



Full wwPDB EM Validation Report ⓘ

Jul 24, 2025 – 04:45 pm BST

PDB ID : 9G6G / pdb_00009g6g
EMDB ID : EMD-51101
Title : Semi-active PSII dimer from native Peak4 PSII dimers
Authors : Zhao, Z.; Vercellino, I.; Nixon, P.J.; Sazanov, L.A.
Deposited on : 2024-07-18
Resolution : 2.20 Å (reported)
Based on initial models : 7NHO, 3KZI

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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

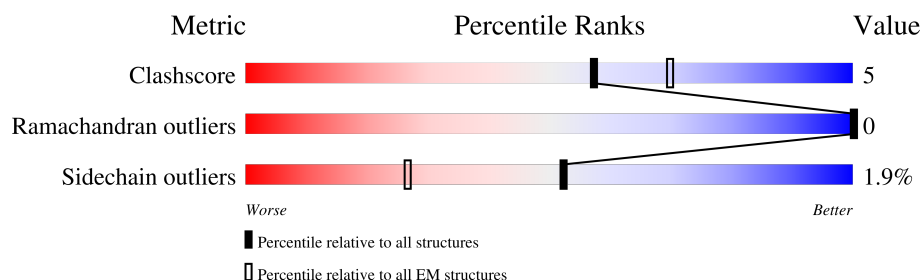
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	360	
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	

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Mol	Chain	Length	Quality of chain
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
14	T	32	
14	t	32	
15	U	134	
16	V	163	
17	X	41	
17	x	41	
18	Y	46	
18	y	46	
19	Z	62	

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Mol	Chain	Length	Quality of chain
19	z	62	
20	a	360	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	C	515	X	-	-	-
23	CLA	C	516	X	-	-	-
23	CLA	C	517	X	-	-	-
23	CLA	C	518	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	D	404	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	402	X	-	-	-
23	CLA	a	403	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	401	X	-	-	-
23	CLA	d	404	X	-	-	-
23	CLA	d	405	X	-	-	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 47004 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	333	Total	C	N	O	S	0	0
			2599	1707	430	447	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	505	Total	C	N	O	S	0	0
			3941	2589	662	677	13		
2	b	504	Total	C	N	O	S	0	0
			3949	2595	655	686	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	451	Total	C	N	O	S	0	0
			3460	2268	581	598	13		
3	c	437	Total	C	N	O	S	0	0
			3362	2211	562	576	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2709	1796	444	457	12		
4	d	341	Total	C	N	O	S	0	0
			2712	1798	444	458	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	80	Total	C	N	O	0	0
			644	422	105	117		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	e	76	Total	C	N	O	0	0
			603	400	96	107		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	35	Total	C	N	O	S	0	0
			280	190	46	43	1		
6	f	34	Total	C	N	O	S	0	0
			274	187	45	41	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			284	194	45	44	1		
8	i	35	Total	C	N	O	S	0	0
			288	196	45	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	35	Total	C	N	O	S	0	0
			253	172	39	41	1		
9	j	29	Total	C	N	O	S	0	0
			216	150	33	32	1		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	35	Total	C	N	O	0	0
			281	189	43	49		
11	l	35	Total	C	N	O	0	0
			287	192	46	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	33	Total	C	N	O	S	0	0
			254	170	38	45	1		
12	m	33	Total	C	N	O	S	0	0
			254	170	37	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	243	Total	C	N	O	S	0	0
			1794	1128	303	359	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	30	Total	C	N	O	S	0	0
			250	177	33	38	2		
14	t	30	Total	C	N	O	S	0	0
			254	179	36	37	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	U	97	Total	C	N	O	0	0
			755	481	128	146		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	X	38	Total	C	N	O	0	0
			279	187	45	47		
17	x	38	Total	C	N	O	0	0
			278	187	45	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	31	Total	C	N	O	S	0	0
			227	152	39	34	2		
18	y	29	Total	C	N	O	S	0	0
			206	136	34	33	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			455	316	67	70	2		
19	z	61	Total	C	N	O	S	0	0
			459	317	68	73	1		

- Molecule 20 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	323	Total	C	N	O	S	0	0
			2531	1660	416	440	15		

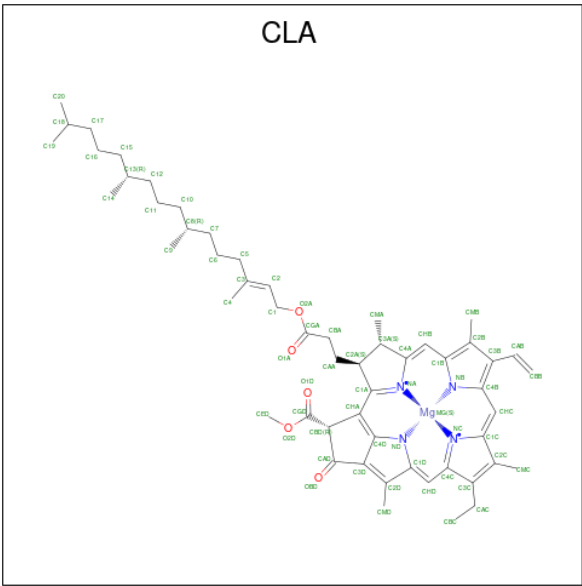
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
22	A	2	Total	Cl	0
			2	2	
22	a	1	Total	Cl	0
			1	1	

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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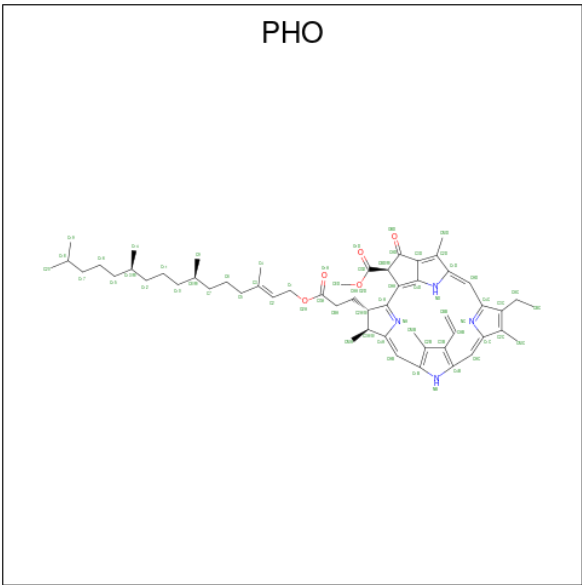
Mol	Chain	Residues	Atoms					AltConf
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	b	1	Total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

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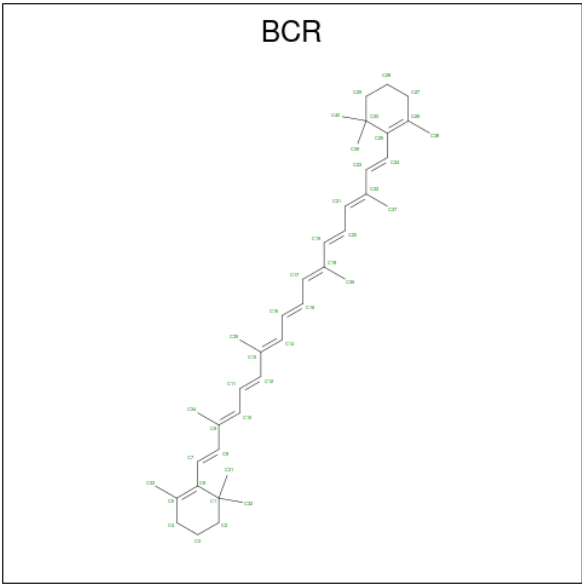
Mol	Chain	Residues	Atoms					AltConf
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0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

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



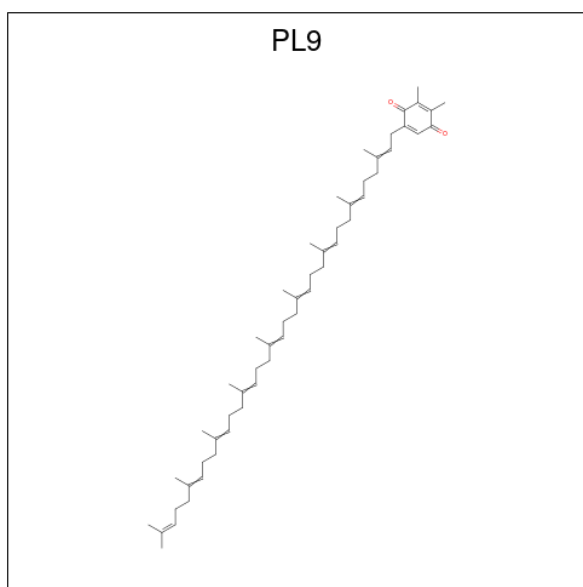
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	
24	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



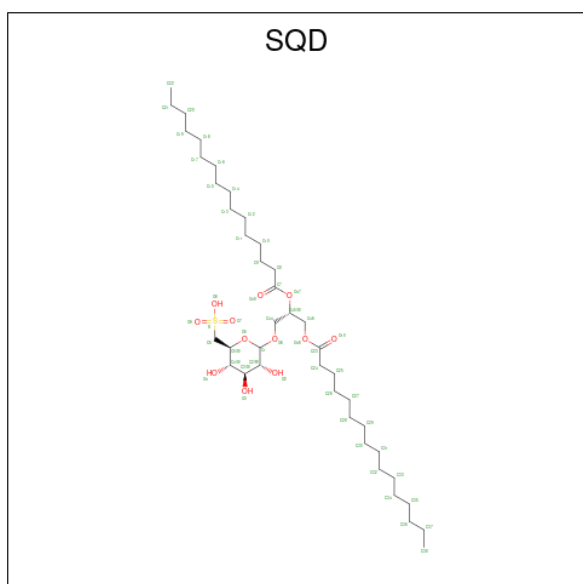
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	D	1	Total C 40 40	0
25	T	1	Total C 40 40	0
25	Y	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	f	1	Total C 40 40	0
25	i	1	Total C 40 40	0
25	j	1	Total C 40 40	0
25	k	1	Total C 40 40	0
25	t	1	Total C 40 40	0
25	z	1	Total C 40 40	0

- Molecule 26 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).



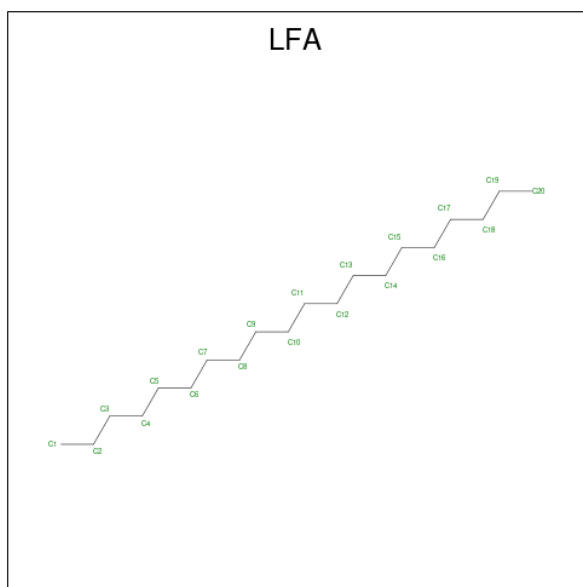
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			55	53	2	
26	D	1	Total	C	O	0
			55	53	2	
26	a	1	Total	C	O	0
			55	53	2	
26	d	1	Total	C	O	0
			55	53	2	

- Molecule 27 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
27	A	1	Total	C	O	S	0
			54	41	12	1	
27	A	1	Total	C	O	S	0
			51	38	12	1	
27	B	1	Total	C	O	S	0
			54	41	12	1	
27	D	1	Total	C	O	S	0
			43	30	12	1	
27	F	1	Total	C	O	S	0
			45	32	12	1	
27	a	1	Total	C	O	S	0
			51	38	12	1	
27	a	1	Total	C	O	S	0
			45	32	12	1	
27	b	1	Total	C	O	S	0
			54	41	12	1	
27	d	1	Total	C	O	S	0
			45	32	12	1	

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



Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	C	0
			7	7	
28	A	1	Total	C	0
			7	7	
28	B	1	Total	C	0
			13	13	

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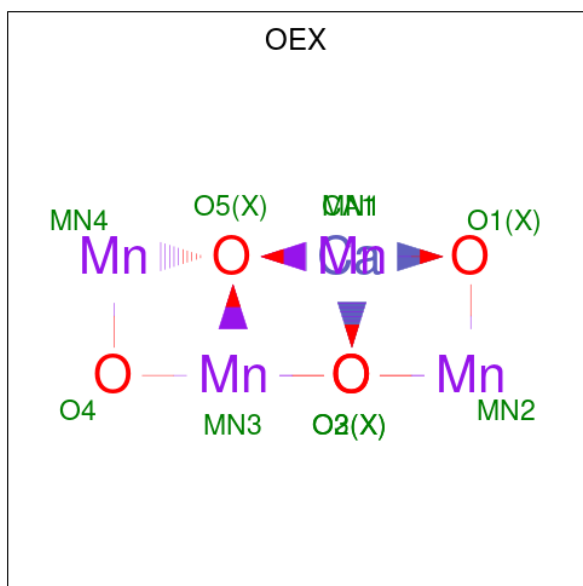
Mol	Chain	Residues	Atoms	AltConf
28	B	1	Total C 6 6	0
28	B	1	Total C 8 8	0
28	B	1	Total C 6 6	0
28	B	1	Total C 7 7	0
28	C	1	Total C 12 12	0
28	C	1	Total C 9 9	0
28	C	1	Total C 13 13	0
28	D	1	Total C 12 12	0
28	D	1	Total C 10 10	0
28	D	1	Total C 8 8	0
28	E	1	Total C 6 6	0
28	H	1	Total C 9 9	0
28	I	1	Total C 13 13	0
28	I	1	Total C 7 7	0
28	I	1	Total C 8 8	0
28	I	1	Total C 8 8	0
28	a	1	Total C 9 9	0
28	a	1	Total C 10 10	0
28	b	1	Total C 8 8	0
28	b	1	Total C 8 8	0
28	b	1	Total C 7 7	0

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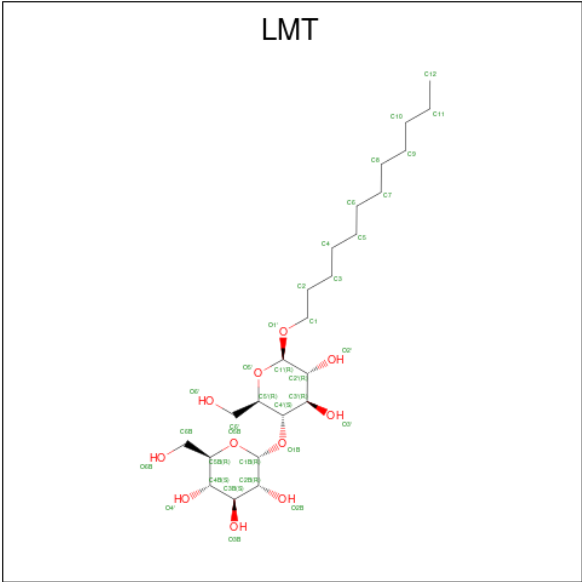
Mol	Chain	Residues	Atoms	AltConf
28	d	1	Total C 10 10	0
28	d	1	Total C 9 9	0
28	e	1	Total C 17 17	0
28	h	1	Total C 10 10	0
28	i	1	Total C 13 13	0
28	m	1	Total C 9 9	0

- Molecule 29 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



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

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



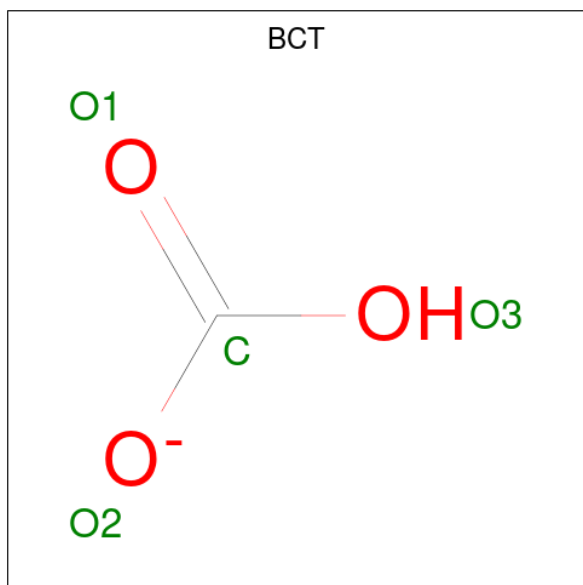
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			35	24	11	
30	B	1	Total	C	O	0
			35	24	11	
30	B	1	Total	C	O	0
			35	24	11	
30	C	1	Total	C	O	0
			35	24	11	
30	D	1	Total	C	O	0
			33	22	11	
30	E	1	Total	C	O	0
			35	24	11	
30	J	1	Total	C	O	0
			24	18	6	
30	M	1	Total	C	O	0
			35	24	11	
30	M	1	Total	C	O	0
			35	24	11	
30	T	1	Total	C	O	0
			24	18	6	
30	T	1	Total	C	O	0
			35	24	11	
30	a	1	Total	C	O	0
			35	24	11	
30	a	1	Total	C	O	0
			24	18	6	
30	c	1	Total	C	O	0
			29	18	11	

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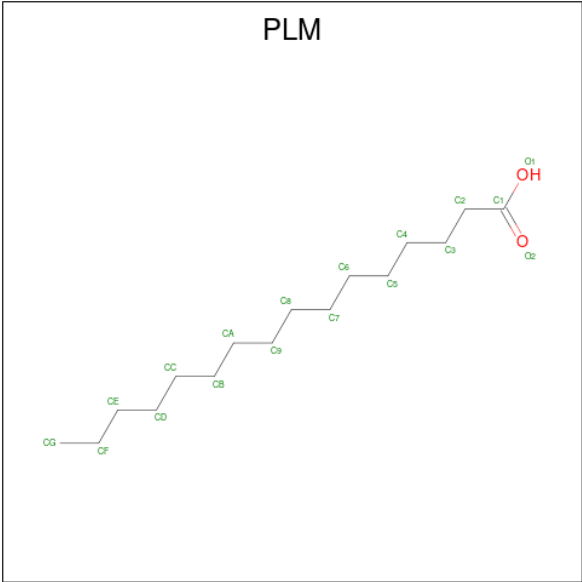
Mol	Chain	Residues	Atoms			AltConf
30	d	1	Total	C	O	0
			24	18	6	
30	f	1	Total	C	O	0
			34	23	11	
30	z	1	Total	C	O	0
			35	24	11	

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



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

- Molecule 32 is PALMITIC ACID (CCD ID: PLM) (formula: $\text{C}_{16}\text{H}_{32}\text{O}_2$).



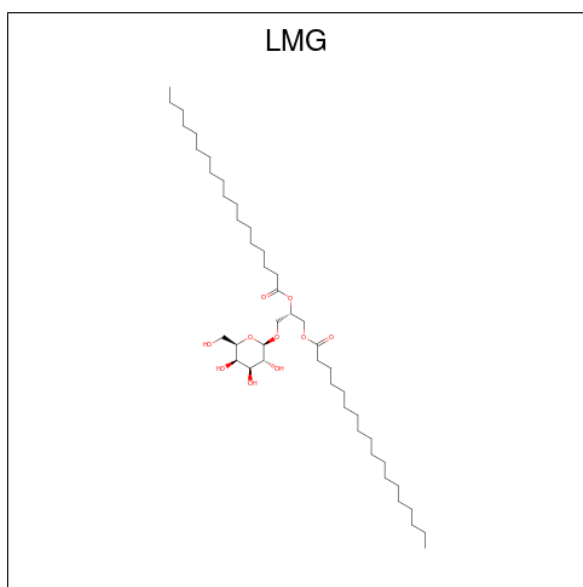
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			13	11	2	
32	B	1	Total	C	O	0
			15	13	2	
32	B	1	Total	C	O	0
			13	11	2	
32	C	1	Total	C	O	0
			13	11	2	
32	C	1	Total	C	O	0
			13	11	2	
32	C	1	Total	C	O	0
			13	11	2	
32	D	1	Total	C	O	0
			18	16	2	
32	D	1	Total	C	O	0
			11	9	2	
32	E	1	Total	C	O	0
			15	13	2	
32	E	1	Total	C	O	0
			16	14	2	
32	E	1	Total	C	O	0
			18	16	2	
32	J	1	Total	C	O	0
			16	14	2	
32	K	1	Total	C	O	0
			14	12	2	
32	a	1	Total	C	O	0
			11	9	2	

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Mol	Chain	Residues	Atoms			AltConf
32	b	1	Total	C	O	0
			15	13	2	
32	b	1	Total	C	O	0
			16	14	2	
32	b	1	Total	C	O	0
			11	9	2	
32	b	1	Total	C	O	0
			12	10	2	
32	c	1	Total	C	O	0
			9	7	2	
32	c	1	Total	C	O	0
			15	13	2	
32	c	1	Total	C	O	0
			10	8	2	
32	c	1	Total	C	O	0
			13	11	2	
32	d	1	Total	C	O	0
			16	14	2	
32	h	1	Total	C	O	0
			11	9	2	
32	i	1	Total	C	O	0
			15	13	2	
32	i	1	Total	C	O	0
			13	11	2	
32	k	1	Total	C	O	0
			12	10	2	
32	l	1	Total	C	O	0
			14	12	2	
32	x	1	Total	C	O	0
			18	16	2	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



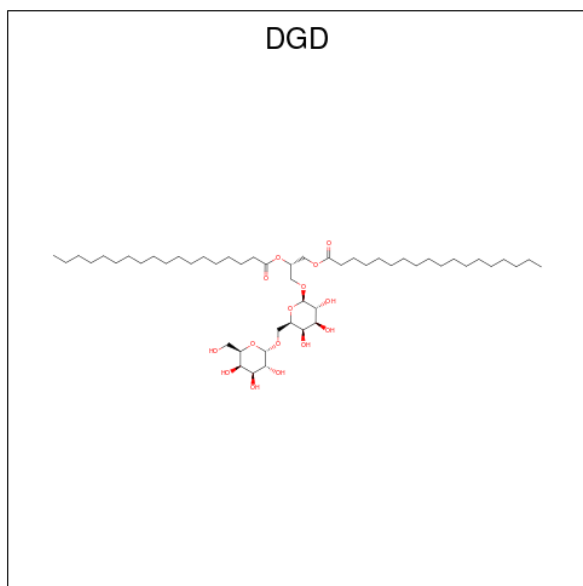
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			51	41	10	
33	C	1	Total	C	O	0
			48	38	10	
33	D	1	Total	C	O	0
			51	41	10	
33	I	1	Total	C	O	0
			51	41	10	
33	Y	1	Total	C	O	0
			51	41	10	
33	a	1	Total	C	O	0
			51	41	10	
33	b	1	Total	C	O	0
			51	41	10	
33	c	1	Total	C	O	0
			51	41	10	
33	d	1	Total	C	O	0
			51	41	10	
33	y	1	Total	C	O	0
			51	41	10	

- Molecule 34 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			6	3	3	

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



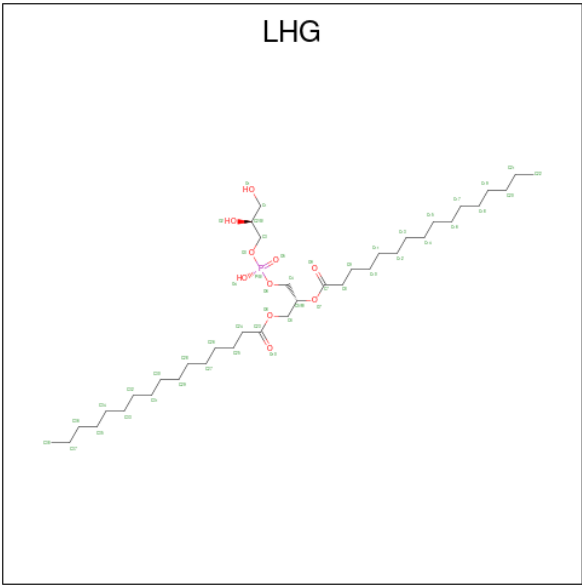
Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			53	38	15	
35	C	1	Total	C	O	0
			62	47	15	

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Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			61	46	15	
35	D	1	Total	C	O	0
			47	36	11	
35	H	1	Total	C	O	0
			58	43	15	
35	c	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			51	41	10	
35	c	1	Total	C	O	0
			62	47	15	
35	d	1	Total	C	O	0
			46	35	11	
35	h	1	Total	C	O	0
			62	47	15	

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



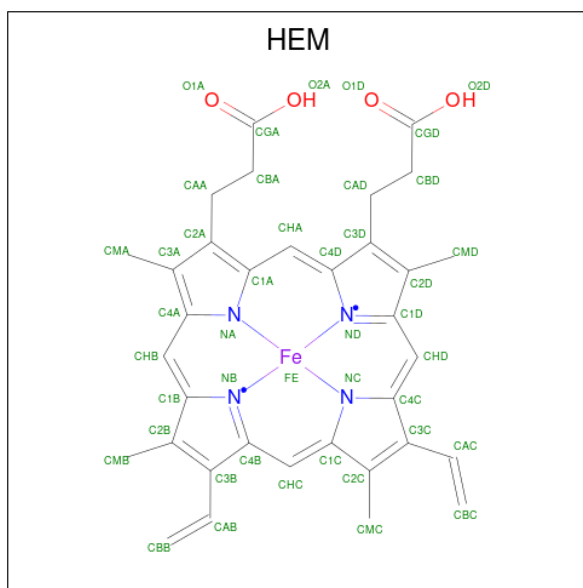
Mol	Chain	Residues	Atoms				AltConf
36	D	1	Total	C	O	P	0
			49	38	10	1	
36	D	1	Total	C	O	P	0
			49	38	10	1	
36	D	1	Total	C	O	P	0
			46	35	10	1	

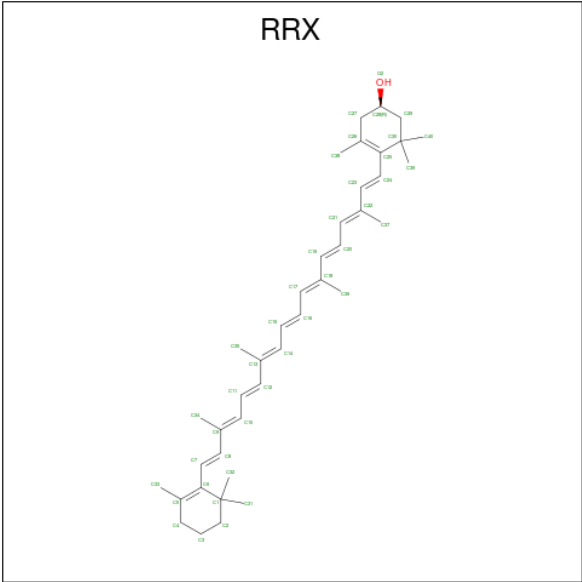
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Mol	Chain	Residues	Atoms				AltConf
36	E	1	Total	C	O	P	0
			49	38	10	1	
36	L	1	Total	C	O	P	0
			49	38	10	1	
36	a	1	Total	C	O	P	0
			46	35	10	1	
36	a	1	Total	C	O	P	0
			49	38	10	1	
36	d	1	Total	C	O	P	0
			49	38	10	1	
36	d	1	Total	C	O	P	0
			49	38	10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

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





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

- Molecule 39 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
39	O	1	Total	Ca	0
			1	1	

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	A	113	Total	O	0
			113	113	
40	B	135	Total	O	0
			135	135	
40	C	118	Total	O	1
			118	118	
40	D	103	Total	O	0
			103	103	
40	E	11	Total	O	0
			11	11	
40	F	4	Total	O	0
			4	4	

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Mol	Chain	Residues	Atoms		AltConf
40	H	15	Total 15	O 15	0
40	I	1	Total 1	O 1	0
40	J	3	Total 3	O 3	0
40	K	2	Total 2	O 2	0
40	L	5	Total 5	O 5	0
40	M	5	Total 5	O 5	0
40	O	38	Total 38	O 38	0
40	T	5	Total 5	O 5	0
40	U	24	Total 24	O 24	0
40	V	36	Total 36	O 36	0
40	X	5	Total 5	O 5	0
40	Y	3	Total 3	O 3	0
40	Z	1	Total 1	O 1	0
40	a	64	Total 64	O 64	0
40	b	107	Total 107	O 107	0
40	c	52	Total 52	O 52	0
40	d	75	Total 75	O 75	0
40	e	6	Total 6	O 6	0
40	f	1	Total 1	O 1	0
40	h	8	Total 8	O 8	0
40	i	1	Total 1	O 1	0

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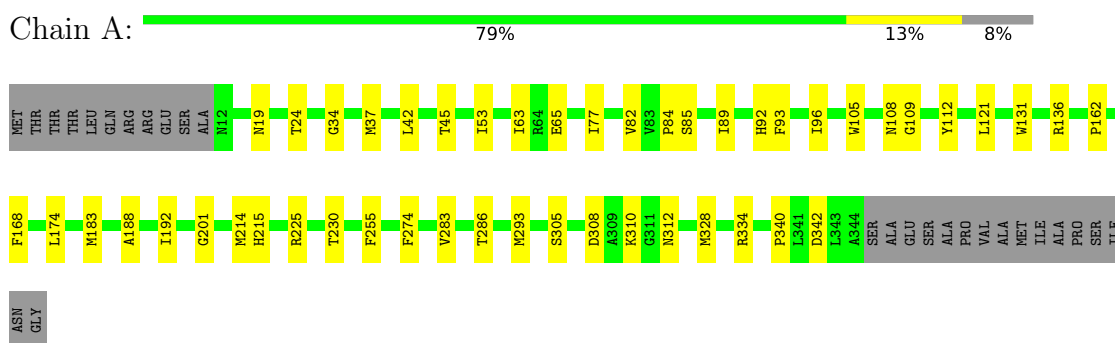
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Mol	Chain	Residues	Atoms		AltConf
40	j	3	Total 3	O 3	0
40	k	1	Total 1	O 1	0
40	l	7	Total 7	O 7	0
40	m	1	Total 1	O 1	0
40	t	3	Total 3	O 3	0
40	x	4	Total 4	O 4	0

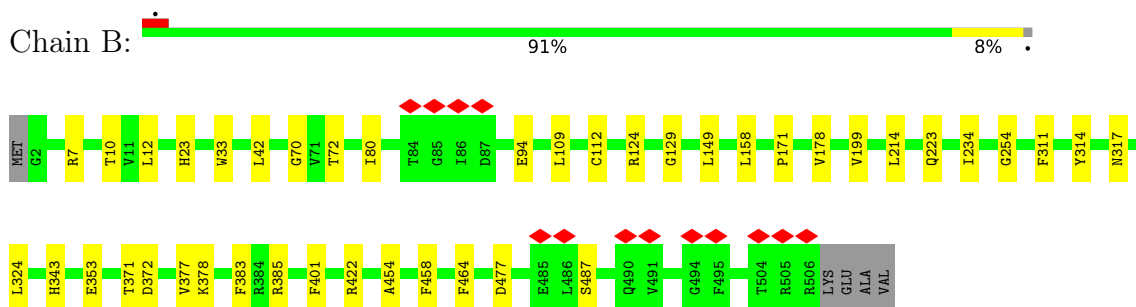
3 Residue-property plots

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

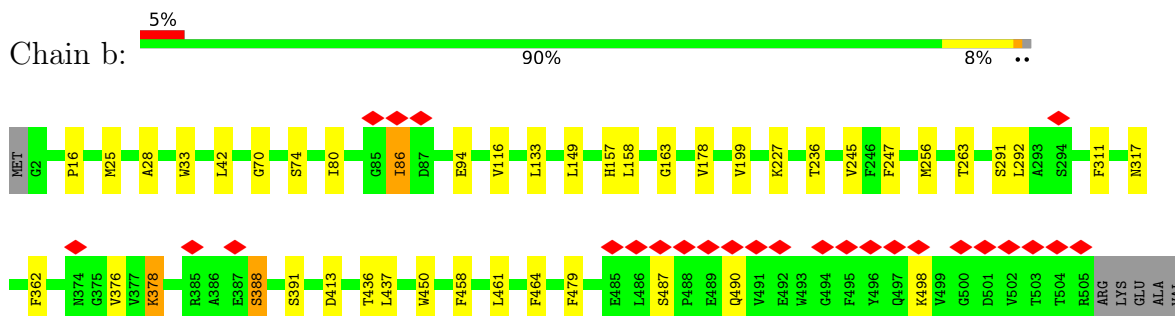
- Molecule 1: Photosystem II protein D1 1




- Molecule 2: Photosystem II CP47 reaction center protein

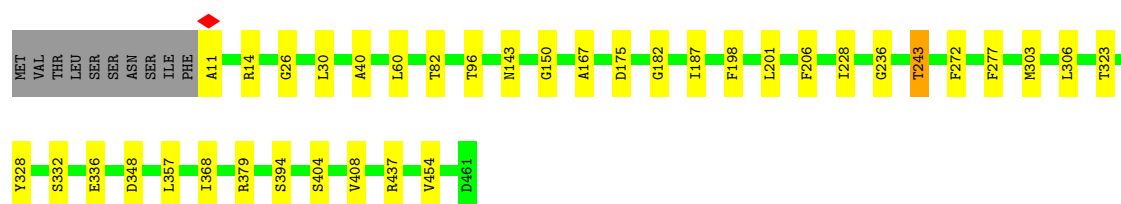


- Molecule 2: Photosystem II CP47 reaction center protein




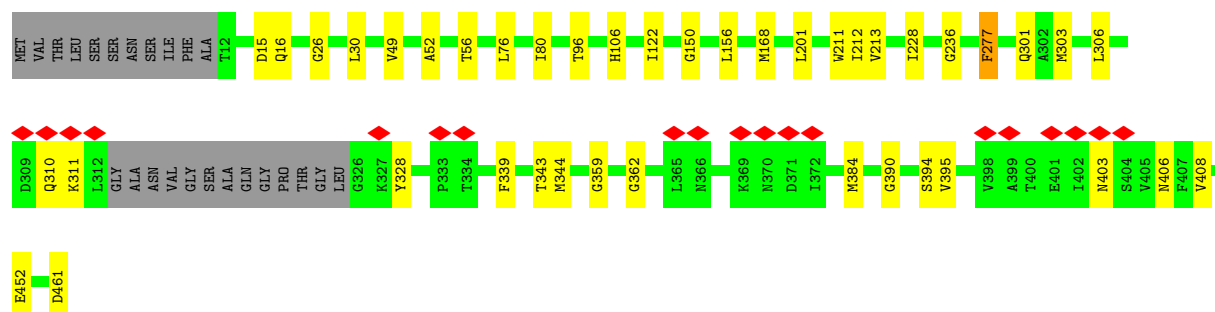
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  90% 8% .




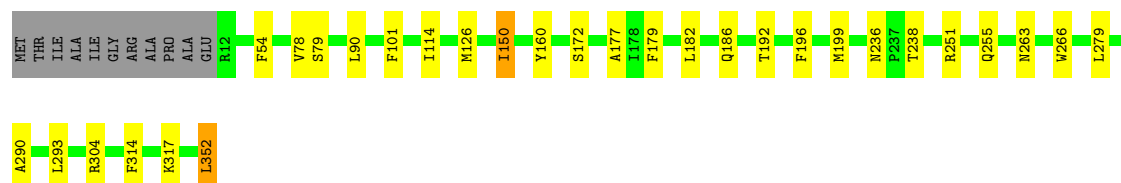
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  86% 9% 5%




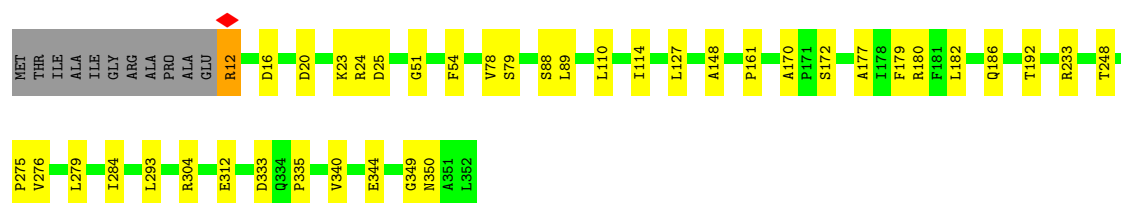
- Molecule 4: Photosystem II D2 protein

Chain D:  88% 8% . .




- Molecule 4: Photosystem II D2 protein

Chain d:  86% 11% .

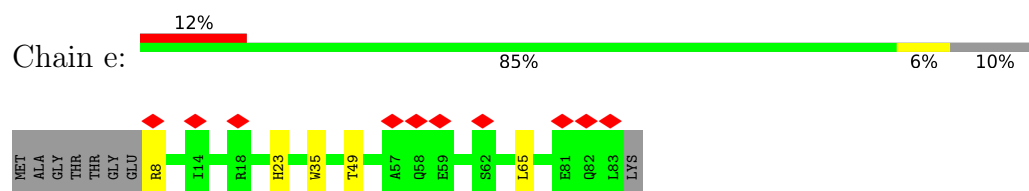


- Molecule 5: Cytochrome b559 subunit alpha

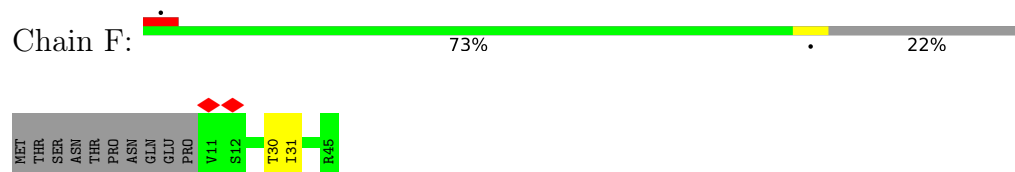
Chain E:  87% 8% 5%



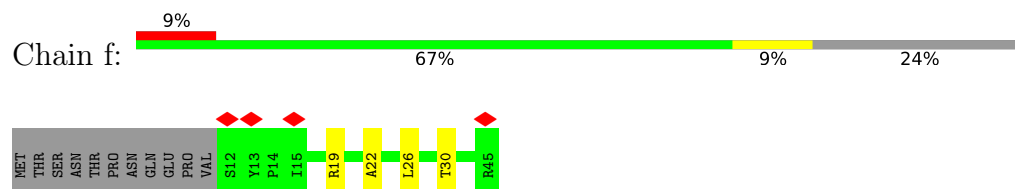
- Molecule 5: Cytochrome b559 subunit alpha



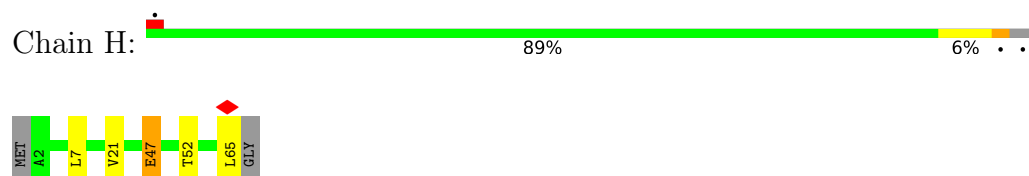
- Molecule 6: Cytochrome b559 subunit beta



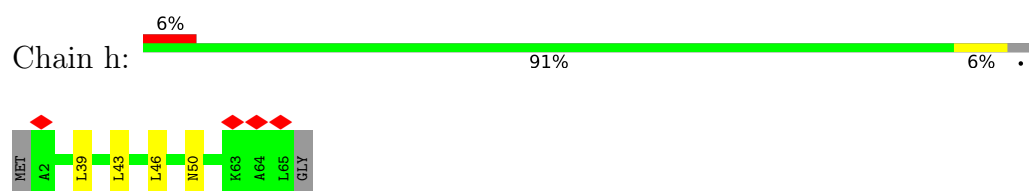
- Molecule 6: Cytochrome b559 subunit beta



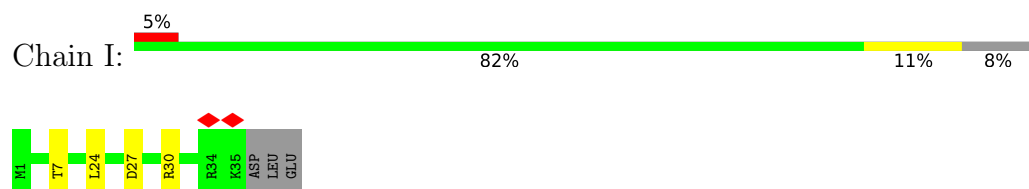
- Molecule 7: Photosystem II reaction center protein H



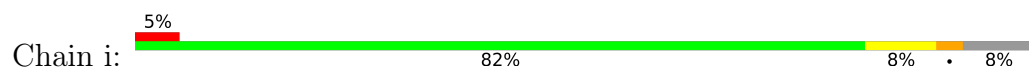
- Molecule 7: Photosystem II reaction center protein H

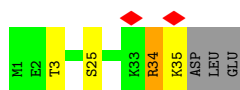


- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I





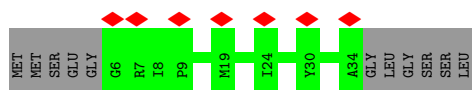
- Molecule 9: Photosystem II reaction center protein J

Chain J: 75% 12% 12%



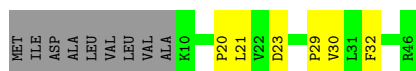
- Molecule 9: Photosystem II reaction center protein J

Chain j: 18% 72% 28%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 67% 13% 20%



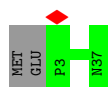
- Molecule 10: Photosystem II reaction center protein K

Chain k: 7% 63% 17% 20%



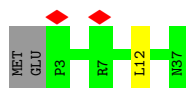
- Molecule 11: Photosystem II reaction center protein L

Chain L: 95% 5%




- Molecule 11: Photosystem II reaction center protein L

Chain l: 5% 92% 5% 5%



- Molecule 12: Photosystem II reaction center protein M

Chain M:  75% 14% 8%




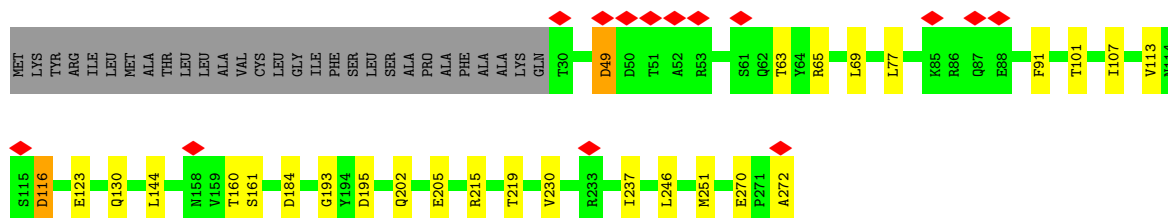
- Molecule 12: Photosystem II reaction center protein M

Chain m:  6% 64% 28% 8%




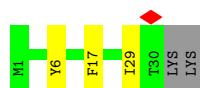
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  5% 79% 10% 11%




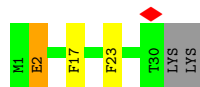
- Molecule 14: Photosystem II reaction center protein T

Chain T:  84% 9% 6%



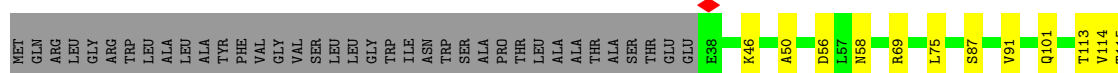
- Molecule 14: Photosystem II reaction center protein T

Chain t:  84% 6% 6%

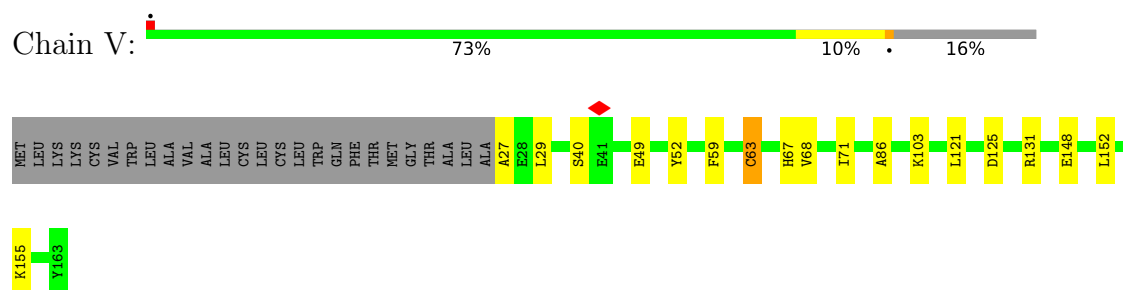


- Molecule 15: Photosystem II 12 kDa extrinsic protein

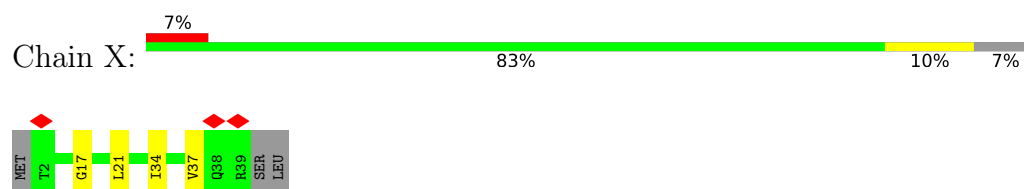
Chain U:  61% 11% 28%



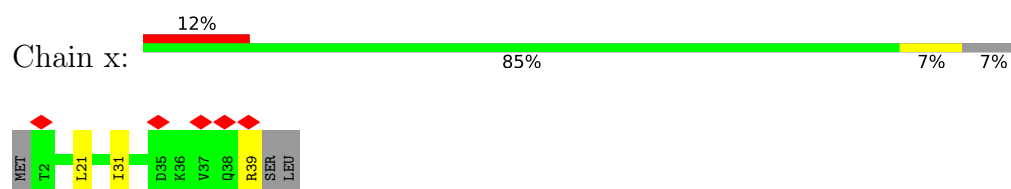
- Molecule 16: Cytochrome c-550



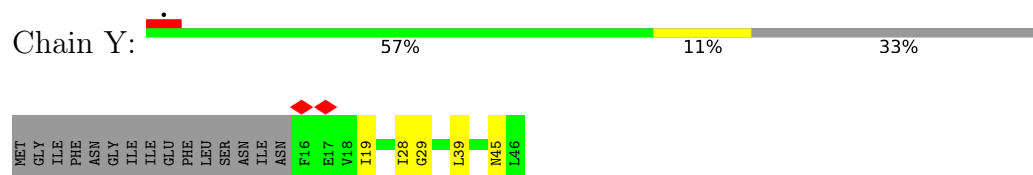
- Molecule 17: Photosystem II reaction center X protein



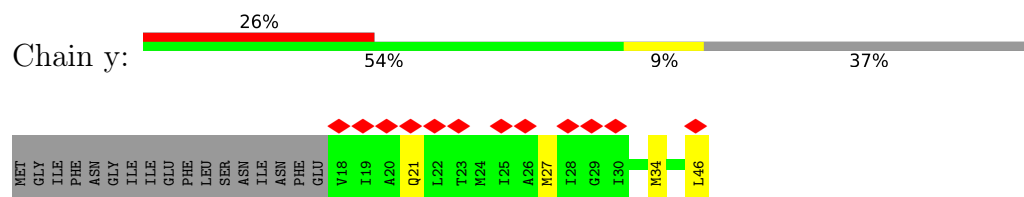
- Molecule 17: Photosystem II reaction center X protein



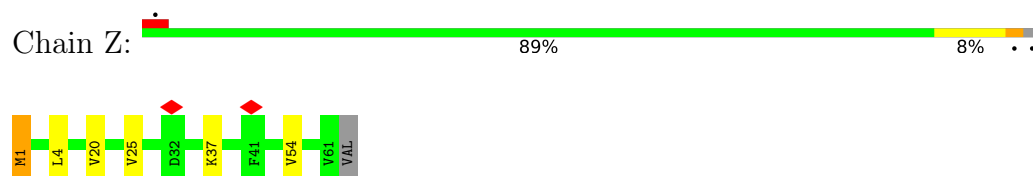
- Molecule 18: Photosystem II reaction center protein Ycf12



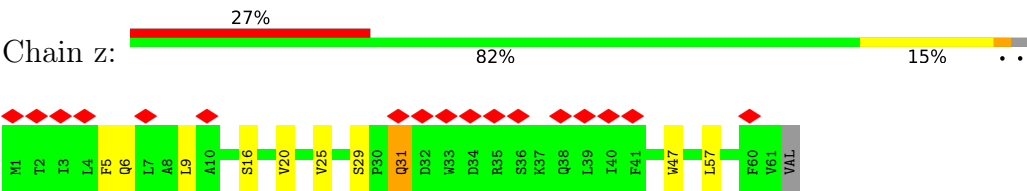
- Molecule 18: Photosystem II reaction center protein Ycf12



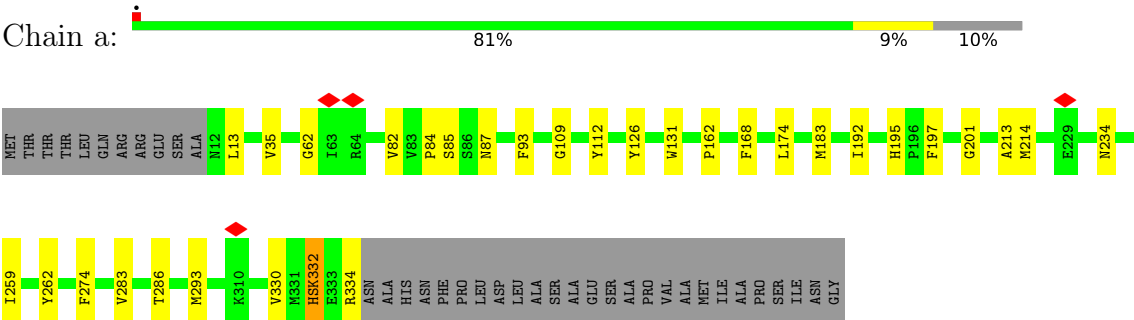
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein D1 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	272215	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.383	Depositor
Minimum map value	-0.129	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.039	Depositor
Map size (Å)	137.0, 208.5, 119.0	wwPDB
Map dimensions	238, 417, 274	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	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: LFA, CL, FE2, CA, LMG, PHO, PLM, LMT, GOL, HSK, FME, BCT, HEM, PL9, DGD, RRX, CLA, BCR, OEX, SQD, LHG

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	0.24	0/2684	0.44	0/3663
2	B	0.22	0/4081	0.39	0/5565
2	b	0.22	0/4089	0.39	0/5576
3	C	0.22	0/3573	0.39	0/4868
3	c	0.20	0/3473	0.38	0/4734
4	D	0.24	0/2804	0.43	0/3822
4	d	0.22	0/2807	0.41	0/3827
5	E	0.20	0/663	0.38	0/907
5	e	0.22	0/622	0.44	0/853
6	F	0.24	0/289	0.44	0/394
6	f	0.22	0/283	0.45	0/387
7	H	0.21	0/519	0.39	0/708
7	h	0.20	0/519	0.39	0/708
8	I	0.20	0/281	0.42	0/380
8	i	0.23	0/285	0.56	0/385
9	J	0.20	0/259	0.42	0/351
9	j	0.15	0/222	0.33	0/303
10	K	0.30	0/299	0.49	0/412
10	k	0.28	0/299	0.54	0/412
11	L	0.18	0/288	0.32	0/392
11	l	0.18	0/294	0.33	0/399
12	M	0.27	0/257	0.49	0/351
12	m	0.31	0/257	0.56	0/351
13	O	0.19	0/1825	0.37	0/2485
14	T	0.21	0/249	0.36	0/339
14	t	0.20	0/253	0.34	0/344
15	U	0.17	0/766	0.36	0/1041
16	V	0.20	0/1073	0.35	0/1459
17	X	0.16	0/282	0.30	0/381
17	x	0.15	0/281	0.28	0/380
18	Y	0.28	0/229	0.45	0/309

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	y	0.25	0/207	0.44	0/278
19	Z	0.22	0/466	0.42	0/639
19	z	0.19	0/470	0.36	0/645
20	a	0.22	0/2600	0.43	0/3545
All	All	0.22	0/37848	0.40	0/51593

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
20	a	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	a	332	HSK	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2599	0	2500	35	0
2	B	3941	0	3786	30	0
2	b	3949	0	3798	29	0
3	C	3460	0	3376	26	0
3	c	3362	0	3267	27	0
4	D	2709	0	2613	22	0
4	d	2712	0	2617	32	0
5	E	644	0	627	5	0
5	e	603	0	581	4	0
6	F	280	0	284	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	274	0	282	3	0
7	H	506	0	529	4	0
7	h	506	0	529	5	0
8	I	284	0	303	4	0
8	i	288	0	307	2	0
9	J	253	0	265	4	0
9	j	216	0	227	0	0
10	K	289	0	294	4	0
10	k	289	0	294	4	0
11	L	281	0	288	0	0
11	l	287	0	299	0	0
12	M	254	0	272	5	0
12	m	254	0	270	9	0
13	O	1794	0	1736	14	0
14	T	250	0	245	2	0
14	t	254	0	257	3	0
15	U	755	0	748	9	0
16	V	1052	0	1053	11	0
17	X	279	0	307	2	0
17	x	278	0	310	3	0
18	Y	227	0	250	3	0
18	y	206	0	226	4	0
19	Z	455	0	486	3	0
19	z	459	0	487	5	0
20	a	2531	0	2434	24	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	1	0	0	0	0
23	A	260	0	288	10	0
23	B	1020	0	1113	23	0
23	C	845	0	936	23	0
23	D	130	0	144	6	0
23	a	195	0	216	7	0
23	b	1040	0	1152	23	0
23	c	845	0	936	25	0
23	d	195	0	216	7	0
24	A	64	0	74	1	0
24	D	64	0	74	2	0
24	a	64	0	74	2	0
24	d	64	0	74	2	0
25	A	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	120	0	168	4	0
25	C	120	0	168	6	0
25	D	40	0	56	1	0
25	T	40	0	56	3	0
25	Y	40	0	56	4	0
25	a	40	0	56	1	0
25	b	120	0	168	8	0
25	f	40	0	56	0	0
25	i	40	0	56	1	0
25	j	40	0	56	0	0
25	k	40	0	56	2	0
25	t	40	0	56	1	0
25	z	40	0	56	2	0
26	A	55	0	80	5	0
26	D	55	0	80	3	0
26	a	55	0	80	4	0
26	d	55	0	80	1	0
27	A	105	0	147	7	0
27	B	54	0	78	4	0
27	D	43	0	50	0	0
27	F	45	0	57	1	0
27	a	96	0	126	5	0
27	b	54	0	78	2	0
27	d	45	0	57	2	0
28	A	14	0	20	0	0
28	B	40	0	63	1	0
28	C	34	0	59	1	0
28	D	30	0	48	0	0
28	E	6	0	8	0	0
28	H	9	0	14	0	0
28	I	36	0	56	1	0
28	a	19	0	30	0	0
28	b	23	0	37	0	0
28	d	19	0	30	0	0
28	e	17	0	33	0	0
28	h	10	0	19	1	0
28	i	13	0	22	0	0
28	m	9	0	14	0	0
29	A	10	0	0	0	0
30	A	35	0	46	1	0
30	B	70	0	92	2	0
30	C	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	D	33	0	39	3	0
30	E	35	0	46	0	0
30	J	24	0	35	0	0
30	M	70	0	92	3	0
30	T	59	0	81	0	0
30	a	59	0	81	1	0
30	c	29	0	31	1	0
30	d	24	0	35	1	0
30	f	34	0	41	1	0
30	z	35	0	46	0	0
31	A	4	0	0	0	0
31	a	4	0	0	0	0
32	A	13	0	18	2	0
32	B	28	0	40	0	0
32	C	39	0	54	1	0
32	D	29	0	45	4	0
32	E	49	0	77	1	0
32	J	16	0	24	0	0
32	K	14	0	20	1	0
32	a	11	0	14	0	0
32	b	54	0	76	1	0
32	c	47	0	62	2	0
32	d	16	0	24	1	0
32	h	11	0	14	0	0
32	i	28	0	40	0	0
32	k	12	0	16	0	0
32	l	14	0	20	0	0
32	x	18	0	31	0	0
33	B	51	0	72	5	0
33	C	48	0	66	1	0
33	D	51	0	72	4	0
33	I	51	0	72	3	0
33	Y	51	0	72	0	0
33	a	51	0	72	2	0
33	b	51	0	72	1	0
33	c	51	0	72	1	0
33	d	51	0	72	1	0
33	y	51	0	72	2	0
34	B	6	0	8	0	0
35	C	176	0	232	6	0
35	D	47	0	59	2	0
35	H	58	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	c	175	0	235	3	0
35	d	46	0	57	0	0
35	h	62	0	82	1	0
36	D	144	0	213	7	0
36	E	49	0	74	2	0
36	L	49	0	74	1	0
36	a	95	0	139	4	0
36	d	98	0	148	3	0
36	l	49	0	74	5	0
37	E	43	0	30	2	0
37	V	43	0	30	0	0
37	f	43	0	30	2	0
38	H	41	0	56	0	0
38	x	41	0	56	1	0
39	O	1	0	0	0	0
40	A	113	0	0	0	0
40	B	135	0	0	0	0
40	C	118	0	0	2	0
40	D	103	0	0	0	0
40	E	11	0	0	0	0
40	F	4	0	0	0	0
40	H	15	0	0	0	0
40	I	1	0	0	0	0
40	J	3	0	0	0	0
40	K	2	0	0	0	0
40	L	5	0	0	0	0
40	M	5	0	0	0	0
40	O	38	0	0	1	0
40	T	5	0	0	0	0
40	U	24	0	0	0	0
40	V	36	0	0	0	0
40	X	5	0	0	0	0
40	Y	3	0	0	0	0
40	Z	1	0	0	0	0
40	a	64	0	0	0	0
40	b	107	0	0	0	0
40	c	52	0	0	0	0
40	d	75	0	0	0	0
40	e	6	0	0	0	0
40	f	1	0	0	0	0
40	h	8	0	0	0	0
40	i	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	j	3	0	0	0	0
40	k	1	0	0	0	0
40	l	7	0	0	0	0
40	m	1	0	0	0	0
40	t	3	0	0	0	0
40	x	4	0	0	0	0
All	All	47004	0	47601	433	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 (433) 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)
25:T:101:BCR:H19C	25:b:619:BCR:H363	1.69	0.74
4:D:192:THR:HG23	23:D:404:CLA:HBC2	1.75	0.68
3:c:30:LEU:HD21	23:c:511:CLA:H2A	1.75	0.67
20:a:192:ILE:HG13	20:a:293:MET:HE1	1.77	0.67
30:a:411:LMT:O3B	4:d:304:ARG:NH2	2.28	0.66
4:d:304:ARG:NH1	12:m:1:MET:SD	2.69	0.66
3:C:30:LEU:HD21	23:C:516:CLA:H2A	1.77	0.65
4:d:192:THR:HG23	23:d:404:CLA:HBC2	1.78	0.65
20:a:195:HIS:HD2	20:a:197:PHE:H	1.43	0.64
20:a:334:ARG:HG3	4:d:350:ASN:HB3	1.79	0.64
4:D:199:MET:HG2	26:D:402:PL9:H311	1.79	0.64
3:c:306:LEU:HD12	3:c:328:TYR:HB2	1.79	0.63
2:B:124:ARG:NH1	2:B:129:GLY:O	2.31	0.63
23:b:616:CLA:H2	23:b:617:CLA:HBB2	1.79	0.62
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.81	0.62
15:U:46:LYS:HE2	15:U:118:GLU:HB2	1.83	0.61
4:d:186:GLN:HB2	23:d:404:CLA:HBC1	1.83	0.60
23:B:601:CLA:HAB	23:B:601:CLA:H171	1.84	0.60
3:c:390:GLY:HA3	3:c:408:VAL:HG22	1.83	0.60
23:c:502:CLA:H61	23:c:512:CLA:H42	1.82	0.60
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.84	0.59
4:D:186:GLN:HB2	23:D:404:CLA:HBC1	1.84	0.58
4:D:304:ARG:NH2	30:D:417:LMT:O3B	2.34	0.58
2:b:498:LYS:HA	4:d:24:ARG:HA	1.85	0.58
15:U:75:LEU:HD21	15:U:101:GLN:HB3	1.86	0.58
33:a:408:LMG:H382	35:c:514:DGD:HB42	1.86	0.57
23:c:513:CLA:HAB	25:k:101:BCR:H371	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:279:LEU:HD22	24:D:401:PHO:HBC3	1.86	0.57
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.37	0.57
3:c:52:ALA:O	3:c:56:THR:OG1	2.20	0.57
36:l:102:LHG:H322	12:m:18:PRO:HB3	1.87	0.57
4:d:279:LEU:HD22	24:d:402:PHO:HBC3	1.86	0.56
15:U:87:SER:HA	15:U:114:VAL:HG21	1.86	0.56
2:B:311:PHE:O	2:B:317:ASN:ND2	2.38	0.56
32:D:414:PLM:HC2	17:X:17:GLY:HA2	1.87	0.56
2:B:12:LEU:HB2	23:B:612:CLA:HMC2	1.86	0.56
27:B:630:SQD:H201	25:B:631:BCR:H351	1.86	0.56
2:B:23:HIS:HE1	23:B:610:CLA:H193	1.70	0.56
3:C:437:ARG:NH2	40:C:606:HOH:O	2.37	0.56
1:A:215:HIS:ND1	26:A:410:PL9:O2	2.34	0.56
33:B:619:LMG:O10	12:M:4:ASN:ND2	2.38	0.56
13:O:65:ARG:HG3	13:O:272:ALA:HB2	1.89	0.55
36:L:101:LHG:H271	12:M:22:LEU:HD21	1.88	0.55
3:c:76:LEU:HB3	23:c:503:CLA:HED3	1.88	0.55
13:O:49:ASP:N	13:O:49:ASP:OD1	2.40	0.55
18:y:21:GLN:HE22	33:y:101:LMG:HC61	1.72	0.55
3:C:306:LEU:HD12	3:C:328:TYR:HB3	1.89	0.55
1:A:63:ILE:HB	3:C:323:THR:HG21	1.88	0.55
18:Y:39:LEU:HD21	19:Z:25:VAL:HA	1.89	0.55
2:b:116:VAL:HG21	25:b:620:BCR:H292	1.89	0.54
20:a:85:SER:HA	20:a:109:GLY:HA3	1.89	0.54
7:H:47:GLU:HG3	7:H:52:THR:HB	1.89	0.54
3:C:11:ALA:HB1	3:C:14:ARG:HB2	1.90	0.54
2:B:234:ILE:HD11	23:B:610:CLA:H191	1.89	0.53
33:y:101:LMG:H291	33:y:101:LMG:H151	1.90	0.53
1:A:201:GLY:HA3	1:A:286:THR:HB	1.89	0.53
23:C:507:CLA:H61	23:C:517:CLA:H42	1.91	0.53
3:c:26:GLY:HA3	23:c:511:CLA:HMD2	1.90	0.53
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.38	0.53
23:A:406:CLA:H112	33:D:409:LMG:H232	1.90	0.53
23:b:616:CLA:H71	23:b:617:CLA:H18	1.90	0.53
19:z:31:GLN:O	19:z:31:GLN:NE2	2.42	0.53
35:c:516:DGD:HAH1	33:d:411:LMG:H191	1.91	0.53
4:d:54:PHE:O	5:e:49:THR:OG1	2.25	0.53
28:C:520:LFA:H162	32:K:101:PLM:H32	1.91	0.53
20:a:84:PRO:HA	20:a:112:TYR:CG	2.44	0.53
5:E:10:PHE:H	36:E:101:LHG:HC32	1.74	0.53
3:c:452:GLU:OE2	4:d:248:THR:OG1	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:93:PHE:HZ	23:a:405:CLA:HAA1	1.74	0.53
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.91	0.52
3:c:168:MET:HE1	32:c:519:PLM:H72	1.90	0.52
4:d:89:LEU:H	7:h:50:ASN:HD21	1.55	0.52
23:C:511:CLA:H18	23:C:511:CLA:H122	1.91	0.52
2:b:42:LEU:HD13	2:b:94:GLU:HG3	1.91	0.52
12:m:18:PRO:O	12:m:21:PHE:HB3	2.09	0.52
2:B:149:LEU:HD11	28:B:622:LFA:H162	1.92	0.52
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.52
1:A:283:VAL:HA	1:A:286:THR:HG22	1.91	0.52
23:b:617:CLA:H171	25:b:620:BCR:H331	1.91	0.52
3:C:303:MET:HE1	3:C:357:LEU:HD12	1.93	0.51
23:b:602:CLA:H193	38:x:102:RRX:H37	1.92	0.51
33:B:619:LMG:HC5	30:B:620:LMT:H12	1.92	0.51
15:U:58:ASN:HB3	15:U:117:VAL:HG22	1.92	0.51
3:C:379:ARG:NH1	40:C:607:HOH:O	2.38	0.51
3:c:303:MET:HE2	3:c:339:PHE:HZ	1.75	0.51
12:M:33:GLN:OE1	30:M:101:LMT:O3B	2.28	0.51
3:c:395:VAL:HG11	3:c:403:ASN:HD22	1.74	0.51
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.93	0.51
10:k:39:TRP:NE1	18:y:46:LEU:OXT	2.36	0.51
4:d:20:ASP:OD2	17:x:39:ARG:NH2	2.43	0.51
2:b:247:PHE:HB2	23:b:609:CLA:HBC1	1.92	0.51
3:c:122:ILE:HD11	23:c:511:CLA:H92	1.93	0.51
23:B:607:CLA:H2	33:B:619:LMG:H152	1.93	0.50
20:a:62:GLY:HA3	3:c:344:MET:HE1	1.92	0.50
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.92	0.50
36:l:102:LHG:H241	36:l:102:LHG:H111	1.92	0.50
2:B:314:TYR:OH	13:O:202:GLN:NE2	2.42	0.50
20:a:201:GLY:HA3	20:a:286:THR:HB	1.93	0.50
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.94	0.50
15:U:50:ALA:HB1	15:U:113:THR:HG21	1.94	0.50
20:a:82:VAL:HB	20:a:174:LEU:HB2	1.92	0.50
13:O:116:ASP:OD1	13:O:116:ASP:N	2.44	0.50
20:a:283:VAL:HA	20:a:286:THR:HG22	1.93	0.50
1:A:214:MET:HB3	26:A:410:PL9:H103	1.93	0.50
2:B:109:LEU:HD13	27:a:410:SQD:H262	1.93	0.50
3:c:156:LEU:HD21	23:c:509:CLA:H61	1.94	0.50
32:A:418:PLM:H61	2:b:94:GLU:HG2	1.94	0.50
2:B:254:GLY:HA3	35:H:101:DGD:HB52	1.94	0.49
1:A:308:ASP:OD1	1:A:312:ASN:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:411:SQD:H342	25:b:619:BCR:H291	1.93	0.49
2:b:158:LEU:HB3	2:b:199:VAL:HG22	1.94	0.49
26:a:409:PL9:H252	36:a:417:LHG:H182	1.94	0.49
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.94	0.49
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.93	0.49
1:A:85:SER:HA	1:A:109:GLY:HA3	1.95	0.49
33:D:409:LMG:H412	6:F:30:THR:HG21	1.95	0.49
2:b:436:THR:HG23	2:b:437:LEU:HG	1.94	0.49
23:b:603:CLA:H101	23:b:610:CLA:H193	1.94	0.49
1:A:274:PHE:HD1	27:A:415:SQD:H112	1.77	0.49
3:C:394:SER:HA	3:C:408:VAL:HG23	1.94	0.49
1:A:93:PHE:HZ	23:A:408:CLA:HAA1	1.78	0.48
1:A:342:ASP:HB2	4:D:352:LEU:HD11	1.95	0.48
15:U:69:ARG:NH2	16:V:86:ALA:O	2.46	0.48
2:b:256:MET:HA	2:b:263:THR:HG21	1.96	0.48
2:B:454:ALA:HB2	33:B:619:LMG:H172	1.95	0.48
23:C:513:CLA:H93	36:D:408:LHG:H151	1.93	0.48
20:a:87:ASN:HD22	3:c:344:MET:HE2	1.78	0.48
25:B:617:BCR:H363	25:B:631:BCR:H19C	1.96	0.48
2:b:25:MET:HG2	25:b:618:BCR:H23C	1.95	0.48
23:A:405:CLA:HED1	26:D:402:PL9:H372	1.94	0.48
13:O:215:ARG:NH1	40:O:405:HOH:O	2.39	0.48
23:c:501:CLA:C3D	23:c:503:CLA:H2	2.44	0.48
23:c:511:CLA:HBA1	25:z:101:BCR:H271	1.95	0.48
3:C:206:PHE:HZ	33:I:103:LMG:H161	1.79	0.48
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.95	0.48
13:O:195:ASP:OD1	13:O:195:ASP:N	2.43	0.48
36:d:409:LHG:H152	36:l:102:LHG:H281	1.95	0.48
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.25	0.48
1:A:92:HIS:NE2	3:C:348:ASP:OD2	2.42	0.47
13:O:219:THR:HG21	13:O:246:LEU:HD12	1.95	0.47
2:b:413:ASP:N	2:b:413:ASP:OD1	2.42	0.47
23:b:605:CLA:H93	23:b:606:CLA:HAB	1.95	0.47
1:A:305:SER:HA	9:J:39:SER:HB3	1.96	0.47
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.44	0.47
20:a:214:MET:HE1	24:d:402:PHO:CAD	2.44	0.47
23:b:604:CLA:H61	23:b:604:CLA:H41	1.78	0.47
1:A:19:ASN:OD1	8:I:30:ARG:NH2	2.46	0.47
4:D:54:PHE:O	5:E:49:THR:OG1	2.23	0.47
36:D:408:LHG:H302	36:D:408:LHG:H331	1.72	0.47
2:B:458:PHE:HB3	23:B:604:CLA:HBC2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:630:SQD:H461	14:t:23:PHE:HB3	1.97	0.47
3:C:454:VAL:HG13	4:D:251:ARG:HD2	1.96	0.47
36:E:101:LHG:H291	36:E:101:LHG:H261	1.80	0.47
10:K:21:LEU:HD21	25:Y:102:BCR:HC31	1.97	0.47
3:c:359:GLY:N	3:c:362:GLY:O	2.42	0.47
2:B:464:PHE:HD2	23:B:611:CLA:HAC2	1.79	0.47
36:D:407:LHG:H182	14:T:17:PHE:HZ	1.80	0.47
32:E:102:PLM:H21	9:J:10:LEU:HD21	1.97	0.47
25:T:101:BCR:H351	27:b:601:SQD:H181	1.96	0.47
2:b:498:LYS:NZ	4:d:20:ASP:OD1	2.42	0.47
2:B:422:ARG:NH1	13:O:205:GLU:OE2	2.47	0.47
23:B:604:CLA:H61	23:B:604:CLA:H92	1.77	0.46
23:B:613:CLA:HED3	23:B:613:CLA:H2	1.97	0.46
30:M:102:LMT:H3B	12:m:31:SER:HA	1.97	0.46
25:b:619:BCR:H20C	25:b:619:BCR:H361	1.76	0.46
3:c:80:ILE:HD11	23:c:503:CLA:HED2	1.97	0.46
4:d:180:ARG:NE	4:d:333:ASP:OD1	2.46	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.50	0.46
35:C:503:DGD:HB72	33:I:103:LMG:H171	1.97	0.46
20:a:162:PRO:HB3	20:a:168:PHE:HA	1.97	0.46
2:b:86:ILE:H	2:b:86:ILE:HG13	1.50	0.46
2:b:498:LYS:HE3	4:d:23:LYS:HB2	1.97	0.46
3:C:26:GLY:HA3	23:C:516:CLA:HMD2	1.96	0.46
2:b:28:ALA:HB1	27:b:601:SQD:H221	1.98	0.46
5:e:23:HIS:CD2	37:f:102:HEM:NC	2.83	0.46
32:C:524:PLM:H82	33:C:525:LMG:H151	1.97	0.46
3:c:49:VAL:HG13	3:c:106:HIS:HD2	1.80	0.46
23:c:502:CLA:H161	23:c:502:CLA:H141	1.73	0.46
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.51	0.46
3:C:175:ASP:O	3:C:182:GLY:HA2	2.16	0.46
26:a:409:PL9:H251	26:a:409:PL9:H302	1.98	0.46
23:A:406:CLA:H91	33:D:409:LMG:H212	1.97	0.46
26:A:410:PL9:H43	26:A:410:PL9:H471	1.74	0.46
27:A:415:SQD:H311	35:C:504:DGD:HBS1	1.96	0.46
27:d:408:SQD:H242	17:x:31:ILE:HD13	1.97	0.46
20:a:126:TYR:CZ	24:a:404:PHO:HBA1	2.50	0.46
3:c:213:VAL:HG13	3:c:277:PHE:HA	1.98	0.46
23:c:504:CLA:H42	35:c:515:DGD:HB31	1.97	0.46
30:d:403:LMT:H123	28:h:101:LFA:H13	1.96	0.46
23:C:506:CLA:C2D	23:C:508:CLA:H2	2.46	0.46
25:C:527:BCR:H332	19:Z:54:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:a:131:TRP:CZ3	23:c:505:CLA:HAA2	2.51	0.46
6:f:19:ARG:NH2	37:f:102:HEM:O2D	2.48	0.46
33:a:408:LMG:H182	33:a:408:LMG:H151	1.77	0.45
26:a:409:PL9:H261	23:d:404:CLA:H141	1.98	0.45
3:c:15:ASP:N	3:c:15:ASP:OD1	2.49	0.45
23:d:405:CLA:H62	23:d:405:CLA:H41	1.81	0.45
23:D:405:CLA:H43	32:D:414:PLM:HF1	1.98	0.45
36:a:416:LHG:H152	36:a:416:LHG:H332	1.99	0.45
4:d:12:ARG:HG3	4:d:16:ASP:HB2	1.98	0.45
27:B:630:SQD:H302	27:B:630:SQD:H332	1.79	0.45
23:c:513:CLA:HAB	25:k:101:BCR:H24C	1.98	0.45
4:d:79:SER:HA	4:d:172:SER:HB3	1.99	0.45
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.52	0.45
3:C:198:PHE:HA	3:C:201:LEU:HB2	1.98	0.45
4:D:126:MET:HE3	4:D:150:ILE:HD12	1.99	0.45
23:c:511:CLA:H52	18:y:46:LEU:HD12	1.99	0.45
3:C:167:ALA:HB1	3:C:187:ILE:HD13	1.98	0.45
2:B:371:THR:HG22	2:B:377:VAL:HA	1.98	0.45
23:B:614:CLA:H3A	23:B:614:CLA:HBA2	1.76	0.45
23:B:615:CLA:H161	7:H:7:LEU:HD21	1.97	0.45
3:C:60:LEU:HD11	3:C:96:THR:HB	1.99	0.45
23:c:503:CLA:H18	23:c:510:CLA:HBB2	1.98	0.45
23:B:604:CLA:H91	23:B:604:CLA:H111	1.75	0.45
3:C:404:SER:HB2	16:V:68:VAL:HG23	1.99	0.45
4:D:179:PHE:HA	4:D:182:LEU:HD12	1.98	0.45
20:a:259:ILE:HA	36:a:417:LHG:H202	1.99	0.45
2:B:112:CYS:HA	25:t:101:BCR:H282	1.99	0.45
2:B:223:GLN:HG2	7:H:21:VAL:HG21	1.99	0.45
23:B:605:CLA:H62	23:B:605:CLA:H41	1.81	0.45
23:a:403:CLA:H13	23:a:403:CLA:H172	1.76	0.45
23:b:609:CLA:H141	23:b:609:CLA:H161	1.82	0.45
3:C:143:ASN:HD21	3:C:243:THR:HB	1.82	0.44
36:D:408:LHG:H152	36:D:408:LHG:H332	1.99	0.44
20:a:183:MET:HA	23:a:402:CLA:HMD1	1.99	0.44
23:b:616:CLA:H2	23:b:617:CLA:CBB	2.46	0.44
25:b:619:BCR:H24C	25:b:619:BCR:H371	1.88	0.44
23:B:604:CLA:H11	23:B:605:CLA:C1D	2.47	0.44
20:a:262:TYR:HA	36:a:417:LHG:H383	1.99	0.44
33:b:621:LMG:H412	12:m:17:VAL:HG21	1.98	0.44
5:E:30:LEU:HD11	37:E:105:HEM:HAB	1.99	0.44
18:Y:28:ILE:HG23	25:Y:102:BCR:H12C	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:504:CLA:H151	23:c:508:CLA:H143	1.99	0.44
4:d:148:ALA:HB2	4:d:276:VAL:HG13	1.99	0.44
18:y:27:MET:HE3	18:y:27:MET:HB3	1.82	0.44
25:C:501:BCR:H271	23:C:516:CLA:HBA1	1.99	0.44
23:a:402:CLA:H202	36:d:410:LHG:H161	1.99	0.44
23:c:512:CLA:H203	23:c:512:CLA:H161	1.85	0.44
5:e:35:TRP:HE1	30:f:103:LMT:H6D	1.82	0.44
2:B:33:TRP:CD1	25:B:631:BCR:H381	2.53	0.44
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.99	0.44
20:a:234:ASN:ND2	36:l:102:LHG:O4	2.48	0.44
10:k:29:PRO:O	10:k:32:PHE:HB2	2.18	0.44
36:l:102:LHG:H171	36:l:102:LHG:H142	1.77	0.44
24:A:407:PHO:H51	27:A:411:SQD:H201	2.00	0.44
2:B:149:LEU:HD23	23:B:603:CLA:HBC1	2.00	0.44
5:E:57:ALA:H	5:E:60:GLN:HE21	1.65	0.44
10:K:20:PRO:O	10:K:23:ASP:HB2	2.17	0.44
4:D:236:ASN:OD1	4:D:238:THR:OG1	2.31	0.44
2:b:74:SER:OG	2:b:94:GLU:OE2	2.29	0.44
23:A:406:CLA:H112	23:A:406:CLA:H142	1.84	0.44
26:A:410:PL9:H271	26:A:410:PL9:H251	1.59	0.44
27:A:415:SQD:H341	23:C:513:CLA:H202	2.00	0.44
23:C:517:CLA:H62	23:C:517:CLA:H41	1.64	0.44
13:O:69:LEU:HB3	13:O:107:ILE:HB	2.00	0.44
20:a:214:MET:HE2	20:a:214:MET:HB2	1.64	0.44
3:c:150:GLY:HA2	3:c:236:GLY:HA2	1.98	0.44
30:c:517:LMT:H2B	8:i:25:SER:HB3	2.00	0.44
1:A:53:ILE:HG21	30:D:417:LMT:H82	1.99	0.43
2:B:171:PRO:HD3	7:H:65:LEU:HD12	1.99	0.43
2:b:487:SER:HB3	2:b:490:GLN:HB2	1.98	0.43
1:A:131:TRP:CH2	23:C:510:CLA:HAA2	2.53	0.43
4:D:79:SER:HA	4:D:172:SER:HB3	2.00	0.43
23:D:405:CLA:NB	32:D:414:PLM:HD1	2.33	0.43
36:D:406:LHG:H351	36:D:406:LHG:H102	1.99	0.43
23:d:401:CLA:H52	26:d:406:PL9:H151	2.00	0.43
3:C:306:LEU:HD21	3:C:368:ILE:HG23	1.98	0.43
37:E:105:HEM:HMC2	6:F:31:ILE:HG13	2.00	0.43
23:d:405:CLA:H142	23:d:405:CLA:H112	1.81	0.43
27:a:407:SQD:H331	27:a:407:SQD:H302	1.78	0.43
2:b:464:PHE:HD2	23:b:612:CLA:HAC2	1.83	0.43
4:d:78:VAL:HG11	4:d:114:ILE:HD12	2.00	0.43
23:C:517:CLA:H142	23:C:517:CLA:H111	1.91	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	1.89	0.43
2:B:72:THR:HG22	2:B:80:ILE:HD11	2.00	0.43
2:B:372:ASP:OD2	2:B:378:LYS:NZ	2.50	0.43
4:D:293:LEU:HD23	4:D:293:LEU:HA	1.93	0.43
3:c:394:SER:OG	3:c:406:ASN:ND2	2.52	0.43
23:d:405:CLA:H42	7:h:43:LEU:HD11	2.01	0.43
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.99	0.43
3:C:332:SER:OG	3:C:336:GLU:OE1	2.35	0.43
23:C:515:CLA:H61	23:C:515:CLA:H2	1.73	0.43
5:E:12:ASP:O	9:J:7:ARG:NH1	2.44	0.43
16:V:29:LEU:HD23	16:V:49:GLU:HG2	2.01	0.43
20:a:330:VAL:O	4:d:349:GLY:N	2.50	0.43
24:a:404:PHO:H92	24:a:404:PHO:H62	1.82	0.43
23:b:616:CLA:H8	23:b:617:CLA:HBB1	2.00	0.43
3:c:301:GLN:HB2	3:c:384:MET:HG3	2.01	0.43
1:A:45:THR:HG23	23:A:405:CLA:H201	1.99	0.43
20:a:183:MET:HB3	23:a:402:CLA:HBC2	2.01	0.43
3:c:311:LYS:HD2	3:c:311:LYS:HA	1.78	0.43
25:z:101:BCR:H371	25:z:101:BCR:H24C	1.75	0.43
2:B:385:ARG:NH2	13:O:193:GLY:O	2.52	0.43
25:C:501:BCR:H343	25:Y:102:BCR:HC32	2.00	0.43
23:c:508:CLA:HBC3	23:c:510:CLA:H71	2.01	0.43
4:d:161:PRO:HB3	4:d:170:ALA:HB2	2.00	0.43
23:A:408:CLA:H41	23:A:408:CLA:H62	1.78	0.43
23:C:513:CLA:H203	10:K:30:VAL:HG13	2.00	0.43
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.00	0.42
23:A:404:CLA:H192	23:A:404:CLA:H161	1.85	0.42
23:B:612:CLA:H102	23:B:612:CLA:H61	1.86	0.42
23:B:614:CLA:H62	23:B:614:CLA:H41	1.76	0.42
4:D:101:PHE:HB2	35:D:411:DGD:HA22	2.01	0.42
23:c:505:CLA:HBC2	25:i:103:BCR:H341	2.00	0.42
23:c:506:CLA:H151	23:c:506:CLA:H18	1.77	0.42
9:J:9:PRO:HD2	9:J:12:ILE:HD12	2.00	0.42
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.84	0.42
19:z:5:PHE:HB2	19:z:57:LEU:HB3	2.00	0.42
16:V:103:LYS:HG2	16:V:121:LEU:HD12	2.01	0.42
8:i:34:ARG:HE	8:i:35:LYS:HZ2	1.67	0.42
30:A:416:LMT:H12	8:I:24:LEU:HD13	2.00	0.42
2:B:343:HIS:O	2:B:401:PHE:HA	2.20	0.42
23:B:603:CLA:H141	23:B:603:CLA:H161	1.83	0.42
35:C:504:DGD:HGB3	36:D:408:LHG:H212	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:D:414:PLM:HG3	17:X:21:LEU:HD11	2.01	0.42
10:K:29:PRO:O	10:K:32:PHE:HB2	2.19	0.42
30:M:102:LMT:H5'	12:m:31:SER:HB3	2.01	0.42
13:O:230:VAL:HG13	13:O:237:ILE:HG22	2.00	0.42
2:b:311:PHE:O	2:b:317:ASN:ND2	2.51	0.42
25:C:501:BCR:H20C	25:C:501:BCR:H361	1.94	0.42
1:A:24:THR:O	4:D:255:GLN:NE2	2.50	0.42
1:A:121:LEU:HD11	23:C:510:CLA:H152	2.02	0.42
2:b:461:LEU:HD21	4:d:284:ILE:HD11	2.02	0.42
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.01	0.42
25:D:403:BCR:H20C	25:D:403:BCR:H361	1.90	0.42
23:D:405:CLA:H93	23:D:405:CLA:H112	1.84	0.42
27:a:410:SQD:H141	27:a:410:SQD:H112	1.82	0.42
3:c:394:SER:O	3:c:406:ASN:ND2	2.53	0.42
3:C:198:PHE:HD1	3:C:201:LEU:HD12	1.85	0.42
23:C:506:CLA:H143	23:C:506:CLA:H161	1.85	0.42
23:b:606:CLA:H62	23:b:606:CLA:H41	1.80	0.42
23:b:615:CLA:H112	23:b:615:CLA:H71	1.87	0.42
1:A:34:GLY:HA2	1:A:37:MET:HB3	2.02	0.42
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.02	0.42
3:C:40:ALA:HB2	23:C:516:CLA:HMA2	2.02	0.42
3:C:206:PHE:HE2	33:I:103:LMG:H132	1.85	0.42
4:D:101:PHE:HB3	35:D:411:DGD:HG2	2.02	0.42
23:b:613:CLA:H61	23:b:613:CLA:H102	1.71	0.42
27:A:415:SQD:H151	36:D:408:LHG:H172	2.02	0.41
33:B:619:LMG:H321	33:B:619:LMG:H291	1.92	0.41
16:V:52:TYR:OH	16:V:148:GLU:OE2	2.32	0.41
16:V:59:PHE:HA	16:V:63:CYS:SG	2.60	0.41
27:a:410:SQD:H191	27:a:410:SQD:H161	1.93	0.41
10:k:12:PRO:HB2	10:k:15:TYR:HD1	1.85	0.41
23:A:408:CLA:H62	23:A:408:CLA:H101	1.67	0.41
2:B:7:ARG:O	2:B:10:THR:OG1	2.33	0.41
23:B:603:CLA:H41	23:B:603:CLA:H61	1.74	0.41
25:B:617:BCR:H24C	25:B:617:BCR:H371	1.85	0.41
23:C:512:CLA:H92	23:C:512:CLA:H61	1.90	0.41
23:C:518:CLA:HAB	25:C:527:BCR:H371	2.03	0.41
4:D:263:ASN:HB3	4:D:266:TRP:HB3	2.02	0.41
19:Z:1:MET:HB2	19:Z:4:LEU:HB3	2.01	0.41
26:D:402:PL9:H422	26:D:402:PL9:H401	1.80	0.41
25:T:101:BCR:H381	2:b:33:TRP:CD1	2.55	0.41
23:c:507:CLA:H61	23:c:507:CLA:H41	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.55	0.41
3:C:82:THR:HG22	23:C:506:CLA:HED1	2.03	0.41
3:C:150:GLY:HA2	3:C:236:GLY:HA2	2.03	0.41
23:a:405:CLA:H162	23:a:405:CLA:H122	1.67	0.41
26:a:409:PL9:H403	6:f:22:ALA:HB2	2.02	0.41
2:b:16:PRO:HB3	2:b:133:LEU:HD21	2.01	0.41
1:A:42:LEU:HD13	25:A:409:BCR:H353	2.02	0.41
23:B:601:CLA:H93	23:B:601:CLA:H111	1.93	0.41
3:C:272:PHE:HB3	35:C:503:DGD:HA42	2.03	0.41
16:V:67:HIS:HA	16:V:71:ILE:O	2.20	0.41
23:b:612:CLA:H72	23:b:612:CLA:H112	1.68	0.41
23:c:513:CLA:H203	33:c:521:LMG:H412	2.03	0.41
26:A:410:PL9:H371	26:A:410:PL9:H351	1.76	0.41
8:I:7:THR:HG21	28:I:104:LFA:H91	2.02	0.41
2:b:70:GLY:HA2	2:b:178:VAL:HG21	2.01	0.41
23:b:604:CLA:HAB	23:b:606:CLA:H152	2.02	0.41
1:A:183:MET:HA	23:A:404:CLA:HMD1	2.01	0.41
23:C:517:CLA:H112	23:C:517:CLA:H91	1.82	0.41
4:D:314:PHE:HA	4:D:317:LYS:HD3	2.02	0.41
13:O:101:THR:O	13:O:130:GLN:NE2	2.54	0.41
25:a:406:BCR:H20C	25:a:406:BCR:H361	1.89	0.41
2:b:388:SER:HB2	2:b:391:SER:HB2	2.02	0.41
32:A:418:PLM:H51	30:D:417:LMT:H21	2.03	0.41
20:a:213:ALA:HB2	4:d:275:PRO:HG2	2.02	0.41
3:c:16:GLN:HG2	4:d:233:ARG:HH21	1.86	0.41
4:d:127:LEU:HD13	32:d:413:PLM:H62	2.02	0.41
4:d:344:GLU:H	4:d:344:GLU:HG2	1.70	0.41
27:d:408:SQD:H111	17:x:31:ILE:HD11	2.02	0.41
19:z:25:VAL:O	19:z:29:SER:OG	2.32	0.41
27:A:415:SQD:H162	27:A:415:SQD:H132	1.82	0.41
2:B:42:LEU:HD13	2:B:94:GLU:HG3	2.03	0.41
2:B:324:LEU:HD21	4:D:196:PHE:HE2	1.86	0.41
35:C:504:DGD:HA21	35:C:504:DGD:HA52	1.93	0.41
23:C:518:CLA:HAB	25:C:527:BCR:H24C	2.03	0.41
15:U:75:LEU:HD23	15:U:75:LEU:HA	1.95	0.41
2:b:378:LYS:HE3	2:b:378:LYS:HB3	1.82	0.41
23:b:602:CLA:H192	23:b:602:CLA:H162	1.90	0.41
23:b:609:CLA:H142	7:h:39:LEU:HD11	2.03	0.41
23:b:615:CLA:H41	23:b:615:CLA:H62	1.78	0.41
23:b:616:CLA:H121	23:b:617:CLA:H111	2.03	0.41
23:c:513:CLA:H2	32:c:518:PLM:H41	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:335:PRO:HB2	5:e:65:LEU:HD11	2.01	0.41
1:A:310:LYS:HD2	16:V:27:ALA:HB1	2.02	0.41
30:B:620:LMT:H102	12:m:8:LEU:HD11	2.03	0.41
23:C:517:CLA:H62	23:C:517:CLA:H92	1.80	0.41
23:D:405:CLA:H41	23:D:405:CLA:H62	1.84	0.41
12:M:18:PRO:O	12:M:21:PHE:HB3	2.21	0.41
12:M:28:GLN:HB3	12:m:27:VAL:HG12	2.03	0.41
2:b:227:LYS:HA	2:b:227:LYS:HD3	1.87	0.41
2:b:458:PHE:HB3	23:b:605:CLA:HBC2	2.03	0.41
4:d:51:GLY:HA3	4:d:78:VAL:HG22	2.02	0.41
19:z:16:SER:OG	19:z:47:TRP:NE1	2.41	0.41
1:A:89:ILE:HD11	1:A:108:ASN:HB3	2.03	0.40
1:A:131:TRP:CZ3	23:C:510:CLA:HAA2	2.57	0.40
23:B:614:CLA:H43	27:B:630:SQD:H122	2.03	0.40
35:C:505:DGD:HBS1	33:D:409:LMG:H202	2.03	0.40
2:b:450:TRP:NE1	23:b:608:CLA:HBA1	2.36	0.40
36:d:410:LHG:H192	14:t:17:PHE:HZ	1.85	0.40
10:k:17:ILE:HG12	19:z:6:GLN:HE21	1.86	0.40
24:D:401:PHO:H41	24:D:401:PHO:H62	1.80	0.40
23:a:405:CLA:H102	23:a:405:CLA:H61	1.75	0.40
2:b:149:LEU:HD11	32:b:622:PLM:HC2	2.03	0.40
3:c:211:TRP:CG	3:c:212:ILE:H	2.39	0.40
4:d:293:LEU:HD23	4:d:293:LEU:HA	1.91	0.40
7:h:46:LEU:HD11	35:h:102:DGD:HA31	2.03	0.40
27:F:101:SQD:H383	27:F:101:SQD:H352	1.91	0.40
16:V:152:LEU:HB3	16:V:155:LYS:HB2	2.02	0.40
18:Y:29:GLY:HA2	25:Y:102:BCR:H16C	2.04	0.40
20:a:274:PHE:HD1	27:a:407:SQD:H111	1.85	0.40
4:d:88:SER:HA	7:h:50:ASN:HD21	1.86	0.40
4:d:179:PHE:HA	4:d:182:LEU:HD12	2.03	0.40
6:f:26:LEU:O	6:f:30:THR:OG1	2.33	0.40
2:B:477:ASP:OD1	2:B:477:ASP:N	2.50	0.40
2:b:157:HIS:HA	2:b:163:GLY:HA3	2.03	0.40
3:c:201:LEU:HD23	3:c:201:LEU:HA	1.91	0.40
16:V:29:LEU:HD12	16:V:29:LEU:HA	1.96	0.40
25:b:619:BCR:H15C	25:b:619:BCR:H351	1.98	0.40
23:c:501:CLA:C2D	23:c:503:CLA:H2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/360 (92%)	328 (99%)	3 (1%)	0	100	100
2	B	503/510 (99%)	496 (99%)	7 (1%)	0	100	100
2	b	502/510 (98%)	493 (98%)	9 (2%)	0	100	100
3	C	449/461 (97%)	440 (98%)	9 (2%)	0	100	100
3	c	433/461 (94%)	425 (98%)	8 (2%)	0	100	100
4	D	339/352 (96%)	334 (98%)	5 (2%)	0	100	100
4	d	339/352 (96%)	335 (99%)	4 (1%)	0	100	100
5	E	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
5	e	74/84 (88%)	72 (97%)	2 (3%)	0	100	100
6	F	33/45 (73%)	33 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	62/66 (94%)	59 (95%)	3 (5%)	0	100	100
7	h	62/66 (94%)	59 (95%)	3 (5%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	31 (94%)	2 (6%)	0	100	100
9	J	33/40 (82%)	33 (100%)	0	0	100	100
9	j	27/40 (68%)	27 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	33/37 (89%)	33 (100%)	0	0	100	100
11	l	33/37 (89%)	33 (100%)	0	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	31/36 (86%)	31 (100%)	0	0	100	100
13	O	241/272 (89%)	235 (98%)	6 (2%)	0	100	100
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	V	135/163 (83%)	134 (99%)	1 (1%)	0	100	100
17	X	36/41 (88%)	36 (100%)	0	0	100	100
17	x	36/41 (88%)	36 (100%)	0	0	100	100
18	Y	29/46 (63%)	29 (100%)	0	0	100	100
18	y	27/46 (59%)	26 (96%)	1 (4%)	0	100	100
19	Z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
19	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
20	a	320/360 (89%)	316 (99%)	4 (1%)	0	100	100
All	All	4654/5081 (92%)	4576 (98%)	78 (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	265/291 (91%)	263 (99%)	2 (1%)	79	88
2	B	393/407 (97%)	390 (99%)	3 (1%)	79	88
2	b	398/407 (98%)	387 (97%)	11 (3%)	38	51
3	C	346/362 (96%)	343 (99%)	3 (1%)	75	86
3	c	335/362 (92%)	329 (98%)	6 (2%)	54	69
4	D	274/283 (97%)	271 (99%)	3 (1%)	70	82
4	d	275/283 (97%)	271 (98%)	4 (2%)	60	75
5	E	69/73 (94%)	68 (99%)	1 (1%)	62	77
5	e	63/73 (86%)	62 (98%)	1 (2%)	58	73
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	54/55 (98%)	53 (98%)	1 (2%)	52	67
7	h	54/55 (98%)	54 (100%)	0	100	100
8	I	30/34 (88%)	30 (100%)	0	100	100
8	i	31/34 (91%)	29 (94%)	2 (6%)	14	16
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	20/28 (71%)	20 (100%)	0	100	100
10	K	29/37 (78%)	29 (100%)	0	100	100
10	k	29/37 (78%)	27 (93%)	2 (7%)	13	14
11	L	32/35 (91%)	32 (100%)	0	100	100
11	l	33/35 (94%)	32 (97%)	1 (3%)	36	48
12	M	29/33 (88%)	28 (97%)	1 (3%)	32	42
12	m	29/33 (88%)	27 (93%)	2 (7%)	13	14
13	O	189/228 (83%)	178 (94%)	11 (6%)	17	20
14	T	24/28 (86%)	23 (96%)	1 (4%)	25	33
14	t	25/28 (89%)	24 (96%)	1 (4%)	27	35
15	U	79/112 (70%)	78 (99%)	1 (1%)	65	78
16	V	114/138 (83%)	112 (98%)	2 (2%)	54	69
17	X	30/34 (88%)	28 (93%)	2 (7%)	13	15
17	x	30/34 (88%)	29 (97%)	1 (3%)	33	44
18	Y	22/37 (60%)	20 (91%)	2 (9%)	7	8
18	y	20/37 (54%)	19 (95%)	1 (5%)	20	26
19	Z	47/52 (90%)	44 (94%)	3 (6%)	14	17
19	z	48/52 (92%)	45 (94%)	3 (6%)	15	17
20	a	259/290 (89%)	257 (99%)	2 (1%)	79	88
All	All	3755/4133 (91%)	3682 (98%)	73 (2%)	52	67

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	ARG
1	A	230	THR
2	B	214	LEU
2	B	353	GLU
2	B	487	SER

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Mol	Chain	Res	Type
3	C	228	ILE
3	C	243	THR
3	C	277	PHE
4	D	90	LEU
4	D	150	ILE
4	D	352	LEU
5	E	5	THR
7	H	47	GLU
12	M	33	GLN
13	O	49	ASP
13	O	63	THR
13	O	113	VAL
13	O	116	ASP
13	O	123	GLU
13	O	144	LEU
13	O	160	THR
13	O	161	SER
13	O	184	ASP
13	O	251	MET
13	O	270	GLU
14	T	29	ILE
15	U	91	VAL
16	V	40	SER
16	V	63	CYS
17	X	34	ILE
17	X	37	VAL
18	Y	19	ILE
18	Y	45	ASN
19	Z	1	MET
19	Z	20	VAL
19	Z	37	LYS
20	a	13	LEU
20	a	35	VAL
2	b	80	ILE
2	b	86	ILE
2	b	236	THR
2	b	245	VAL
2	b	291	SER
2	b	292	LEU
2	b	362	PHE
2	b	376	VAL
2	b	378	LYS

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Mol	Chain	Res	Type
2	b	388	SER
2	b	479	PHE
3	c	96	THR
3	c	228	ILE
3	c	277	PHE
3	c	310	GLN
3	c	343	THR
3	c	461	ASP
4	d	12	ARG
4	d	25	ASP
4	d	312	GLU
4	d	340	VAL
5	e	8	ARG
8	i	3	THR
8	i	34	ARG
10	k	11	LEU
10	k	46	ARG
11	l	12	LEU
12	m	4	ASN
12	m	9	ILE
14	t	2	GLU
17	x	21	LEU
18	y	34	MET
19	z	9	LEU
19	z	20	VAL
19	z	31	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	HIS
2	B	438	ASN
2	B	497	GLN
3	C	44	HIS
3	C	143	ASN
3	C	320	GLN
4	D	186	GLN
4	D	224	GLN
4	D	250	ASN
5	E	74	GLN
5	E	82	GLN
7	H	59	ASN

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Mol	Chain	Res	Type
13	O	62	GLN
13	O	114	ASN
13	O	130	GLN
13	O	135	GLN
13	O	254	HIS
15	U	103	GLN
15	U	108	ASN
15	U	111	HIS
16	V	51	GLN
16	V	132	ASN
18	Y	21	GLN
20	a	12	ASN
20	a	195	HIS
20	a	312	ASN
20	a	315	ASN
2	b	497	GLN
3	c	44	HIS
3	c	299	GLN
3	c	403	ASN
4	d	98	GLN
4	d	186	GLN
4	d	322	ASN
5	e	82	GLN
7	h	50	ASN
12	m	4	ASN
17	x	33	GLN
18	y	21	GLN
19	z	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	$\# Z > 2$
14	FME	t	1	14	8,9,10	0.34	0	7,9,11	0.99	0
8	FME	I	1	8	8,9,10	0.38	0	7,9,11	0.86	0
20	HSK	a	332	20	7,11,12	1.27	1 (14%)	3,14,16	0.92	0
14	FME	T	1	14	8,9,10	0.39	0	7,9,11	1.09	0
8	FME	i	1	8	8,9,10	0.37	0	7,9,11	0.99	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
14	FME	t	1	14	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
20	HSK	a	332	20	-	2/5/6/8	0/1/1/1
14	FME	T	1	14	-	0/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	332	HSK	CE1-ND1	-2.14	1.34	1.36

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	a	332	HSK	C-CA-CB-CG
8	i	1	FME	CA-CB-CG-SD
20	a	332	HSK	N-CA-CB-CG
8	i	1	FME	C-CA-CB-CG
14	t	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 228 ligands modelled in this entry, 6 are monoatomic - leaving 222 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
32	PLM	b	626	-	10,10,17	0.80	0	10,10,17	0.82	0
30	LMT	C	526	-	36,36,36	0.57	0	47,47,47	0.76	2 (4%)
32	PLM	A	418	-	12,12,17	0.76	0	12,12,17	0.72	0
28	LFA	C	523	-	12,12,19	0.22	0	11,11,18	0.25	0
23	CLA	b	609	-	65,73,73	1.40	7 (10%)	76,113,113	1.48	10 (13%)
23	CLA	B	610	40	65,73,73	1.47	6 (9%)	76,113,113	1.51	9 (11%)
25	BCR	k	101	-	41,41,41	0.34	0	56,56,56	0.64	0
30	LMT	c	517	-	30,30,36	0.59	0	41,41,47	0.80	0
23	CLA	B	613	-	65,73,73	1.41	7 (10%)	76,113,113	1.47	8 (10%)
28	LFA	a	418	-	9,9,19	0.24	0	8,8,18	0.26	0
23	CLA	C	517	-	65,73,73	1.43	6 (9%)	76,113,113	1.49	7 (9%)
27	SQD	A	411	-	53,54,54	1.55	8 (15%)	62,65,65	1.37	8 (12%)
30	LMT	D	417	-	34,34,36	0.55	0	45,45,47	0.77	0
32	PLM	i	102	-	12,12,17	0.74	0	12,12,17	0.71	0
25	BCR	b	619	-	41,41,41	0.36	0	56,56,56	0.80	0
30	LMT	d	403	-	24,24,36	0.54	0	29,29,47	0.61	0
35	DGD	D	411	-	47,47,67	0.50	0	54,55,81	0.66	1 (1%)
35	DGD	d	407	-	46,46,67	0.55	0	53,54,81	0.71	0
30	LMT	J	101	-	24,24,36	0.49	0	29,29,47	0.59	0
33	LMG	B	619	-	51,51,55	0.52	0	59,59,63	0.57	0
27	SQD	a	407	-	50,51,54	1.52	6 (12%)	59,62,65	1.63	8 (13%)
33	LMG	D	409	-	51,51,55	0.56	0	59,59,63	0.64	0
33	LMG	y	101	-	51,51,55	0.51	0	59,59,63	0.63	0
32	PLM	c	519	-	14,14,17	0.72	0	14,14,17	0.66	0
32	PLM	x	101	-	17,17,17	0.66	0	17,17,17	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMT	f	103	-	35,35,36	0.54	0	46,46,47	0.69	1 (2%)
28	LFA	b	624	-	7,7,19	0.26	0	6,6,18	0.12	0
32	PLM	c	520	-	9,9,17	0.86	0	9,9,17	0.86	0
30	LMT	T	102	-	24,24,36	0.49	0	29,29,47	0.59	0
23	CLA	B	615	-	65,73,73	1.40	7 (10%)	76,113,113	1.43	7 (9%)
27	SQD	d	408	-	44,45,54	1.61	8 (18%)	53,56,65	1.51	8 (15%)
23	CLA	B	602	-	65,73,73	1.42	7 (10%)	76,113,113	1.47	8 (10%)
30	LMT	B	626	-	36,36,36	0.54	0	47,47,47	1.04	2 (4%)
23	CLA	B	612	-	65,73,73	1.37	7 (10%)	76,113,113	1.51	6 (7%)
35	DGD	C	504	-	63,63,67	0.59	0	77,77,81	1.22	8 (10%)
23	CLA	b	608	40	65,73,73	1.44	7 (10%)	76,113,113	1.51	8 (10%)
23	CLA	d	405	-	65,73,73	1.43	7 (10%)	76,113,113	1.48	9 (11%)
30	LMT	T	103	-	36,36,36	0.51	0	47,47,47	0.89	1 (2%)
33	LMG	c	521	-	51,51,55	0.49	0	59,59,63	0.60	0
26	PL9	D	402	-	55,55,55	1.26	5 (9%)	68,69,69	1.52	14 (20%)
36	LHG	a	416	-	45,45,48	0.53	0	48,51,54	0.49	0
23	CLA	C	506	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	10 (13%)
25	BCR	a	406	-	41,41,41	0.37	0	56,56,56	0.79	0
25	BCR	z	101	-	41,41,41	0.40	0	56,56,56	0.98	1 (1%)
23	CLA	b	603	-	65,73,73	1.44	7 (10%)	76,113,113	1.46	7 (9%)
30	LMT	M	101	-	36,36,36	0.59	0	47,47,47	0.79	1 (2%)
33	LMG	a	408	-	51,51,55	0.54	0	59,59,63	0.68	0
23	CLA	A	405	40	65,73,73	1.38	6 (9%)	76,113,113	1.59	10 (13%)
23	CLA	B	605	-	65,73,73	1.44	7 (10%)	76,113,113	1.46	7 (9%)
23	CLA	B	606	-	65,73,73	1.43	6 (9%)	76,113,113	1.52	9 (11%)
23	CLA	D	404	-	65,73,73	1.43	7 (10%)	76,113,113	1.41	6 (7%)
25	BCR	b	620	-	41,41,41	0.35	0	56,56,56	0.77	0
23	CLA	b	604	-	65,73,73	1.43	7 (10%)	76,113,113	1.45	8 (10%)
30	LMT	M	102	-	36,36,36	0.58	0	47,47,47	0.71	0
36	LHG	E	101	-	48,48,48	0.51	0	51,54,54	0.50	0
24	PHO	d	402	-	51,69,69	0.67	0	47,99,99	1.06	5 (10%)
32	PLM	B	624	-	14,14,17	0.71	0	14,14,17	0.66	0
25	BCR	A	409	-	41,41,41	0.34	0	56,56,56	0.67	0
35	DGD	c	516	-	63,63,67	0.57	0	77,77,81	0.70	1 (1%)
29	OEX	A	414	40,1,3	0,15,15	-	-	-	-	-
25	BCR	j	101	-	41,41,41	0.36	0	56,56,56	1.05	5 (8%)
35	DGD	C	505	-	62,62,67	0.61	0	76,76,81	1.39	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	C	525	-	48,48,55	0.50	0	56,56,63	0.83	3 (5%)
32	PLM	C	524	-	12,12,17	0.77	0	12,12,17	0.78	1 (8%)
36	LHG	d	409	-	48,48,48	0.52	0	51,54,54	0.50	0
23	CLA	b	610	-	65,73,73	1.48	7 (10%)	76,113,113	1.41	8 (10%)
38	RRX	x	102	-	42,42,42	0.26	0	57,58,58	0.41	0
36	LHG	l	102	-	48,48,48	0.51	0	51,54,54	0.56	1 (1%)
23	CLA	C	514	-	65,73,73	1.39	6 (9%)	76,113,113	1.54	7 (9%)
23	CLA	a	405	-	65,73,73	1.44	7 (10%)	76,113,113	1.44	8 (10%)
23	CLA	B	603	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	9 (11%)
23	CLA	D	405	-	65,73,73	1.43	6 (9%)	76,113,113	1.42	8 (10%)
25	BCR	i	103	-	41,41,41	0.34	0	56,56,56	0.65	0
28	LFA	B	629	-	6,6,19	0.25	0	5,5,18	0.16	0
36	LHG	D	408	-	45,45,48	0.53	0	48,51,54	0.50	0
36	LHG	L	101	-	48,48,48	0.51	0	51,54,54	0.57	0
23	CLA	B	604	-	65,73,73	1.40	6 (9%)	76,113,113	1.55	8 (10%)
23	CLA	d	401	40	65,73,73	1.40	6 (9%)	76,113,113	1.61	8 (10%)
25	BCR	C	527	-	41,41,41	0.36	0	56,56,56	0.71	0
25	BCR	b	618	-	41,41,41	0.39	0	56,56,56	0.76	0
28	LFA	m	101	-	8,8,19	0.23	0	7,7,18	0.20	0
25	BCR	f	101	-	41,41,41	0.33	0	56,56,56	0.89	3 (5%)
28	LFA	h	101	-	9,9,19	0.23	0	8,8,18	0.21	0
35	DGD	c	514	-	63,63,67	0.59	0	77,77,81	0.76	2 (2%)
28	LFA	D	412	-	11,11,19	0.24	0	10,10,18	0.21	0
28	LFA	B	625	-	7,7,19	0.24	0	6,6,18	0.21	0
23	CLA	C	518	-	65,73,73	1.41	6 (9%)	76,113,113	1.49	8 (10%)
23	CLA	c	505	-	65,73,73	1.44	8 (12%)	76,113,113	1.42	8 (10%)
27	SQD	A	415	-	50,51,54	1.49	5 (10%)	59,62,65	1.72	10 (16%)
28	LFA	B	622	-	12,12,19	0.23	0	11,11,18	0.30	0
23	CLA	C	510	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
32	PLM	b	623	-	15,15,17	0.70	0	15,15,17	0.64	0
30	LMT	E	106	-	36,36,36	0.54	0	47,47,47	0.76	1 (2%)
25	BCR	B	631	-	41,41,41	0.36	0	56,56,56	1.37	6 (10%)
30	LMT	A	416	-	36,36,36	0.50	0	47,47,47	1.26	5 (10%)
27	SQD	F	101	-	44,45,54	1.61	9 (20%)	53,56,65	1.57	9 (16%)
35	DGD	h	102	-	63,63,67	0.57	0	77,77,81	0.76	1 (1%)
23	CLA	C	511	-	65,73,73	1.44	7 (10%)	76,113,113	1.49	9 (11%)
28	LFA	I	101	-	12,12,19	0.24	0	11,11,18	0.30	0
32	PLM	J	102	-	15,15,17	0.70	0	15,15,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PLM	i	101	-	14,14,17	0.73	0	14,14,17	0.65	0
32	PLM	b	622	-	14,14,17	0.69	0	14,14,17	0.67	0
27	SQD	b	601	-	53,54,54	1.48	9 (16%)	62,65,65	1.49	7 (11%)
33	LMG	d	411	-	51,51,55	0.53	0	59,59,63	0.60	0
28	LFA	I	104	-	7,7,19	0.24	0	6,6,18	0.19	0
23	CLA	c	513	-	65,73,73	1.43	8 (12%)	76,113,113	1.43	6 (7%)
23	CLA	A	404	-	65,73,73	1.41	6 (9%)	76,113,113	1.51	8 (10%)
23	CLA	c	509	-	65,73,73	1.40	6 (9%)	76,113,113	1.51	7 (9%)
28	LFA	A	413	-	6,6,19	0.26	0	5,5,18	0.17	0
27	SQD	a	410	-	44,45,54	1.63	7 (15%)	53,56,65	1.44	7 (13%)
36	LHG	D	406	-	48,48,48	0.51	0	51,54,54	0.47	0
27	SQD	D	410	-	42,43,54	1.67	8 (19%)	51,54,65	1.53	8 (15%)
37	HEM	E	105	5,6	41,50,50	1.45	4 (9%)	45,82,82	1.48	8 (17%)
30	LMT	a	411	-	36,36,36	0.53	0	47,47,47	0.90	3 (6%)
32	PLM	k	102	-	11,11,17	0.78	0	11,11,17	0.76	0
25	BCR	C	502	-	41,41,41	0.36	0	56,56,56	0.74	1 (1%)
23	CLA	d	404	-	65,73,73	1.44	7 (10%)	76,113,113	1.40	6 (7%)
28	LFA	b	625	-	7,7,19	0.26	0	6,6,18	0.22	0
25	BCR	B	618	-	41,41,41	0.32	0	56,56,56	0.83	2 (3%)
23	CLA	A	408	-	65,73,73	1.44	7 (10%)	76,113,113	1.43	8 (10%)
23	CLA	B	601	40	65,73,73	1.47	7 (10%)	76,113,113	1.38	6 (7%)
36	LHG	d	410	-	48,48,48	0.52	0	51,54,54	0.51	0
23	CLA	a	403	40	65,73,73	1.42	6 (9%)	76,113,113	1.47	10 (13%)
32	PLM	l	101	-	13,13,17	0.78	0	13,13,17	0.67	0
30	LMT	z	102	-	36,36,36	0.53	0	47,47,47	0.77	1 (2%)
32	PLM	d	413	-	15,15,17	0.68	0	15,15,17	0.65	0
37	HEM	f	102	5,6	41,50,50	1.46	4 (9%)	45,82,82	1.41	7 (15%)
26	PL9	d	406	-	55,55,55	1.23	5 (9%)	68,69,69	1.52	15 (22%)
23	CLA	B	611	-	65,73,73	1.43	7 (10%)	76,113,113	1.53	9 (11%)
23	CLA	c	510	-	65,73,73	1.46	7 (10%)	76,113,113	1.37	5 (6%)
33	LMG	Y	101	-	51,51,55	0.52	0	59,59,63	0.67	0
28	LFA	D	416	-	7,7,19	0.25	0	6,6,18	0.21	0
23	CLA	b	611	40	65,73,73	1.47	8 (12%)	76,113,113	1.40	9 (11%)
30	LMT	B	620	-	36,36,36	0.55	0	47,47,47	0.71	0
23	CLA	b	605	-	65,73,73	1.45	6 (9%)	76,113,113	1.53	9 (11%)
36	LHG	D	407	-	48,48,48	0.52	0	51,54,54	0.47	0
32	PLM	E	107	-	17,17,17	0.65	0	17,17,17	0.61	0
32	PLM	E	102	-	14,14,17	0.75	0	14,14,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	616	-	65,73,73	1.43	7 (10%)	76,113,113	1.43	7 (9%)
32	PLM	C	519	-	12,12,17	0.74	0	12,12,17	0.77	1 (8%)
23	CLA	B	614	-	65,73,73	1.45	7 (10%)	76,113,113	1.48	10 (13%)
23	CLA	C	513	-	65,73,73	1.39	7 (10%)	76,113,113	1.50	9 (11%)
32	PLM	B	628	-	12,12,17	0.76	0	12,12,17	0.73	0
32	PLM	D	414	-	17,17,17	0.62	0	17,17,17	0.65	0
28	LFA	d	412	-	9,9,19	0.21	0	8,8,18	0.25	0
23	CLA	C	507	-	65,73,73	1.44	7 (10%)	76,113,113	1.44	6 (7%)
23	CLA	b	607	-	65,73,73	1.45	7 (10%)	76,113,113	1.49	9 (11%)
35	DGD	c	515	-	51,51,67	0.52	0	59,59,81	0.75	2 (3%)
23	CLA	b	617	-	65,73,73	1.43	7 (10%)	76,113,113	1.46	7 (9%)
31	BCT	a	415	21	2,3,3	0.89	0	2,3,3	3.22	2 (100%)
32	PLM	D	415	-	10,10,17	0.83	0	10,10,17	0.79	0
23	CLA	C	508	-	65,73,73	1.44	6 (9%)	76,113,113	1.41	8 (10%)
28	LFA	C	520	-	11,11,19	0.26	0	10,10,18	0.19	0
36	LHG	a	417	-	48,48,48	0.50	0	51,54,54	0.49	0
27	SQD	B	630	-	53,54,54	1.51	8 (15%)	62,65,65	1.49	6 (9%)
28	LFA	B	623	-	5,5,19	0.25	0	4,4,18	0.16	0
23	CLA	B	608	-	65,73,73	1.41	6 (9%)	76,113,113	1.51	8 (10%)
32	PLM	K	101	-	13,13,17	0.74	0	13,13,17	0.70	0
32	PLM	b	628	-	11,11,17	0.78	0	11,11,17	0.74	0
23	CLA	A	406	40	65,73,73	1.44	6 (9%)	76,113,113	1.45	11 (14%)
23	CLA	C	516	3	65,73,73	1.40	7 (10%)	76,113,113	1.54	8 (10%)
28	LFA	H	103	-	8,8,19	0.24	0	7,7,18	0.18	0
23	CLA	C	512	40	65,73,73	1.40	6 (9%)	76,113,113	1.55	8 (10%)
32	PLM	E	103	-	15,15,17	0.67	0	15,15,17	0.68	0
32	PLM	a	413	-	10,10,17	0.85	0	10,10,17	0.76	0
28	LFA	d	414	-	8,8,19	0.25	0	7,7,18	0.19	0
28	LFA	a	412	-	8,8,19	0.25	0	7,7,18	0.19	0
23	CLA	c	511	3	65,73,73	1.43	7 (10%)	76,113,113	1.54	8 (10%)
24	PHO	D	401	-	51,69,69	0.68	0	47,99,99	1.15	5 (10%)
23	CLA	c	502	-	65,73,73	1.42	7 (10%)	76,113,113	1.47	7 (9%)
33	LMG	b	621	-	51,51,55	0.53	0	59,59,63	0.61	0
32	PLM	c	518	-	8,8,17	0.92	0	8,8,17	0.88	0
32	PLM	C	522	-	12,12,17	0.76	0	12,12,17	0.70	0
25	BCR	T	101	-	41,41,41	0.36	0	56,56,56	1.50	6 (10%)
25	BCR	C	501	-	41,41,41	0.40	0	56,56,56	0.98	1 (1%)
23	CLA	C	515	-	65,73,73	1.42	6 (9%)	76,113,113	1.41	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LFA	A	412	-	6,6,19	0.26	0	5,5,18	0.18	0
23	CLA	B	616	-	45,53,73	1.72	7 (15%)	52,89,113	1.75	7 (13%)
23	CLA	c	503	-	65,73,73	1.45	6 (9%)	76,113,113	1.39	8 (10%)
23	CLA	b	613	-	65,73,73	1.38	7 (10%)	76,113,113	1.55	7 (9%)
23	CLA	c	506	-	65,73,73	1.45	7 (10%)	76,113,113	1.53	7 (9%)
35	DGD	C	503	-	54,54,67	0.67	0	68,68,81	0.73	1 (1%)
28	LFA	I	105	-	7,7,19	0.24	0	6,6,18	0.20	0
23	CLA	B	609	-	65,73,73	1.45	7 (10%)	76,113,113	1.46	7 (9%)
34	GOL	B	621	-	5,5,5	0.38	0	5,5,5	0.41	0
23	CLA	c	512	-	65,73,73	1.41	6 (9%)	76,113,113	1.48	6 (7%)
31	BCT	A	417	21	2,3,3	0.89	0	2,3,3	3.28	2 (100%)
32	PLM	h	103	-	10,10,17	0.82	0	10,10,17	0.78	0
33	LMG	I	103	-	51,51,55	0.53	0	59,59,63	0.64	0
38	RRX	H	102	-	42,42,42	0.24	0	57,58,58	0.43	0
25	BCR	D	403	-	41,41,41	0.35	0	56,56,56	0.87	2 (3%)
37	HEM	V	201	16	41,50,50	1.43	3 (7%)	45,82,82	1.52	10 (22%)
24	PHO	A	407	-	51,69,69	0.72	2 (3%)	47,99,99	0.95	3 (6%)
23	CLA	B	607	40	65,73,73	1.43	7 (10%)	76,113,113	1.49	8 (10%)
28	LFA	B	627	-	5,5,19	0.26	0	4,4,18	0.15	0
28	LFA	I	102	-	6,6,19	0.26	0	5,5,18	0.20	0
23	CLA	b	614	-	65,73,73	1.41	6 (9%)	76,113,113	1.41	8 (10%)
23	CLA	b	606	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	7 (9%)
23	CLA	c	507	40	65,73,73	1.39	6 (9%)	76,113,113	1.53	8 (10%)
23	CLA	b	615	-	65,73,73	1.41	7 (10%)	76,113,113	1.43	8 (10%)
30	LMT	a	419	-	24,24,36	0.57	0	29,29,47	0.75	1 (3%)
32	PLM	c	522	-	12,12,17	0.79	0	12,12,17	0.69	0
23	CLA	c	504	40	65,73,73	1.42	7 (10%)	76,113,113	1.53	8 (10%)
23	CLA	b	602	40	65,73,73	1.47	6 (9%)	76,113,113	1.37	6 (7%)
23	CLA	b	612	-	65,73,73	1.42	7 (10%)	76,113,113	1.52	10 (13%)
28	LFA	E	104	-	5,5,19	0.27	0	4,4,18	0.17	0
26	PL9	A	410	-	55,55,55	1.27	5 (9%)	68,69,69	1.62	14 (20%)
23	CLA	a	402	-	65,73,73	1.39	6 (9%)	76,113,113	1.50	8 (10%)
28	LFA	b	627	-	6,6,19	0.27	0	5,5,18	0.17	0
26	PL9	a	409	-	55,55,55	1.17	3 (5%)	68,69,69	1.48	12 (17%)
25	BCR	t	101	-	41,41,41	0.37	0	56,56,56	0.86	1 (1%)
25	BCR	B	617	-	41,41,41	0.37	0	56,56,56	0.71	0
25	BCR	Y	102	-	41,41,41	0.36	0	56,56,56	0.95	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PHO	a	404	-	51,69,69	0.70	0	47,99,99	0.95	3 (6%)
28	LFA	i	104	-	12,12,19	0.23	0	11,11,18	0.19	0
23	CLA	c	501	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	10 (13%)
28	LFA	C	521	-	8,8,19	0.21	0	7,7,18	0.24	0
23	CLA	C	509	40	65,73,73	1.41	7 (10%)	76,113,113	1.55	8 (10%)
28	LFA	D	413	-	9,9,19	0.26	0	8,8,18	0.20	0
35	DGD	H	101	-	59,59,67	0.58	0	73,73,81	0.81	0
28	LFA	e	101	-	16,16,19	0.23	0	15,15,18	0.21	0
23	CLA	c	508	-	65,73,73	1.40	7 (10%)	76,113,113	1.52	9 (11%)

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
32	PLM	b	626	-	-	0/8/8/15	-
30	LMT	C	526	-	-	11/21/61/61	0/2/2/2
32	PLM	A	418	-	-	5/10/10/15	-
28	LFA	C	523	-	-	1/10/10/17	-
23	CLA	b	609	-	1/1/15/20	5/37/115/115	-
23	CLA	B	610	40	1/1/15/20	10/37/115/115	-
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
30	LMT	c	517	-	-	10/15/55/61	0/2/2/2
23	CLA	B	613	-	1/1/15/20	10/37/115/115	-
28	LFA	a	418	-	-	5/7/7/17	-
23	CLA	C	517	-	1/1/15/20	17/37/115/115	-
27	SQD	A	411	-	-	19/49/69/69	0/1/1/1
30	LMT	D	417	-	-	5/19/59/61	0/2/2/2
32	PLM	i	102	-	-	2/10/10/15	-
25	BCR	b	619	-	-	0/29/63/63	0/2/2/2
30	LMT	d	403	-	-	4/15/35/61	0/1/1/2
35	DGD	D	411	-	-	22/41/62/95	0/1/1/2
35	DGD	d	407	-	-	18/40/61/95	0/1/1/2
30	LMT	J	101	-	-	9/15/35/61	0/1/1/2
33	LMG	B	619	-	-	16/46/66/70	0/1/1/1
27	SQD	a	407	-	-	17/46/66/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	D	409	-	-	9/46/66/70	0/1/1/1
33	LMG	y	101	-	-	27/46/66/70	0/1/1/1
32	PLM	c	519	-	-	4/12/12/15	-
32	PLM	x	101	-	-	6/15/15/15	-
30	LMT	f	103	-	-	13/20/60/61	0/2/2/2
28	LFA	b	624	-	-	0/5/5/17	-
32	PLM	c	520	-	-	0/7/7/15	-
30	LMT	T	102	-	-	9/15/35/61	0/1/1/2
23	CLA	B	615	-	1/1/15/20	8/37/115/115	-
27	SQD	d	408	-	-	17/40/60/69	0/1/1/1
23	CLA	B	602	-	1/1/15/20	5/37/115/115	-
30	LMT	B	626	-	-	4/21/61/61	0/2/2/2
23	CLA	B	612	-	1/1/15/20	8/37/115/115	-
35	DGD	C	504	-	-	24/51/91/95	0/2/2/2
23	CLA	b	608	40	1/1/15/20	5/37/115/115	-
23	CLA	d	405	-	1/1/15/20	12/37/115/115	-
30	LMT	T	103	-	-	2/21/61/61	0/2/2/2
33	LMG	c	521	-	-	16/46/66/70	0/1/1/1
26	PL9	D	402	-	-	18/53/73/73	0/1/1/1
36	LHG	a	416	-	-	13/50/50/53	-
23	CLA	C	506	-	1/1/15/20	5/37/115/115	-
25	BCR	a	406	-	-	2/29/63/63	0/2/2/2
25	BCR	z	101	-	-	3/29/63/63	0/2/2/2
23	CLA	b	603	-	1/1/15/20	11/37/115/115	-
30	LMT	M	101	-	-	6/21/61/61	0/2/2/2
33	LMG	a	408	-	-	21/46/66/70	0/1/1/1
23	CLA	A	405	40	1/1/15/20	6/37/115/115	-
23	CLA	B	605	-	1/1/15/20	5/37/115/115	-
23	CLA	B	606	-	1/1/15/20	7/37/115/115	-
23	CLA	D	404	-	1/1/15/20	3/37/115/115	-
25	BCR	b	620	-	-	2/29/63/63	0/2/2/2
23	CLA	b	604	-	1/1/15/20	10/37/115/115	-
30	LMT	M	102	-	-	5/21/61/61	0/2/2/2
36	LHG	E	101	-	-	19/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	d	402	-	-	2/37/103/103	0/5/6/6
32	PLM	B	624	-	-	5/12/12/15	-
25	BCR	A	409	-	-	3/29/63/63	0/2/2/2
35	DGD	c	516	-	-	13/51/91/95	0/2/2/2
25	BCR	j	101	-	-	12/29/63/63	0/2/2/2
35	DGD	C	505	-	-	27/50/90/95	0/2/2/2
33	LMG	C	525	-	-	15/43/63/70	0/1/1/1
32	PLM	C	524	-	-	4/10/10/15	-
36	LHG	d	409	-	-	12/53/53/53	-
23	CLA	b	610	-	1/1/15/20	7/37/115/115	-
38	RRX	x	102	-	-	2/29/65/65	0/2/2/2
36	LHG	l	102	-	-	20/53/53/53	-
23	CLA	C	514	-	1/1/15/20	3/37/115/115	-
23	CLA	a	405	-	1/1/15/20	12/37/115/115	-
23	CLA	B	603	-	1/1/15/20	13/37/115/115	-
23	CLA	D	405	-	1/1/15/20	7/37/115/115	-
25	BCR	i	103	-	-	2/29/63/63	0/2/2/2
28	LFA	B	629	-	-	0/4/4/17	-
36	LHG	D	408	-	-	11/50/50/53	-
36	LHG	L	101	-	-	22/53/53/53	-
23	CLA	B	604	-	1/1/15/20	12/37/115/115	-
23	CLA	d	401	40	1/1/15/20	4/37/115/115	-
25	BCR	C	527	-	-	4/29/63/63	0/2/2/2
25	BCR	b	618	-	-	4/29/63/63	0/2/2/2
28	LFA	m	101	-	-	3/6/6/17	-
25	BCR	f	101	-	-	9/29/63/63	0/2/2/2
28	LFA	h	101	-	-	2/7/7/17	-
35	DGD	c	514	-	-	25/51/91/95	0/2/2/2
28	LFA	D	412	-	-	0/9/9/17	-
28	LFA	B	625	-	-	1/5/5/17	-
23	CLA	C	518	-	1/1/15/20	7/37/115/115	-
23	CLA	c	505	-	1/1/15/20	6/37/115/115	-
27	SQD	A	415	-	-	23/46/66/69	0/1/1/1
28	LFA	B	622	-	-	3/10/10/17	-
23	CLA	C	510	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PLM	b	623	-	-	5/13/13/15	-
30	LMT	E	106	-	-	7/21/61/61	0/2/2/2
25	BCR	B	631	-	-	10/29/63/63	0/2/2/2
30	LMT	A	416	-	-	10/21/61/61	0/2/2/2
27	SQD	F	101	-	-	16/40/60/69	0/1/1/1
35	DGD	h	102	-	-	15/51/91/95	0/2/2/2
23	CLA	C	511	-	1/1/15/20	13/37/115/115	-
28	LFA	I	101	-	-	1/10/10/17	-
32	PLM	J	102	-	-	3/13/13/15	-
32	PLM	i	101	-	-	4/12/12/15	-
32	PLM	b	622	-	-	3/12/12/15	-
27	SQD	b	601	-	-	21/49/69/69	0/1/1/1
33	LMG	d	411	-	-	14/46/66/70	0/1/1/1
28	LFA	I	104	-	-	0/5/5/17	-
23	CLA	c	513	-	1/1/15/20	9/37/115/115	-
23	CLA	A	404	-	1/1/15/20	10/37/115/115	-
23	CLA	c	509	-	1/1/15/20	5/37/115/115	-
28	LFA	A	413	-	-	0/4/4/17	-
27	SQD	a	410	-	-	15/40/60/69	0/1/1/1
36	LHG	D	406	-	-	11/53/53/53	-
27	SQD	D	410	-	-	25/38/58/69	0/1/1/1
37	HEM	E	105	5,6	-	3/12/54/54	-
30	LMT	a	411	-	-	9/21/61/61	0/2/2/2
32	PLM	k	102	-	-	7/9/9/15	-
25	BCR	C	502	-	-	2/29/63/63	0/2/2/2
23	CLA	d	404	-	1/1/15/20	5/37/115/115	-
28	LFA	b	625	-	-	0/5/5/17	-
25	BCR	B	618	-	-	3/29/63/63	0/2/2/2
23	CLA	A	408	-	1/1/15/20	9/37/115/115	-
23	CLA	B	601	40	1/1/15/20	10/37/115/115	-
36	LHG	d	410	-	-	16/53/53/53	-
23	CLA	a	403	40	1/1/15/20	6/37/115/115	-
32	PLM	l	101	-	-	7/11/11/15	-
30	LMT	z	102	-	-	8/21/61/61	0/2/2/2
32	PLM	d	413	-	-	8/13/13/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	HEM	f	102	5,6	-	2/12/54/54	-
26	PL9	d	406	-	-	8/53/73/73	0/1/1/1
23	CLA	B	611	-	1/1/15/20	5/37/115/115	-
23	CLA	c	510	-	1/1/15/20	6/37/115/115	-
33	LMG	Y	101	-	-	17/46/66/70	0/1/1/1
28	LFA	D	416	-	-	0/5/5/17	-
23	CLA	b	611	40	1/1/15/20	11/37/115/115	-
30	LMT	B	620	-	-	10/21/61/61	0/2/2/2
23	CLA	b	605	-	1/1/15/20	10/37/115/115	-
36	LHG	D	407	-	-	16/53/53/53	-
32	PLM	E	107	-	-	5/15/15/15	-
32	PLM	E	102	-	-	6/12/12/15	-
23	CLA	b	616	-	1/1/15/20	4/37/115/115	-
32	PLM	C	519	-	-	3/10/10/15	-
23	CLA	B	614	-	1/1/15/20	16/37/115/115	-
23	CLA	C	513	-	1/1/15/20	5/37/115/115	-
32	PLM	B	628	-	-	4/10/10/15	-
32	PLM	D	414	-	-	9/15/15/15	-
28	LFA	d	412	-	-	0/7/7/17	-
23	CLA	C	507	-	1/1/15/20	8/37/115/115	-
23	CLA	b	607	-	1/1/15/20	5/37/115/115	-
35	DGD	c	515	-	-	16/46/66/95	0/1/1/2
23	CLA	b	617	-	1/1/15/20	15/37/115/115	-
32	PLM	D	415	-	-	3/8/8/15	-
23	CLA	C	508	-	1/1/15/20	6/37/115/115	-
28	LFA	C	520	-	-	0/9/9/17	-
36	LHG	a	417	-	-	26/53/53/53	-
27	SQD	B	630	-	-	23/49/69/69	0/1/1/1
28	LFA	B	623	-	-	0/3/3/17	-
23	CLA	B	608	-	1/1/15/20	5/37/115/115	-
32	PLM	K	101	-	-	2/11/11/15	-
32	PLM	b	628	-	-	5/9/9/15	-
23	CLA	A	406	40	1/1/15/20	10/37/115/115	-
23	CLA	C	516	3	1/1/15/20	6/37/115/115	-
28	LFA	H	103	-	-	0/6/6/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	512	40	1/1/15/20	11/37/115/115	-
32	PLM	E	103	-	-	5/13/13/15	-
32	PLM	a	413	-	-	3/8/8/15	-
28	LFA	d	414	-	-	2/6/6/17	-
28	LFA	a	412	-	-	2/6/6/17	-
23	CLA	c	511	3	1/1/15/20	6/37/115/115	-
24	PHO	D	401	-	-	9/37/103/103	0/5/6/6
23	CLA	c	502	-	1/1/15/20	12/37/115/115	-
33	LMG	b	621	-	-	12/46/66/70	0/1/1/1
32	PLM	c	518	-	-	2/6/6/15	-
32	PLM	C	522	-	-	6/10/10/15	-
25	BCR	T	101	-	-	8/29/63/63	0/2/2/2
25	BCR	C	501	-	-	4/29/63/63	0/2/2/2
23	CLA	C	515	-	1/1/15/20	7/37/115/115	-
28	LFA	A	412	-	-	0/4/4/17	-
23	CLA	B	616	-	1/1/11/20	5/13/91/115	-
23	CLA	c	503	-	1/1/15/20	3/37/115/115	-
23	CLA	b	613	-	1/1/15/20	5/37/115/115	-
23	CLA	c	506	-	1/1/15/20	17/37/115/115	-
35	DGD	C	503	-	-	21/42/82/95	0/2/2/2
28	LFA	I	105	-	-	0/5/5/17	-
23	CLA	B	609	-	1/1/15/20	7/37/115/115	-
34	GOL	B	621	-	-	2/4/4/4	-
23	CLA	c	512	-	1/1/15/20	10/37/115/115	-
32	PLM	h	103	-	-	5/8/8/15	-
33	LMG	I	103	-	-	22/46/66/70	0/1/1/1
38	RRX	H	102	-	-	2/29/65/65	0/2/2/2
25	BCR	D	403	-	-	9/29/63/63	0/2/2/2
37	HEM	V	201	16	-	2/12/54/54	-
24	PHO	A	407	-	-	3/37/103/103	0/5/6/6
23	CLA	B	607	40	1/1/15/20	8/37/115/115	-
28	LFA	B	627	-	-	0/3/3/17	-
28	LFA	I	102	-	-	0/4/4/17	-
23	CLA	b	614	-	1/1/15/20	6/37/115/115	-
23	CLA	b	606	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	507	40	1/1/15/20	14/37/115/115	-
23	CLA	b	615	-	1/1/15/20	19/37/115/115	-
30	LMT	a	419	-	-	11/15/35/61	0/1/1/2
32	PLM	c	522	-	-	3/10/10/15	-
23	CLA	c	504	40	1/1/15/20	7/37/115/115	-
23	CLA	b	602	40	1/1/15/20	17/37/115/115	-
23	CLA	b	612	-	1/1/15/20	3/37/115/115	-
28	LFA	E	104	-	-	0/3/3/17	-
26	PL9	A	410	-	-	28/53/73/73	0/1/1/1
23	CLA	a	402	-	1/1/15/20	8/37/115/115	-
28	LFA	b	627	-	-	0/4/4/17	-
26	PL9	a	409	-	-	14/53/73/73	0/1/1/1
25	BCR	t	101	-	-	6/29/63/63	0/2/2/2
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
25	BCR	Y	102	-	-	6/29/63/63	0/2/2/2
24	PHO	a	404	-	-	6/37/103/103	0/5/6/6
28	LFA	i	104	-	-	1/10/10/17	-
23	CLA	c	501	-	1/1/15/20	4/37/115/115	-
28	LFA	C	521	-	-	1/6/6/17	-
23	CLA	C	509	40	1/1/15/20	10/37/115/115	-
28	LFA	D	413	-	-	1/7/7/17	-
35	DGD	H	101	-	-	7/47/87/95	0/2/2/2
28	LFA	e	101	-	-	6/14/14/17	-
23	CLA	c	508	-	1/1/15/20	6/37/115/115	-

All (567) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C4B-NB	7.30	1.41	1.35
23	B	610	CLA	C4B-NB	7.27	1.41	1.35
23	b	607	CLA	C4B-NB	7.26	1.41	1.35
23	B	601	CLA	C4B-NB	7.24	1.41	1.35
23	b	610	CLA	C4B-NB	7.22	1.41	1.35
23	B	614	CLA	C4B-NB	7.17	1.41	1.35
23	c	510	CLA	C4B-NB	7.14	1.41	1.35
23	c	501	CLA	C4B-NB	7.13	1.41	1.35
23	C	506	CLA	C4B-NB	7.12	1.41	1.35
23	C	510	CLA	C4B-NB	7.11	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C4B-NB	7.06	1.41	1.35
23	c	506	CLA	C4B-NB	7.06	1.41	1.35
23	B	603	CLA	C4B-NB	7.06	1.41	1.35
23	c	503	CLA	C4B-NB	7.05	1.41	1.35
23	B	605	CLA	C4B-NB	7.01	1.41	1.35
23	b	608	CLA	C4B-NB	7.00	1.41	1.35
23	c	505	CLA	C4B-NB	6.99	1.41	1.35
23	C	517	CLA	C4B-NB	6.96	1.41	1.35
23	c	504	CLA	C4B-NB	6.96	1.41	1.35
23	B	607	CLA	C4B-NB	6.95	1.41	1.35
23	C	508	CLA	C4B-NB	6.95	1.41	1.35
23	a	405	CLA	C4B-NB	6.94	1.41	1.35
23	d	404	CLA	C4B-NB	6.94	1.41	1.35
23	B	611	CLA	C4B-NB	6.93	1.41	1.35
23	b	606	CLA	C4B-NB	6.93	1.41	1.35
23	d	405	CLA	C4B-NB	6.89	1.41	1.35
23	B	606	CLA	C4B-NB	6.88	1.41	1.35
23	b	603	CLA	C4B-NB	6.88	1.41	1.35
23	b	612	CLA	C4B-NB	6.88	1.41	1.35
23	D	405	CLA	C4B-NB	6.87	1.41	1.35
23	C	511	CLA	C4B-NB	6.87	1.41	1.35
23	b	616	CLA	C4B-NB	6.86	1.41	1.35
23	c	511	CLA	C4B-NB	6.86	1.41	1.35
23	c	512	CLA	C4B-NB	6.86	1.41	1.35
23	C	507	CLA	C4B-NB	6.84	1.41	1.35
23	b	605	CLA	C4B-NB	6.83	1.41	1.35
23	C	518	CLA	C4B-NB	6.80	1.41	1.35
23	C	509	CLA	C4B-NB	6.80	1.41	1.35
23	b	615	CLA	C4B-NB	6.80	1.41	1.35
23	B	609	CLA	C4B-NB	6.80	1.41	1.35
23	D	404	CLA	C4B-NB	6.80	1.41	1.35
23	c	513	CLA	C4B-NB	6.78	1.41	1.35
23	B	602	CLA	C4B-NB	6.78	1.41	1.35
23	C	515	CLA	C4B-NB	6.74	1.41	1.35
23	A	408	CLA	C4B-NB	6.72	1.41	1.35
23	c	502	CLA	C4B-NB	6.72	1.41	1.35
23	b	604	CLA	C4B-NB	6.72	1.41	1.35
23	C	516	CLA	C4B-NB	6.72	1.41	1.35
23	c	507	CLA	C4B-NB	6.68	1.41	1.35
23	A	406	CLA	C4B-NB	6.67	1.41	1.35
23	b	609	CLA	C4B-NB	6.65	1.41	1.35
23	C	513	CLA	C4B-NB	6.64	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	C4B-NB	6.63	1.41	1.35
23	B	616	CLA	C4B-NB	6.62	1.41	1.35
23	d	401	CLA	C4B-NB	6.59	1.41	1.35
23	c	509	CLA	C4B-NB	6.56	1.41	1.35
23	B	615	CLA	C4B-NB	6.53	1.41	1.35
23	c	508	CLA	C4B-NB	6.53	1.41	1.35
23	B	608	CLA	C4B-NB	6.52	1.41	1.35
23	b	614	CLA	C4B-NB	6.49	1.41	1.35
23	b	617	CLA	C4B-NB	6.48	1.41	1.35
23	C	512	CLA	C4B-NB	6.47	1.41	1.35
23	B	613	CLA	C4B-NB	6.45	1.41	1.35
23	a	403	CLA	C4B-NB	6.43	1.40	1.35
23	A	404	CLA	C4B-NB	6.40	1.40	1.35
23	B	612	CLA	C4B-NB	6.40	1.40	1.35
23	C	514	CLA	C4B-NB	6.39	1.40	1.35
23	a	402	CLA	C4B-NB	6.37	1.40	1.35
23	b	613	CLA	C4B-NB	6.32	1.40	1.35
23	A	405	CLA	C4B-NB	6.22	1.40	1.35
26	A	410	PL9	C7-C3	-5.04	1.46	1.51
27	a	410	SQD	O48-C23	4.84	1.47	1.33
26	a	409	PL9	C7-C3	-4.73	1.46	1.51
27	A	411	SQD	O48-C23	4.72	1.47	1.33
27	d	408	SQD	O48-C23	4.72	1.47	1.33
27	D	410	SQD	O48-C23	4.61	1.46	1.33
27	a	407	SQD	O48-C23	4.60	1.46	1.33
27	F	101	SQD	O48-C23	4.58	1.46	1.33
27	B	630	SQD	O48-C23	4.56	1.46	1.33
27	A	415	SQD	O48-C23	4.44	1.46	1.33
27	b	601	SQD	O48-C23	4.37	1.46	1.33
26	D	402	PL9	C7-C3	-4.22	1.47	1.51
37	f	102	HEM	C3C-CAC	3.93	1.55	1.47
37	E	105	HEM	C3C-CAC	3.92	1.55	1.47
37	E	105	HEM	C3C-C2C	-3.92	1.34	1.40
37	V	201	HEM	C3C-CAC	3.83	1.55	1.47
26	D	402	PL9	C3-C4	-3.79	1.43	1.49
27	a	407	SQD	O47-C45	-3.77	1.37	1.46
37	V	201	HEM	C3C-C2C	-3.77	1.35	1.40
27	F	101	SQD	O5-C1	3.72	1.51	1.41
23	b	602	CLA	C1D-ND	3.70	1.42	1.37
27	B	630	SQD	O47-C45	-3.69	1.37	1.46
37	f	102	HEM	C3C-C2C	-3.68	1.35	1.40
27	D	410	SQD	O5-C1	3.67	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	403	CLA	C1D-ND	3.67	1.42	1.37
23	A	405	CLA	C1D-ND	3.67	1.42	1.37
26	d	406	PL9	C3-C4	-3.64	1.43	1.49
23	c	503	CLA	C1D-ND	3.64	1.42	1.37
27	A	411	SQD	O5-C1	3.63	1.51	1.41
23	B	616	CLA	C1D-ND	3.63	1.42	1.37
23	b	603	CLA	C1D-ND	3.62	1.42	1.37
23	B	601	CLA	C1D-ND	3.61	1.42	1.37
23	A	404	CLA	C1D-ND	3.60	1.42	1.37
23	c	511	CLA	C1D-ND	3.59	1.42	1.37
26	A	410	PL9	C3-C4	-3.58	1.43	1.49
23	A	408	CLA	C1D-ND	3.57	1.42	1.37
23	b	614	CLA	C1D-ND	3.57	1.42	1.37
23	b	617	CLA	C1D-ND	3.56	1.42	1.37
23	b	617	CLA	C4D-ND	-3.56	1.32	1.37
23	d	404	CLA	C4D-ND	-3.56	1.32	1.37
23	B	602	CLA	C1D-ND	3.56	1.42	1.37
23	B	609	CLA	C1D-ND	3.55	1.42	1.37
27	A	415	SQD	O47-C45	-3.55	1.37	1.46
23	b	616	CLA	C1D-ND	3.55	1.42	1.37
23	B	613	CLA	C1D-ND	3.54	1.42	1.37
23	b	610	CLA	C1D-ND	3.53	1.42	1.37
23	c	513	CLA	C1D-ND	3.53	1.42	1.37
23	C	511	CLA	C1D-ND	3.53	1.42	1.37
27	a	410	SQD	O47-C45	-3.53	1.37	1.46
23	b	606	CLA	C4D-ND	-3.50	1.32	1.37
27	b	601	SQD	O47-C7	3.50	1.44	1.34
23	B	607	CLA	C1D-ND	3.49	1.42	1.37
23	B	605	CLA	C4D-ND	-3.49	1.32	1.37
23	A	406	CLA	C4D-ND	-3.48	1.32	1.37
27	D	410	SQD	O47-C7	3.48	1.44	1.34
23	b	610	CLA	C4D-ND	-3.48	1.32	1.37
23	d	401	CLA	C1D-ND	3.48	1.42	1.37
23	d	405	CLA	C1D-ND	3.47	1.42	1.37
23	a	405	CLA	C1D-ND	3.47	1.42	1.37
23	c	502	CLA	C1D-ND	3.46	1.42	1.37
23	C	506	CLA	C1D-ND	3.46	1.42	1.37
23	C	518	CLA	C1D-ND	3.46	1.42	1.37
27	F	101	SQD	O47-C45	-3.46	1.37	1.46
23	b	613	CLA	C4D-ND	-3.45	1.33	1.37
23	c	508	CLA	C4D-ND	-3.45	1.33	1.37
27	A	411	SQD	O47-C45	-3.45	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C4D-ND	-3.45	1.33	1.37
23	A	406	CLA	C1D-ND	3.45	1.42	1.37
23	B	614	CLA	C4D-ND	-3.45	1.33	1.37
23	B	608	CLA	C1D-ND	3.45	1.42	1.37
23	b	611	CLA	C1D-ND	3.44	1.42	1.37
23	c	510	CLA	C1D-ND	3.43	1.42	1.37
27	d	408	SQD	O47-C45	-3.43	1.38	1.46
23	C	508	CLA	C4D-ND	-3.43	1.33	1.37
23	B	606	CLA	C1D-ND	3.42	1.42	1.37
23	a	403	CLA	C4D-ND	-3.42	1.33	1.37
23	B	616	CLA	C4D-ND	-3.42	1.33	1.37
23	B	610	CLA	C4D-ND	-3.41	1.33	1.37
23	D	404	CLA	C4D-ND	-3.41	1.33	1.37
23	c	508	CLA	C1D-ND	3.40	1.42	1.37
23	C	512	CLA	C1D-ND	3.40	1.42	1.37
23	B	615	CLA	C1D-ND	3.40	1.42	1.37
23	c	502	CLA	C4D-ND	-3.39	1.33	1.37
23	b	606	CLA	C1D-ND	3.39	1.41	1.37
23	B	614	CLA	C1D-ND	3.39	1.41	1.37
23	B	611	CLA	C4D-ND	-3.38	1.33	1.37
23	C	507	CLA	C4D-ND	-3.38	1.33	1.37
23	C	516	CLA	C1D-ND	3.38	1.41	1.37
23	b	608	CLA	C1D-ND	3.38	1.41	1.37
23	c	501	CLA	C1D-ND	3.38	1.41	1.37
23	d	401	CLA	C4D-ND	-3.38	1.33	1.37
23	B	610	CLA	C1D-ND	3.38	1.41	1.37
23	b	607	CLA	C1D-ND	3.38	1.41	1.37
23	c	504	CLA	C1D-ND	3.38	1.41	1.37
23	C	512	CLA	C4D-ND	-3.38	1.33	1.37
23	b	612	CLA	C4D-ND	-3.37	1.33	1.37
26	d	406	PL9	C7-C3	-3.37	1.47	1.51
23	C	506	CLA	C4D-ND	-3.37	1.33	1.37
23	a	402	CLA	C1D-ND	3.37	1.41	1.37
23	A	405	CLA	C4D-ND	-3.36	1.33	1.37
23	B	609	CLA	C4D-ND	-3.36	1.33	1.37
23	B	604	CLA	C1D-ND	3.36	1.41	1.37
23	B	613	CLA	C4D-ND	-3.35	1.33	1.37
23	c	506	CLA	C1D-ND	3.35	1.41	1.37
23	B	605	CLA	C1D-ND	3.35	1.41	1.37
23	b	611	CLA	C4D-ND	-3.35	1.33	1.37
23	A	404	CLA	C4D-ND	-3.34	1.33	1.37
23	c	509	CLA	C1D-ND	3.33	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	630	SQD	O5-C1	3.32	1.50	1.41
26	a	409	PL9	C3-C4	-3.32	1.44	1.49
23	b	605	CLA	C1D-ND	3.32	1.41	1.37
23	D	405	CLA	C1D-ND	3.32	1.41	1.37
23	C	514	CLA	C1D-ND	3.32	1.41	1.37
23	C	509	CLA	C1D-ND	3.32	1.41	1.37
23	C	513	CLA	C1D-ND	3.32	1.41	1.37
23	C	515	CLA	C4D-ND	-3.32	1.33	1.37
23	B	607	CLA	C4D-ND	-3.32	1.33	1.37
23	b	615	CLA	C4D-ND	-3.32	1.33	1.37
23	c	512	CLA	C1D-ND	3.30	1.41	1.37
23	B	608	CLA	C4D-ND	-3.30	1.33	1.37
23	C	507	CLA	C1D-ND	3.29	1.41	1.37
23	B	602	CLA	C4D-ND	-3.29	1.33	1.37
23	C	513	CLA	C4D-ND	-3.29	1.33	1.37
23	C	508	CLA	C1D-ND	3.28	1.41	1.37
23	C	510	CLA	C4D-ND	-3.28	1.33	1.37
27	d	408	SQD	O47-C7	3.28	1.43	1.34
23	c	506	CLA	C4D-ND	-3.28	1.33	1.37
23	b	614	CLA	C4D-ND	-3.27	1.33	1.37
27	F	101	SQD	O47-C7	3.26	1.43	1.34
27	A	415	SQD	O47-C7	3.26	1.43	1.34
23	b	615	CLA	C1D-ND	3.25	1.41	1.37
23	b	609	CLA	C1D-ND	3.24	1.41	1.37
23	B	611	CLA	C1D-ND	3.24	1.41	1.37
23	b	604	CLA	C1D-ND	3.24	1.41	1.37
23	D	405	CLA	C4D-ND	-3.24	1.33	1.37
23	C	514	CLA	C4D-ND	-3.23	1.33	1.37
23	b	604	CLA	C4D-ND	-3.23	1.33	1.37
23	a	405	CLA	C4D-ND	-3.23	1.33	1.37
23	C	511	CLA	C4D-ND	-3.22	1.33	1.37
23	B	603	CLA	C4D-ND	-3.22	1.33	1.37
23	C	510	CLA	C1D-ND	3.22	1.41	1.37
23	B	615	CLA	C4D-ND	-3.22	1.33	1.37
27	A	411	SQD	O47-C7	3.21	1.43	1.34
23	C	517	CLA	C4D-ND	-3.21	1.33	1.37
23	B	614	CLA	CHC-C1C	3.21	1.43	1.35
23	C	515	CLA	C1D-ND	3.21	1.41	1.37
23	c	503	CLA	C4D-ND	-3.20	1.33	1.37
23	c	505	CLA	C4D-ND	-3.20	1.33	1.37
23	b	612	CLA	C1D-ND	3.20	1.41	1.37
23	A	408	CLA	C4D-ND	-3.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C4D-ND	-3.20	1.33	1.37
23	b	607	CLA	C4D-ND	-3.20	1.33	1.37
23	c	507	CLA	C4D-ND	-3.19	1.33	1.37
27	d	408	SQD	O5-C1	3.19	1.50	1.41
23	C	518	CLA	C4D-ND	-3.18	1.33	1.37
23	B	603	CLA	C1D-ND	3.18	1.41	1.37
23	B	612	CLA	C4D-ND	-3.18	1.33	1.37
23	d	405	CLA	C4D-ND	-3.18	1.33	1.37
23	B	606	CLA	C4D-ND	-3.18	1.33	1.37
23	b	616	CLA	C4D-ND	-3.17	1.33	1.37
23	c	509	CLA	C4D-ND	-3.17	1.33	1.37
27	a	410	SQD	O5-C1	3.17	1.49	1.41
23	b	609	CLA	C4D-ND	-3.16	1.33	1.37
23	c	511	CLA	C4D-ND	-3.15	1.33	1.37
23	c	510	CLA	C4D-ND	-3.15	1.33	1.37
23	C	518	CLA	CHC-C1C	3.15	1.43	1.35
23	B	601	CLA	C4D-ND	-3.14	1.33	1.37
23	c	512	CLA	C4D-ND	-3.14	1.33	1.37
27	a	410	SQD	O47-C7	3.14	1.43	1.34
37	f	102	HEM	CAB-C3B	3.13	1.56	1.47
23	b	605	CLA	C4D-ND	-3.12	1.33	1.37
23	C	513	CLA	CHC-C1C	3.12	1.43	1.35
23	B	605	CLA	CHC-C1C	3.12	1.43	1.35
23	a	402	CLA	C4D-ND	-3.12	1.33	1.37
23	c	513	CLA	CHC-C1C	3.12	1.43	1.35
23	c	513	CLA	C4D-ND	-3.12	1.33	1.37
23	b	606	CLA	CHC-C1C	3.12	1.43	1.35
23	b	603	CLA	CHC-C1C	3.11	1.42	1.35
23	C	514	CLA	CHC-C1C	3.11	1.42	1.35
23	c	504	CLA	C4D-ND	-3.09	1.33	1.37
23	B	601	CLA	CHC-C1C	3.08	1.42	1.35
23	c	503	CLA	CHC-C1C	3.08	1.42	1.35
27	B	630	SQD	O47-C7	3.08	1.43	1.34
23	c	512	CLA	CHC-C1C	3.07	1.42	1.35
23	C	509	CLA	C4D-ND	-3.07	1.33	1.37
23	D	405	CLA	CHC-C1C	3.07	1.42	1.35
23	C	517	CLA	C1D-ND	3.07	1.41	1.37
23	c	501	CLA	C4D-ND	-3.07	1.33	1.37
23	b	615	CLA	CHC-C1C	3.07	1.42	1.35
23	C	510	CLA	CHC-C1C	3.06	1.42	1.35
23	B	604	CLA	C4D-ND	-3.06	1.33	1.37
23	b	610	CLA	CHC-C1C	3.06	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	CHC-C1C	3.06	1.42	1.35
27	a	407	SQD	C24-C23	3.06	1.59	1.50
27	a	407	SQD	O47-C7	3.05	1.42	1.34
23	B	612	CLA	CHC-C1C	3.05	1.42	1.35
23	D	404	CLA	CHC-C1C	3.05	1.42	1.35
23	b	611	CLA	CHC-C1C	3.05	1.42	1.35
23	b	602	CLA	CHC-C1C	3.04	1.42	1.35
23	c	508	CLA	CHC-C1C	3.04	1.42	1.35
23	B	611	CLA	CHC-C1C	3.04	1.42	1.35
23	B	608	CLA	CHC-C1C	3.04	1.42	1.35
23	c	509	CLA	CHC-C1C	3.04	1.42	1.35
23	B	606	CLA	CHC-C1C	3.04	1.42	1.35
23	c	507	CLA	C1D-ND	3.03	1.41	1.37
23	B	602	CLA	CHC-C1C	3.03	1.42	1.35
23	d	405	CLA	CHC-C1C	3.03	1.42	1.35
23	C	516	CLA	C4D-ND	-3.03	1.33	1.37
27	d	408	SQD	C24-C23	3.03	1.59	1.50
23	C	507	CLA	CHC-C1C	3.03	1.42	1.35
23	c	505	CLA	C1D-ND	3.03	1.41	1.37
23	C	508	CLA	CHC-C1C	3.02	1.42	1.35
26	A	410	PL9	C6-C1	-3.02	1.43	1.48
27	D	410	SQD	C24-C23	3.02	1.59	1.50
27	a	410	SQD	C24-C23	3.02	1.59	1.50
23	c	501	CLA	CHC-C1C	3.02	1.42	1.35
23	B	609	CLA	CHC-C1C	3.02	1.42	1.35
23	b	612	CLA	CHC-C1C	3.01	1.42	1.35
27	D	410	SQD	O47-C45	-3.01	1.39	1.46
23	C	511	CLA	CHC-C1C	3.01	1.42	1.35
27	A	411	SQD	C24-C23	3.01	1.59	1.50
23	b	602	CLA	C4D-ND	-3.01	1.33	1.37
23	C	506	CLA	CHC-C1C	3.01	1.42	1.35
23	c	510	CLA	CHC-C1C	3.01	1.42	1.35
23	b	604	CLA	CHC-C1C	3.00	1.42	1.35
23	d	404	CLA	CHC-C1C	3.00	1.42	1.35
23	c	506	CLA	CHC-C1C	3.00	1.42	1.35
23	c	505	CLA	CHC-C1C	2.99	1.42	1.35
23	a	403	CLA	CHC-C1C	2.99	1.42	1.35
23	A	408	CLA	CHC-C1C	2.99	1.42	1.35
23	a	405	CLA	CHC-C1C	2.99	1.42	1.35
23	C	517	CLA	CHC-C1C	2.99	1.42	1.35
27	b	601	SQD	O5-C1	2.99	1.49	1.41
23	C	516	CLA	CHC-C1C	2.98	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	601	SQD	O47-C45	-2.98	1.39	1.46
23	b	609	CLA	CHC-C1C	2.98	1.42	1.35
23	b	614	CLA	CHC-C1C	2.97	1.42	1.35
23	b	613	CLA	CHC-C1C	2.97	1.42	1.35
27	A	415	SQD	C24-C23	2.97	1.59	1.50
23	C	509	CLA	CHC-C1C	2.96	1.42	1.35
37	V	201	HEM	CAB-C3B	2.96	1.55	1.47
23	c	511	CLA	CHC-C1C	2.95	1.42	1.35
37	E	105	HEM	CAB-C3B	2.95	1.55	1.47
23	B	613	CLA	CHC-C1C	2.93	1.42	1.35
23	b	608	CLA	CHC-C1C	2.92	1.42	1.35
23	B	603	CLA	CHC-C1C	2.92	1.42	1.35
23	c	504	CLA	CHC-C1C	2.92	1.42	1.35
23	c	502	CLA	CHC-C1C	2.92	1.42	1.35
23	B	616	CLA	CHC-C1C	2.91	1.42	1.35
23	b	605	CLA	CMB-C2B	-2.91	1.45	1.51
23	a	402	CLA	CHC-C1C	2.91	1.42	1.35
23	A	406	CLA	CHC-C1C	2.91	1.42	1.35
23	d	404	CLA	C1D-ND	2.90	1.41	1.37
23	C	510	CLA	CMD-C2D	-2.90	1.44	1.50
23	B	610	CLA	CHC-C1C	2.89	1.42	1.35
27	F	101	SQD	C24-C23	2.88	1.59	1.50
23	d	401	CLA	CHC-C1C	2.88	1.42	1.35
23	C	515	CLA	CHC-C1C	2.88	1.42	1.35
23	B	607	CLA	CHC-C1C	2.88	1.42	1.35
27	A	415	SQD	O5-C1	2.87	1.49	1.41
27	B	630	SQD	C24-C23	2.86	1.59	1.50
23	c	507	CLA	CHC-C1C	2.86	1.42	1.35
23	D	404	CLA	C1D-ND	2.86	1.41	1.37
23	C	512	CLA	CHC-C1C	2.85	1.42	1.35
23	B	603	CLA	CMB-C2B	-2.84	1.45	1.51
26	D	402	PL9	C6-C1	-2.84	1.43	1.48
23	A	404	CLA	CHC-C1C	2.84	1.42	1.35
23	b	617	CLA	CHC-C1C	2.83	1.42	1.35
23	B	615	CLA	CHC-C1C	2.82	1.42	1.35
23	b	616	CLA	CHC-C1C	2.82	1.42	1.35
23	b	613	CLA	C1D-ND	2.80	1.41	1.37
27	b	601	SQD	C24-C23	2.79	1.58	1.50
23	A	405	CLA	CHC-C1C	2.79	1.42	1.35
23	b	605	CLA	CHC-C1C	2.78	1.42	1.35
23	C	511	CLA	CMB-C2B	-2.77	1.45	1.51
27	a	407	SQD	O5-C1	2.77	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	CMB-C2B	-2.77	1.45	1.51
23	B	609	CLA	CMB-C2B	-2.76	1.45	1.51
23	B	604	CLA	CMB-C2B	-2.76	1.45	1.51
23	B	612	CLA	C1D-ND	2.73	1.41	1.37
23	b	609	CLA	CMB-C2B	-2.72	1.46	1.51
23	B	604	CLA	CHC-C1C	2.72	1.41	1.35
23	b	604	CLA	CMB-C2B	-2.70	1.46	1.51
23	A	408	CLA	CMB-C2B	-2.69	1.46	1.51
23	c	505	CLA	CMD-C2D	-2.69	1.45	1.50
23	B	610	CLA	CMB-C2B	-2.69	1.46	1.51
23	C	515	CLA	CMD-C2D	-2.65	1.45	1.50
23	B	608	CLA	CMB-C2B	-2.65	1.46	1.51
23	C	515	CLA	CMB-C2B	-2.65	1.46	1.51
23	b	605	CLA	CMD-C2D	-2.65	1.45	1.50
23	A	404	CLA	CMB-C2B	-2.65	1.46	1.51
23	D	404	CLA	CMD-C2D	-2.64	1.45	1.50
23	b	613	CLA	CMD-C2D	-2.64	1.45	1.50
23	A	406	CLA	CMB-C2B	-2.64	1.46	1.51
23	b	610	CLA	CMB-C2B	-2.62	1.46	1.51
23	B	612	CLA	CMD-C2D	-2.61	1.45	1.50
23	B	616	CLA	CMC-C2C	-2.60	1.45	1.50
23	b	611	CLA	CMB-C2B	-2.60	1.46	1.51
23	A	405	CLA	CMB-C2B	-2.60	1.46	1.51
23	a	405	CLA	CMB-C2B	-2.59	1.46	1.51
23	a	402	CLA	CMD-C2D	-2.59	1.45	1.50
23	c	510	CLA	CMB-C2B	-2.59	1.46	1.51
23	c	501	CLA	CMB-C2B	-2.58	1.46	1.51
23	C	506	CLA	CMB-C2B	-2.58	1.46	1.51
23	b	608	CLA	CMB-C2B	-2.58	1.46	1.51
23	b	614	CLA	CMB-C2B	-2.58	1.46	1.51
23	b	617	CLA	CMC-C2C	-2.57	1.45	1.50
23	d	401	CLA	CMB-C2B	-2.57	1.46	1.51
23	C	507	CLA	CMB-C2B	-2.56	1.46	1.51
23	B	613	CLA	CMB-C2B	-2.56	1.46	1.51
23	b	607	CLA	CMB-C2B	-2.56	1.46	1.51
23	c	508	CLA	CMB-C2B	-2.56	1.46	1.51
23	b	604	CLA	CMD-C2D	-2.56	1.45	1.50
23	B	602	CLA	CMB-C2B	-2.54	1.46	1.51
23	b	617	CLA	CMB-C2B	-2.54	1.46	1.51
23	C	508	CLA	CMB-C2B	-2.54	1.46	1.51
26	d	406	PL9	C6-C1	-2.53	1.44	1.48
23	b	612	CLA	CMB-C2B	-2.53	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	CMD-C2D	-2.53	1.45	1.50
23	C	512	CLA	CMB-C2B	-2.53	1.46	1.51
23	C	517	CLA	CMB-C2B	-2.53	1.46	1.51
23	B	616	CLA	CMB-C2B	-2.53	1.46	1.51
23	c	505	CLA	CMB-C2B	-2.52	1.46	1.51
23	b	616	CLA	CMB-C2B	-2.51	1.46	1.51
23	b	602	CLA	CMB-C2B	-2.51	1.46	1.51
23	c	502	CLA	CMB-C2B	-2.50	1.46	1.51
23	c	511	CLA	CMB-C2B	-2.50	1.46	1.51
23	B	607	CLA	CMB-C2B	-2.50	1.46	1.51
23	C	513	CLA	CMB-C2B	-2.50	1.46	1.51
23	b	613	CLA	CMB-C2B	-2.50	1.46	1.51
23	C	509	CLA	CMB-C2B	-2.50	1.46	1.51
23	B	615	CLA	CMB-C2B	-2.50	1.46	1.51
23	c	504	CLA	CMB-C2B	-2.49	1.46	1.51
23	B	611	CLA	CMB-C2B	-2.49	1.46	1.51
23	a	402	CLA	CMB-C2B	-2.49	1.46	1.51
23	b	603	CLA	CMB-C2B	-2.48	1.46	1.51
26	d	406	PL9	C53-C6	-2.48	1.45	1.50
23	B	606	CLA	CMB-C2B	-2.47	1.46	1.51
26	a	409	PL9	C53-C6	-2.47	1.45	1.50
23	d	404	CLA	CMB-C2B	-2.46	1.46	1.51
23	d	404	CLA	CMD-C2D	-2.46	1.45	1.50
23	C	510	CLA	CMB-C2B	-2.46	1.46	1.51
23	c	503	CLA	CMB-C2B	-2.45	1.46	1.51
23	B	612	CLA	CMB-C2B	-2.44	1.46	1.51
23	C	516	CLA	CMB-C2B	-2.44	1.46	1.51
23	B	601	CLA	CMB-C2B	-2.44	1.46	1.51
23	b	615	CLA	CMB-C2B	-2.42	1.46	1.51
23	D	405	CLA	CMB-C2B	-2.42	1.46	1.51
23	A	404	CLA	CMD-C2D	-2.42	1.45	1.50
23	c	512	CLA	CMB-C2B	-2.42	1.46	1.51
23	c	502	CLA	CMC-C2C	-2.41	1.45	1.50
23	B	614	CLA	CMB-C2B	-2.41	1.46	1.51
23	c	507	CLA	CMB-C2B	-2.40	1.46	1.51
23	D	404	CLA	CMB-C2B	-2.40	1.46	1.51
23	d	405	CLA	CMB-C2B	-2.40	1.46	1.51
23	B	605	CLA	CMB-C2B	-2.40	1.46	1.51
23	b	606	CLA	CMB-C2B	-2.40	1.46	1.51
23	c	510	CLA	CMD-C2D	-2.39	1.45	1.50
23	a	403	CLA	CMB-C2B	-2.38	1.46	1.51
23	B	604	CLA	CMD-C2D	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	410	PL9	C53-C6	-2.37	1.45	1.50
23	C	518	CLA	CMB-C2B	-2.37	1.46	1.51
23	c	509	CLA	CMB-C2B	-2.36	1.46	1.51
23	b	612	CLA	CMC-C2C	-2.36	1.45	1.50
23	B	608	CLA	CMD-C2D	-2.36	1.45	1.50
23	C	514	CLA	CMB-C2B	-2.36	1.46	1.51
26	d	406	PL9	C52-C5	-2.36	1.45	1.50
23	B	615	CLA	CMC-C2C	-2.35	1.45	1.50
23	b	609	CLA	CMD-C2D	-2.34	1.45	1.50
23	c	513	CLA	CMB-C2B	-2.33	1.46	1.51
26	A	410	PL9	C52-C5	-2.31	1.45	1.50
23	B	611	CLA	CMC-C2C	-2.30	1.45	1.50
23	C	507	CLA	CMC-C2C	-2.30	1.45	1.50
23	C	509	CLA	CMC-C2C	-2.27	1.46	1.50
23	b	613	CLA	CMC-C2C	-2.26	1.46	1.50
23	C	506	CLA	CMD-C2D	-2.24	1.46	1.50
23	C	517	CLA	CMD-C2D	-2.24	1.46	1.50
23	b	606	CLA	CMD-C2D	-2.24	1.46	1.50
23	a	403	CLA	CMD-C2D	-2.23	1.46	1.50
23	D	404	CLA	CMC-C2C	-2.23	1.46	1.50
23	b	603	CLA	CMD-C2D	-2.22	1.46	1.50
23	c	509	CLA	CMD-C2D	-2.22	1.46	1.50
23	B	612	CLA	CMC-C2C	-2.20	1.46	1.50
23	c	501	CLA	CMD-C2D	-2.19	1.46	1.50
23	B	613	CLA	CMD-C2D	-2.19	1.46	1.50
27	B	630	SQD	C6-S	2.18	1.85	1.77
23	B	602	CLA	CMD-C2D	-2.18	1.46	1.50
23	c	505	CLA	CMC-C2C	-2.18	1.46	1.50
23	b	611	CLA	C3B-C2B	-2.17	1.37	1.40
23	B	606	CLA	CMC-C2C	-2.17	1.46	1.50
23	d	405	CLA	CMD-C2D	-2.17	1.46	1.50
23	B	605	CLA	CMD-C2D	-2.17	1.46	1.50
27	b	601	SQD	O7-S	2.17	1.51	1.45
23	c	513	CLA	CMC-C2C	-2.17	1.46	1.50
23	D	405	CLA	CMD-C2D	-2.17	1.46	1.50
23	B	607	CLA	CMD-C2D	-2.16	1.46	1.50
27	A	411	SQD	O9-S	2.15	1.51	1.45
23	A	406	CLA	CMD-C2D	-2.15	1.46	1.50
27	b	601	SQD	O9-S	2.15	1.51	1.45
23	B	602	CLA	CMC-C2C	-2.15	1.46	1.50
23	B	614	CLA	CMC-C2C	-2.15	1.46	1.50
23	b	616	CLA	CMC-C2C	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	CMD-C2D	-2.15	1.46	1.50
23	C	507	CLA	CMD-C2D	-2.14	1.46	1.50
23	C	514	CLA	CMD-C2D	-2.14	1.46	1.50
23	C	513	CLA	CMC-C2C	-2.14	1.46	1.50
23	b	604	CLA	CMC-C2C	-2.13	1.46	1.50
27	F	101	SQD	O5-C5	2.13	1.49	1.44
23	a	405	CLA	CMD-C2D	-2.13	1.46	1.50
23	C	506	CLA	C3B-C2B	-2.13	1.37	1.40
23	b	611	CLA	CMD-C2D	-2.13	1.46	1.50
23	b	615	CLA	CMD-C2D	-2.13	1.46	1.50
23	B	615	CLA	CMD-C2D	-2.13	1.46	1.50
23	b	616	CLA	CMD-C2D	-2.12	1.46	1.50
23	c	504	CLA	CMC-C2C	-2.12	1.46	1.50
27	B	630	SQD	O9-S	2.12	1.51	1.45
23	C	516	CLA	CMD-C2D	-2.12	1.46	1.50
23	b	606	CLA	CMC-C2C	-2.12	1.46	1.50
23	A	408	CLA	CMD-C2D	-2.12	1.46	1.50
23	B	614	CLA	CMD-C2D	-2.12	1.46	1.50
23	B	616	CLA	CMD-C2D	-2.12	1.46	1.50
23	C	508	CLA	CMD-C2D	-2.12	1.46	1.50
23	c	506	CLA	CMC-C2C	-2.12	1.46	1.50
23	c	506	CLA	CMD-C2D	-2.10	1.46	1.50
23	c	511	CLA	CMD-C2D	-2.10	1.46	1.50
23	B	610	CLA	CMD-C2D	-2.10	1.46	1.50
23	d	404	CLA	CMC-C2C	-2.10	1.46	1.50
23	c	513	CLA	C3B-CAB	-2.10	1.43	1.47
23	c	508	CLA	CMC-C2C	-2.10	1.46	1.50
23	c	508	CLA	CMD-C2D	-2.10	1.46	1.50
27	d	408	SQD	O9-S	2.10	1.51	1.45
27	a	410	SQD	O9-S	2.10	1.51	1.45
23	A	405	CLA	CMD-C2D	-2.10	1.46	1.50
23	c	511	CLA	CMC-C2C	-2.10	1.46	1.50
27	A	411	SQD	O5-C5	2.10	1.49	1.44
23	B	611	CLA	CMD-C2D	-2.09	1.46	1.50
26	D	402	PL9	C52-C5	-2.09	1.46	1.50
23	C	512	CLA	CMD-C2D	-2.09	1.46	1.50
23	C	511	CLA	CMD-C2D	-2.08	1.46	1.50
23	B	601	CLA	CMD-C2D	-2.08	1.46	1.50
23	b	608	CLA	CMD-C2D	-2.08	1.46	1.50
23	b	614	CLA	CMD-C2D	-2.08	1.46	1.50
23	c	513	CLA	CMD-C2D	-2.08	1.46	1.50
23	b	607	CLA	CMC-C2C	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	405	CLA	CMC-C2C	-2.08	1.46	1.50
23	c	501	CLA	C3B-C2B	-2.08	1.37	1.40
23	C	518	CLA	CMD-C2D	-2.08	1.46	1.50
27	b	601	SQD	C6-S	2.08	1.85	1.77
26	D	402	PL9	C53-C6	-2.08	1.46	1.50
23	b	608	CLA	CMC-C2C	-2.07	1.46	1.50
23	B	607	CLA	CMC-C2C	-2.07	1.46	1.50
23	B	609	CLA	CMC-C2C	-2.07	1.46	1.50
23	c	510	CLA	CMC-C2C	-2.07	1.46	1.50
23	b	610	CLA	CMD-C2D	-2.07	1.46	1.50
27	D	410	SQD	C46-C45	2.07	1.57	1.50
23	c	505	CLA	C3B-CAB	-2.07	1.43	1.47
23	b	612	CLA	CMD-C2D	-2.06	1.46	1.50
37	f	102	HEM	CMB-C2B	2.06	1.55	1.50
27	d	408	SQD	O7-S	2.06	1.51	1.45
23	b	607	CLA	CMD-C2D	-2.06	1.46	1.50
27	D	410	SQD	O7-S	2.06	1.51	1.45
23	A	408	CLA	C3B-C2B	-2.06	1.37	1.40
23	B	603	CLA	CMC-C2C	-2.05	1.46	1.50
23	C	511	CLA	CMC-C2C	-2.05	1.46	1.50
23	C	513	CLA	CMD-C2D	-2.05	1.46	1.50
23	B	609	CLA	CMD-C2D	-2.05	1.46	1.50
24	A	407	PHO	C1C-NC	-2.05	1.32	1.38
27	a	410	SQD	O7-S	2.04	1.51	1.45
27	A	411	SQD	O7-S	2.04	1.51	1.45
23	d	401	CLA	CMD-C2D	-2.04	1.46	1.50
24	A	407	PHO	C3B-C2B	-2.04	1.37	1.40
23	b	615	CLA	CMC-C2C	-2.04	1.46	1.50
27	F	101	SQD	O9-S	2.04	1.51	1.45
23	C	509	CLA	CMD-C2D	-2.03	1.46	1.50
27	a	407	SQD	O9-S	2.03	1.51	1.45
23	b	603	CLA	CMC-C2C	-2.03	1.46	1.50
23	c	502	CLA	CMD-C2D	-2.03	1.46	1.50
27	D	410	SQD	O9-S	2.03	1.51	1.45
23	b	609	CLA	CMC-C2C	-2.02	1.46	1.50
27	d	408	SQD	C46-C45	2.02	1.56	1.50
23	c	512	CLA	CMC-C2C	-2.02	1.46	1.50
23	c	507	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	602	CLA	CMD-C2D	-2.02	1.46	1.50
27	b	601	SQD	C8-C7	2.02	1.56	1.50
27	F	101	SQD	C8-C7	2.02	1.56	1.50
23	c	504	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	630	SQD	O7-S	2.02	1.51	1.45
23	B	605	CLA	CMC-C2C	-2.01	1.46	1.50
23	C	516	CLA	CMC-C2C	-2.01	1.46	1.50
27	F	101	SQD	O7-S	2.01	1.51	1.45
23	b	610	CLA	CMC-C2C	-2.01	1.46	1.50
23	B	601	CLA	CMC-C2C	-2.01	1.46	1.50
23	B	613	CLA	CMC-C2C	-2.01	1.46	1.50
23	b	617	CLA	CMD-C2D	-2.01	1.46	1.50
23	b	611	CLA	CMC-C2C	-2.01	1.46	1.50
37	E	105	HEM	CMB-C2B	2.00	1.55	1.50
23	a	405	CLA	CMC-C2C	-2.00	1.46	1.50

All (800) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C4A-NA-C1A	8.39	110.48	106.71
23	B	604	CLA	C4A-NA-C1A	8.26	110.42	106.71
23	C	512	CLA	C4A-NA-C1A	8.15	110.37	106.71
23	b	608	CLA	C4A-NA-C1A	8.09	110.34	106.71
23	B	607	CLA	C4A-NA-C1A	7.94	110.28	106.71
23	c	504	CLA	C4A-NA-C1A	7.92	110.27	106.71
23	b	605	CLA	C4A-NA-C1A	7.79	110.21	106.71
23	b	613	CLA	C4A-NA-C1A	7.76	110.19	106.71
23	c	505	CLA	C4A-NA-C1A	7.75	110.19	106.71
23	B	615	CLA	C4A-NA-C1A	7.70	110.17	106.71
23	c	506	CLA	C4A-NA-C1A	7.69	110.17	106.71
23	B	612	CLA	C4A-NA-C1A	7.64	110.14	106.71
23	C	516	CLA	C4A-NA-C1A	7.56	110.10	106.71
23	c	511	CLA	C4A-NA-C1A	7.51	110.08	106.71
23	C	509	CLA	C4A-NA-C1A	7.50	110.08	106.71
23	C	514	CLA	C4A-NA-C1A	7.40	110.03	106.71
23	b	616	CLA	C4A-NA-C1A	7.40	110.03	106.71
23	b	607	CLA	C4A-NA-C1A	7.37	110.02	106.71
23	b	606	CLA	C4A-NA-C1A	7.36	110.01	106.71
23	b	612	CLA	C4A-NA-C1A	7.33	110.00	106.71
23	d	404	CLA	C4A-NA-C1A	7.32	110.00	106.71
23	B	611	CLA	C4A-NA-C1A	7.31	109.99	106.71
23	B	616	CLA	C4A-NA-C1A	7.30	109.99	106.71
23	A	404	CLA	C4A-NA-C1A	7.29	109.98	106.71
23	C	517	CLA	C4A-NA-C1A	7.28	109.98	106.71
23	A	408	CLA	C4A-NA-C1A	7.22	109.95	106.71
23	B	603	CLA	C4A-NA-C1A	7.22	109.95	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	C4A-NA-C1A	7.19	109.94	106.71
23	A	405	CLA	C4A-NA-C1A	7.18	109.94	106.71
23	D	404	CLA	C4A-NA-C1A	7.18	109.93	106.71
23	c	502	CLA	C4A-NA-C1A	7.18	109.93	106.71
23	d	401	CLA	C4A-NA-C1A	7.15	109.92	106.71
23	B	609	CLA	C4A-NA-C1A	7.13	109.91	106.71
23	C	507	CLA	C4A-NA-C1A	7.13	109.91	106.71
23	d	405	CLA	C4A-NA-C1A	7.12	109.91	106.71
23	C	510	CLA	C4A-NA-C1A	7.11	109.90	106.71
23	B	605	CLA	C4A-NA-C1A	7.10	109.90	106.71
23	B	610	CLA	C4A-NA-C1A	7.09	109.89	106.71
23	B	606	CLA	C4A-NA-C1A	7.09	109.89	106.71
23	B	601	CLA	C4A-NA-C1A	7.07	109.88	106.71
23	b	604	CLA	C4A-NA-C1A	7.06	109.88	106.71
23	b	615	CLA	C4A-NA-C1A	7.06	109.88	106.71
23	C	511	CLA	C4A-NA-C1A	7.05	109.88	106.71
23	D	405	CLA	C4A-NA-C1A	7.04	109.87	106.71
23	C	508	CLA	C4A-NA-C1A	7.01	109.86	106.71
23	c	508	CLA	C4A-NA-C1A	6.96	109.84	106.71
23	C	515	CLA	C4A-NA-C1A	6.96	109.83	106.71
23	C	518	CLA	C4A-NA-C1A	6.92	109.82	106.71
23	b	617	CLA	C4A-NA-C1A	6.92	109.82	106.71
23	B	613	CLA	C4A-NA-C1A	6.90	109.81	106.71
23	C	506	CLA	C4A-NA-C1A	6.90	109.81	106.71
23	b	614	CLA	C4A-NA-C1A	6.88	109.80	106.71
23	b	602	CLA	C4A-NA-C1A	6.87	109.80	106.71
23	b	610	CLA	C4A-NA-C1A	6.85	109.79	106.71
23	c	513	CLA	C4A-NA-C1A	6.84	109.78	106.71
23	c	512	CLA	C4A-NA-C1A	6.82	109.77	106.71
23	a	403	CLA	C4A-NA-C1A	6.82	109.77	106.71
23	a	405	CLA	C4A-NA-C1A	6.80	109.76	106.71
23	B	608	CLA	C4A-NA-C1A	6.80	109.76	106.71
23	c	509	CLA	C4A-NA-C1A	6.78	109.75	106.71
23	B	602	CLA	C4A-NA-C1A	6.75	109.74	106.71
23	b	603	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	C	513	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	a	402	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	A	406	CLA	C4A-NA-C1A	6.64	109.69	106.71
23	c	501	CLA	C4A-NA-C1A	6.62	109.68	106.71
23	c	510	CLA	C4A-NA-C1A	6.56	109.65	106.71
23	b	609	CLA	C4A-NA-C1A	6.51	109.63	106.71
23	c	503	CLA	C4A-NA-C1A	6.44	109.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	505	DGD	O5D-C1E-C2E	6.35	118.22	108.30
23	b	611	CLA	C4A-NA-C1A	6.04	109.42	106.71
35	C	505	DGD	C6D-O5D-C1E	6.00	125.46	113.74
25	T	101	BCR	C15-C14-C13	5.96	135.81	127.31
26	A	410	PL9	C7-C3-C4	5.81	121.60	116.88
35	C	504	DGD	C6D-O5D-C1E	5.49	124.47	113.74
27	B	630	SQD	O7-S-C6	5.39	113.34	106.94
27	A	415	SQD	O6-C1-C2	5.24	116.49	108.30
23	d	401	CLA	CMB-C2B-C1B	-5.19	120.49	128.46
27	b	601	SQD	O7-S-C6	5.18	113.10	106.94
23	c	508	CLA	CMB-C2B-C1B	-5.14	120.56	128.46
35	C	505	DGD	O5D-C6D-C5D	5.13	118.53	109.05
23	C	513	CLA	CMB-C2B-C1B	-5.11	120.61	128.46
23	C	511	CLA	CMB-C2B-C1B	-5.09	120.65	128.46
23	c	506	CLA	CMB-C2B-C1B	-5.08	120.66	128.46
23	c	509	CLA	CMB-C2B-C1B	-5.01	120.76	128.46
23	b	609	CLA	CMB-C2B-C1B	-4.94	120.87	128.46
23	b	612	CLA	CMB-C2B-C1B	-4.94	120.87	128.46
23	b	613	CLA	CMB-C2B-C1B	-4.94	120.88	128.46
23	B	606	CLA	CMB-C2B-C1B	-4.91	120.92	128.46
23	C	514	CLA	CMB-C2B-C1B	-4.89	120.95	128.46
23	B	608	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
26	a	409	PL9	C7-C3-C4	4.83	120.80	116.88
23	a	402	CLA	CMB-C2B-C1B	-4.82	121.06	128.46
23	B	611	CLA	CMB-C2B-C1B	-4.76	121.14	128.46
25	B	631	BCR	C15-C14-C13	4.75	134.09	127.31
23	B	613	CLA	CMB-C2B-C1B	-4.72	121.20	128.46
23	A	405	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
27	B	630	SQD	O9-S-C6	4.65	112.46	106.94
23	A	404	CLA	CMB-C2B-C1B	-4.65	121.32	128.46
26	d	406	PL9	C7-C3-C4	4.60	120.62	116.88
23	C	509	CLA	CMB-C2B-C1B	-4.58	121.42	128.46
23	b	614	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
23	B	602	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
26	D	402	PL9	C7-C3-C4	4.49	120.53	116.88
23	B	616	CLA	CMB-C2B-C1B	-4.48	121.57	128.46
23	C	516	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
23	C	518	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
23	b	607	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
23	c	512	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
23	c	509	CLA	CMB-C2B-C3B	4.38	132.88	124.68
23	B	612	CLA	CMB-C2B-C1B	-4.36	121.76	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
23	c	507	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
23	d	401	CLA	CMB-C2B-C3B	4.31	132.75	124.68
23	C	514	CLA	CMB-C2B-C3B	4.29	132.70	124.68
27	a	407	SQD	O6-C1-C2	4.27	114.96	108.30
27	a	407	SQD	O8-S-C6	4.26	112.54	105.74
27	d	408	SQD	O9-S-C6	4.26	112.01	106.94
23	c	508	CLA	CMB-C2B-C3B	4.26	132.65	124.68
23	C	517	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
35	C	504	DGD	C1E-O6E-C5E	4.26	122.04	113.69
23	C	512	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
23	C	513	CLA	CMB-C2B-C3B	4.25	132.63	124.68
23	B	604	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
23	c	511	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
23	B	610	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
27	A	415	SQD	O9-S-C6	4.22	111.96	106.94
23	B	609	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
27	b	601	SQD	O9-S-C6	4.22	111.95	106.94
23	c	503	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
23	b	615	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
23	b	613	CLA	CMB-C2B-C3B	4.18	132.49	124.68
23	C	515	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
23	d	405	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
23	b	608	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
27	F	101	SQD	O47-C7-C8	4.17	120.48	111.50
23	b	610	CLA	CMB-C2B-C1B	-4.16	122.08	128.46
25	T	101	BCR	C16-C15-C14	4.15	131.98	123.47
23	b	603	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
23	B	614	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
23	c	510	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
23	c	502	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
27	A	411	SQD	O9-S-C6	4.10	111.81	106.94
26	A	410	PL9	C7-C3-C2	-4.08	117.93	123.30
23	a	402	CLA	CMB-C2B-C3B	4.08	132.31	124.68
23	B	606	CLA	CMB-C2B-C3B	4.07	132.30	124.68
23	B	605	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
31	A	417	BCT	O2-C-O1	4.03	130.01	119.55
23	A	405	CLA	CMB-C2B-C3B	4.03	132.21	124.68
27	a	410	SQD	O7-S-C6	4.02	111.72	106.94
23	b	612	CLA	CMB-C2B-C3B	4.02	132.19	124.68
30	A	416	LMT	C1B-O5B-C5B	4.00	121.54	113.69
27	D	410	SQD	O47-C7-C8	4.00	120.11	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	CMB-C2B-C3B	4.00	132.15	124.68
23	c	513	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
37	E	105	HEM	CBA-CAA-C2A	-3.98	105.83	112.62
31	a	415	BCT	O2-C-O1	3.98	129.87	119.55
27	a	407	SQD	O47-C7-C8	3.98	120.07	111.50
27	A	411	SQD	O47-C7-C8	3.97	120.06	111.50
25	T	101	BCR	C15-C16-C17	-3.97	115.34	123.47
23	b	606	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
23	C	507	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
23	B	607	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
23	b	604	CLA	CMB-C2B-C1B	-3.92	122.45	128.46
23	B	611	CLA	CMB-C2B-C3B	3.89	131.96	124.68
23	B	608	CLA	CMB-C2B-C3B	3.89	131.95	124.68
23	c	506	CLA	CMB-C2B-C3B	3.89	131.95	124.68
23	C	508	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
23	B	613	CLA	CMB-C2B-C3B	3.88	131.94	124.68
23	C	518	CLA	CMB-C2B-C3B	3.87	131.93	124.68
23	b	611	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
23	C	511	CLA	CMB-C2B-C3B	3.87	131.92	124.68
23	a	403	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
27	D	410	SQD	O7-S-C6	3.87	111.54	106.94
23	B	603	CLA	CMB-C2B-C1B	-3.86	122.52	128.46
23	a	405	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
27	d	408	SQD	O9-S-O7	-3.85	100.62	113.95
23	D	404	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
23	d	404	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
23	A	404	CLA	CMB-C2B-C3B	3.83	131.85	124.68
23	b	617	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
23	C	516	CLA	CMB-C2B-C3B	3.83	131.84	124.68
23	B	612	CLA	CMB-C2B-C3B	3.82	131.83	124.68
23	C	509	CLA	CMB-C2B-C3B	3.82	131.83	124.68
23	b	605	CLA	CMB-C2B-C1B	-3.81	122.60	128.46
23	B	616	CLA	CMB-C2B-C3B	3.81	131.81	124.68
23	B	602	CLA	CMB-C2B-C3B	3.79	131.76	124.68
23	c	512	CLA	CMB-C2B-C3B	3.78	131.74	124.68
27	F	101	SQD	O7-S-C6	3.76	111.41	106.94
27	D	410	SQD	O9-S-O7	-3.74	100.99	113.95
27	d	408	SQD	O47-C7-C8	3.74	119.56	111.50
27	b	601	SQD	O47-C7-C8	3.73	119.55	111.50
23	C	512	CLA	CMB-C2B-C3B	3.72	131.63	124.68
27	F	101	SQD	O9-S-O7	-3.71	101.11	113.95
23	c	507	CLA	CMB-C2B-C3B	3.69	131.57	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	407	SQD	O9-S-C6	3.68	111.31	106.94
27	B	630	SQD	O9-S-O7	-3.67	101.25	113.95
23	b	614	CLA	CMB-C2B-C3B	3.66	131.53	124.68
27	A	415	SQD	O47-C7-C8	3.66	119.39	111.50
23	c	504	CLA	CMB-C2B-C3B	3.63	131.48	124.68
23	D	405	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
27	a	407	SQD	O9-S-O7	-3.63	101.40	113.95
23	c	513	CLA	CMB-C2B-C3B	3.58	131.37	124.68
25	B	631	BCR	C15-C16-C17	-3.57	116.16	123.47
23	C	517	CLA	CMB-C2B-C3B	3.57	131.36	124.68
23	c	503	CLA	CMB-C2B-C3B	3.57	131.35	124.68
23	d	405	CLA	CMB-C2B-C3B	3.56	131.34	124.68
27	A	415	SQD	O9-S-O7	-3.56	101.63	113.95
23	c	511	CLA	CMB-C2B-C3B	3.56	131.33	124.68
27	F	101	SQD	O9-S-C6	3.55	111.16	106.94
23	b	603	CLA	CMB-C2B-C3B	3.55	131.32	124.68
27	A	411	SQD	O9-S-O7	-3.55	101.67	113.95
24	d	402	PHO	CMB-C2B-C3B	3.55	131.31	124.68
23	b	607	CLA	CMB-C2B-C3B	3.54	131.31	124.68
27	a	410	SQD	O9-S-O7	-3.54	101.69	113.95
30	B	626	LMT	O1B-C1B-C2B	3.54	117.27	108.10
23	b	602	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
27	B	630	SQD	O47-C7-C8	3.52	119.08	111.50
27	A	415	SQD	O8-S-C6	3.51	111.34	105.74
23	b	615	CLA	CMB-C2B-C3B	3.51	131.25	124.68
27	D	410	SQD	O9-S-C6	3.51	111.11	106.94
37	f	102	HEM	CMC-C2C-C3C	3.51	131.24	124.68
23	B	605	CLA	CMB-C2B-C3B	3.50	131.22	124.68
23	b	603	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
27	a	410	SQD	O47-C7-C8	3.49	119.02	111.50
23	B	614	CLA	CMB-C2B-C3B	3.49	131.21	124.68
23	A	406	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
26	a	409	PL9	C7-C3-C2	-3.47	118.74	123.30
23	b	608	CLA	CMB-C2B-C3B	3.46	131.15	124.68
23	c	501	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
24	D	401	PHO	CMB-C2B-C3B	3.43	131.09	124.68
23	c	502	CLA	CMB-C2B-C3B	3.42	131.07	124.68
23	C	510	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
23	b	606	CLA	CMB-C2B-C3B	3.42	131.07	124.68
23	C	508	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
25	B	631	BCR	C16-C17-C18	3.41	132.17	127.31
27	b	601	SQD	O9-S-O7	-3.40	102.17	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
23	B	601	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
25	B	631	BCR	C16-C15-C14	3.36	130.36	123.47
27	a	410	SQD	O9-S-C6	3.35	110.93	106.94
23	c	510	CLA	CMB-C2B-C3B	3.34	130.92	124.68
23	B	604	CLA	CMB-C2B-C3B	3.33	130.92	124.68
23	C	507	CLA	CMB-C2B-C3B	3.33	130.92	124.68
23	b	610	CLA	CMB-C2B-C3B	3.33	130.91	124.68
23	B	609	CLA	CMB-C2B-C3B	3.32	130.90	124.68
23	B	606	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
23	a	403	CLA	CMB-C2B-C3B	3.31	130.88	124.68
23	B	607	CLA	CMB-C2B-C3B	3.31	130.88	124.68
23	B	614	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
23	C	515	CLA	CMB-C2B-C3B	3.30	130.86	124.68
23	D	404	CLA	CMB-C2B-C3B	3.30	130.85	124.68
23	A	408	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
27	d	408	SQD	O7-S-C6	3.29	110.84	106.94
23	B	615	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
23	C	508	CLA	CMB-C2B-C3B	3.27	130.80	124.68
23	d	404	CLA	CMB-C2B-C3B	3.25	130.75	124.68
23	b	617	CLA	CMB-C2B-C3B	3.24	130.74	124.68
27	A	415	SQD	C44-O6-C1	-3.23	107.43	113.74
23	b	607	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
35	c	515	DGD	C4D-C3D-C2D	3.22	116.45	110.82
23	C	509	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
23	C	512	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
23	a	405	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
23	B	602	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
23	a	405	CLA	CMB-C2B-C3B	3.21	130.68	124.68
23	b	604	CLA	CMB-C2B-C3B	3.19	130.65	124.68
23	c	502	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
23	c	511	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
27	F	101	SQD	O8-S-C6	3.18	110.81	105.74
23	B	610	CLA	CMB-C2B-C3B	3.17	130.62	124.68
25	f	101	BCR	C24-C23-C22	-3.17	121.45	126.23
23	b	604	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
23	C	518	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
23	B	611	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
27	a	407	SQD	O7-S-C6	3.15	110.69	106.94
27	d	408	SQD	O8-S-C6	3.14	110.75	105.74
37	V	201	HEM	CBA-CAA-C2A	-3.14	107.26	112.62
26	D	402	PL9	C7-C8-C9	-3.14	121.57	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	CMB-C2B-C3B	3.13	130.54	124.68
26	d	406	PL9	C7-C8-C9	-3.13	121.58	126.79
23	c	507	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
23	d	401	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
27	D	410	SQD	O8-S-C6	3.12	110.70	105.74
23	c	508	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
23	D	405	CLA	CMB-C2B-C3B	3.11	130.50	124.68
23	c	505	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
23	b	615	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
23	A	405	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
37	E	105	HEM	C4B-CHC-C1C	3.09	126.64	122.56
23	b	616	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
23	D	405	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
37	V	201	HEM	CMB-C2B-C1B	-3.08	120.34	125.04
23	b	602	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
23	C	517	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	B	612	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	C	507	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	B	608	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
23	b	609	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
23	C	516	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	b	613	CLA	CHB-C4A-NA	3.04	128.72	124.51
25	T	101	BCR	C16-C17-C18	3.04	131.64	127.31
23	A	406	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
26	D	402	PL9	C40-C39-C41	3.03	120.37	115.27
23	B	604	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
23	c	501	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
37	E	105	HEM	CMC-C2C-C3C	3.01	130.30	124.68
27	A	415	SQD	C1-O5-C5	-3.00	107.79	113.69
23	b	608	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
33	C	525	LMG	C4-C3-C2	3.00	116.06	110.82
35	C	504	DGD	O6E-C1E-O5D	3.00	117.07	109.97
23	c	513	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
23	b	605	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
23	C	513	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
23	B	610	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
23	b	617	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
26	D	402	PL9	C7-C3-C2	-2.98	119.38	123.30
26	d	406	PL9	C7-C3-C2	-2.97	119.39	123.30
23	b	616	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	B	603	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	B	601	CLA	O2D-CGD-O1D	-2.97	118.03	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
23	a	403	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	b	613	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
23	B	603	CLA	CMB-C2B-C3B	2.95	130.19	124.68
23	B	612	CLA	CHB-C4A-NA	2.94	128.58	124.51
23	C	514	CLA	CHB-C4A-NA	2.94	128.57	124.51
23	c	509	CLA	CHB-C4A-NA	2.93	128.57	124.51
23	D	404	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
23	c	512	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
23	A	406	CLA	CMB-C2B-C3B	2.92	130.14	124.68
23	C	510	CLA	CMB-C2B-C3B	2.91	130.13	124.68
23	d	405	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
30	B	626	LMT	C1B-O1B-C4'	2.91	125.16	117.96
23	c	507	CLA	CHB-C4A-NA	2.91	128.53	124.51
23	c	506	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
23	C	510	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
24	D	401	PHO	C1A-C2A-C3A	-2.90	100.08	102.84
23	c	504	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	c	503	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
27	A	415	SQD	O7-S-C6	2.87	110.36	106.94
37	V	201	HEM	C1B-NB-C4B	2.87	108.04	105.07
23	C	512	CLA	CHB-C4A-NA	2.87	128.48	124.51
23	c	511	CLA	CHB-C4A-NA	2.86	128.47	124.51
23	C	506	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
23	B	615	CLA	CHB-C4A-NA	2.86	128.46	124.51
23	b	608	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	C	516	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	T	101	BCR	C12-C13-C14	-2.84	114.58	118.94
23	b	602	CLA	CMB-C2B-C3B	2.84	129.99	124.68
23	c	512	CLA	CHB-C4A-NA	2.84	128.44	124.51
24	D	401	PHO	C4A-C3A-C2A	-2.84	100.14	102.84
23	b	616	CLA	CHB-C4A-NA	2.83	128.43	124.51
27	d	408	SQD	O48-C23-C24	2.83	120.78	111.91
30	a	411	LMT	C2'-C3'-C4'	2.83	116.13	109.68
23	c	504	CLA	CHB-C4A-NA	2.83	128.42	124.51
23	b	605	CLA	CMB-C2B-C3B	2.82	129.96	124.68
23	C	511	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	B	615	CLA	CMB-C2B-C3B	2.81	129.94	124.68
26	d	406	PL9	C22-C23-C24	-2.81	120.90	127.66
26	a	409	PL9	C40-C39-C41	2.80	119.98	115.27
23	A	408	CLA	CMB-C2B-C3B	2.79	129.90	124.68
27	A	411	SQD	O7-S-C6	2.79	110.25	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
27	b	601	SQD	O6-C1-C2	2.78	112.65	108.30
37	V	201	HEM	CBD-CAD-C3D	-2.78	104.91	112.63
25	j	101	BCR	C7-C8-C9	2.78	130.43	126.23
37	f	102	HEM	C4B-CHC-C1C	2.77	126.22	122.56
23	C	514	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	B	605	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
24	a	404	PHO	C4A-C3A-C2A	-2.76	100.21	102.84
23	c	501	CLA	CMB-C2B-C3B	2.76	129.84	124.68
23	C	517	CLA	CHB-C4A-NA	2.76	128.32	124.51
33	C	525	LMG	O6-C5-C4	2.74	114.68	109.69
23	b	612	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	B	609	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	d	405	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	B	607	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
23	B	601	CLA	CMB-C2B-C3B	2.72	129.76	124.68
35	C	504	DGD	O6E-C1E-C2E	2.72	116.10	110.35
25	C	501	BCR	C7-C8-C9	-2.72	122.13	126.23
23	c	505	CLA	CMB-C2B-C3B	2.72	129.76	124.68
26	d	406	PL9	C40-C39-C41	2.71	119.84	115.27
23	C	509	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	d	401	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	B	615	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
27	F	101	SQD	O48-C23-C24	2.70	120.39	111.91
23	c	505	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
27	D	410	SQD	O48-C23-C24	2.69	120.35	111.91
23	A	406	CLA	CHB-C4A-NA	2.69	128.23	124.51
23	B	607	CLA	CHB-C4A-NA	2.69	128.23	124.51
23	b	610	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
23	A	405	CLA	CHB-C4A-NA	2.68	128.22	124.51
23	B	601	CLA	CHB-C4A-NA	2.68	128.21	124.51
26	d	406	PL9	C36-C34-C33	-2.67	115.70	121.12
26	A	410	PL9	C40-C39-C41	2.67	119.76	115.27
27	a	410	SQD	O48-C23-C24	2.66	120.26	111.91
23	B	610	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
24	A	407	PHO	CMB-C2B-C3B	2.66	129.65	124.68
27	B	630	SQD	O48-C23-C24	2.65	120.24	111.91
23	b	605	CLA	CHB-C4A-NA	2.65	128.18	124.51
27	F	101	SQD	O5-C5-C4	2.65	114.50	109.69
23	A	408	CLA	CHB-C4A-NA	2.65	128.17	124.51
26	D	402	PL9	C22-C23-C24	-2.64	121.30	127.66
23	a	403	CLA	CHB-C4A-NA	2.64	128.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	a	402	CLA	CHB-C4A-NA	2.63	128.15	124.51
30	A	416	LMT	C1'-O5'-C5'	2.63	118.85	113.69
24	a	404	PHO	C1B-NB-C4B	2.63	112.48	107.09
23	a	405	CLA	CHB-C4A-NA	2.62	128.14	124.51
23	D	405	CLA	CHB-C4A-NA	2.62	128.14	124.51
23	b	602	CLA	CHB-C4A-NA	2.62	128.14	124.51
23	b	603	CLA	CHB-C4A-NA	2.62	128.14	124.51
27	A	415	SQD	O48-C23-C24	2.62	120.14	111.91
23	b	616	CLA	CMB-C2B-C3B	2.62	129.58	124.68
33	C	525	LMG	C1-O6-C5	2.62	118.83	113.69
23	A	404	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
23	c	513	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	B	616	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
35	C	504	DGD	O3E-C3E-C2E	-2.60	104.33	110.35
37	f	102	HEM	CBA-CAA-C2A	-2.60	108.18	112.62
23	c	508	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	b	606	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
35	C	504	DGD	C3D-C4D-C5D	-2.60	105.60	110.24
23	d	404	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
23	C	518	CLA	CHB-C4A-NA	2.60	128.10	124.51
30	A	416	LMT	O1B-C4'-C3'	2.59	114.18	107.28
23	b	614	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
23	b	608	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
23	c	503	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	C	511	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
27	D	410	SQD	O5-C1-C2	2.58	115.82	110.35
23	c	506	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	B	611	CLA	C1-C2-C3	-2.57	121.60	126.04
23	B	604	CLA	CHB-C4A-NA	2.57	128.06	124.51
27	A	411	SQD	O8-S-C6	2.56	109.83	105.74
37	V	201	HEM	C3B-C2B-C1B	2.56	108.39	106.49
23	C	510	CLA	O2D-CGD-CBD	2.56	115.81	111.27
23	C	507	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	a	402	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
23	c	506	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
23	b	617	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	B	608	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
27	a	407	SQD	O48-C23-C24	2.55	119.91	111.91
37	f	102	HEM	CBD-CAD-C3D	-2.55	105.55	112.63
23	B	613	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
26	A	410	PL9	C7-C8-C9	-2.55	122.55	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	O2D-CGD-CBD	2.55	115.79	111.27
23	b	609	CLA	CHB-C4A-NA	2.54	128.03	124.51
37	f	102	HEM	C4D-ND-C1D	2.54	107.70	105.07
23	d	401	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
23	c	502	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	b	604	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
23	c	510	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
23	B	610	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	a	409	PL9	C22-C23-C24	-2.52	121.58	127.66
30	T	103	LMT	C1B-O5B-C5B	2.52	118.64	113.69
23	a	402	CLA	C2D-C1D-ND	-2.52	108.25	110.10
23	A	404	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	b	615	CLA	CHB-C4A-NA	2.52	128.00	124.51
37	E	105	HEM	C4D-ND-C1D	2.52	107.67	105.07
23	B	608	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	B	602	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	d	401	CLA	CHD-C1D-ND	-2.51	122.15	124.45
23	B	614	CLA	C1-C2-C3	-2.51	121.70	126.04
23	A	408	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
23	B	605	CLA	CHD-C1D-ND	-2.50	122.15	124.45
23	b	612	CLA	C1-C2-C3	-2.50	121.71	126.04
24	D	401	PHO	C1B-NB-C4B	2.50	112.22	107.09
23	b	607	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	c	501	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	B	611	CLA	O2D-CGD-CBD	2.50	115.70	111.27
37	V	201	HEM	C4D-ND-C1D	2.50	107.65	105.07
23	C	511	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	b	611	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
23	B	616	CLA	CHB-C4A-NA	2.48	127.95	124.51
23	b	611	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	A	405	CLA	CHD-C1D-ND	-2.48	122.17	124.45
23	b	606	CLA	CHB-C4A-NA	2.48	127.94	124.51
24	d	402	PHO	C1A-C2A-C3A	-2.48	100.48	102.84
23	b	612	CLA	CHB-C4A-NA	2.48	127.94	124.51
35	C	503	DGD	C6D-O5D-C1E	2.47	118.57	113.74
23	C	508	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	C	515	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
35	C	505	DGD	C6D-C5D-C4D	-2.47	106.94	112.09
23	B	605	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	A	406	CLA	O2D-CGD-CBD	2.47	115.65	111.27
23	a	403	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
23	C	518	CLA	C1B-CHB-C4A	-2.46	125.24	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	E	105	HEM	C1B-NB-C4B	2.46	107.62	105.07
23	c	508	CLA	O2D-CGD-CBD	2.45	115.63	111.27
23	C	513	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	A	405	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
23	A	404	CLA	C2D-C1D-ND	-2.45	108.30	110.10
23	a	402	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
23	B	614	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	d	402	PHO	C1B-NB-C4B	2.45	112.11	107.09
24	A	407	PHO	C1B-NB-C4B	2.44	112.10	107.09
23	d	405	CLA	C1-C2-C3	-2.44	121.83	126.04
23	B	606	CLA	CHB-C4A-NA	2.44	127.88	124.51
25	D	403	BCR	C24-C23-C22	-2.43	122.56	126.23
23	B	609	CLA	CHB-C4A-NA	2.43	127.88	124.51
23	B	602	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	a	405	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
23	c	508	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	b	604	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	A	406	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
35	C	504	DGD	O5D-C1E-C2E	2.42	112.09	108.30
27	d	408	SQD	C4-C3-C2	2.42	115.06	110.82
23	c	513	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
23	c	509	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
27	A	411	SQD	O48-C23-C24	2.41	119.46	111.91
23	d	405	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
23	C	508	CLA	O2D-CGD-CBD	2.40	115.54	111.27
23	C	512	CLA	O2D-CGD-CBD	2.40	115.53	111.27
23	b	617	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
27	a	410	SQD	O6-C1-C2	2.40	112.05	108.30
23	C	510	CLA	C2D-C1D-ND	-2.40	108.34	110.10
26	A	410	PL9	C22-C23-C24	-2.40	121.89	127.66
23	a	403	CLA	O2D-CGD-CBD	2.40	115.53	111.27
23	B	603	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
26	D	402	PL9	O1-C4-C3	-2.39	118.09	120.72
24	a	404	PHO	CMB-C2B-C3B	2.38	129.14	124.68
23	c	505	CLA	CHB-C4A-NA	2.38	127.81	124.51
26	A	410	PL9	C37-C38-C39	-2.38	121.94	127.66
35	C	504	DGD	C1E-C2E-C3E	2.37	114.94	110.00
37	E	105	HEM	CMA-C3A-C4A	-2.37	124.82	128.46
27	A	411	SQD	O5-C5-C4	2.37	114.00	109.69
26	A	410	PL9	C27-C28-C29	-2.37	121.96	127.66
23	D	404	CLA	CHB-C4A-NA	2.37	127.78	124.51
23	B	610	CLA	CHD-C1D-ND	-2.37	122.28	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
23	C	512	CLA	C2A-C1A-CHA	2.36	127.99	123.86
26	a	409	PL9	C7-C8-C9	-2.36	122.86	126.79
23	b	612	CLA	O2D-CGD-CBD	2.36	115.47	111.27
23	C	506	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	B	603	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	b	605	CLA	C2D-C1D-ND	-2.36	108.37	110.10
23	C	513	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
23	b	611	CLA	CAA-C2A-C3A	-2.36	106.33	112.78
23	b	615	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
23	b	606	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
23	B	614	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
37	V	201	HEM	C4C-CHD-C1D	2.35	125.66	122.56
23	b	603	CLA	O2D-CGD-CBD	2.35	115.44	111.27
23	c	512	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
26	D	402	PL9	C20-C19-C21	2.34	119.21	115.27
23	b	605	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
23	b	612	CLA	CHD-C1D-ND	-2.34	122.31	124.45
23	B	613	CLA	CHB-C4A-NA	2.33	127.74	124.51
23	B	609	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	c	509	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
37	E	105	HEM	CBD-CAD-C3D	-2.33	106.16	112.63
23	B	613	CLA	C1-C2-C3	-2.33	122.02	126.04
23	b	610	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
26	a	409	PL9	O2-C1-C6	2.33	124.62	120.59
23	B	607	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
23	B	604	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
23	C	515	CLA	C2D-C1D-ND	-2.32	108.39	110.10
23	b	604	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
23	C	515	CLA	CHB-C4A-NA	2.31	127.71	124.51
26	D	402	PL9	C27-C28-C29	-2.31	122.09	127.66
23	C	509	CLA	CHD-C1D-ND	-2.31	122.33	124.45
27	B	630	SQD	O8-S-C6	2.31	109.42	105.74
23	C	506	CLA	CMB-C2B-C3B	2.31	128.99	124.68
23	b	603	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
26	d	406	PL9	O1-C4-C3	-2.30	118.18	120.72
31	A	417	BCT	O3-C-O1	-2.30	113.57	119.55
23	d	404	CLA	CHB-C4A-NA	2.30	127.69	124.51
23	B	603	CLA	CHB-C4A-NA	2.30	127.69	124.51
23	A	405	CLA	O2D-CGD-CBD	2.30	115.35	111.27
26	a	409	PL9	C20-C19-C21	2.29	119.13	115.27
30	A	416	LMT	C3'-C4'-C5'	-2.29	105.67	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C2A-C1A-CHA	2.29	127.87	123.86
26	A	410	PL9	C25-C24-C26	2.29	119.12	115.27
23	B	605	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
26	D	402	PL9	C37-C38-C39	-2.29	122.15	127.66
25	t	101	BCR	C29-C30-C25	2.29	114.01	110.48
25	T	101	BCR	C35-C13-C14	2.28	126.12	122.92
23	C	506	CLA	CHD-C1D-ND	-2.28	122.36	124.45
26	d	406	PL9	C8-C7-C3	2.28	118.43	111.98
23	b	602	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
23	A	406	CLA	C2D-C1D-ND	-2.28	108.42	110.10
23	C	510	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
23	a	405	CLA	O2D-CGD-CBD	2.28	115.31	111.27
23	B	610	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
23	C	512	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
30	A	416	LMT	C1B-O1B-C4'	2.28	123.60	117.96
23	b	611	CLA	CAA-CBA-CGA	-2.27	106.61	113.25
23	b	613	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
27	D	410	SQD	C1-C2-C3	2.27	114.73	110.00
23	d	404	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
23	b	607	CLA	O2D-CGD-CBD	2.27	115.30	111.27
27	b	601	SQD	O48-C23-C24	2.27	119.02	111.91
23	C	510	CLA	CHB-C4A-NA	2.27	127.65	124.51
23	b	605	CLA	O2D-CGD-CBD	2.27	115.29	111.27
23	C	511	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
27	A	415	SQD	C3-C4-C5	2.26	114.28	110.24
30	a	411	LMT	C1B-O5B-C5B	2.26	118.13	113.69
23	A	404	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	C	516	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
23	c	511	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
23	B	606	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
23	b	613	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
25	B	618	BCR	C29-C30-C25	2.25	113.95	110.48
23	c	503	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	C	506	CLA	O2D-CGD-CBD	2.25	115.26	111.27
26	a	409	PL9	C27-C28-C29	-2.25	122.25	127.66
23	c	505	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
23	C	513	CLA	CHD-C1D-ND	-2.24	122.39	124.45
27	b	601	SQD	O8-S-C6	2.24	109.32	105.74
23	B	601	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
23	c	510	CLA	CHB-C4A-NA	2.24	127.61	124.51
23	b	607	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
26	A	410	PL9	C32-C33-C34	-2.24	122.28	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
25	j	101	BCR	C20-C21-C22	2.23	130.49	127.31
31	a	415	BCT	O3-C-O1	-2.23	113.76	119.55
23	b	612	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
23	b	607	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
37	f	102	HEM	C1B-NB-C4B	2.23	107.37	105.07
37	V	201	HEM	C3D-C4D-ND	-2.22	107.69	110.17
23	b	610	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
27	d	408	SQD	O6-C1-C2	2.22	111.77	108.30
23	c	502	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	c	503	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
25	C	502	BCR	C23-C22-C21	-2.22	115.54	118.94
23	C	507	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
23	c	501	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
23	b	610	CLA	CHB-C4A-NA	2.21	127.57	124.51
25	f	101	BCR	C38-C26-C25	-2.21	122.04	124.53
23	c	504	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
23	c	505	CLA	O2D-CGD-CBD	2.21	115.20	111.27
23	C	517	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
23	B	611	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	C	513	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
25	z	101	BCR	C20-C21-C22	-2.21	124.16	127.31
23	D	405	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
37	V	201	HEM	C4B-CHC-C1C	2.20	125.47	122.56
23	a	403	CLA	C2D-C1D-ND	-2.20	108.48	110.10
23	B	611	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
35	C	505	DGD	O3G-C3G-C2G	2.20	116.21	110.90
23	b	604	CLA	O2D-CGD-CBD	2.20	115.18	111.27
23	c	504	CLA	CHD-C1D-ND	-2.20	122.43	124.45
23	C	509	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
25	j	101	BCR	C2-C1-C6	2.20	113.86	110.48
23	B	604	CLA	O2D-CGD-CBD	2.19	115.17	111.27
23	A	406	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
23	b	614	CLA	CHB-C4A-NA	2.18	127.53	124.51
37	V	201	HEM	CMC-C2C-C3C	2.18	128.76	124.68
25	j	101	BCR	C8-C9-C10	-2.18	115.59	118.94
23	B	608	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
23	C	514	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
25	j	101	BCR	C23-C22-C21	-2.18	115.60	118.94
23	B	614	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
23	B	612	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
24	D	401	PHO	C1-C2-C3	-2.18	122.28	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	E	105	HEM	CMB-C2B-C1B	-2.18	121.72	125.04
26	d	406	PL9	C27-C28-C29	-2.18	122.42	127.66
23	C	508	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
26	A	410	PL9	O2-C1-C2	-2.17	116.80	121.78
25	B	618	BCR	C29-C28-C27	2.17	116.23	111.38
23	d	401	CLA	O2D-CGD-CBD	2.17	115.13	111.27
23	b	615	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	c	507	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
23	B	607	CLA	CHD-C1D-ND	-2.17	122.46	124.45
26	a	409	PL9	O2-C1-C2	-2.17	116.81	121.78
23	b	614	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
24	A	407	PHO	C4A-C3A-C2A	-2.17	100.78	102.84
23	a	405	CLA	CHD-C1D-ND	-2.17	122.46	124.45
26	a	409	PL9	O1-C4-C3	-2.17	118.33	120.72
26	a	409	PL9	C32-C33-C34	-2.16	122.45	127.66
35	c	514	DGD	C6D-O5D-C1E	2.16	117.96	113.74
23	C	513	CLA	O2D-CGD-CBD	2.16	115.11	111.27
23	C	515	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
30	z	102	LMT	C1B-O5B-C5B	2.16	117.93	113.69
23	B	615	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
23	B	606	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
23	B	614	CLA	CHD-C1D-ND	-2.16	122.47	124.45
23	b	609	CLA	CHD-C1D-ND	-2.15	122.48	124.45
23	A	406	CLA	CHD-C1D-ND	-2.15	122.48	124.45
23	A	405	CLA	C3C-C4C-NC	-2.15	108.16	110.57
23	c	507	CLA	O2D-CGD-CBD	2.15	115.08	111.27
23	B	613	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
26	d	406	PL9	C20-C19-C21	2.15	118.88	115.27
23	c	506	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
23	C	516	CLA	C2A-C1A-CHA	2.14	127.61	123.86
23	C	511	CLA	CHD-C1D-ND	-2.14	122.48	124.45
25	B	631	BCR	C12-C13-C14	-2.14	115.66	118.94
26	A	410	PL9	C36-C34-C33	-2.13	116.81	121.12
25	B	631	BCR	C35-C13-C14	2.13	125.91	122.92
26	d	406	PL9	C50-C49-C48	-2.13	116.49	122.65
25	Y	102	BCR	C20-C21-C22	2.13	130.34	127.31
27	F	101	SQD	C1-O5-C5	2.13	117.86	113.69
23	c	508	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	C	508	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
23	c	503	CLA	CHD-C1D-ND	-2.12	122.51	124.45
27	F	101	SQD	O5-C1-C2	2.11	114.81	110.35
26	d	406	PL9	C12-C13-C14	-2.11	122.58	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	405	CLA	O2D-CGD-CBD	2.11	115.01	111.27
23	b	609	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
30	a	419	LMT	C4'-C3'-C2'	2.10	114.49	110.82
26	D	402	PL9	C8-C7-C3	2.10	117.92	111.98
23	B	613	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
27	a	407	SQD	C3-C4-C5	2.10	113.99	110.24
23	A	408	CLA	O2D-CGD-CBD	2.10	115.00	111.27
23	C	514	CLA	CHD-C1D-ND	-2.10	122.52	124.45
23	A	406	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
23	b	616	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
23	b	610	CLA	CHD-C1D-ND	-2.10	122.53	124.45
23	B	603	CLA	C2D-C1D-ND	-2.10	108.56	110.10
23	B	603	CLA	O2D-CGD-CBD	2.10	114.99	111.27
30	M	101	LMT	C1B-O5B-C5B	2.09	117.80	113.69
23	d	405	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	C	518	CLA	CHD-C1D-ND	-2.09	122.53	124.45
23	b	606	CLA	CHD-C1D-ND	-2.09	122.53	124.45
23	B	610	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
23	c	501	CLA	CHD-C1D-ND	-2.09	122.53	124.45
23	b	605	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
24	d	402	PHO	C4A-C3A-C2A	-2.09	100.85	102.84
23	b	609	CLA	O1D-CGD-CBD	2.09	128.76	124.48
23	B	609	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
26	A	410	PL9	O2-C1-C6	2.08	124.20	120.59
30	a	411	LMT	O3'-C3'-C2'	-2.08	105.54	110.35
23	C	506	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
35	C	505	DGD	C1E-O6E-C5E	2.08	117.77	113.69
23	c	501	CLA	O2D-CGD-CBD	2.08	114.96	111.27
30	E	106	LMT	C1B-O5B-C5B	2.08	117.77	113.69
23	b	611	CLA	CHD-C1D-ND	-2.08	122.55	124.45
37	f	102	HEM	CMB-C2B-C1B	-2.07	121.88	125.04
23	B	608	CLA	C2D-C1D-ND	-2.07	108.58	110.10
23	C	506	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
24	d	402	PHO	CMC-C2C-C3C	2.07	128.84	124.94
23	c	509	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
23	a	403	CLA	CHD-C1D-ND	-2.06	122.56	124.45
26	a	409	PL9	C50-C49-C48	-2.06	116.69	122.65
26	d	406	PL9	O2-C1-C2	-2.06	117.05	121.78
23	C	516	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	b	612	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	A	408	CLA	C1-C2-C3	-2.06	122.48	126.04
26	d	406	PL9	C36-C37-C38	-2.06	105.11	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	402	PL9	O2-C1-C2	-2.06	117.06	121.78
35	c	515	DGD	O6D-C1D-C2D	2.06	114.71	110.35
23	b	616	CLA	C2A-C1A-CHA	2.06	127.45	123.86
23	B	604	CLA	CBC-CAC-C3C	2.06	118.10	112.43
23	C	517	CLA	C1-C2-C3	-2.06	122.49	126.04
35	D	411	DGD	C3G-O3G-C1D	2.06	117.75	113.74
23	b	609	CLA	C2D-C1D-ND	-2.05	108.59	110.10
30	f	103	LMT	C1B-O5B-C5B	2.05	117.71	113.69
27	a	410	SQD	O8-S-C6	2.05	109.01	105.74
26	A	410	PL9	C42-C43-C44	-2.05	122.72	127.66
23	B	606	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	C	506	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
23	A	405	CLA	CMC-C2C-C3C	2.05	131.68	126.12
26	A	410	PL9	C26-C24-C23	-2.05	116.97	121.12
23	c	505	CLA	C2D-C1D-ND	-2.05	108.59	110.10
23	c	501	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
25	D	403	BCR	C23-C22-C21	-2.04	115.80	118.94
23	C	511	CLA	O1D-CGD-CBD	2.04	128.67	124.48
30	C	526	LMT	C1'-O5'-C5'	2.04	117.70	113.69
23	C	518	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
23	B	607	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
35	c	516	DGD	C6D-O5D-C1E	2.04	117.73	113.74
23	C	509	CLA	C3C-C4C-NC	-2.04	108.28	110.57
23	B	602	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	b	614	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
23	B	614	CLA	O2D-CGD-CBD	2.04	114.89	111.27
23	b	608	CLA	CHD-C1D-ND	-2.03	122.58	124.45
26	D	402	PL9	O2-C1-C6	2.03	124.11	120.59
23	B	615	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
23	D	405	CLA	C1-C2-C3	-2.03	122.54	126.04
23	b	615	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
23	b	614	CLA	C1-C2-C3	-2.02	122.54	126.04
23	c	502	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
23	B	602	CLA	O2D-CGD-CBD	2.02	114.86	111.27
23	D	404	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
26	D	402	PL9	C42-C43-C44	-2.02	122.79	127.66
36	l	102	LHG	O4-P-O5	2.02	122.23	112.24
23	c	511	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
23	b	617	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
23	a	402	CLA	O1D-CGD-CBD	2.02	128.62	124.48
23	d	405	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	c	504	CLA	C3C-C4C-NC	-2.02	108.31	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	519	PLM	O2-C1-C2	-2.02	116.60	123.08
23	a	403	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	b	607	CLA	CHD-C1D-ND	-2.01	122.60	124.45
27	A	411	SQD	O5-C1-C2	2.01	114.61	110.35
23	c	501	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
25	f	101	BCR	C7-C8-C9	-2.01	123.20	126.23
35	c	514	DGD	C3G-O3G-C1D	2.01	117.67	113.74
26	d	406	PL9	C31-C32-C33	-2.01	105.28	111.88
30	C	526	LMT	C1'-C2'-C3'	-2.01	105.81	110.00
23	A	404	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
35	h	102	DGD	C6D-O5D-C1E	2.01	117.66	113.74
23	c	511	CLA	C1-C2-C3	-2.00	122.58	126.04
23	B	616	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
23	b	608	CLA	O2D-CGD-CBD	2.00	114.83	111.27
26	D	402	PL9	C31-C32-C33	-2.00	105.30	111.88
32	C	524	PLM	O2-C1-C2	-2.00	116.65	123.08
23	c	508	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	406	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	608	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	506	CLA	ND

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Mol	Chain	Res	Type	Atom
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	C	515	CLA	ND
23	C	516	CLA	ND
23	C	517	CLA	ND
23	C	518	CLA	ND
23	D	404	CLA	ND
23	D	405	CLA	ND
23	a	402	CLA	ND
23	a	403	CLA	ND
23	a	405	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	608	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	b	617	CLA	ND
23	c	501	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	d	401	CLA	ND
23	d	404	CLA	ND
23	d	405	CLA	ND

All (1761) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404	CLA	CBD-CGD-O2D-CED
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
23	A	406	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	603	CLA	C2-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
23	B	614	CLA	C1A-C2A-CAA-CBA
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	C2-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CBD-CGD-O2D-CED
23	C	509	CLA	C2-C3-C5-C6
23	C	509	CLA	C4-C3-C5-C6
23	C	513	CLA	CHA-CBD-CGD-O1D
23	C	513	CLA	CHA-CBD-CGD-O2D
23	a	402	CLA	CBD-CGD-O2D-CED
23	b	602	CLA	CHA-CBD-CGD-O1D
23	b	602	CLA	CHA-CBD-CGD-O2D
23	b	603	CLA	CHA-CBD-CGD-O1D
23	b	604	CLA	C2-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	b	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	b	615	CLA	CHA-CBD-CGD-O1D
23	b	615	CLA	CHA-CBD-CGD-O2D
23	b	615	CLA	CAD-CBD-CGD-O1D
23	b	615	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O1D
23	c	502	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	512	CLA	C1A-C2A-CAA-CBA
23	d	401	CLA	CHA-CBD-CGD-O1D
23	d	401	CLA	CHA-CBD-CGD-O2D
25	B	618	BCR	C37-C22-C23-C24
25	B	631	BCR	C5-C6-C7-C8
25	B	631	BCR	C13-C14-C15-C16
25	D	403	BCR	C23-C24-C25-C26
25	T	101	BCR	C13-C14-C15-C16
25	Y	102	BCR	C5-C6-C7-C8
25	Y	102	BCR	C36-C18-C19-C20
25	b	618	BCR	C5-C6-C7-C8
25	b	618	BCR	C17-C18-C19-C20
25	b	618	BCR	C36-C18-C19-C20
25	b	620	BCR	C37-C22-C23-C24
25	f	101	BCR	C7-C8-C9-C10
25	f	101	BCR	C7-C8-C9-C34
25	f	101	BCR	C23-C24-C25-C26
25	j	101	BCR	C5-C6-C7-C8
25	j	101	BCR	C21-C22-C23-C24
25	j	101	BCR	C37-C22-C23-C24
25	z	101	BCR	C7-C8-C9-C10
25	z	101	BCR	C7-C8-C9-C34
26	A	410	PL9	C7-C8-C9-C10
26	A	410	PL9	C7-C8-C9-C11
26	A	410	PL9	C12-C13-C14-C15
26	A	410	PL9	C12-C13-C14-C16
26	A	410	PL9	C17-C18-C19-C21
26	A	410	PL9	C32-C33-C34-C36
26	A	410	PL9	C33-C34-C36-C37
26	A	410	PL9	C34-C36-C37-C38
26	A	410	PL9	C37-C38-C39-C41
26	A	410	PL9	C44-C46-C47-C48
26	D	402	PL9	C27-C28-C29-C31
26	D	402	PL9	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
26	D	402	PL9	C32-C33-C34-C35
26	D	402	PL9	C32-C33-C34-C36
26	D	402	PL9	C40-C39-C41-C42
26	D	402	PL9	C42-C43-C44-C46
26	D	402	PL9	C44-C46-C47-C48
26	a	409	PL9	C12-C13-C14-C16
26	a	409	PL9	C24-C26-C27-C28
26	a	409	PL9	C34-C36-C37-C38
27	A	415	SQD	O6-C44-C45-O47
27	A	415	SQD	C5-C6-S-O8
27	A	415	SQD	C5-C6-S-O9
27	B	630	SQD	O10-C23-O48-C46
27	B	630	SQD	C24-C23-O48-C46
27	D	410	SQD	O5-C1-O6-C44
27	D	410	SQD	C5-C6-S-O7
27	F	101	SQD	O6-C44-C45-O47
27	a	410	SQD	O6-C44-C45-O47
27	b	601	SQD	C8-C7-O47-C45
27	b	601	SQD	O5-C5-C6-S
30	A	416	LMT	C2'-C1'-O1'-C1
30	A	416	LMT	O5'-C1'-O1'-C1
30	B	620	LMT	O5'-C1'-O1'-C1
30	B	626	LMT	C2B-C1B-O1B-C4'
30	C	526	LMT	C2'-C1'-O1'-C1
30	C	526	LMT	O5'-C1'-O1'-C1
30	J	101	LMT	O5'-C1'-O1'-C1
30	J	101	LMT	C2-C1-O1'-C1'
30	T	102	LMT	C2'-C1'-O1'-C1
30	T	102	LMT	O5'-C1'-O1'-C1
30	T	103	LMT	O5'-C1'-O1'-C1
30	a	411	LMT	O5'-C1'-O1'-C1
30	a	419	LMT	C2'-C1'-O1'-C1
30	a	419	LMT	O5'-C1'-O1'-C1
30	a	419	LMT	C2-C1-O1'-C1'
30	f	103	LMT	C2'-C1'-O1'-C1
30	f	103	LMT	O5'-C1'-O1'-C1
30	z	102	LMT	C2'-C1'-O1'-C1
30	z	102	LMT	O5'-C1'-O1'-C1
35	C	503	DGD	O2G-C2G-C3G-O3G
35	C	504	DGD	C2B-C1B-O2G-C2G
35	C	504	DGD	C2D-C1D-O3G-C3G
35	C	504	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
35	C	504	DGD	C2E-C1E-O5D-C6D
35	C	505	DGD	O2G-C2G-C3G-O3G
35	D	411	DGD	C2B-C1B-O2G-C2G
35	c	515	DGD	C2D-C1D-O3G-C3G
35	c	515	DGD	O6D-C1D-O3G-C3G
36	D	406	LHG	C1-C2-C3-O3
36	D	406	LHG	O2-C2-C3-O3
36	D	407	LHG	O1-C1-C2-C3
36	D	407	LHG	C4-O6-P-O4
36	E	101	LHG	C3-O3-P-O4
36	L	101	LHG	O1-C1-C2-C3
36	L	101	LHG	C3-O3-P-O4
36	L	101	LHG	C4-O6-P-O4
36	a	417	LHG	O1-C1-C2-C3
36	a	417	LHG	O7-C5-C6-O8
36	d	409	LHG	C1-C2-C3-O3
36	d	410	LHG	O1-C1-C2-C3
36	d	410	LHG	O2-C2-C3-O3
36	d	410	LHG	C3-O3-P-O4
36	d	410	LHG	C4-O6-P-O4
23	C	508	CLA	O1D-CGD-O2D-CED
23	b	617	CLA	CBD-CGD-O2D-CED
27	D	410	SQD	O10-C23-O48-C46
27	b	601	SQD	O10-C23-O48-C46
27	d	408	SQD	O10-C23-O48-C46
23	A	404	CLA	O1D-CGD-O2D-CED
23	a	402	CLA	O1D-CGD-O2D-CED
23	b	610	CLA	O1D-CGD-O2D-CED
27	D	410	SQD	C24-C23-O48-C46
27	d	408	SQD	C24-C23-O48-C46
23	B	603	CLA	CBD-CGD-O2D-CED
23	B	610	CLA	CBD-CGD-O2D-CED
23	b	604	CLA	CBD-CGD-O2D-CED
23	c	502	CLA	CBD-CGD-O2D-CED
27	A	415	SQD	O10-C23-O48-C46
33	I	103	LMG	O10-C28-O8-C9
35	c	514	DGD	O1A-C1A-O1G-C1G
30	C	526	LMT	O5'-C5'-C6'-O6'
23	b	608	CLA	CBD-CGD-O2D-CED
27	D	410	SQD	O49-C7-O47-C45
27	b	601	SQD	O49-C7-O47-C45
27	d	408	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
35	C	504	DGD	O1B-C1B-O2G-C2G
35	D	411	DGD	O1B-C1B-O2G-C2G
23	B	614	CLA	C3-C5-C6-C7
27	A	415	SQD	C24-C23-O48-C46
27	b	601	SQD	C24-C23-O48-C46
35	c	514	DGD	C2A-C1A-O1G-C1G
30	c	517	LMT	O5'-C5'-C6'-O6'
30	T	102	LMT	C4'-C5'-C6'-O6'
27	D	410	SQD	C8-C7-O47-C45
27	d	408	SQD	C8-C7-O47-C45
23	C	518	CLA	O1A-CGA-O2A-C1
35	C	505	DGD	O1A-C1A-O1G-C1G
33	Y	101	LMG	O6-C5-C6-O5
33	a	408	LMG	O6-C5-C6-O5
33	y	101	LMG	O6-C5-C6-O5
23	B	605	CLA	C4-C3-C5-C6
23	B	609	CLA	CBD-CGD-O2D-CED
23	b	609	CLA	CBD-CGD-O2D-CED
23	B	610	CLA	C2A-CAA-CBA-CGA
23	C	517	CLA	C2A-CAA-CBA-CGA
23	D	405	CLA	O1A-CGA-O2A-C1
23	d	405	CLA	O1A-CGA-O2A-C1
23	b	615	CLA	C3-C5-C6-C7
23	D	405	CLA	CBA-CGA-O2A-C1
23	d	405	CLA	CBA-CGA-O2A-C1
33	I	103	LMG	C29-C28-O8-C9
30	c	517	LMT	O5B-C5B-C6B-O6B
35	D	411	DGD	C4D-C5D-C6D-O5D
26	A	410	PL9	C37-C38-C39-C40
26	a	409	PL9	C37-C38-C39-C40
23	C	506	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	O1D-CGD-O2D-CED
26	a	409	PL9	C37-C38-C39-C41
30	B	626	LMT	O5B-C5B-C6B-O6B
30	T	102	LMT	O5'-C5'-C6'-O6'
30	z	102	LMT	O5'-C5'-C6'-O6'
23	b	611	CLA	CBD-CGD-O2D-CED
36	d	409	LHG	O2-C2-C3-O3
23	C	517	CLA	CBA-CGA-O2A-C1
23	C	518	CLA	CBA-CGA-O2A-C1
35	C	505	DGD	C2A-C1A-O1G-C1G
26	a	409	PL9	C47-C48-C49-C50

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Mol	Chain	Res	Type	Atoms
23	B	616	CLA	CBD-CGD-O2D-CED
23	C	509	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	CBD-CGD-O2D-CED
30	d	403	LMT	O5'-C5'-C6'-O6'
30	c	517	LMT	C3'-C4'-O1B-C1B
30	a	419	LMT	O5'-C5'-C6'-O6'
30	c	517	LMT	C4'-C5'-C6'-O6'
30	A	416	LMT	C3'-C4'-O1B-C1B
30	E	106	LMT	O5B-C5B-C6B-O6B
35	c	516	DGD	O6E-C5E-C6E-O5E
30	B	620	LMT	C4B-C5B-C6B-O6B
33	y	101	LMG	C4-C5-C6-O5
30	T	102	LMT	C7-C8-C9-C10
23	C	517	CLA	O1A-CGA-O2A-C1
26	a	409	PL9	C47-C48-C49-C51
30	f	103	LMT	O5'-C5'-C6'-O6'
33	c	521	LMG	O6-C5-C6-O5
23	C	517	CLA	C4-C3-C5-C6
26	A	410	PL9	C25-C24-C26-C27
33	Y	101	LMG	C4-C5-C6-O5
33	a	408	LMG	C4-C5-C6-O5
23	B	605	CLA	C2-C3-C5-C6
23	C	517	CLA	C2-C3-C5-C6
26	A	410	PL9	C23-C24-C26-C27
26	D	402	PL9	C38-C39-C41-C42
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	607	CLA	C2A-CAA-CBA-CGA
30	C	526	LMT	C4'-C5'-C6'-O6'
30	z	102	LMT	C4'-C5'-C6'-O6'
27	d	408	SQD	O5-C1-O6-C44
30	c	517	LMT	O5'-C1'-O1'-C1
33	Y	101	LMG	O6-C1-O1-C7
26	a	409	PL9	C39-C41-C42-C43
26	d	406	PL9	C39-C41-C42-C43
35	d	407	DGD	C2A-C1A-O1G-C1G
23	c	511	CLA	CBD-CGD-O2D-CED
30	B	620	LMT	O5'-C5'-C6'-O6'
26	d	406	PL9	C47-C48-C49-C51
30	a	419	LMT	C4'-C5'-C6'-O6'
26	A	410	PL9	C27-C28-C29-C30
26	D	402	PL9	C42-C43-C44-C45
36	a	417	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
36	l	102	LHG	C1-C2-C3-O3
26	A	410	PL9	C27-C28-C29-C31
35	d	407	DGD	O1A-C1A-O1G-C1G
23	B	607	CLA	C3-C5-C6-C7
23	C	517	CLA	C3-C5-C6-C7
23	B	610	CLA	O1D-CGD-O2D-CED
23	c	502	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	CBA-CGA-O2A-C1
36	E	101	LHG	C24-C23-O8-C6
33	b	621	LMG	O6-C5-C6-O5
23	B	607	CLA	CBD-CGD-O2D-CED
30	c	517	LMT	C4B-C5B-C6B-O6B
30	f	103	LMT	C4'-C5'-C6'-O6'
36	a	417	LHG	C7-C8-C9-C10
23	C	518	CLA	C10-C11-C12-C13
30	B	620	LMT	C4'-C5'-C6'-O6'
33	c	521	LMG	C4-C5-C6-O5
35	C	505	DGD	O6D-C5D-C6D-O5D
36	l	102	LHG	O2-C2-C3-O3
30	B	620	LMT	C2'-C1'-O1'-C1
35	C	505	DGD	C2E-C1E-O5D-C6D
35	C	504	DGD	O1G-C1G-C2G-O2G
30	B	620	LMT	O5B-C5B-C6B-O6B
30	d	403	LMT	C4'-C5'-C6'-O6'
33	b	621	LMG	C4-C5-C6-O5
23	A	408	CLA	C11-C10-C8-C9
23	C	514	CLA	C6-C7-C8-C9
23	C	517	CLA	C6-C7-C8-C9
23	b	602	CLA	C11-C10-C8-C9
23	b	605	CLA	C11-C10-C8-C9
23	b	611	CLA	C11-C12-C13-C14
23	c	502	CLA	C14-C13-C15-C16
23	B	614	CLA	CBD-CGD-O2D-CED
25	B	631	BCR	C7-C8-C9-C34
25	B	631	BCR	C37-C22-C23-C24
25	C	501	BCR	C7-C8-C9-C34
25	D	403	BCR	C37-C22-C23-C24
25	T	101	BCR	C7-C8-C9-C34
25	T	101	BCR	C37-C22-C23-C24
25	j	101	BCR	C36-C18-C19-C20
25	B	631	BCR	C7-C8-C9-C10
25	D	403	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	T	101	BCR	C7-C8-C9-C10
30	M	102	LMT	O5'-C5'-C6'-O6'
33	I	103	LMG	O6-C5-C6-O5
35	C	503	DGD	C2B-C1B-O2G-C2G
35	H	101	DGD	C7B-C8B-C9B-CAB
30	E	106	LMT	C4B-C5B-C6B-O6B
35	c	516	DGD	C4E-C5E-C6E-O5E
27	A	415	SQD	C7-C8-C9-C10
33	C	525	LMG	C28-C29-C30-C31
23	a	405	CLA	C10-C11-C12-C13
23	B	603	CLA	O1D-CGD-O2D-CED
35	d	407	DGD	C4D-C5D-C6D-O5D
30	C	526	LMT	O5B-C5B-C6B-O6B
23	A	408	CLA	C5-C6-C7-C8
23	C	517	CLA	C5-C6-C7-C8
23	a	402	CLA	C15-C16-C17-C18
32	d	413	PLM	C1-C2-C3-C4
23	b	614	CLA	CBD-CGD-O2D-CED
23	A	408	CLA	C10-C11-C12-C13
23	B	604	CLA	C8-C10-C11-C12
23	B	606	CLA	C13-C15-C16-C17
23	B	606	CLA	C15-C16-C17-C18
23	D	405	CLA	C8-C10-C11-C12
23	a	403	CLA	C8-C10-C11-C12
23	b	603	CLA	C5-C6-C7-C8
23	b	611	CLA	C15-C16-C17-C18
23	b	616	CLA	C10-C11-C12-C13
35	D	411	DGD	C9B-CAB-CBB-CCB
36	D	407	LHG	O1-C1-C2-O2
27	A	415	SQD	C23-C24-C25-C26
27	F	101	SQD	C23-C24-C25-C26
32	C	522	PLM	C1-C2-C3-C4
32	k	102	PLM	C1-C2-C3-C4
33	c	521	LMG	C28-C29-C30-C31
35	C	504	DGD	C1B-C2B-C3B-C4B
35	C	505	DGD	C1B-C2B-C3B-C4B
35	c	515	DGD	C1B-C2B-C3B-C4B
23	b	615	CLA	CBD-CGD-O2D-CED
23	d	405	CLA	CBD-CGD-O2D-CED
23	a	405	CLA	C13-C15-C16-C17
23	b	602	CLA	C8-C10-C11-C12
23	b	614	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	c	502	CLA	C13-C15-C16-C17
23	c	508	CLA	C5-C6-C7-C8
27	F	101	SQD	C24-C23-O48-C46
35	D	411	DGD	O6D-C5D-C6D-O5D
23	B	602	CLA	C13-C15-C16-C17
23	B	614	CLA	C10-C11-C12-C13
23	b	615	CLA	C5-C6-C7-C8
23	b	617	CLA	C8-C10-C11-C12
27	D	410	SQD	C7-C8-C9-C10
32	B	624	PLM	C1-C2-C3-C4
33	y	101	LMG	C28-C29-C30-C31
23	A	408	CLA	C6-C7-C8-C10
23	B	613	CLA	C11-C10-C8-C7
23	C	514	CLA	C6-C7-C8-C10
23	c	513	CLA	C11-C10-C8-C7
36	E	101	LHG	O10-C23-O8-C6
25	B	631	BCR	C9-C10-C11-C12
23	b	602	CLA	C2A-CAA-CBA-CGA
23	b	604	CLA	O1D-CGD-O2D-CED
23	b	608	CLA	O1D-CGD-O2D-CED
33	y	101	LMG	O6-C1-O1-C7
23	b	615	CLA	C10-C11-C12-C13
26	D	402	PL9	C29-C31-C32-C33
26	a	409	PL9	C9-C11-C12-C13
26	a	409	PL9	C14-C16-C17-C18
26	a	409	PL9	C29-C31-C32-C33
36	a	417	LHG	O2-C2-C3-O3
35	C	505	DGD	C4D-C5D-C6D-O5D
23	A	404	CLA	C15-C16-C17-C18
30	C	526	LMT	C4-C5-C6-C7
23	D	405	CLA	CBD-CGD-O2D-CED
23	B	604	CLA	O1A-CGA-O2A-C1
23	B	613	CLA	C8-C10-C11-C12
23	C	511	CLA	C10-C11-C12-C13
23	b	602	CLA	C10-C11-C12-C13
23	b	614	CLA	C15-C16-C17-C18
36	D	407	LHG	C4-O6-P-O3
36	L	101	LHG	C4-O6-P-O3
36	d	410	LHG	C3-O3-P-O6
36	l	102	LHG	C4-O6-P-O3
23	C	511	CLA	CBA-CGA-O2A-C1
33	d	411	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
30	B	626	LMT	C4B-C5B-C6B-O6B
30	M	102	LMT	C4'-C5'-C6'-O6'
23	B	609	CLA	O1D-CGD-O2D-CED
36	d	410	LHG	C1-C2-C3-O3
35	C	503	DGD	O1B-C1B-O2G-C2G
23	b	615	CLA	C4-C3-C5-C6
35	C	503	DGD	C2B-C3B-C4B-C5B
23	c	507	CLA	C2A-CAA-CBA-CGA
23	B	611	CLA	C16-C17-C18-C20
23	B	608	CLA	CBA-CGA-O2A-C1
23	c	502	CLA	CBA-CGA-O2A-C1
33	a	408	LMG	C20-C21-C22-C23
35	D	411	DGD	C1B-C2B-C3B-C4B
32	k	102	PLM	C5-C6-C7-C8
27	F	101	SQD	C8-C7-O47-C45
36	D	406	LHG	C8-C7-O7-C5
35	d	407	DGD	O6D-C5D-C6D-O5D
30	z	102	LMT	C11-C10-C9-C8
32	d	413	PLM	C4-C5-C6-C7
33	C	525	LMG	C15-C16-C17-C18
33	I	103	LMG	C18-C19-C20-C21
33	Y	101	LMG	C17-C18-C19-C20
33	Y	101	LMG	C34-C35-C36-C37
35	C	504	DGD	CCB-CDB-CEB-CFB
36	D	406	LHG	C25-C26-C27-C28
36	L	101	LHG	C31-C32-C33-C34
36	a	417	LHG	C30-C31-C32-C33
23	b	609	CLA	O1D-CGD-O2D-CED
23	C	507	CLA	C16-C17-C18-C20
23	b	617	CLA	C16-C17-C18-C19
27	B	630	SQD	C34-C35-C36-C37
27	D	410	SQD	C14-C15-C16-C17
27	F	101	SQD	C26-C27-C28-C29
27	a	407	SQD	C15-C16-C17-C18
27	a	407	SQD	C26-C27-C28-C29
28	a	412	LFA	C11-C10-C9-C8
32	E	102	PLM	C6-C7-C8-C9
32	k	102	PLM	C2-C3-C4-C5
35	H	101	DGD	C5B-C6B-C7B-C8B
36	D	407	LHG	C11-C10-C9-C8
36	E	101	LHG	C28-C29-C30-C31
27	b	601	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
23	C	506	CLA	O1D-CGD-O2D-CED
27	F	101	SQD	O49-C7-O47-C45
36	D	406	LHG	O9-C7-O7-C5
33	Y	101	LMG	C28-C29-C30-C31
23	c	504	CLA	CBD-CGD-O2D-CED
27	A	415	SQD	C9-C10-C11-C12
27	a	407	SQD	C11-C12-C13-C14
30	d	403	LMT	C2-C3-C4-C5
32	i	102	PLM	C5-C6-C7-C8
35	d	407	DGD	C2A-C3A-C4A-C5A
27	B	630	SQD	C10-C11-C12-C13
27	B	630	SQD	C32-C33-C34-C35
27	d	408	SQD	C25-C26-C27-C28
28	d	414	LFA	C9-C10-C11-C12
30	f	103	LMT	C7-C8-C9-C10
33	y	101	LMG	C20-C21-C22-C23
35	C	505	DGD	C2B-C3B-C4B-C5B
36	a	416	LHG	C30-C31-C32-C33
30	A	416	LMT	C2-C3-C4-C5
35	C	504	DGD	C7A-C8A-C9A-CAA
35	C	505	DGD	C6B-C7B-C8B-C9B
36	E	101	LHG	C34-C35-C36-C37
23	B	601	CLA	C3-C5-C6-C7
27	a	410	SQD	C2-C1-O6-C44
33	I	103	LMG	C2-C1-O1-C7
35	c	514	DGD	C2D-C1D-O3G-C3G
27	A	415	SQD	C14-C15-C16-C17
30	z	102	LMT	C3-C4-C5-C6
32	C	522	PLM	C4-C5-C6-C7
32	E	107	PLM	C6-C7-C8-C9
33	y	101	LMG	C11-C12-C13-C14
35	C	505	DGD	C5B-C6B-C7B-C8B
35	d	407	DGD	C7B-C8B-C9B-CAB
35	h	102	DGD	CBA-CCA-CDA-CEA
36	D	408	LHG	C29-C30-C31-C32
36	L	101	LHG	C29-C30-C31-C32
23	C	517	CLA	C10-C11-C12-C13
23	c	502	CLA	O1A-CGA-O2A-C1
27	F	101	SQD	O10-C23-O48-C46
23	C	511	CLA	C16-C17-C18-C19
23	c	506	CLA	C16-C17-C18-C19
26	A	410	PL9	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
27	B	630	SQD	C9-C10-C11-C12
27	B	630	SQD	C25-C26-C27-C28
30	C	526	LMT	O1'-C1-C2-C3
30	J	101	LMT	C11-C10-C9-C8
30	f	103	LMT	C3-C4-C5-C6
33	b	621	LMG	C14-C15-C16-C17
35	D	411	DGD	C6B-C7B-C8B-C9B
36	D	408	LHG	C16-C17-C18-C19
36	L	101	LHG	C12-C13-C14-C15
36	l	102	LHG	C10-C11-C12-C13
33	C	525	LMG	C4-C5-C6-O5
26	d	406	PL9	C43-C44-C46-C47
23	D	405	CLA	C14-C13-C15-C16
23	b	607	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C10-C8-C9
27	B	630	SQD	C7-C8-C9-C10
27	d	408	SQD	C27-C28-C29-C30
32	B	624	PLM	C7-C8-C9-CA
33	I	103	LMG	C34-C35-C36-C37
33	c	521	LMG	C16-C17-C18-C19
35	C	504	DGD	C3A-C4A-C5A-C6A
36	D	407	LHG	C18-C19-C20-C21
36	E	101	LHG	C11-C10-C9-C8
23	C	512	CLA	C2A-CAA-CBA-CGA
25	f	101	BCR	C37-C22-C23-C24
27	B	630	SQD	C12-C13-C14-C15
27	a	410	SQD	C25-C26-C27-C28
32	b	622	PLM	C2-C3-C4-C5
32	k	102	PLM	C3-C4-C5-C6
36	a	416	LHG	C11-C12-C13-C14
36	d	409	LHG	C25-C26-C27-C28
34	B	621	GOL	C1-C2-C3-O3
36	D	406	LHG	O1-C1-C2-C3
36	D	408	LHG	O1-C1-C2-C3
36	d	409	LHG	O1-C1-C2-C3
25	B	618	BCR	C21-C22-C23-C24
25	C	501	BCR	C7-C8-C9-C10
25	Y	102	BCR	C17-C18-C19-C20
25	b	620	BCR	C21-C22-C23-C24
25	f	101	BCR	C21-C22-C23-C24
25	j	101	BCR	C17-C18-C19-C20
30	J	101	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
33	Y	101	LMG	O9-C10-O7-C8
33	Y	101	LMG	C11-C10-O7-C8
27	B	630	SQD	C15-C16-C17-C18
27	a	407	SQD	C9-C10-C11-C12
33	C	525	LMG	C16-C17-C18-C19
33	D	409	LMG	C15-C16-C17-C18
35	h	102	DGD	CBB-CCB-CDB-CEB
36	l	102	LHG	C29-C30-C31-C32
36	E	101	LHG	C7-C8-C9-C10
36	d	409	LHG	C23-C24-C25-C26
27	B	630	SQD	C16-C17-C18-C19
27	D	410	SQD	C12-C13-C14-C15
27	F	101	SQD	C9-C10-C11-C12
27	F	101	SQD	C34-C35-C36-C37
27	a	407	SQD	C24-C25-C26-C27
27	b	601	SQD	C27-C28-C29-C30
27	b	601	SQD	C28-C29-C30-C31
27	d	408	SQD	C9-C10-C11-C12
28	e	101	LFA	C10-C11-C12-C13
30	a	419	LMT	O1'-C1-C2-C3
33	d	411	LMG	C17-C18-C19-C20
35	C	505	DGD	C9A-CAA-CBA-CCA
35	D	411	DGD	C8B-C9B-CAB-CBB
35	c	514	DGD	CBA-CCA-CDA-CEA
36	E	101	LHG	C13-C14-C15-C16
36	L	101	LHG	C27-C28-C29-C30
36	a	416	LHG	C16-C17-C18-C19
23	B	606	CLA	C16-C17-C18-C19
23	b	617	CLA	C16-C17-C18-C20
35	c	514	DGD	O6D-C1D-O3G-C3G
26	A	410	PL9	C24-C26-C27-C28
26	d	406	PL9	C44-C46-C47-C48
32	E	102	PLM	C7-C8-C9-CA
35	C	505	DGD	C7B-C8B-C9B-CAB
36	E	101	LHG	C24-C25-C26-C27
36	a	417	LHG	C12-C13-C14-C15
23	C	516	CLA	CBD-CGD-O2D-CED
27	a	407	SQD	C27-C28-C29-C30
27	b	601	SQD	C12-C13-C14-C15
27	d	408	SQD	C33-C34-C35-C36
35	C	503	DGD	C5B-C6B-C7B-C8B
35	H	101	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
36	D	407	LHG	C13-C14-C15-C16
36	l	102	LHG	C11-C12-C13-C14
23	B	615	CLA	C13-C15-C16-C17
23	C	511	CLA	O1A-CGA-O2A-C1
27	b	601	SQD	C10-C11-C12-C13
30	C	526	LMT	C6-C7-C8-C9
30	C	526	LMT	C7-C8-C9-C10
33	y	101	LMG	C38-C39-C40-C41
36	a	416	LHG	C12-C13-C14-C15
23	b	611	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	C3A-C2A-CAA-CBA
24	D	401	PHO	C3A-C2A-CAA-CBA
23	A	404	CLA	C13-C15-C16-C17
23	B	604	CLA	C5-C6-C7-C8
23	B	615	CLA	C10-C11-C12-C13
27	A	411	SQD	C11-C12-C13-C14
32	c	522	PLM	C7-C8-C9-CA
35	H	101	DGD	C2B-C3B-C4B-C5B
36	a	416	LHG	C27-C28-C29-C30
35	d	407	DGD	C1A-C2A-C3A-C4A
23	B	606	CLA	C16-C17-C18-C20
23	C	507	CLA	C16-C17-C18-C19
23	C	511	CLA	C16-C17-C18-C20
23	b	605	CLA	C16-C17-C18-C19
23	b	605	CLA	C16-C17-C18-C20
27	d	408	SQD	C11-C10-C9-C8
33	d	411	LMG	C20-C21-C22-C23
35	C	504	DGD	C9A-CAA-CBA-CCA
36	D	407	LHG	C11-C12-C13-C14
33	I	103	LMG	O1-C7-C8-C9
32	D	414	PLM	C6-C7-C8-C9
35	c	514	DGD	C1A-C2A-C3A-C4A
35	c	515	DGD	C9A-CAA-CBA-CCA
23	B	608	CLA	O1A-CGA-O2A-C1
26	a	409	PL9	C45-C44-C46-C47
23	c	506	CLA	CBA-CGA-O2A-C1
26	d	406	PL9	C13-C14-C16-C17
27	D	410	SQD	C10-C11-C12-C13
32	d	413	PLM	C6-C7-C8-C9
36	l	102	LHG	C11-C10-C9-C8
36	a	417	LHG	O1-C1-C2-O2
36	d	410	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
27	A	415	SQD	C31-C32-C33-C34
27	D	410	SQD	C11-C12-C13-C14
27	a	410	SQD	C18-C19-C20-C21
27	b	601	SQD	C11-C10-C9-C8
33	C	525	LMG	C17-C18-C19-C20
33	D	409	LMG	C16-C17-C18-C19
33	c	521	LMG	C32-C33-C34-C35
35	C	504	DGD	CEB-CFB-CGB-CHB
27	b	601	SQD	C16-C17-C18-C19
36	l	102	LHG	C12-C13-C14-C15
23	C	511	CLA	C5-C6-C7-C8
32	h	103	PLM	C2-C3-C4-C5
30	C	526	LMT	C1-C2-C3-C4
23	C	510	CLA	CBA-CGA-O2A-C1
27	b	601	SQD	C29-C30-C31-C32
36	d	409	LHG	C7-C8-C9-C10
27	a	410	SQD	C11-C10-C9-C8
27	a	410	SQD	C14-C15-C16-C17
35	H	101	DGD	C7A-C8A-C9A-CAA
35	h	102	DGD	C9B-CAB-CBB-CCB
27	A	411	SQD	C9-C10-C11-C12
27	A	415	SQD	C27-C28-C29-C30
32	C	522	PLM	C3-C4-C5-C6
28	a	418	LFA	C12-C13-C14-C15
35	c	514	DGD	CCA-CDA-CEA-CFA
35	h	102	DGD	C7A-C8A-C9A-CAA
25	B	618	BCR	C23-C24-C25-C26
25	B	631	BCR	C1-C6-C7-C8
25	C	527	BCR	C5-C6-C7-C8
25	D	403	BCR	C5-C6-C7-C8
25	D	403	BCR	C23-C24-C25-C30
25	T	101	BCR	C1-C6-C7-C8
25	T	101	BCR	C5-C6-C7-C8
25	Y	102	BCR	C1-C6-C7-C8
25	a	406	BCR	C23-C24-C25-C26
25	b	618	BCR	C1-C6-C7-C8
25	f	101	BCR	C5-C6-C7-C8
25	f	101	BCR	C23-C24-C25-C30
25	j	101	BCR	C1-C6-C7-C8
25	t	101	BCR	C1-C6-C7-C8
25	t	101	BCR	C5-C6-C7-C8
23	c	511	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	c	513	CLA	CBA-CGA-O2A-C1
37	E	105	HEM	C3D-CAD-CBD-CGD
33	a	408	LMG	C11-C10-O7-C8
28	a	418	LFA	C11-C10-C9-C8
32	d	413	PLM	C7-C8-C9-CA
32	h	103	PLM	C5-C6-C7-C8
33	d	411	LMG	C18-C19-C20-C21
35	C	503	DGD	C4A-C5A-C6A-C7A
30	E	106	LMT	C5-C6-C7-C8
32	B	628	PLM	C7-C8-C9-CA
27	D	410	SQD	C9-C10-C11-C12
33	y	101	LMG	C36-C37-C38-C39
23	A	408	CLA	C4-C3-C5-C6
23	B	616	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	O1D-CGD-O2D-CED
23	B	615	CLA	C11-C10-C8-C7
23	C	517	CLA	C12-C13-C15-C16
23	D	405	CLA	C12-C13-C15-C16
23	b	607	CLA	C12-C13-C15-C16
23	c	506	CLA	C11-C10-C8-C7
23	c	510	CLA	C6-C7-C8-C10
23	c	511	CLA	C6-C7-C8-C10
24	D	401	PHO	C11-C10-C8-C7
32	K	101	PLM	C7-C8-C9-CA
23	c	506	CLA	C13-C15-C16-C17
23	B	611	CLA	C16-C17-C18-C19
27	B	630	SQD	O49-C7-O47-C45
35	d	407	DGD	O1B-C1B-O2G-C2G
23	b	609	CLA	CBA-CGA-O2A-C1
23	c	505	CLA	CBA-CGA-O2A-C1
33	C	525	LMG	C29-C28-O8-C9
36	a	417	LHG	C24-C23-O8-C6
33	I	103	LMG	C12-C13-C14-C15
35	D	411	DGD	C4A-C5A-C6A-C7A
33	y	101	LMG	C12-C13-C14-C15
35	c	514	DGD	C9A-CAA-CBA-CCA
27	A	415	SQD	C15-C16-C17-C18
27	B	630	SQD	C28-C29-C30-C31
35	c	514	DGD	C4B-C5B-C6B-C7B
35	c	515	DGD	C7A-C8A-C9A-CAA
23	c	506	CLA	O1D-CGD-O2D-CED
35	c	515	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
27	D	410	SQD	C13-C14-C15-C16
33	a	408	LMG	C21-C22-C23-C24
23	B	604	CLA	C16-C17-C18-C20
23	c	506	CLA	C16-C17-C18-C20
33	I	103	LMG	C4-C5-C6-O5
27	a	410	SQD	O5-C1-O6-C44
33	I	103	LMG	O6-C1-O1-C7
27	b	601	SQD	C9-C10-C11-C12
35	c	516	DGD	C2A-C3A-C4A-C5A
35	c	516	DGD	CCA-CDA-CEA-CFA
36	D	407	LHG	C34-C35-C36-C37
27	B	630	SQD	C8-C7-O47-C45
35	d	407	DGD	C2B-C1B-O2G-C2G
36	E	101	LHG	C8-C7-O7-C5
28	e	101	LFA	C6-C7-C8-C9
36	E	101	LHG	O9-C7-O7-C5
36	D	406	LHG	C24-C25-C26-C27
33	y	101	LMG	O7-C8-C9-O8
35	C	504	DGD	O6E-C5E-C6E-O5E
33	y	101	LMG	C37-C38-C39-C40
32	E	102	PLM	C9-CA-CB-CC
23	C	511	CLA	C13-C15-C16-C17
33	B	619	LMG	C28-C29-C30-C31
23	b	615	CLA	C2-C3-C5-C6
26	D	402	PL9	C4-C3-C7-C8
23	A	406	CLA	C6-C7-C8-C9
23	B	614	CLA	C11-C12-C13-C14
23	B	615	CLA	C11-C10-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	C	517	CLA	C14-C13-C15-C16
23	b	605	CLA	C11-C12-C13-C14
23	c	510	CLA	C6-C7-C8-C9
23	c	513	CLA	C11-C10-C8-C9
24	D	401	PHO	C11-C10-C8-C9
33	D	409	LMG	O6-C5-C6-O5
27	B	630	SQD	C27-C28-C29-C30
27	F	101	SQD	C32-C33-C34-C35
35	C	505	DGD	C5A-C6A-C7A-C8A
35	c	515	DGD	C6B-C7B-C8B-C9B
35	h	102	DGD	C5B-C6B-C7B-C8B
23	C	506	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	T	102	LMT	C1-C2-C3-C4
28	h	101	LFA	C5-C6-C7-C8
33	c	521	LMG	C17-C18-C19-C20
36	L	101	LHG	C13-C14-C15-C16
30	B	626	LMT	O5'-C5'-C6'-O6'
32	D	414	PLM	C5-C6-C7-C8
35	C	503	DGD	C6A-C7A-C8A-C9A
23	C	510	CLA	O1A-CGA-O2A-C1
23	c	506	CLA	O1A-CGA-O2A-C1
23	c	511	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	O1A-CGA-O2A-C1
23	c	511	CLA	O1D-CGD-O2D-CED
23	A	405	CLA	C1A-C2A-CAA-CBA
23	A	406	CLA	C1A-C2A-CAA-CBA
23	A	408	CLA	C1A-C2A-CAA-CBA
23	C	506	CLA	C1A-C2A-CAA-CBA
23	a	403	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C1A-C2A-CAA-CBA
23	d	401	CLA	C1A-C2A-CAA-CBA
23	B	604	CLA	C16-C17-C18-C19
33	a	408	LMG	O9-C10-O7-C8
27	a	407	SQD	C10-C11-C12-C13
36	L	101	LHG	C3-O3-P-O6
36	d	410	LHG	C4-O6-P-O3
27	D	410	SQD	C23-C24-C25-C26
32	E	102	PLM	C5-C6-C7-C8
35	C	505	DGD	CAB-CBB-CCB-CDB
35	d	407	DGD	C5B-C6B-C7B-C8B
36	l	102	LHG	O6-C4-C5-C6
23	B	607	CLA	O1D-CGD-O2D-CED
36	D	407	LHG	C9-C10-C11-C12
35	c	514	DGD	O6E-C5E-C6E-O5E
23	b	612	CLA	C8-C10-C11-C12
32	K	101	PLM	C5-C6-C7-C8
30	D	417	LMT	C3-C4-C5-C6
33	y	101	LMG	C34-C35-C36-C37
35	C	504	DGD	C2B-C3B-C4B-C5B
30	J	101	LMT	O5'-C5'-C6'-O6'
30	A	416	LMT	O1'-C1-C2-C3
32	A	418	PLM	C5-C6-C7-C8
33	C	525	LMG	C18-C19-C20-C21
23	b	603	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
35	H	101	DGD	CBA-CCA-CDA-CEA
23	c	505	CLA	O1A-CGA-O2A-C1
27	F	101	SQD	C25-C26-C27-C28
30	M	101	LMT	C11-C10-C9-C8
36	a	417	LHG	C10-C11-C12-C13
23	C	512	CLA	C16-C17-C18-C19
23	c	513	CLA	C16-C17-C18-C19
33	d	411	LMG	O6-C5-C6-O5
27	B	630	SQD	O6-C44-C45-C46
27	F	101	SQD	O6-C44-C45-C46
27	a	407	SQD	C32-C33-C34-C35
27	a	410	SQD	O6-C44-C45-C46
27	b	601	SQD	C19-C20-C21-C22
33	a	408	LMG	C7-C8-C9-O8
33	a	408	LMG	C12-C13-C14-C15
33	d	411	LMG	C38-C39-C40-C41
33	y	101	LMG	C7-C8-C9-O8
35	C	505	DGD	O1G-C1G-C2G-C3G
35	D	411	DGD	O1G-C1G-C2G-C3G
35	c	514	DGD	C1G-C2G-C3G-O3G
36	a	417	LHG	C4-C5-C6-O8
35	C	504	DGD	C4A-C5A-C6A-C7A
35	h	102	DGD	CCA-CDA-CEA-CFA
27	A	411	SQD	C45-C44-O6-C1
33	c	521	LMG	C8-C7-O1-C1
35	C	504	DGD	C5D-C6D-O5D-C1E
35	c	515	DGD	C2G-C3G-O3G-C1D
27	d	408	SQD	C10-C11-C12-C13
32	E	107	PLM	CA-CB-CC-CD
33	a	408	LMG	C40-C41-C42-C43
23	d	405	CLA	C10-C11-C12-C13
30	T	102	LMT	C3-C4-C5-C6
35	c	515	DGD	O6D-C5D-C6D-O5D
36	D	406	LHG	C23-C24-C25-C26
35	c	514	DGD	C4A-C5A-C6A-C7A
23	c	501	CLA	C16-C17-C18-C19
30	z	102	LMT	C6-C7-C8-C9
35	C	503	DGD	CAA-CBA-CCA-CDA
36	D	406	LHG	O1-C1-C2-O2
36	D	408	LHG	O1-C1-C2-O2
36	d	409	LHG	O1-C1-C2-O2
30	A	416	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
36	a	417	LHG	O10-C23-O8-C6
32	b	623	PLM	C7-C8-C9-CA
35	c	515	DGD	CDB-CEB-CFB-CGB
23	b	614	CLA	O1D-CGD-O2D-CED
26	d	406	PL9	C45-C44-C46-C47
27	B	630	SQD	C33-C34-C35-C36
33	b	621	LMG	C37-C38-C39-C40
27	d	408	SQD	C23-C24-C25-C26
23	a	405	CLA	CBA-CGA-O2A-C1
35	D	411	DGD	C2A-C1A-O1G-C1G
35	C	503	DGD	O6E-C5E-C6E-O5E
30	A	416	LMT	C3-C4-C5-C6
32	h	103	PLM	C6-C7-C8-C9
23	c	504	CLA	C13-C15-C16-C17
30	c	517	LMT	C5'-C4'-O1B-C1B
32	l	101	PLM	C9-CA-CB-CC
35	C	503	DGD	C6B-C7B-C8B-C9B
36	a	417	LHG	C19-C20-C21-C22
27	D	410	SQD	C46-C45-O47-C7
23	C	508	CLA	C8-C10-C11-C12
28	B	625	LFA	C10-C11-C12-C13
36	D	406	LHG	C12-C13-C14-C15
24	D	401	PHO	C10-C11-C12-C13
33	C	525	LMG	O10-C28-O8-C9
23	C	512	CLA	C16-C17-C18-C20
23	c	513	CLA	C16-C17-C18-C20
30	f	103	LMT	C2-C3-C4-C5
35	C	503	DGD	C9A-CAA-CBA-CCA
23	B	613	CLA	C15-C16-C17-C18
23	c	506	CLA	C10-C11-C12-C13
23	B	614	CLA	O1D-CGD-O2D-CED
23	b	609	CLA	O1A-CGA-O2A-C1
32	D	415	PLM	C1-C2-C3-C4
30	a	411	LMT	C2'-C1'-O1'-C1
33	D	409	LMG	C35-C36-C37-C38
23	b	615	CLA	O1D-CGD-O2D-CED
36	a	416	LHG	C32-C33-C34-C35
35	C	503	DGD	O6D-C5D-C6D-O5D
32	l	101	PLM	C5-C6-C7-C8
33	I	103	LMG	C13-C14-C15-C16
27	a	410	SQD	C10-C11-C12-C13
28	C	523	LFA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
32	E	102	PLM	C3-C4-C5-C6
23	A	406	CLA	C6-C7-C8-C10
23	A	406	CLA	C12-C13-C15-C16
23	A	408	CLA	C11-C10-C8-C7
23	B	603	CLA	C6-C7-C8-C10
23	B	614	CLA	C11-C12-C13-C15
23	C	509	CLA	C6-C7-C8-C10
23	C	510	CLA	C11-C12-C13-C15
23	C	512	CLA	C11-C10-C8-C7
23	C	513	CLA	C11-C10-C8-C7
23	b	602	CLA	C6-C7-C8-C10
23	b	602	CLA	C11-C10-C8-C7
23	b	605	CLA	C11-C12-C13-C15
23	b	616	CLA	C12-C13-C15-C16
23	b	617	CLA	C11-C12-C13-C15
23	b	617	CLA	C12-C13-C15-C16
23	c	505	CLA	C11-C12-C13-C15
23	c	508	CLA	C11-C10-C8-C7
23	c	512	CLA	C12-C13-C15-C16
23	d	405	CLA	C11-C10-C8-C7
23	A	404	CLA	C3-C5-C6-C7
23	B	603	CLA	C6-C7-C8-C9
23	B	604	CLA	C11-C10-C8-C9
23	B	613	CLA	C11-C10-C8-C9
23	C	510	CLA	C11-C12-C13-C14
23	C	515	CLA	C6-C7-C8-C9
23	b	615	CLA	C11-C12-C13-C14
23	b	617	CLA	C11-C12-C13-C14
23	c	505	CLA	C11-C12-C13-C14
23	c	508	CLA	C11-C10-C8-C9
23	c	511	CLA	C6-C7-C8-C9
23	c	512	CLA	C14-C13-C15-C16
23	d	405	CLA	C11-C10-C8-C9
23	B	612	CLA	CBA-CGA-O2A-C1
23	C	516	CLA	CBA-CGA-O2A-C1
27	A	411	SQD	C24-C23-O48-C46
23	C	517	CLA	C13-C15-C16-C17
23	d	405	CLA	O1D-CGD-O2D-CED
23	b	608	CLA	C2A-CAA-CBA-CGA
28	i	104	LFA	C11-C12-C13-C14
30	c	517	LMT	C1-C2-C3-C4
36	D	408	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	a	408	LMG	C17-C18-C19-C20
23	B	614	CLA	C5-C6-C7-C8
23	C	512	CLA	C5-C6-C7-C8
23	C	517	CLA	C15-C16-C17-C18
23	b	613	CLA	C10-C11-C12-C13
23	c	503	CLA	C8-C10-C11-C12
27	A	411	SQD	C19-C20-C21-C22
32	D	414	PLM	C7-C8-C9-CA
36	d	409	LHG	C24-C25-C26-C27
23	C	513	CLA	C5-C6-C7-C8
35	C	505	DGD	CBB-CCB-CDB-CEB
28	h	101	LFA	C6-C7-C8-C9
26	A	410	PL9	C39-C41-C42-C43
33	d	411	LMG	C19-C20-C21-C22
23	a	405	CLA	C8-C10-C11-C12
23	c	504	CLA	O1D-CGD-O2D-CED
27	A	411	SQD	C33-C34-C35-C36
23	b	606	CLA	C4-C3-C5-C6
35	c	514	DGD	C6B-C7B-C8B-C9B
23	D	405	CLA	O1D-CGD-O2D-CED
28	a	412	LFA	C9-C10-C11-C12
33	c	521	LMG	C37-C38-C39-C40
35	C	504	DGD	C8A-C9A-CAA-CBA
36	E	101	LHG	C30-C31-C32-C33
23	c	507	CLA	C5-C6-C7-C8
23	b	606	CLA	CBA-CGA-O2A-C1
33	B	619	LMG	C29-C28-O8-C9
35	c	516	DGD	C2A-C1A-O1G-C1G
30	A	416	LMT	C9-C10-C11-C12
33	d	411	LMG	C12-C13-C14-C15
23	B	614	CLA	C3A-C2A-CAA-CBA
28	e	101	LFA	C1-C2-C3-C4
33	B	619	LMG	C34-C35-C36-C37
30	E	106	LMT	C2-C1-O1'-C1'
30	M	102	LMT	C2-C1-O1'-C1'
30	T	103	LMT	C2-C1-O1'-C1'
30	c	517	LMT	C2-C1-O1'-C1'
27	A	415	SQD	C26-C27-C28-C29
27	b	601	SQD	C32-C33-C34-C35
35	c	514	DGD	C7B-C8B-C9B-CAB
27	D	410	SQD	O6-C44-C45-C46
35	C	503	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
35	C	504	DGD	O1G-C1G-C2G-C3G
35	C	505	DGD	C1G-C2G-C3G-O3G
35	c	514	DGD	O1G-C1G-C2G-C3G
35	c	516	DGD	O1G-C1G-C2G-C3G
33	I	103	LMG	C10-C11-C12-C13
23	a	405	CLA	O1A-CGA-O2A-C1
36	L	101	LHG	C32-C33-C34-C35
33	y	101	LMG	C29-C30-C31-C32
33	D	409	LMG	C17-C18-C19-C20
23	d	405	CLA	C4-C3-C5-C6
23	A	408	CLA	C2-C3-C5-C6
36	E	101	LHG	C25-C26-C27-C28
32	E	102	PLM	CA-CB-CC-CD
23	b	616	CLA	C13-C15-C16-C17
35	D	411	DGD	O1A-C1A-O1G-C1G
30	C	526	LMT	C4B-C5B-C6B-O6B
27	A	411	SQD	C25-C26-C27-C28
35	D	411	DGD	C7A-C8A-C9A-CAA
32	C	524	PLM	C6-C7-C8-C9
33	I	103	LMG	C17-C18-C19-C20
23	C	516	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	O1A-CGA-O2A-C1
27	b	601	SQD	C7-C8-C9-C10
30	B	620	LMT	C5-C6-C7-C8
27	A	411	SQD	O10-C23-O48-C46
26	A	410	PL9	C47-C48-C49-C51
32	c	518	PLM	C4-C5-C6-C7
32	D	414	PLM	C1-C2-C3-C4
33	I	103	LMG	O1-C7-C8-O7
33	a	408	LMG	O1-C7-C8-O7
35	D	411	DGD	O2G-C2G-C3G-O3G
35	c	514	DGD	O2G-C2G-C3G-O3G
35	d	407	DGD	O2G-C2G-C3G-O3G
24	a	404	PHO	C8-C10-C11-C12
27	A	411	SQD	C32-C33-C34-C35
23	c	501	CLA	C16-C17-C18-C20
36	d	410	LHG	C11-C10-C9-C8
35	D	411	DGD	O6D-C1D-O3G-C3G
27	A	411	SQD	C12-C13-C14-C15
35	h	102	DGD	CDB-CEB-CFB-CGB
23	C	515	CLA	C4-C3-C5-C6
23	D	404	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
23	C	516	CLA	O1A-CGA-O2A-C1
23	A	406	CLA	C11-C10-C8-C9
23	C	507	CLA	C6-C7-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	b	602	CLA	C6-C7-C8-C9
23	c	506	CLA	C11-C12-C13-C14
23	c	509	CLA	C6-C7-C8-C9
23	c	513	CLA	C14-C13-C15-C16
23	d	405	CLA	C14-C13-C15-C16
27	A	415	SQD	C30-C31-C32-C33
33	B	619	LMG	C19-C20-C21-C22
33	c	521	LMG	C15-C16-C17-C18
23	a	405	CLA	C15-C16-C17-C18
24	D	401	PHO	C1A-C2A-CAA-CBA
36	D	408	LHG	C2-C3-O3-P
30	M	102	LMT	C5-C6-C7-C8
36	L	101	LHG	C11-C10-C9-C8
36	L	101	LHG	C10-C11-C12-C13
25	A	409	BCR	C23-C24-C25-C26
25	C	502	BCR	C23-C24-C25-C26
25	C	527	BCR	C23-C24-C25-C26
25	D	403	BCR	C1-C6-C7-C8
25	f	101	BCR	C1-C6-C7-C8
25	i	103	BCR	C5-C6-C7-C8
25	j	101	BCR	C23-C24-C25-C26
25	k	101	BCR	C23-C24-C25-C26
25	t	101	BCR	C23-C24-C25-C26
38	H	102	RRX	C23-C24-C25-C30
38	H	102	RRX	C23-C24-C25-C26
38	x	102	RRX	C23-C24-C25-C30
38	x	102	RRX	C23-C24-C25-C26
23	B	612	CLA	C10-C11-C12-C13
23	C	506	CLA	C13-C15-C16-C17
32	c	519	PLM	C8-C9-CA-CB
26	A	410	PL9	C47-C48-C49-C50
32	E	107	PLM	C2-C3-C4-C5
33	c	521	LMG	C13-C14-C15-C16
25	B	631	BCR	C21-C22-C23-C24
25	T	101	BCR	C21-C22-C23-C24
35	C	503	DGD	C4D-C5D-C6D-O5D
23	b	617	CLA	C10-C11-C12-C13
30	d	403	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
32	b	623	PLM	CB-CC-CD-CE
27	A	411	SQD	O49-C7-O47-C45
27	a	407	SQD	O49-C7-O47-C45
27	A	411	SQD	C8-C7-O47-C45
27	a	407	SQD	C8-C7-O47-C45
28	m	101	LFA	C11-C12-C13-C14
33	a	408	LMG	C18-C19-C20-C21
35	h	102	DGD	CAB-CBB-CCB-CDB
36	l	102	LHG	C27-C28-C29-C30
36	a	417	LHG	C18-C19-C20-C21
33	b	621	LMG	C12-C13-C14-C15
35	D	411	DGD	C2A-C3A-C4A-C5A
30	M	101	LMT	C9-C10-C11-C12
23	B	604	CLA	C10-C11-C12-C13
23	b	617	CLA	C15-C16-C17-C18
35	h	102	DGD	O2G-C1B-C2B-C3B
27	A	411	SQD	C11-C10-C9-C8
28	e	101	LFA	C9-C10-C11-C12
32	b	628	PLM	C5-C6-C7-C8
23	A	406	CLA	C11-C10-C8-C7
23	B	601	CLA	C6-C7-C8-C10
23	C	511	CLA	C6-C7-C8-C10
23	C	511	CLA	C11-C12-C13-C15
23	C	515	CLA	C6-C7-C8-C10
23	D	404	CLA	C11-C12-C13-C15
23	a	403	CLA	C12-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C10
23	b	604	CLA	C11-C10-C8-C7
23	b	615	CLA	C11-C12-C13-C15
23	b	615	CLA	C12-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C15
23	c	513	CLA	C12-C13-C15-C16
23	d	405	CLA	C12-C13-C15-C16
27	A	415	SQD	C32-C33-C34-C35
32	D	414	PLM	C8-C9-CA-CB
25	B	631	BCR	C15-C16-C17-C18
25	C	501	BCR	C9-C10-C11-C12
25	T	101	BCR	C15-C16-C17-C18
25	Y	102	BCR	C19-C20-C21-C22
25	j	101	BCR	C19-C20-C21-C22
23	C	517	CLA	CBD-CGD-O2D-CED
23	B	601	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
27	d	408	SQD	C26-C27-C28-C29
32	b	628	PLM	C4-C5-C6-C7
33	a	408	LMG	C34-C35-C36-C37
36	d	409	LHG	C13-C14-C15-C16
35	C	503	DGD	C1A-C2A-C3A-C4A
35	C	504	DGD	CFB-CGB-CHB-CIB
23	B	607	CLA	C2A-CAA-CBA-CGA
27	A	415	SQD	C29-C30-C31-C32
35	d	407	DGD	C6B-C7B-C8B-C9B
36	d	410	LHG	C11-C12-C13-C14
23	A	405	CLA	C15-C16-C17-C18
23	b	611	CLA	C13-C15-C16-C17
33	d	411	LMG	C34-C35-C36-C37
36	a	417	LHG	C23-C24-C25-C26
33	c	521	LMG	C35-C36-C37-C38
35	C	505	DGD	C3B-C4B-C5B-C6B
27	D	410	SQD	C25-C26-C27-C28
27	a	407	SQD	C16-C17-C18-C19
33	C	525	LMG	C30-C31-C32-C33
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	514	CLA	CAD-CBD-CGD-O2D
23	C	515	CLA	CAD-CBD-CGD-O2D
23	C	518	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
24	A	407	PHO	CAD-CBD-CGD-O2D
27	A	415	SQD	C12-C13-C14-C15
23	B	601	CLA	C8-C10-C11-C12
24	D	401	PHO	C8-C10-C11-C12
30	a	419	LMT	C6-C7-C8-C9
35	c	516	DGD	C8A-C9A-CAA-CBA
35	C	504	DGD	O6E-C1E-O5D-C6D
27	D	410	SQD	C15-C16-C17-C18
27	A	415	SQD	O6-C44-C45-C46
33	a	408	LMG	O1-C7-C8-C9
30	D	417	LMT	C4'-C5'-C6'-O6'
36	l	102	LHG	O6-C4-C5-O7
23	B	601	CLA	C2A-CAA-CBA-CGA
23	a	402	CLA	C2A-CAA-CBA-CGA
24	a	404	PHO	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
28	m	101	LFA	C10-C11-C12-C13
35	C	505	DGD	C7A-C8A-C9A-CAA
23	C	507	CLA	CBD-CGD-O2D-CED
23	A	406	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	609	CLA	CHA-CBD-CGD-O1D
23	B	609	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	a	403	CLA	CHA-CBD-CGD-O1D
23	b	603	CLA	CHA-CBD-CGD-O2D
23	b	607	CLA	CHA-CBD-CGD-O1D
23	b	607	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CHA-CBD-CGD-O1D
23	c	506	CLA	CHA-CBD-CGD-O2D
23	B	604	CLA	C3-C5-C6-C7
23	b	606	CLA	O1A-CGA-O2A-C1
33	b	621	LMG	C16-C17-C18-C19
35	D	411	DGD	C2D-C1D-O3G-C3G
32	l	101	PLM	C2-C3-C4-C5
33	a	408	LMG	C14-C15-C16-C17
27	A	411	SQD	O47-C45-C46-O48
27	D	410	SQD	O6-C44-C45-O47
33	a	408	LMG	O7-C8-C9-O8
35	D	411	DGD	O1G-C1G-C2G-O2G
35	c	514	DGD	O1G-C1G-C2G-O2G
23	b	613	CLA	CBA-CGA-O2A-C1
33	C	525	LMG	C12-C13-C14-C15
33	B	619	LMG	O10-C28-O8-C9
35	c	516	DGD	O1A-C1A-O1G-C1G
28	B	622	LFA	C11-C12-C13-C14
33	B	619	LMG	C31-C32-C33-C34
27	F	101	SQD	C33-C34-C35-C36
35	C	505	DGD	C8A-C9A-CAA-CBA
36	D	408	LHG	C15-C16-C17-C18
26	D	402	PL9	C27-C28-C29-C30
35	d	407	DGD	C5A-C6A-C7A-C8A
35	C	503	DGD	C1B-C2B-C3B-C4B
23	B	601	CLA	C6-C7-C8-C9
23	b	604	CLA	C11-C10-C8-C9
23	c	512	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
35	D	411	DGD	CCB-CDB-CEB-CFB
23	b	605	CLA	C13-C15-C16-C17
30	a	419	LMT	C2-C3-C4-C5
32	B	624	PLM	C6-C7-C8-C9
33	a	408	LMG	C19-C20-C21-C22
25	D	403	BCR	C7-C8-C9-C34
25	j	101	BCR	C7-C8-C9-C34
25	t	101	BCR	C36-C18-C19-C20
32	c	518	PLM	C1-C2-C3-C4
35	C	505	DGD	C9B-CAB-CBB-CCB
36	E	101	LHG	C26-C27-C28-C29
23	C	518	CLA	C15-C16-C17-C18
23	b	603	CLA	C15-C16-C17-C18
35	D	411	DGD	C5A-C6A-C7A-C8A
36	E	101	LHG	C9-C10-C11-C12
23	a	405	CLA	C1A-C2A-CAA-CBA
23	c	503	CLA	C1A-C2A-CAA-CBA
23	b	609	CLA	C13-C15-C16-C17
32	D	414	PLM	CD-CE-CF-CG
32	c	522	PLM	C6-C7-C8-C9
35	c	515	DGD	C8A-C9A-CAA-CBA
23	d	404	CLA	C2-C1-O2A-CGA
25	A	409	BCR	C19-C20-C21-C22
35	C	505	DGD	O6E-C5E-C6E-O5E
27	d	408	SQD	C29-C30-C31-C32
36	a	416	LHG	C2-C3-O3-P
26	A	410	PL9	C12-C11-C9-C8
30	z	102	LMT	C7-C8-C9-C10
32	D	414	PLM	C9-CA-CB-CC
33	B	619	LMG	C20-C21-C22-C23
36	d	409	LHG	C17-C18-C19-C20
23	b	613	CLA	O1A-CGA-O2A-C1
36	D	407	LHG	C4-O6-P-O5
36	L	101	LHG	C4-O6-P-O5
36	d	410	LHG	C4-O6-P-O5
36	l	102	LHG	C4-O6-P-O5
30	f	103	LMT	C11-C10-C9-C8
23	b	617	CLA	CBA-CGA-O2A-C1
36	a	417	LHG	O6-C4-C5-C6
30	T	102	LMT	C5-C6-C7-C8
36	a	417	LHG	C25-C26-C27-C28
33	a	408	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
36	a	416	LHG	C17-C18-C19-C20
32	i	102	PLM	C2-C3-C4-C5
36	a	416	LHG	C25-C26-C27-C28
23	c	507	CLA	C16-C17-C18-C19
33	I	103	LMG	C21-C22-C23-C24
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	C	508	CLA	CAD-CBD-CGD-O1D
23	b	602	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
27	A	415	SQD	C5-C6-S-O7
27	B	630	SQD	O5-C5-C6-S
27	d	408	SQD	C5-C6-S-O9
33	b	621	LMG	C28-C29-C30-C31
32	b	623	PLM	C8-C9-CA-CB
33	d	411	LMG	C15-C16-C17-C18
23	A	406	CLA	C10-C11-C12-C13
33	y	101	LMG	C16-C17-C18-C19
27	A	415	SQD	O47-C7-C8-C9
36	d	410	LHG	C26-C27-C28-C29
24	A	407	PHO	C4-C3-C5-C6
23	B	603	CLA	C11-C10-C8-C7
23	B	608	CLA	C6-C7-C8-C10
23	B	615	CLA	C12-C13-C15-C16
23	C	515	CLA	C2-C3-C5-C6
23	a	405	CLA	C11-C10-C8-C7
23	b	603	CLA	C11-C10-C8-C7
23	b	613	CLA	C11-C10-C8-C7
23	c	504	CLA	C12-C13-C15-C16
23	c	512	CLA	C11-C10-C8-C7
26	A	410	PL9	C43-C44-C46-C47
32	B	628	PLM	C6-C7-C8-C9
36	a	417	LHG	C31-C32-C33-C34
23	C	517	CLA	O1D-CGD-O2D-CED
26	D	402	PL9	C47-C48-C49-C50
27	A	415	SQD	C13-C14-C15-C16
30	a	411	LMT	C7-C8-C9-C10
35	c	514	DGD	CDA-CEA-CFA-CGA
32	x	101	PLM	C1-C2-C3-C4
33	I	103	LMG	C29-C30-C31-C32
23	B	601	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
32	E	103	PLM	C5-C6-C7-C8
27	A	411	SQD	C44-C45-C46-O48
33	a	408	LMG	C32-C33-C34-C35
33	y	101	LMG	O1-C7-C8-C9
33	I	103	LMG	O7-C8-C9-O8
33	Y	101	LMG	O1-C7-C8-O7
33	y	101	LMG	O1-C7-C8-O7
35	C	505	DGD	O1G-C1G-C2G-O2G
35	c	516	DGD	O1G-C1G-C2G-O2G
32	C	519	PLM	C5-C6-C7-C8
32	i	101	PLM	C9-CA-CB-CC
32	l	101	PLM	C6-C7-C8-C9
32	c	519	PLM	C6-C7-C8-C9
33	C	525	LMG	C8-C7-O1-C1
35	C	505	DGD	C5D-C6D-O5D-C1E
27	A	415	SQD	C17-C18-C19-C20
23	B	609	CLA	CBA-CGA-O2A-C1
27	a	407	SQD	C29-C30-C31-C32
23	b	606	CLA	C13-C15-C16-C17
23	A	408	CLA	C6-C7-C8-C9
23	C	509	CLA	C6-C7-C8-C9
23	D	404	CLA	C11-C12-C13-C14
23	a	405	CLA	C11-C10-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	b	616	CLA	C14-C13-C15-C16
33	D	409	LMG	C14-C15-C16-C17
33	d	411	LMG	C31-C32-C33-C34
27	a	407	SQD	C30-C31-C32-C33
28	I	101	LFA	C14-C15-C16-C17
35	C	503	DGD	O6D-C1D-O3G-C3G
35	C	504	DGD	C4D-C5D-C6D-O5D
23	b	617	CLA	O1A-CGA-O2A-C1
36	L	101	LHG	O1-C1-C2-O2
30	B	620	LMT	O1'-C1-C2-C3
32	E	103	PLM	C2-C3-C4-C5
35	h	102	DGD	C1A-C2A-C3A-C4A
35	c	514	DGD	C3A-C4A-C5A-C6A
25	D	403	BCR	C7-C8-C9-C10
27	D	410	SQD	C26-C27-C28-C29
32	c	522	PLM	C4-C5-C6-C7
28	m	101	LFA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	a	411	LMT	C9-C10-C11-C12
35	c	516	DGD	C9B-CAB-CBB-CCB
23	b	606	CLA	C2-C3-C5-C6
30	a	419	LMT	C7-C8-C9-C10
23	b	608	CLA	C3-C5-C6-C7
23	B	614	CLA	CAA-CBA-CGA-O2A
36	D	407	LHG	C35-C36-C37-C38
33	Y	101	LMG	C7-C8-O7-C10
23	A	404	CLA	C2-C1-O2A-CGA
23	c	504	CLA	C2-C1-O2A-CGA
24	D	401	PHO	C2-C1-O2A-CGA
24	a	404	PHO	C2-C1-O2A-CGA
27	d	408	SQD	C30-C31-C32-C33
30	A	416	LMT	C4-C5-C6-C7
27	A	415	SQD	C11-C10-C9-C8
30	J	101	LMT	O1'-C1-C2-C3
33	a	408	LMG	O8-C28-C29-C30
23	b	605	CLA	C3-C5-C6-C7
30	D	417	LMT	C6-C7-C8-C9
32	D	415	PLM	C4-C5-C6-C7
25	j	101	BCR	C9-C10-C11-C12
23	B	609	CLA	O1A-CGA-O2A-C1
23	c	508	CLA	C16-C17-C18-C19
23	c	507	CLA	C4-C3-C5-C6
26	D	402	PL9	C25-C24-C26-C27
28	d	414	LFA	C10-C11-C12-C13
25	C	527	BCR	C1-C6-C7-C8
25	k	101	BCR	C1-C6-C7-C8
23	b	602	CLA	O1A-CGA-O2A-C1
30	B	620	LMT	C4-C5-C6-C7
23	B	612	CLA	C8-C10-C11-C12
33	B	619	LMG	C35-C36-C37-C38
33	c	521	LMG	C34-C35-C36-C37
35	c	516	DGD	C3B-C4B-C5B-C6B
23	c	507	CLA	C16-C17-C18-C20
35	C	503	DGD	O6E-C1E-O5D-C6D
27	B	630	SQD	O6-C44-C45-O47
35	d	407	DGD	C4B-C5B-C6B-C7B
36	d	410	LHG	C14-C15-C16-C17
36	D	407	LHG	C3-O3-P-O6
36	E	101	LHG	C4-O6-P-O3
36	a	417	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
23	b	602	CLA	C13-C15-C16-C17
30	J	101	LMT	C5-C6-C7-C8
30	a	419	LMT	C4-C5-C6-C7
27	D	410	SQD	C11-C10-C9-C8
28	a	418	LFA	C13-C14-C15-C16
30	J	101	LMT	C3-C4-C5-C6
27	d	408	SQD	O6-C44-C45-C46
33	I	103	LMG	C7-C8-C9-O8
33	Y	101	LMG	O1-C7-C8-C9
27	A	411	SQD	C30-C31-C32-C33
30	D	417	LMT	O5'-C5'-C6'-O6'
23	C	517	CLA	C6-C7-C8-C10
23	b	603	CLA	C11-C12-C13-C15
23	A	406	CLA	C14-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C14
23	C	512	CLA	C11-C10-C8-C9
23	a	403	CLA	C14-C13-C15-C16
23	b	617	CLA	C14-C13-C15-C16
23	B	613	CLA	C13-C15-C16-C17
25	C	527	BCR	C15-C16-C17-C18
25	i	103	BCR	C19-C20-C21-C22
30	a	411	LMT	C3'-C4'-O1B-C1B
23	c	502	CLA	C15-C16-C17-C18
30	E	106	LMT	C7-C8-C9-C10
23	b	615	CLA	CBA-CGA-O2A-C1
30	c	517	LMT	O1'-C1-C2-C3
32	C	522	PLM	C7-C8-C9-CA
35	c	515	DGD	C9B-CAB-CBB-CCB
36	a	416	LHG	C24-C25-C26-C27
23	c	509	CLA	C3-C5-C6-C7
23	d	405	CLA	C2-C3-C5-C6
24	A	407	PHO	C2-C3-C5-C6
23	b	602	CLA	CBA-CGA-O2A-C1
24	a	404	PHO	CBA-CGA-O2A-C1
35	C	504	DGD	C2A-C1A-O1G-C1G
30	D	417	LMT	C2-C3-C4-C5
30	M	101	LMT	O5'-C5'-C6'-O6'
35	C	504	DGD	O1A-C1A-O1G-C1G
23	C	511	CLA	C3-C5-C6-C7
36	D	408	LHG	C30-C31-C32-C33
32	E	107	PLM	C8-C9-CA-CB
32	k	102	PLM	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
35	h	102	DGD	CCB-CDB-CEB-CFB
23	b	610	CLA	CBA-CGA-O2A-C1
35	d	407	DGD	O6D-C1D-O3G-C3G
25	C	501	BCR	C19-C20-C21-C22
25	z	101	BCR	C19-C20-C21-C22
35	c	514	DGD	C3B-C4B-C5B-C6B
24	a	404	PHO	O1A-CGA-O2A-C1
36	a	417	LHG	C11-C10-C9-C8
30	M	101	LMT	C4B-C5B-C6B-O6B
35	c	514	DGD	O6D-C5D-C6D-O5D
27	A	411	SQD	C24-C25-C26-C27
30	a	411	LMT	C6-C7-C8-C9
33	b	621	LMG	C40-C41-C42-C43
36	d	410	LHG	C13-C14-C15-C16
36	l	102	LHG	C30-C31-C32-C33
23	b	603	CLA	C4-C3-C5-C6
26	A	410	PL9	C35-C34-C36-C37
26	d	406	PL9	C15-C14-C16-C17
35	c	516	DGD	C2B-C3B-C4B-C5B
26	a	409	PL9	C43-C44-C46-C47
28	D	413	LFA	C5-C6-C7-C8
32	A	418	PLM	C3-C4-C5-C6
36	a	416	LHG	C29-C30-C31-C32
23	B	610	CLA	C13-C15-C16-C17
30	T	102	LMT	C2-C3-C4-C5
30	f	103	LMT	C4-C5-C6-C7
33	b	621	LMG	C15-C16-C17-C18
32	c	519	PLM	O2-C1-C2-C3
23	C	509	CLA	C15-C16-C17-C18
23	C	510	CLA	C2A-CAA-CBA-CGA
23	b	611	CLA	C2A-CAA-CBA-CGA
35	H	101	DGD	O2G-C1B-C2B-C3B
23	c	507	CLA	CBD-CGD-O2D-CED
36	l	102	LHG	C14-C15-C16-C17
23	B	607	CLA	C3A-C2A-CAA-CBA
23	B	612	CLA	C3A-C2A-CAA-CBA
35	c	516	DGD	CAA-CBA-CCA-CDA
23	B	604	CLA	C4-C3-C5-C6
26	D	402	PL9	C15-C14-C16-C17
32	b	622	PLM	CA-CB-CC-CD
26	D	402	PL9	C23-C24-C26-C27
26	A	410	PL9	C4-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
36	L	101	LHG	C17-C18-C19-C20
27	B	630	SQD	O47-C7-C8-C9
23	B	603	CLA	C11-C10-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C9
23	c	502	CLA	C6-C7-C8-C9
33	D	409	LMG	C33-C34-C35-C36
35	c	514	DGD	CAB-CBB-CCB-CDB
32	E	103	PLM	C3-C4-C5-C6
27	a	410	SQD	C44-C45-C46-O48
36	D	408	LHG	C4-C5-C6-O8
23	b	606	CLA	C3-C5-C6-C7
33	B	619	LMG	C32-C33-C34-C35
32	B	624	PLM	O2-C1-C2-C3
32	B	628	PLM	C8-C9-CA-CB
23	b	615	CLA	C16-C17-C18-C19
33	b	621	LMG	O6-C1-O1-C7
23	B	608	CLA	C13-C15-C16-C17
32	A	418	PLM	C4-C5-C6-C7
33	c	521	LMG	C33-C34-C35-C36
32	c	519	PLM	O1-C1-C2-C3
32	E	107	PLM	C5-C6-C7-C8
33	Y	101	LMG	C33-C34-C35-C36
27	B	630	SQD	C14-C15-C16-C17
30	M	101	LMT	C5-C6-C7-C8
36	D	407	LHG	C26-C27-C28-C29
23	B	615	CLA	C4-C3-C5-C6
23	B	612	CLA	C1A-C2A-CAA-CBA
28	e	101	LFA	C5-C6-C7-C8
23	B	610	CLA	C11-C12-C13-C15
23	C	509	CLA	C12-C13-C15-C16
23	C	510	CLA	C12-C13-C15-C16
23	b	602	CLA	C11-C12-C13-C15
23	c	507	CLA	C6-C7-C8-C10
23	c	507	CLA	C12-C13-C15-C16
23	d	404	CLA	C12-C13-C15-C16
33	I	103	LMG	C40-C41-C42-C43
32	a	413	PLM	O2-C1-C2-C3
36	E	101	LHG	C3-O3-P-O6
32	D	414	PLM	O1-C1-C2-C3
32	D	414	PLM	O2-C1-C2-C3
27	B	630	SQD	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
23	a	402	CLA	C3-C5-C6-C7
23	C	507	CLA	O1D-CGD-O2D-CED
23	A	404	CLA	C2A-CAA-CBA-CGA
23	b	615	CLA	C2A-CAA-CBA-CGA
23	c	504	CLA	C2A-CAA-CBA-CGA
23	d	405	CLA	C13-C15-C16-C17
23	b	615	CLA	O1A-CGA-O2A-C1
36	a	417	LHG	O6-C4-C5-O7
33	y	101	LMG	C14-C15-C16-C17
32	l	101	PLM	C3-C4-C5-C6
35	c	514	DGD	C4D-C5D-C6D-O5D
33	c	521	LMG	C29-C30-C31-C32
23	b	610	CLA	O1A-CGA-O2A-C1
23	C	509	CLA	C13-C15-C16-C17
23	c	509	CLA	C10-C11-C12-C13
33	B	619	LMG	C10-C11-C12-C13
36	a	417	LHG	C29-C30-C31-C32
35	c	515	DGD	C2A-C1A-O1G-C1G
23	B	613	CLA	C5-C6-C7-C8
27	b	601	SQD	C14-C15-C16-C17
35	C	504	DGD	C2A-C3A-C4A-C5A
33	y	101	LMG	O9-C10-O7-C8
27	D	410	SQD	C2-C1-O6-C44
33	b	621	LMG	C2-C1-O1-C7
35	C	503	DGD	C2E-C1E-O5D-C6D
37	V	201	HEM	CAD-CBD-CGD-O2D
27	a	410	SQD	O47-C45-C46-O48
28	C	521	LFA	C6-C7-C8-C9
35	c	515	DGD	O1A-C1A-O1G-C1G
23	C	518	CLA	C16-C17-C18-C19
33	Y	101	LMG	C12-C13-C14-C15
36	l	102	LHG	C16-C17-C18-C19
32	d	413	PLM	C3-C4-C5-C6
26	A	410	PL9	C45-C44-C46-C47
23	a	402	CLA	C2-C1-O2A-CGA
23	B	604	CLA	C2-C3-C5-C6
23	c	506	CLA	C15-C16-C17-C18
33	D	409	LMG	C37-C38-C39-C40
23	A	404	CLA	C14-C13-C15-C16
23	C	516	CLA	C6-C7-C8-C9
23	b	611	CLA	C14-C13-C15-C16
32	C	522	PLM	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	a	407	SQD	C18-C19-C20-C21
33	Y	101	LMG	C31-C32-C33-C34
32	a	413	PLM	O1-C1-C2-C3
32	a	413	PLM	C5-C6-C7-C8
33	B	619	LMG	O9-C10-O7-C8
36	d	410	LHG	C16-C17-C18-C19
23	b	606	CLA	C16-C17-C18-C20
36	a	417	LHG	C33-C34-C35-C36
25	A	409	BCR	C23-C24-C25-C30
25	C	502	BCR	C23-C24-C25-C30
25	j	101	BCR	C23-C24-C25-C30
25	k	101	BCR	C5-C6-C7-C8
25	k	101	BCR	C23-C24-C25-C30
32	h	103	PLM	O2-C1-C2-C3
25	B	631	BCR	C19-C20-C21-C22
24	D	401	PHO	C4-C3-C5-C6
23	c	512	CLA	C5-C6-C7-C8
30	E	106	LMT	C9-C10-C11-C12
23	b	602	CLA	CAA-CBA-CGA-O2A
23	B	616	CLA	CAA-CBA-CGA-O2A
32	k	102	PLM	O1-C1-C2-C3
35	C	503	DGD	C2A-C3A-C4A-C5A
36	d	409	LHG	C11-C12-C13-C14
28	a	418	LFA	C11-C12-C13-C14
33	B	619	LMG	C16-C17-C18-C19
35	c	514	DGD	C5A-C6A-C7A-C8A
36	E	101	LHG	C33-C34-C35-C36
37	V	201	HEM	CAD-CBD-CGD-O1D
35	h	102	DGD	C4B-C5B-C6B-C7B
23	A	404	CLA	C12-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C15
23	a	405	CLA	C12-C13-C15-C16
23	b	612	CLA	C2-C3-C5-C6
23	c	509	CLA	C6-C7-C8-C10
26	D	402	PL9	C13-C14-C16-C17
32	C	519	PLM	O1-C1-C2-C3
32	D	415	PLM	C2-C3-C4-C5
33	c	521	LMG	C12-C13-C14-C15
33	y	101	LMG	C13-C14-C15-C16
36	a	417	LHG	C26-C27-C28-C29
30	B	620	LMT	C1-C2-C3-C4
25	D	403	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
25	t	101	BCR	C13-C14-C15-C16
30	f	103	LMT	C5-C6-C7-C8
33	d	411	LMG	C16-C17-C18-C19
35	C	505	DGD	CCB-CDB-CEB-CFB
23	b	604	CLA	C2A-CAA-CBA-CGA
36	d	409	LHG	C18-C19-C20-C21
27	D	410	SQD	O48-C23-C24-C25
27	a	410	SQD	O48-C23-C24-C25
23	C	512	CLA	C4-C3-C5-C6
32	x	101	PLM	CC-CD-CE-CF
32	A	418	PLM	O1-C1-C2-C3
32	J	102	PLM	O2-C1-C2-C3
36	l	102	LHG	C3-O3-P-O6
23	B	613	CLA	O1D-CGD-O2D-CED
33	a	408	LMG	C15-C16-C17-C18
23	B	608	CLA	C6-C7-C8-C9
23	C	509	CLA	C14-C13-C15-C16
23	C	511	CLA	C6-C7-C8-C9
23	b	602	CLA	C14-C13-C15-C16
23	b	613	CLA	C11-C10-C8-C9
23	c	504	CLA	C14-C13-C15-C16
23	c	507	CLA	C14-C13-C15-C16
30	a	411	LMT	C5'-C4'-O1B-C1B
32	B	624	PLM	O1-C1-C2-C3
37	f	102	HEM	CAA-CBA-CGA-O2A
23	d	404	CLA	C3A-C2A-CAA-CBA
23	C	515	CLA	CAA-CBA-CGA-O2A
32	A	418	PLM	O2-C1-C2-C3
32	E	103	PLM	O2-C1-C2-C3
32	d	413	PLM	O1-C1-C2-C3
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	C	511	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	605	CLA	CAD-CBD-CGD-O2D
23	b	606	CLA	CAD-CBD-CGD-O2D
23	b	608	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	b	611	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	CAD-CBD-CGD-O2D
23	C	518	CLA	C16-C17-C18-C20
28	B	622	LFA	C7-C8-C9-C10
23	c	506	CLA	C2-C1-O2A-CGA
32	b	628	PLM	O1-C1-C2-C3
33	C	525	LMG	C36-C37-C38-C39
23	b	617	CLA	CAA-CBA-CGA-O2A
33	B	619	LMG	O8-C28-C29-C30
36	L	101	LHG	O7-C7-C8-C9
35	C	505	DGD	CAA-CBA-CCA-CDA
32	b	628	PLM	C6-C7-C8-C9
26	A	410	PL9	C12-C11-C9-C10
26	A	410	PL9	C15-C14-C16-C17
33	B	619	LMG	C18-C19-C20-C21
33	C	525	LMG	O6-C1-O1-C7
23	B	615	CLA	C2-C3-C5-C6
23	c	510	CLA	CAA-CBA-CGA-O2A
30	M	101	LMT	O5B-C5B-C6B-O6B
35	D	411	DGD	C1G-C2G-C3G-O3G
23	c	507	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	CAA-CBA-CGA-O2A
27	a	407	SQD	O47-C7-C8-C9
23	b	606	CLA	C16-C17-C18-C19
32	b	623	PLM	O1-C1-C2-C3
32	k	102	PLM	O2-C1-C2-C3
27	A	411	SQD	C31-C32-C33-C34
33	I	103	LMG	C20-C21-C22-C23
23	b	603	CLA	O2A-C1-C2-C3
23	c	512	CLA	O2A-C1-C2-C3
36	L	101	LHG	C11-C12-C13-C14
30	f	103	LMT	O5B-C1B-O1B-C4'
27	b	601	SQD	C30-C31-C32-C33
30	J	101	LMT	C6-C7-C8-C9
23	B	616	CLA	CAA-CBA-CGA-O1A
32	C	519	PLM	O2-C1-C2-C3
32	E	103	PLM	O1-C1-C2-C3
32	b	623	PLM	O2-C1-C2-C3
23	B	603	CLA	CHA-CBD-CGD-O2D
23	B	605	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	C	512	CLA	CHA-CBD-CGD-O1D
23	C	512	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	a	403	CLA	CHA-CBD-CGD-O2D
23	b	605	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
32	d	413	PLM	O2-C1-C2-C3
32	i	101	PLM	O1-C1-C2-C3
23	b	614	CLA	CAA-CBA-CGA-O2A
30	A	416	LMT	C11-C10-C9-C8
28	a	418	LFA	C7-C8-C9-C10
33	D	409	LMG	C22-C23-C24-C25
35	C	505	DGD	C8B-C9B-CAB-CBB
27	F	101	SQD	C35-C36-C37-C38
35	h	102	DGD	C8A-C9A-CAA-CBA
27	b	601	SQD	O6-C44-C45-O47
32	C	522	PLM	C8-C9-CA-CB
32	i	101	PLM	CA-CB-CC-CD
33	C	525	LMG	O7-C10-C11-C12
33	Y	101	LMG	O7-C10-C11-C12
36	D	406	LHG	C26-C27-C28-C29
32	i	101	PLM	O2-C1-C2-C3
24	d	402	PHO	CHA-CBD-CGD-O1D
24	d	402	PHO	CHA-CBD-CGD-O2D
34	B	621	GOL	O2-C2-C3-O3
36	a	416	LHG	C26-C27-C28-C29
35	h	102	DGD	O1B-C1B-C2B-C3B
23	c	512	CLA	CAA-CBA-CGA-O2A
36	a	417	LHG	C32-C33-C34-C35
23	c	507	CLA	C2-C3-C5-C6
26	a	409	PL9	C23-C24-C26-C27
35	D	411	DGD	C2B-C3B-C4B-C5B
35	c	514	DGD	O1B-C1B-O2G-C2G
27	F	101	SQD	O5-C1-O6-C44
33	y	101	LMG	O7-C10-C11-C12
23	B	610	CLA	C11-C12-C13-C14
23	B	611	CLA	C14-C13-C15-C16
23	B	615	CLA	C14-C13-C15-C16
23	a	402	CLA	C14-C13-C15-C16
23	a	405	CLA	C11-C12-C13-C14
23	b	606	CLA	C6-C7-C8-C9
23	c	507	CLA	C6-C7-C8-C9
25	a	406	BCR	C19-C20-C21-C22
25	f	101	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
32	h	103	PLM	O1-C1-C2-C3
32	l	101	PLM	O2-C1-C2-C3
33	b	621	LMG	C17-C18-C19-C20
35	C	503	DGD	O2G-C1B-C2B-C3B
27	D	410	SQD	C5-C6-S-O8
27	b	601	SQD	C4-C5-C6-S
33	c	521	LMG	C38-C39-C40-C41
33	B	619	LMG	C11-C10-O7-C8
33	y	101	LMG	C11-C10-O7-C8
32	J	102	PLM	O1-C1-C2-C3
32	b	628	PLM	O2-C1-C2-C3
23	B	603	CLA	C2A-CAA-CBA-CGA
23	C	512	CLA	CBD-CGD-O2D-CED
23	C	515	CLA	CAA-CBA-CGA-O1A
23	c	510	CLA	CAA-CBA-CGA-O1A
23	a	405	CLA	C4-C3-C5-C6
27	F	101	SQD	C28-C29-C30-C31
23	b	610	CLA	C2-C3-C5-C6
37	f	102	HEM	CAA-CBA-CGA-O1A
25	Y	102	BCR	C21-C22-C23-C24
25	j	101	BCR	C7-C8-C9-C10
25	t	101	BCR	C17-C18-C19-C20
23	A	405	CLA	C2C-C3C-CAC-CBC
23	B	607	CLA	C1A-C2A-CAA-CBA
23	d	404	CLA	C1A-C2A-CAA-CBA
36	L	101	LHG	C1-C2-C3-O3
33	y	101	LMG	C19-C20-C21-C22
23	A	405	CLA	C16-C17-C18-C20
32	J	102	PLM	C6-C7-C8-C9
30	a	411	LMT	O5'-C5'-C6'-O6'
23	b	617	CLA	CAA-CBA-CGA-O1A
27	D	410	SQD	O10-C23-C24-C25
27	a	407	SQD	O49-C7-C8-C9
27	a	410	SQD	O10-C23-C24-C25
30	a	419	LMT	C5-C6-C7-C8
35	c	515	DGD	C1G-C2G-C3G-O3G
35	d	407	DGD	C1G-C2G-C3G-O3G
33	y	101	LMG	O8-C28-C29-C30
30	E	106	LMT	C2-C3-C4-C5
36	D	407	LHG	C33-C34-C35-C36
23	b	614	CLA	CAA-CBA-CGA-O1A
33	Y	101	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	y	101	LMG	O9-C10-C11-C12
33	I	103	LMG	C14-C15-C16-C17
37	E	105	HEM	CAA-CBA-CGA-O2A
23	B	613	CLA	CBD-CGD-O2D-CED
23	b	612	CLA	C4-C3-C5-C6
33	B	619	LMG	O10-C28-C29-C30
32	x	101	PLM	O2-C1-C2-C3
35	d	407	DGD	C2D-C1D-O3G-C3G
24	D	401	PHO	C5-C6-C7-C8
27	B	630	SQD	C26-C27-C28-C29
27	a	407	SQD	C19-C20-C21-C22
28	B	622	LFA	C14-C15-C16-C17
36	D	407	LHG	C3-O3-P-O5
36	E	101	LHG	C4-O6-P-O5
36	L	101	LHG	C3-O3-P-O5
36	a	417	LHG	C3-O3-P-O5
36	l	102	LHG	C3-O3-P-O5
23	C	510	CLA	C16-C17-C18-C19
32	x	101	PLM	C3-C4-C5-C6
26	A	410	PL9	C42-C43-C44-C45
23	C	512	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	CAA-CBA-CGA-O1A
36	L	101	LHG	O9-C7-C8-C9
32	d	413	PLM	CB-CC-CD-CE
23	c	505	CLA	C2A-CAA-CBA-CGA
36	a	416	LHG	C10-C11-C12-C13
33	d	411	LMG	C13-C14-C15-C16
23	B	613	CLA	CAA-CBA-CGA-O2A
33	d	411	LMG	C36-C37-C38-C39
36	d	410	LHG	C7-C8-C9-C10
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	610	CLA	CAD-CBD-CGD-O1D
27	a	410	SQD	C5-C6-S-O7
33	y	101	LMG	C32-C33-C34-C35
23	B	603	CLA	C11-C12-C13-C14
23	B	605	CLA	C11-C12-C13-C14
23	C	510	CLA	C14-C13-C15-C16
23	b	602	CLA	C11-C12-C13-C14
33	Y	101	LMG	C16-C17-C18-C19
23	B	603	CLA	C13-C15-C16-C17
32	C	524	PLM	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	l	101	PLM	O1-C1-C2-C3
32	C	524	PLM	C1-C2-C3-C4
23	c	512	CLA	CAA-CBA-CGA-O1A
27	a	410	SQD	C26-C27-C28-C29
32	x	101	PLM	C4-C5-C6-C7
23	d	404	CLA	CAA-CBA-CGA-O2A
36	D	408	LHG	O8-C23-C24-C25
30	f	103	LMT	C5'-C4'-O1B-C1B
33	C	525	LMG	O9-C10-C11-C12
33	y	101	LMG	O10-C28-C29-C30
33	I	103	LMG	C19-C20-C21-C22
23	b	611	CLA	C16-C17-C18-C20
23	A	404	CLA	C4-C3-C5-C6
23	b	610	CLA	C4-C3-C5-C6
32	b	622	PLM	C7-C8-C9-CA
23	B	610	CLA	C12-C13-C15-C16
23	B	611	CLA	C12-C13-C15-C16
23	C	516	CLA	C6-C7-C8-C10
23	a	402	CLA	C12-C13-C15-C16
23	b	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C11-C10-C8-C7
23	b	606	CLA	C6-C7-C8-C10
23	b	611	CLA	C11-C12-C13-C15
23	b	611	CLA	C12-C13-C15-C16
23	c	502	CLA	C12-C13-C15-C16
23	d	401	CLA	C11-C10-C8-C7
24	a	404	PHO	C3A-C2A-CAA-CBA
26	d	406	PL9	C18-C19-C21-C22
30	M	102	LMT	C9-C10-C11-C12
35	h	102	DGD	CDA-CEA-CFA-CGA
27	A	411	SQD	C16-C17-C18-C19
36	l	102	LHG	C35-C36-C37-C38
30	f	103	LMT	C3'-C4'-O1B-C1B
36	l	102	LHG	C7-C8-C9-C10
23	B	613	CLA	CAA-CBA-CGA-O1A
32	C	524	PLM	O1-C1-C2-C3
28	e	101	LFA	C11-C12-C13-C14
35	c	515	DGD	CBA-CCA-CDA-CEA
36	l	102	LHG	O7-C7-C8-C9
23	c	510	CLA	O1D-CGD-O2D-CED
36	D	408	LHG	O10-C23-C24-C25
30	a	411	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
37	E	105	HEM	CAA-CBA-CGA-O1A
26	D	402	PL9	C11-C12-C13-C14
23	C	517	CLA	CAA-CBA-CGA-O2A
35	d	407	DGD	O1G-C1A-C2A-C3A
23	B	611	CLA	C15-C16-C17-C18
32	x	101	PLM	O1-C1-C2-C3
36	L	101	LHG	C26-C27-C28-C29
32	B	628	PLM	C5-C6-C7-C8

There are no ring outliers.

146 monomers are involved in 245 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	A	418	PLM	2	0
23	b	609	CLA	3	0
23	B	610	CLA	2	0
25	k	101	BCR	2	0
30	c	517	LMT	1	0
23	B	613	CLA	1	0
23	C	517	CLA	5	0
27	A	411	SQD	2	0
30	D	417	LMT	3	0
25	b	619	BCR	5	0
30	d	403	LMT	1	0
35	D	411	DGD	2	0
33	B	619	LMG	5	0
27	a	407	SQD	2	0
33	D	409	LMG	4	0
33	y	101	LMG	2	0
32	c	519	PLM	1	0
30	f	103	LMT	1	0
23	B	615	CLA	3	0
27	d	408	SQD	2	0
23	B	612	CLA	2	0
35	C	504	DGD	3	0
23	b	608	CLA	1	0
23	d	405	CLA	3	0
33	c	521	LMG	1	0
26	D	402	PL9	3	0
36	a	416	LHG	1	0
23	C	506	CLA	3	0
25	a	406	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	z	101	BCR	2	0
23	b	603	CLA	1	0
30	M	101	LMT	1	0
33	a	408	LMG	2	0
23	A	405	CLA	2	0
23	B	605	CLA	2	0
23	D	404	CLA	2	0
25	b	620	BCR	2	0
23	b	604	CLA	2	0
30	M	102	LMT	2	0
36	E	101	LHG	2	0
24	d	402	PHO	2	0
25	A	409	BCR	1	0
35	c	516	DGD	1	0
35	C	505	DGD	1	0
33	C	525	LMG	1	0
32	C	524	PLM	1	0
36	d	409	LHG	1	0
23	b	610	CLA	1	0
38	x	102	RRX	1	0
36	l	102	LHG	5	0
23	a	405	CLA	3	0
23	B	603	CLA	3	0
23	D	405	CLA	4	0
25	i	103	BCR	1	0
36	D	408	LHG	5	0
36	L	101	LHG	1	0
23	B	604	CLA	4	0
23	d	401	CLA	1	0
25	C	527	BCR	3	0
25	b	618	BCR	1	0
28	h	101	LFA	1	0
35	c	514	DGD	1	0
23	C	518	CLA	2	0
23	c	505	CLA	2	0
27	A	415	SQD	5	0
28	B	622	LFA	1	0
23	C	510	CLA	3	0
25	B	631	BCR	3	0
30	A	416	LMT	1	0
27	F	101	SQD	1	0
35	h	102	DGD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	511	CLA	1	0
32	b	622	PLM	1	0
27	b	601	SQD	2	0
33	d	411	LMG	1	0
28	I	104	LFA	1	0
23	c	513	CLA	4	0
23	A	404	CLA	2	0
23	c	509	CLA	1	0
27	a	410	SQD	3	0
36	D	406	LHG	1	0
37	E	105	HEM	2	0
30	a	411	LMT	1	0
23	d	404	CLA	3	0
23	A	408	CLA	3	0
23	B	601	CLA	2	0
36	d	410	LHG	2	0
23	a	403	CLA	1	0
32	d	413	PLM	1	0
37	f	102	HEM	2	0
26	d	406	PL9	1	0
23	B	611	CLA	1	0
23	c	510	CLA	2	0
30	B	620	LMT	2	0
23	b	605	CLA	2	0
36	D	407	LHG	1	0
32	E	102	PLM	1	0
23	b	616	CLA	5	0
23	B	614	CLA	3	0
23	C	513	CLA	3	0
32	D	414	PLM	4	0
23	C	507	CLA	1	0
35	c	515	DGD	1	0
23	b	617	CLA	6	0
23	C	508	CLA	1	0
28	C	520	LFA	1	0
36	a	417	LHG	3	0
27	B	630	SQD	4	0
32	K	101	PLM	1	0
23	A	406	CLA	3	0
23	C	516	CLA	4	0
23	C	512	CLA	1	0
23	c	511	CLA	5	0

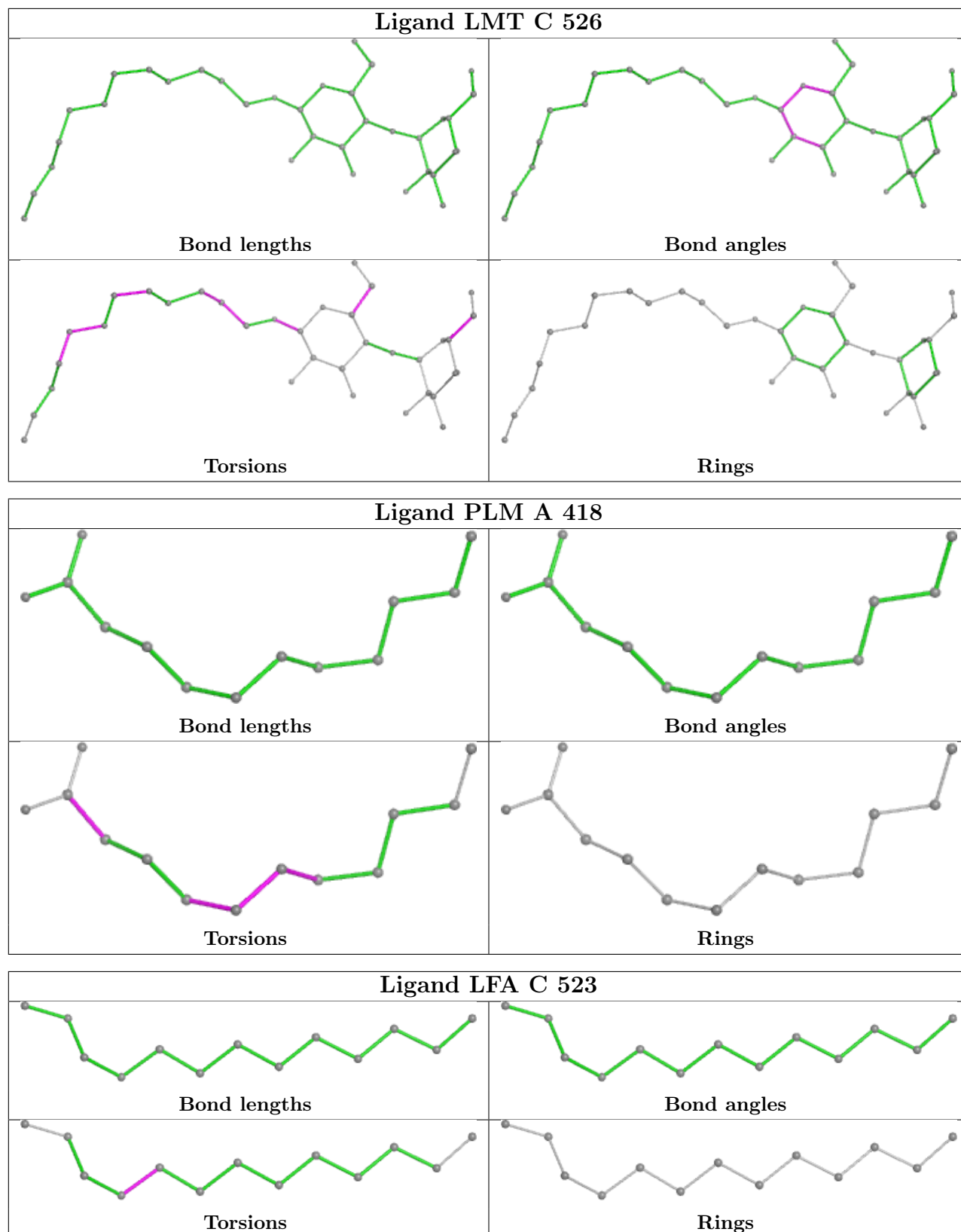
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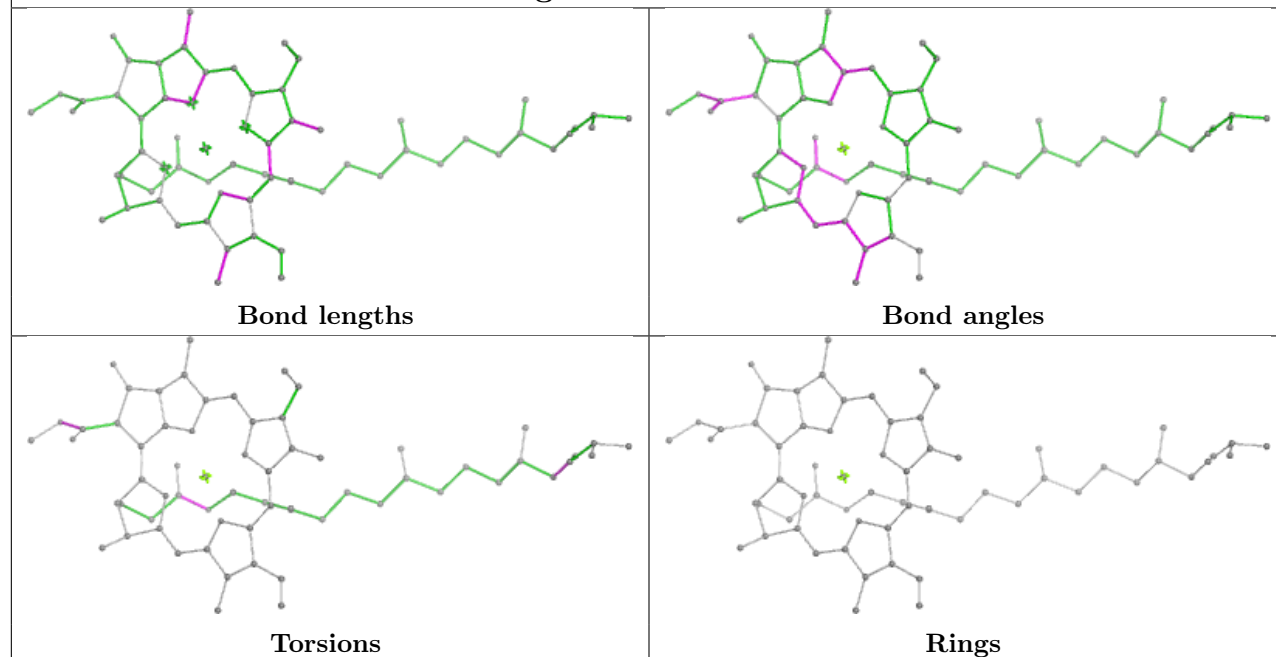
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	401	PHO	2	0
23	c	502	CLA	2	0
33	b	621	LMG	1	0
32	c	518	PLM	1	0
25	T	101	BCR	3	0
25	C	501	BCR	3	0
23	C	515	CLA	1	0
23	B	616	CLA	2	0
23	c	503	CLA	5	0
23	b	613	CLA	1	0
23	c	506	CLA	1	0
35	C	503	DGD	2	0
23	c	512	CLA	2	0
33	I	103	LMG	3	0
25	D	403	BCR	1	0
24	A	407	PHO	1	0
23	B	607	CLA	1	0
23	b	606	CLA	3	0
23	c	507	CLA	1	0
23	b	615	CLA	2	0
23	c	504	CLA	2	0
23	b	602	CLA	2	0
23	b	612	CLA	2	0
26	A	410	PL9	5	0
23	a	402	CLA	3	0
26	a	409	PL9	4	0
25	t	101	BCR	1	0
25	B	617	BCR	2	0
25	Y	102	BCR	4	0
24	a	404	PHO	2	0
23	c	501	CLA	2	0
35	H	101	DGD	1	0
23	c	508	CLA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

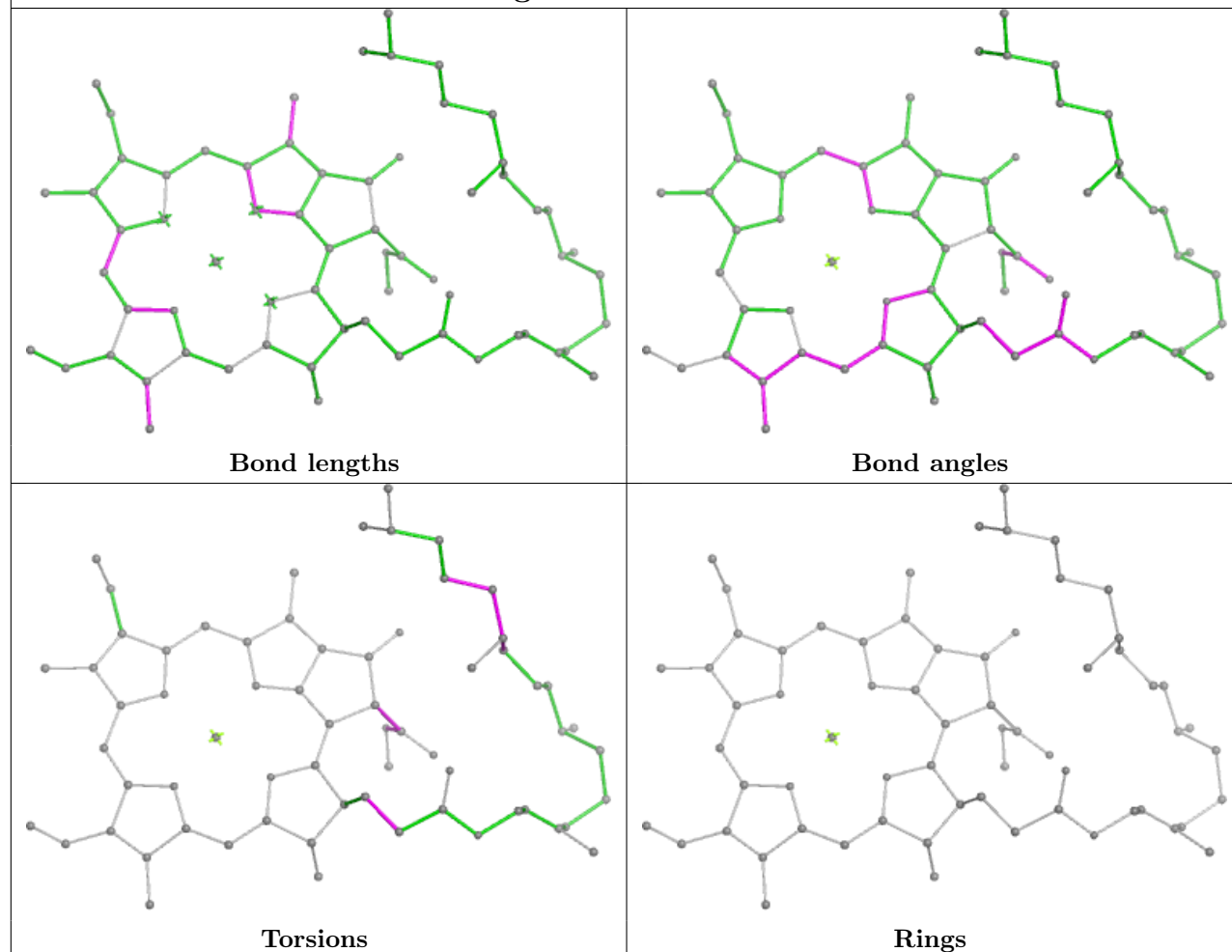
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

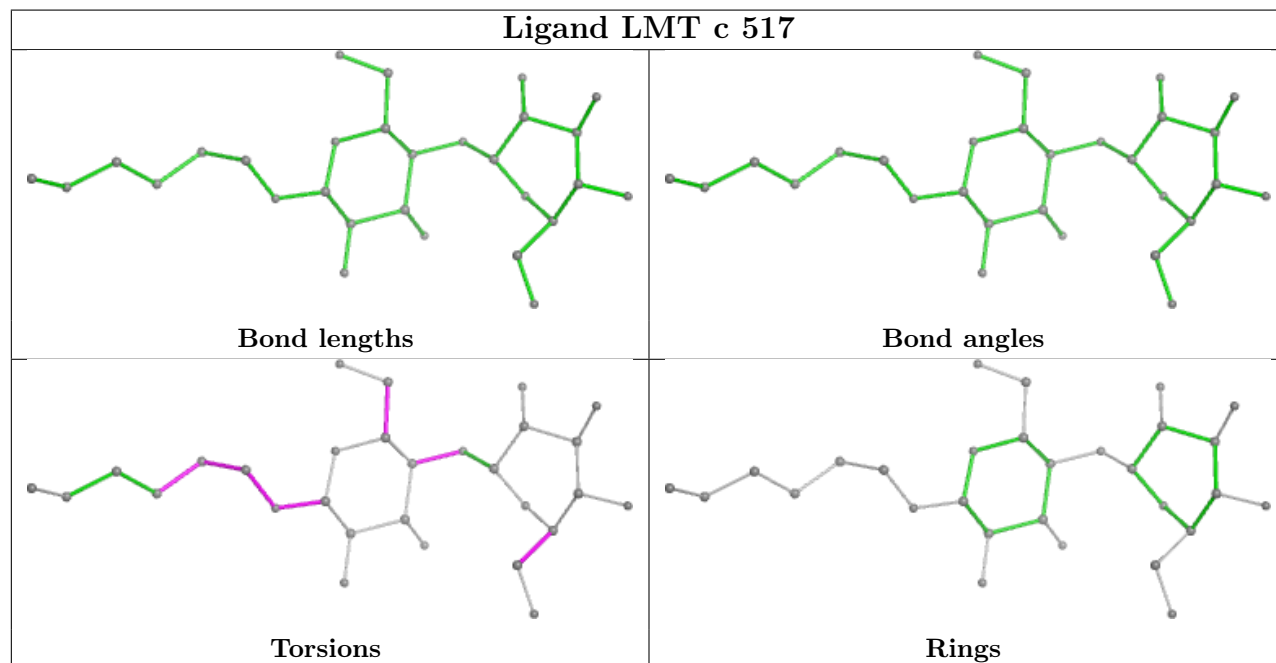
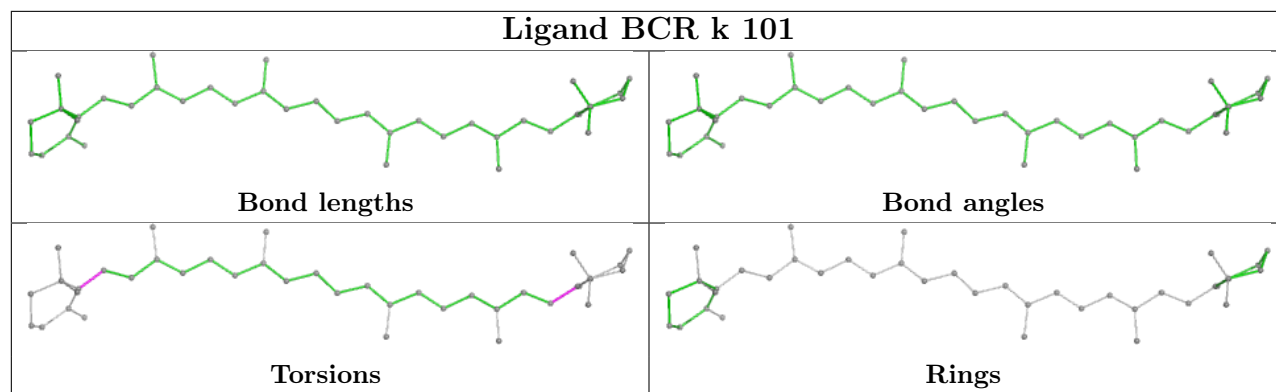


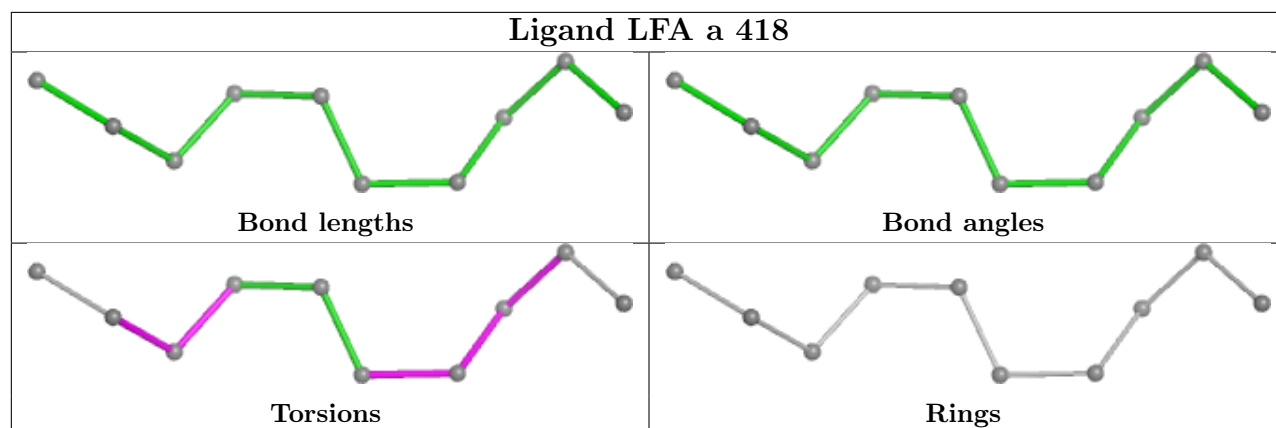
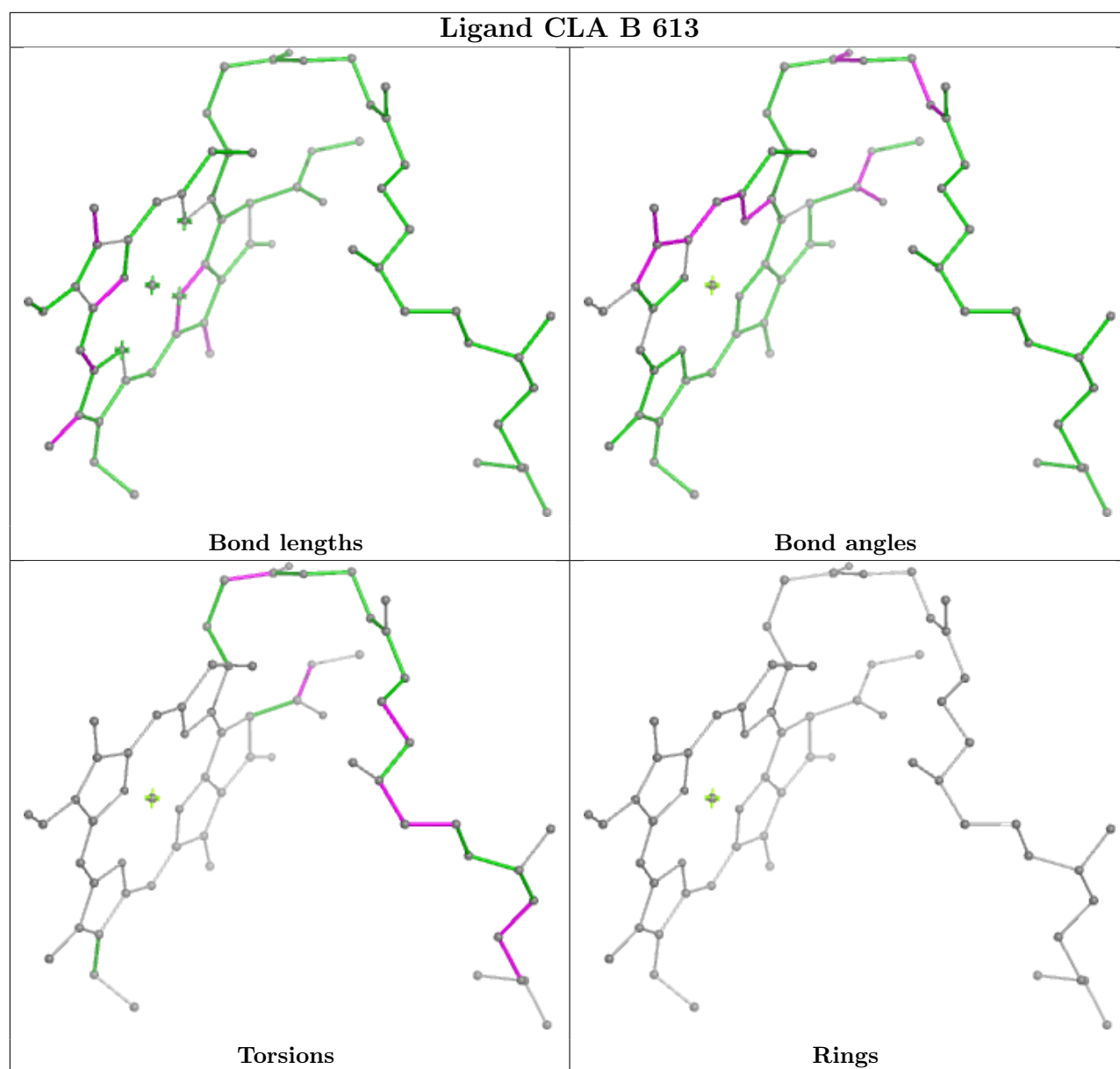
Ligand CLA b 609



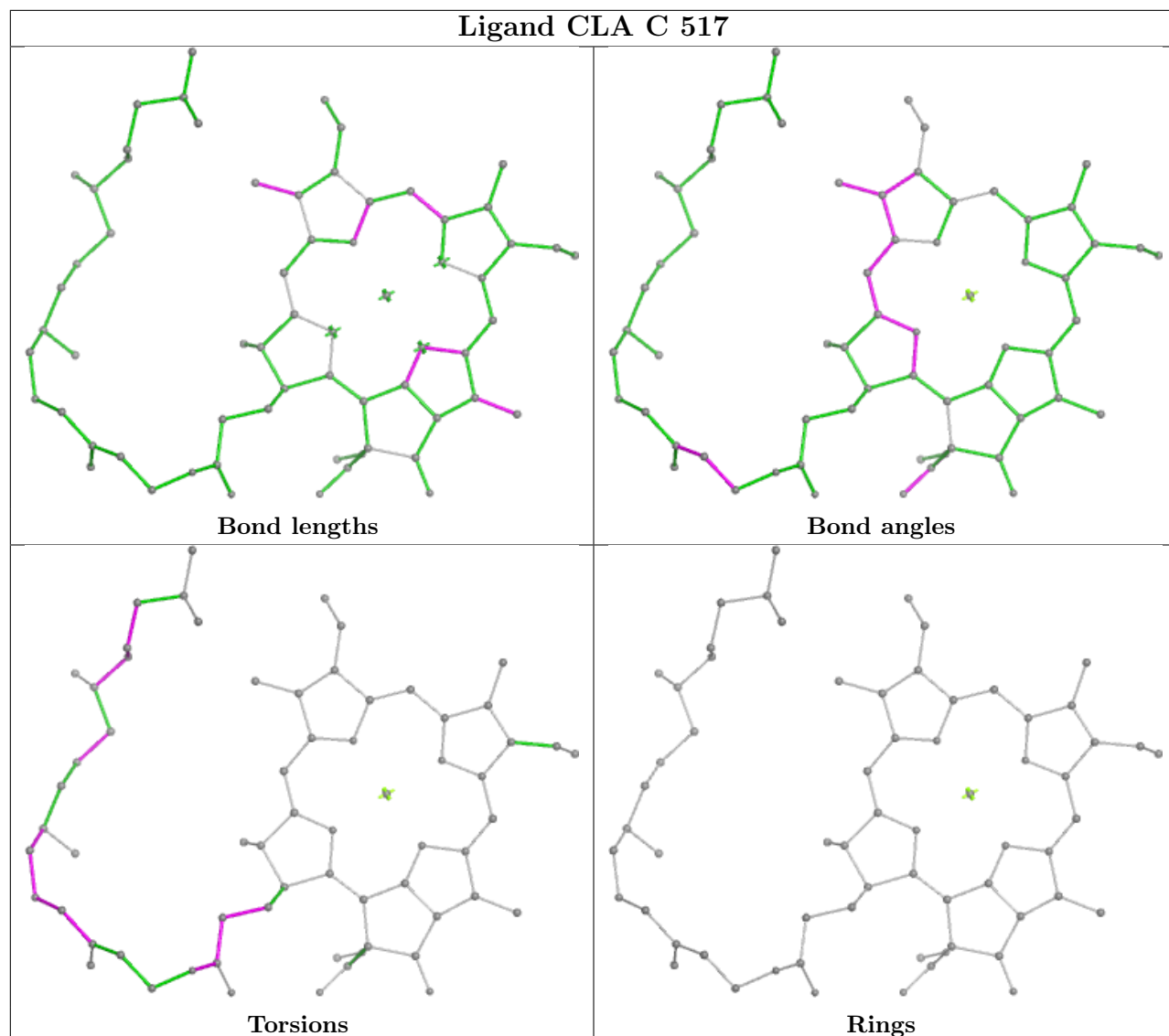
Ligand CLA B 610

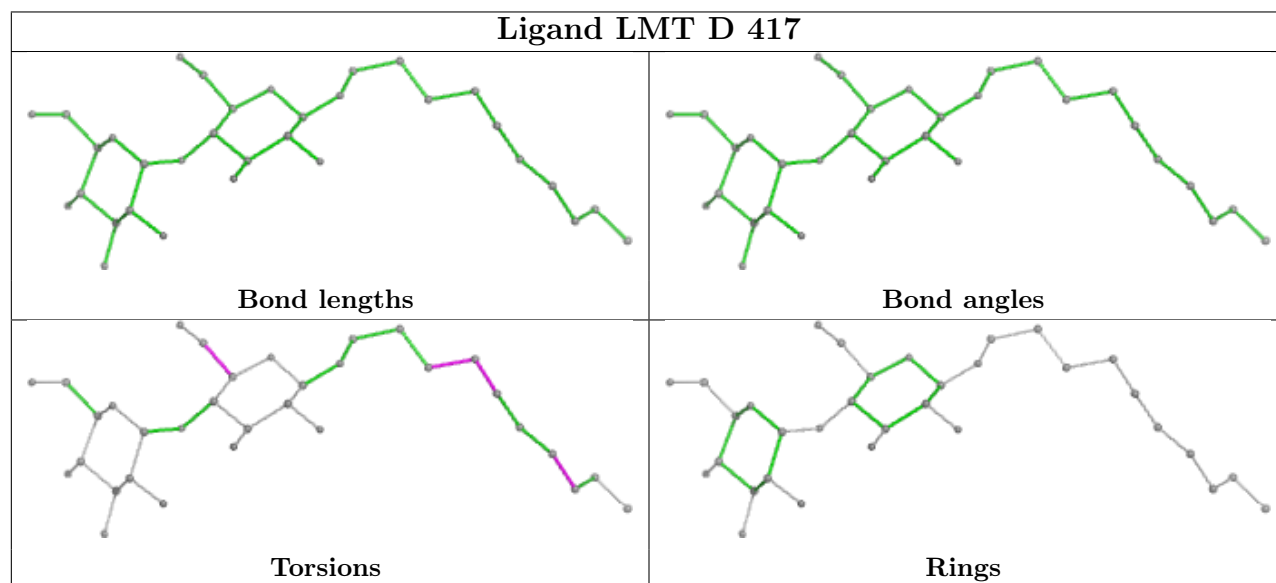
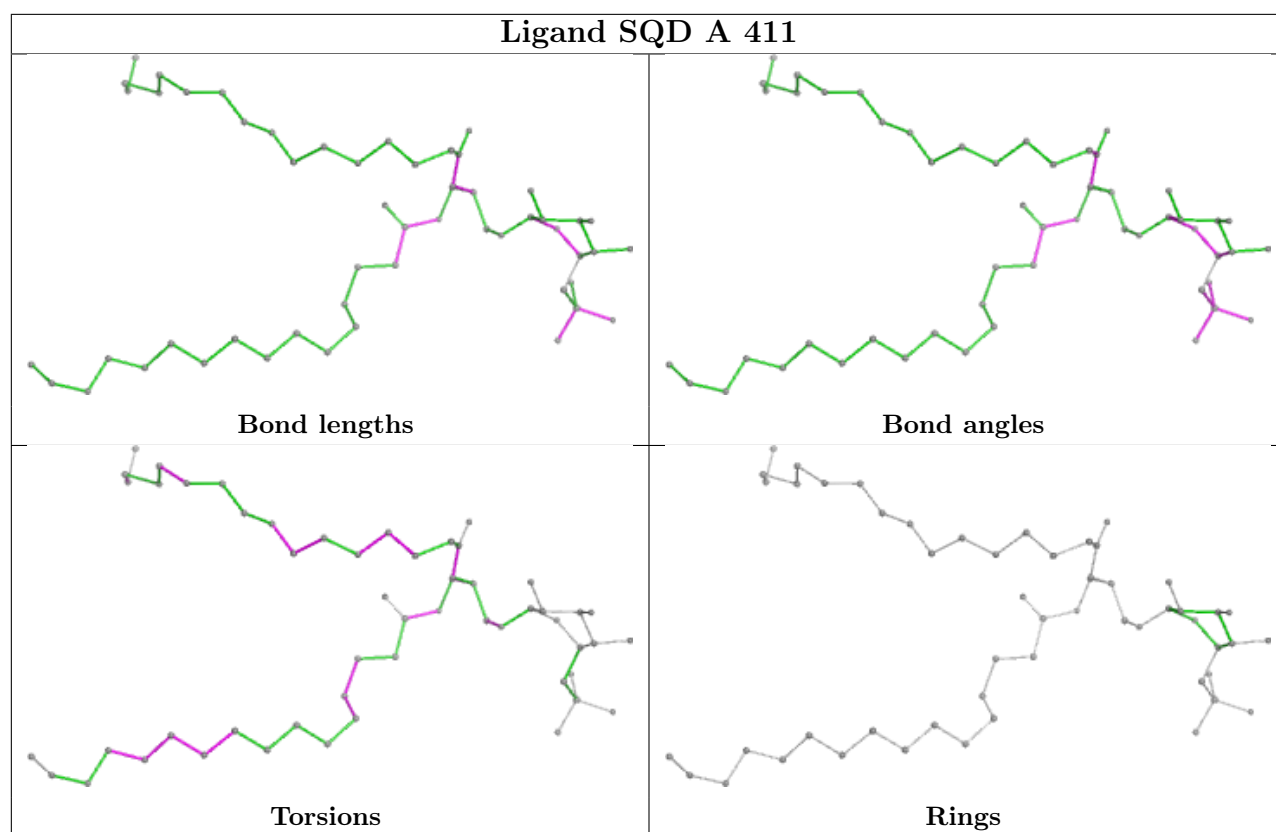


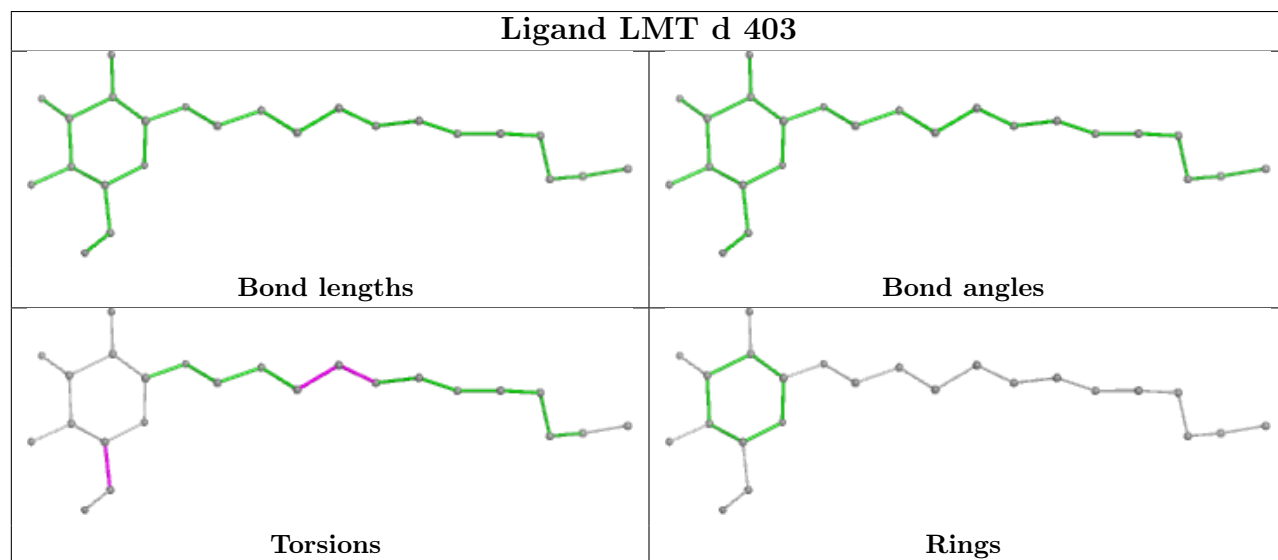
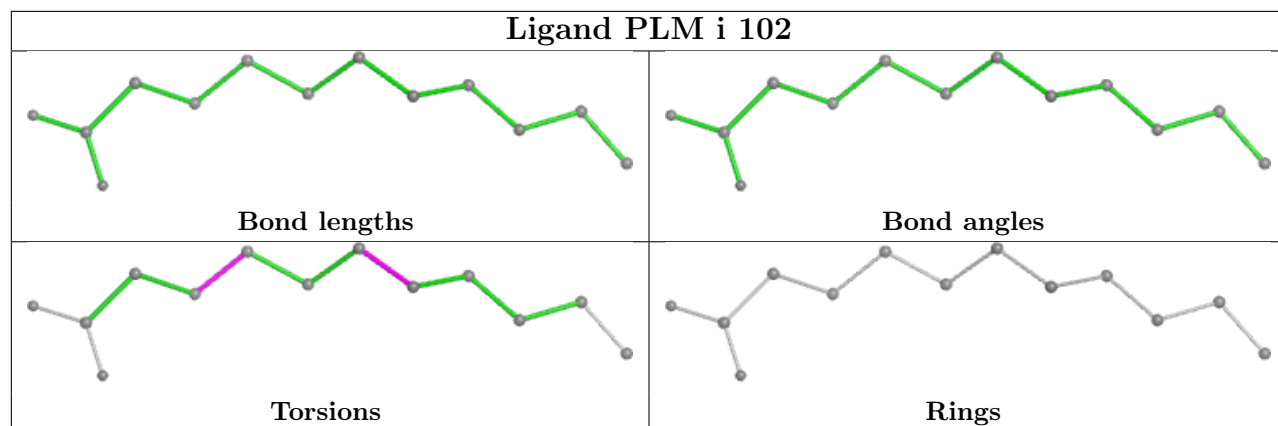


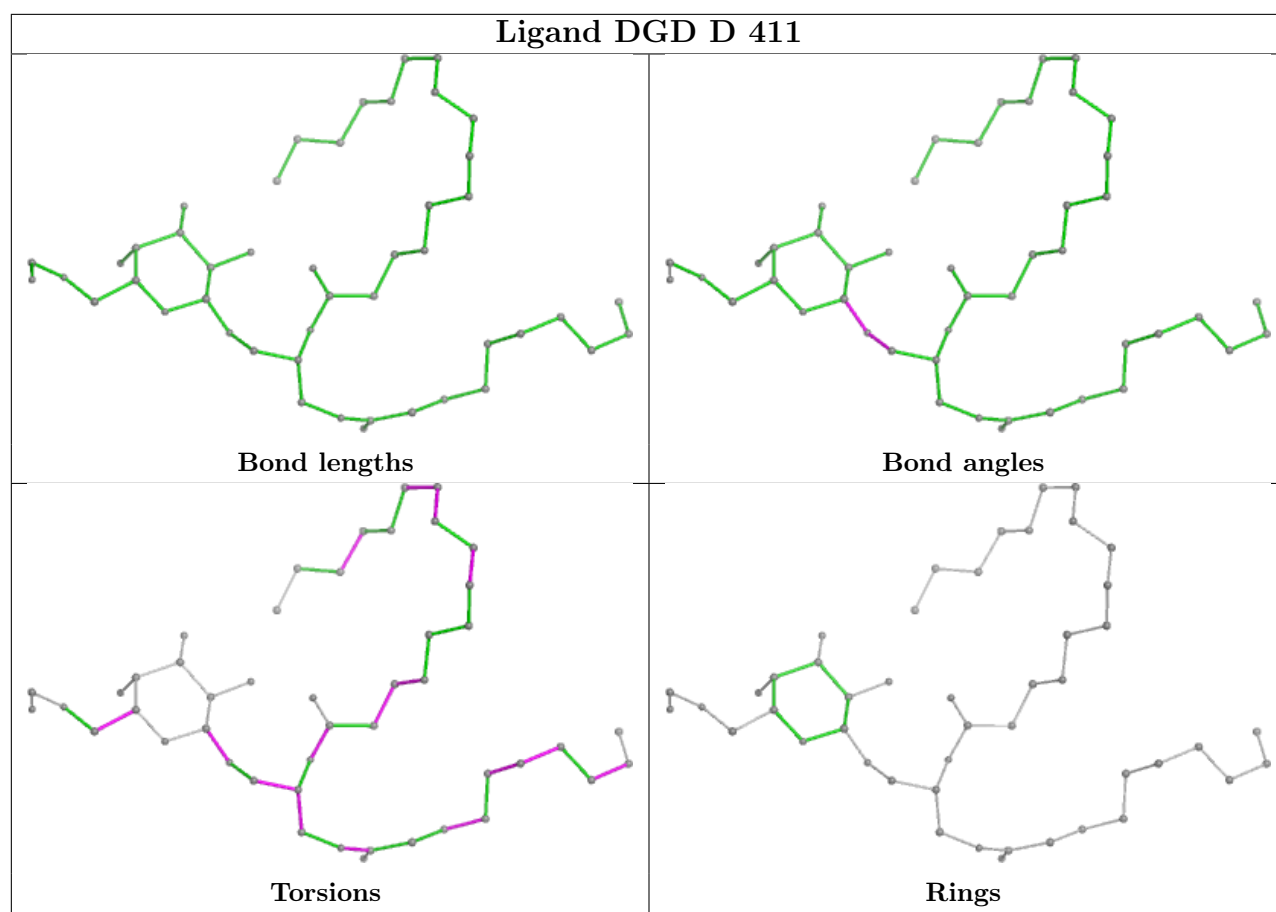


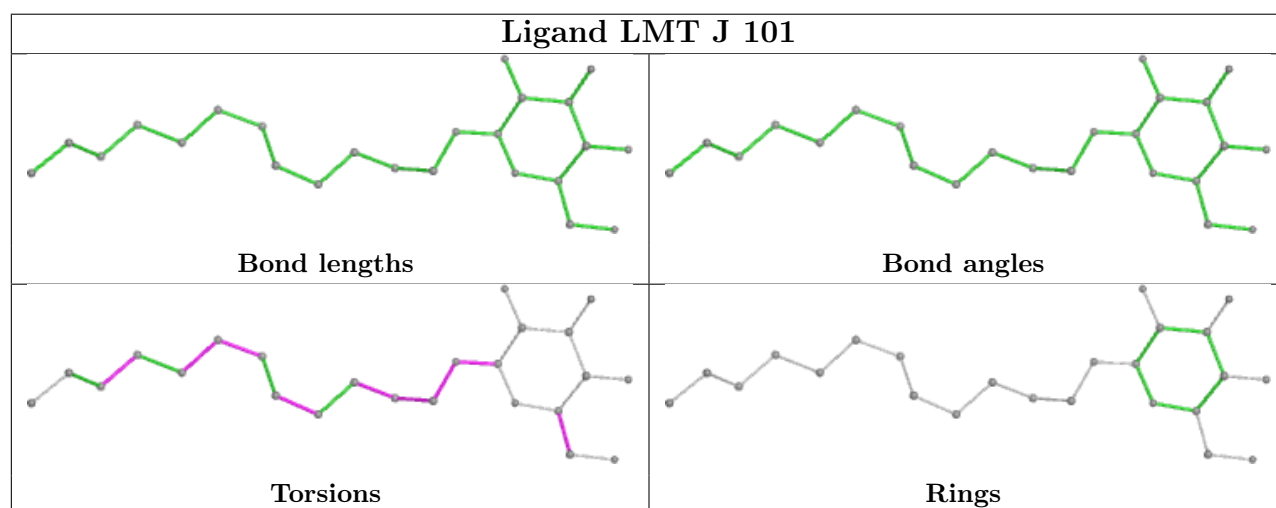
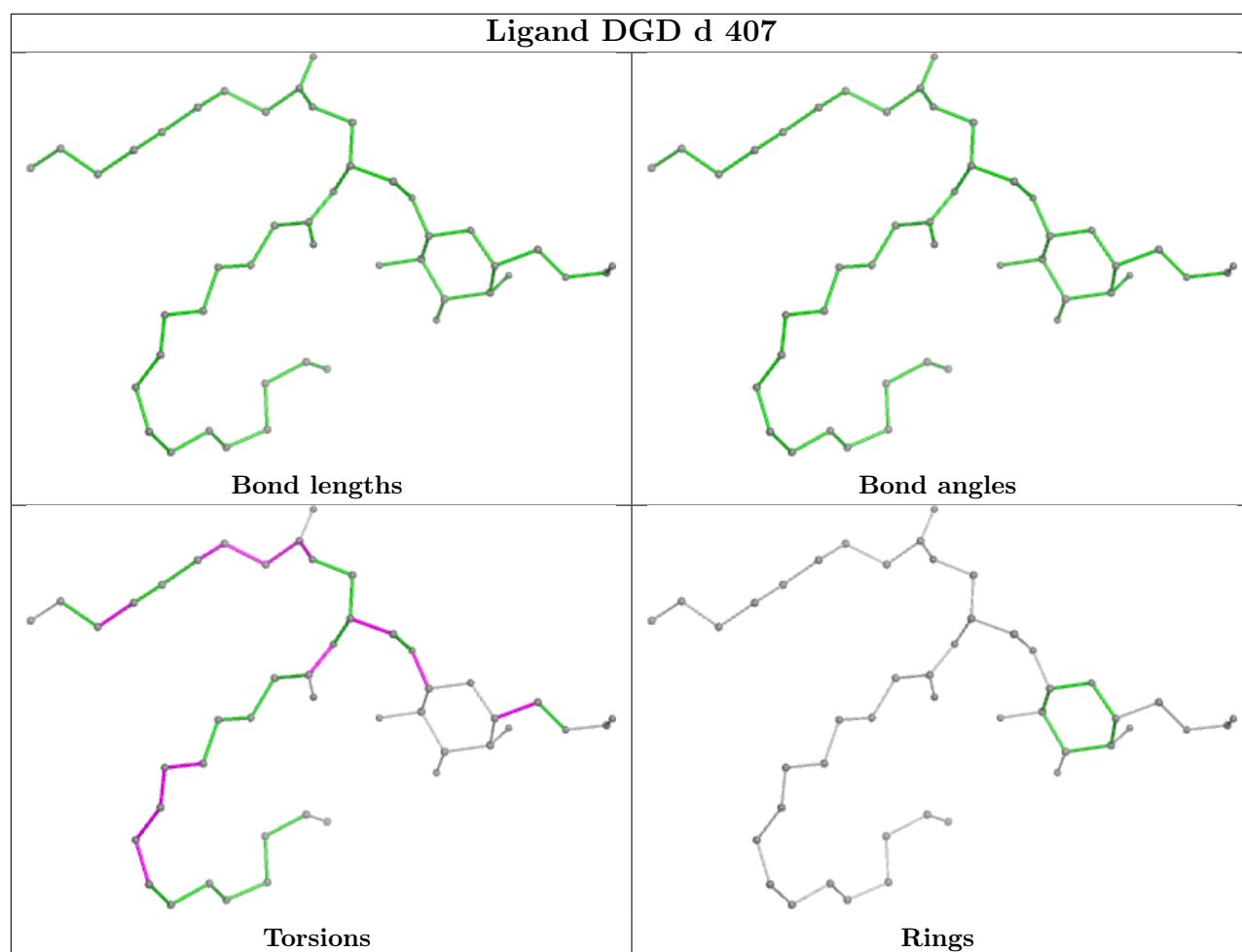
Ligand CLA C 517

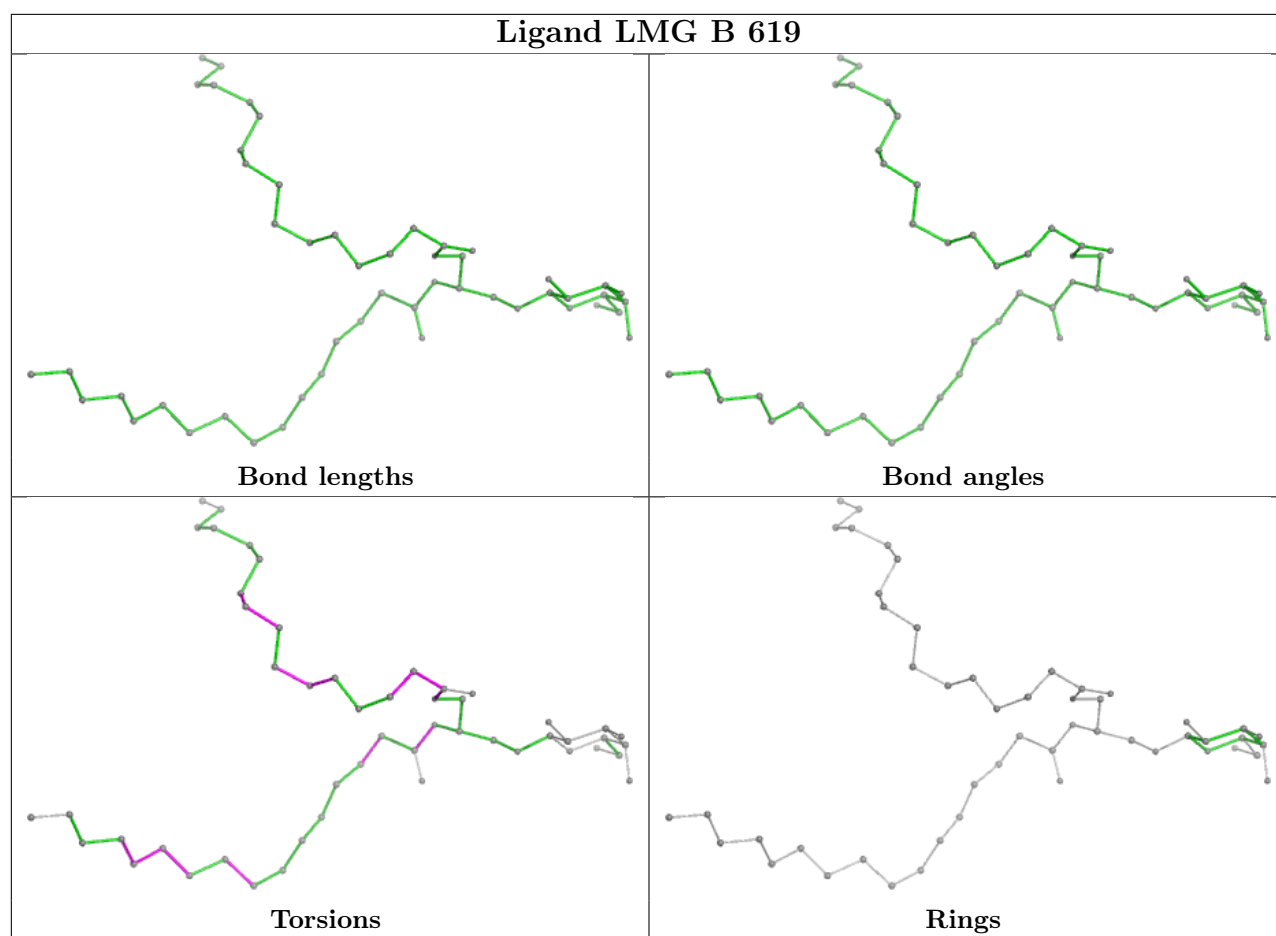


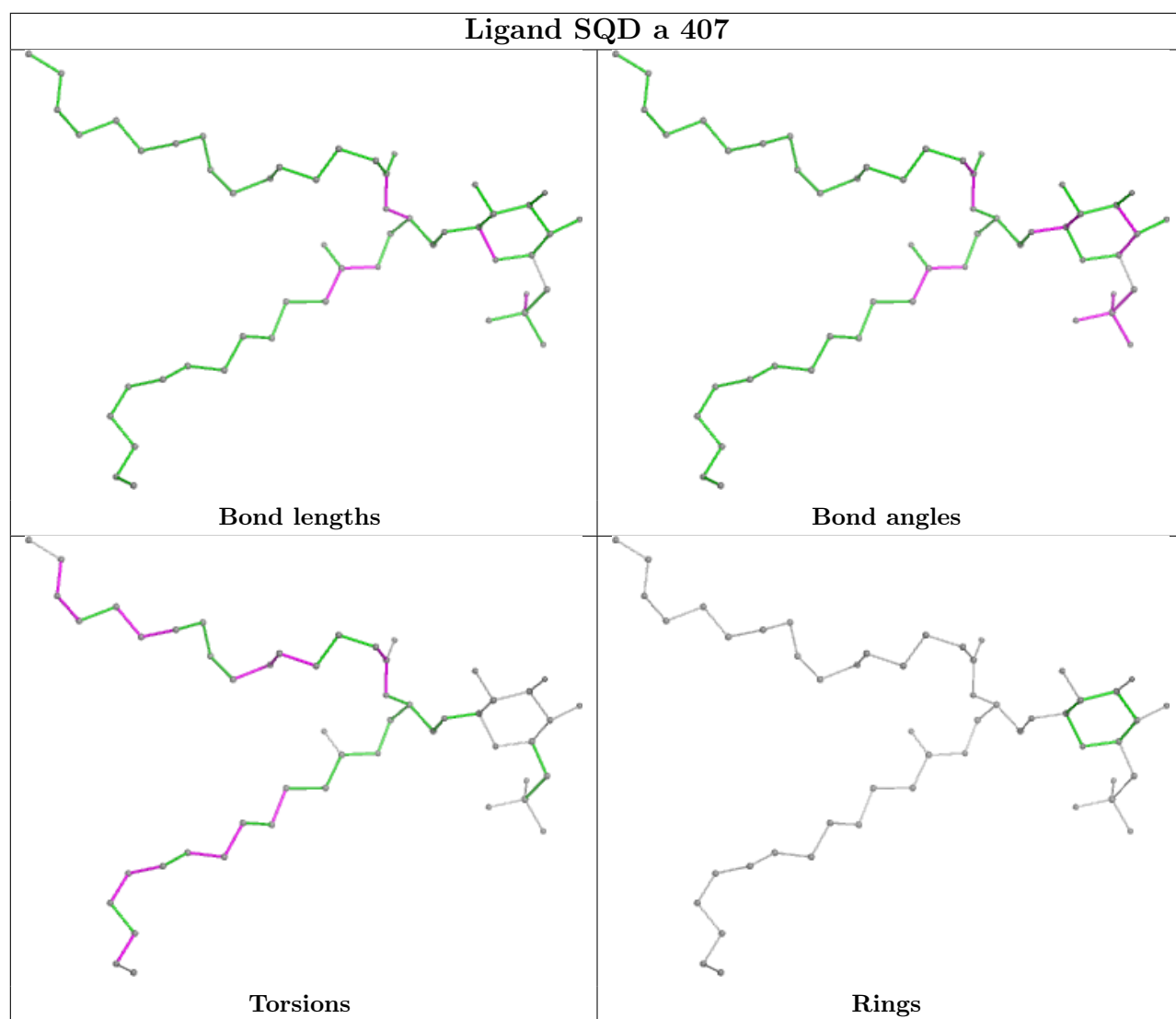


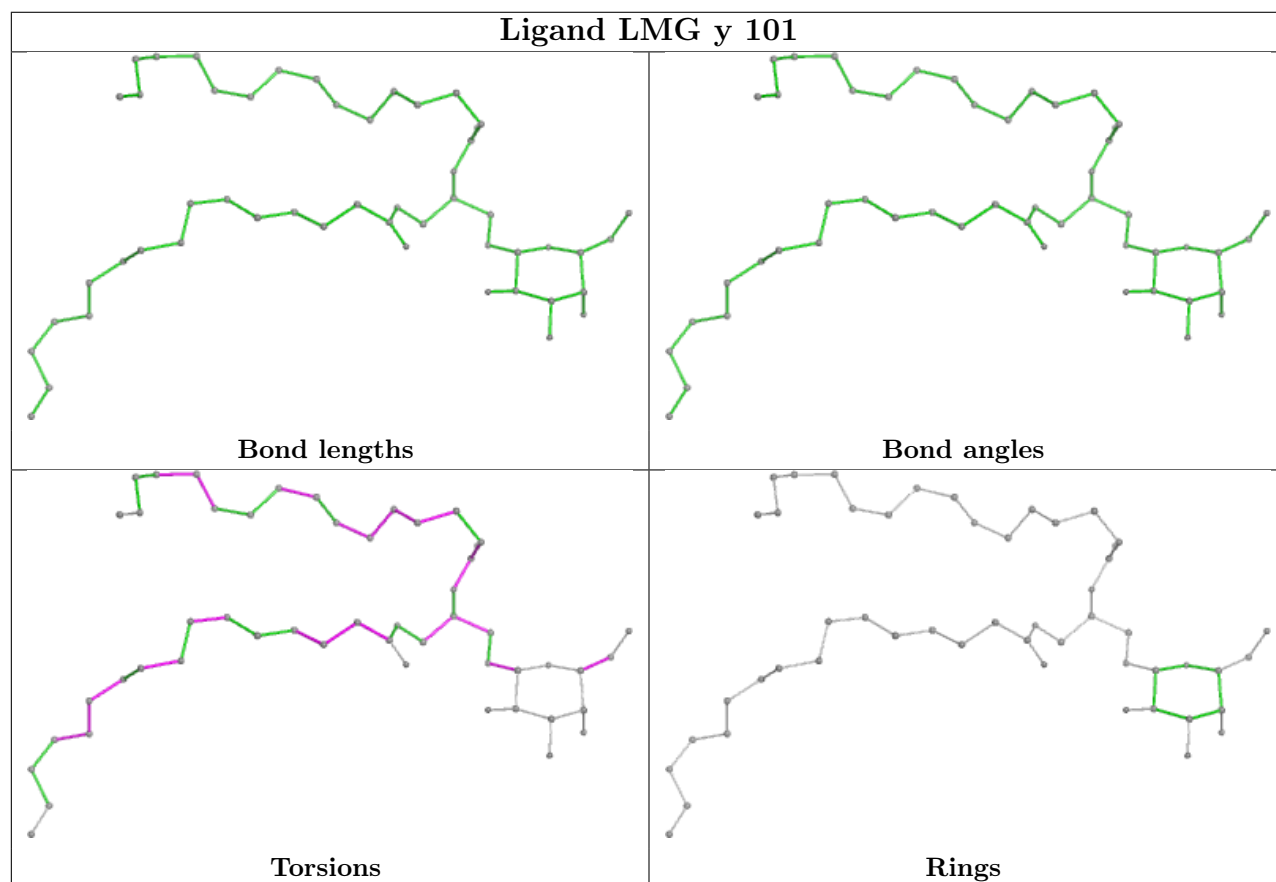
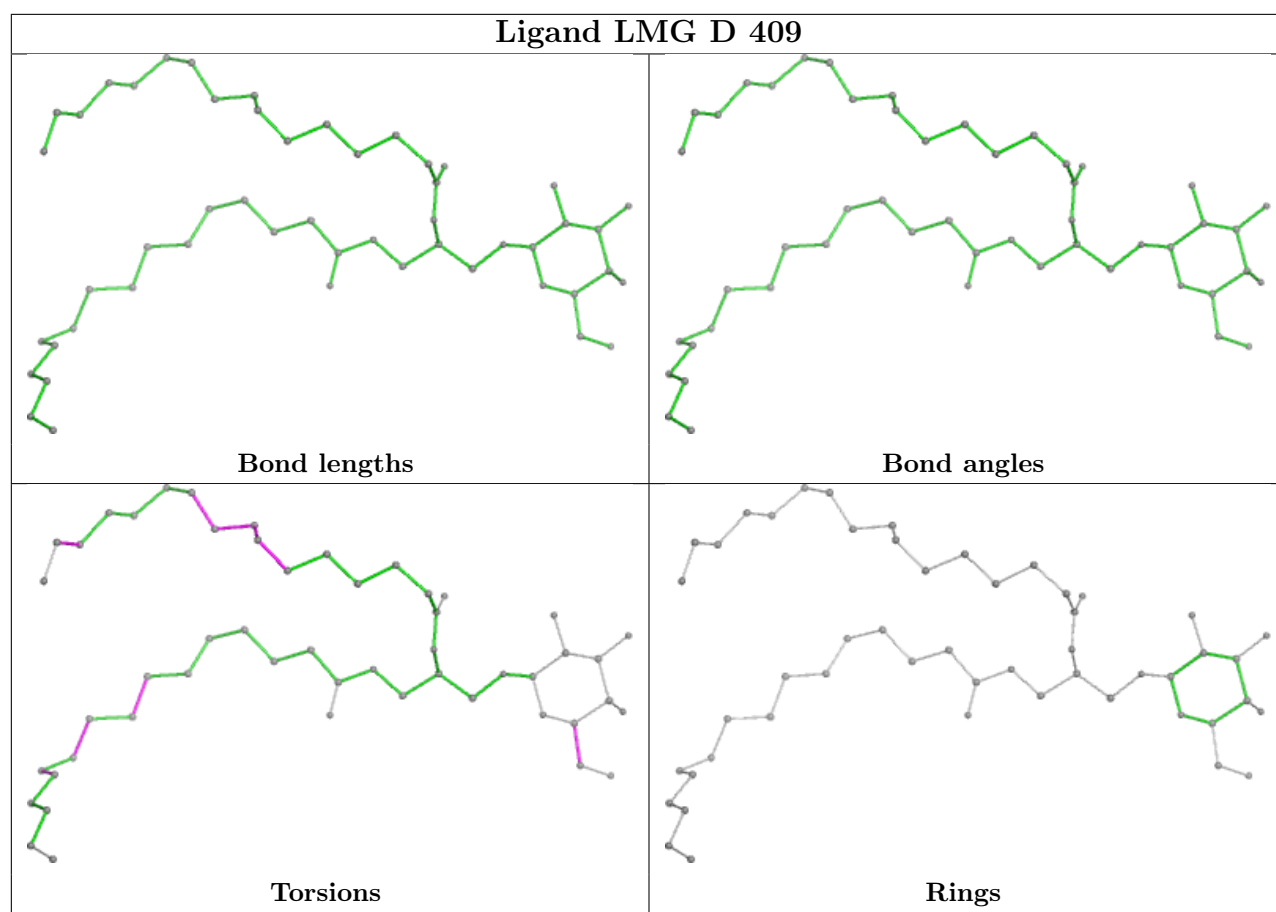


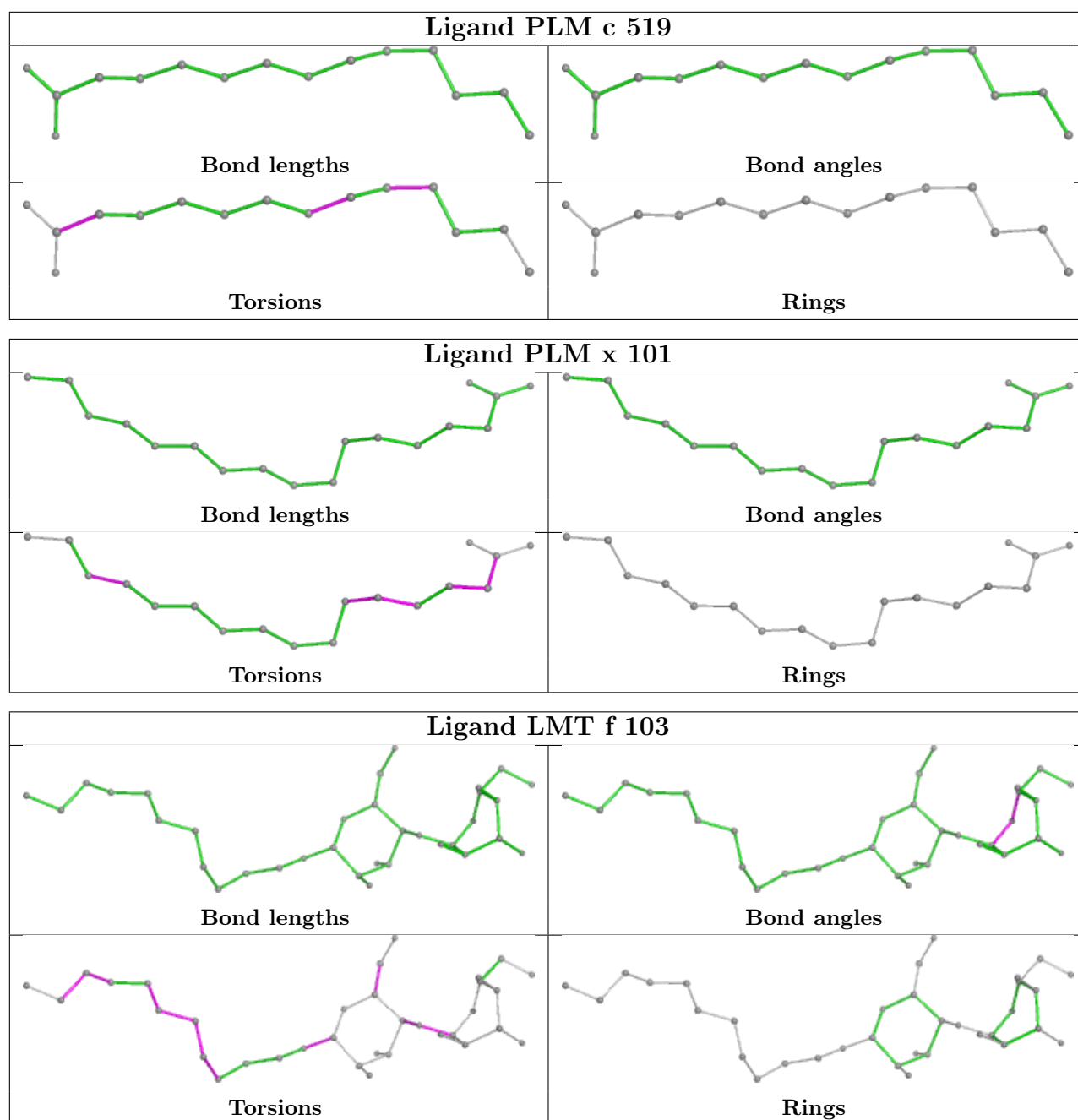


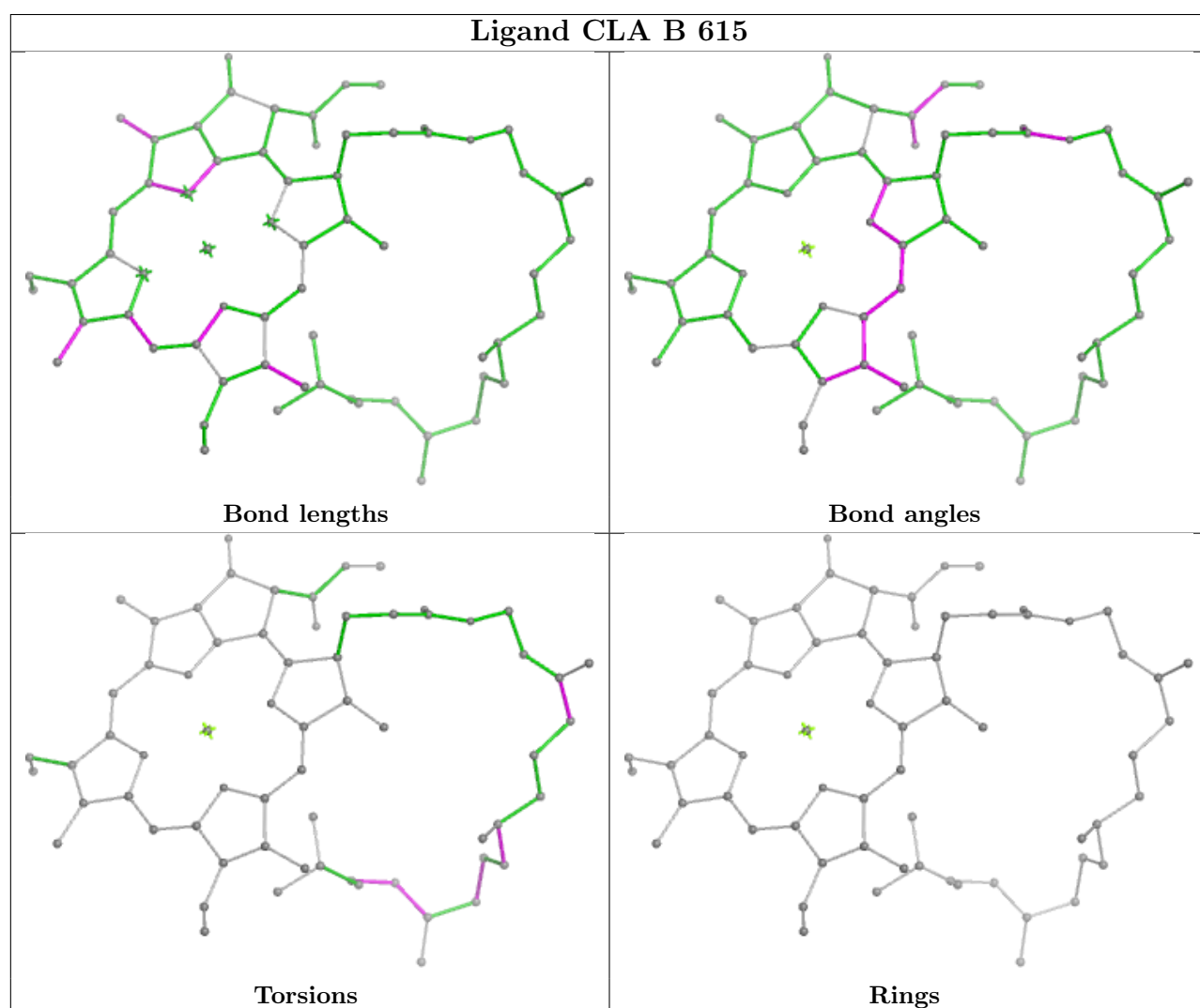
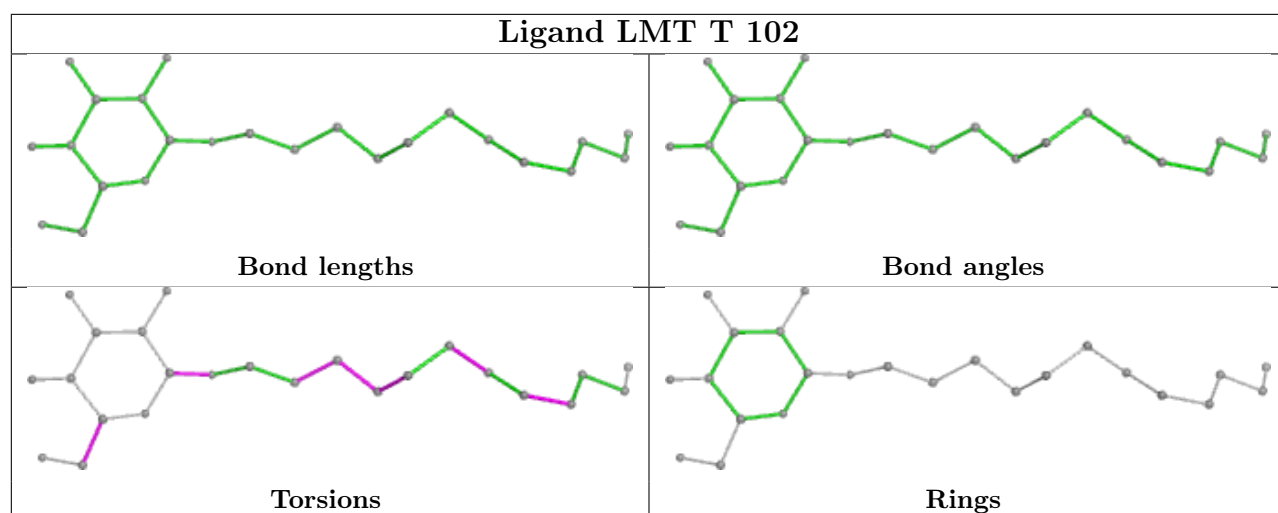




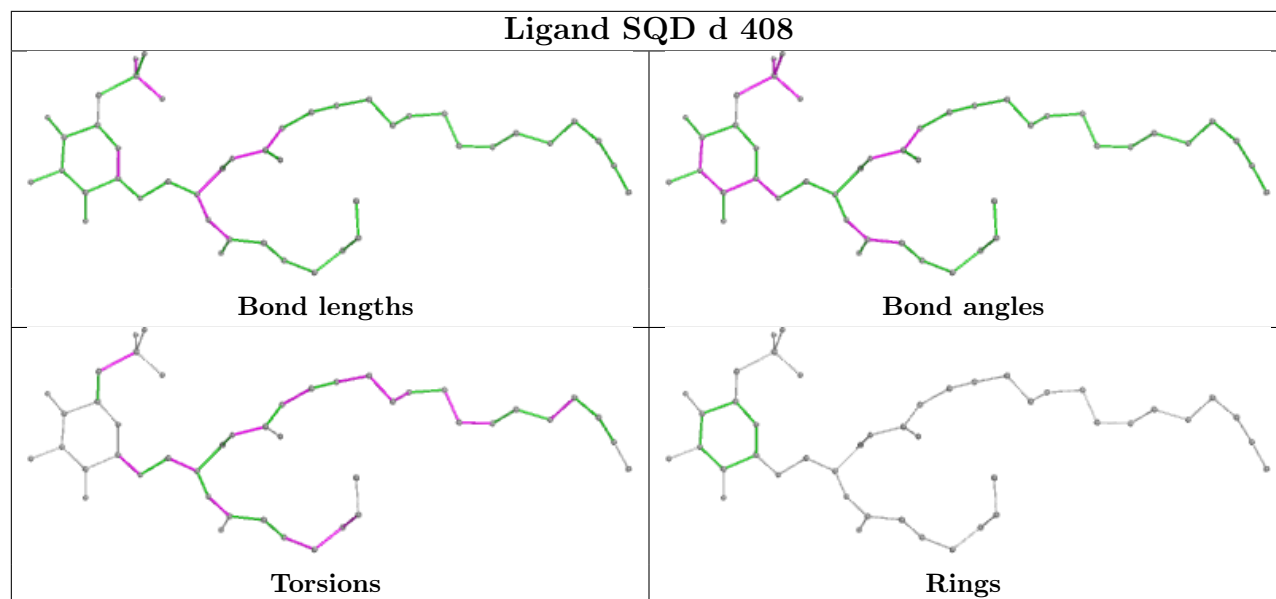




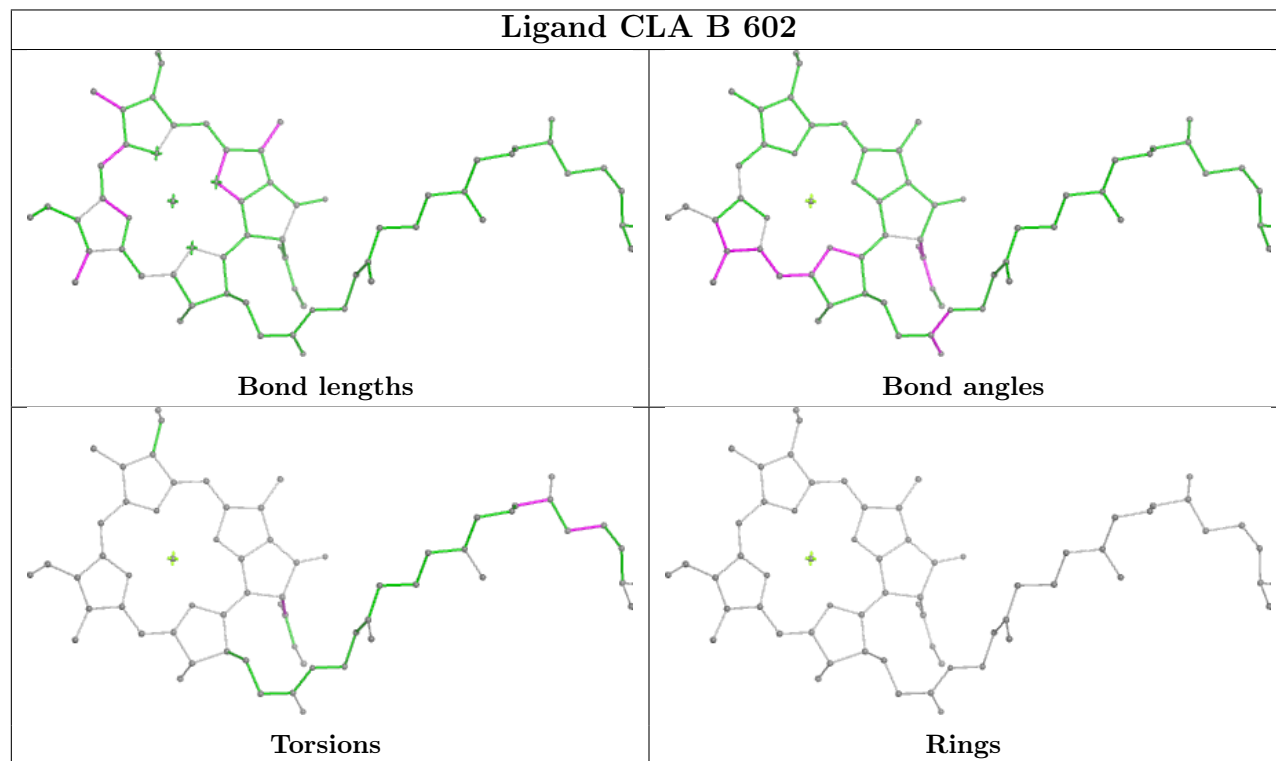


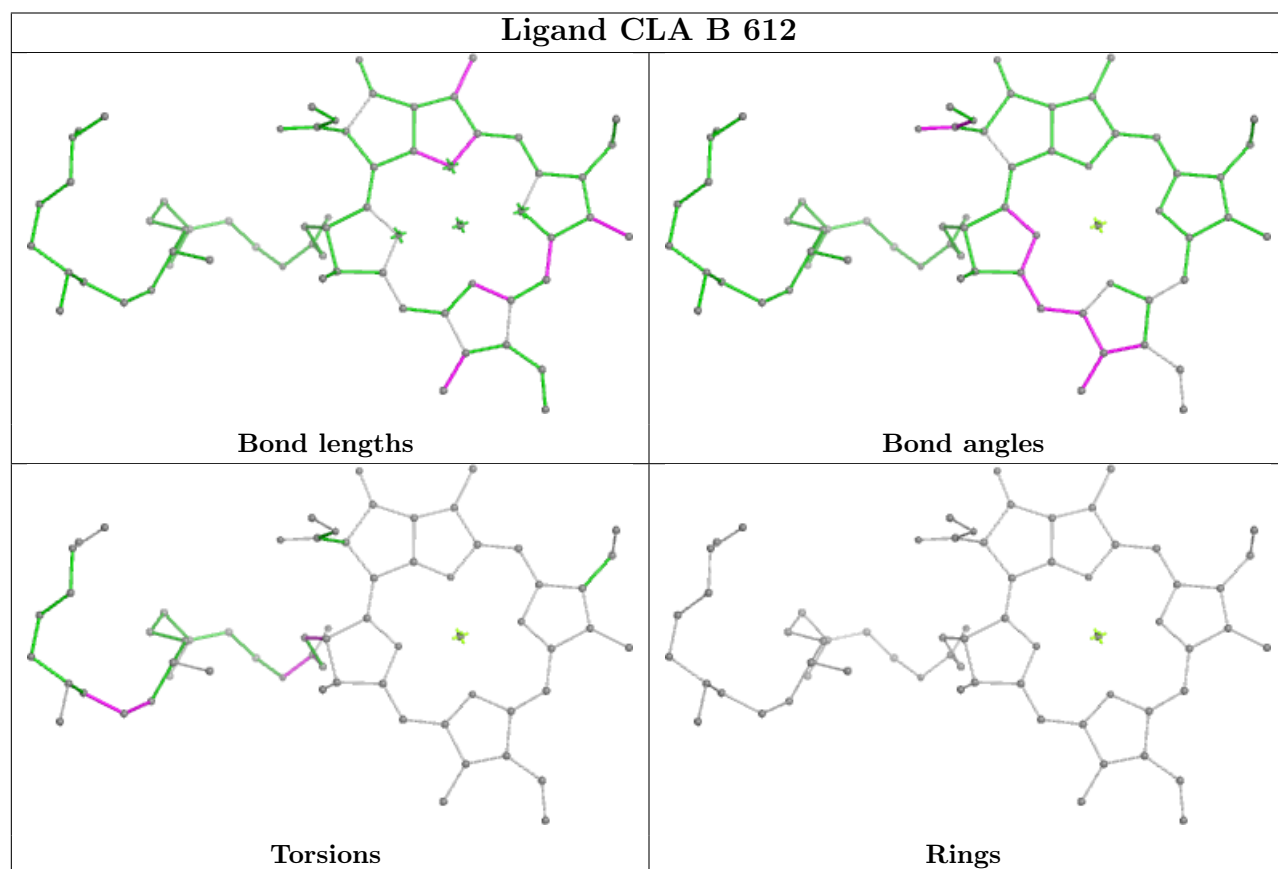
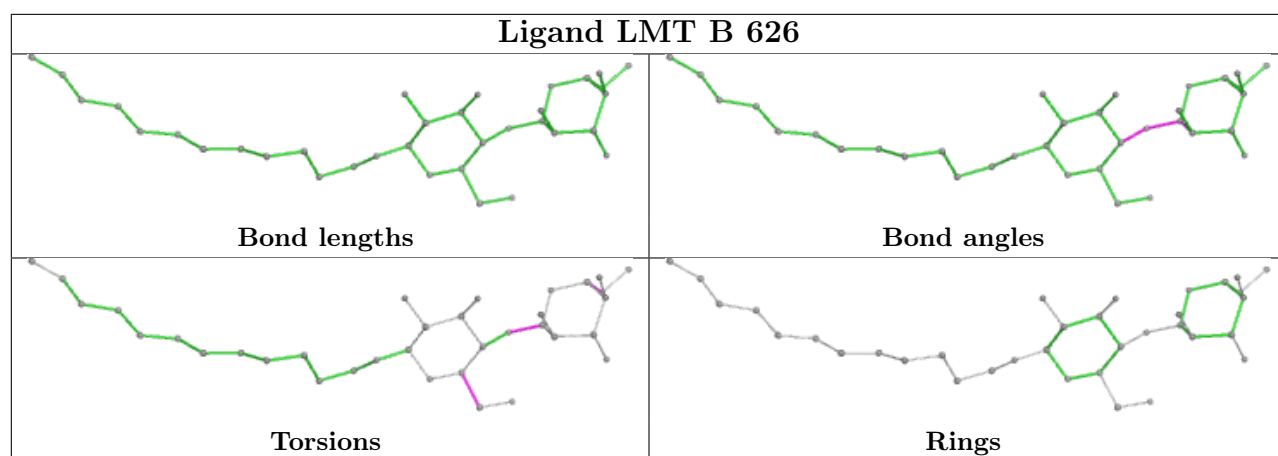


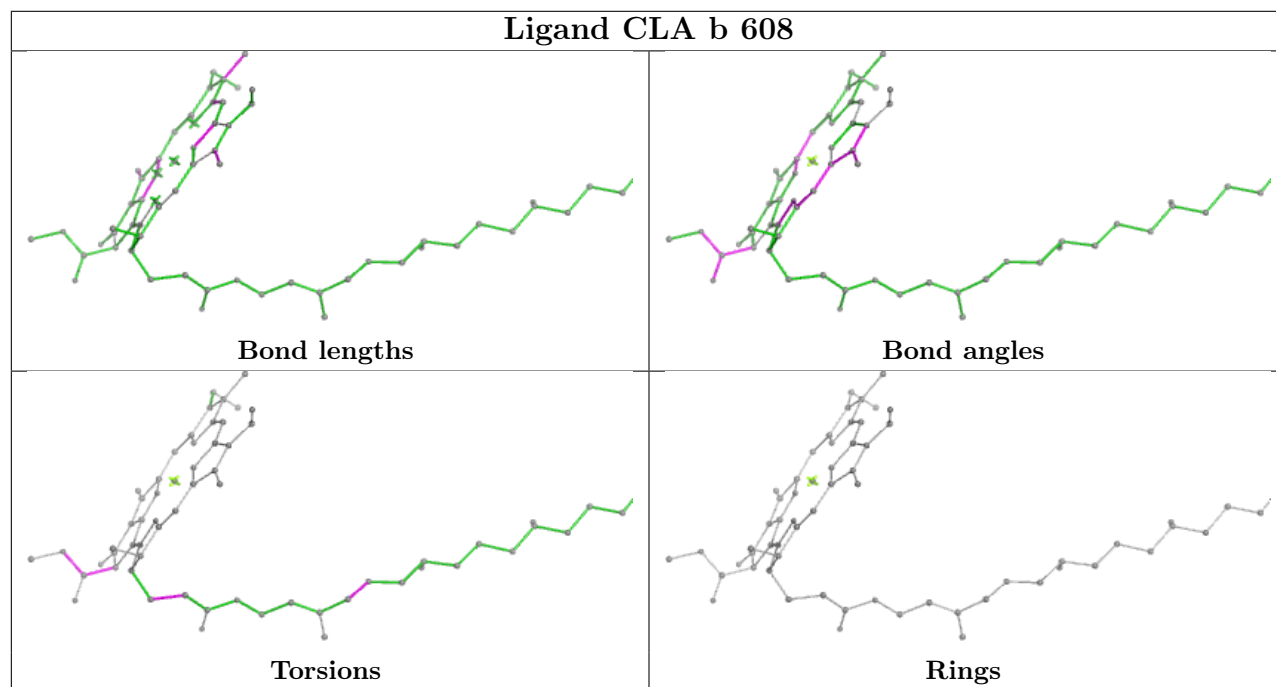
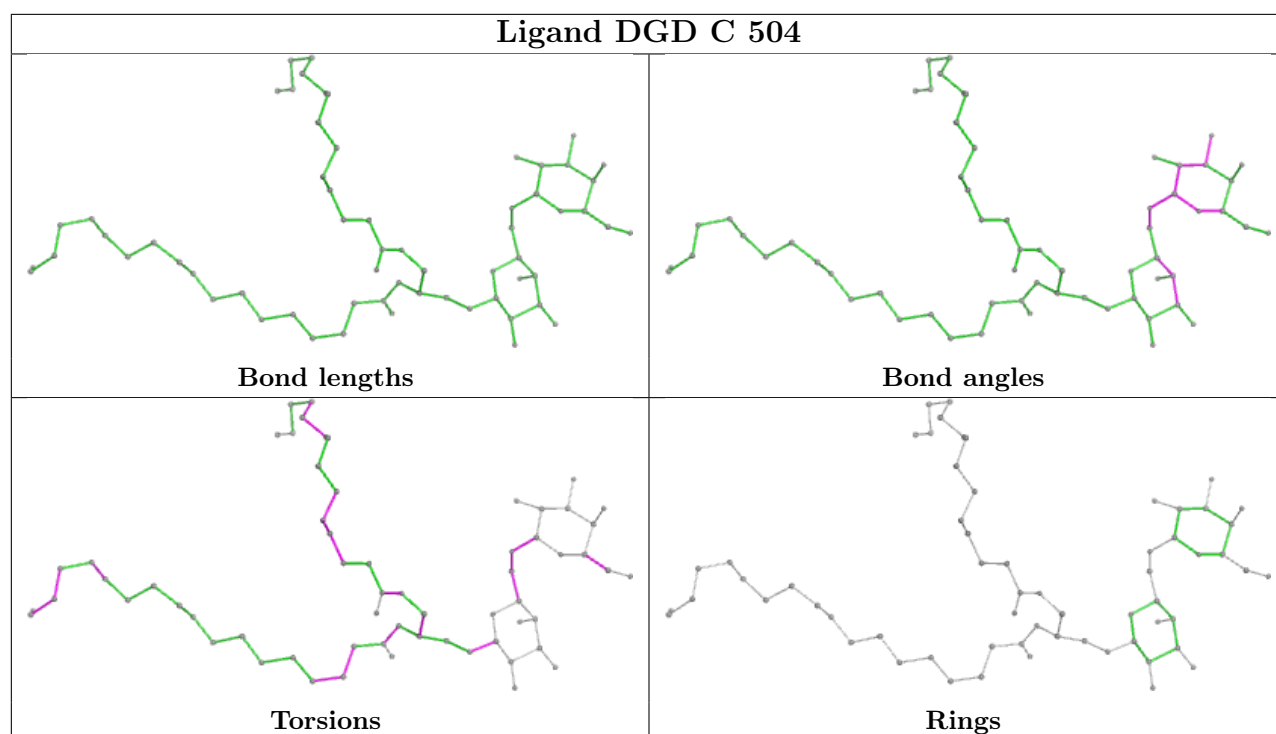
Ligand SQD d 408

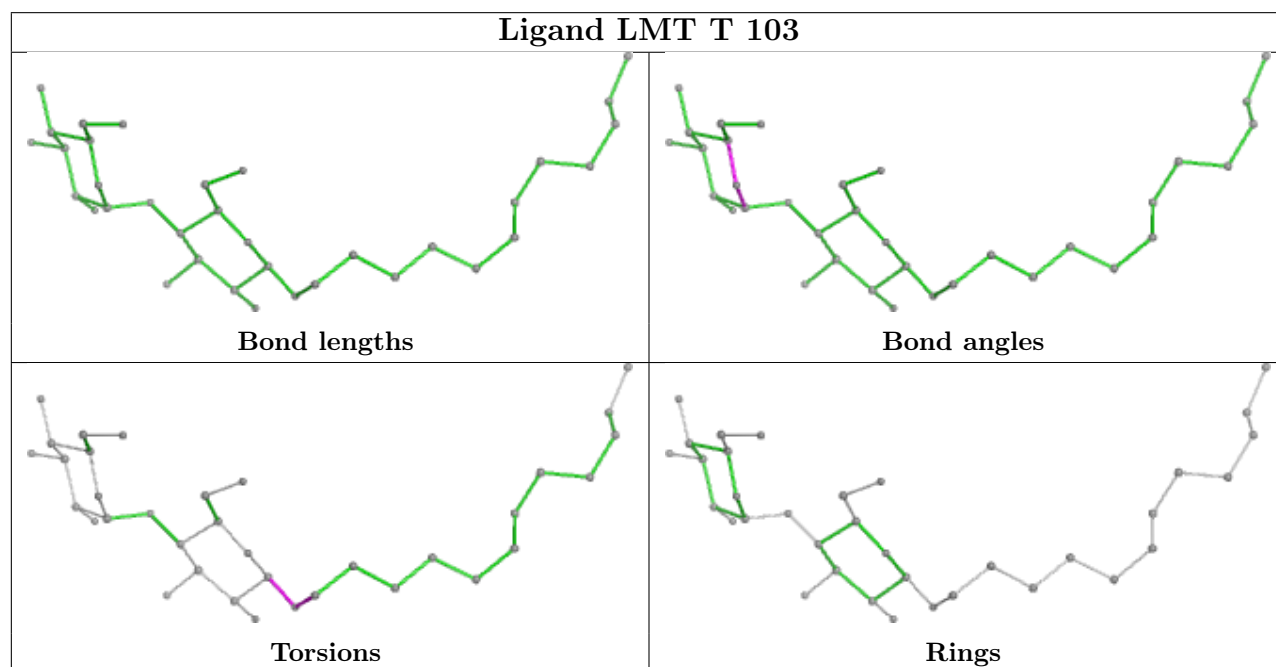
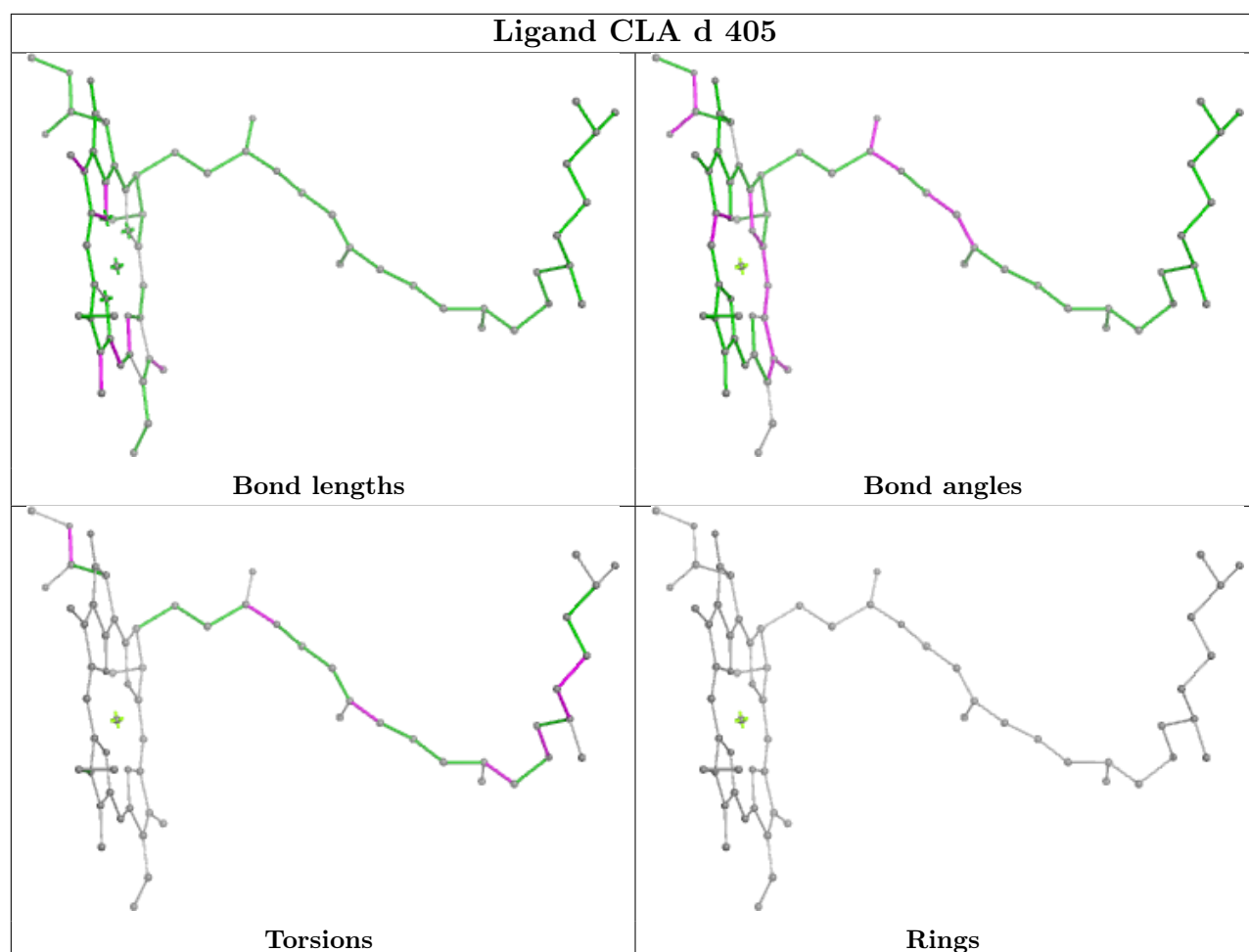


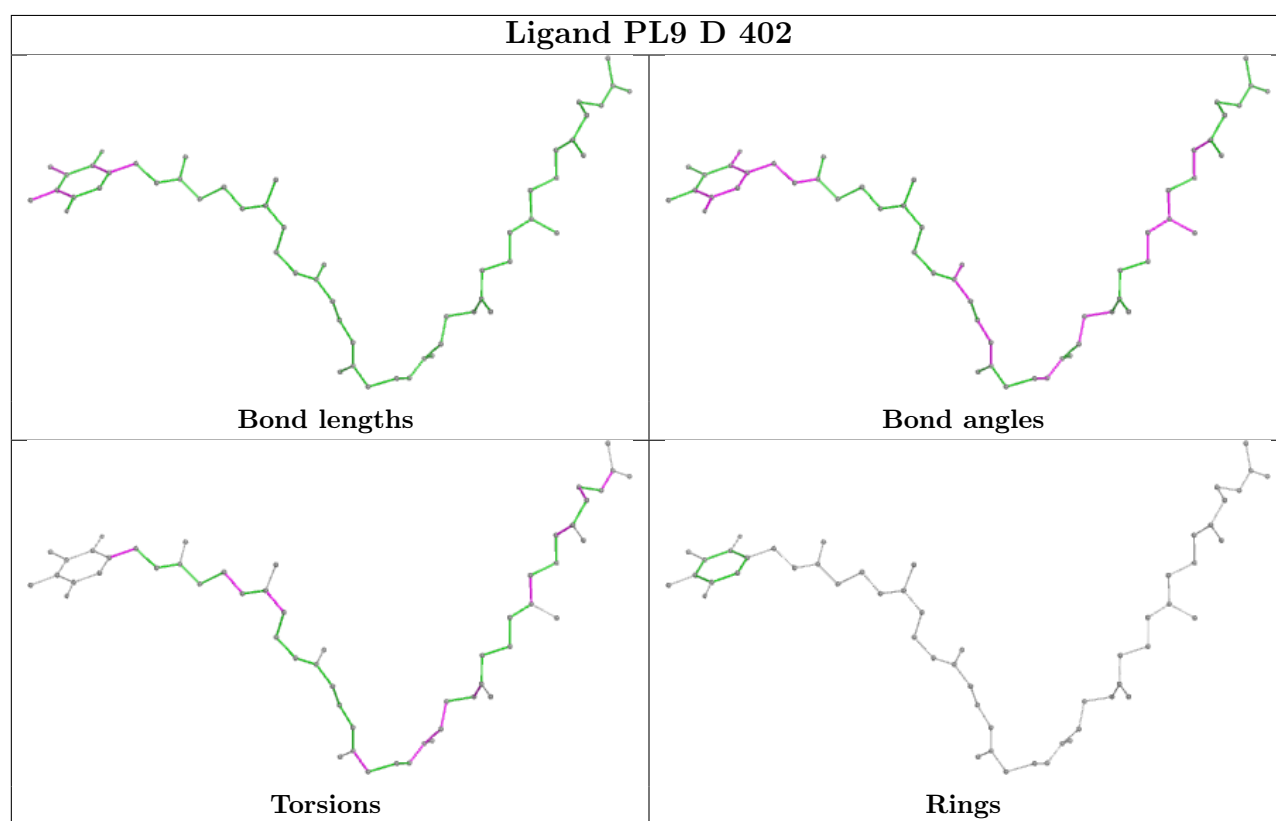
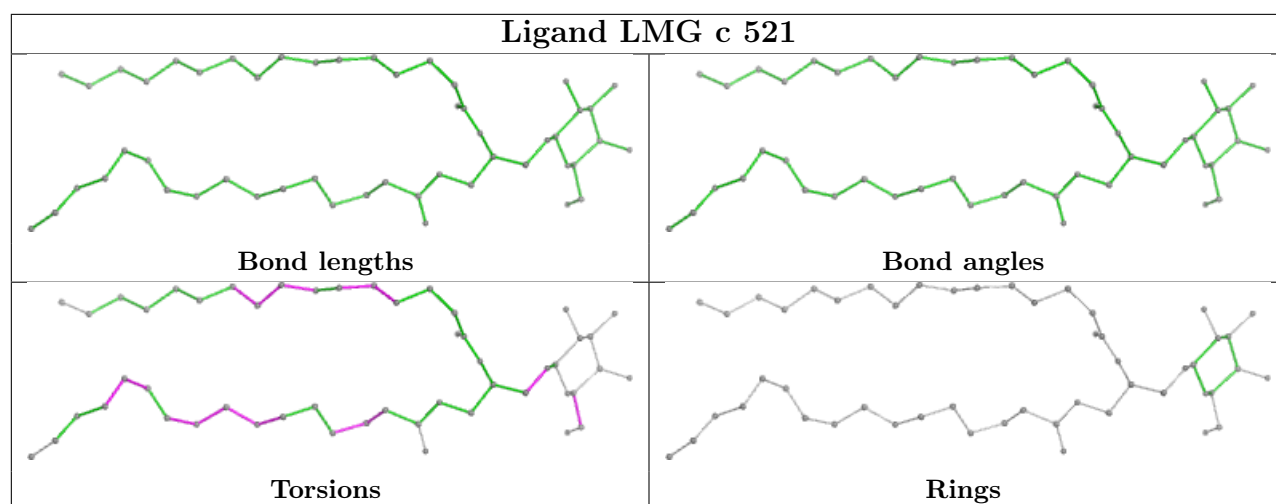
Ligand CLA B 602

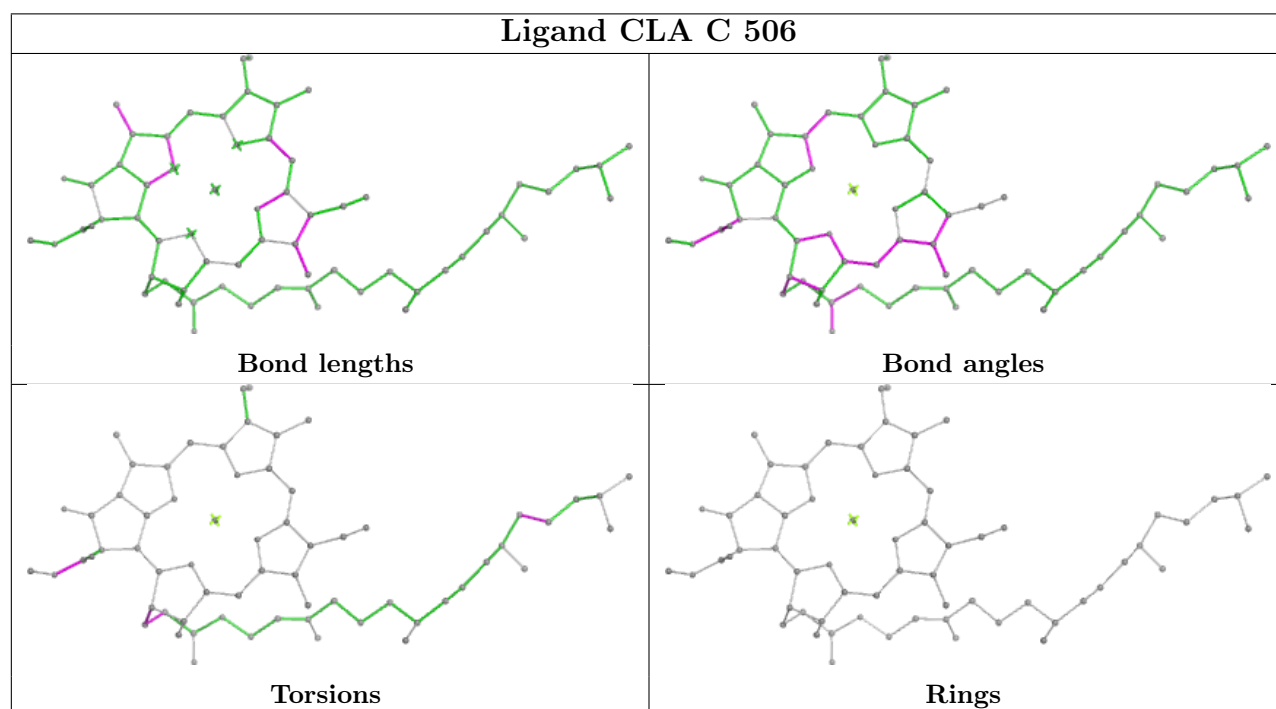
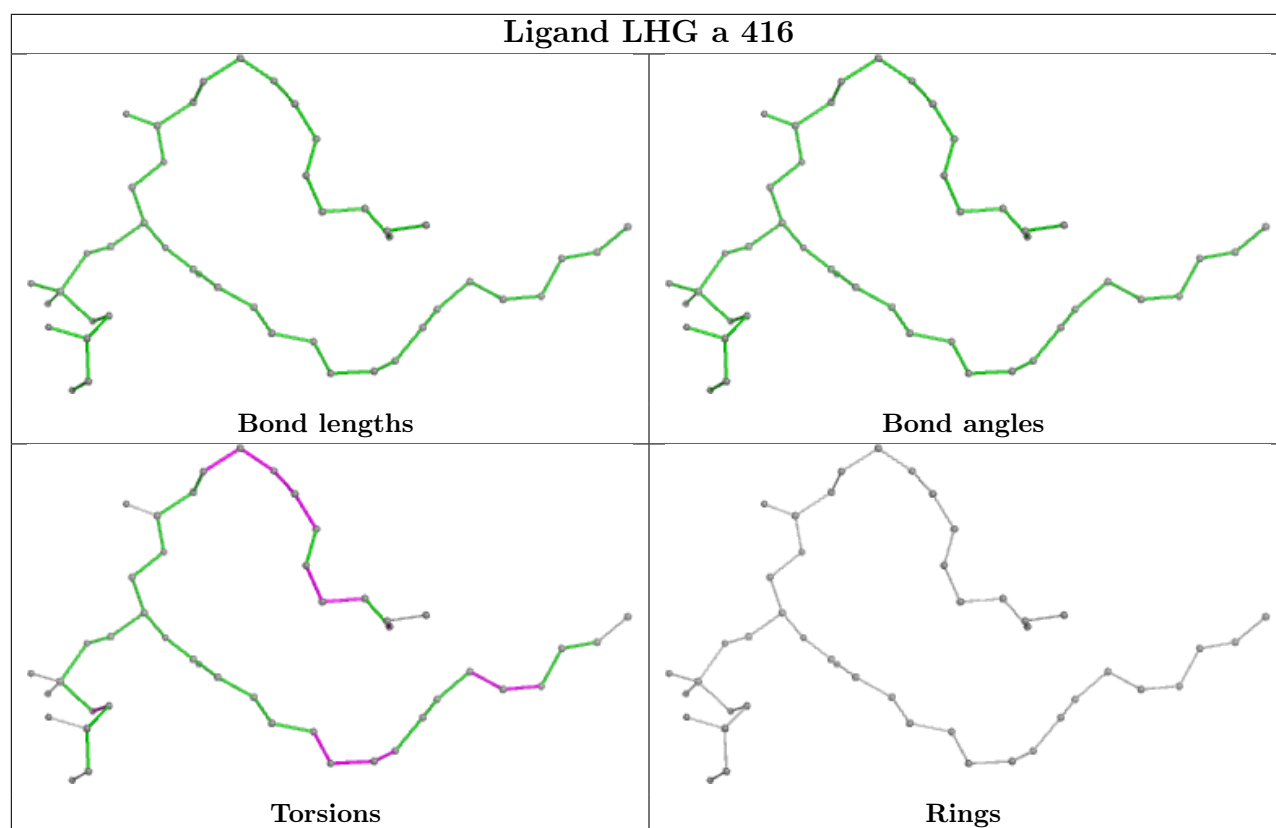


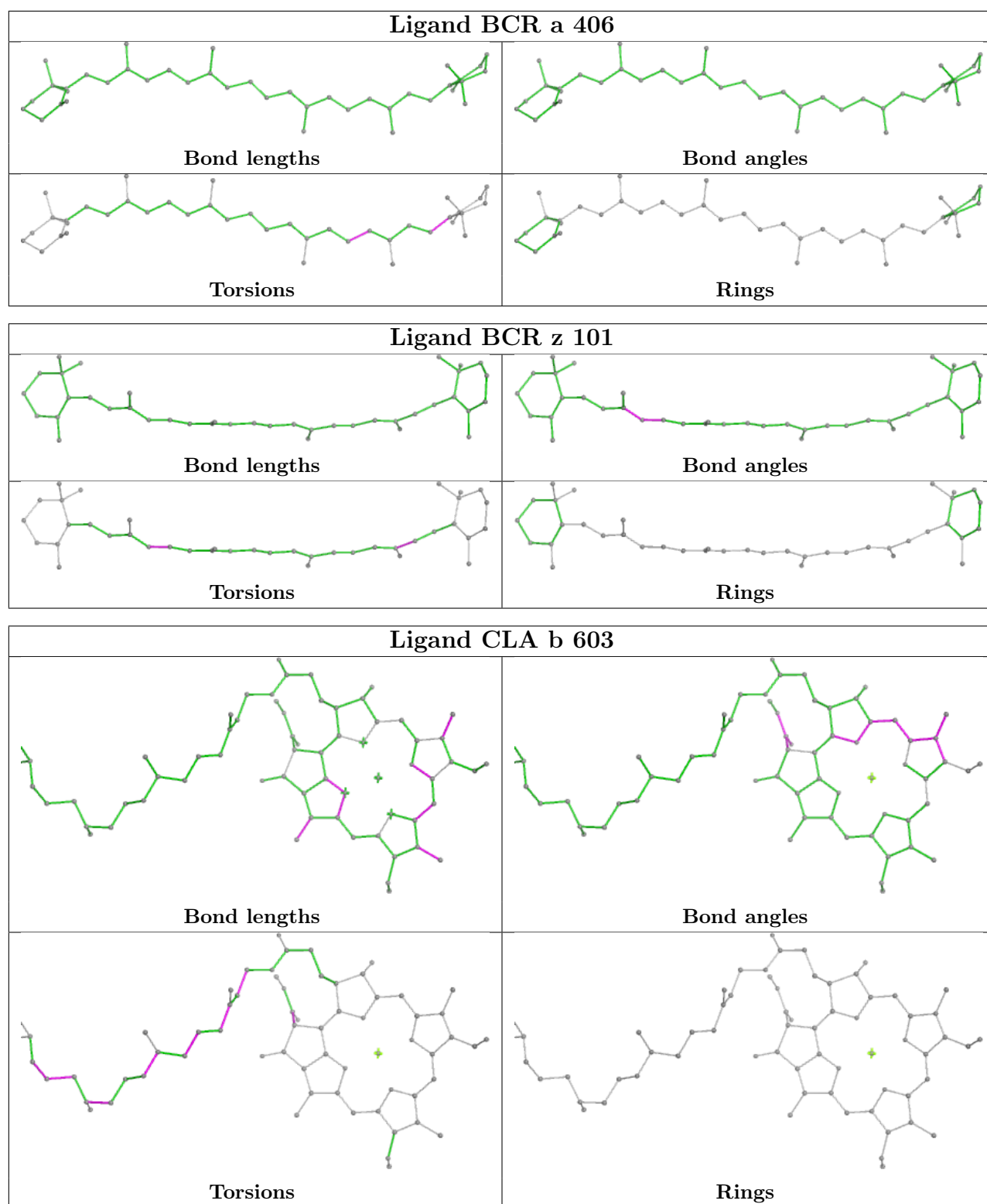


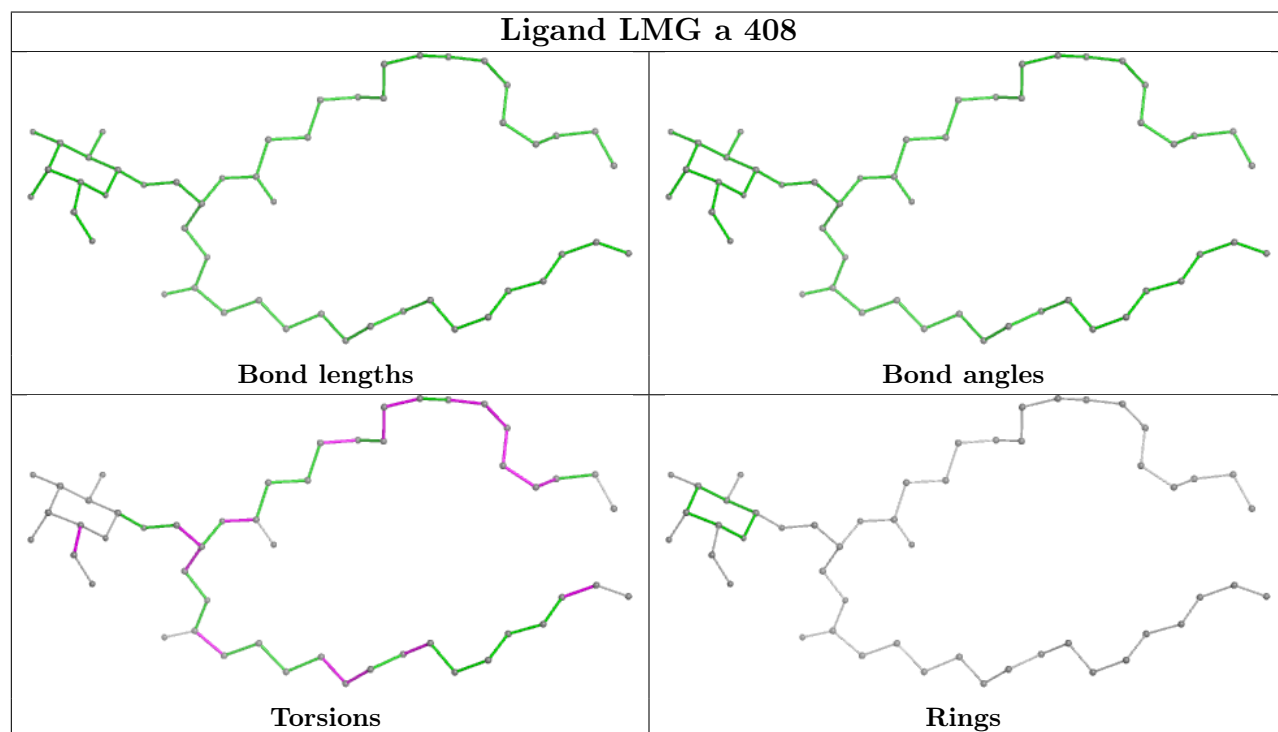
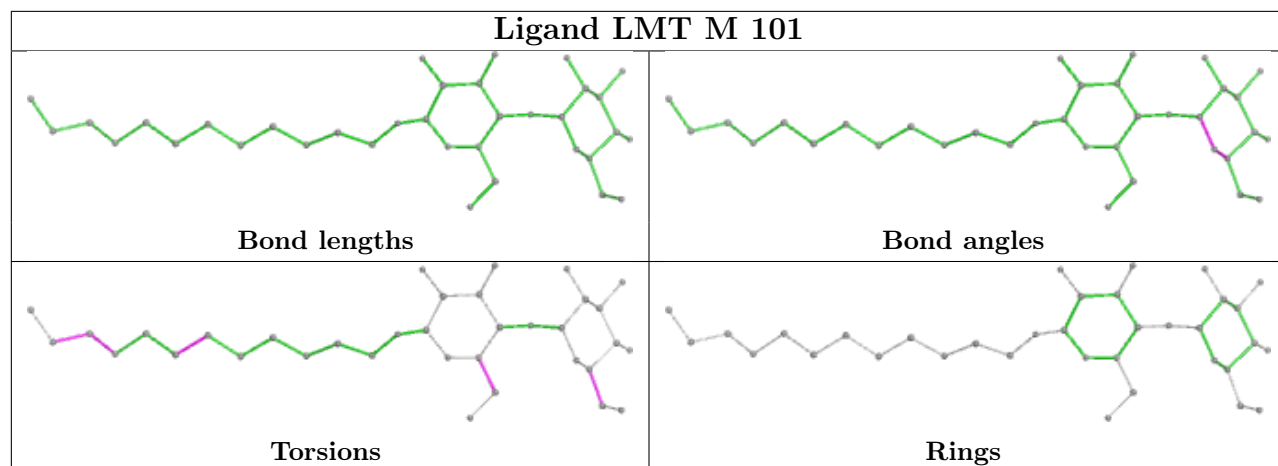




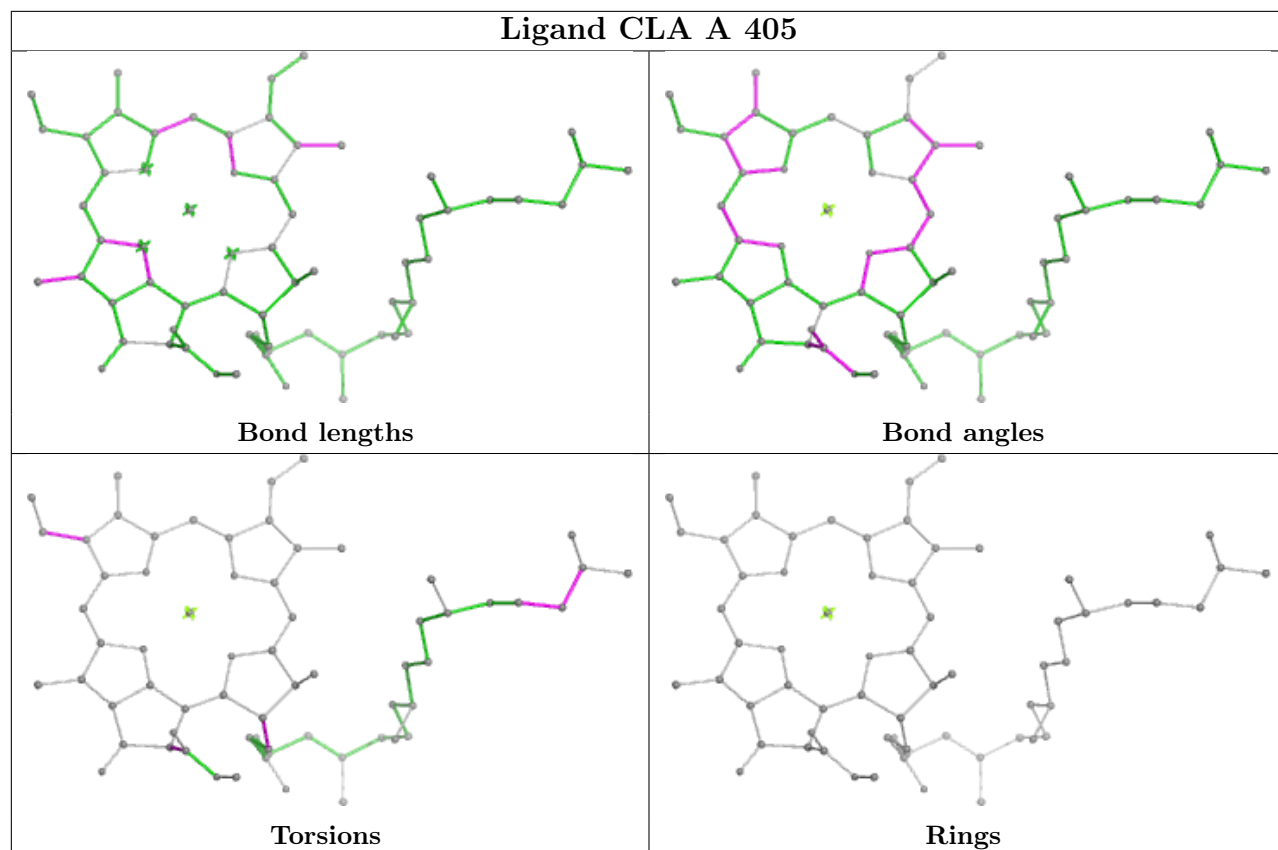




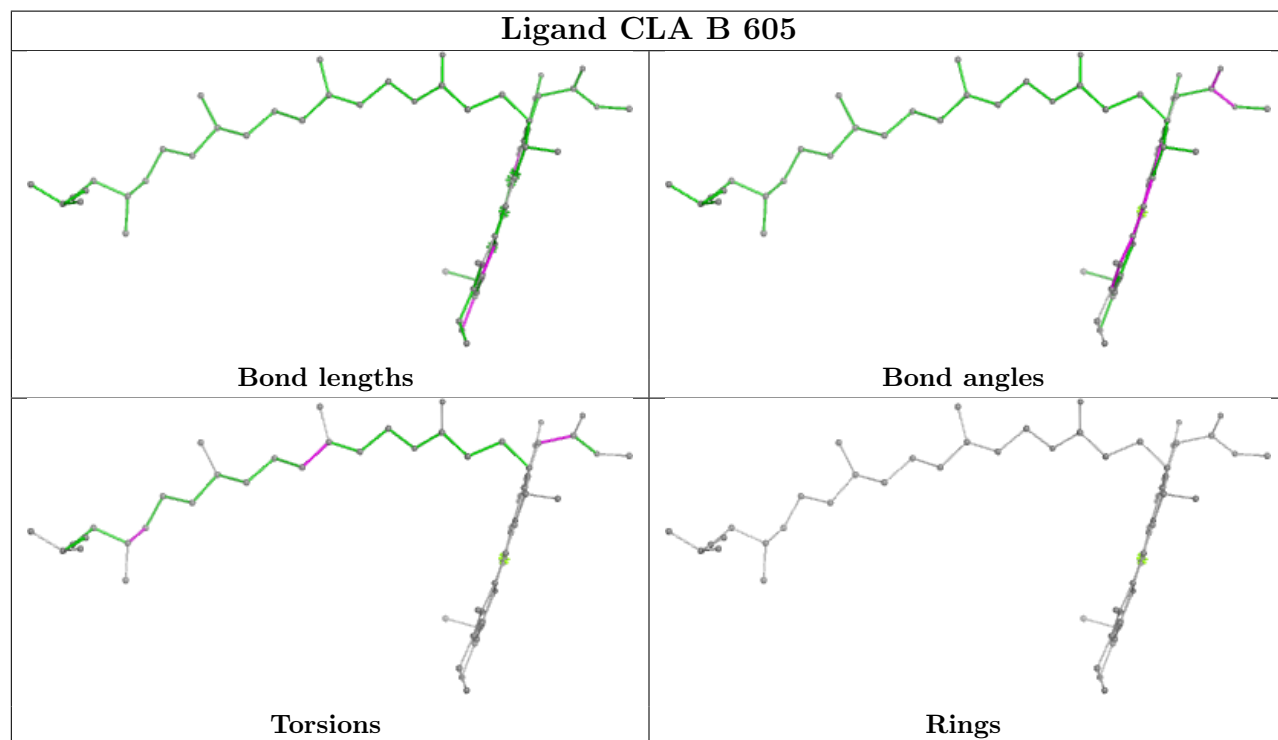


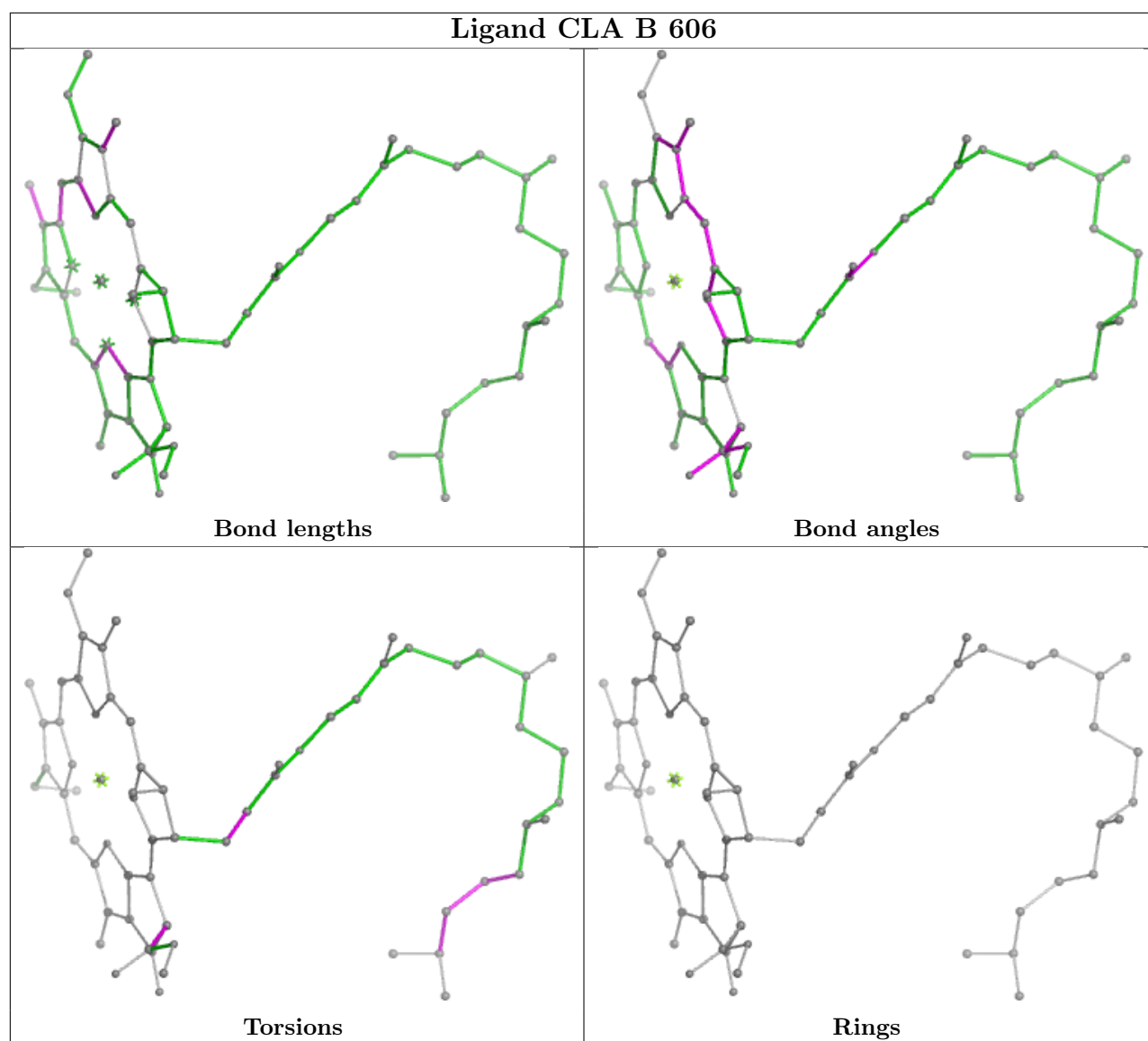


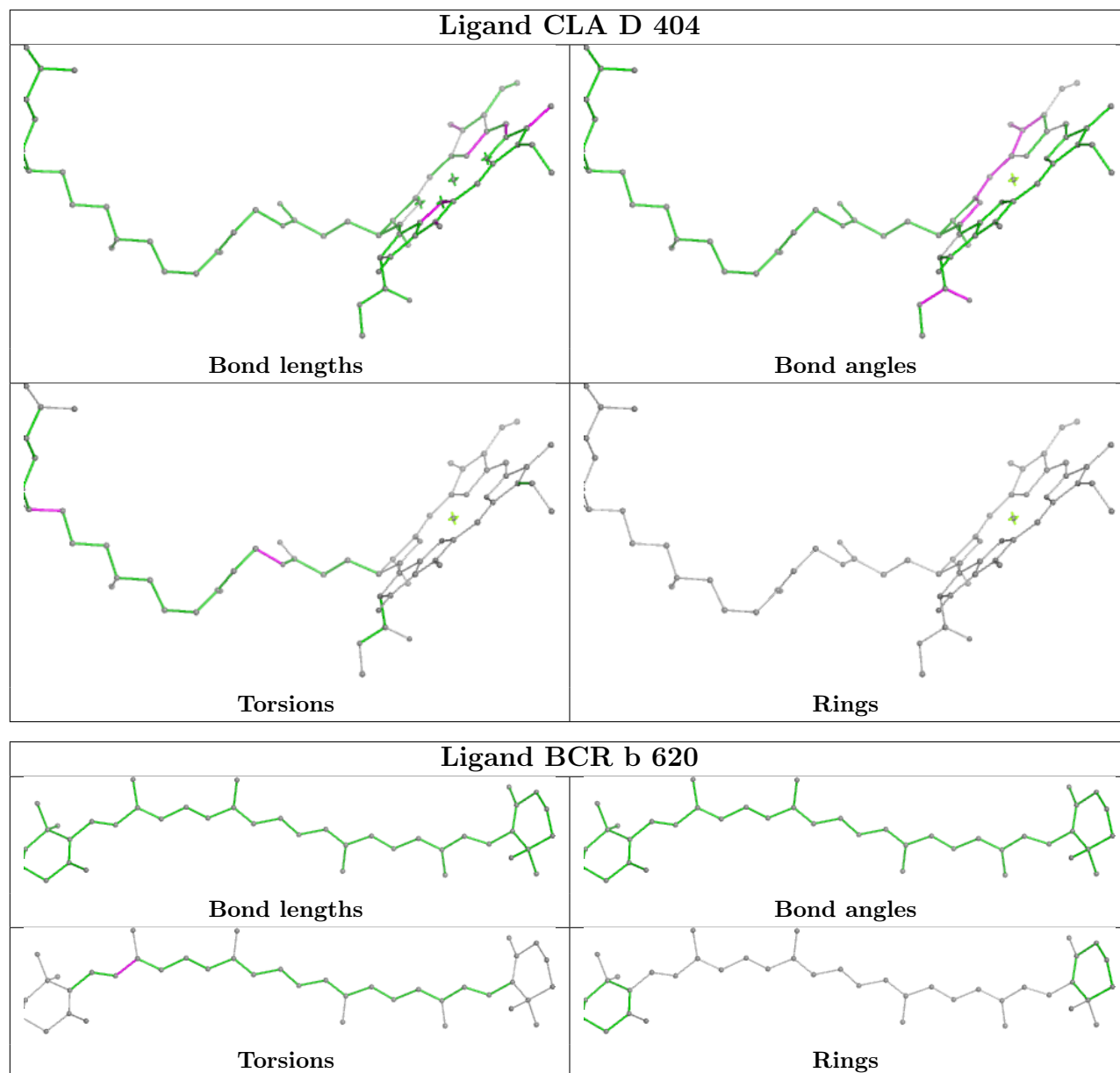
Ligand CLA A 405

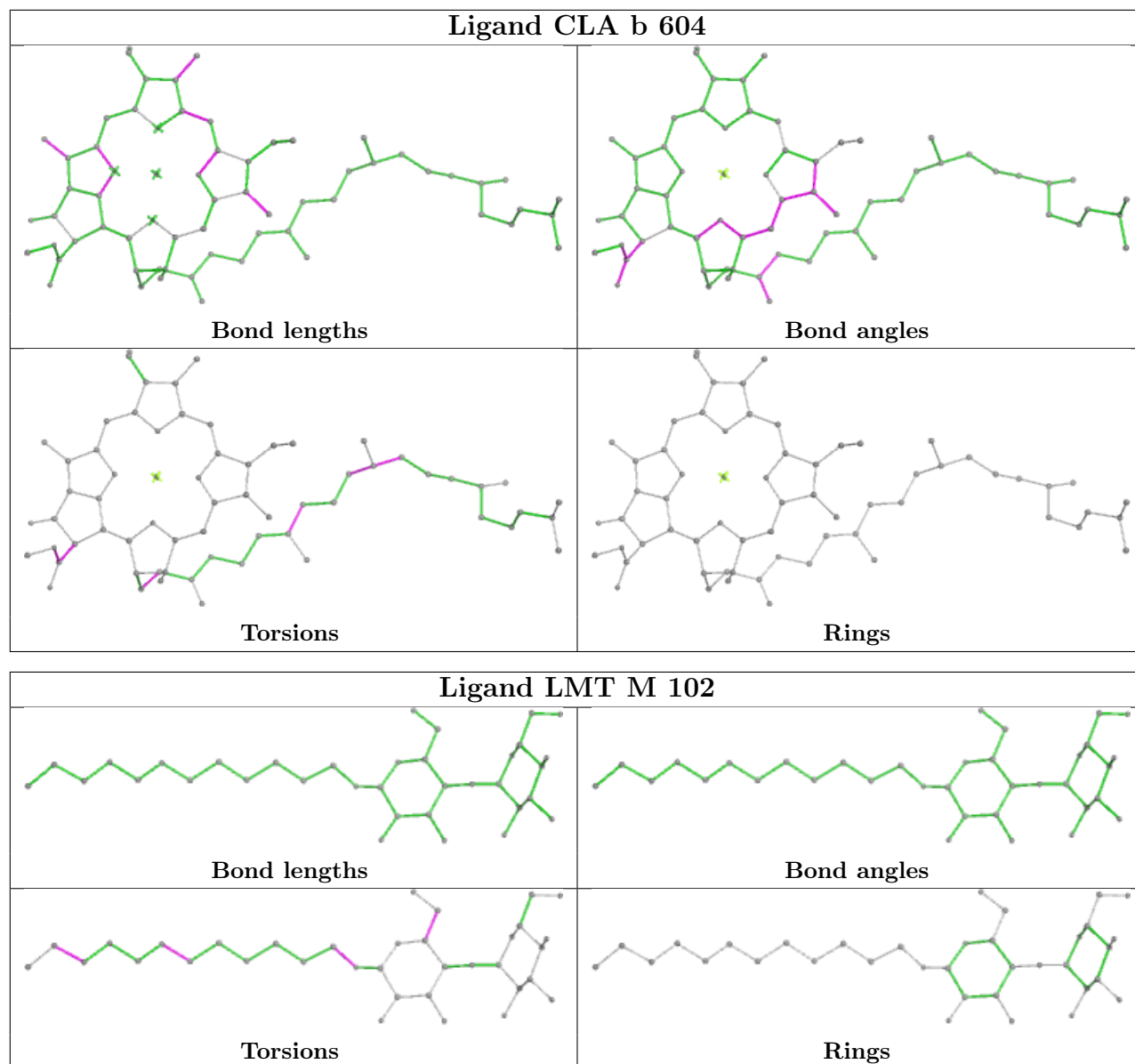


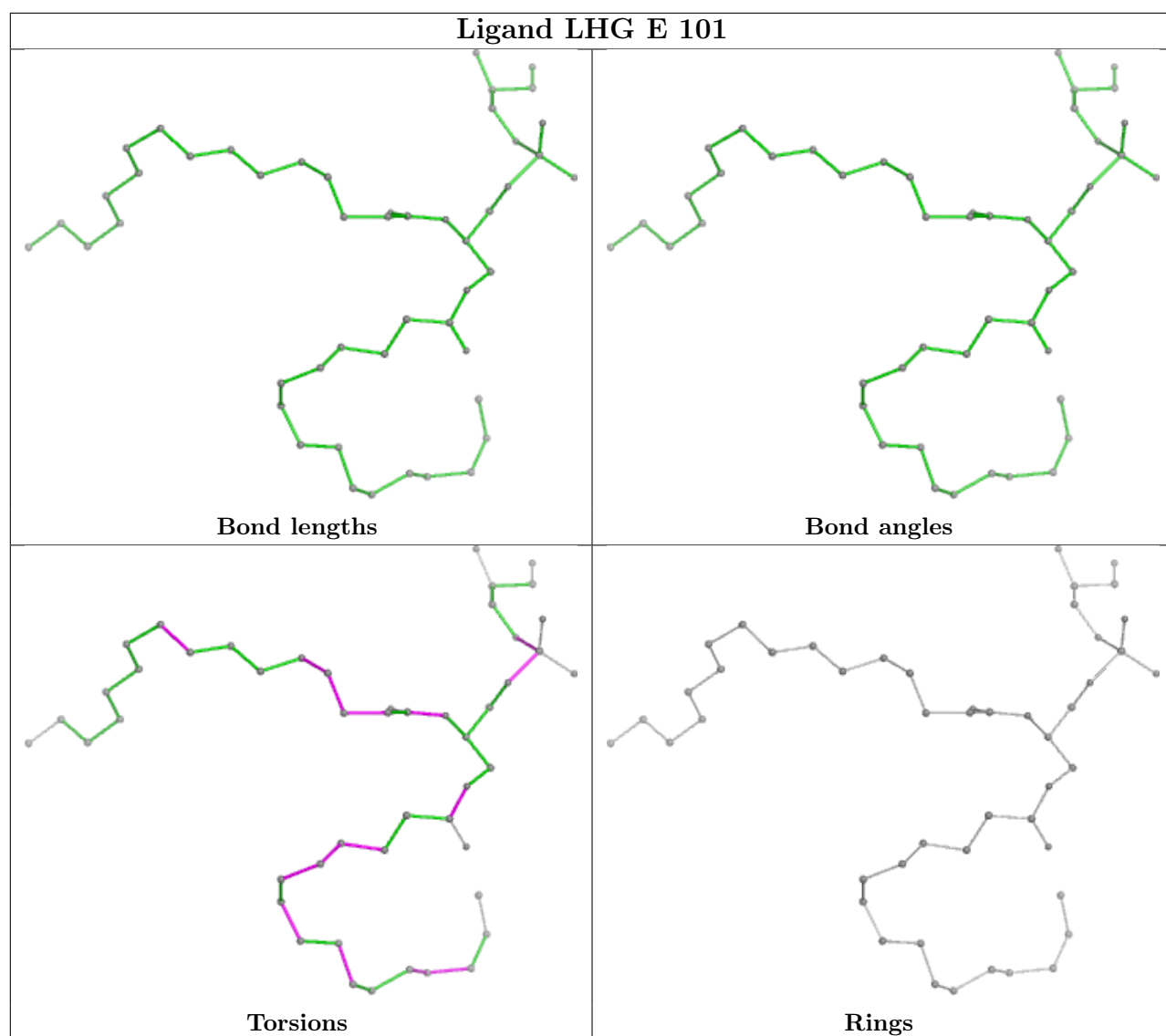
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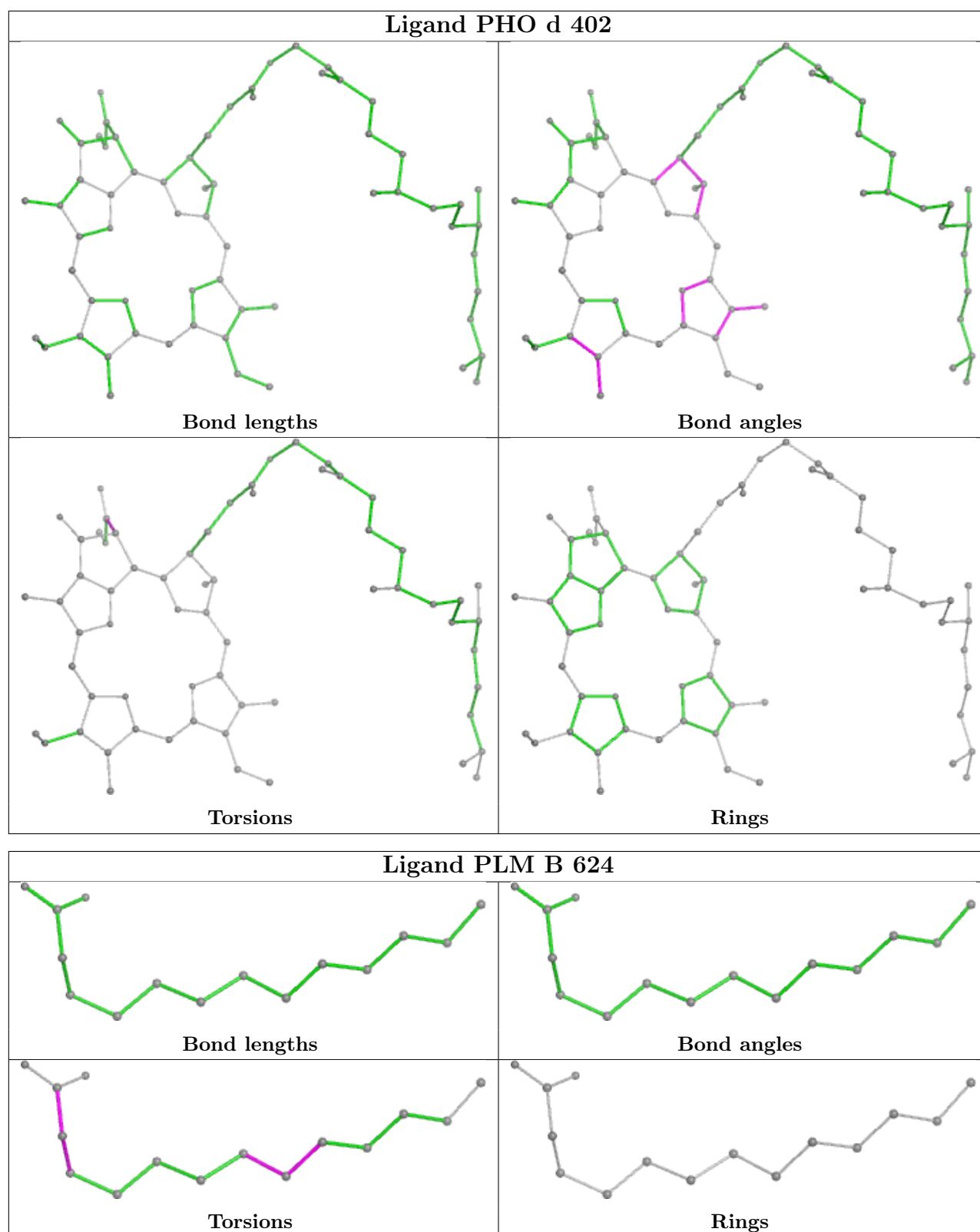


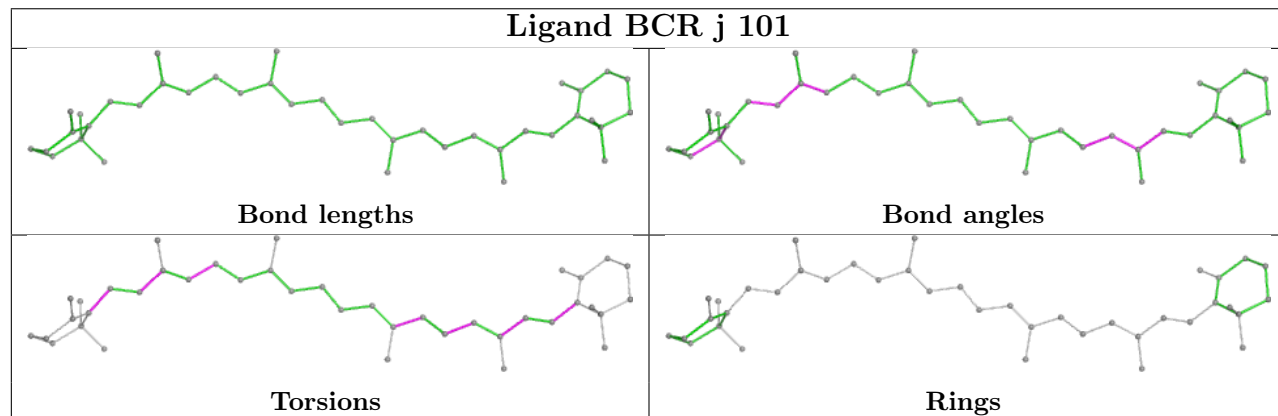
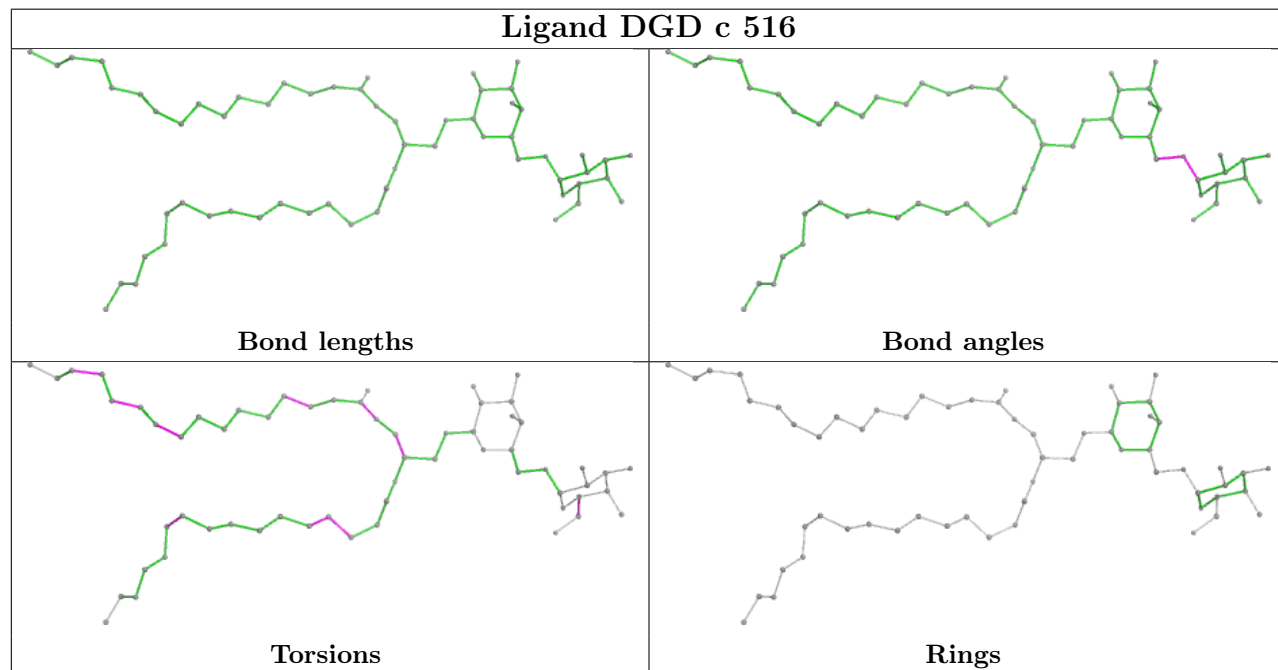
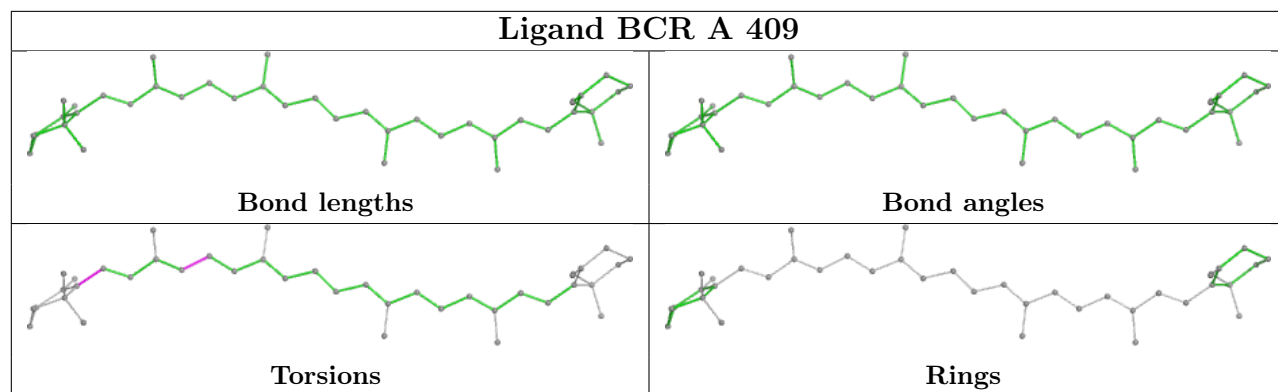


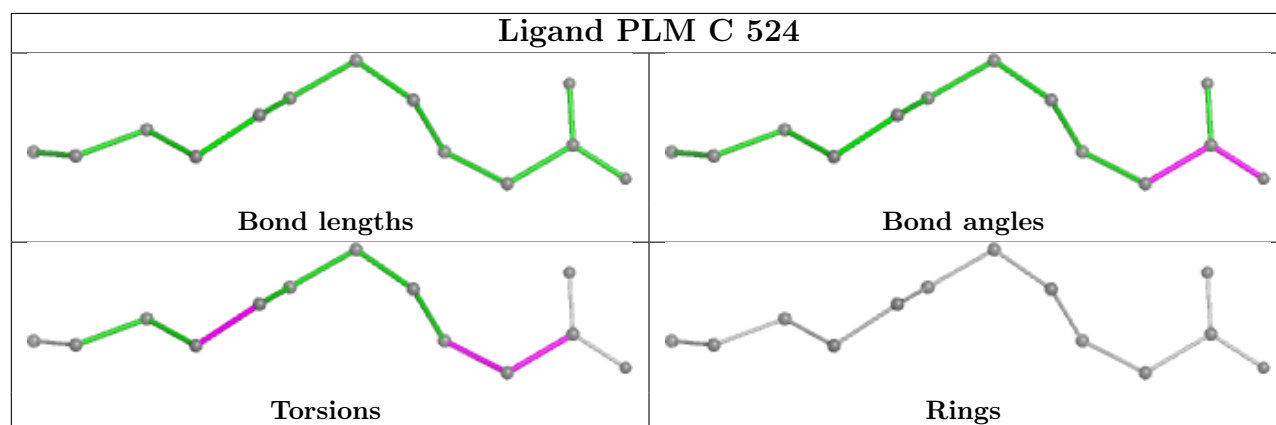
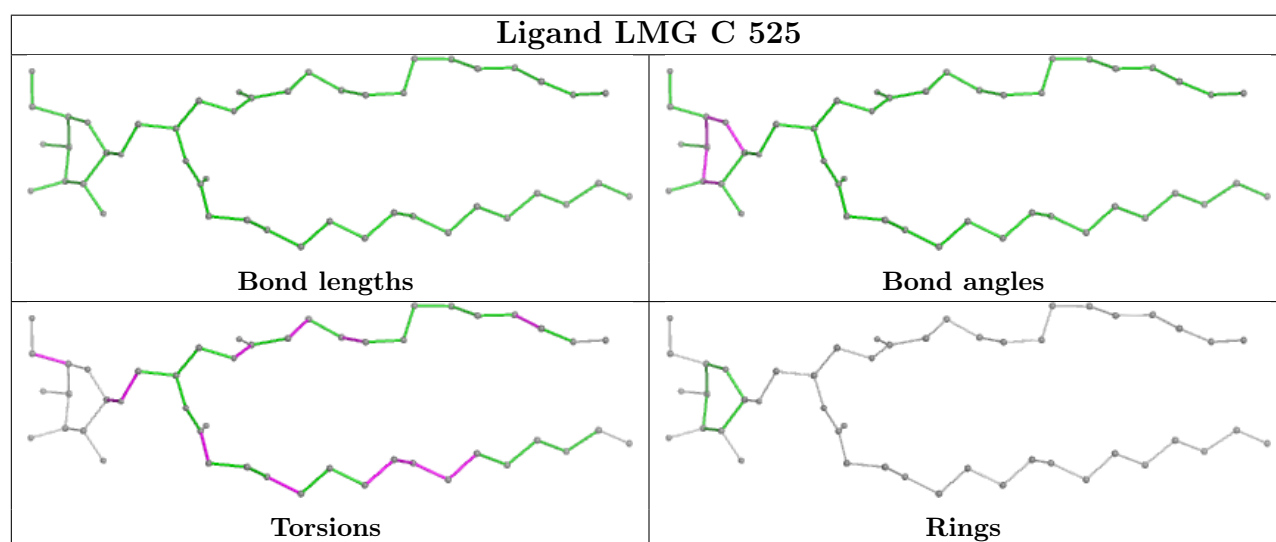
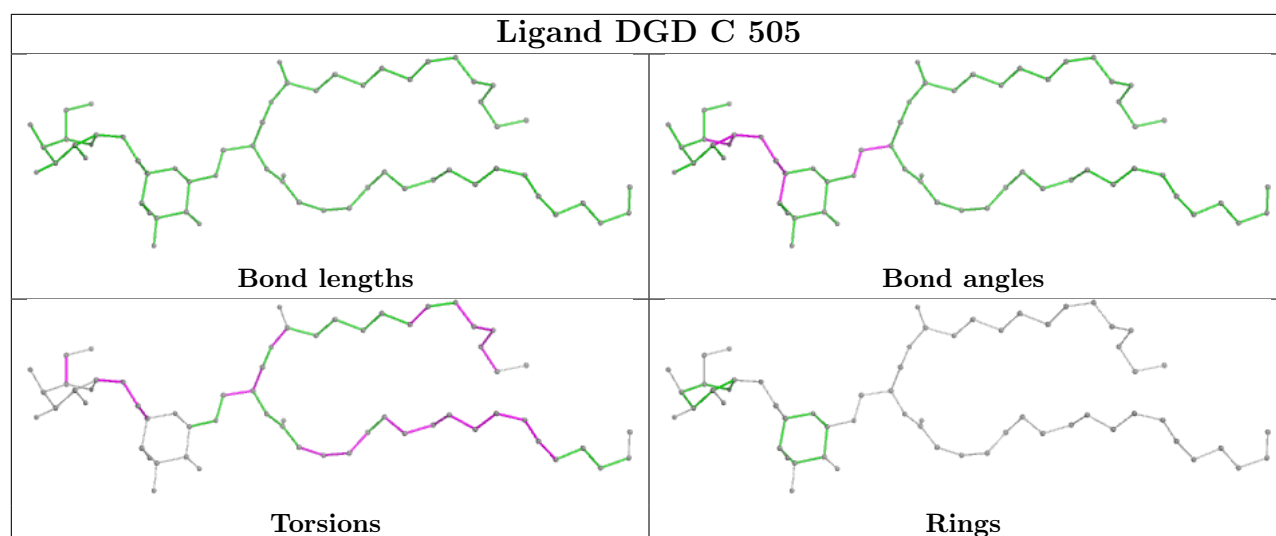


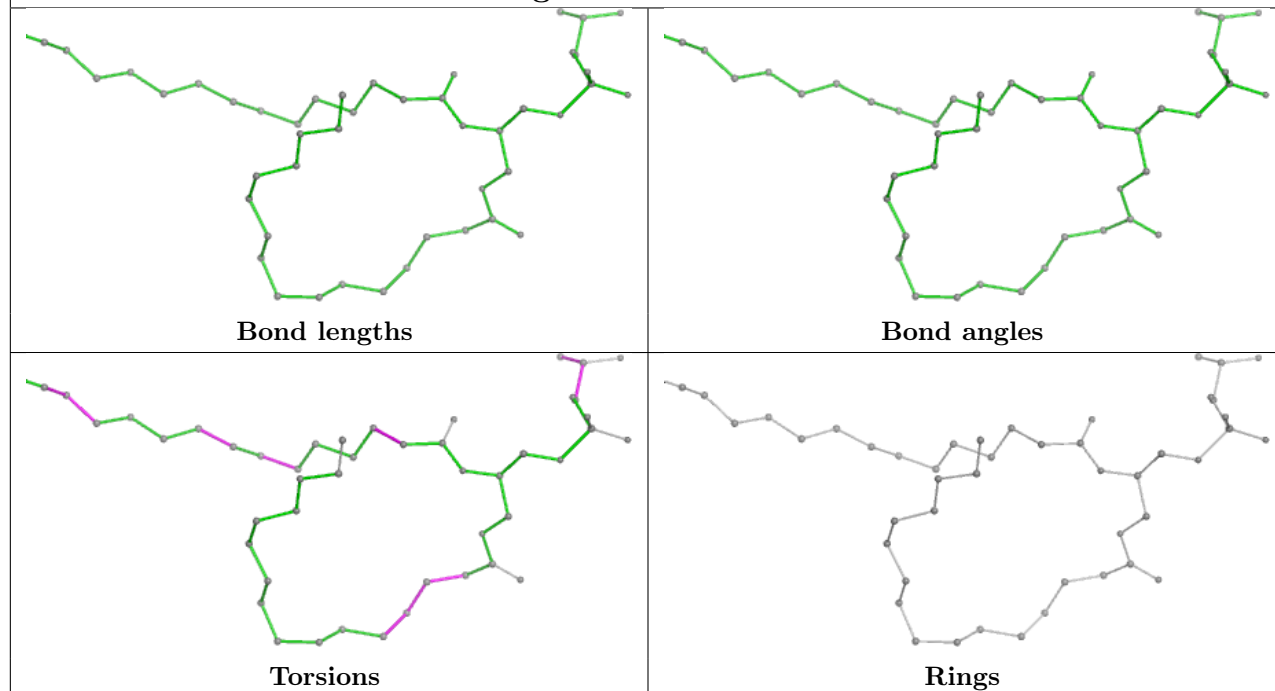
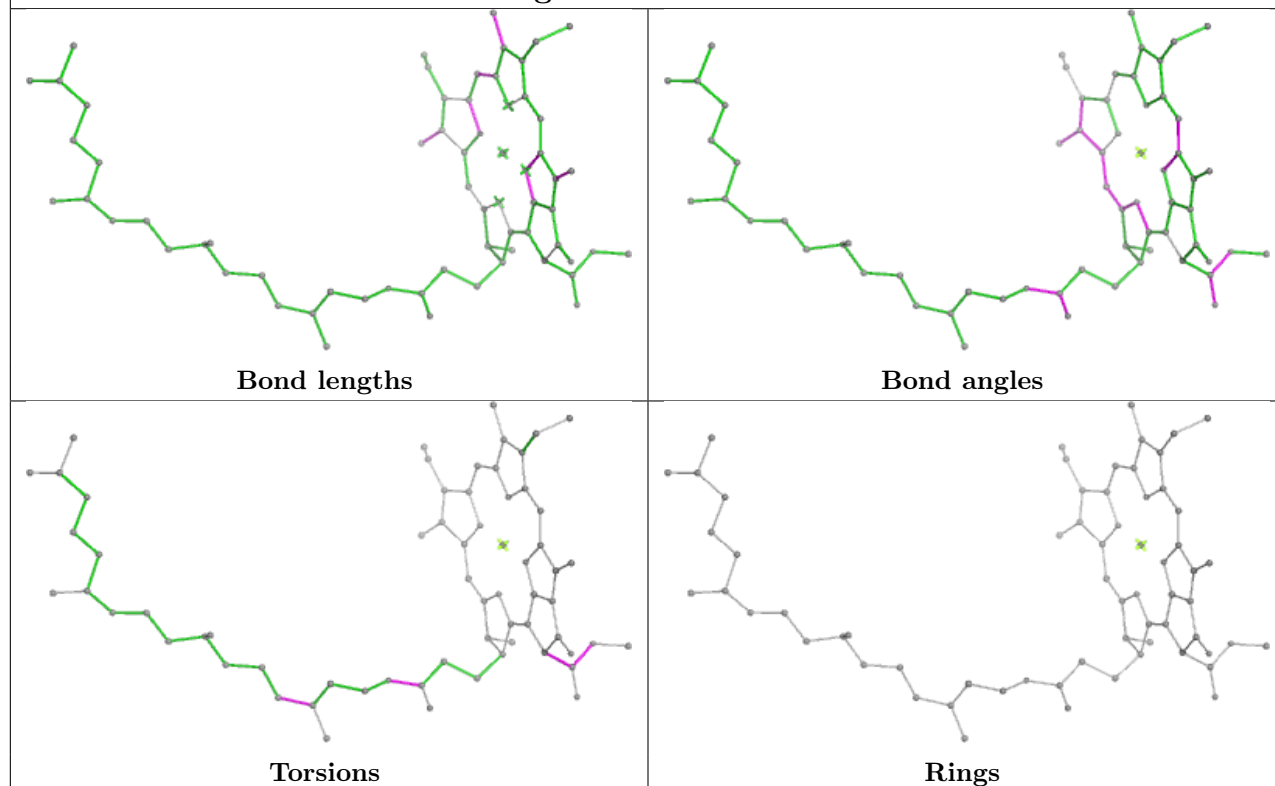


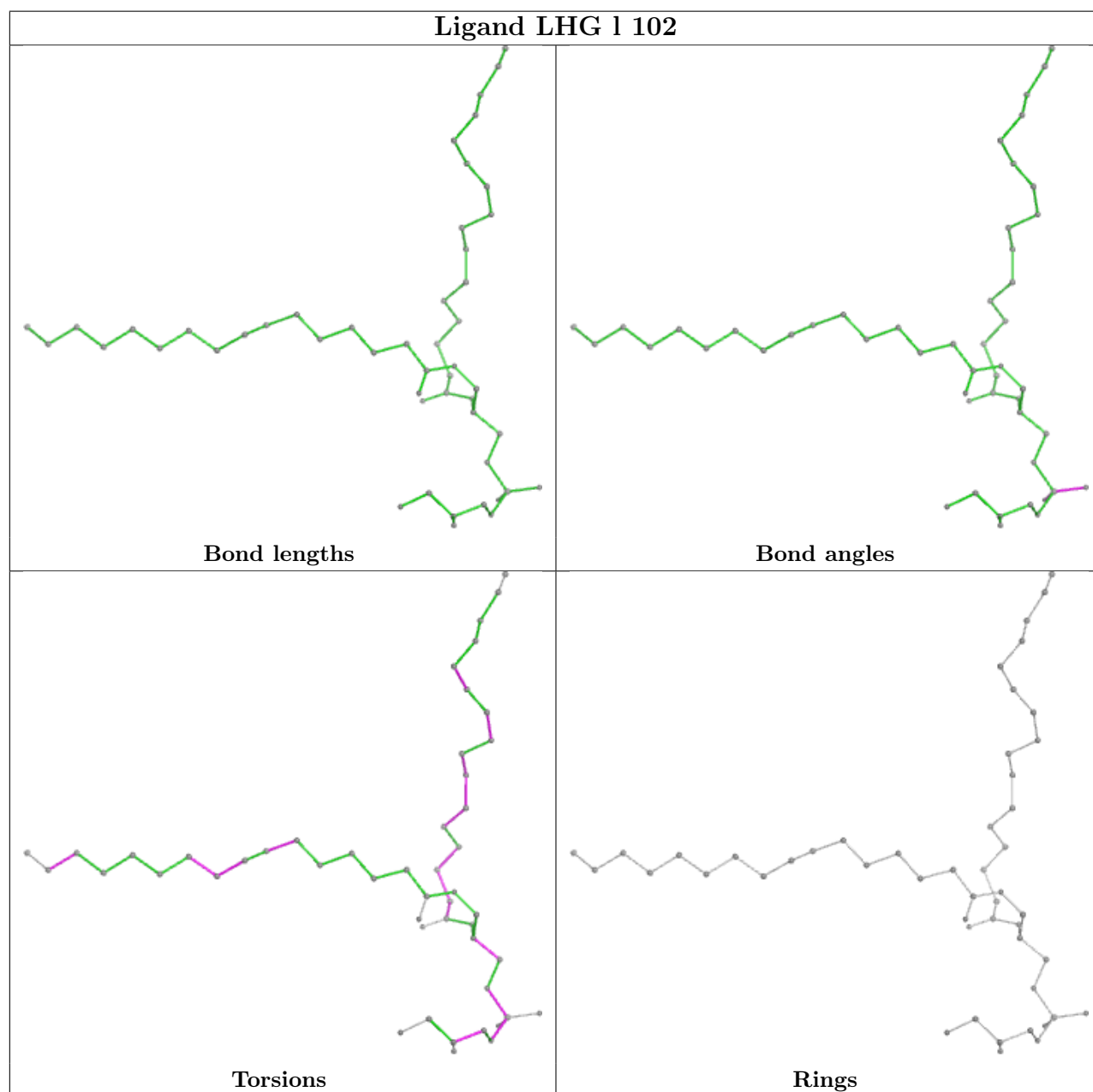
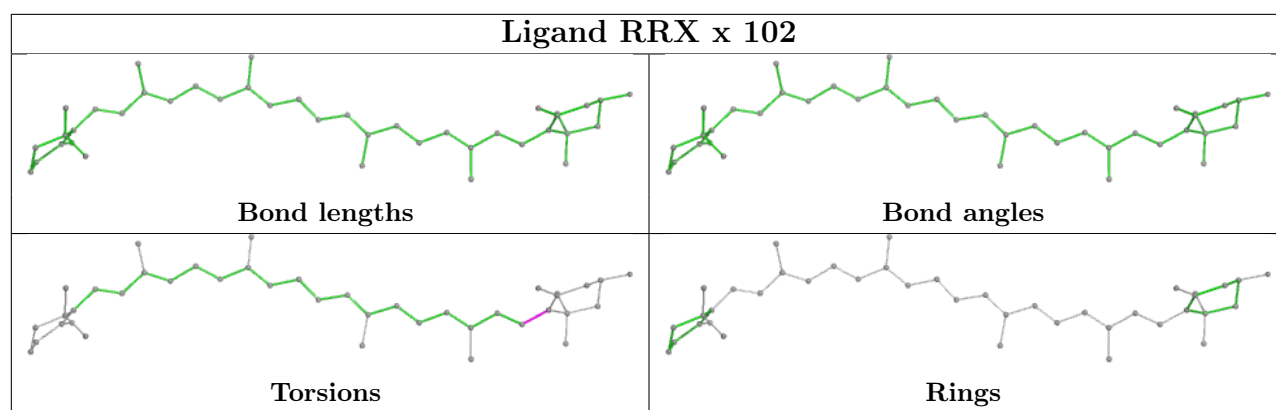




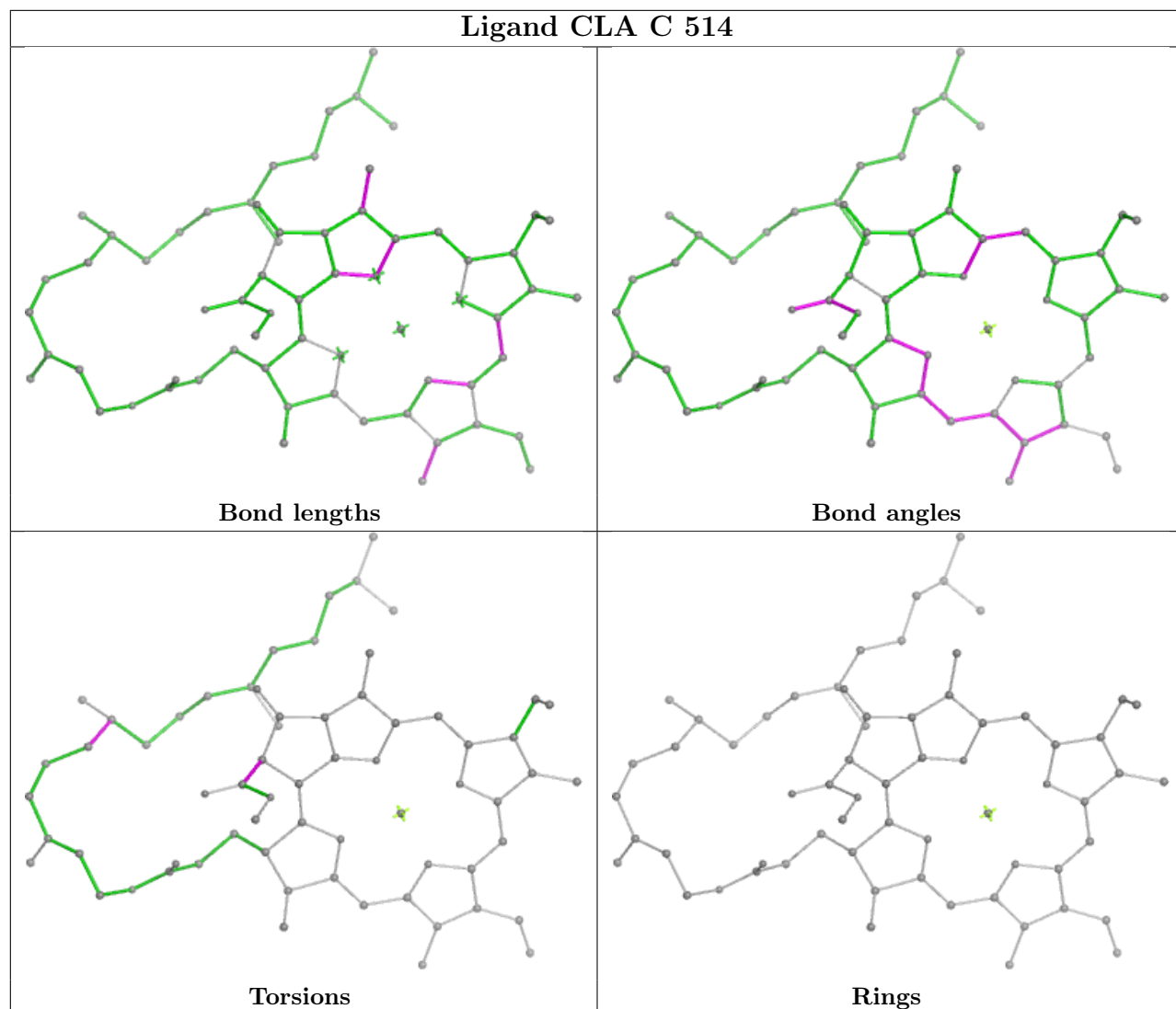


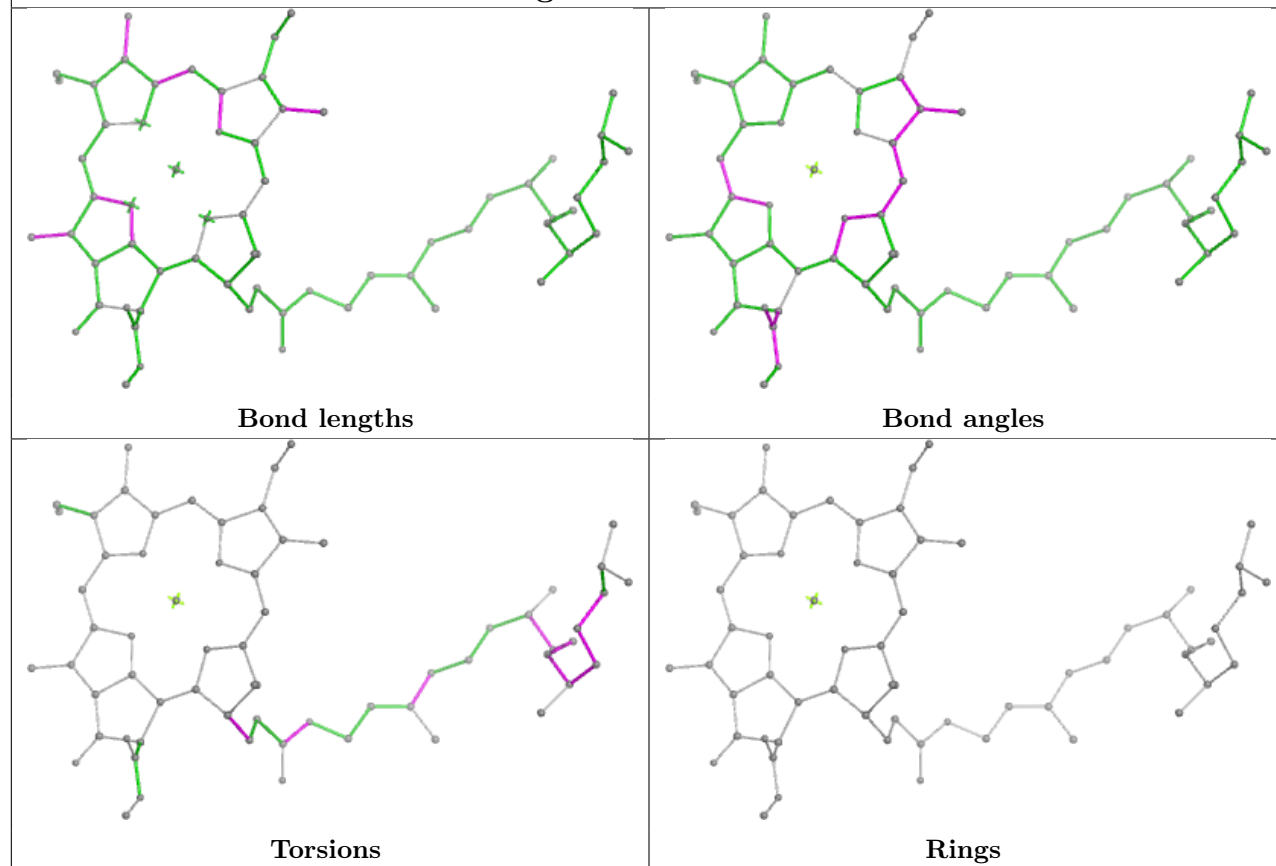
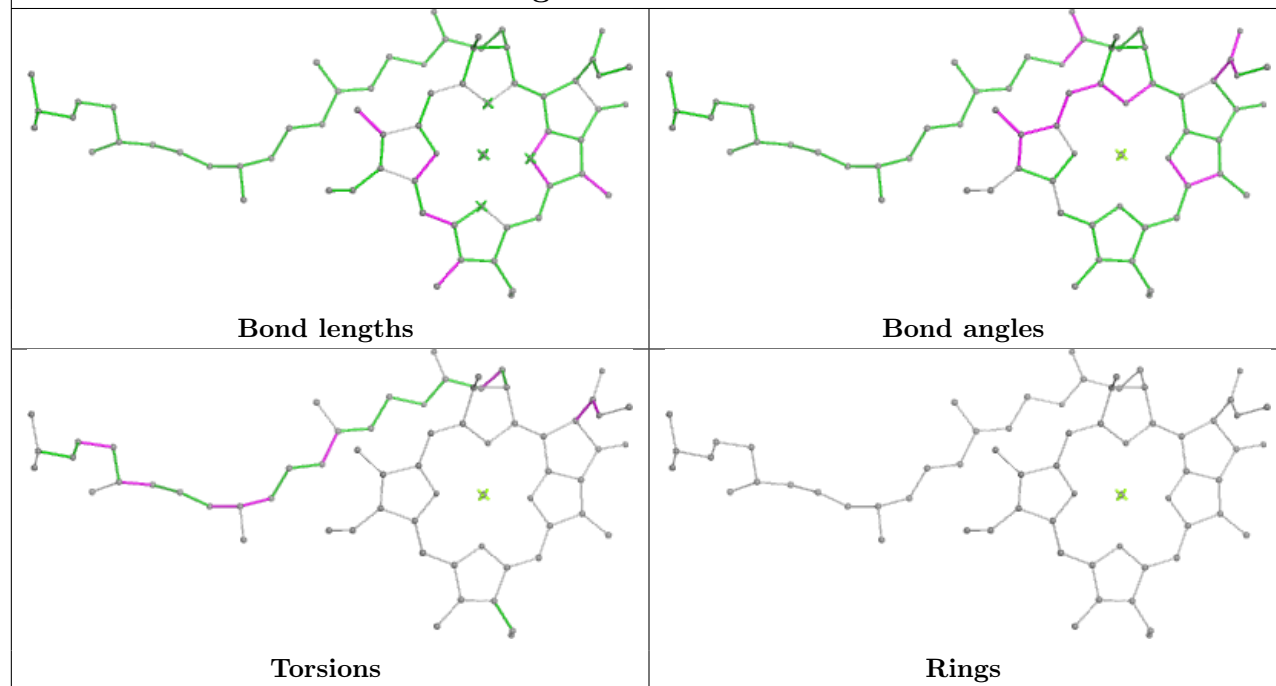


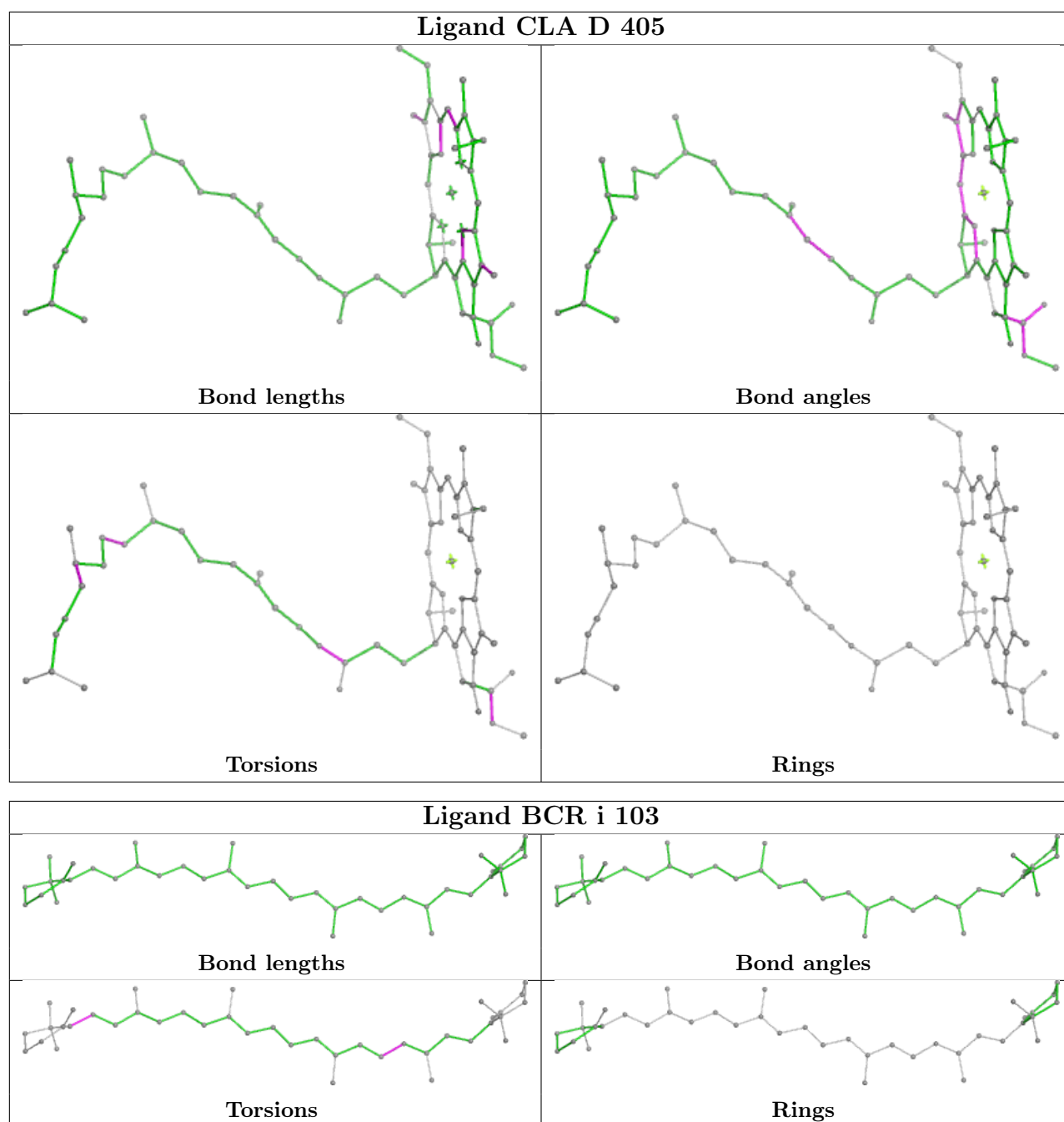
Ligand LHG d 409**Ligand CLA b 610**

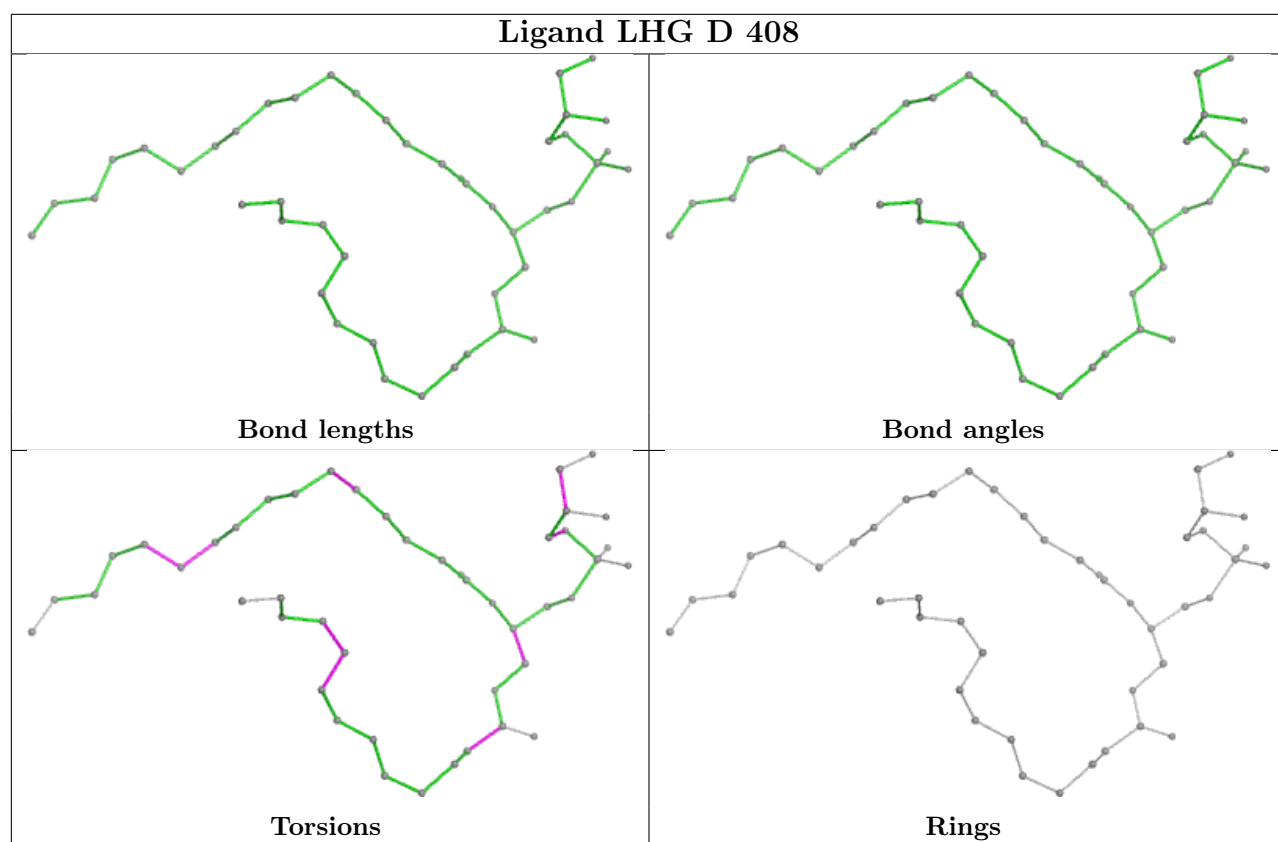


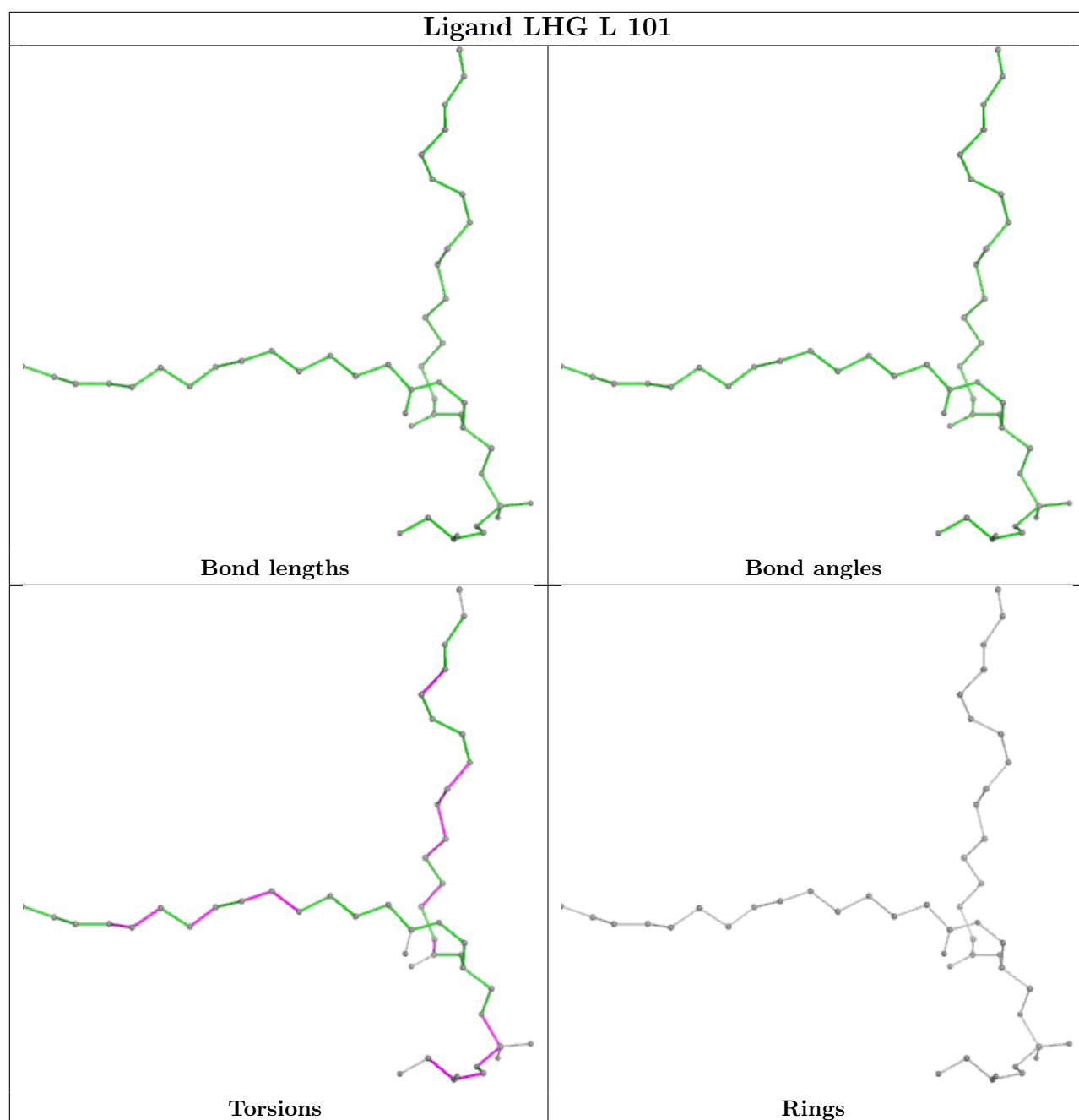
Ligand CLA C 514

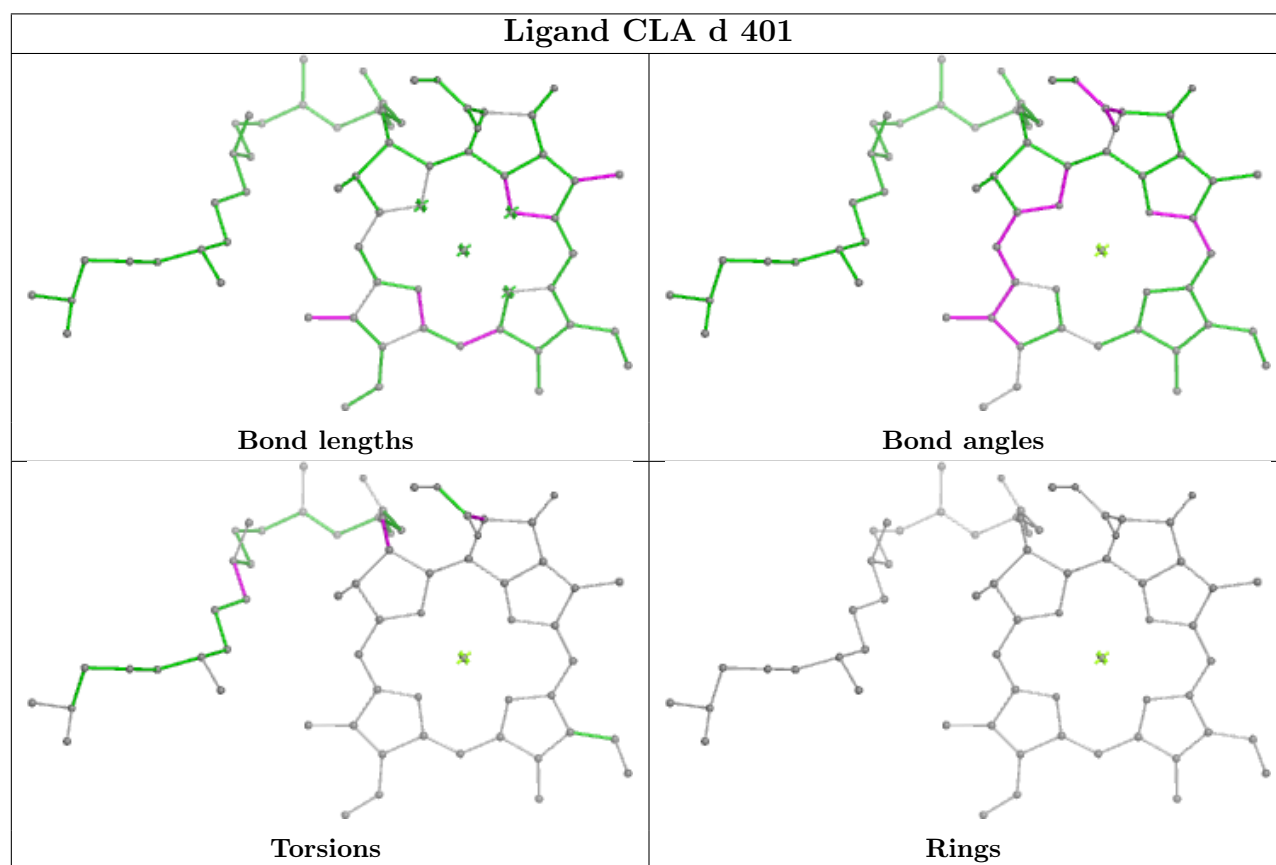
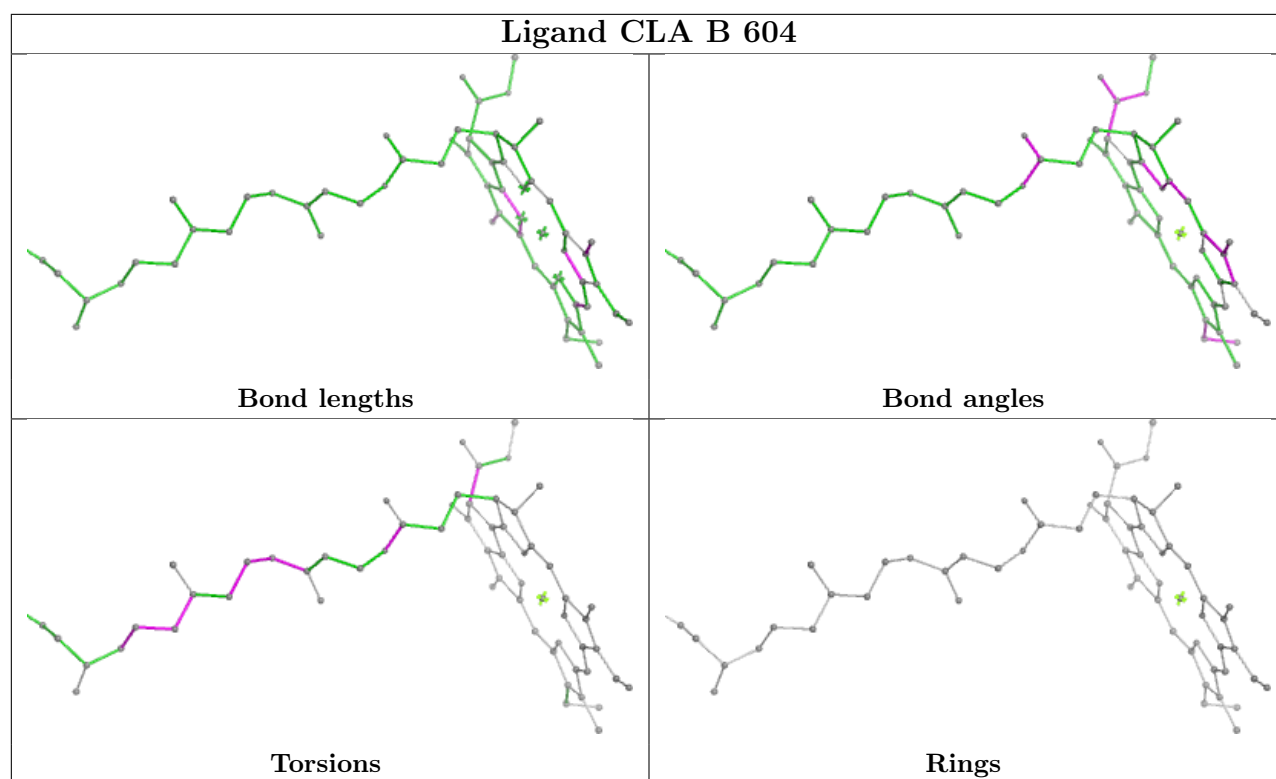


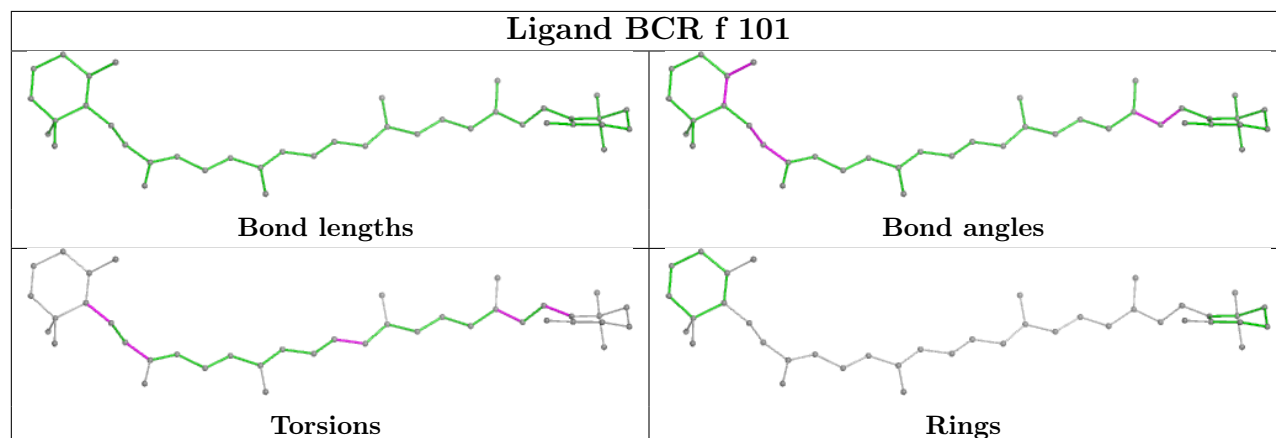
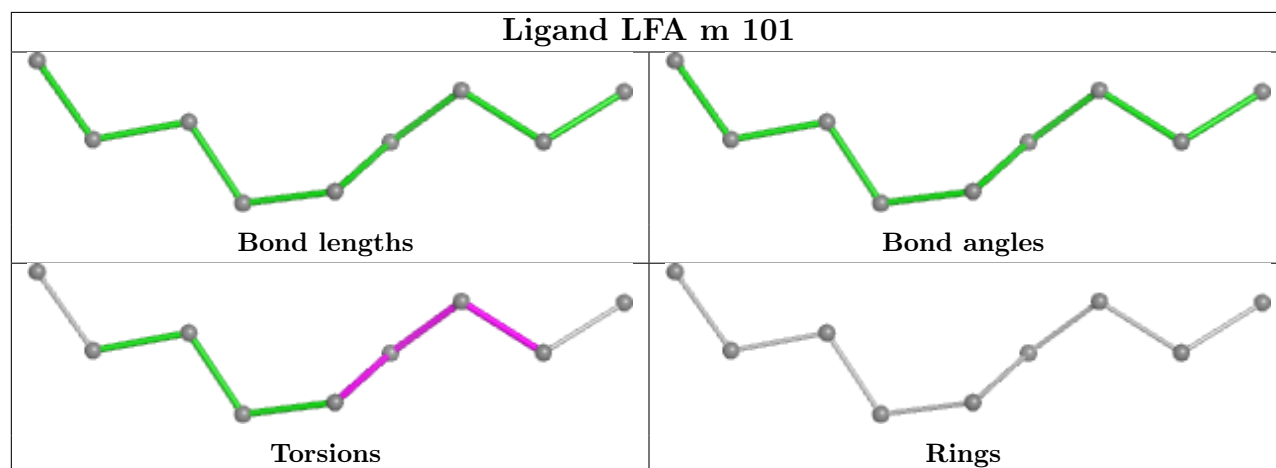
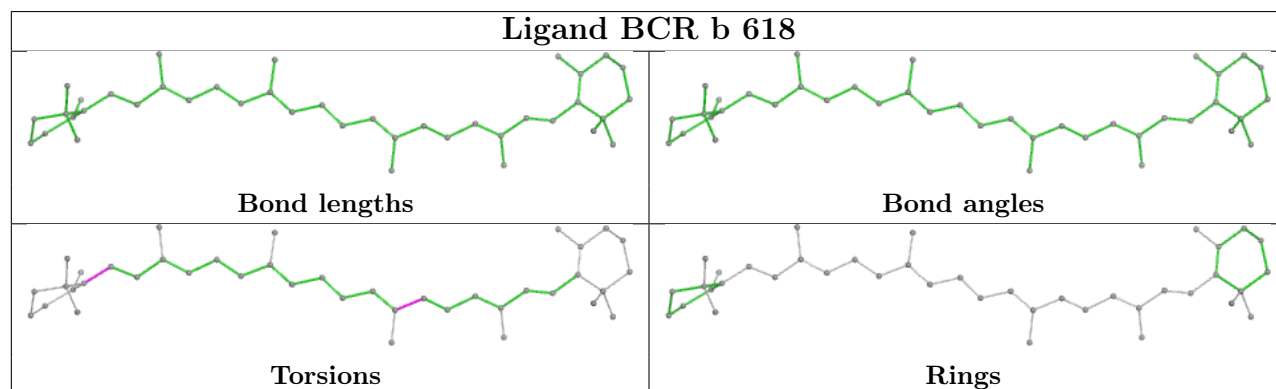
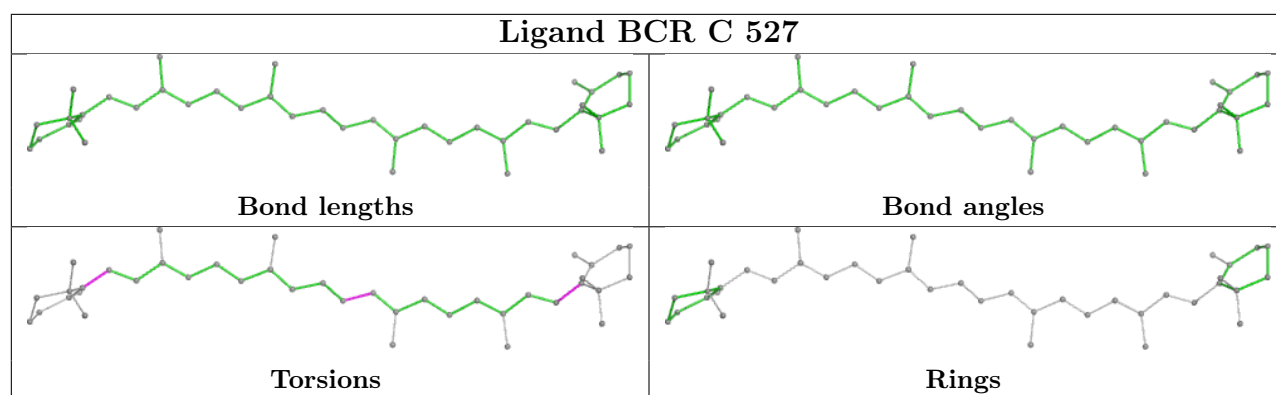
Ligand CLA a 405**Ligand CLA B 603**

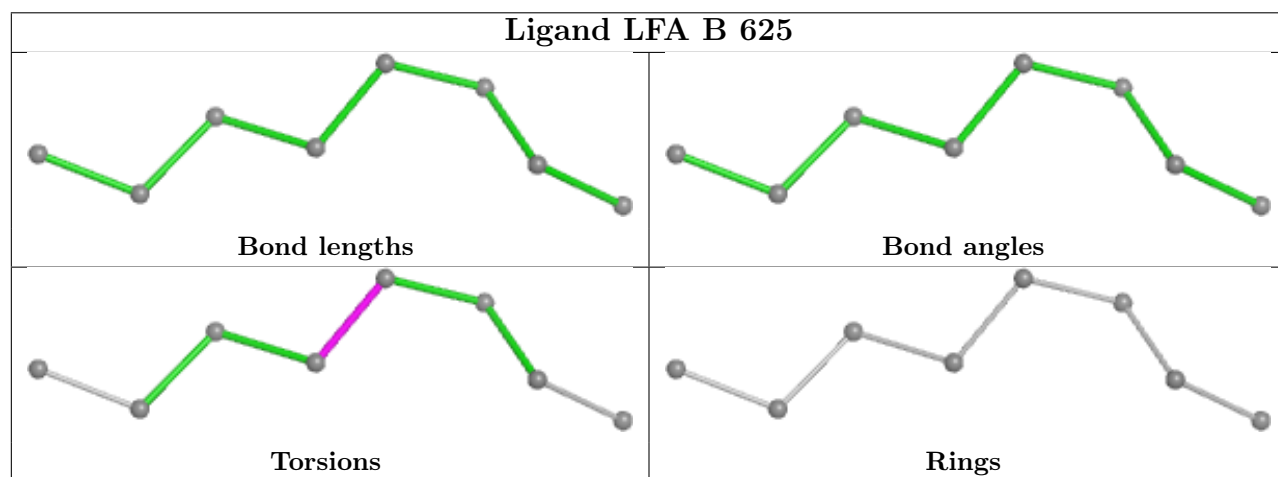
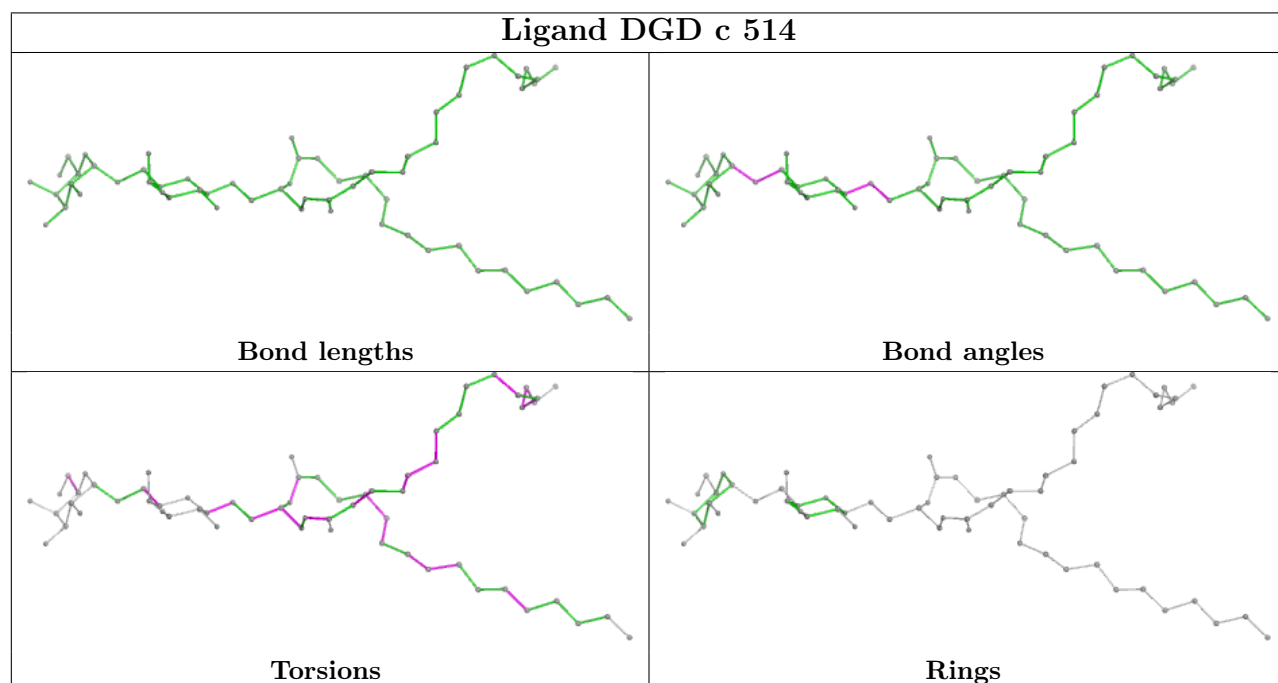
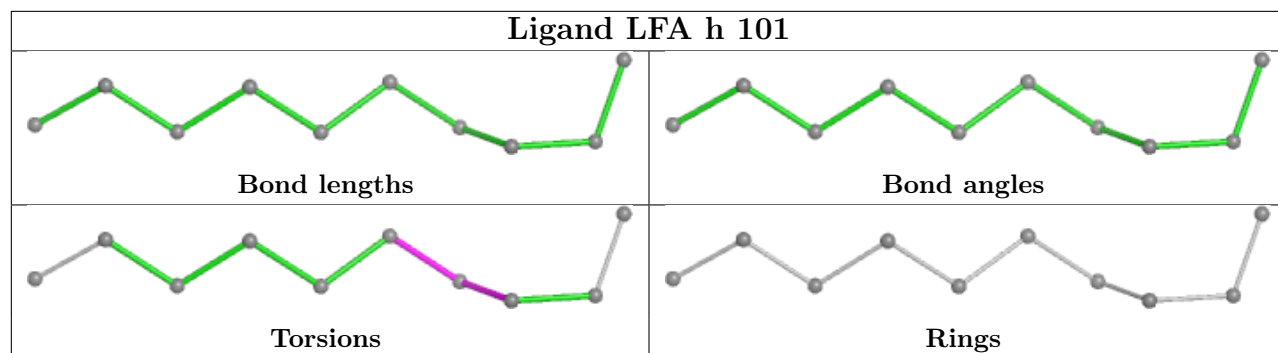


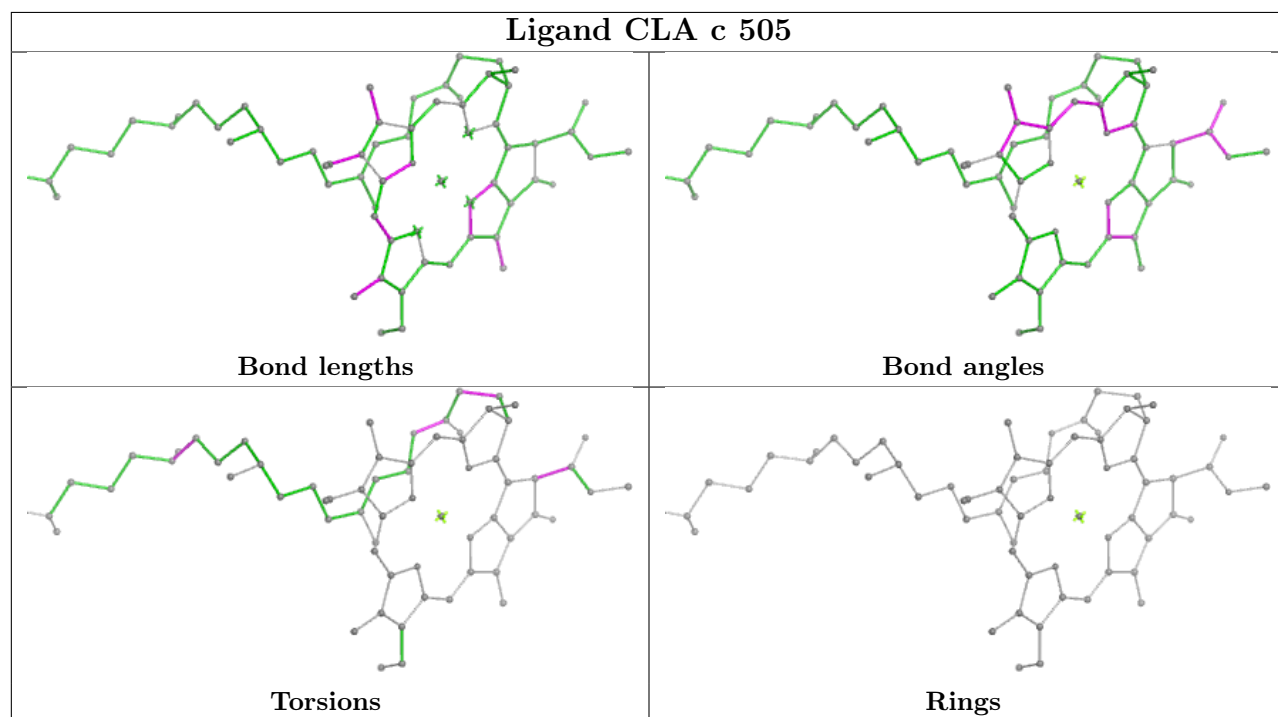
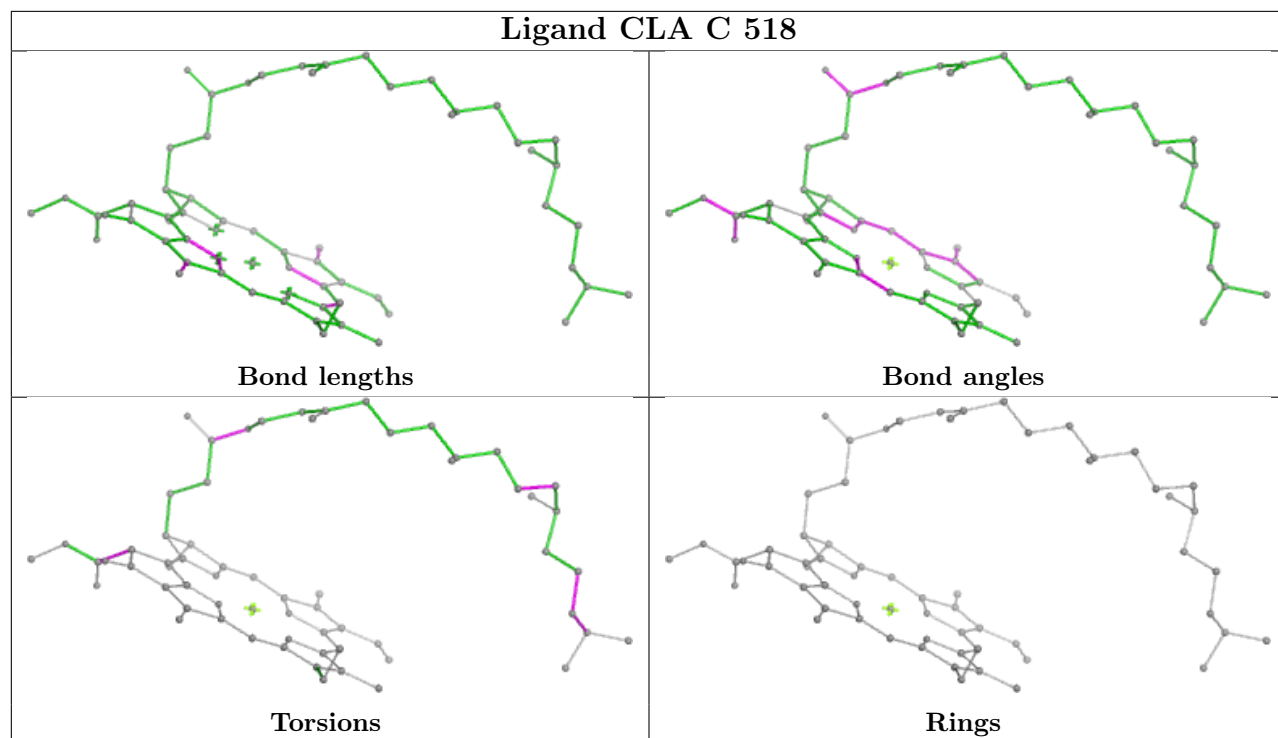


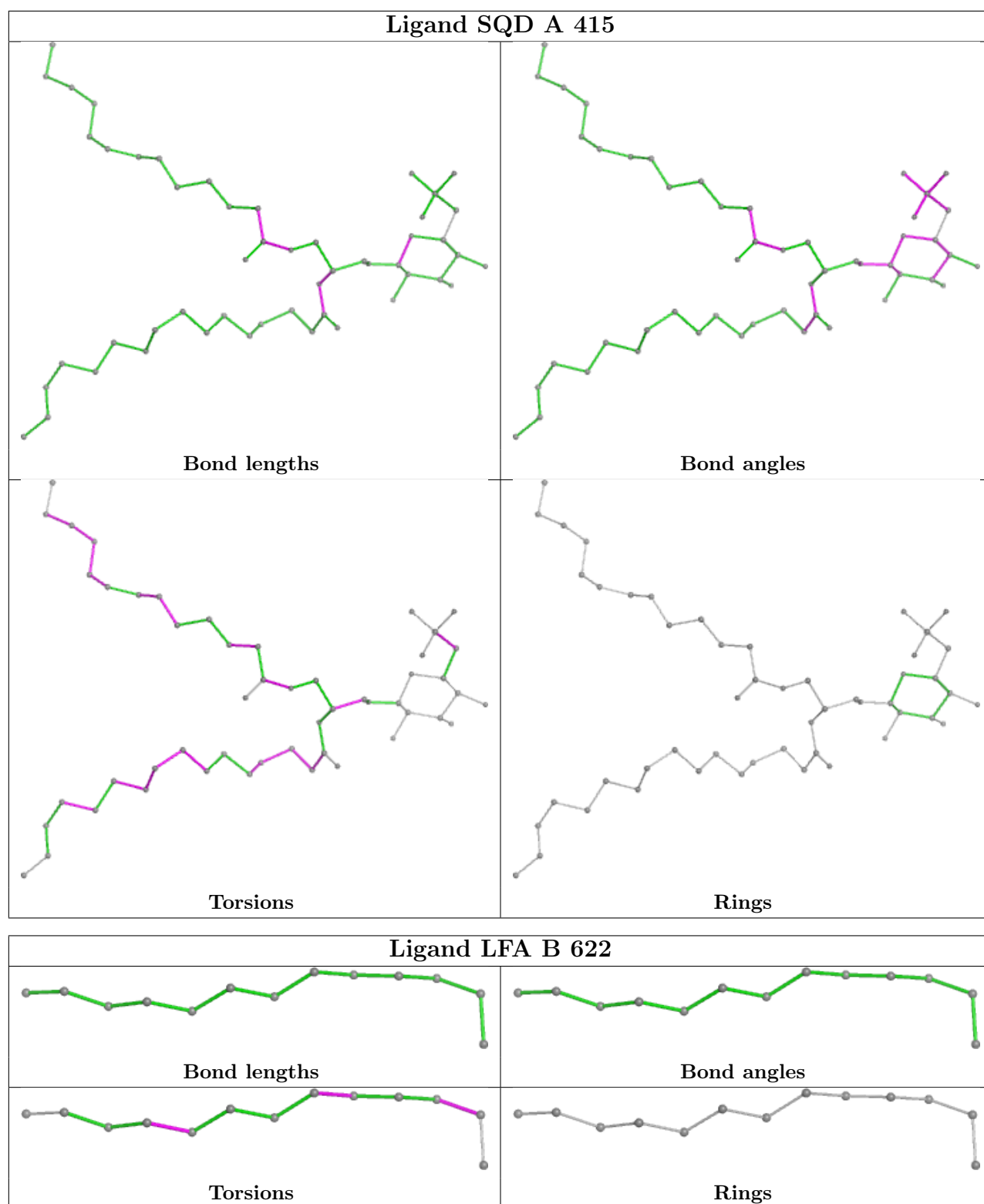


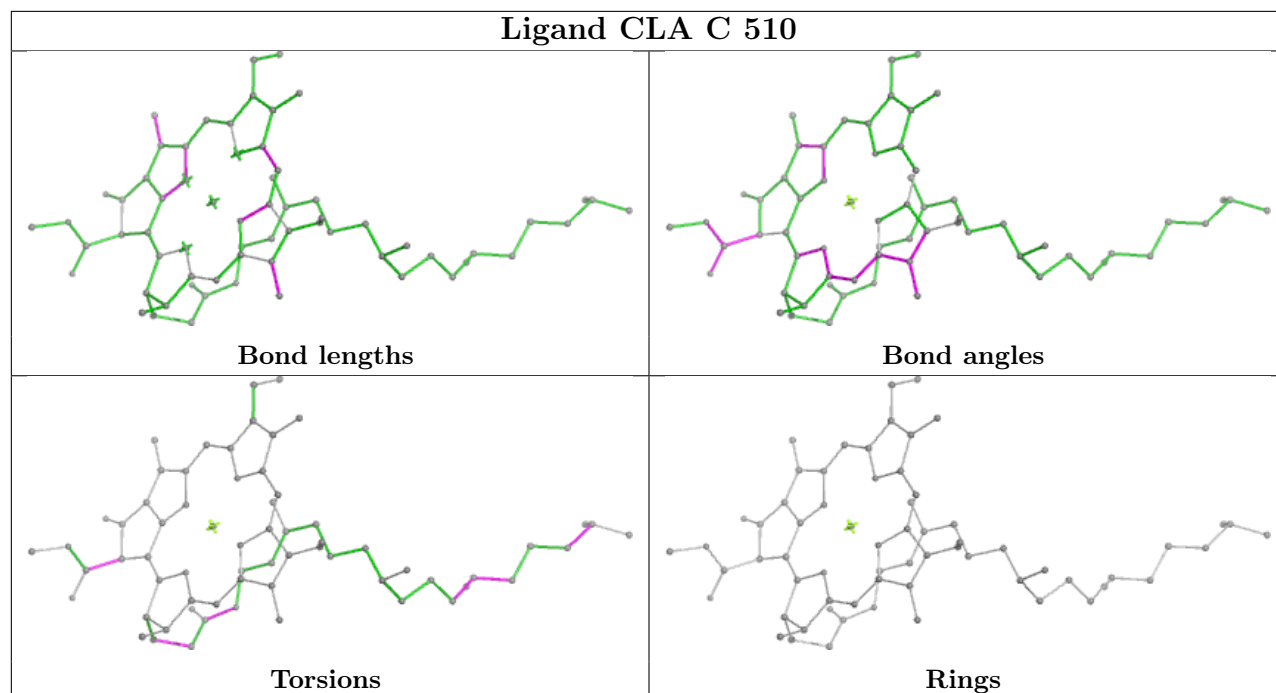
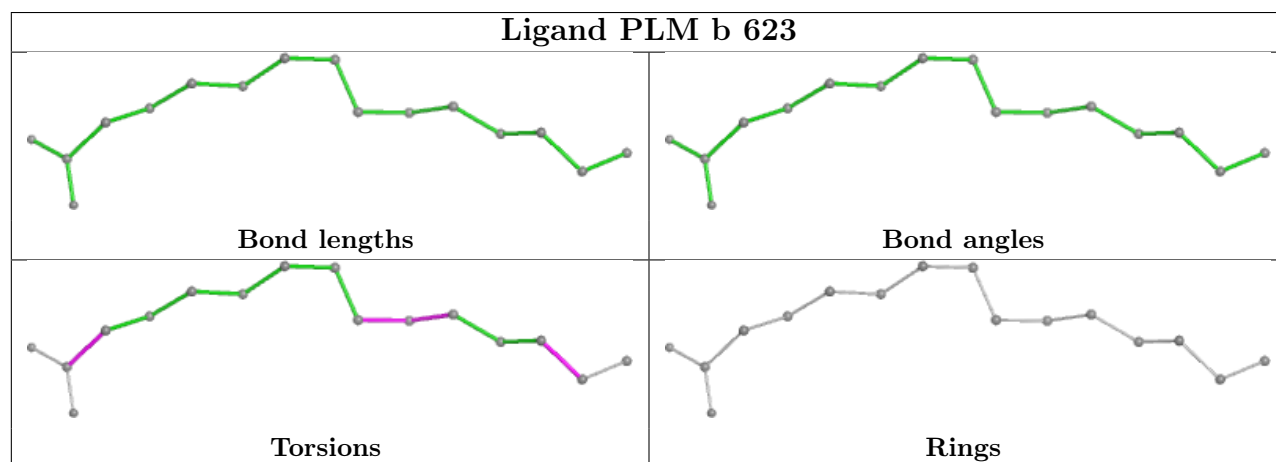
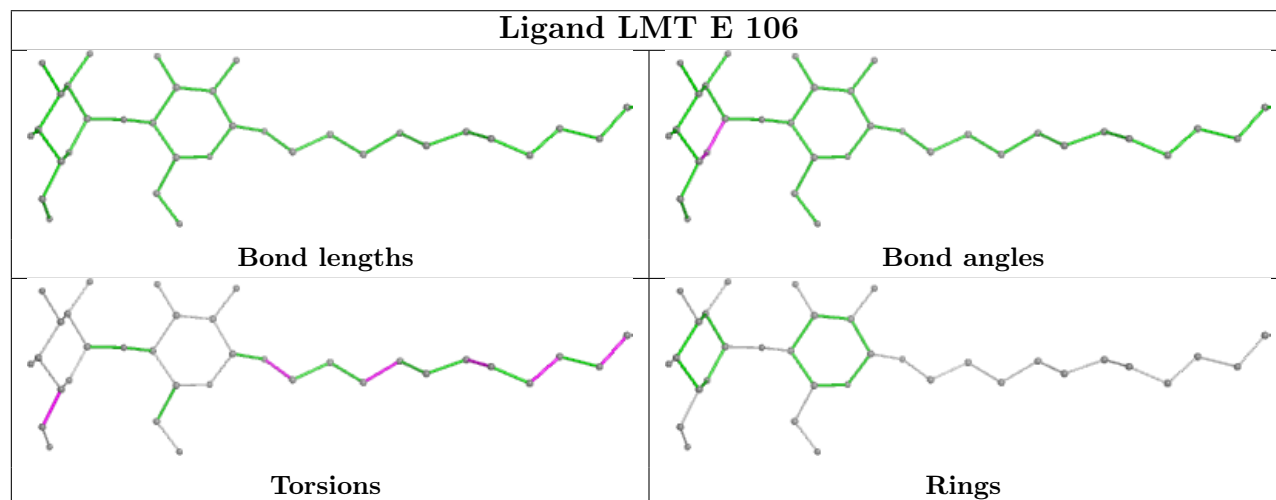


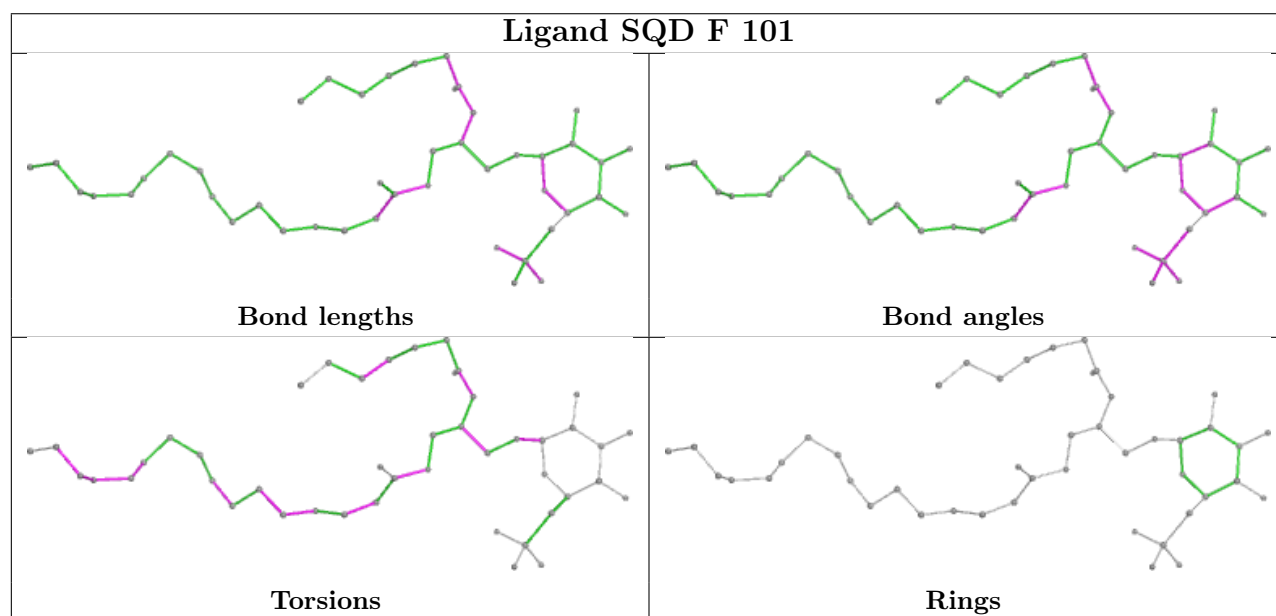
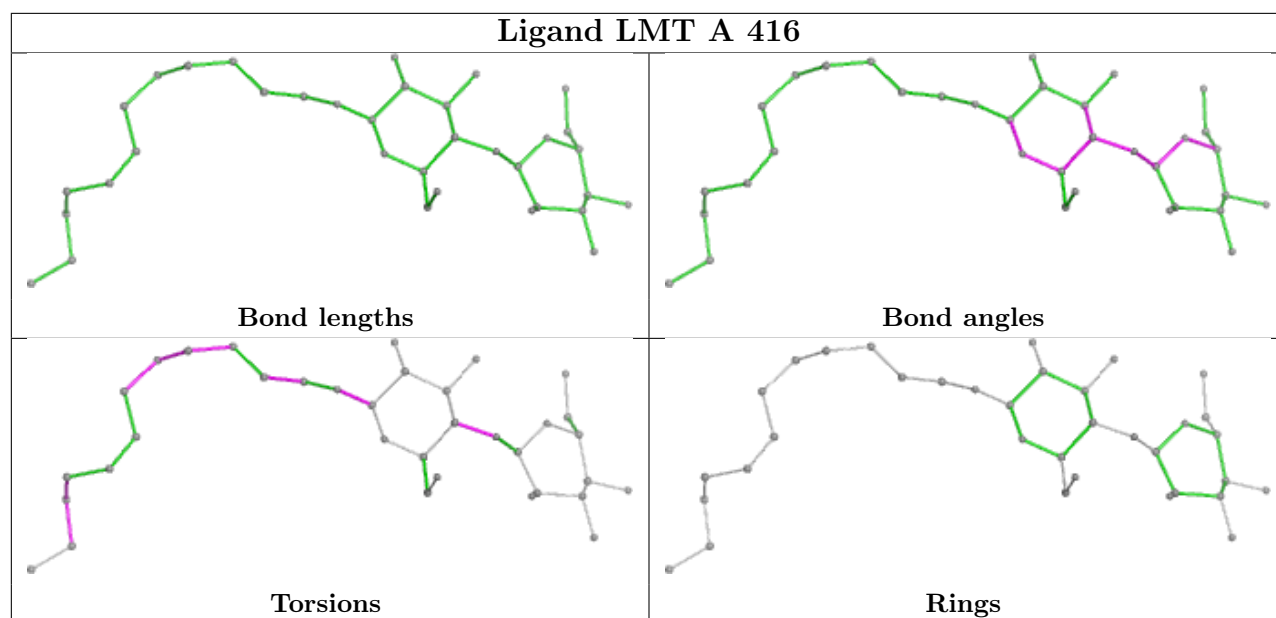
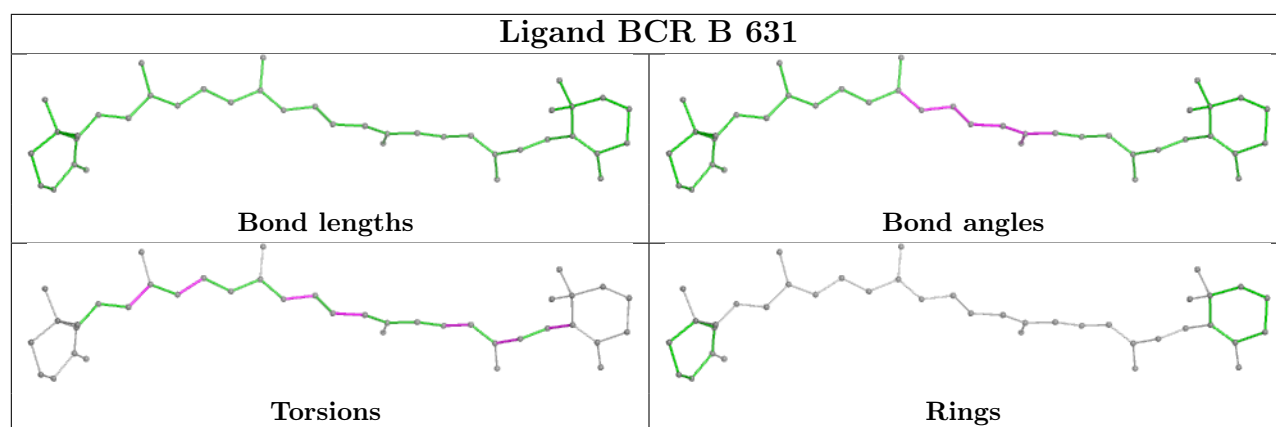


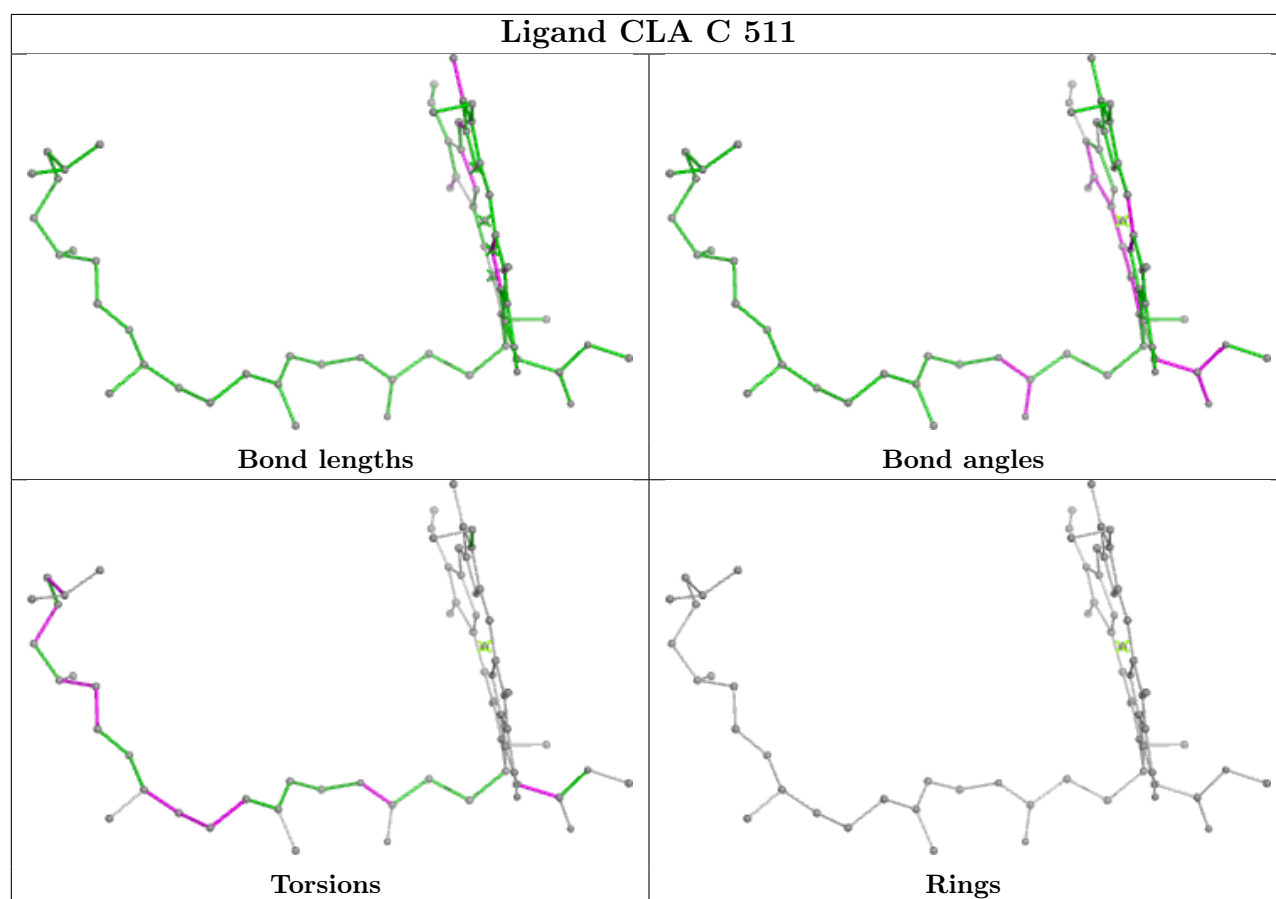
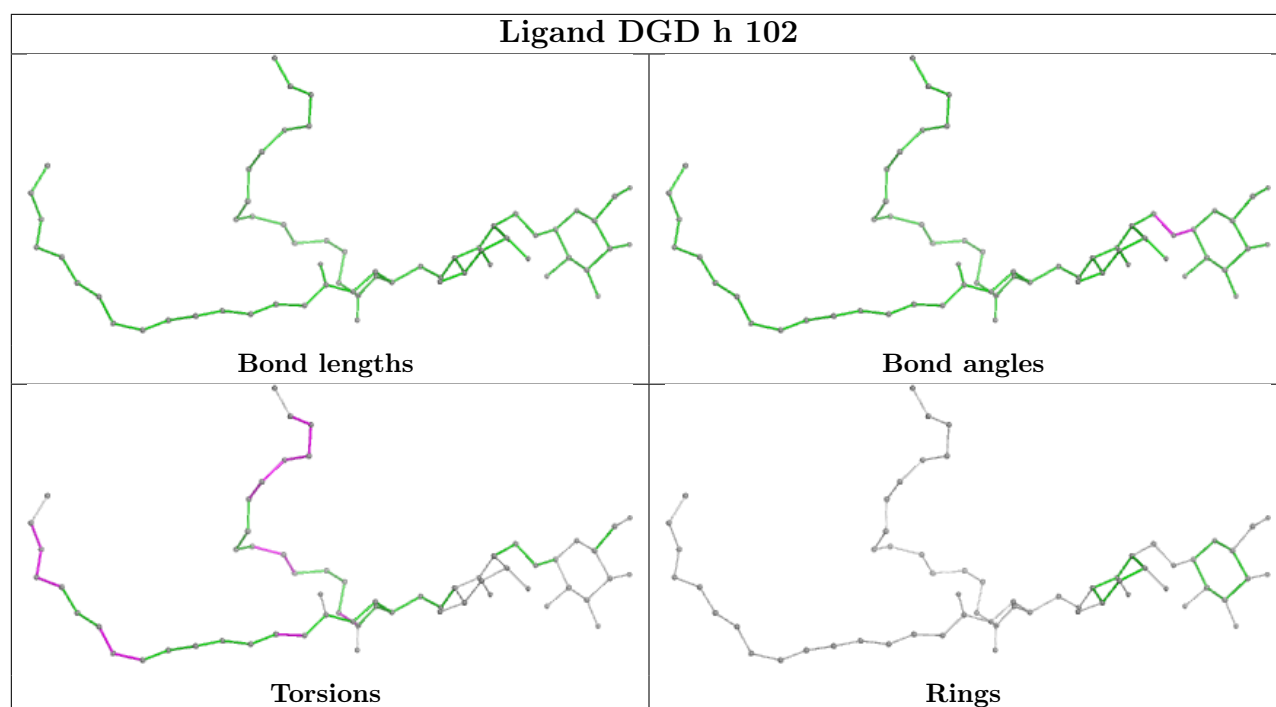


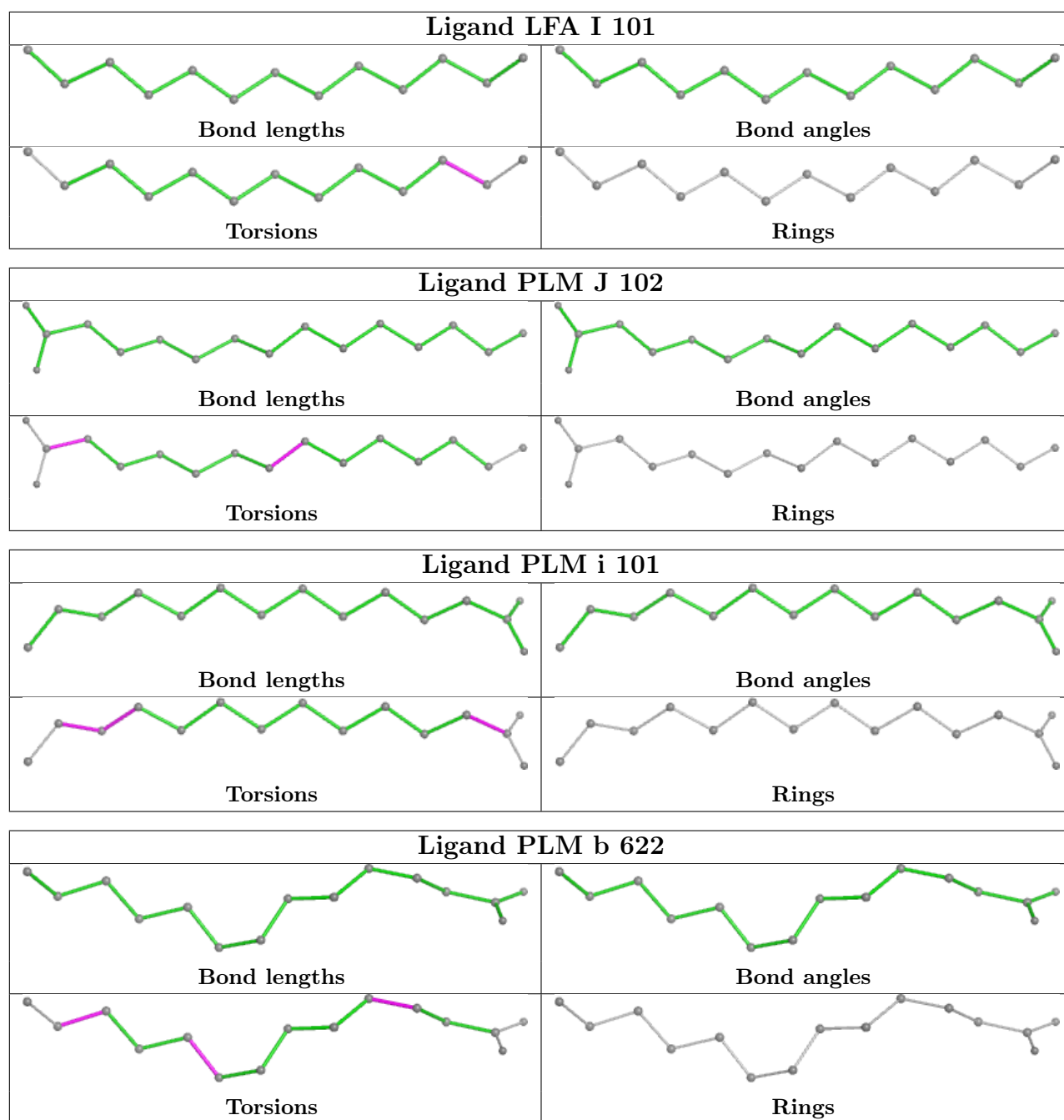


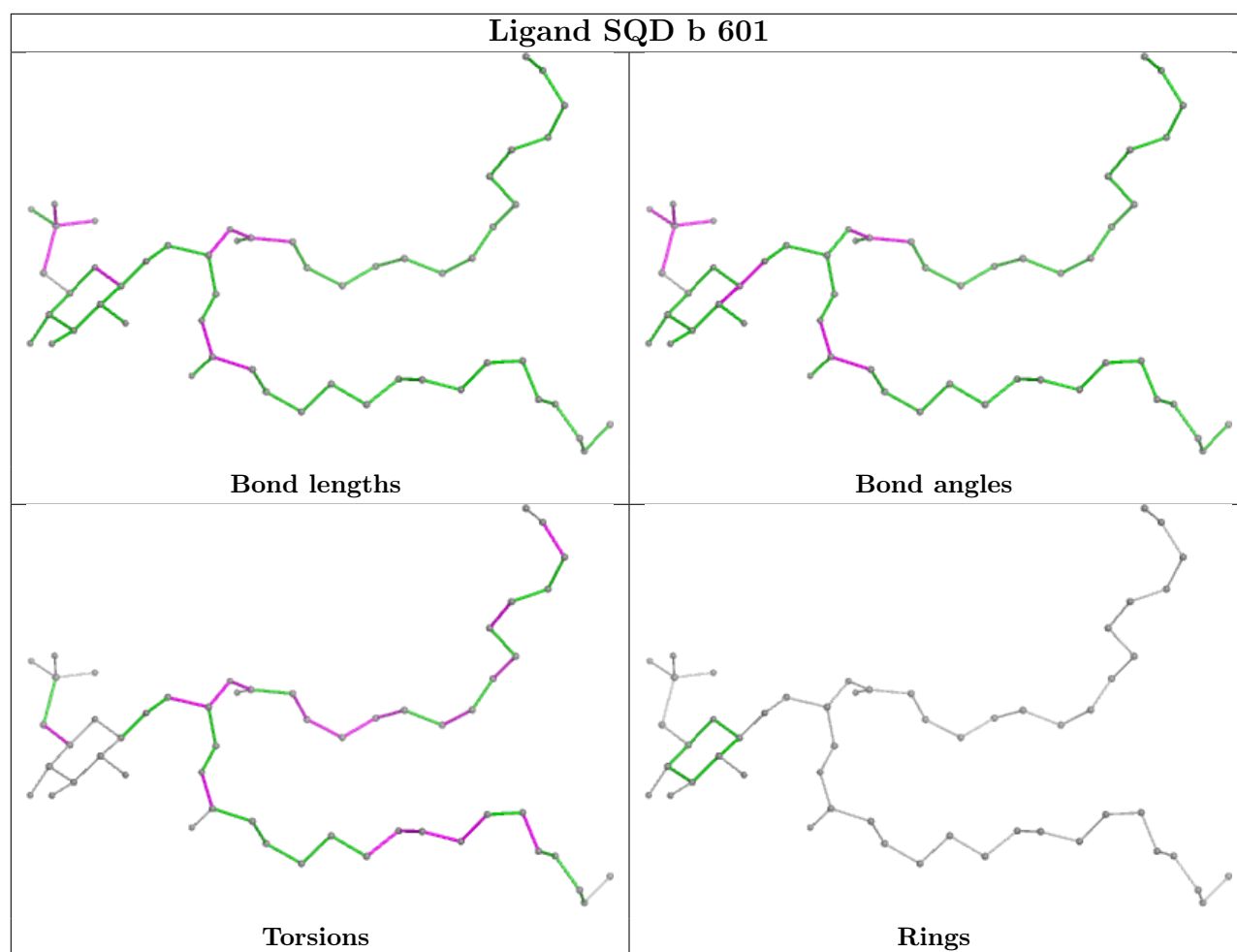


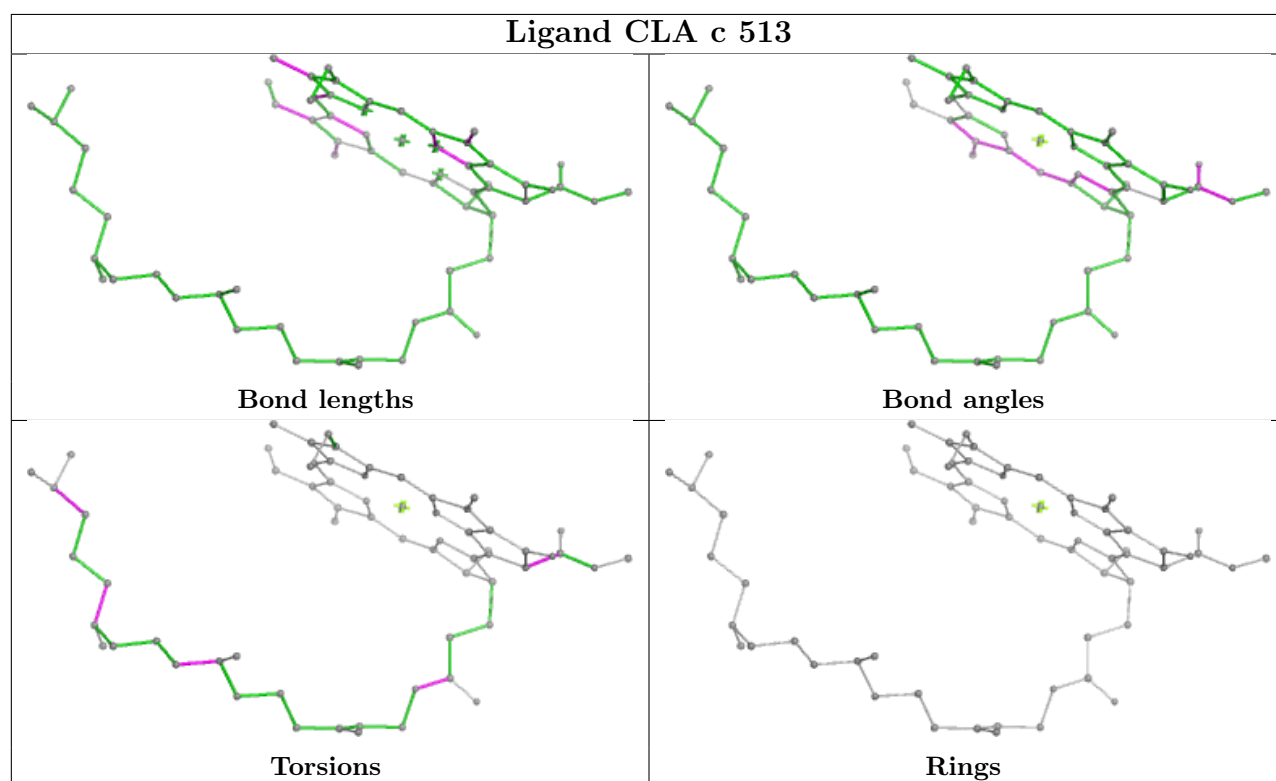
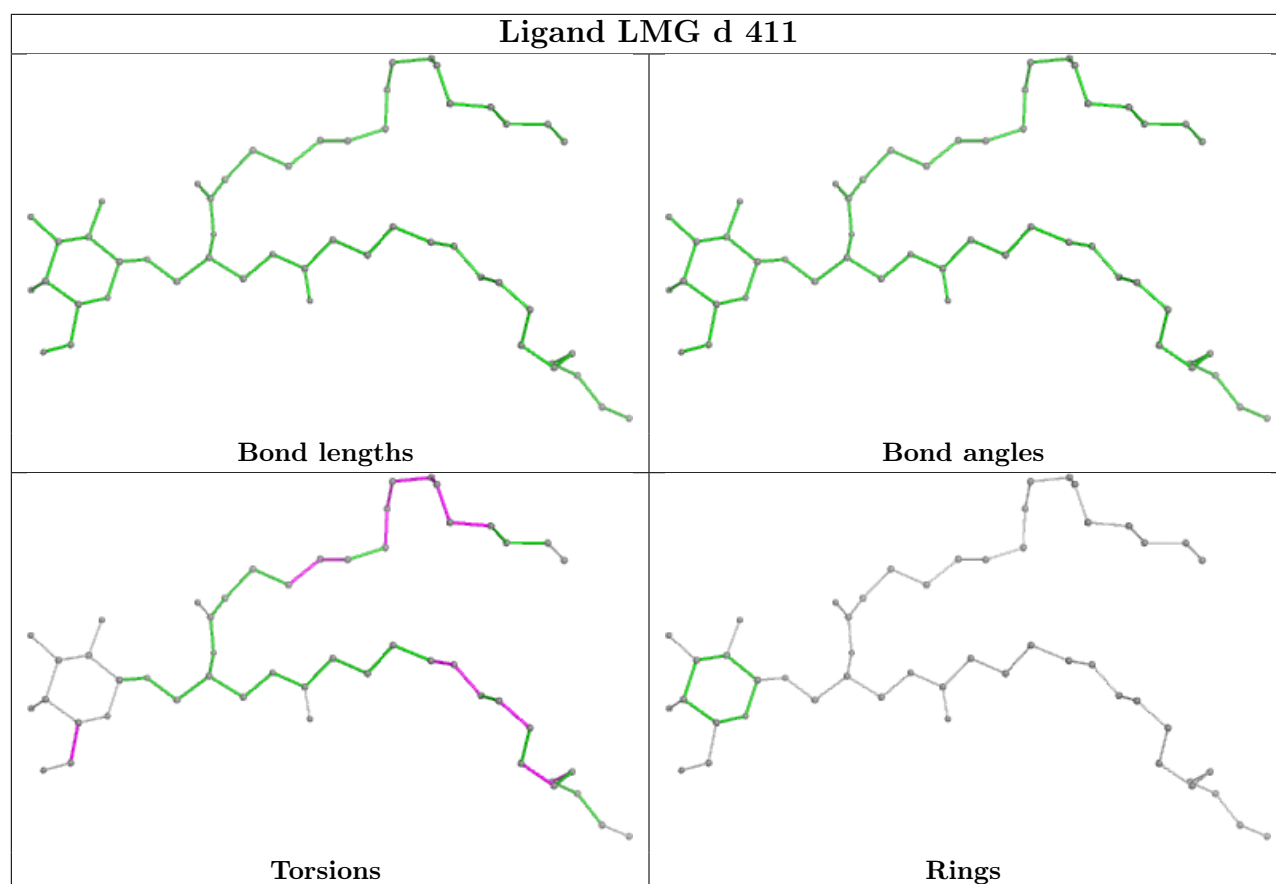
Ligand CLA C 510**Ligand PLM b 623****Ligand LMT E 106**



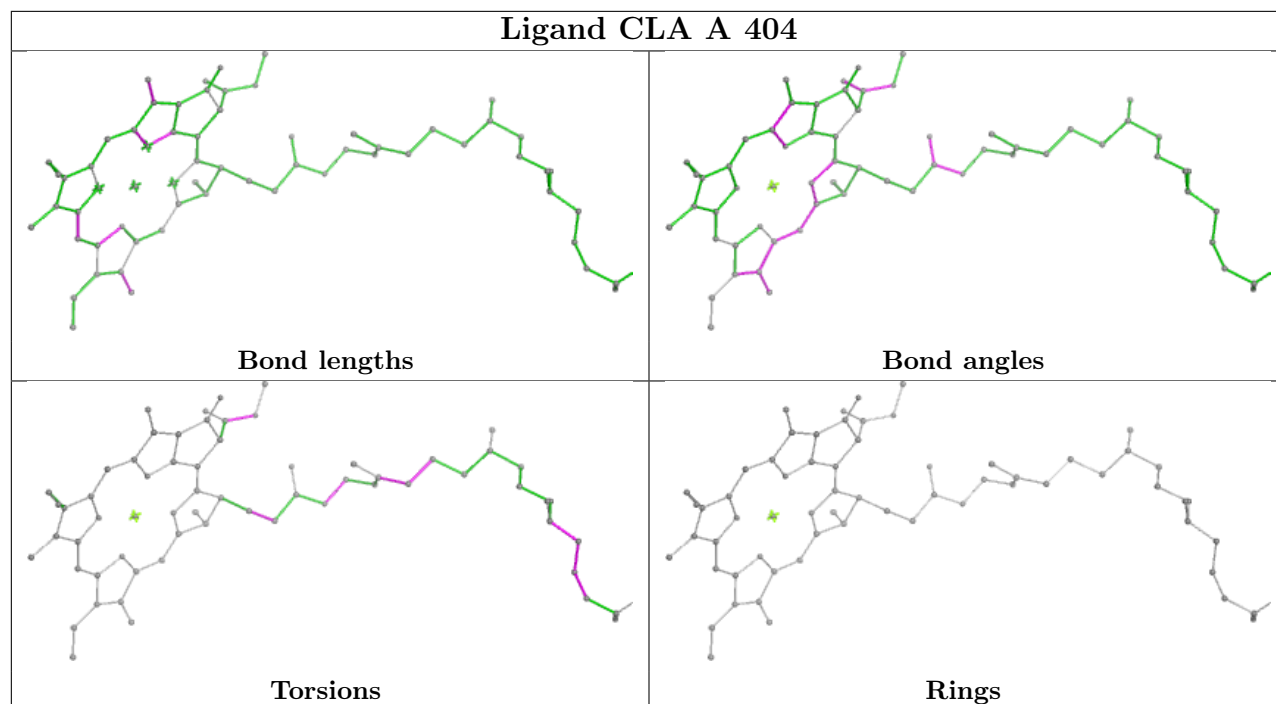




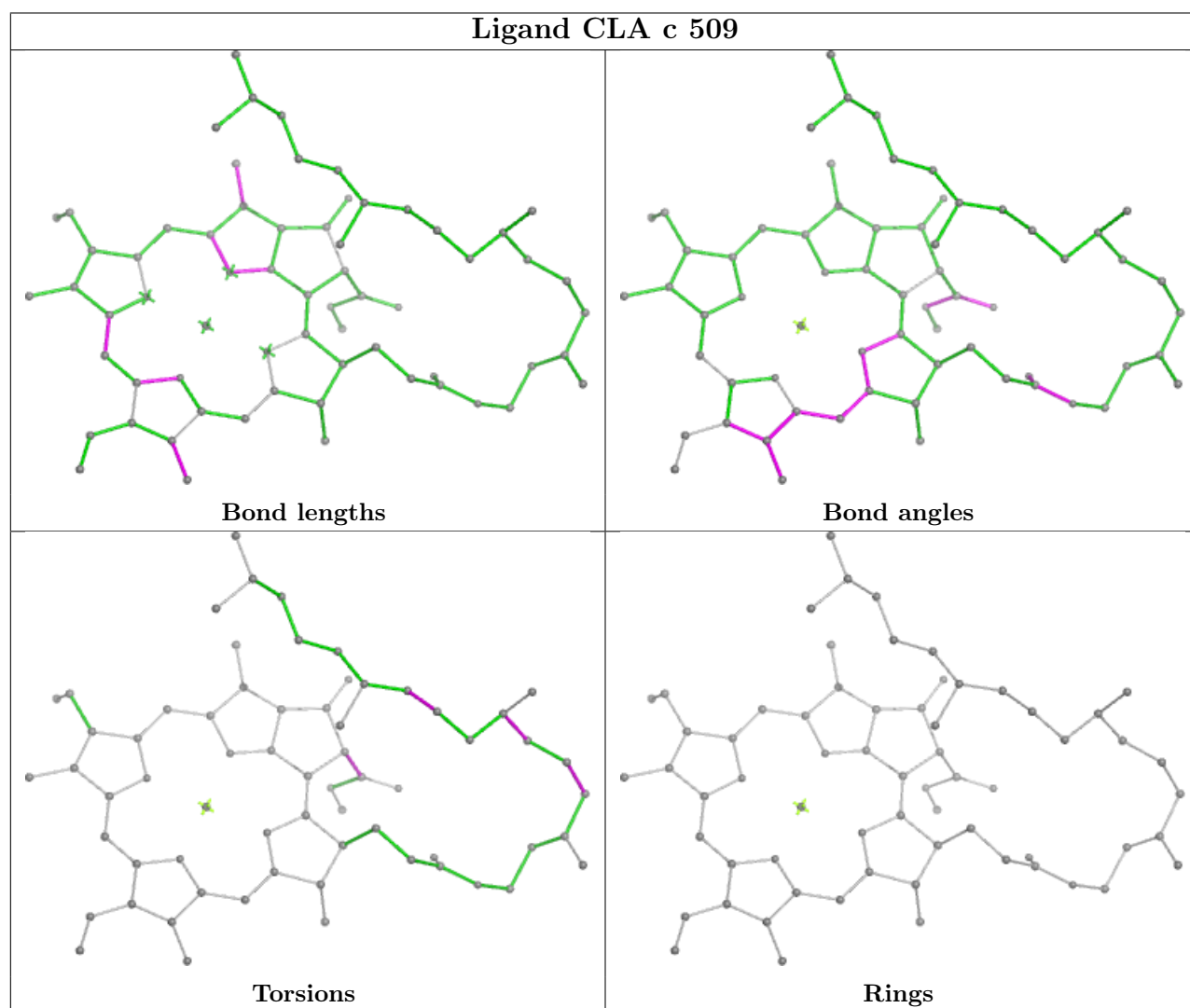




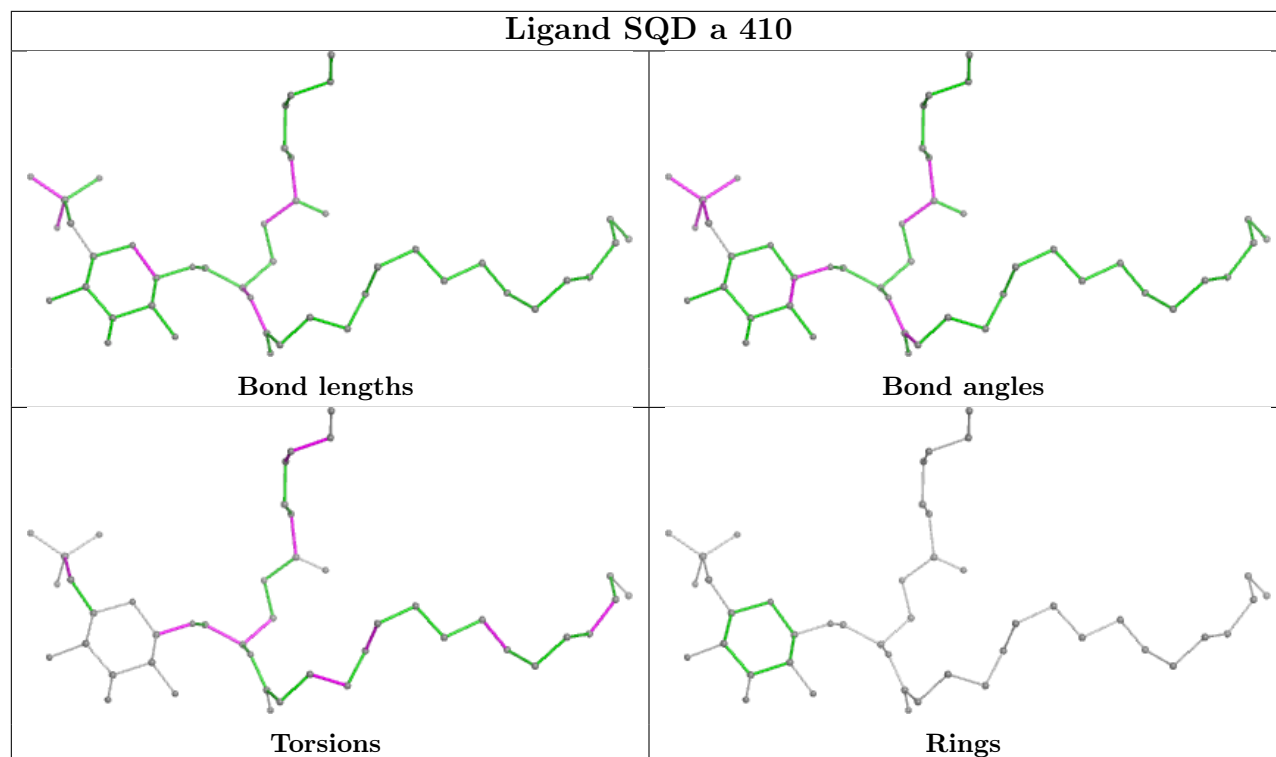
Ligand CLA A 404



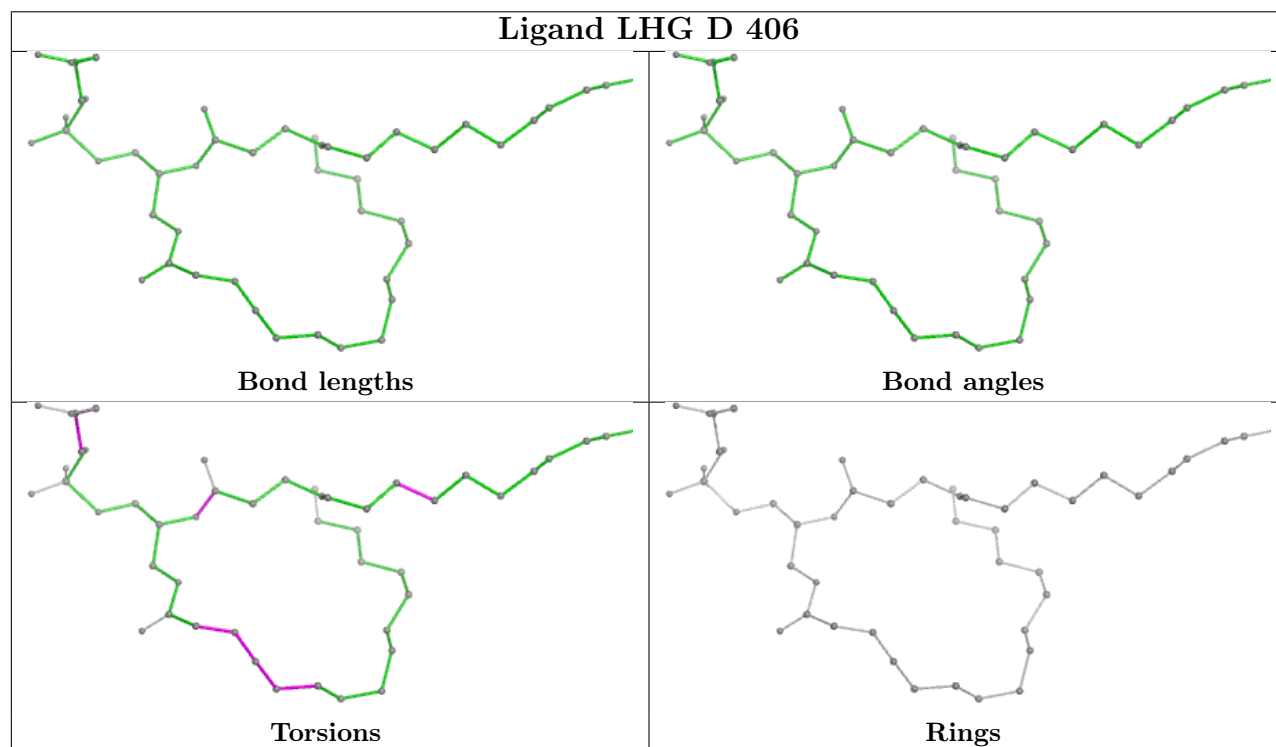
Ligand CLA c 509

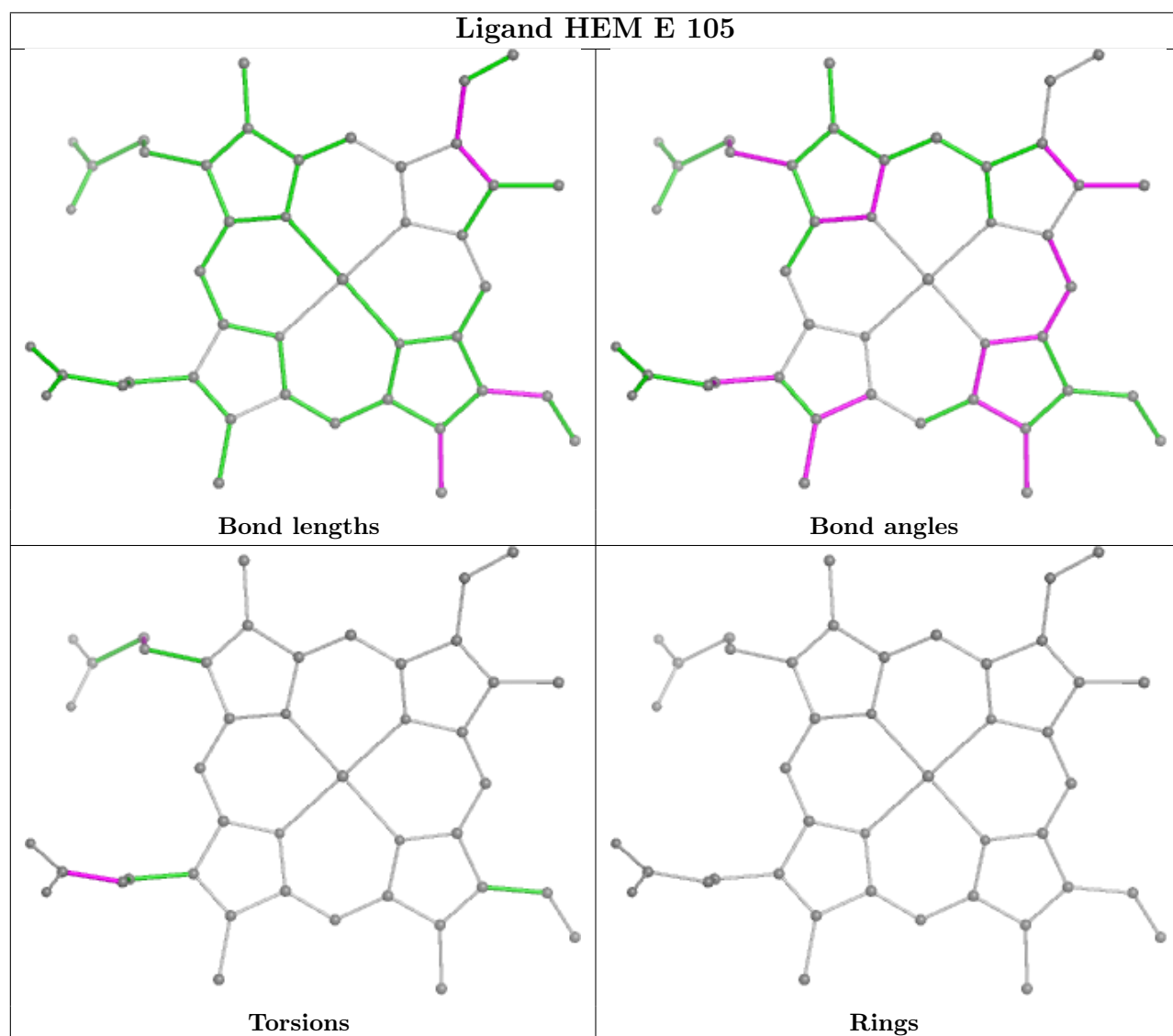
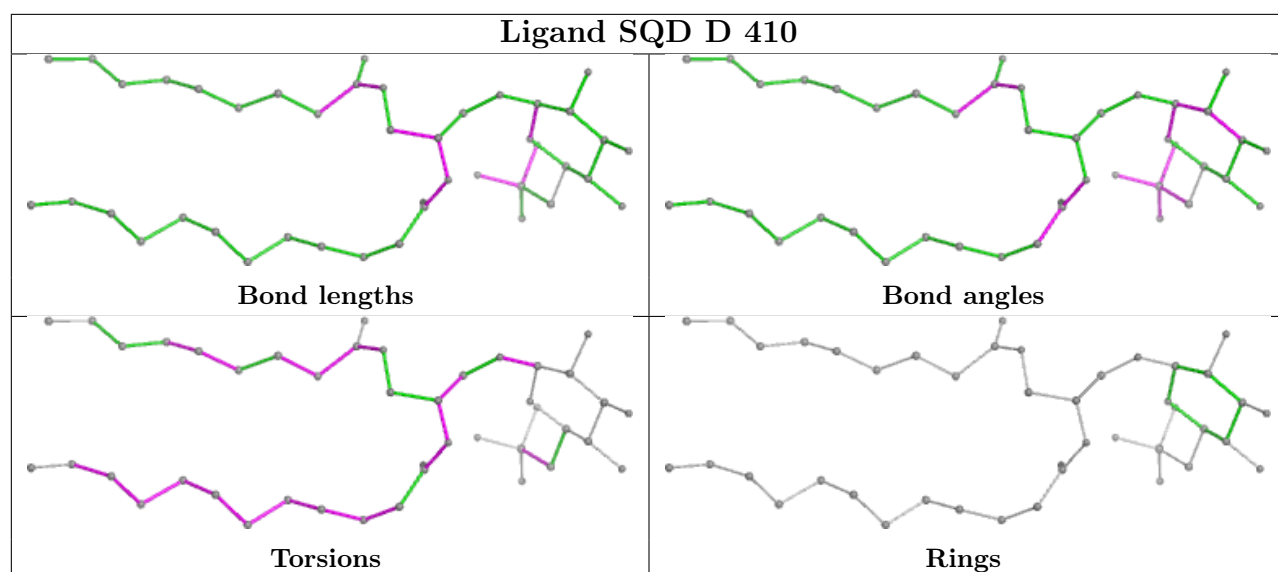


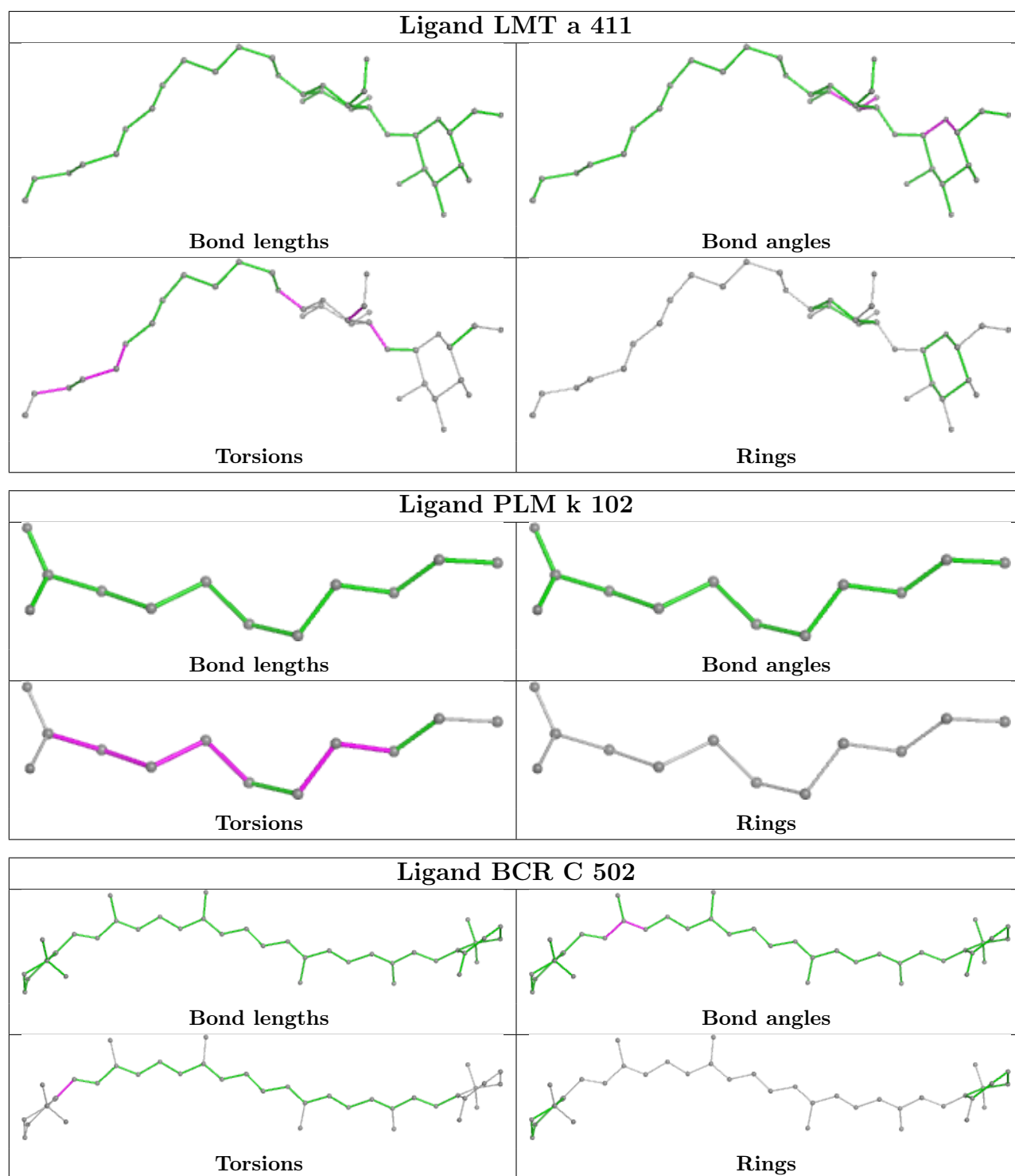
Ligand SQD a 410

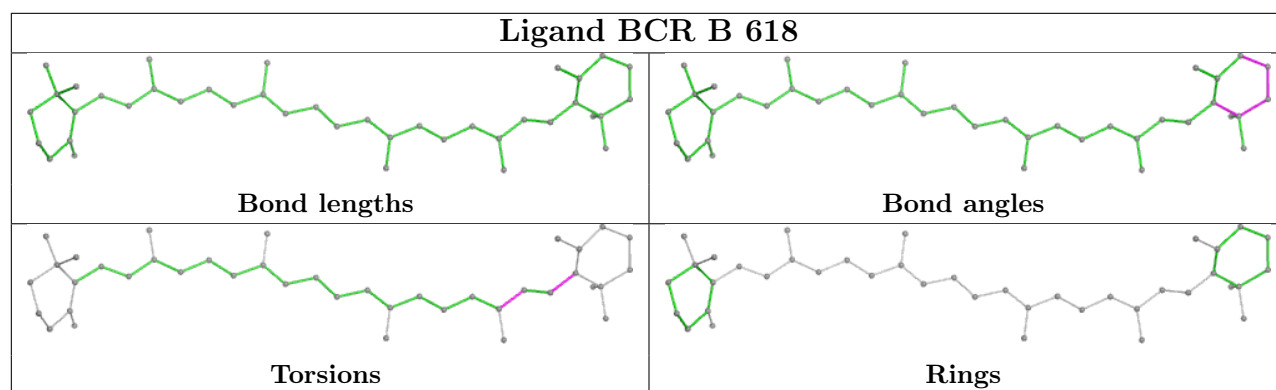
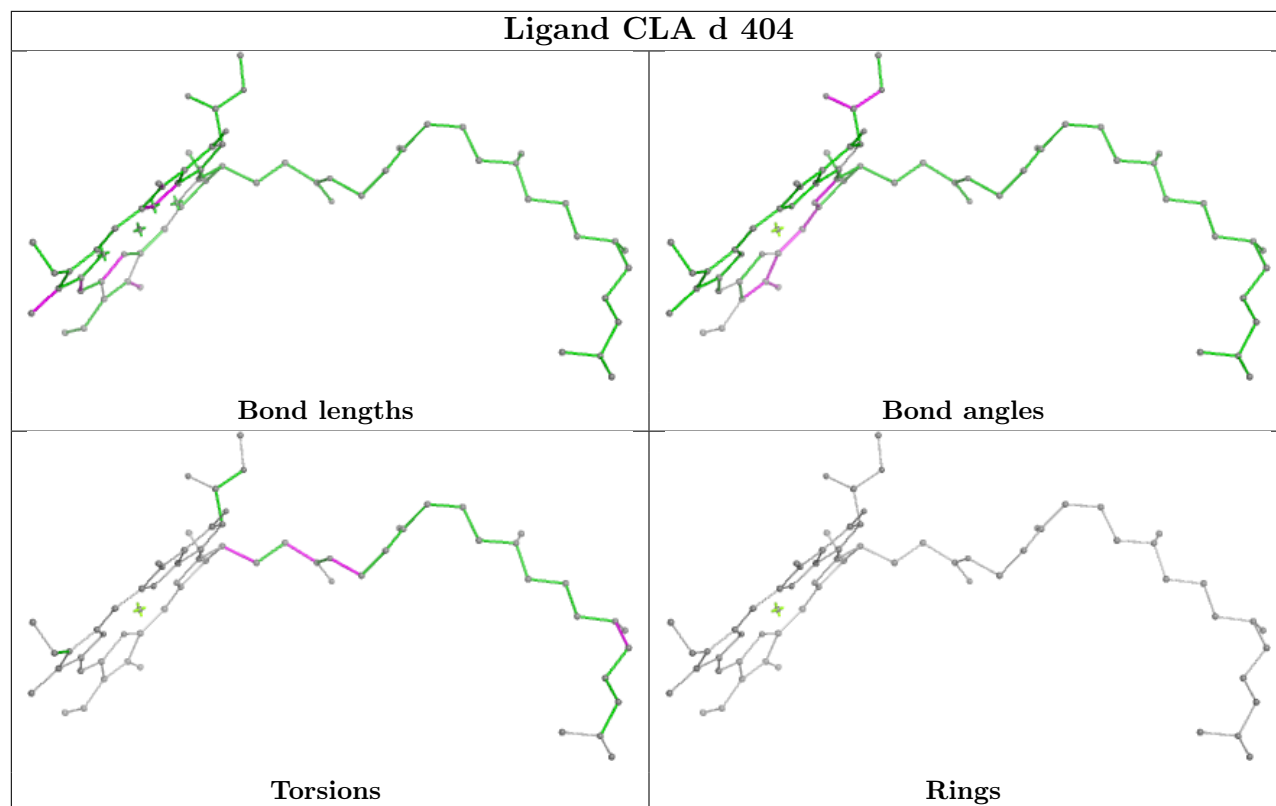


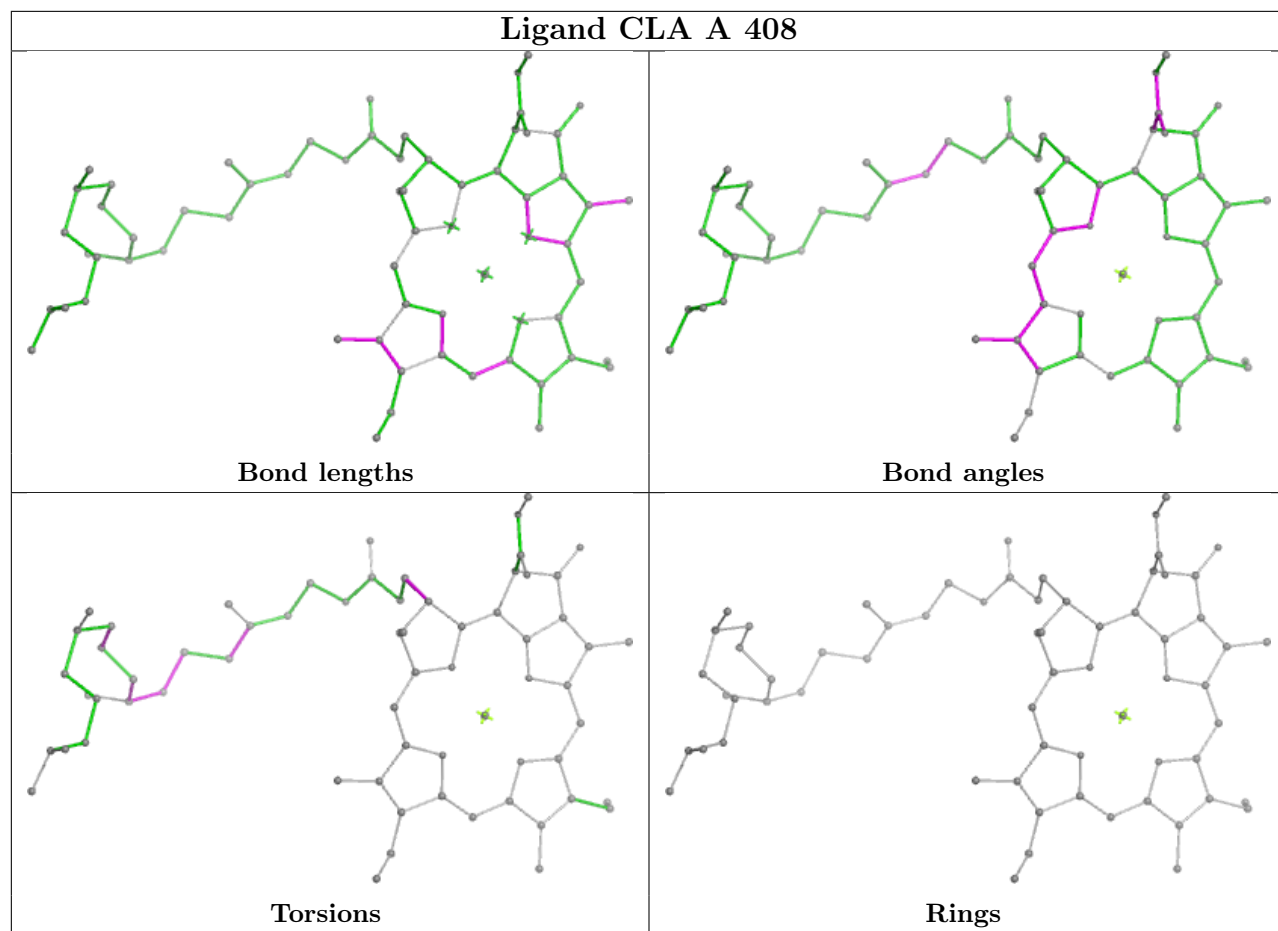
Ligand LHG D 406



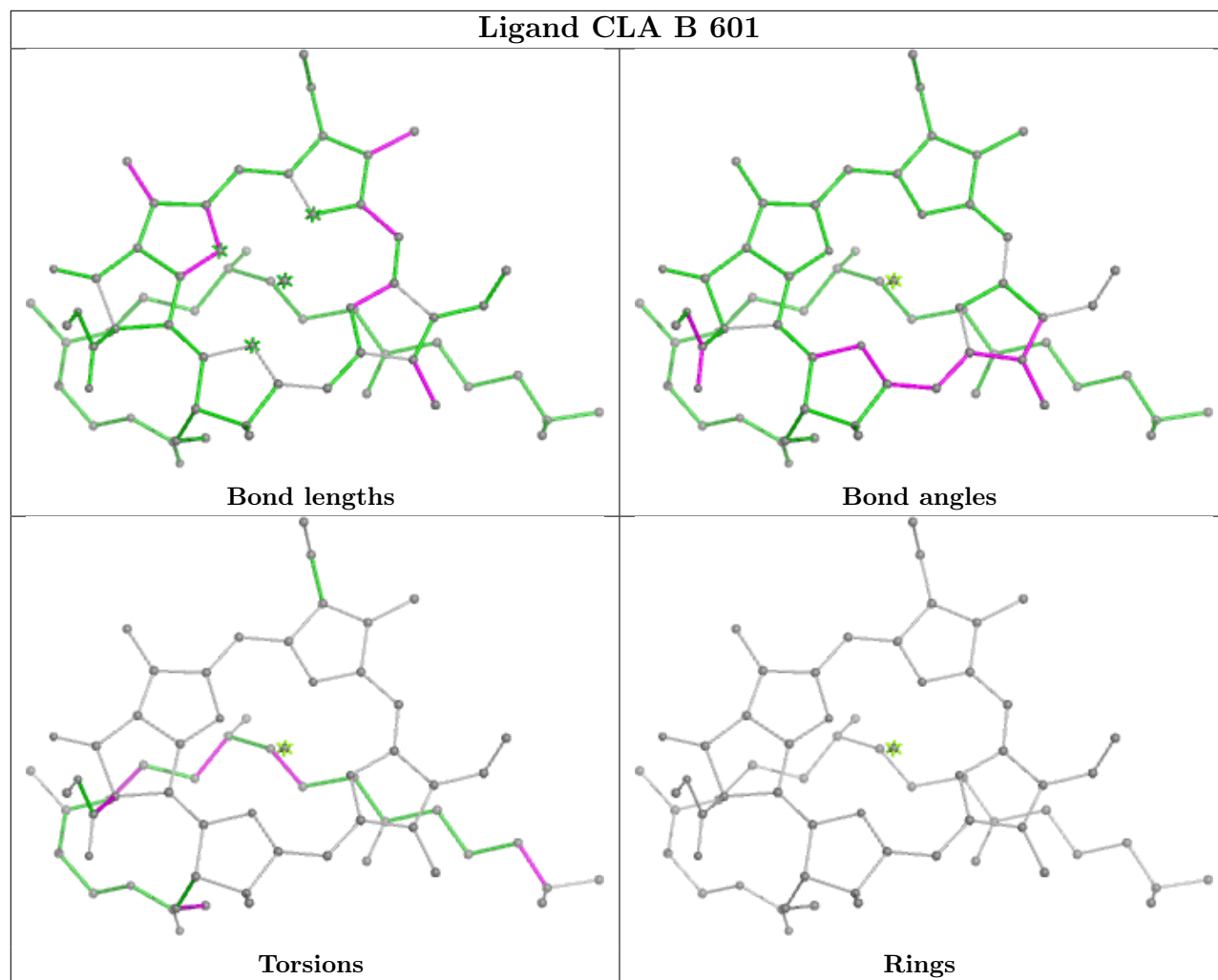


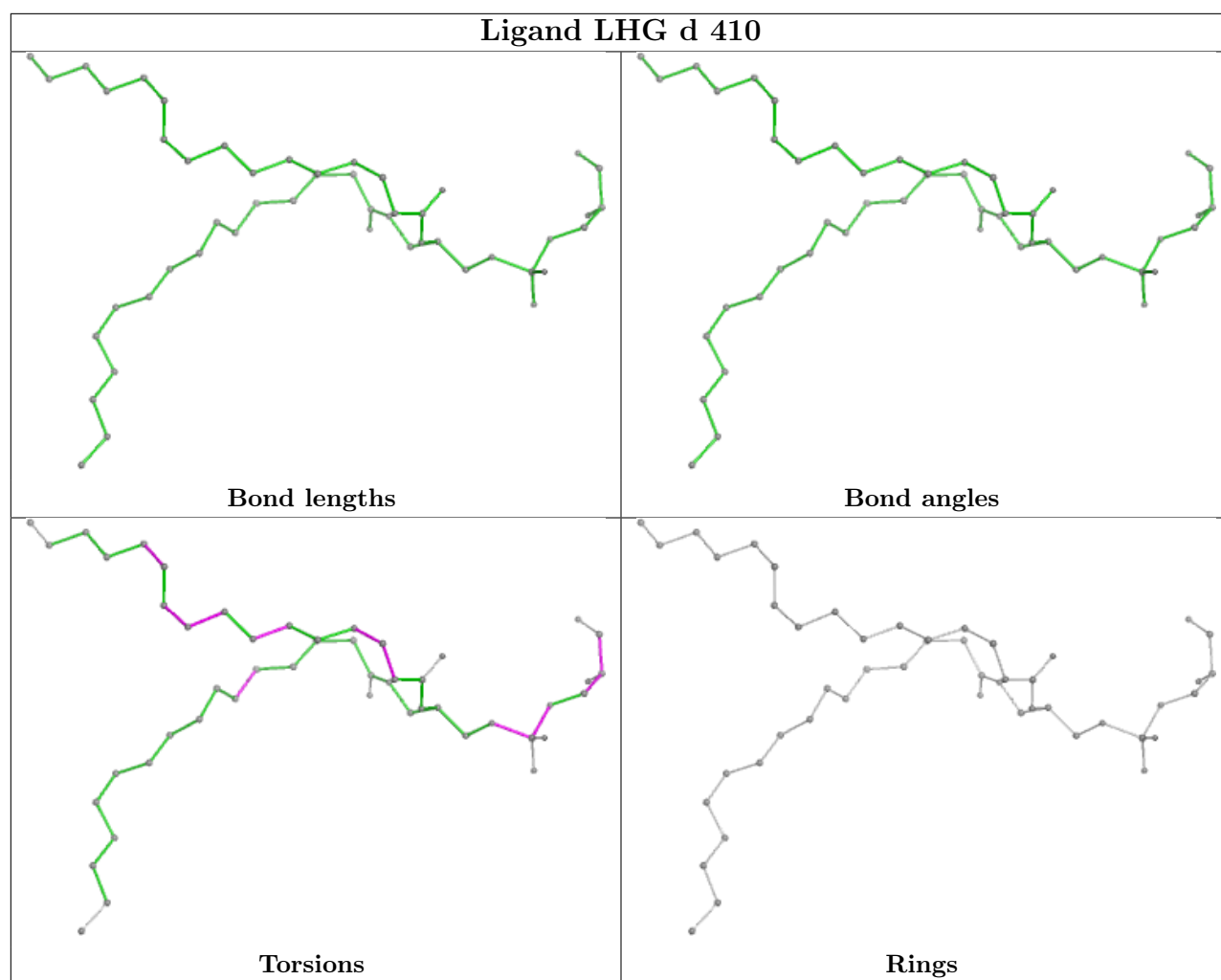




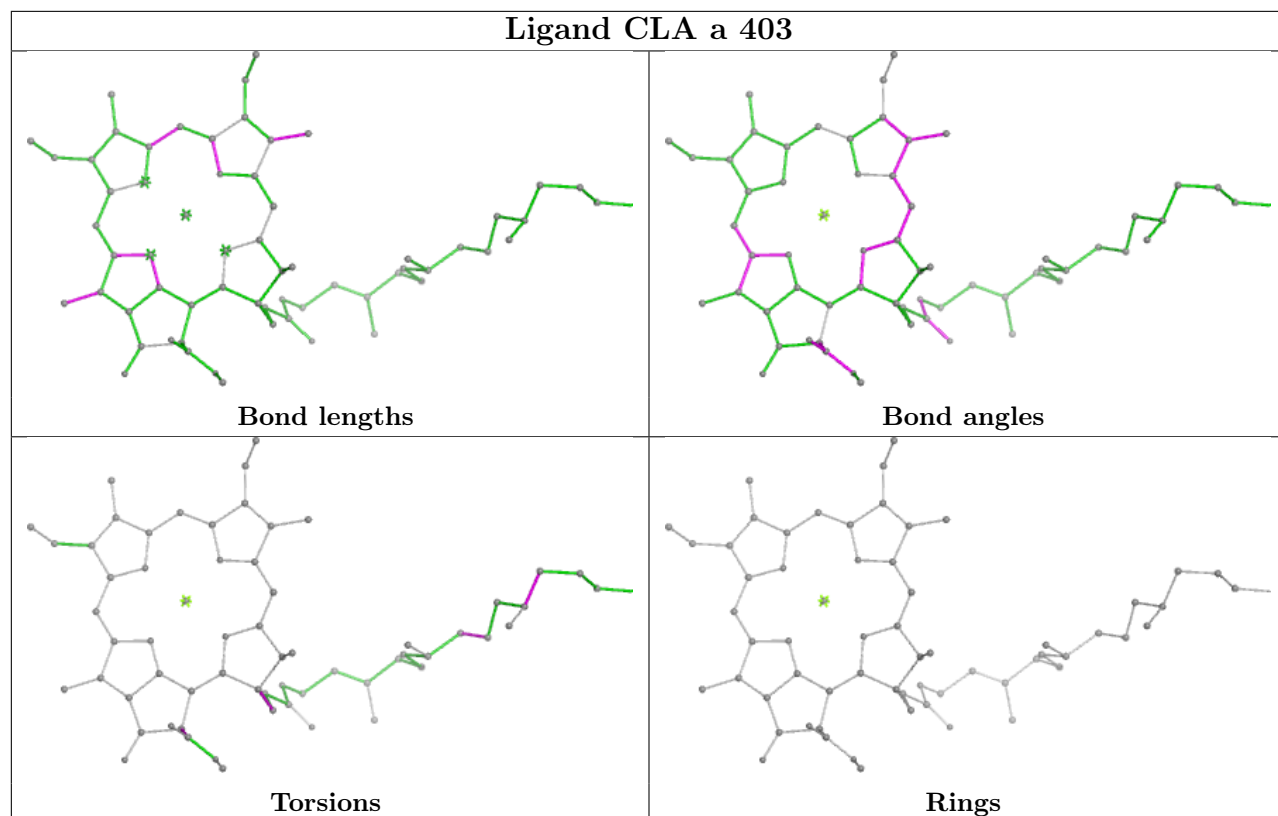


Ligand CLA B 601

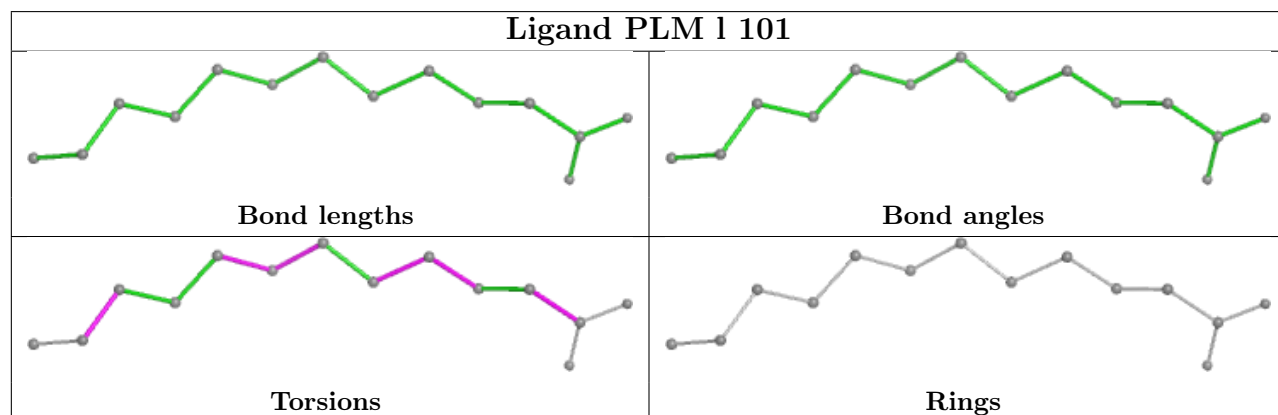


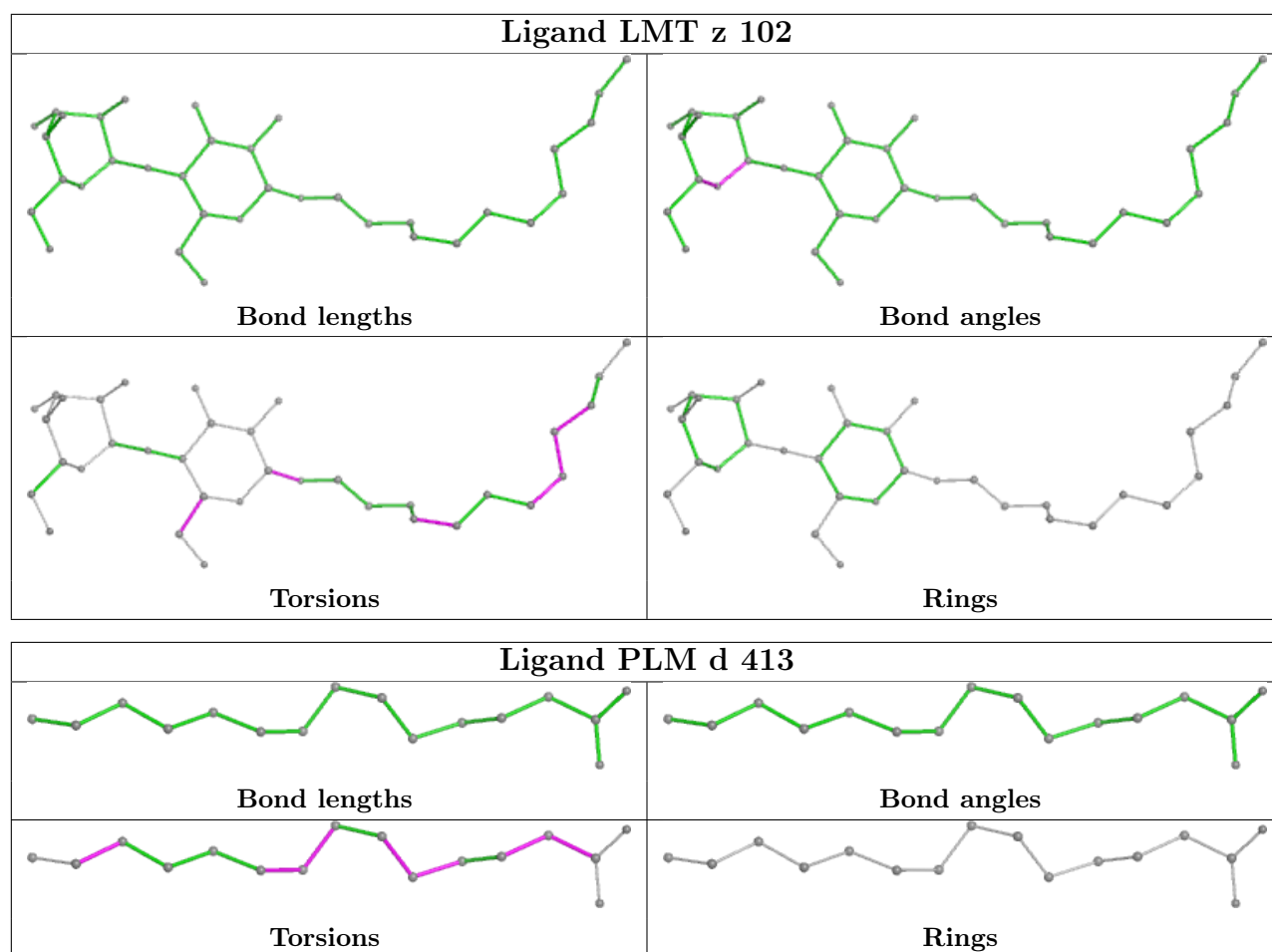


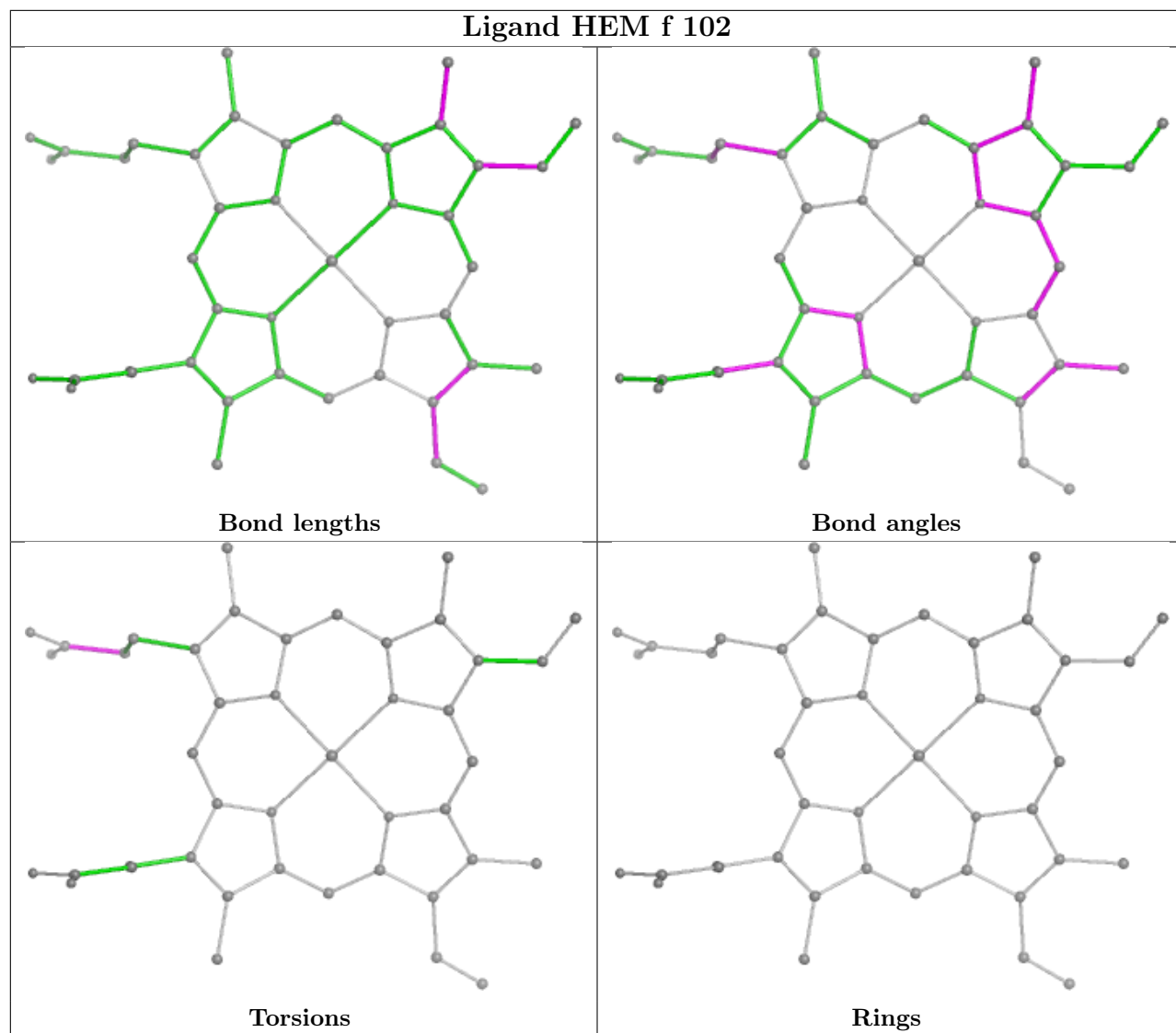
Ligand CLA a 403

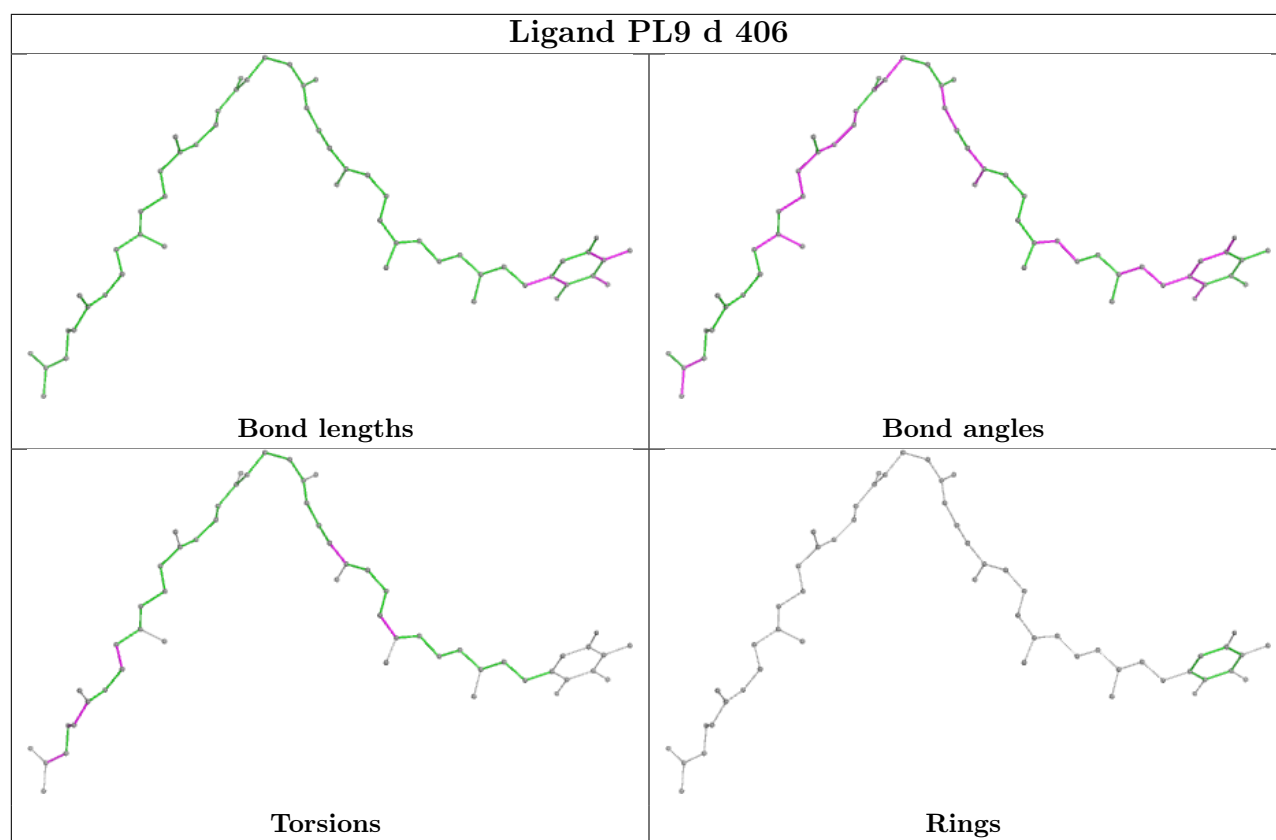


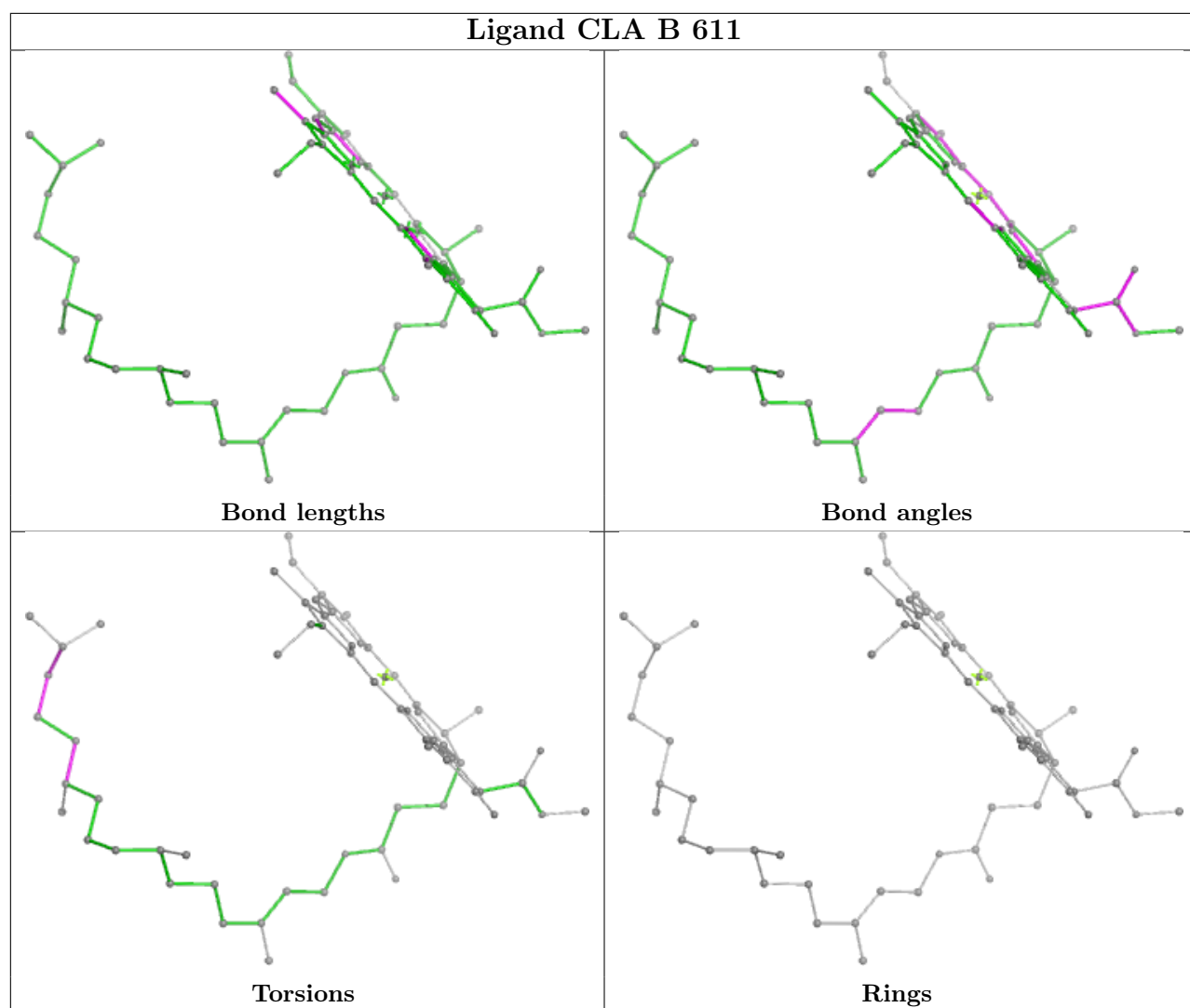
Ligand PLM l 101



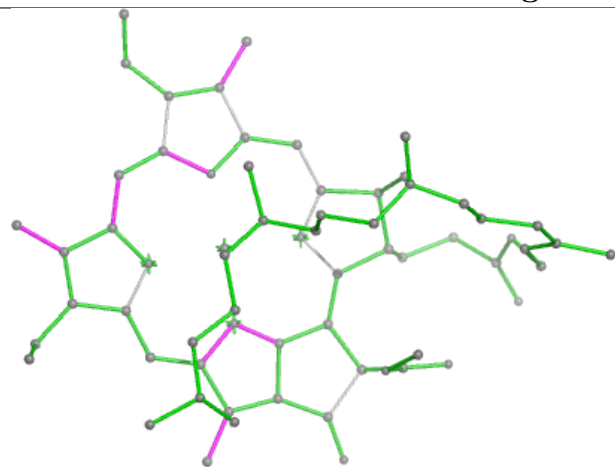




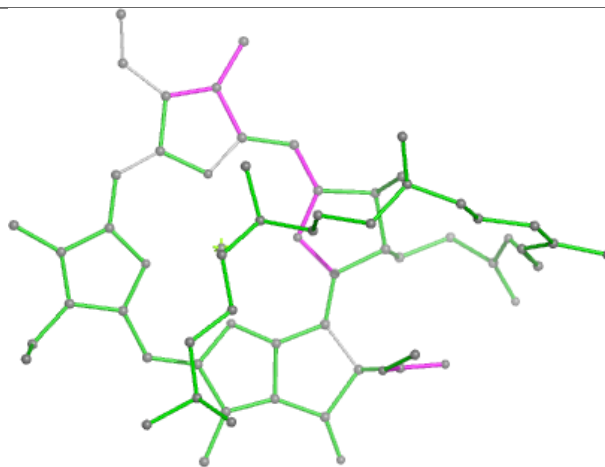




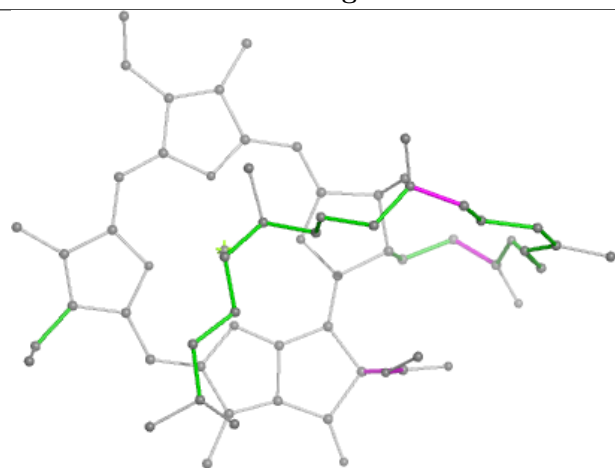
Ligand CLA c 510



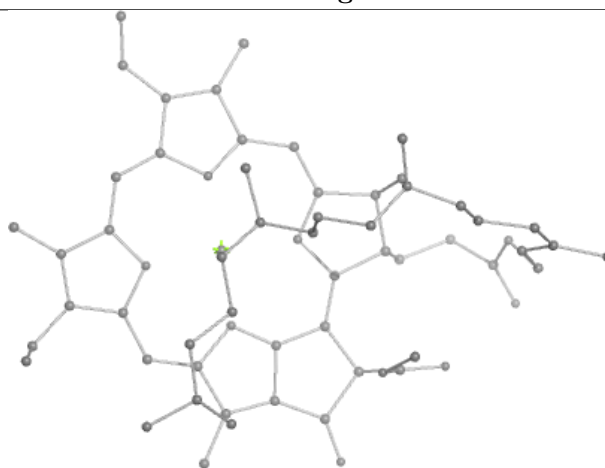
Bond lengths



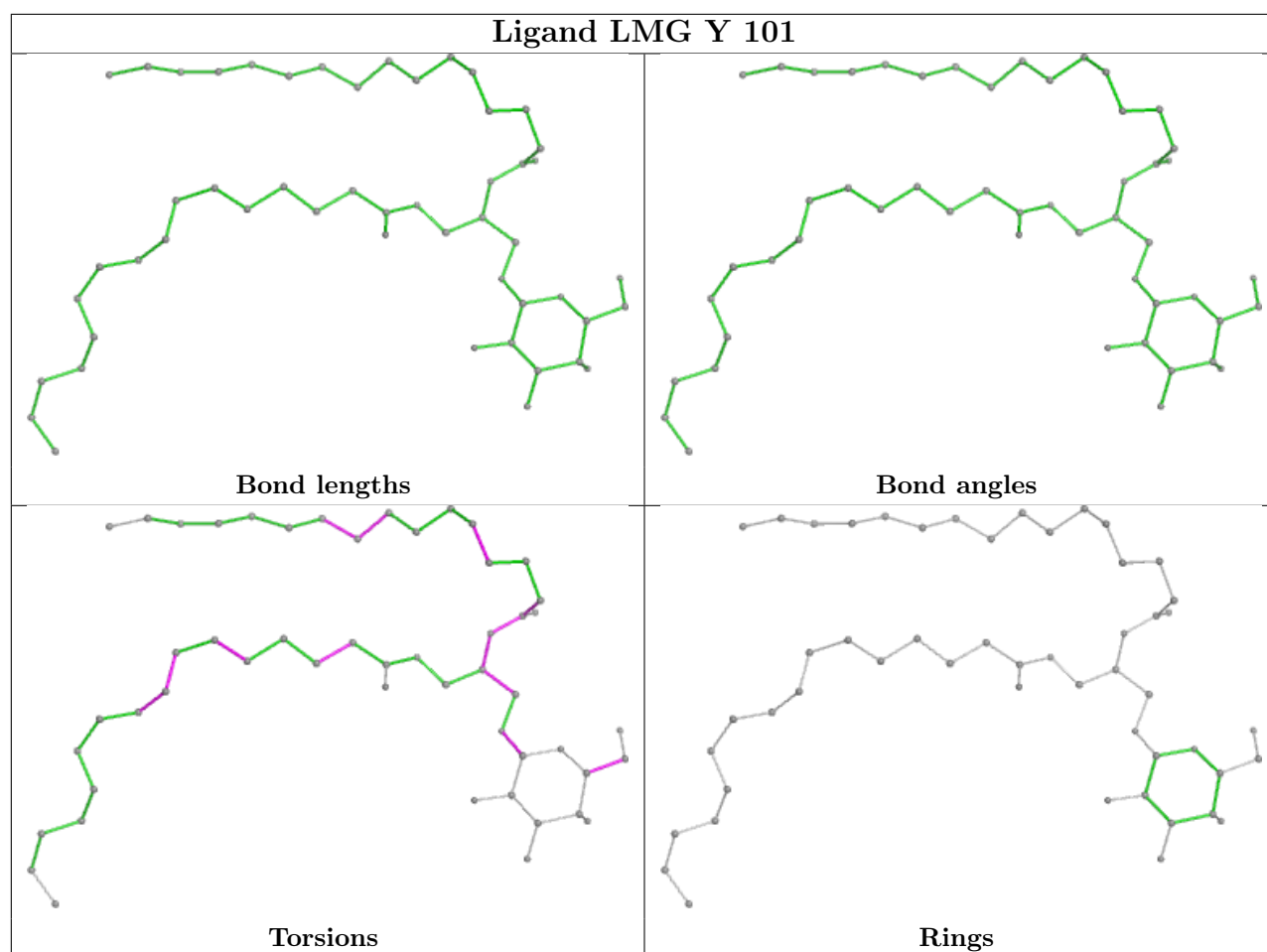
Bond angles



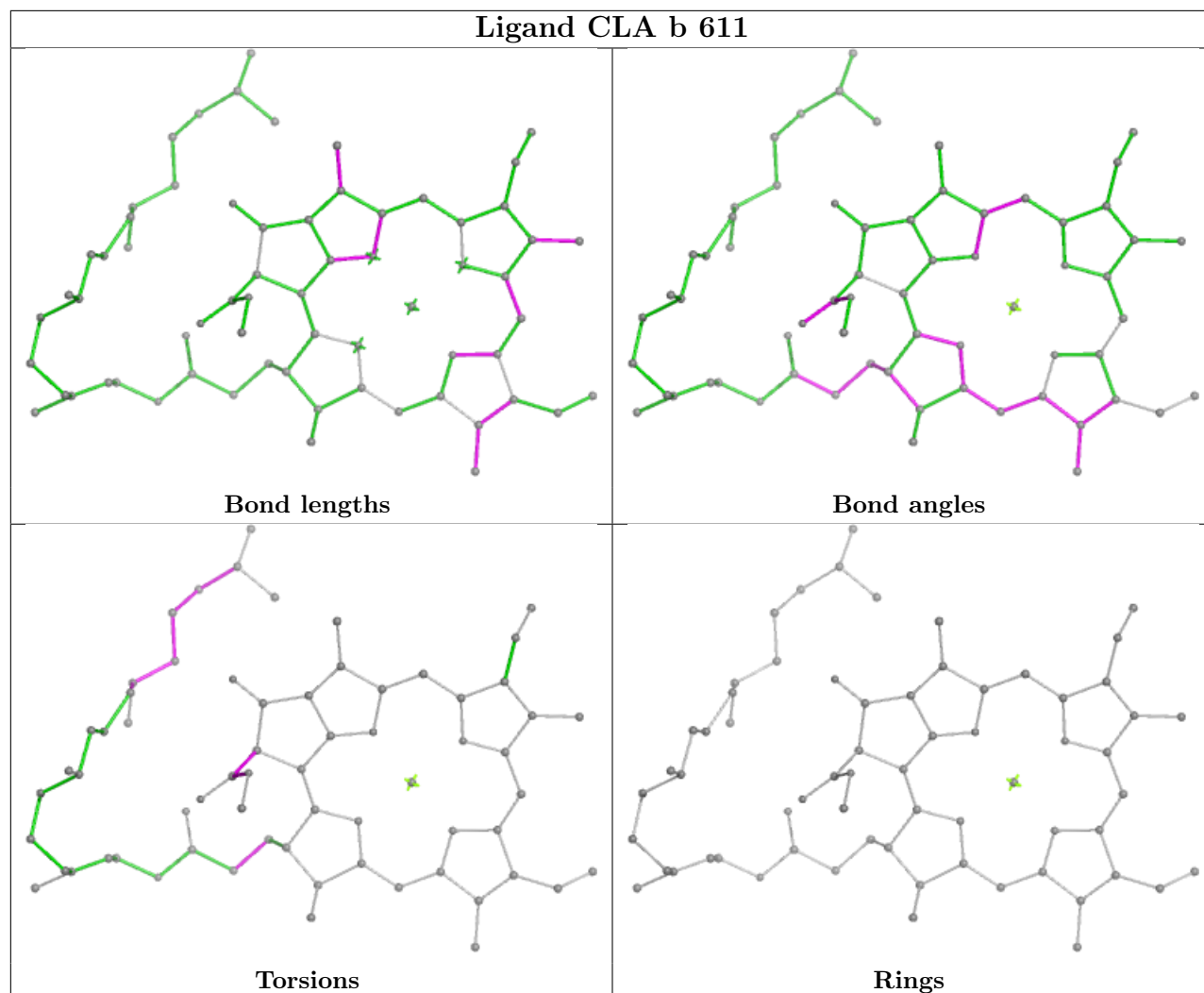
Torsions



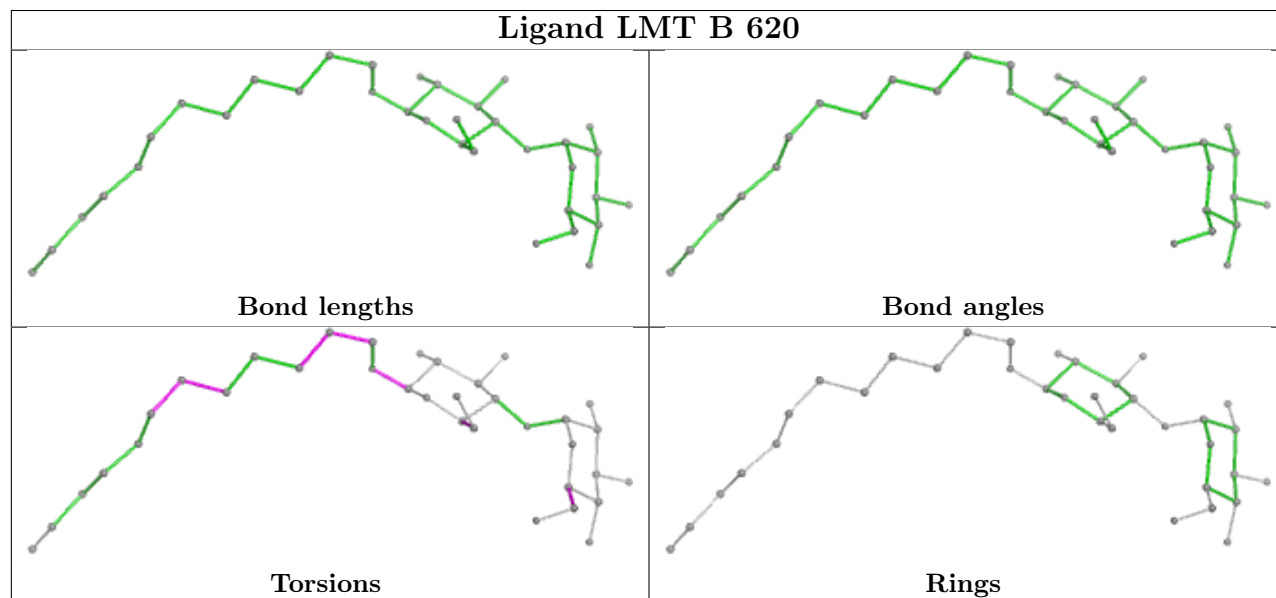
Rings

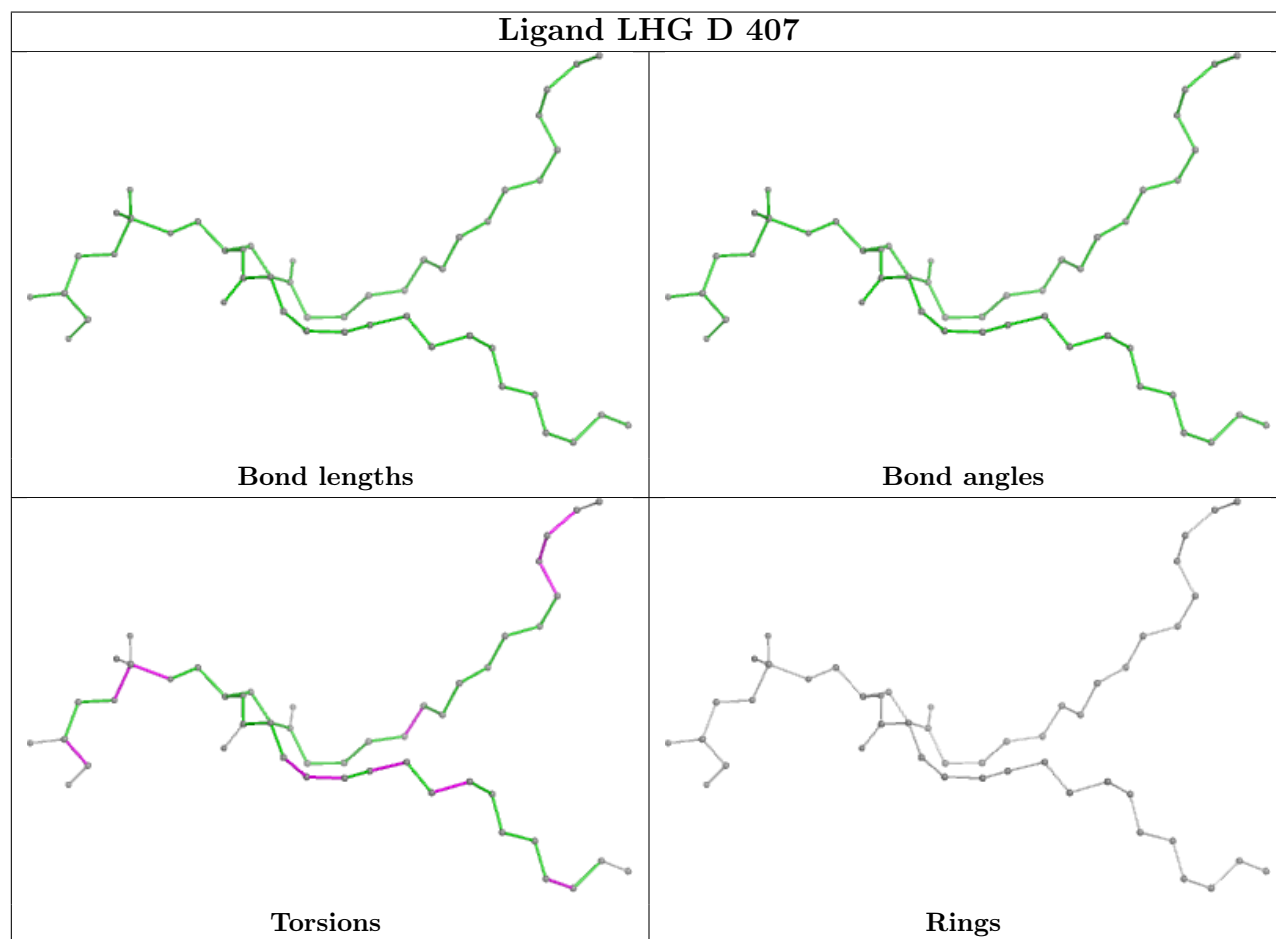
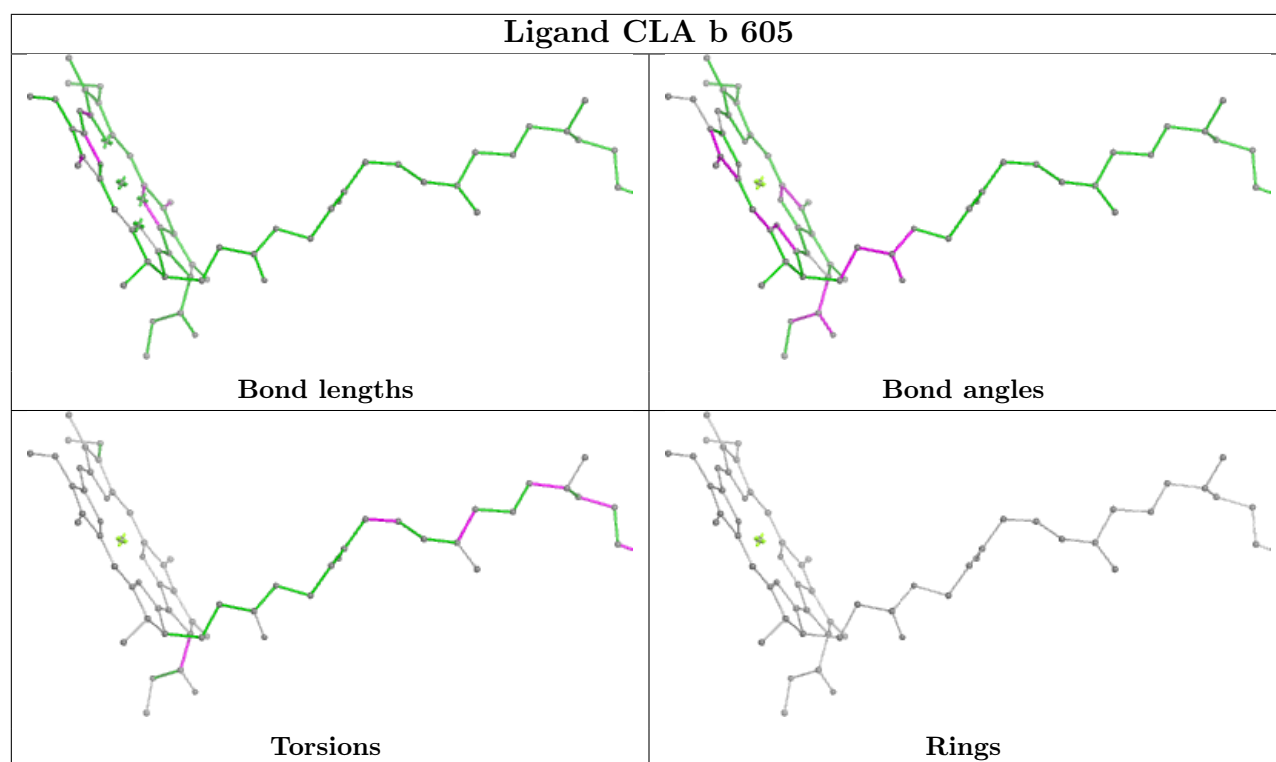


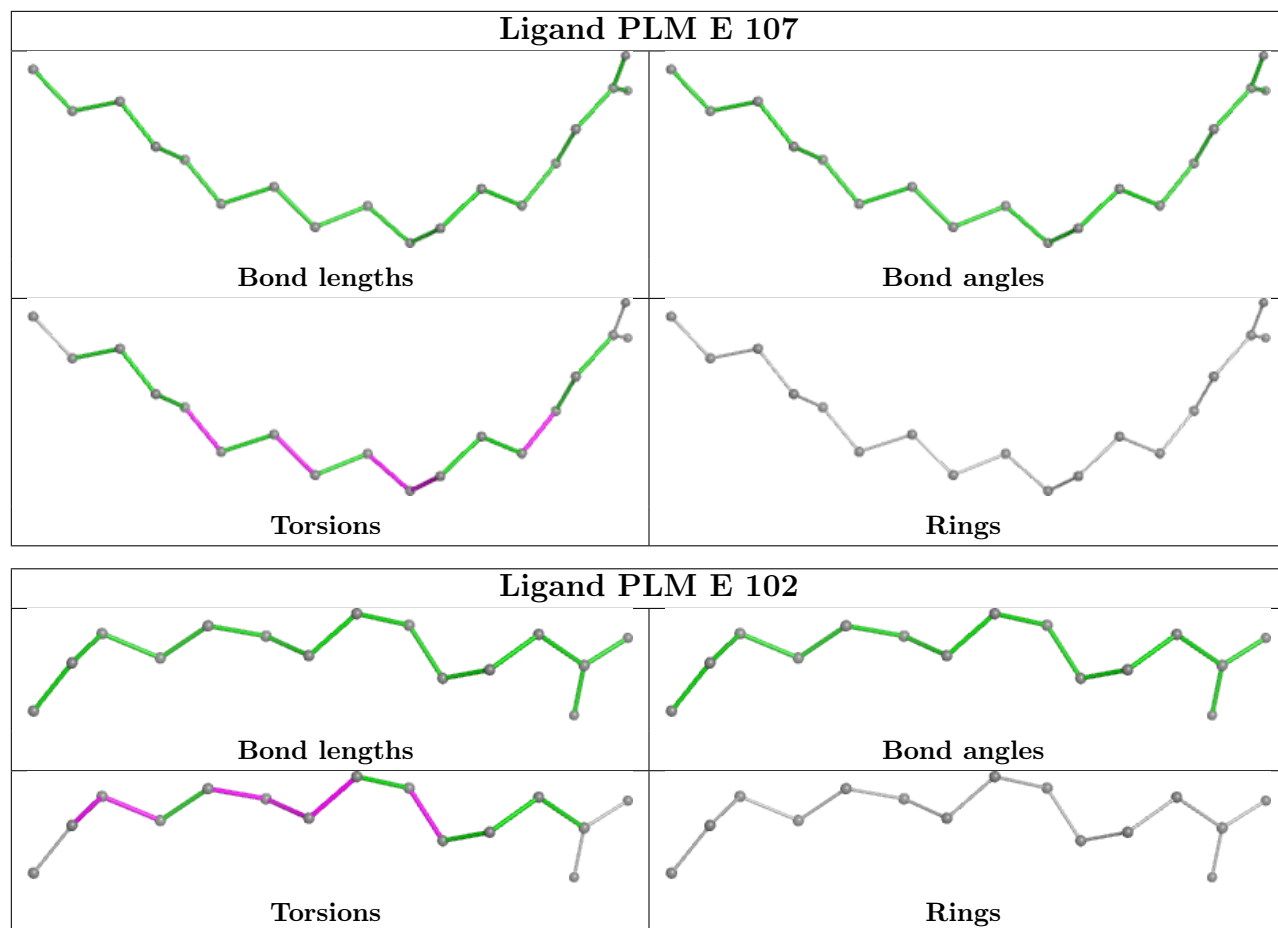
Ligand CLA b 611



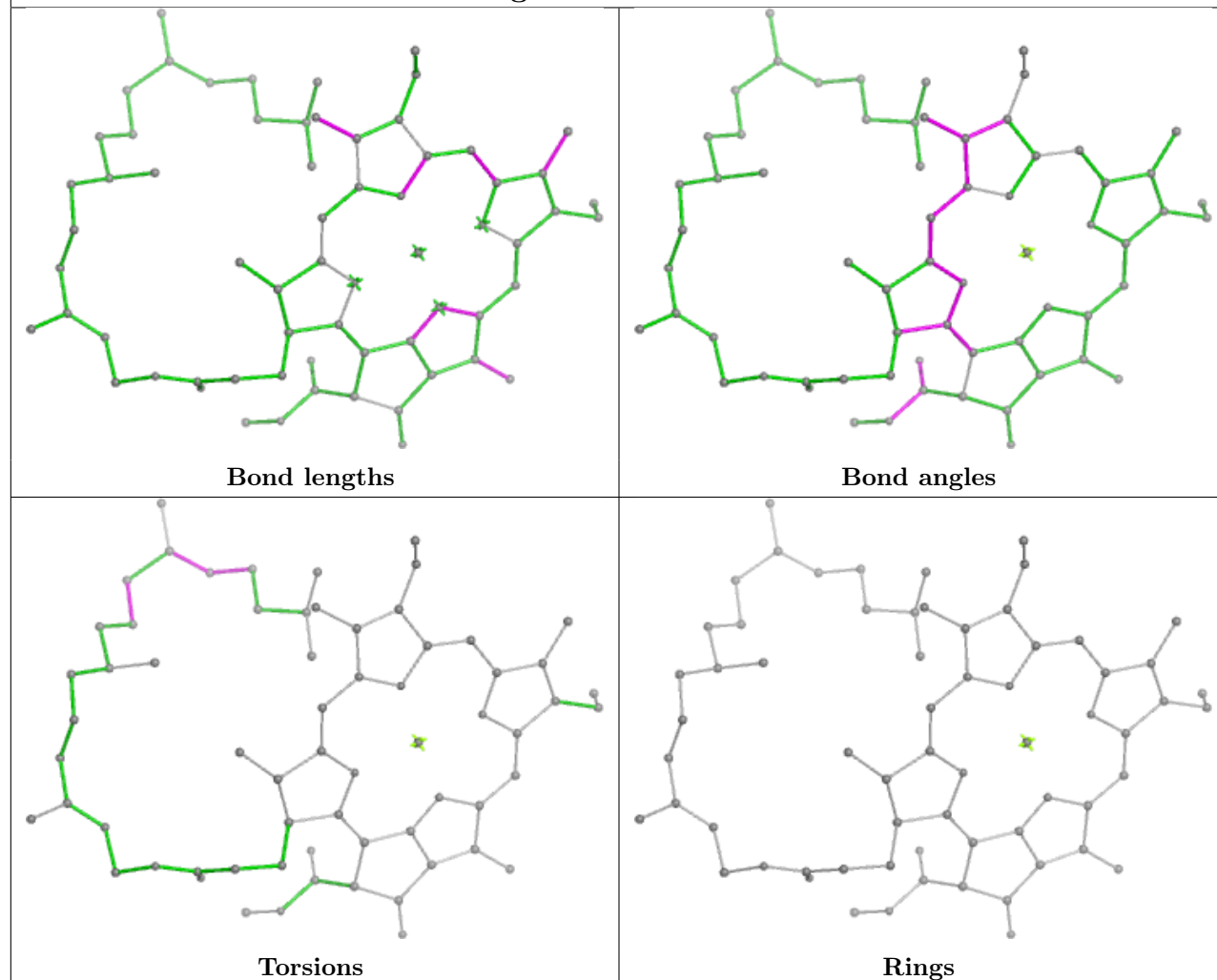
Ligand LMT B 620



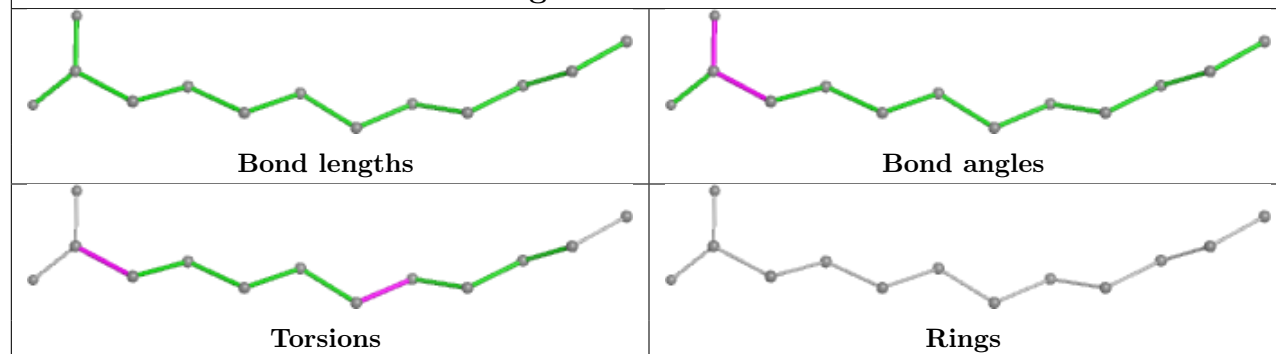


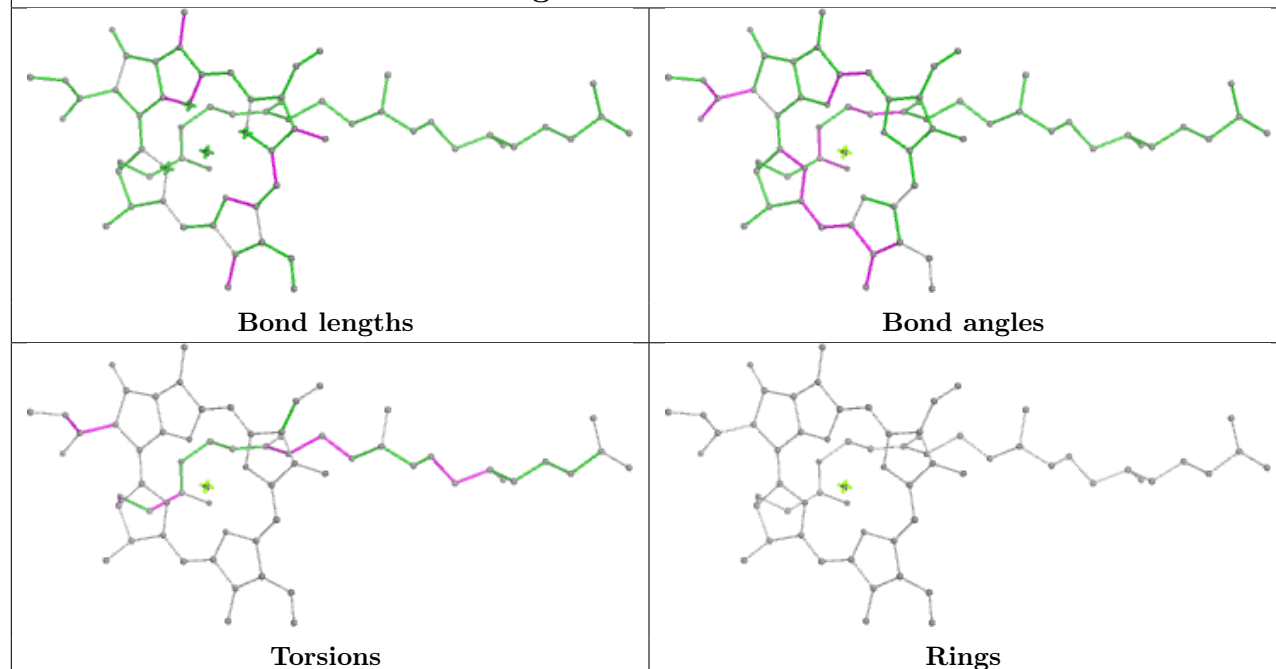
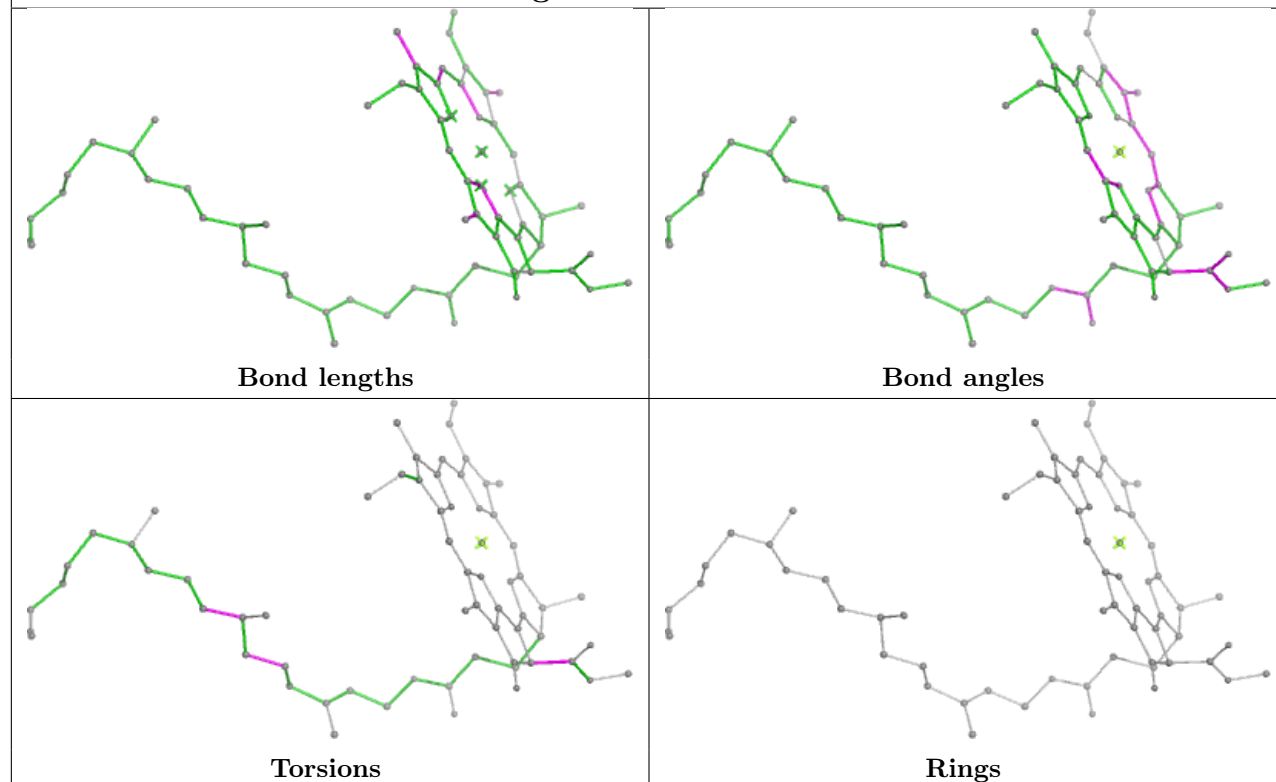


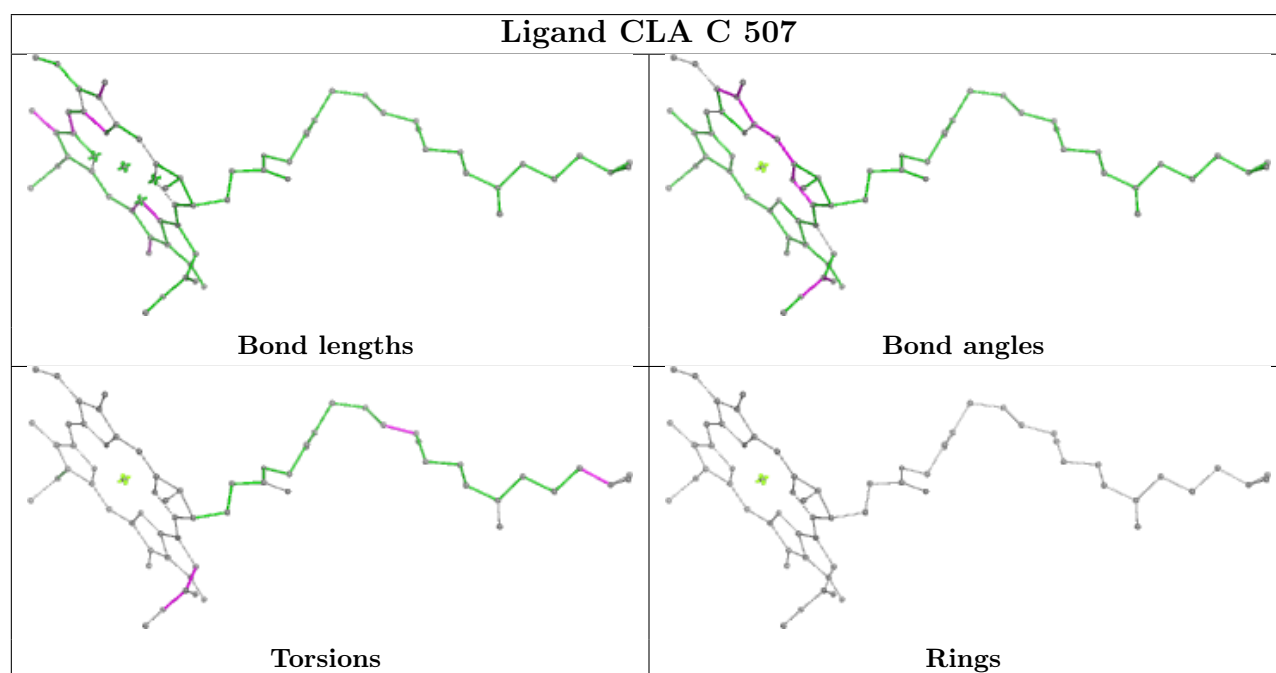
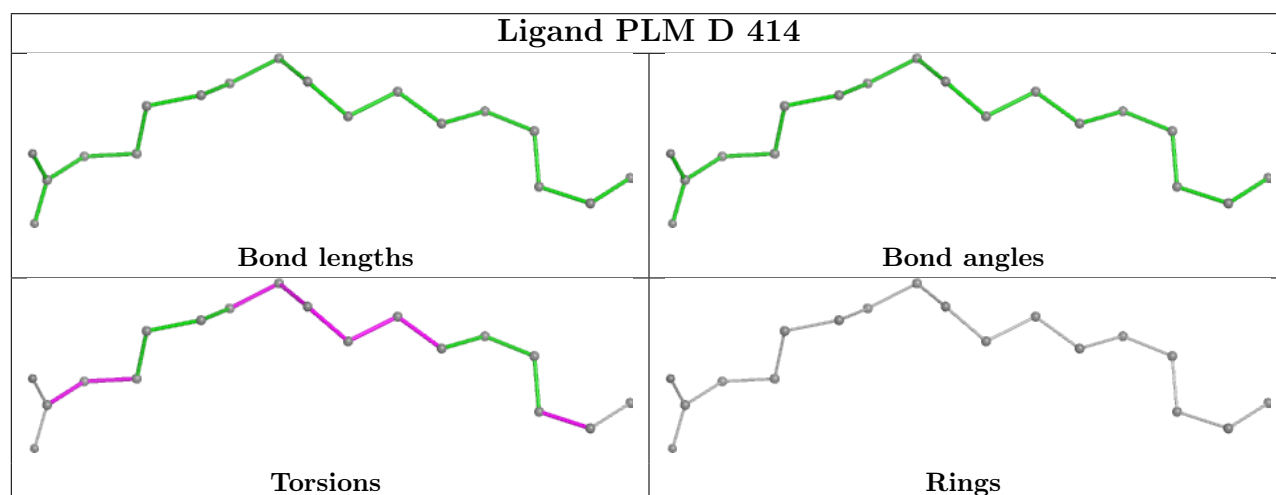
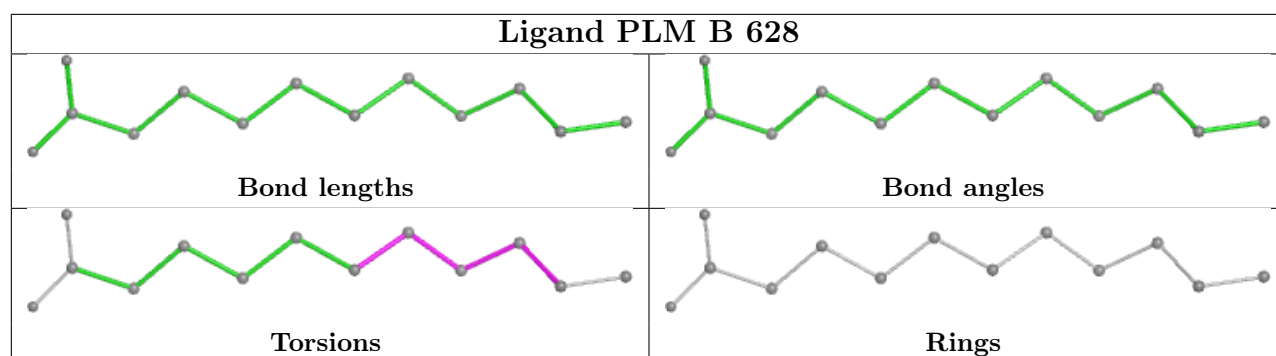
Ligand CLA b 616

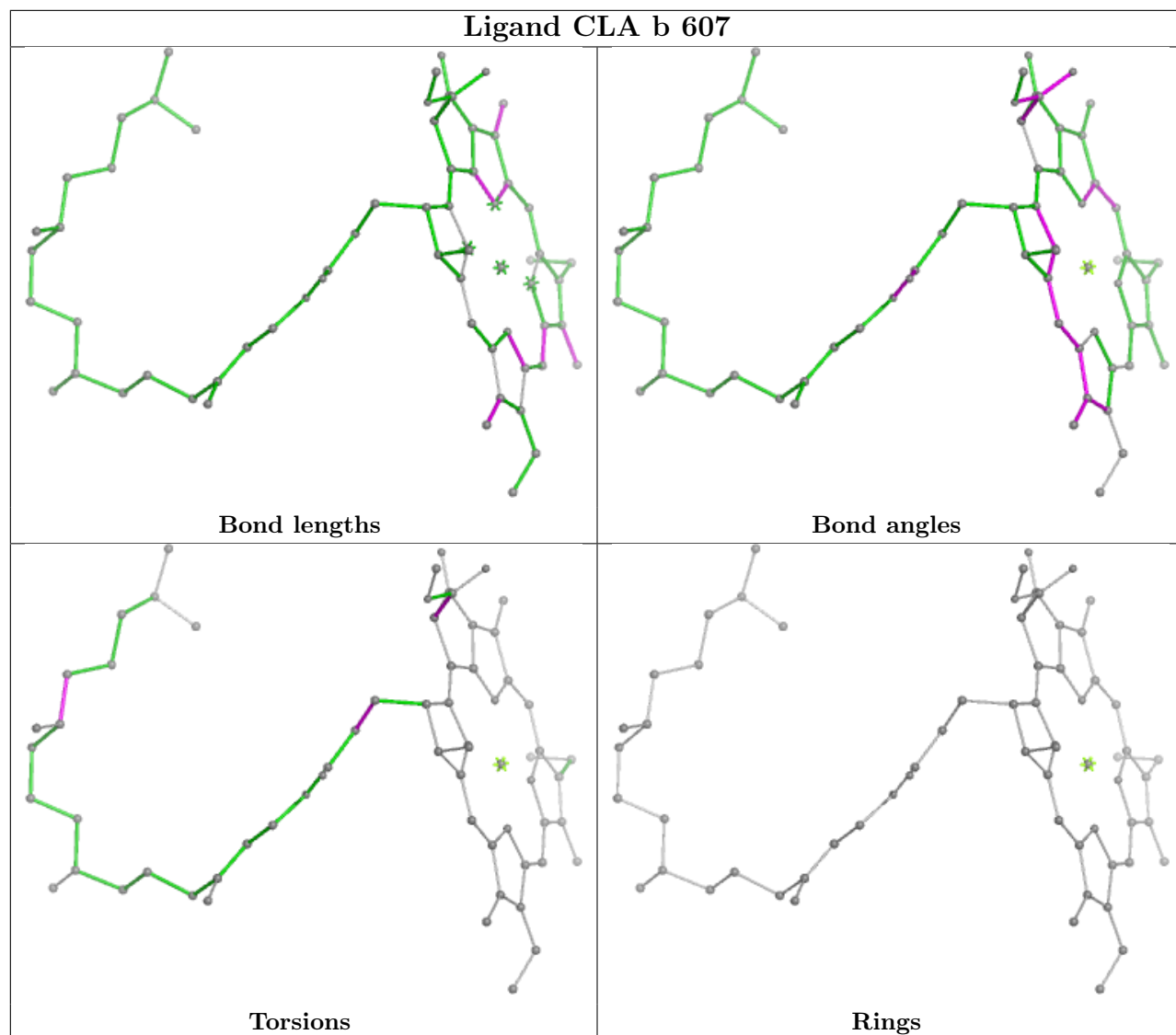


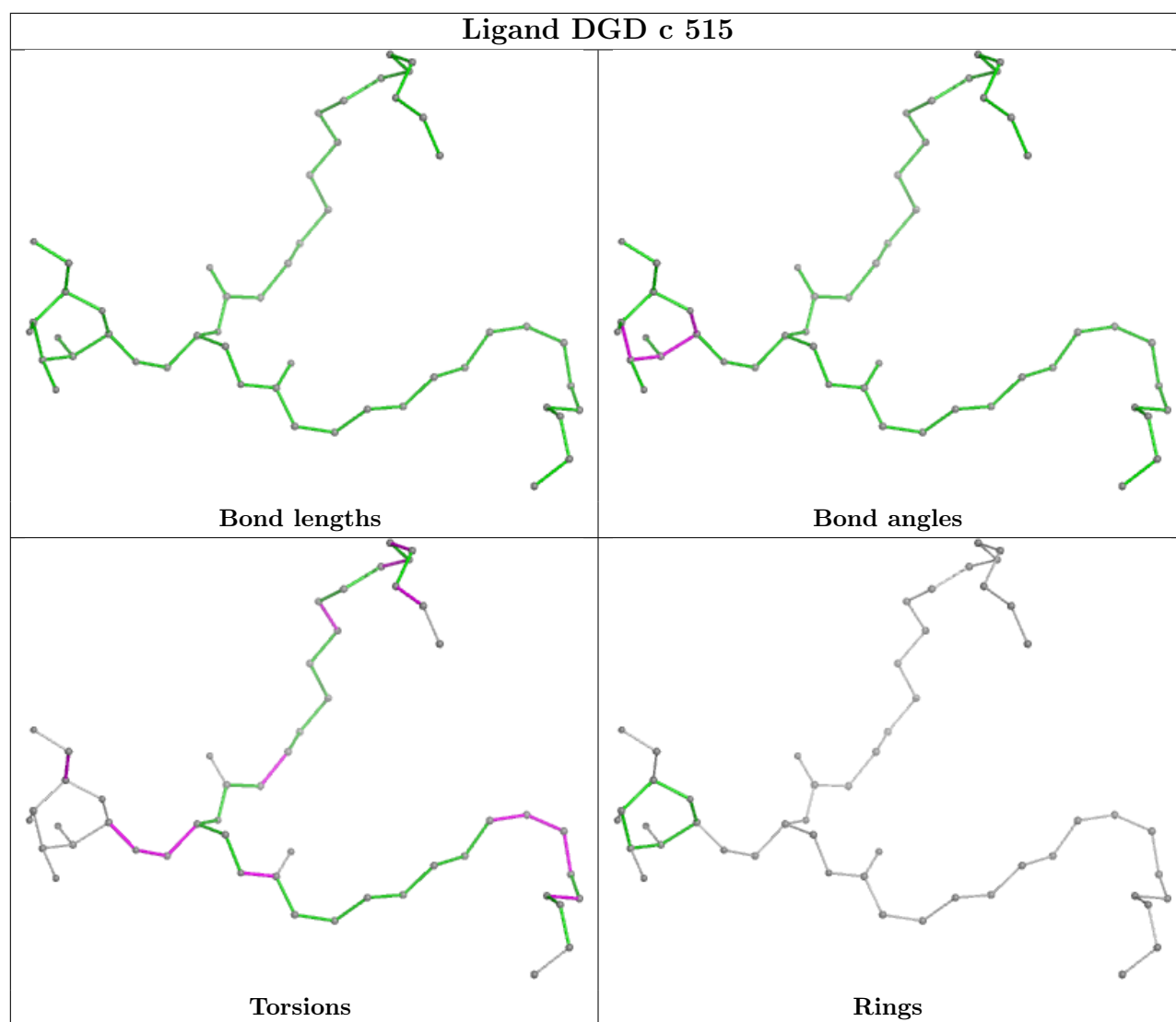
Ligand PLM C 519



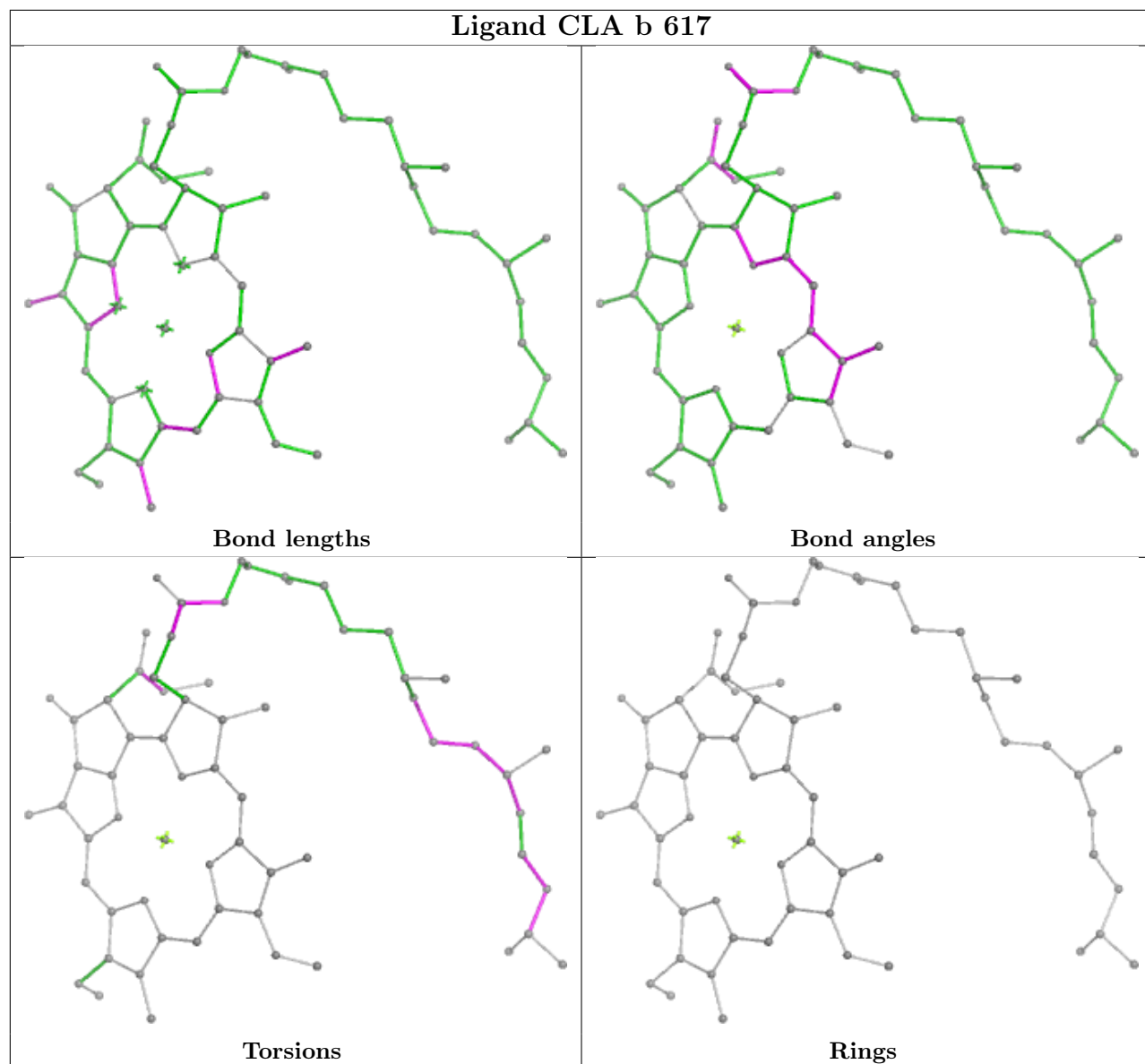
Ligand CLA B 614**Ligand CLA C 513**



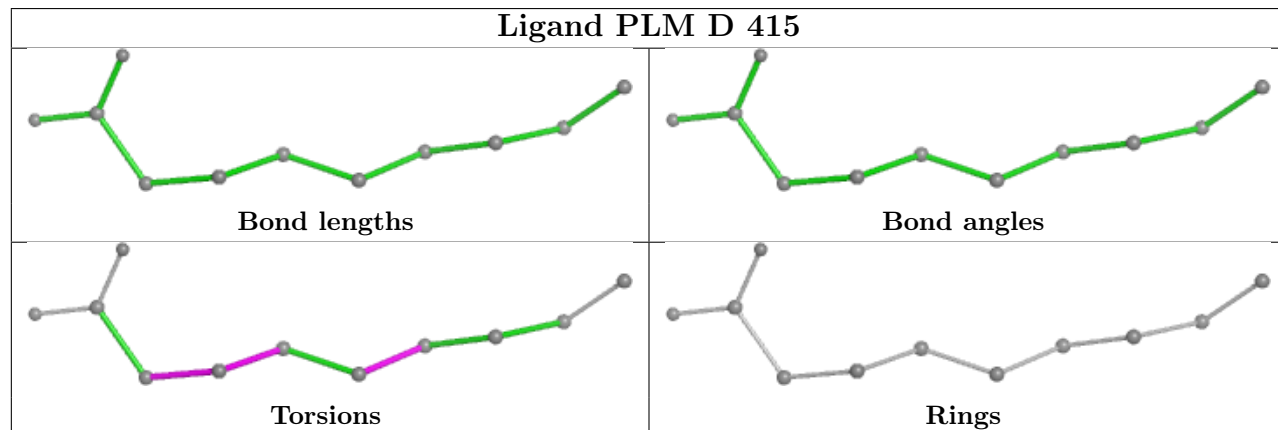




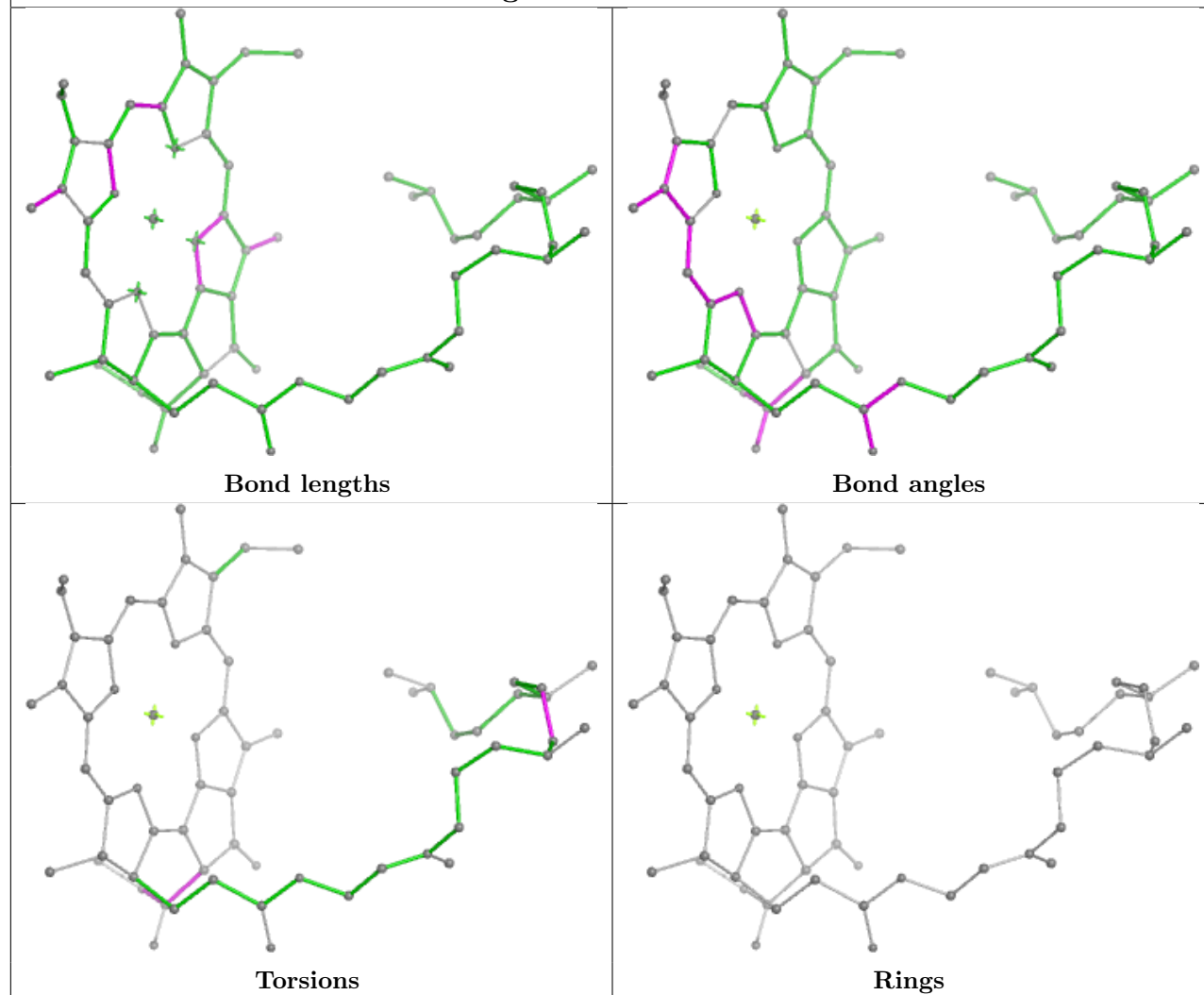
Ligand CLA b 617



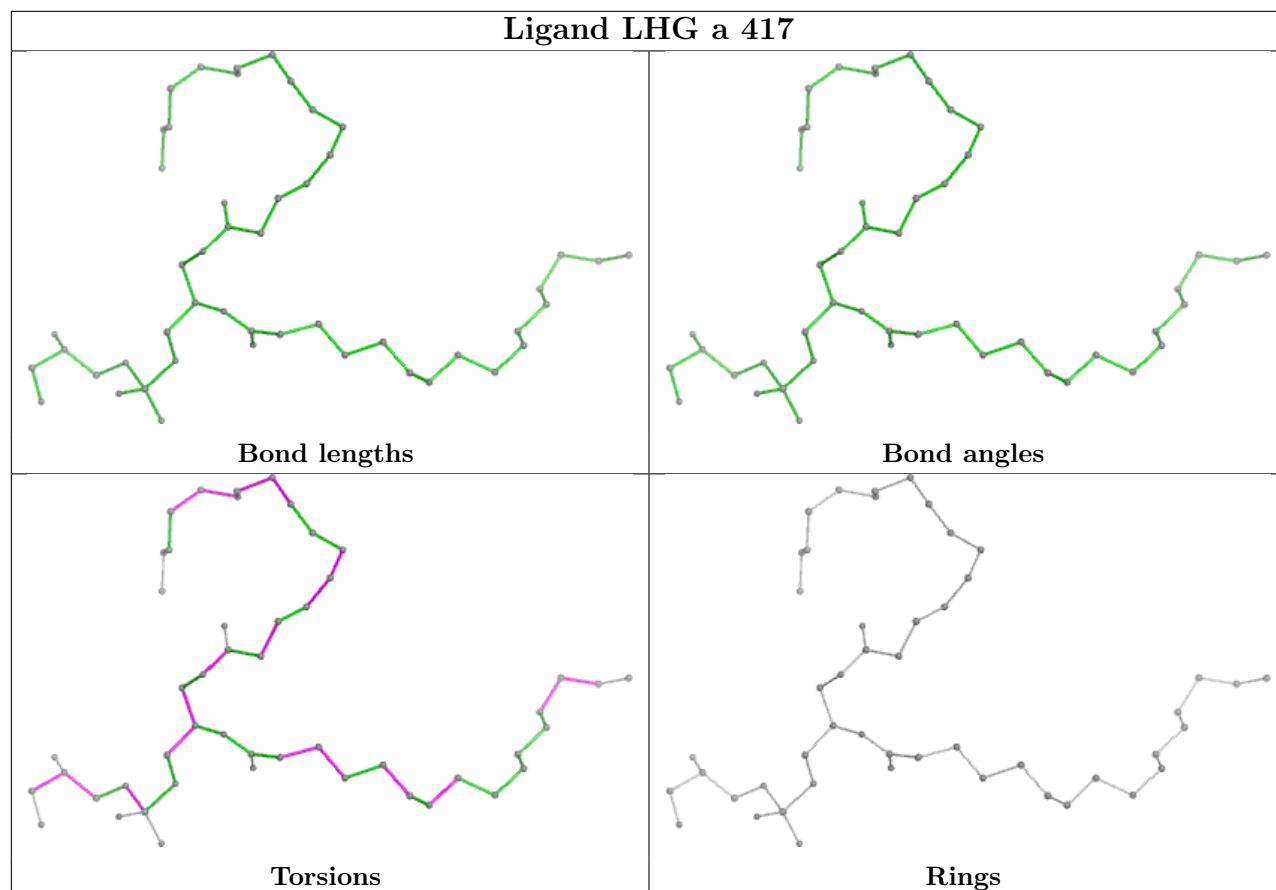
Ligand PLM D 415



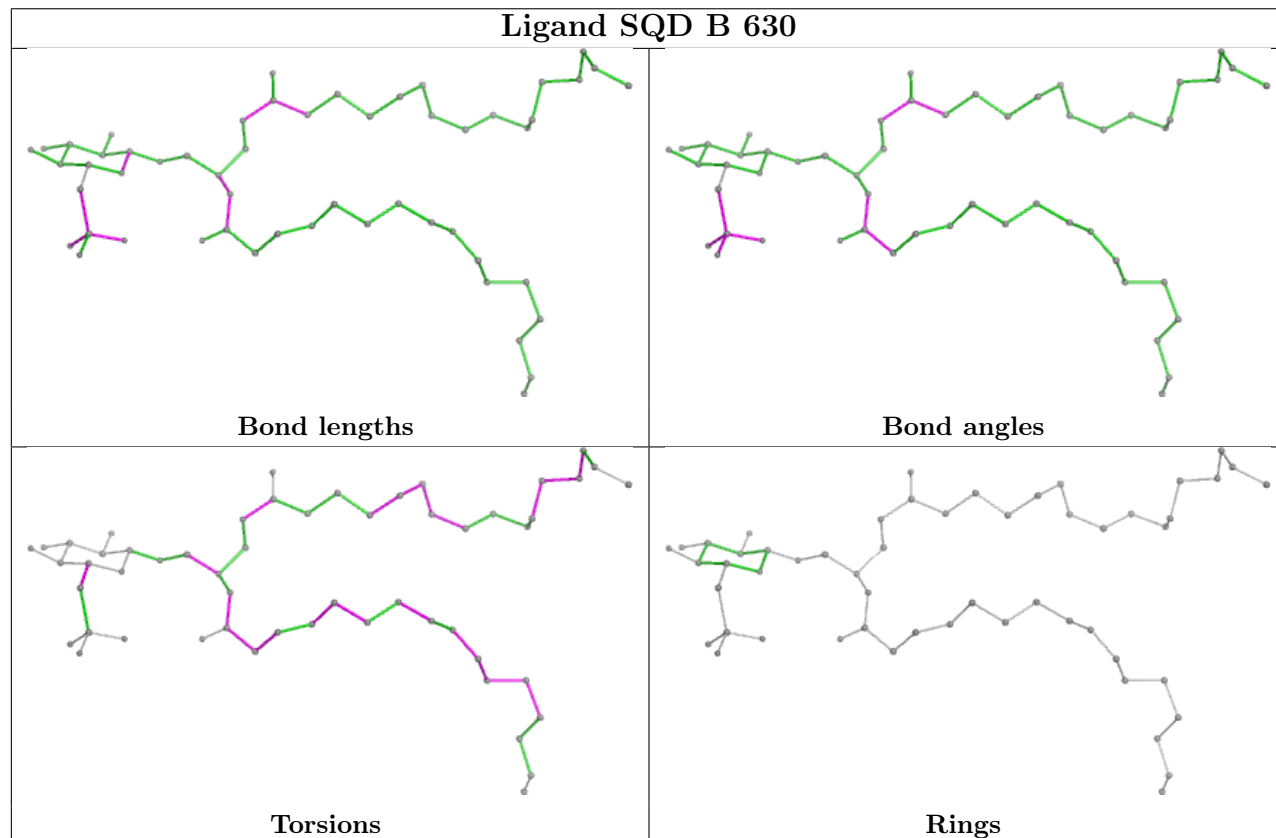
Ligand CLA C 508

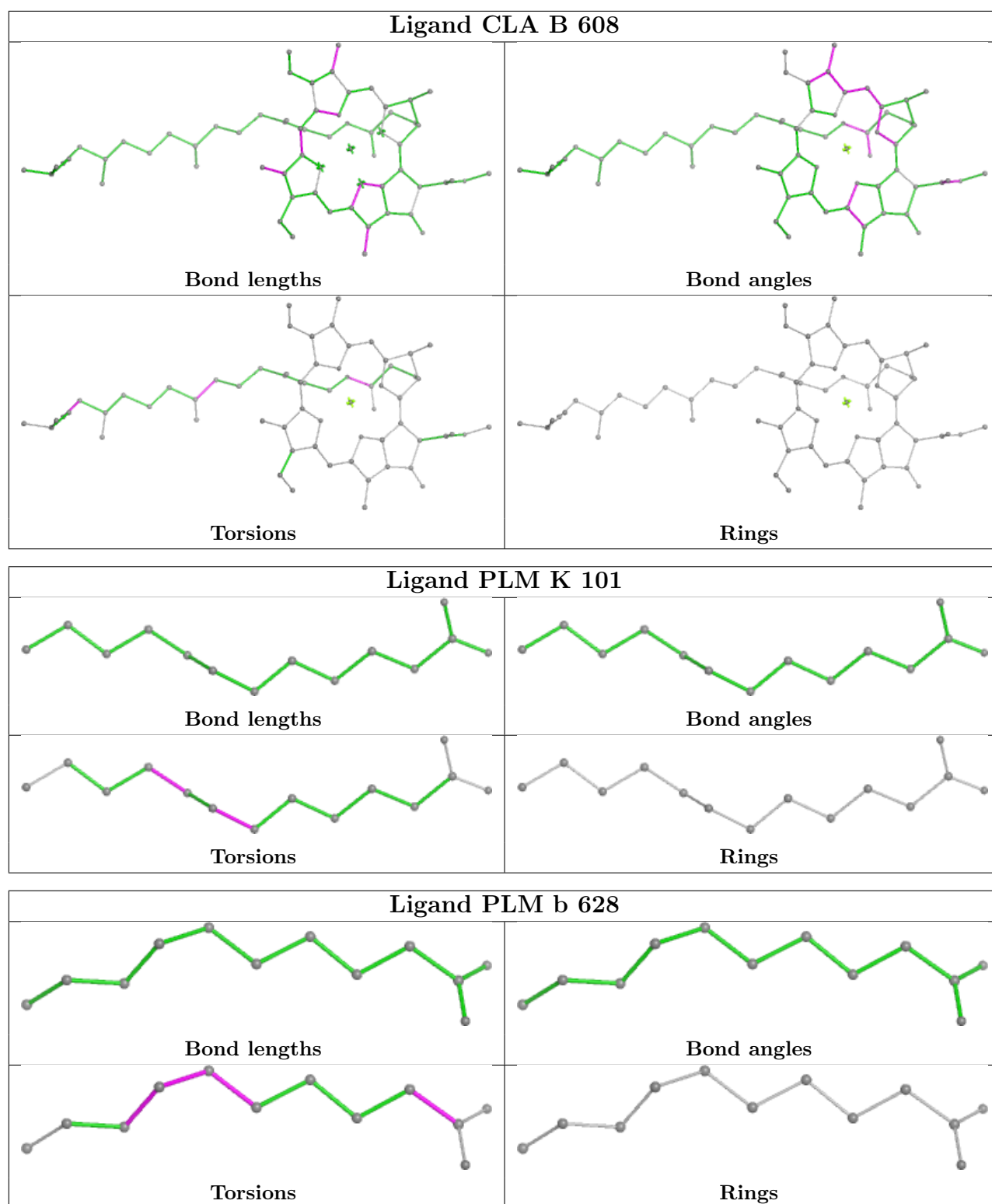


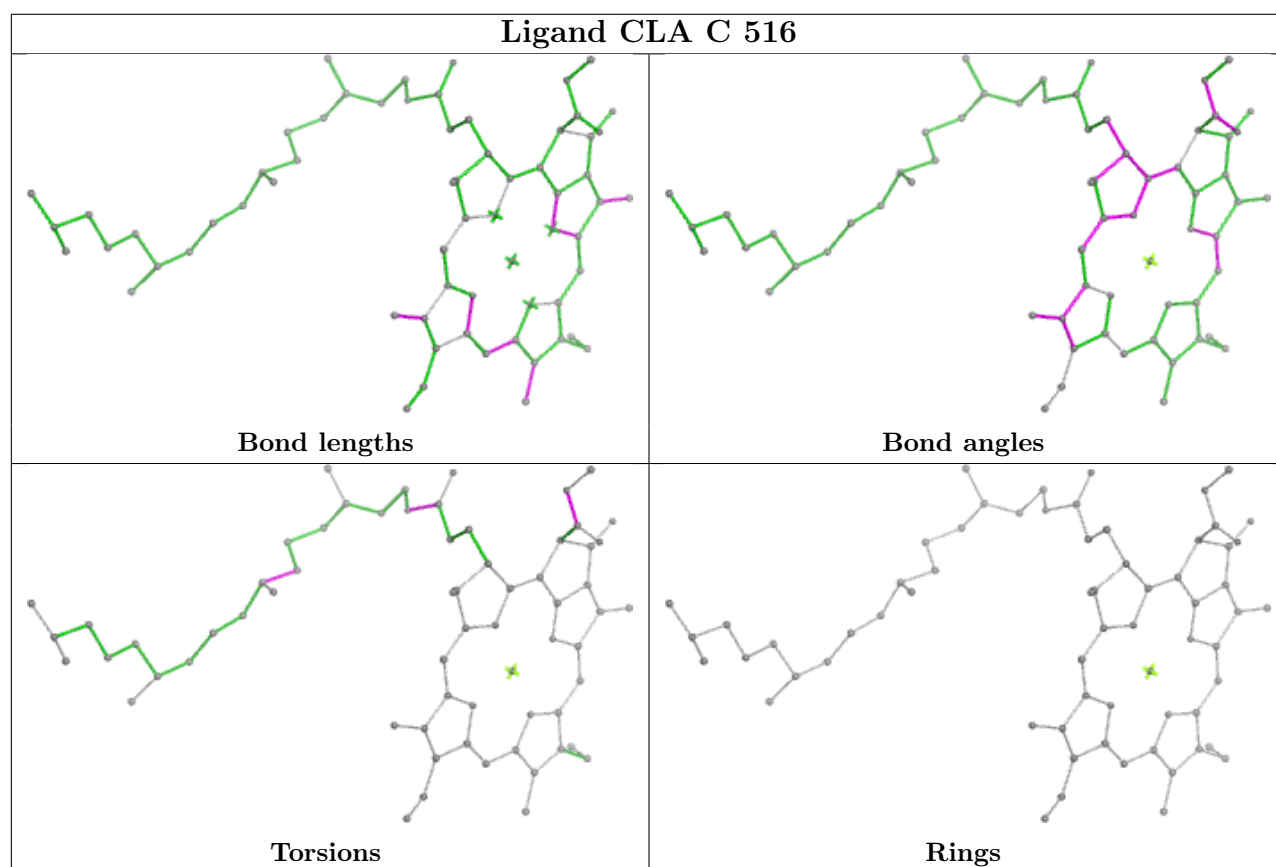
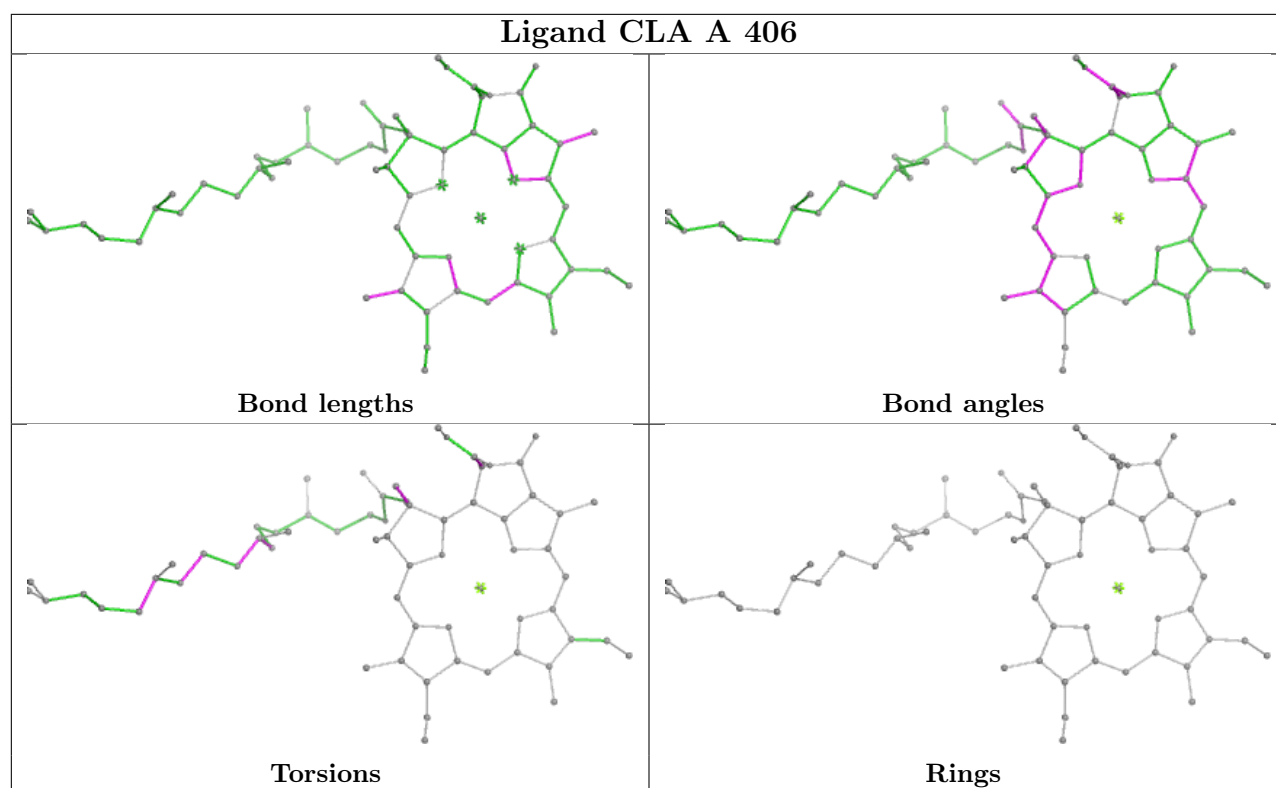
Ligand LHG a 417



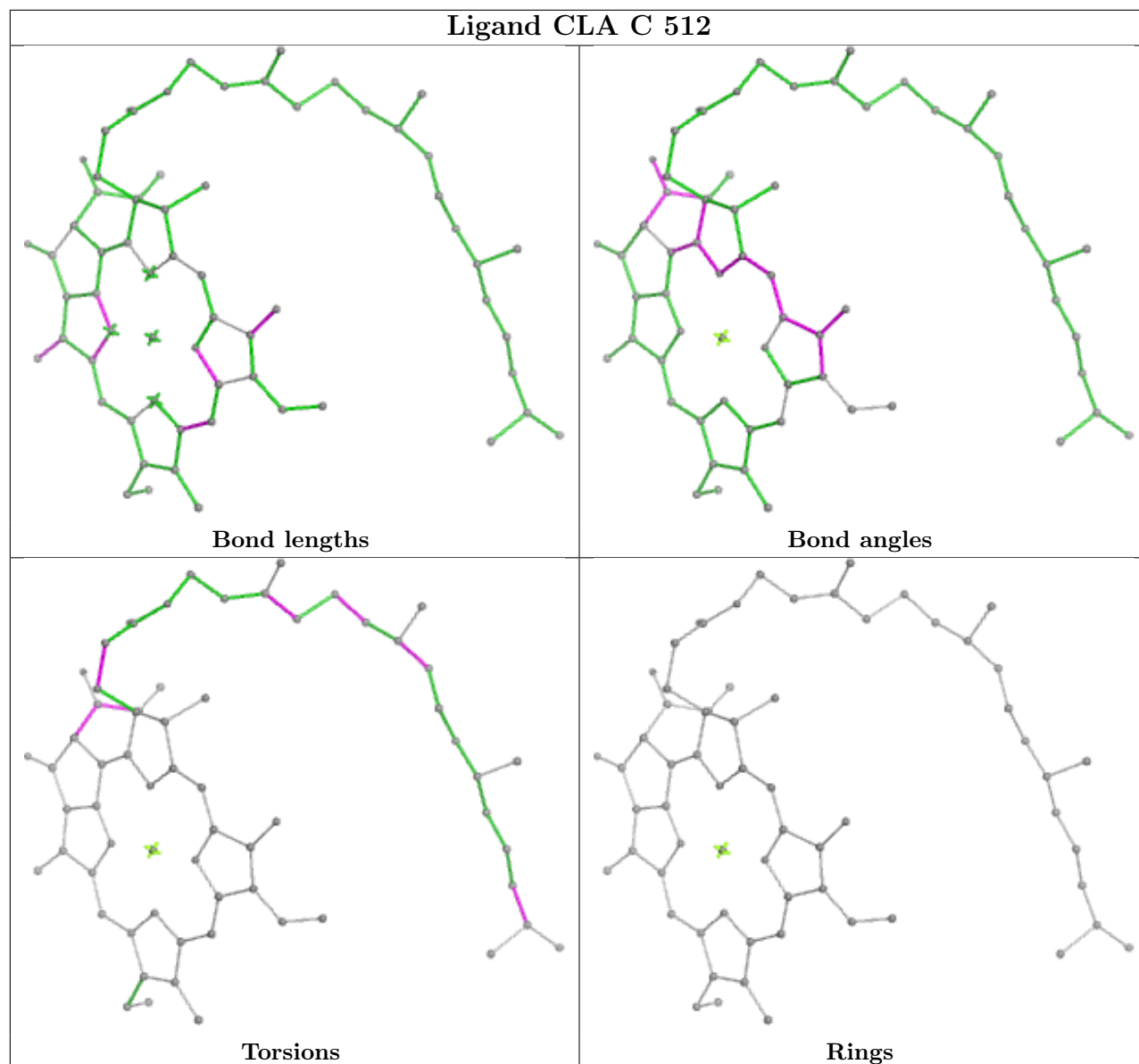
Ligand SQD B 630



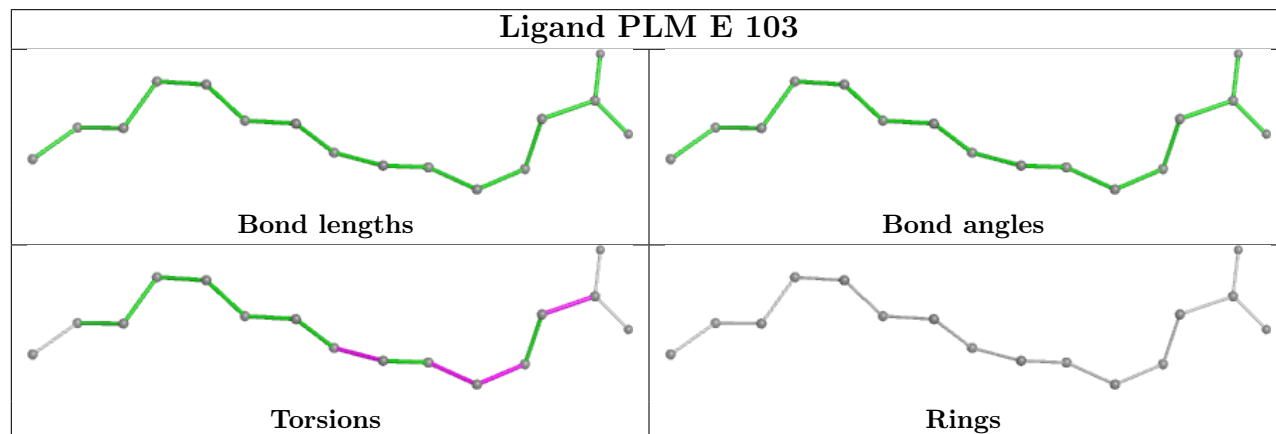


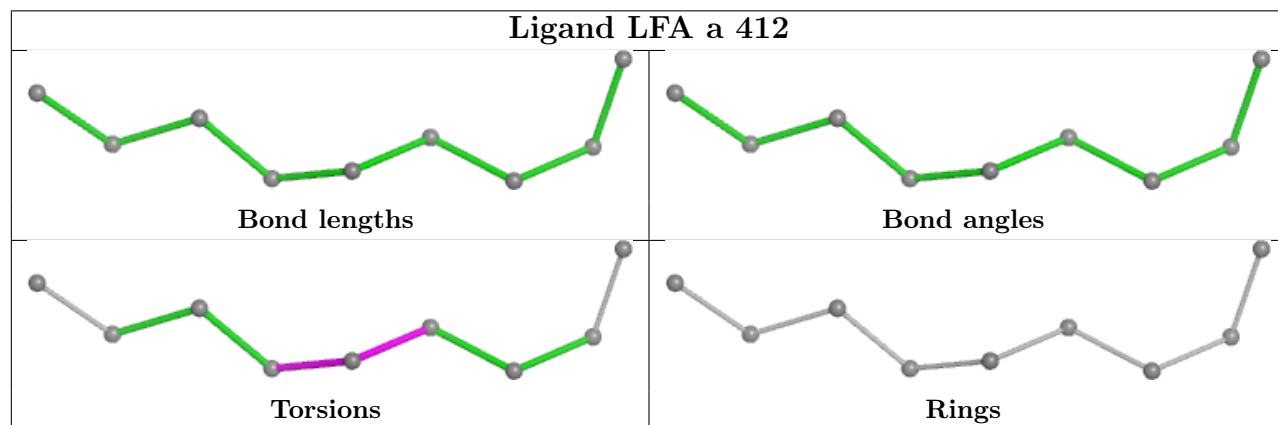
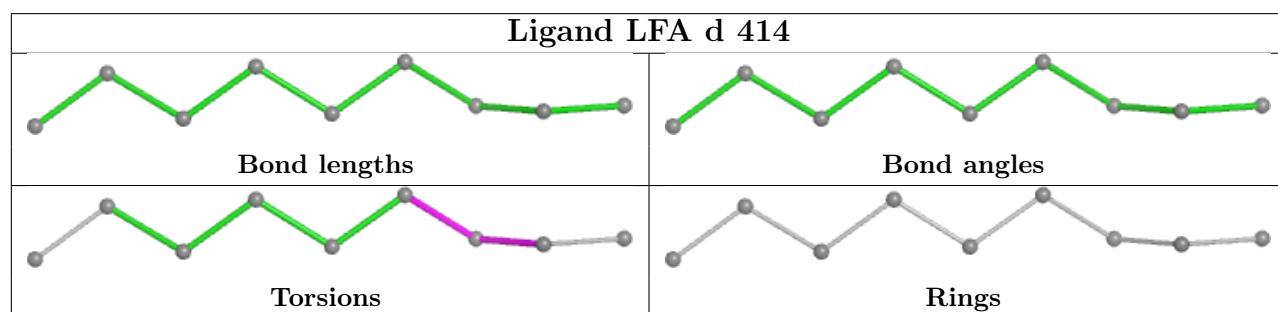
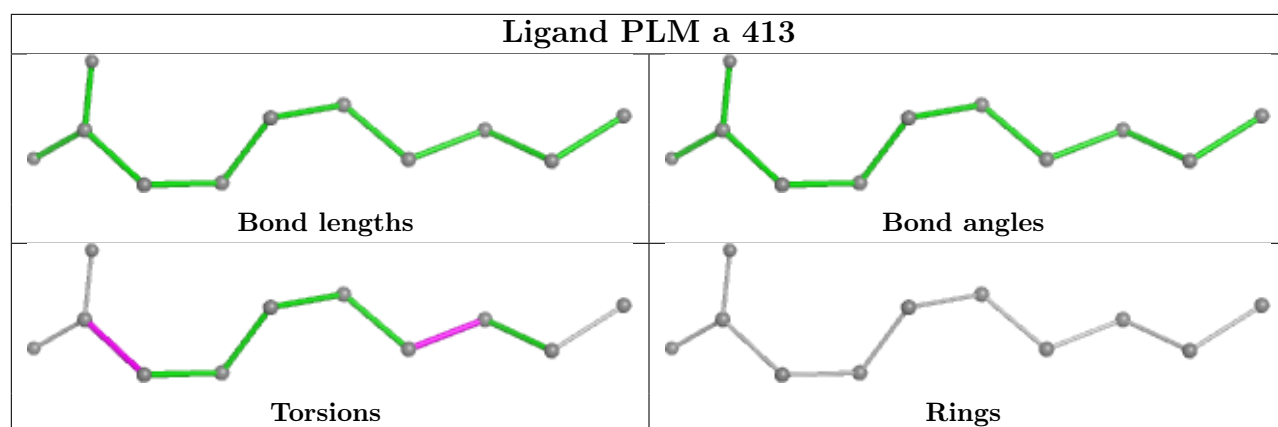


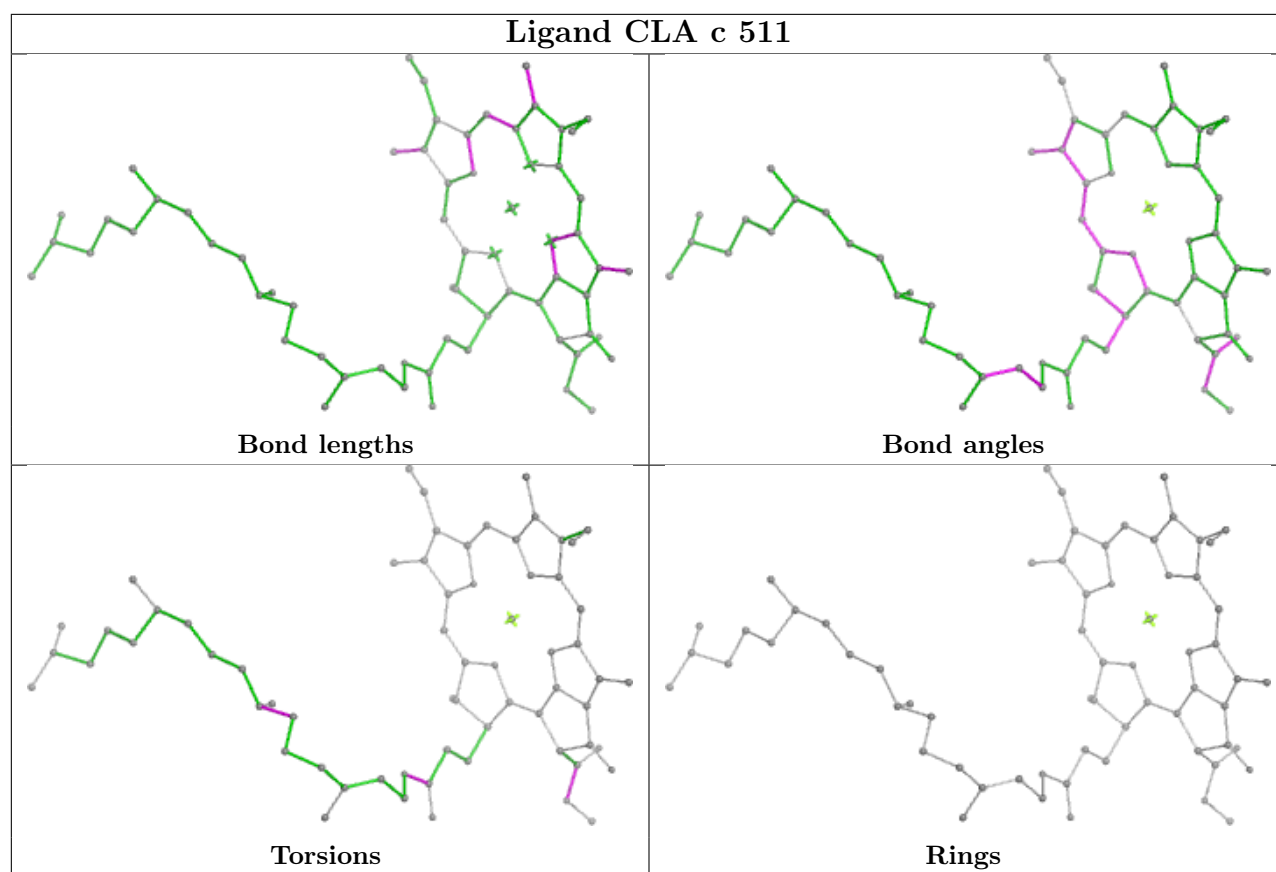
Ligand CLA C 512

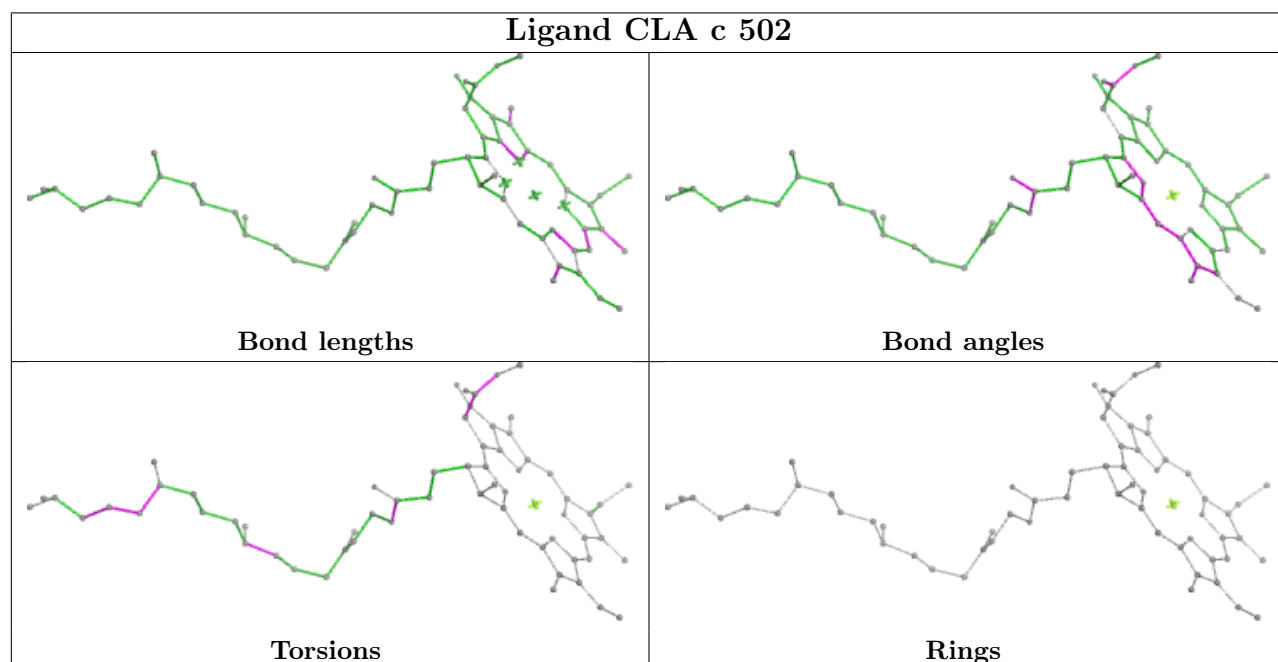
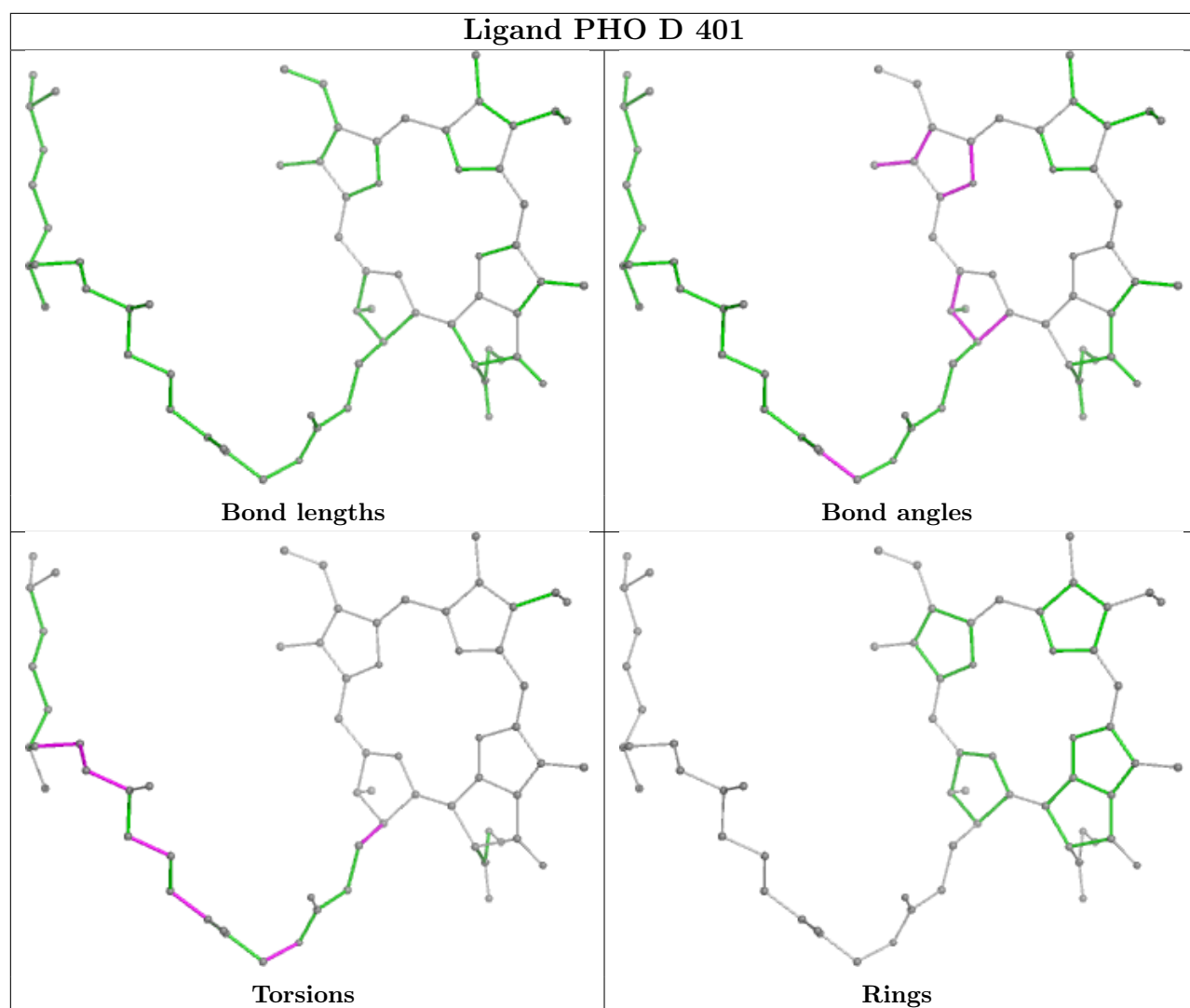


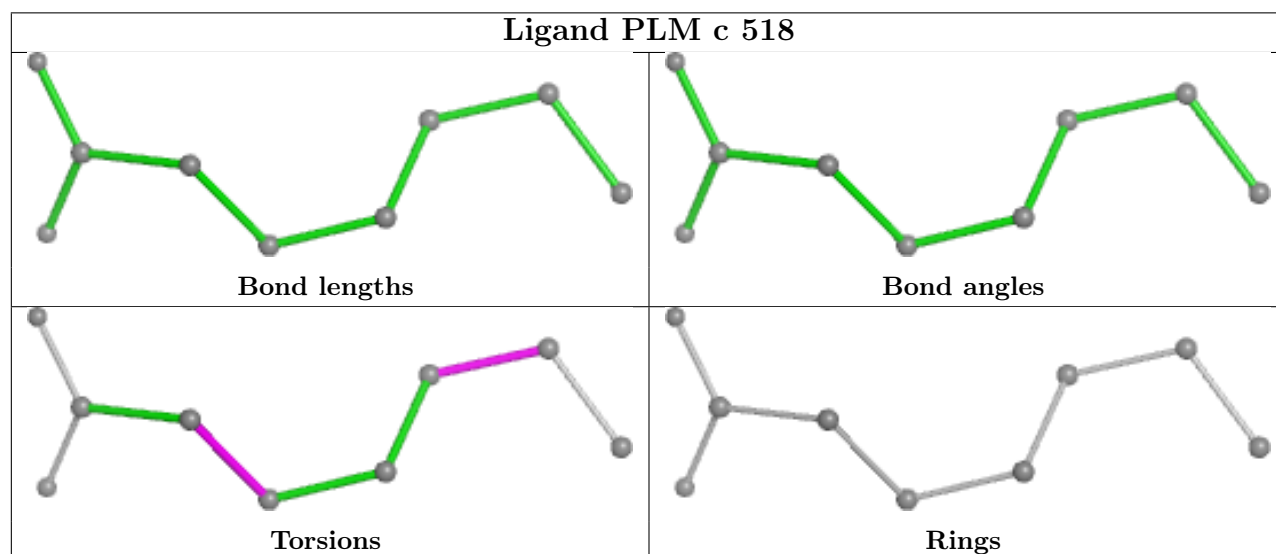
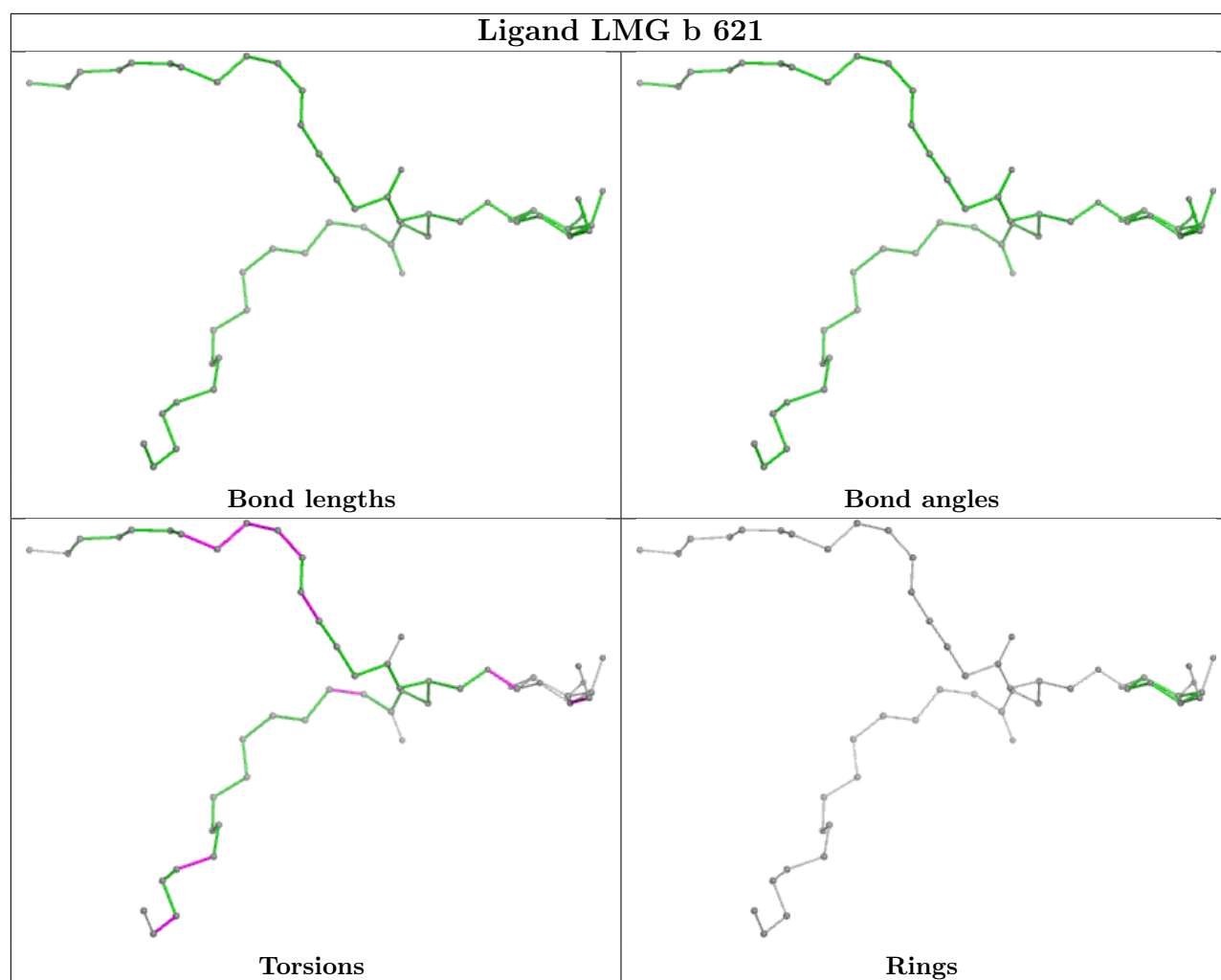
Ligand PLM E 103

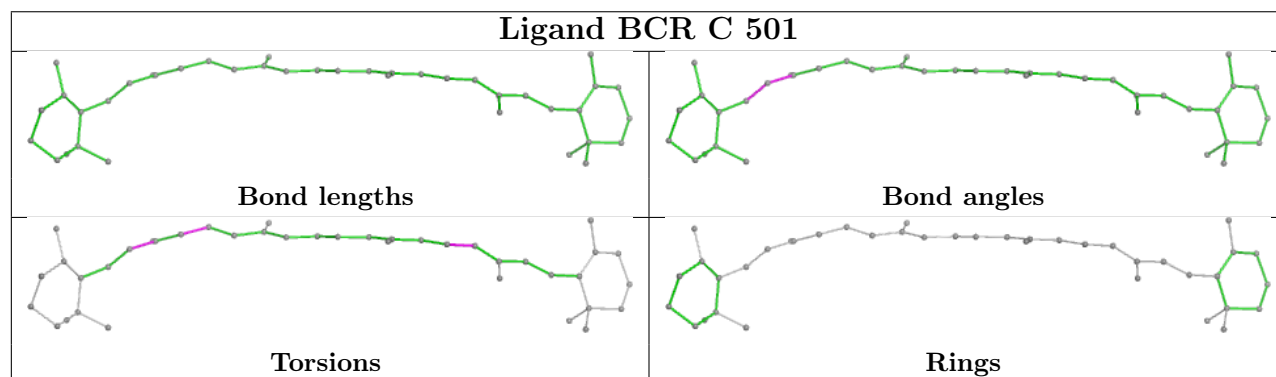
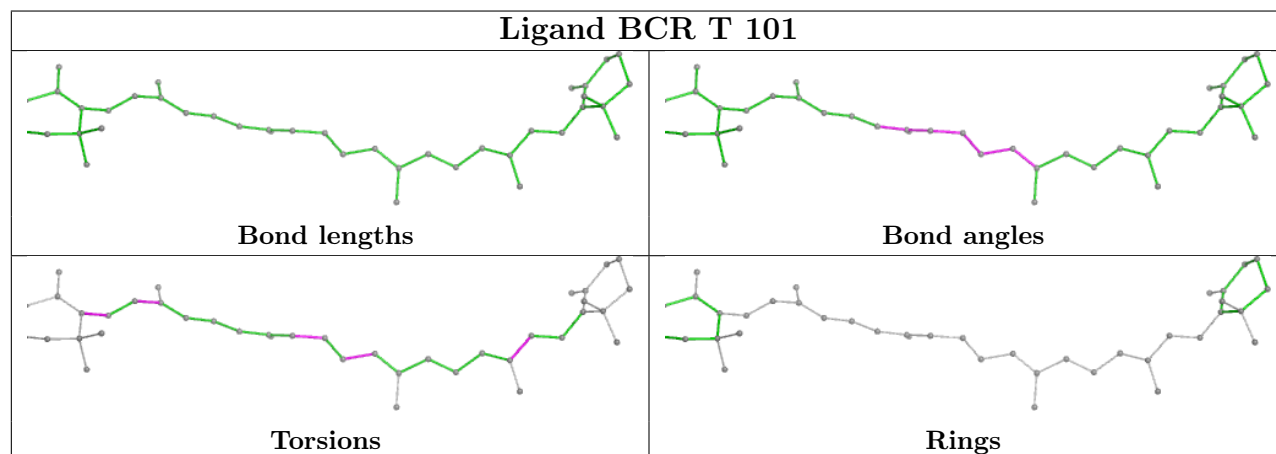
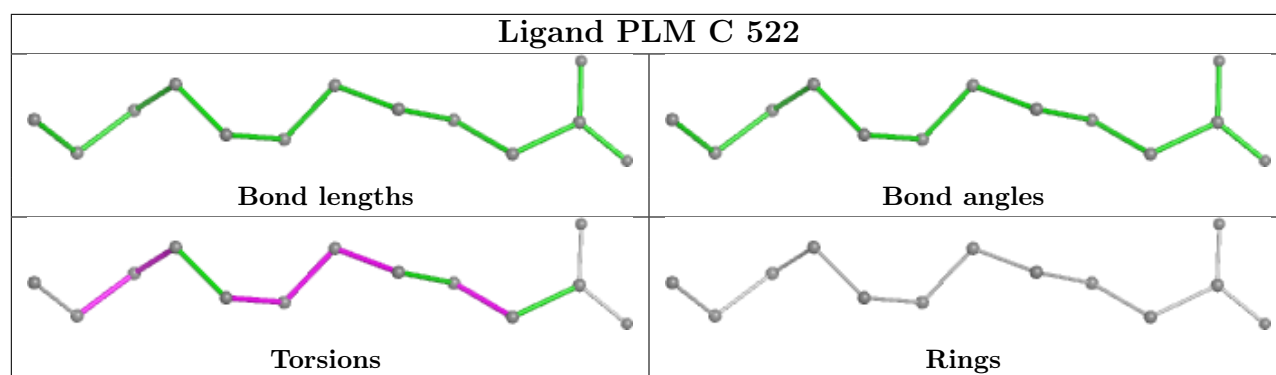


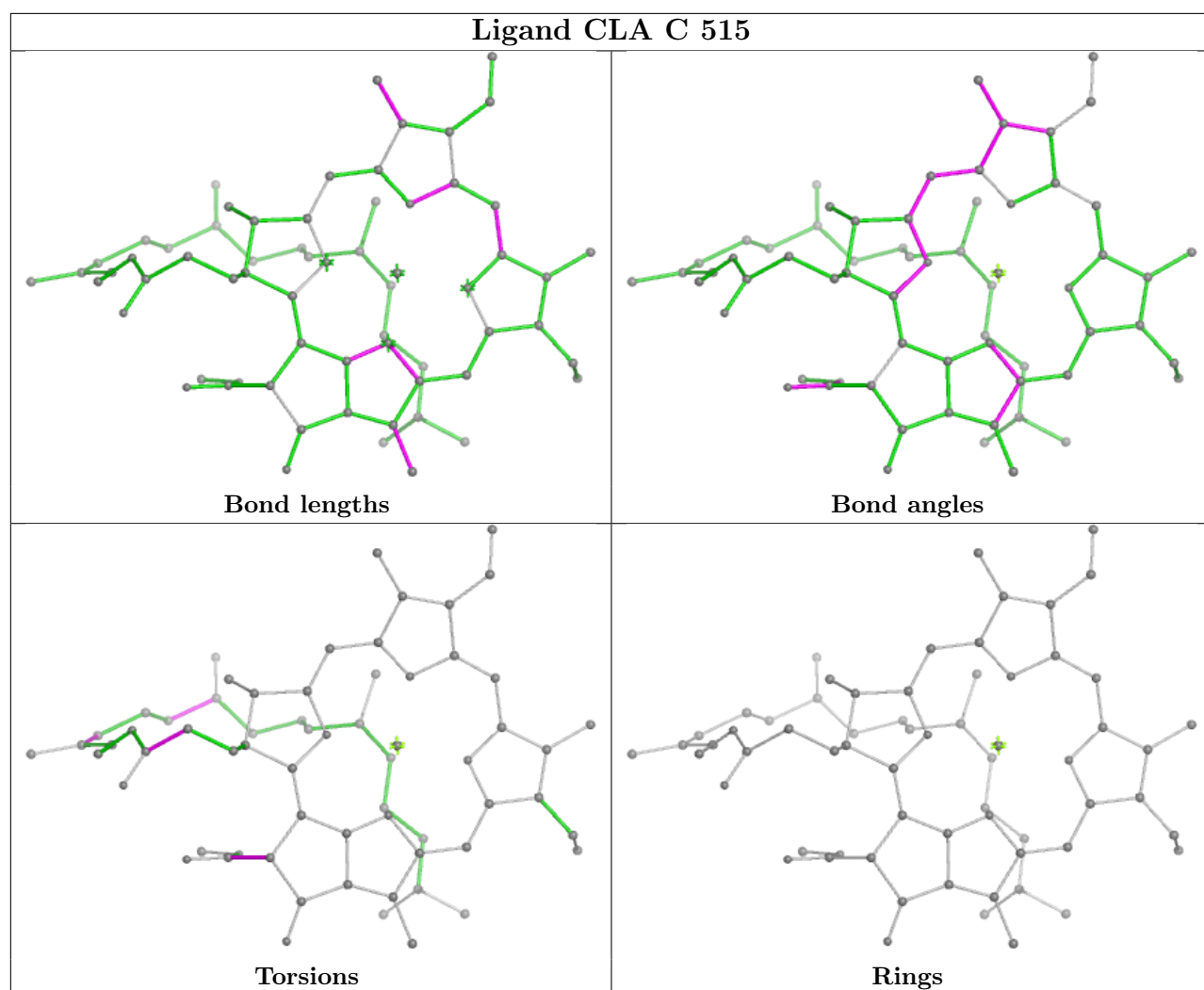




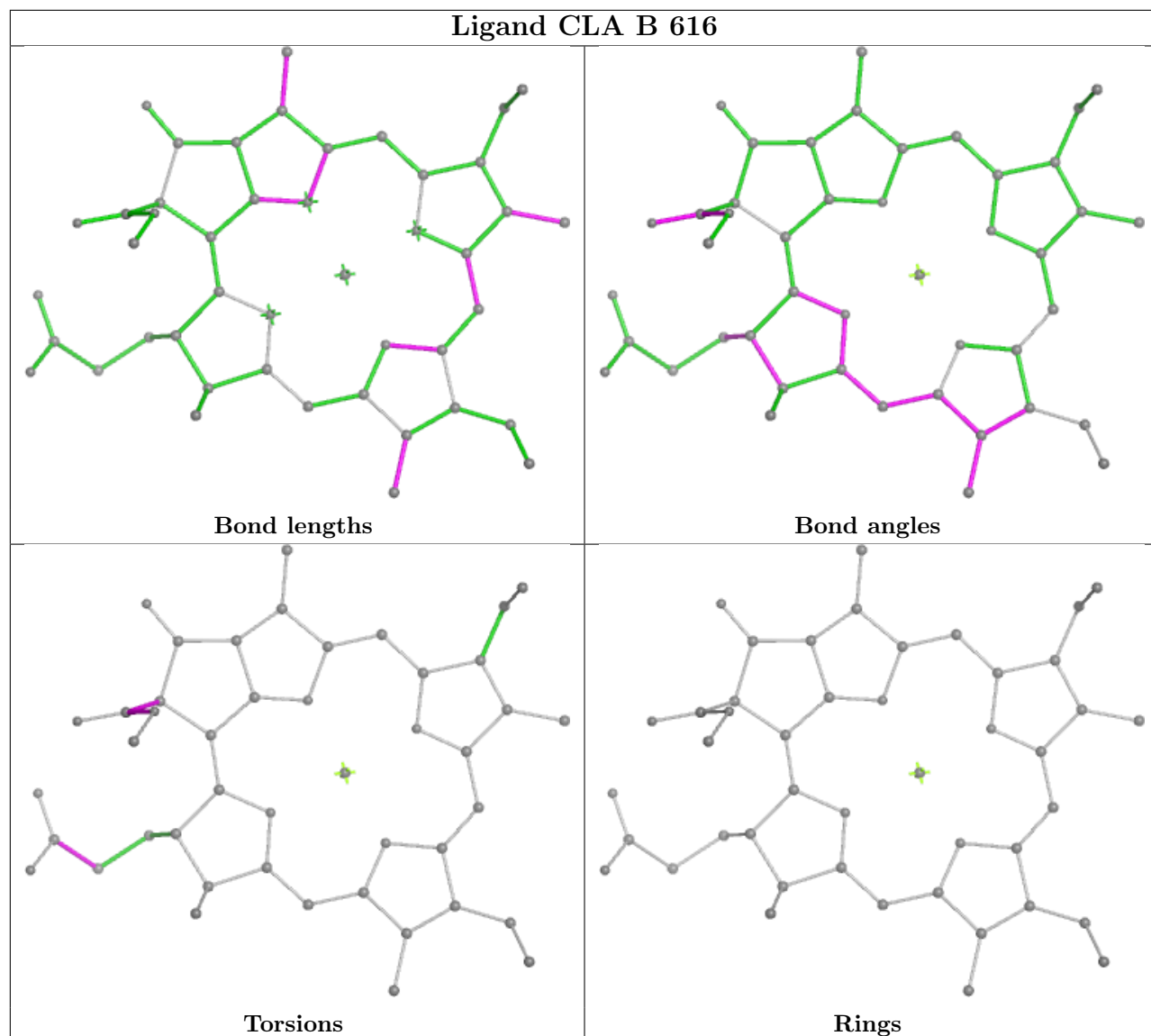




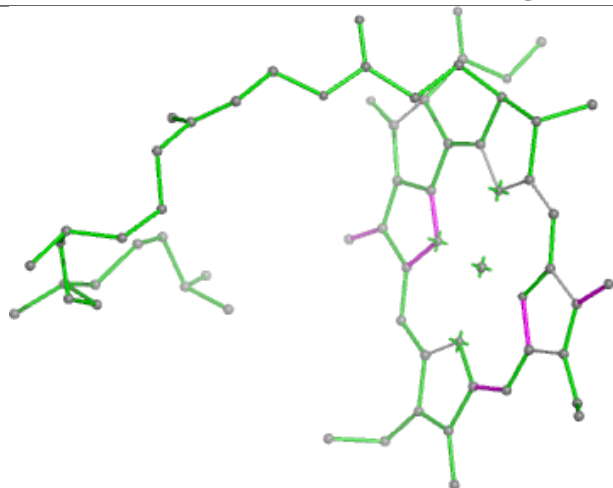




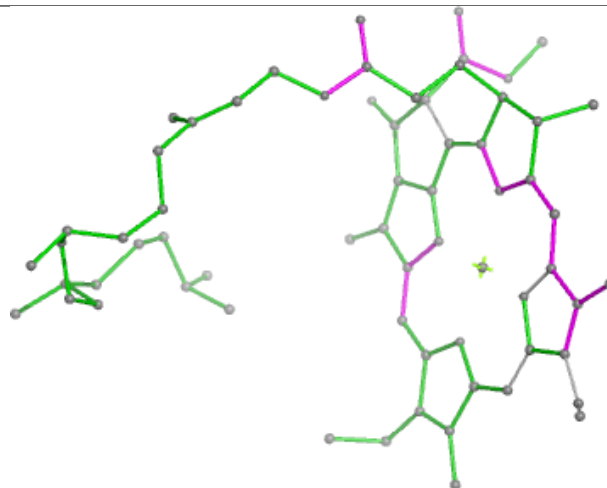
Ligand CLA B 616



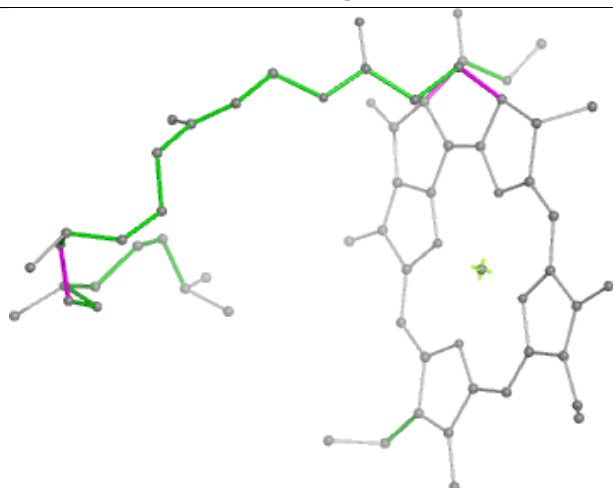
Ligand CLA c 503



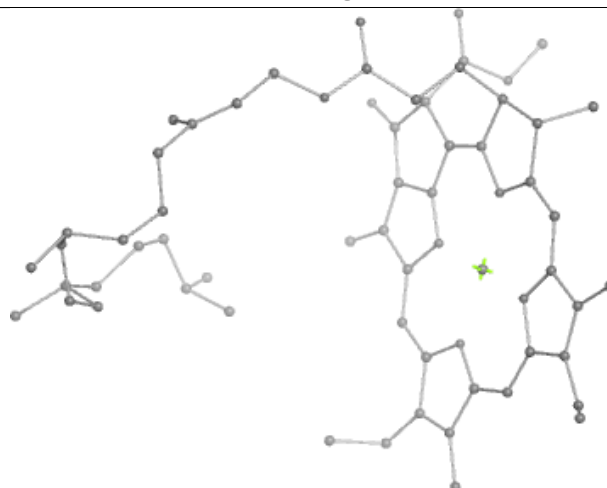
Bond lengths



Bond angles

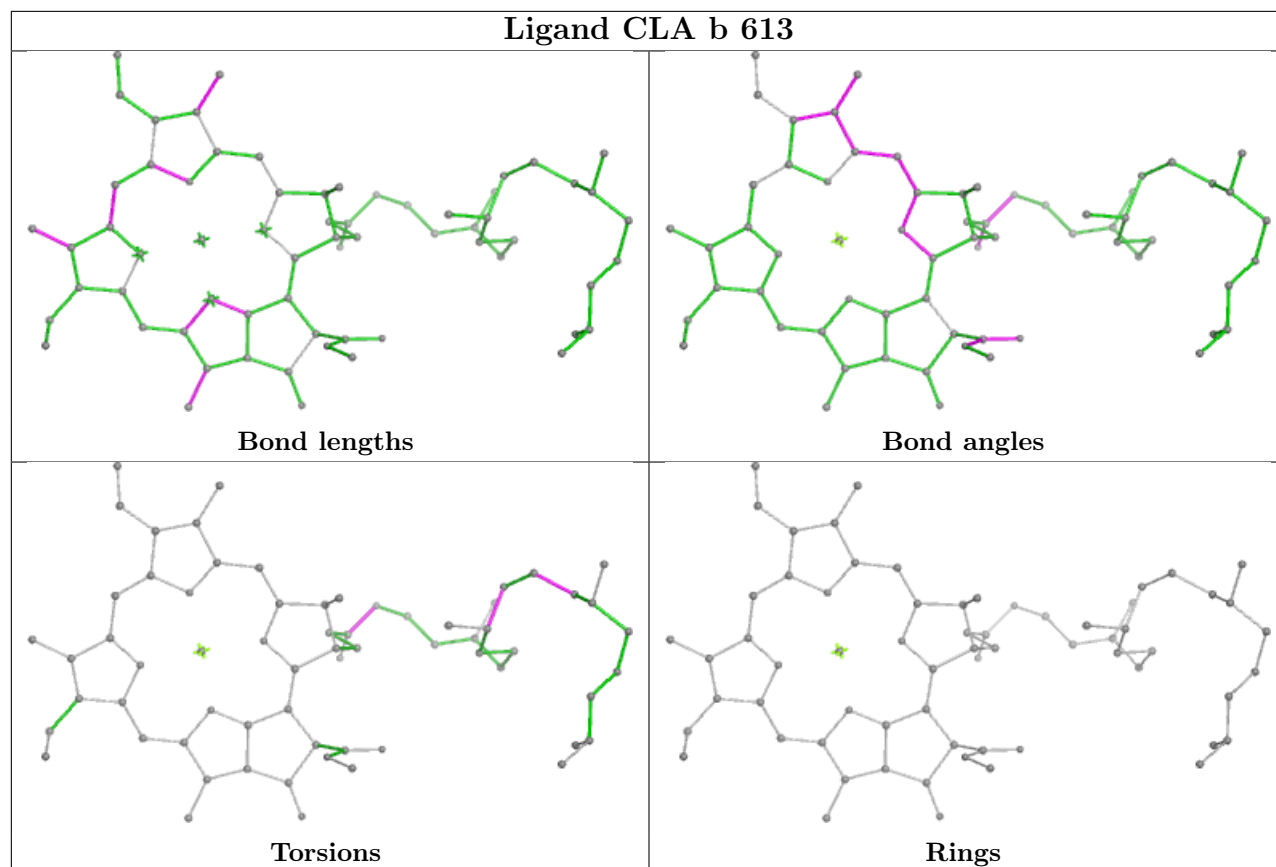


Torsions

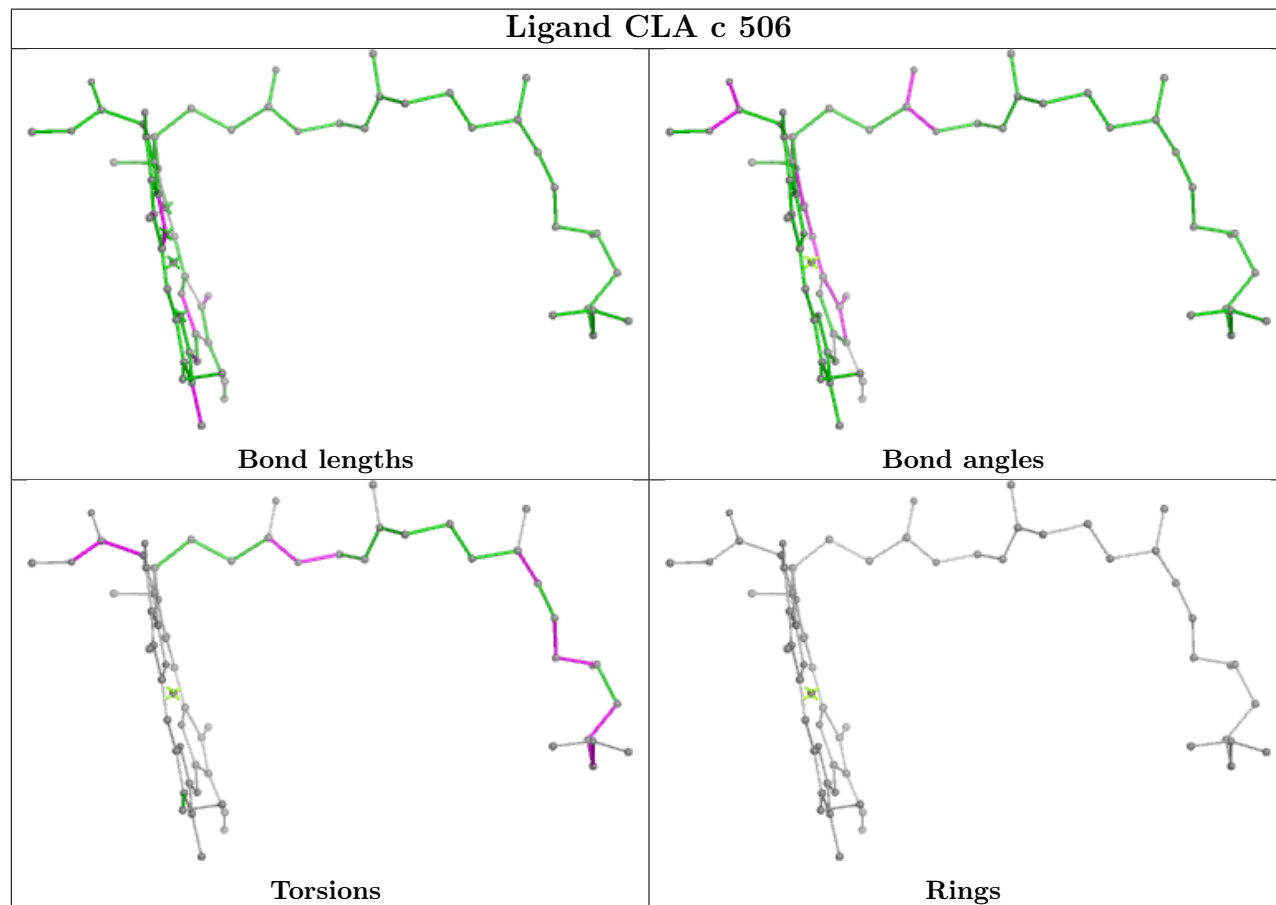


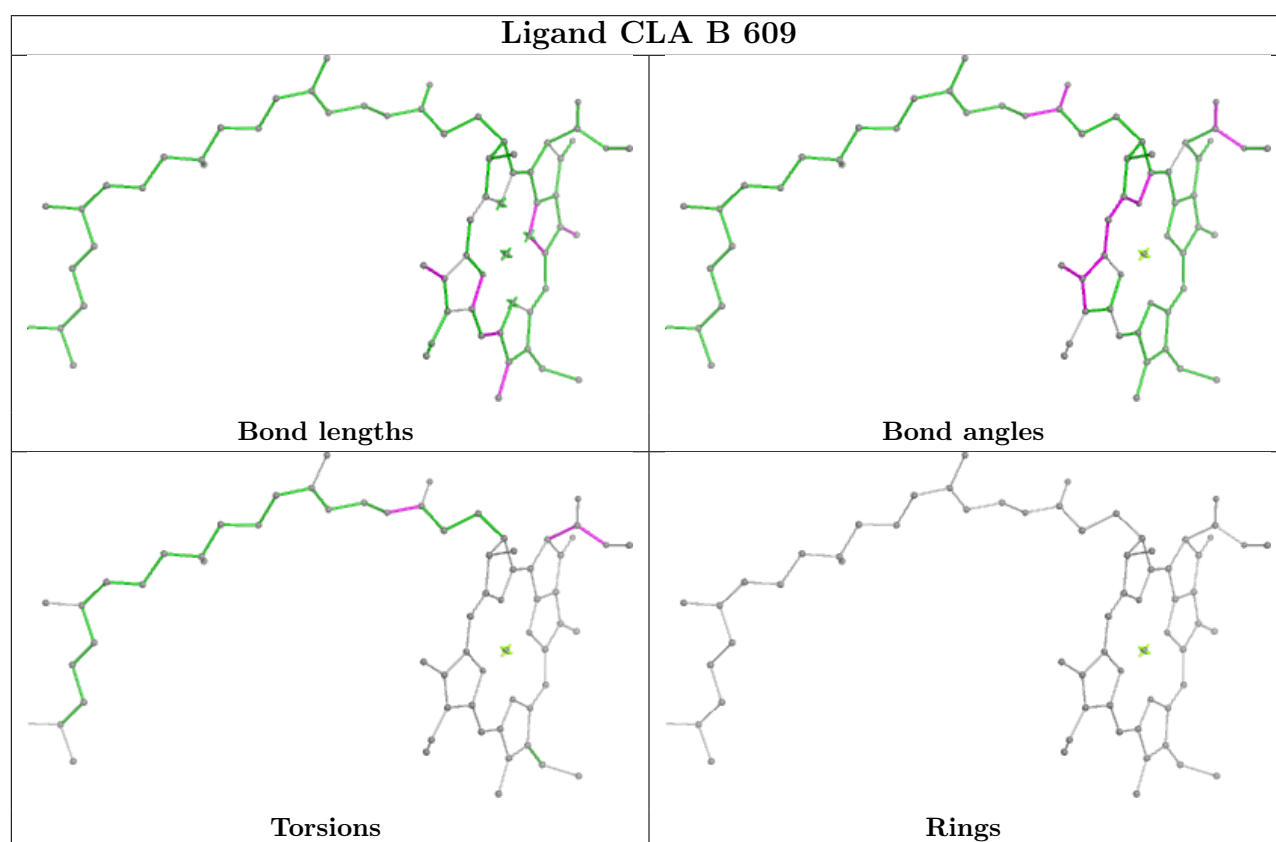
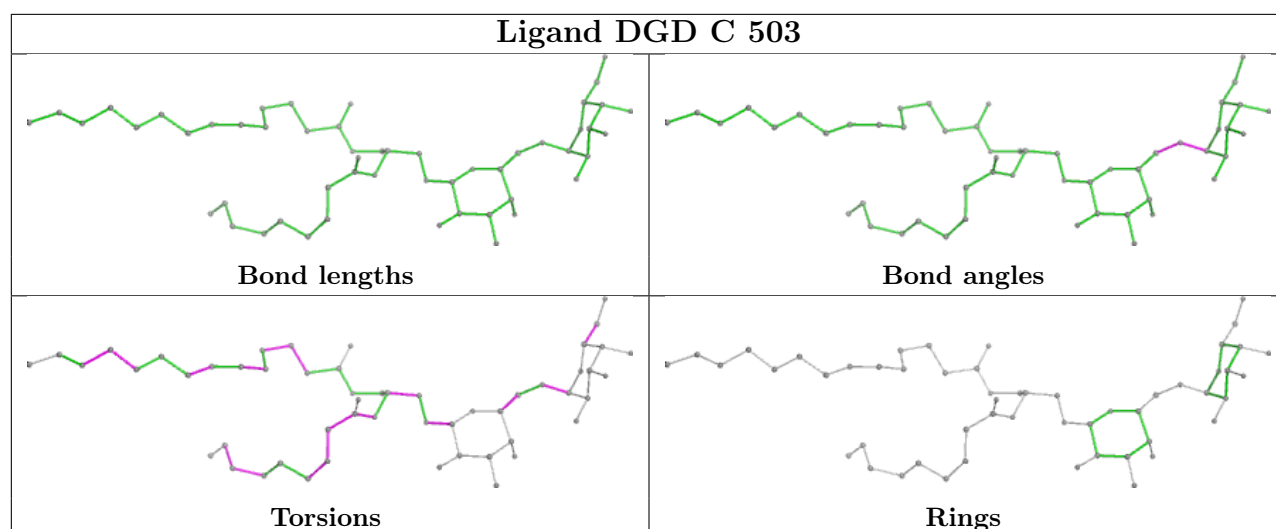
Rings

Ligand CLA b 613

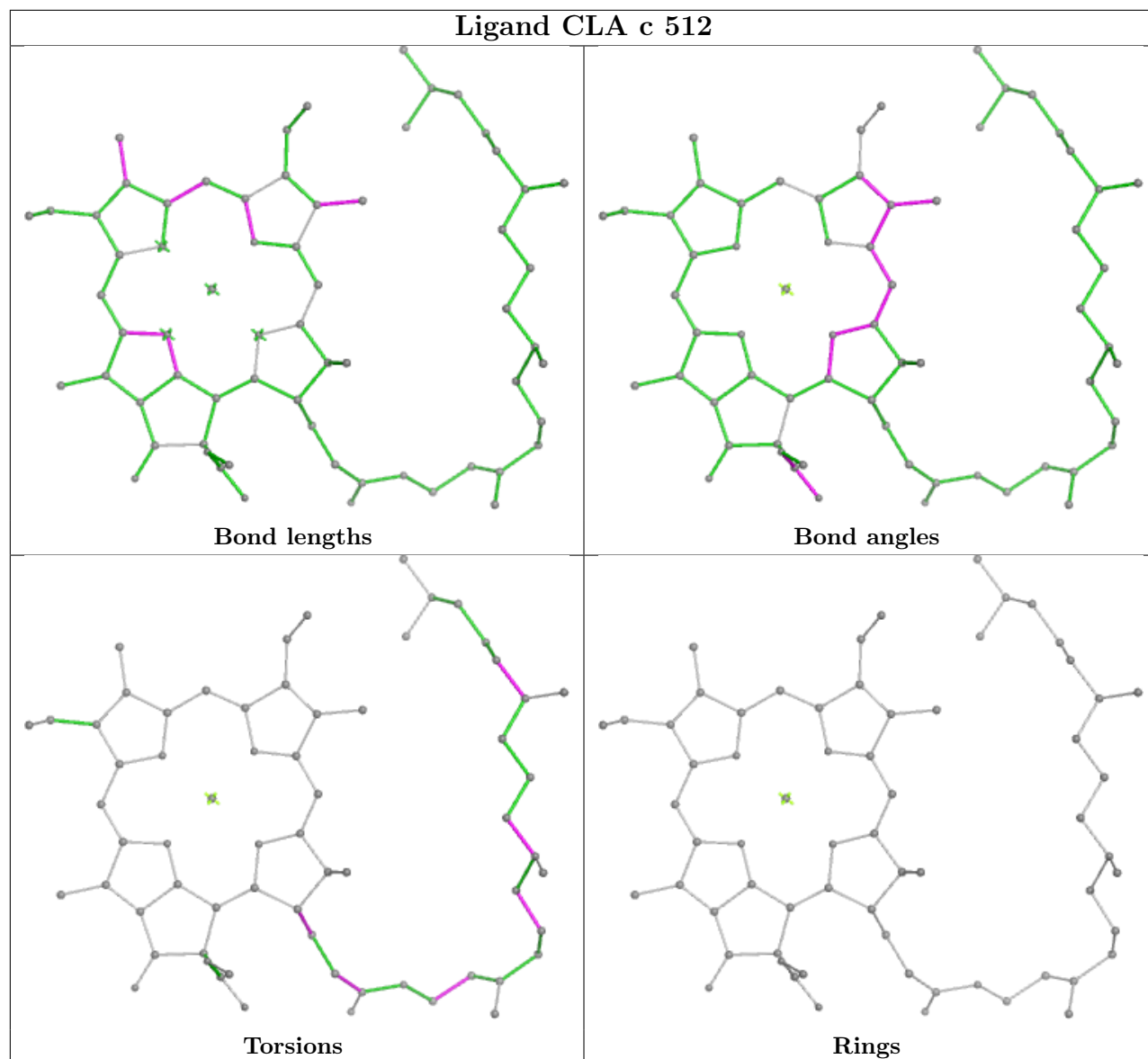


Ligand CLA c 506

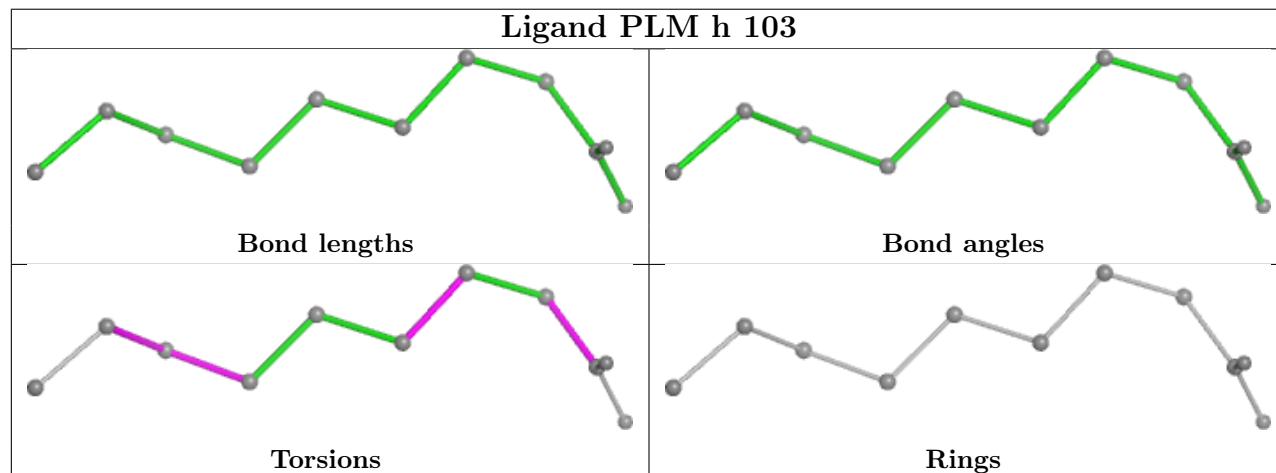




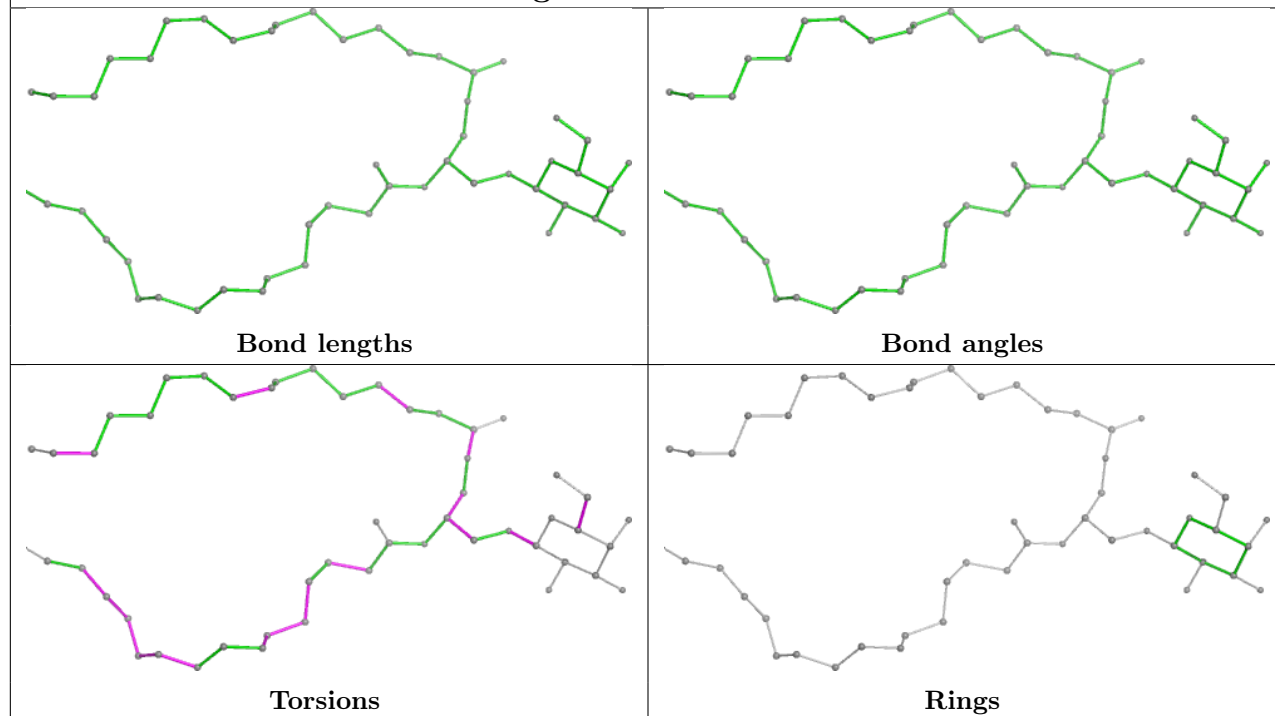
Ligand CLA c 512



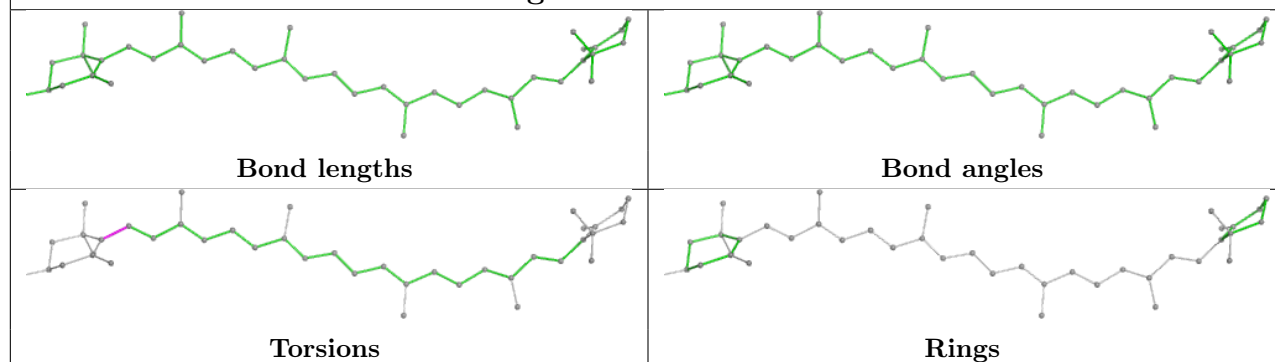
Ligand PLM h 103



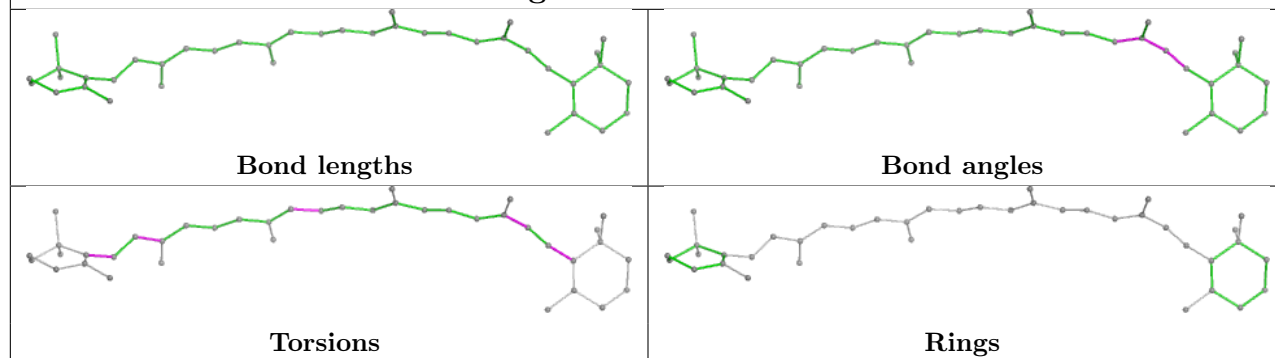
Ligand LMG I 103

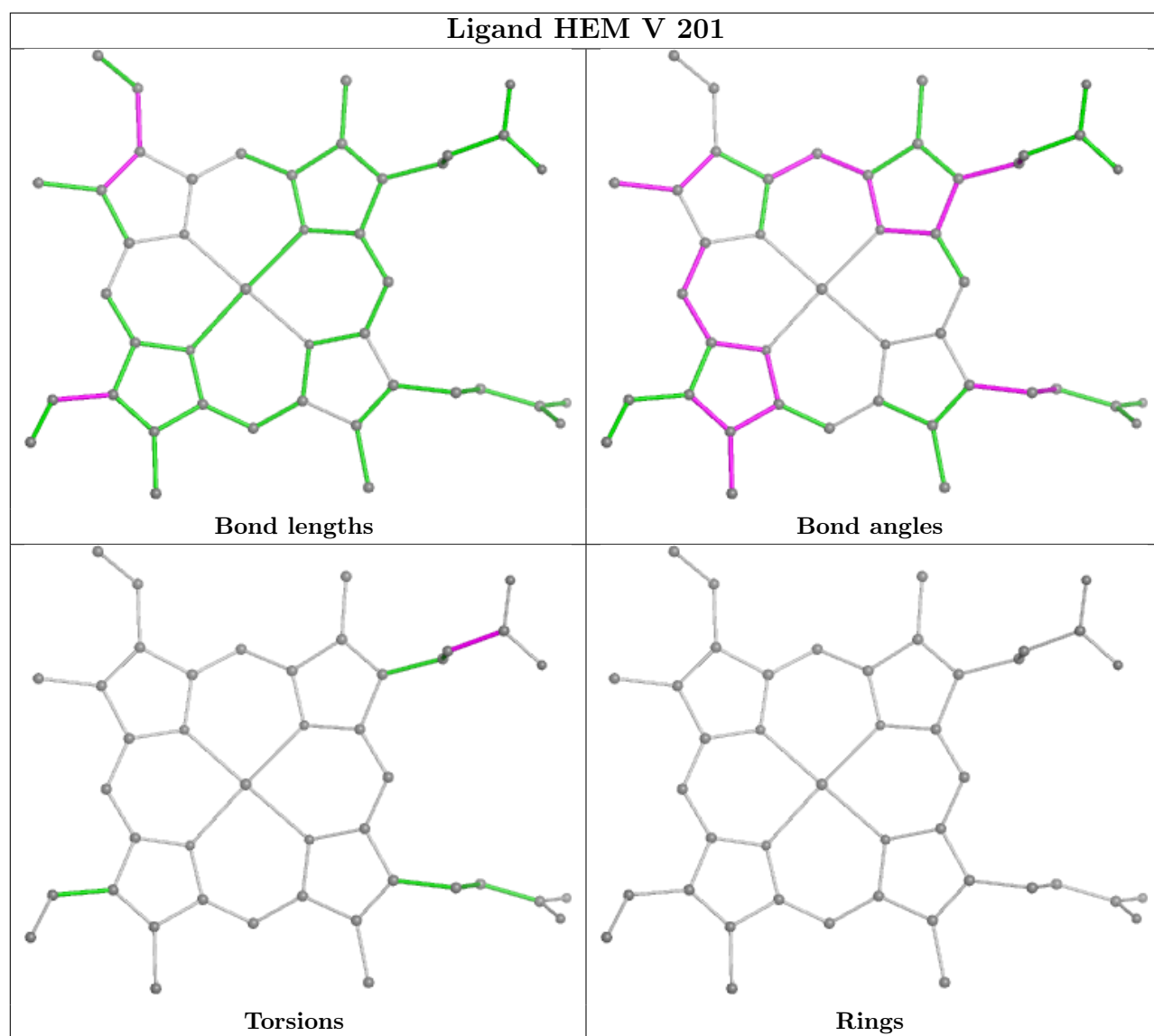


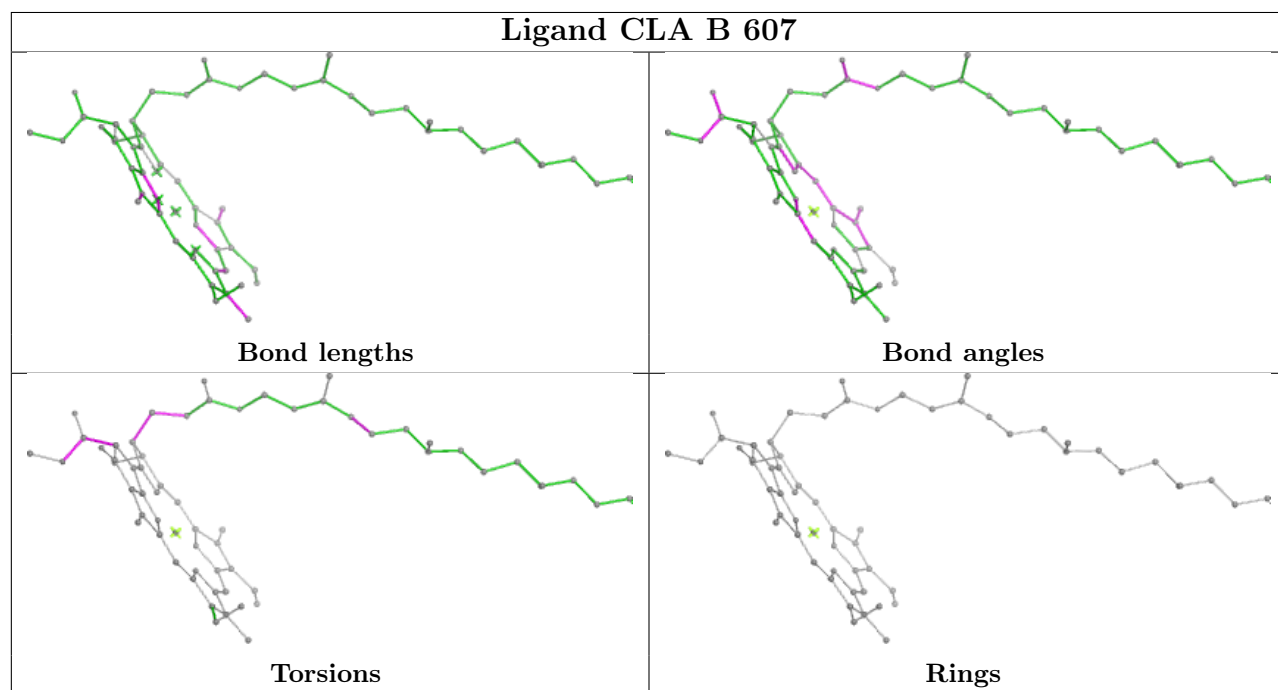
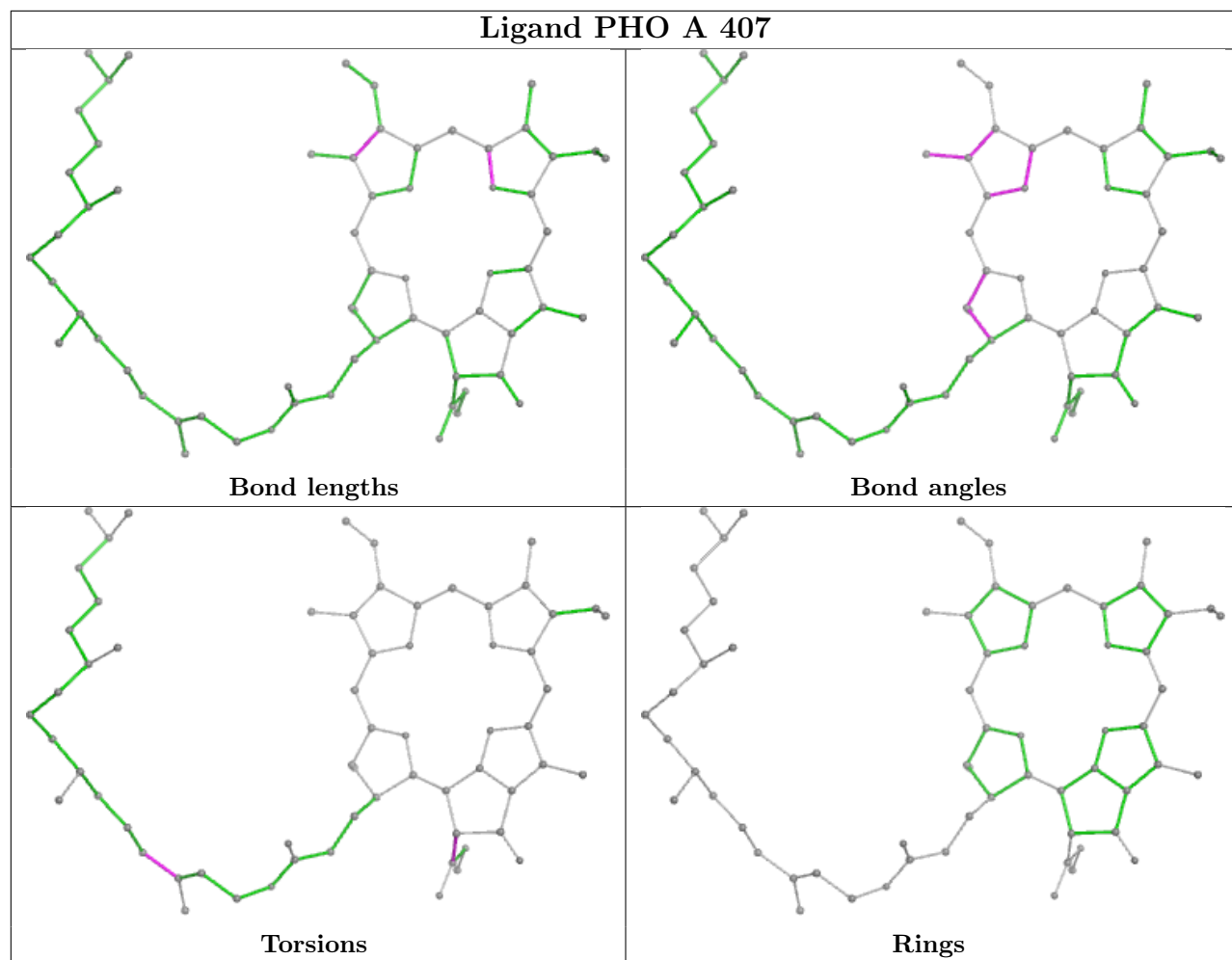
Ligand RRX H 102



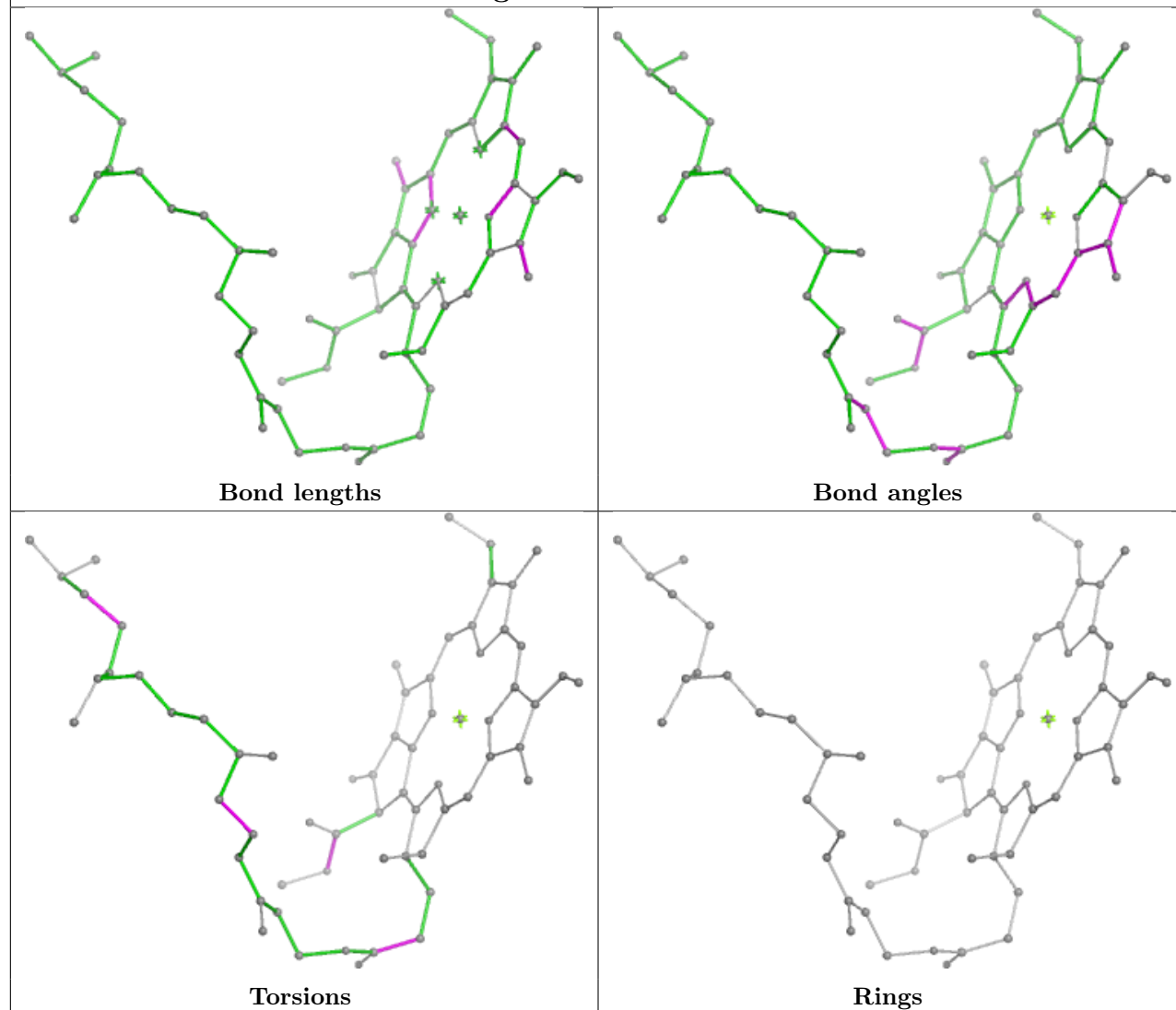
Ligand BCR D 403

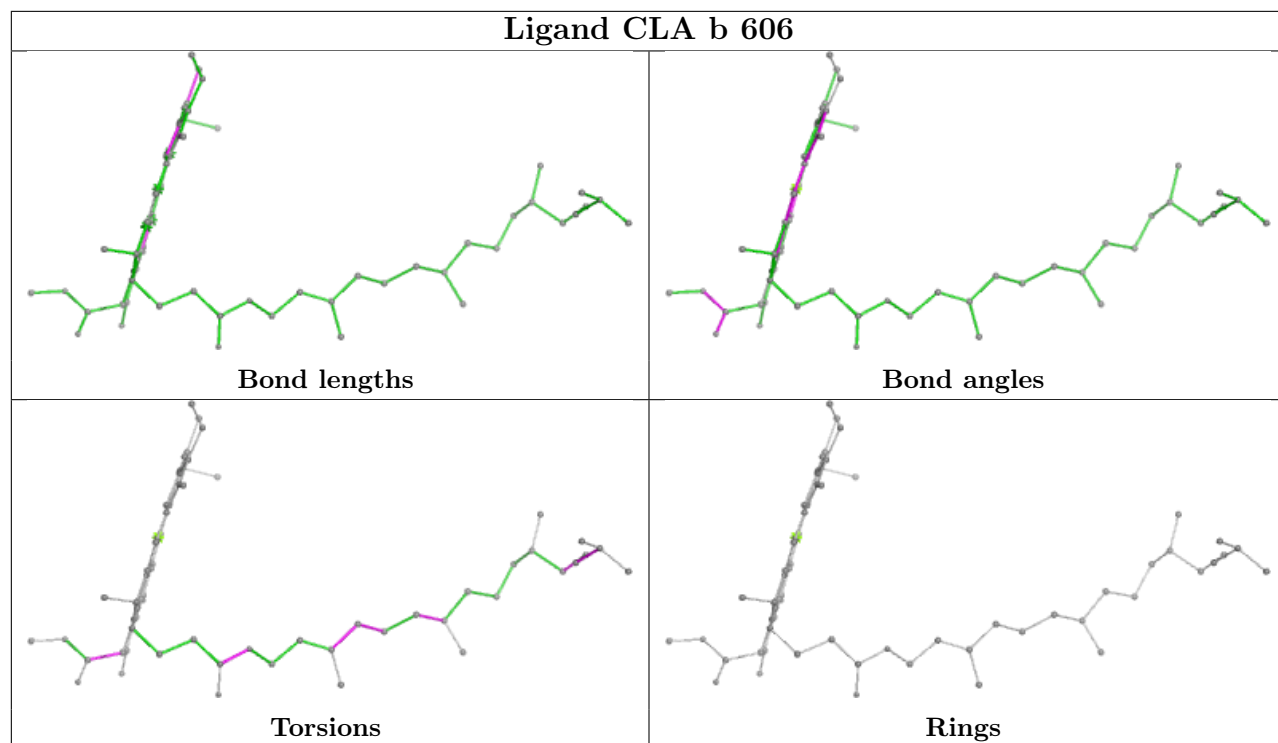




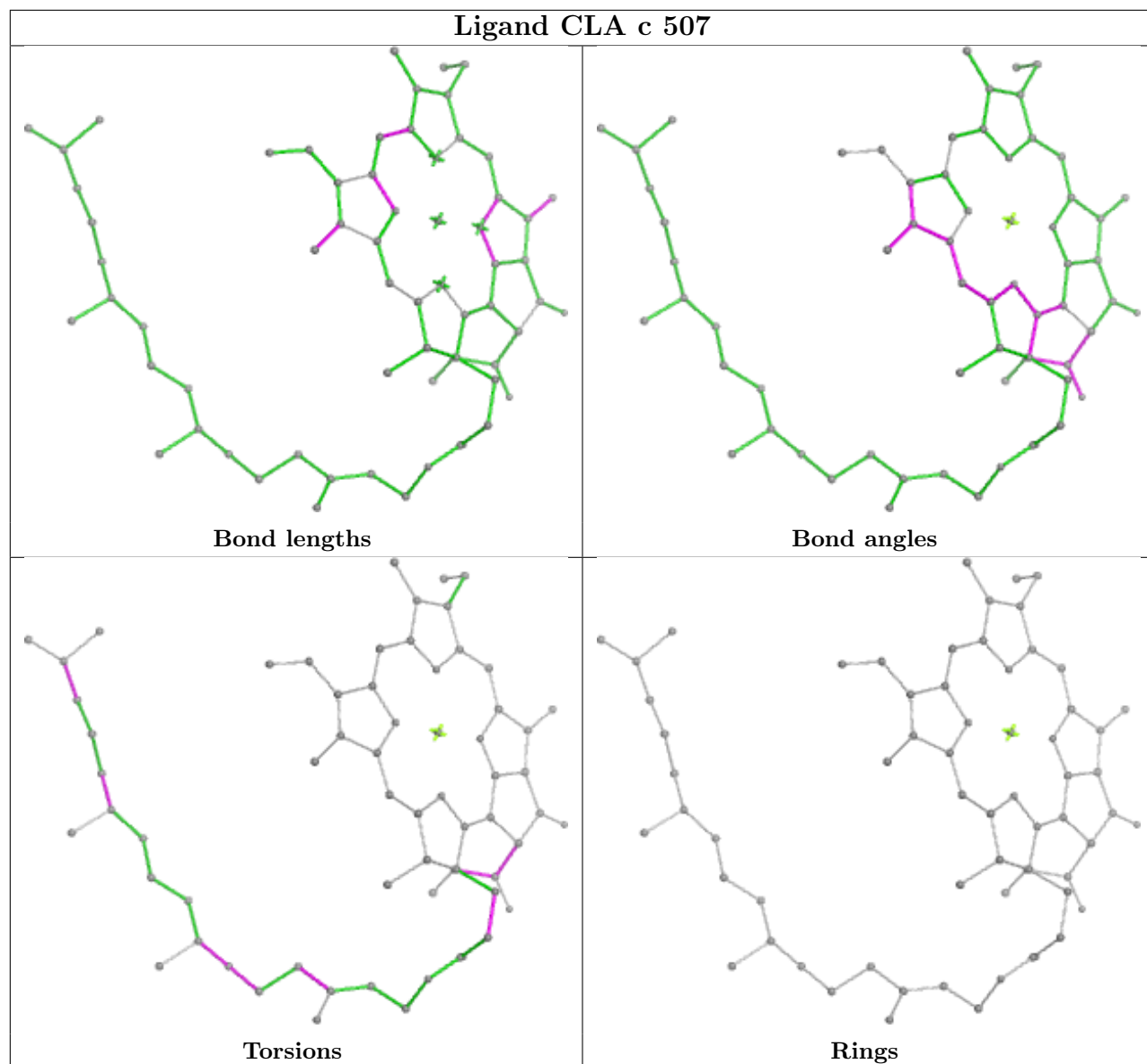


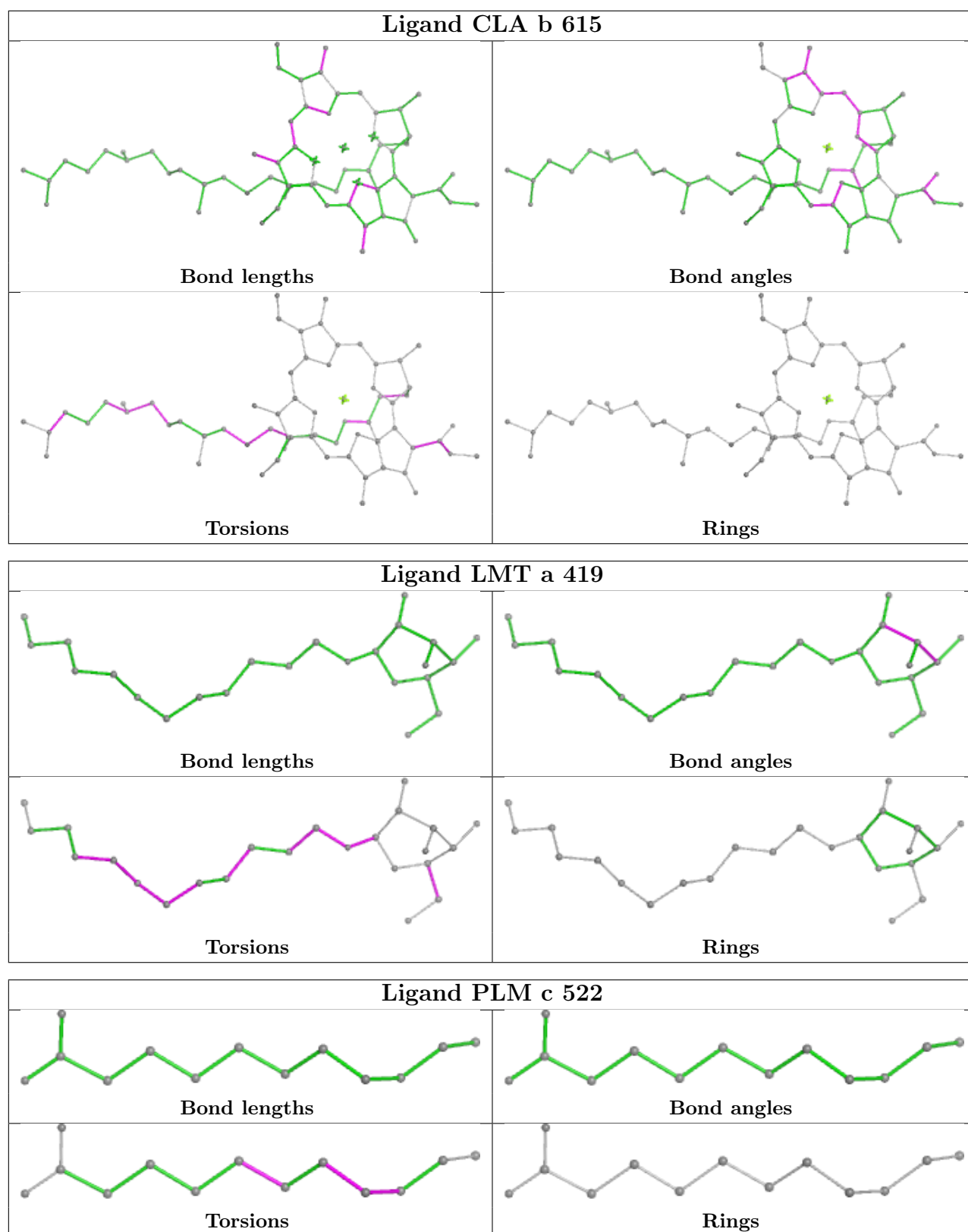
Ligand CLA b 614



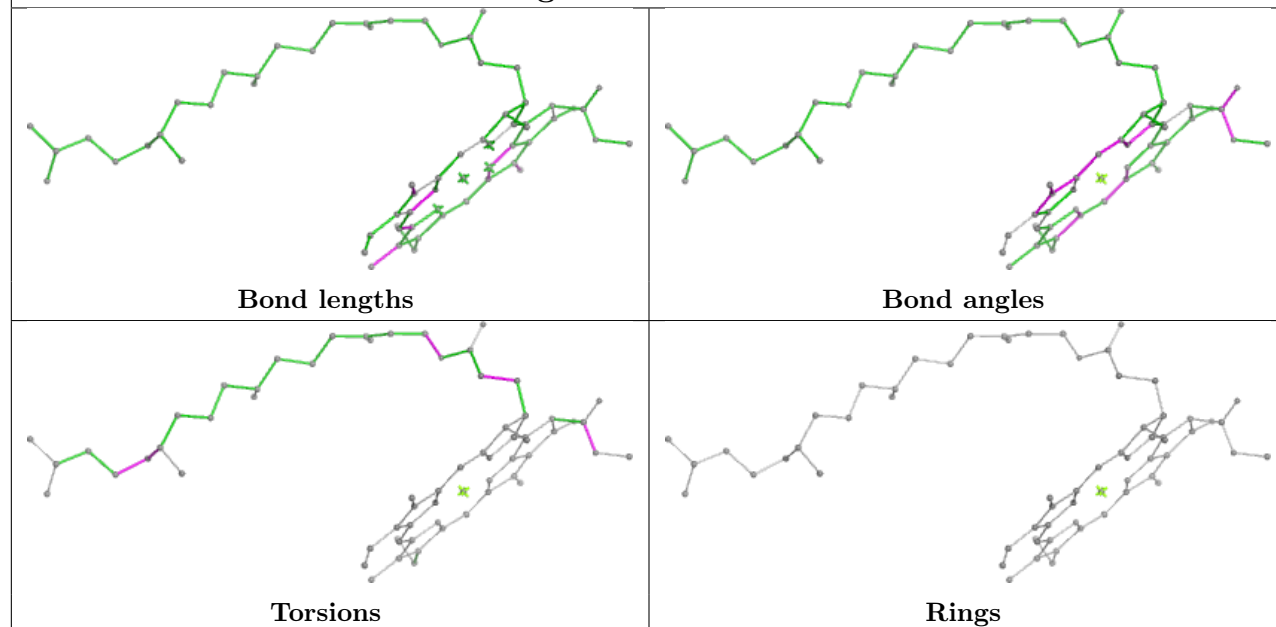


Ligand CLA c 507

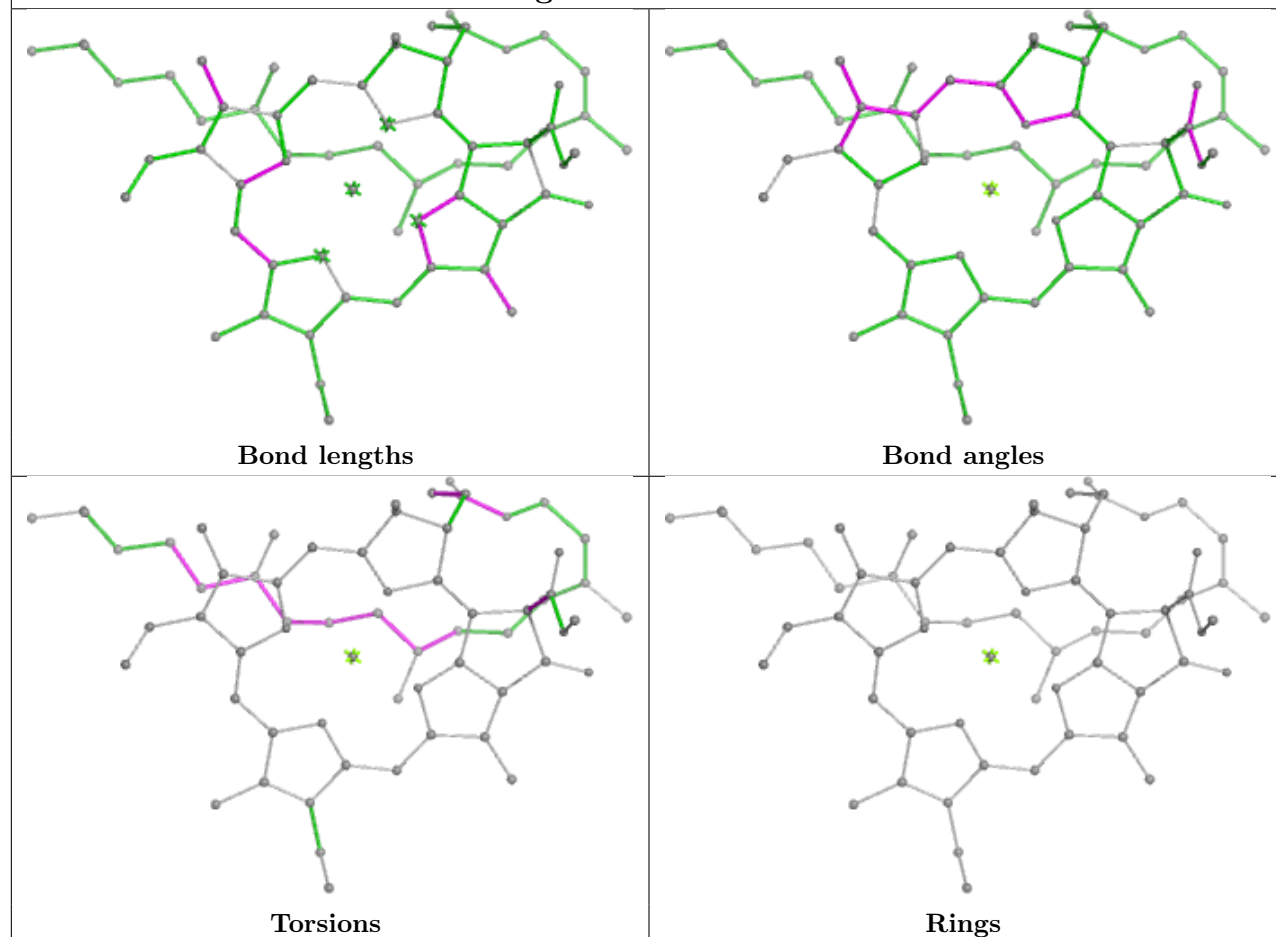




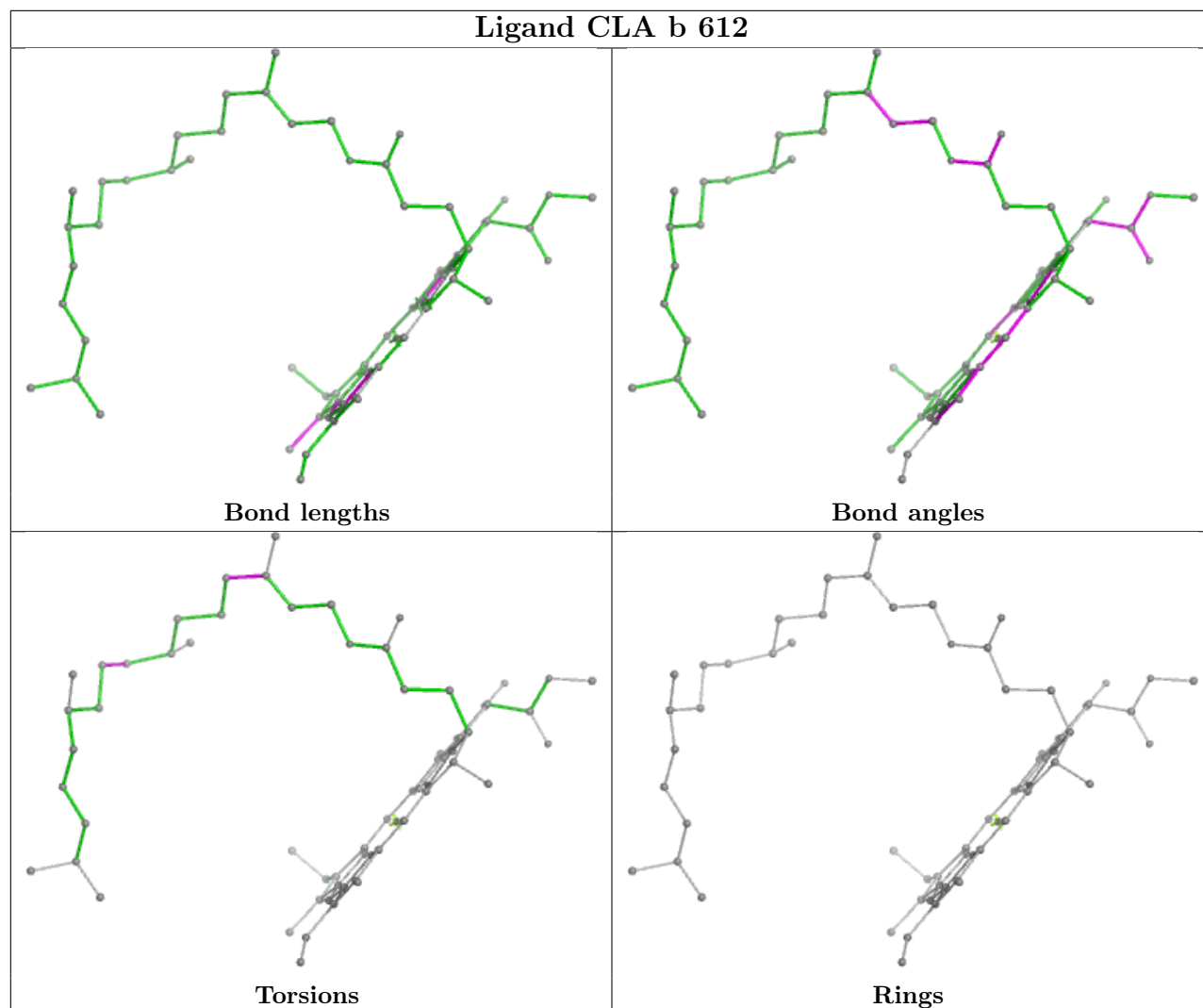
Ligand CLA c 504



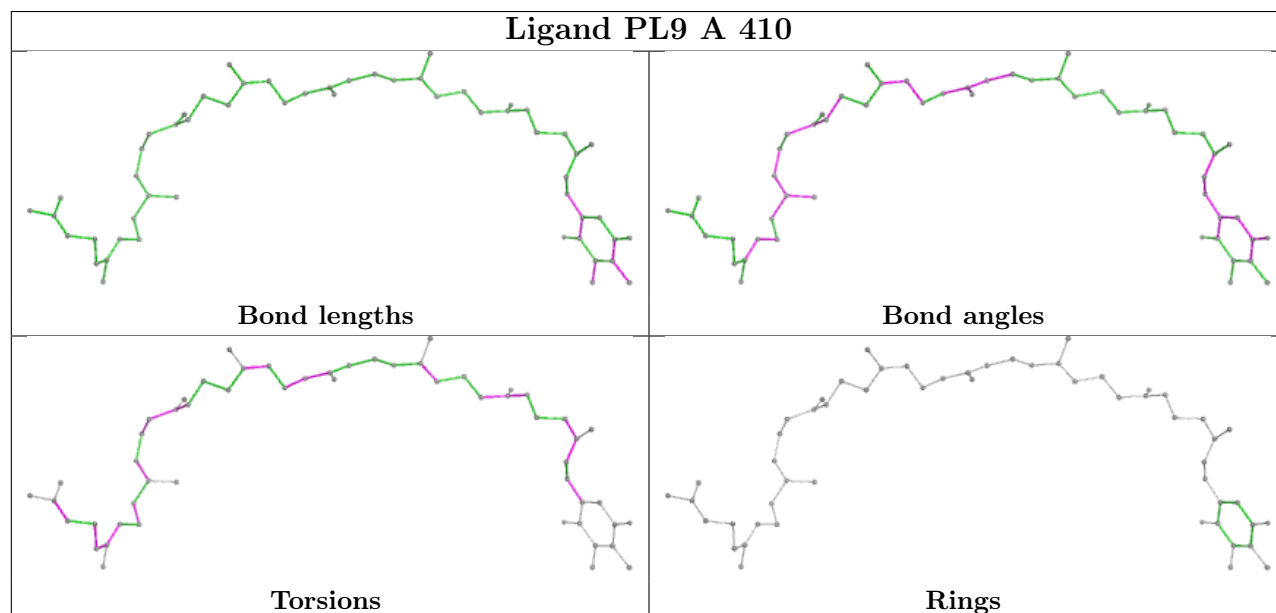
Ligand CLA b 602

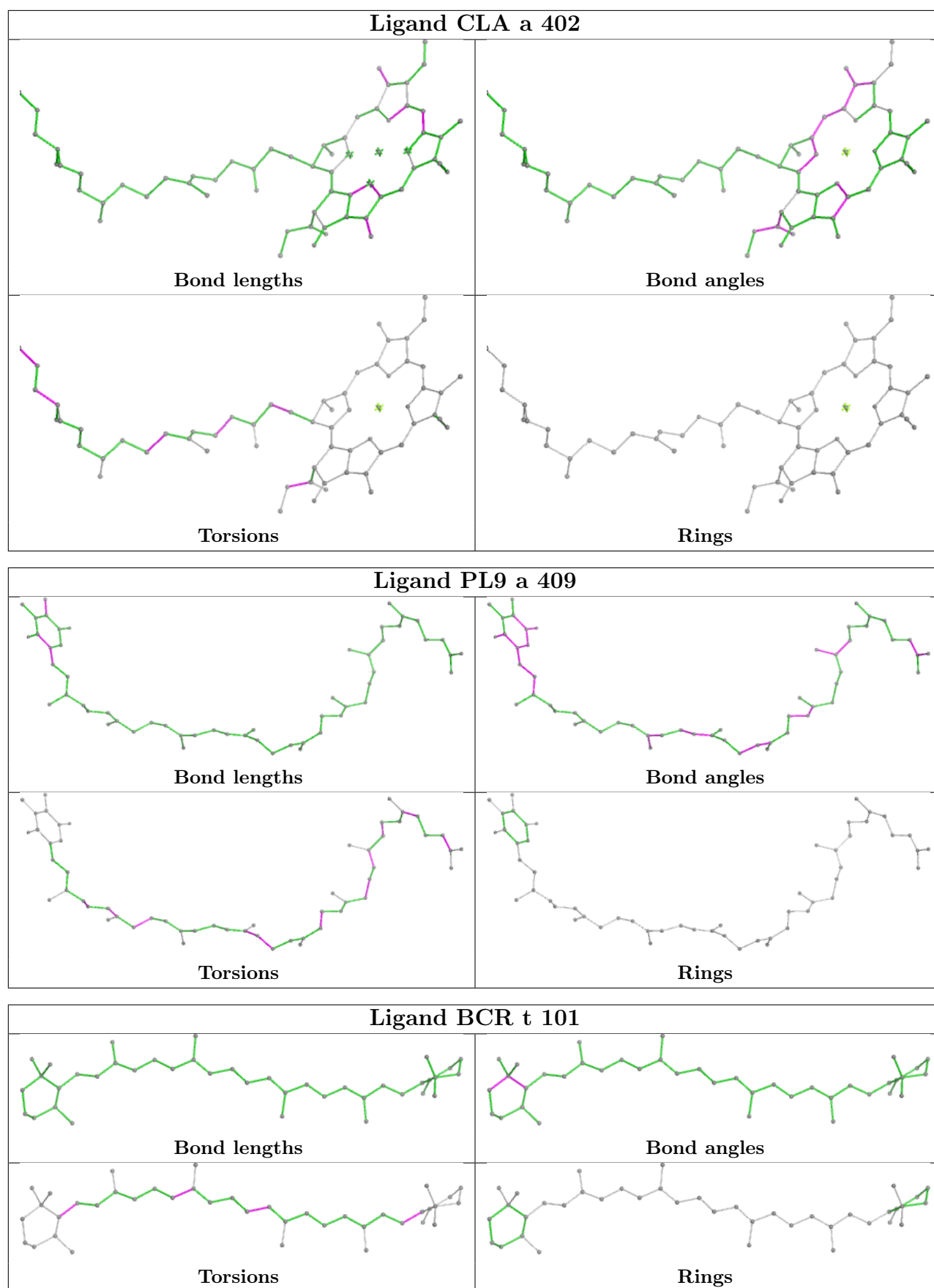


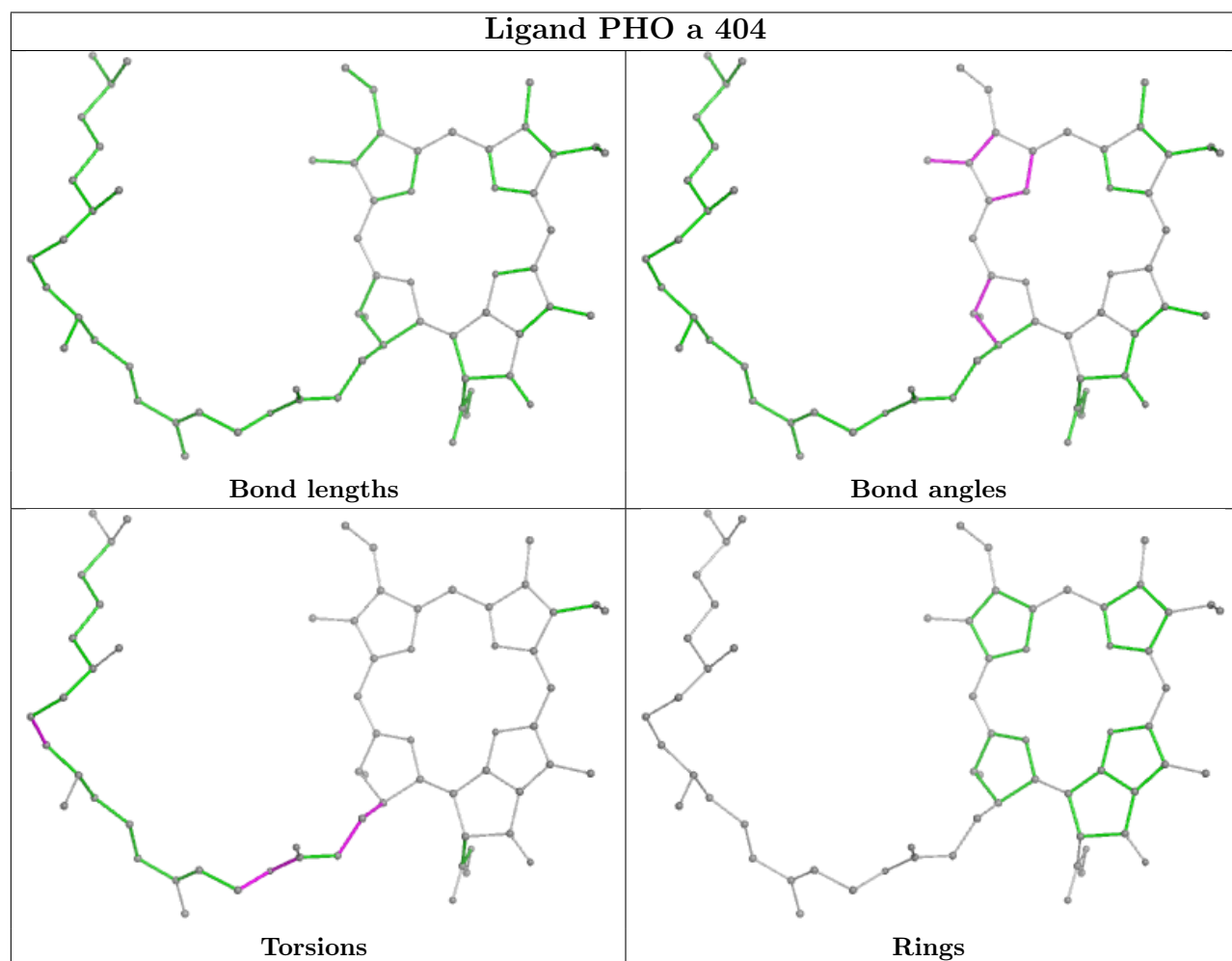
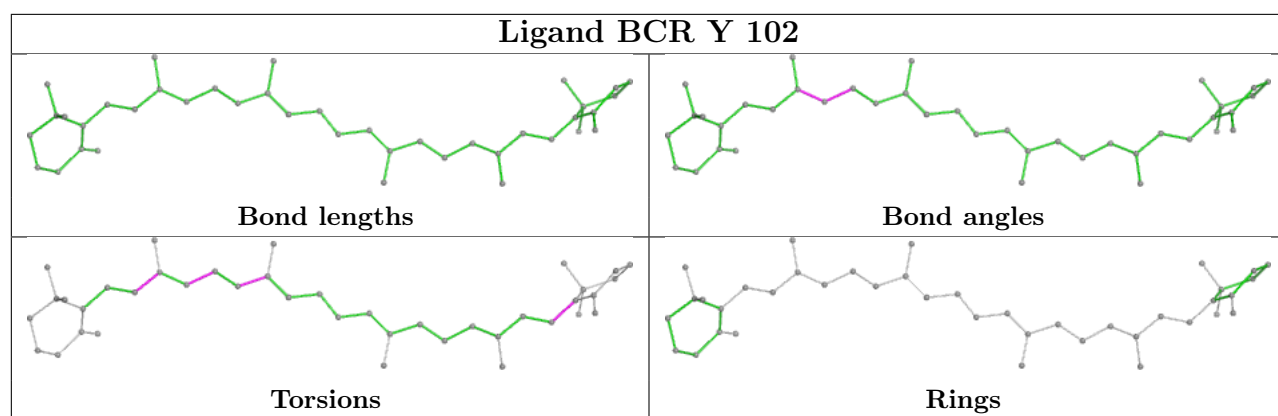
Ligand CLA b 612

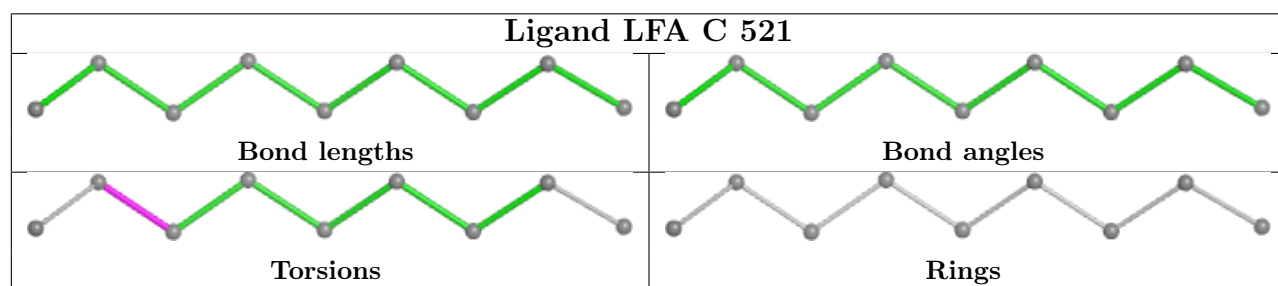
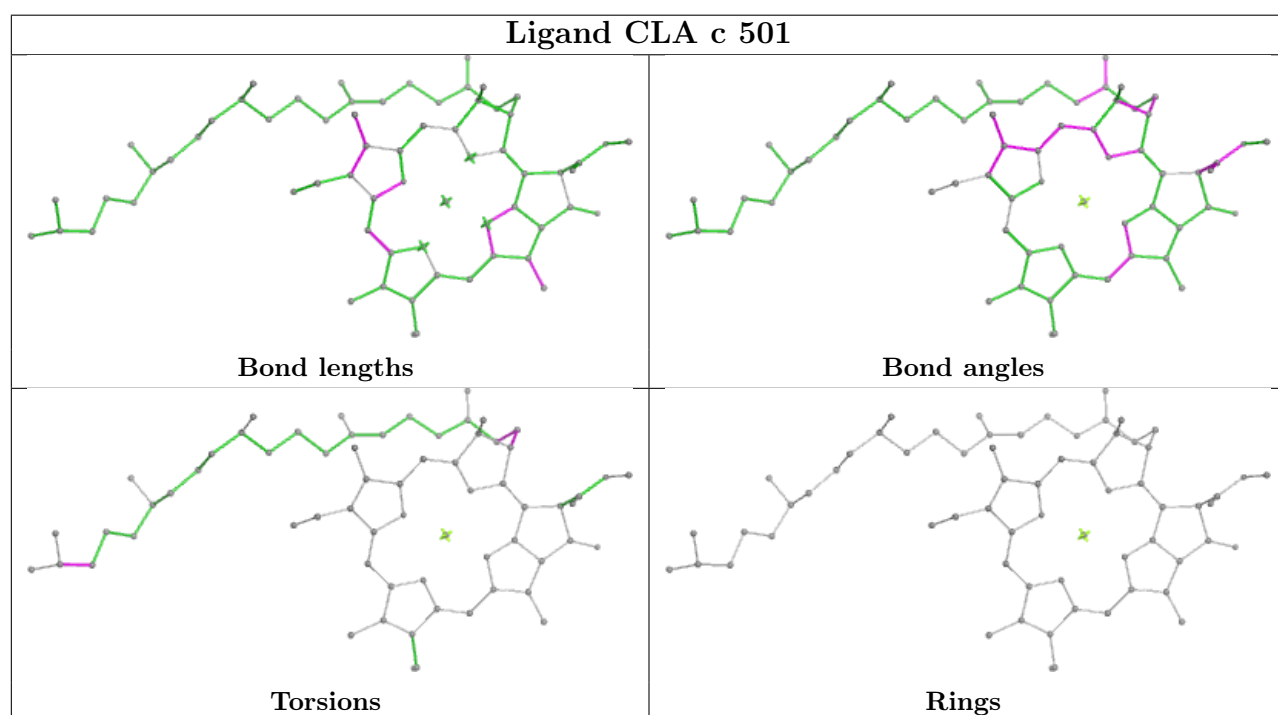
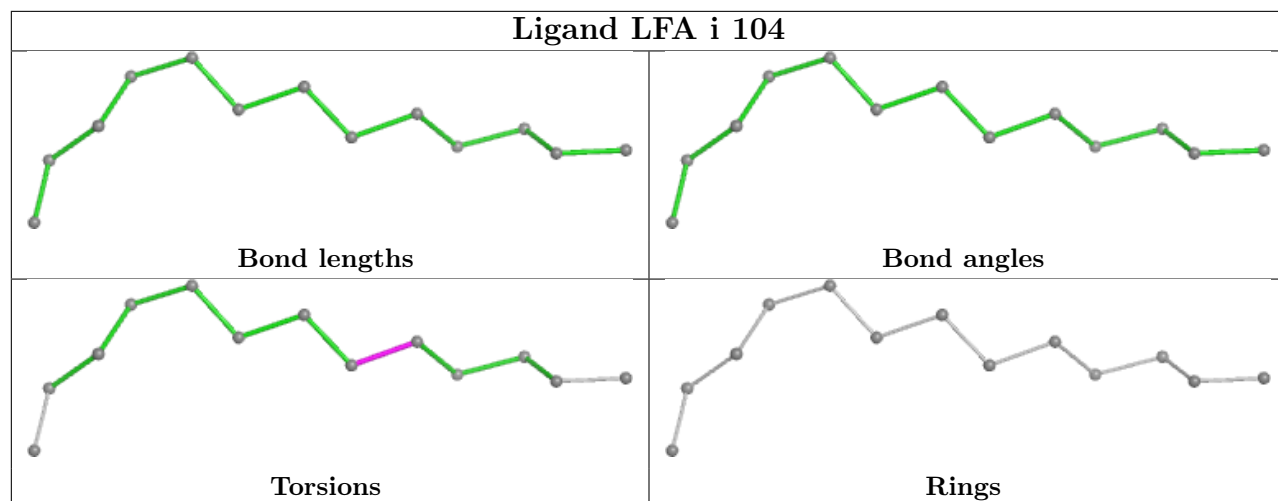


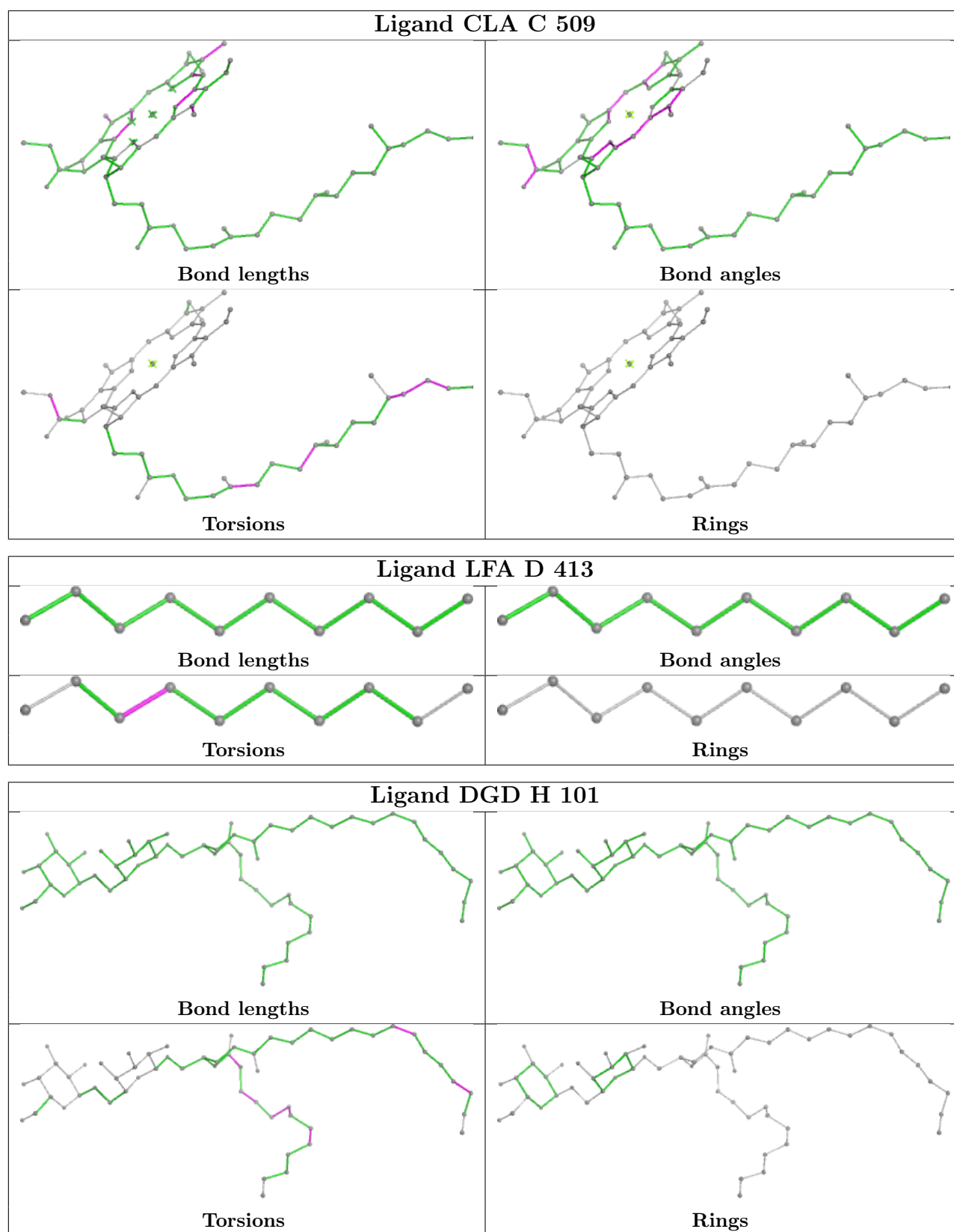
Ligand PL9 A 410

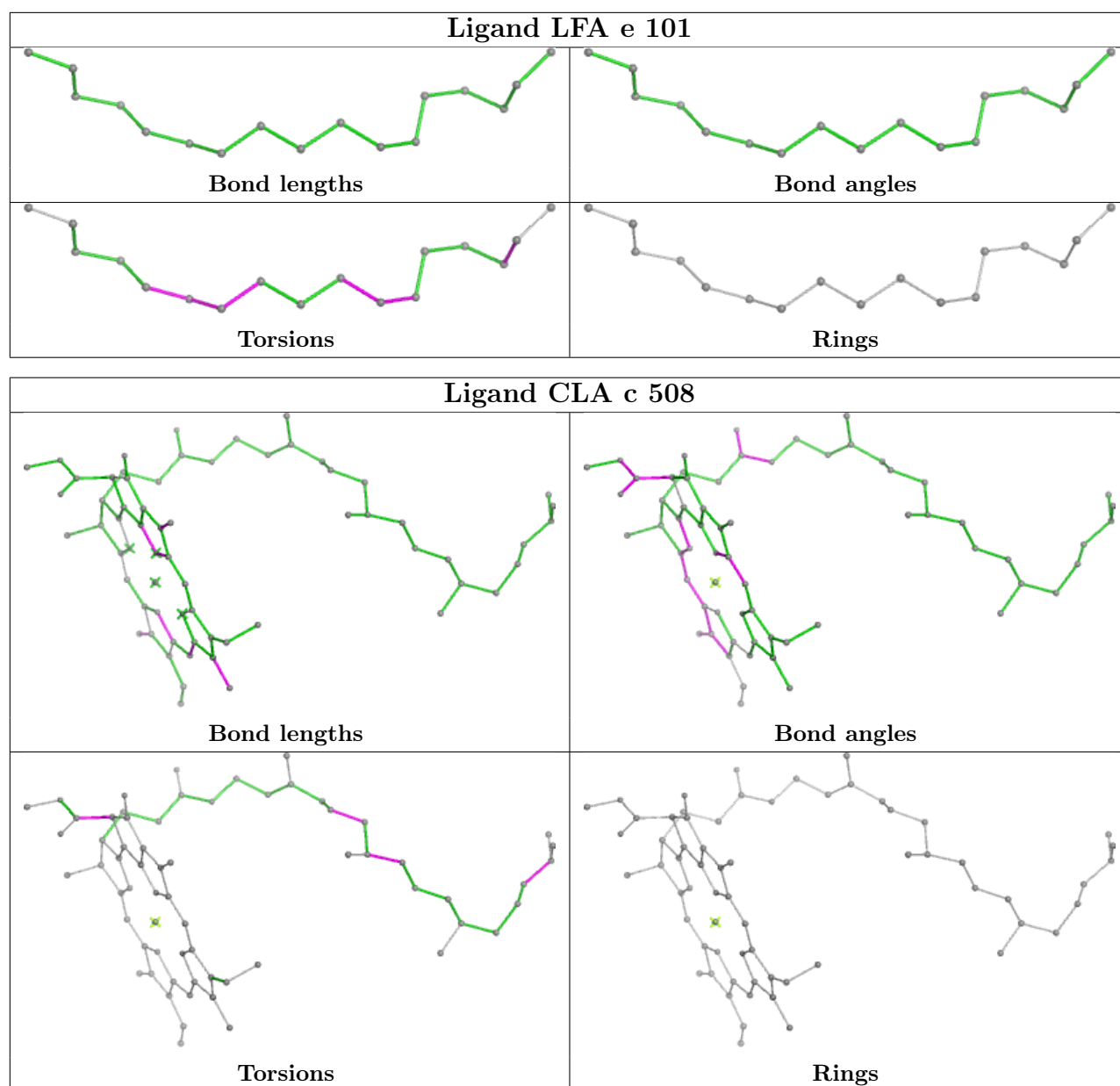












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

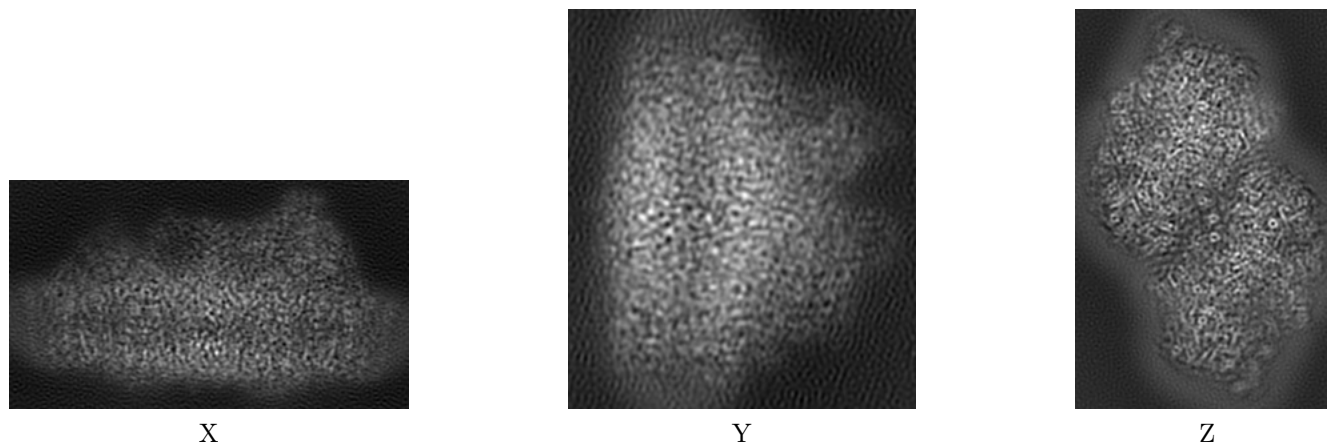
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51101. These allow visual inspection of the internal detail of the map and identification of artifacts.

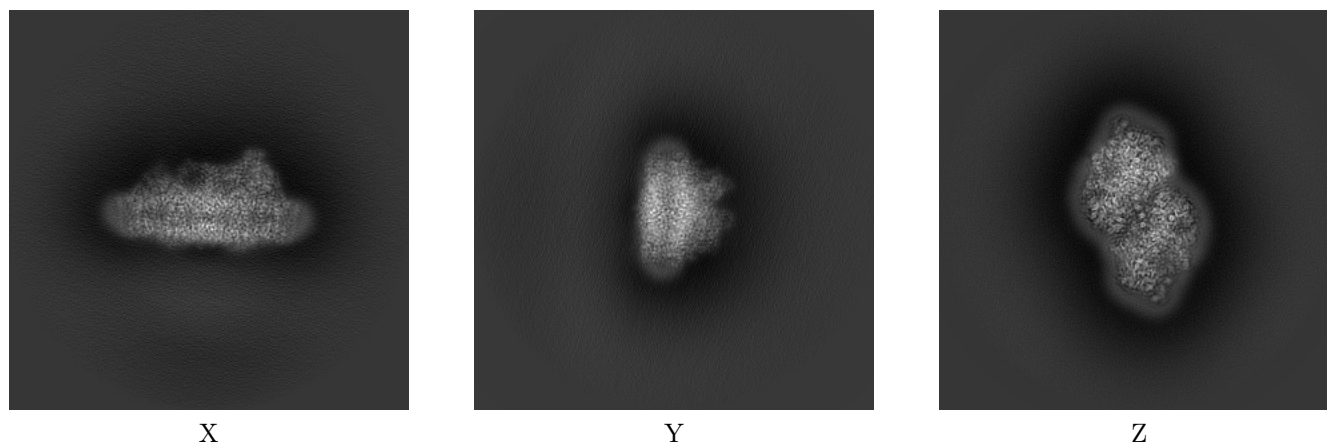
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



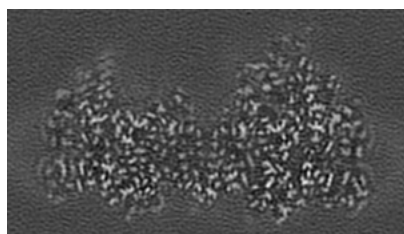
6.1.2 Raw map



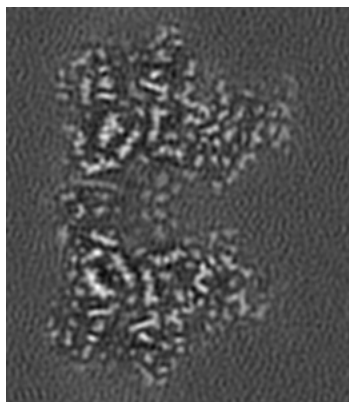
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

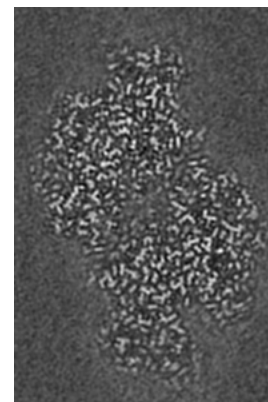
6.2.1 Primary map



X Index: 137

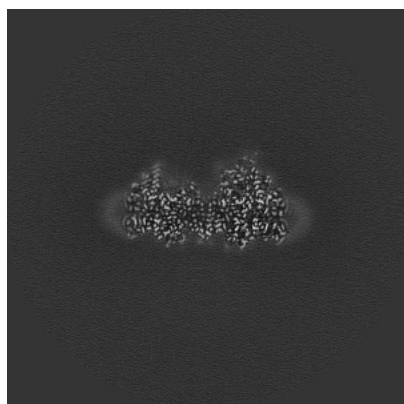


Y Index: 208

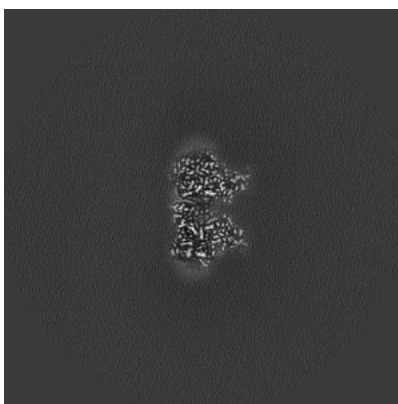


Z Index: 119

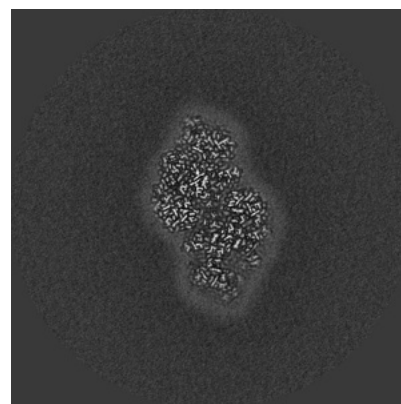
6.2.2 Raw map



X Index: 200



Y Index: 200

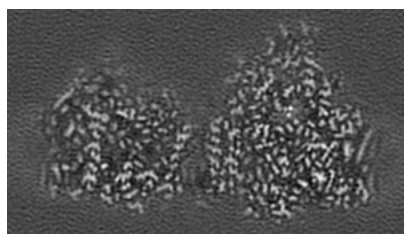


Z Index: 200

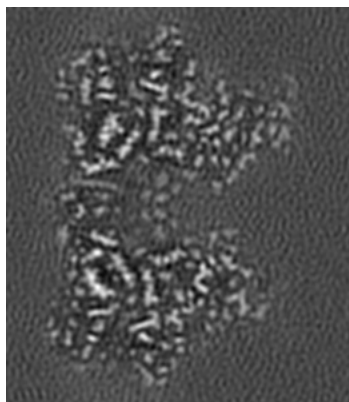
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

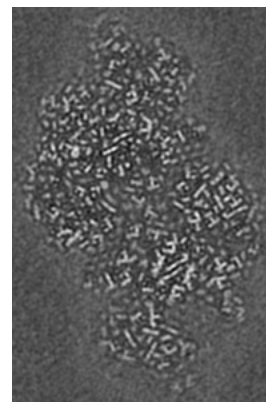
6.3.1 Primary map



X Index: 129

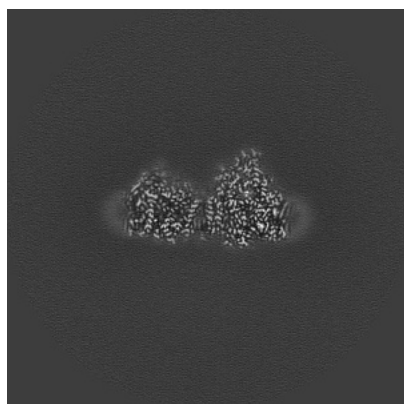


Y Index: 208

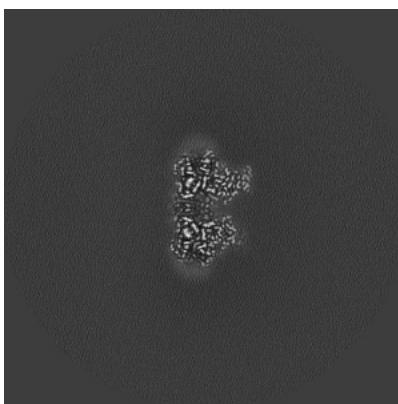


Z Index: 105

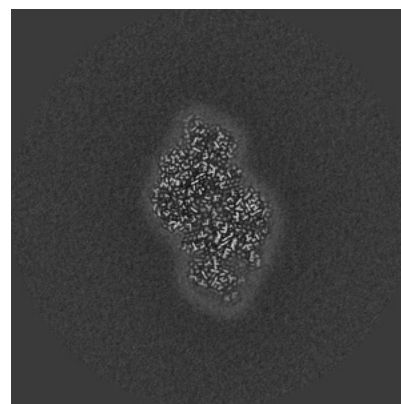
6.3.2 Raw map



X Index: 196



Y Index: 198

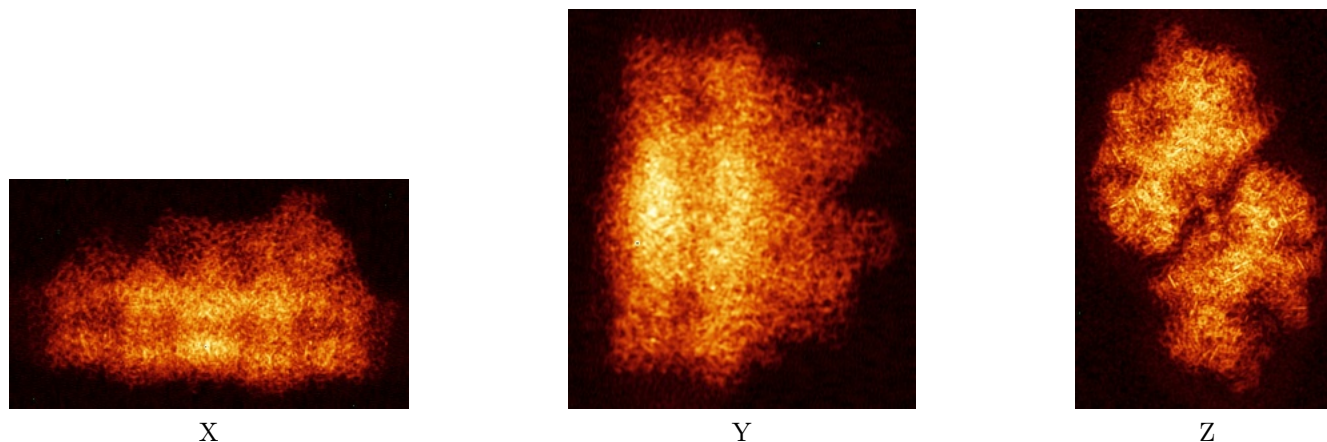


Z Index: 202

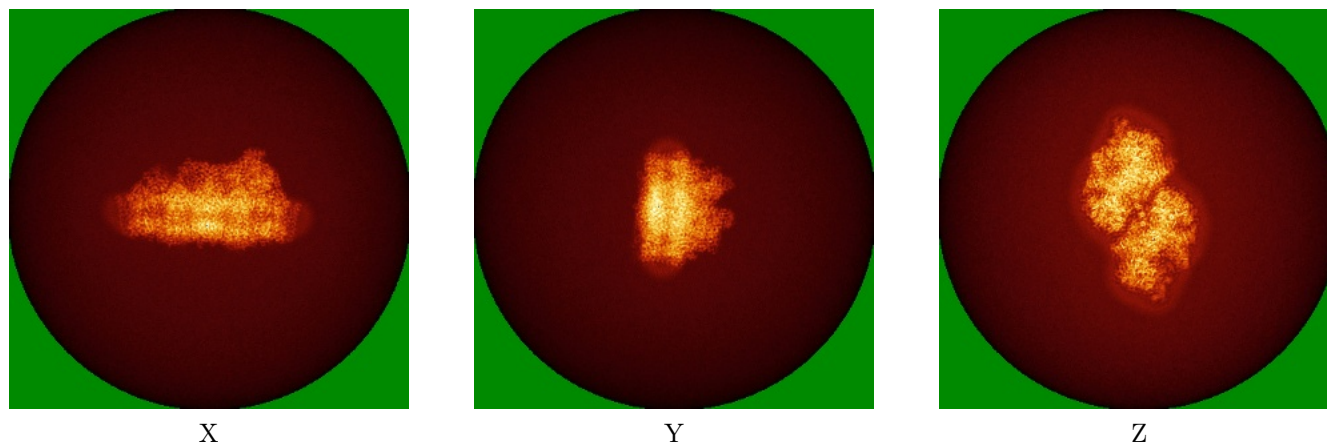
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



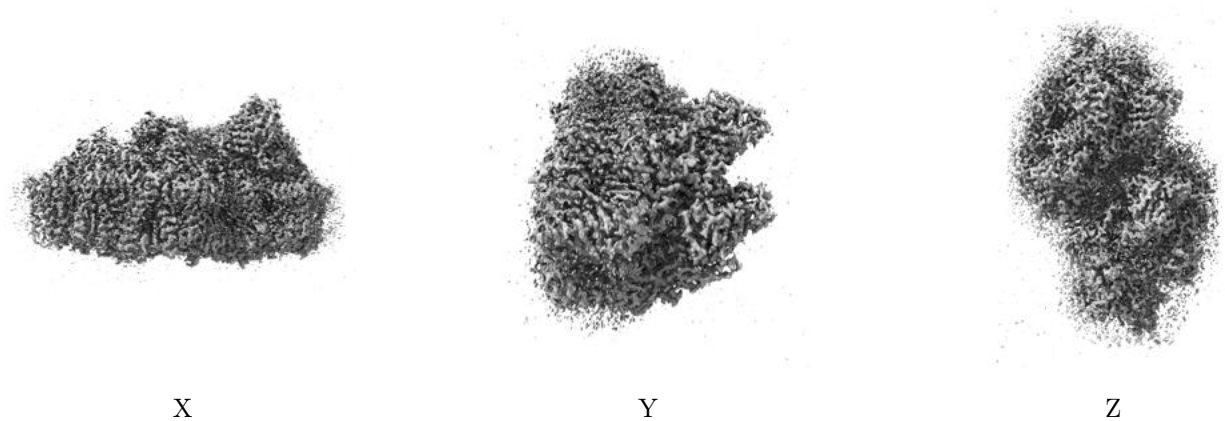
6.4.2 Raw map



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.

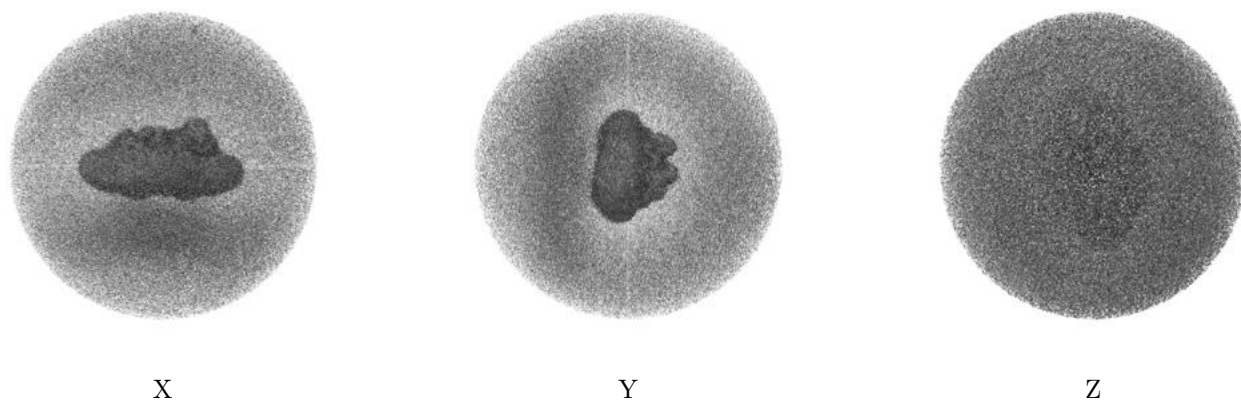
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.039. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

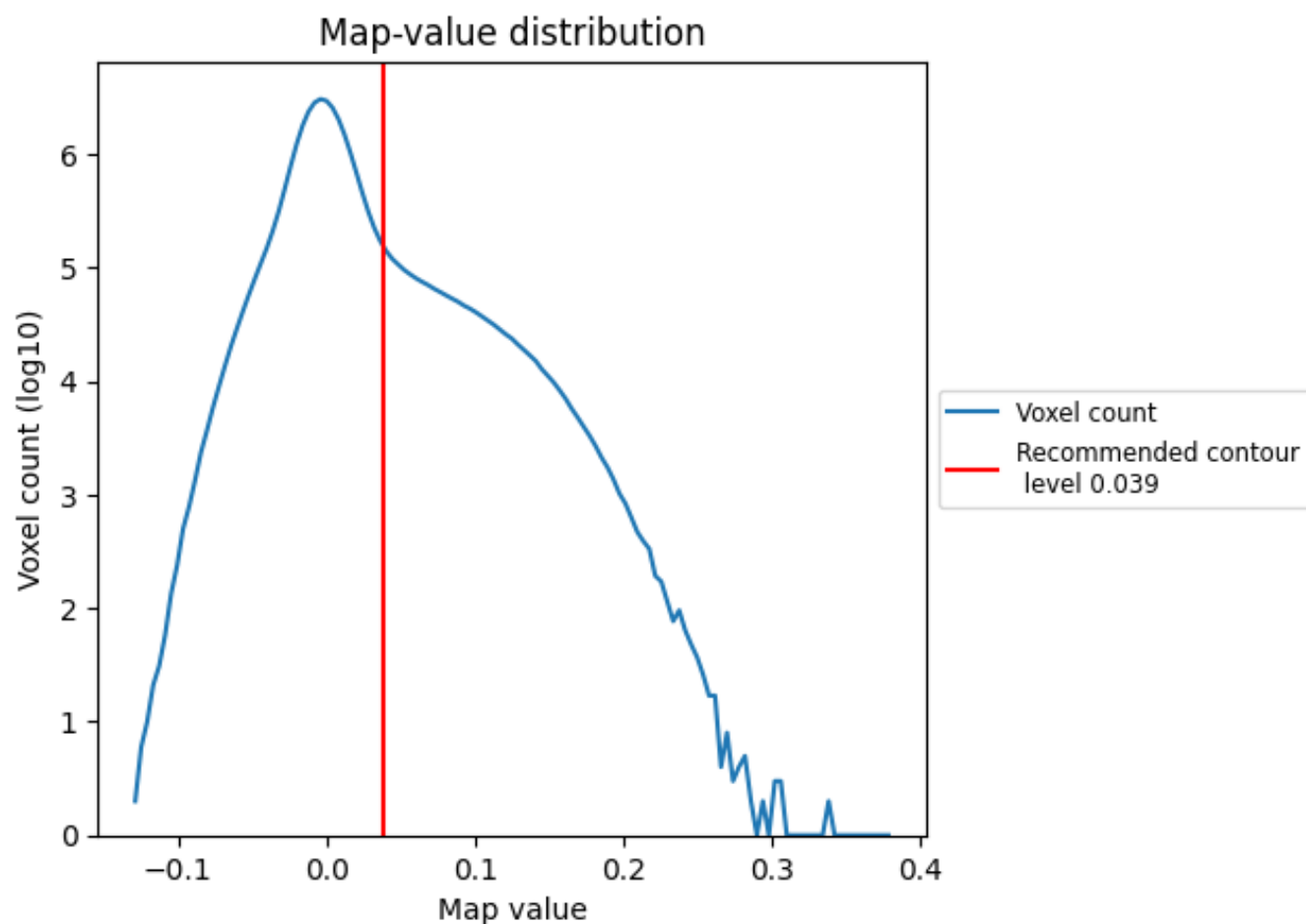
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

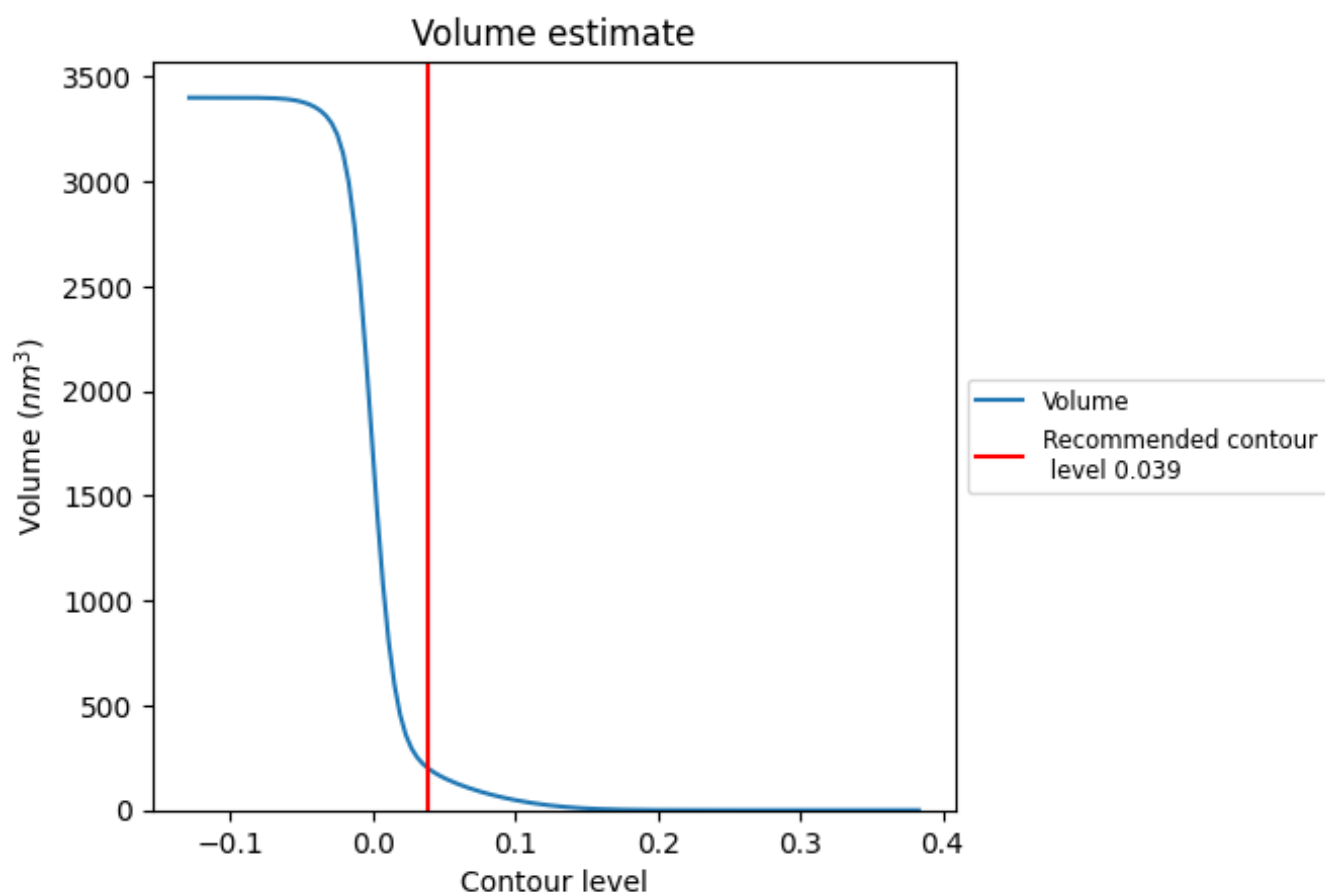
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm³; this corresponds to an approximate mass of 180 kDa.

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

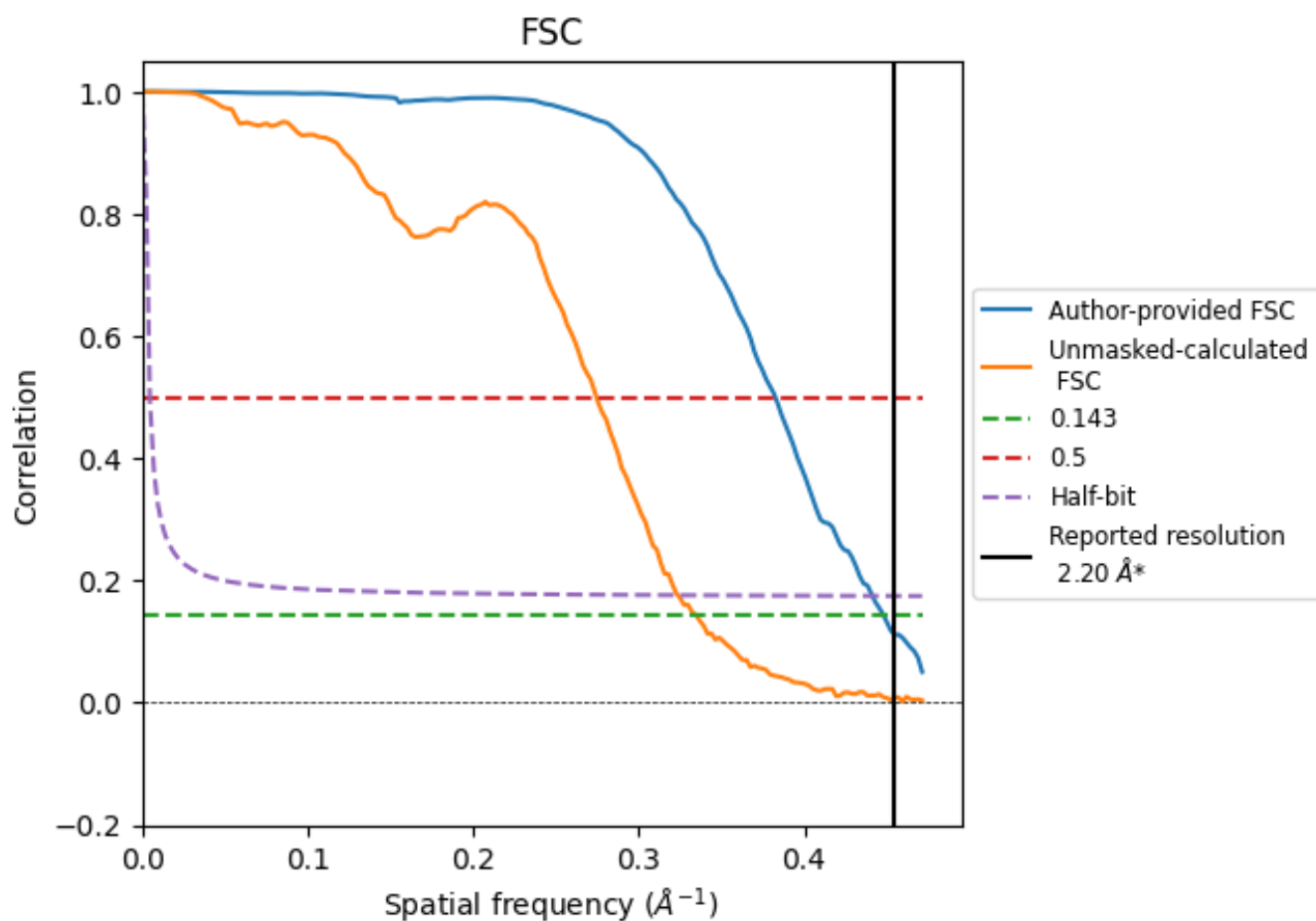
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.455 \AA^{-1}

8.2 Resolution estimates [i](#)

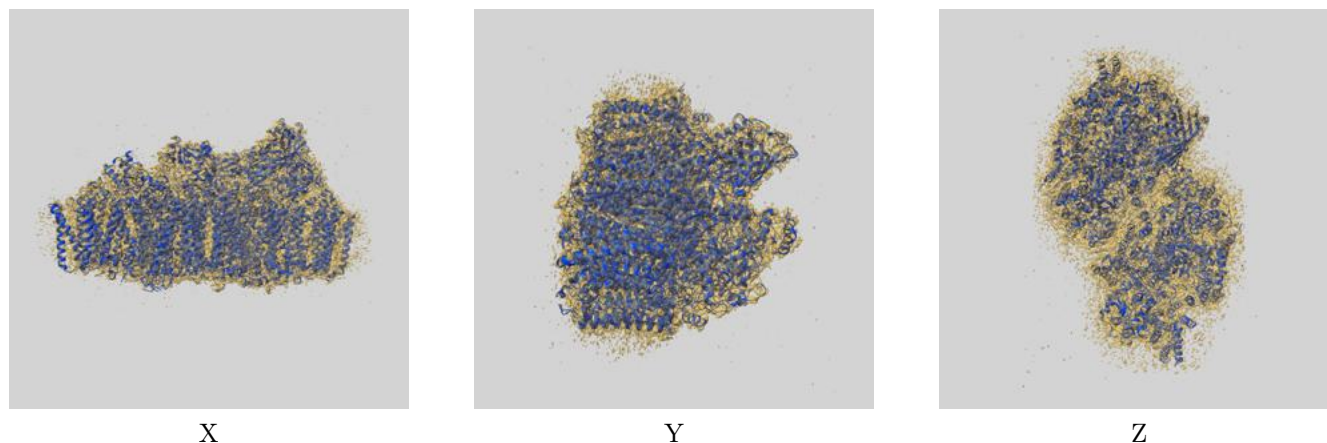
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.23	2.61	2.27
Unmasked-calculated*	2.99	3.64	3.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

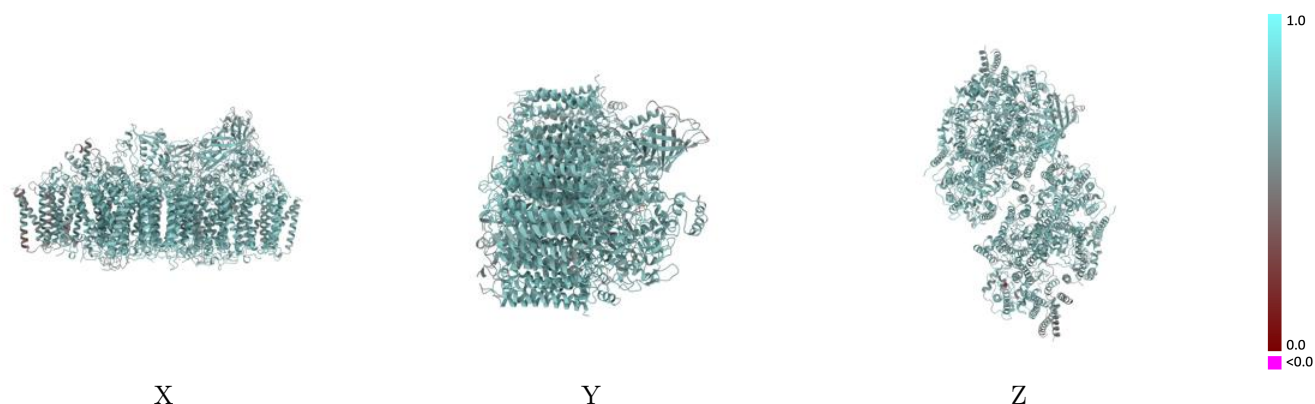
This section contains information regarding the fit between EMDB map EMD-51101 and PDB model 9G6G. Per-residue inclusion information can be found in section 3 on page 31.

9.1 Map-model overlay [i](#)



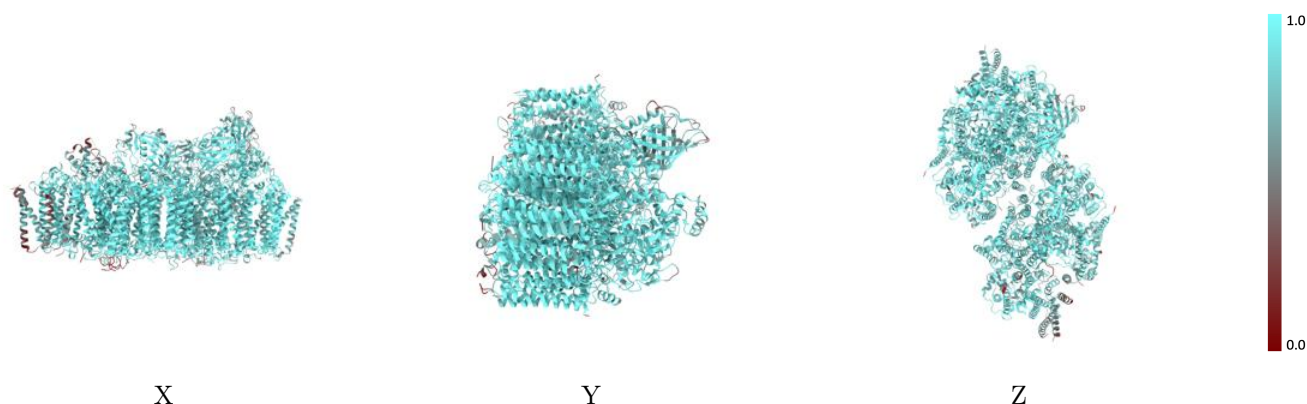
The images above show the 3D surface view of the map at the recommended contour level 0.039 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



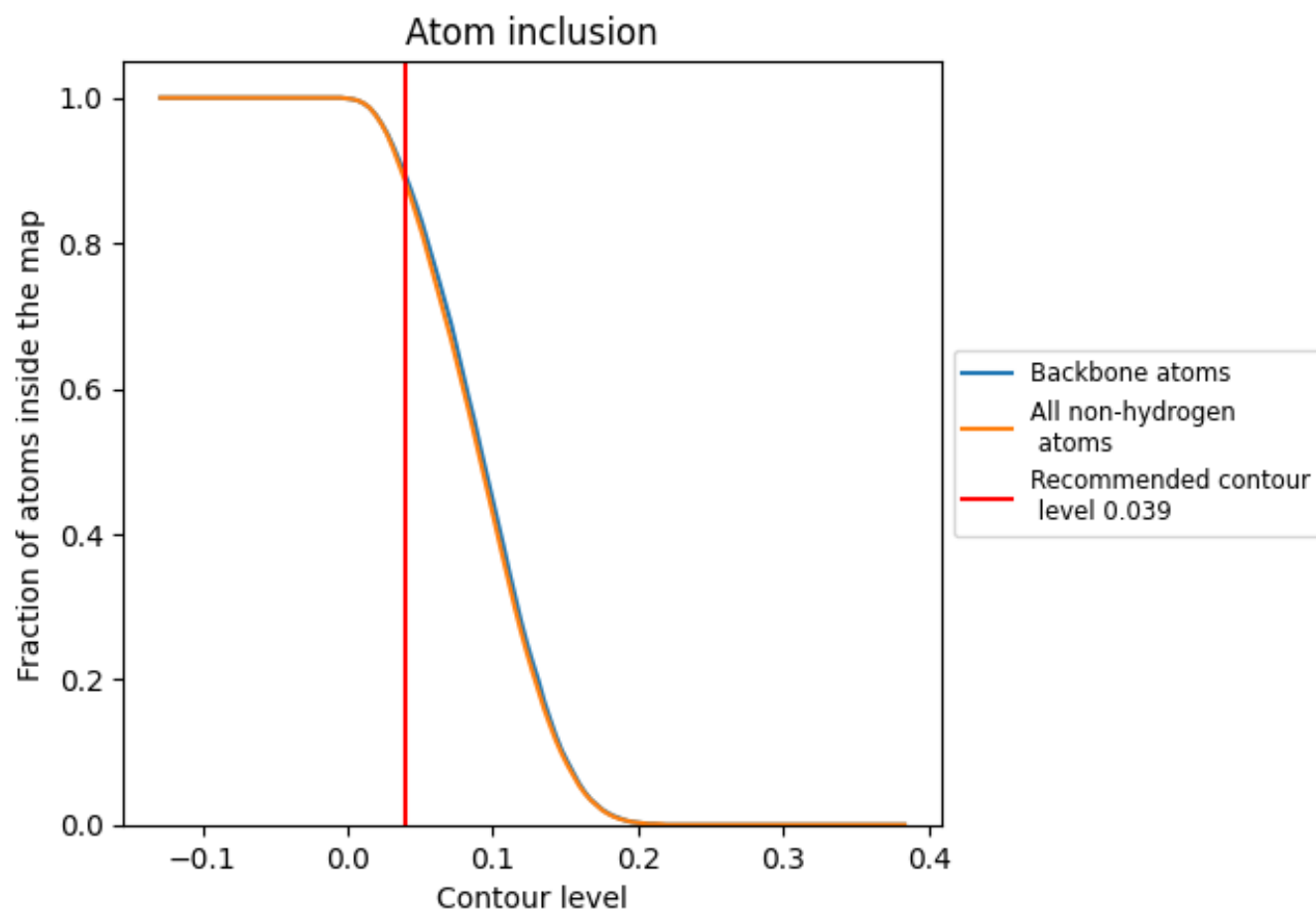
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.039).









































































9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.039) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.6690
A	 0.9490	 0.6990
B	 0.9210	 0.6870
C	 0.9350	 0.6810
D	 0.9400	 0.6980
E	 0.8190	 0.6460
F	 0.8310	 0.6720
H	 0.9300	 0.6870
I	 0.8690	 0.6600
J	 0.8820	 0.6530
K	 0.9360	 0.6660
L	 0.9360	 0.6960
M	 0.8730	 0.6690
O	 0.8310	 0.6340
T	 0.8470	 0.6530
U	 0.8700	 0.6400
V	 0.9050	 0.6600
X	 0.8410	 0.6620
Y	 0.7640	 0.6210
Z	 0.8140	 0.6280
a	 0.9030	 0.6820
b	 0.8910	 0.6710
c	 0.8490	 0.6480
d	 0.9280	 0.6900
e	 0.7440	 0.5950
f	 0.7450	 0.6030
h	 0.9000	 0.6640
i	 0.8850	 0.6640
j	 0.5860	 0.5650
k	 0.8460	 0.6250
l	 0.8890	 0.6970
m	 0.8970	 0.6670
t	 0.9340	 0.6960
x	 0.8060	 0.6400
y	 0.4270	 0.5060
z	 0.5860	 0.5420

