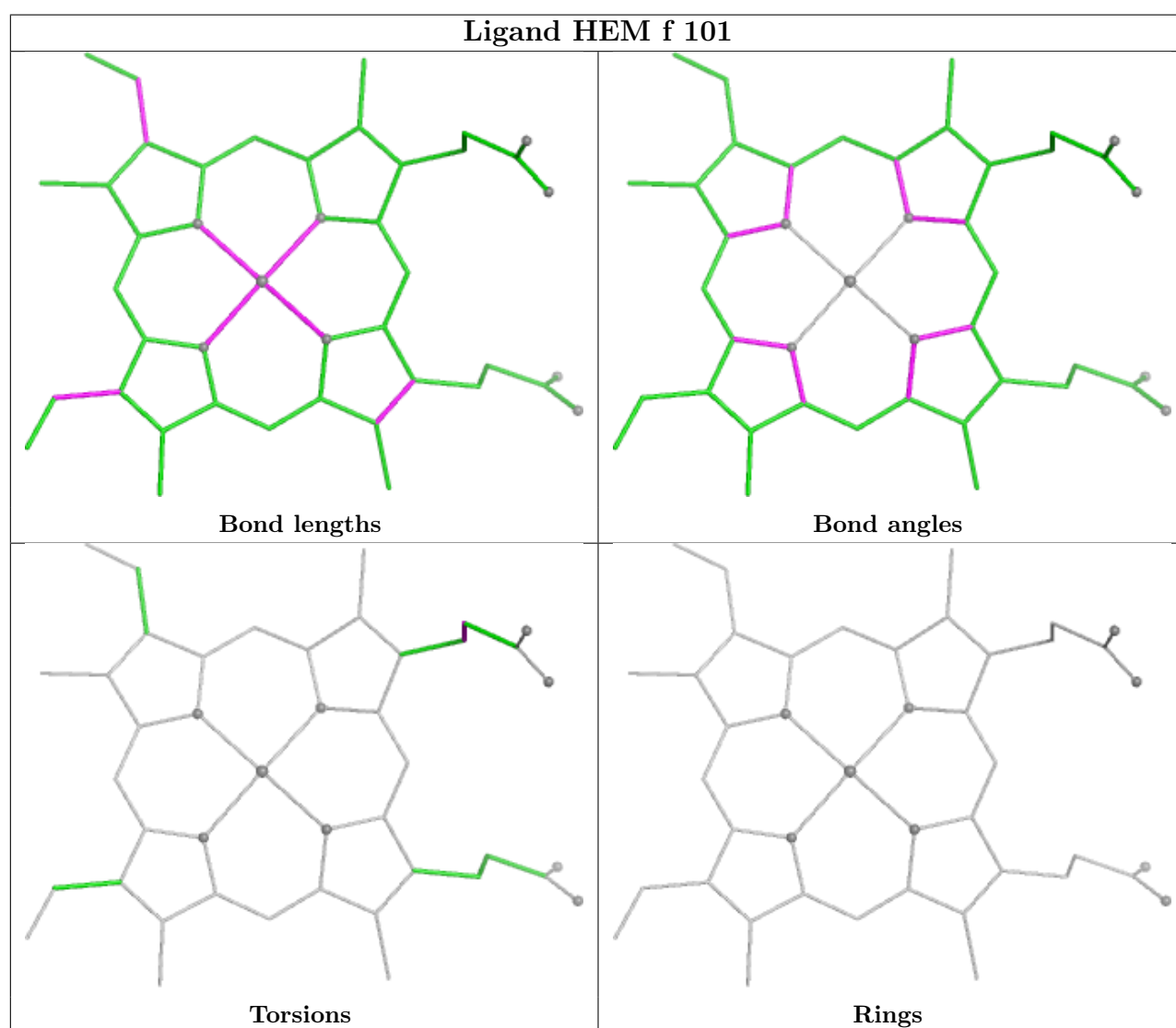
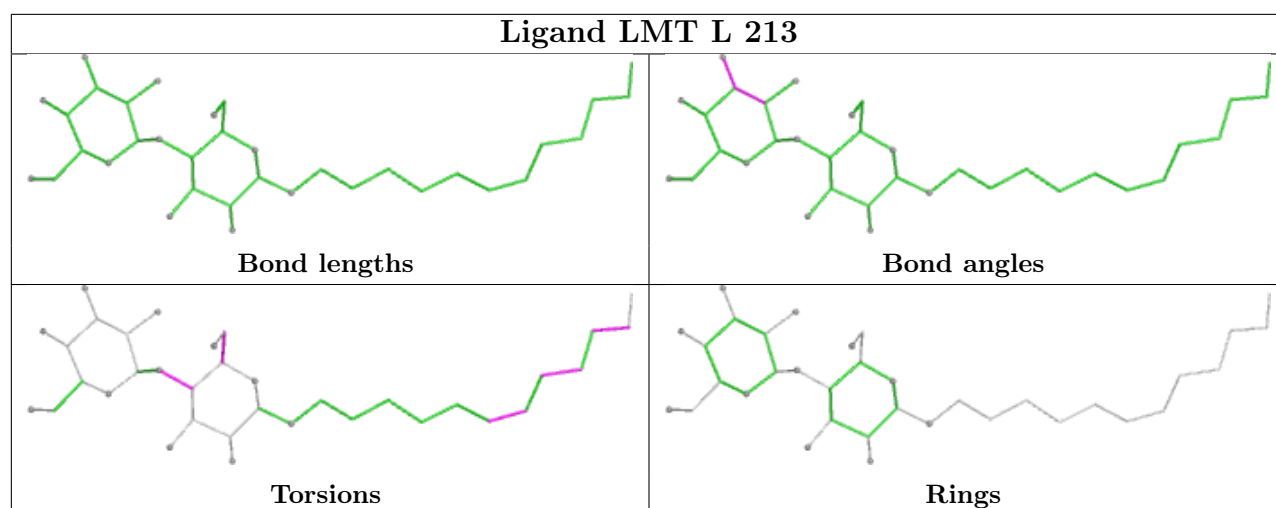


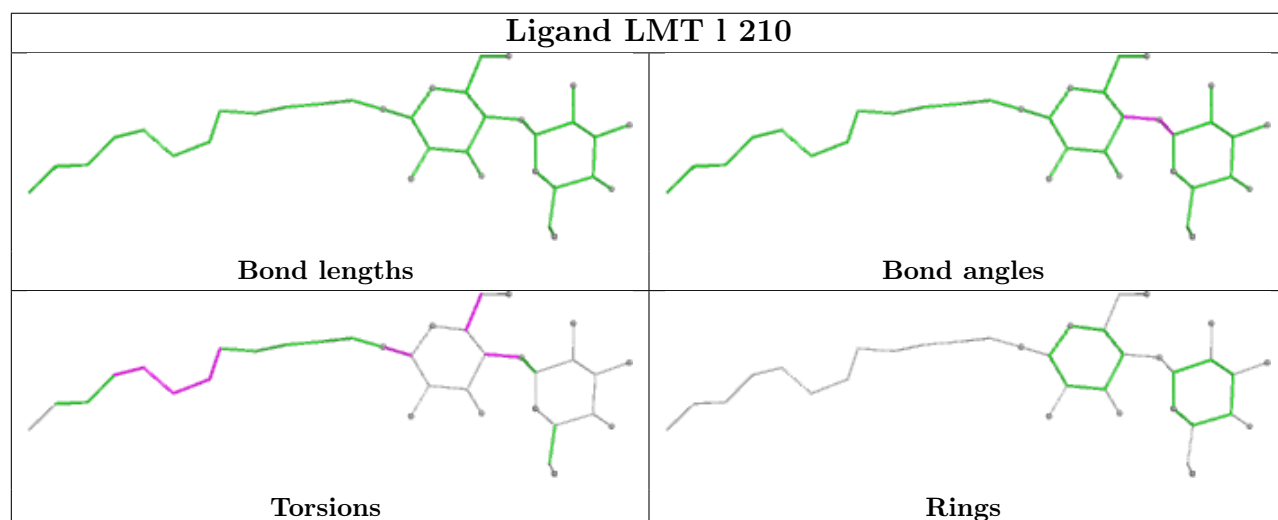
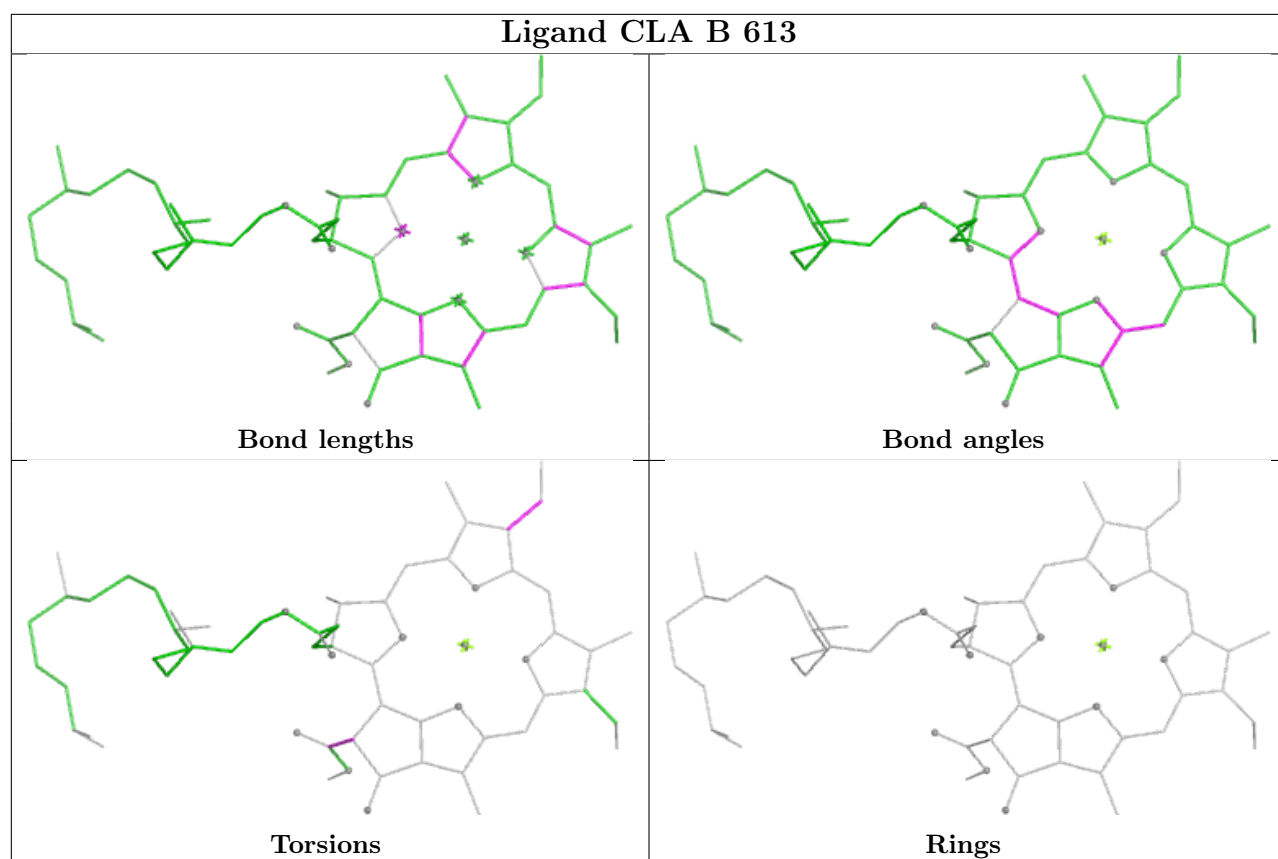
Ligand BCR k 102

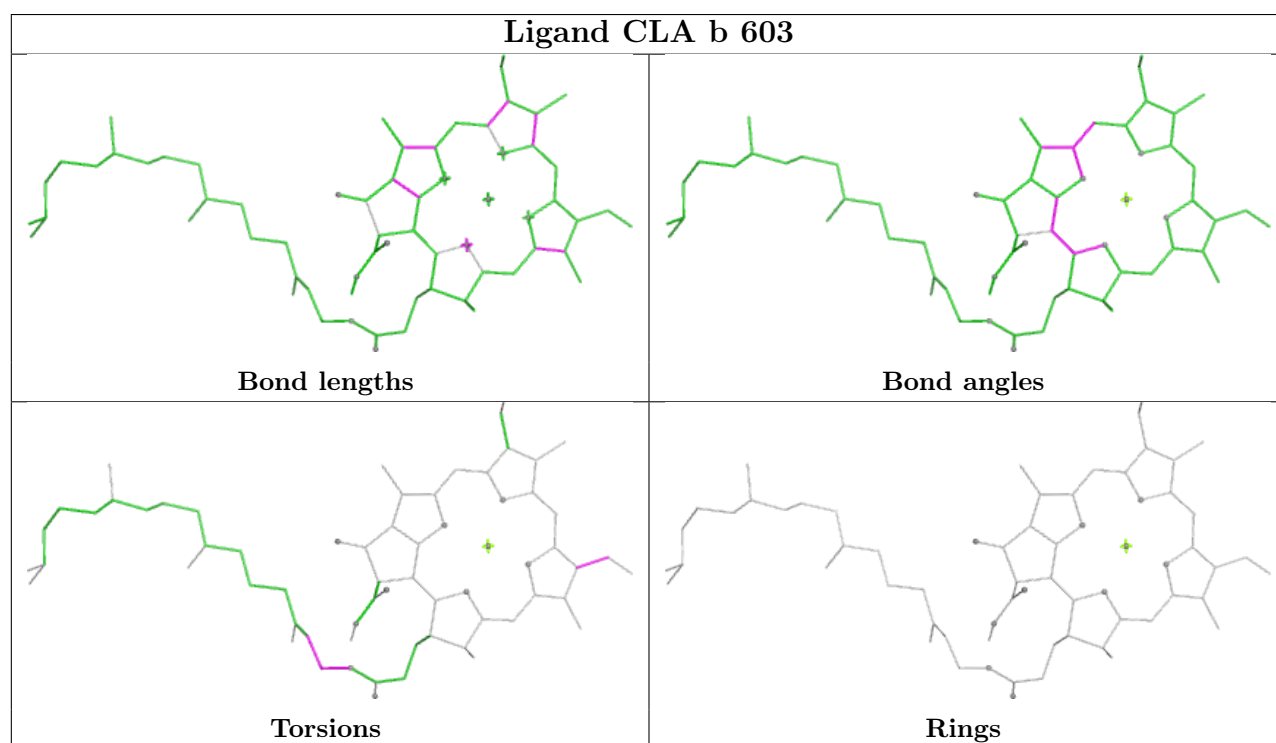
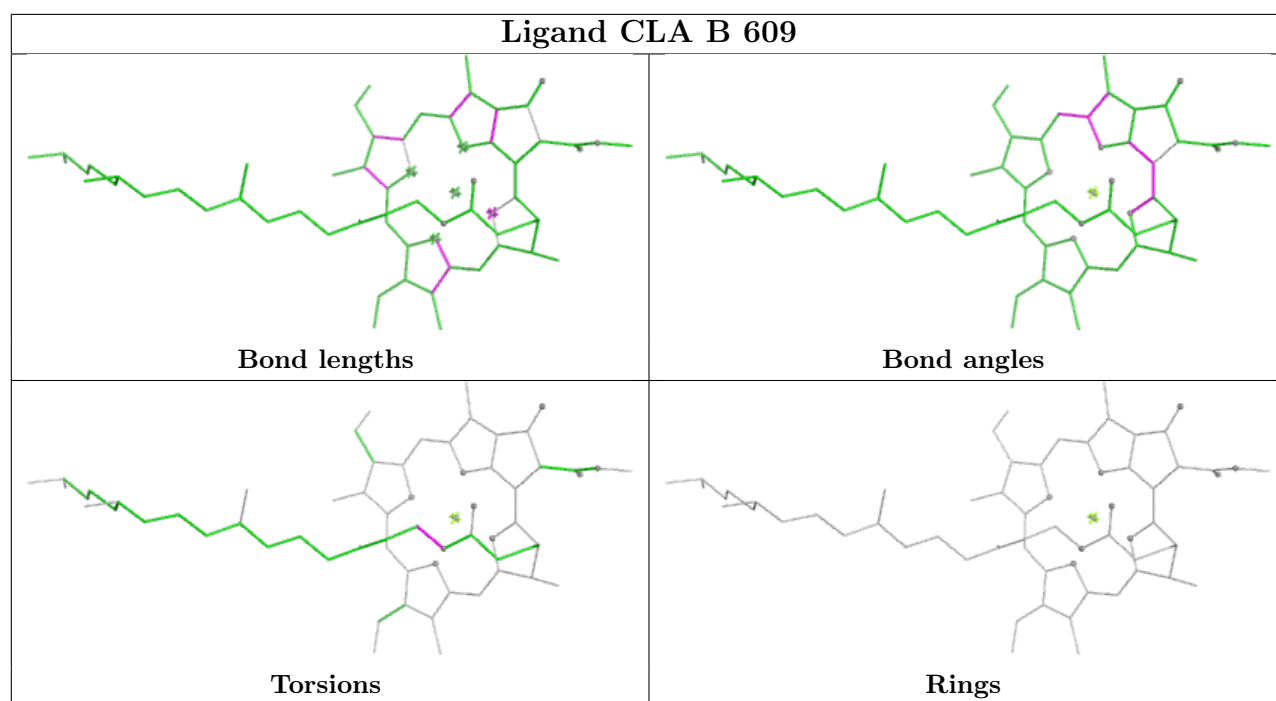


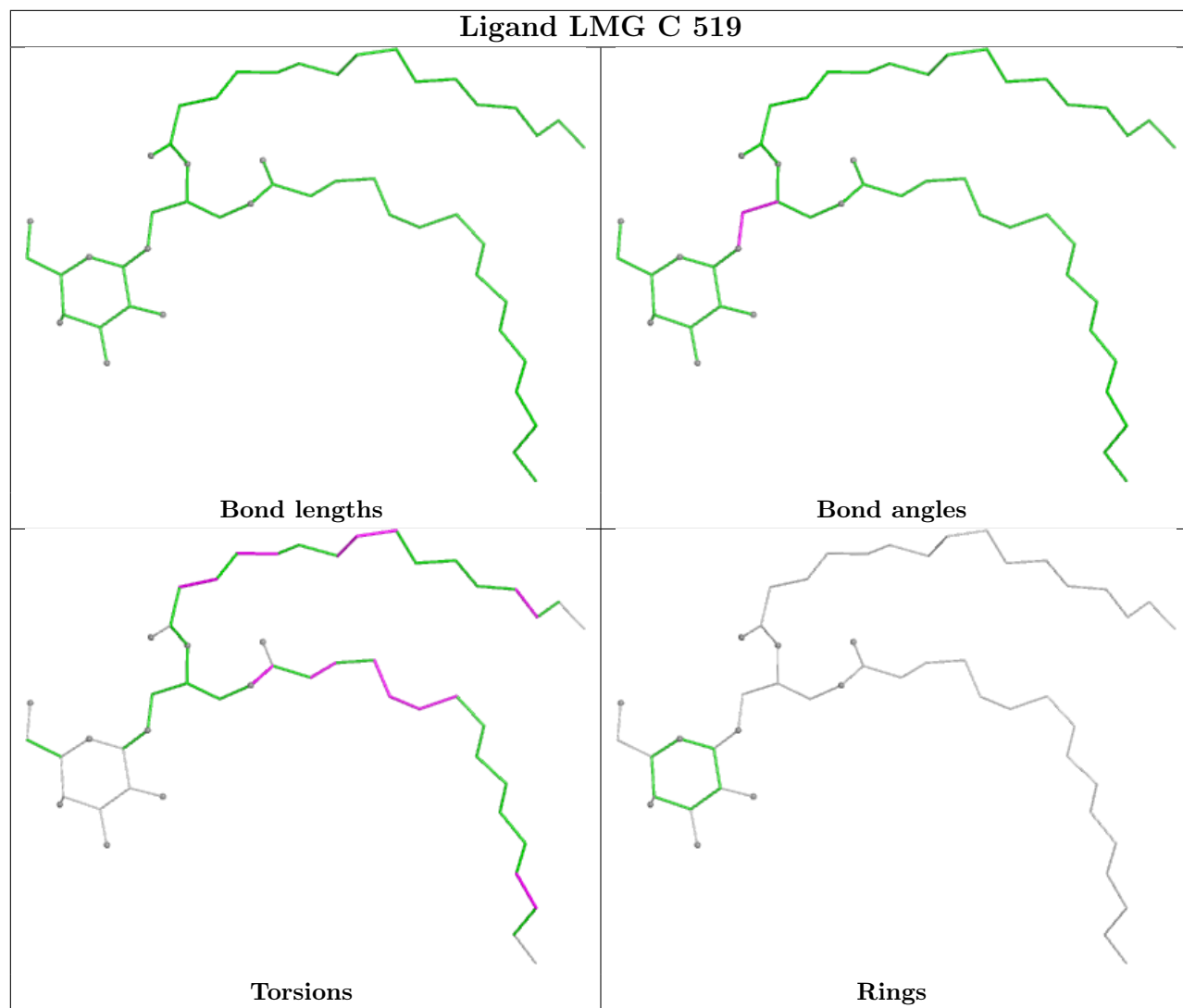


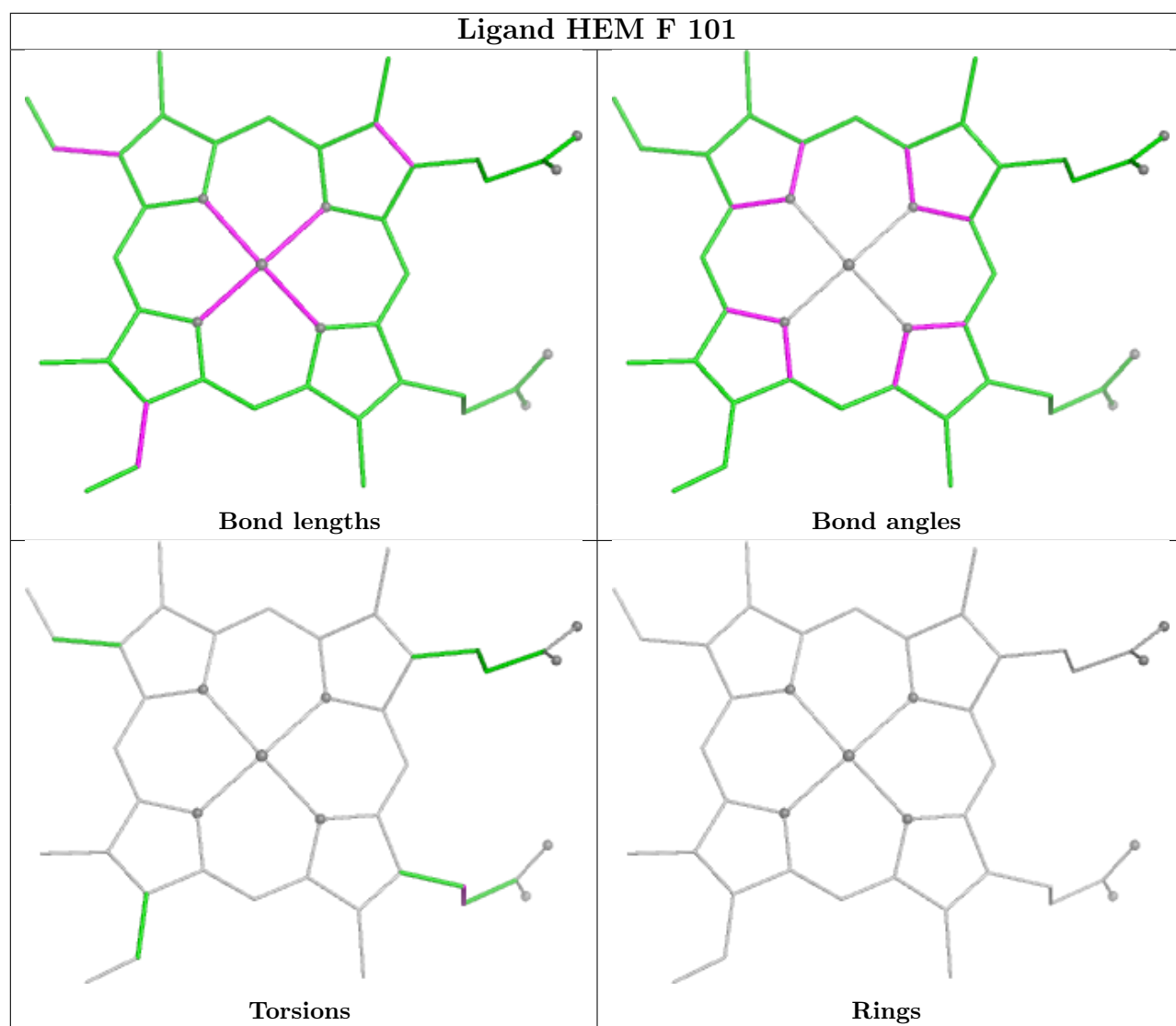


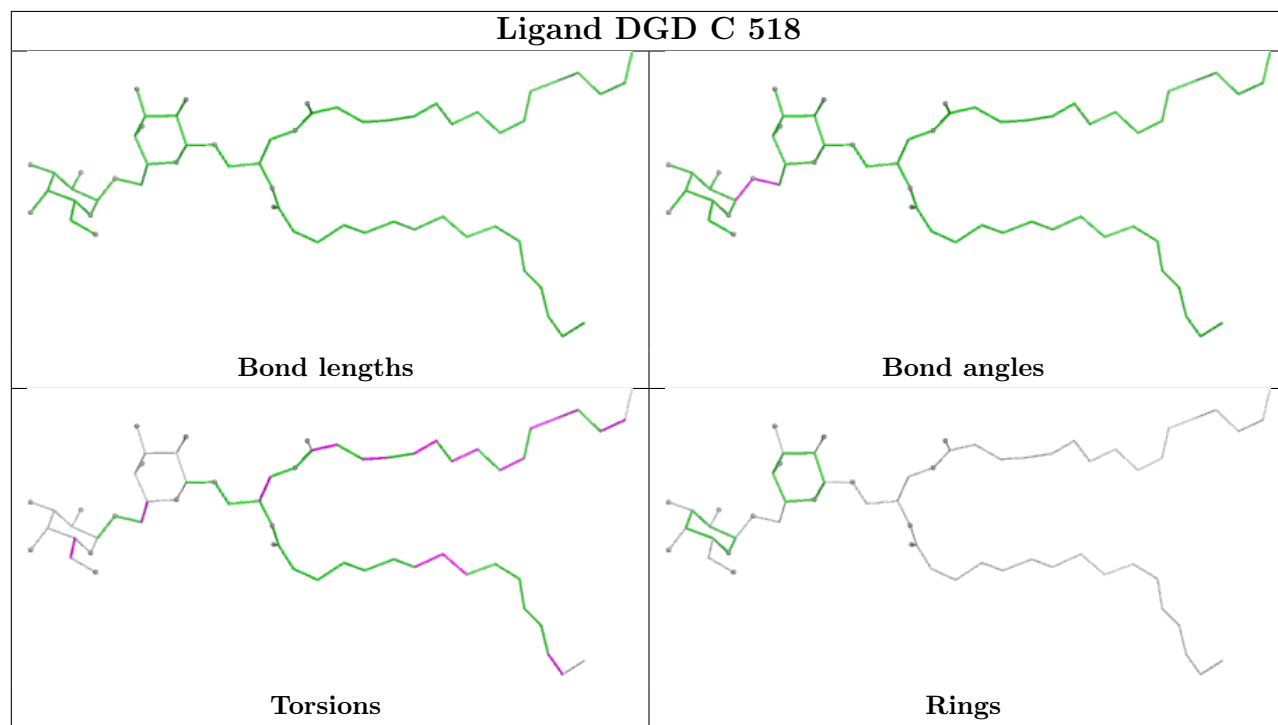
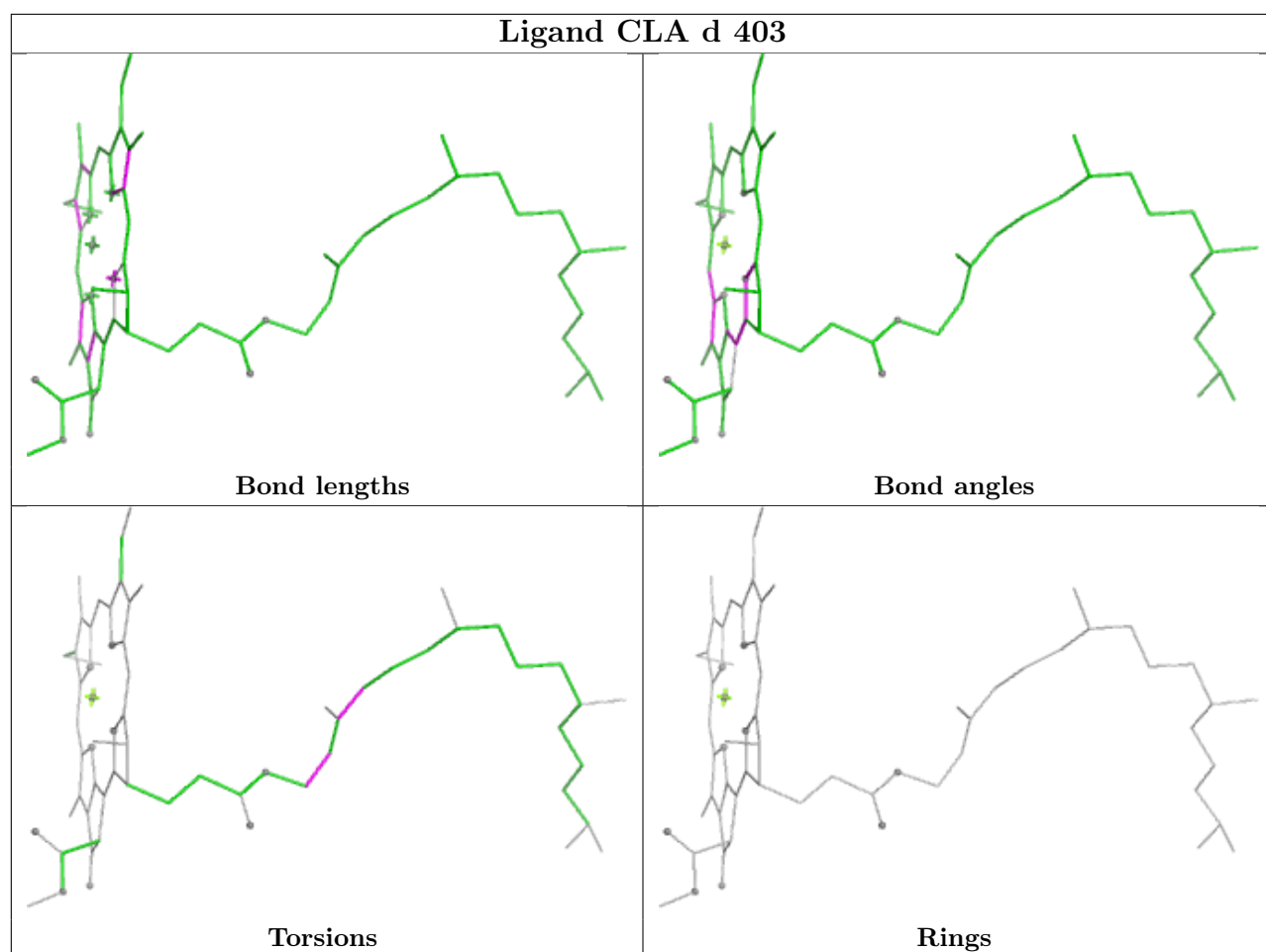


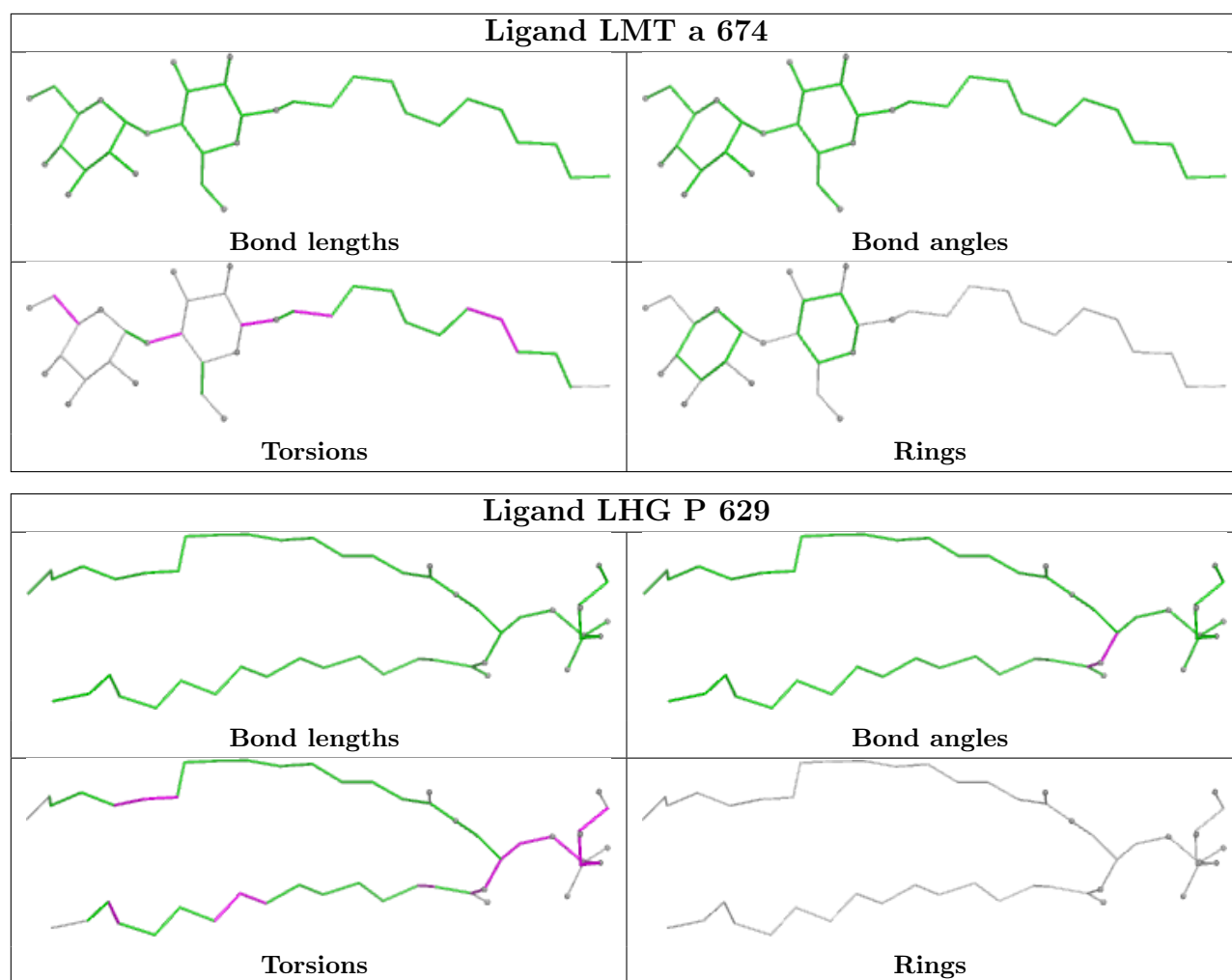


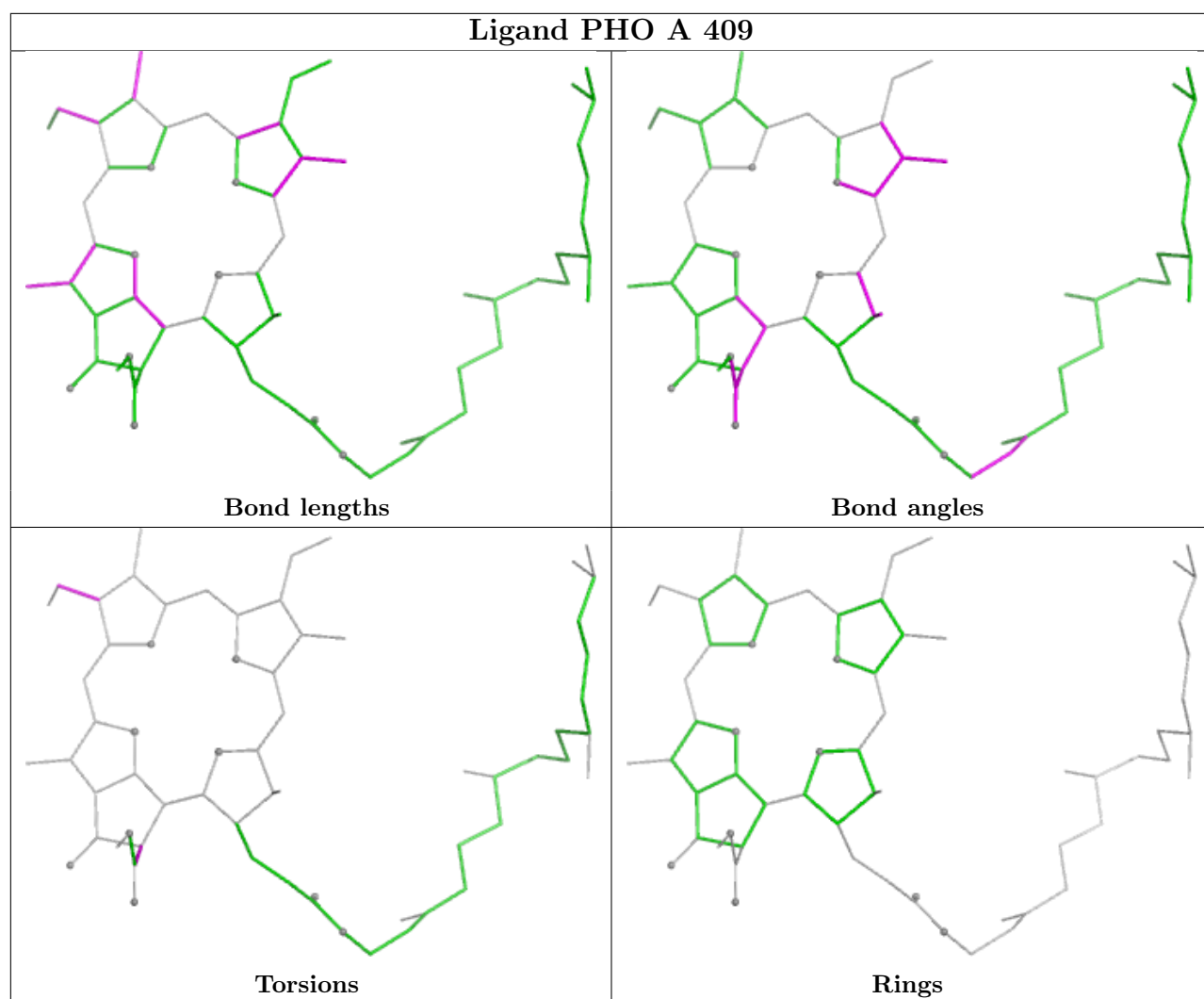


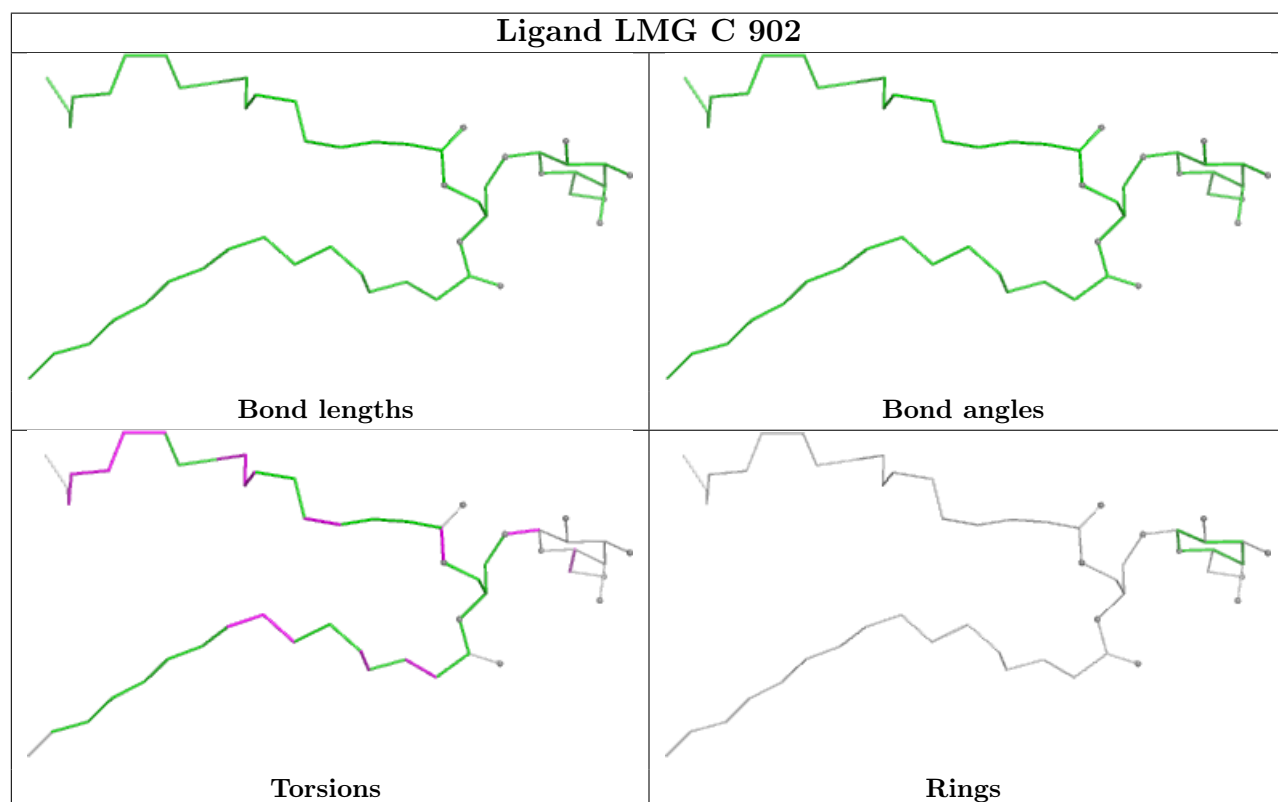
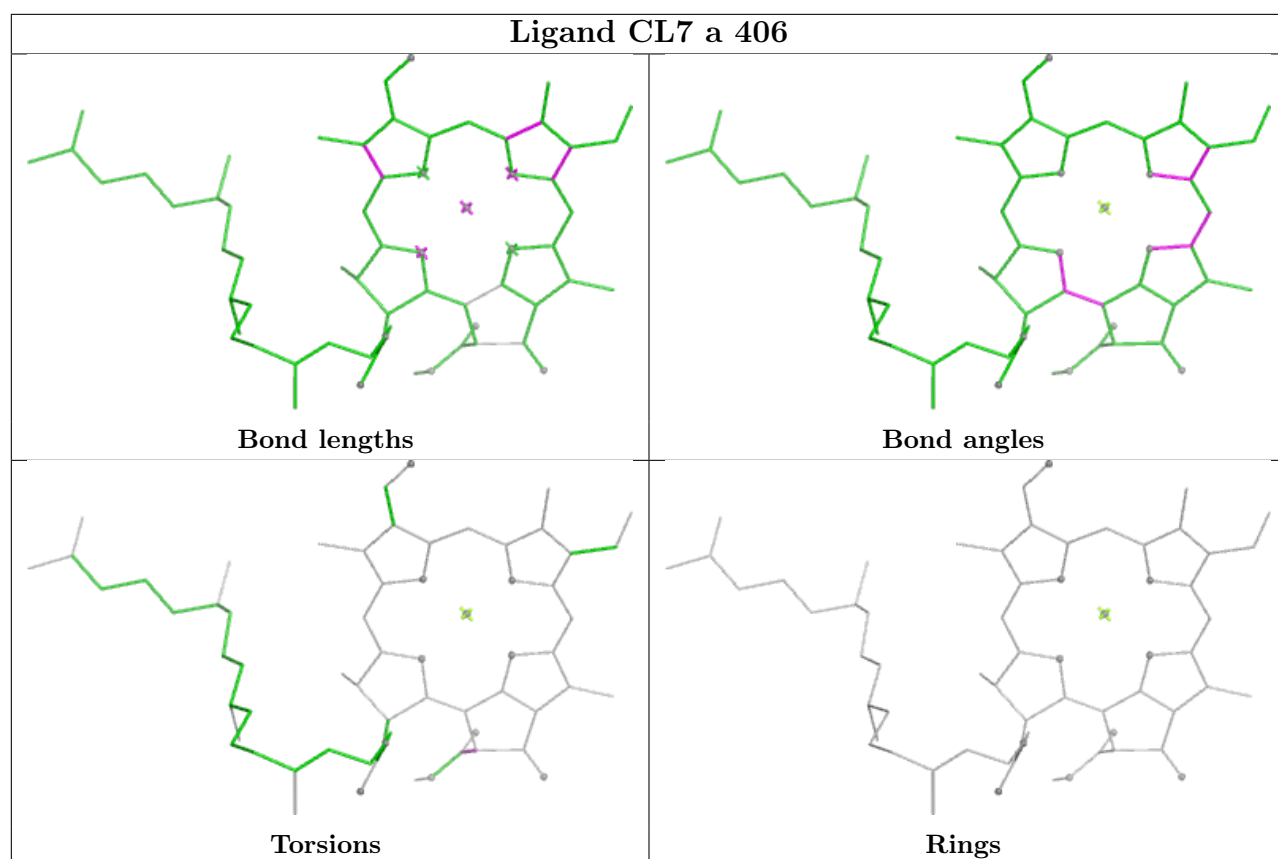


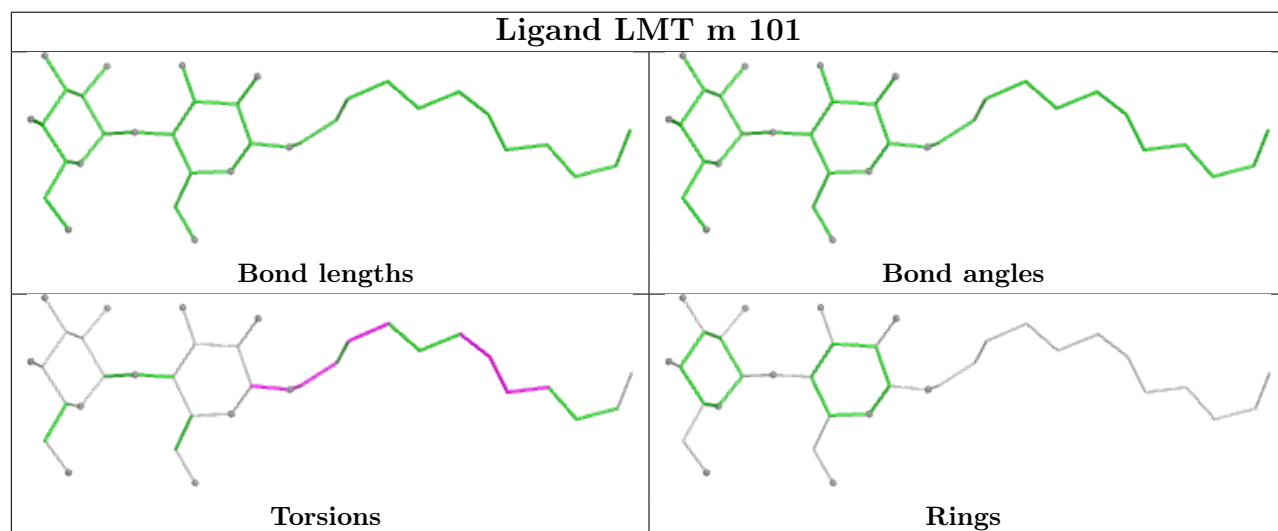
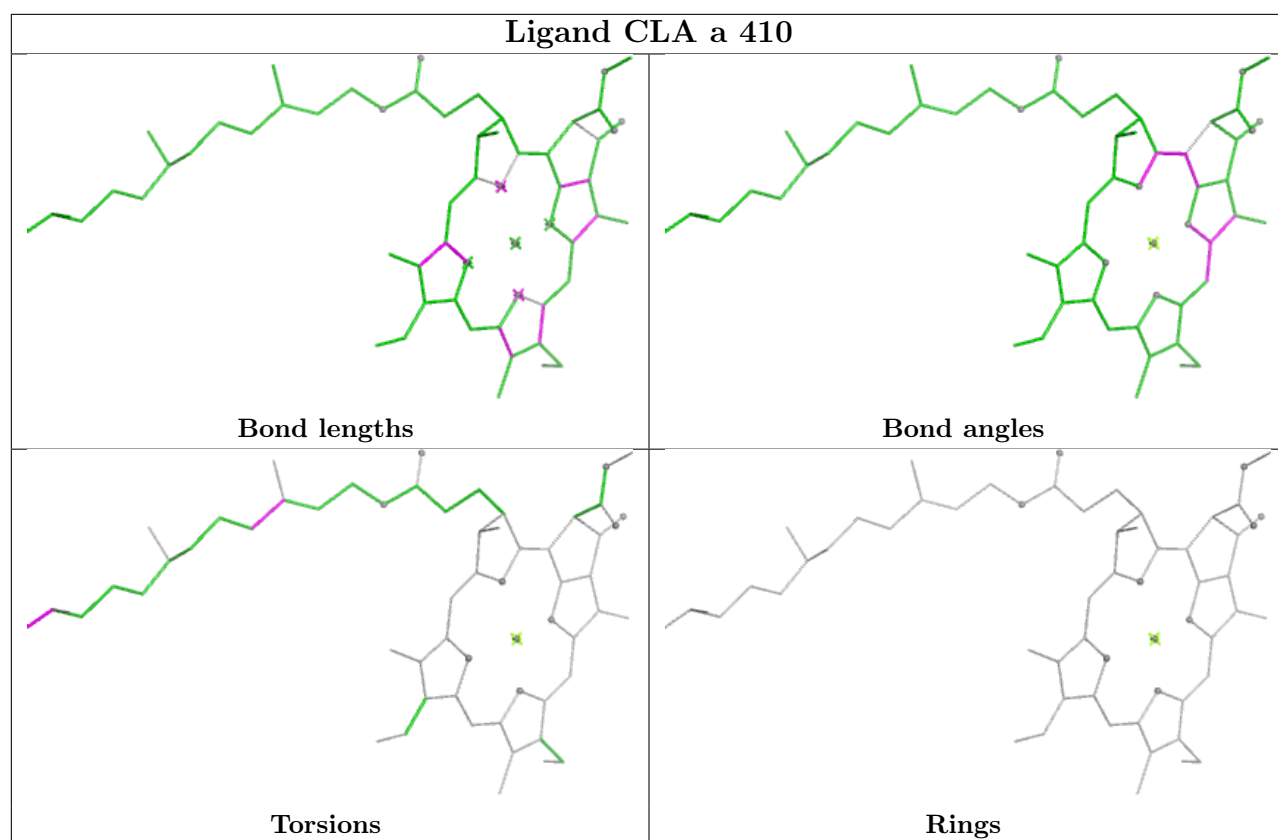


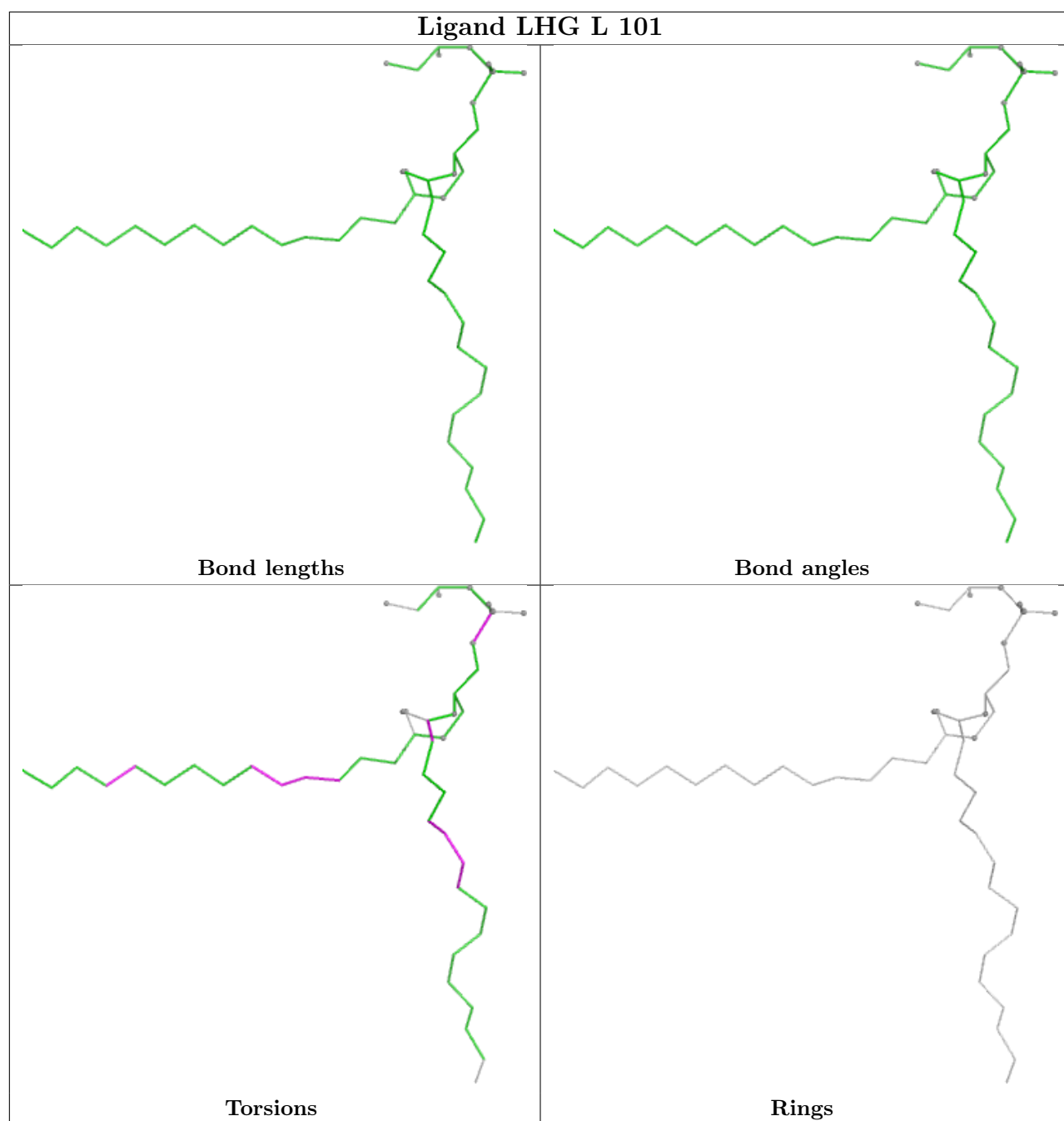




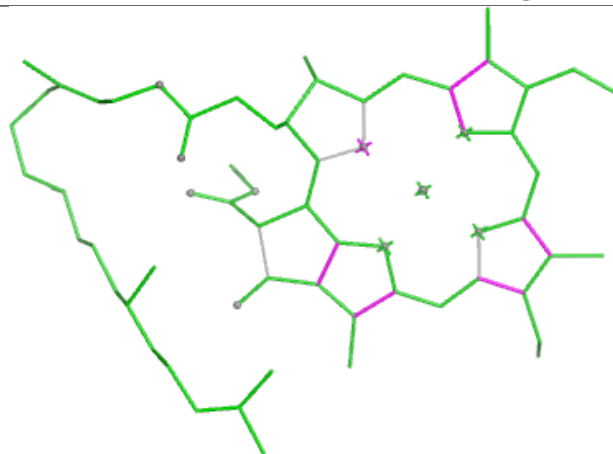




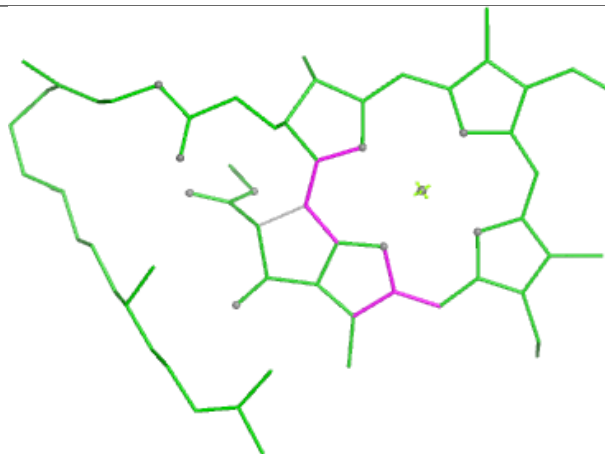




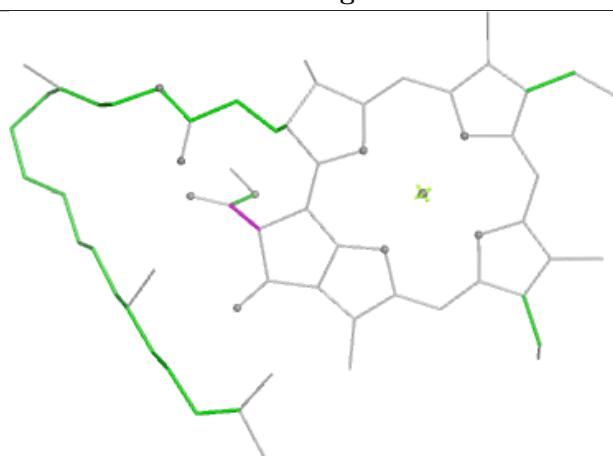
Ligand CLA b 611



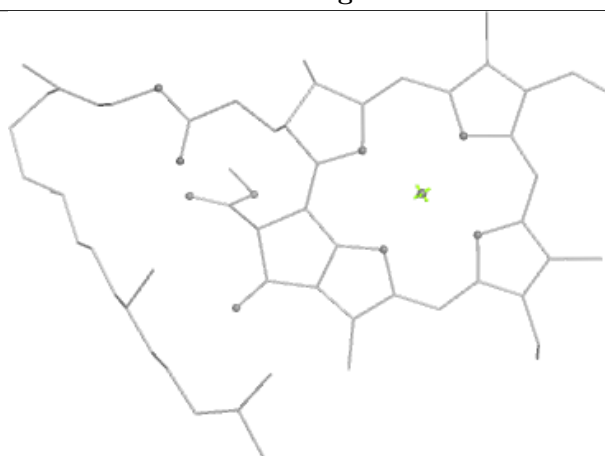
Bond lengths



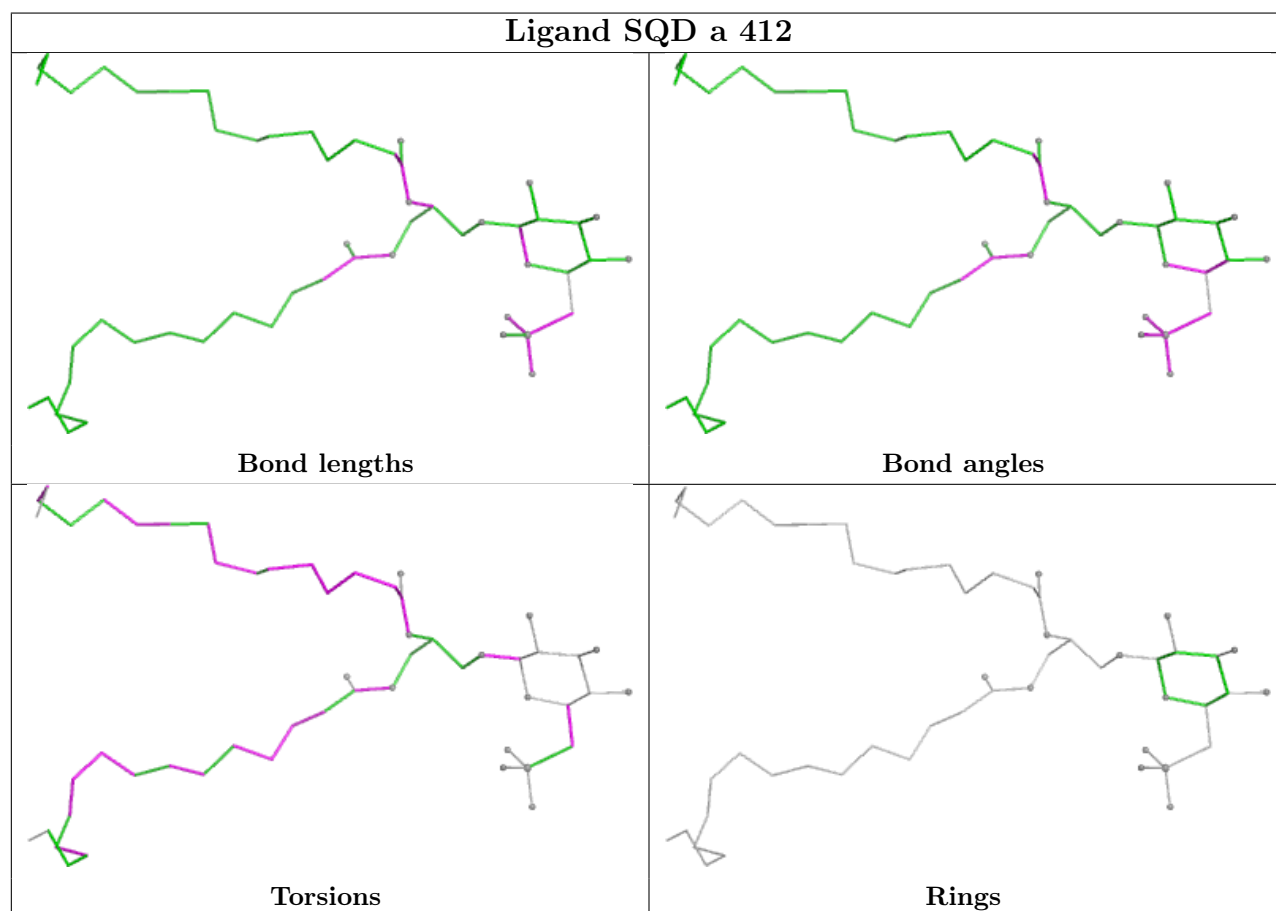
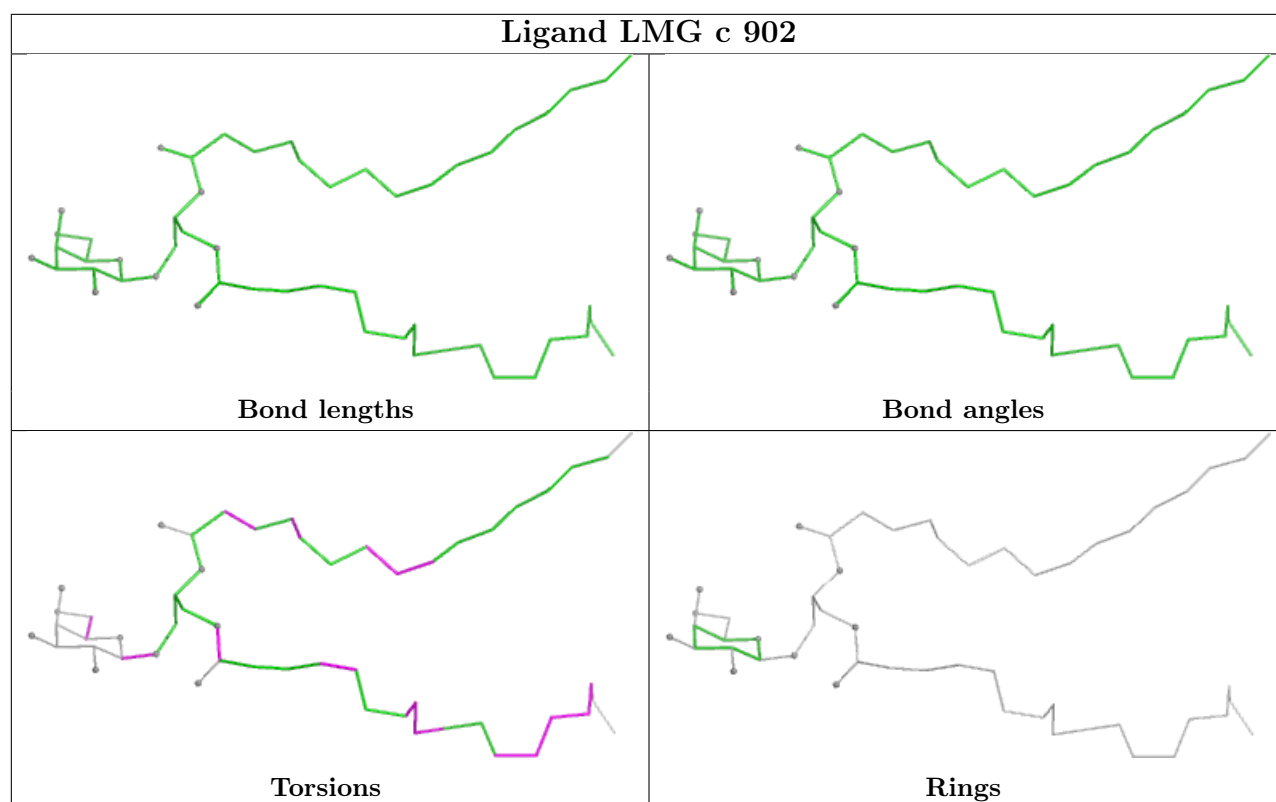
Bond angles

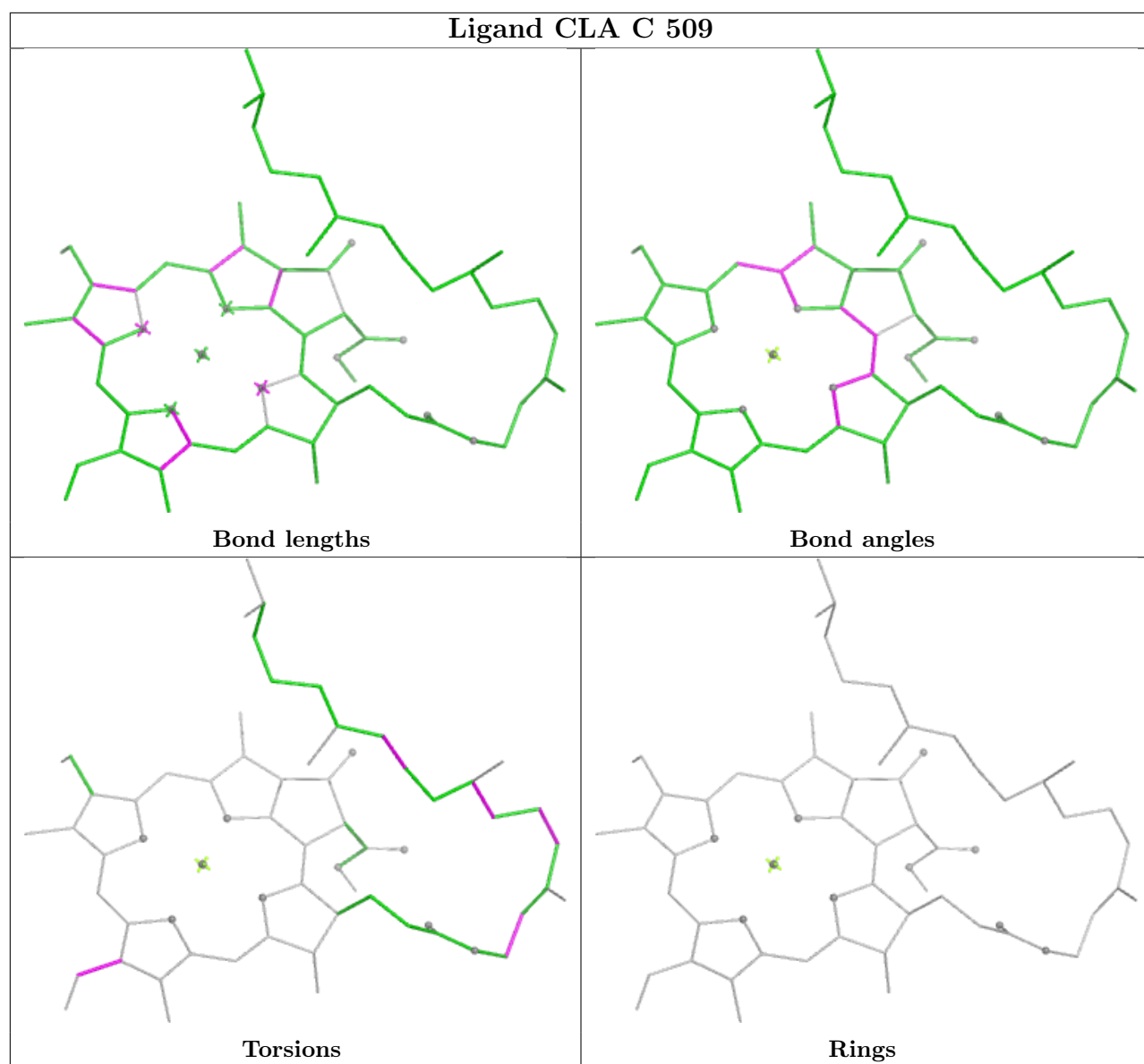


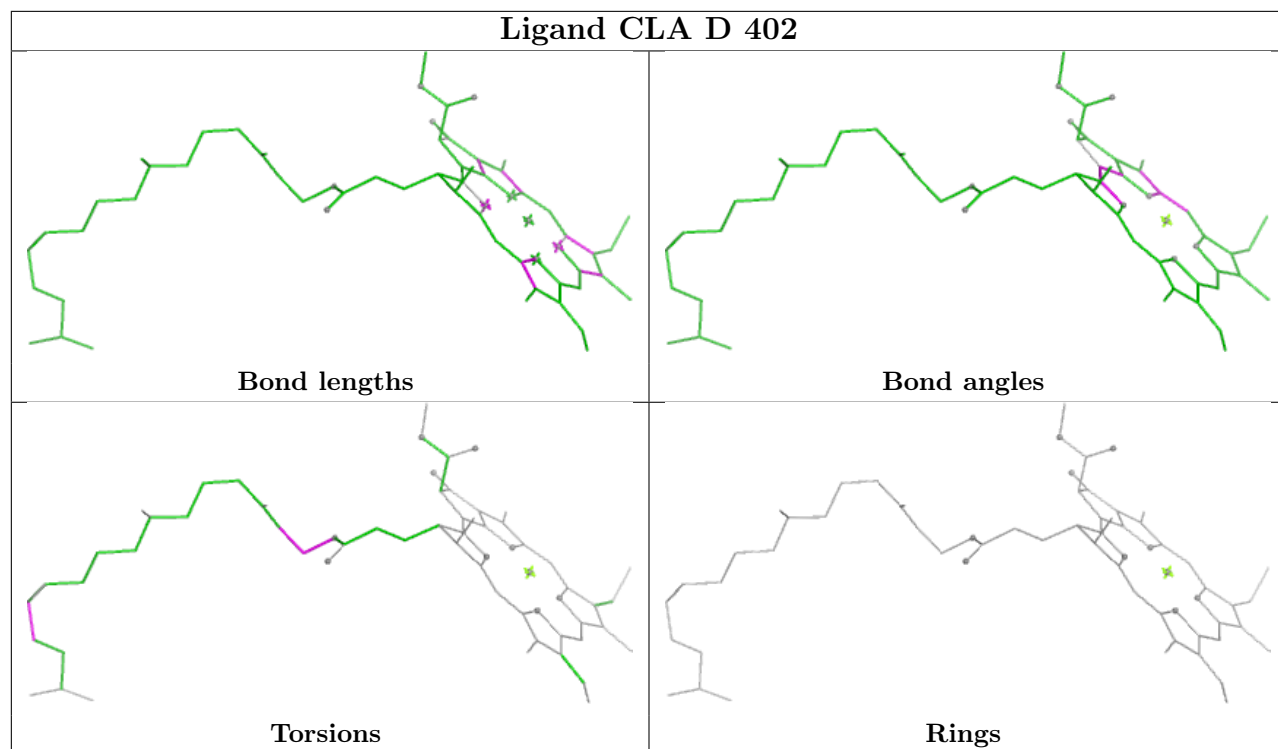
Torsions



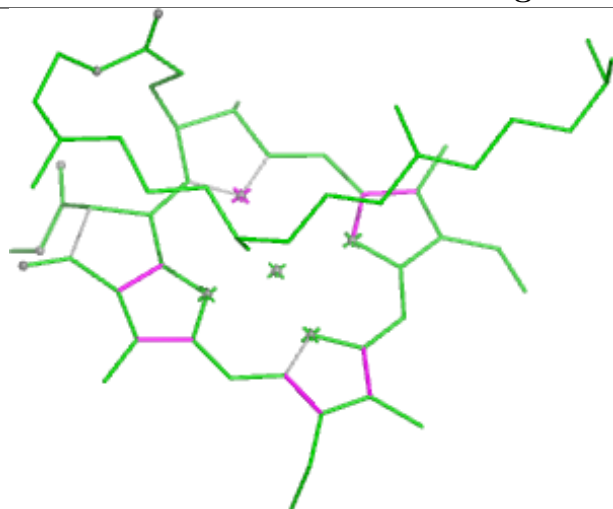
Rings



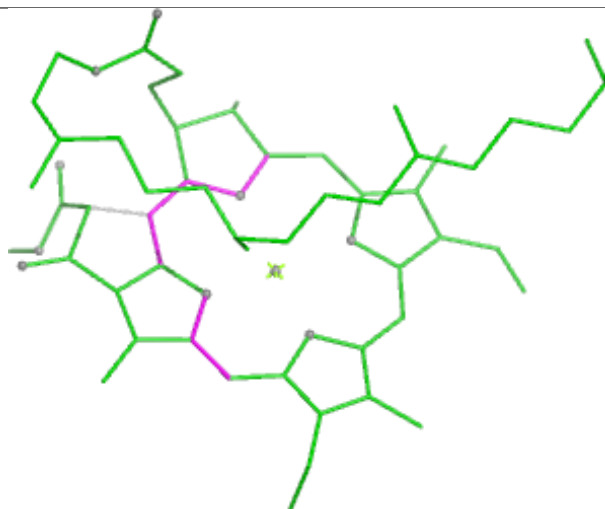




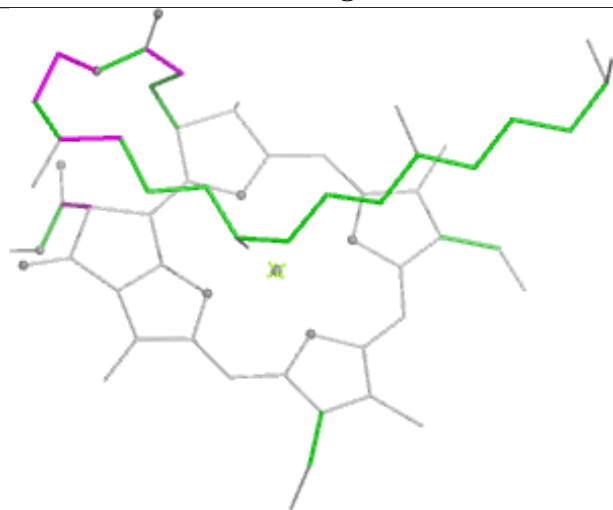
Ligand CLA B 602



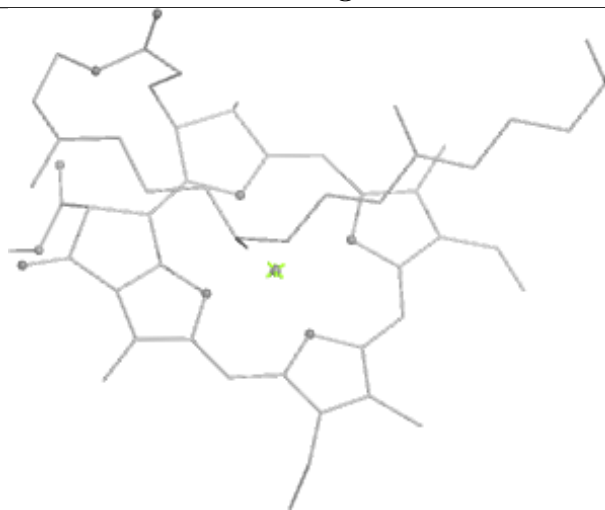
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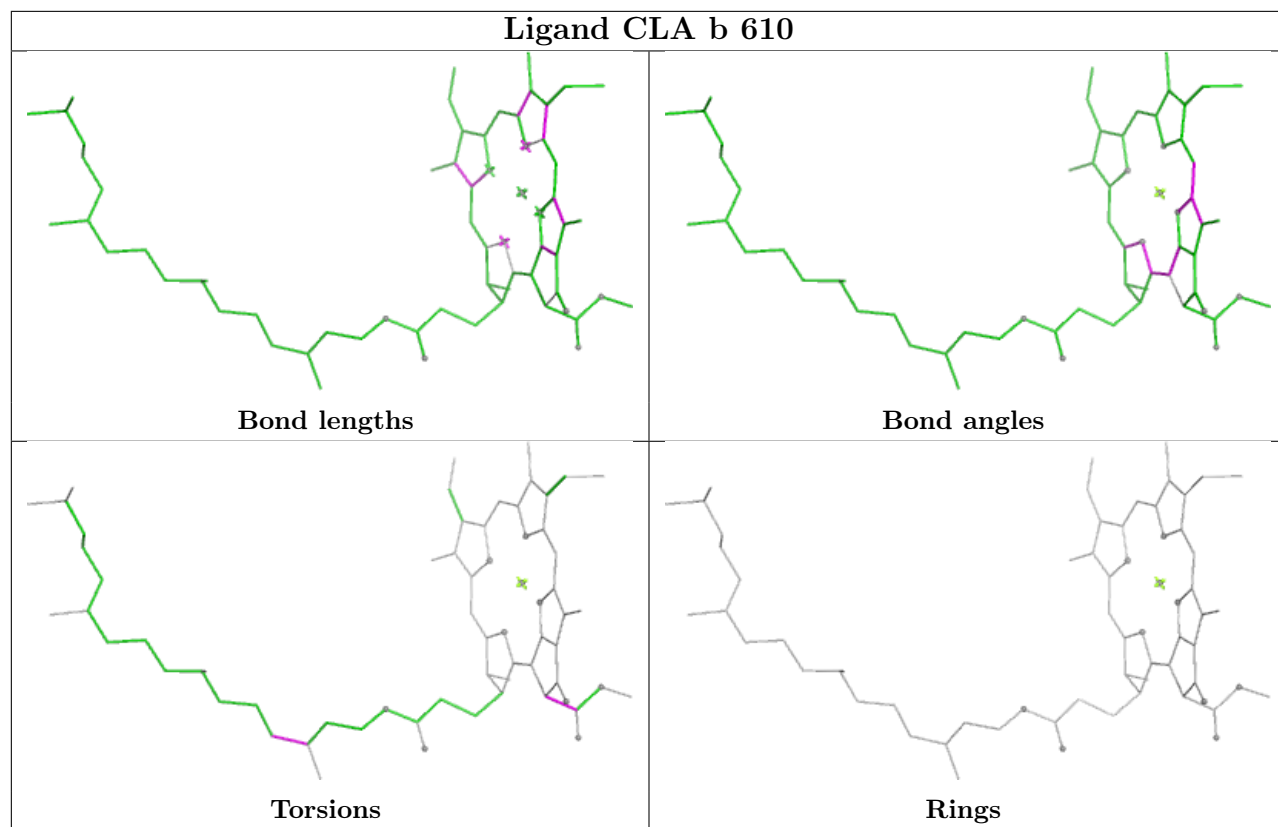
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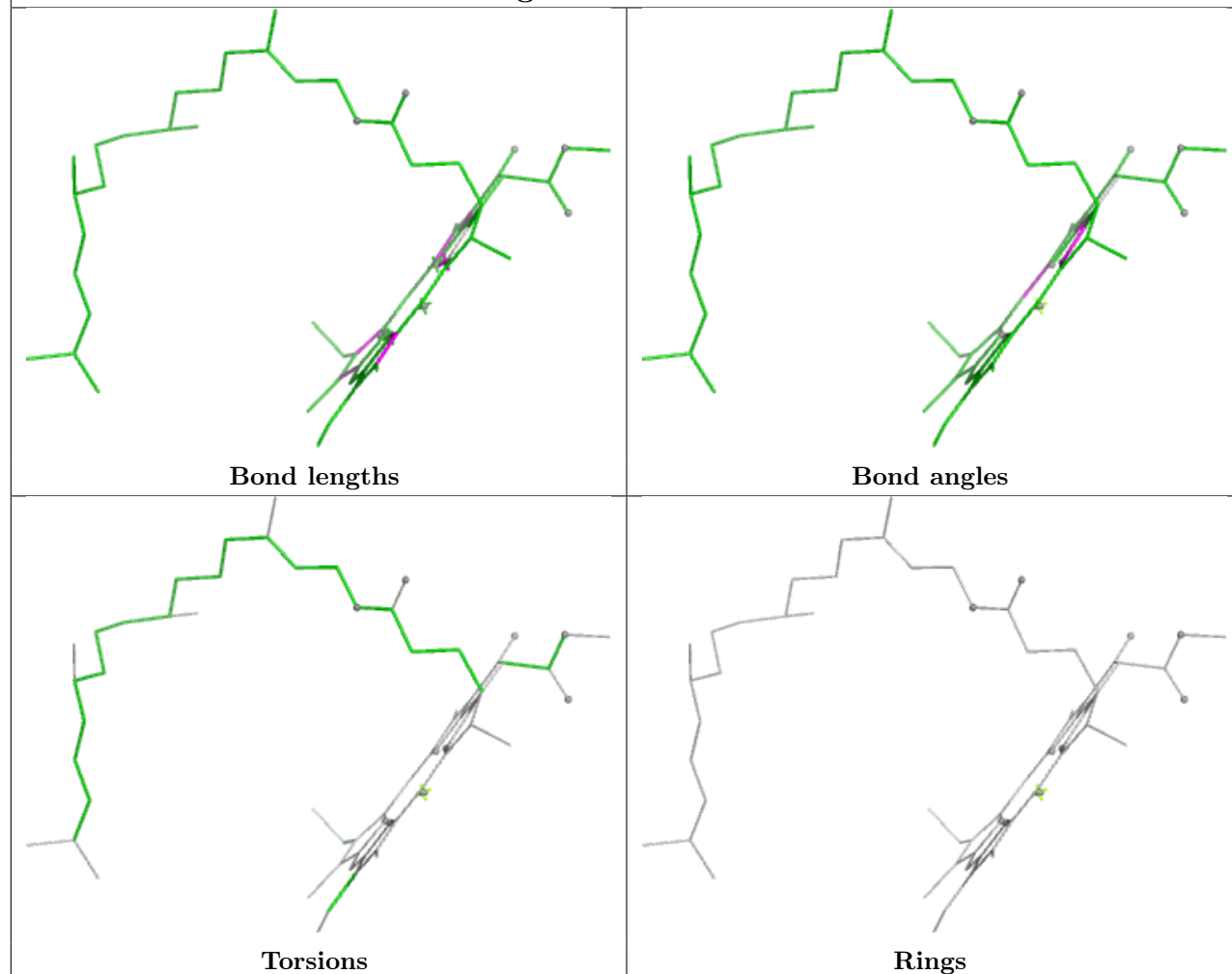
Torsions



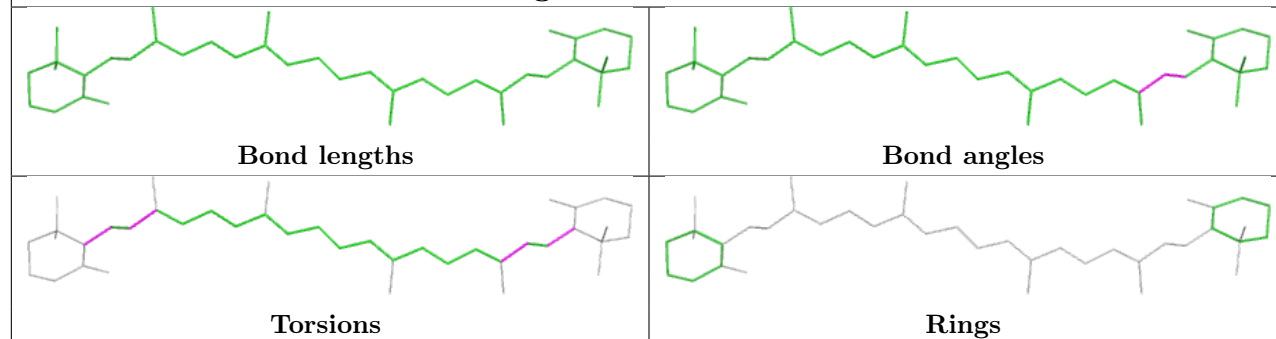
Rings



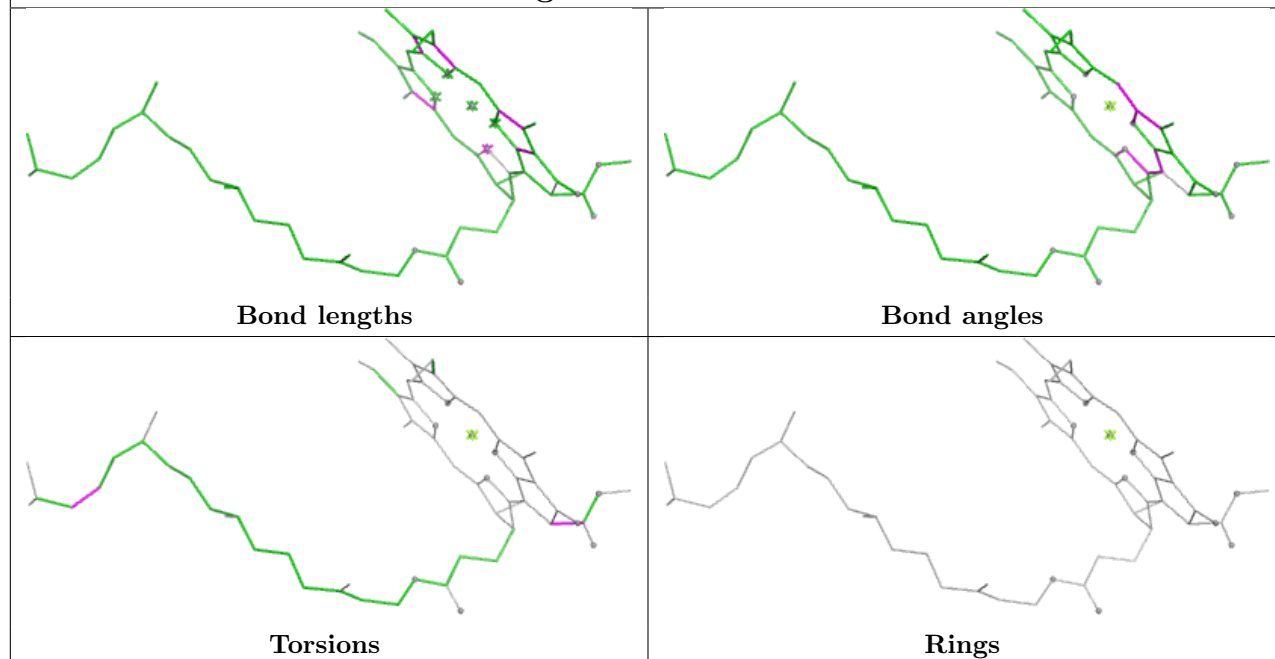
Ligand CLA b 612



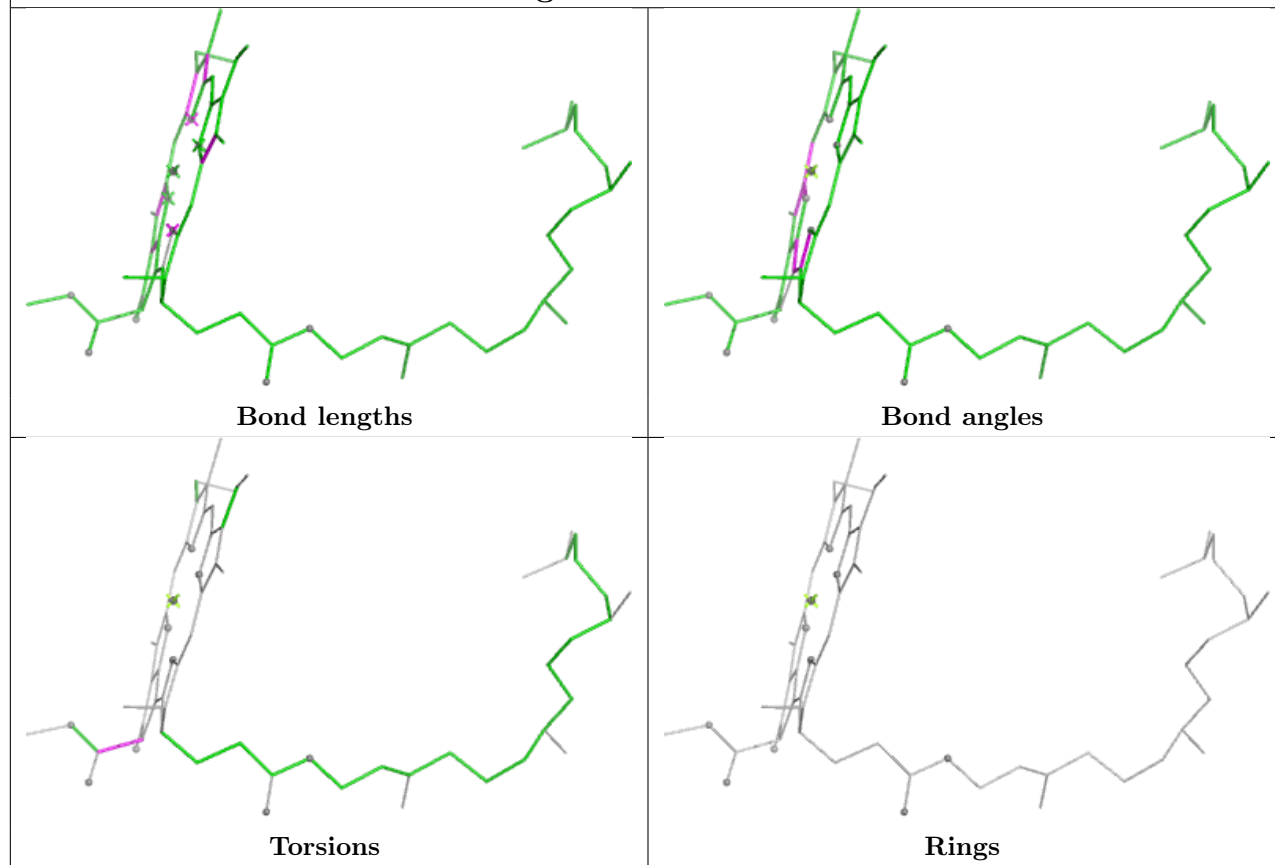
Ligand BCR d 404

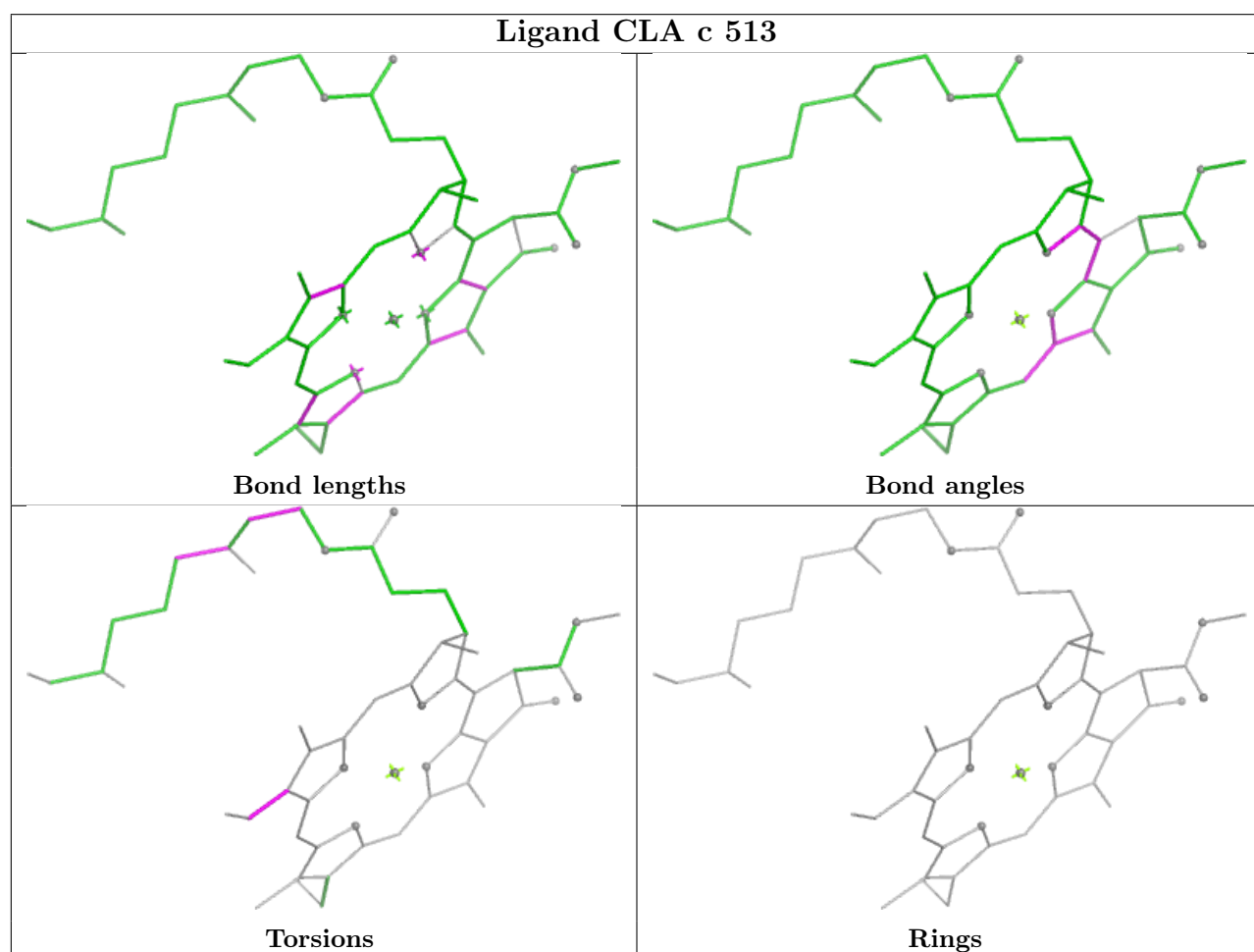
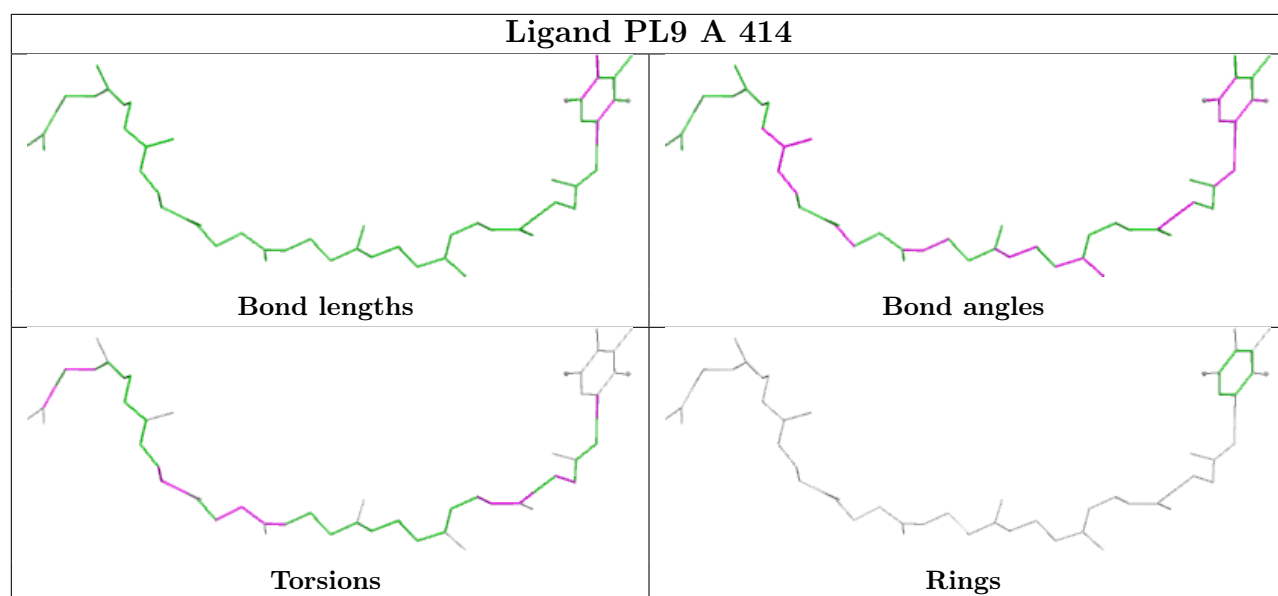


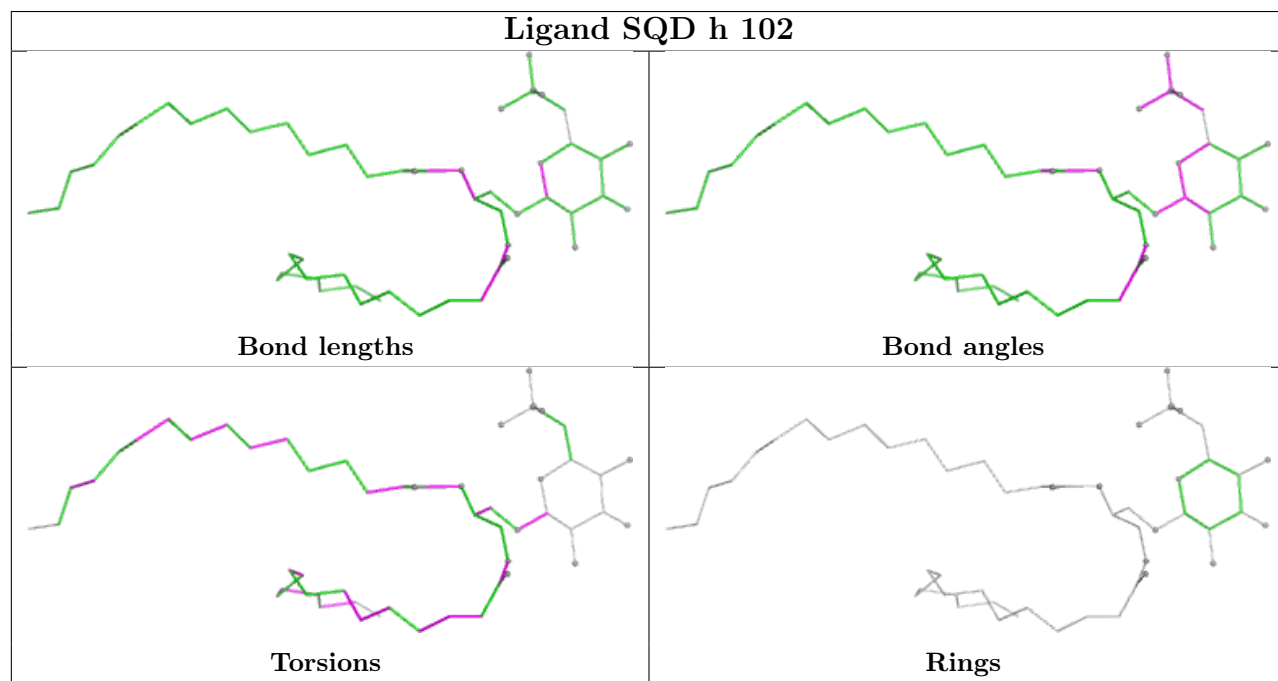
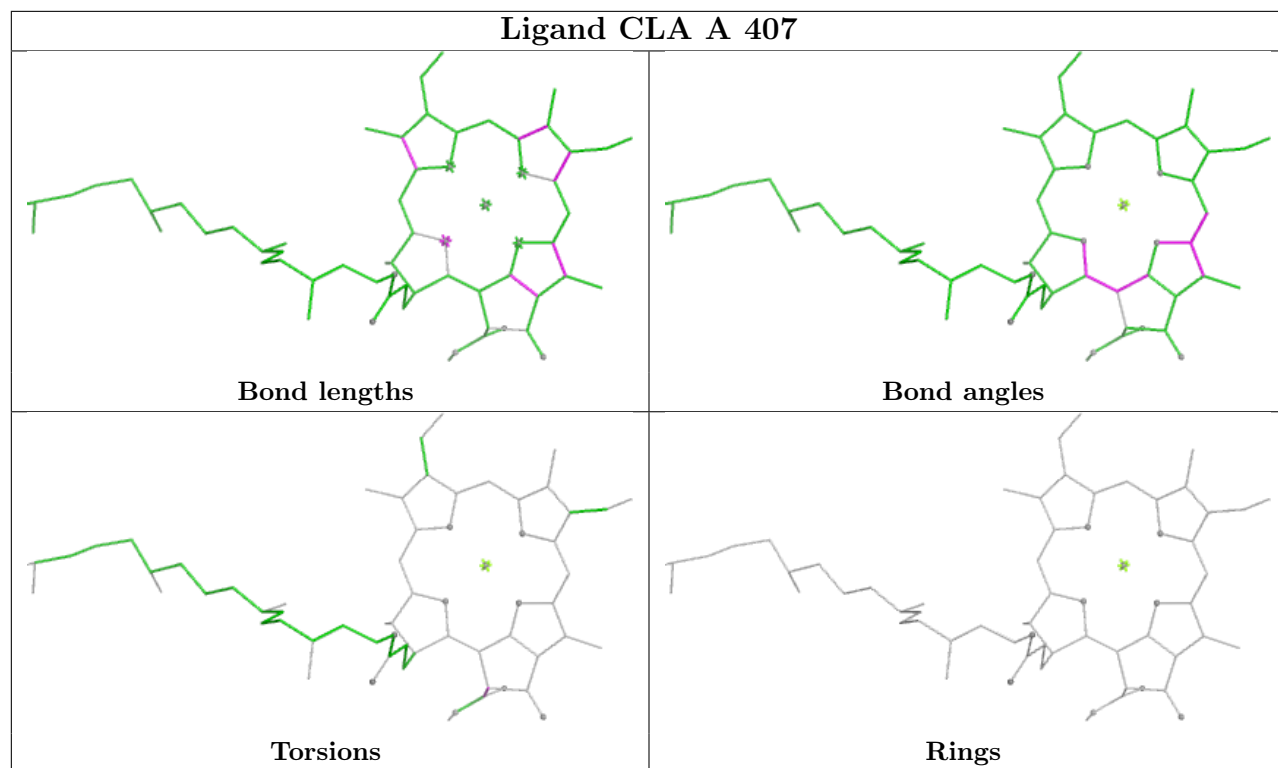
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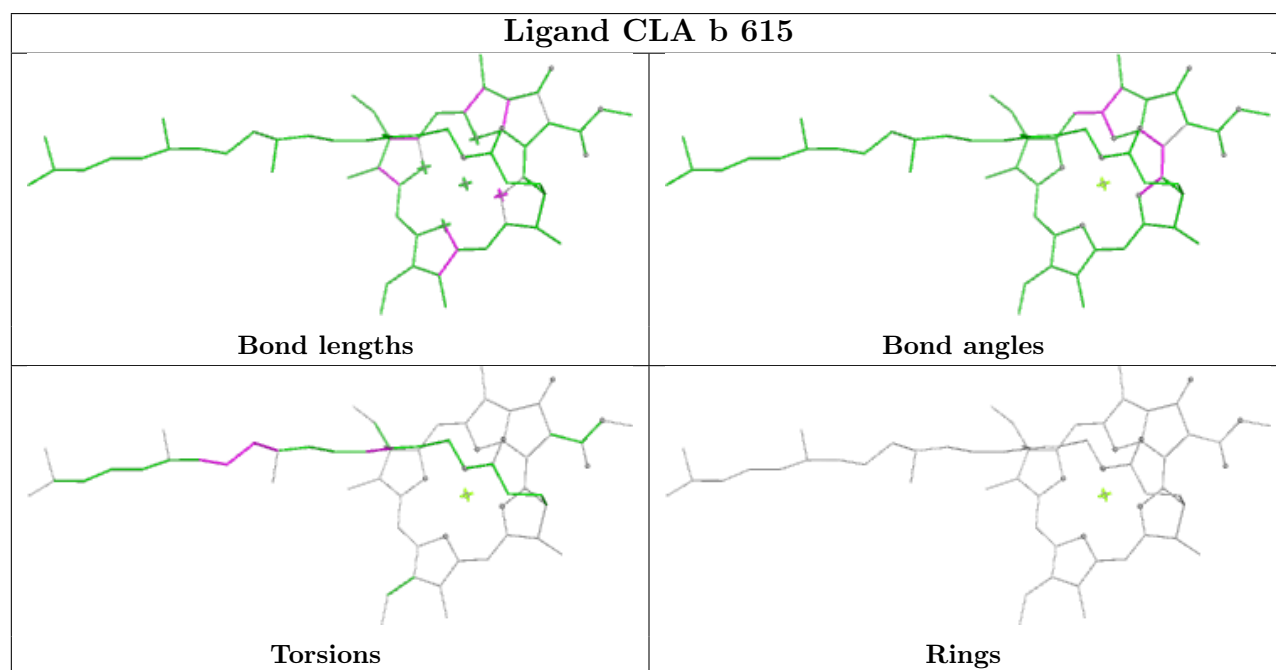
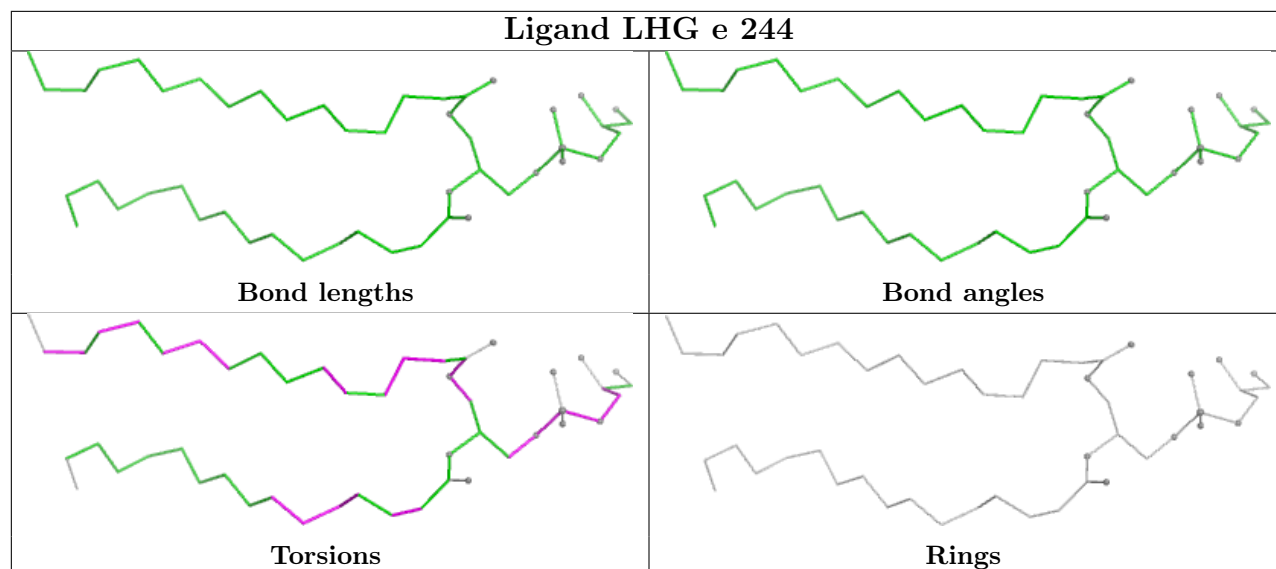


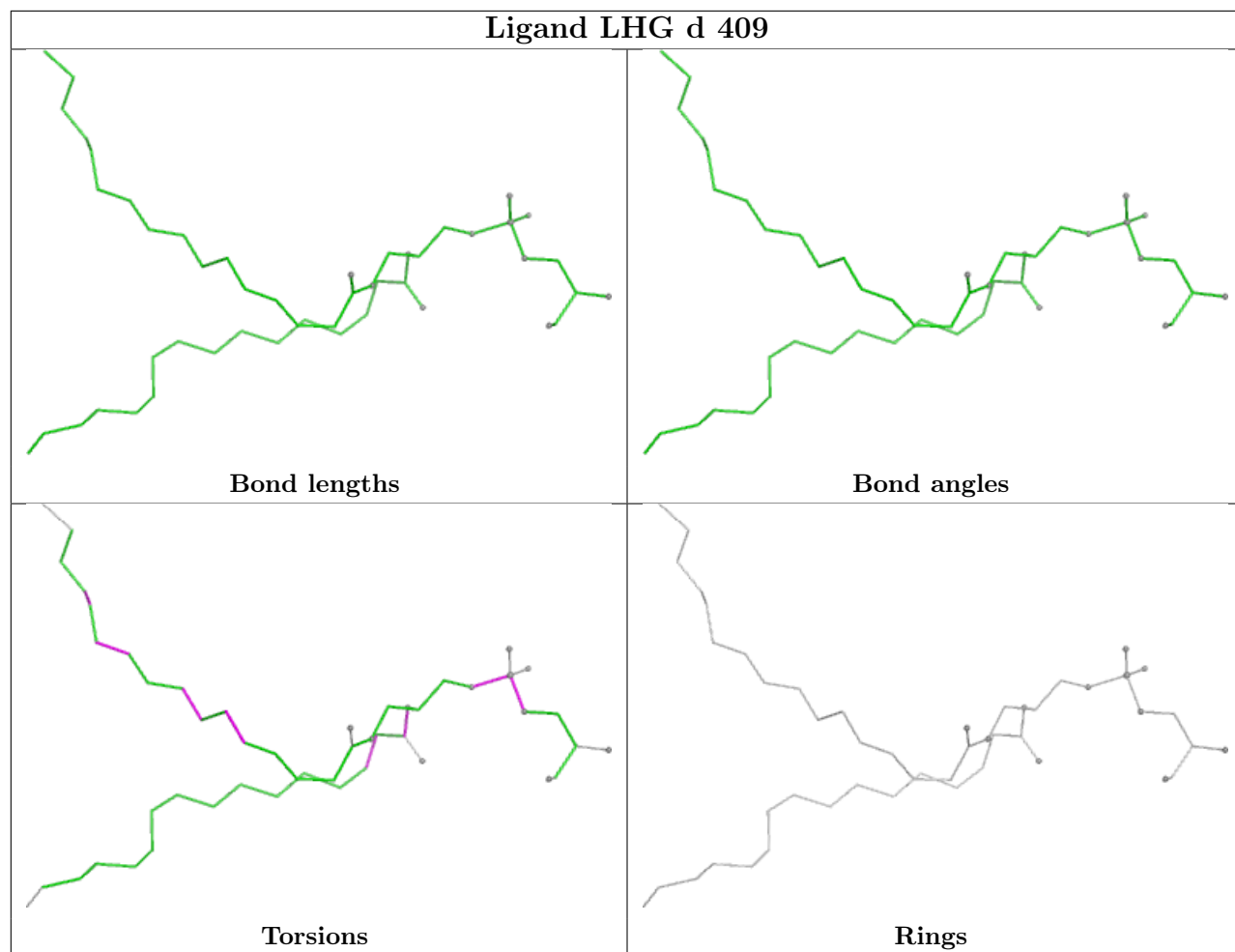
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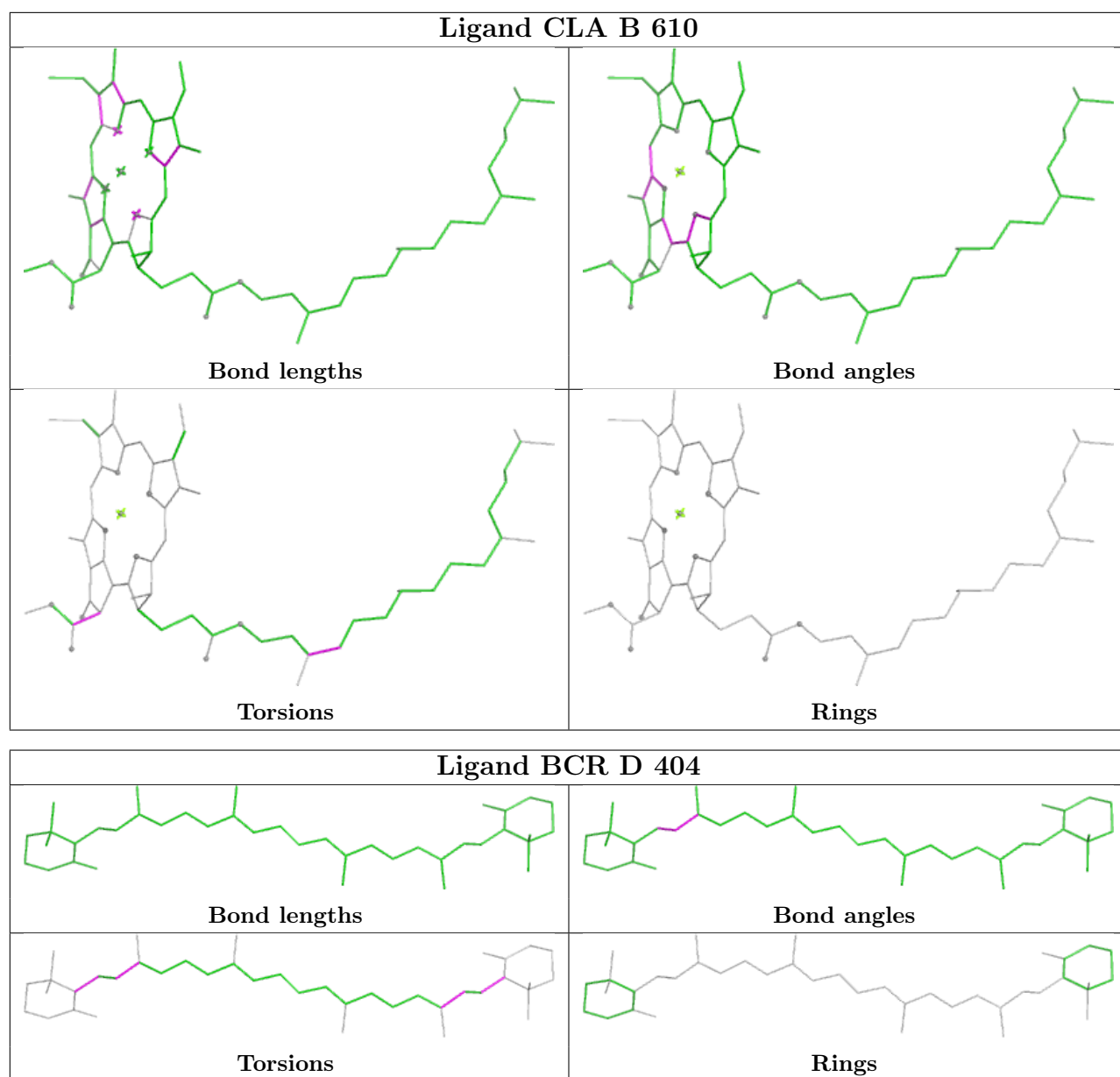


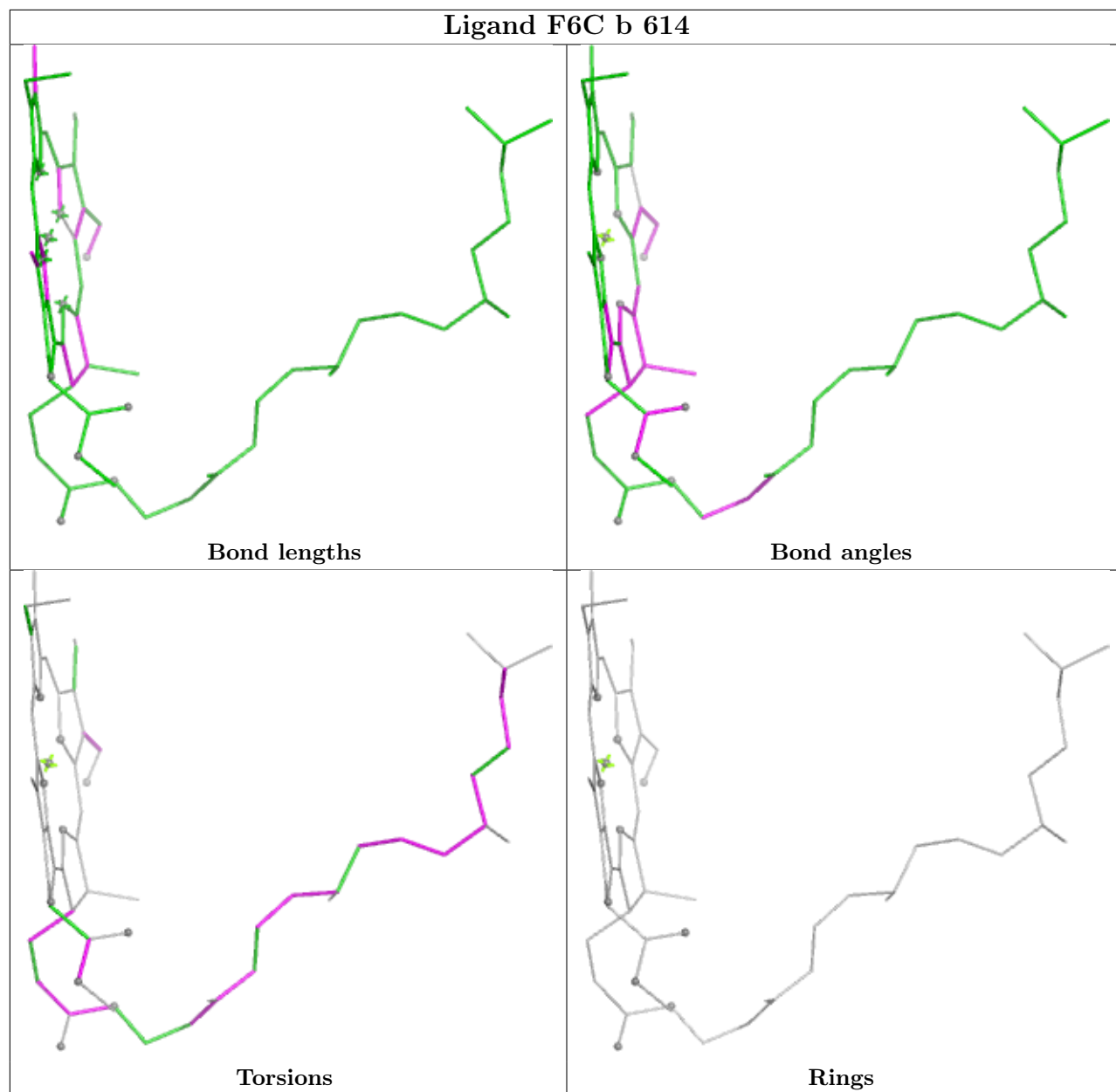


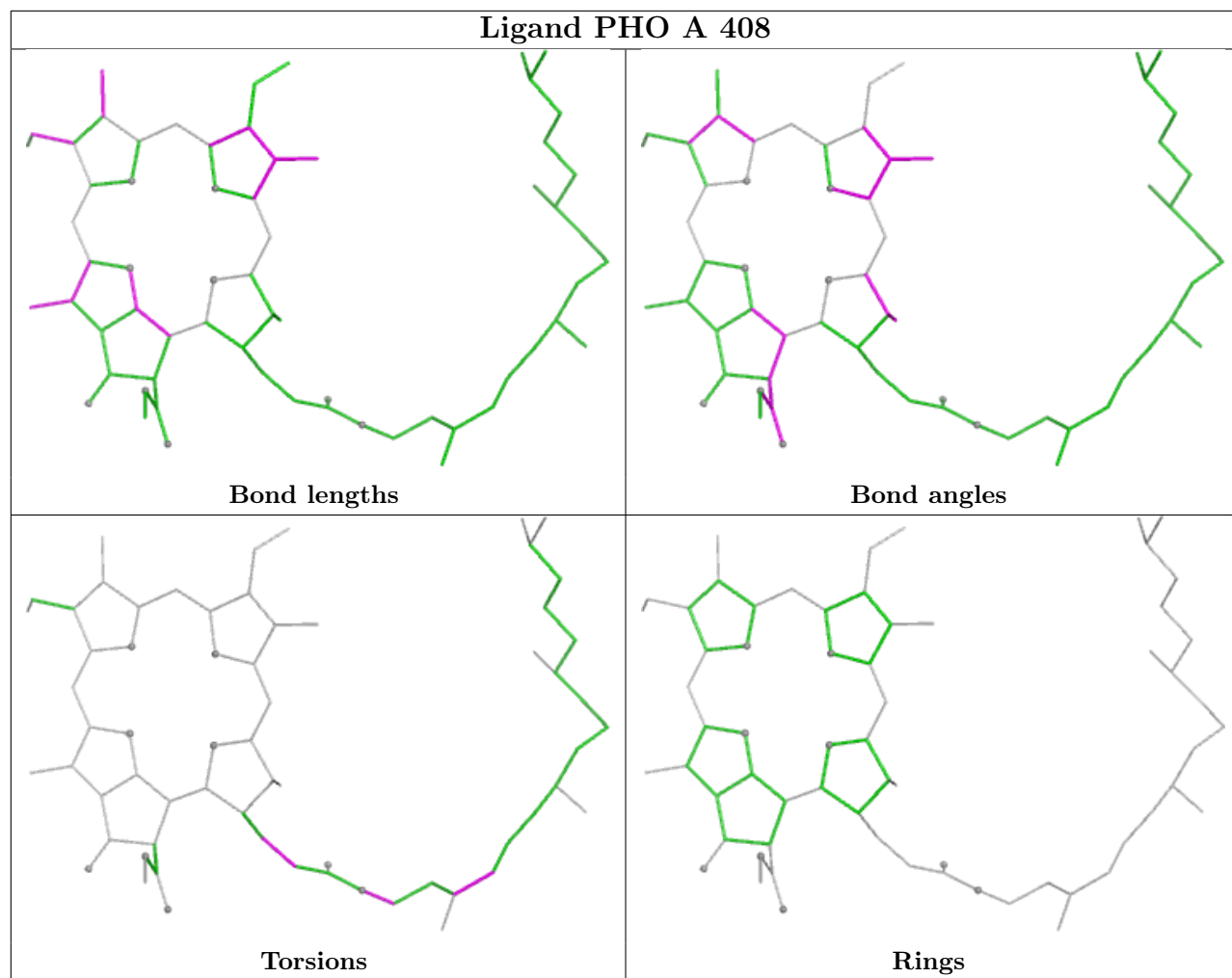


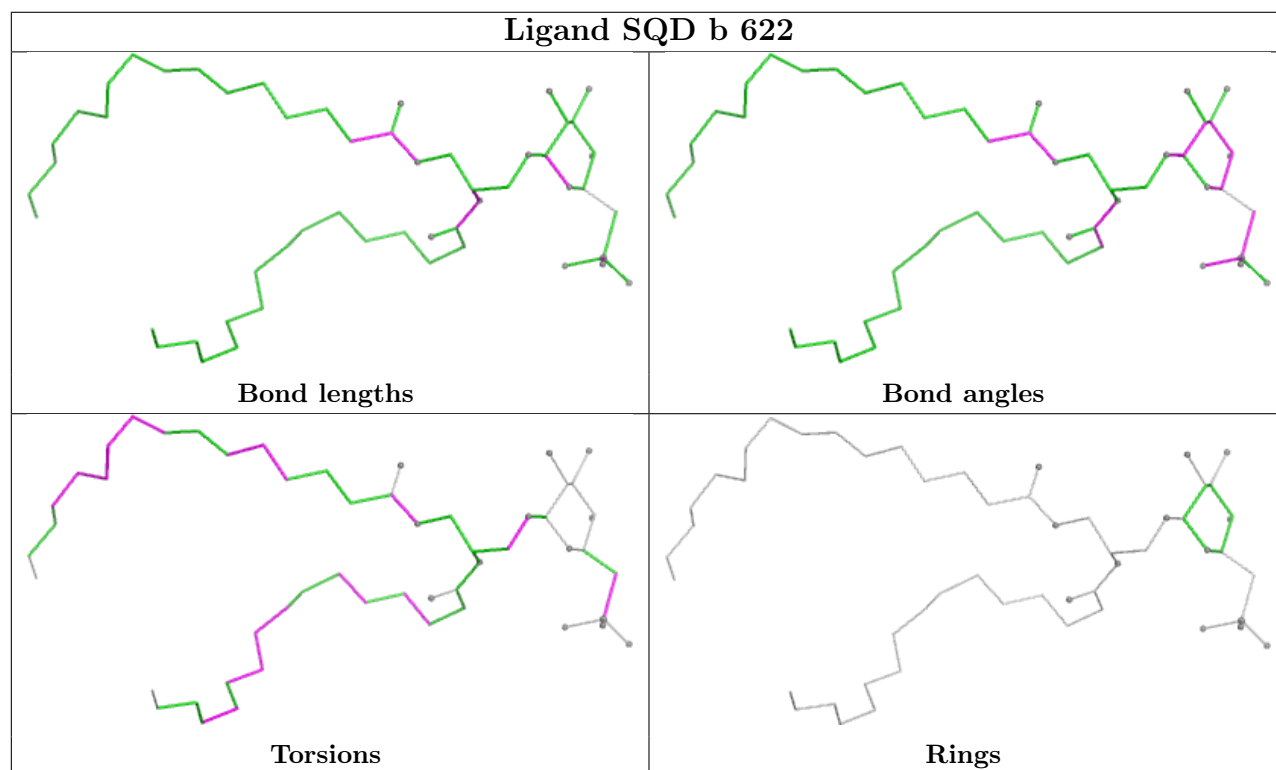
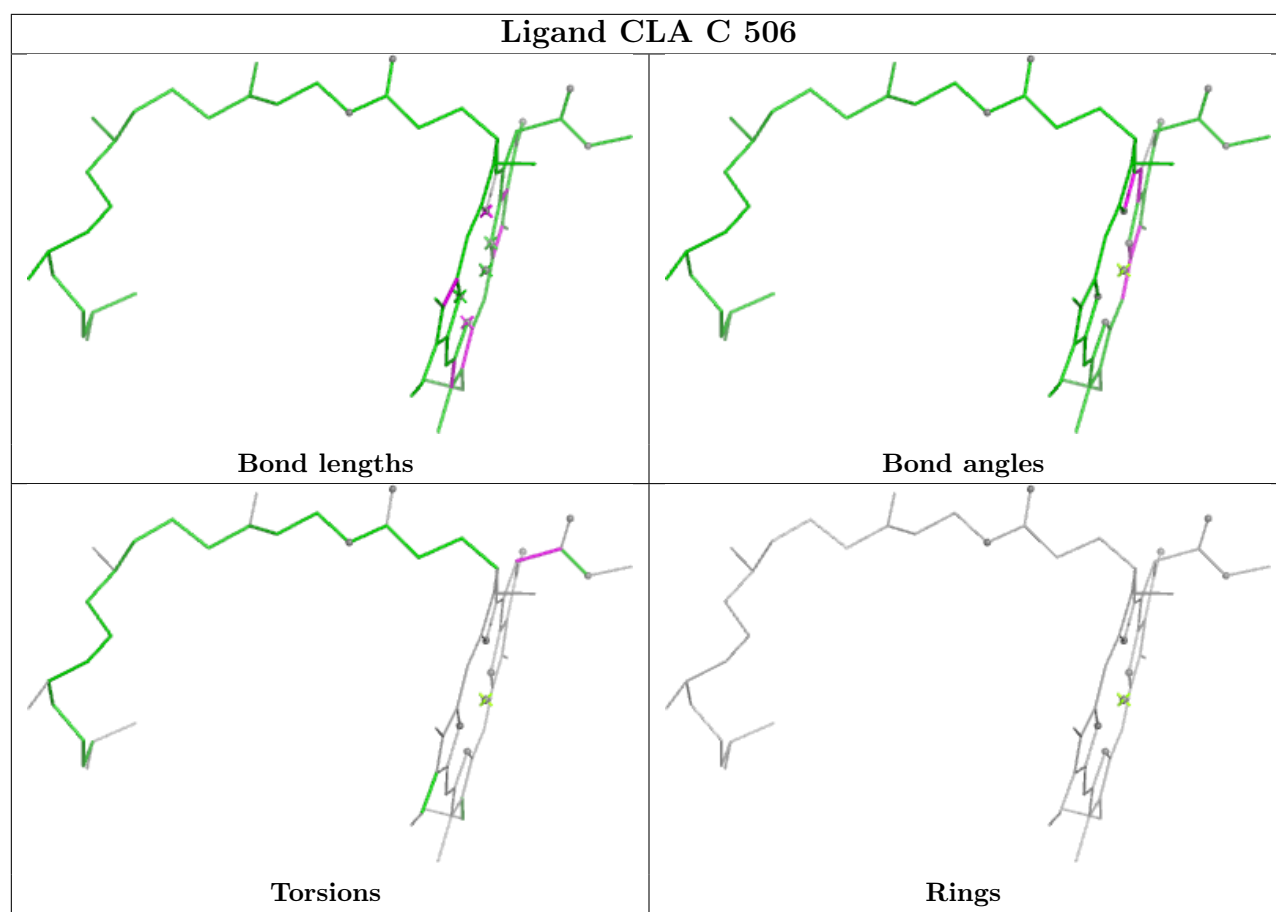


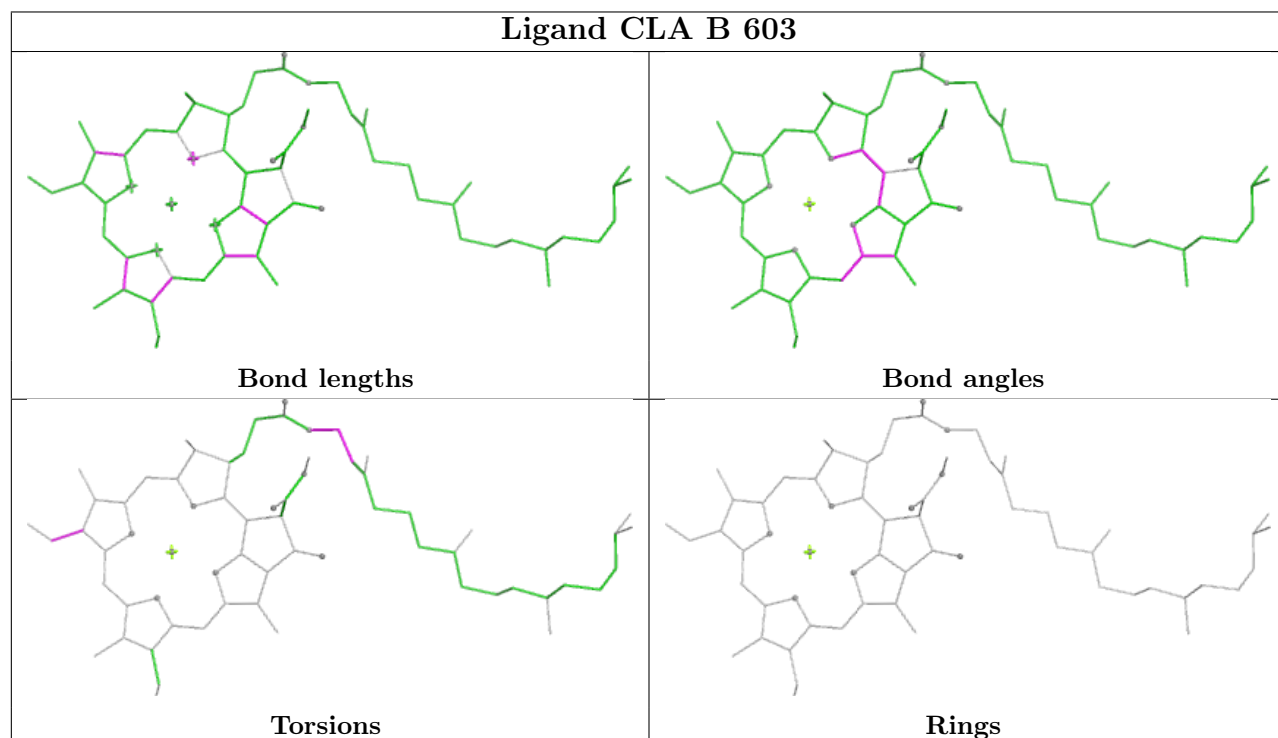
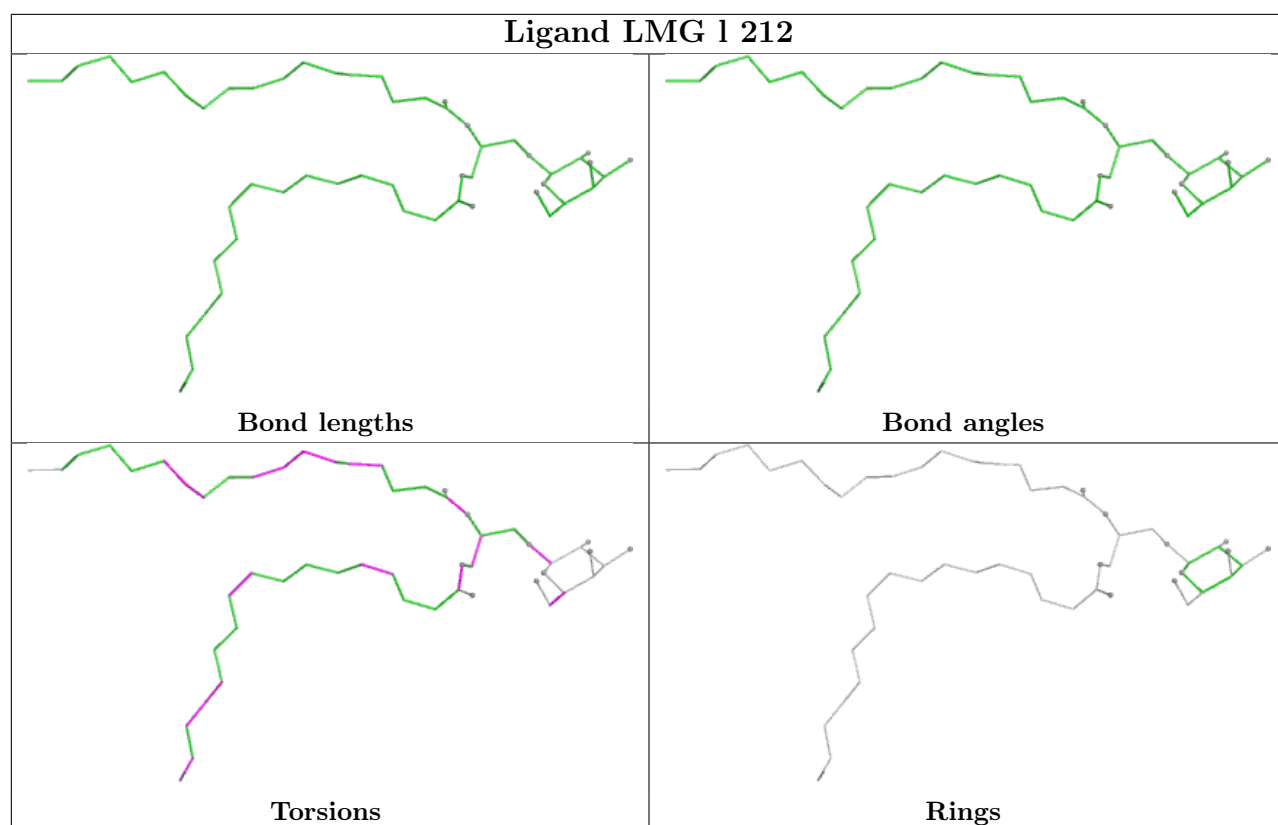


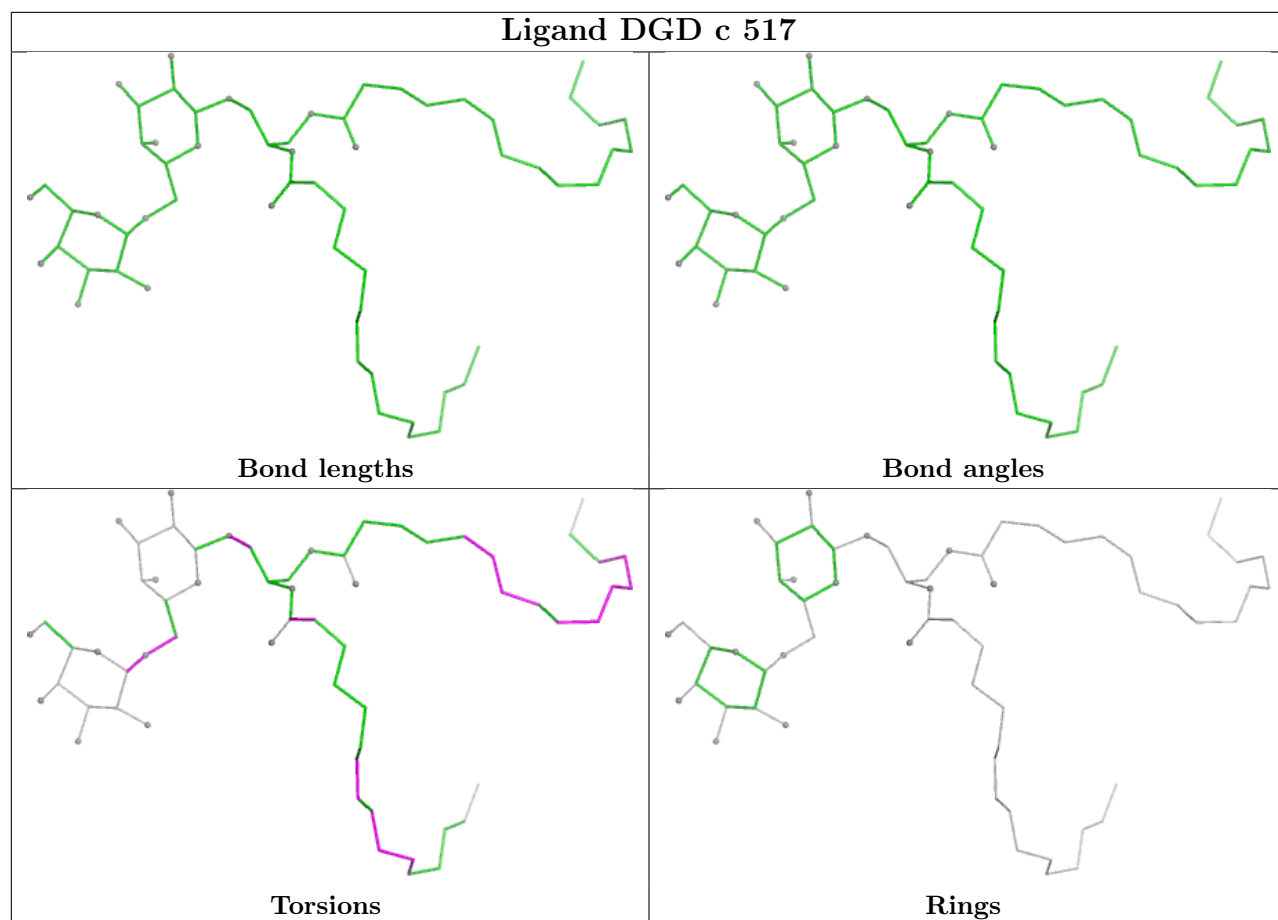
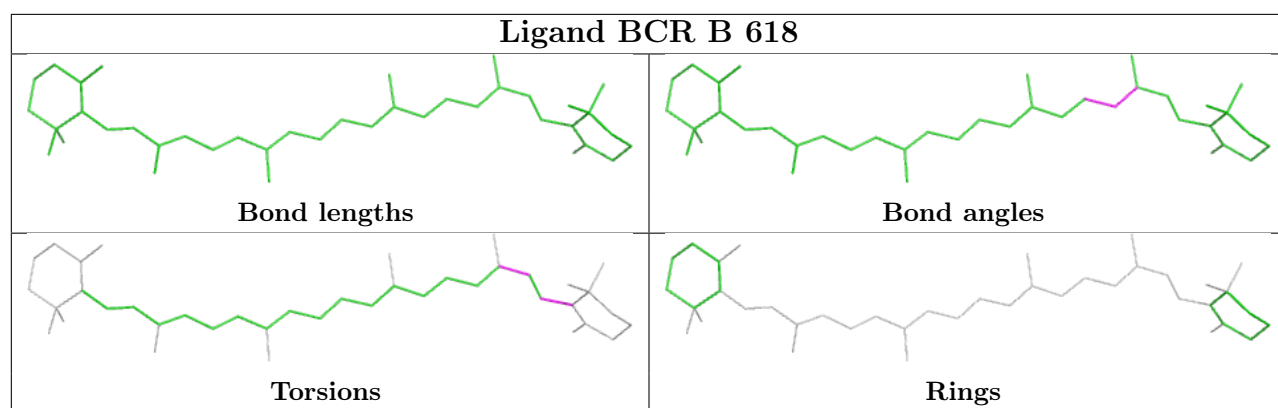


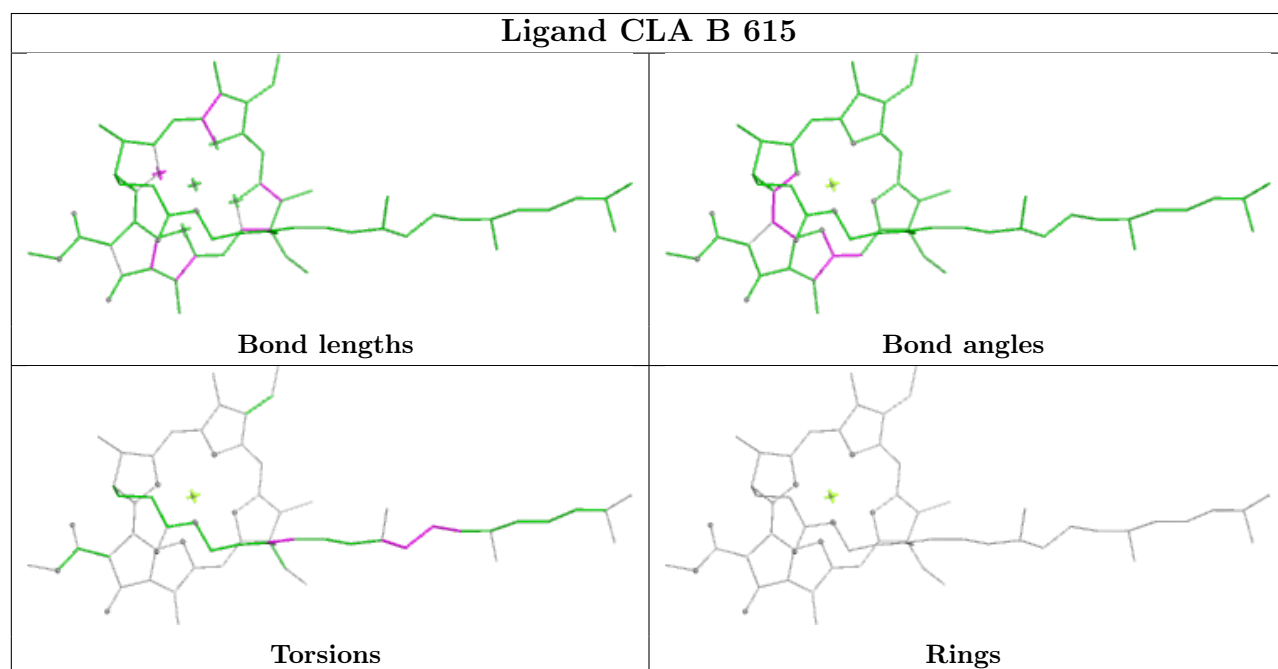
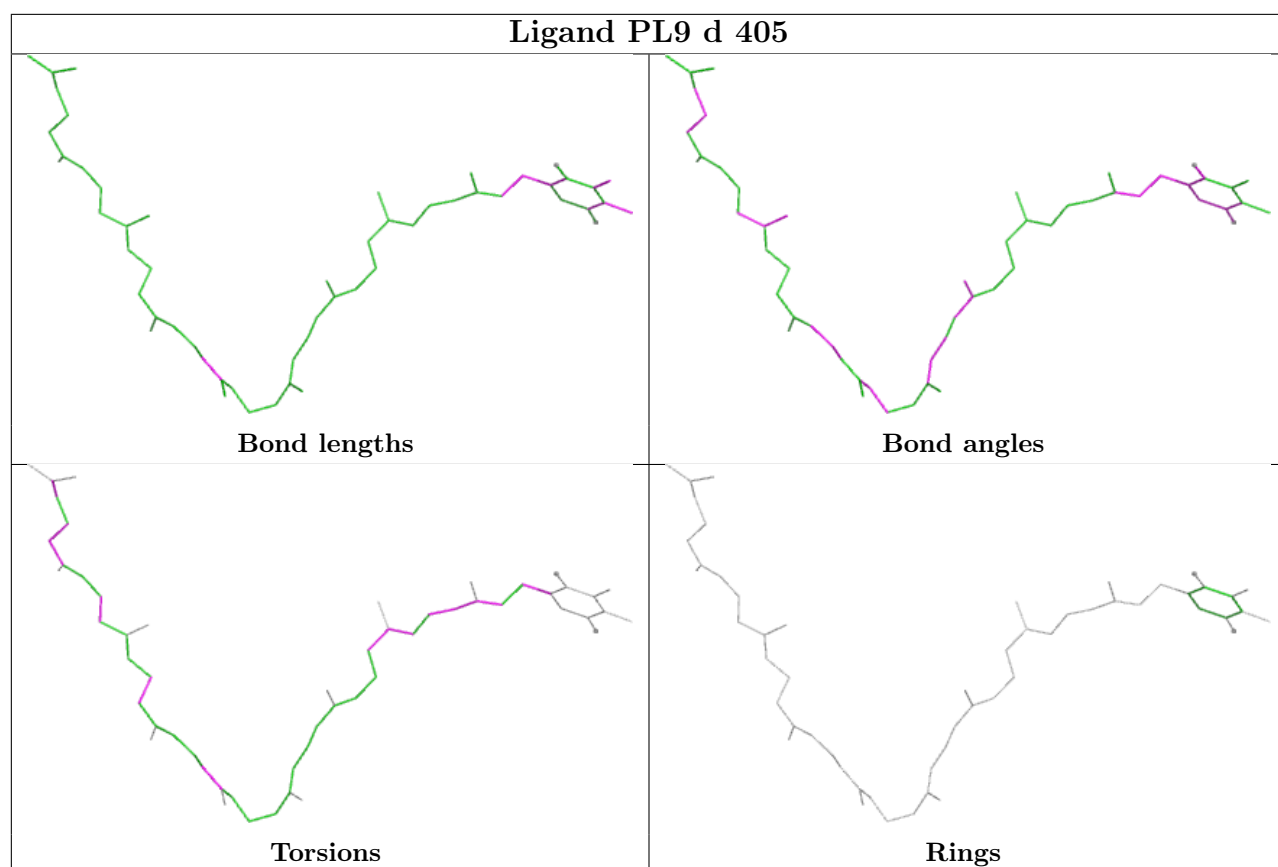


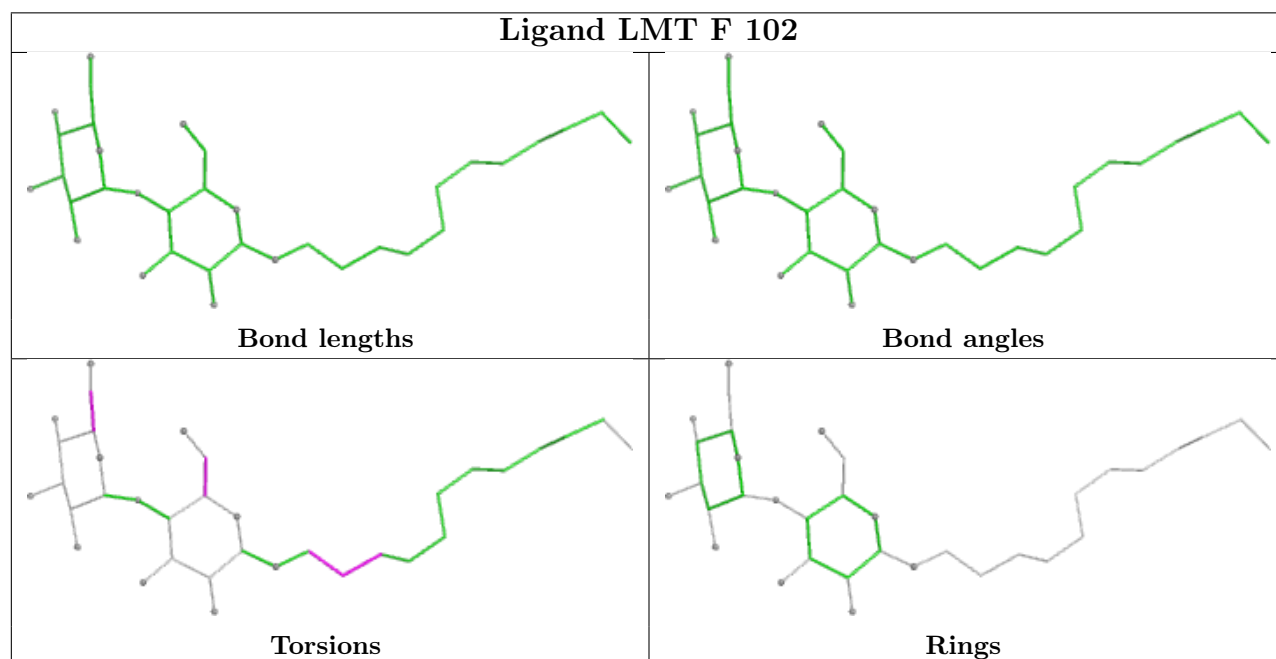
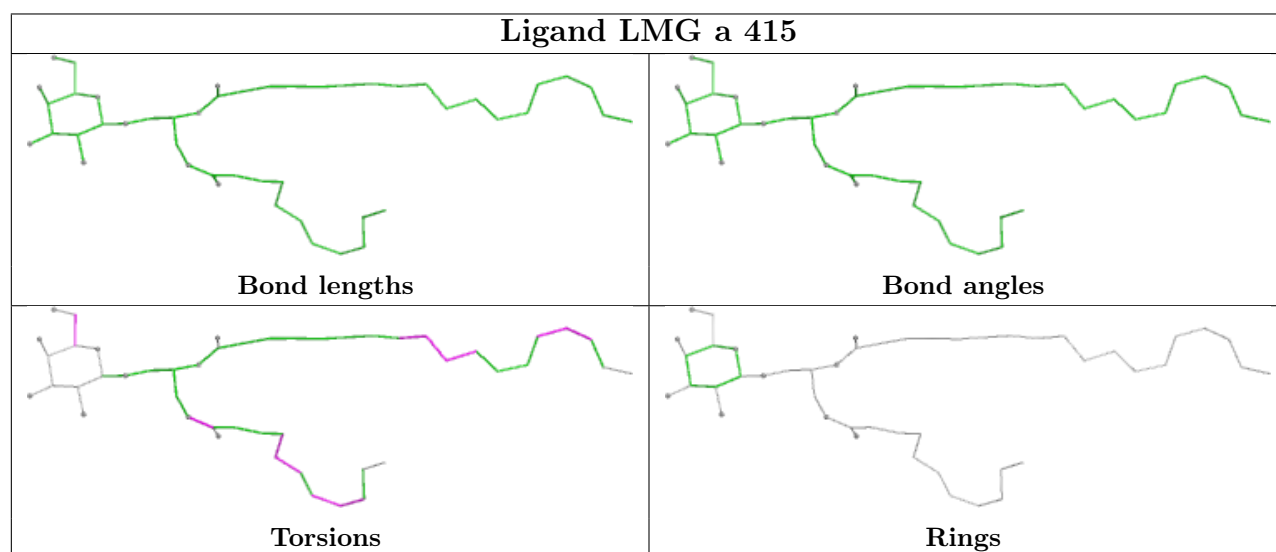
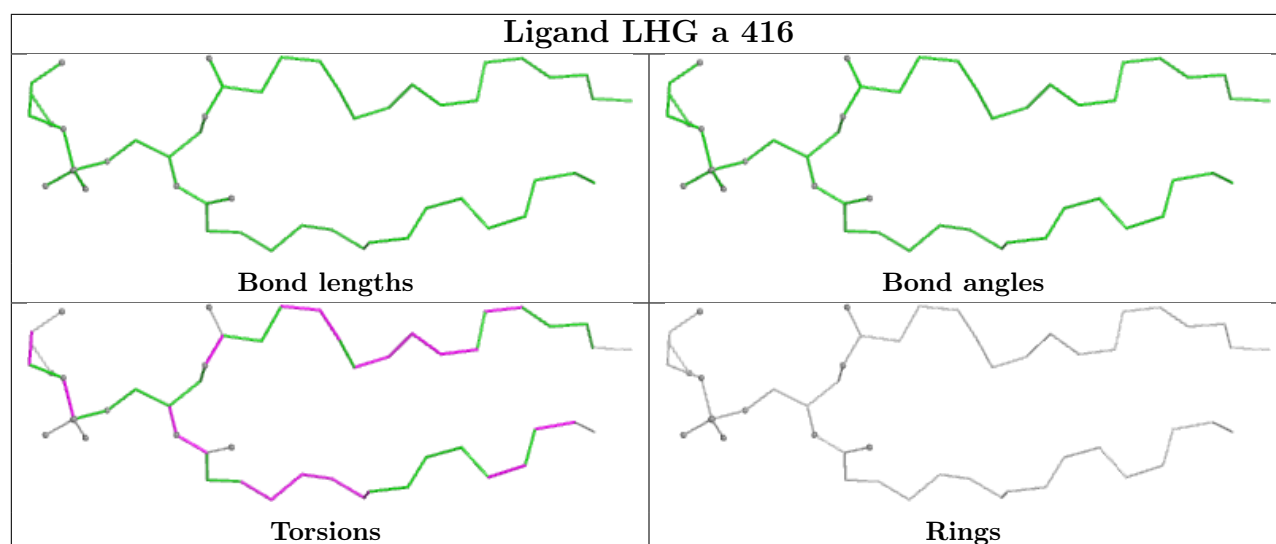


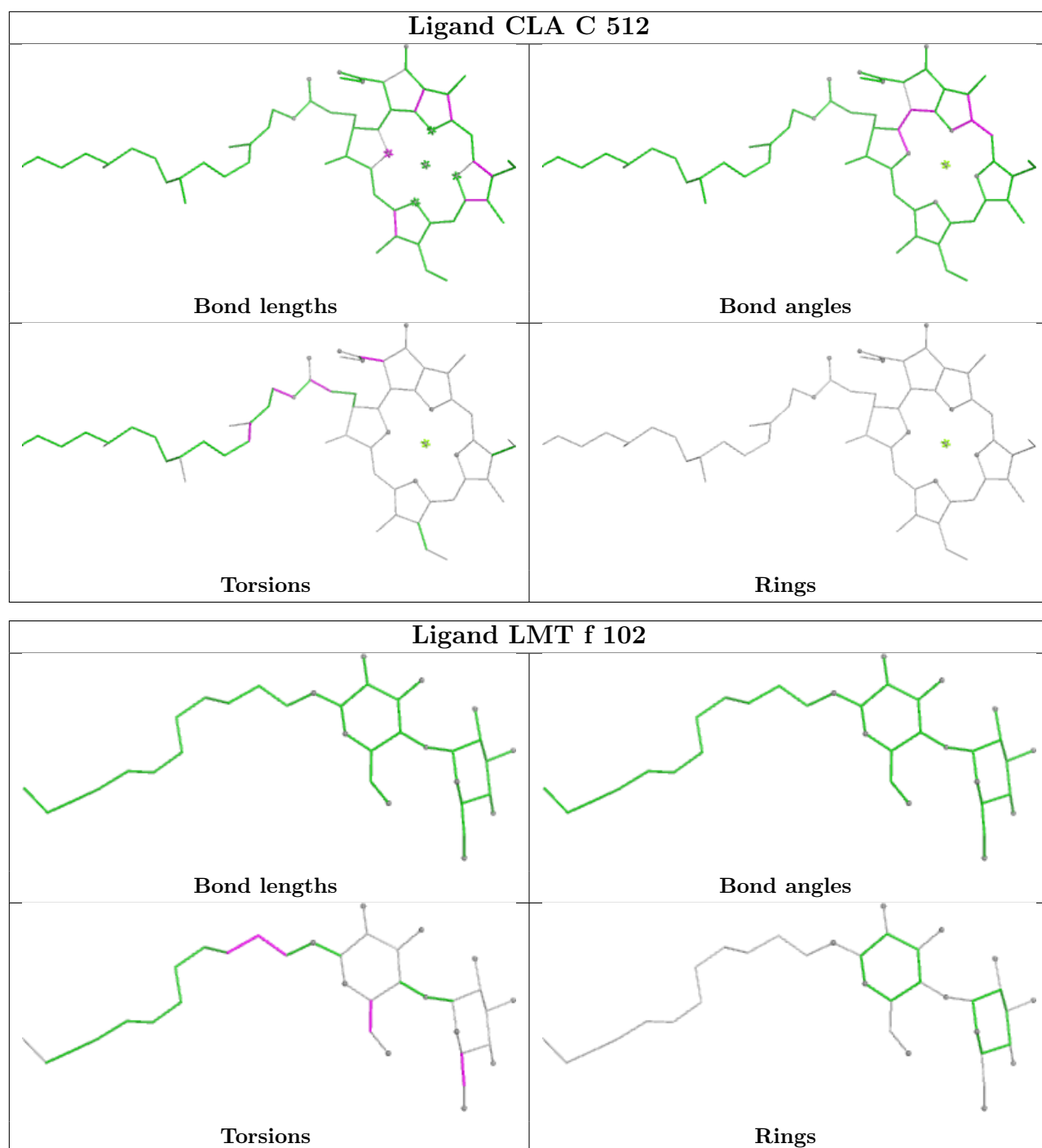




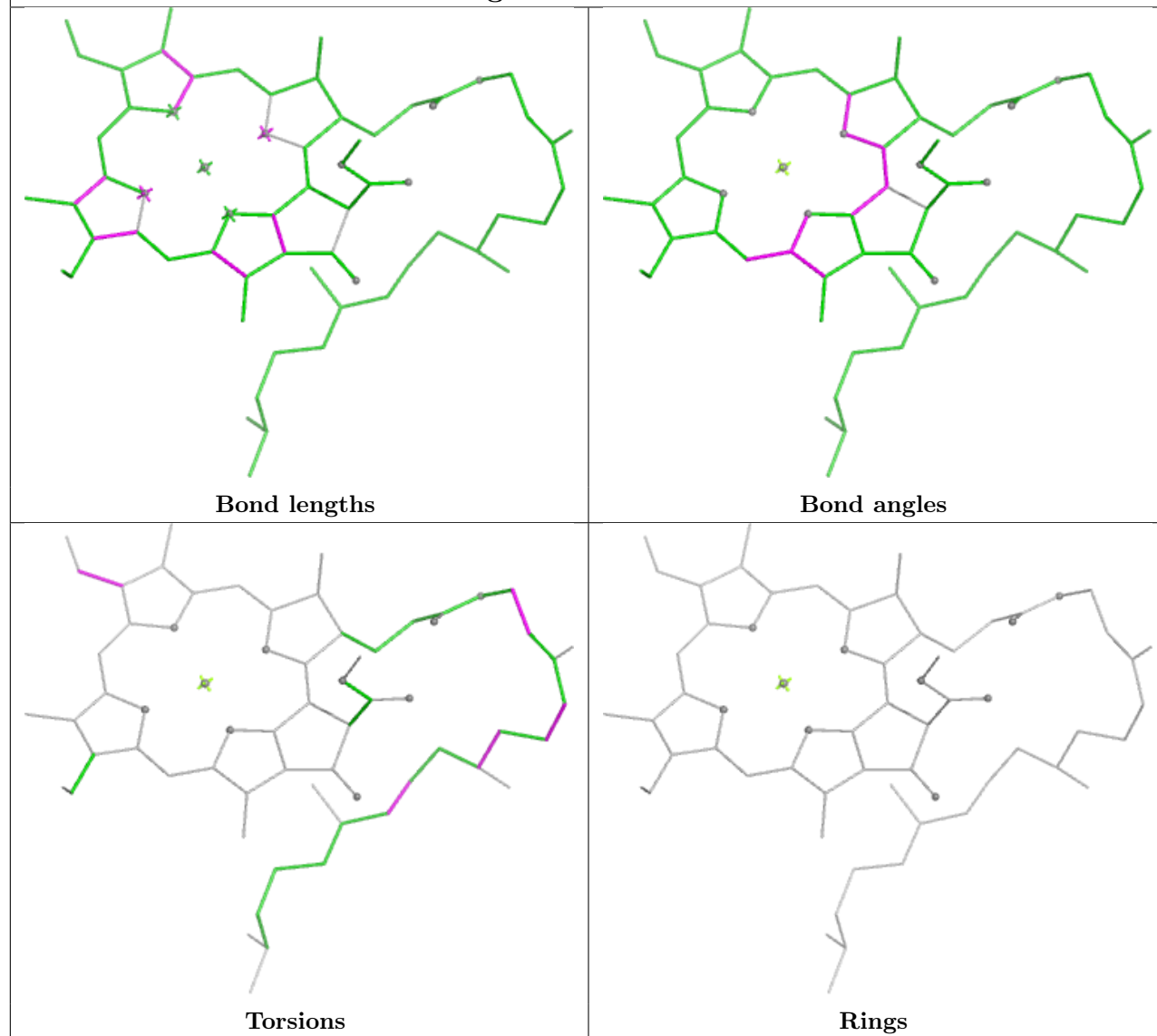




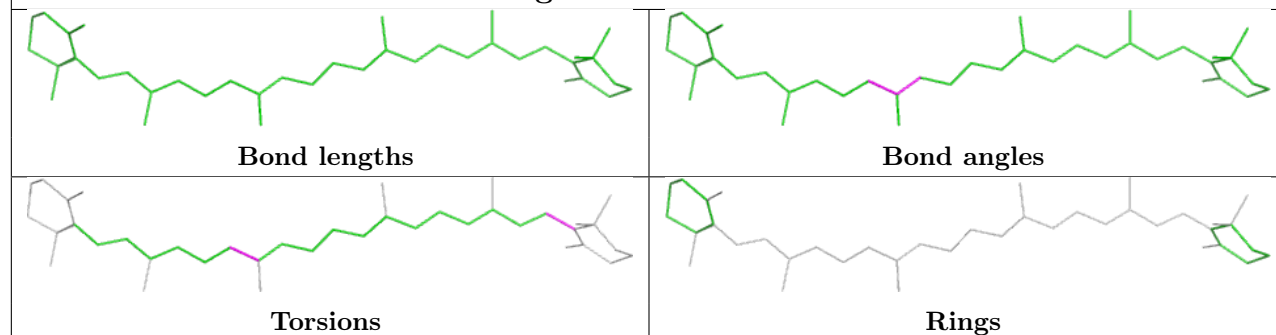




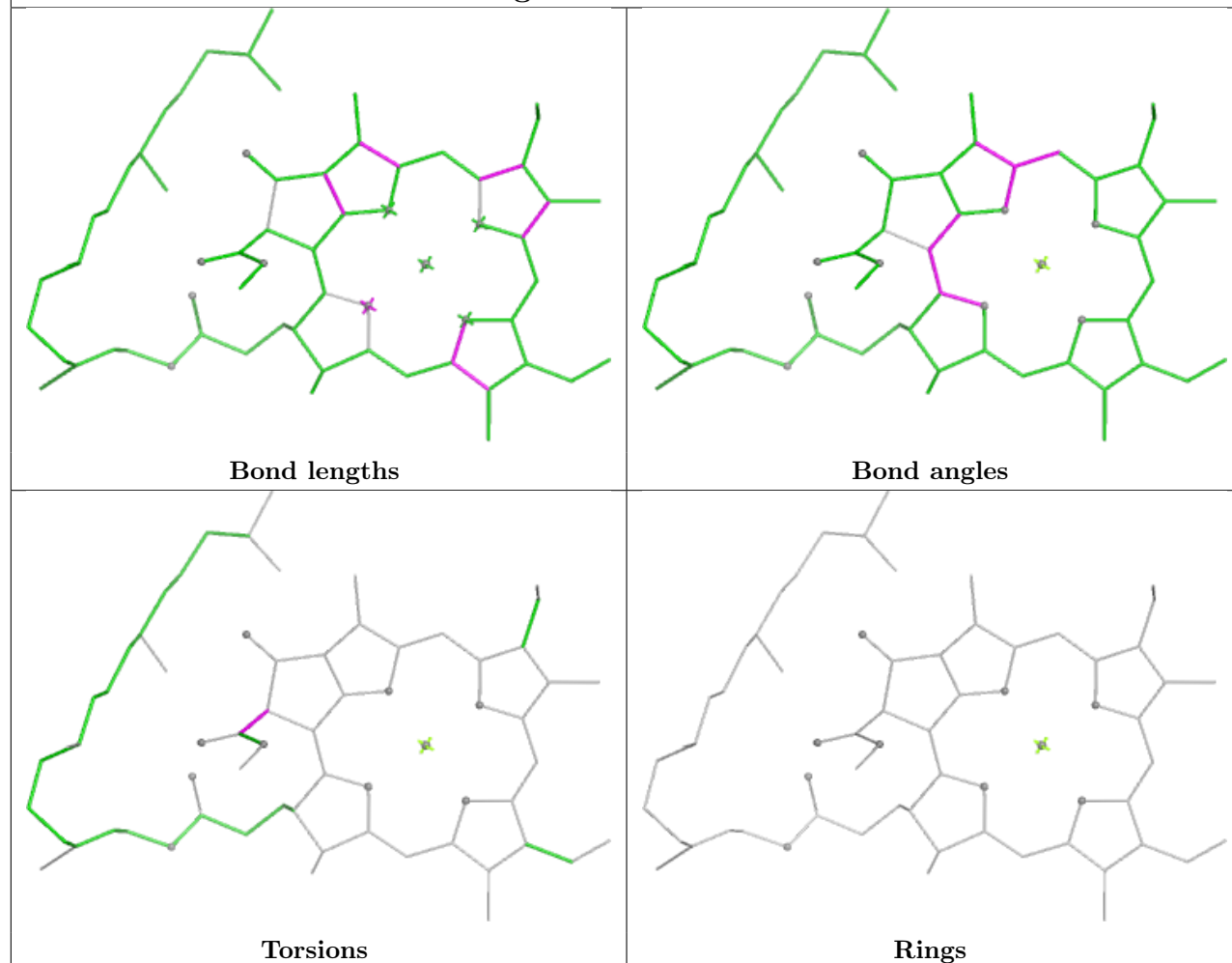
Ligand CLA c 509



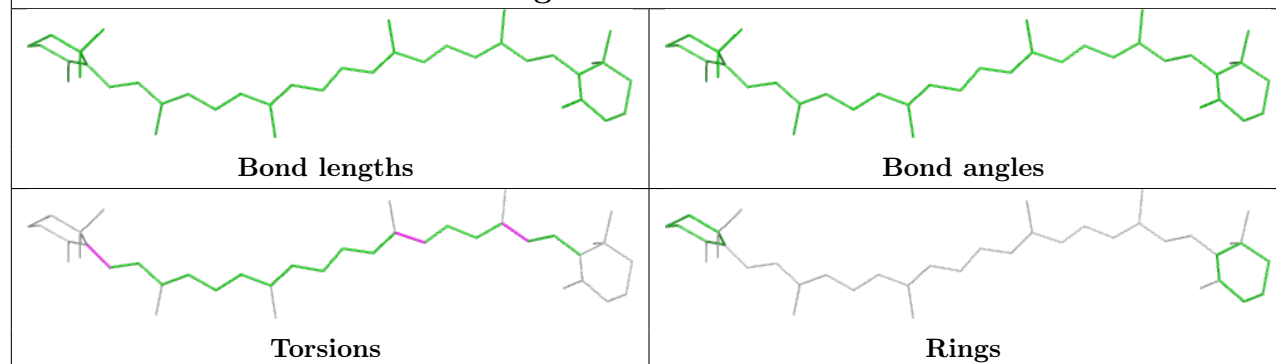
Ligand BCR c 515

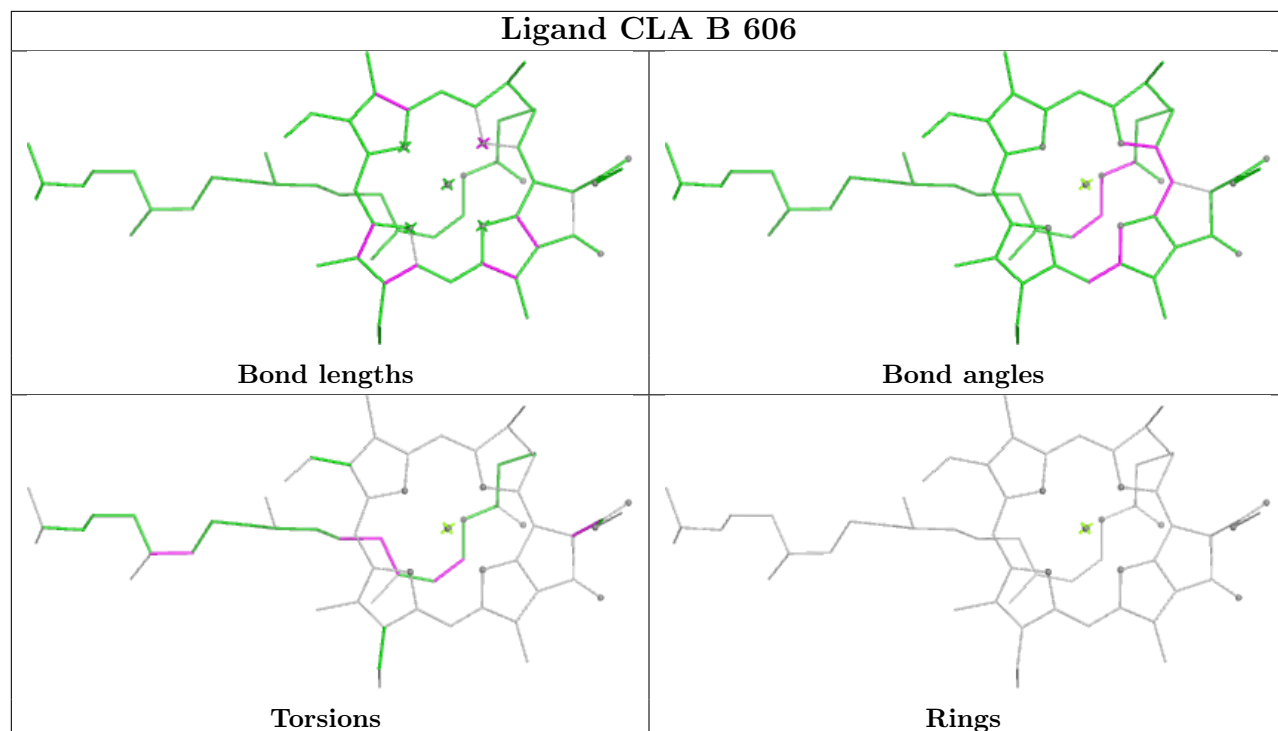
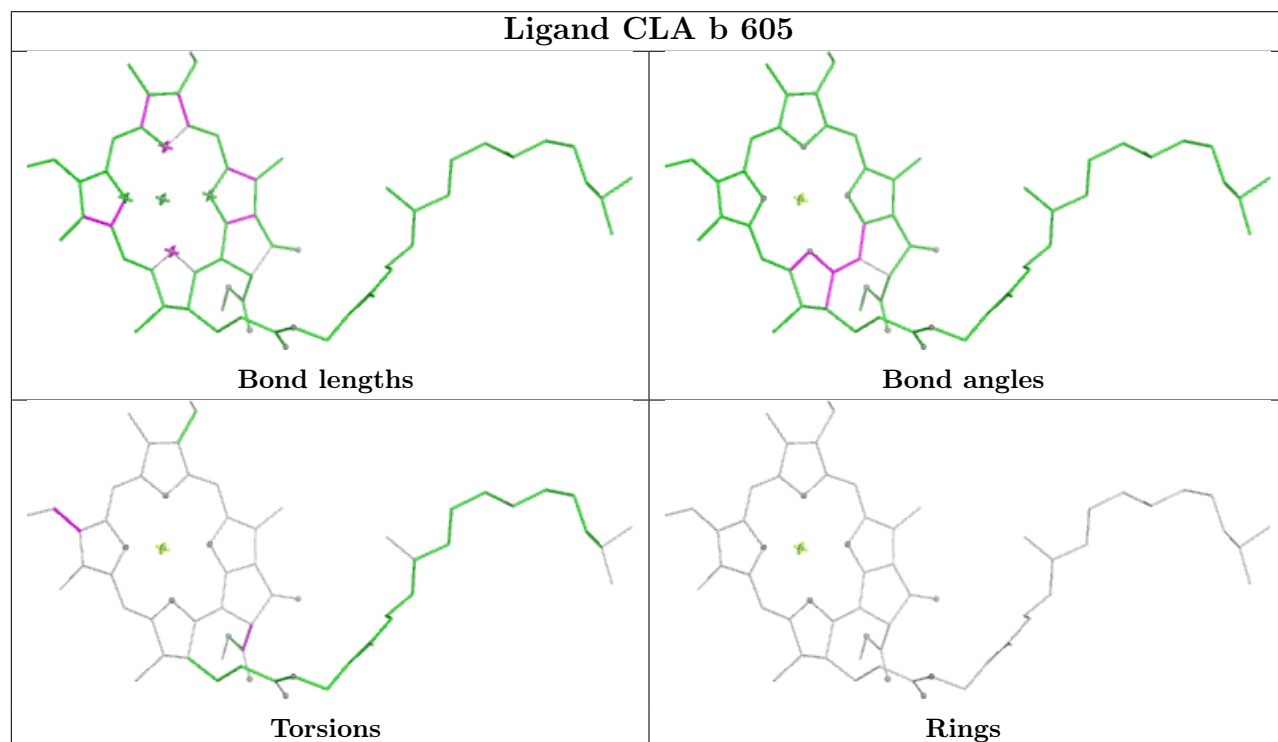


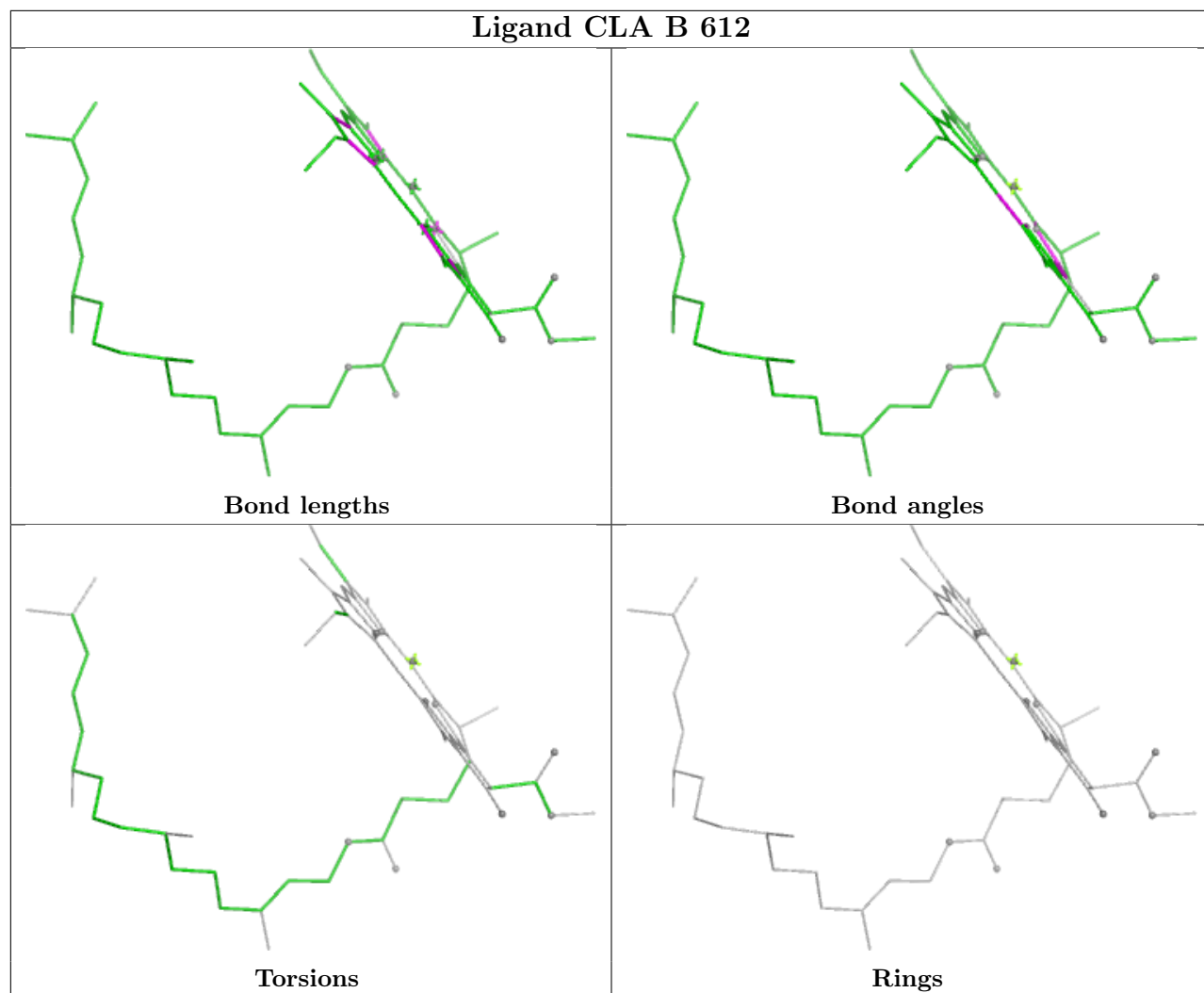
Ligand CLA B 611

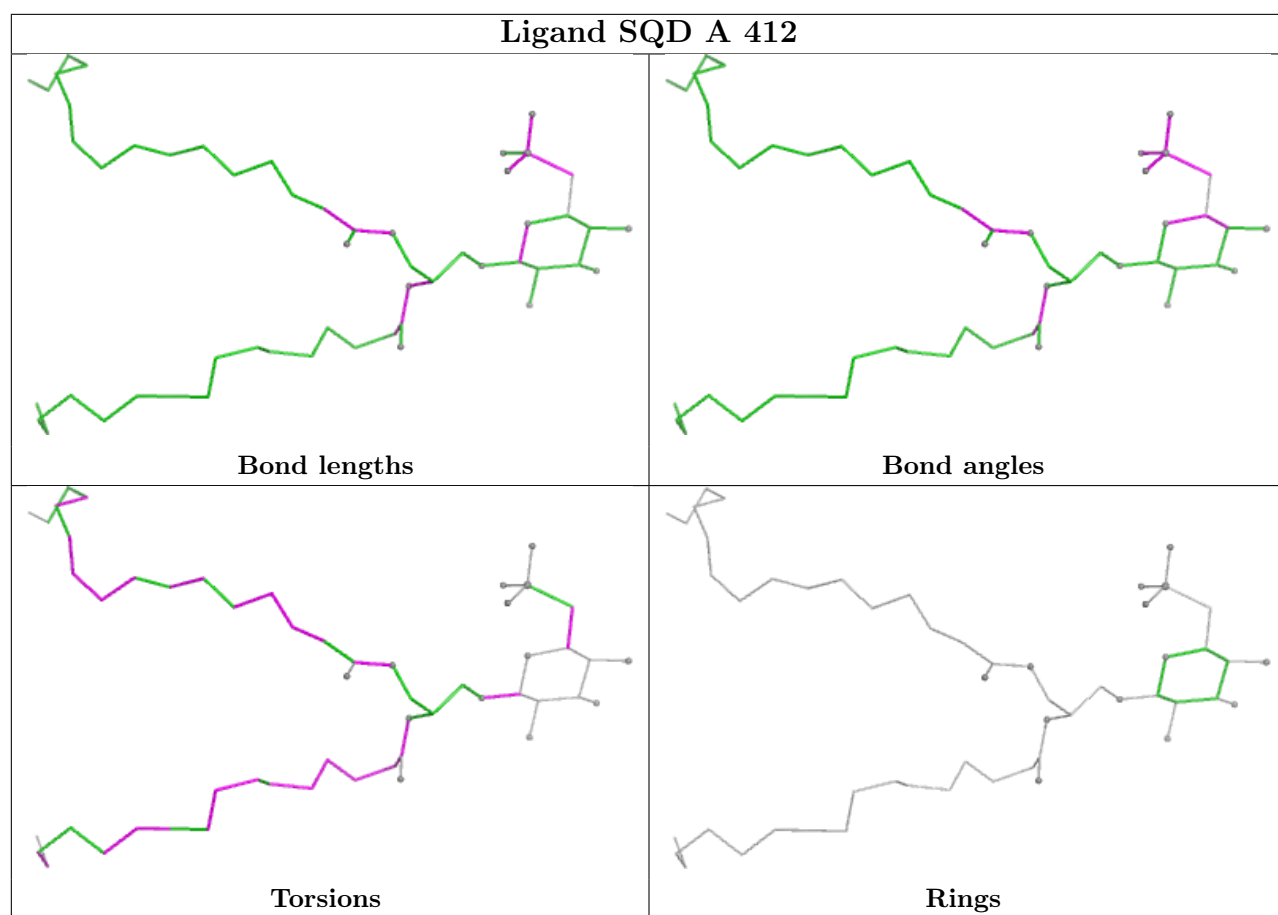


Ligand BCR k 101

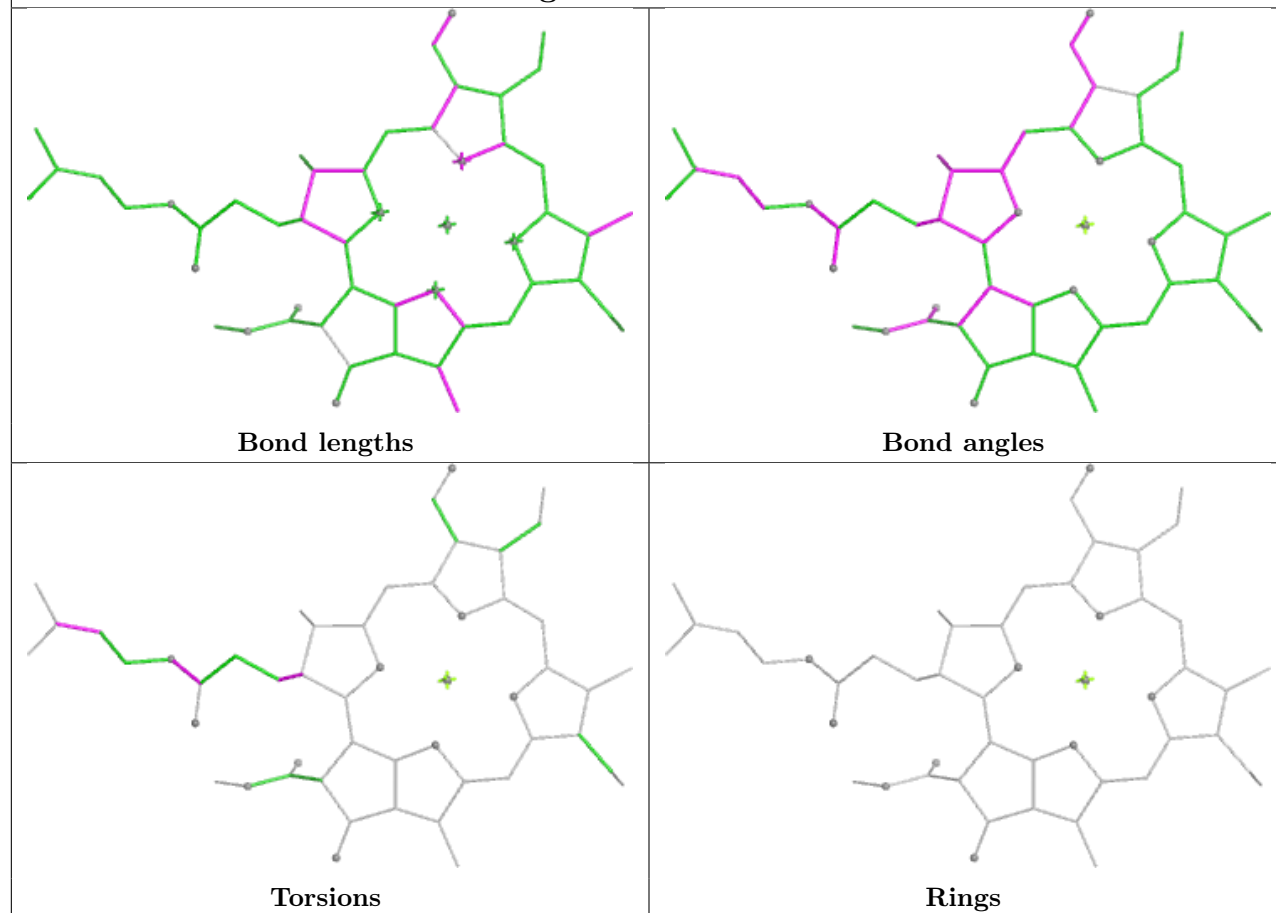


Ligand CLA B 606**Ligand CLA b 605**

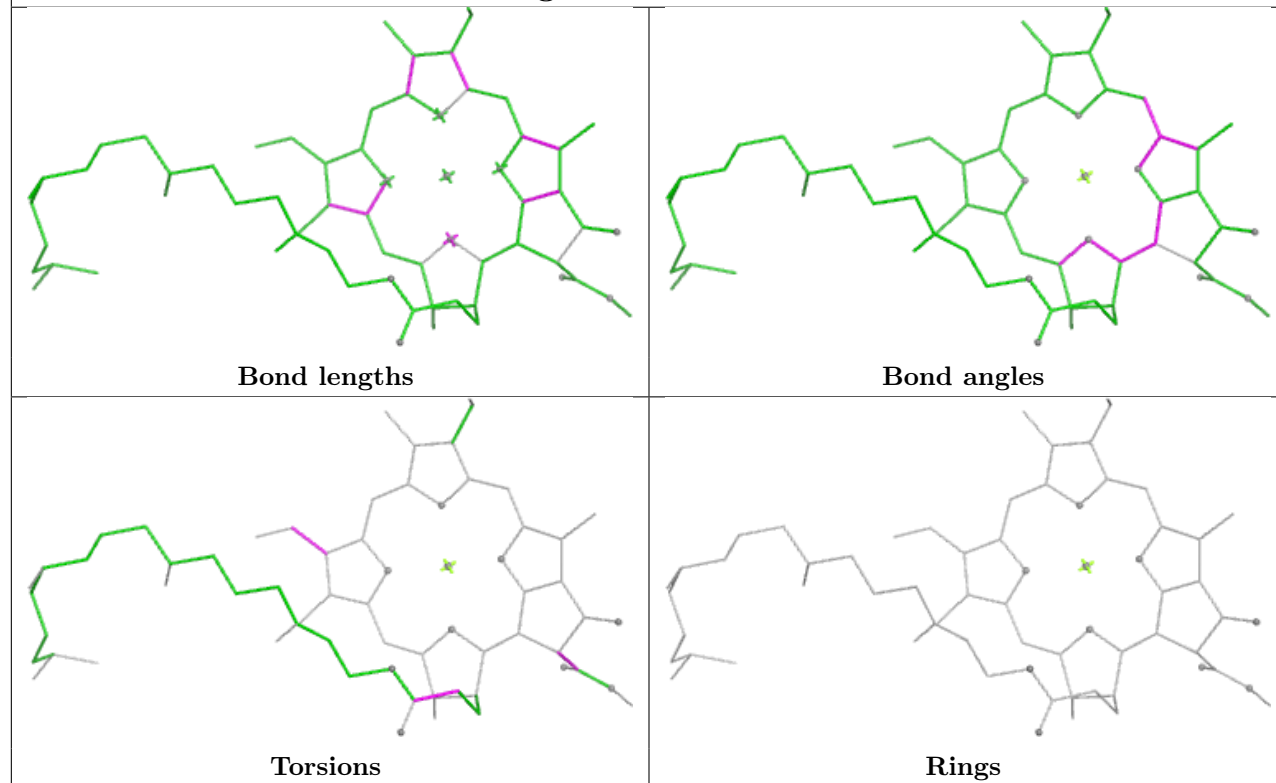


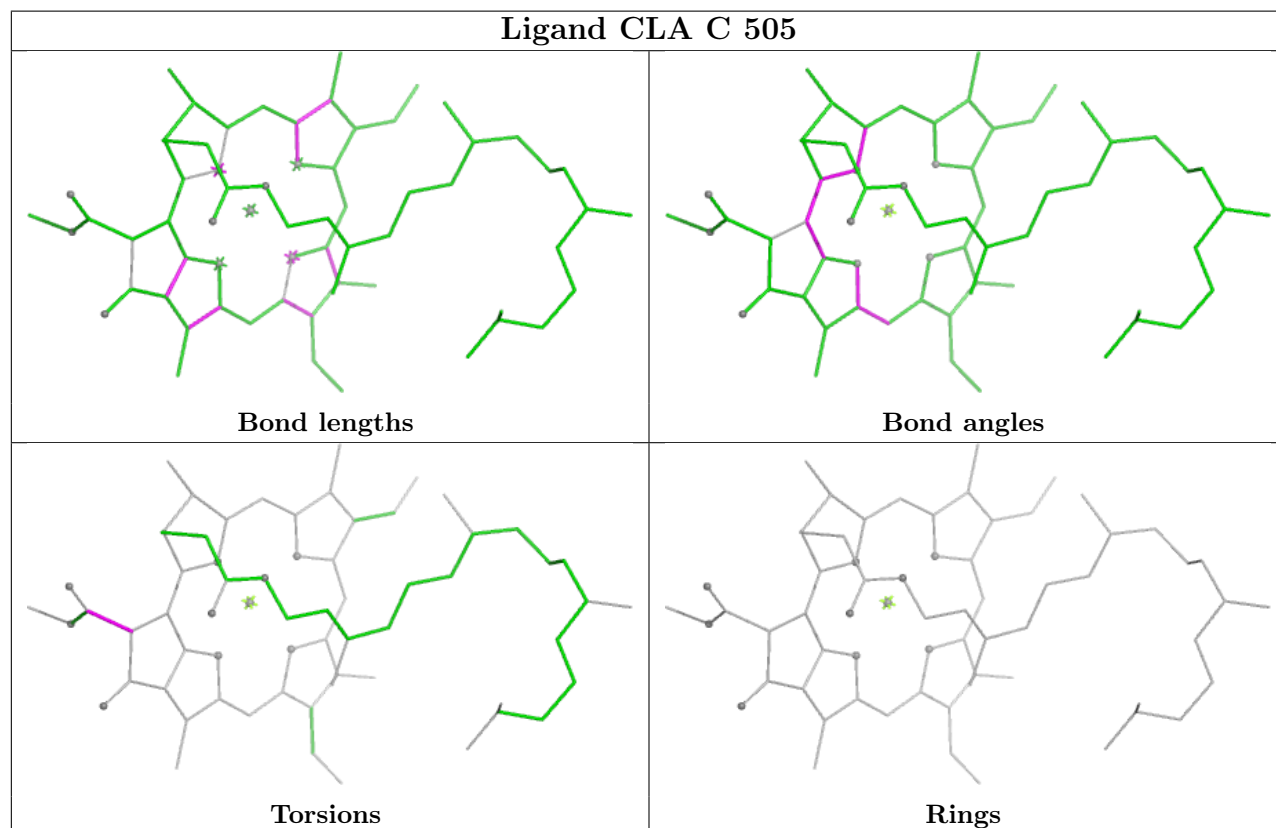
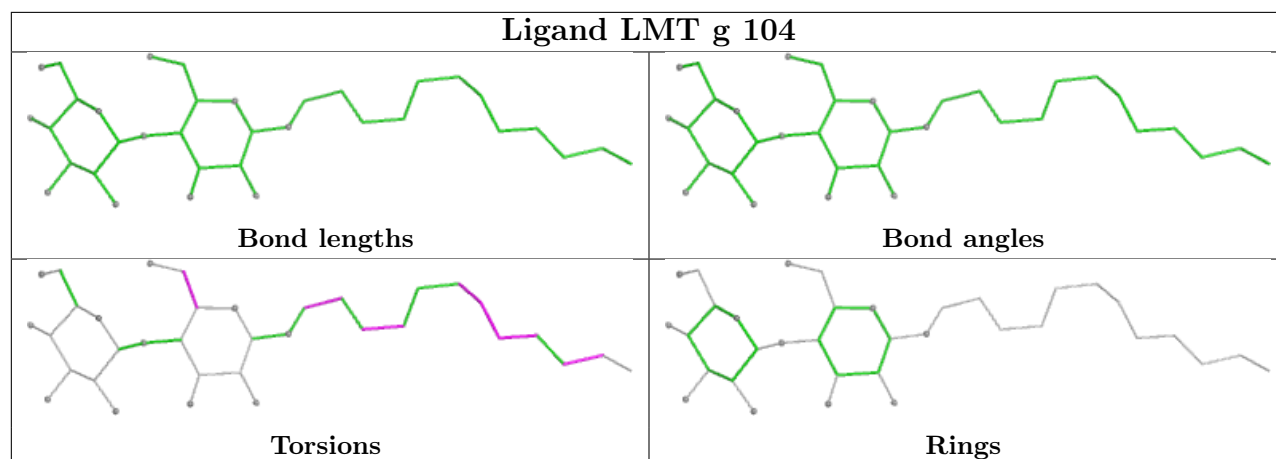
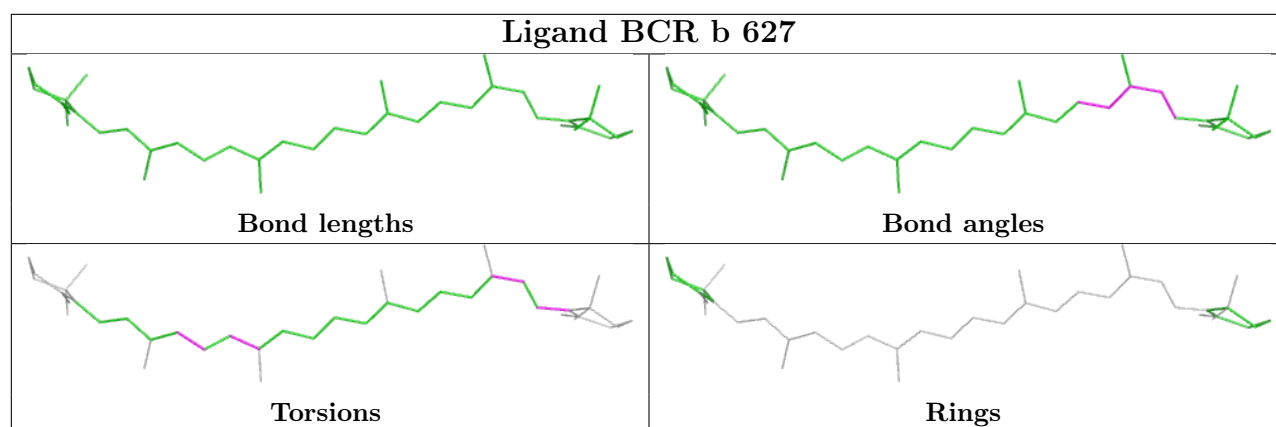


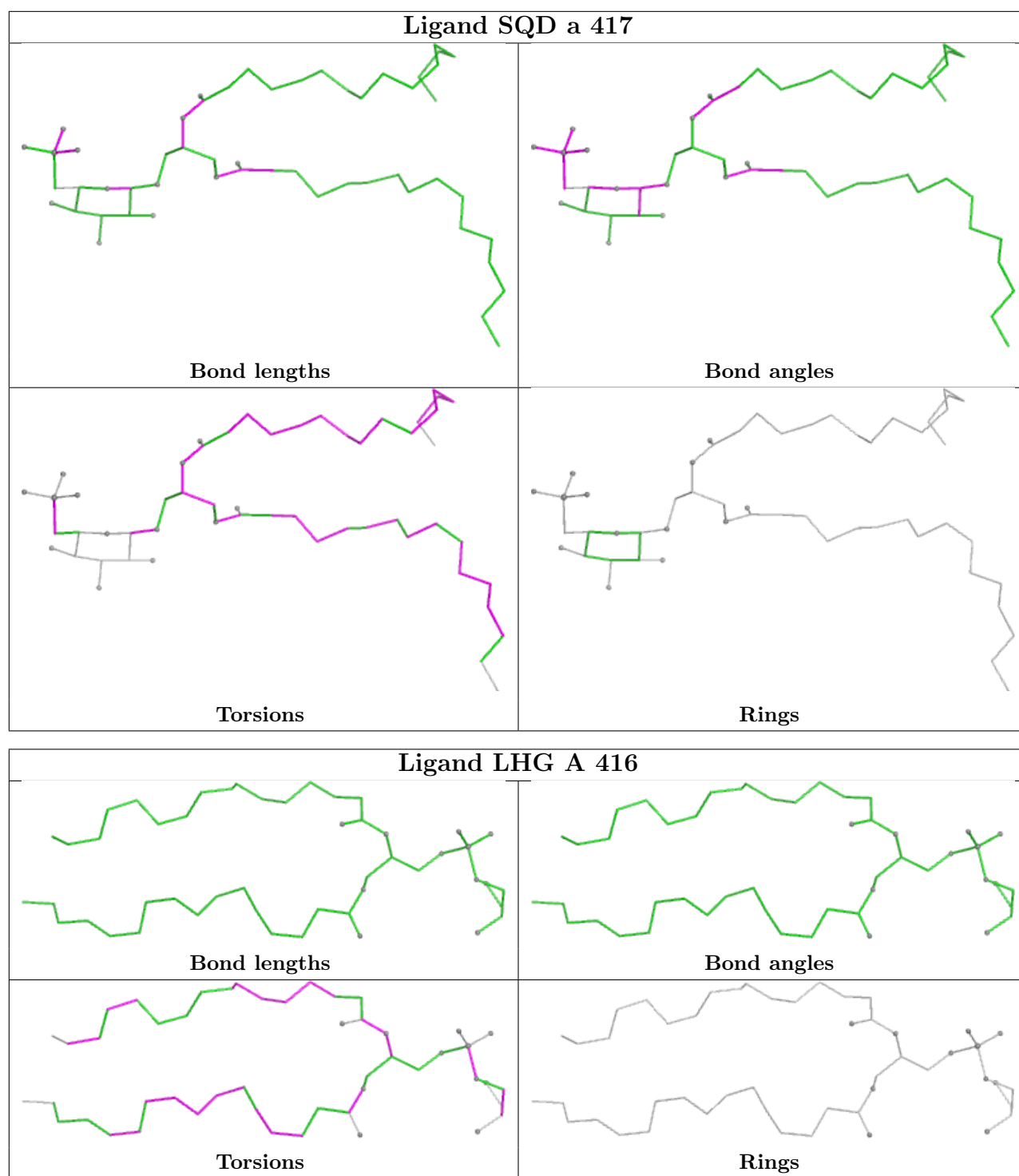
Ligand F6C b 617

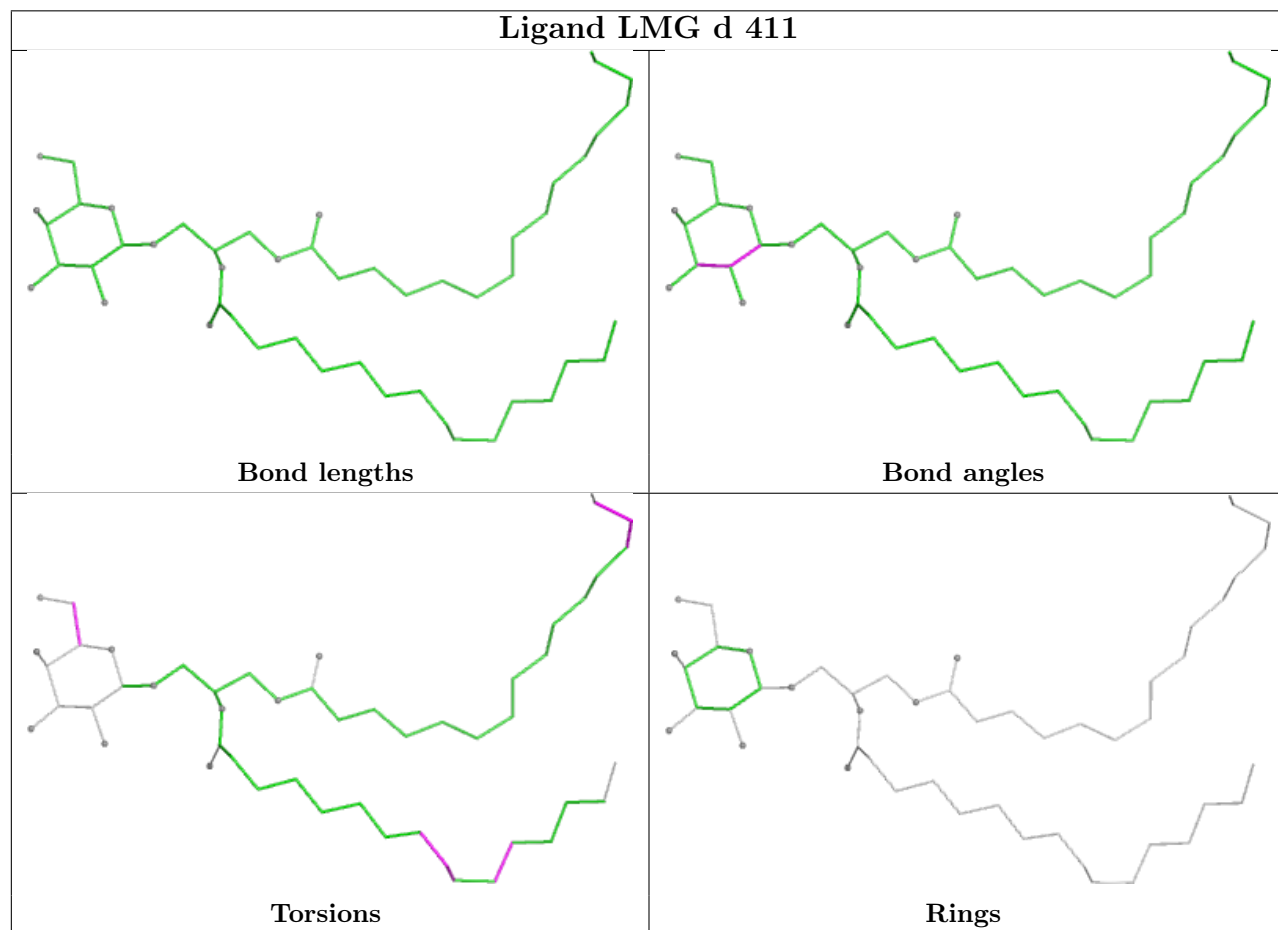
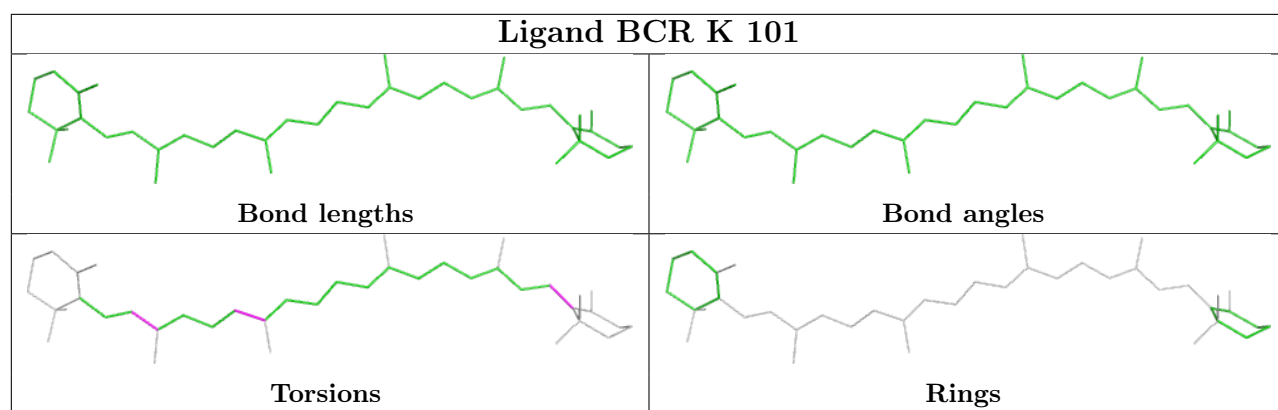


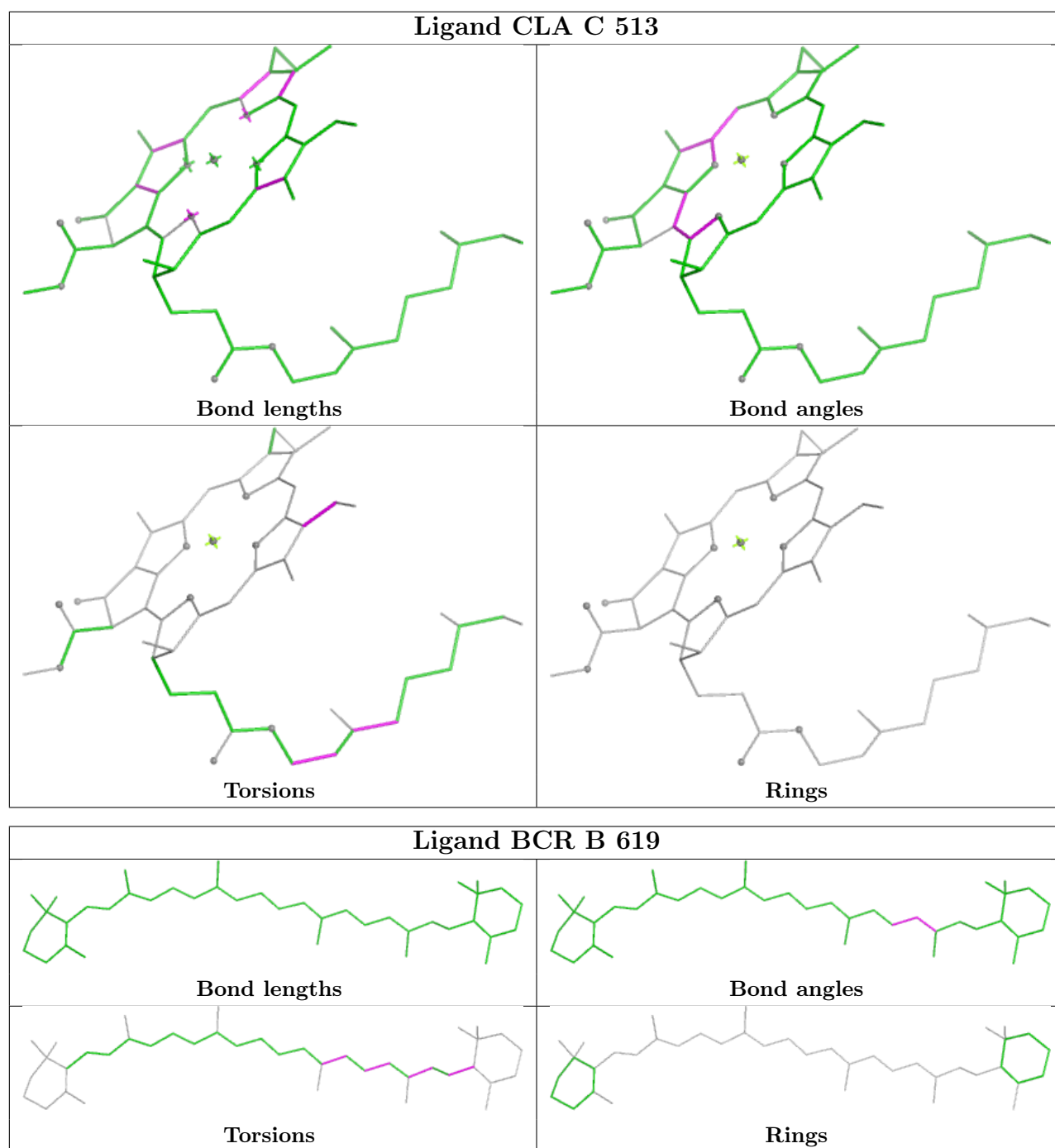
Ligand CLA c 501



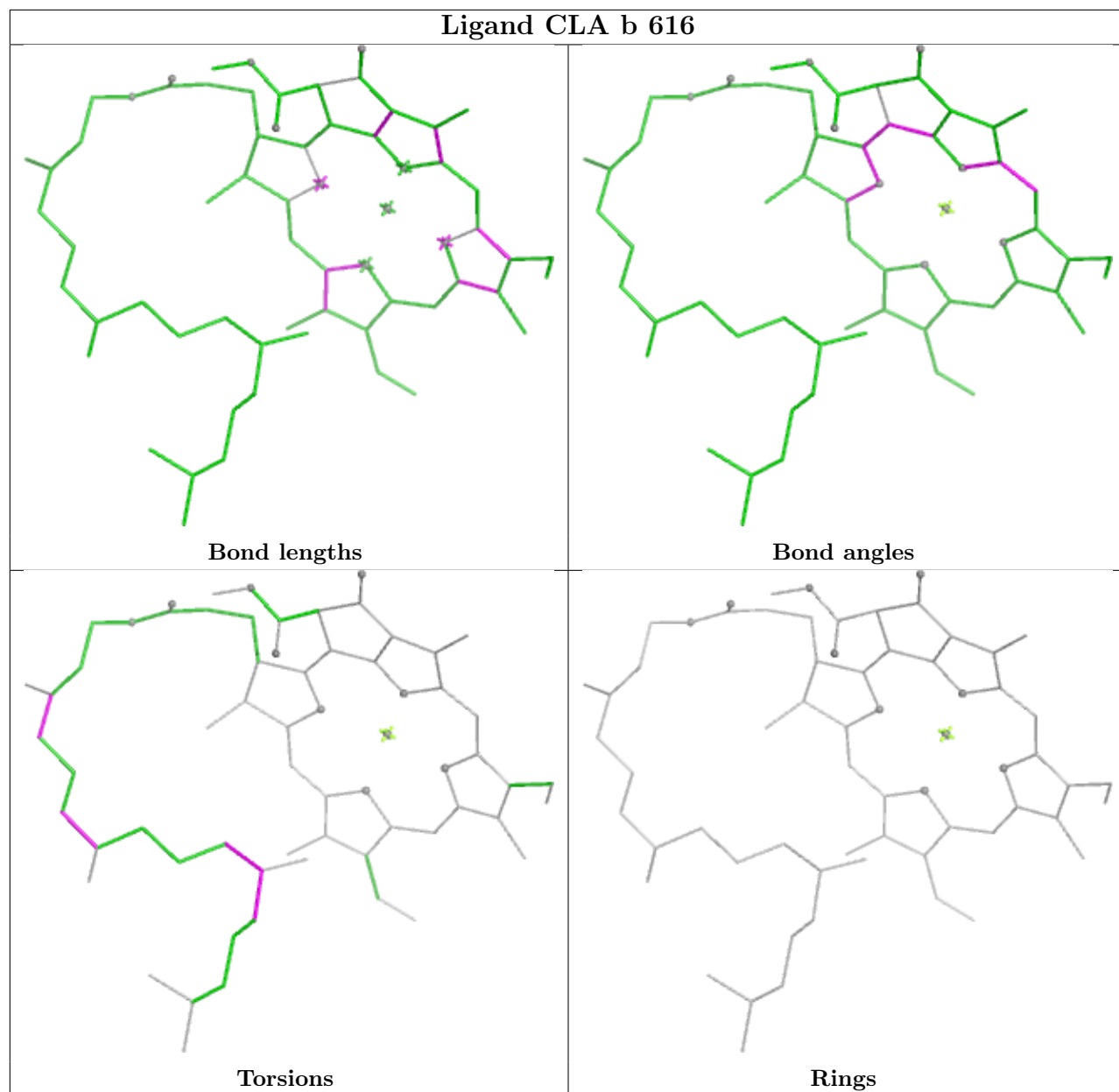


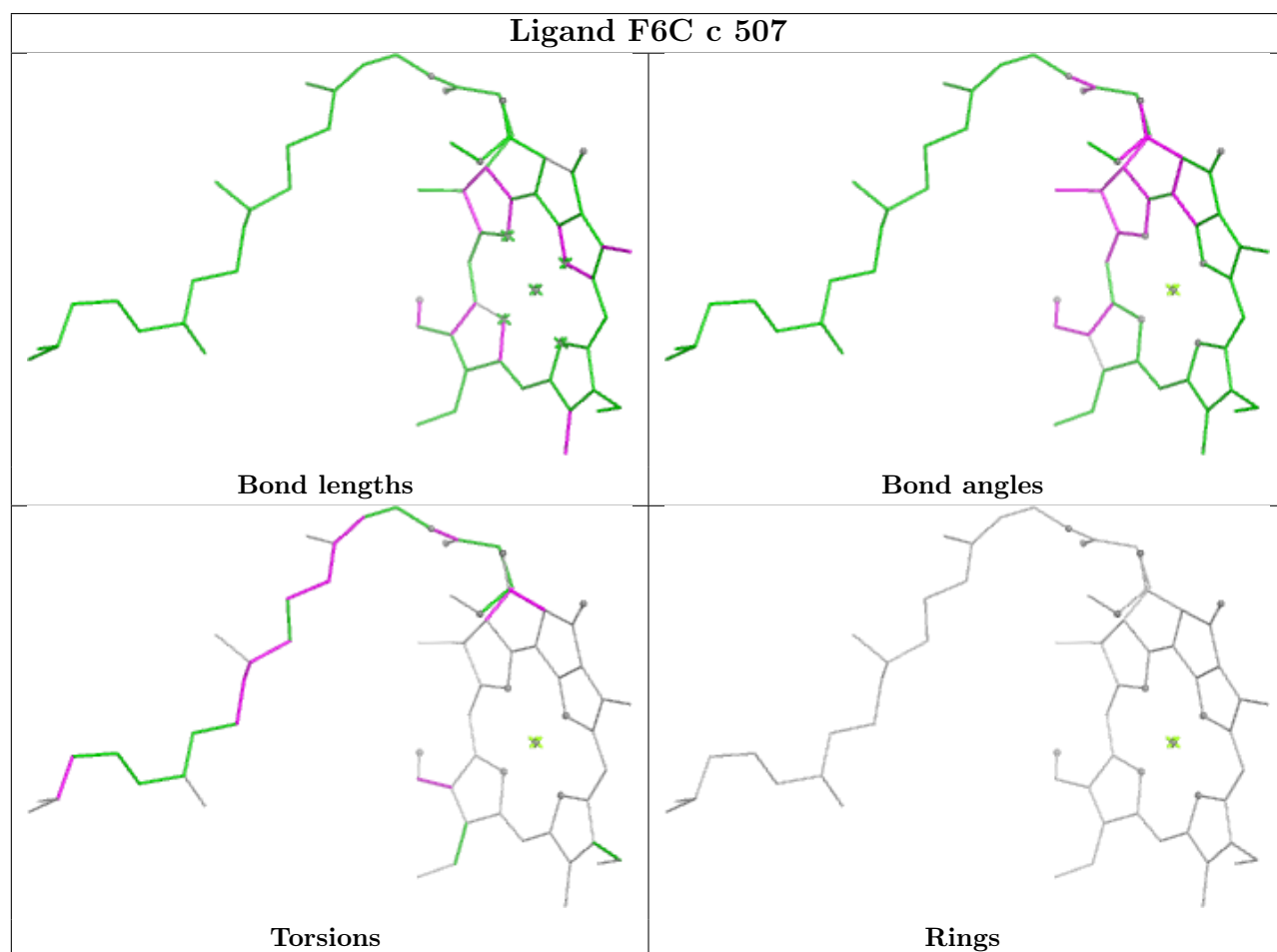
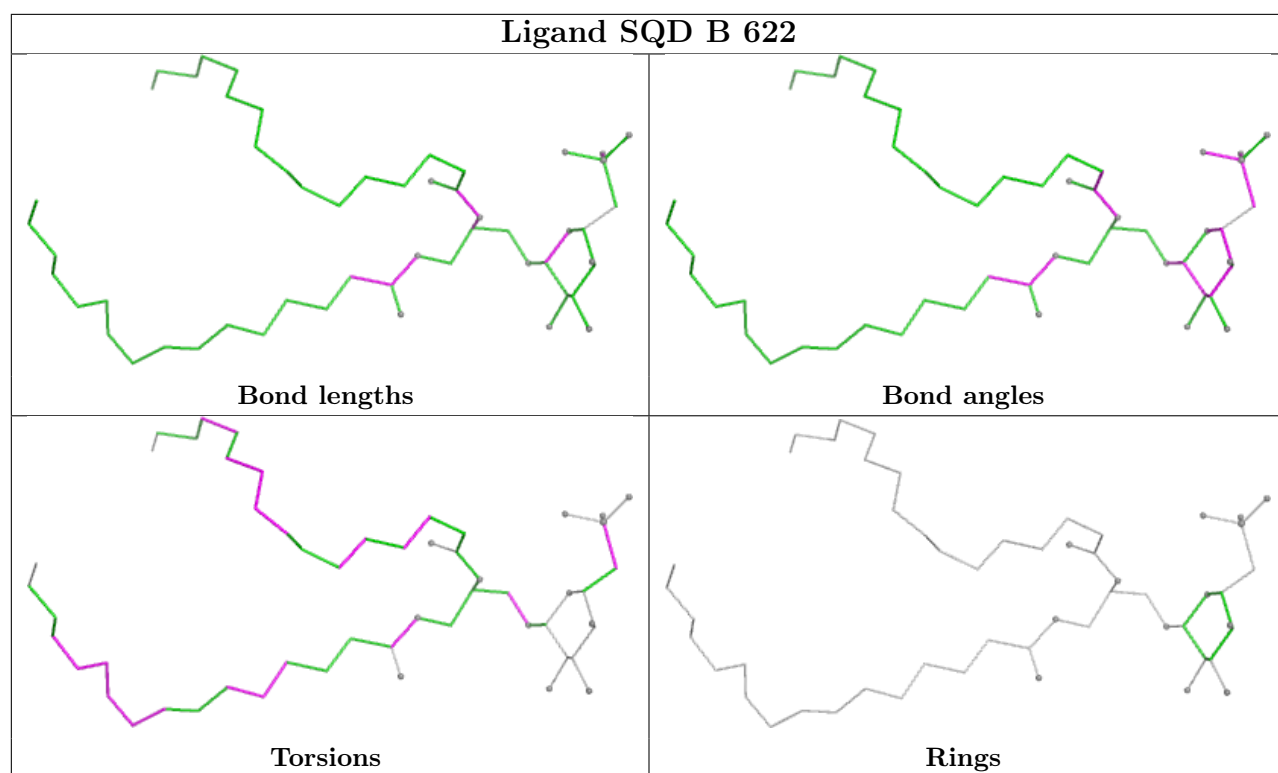


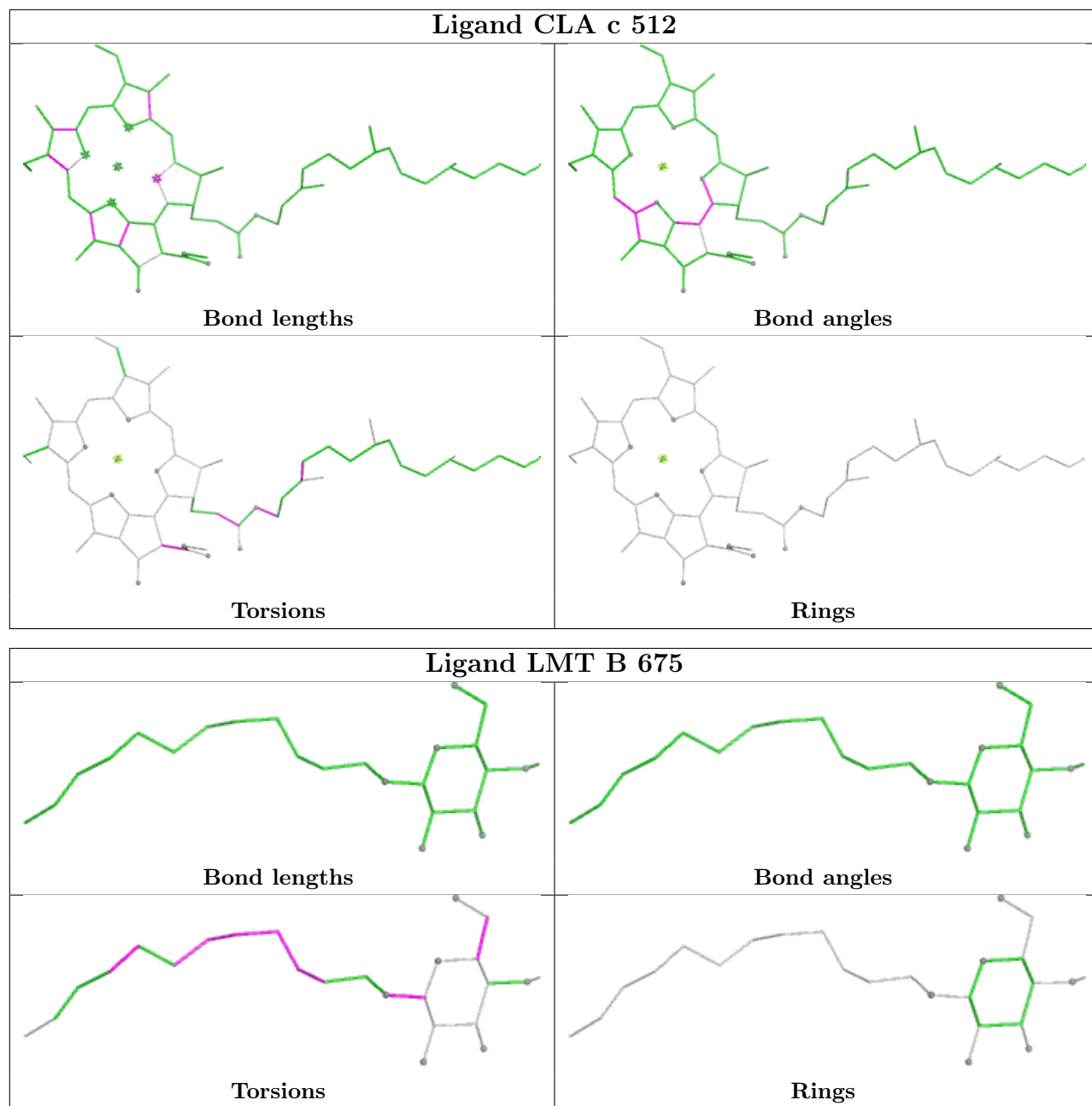


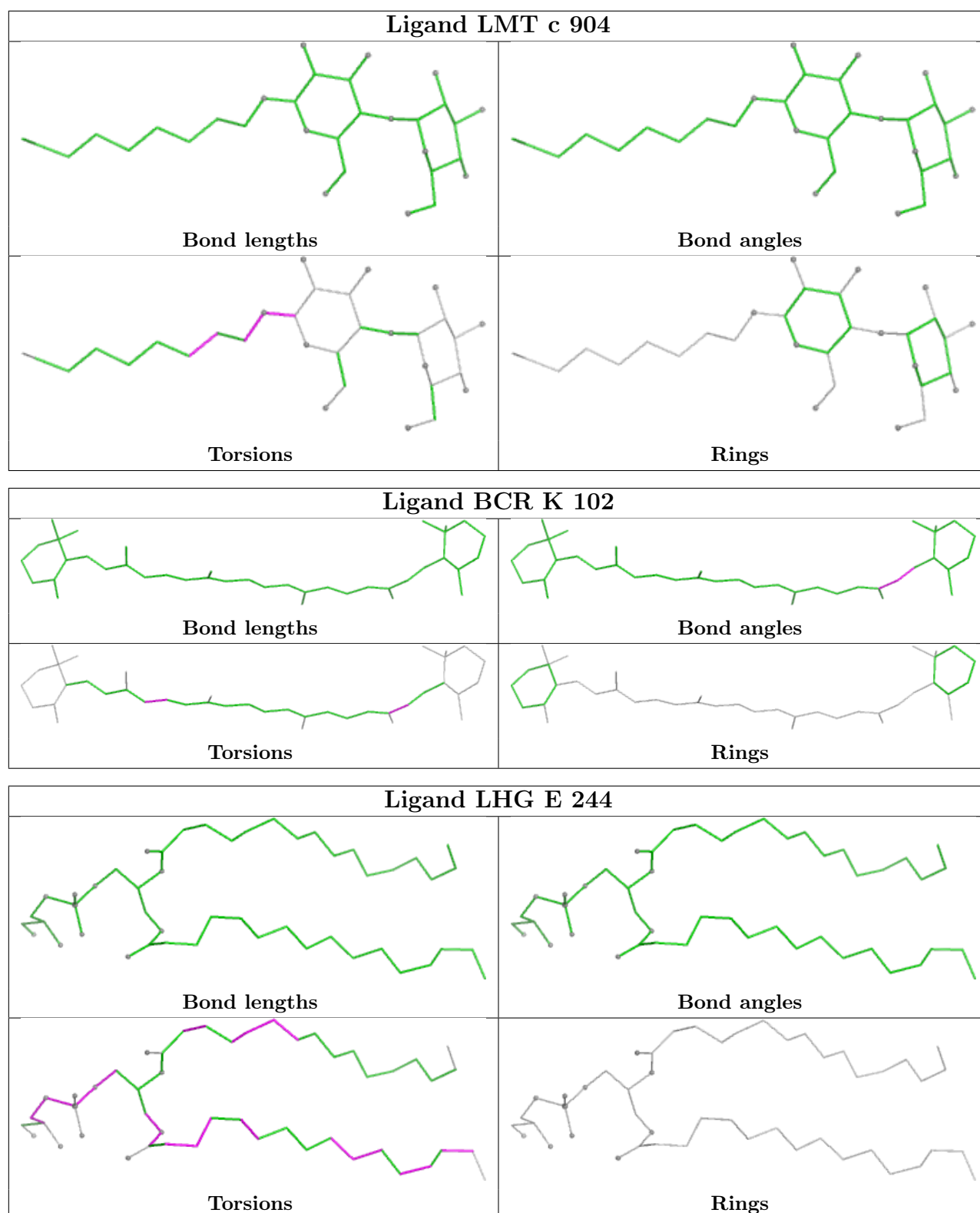


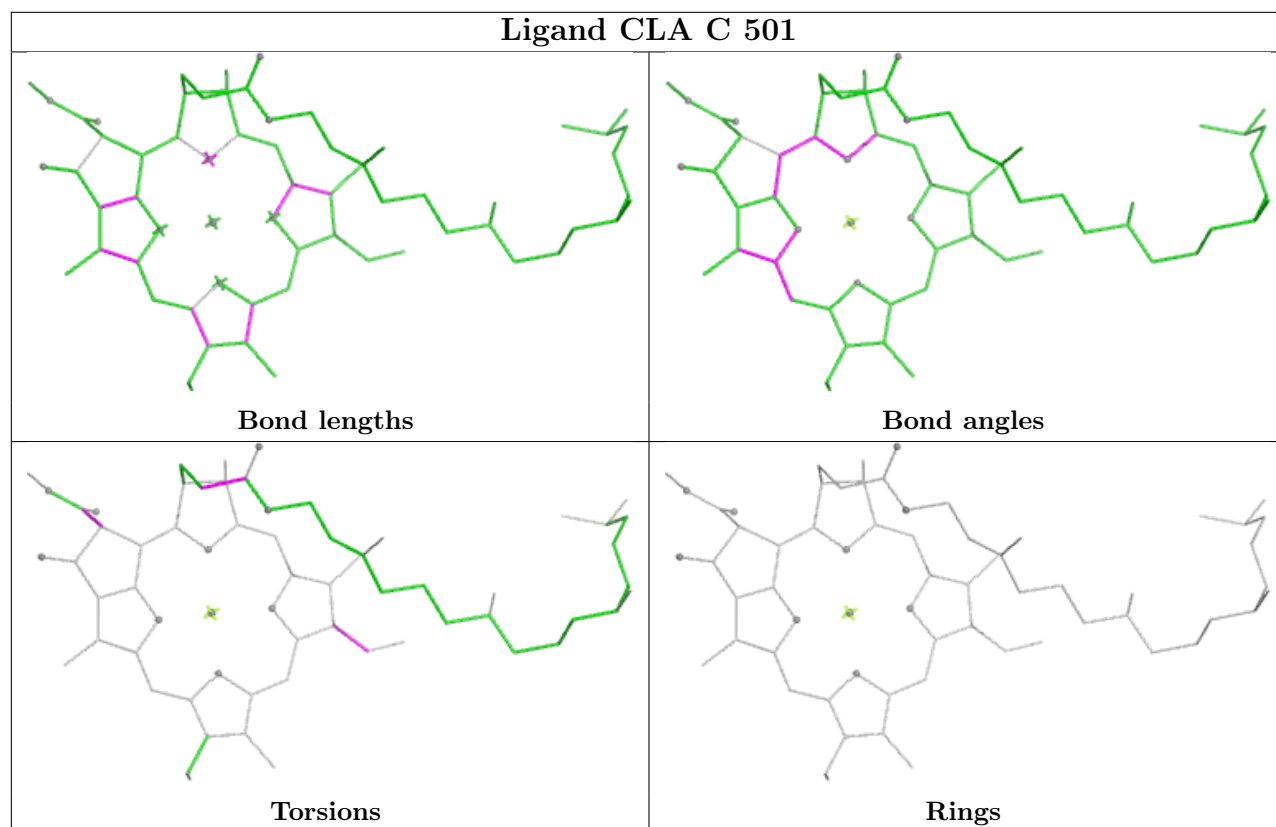
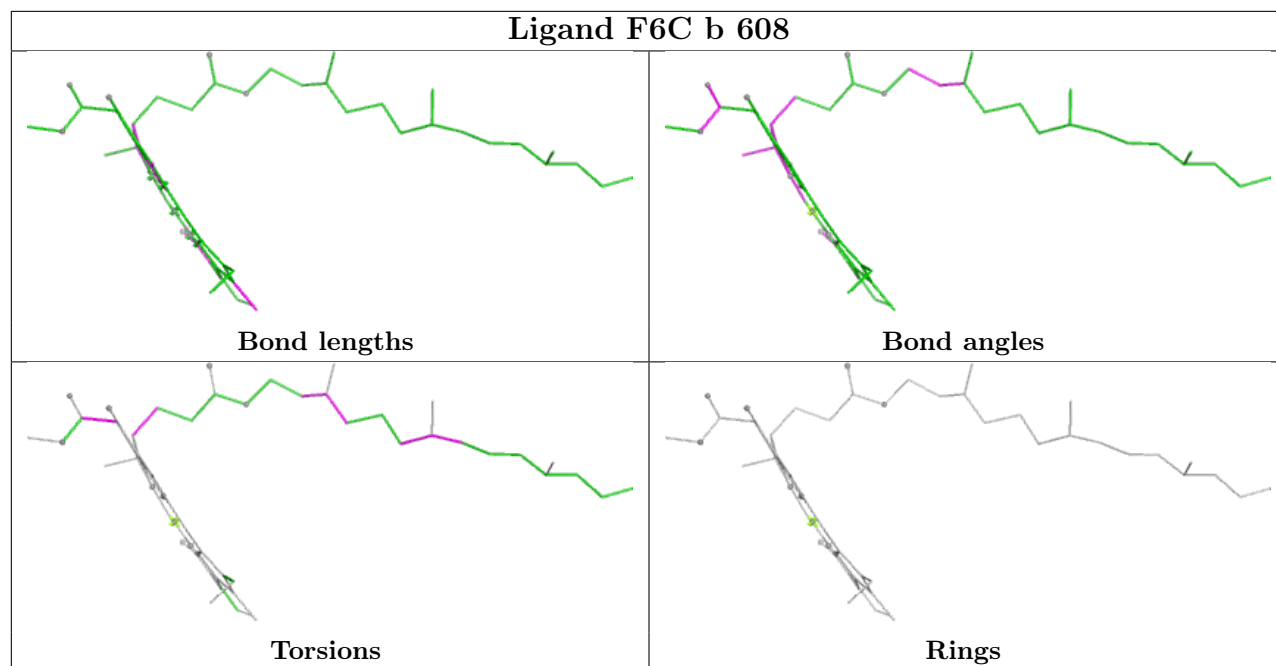
Ligand CLA b 616

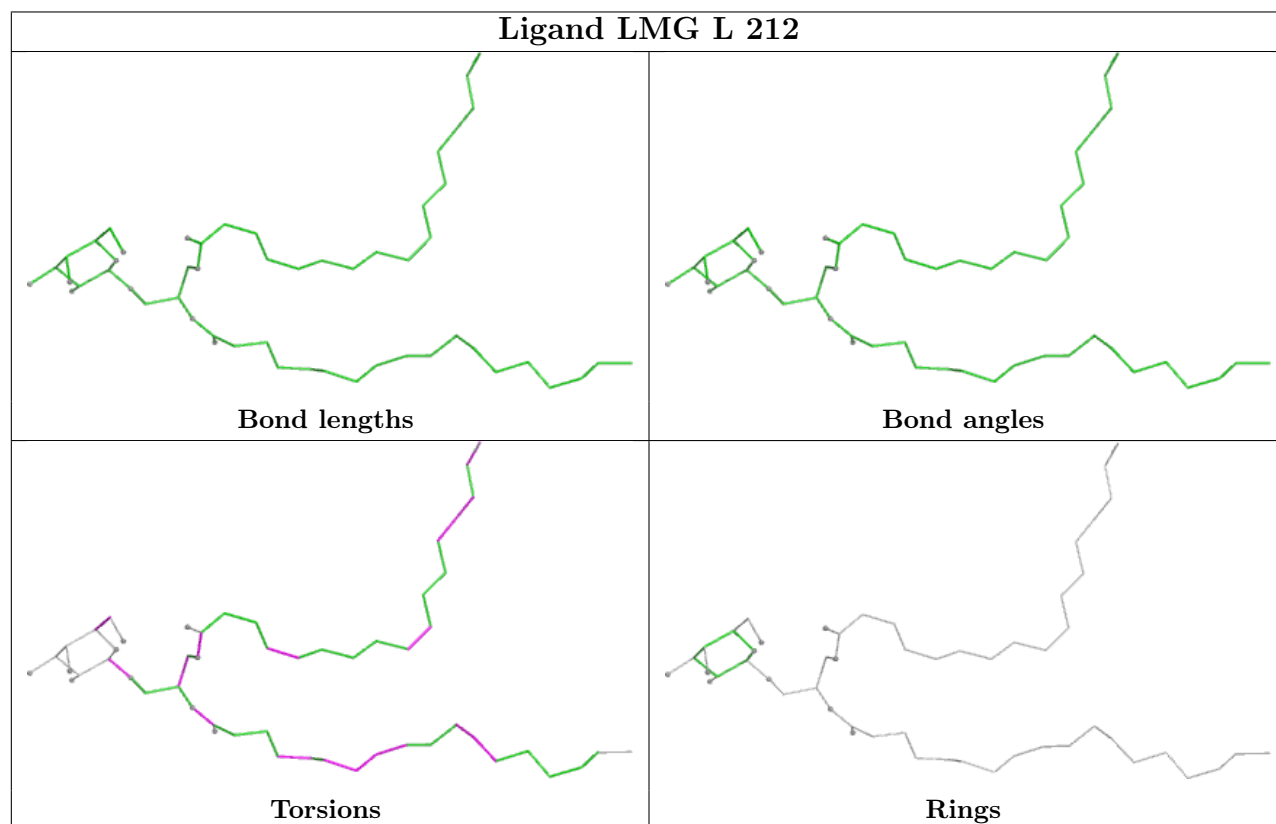
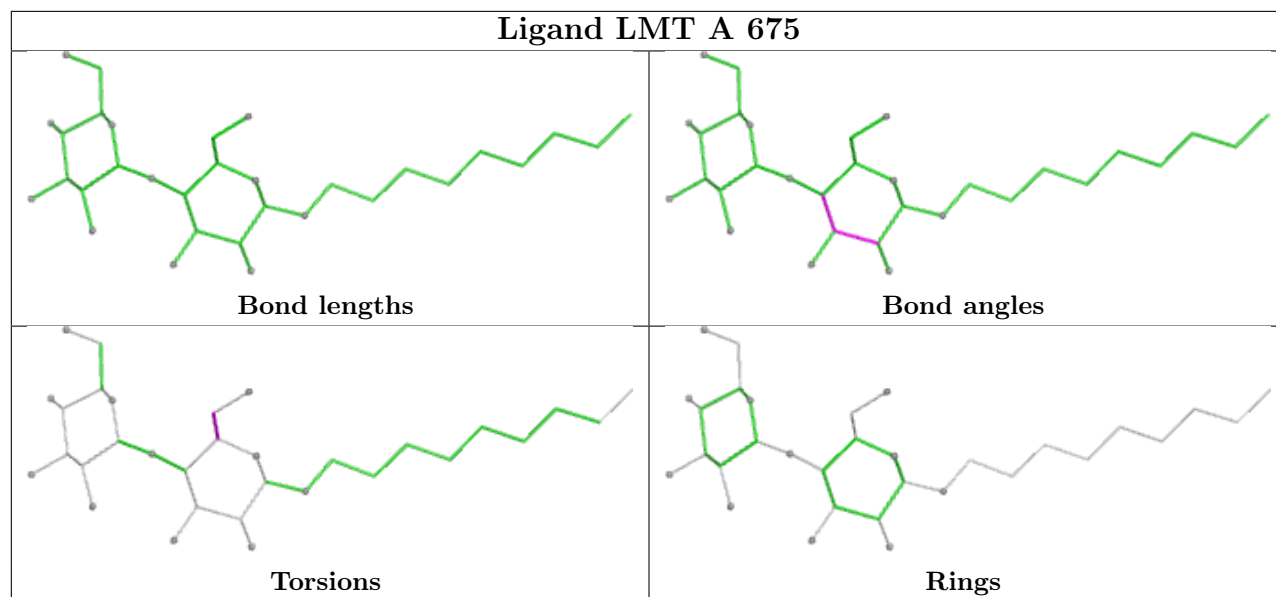


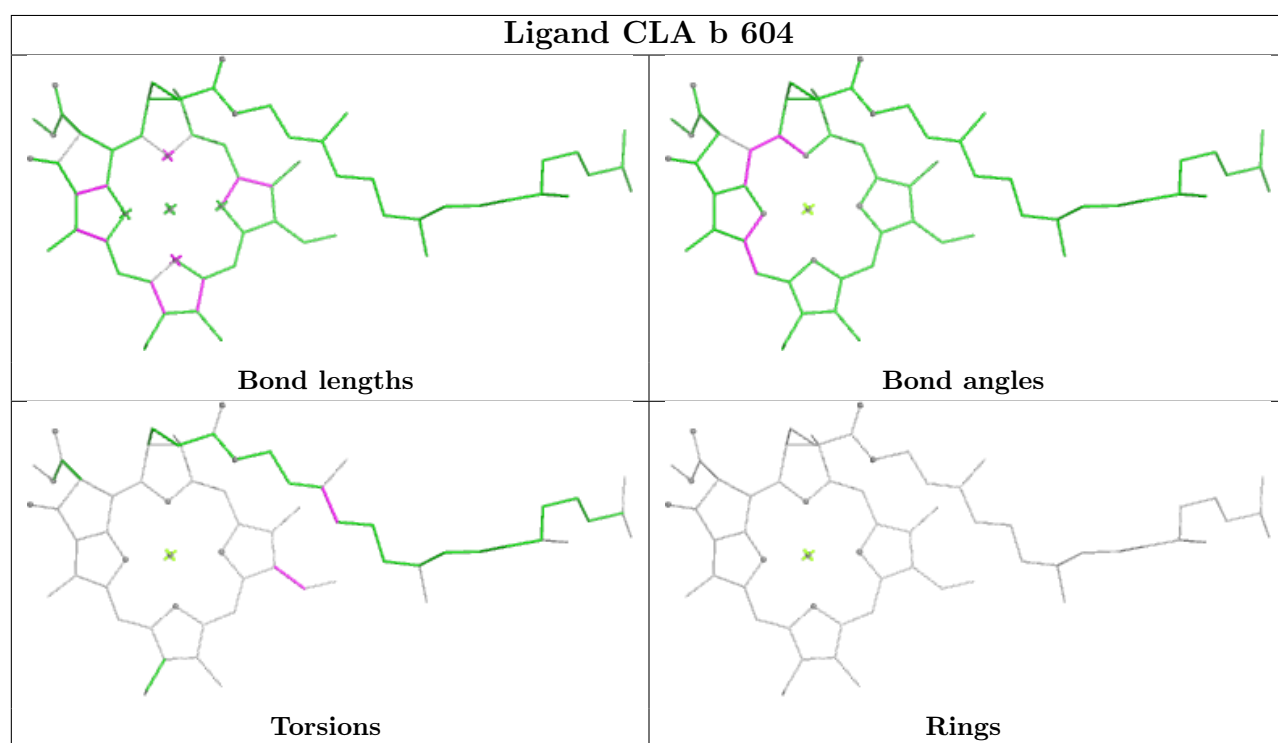
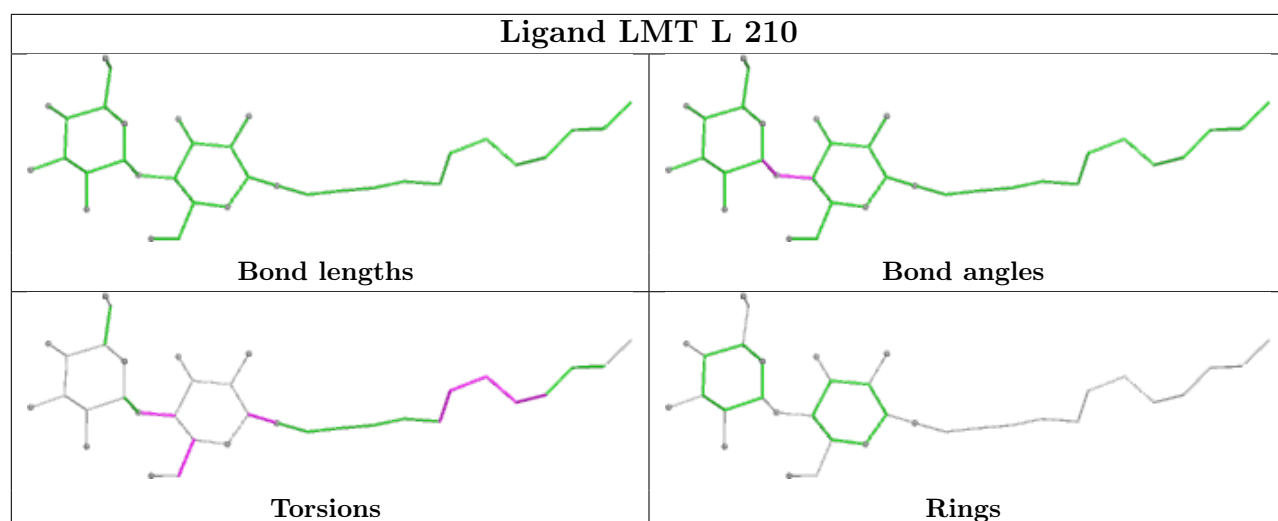


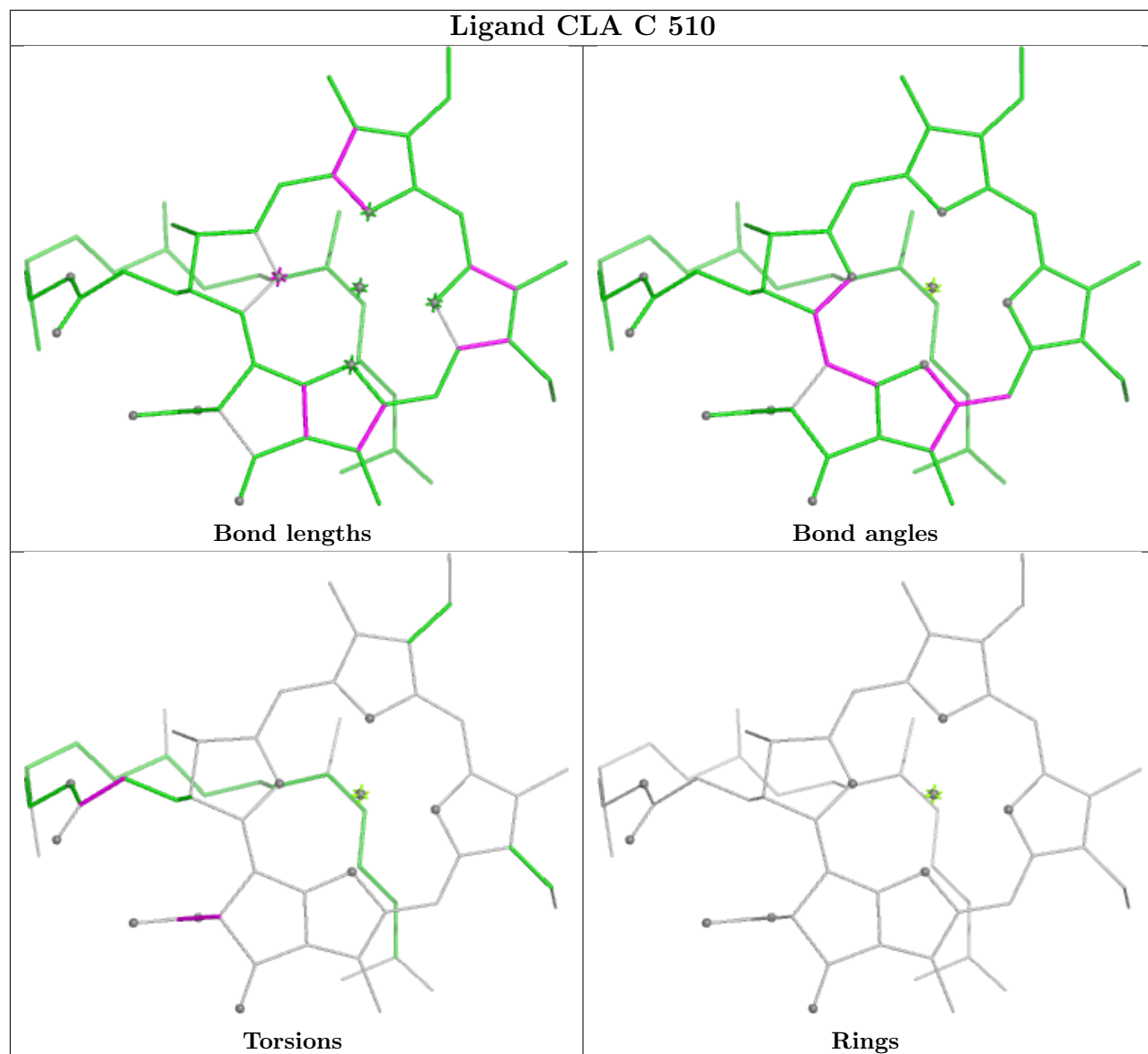


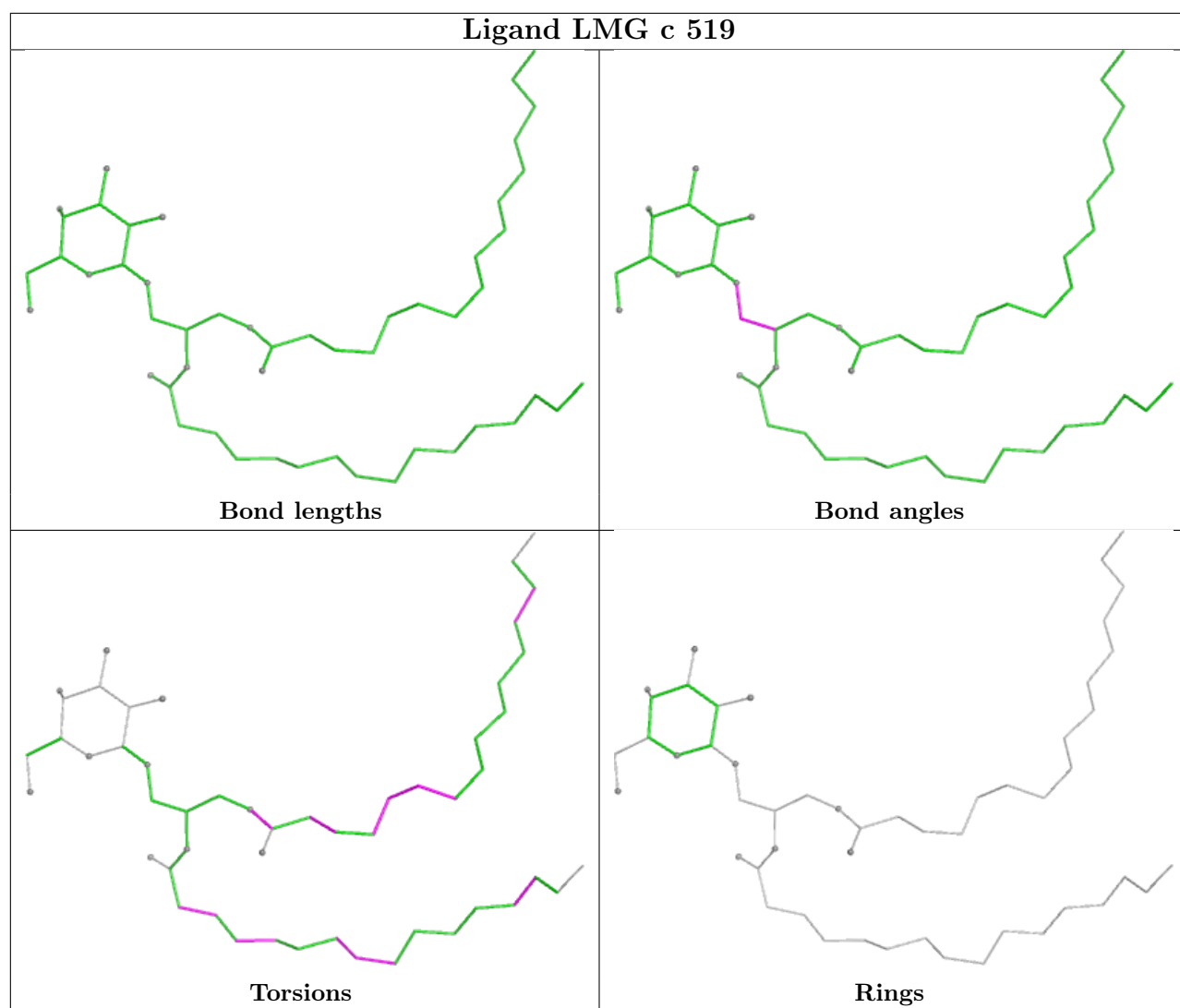


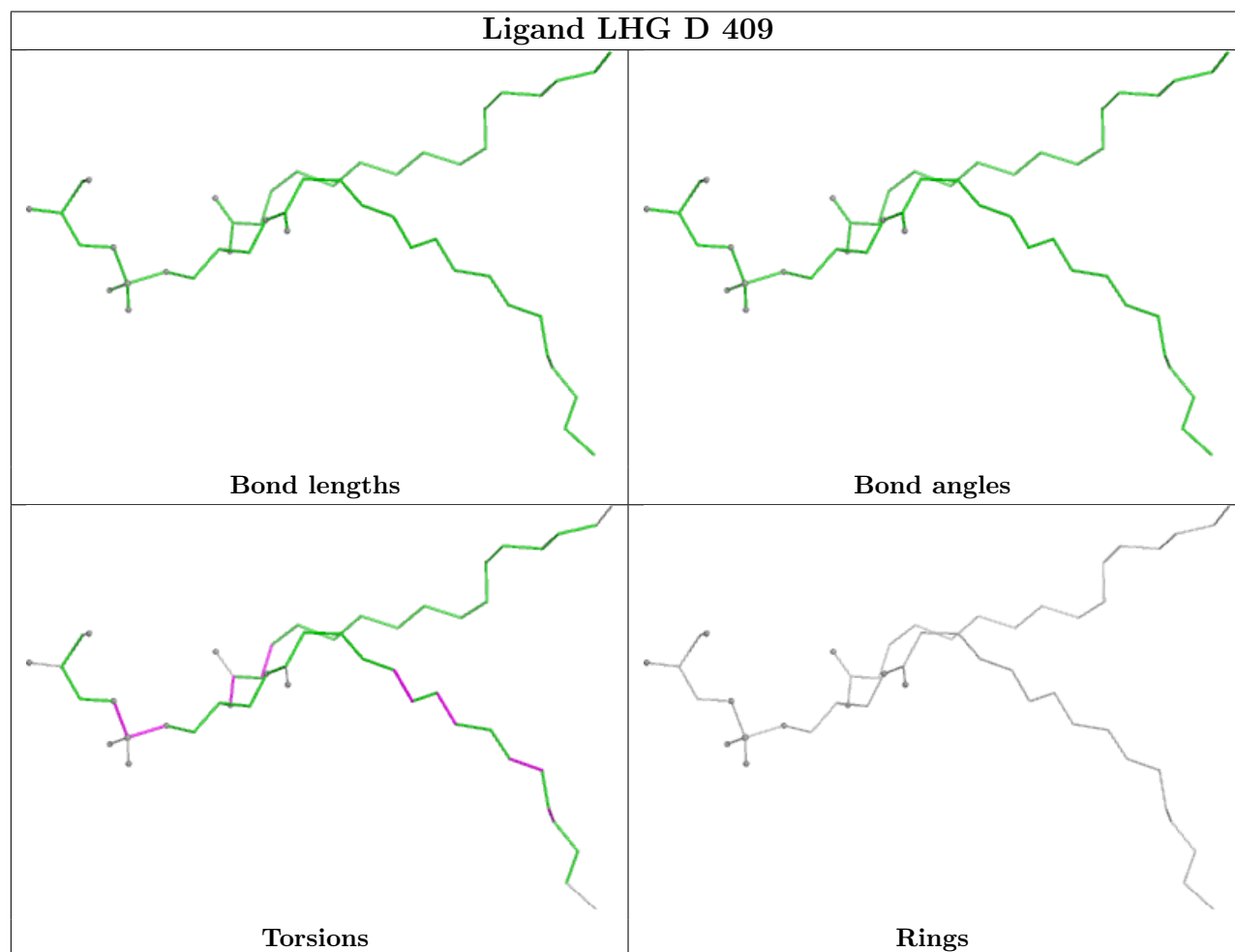
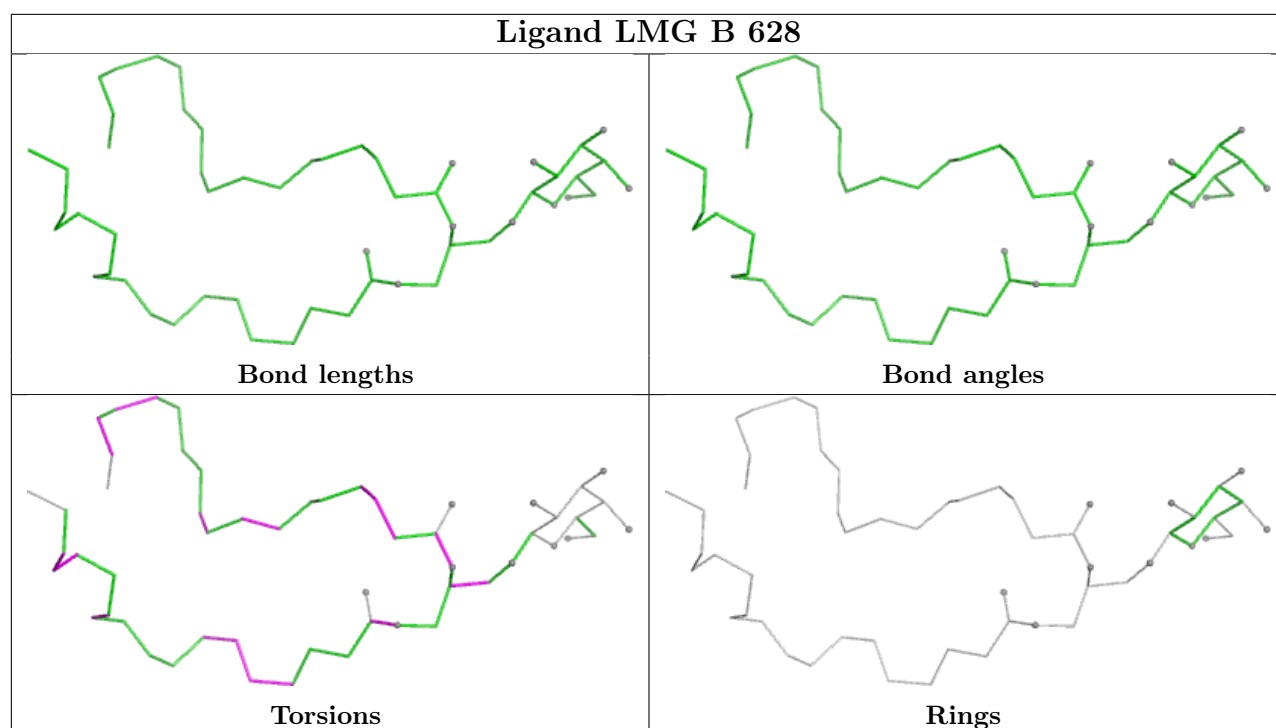




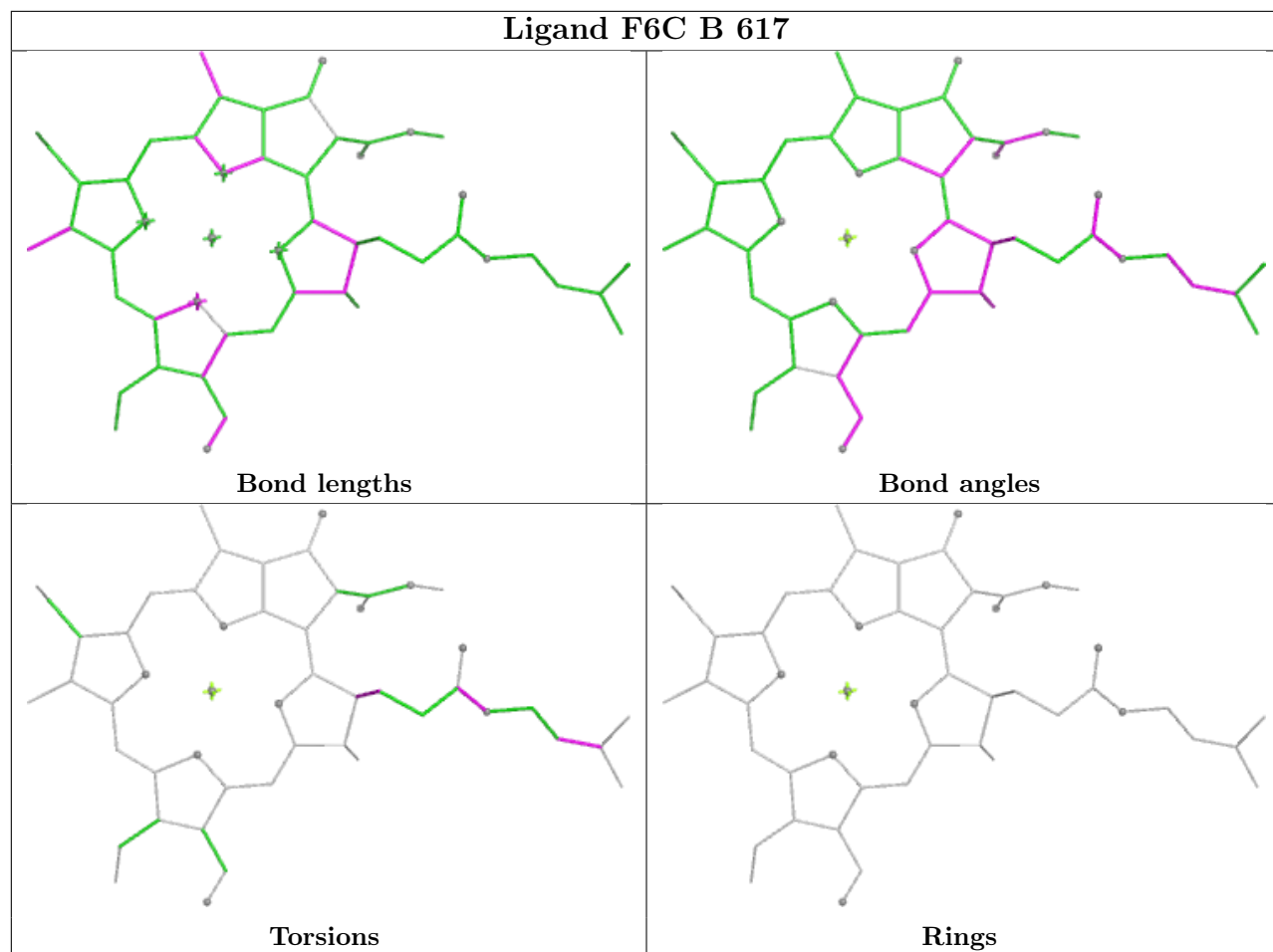




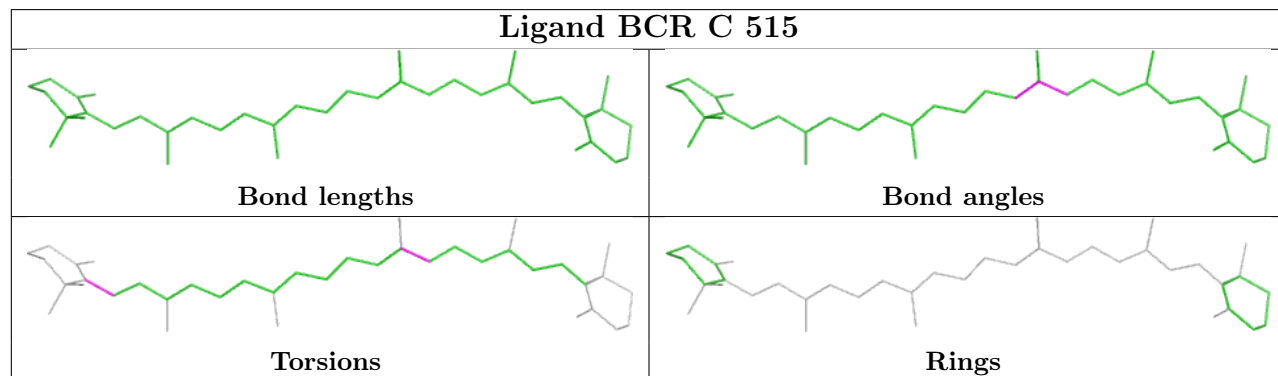




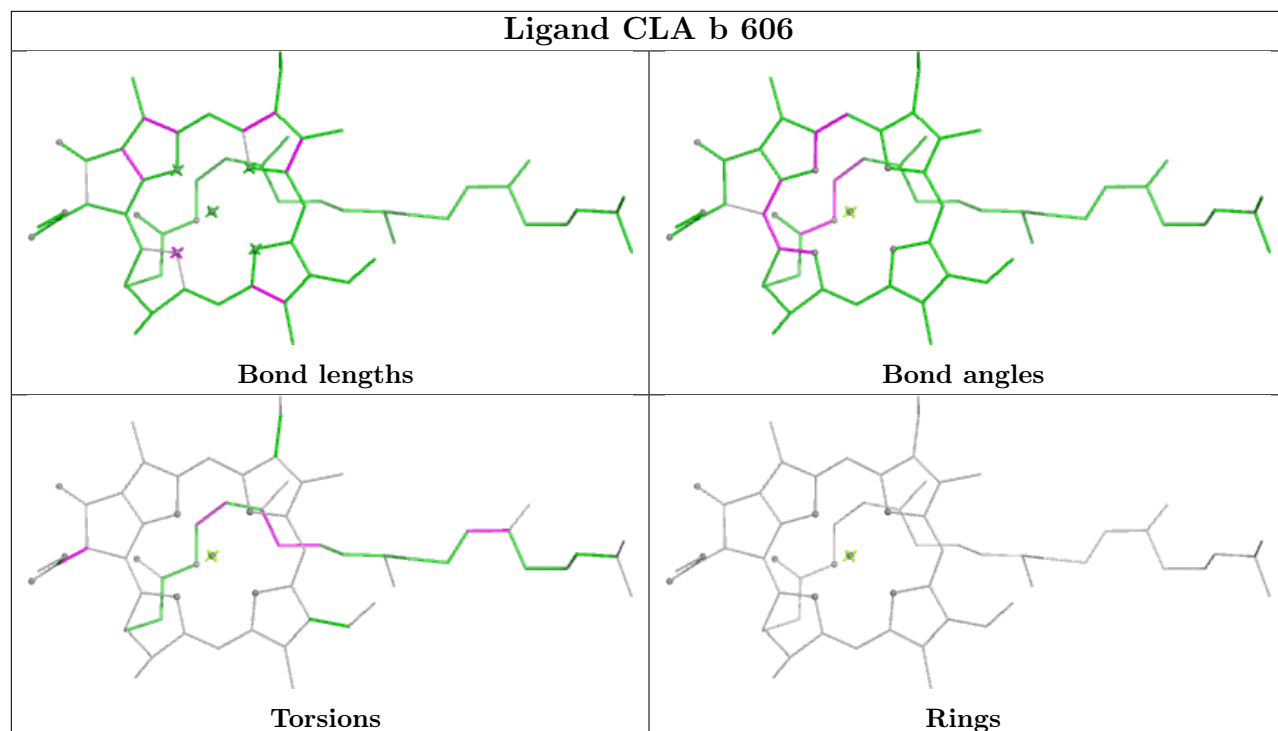
Ligand F6C B 617



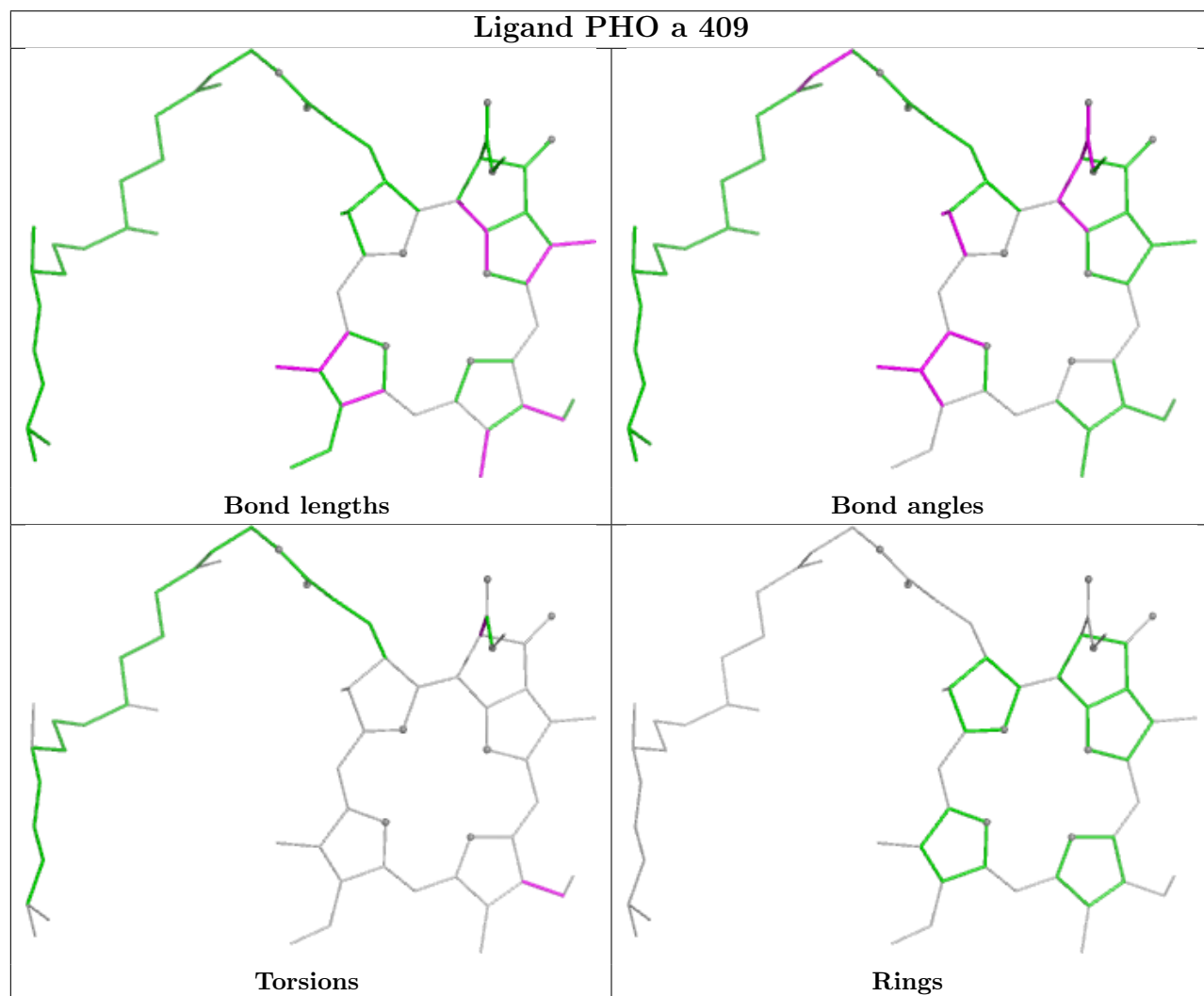
Ligand BCR C 515

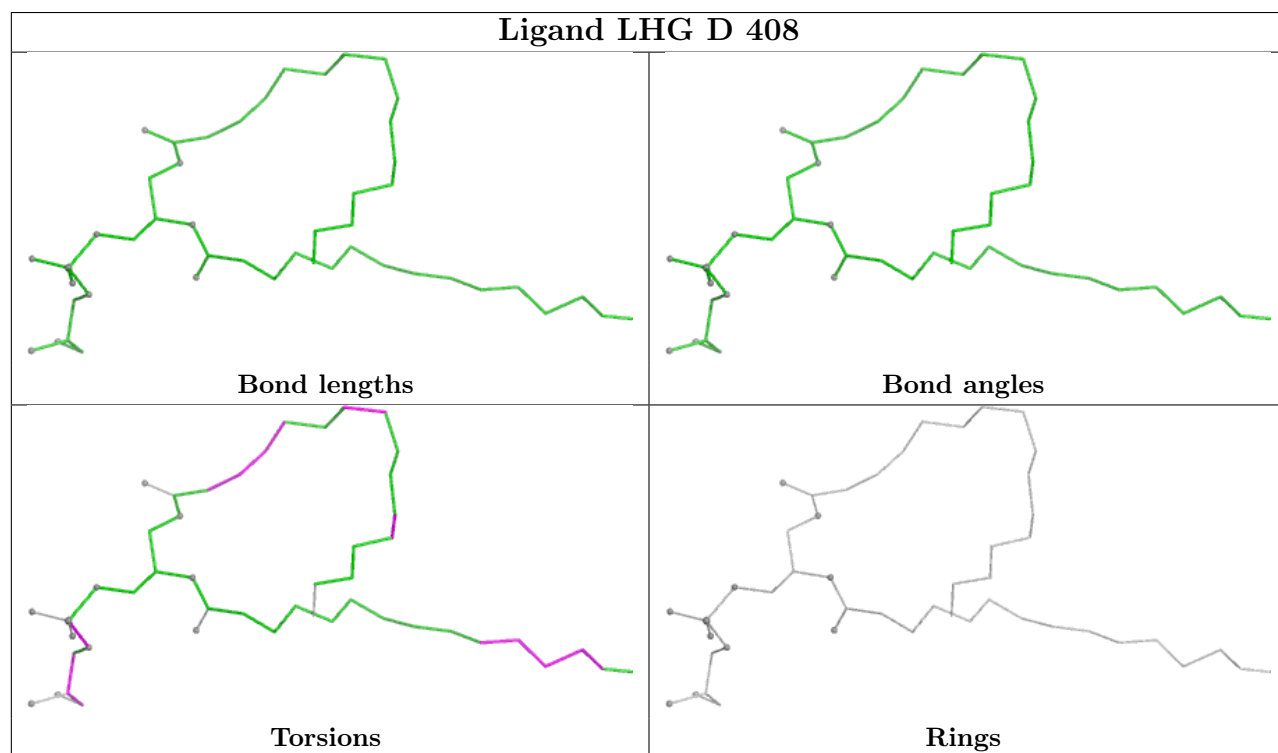
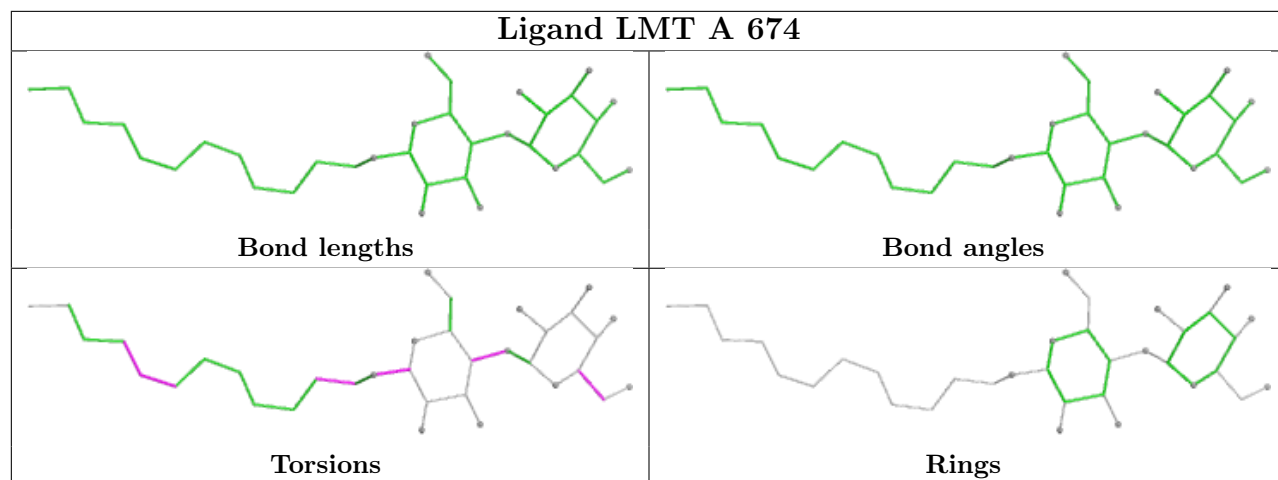


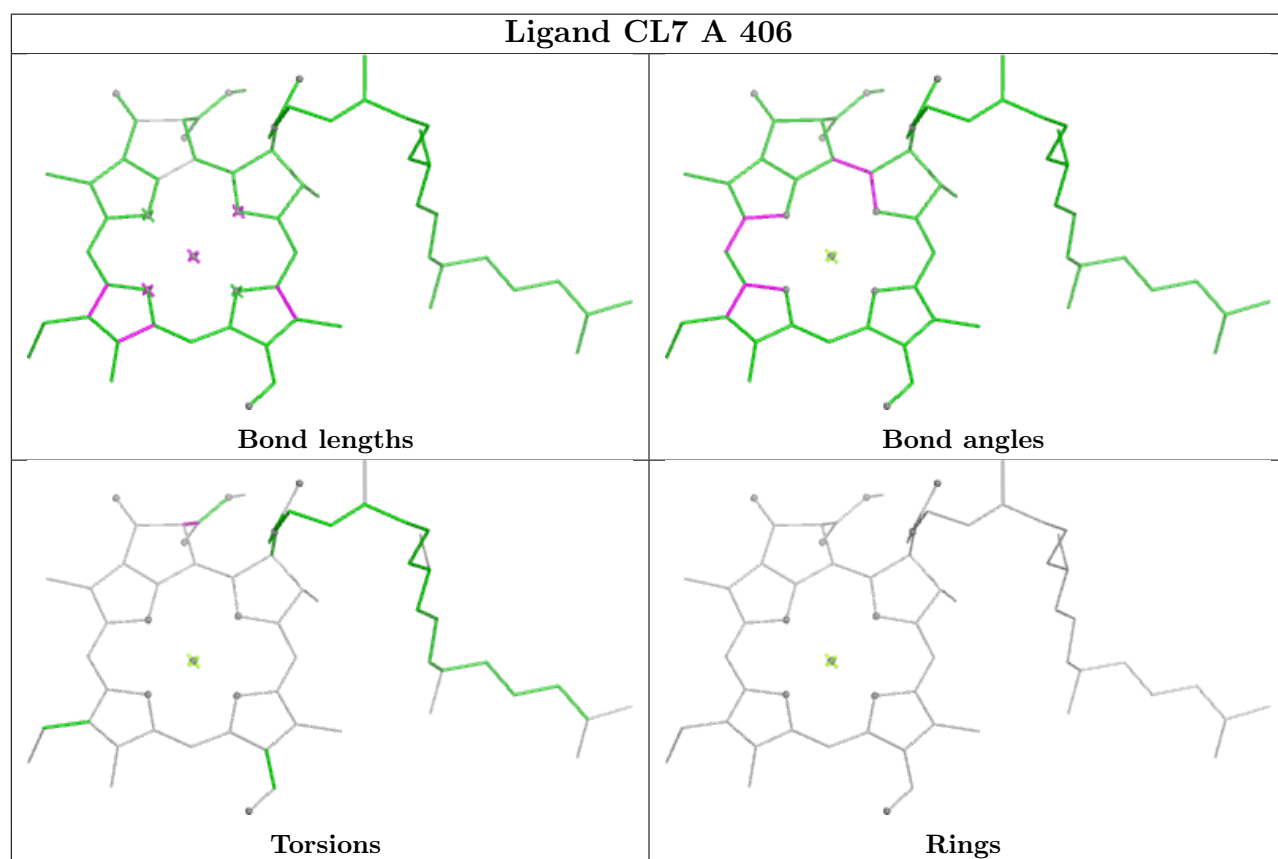
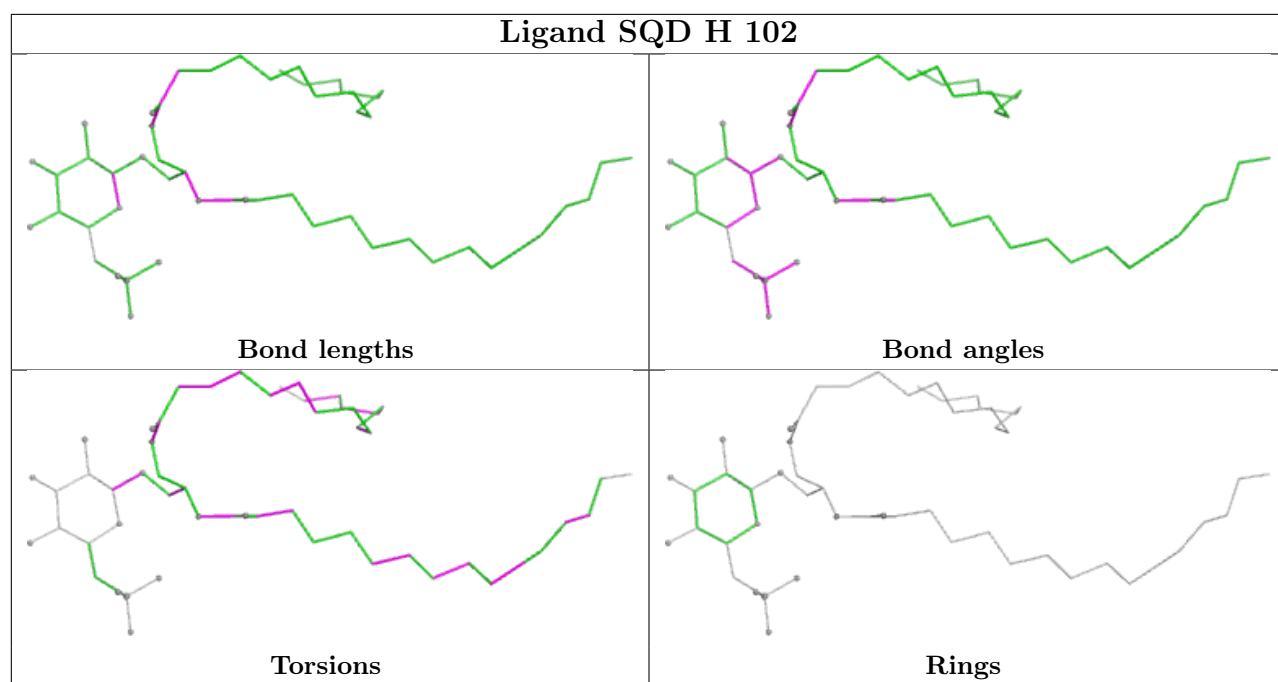
Ligand CLA b 606

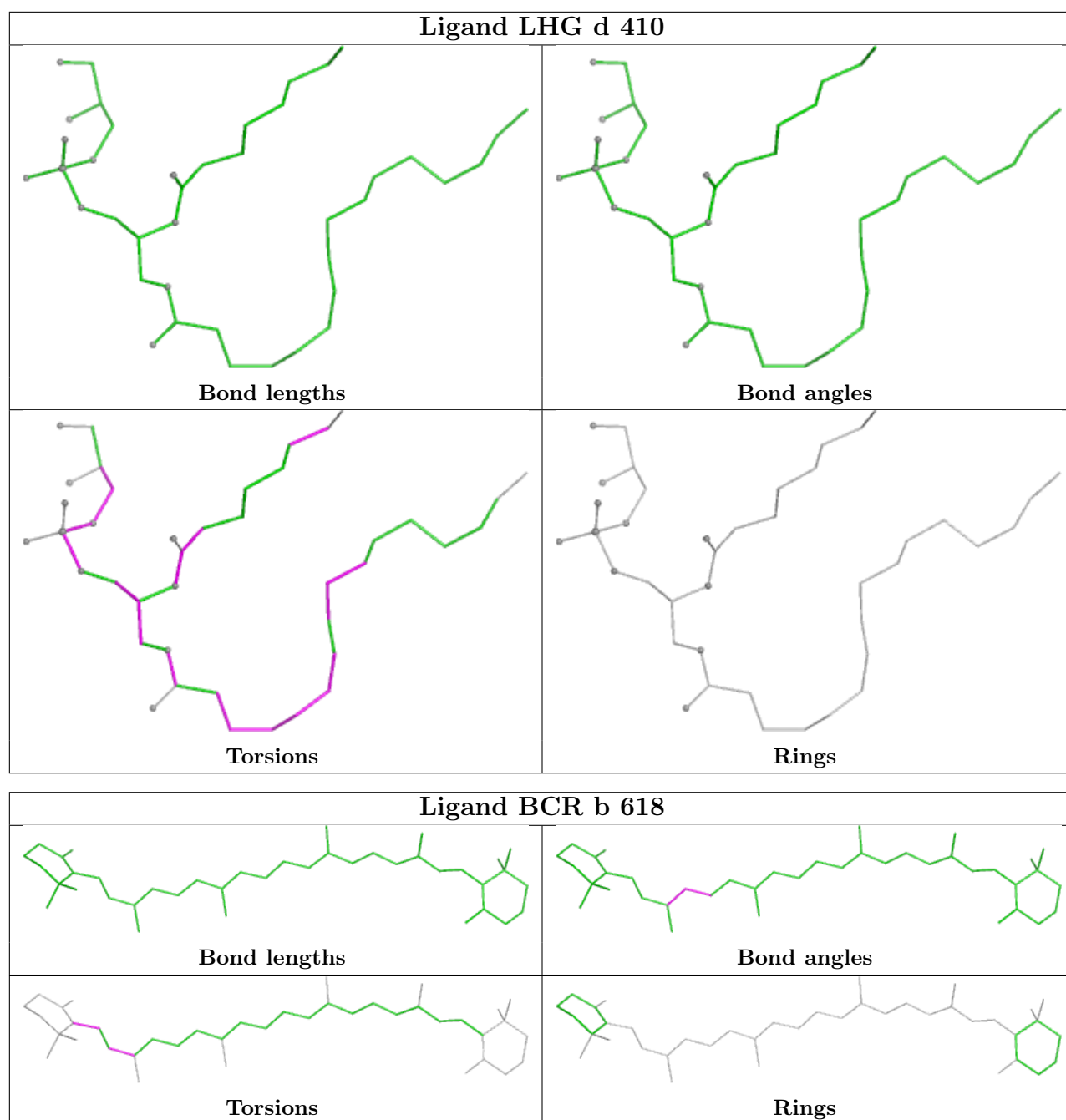


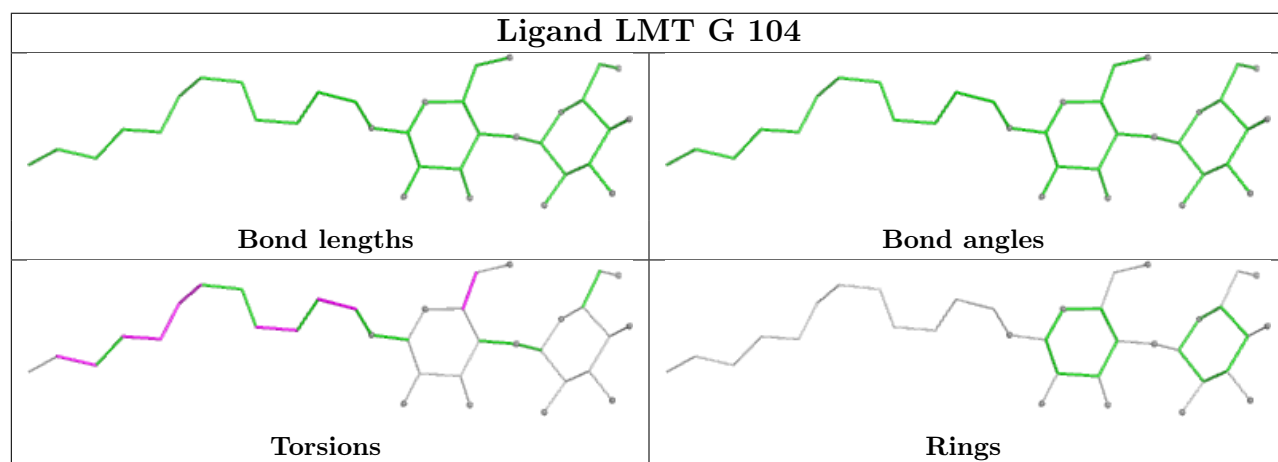
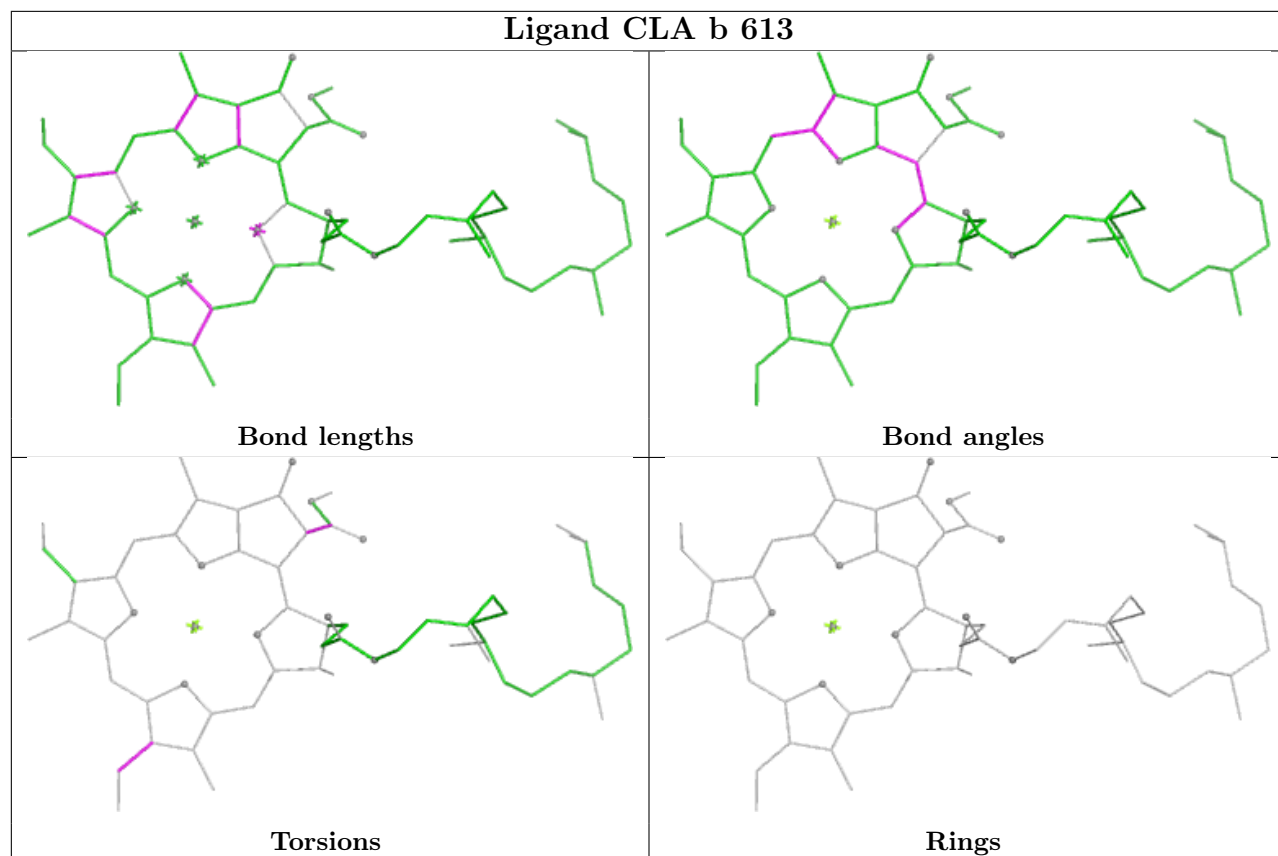
Ligand PHO a 409

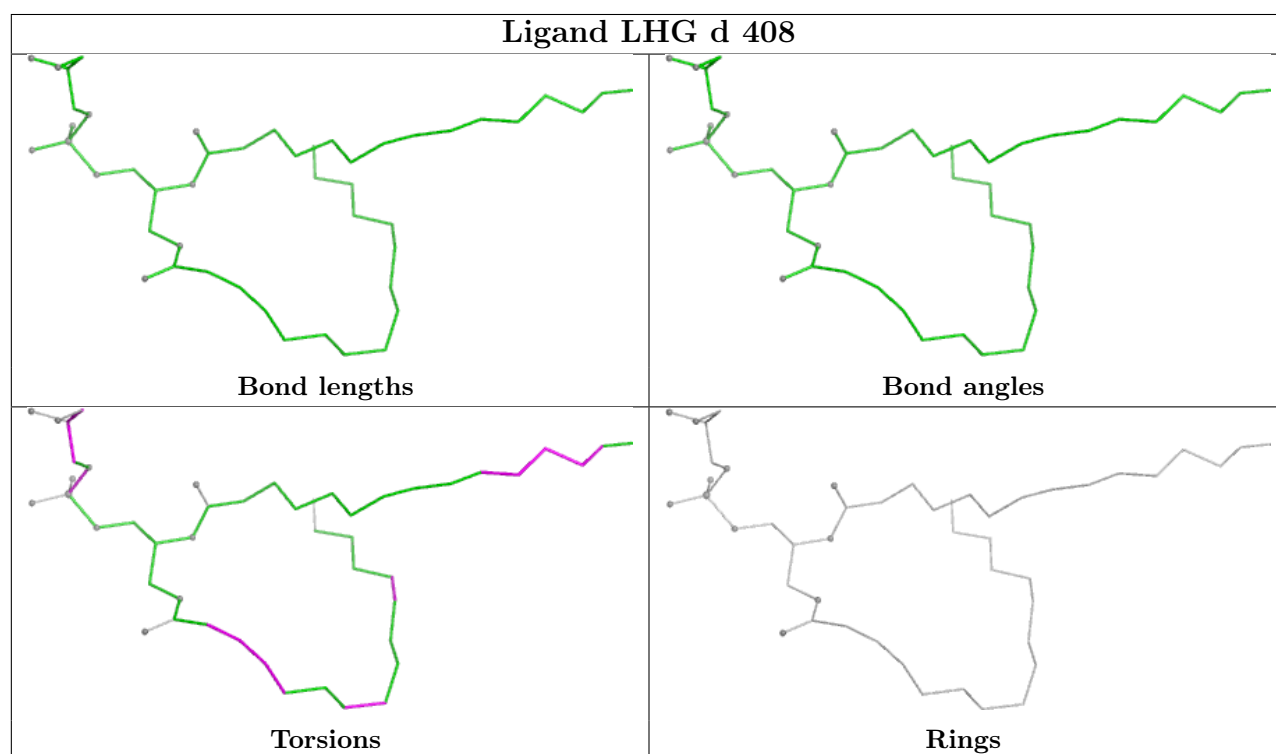
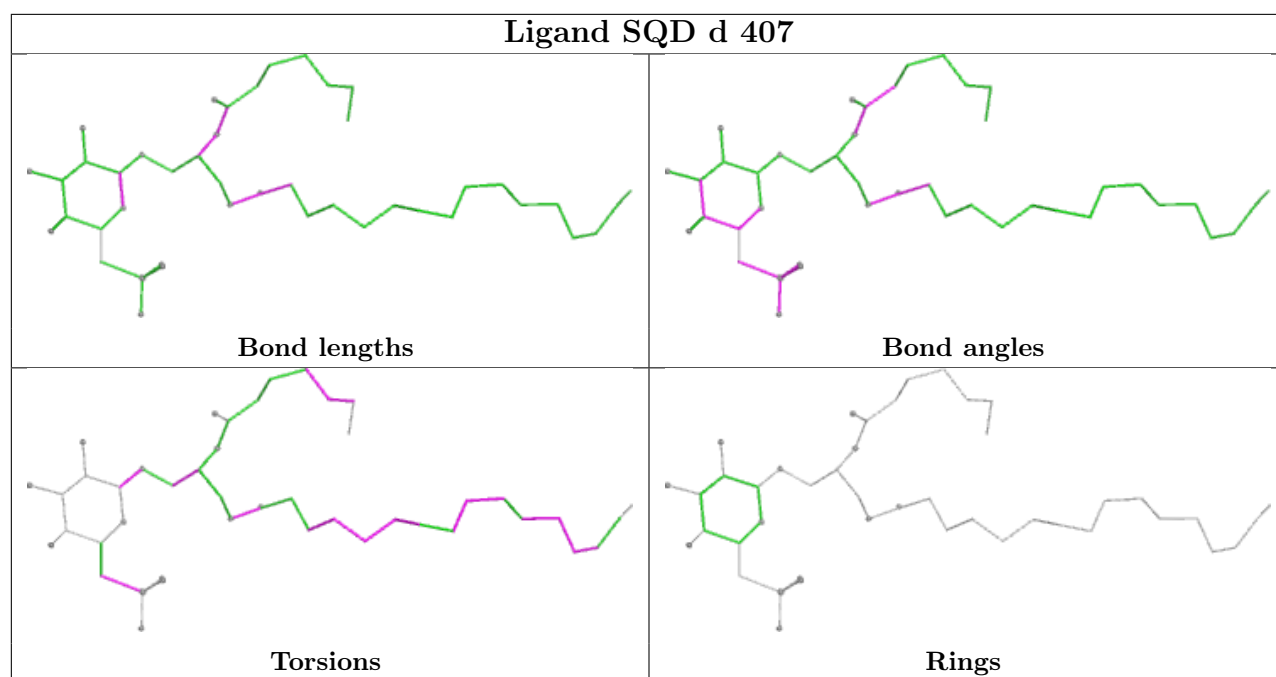


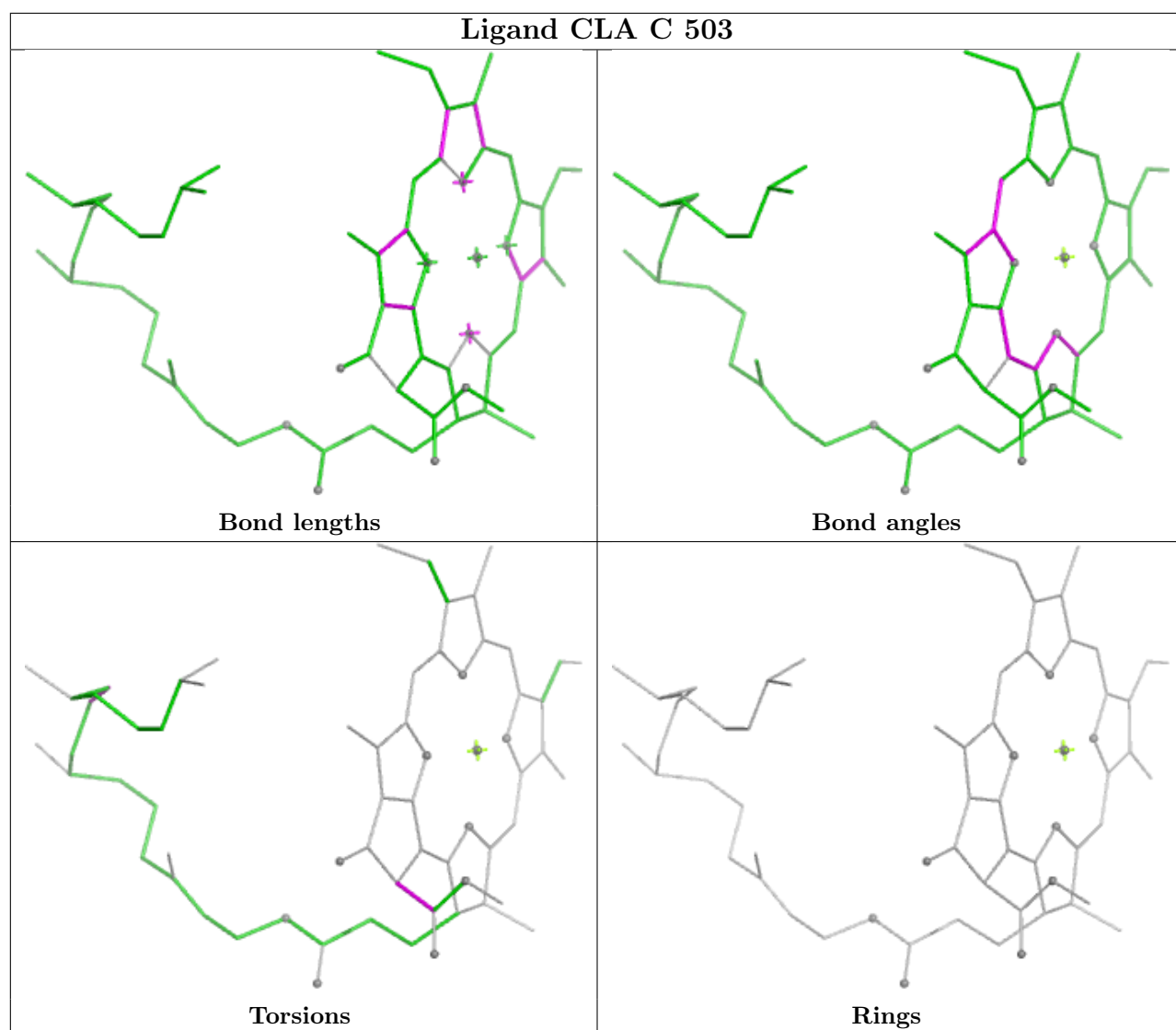


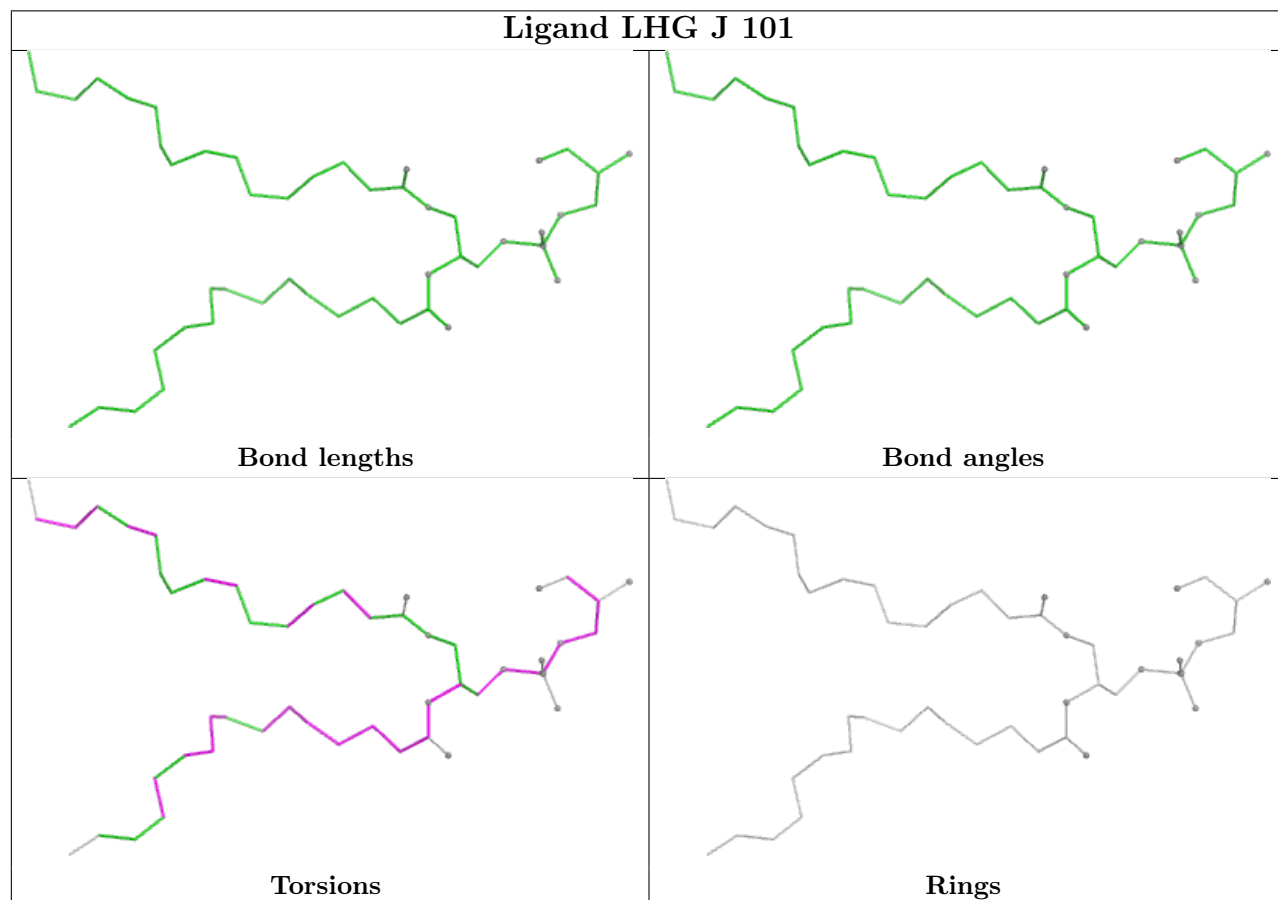
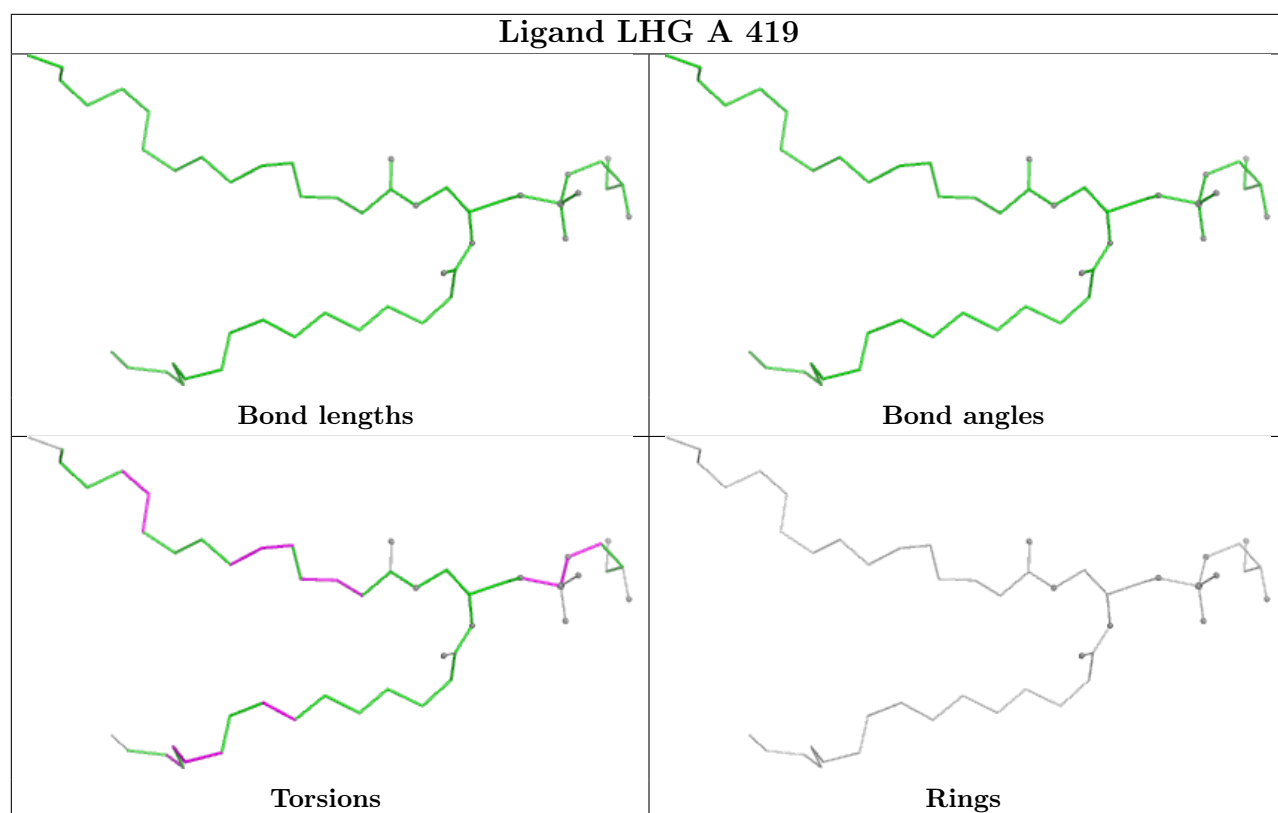


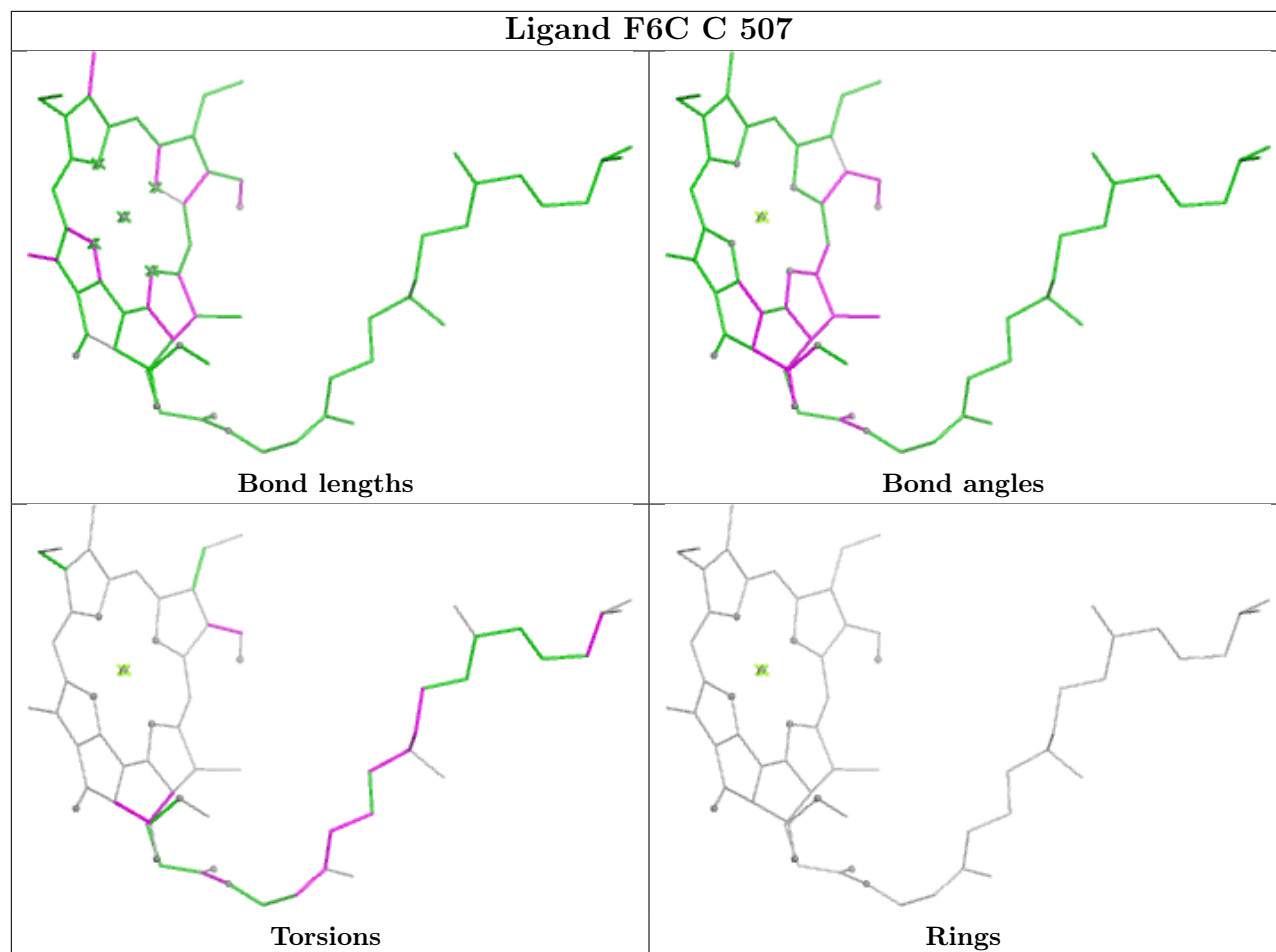




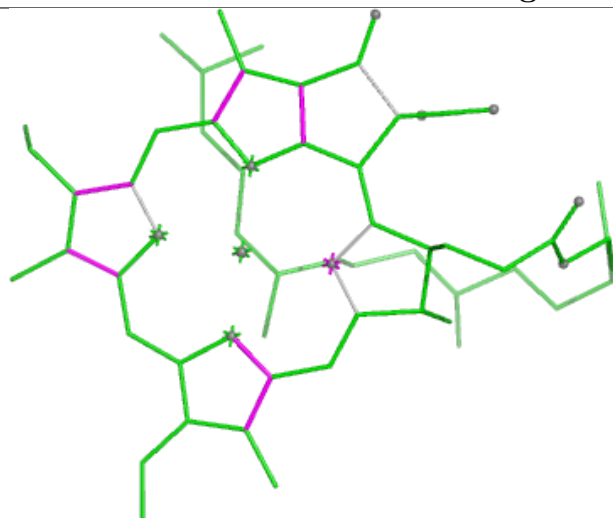




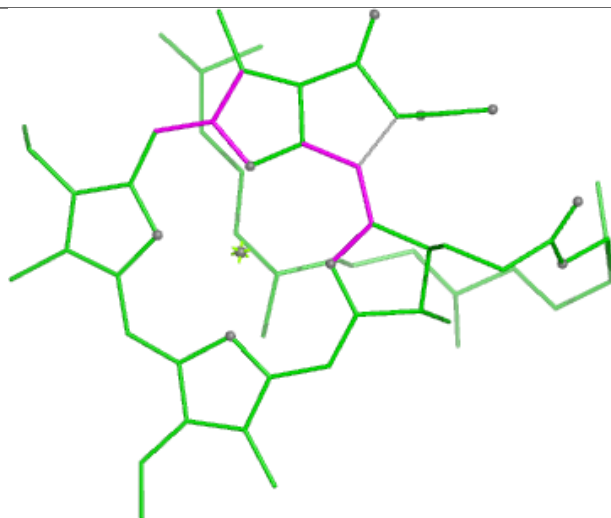




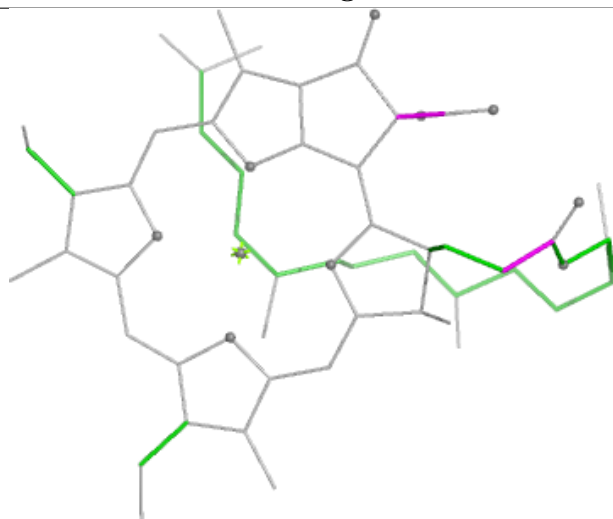
Ligand CLA c 510



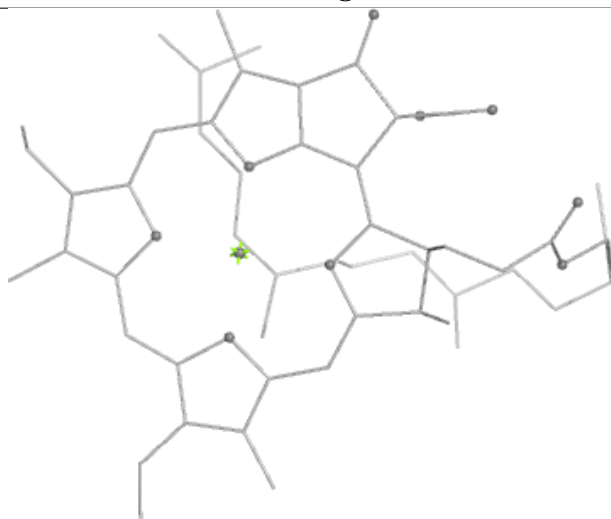
Bond lengths



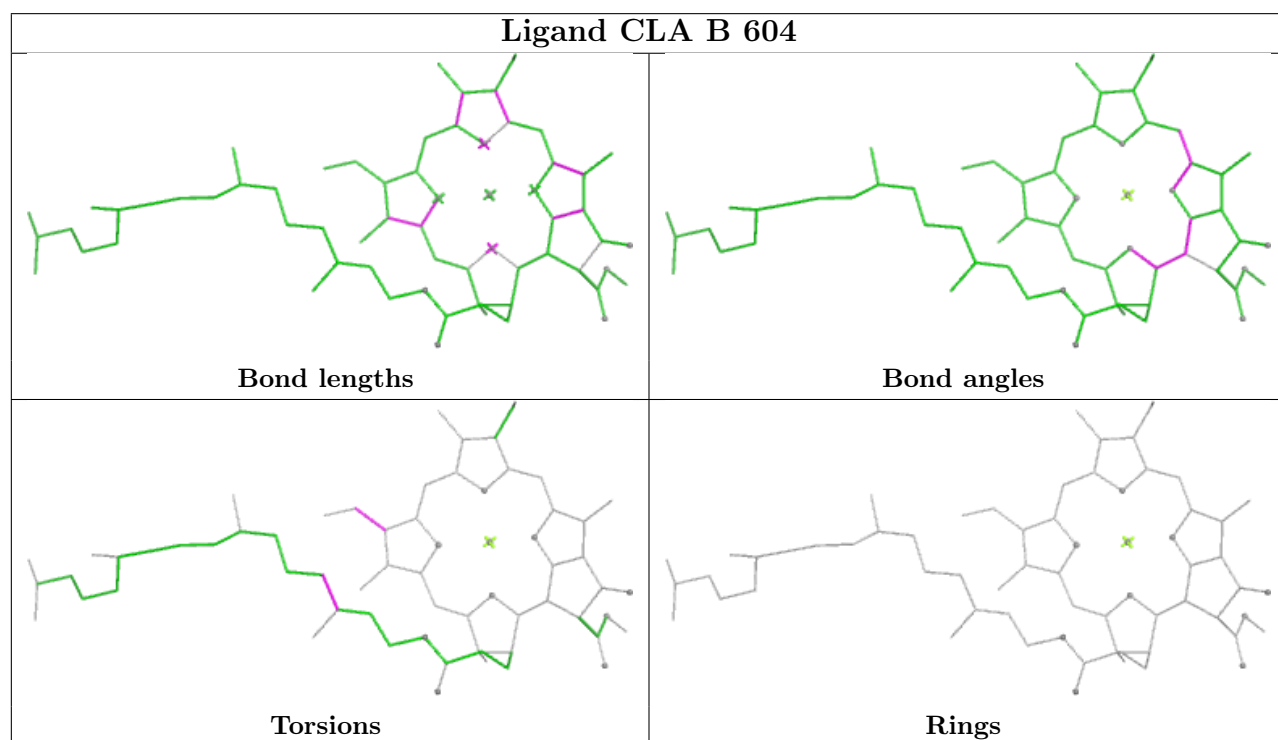
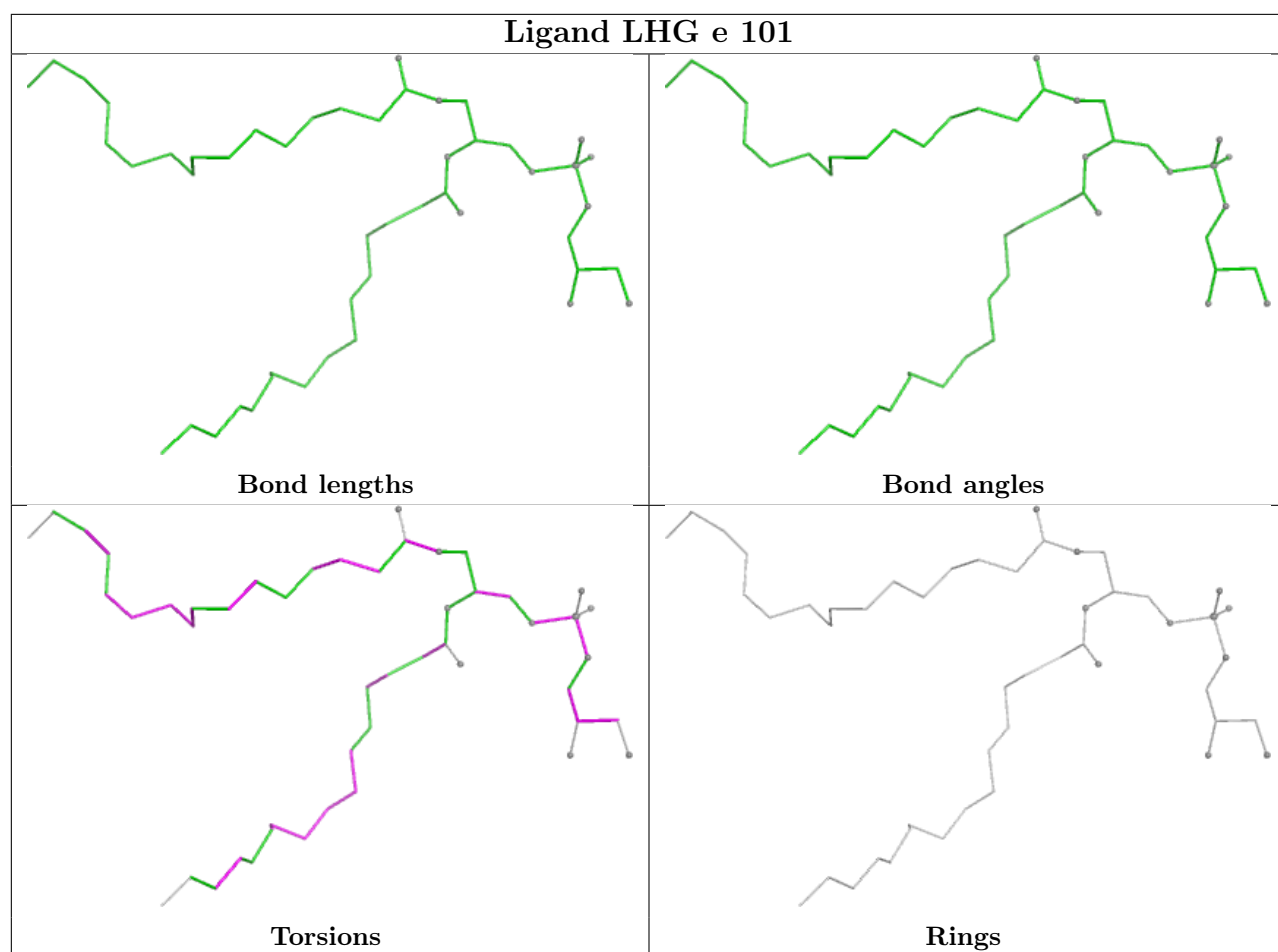
Bond angles

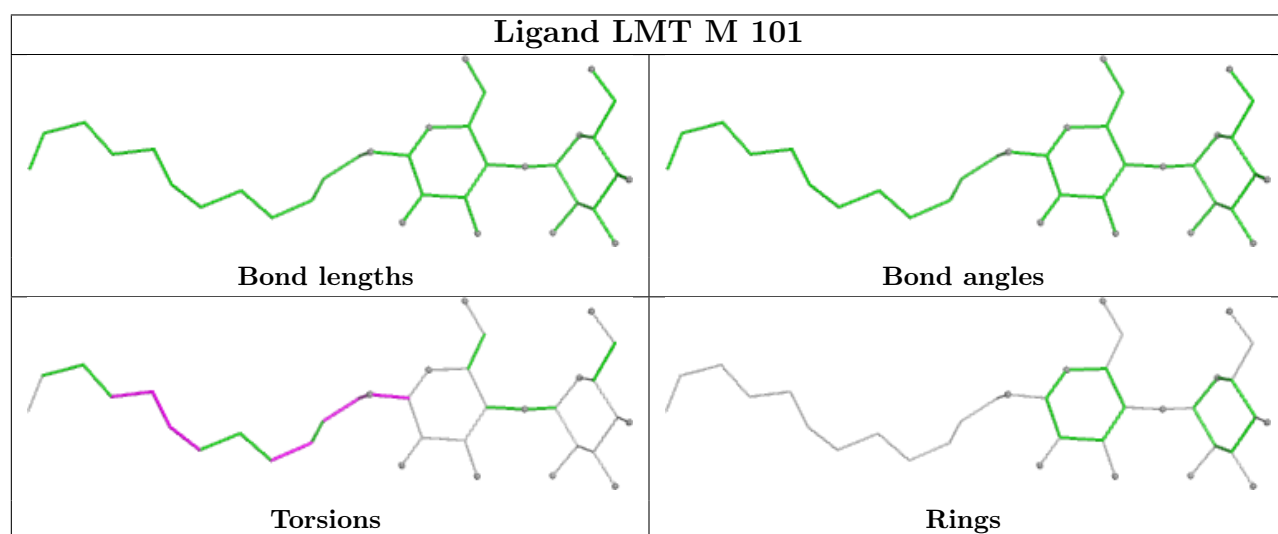
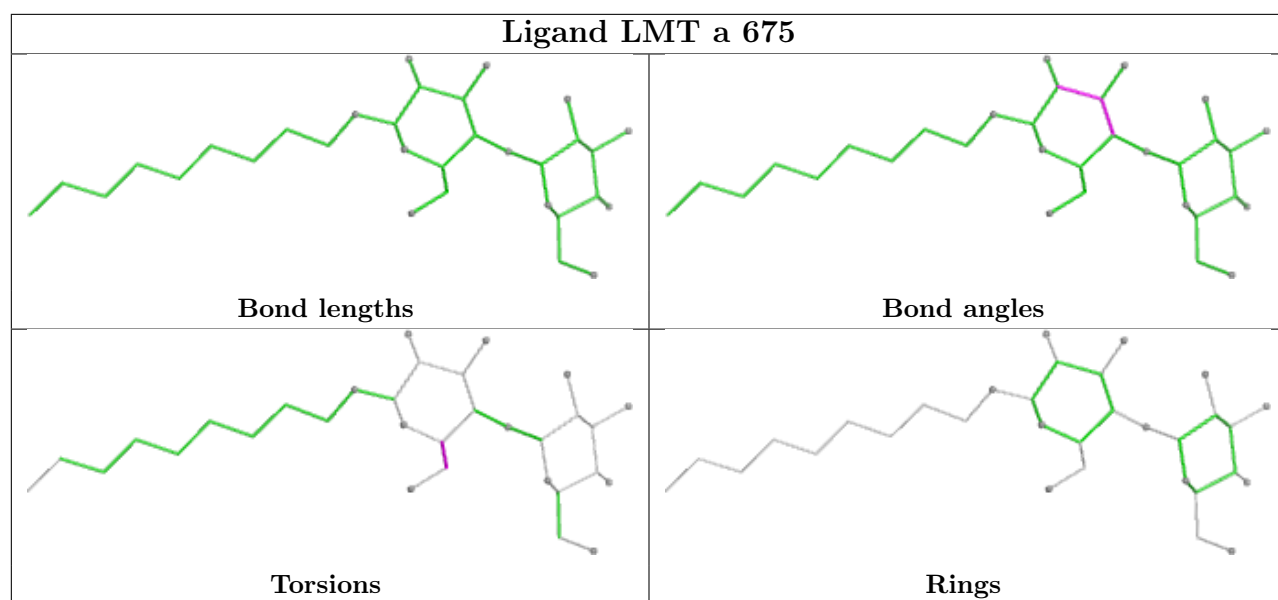


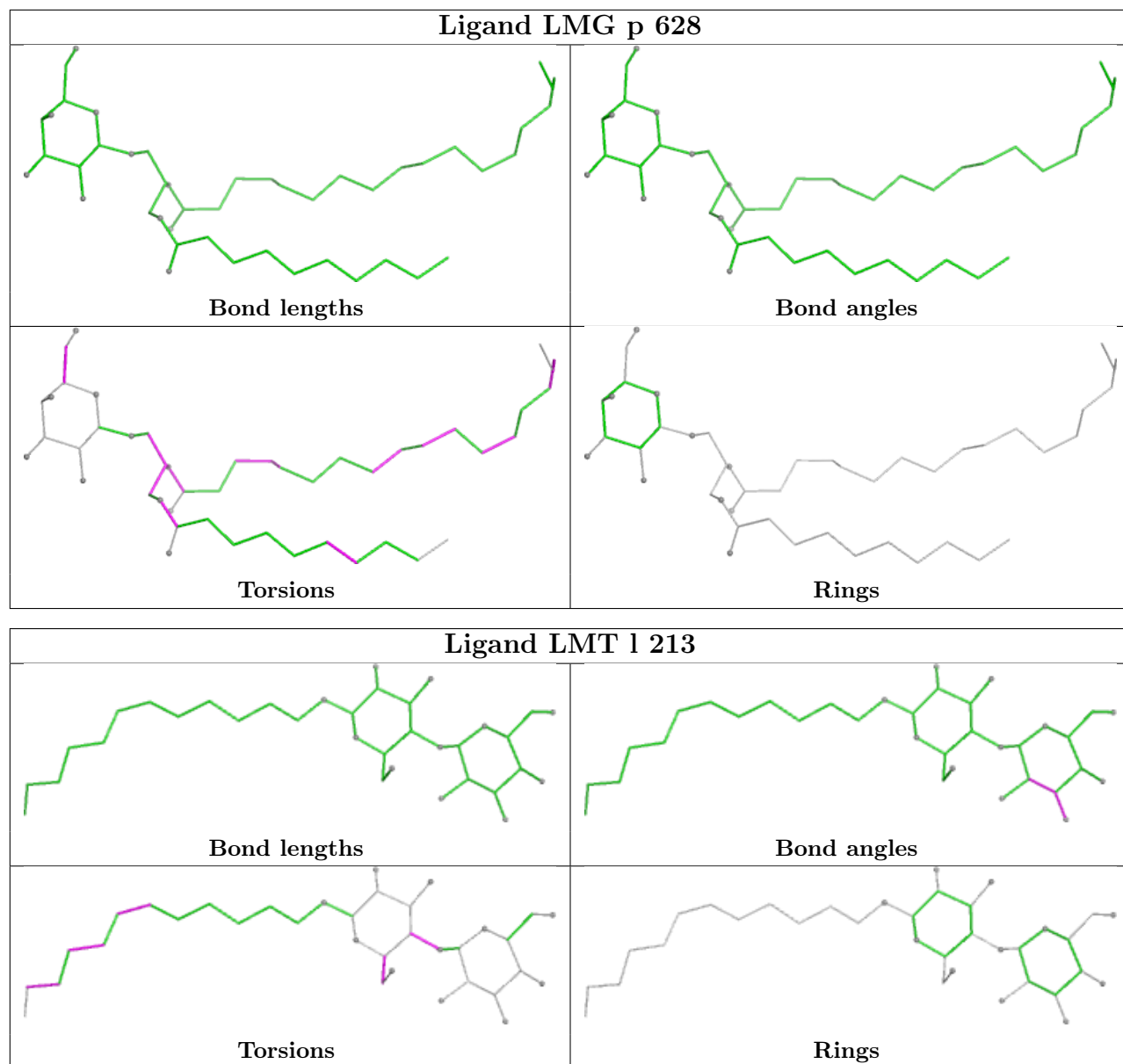
Torsions



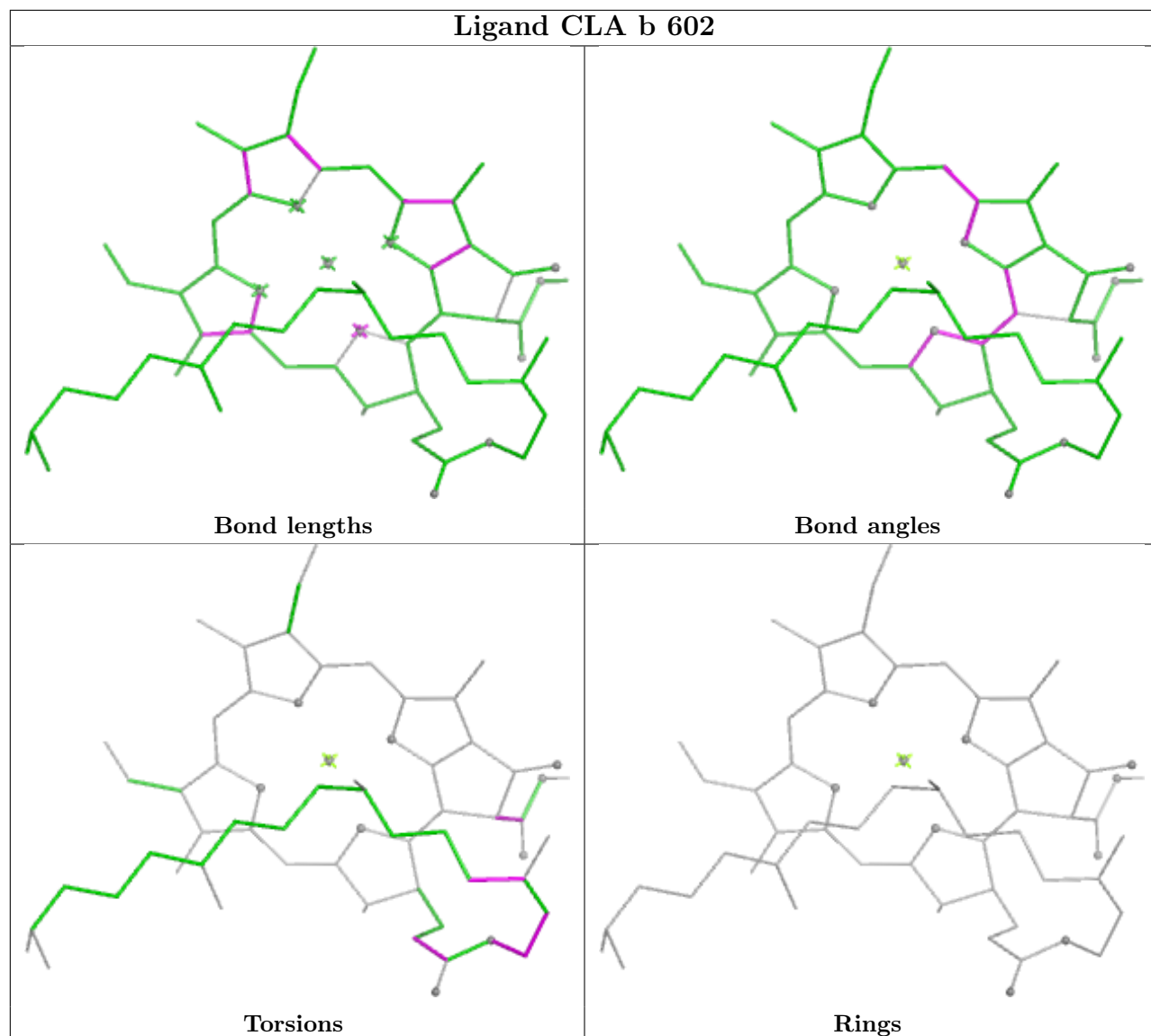
Rings

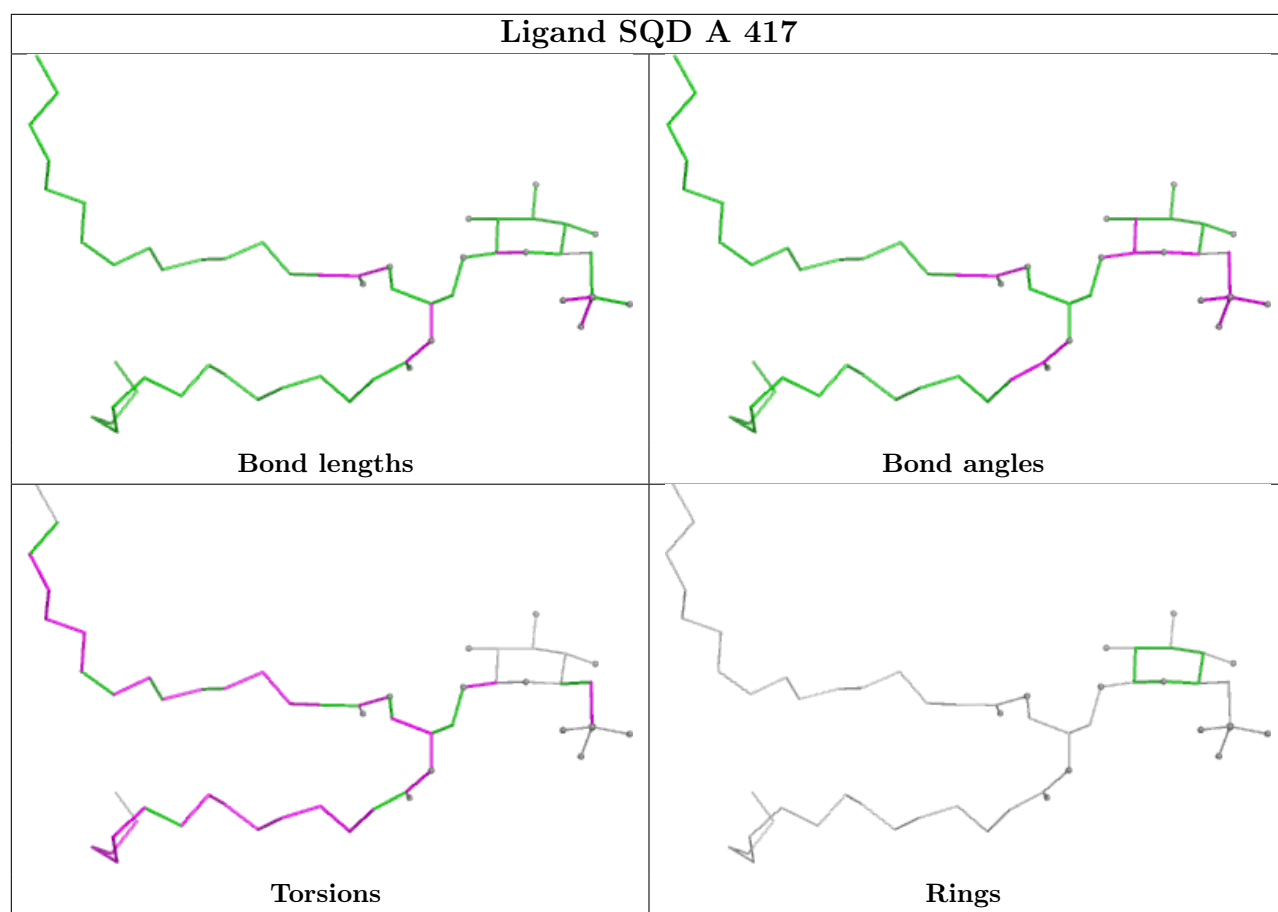


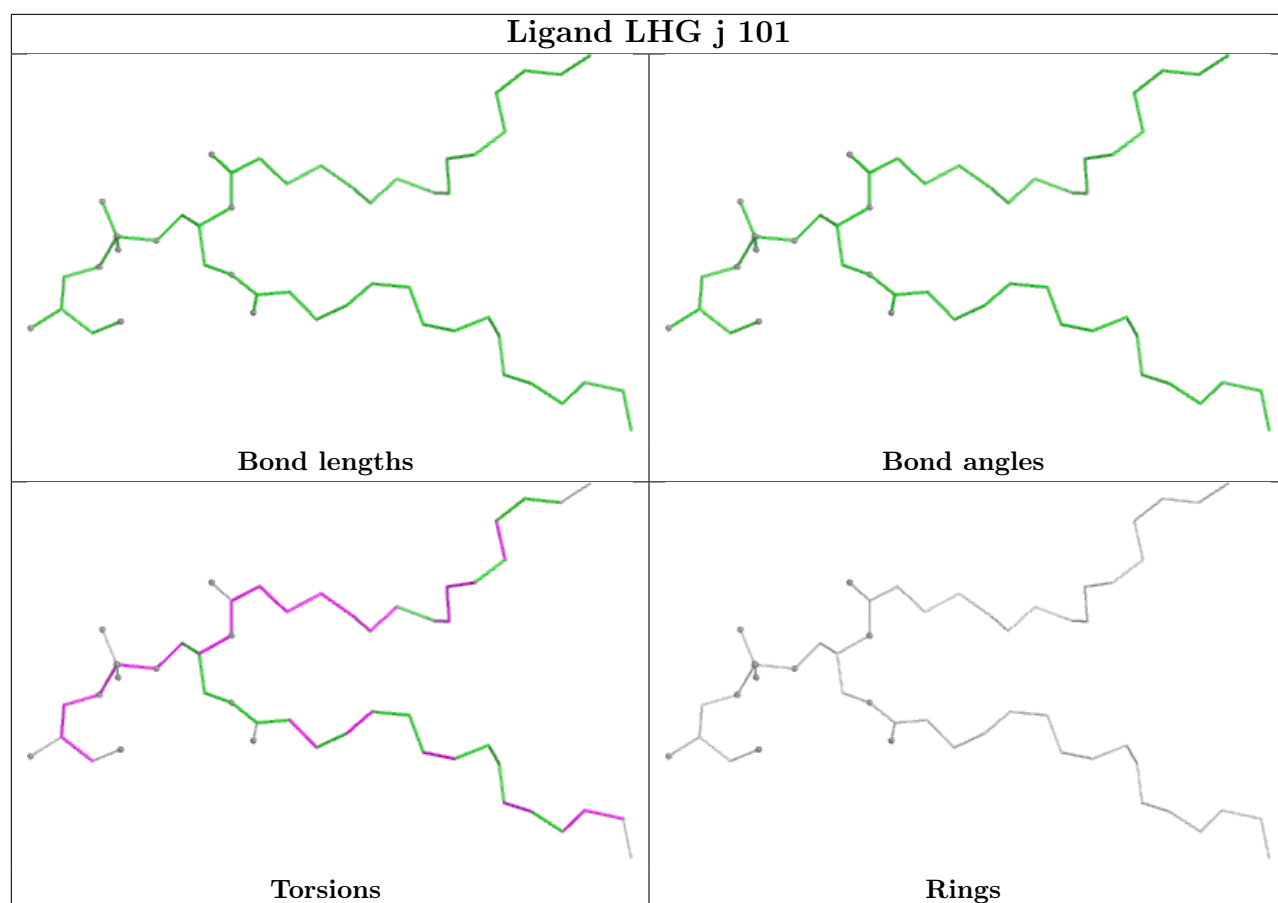


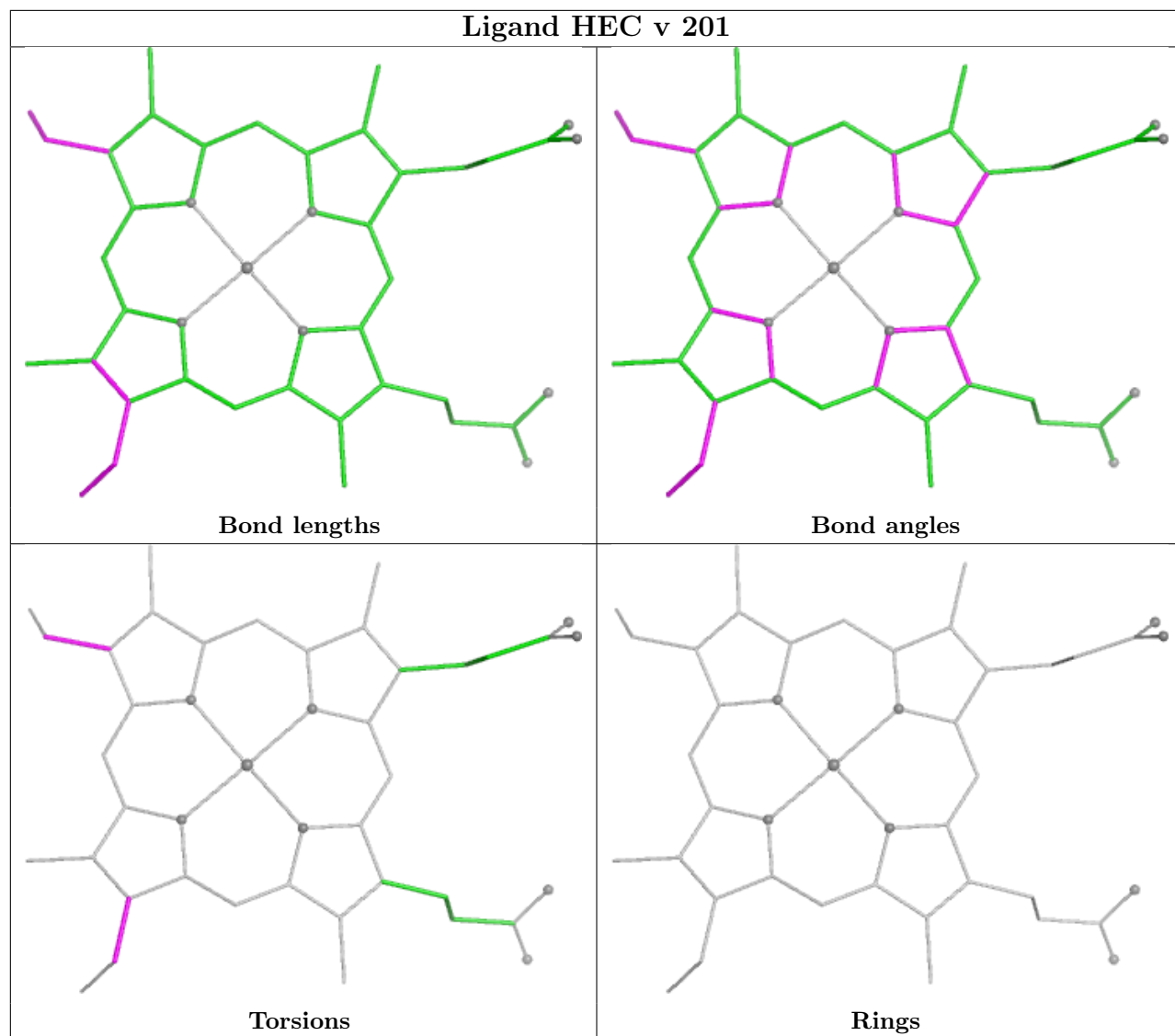


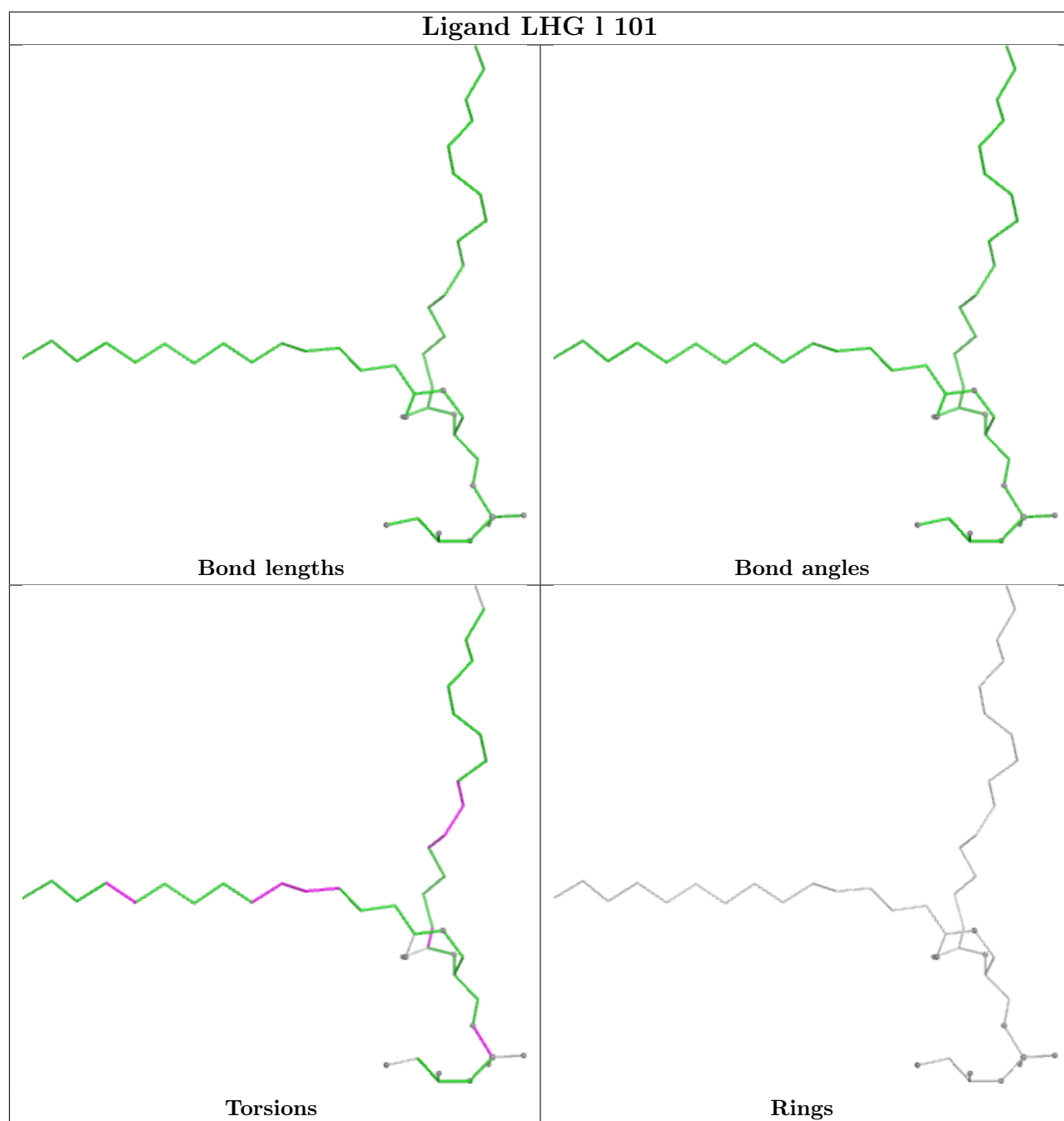
Ligand CLA b 602

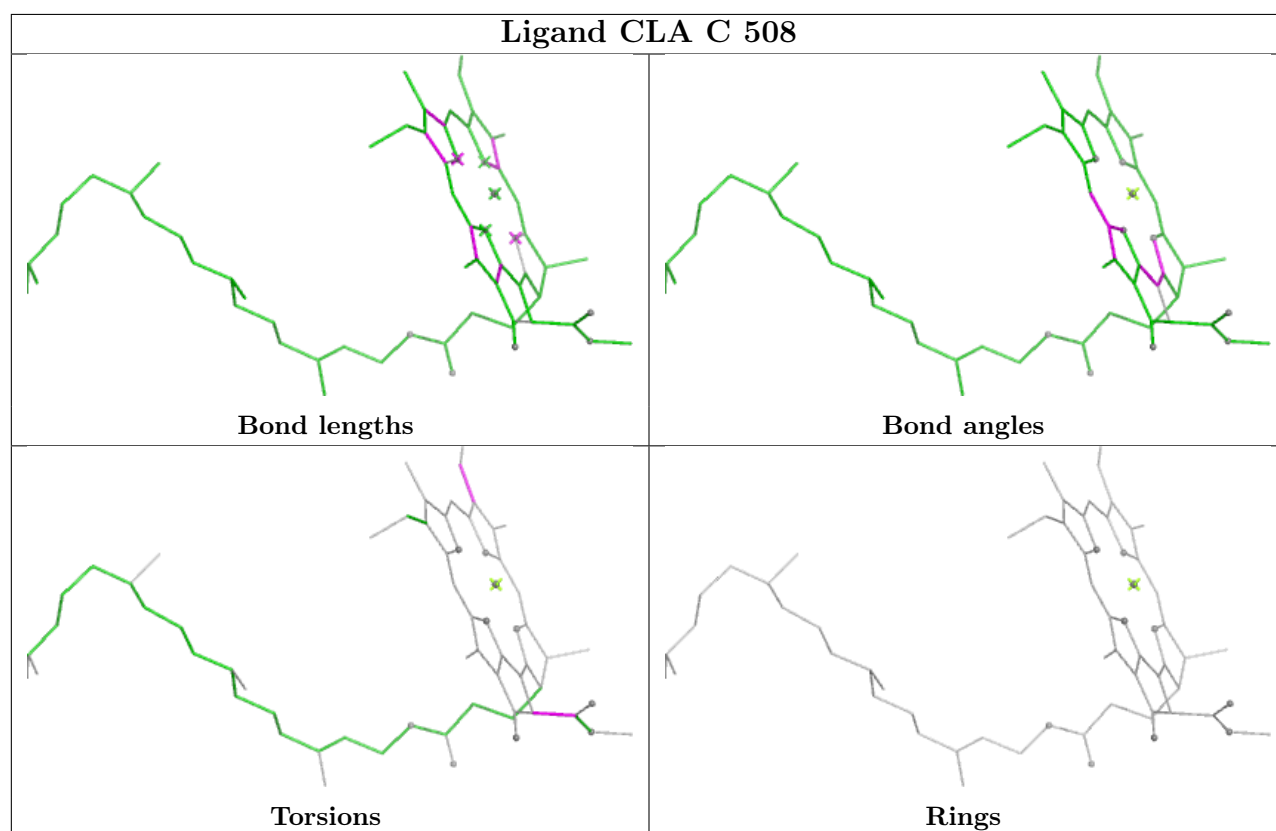
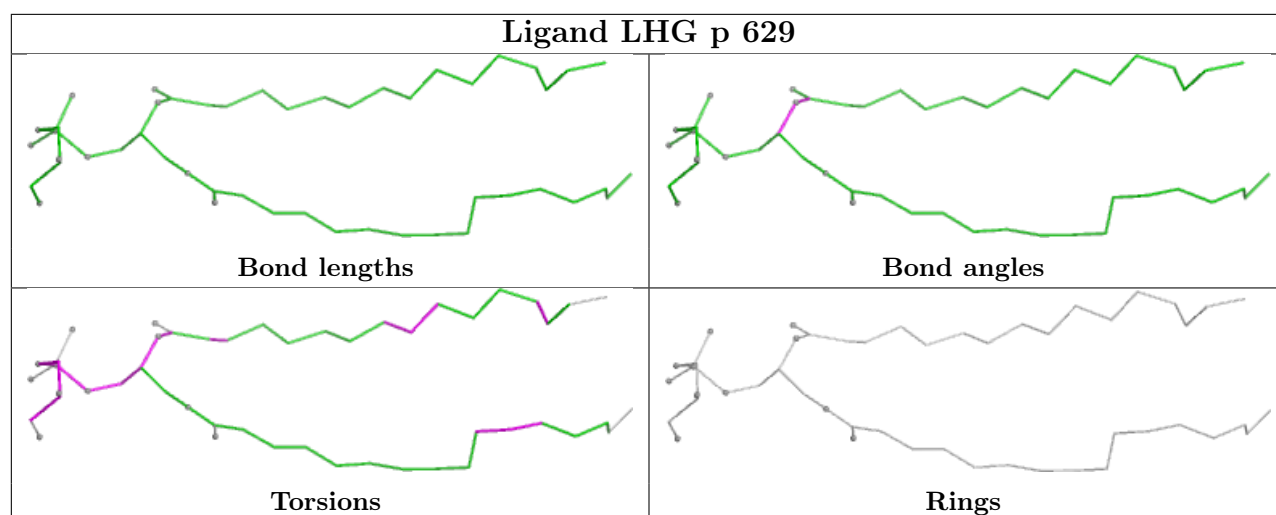


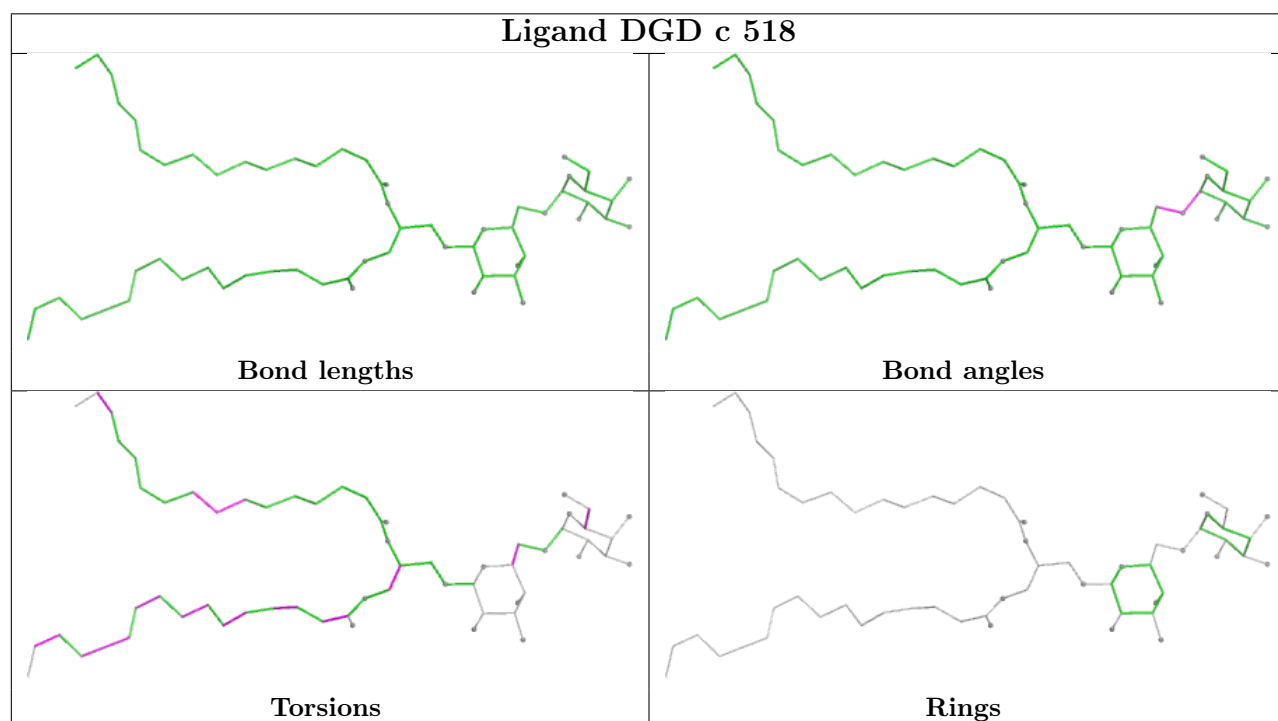
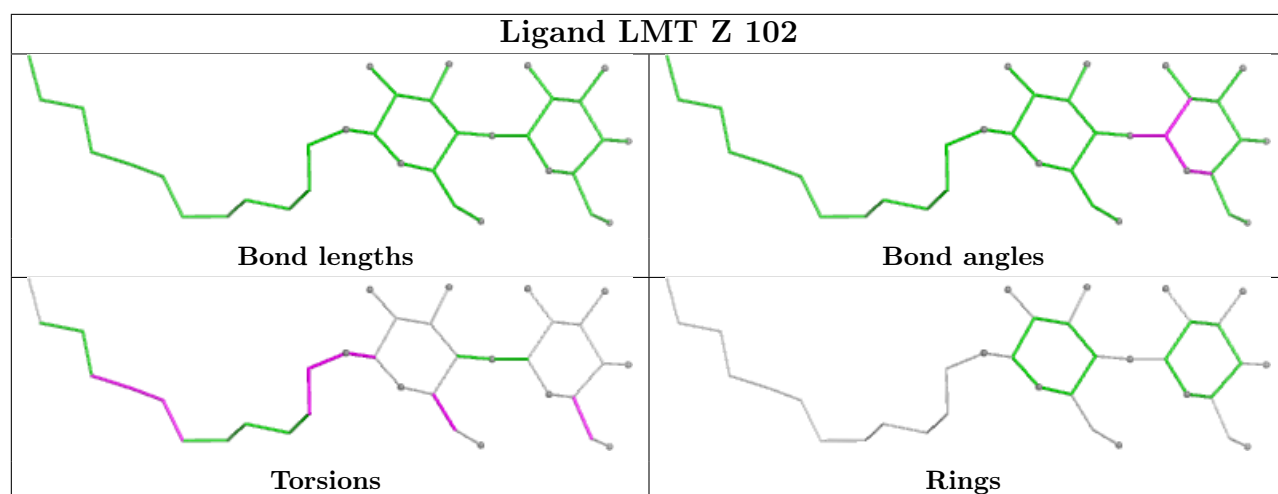


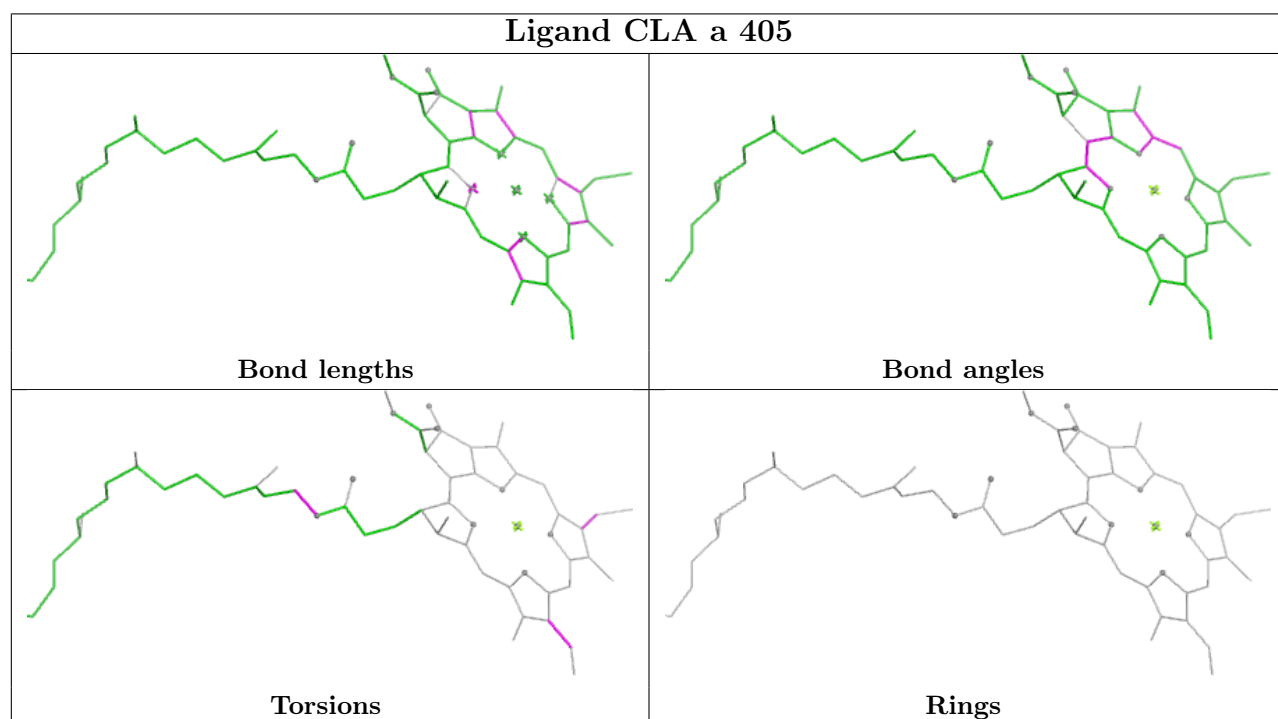
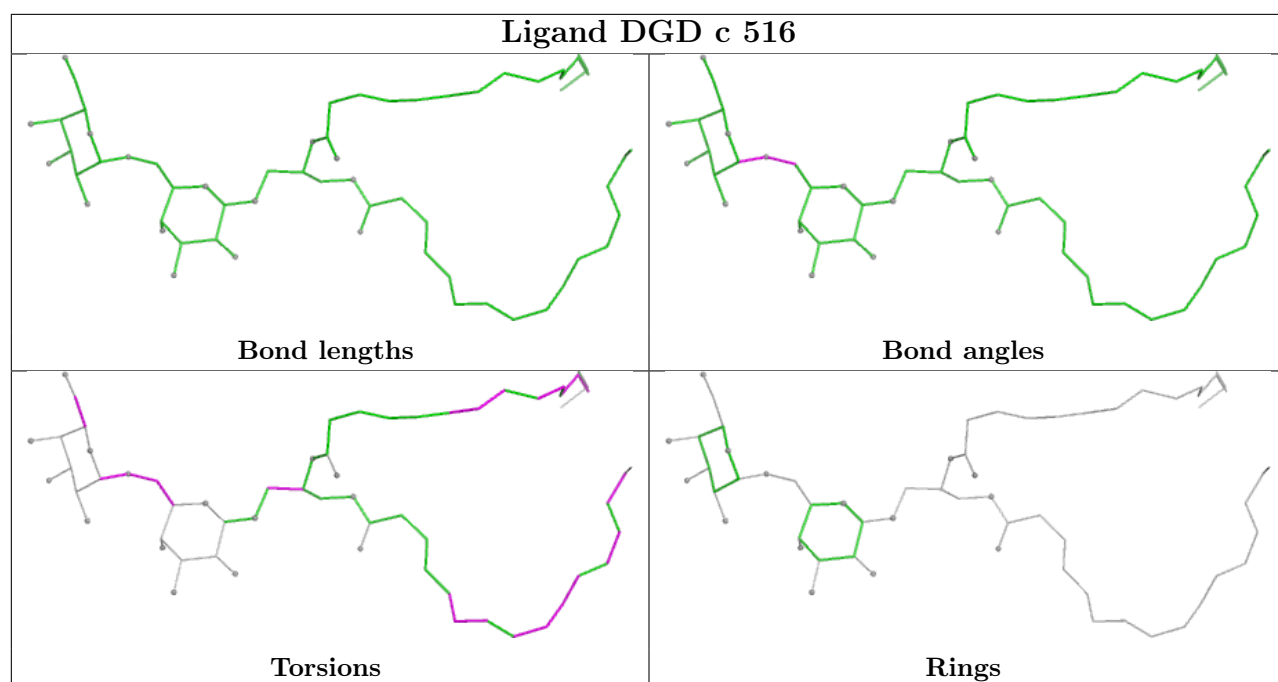


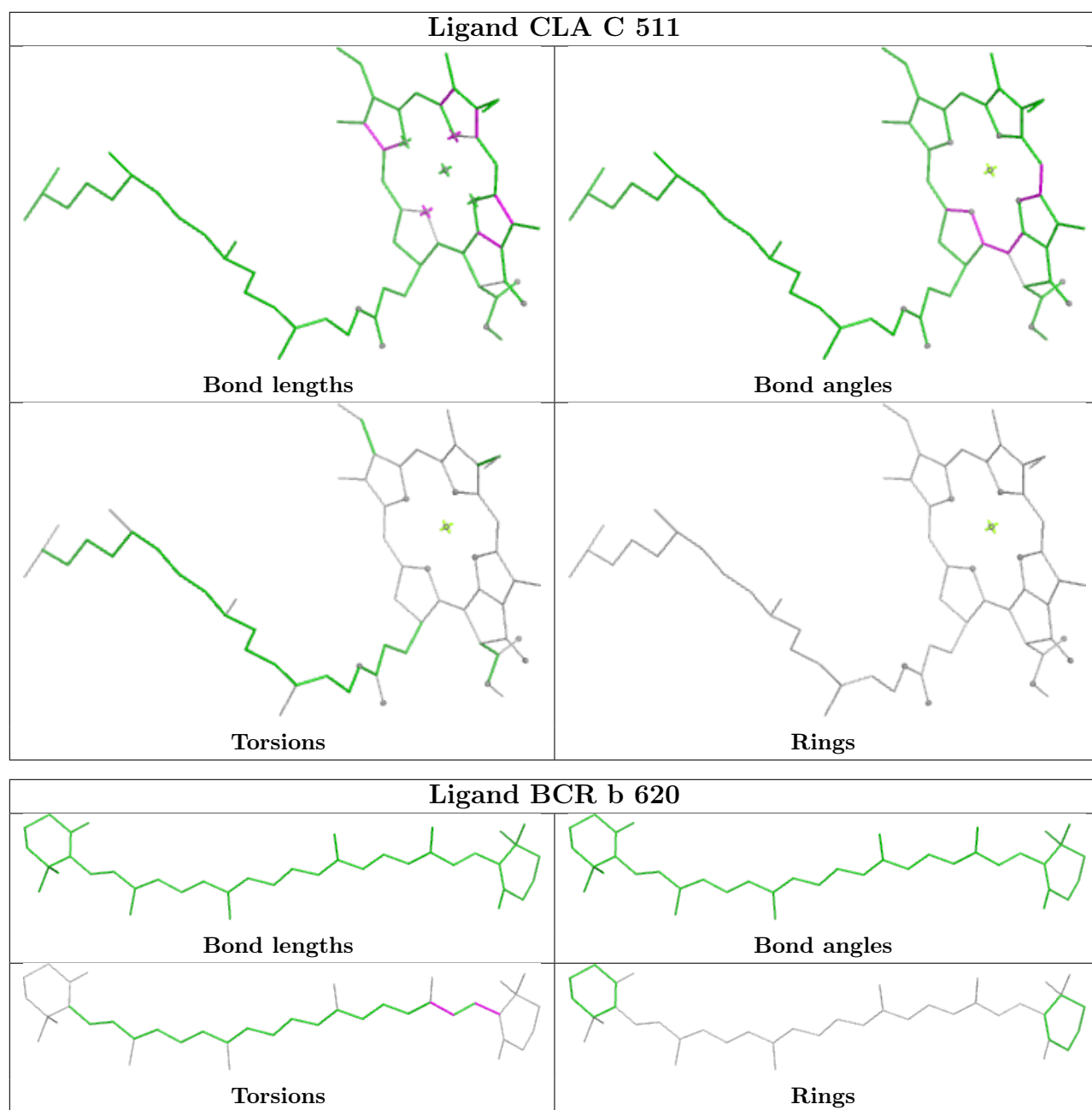


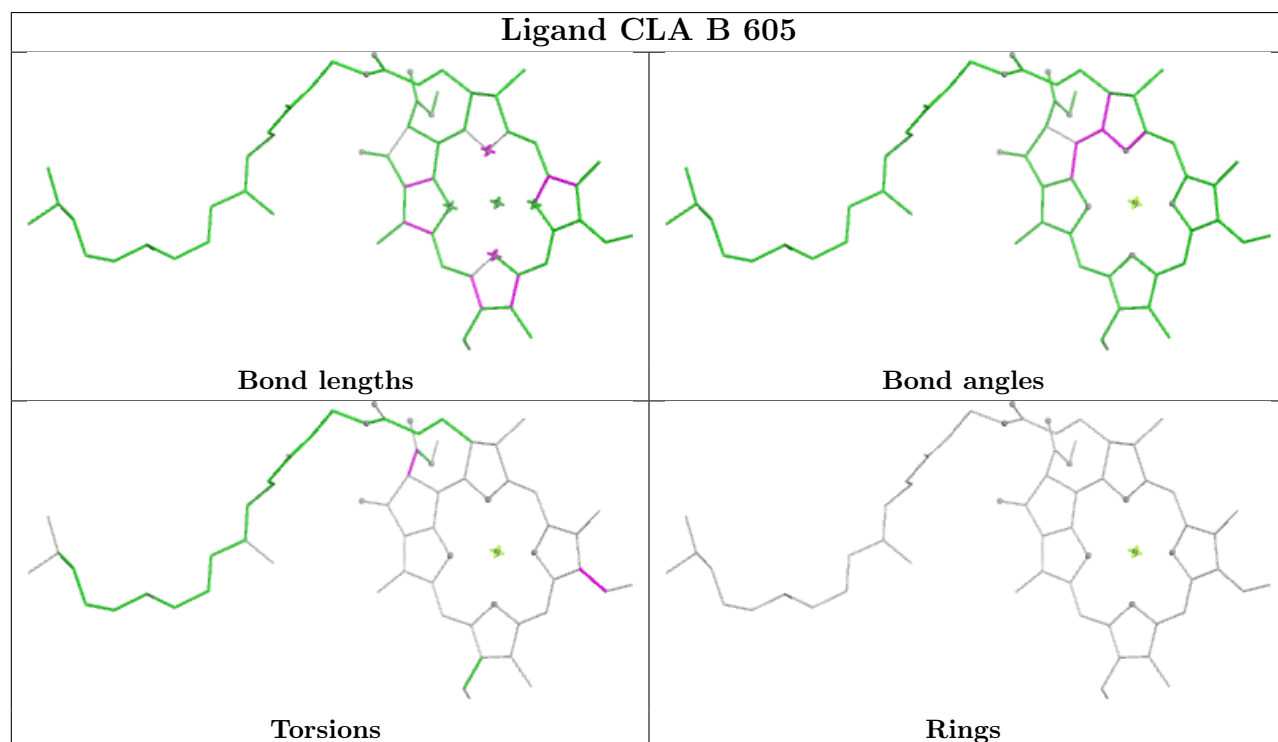
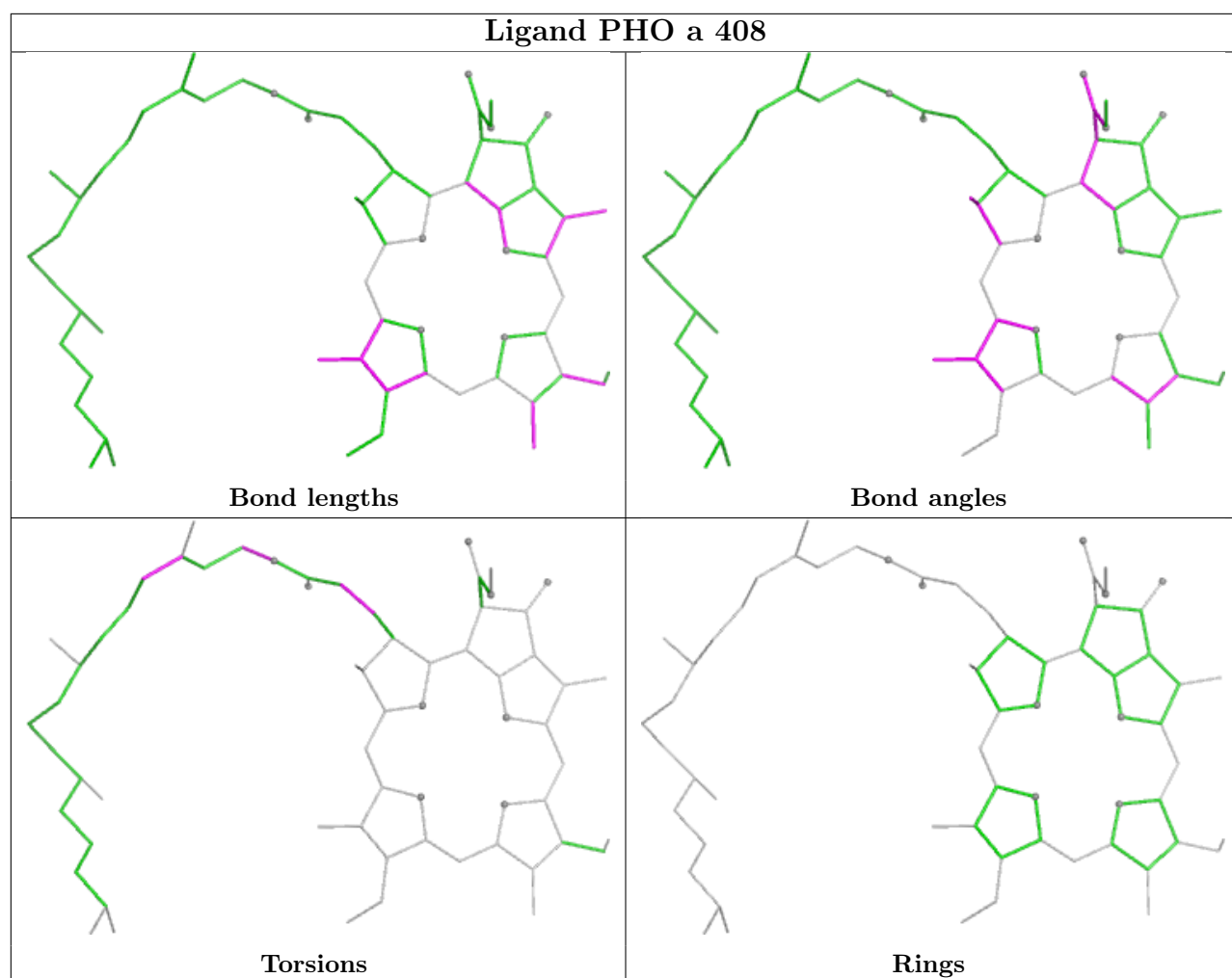


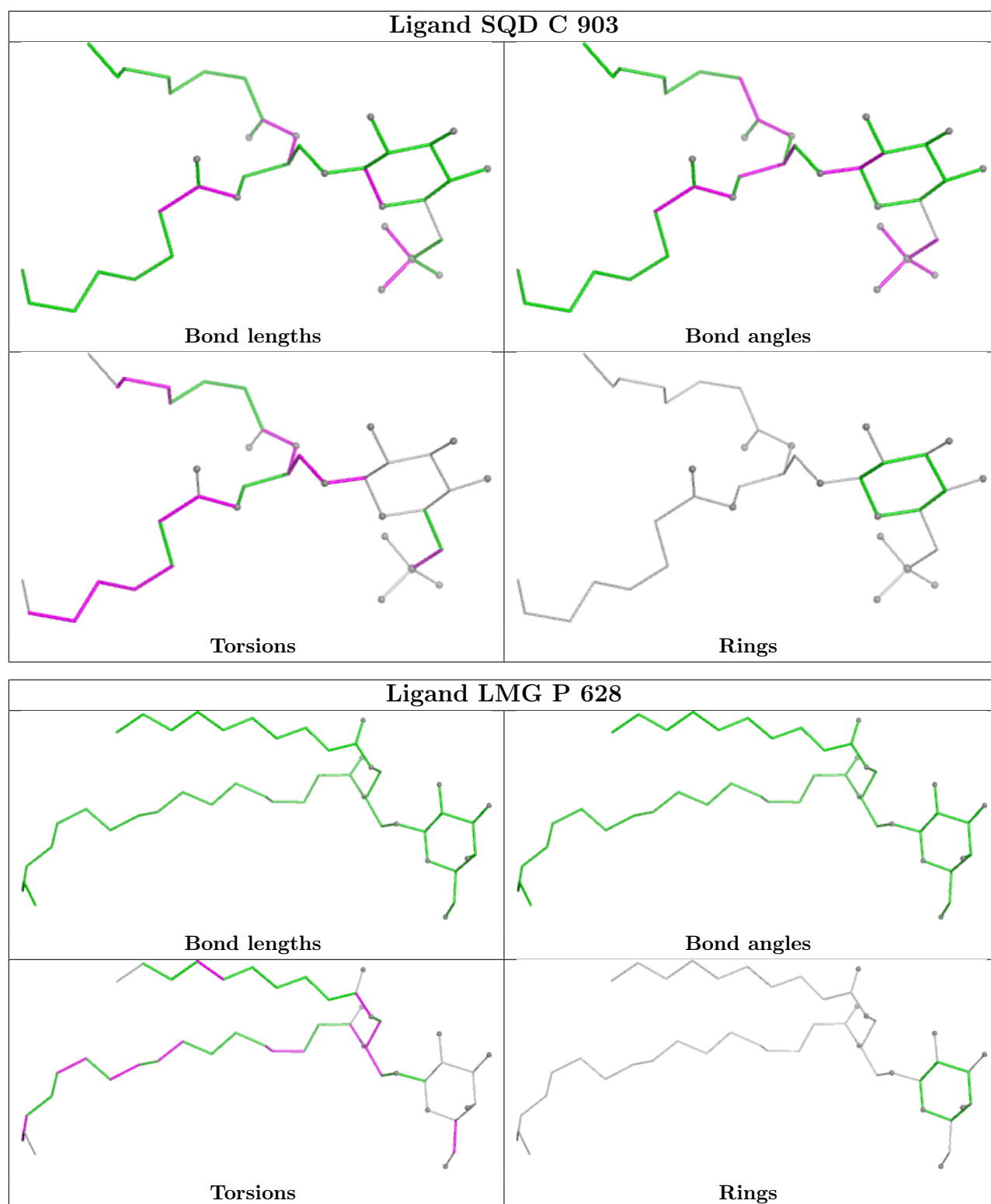












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

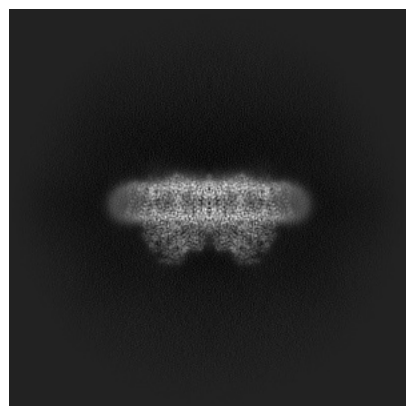
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55593. These allow visual inspection of the internal detail of the map and identification of artifacts.

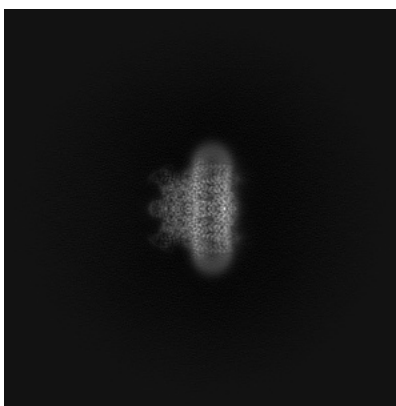
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

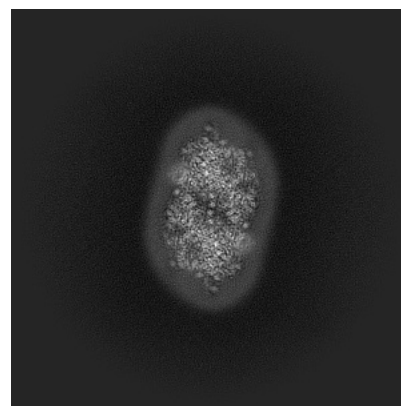
6.1.1 Primary map



X

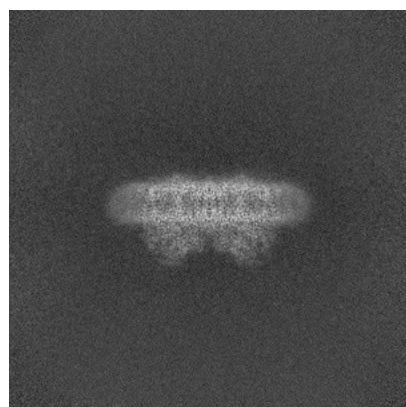


Y

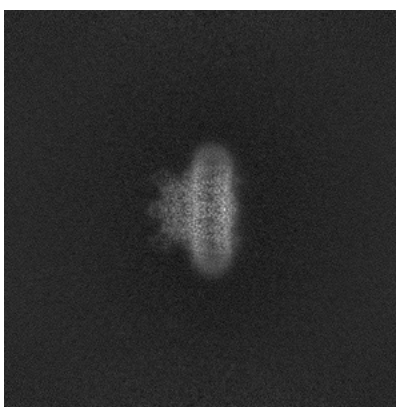


Z

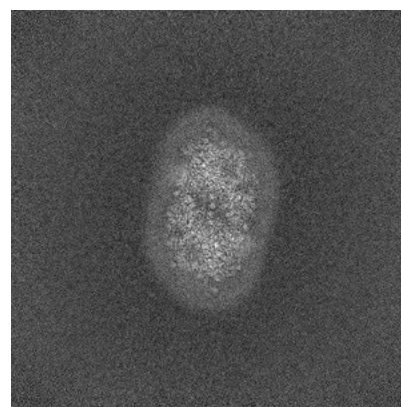
6.1.2 Raw map



X



Y

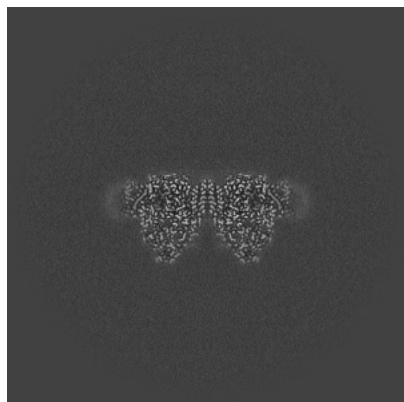


Z

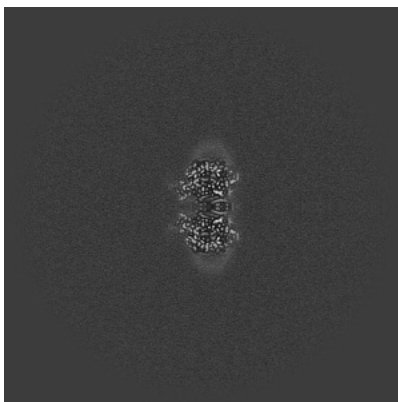
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

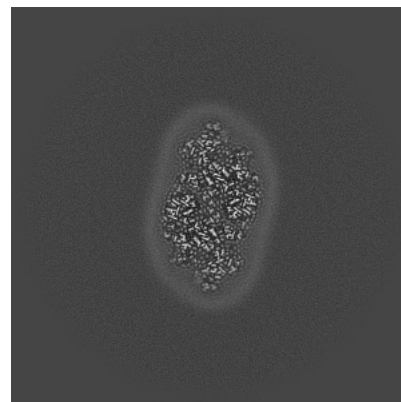
6.2.1 Primary map



X Index: 325

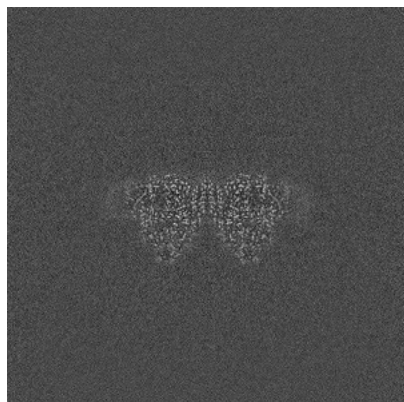


Y Index: 325

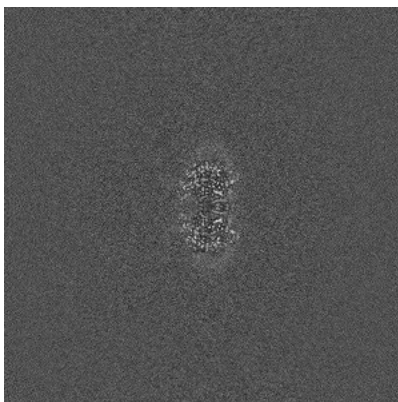


Z Index: 325

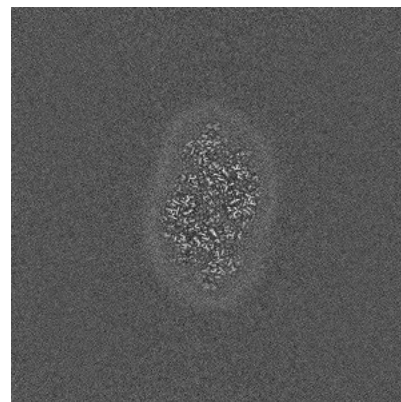
6.2.2 Raw map



X Index: 325



Y Index: 325

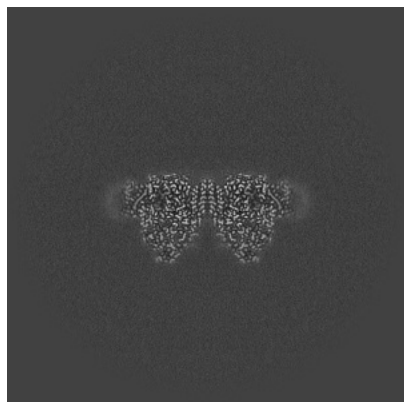


Z Index: 325

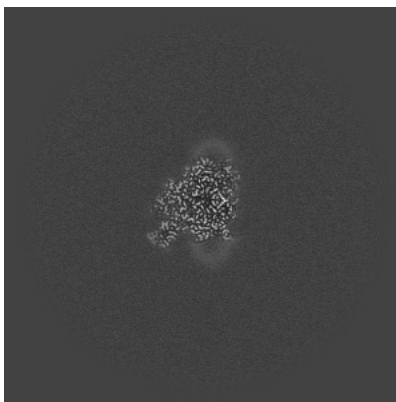
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

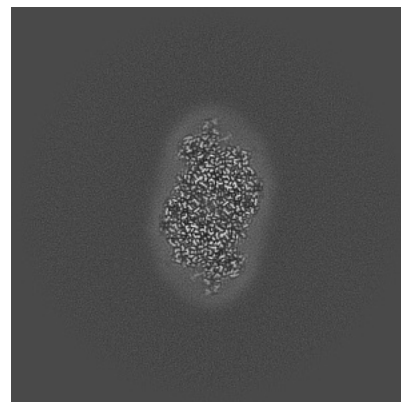
6.3.1 Primary map



X Index: 325

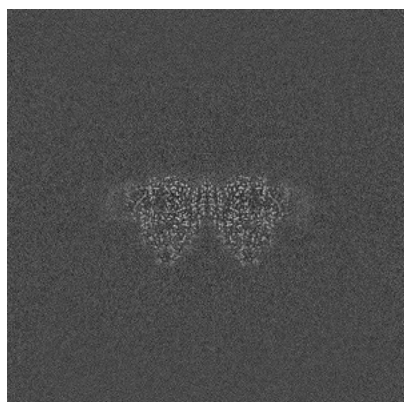


Y Index: 373

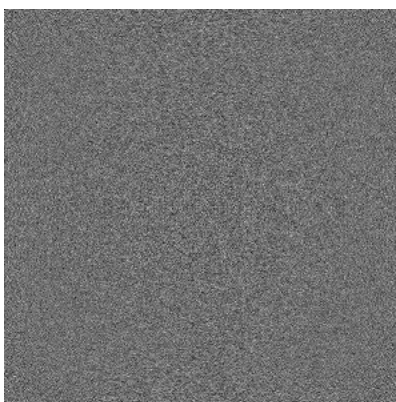


Z Index: 313

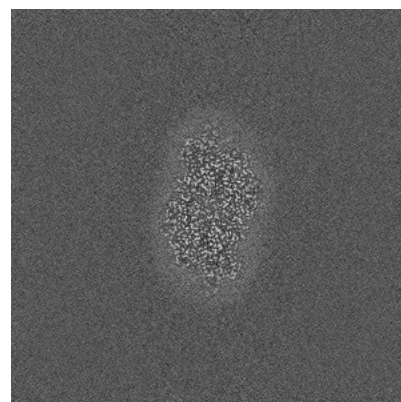
6.3.2 Raw map



X Index: 325



Y Index: 0

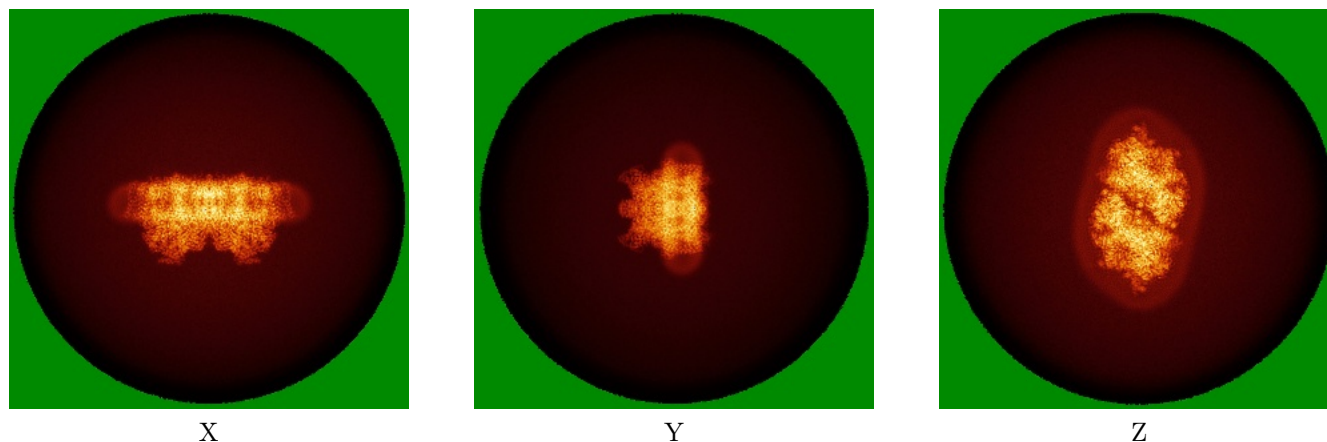


Z Index: 312

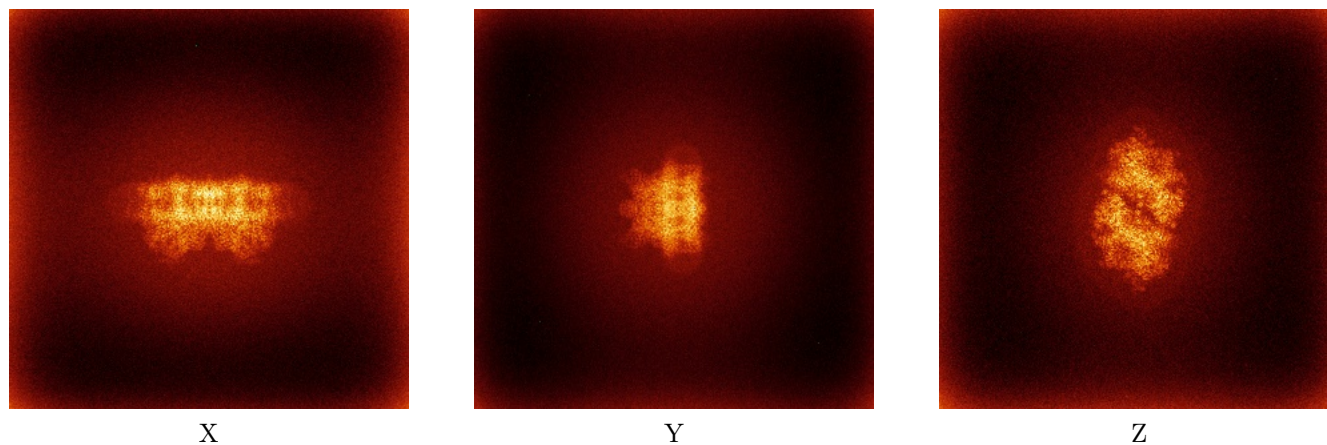
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



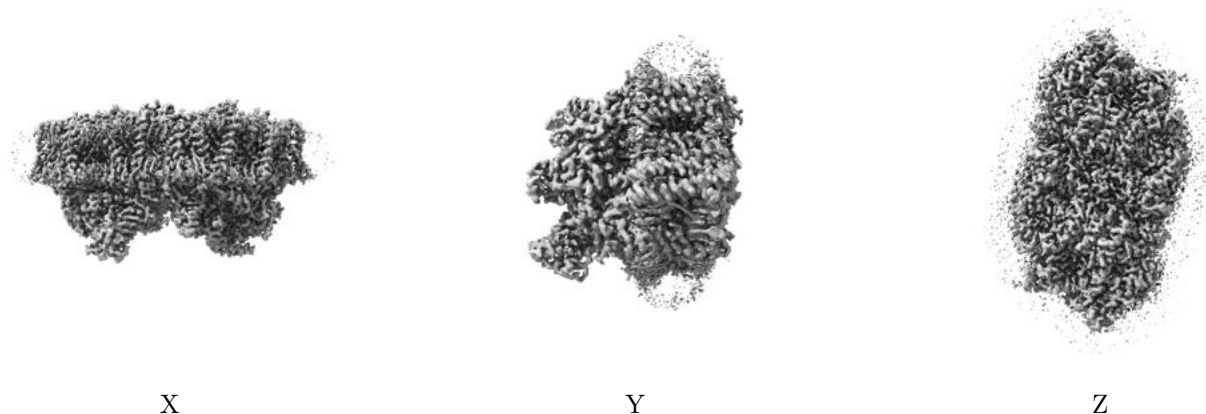
6.4.2 Raw map



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.

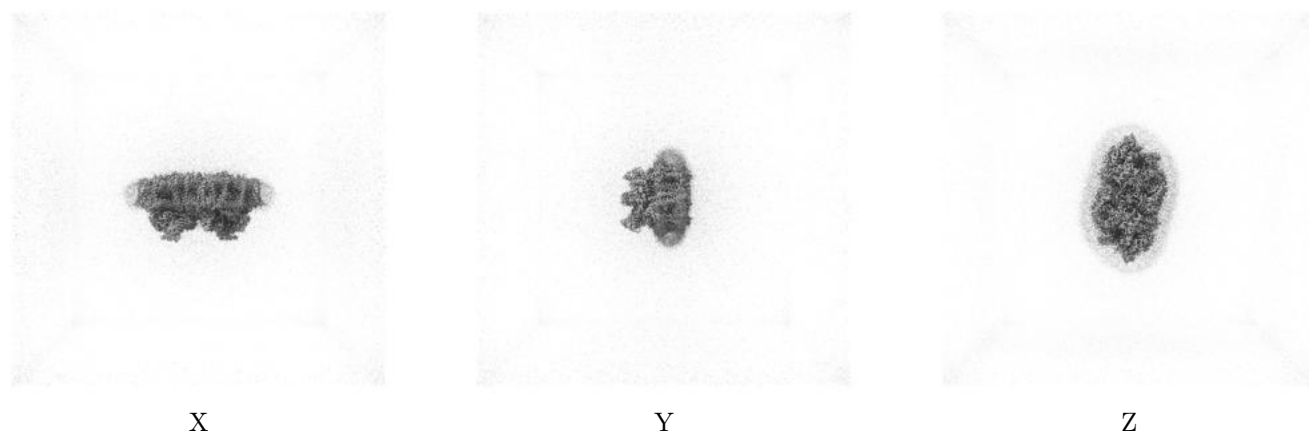
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

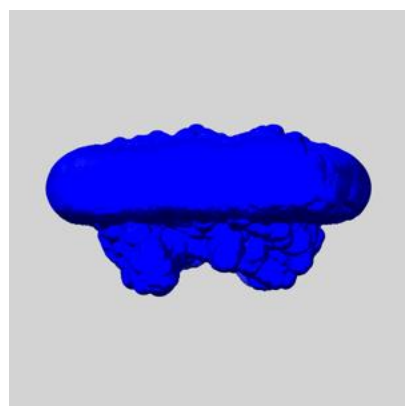
6.6 Mask visualisation [i](#)

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

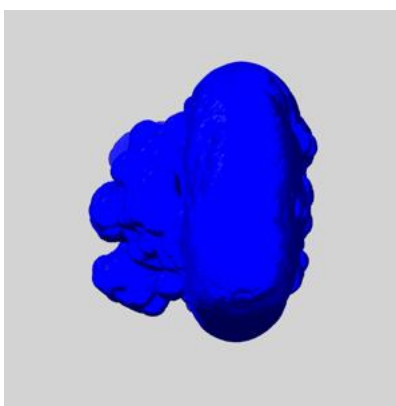
A mask typically either:

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

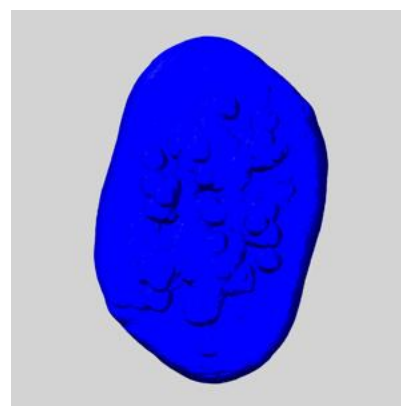
6.6.1 emd_55593_msk_1.map [i](#)



X



Y

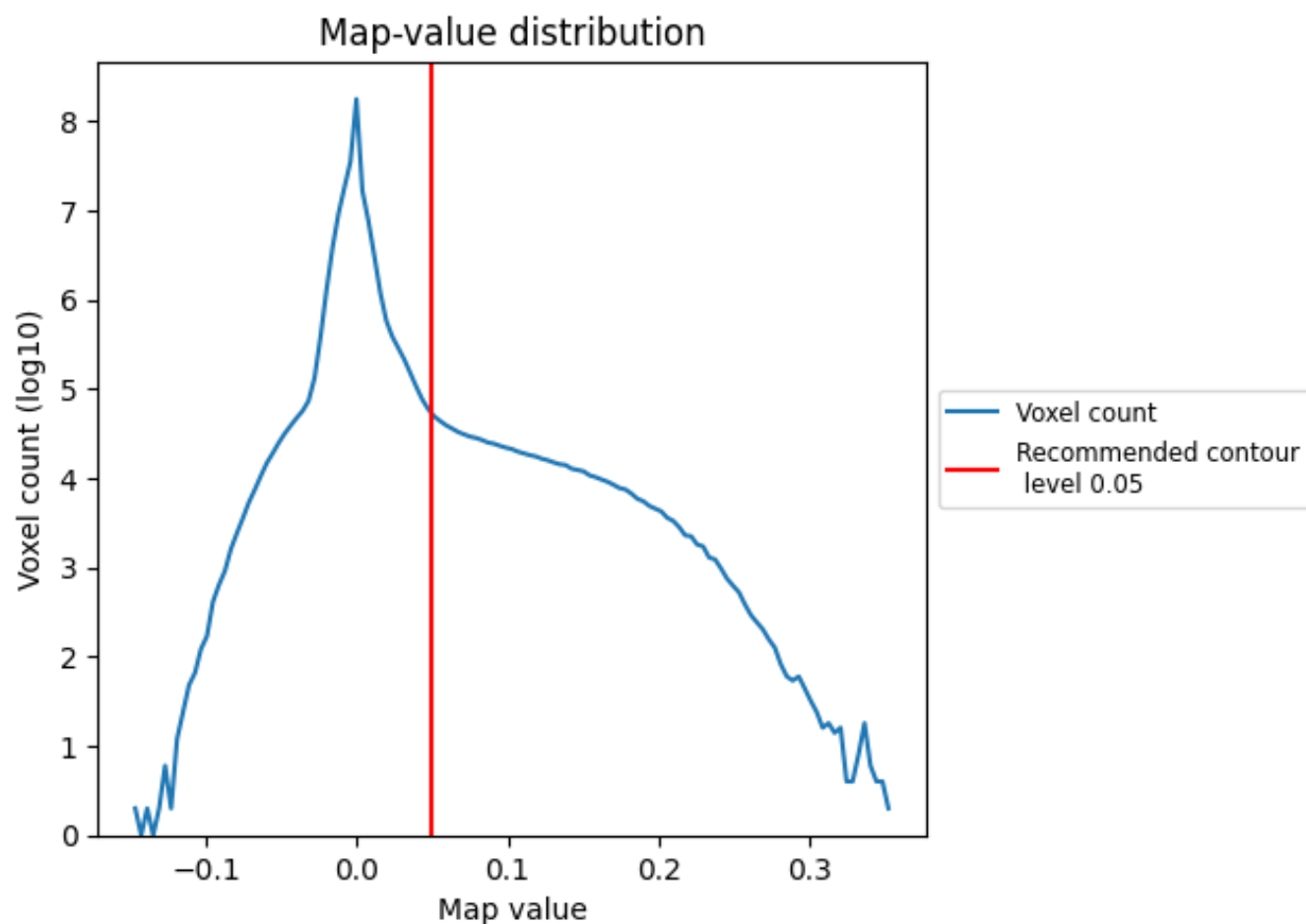


Z

7 Map analysis [i](#)

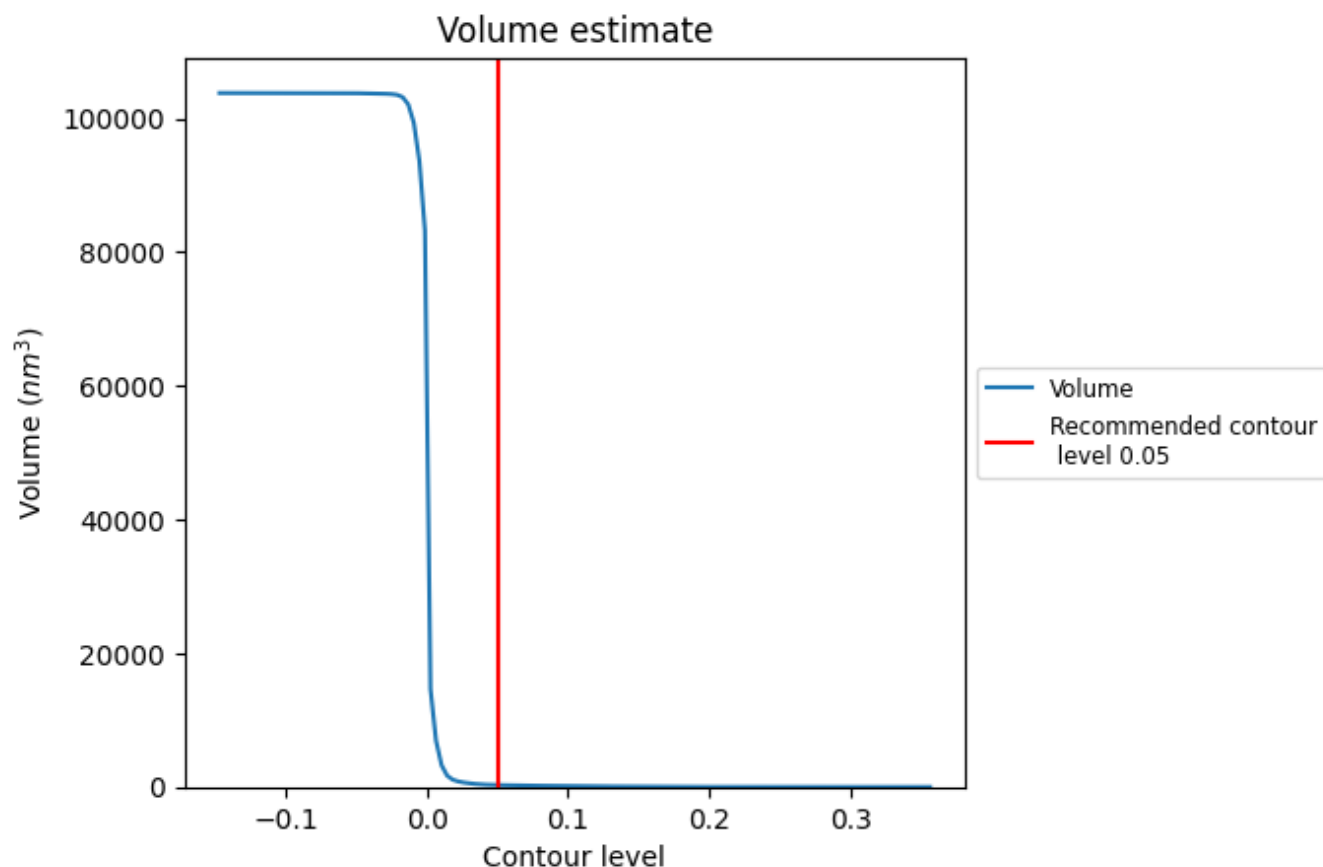
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

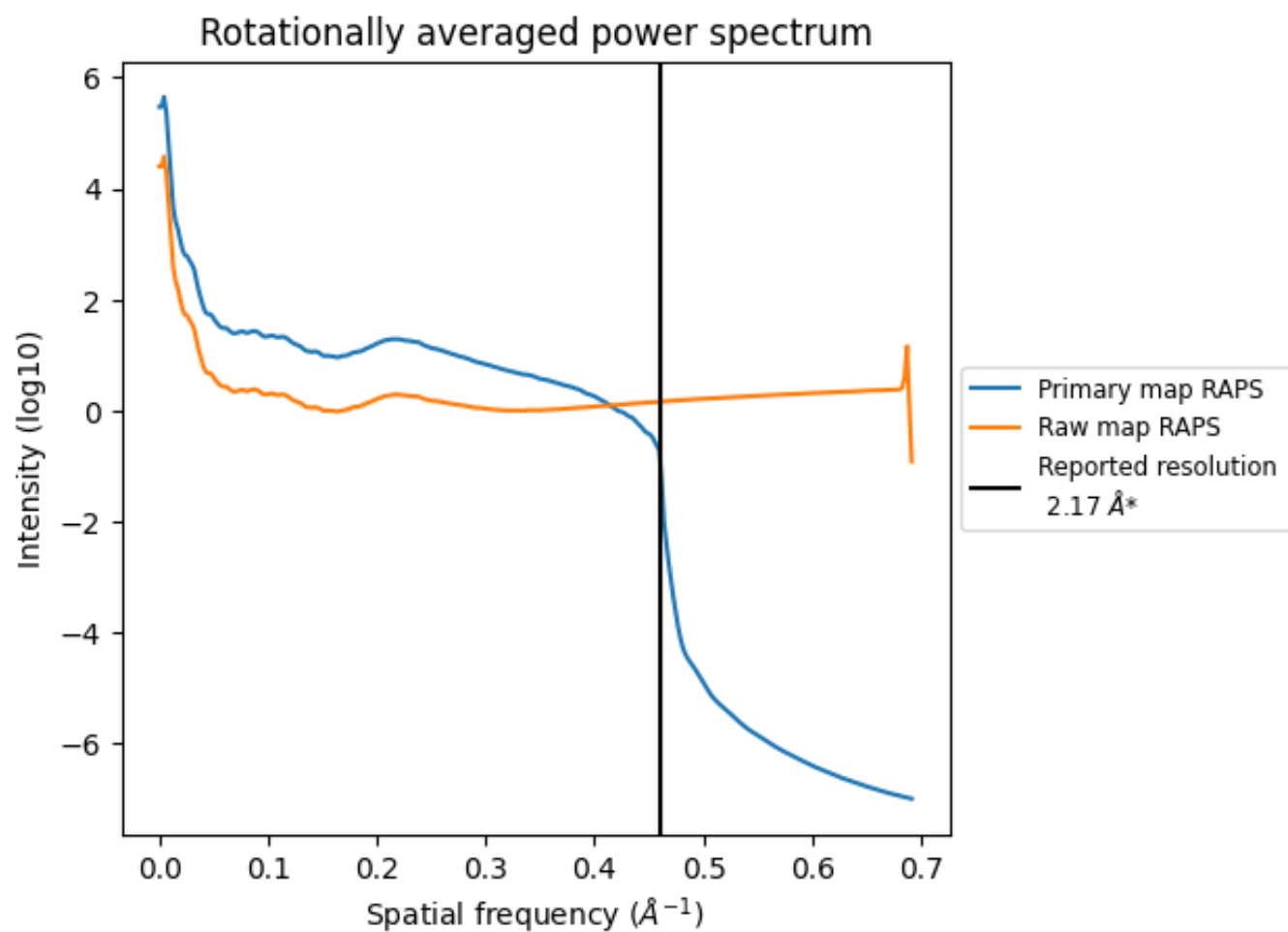
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 285 nm^3 ; this corresponds to an approximate mass of 258 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

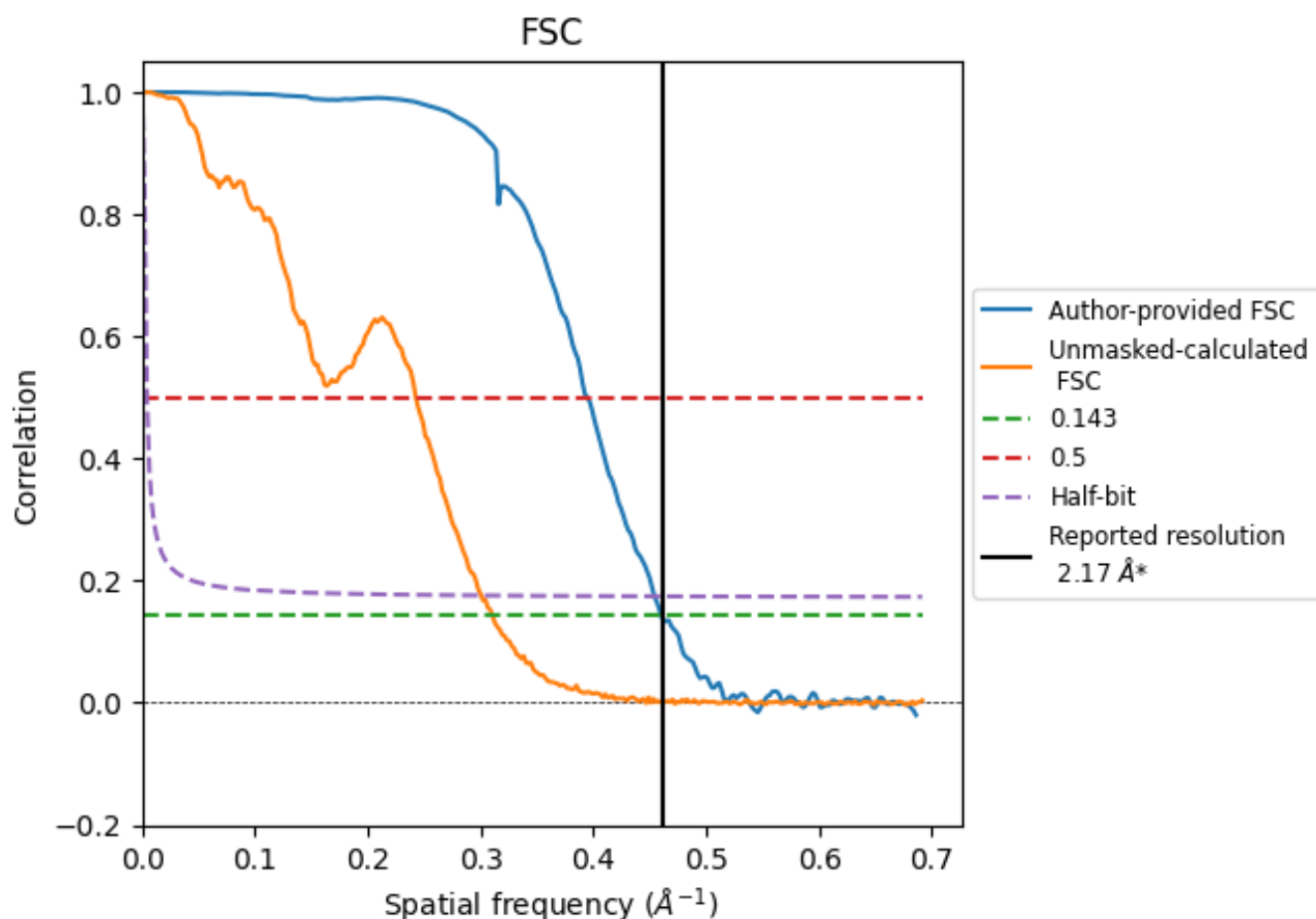


*Reported resolution corresponds to spatial frequency of 0.461 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.461 \AA^{-1}

8.2 Resolution estimates [i](#)

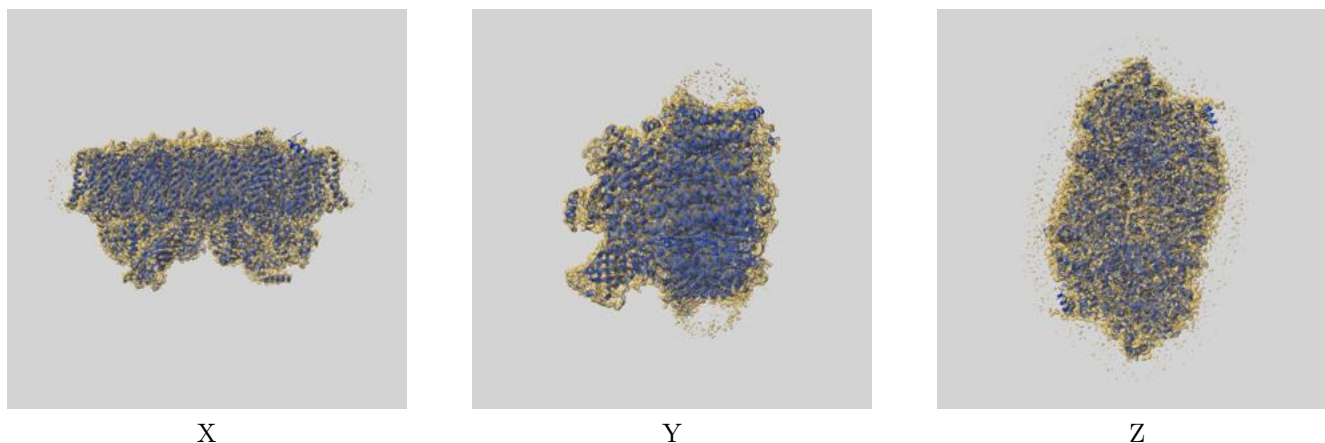
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.17	-	-
Author-provided FSC curve	2.17	2.53	2.20
Unmasked-calculated*	3.22	4.12	3.33

*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 3.22 differs from the reported value 2.17 by more than 10 %

9 Map-model fit [i](#)

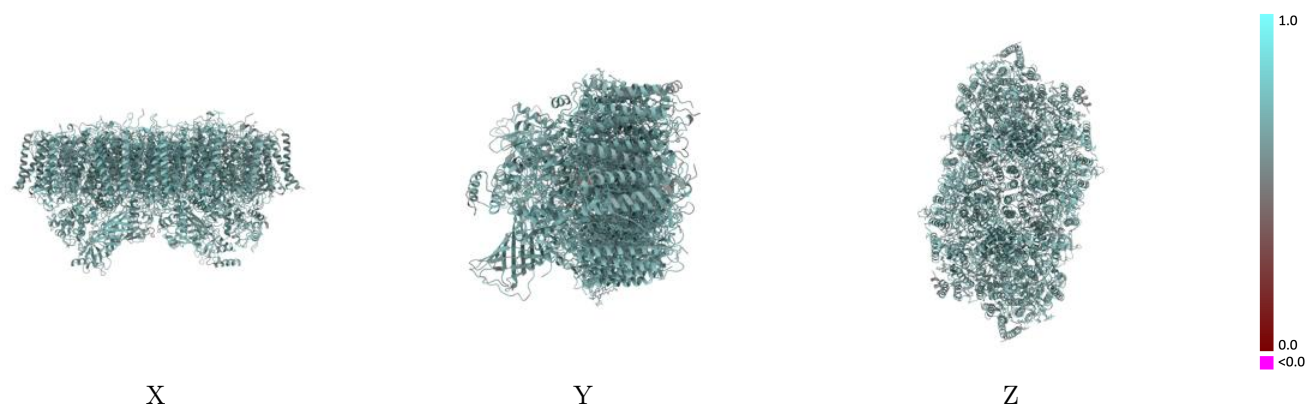
This section contains information regarding the fit between EMDB map EMD-55593 and PDB model 9T5T. Per-residue inclusion information can be found in section [3](#) on page [33](#).

9.1 Map-model overlay [i](#)



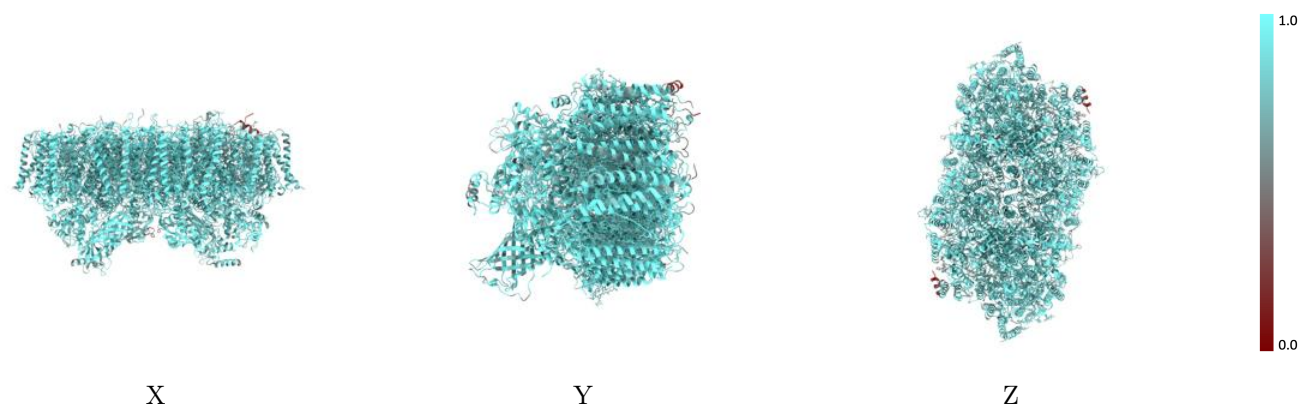
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



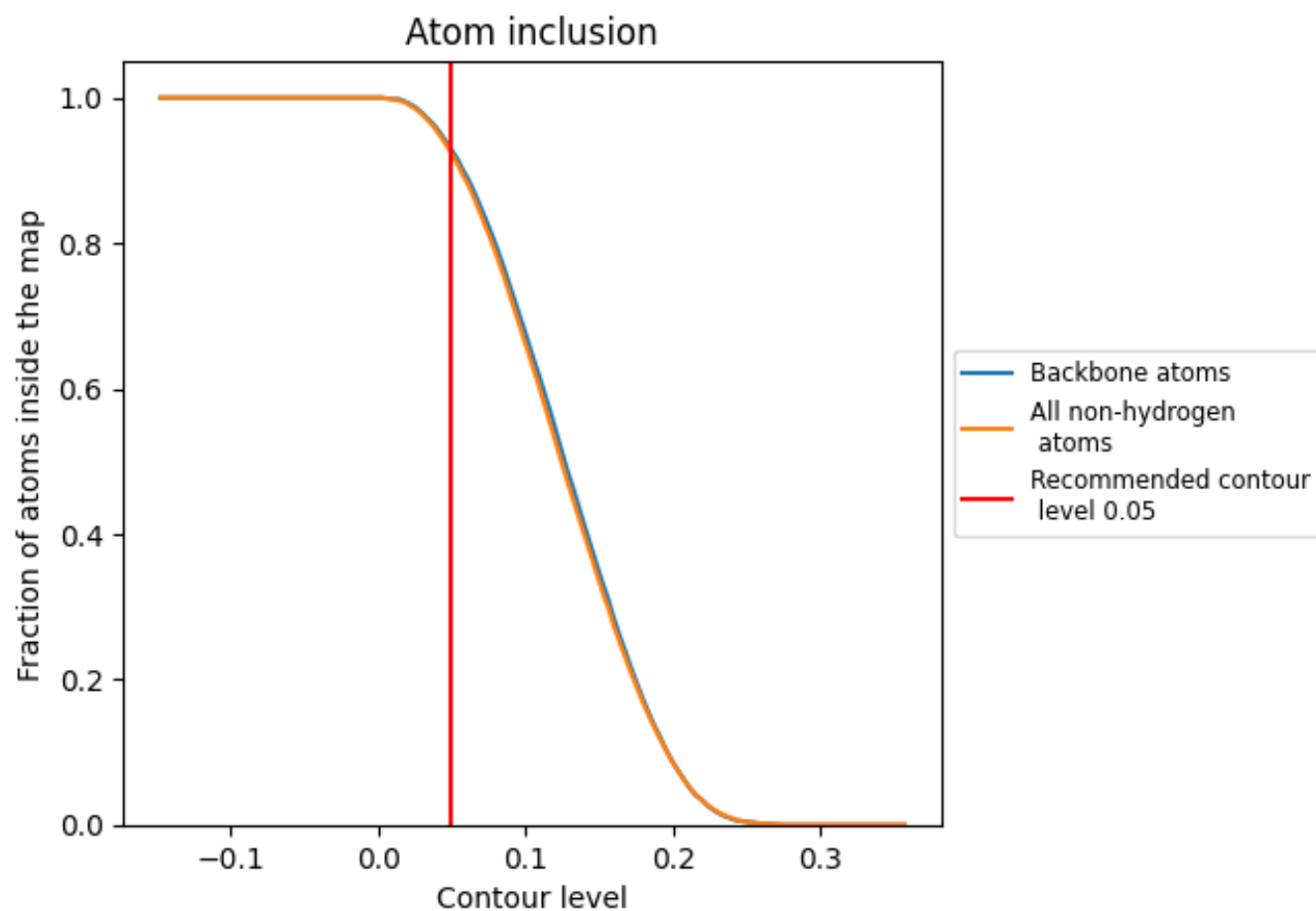
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9230	 0.6620
A	 0.9510	 0.6780
B	 0.9540	 0.6830
C	 0.9420	 0.6640
D	 0.9680	 0.6890
E	 0.8540	 0.6220
F	 0.8750	 0.6310
G	 0.9120	 0.6480
H	 0.9500	 0.6670
I	 0.9700	 0.6710
J	 0.8810	 0.6410
K	 0.9310	 0.6360
L	 0.8990	 0.6540
M	 0.9190	 0.6550
O	 0.8650	 0.6300
P	 0.6040	 0.5400
R	 0.6110	 0.5510
T	 0.9360	 0.6690
U	 0.8710	 0.6360
V	 0.8960	 0.6400
X	 0.8850	 0.6350
Y	 0.7770	 0.5880
Z	 0.8120	 0.5820
a	 0.9510	 0.6780
b	 0.9540	 0.6830
c	 0.9420	 0.6640
d	 0.9680	 0.6900
e	 0.8540	 0.6250
f	 0.8750	 0.6290
g	 0.9120	 0.6520
h	 0.9500	 0.6640
i	 0.9700	 0.6730
j	 0.8810	 0.6390
k	 0.9310	 0.6410
l	 0.8990	 0.6550



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Chain	Atom inclusion	Q-score
m	 0.9190	 0.6530
o	 0.8650	 0.6310
p	 0.6040	 0.5440
r	 0.6110	 0.5530
t	 0.9360	 0.6710
u	 0.8710	 0.6370
v	 0.8960	 0.6400
x	 0.8850	 0.6360
y	 0.7770	 0.5910
z	 0.8120	 0.5810