



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 10:58 PM UTC

PDB ID : 9GAE / pdb_00009gae
EMDB ID : EMD-51181
Title : Respiratory supercomplex CI1-CIII2-CIV2 from alphaproteobacterium
Authors : Yaikhomba, M.; Hirst, J.; Croll, T.I.; Spikes, T.E.; Agip, A.N.A.
Deposited on : 2024-07-26
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

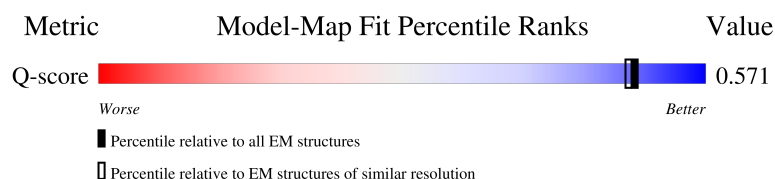
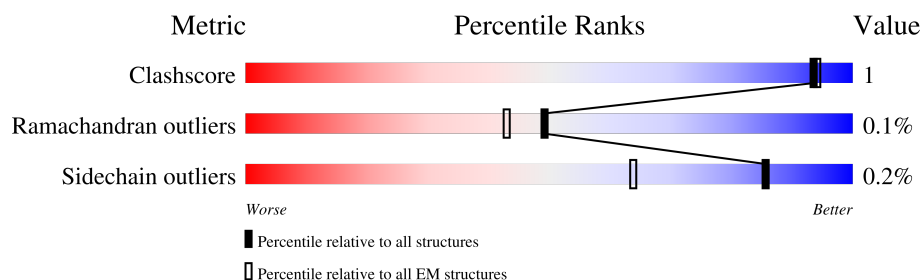
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

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



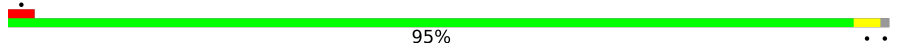
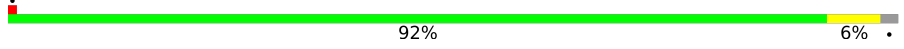
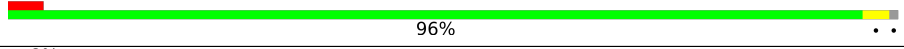
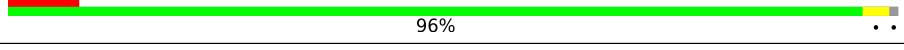
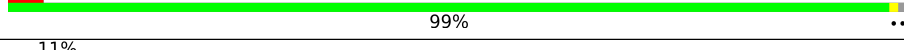
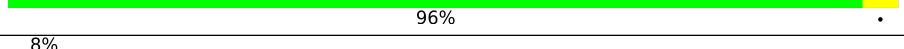
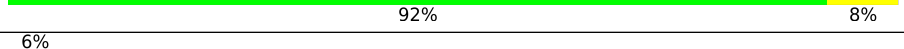
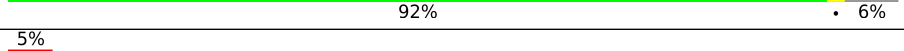
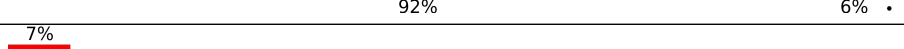
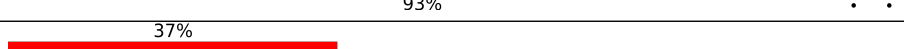
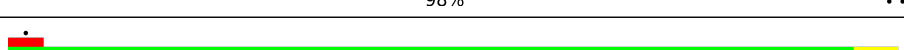
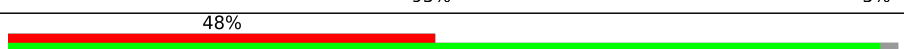
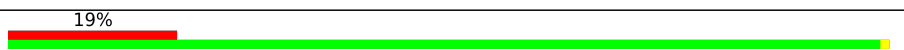
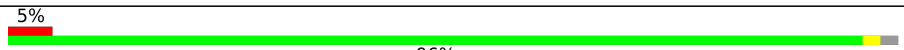
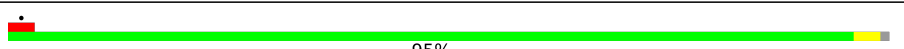




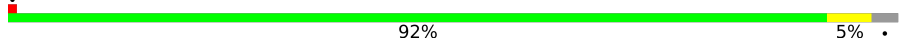
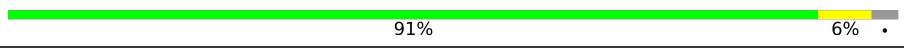
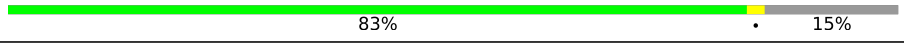

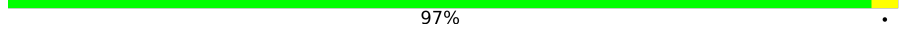

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	121	<div> <div>14%</div> <div>95%</div> <div>5%</div> </div>
2	B	175	<div> <div>10%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>
3	C	208	<div> <div>10%</div> <div>91%</div> <div>7%</div> </div>
4	D	412	<div> <div>11%</div> <div>96%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	239	
6	F	431	
7	G	674	
8	H	345	
9	I	163	
10	J	199	
11	K	101	
12	L	703	
13	M	513	
14	N	499	
15	P	330	
16	Q	103	
17	R	62	
18	Z	217	
19	a	440	
19	d	440	
20	b	450	
20	e	450	
21	c	195	
21	f	195	
22	g	558	
22	k	558	
23	h	298	
23	l	298	
24	i	274	

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Mol	Chain	Length	Quality of chain
24	m	274	<div><div></div><div>95%</div><div>5%</div></div>
25	j	66	<div><div></div><div>64%</div><div>35%</div></div>
25	n	66	<div><div></div><div>65%</div><div>35%</div></div>
26	o	176	<div><div></div><div>25%</div><div>75%</div></div>
26	p	176	<div><div></div><div>24%</div><div>74%</div></div>
27	q	124	<div><div></div><div>98%</div><div>2%</div></div>

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 82894 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 NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	121	Total	C	N	O	S	0	0
			969	658	141	164	6		

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	162	Total	C	N	O	S	0	0
			1270	799	227	231	13		

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	194	Total	C	N	O	S	0	0
			1586	1020	274	290	2		

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	411	Total	C	N	O	S	0	0
			3277	2072	582	601	22		

- Molecule 5 is a protein called NADH dehydrogenase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	237	Total	C	N	O	S	0	0
			1822	1155	314	340	13		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	422	Total	C	N	O	S	0	0
			3241	2027	583	600	31		

- Molecule 7 is a protein called NADH-quinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	665	Total	C	N	O	S	0	0
			5068	3149	917	969	33		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	341	Total	C	N	O	S	0	0
			2722	1848	413	439	22		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	162	Total	C	N	O	S	0	0
			1319	836	230	242	11		

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	199	Total	C	N	O	S	0	0
			1528	1014	246	257	11		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			764	508	123	128	5		

- Molecule 12 is a protein called NADH dehydrogenase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	661	Total	C	N	O	S	0	0
			5215	3472	853	857	33		

- Molecule 13 is a protein called NADH dehydrogenase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	503	Total	C	N	O	S	0	0
			3915	2615	610	658	32		

- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	480	Total	C	N	O	S	0	0
			3556	2342	565	617	32		

- Molecule 15 is a protein called NAD-dependent epimerase/dehydratase.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	328	Total	C	N	O	S	0	0
			2468	1541	463	452	12		

- Molecule 16 is a protein called ETC complex I subunit conserved region.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	103	Total	C	N	O	S	0	0
			849	523	167	156	3		

- Molecule 17 is a protein called Zinc finger CHCC-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	61	Total	C	N	O	S	0	0
			488	304	90	91	3		

- Molecule 18 is a protein called Protein-L-isoaspartate O-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	216	Total	C	N	O	S	0	0
			1642	1033	294	306	9		

- Molecule 19 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	433	Total	C	N	O	S	0	0
			3504	2373	552	561	18		
19	d	434	Total	C	N	O	S	0	0
			3513	2378	553	564	18		

- Molecule 20 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		
20	e	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		

- Molecule 21 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	180	Total	C	N	O	S	0	0
			1353	838	245	263	7		
21	f	181	Total	C	N	O	S	0	0
			1361	842	246	266	7		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		
22	k	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	h	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		
23	l	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		

- Molecule 24 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		
24	m	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		

- Molecule 25 is a protein called Aa3 type cytochrome c oxidase subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	43	Total	C	N	O	S	0	0
			332	214	58	59	1		
25	n	43	Total	C	N	O	S	0	0
			332	214	58	59	1		

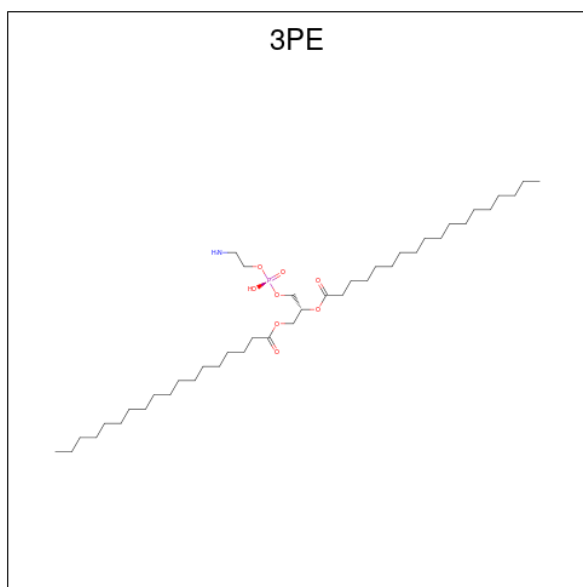
- Molecule 26 is a protein called Cytochrome c, class I.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	o	44	Total	C	N	O	S	0	0
			324	215	49	58	2		
26	p	45	Total	C	N	O	S	0	0
			330	218	50	60	2		

- Molecule 27 is a protein called NADH:ubiquinone oxidoreductase 17.2 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	q	123	Total	C	N	O	S	0	0
			1018	651	181	185	1		

- Molecule 28 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	L	1	Total	C	N	O	P	0
			51	41	1	8	1	

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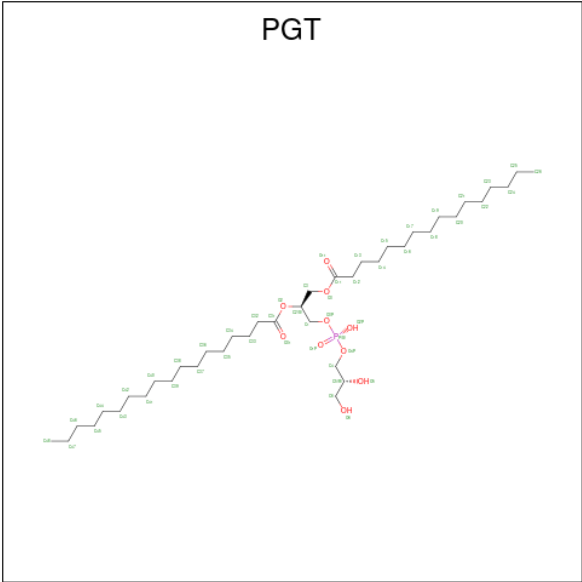
Mol	Chain	Residues	Atoms					AltConf
28	L	1	Total 51	C 41	N 1	O 8	P 1	0
28	L	1	Total 51	C 41	N 1	O 8	P 1	0
28	L	1	Total 51	C 41	N 1	O 8	P 1	0
28	P	1	Total 51	C 41	N 1	O 8	P 1	0
28	a	1	Total 51	C 41	N 1	O 8	P 1	0
28	a	1	Total 51	C 41	N 1	O 8	P 1	0
28	a	1	Total 51	C 41	N 1	O 8	P 1	0
28	a	1	Total 51	C 41	N 1	O 8	P 1	0
28	c	1	Total 51	C 41	N 1	O 8	P 1	0
28	d	1	Total 51	C 41	N 1	O 8	P 1	0
28	d	1	Total 51	C 41	N 1	O 8	P 1	0
28	d	1	Total 51	C 41	N 1	O 8	P 1	0
28	e	1	Total 51	C 41	N 1	O 8	P 1	0
28	e	1	Total 51	C 41	N 1	O 8	P 1	0
28	g	1	Total 51	C 41	N 1	O 8	P 1	0
28	g	1	Total 51	C 41	N 1	O 8	P 1	0
28	g	1	Total 51	C 41	N 1	O 8	P 1	0
28	h	1	Total 51	C 41	N 1	O 8	P 1	0
28	h	1	Total 51	C 41	N 1	O 8	P 1	0
28	i	1	Total 51	C 41	N 1	O 8	P 1	0
28	i	1	Total 51	C 41	N 1	O 8	P 1	0

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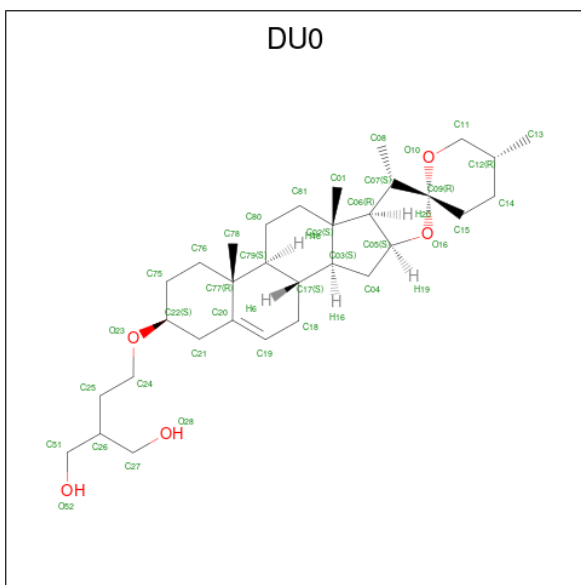
Mol	Chain	Residues	Atoms					AltConf
28	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	k	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	n	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	p	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 29 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O	P	0
			51	40	10	1	
29	H	1	Total	C	O	P	0
			51	40	10	1	
29	J	1	Total	C	O	P	0
			51	40	10	1	
29	J	1	Total	C	O	P	0
			51	40	10	1	
29	K	1	Total	C	O	P	0
			51	40	10	1	
29	L	1	Total	C	O	P	0
			51	40	10	1	
29	M	1	Total	C	O	P	0
			51	40	10	1	
29	N	1	Total	C	O	P	0
			51	40	10	1	
29	P	1	Total	C	O	P	0
			51	40	10	1	
29	a	1	Total	C	O	P	0
			51	40	10	1	
29	g	1	Total	C	O	P	0
			51	40	10	1	
29	q	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 30 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (CCD ID: DU0) (formula: C₃₂H₅₂O₅).



Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total 37	C 32	O 5	0
30	H	1	Total 37	C 32	O 5	0
30	J	1	Total 37	C 32	O 5	0
30	J	1	Total 37	C 32	O 5	0
30	M	1	Total 37	C 32	O 5	0
30	M	1	Total 37	C 32	O 5	0
30	a	1	Total 37	C 32	O 5	0
30	c	1	Total 37	C 32	O 5	0
30	c	1	Total 37	C 32	O 5	0
30	d	1	Total 37	C 32	O 5	0
30	d	1	Total 37	C 32	O 5	0
30	d	1	Total 37	C 32	O 5	0
30	e	1	Total 37	C 32	O 5	0
30	f	1	Total 37	C 32	O 5	0

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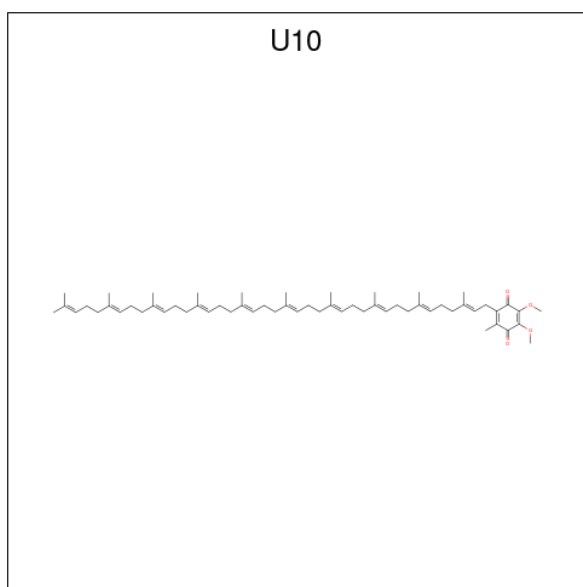
Mol	Chain	Residues	Atoms			AltConf
30	g	1	Total	C	O	0
			37	32	5	
30	g	1	Total	C	O	0
			37	32	5	
30	g	1	Total	C	O	0
			37	32	5	
30	g	1	Total	C	O	0
			37	32	5	
30	h	1	Total	C	O	0
			37	32	5	
30	h	1	Total	C	O	0
			37	32	5	
30	h	1	Total	C	O	0
			37	32	5	
30	i	1	Total	C	O	0
			37	32	5	
30	i	1	Total	C	O	0
			37	32	5	
30	i	1	Total	C	O	0
			37	32	5	
30	i	1	Total	C	O	0
			37	32	5	
30	j	1	Total	C	O	0
			37	32	5	
30	k	1	Total	C	O	0
			37	32	5	
30	m	1	Total	C	O	0
			37	32	5	
30	m	1	Total	C	O	0
			37	32	5	

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



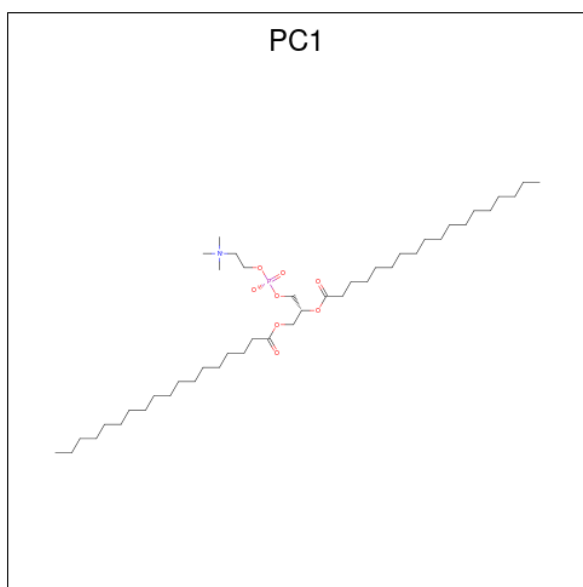
Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	Fe	S	0
			8	4	4	
31	F	1	Total	Fe	S	0
			8	4	4	
31	G	1	Total	Fe	S	0
			8	4	4	
31	G	1	Total	Fe	S	0
			8	4	4	
31	I	1	Total	Fe	S	0
			8	4	4	
31	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 32 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			63	59	4	
32	a	1	Total	C	O	0
			63	59	4	
32	a	1	Total	C	O	0
			63	59	4	
32	d	1	Total	C	O	0
			63	59	4	
32	d	1	Total	C	O	0
			63	59	4	

- Molecule 33 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
33	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	N	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	N	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	N	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	b	1	Total	C	N	O	P	0
			54	44	1	8	1	

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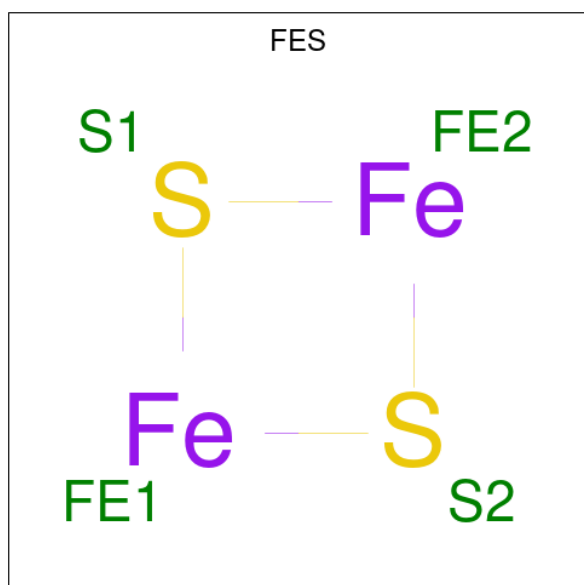
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Mol	Chain	Residues	Atoms					AltConf
33	b	1	Total 54	C 44	N 1	O 8	P 1	0
33	c	1	Total 54	C 44	N 1	O 8	P 1	0
33	d	1	Total 54	C 44	N 1	O 8	P 1	0
33	d	1	Total 54	C 44	N 1	O 8	P 1	0
33	f	1	Total 54	C 44	N 1	O 8	P 1	0
33	g	1	Total 54	C 44	N 1	O 8	P 1	0
33	h	1	Total 54	C 44	N 1	O 8	P 1	0
33	i	1	Total 54	C 44	N 1	O 8	P 1	0
33	i	1	Total 54	C 44	N 1	O 8	P 1	0
33	i	1	Total 54	C 44	N 1	O 8	P 1	0
33	j	1	Total 54	C 44	N 1	O 8	P 1	0
33	k	1	Total 54	C 44	N 1	O 8	P 1	0
33	k	1	Total 54	C 44	N 1	O 8	P 1	0
33	l	1	Total 54	C 44	N 1	O 8	P 1	0
33	l	1	Total 54	C 44	N 1	O 8	P 1	0
33	l	1	Total 54	C 44	N 1	O 8	P 1	0
33	m	1	Total 54	C 44	N 1	O 8	P 1	0
33	m	1	Total 54	C 44	N 1	O 8	P 1	0
33	m	1	Total 54	C 44	N 1	O 8	P 1	0
33	m	1	Total 54	C 44	N 1	O 8	P 1	0
33	n	1	Total 54	C 44	N 1	O 8	P 1	0

- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

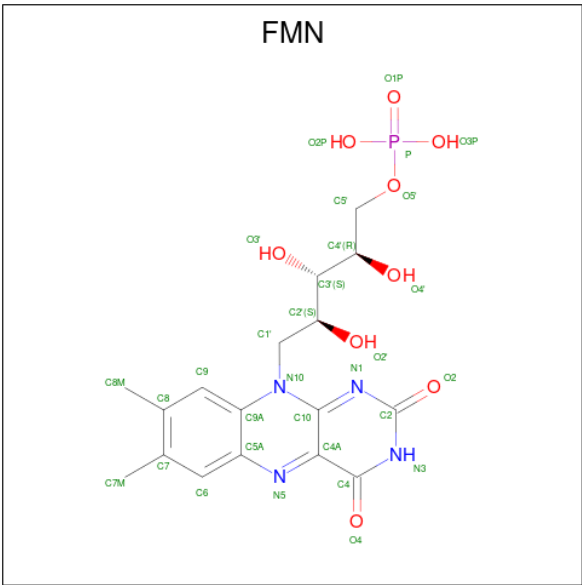
Mol	Chain	Residues	Atoms		AltConf
34	D	1	Total	Ca	0
			1	1	
34	b	1	Total	Ca	0
			1	1	
34	e	1	Total	Ca	0
			1	1	
34	g	1	Total	Ca	0
			1	1	
34	k	1	Total	Ca	0
			1	1	

- Molecule 35 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
35	E	1	Total	Fe	S	0
			4	2	2	
35	G	1	Total	Fe	S	0
			4	2	2	
35	c	1	Total	Fe	S	0
			4	2	2	
35	f	1	Total	Fe	S	0
			4	2	2	

- Molecule 36 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



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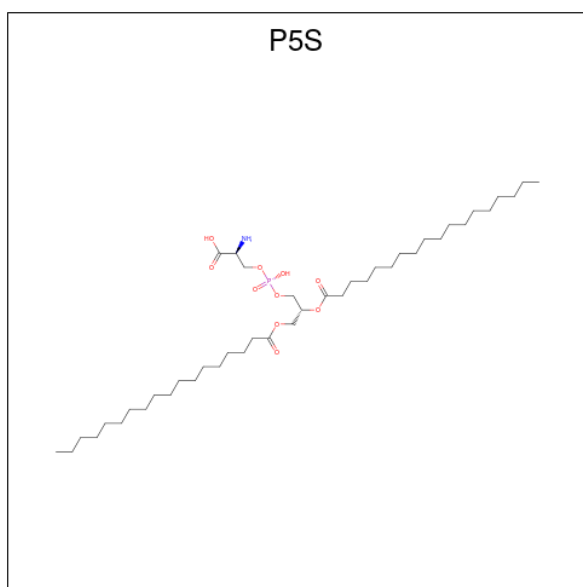
Mol	Chain	Residues	Atoms				AltConf
37	L	1	Total 48	C 39	O 8	P 1	0
37	L	1	Total 48	C 39	O 8	P 1	0
37	L	1	Total 48	C 39	O 8	P 1	0
37	M	1	Total 48	C 39	O 8	P 1	0
37	M	1	Total 48	C 39	O 8	P 1	0
37	M	1	Total 48	C 39	O 8	P 1	0
37	M	1	Total 48	C 39	O 8	P 1	0
37	N	1	Total 48	C 39	O 8	P 1	0
37	P	1	Total 48	C 39	O 8	P 1	0
37	a	1	Total 48	C 39	O 8	P 1	0
37	a	1	Total 48	C 39	O 8	P 1	0
37	a	1	Total 48	C 39	O 8	P 1	0
37	c	1	Total 48	C 39	O 8	P 1	0
37	d	1	Total 48	C 39	O 8	P 1	0
37	d	1	Total 48	C 39	O 8	P 1	0
37	d	1	Total 48	C 39	O 8	P 1	0
37	f	1	Total 48	C 39	O 8	P 1	0
37	f	1	Total 48	C 39	O 8	P 1	0
37	g	1	Total 48	C 39	O 8	P 1	0
37	g	1	Total 48	C 39	O 8	P 1	0
37	i	1	Total 48	C 39	O 8	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
37	i	1	Total	C	O	P	0
			48	39	8	1	
37	i	1	Total	C	O	P	0
			48	39	8	1	
37	i	1	Total	C	O	P	0
			48	39	8	1	
37	i	1	Total	C	O	P	0
			48	39	8	1	
37	j	1	Total	C	O	P	0
			48	39	8	1	
37	k	1	Total	C	O	P	0
			48	39	8	1	
37	k	1	Total	C	O	P	0
			48	39	8	1	
37	m	1	Total	C	O	P	0
			48	39	8	1	
37	m	1	Total	C	O	P	0
			48	39	8	1	
37	o	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 38 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



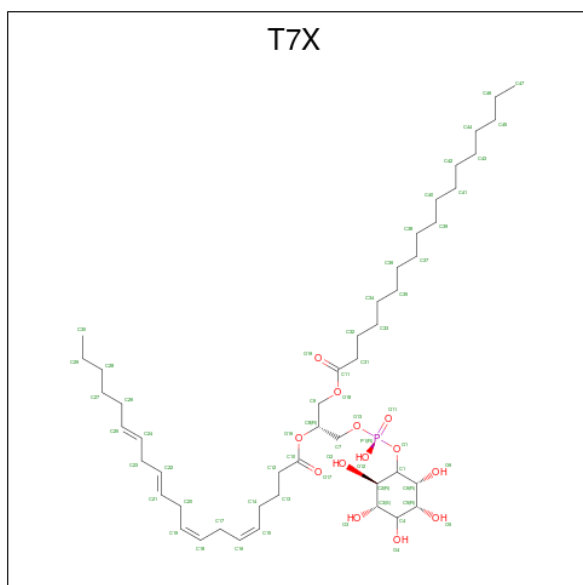
Mol	Chain	Residues	Atoms					AltConf
38	I	1	Total	C	N	O	P	0
			54	42	1	10	1	

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Mol	Chain	Residues	Atoms				AltConf
38	L	1	Total	C	N	O	P
			54	42	1	10	1
38	a	1	Total	C	N	O	P
			54	42	1	10	1

- Molecule 39 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).

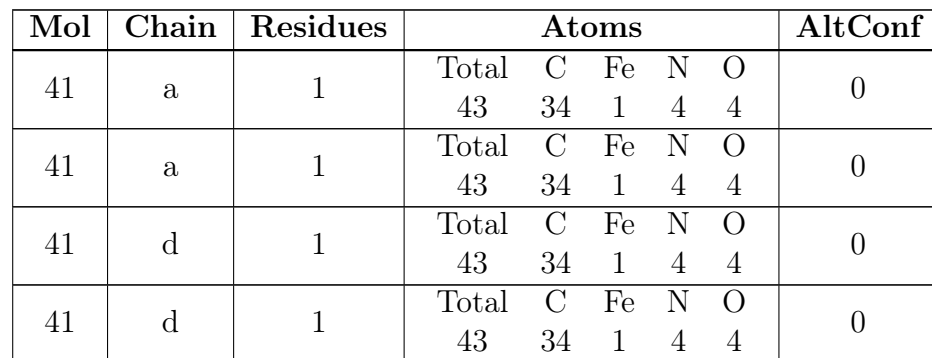


Mol	Chain	Residues	Atoms				AltConf
39	J	1	Total	C	O	P	0
			61	47	13	1	
39	g	1	Total	C	O	P	0
			61	47	13	1	

- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	R	1	Total	Zn	0
			1	1	
40	i	1	Total	Zn	0
			1	1	
40	m	1	Total	Zn	0
			1	1	

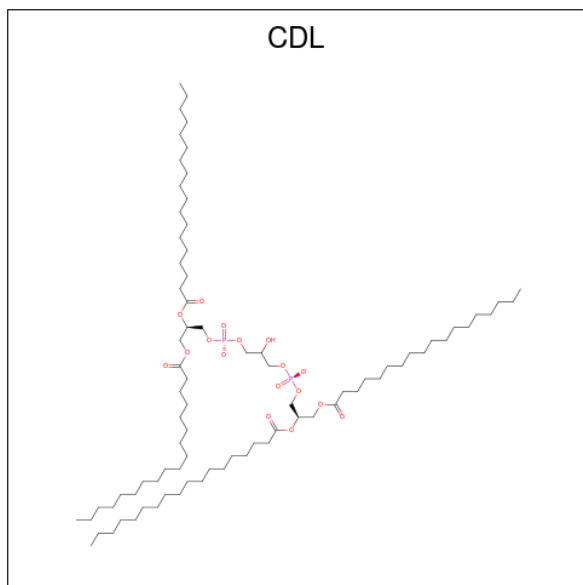
- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



-
- The chemical structure of HEC (Hydroxyethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure is labeled with various side chains and atoms, including C1A, C2A, C3A, C4A, C1B, C2B, C3B, C4B, C1C, C2C, C3C, C4C, C1D, C2D, C3D, C4D, C1E, C2E, C3E, C4E, C1F, C2F, C3F, C4F, C1G, C2G, C3G, C4G, C1H, C2H, C3H, C4H, C1I, C2I, C3I, C4I, C1J, C2J, C3J, C4J, C1K, C2K, C3K, C4K, C1L, C2L, C3L, C4L, C1M, C2M, C3M, C4M, C1N, C2N, C3N, C4N, C1O, C2O, C3O, C4O, C1P, C2P, C3P, C4P, C1Q, C2Q, C3Q, C4Q, C1R, C2R, C3R, C4R, C1S, C2S, C3S, C4S, C1T, C2T, C3T, C4T, C1U, C2U, C3U, C4U, C1V, C2V, C3V, C4V, C1W, C2W, C3W, C4W, C1X, C2X, C3X, C4X, C1Y, C2Y, C3Y, C4Y, C1Z, C2Z, C3Z, C4Z, C1AA, C2AA, C3AA, C4AA, C1AB, C2AB, C3AB, C4AB, C1AC, C2AC, C3AC, C4AC, C1AD, C2AD, C3AD, C4AD, C1AE, C2AE, C3AE, C4AE, C1AF, C2AF, C3AF, C4AF, C1AG, C2AG, C3AG, C4AG, C1AH, C2AH, C3AH, C4AH, C1AI, C2AI, C3AI, C4AI, C1AJ, C2AJ, C3AJ, C4AJ, C1AK, C2AK, C3AK, C4AK, C1AL, C2AL, C3AL, C4AL, C1AM, C2AM, C3AM, C4AM, C1AN, C2AN, C3AN, C4AN, C1AO, C2AO, C3AO, C4AO, C1AP, C2AP, C3AP, C4AP, C1AQ, C2AQ, C3AQ, C4AQ, 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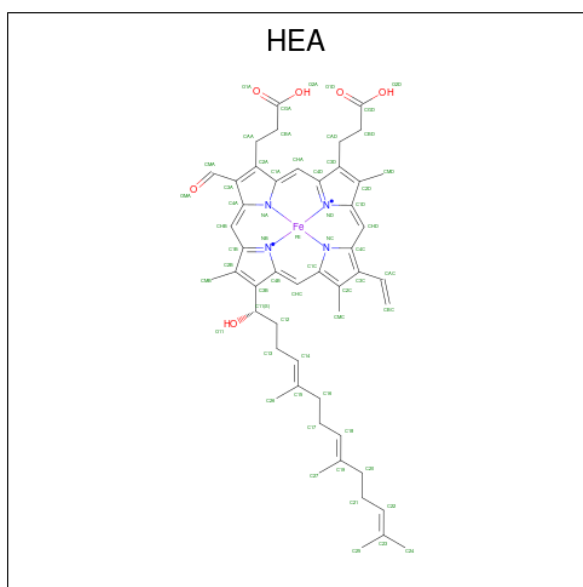
Mol	Chain	Residues	Atoms					AltConf
42	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
42	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 43 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
43	d	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 44 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
44	g	1	Total 60	C 49	Fe 1	N 4	O 6	0
44	g	1	Total 60	C 49	Fe 1	N 4	O 6	0
44	k	1	Total 60	C 49	Fe 1	N 4	O 6	0
44	k	1	Total 60	C 49	Fe 1	N 4	O 6	0

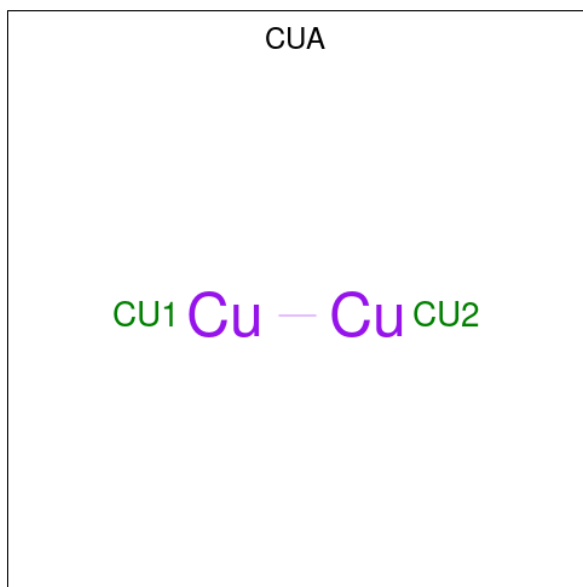
- Molecule 45 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
45	g	1	Total	Cu	0
			1	1	
45	k	1	Total	Cu	0
			1	1	

- Molecule 46 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
46	g	1	Total	Mn	0
			1	1	
46	k	1	Total	Mn	0
			1	1	

- Molecule 47 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

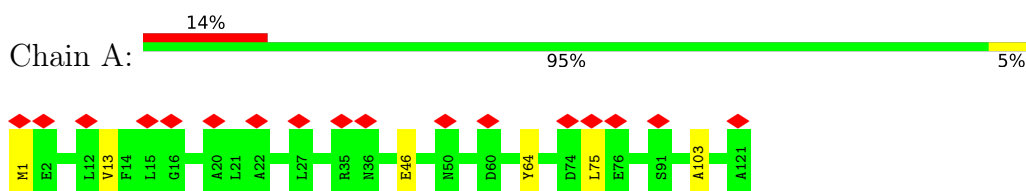


Mol	Chain	Residues	Atoms		AltConf
47	h	1	Total 2	Cu 2	0
47	l	1	Total 2	Cu 2	0

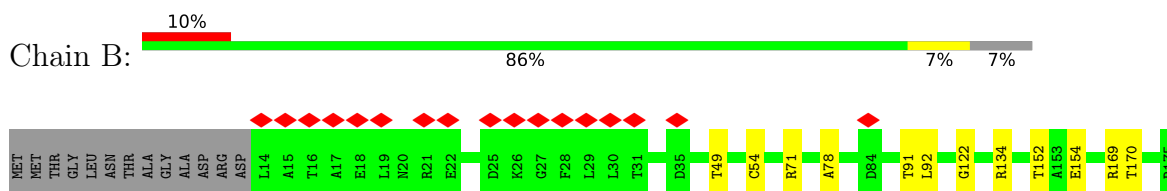
3 Residue-property plots [i](#)

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

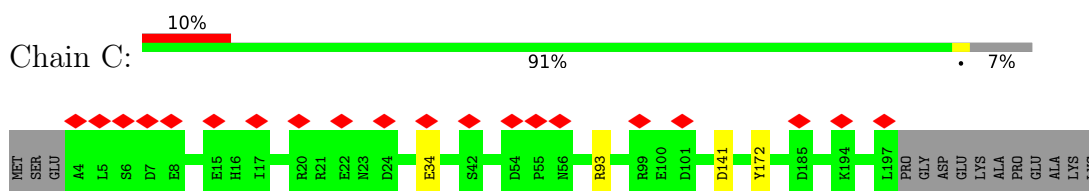
- Molecule 1: NADH-quinone oxidoreductase subunit A



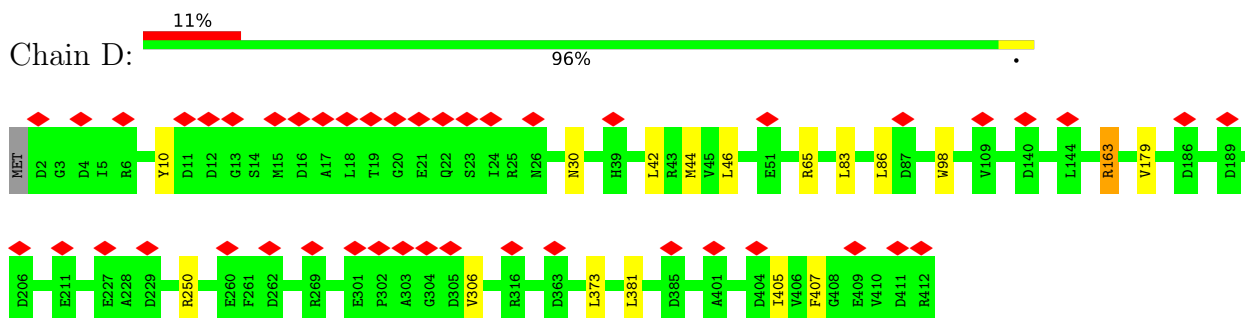
- Molecule 2: NADH-quinone oxidoreductase subunit B



- Molecule 3: NADH-quinone oxidoreductase subunit C

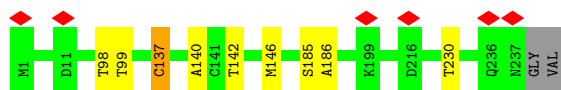


- Molecule 4: NADH-quinone oxidoreductase subunit D



- Molecule 5: NADH dehydrogenase subunit E





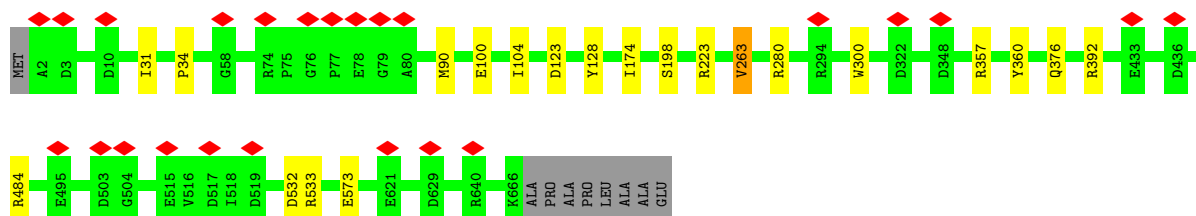
- Molecule 6: NADH-quinone oxidoreductase subunit F

Chain F: 92% 6%



- Molecule 7: NADH-quinone oxidoreductase

Chain G: 96%



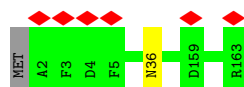
- Molecule 8: NADH-quinone oxidoreductase subunit H

Chain H: 8% 96%



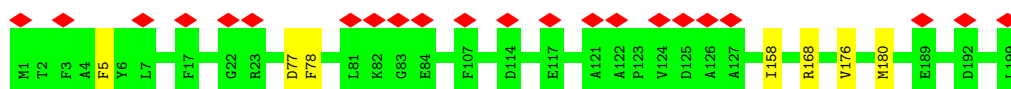
- Molecule 9: NADH-quinone oxidoreductase subunit I

Chain I: 99%

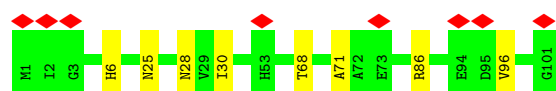


- Molecule 10: NADH-quinone oxidoreductase subunit J

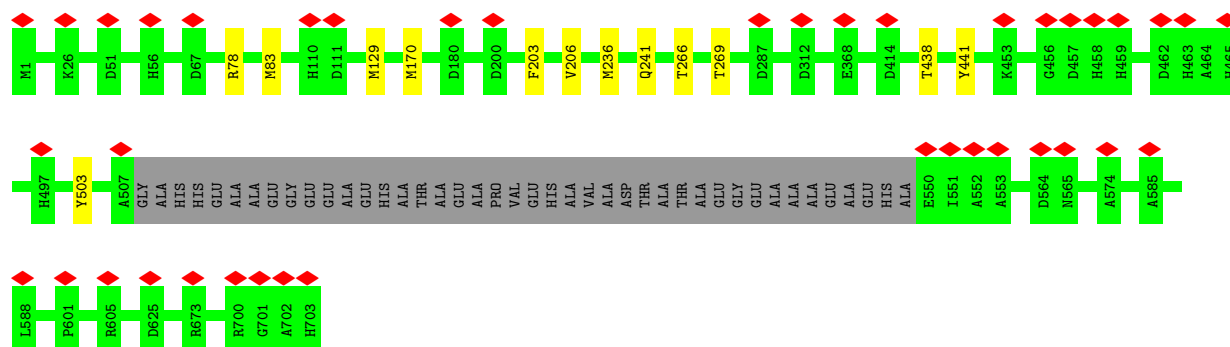
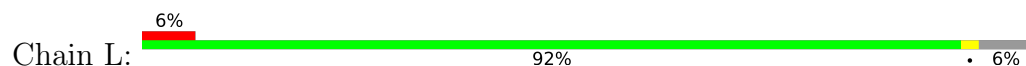
Chain J: 11% 96%



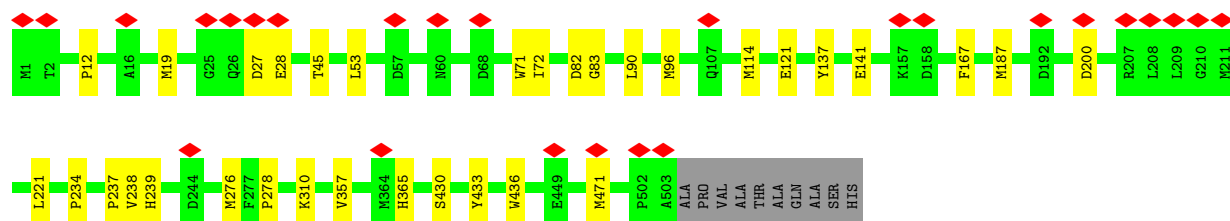
- Molecule 11: NADH-quinone oxidoreductase subunit K



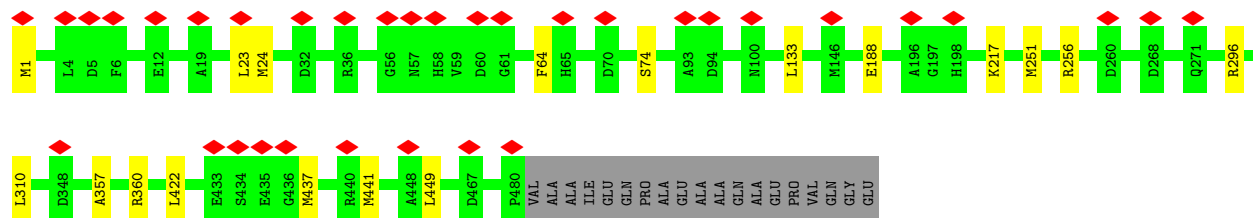
• Molecule 12: NADH dehydrogenase subunit L



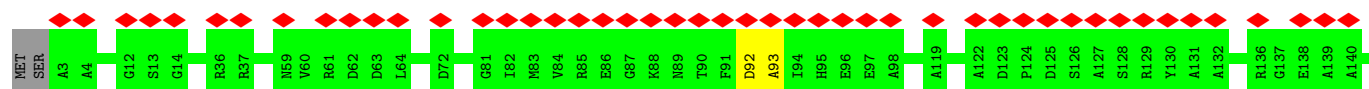
• Molecule 13: NADH dehydrogenase subunit M

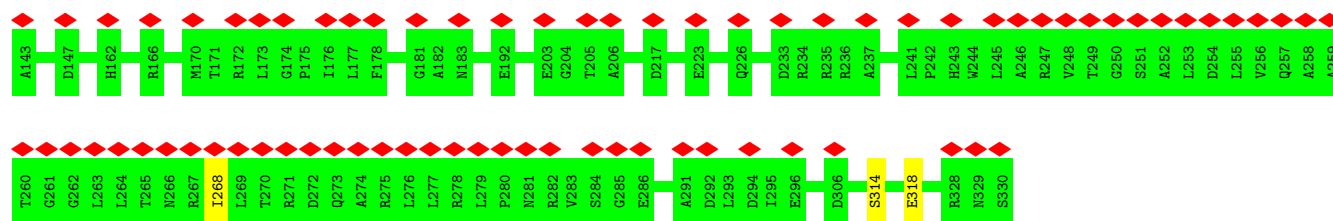


• Molecule 14: NADH-quinone oxidoreductase subunit N

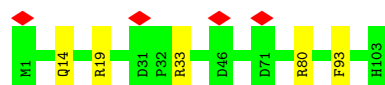


• Molecule 15: NAD-dependent epimerase/dehydratase

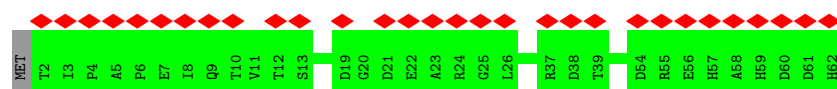




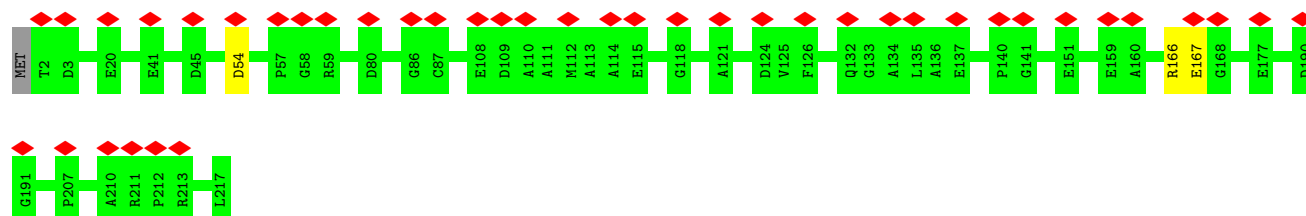
- Molecule 16: ETC complex I subunit conserved region



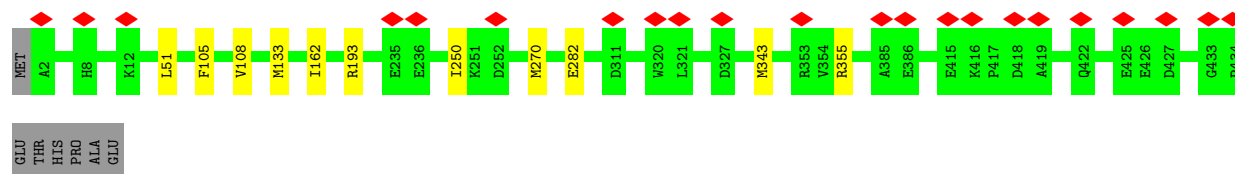
- Molecule 17: Zinc finger CHCC-type domain-containing protein



- Molecule 18: Protein-L-isoaspartate O-methyltransferase

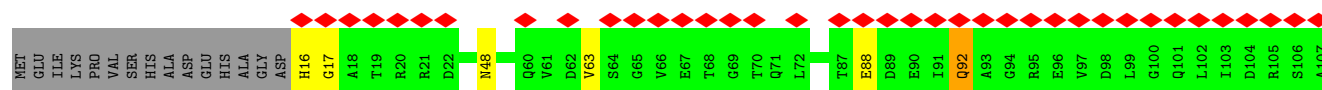


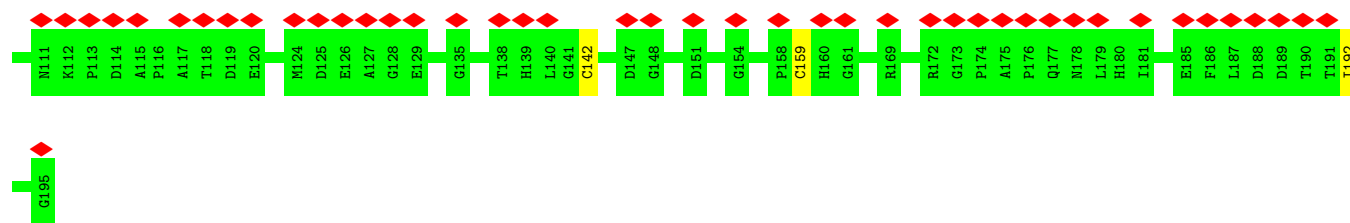
- Molecule 19: Cytochrome b



- Molecule 19: Cytochrome b

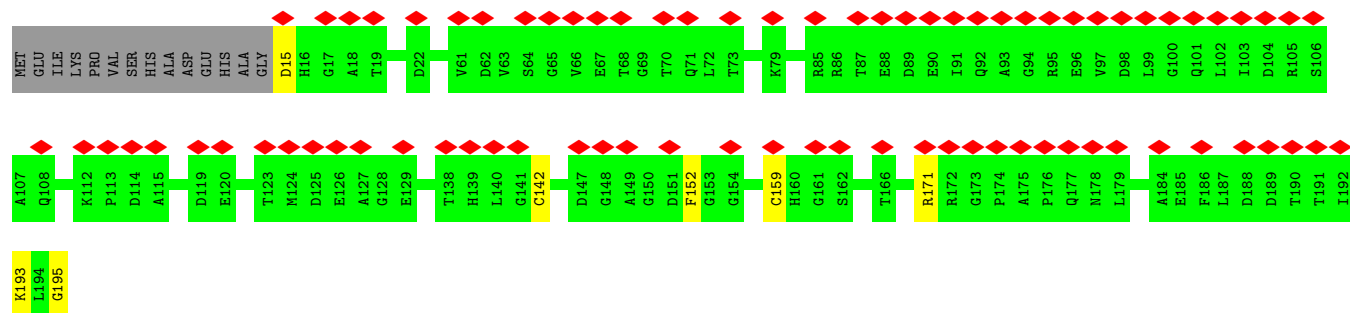






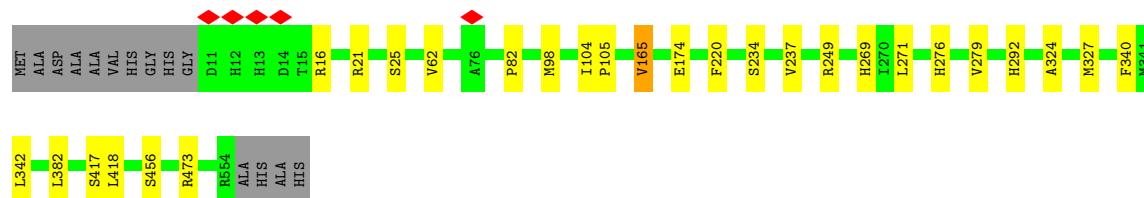
- Molecule 21: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain f: 41% 89% 7%



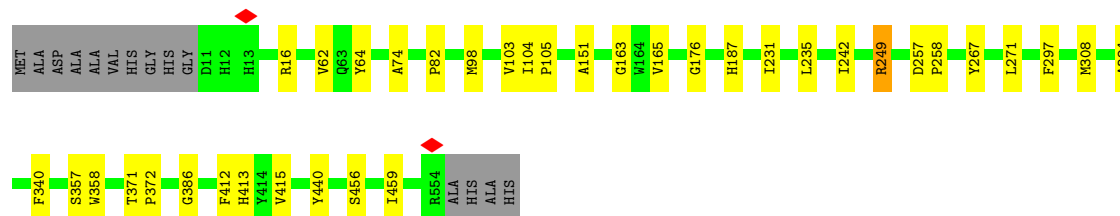
- Molecule 22: Cytochrome c oxidase subunit 1

Chain g: 92% 5% 3%



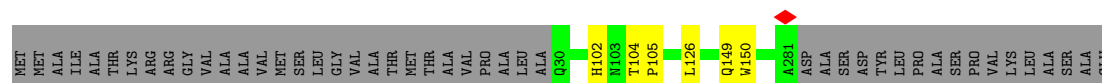
- Molecule 22: Cytochrome c oxidase subunit 1

Chain k: 91% 6% 3%



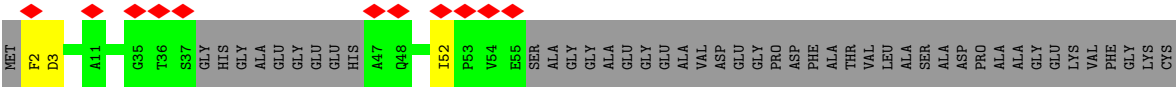
- Molecule 23: Cytochrome c oxidase subunit 2

Chain h: 83% 15% 2%



LEU
PRO
LYS
ILE
GLU
ASP
ARG
ALA
ASN
LEU
ILE
ALA
TYR
LEU
GLU
GLY
GLN
GLN

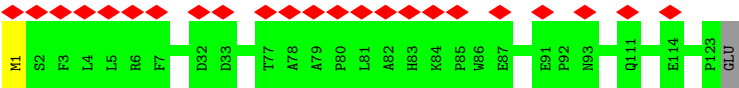
● Molecule 26: Cytochrome c, class I



LYS
ALA
CYS
HIS
LYS
LEU
ASP
GLY
ASN
ASP
GLY
VAL
GLY
GLY
PRO
HIS
LEU
GLY
ASN
GLY
VAL
VAL
VAL
GLY
ARG
THR
VAL
ALA
GLY
VAL
ASP
GLY
PHE
ASN
TYR
SER
ASP
PRO
MET
LYS
ALA
HIS
GLY
ASP
GLY
TRP
THR
PHE
PRO
GLU
ALA
THR
VAL
LEU
ALA
GLN
GLU
PHE
LEU
ASP
THR
ASN
PRO
ALA
LYS
VAL
VAL
PHE
GLY
LYS
CYS

GLY
THR
LYS
MET
ALA
PHE
ALA
GLY
LEU
PRO
LYS
ILE
GLU
ASP
ARG
ALA
ASN
LEU
TLE
ALA
TYR
LEU
GLU
GLY
GLN
GLN

● Molecule 27: NADH:ubiquinone oxidoreductase 17.2 kD subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99946	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.2	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	52.125	Depositor
Minimum map value	-28.966	Depositor
Average map value	0.036	Depositor
Map value standard deviation	1.388	Depositor
Recommended contour level	5.34	Depositor
Map size (Å)	393.0, 393.0, 393.0	wwPDB
Map dimensions	375, 375, 375	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGT, CA, 2MR, MN, CU, CUA, CDL, HEA, 3PE, PC1, T7X, DU0, HEC, HEM, FME, 3PH, FES, SF4, ZN, U10, FMN, P5S

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	0.23	0/988	0.50	0/1345
2	B	0.31	0/1297	0.57	0/1758
3	C	0.26	0/1624	0.56	0/2208
4	D	0.28	0/3339	0.55	0/4520
5	E	0.21	0/1865	0.51	0/2537
6	F	0.21	0/3308	0.52	0/4456
7	G	0.24	0/5156	0.53	0/6982
8	H	0.25	0/2815	0.54	0/3837
9	I	0.30	0/1354	0.57	0/1828
10	J	0.24	0/1548	0.56	0/2104
11	K	0.25	0/775	0.50	0/1050
12	L	0.21	0/5379	0.51	0/7323
13	M	0.23	0/4010	0.53	0/5460
14	N	0.24	0/3634	0.54	0/4935
15	P	0.22	0/2511	0.55	0/3409
16	Q	0.23	0/872	0.51	0/1181
17	R	0.20	0/503	0.50	0/685
18	Z	0.22	0/1669	0.57	0/2266
19	a	0.26	0/3641	0.52	0/4993
19	d	0.24	0/3650	0.51	0/5005
20	b	0.21	0/1906	0.47	0/2592
20	e	0.20	0/1906	0.53	0/2592
21	c	0.17	0/1382	0.44	0/1880
21	f	0.18	0/1390	0.46	0/1891
22	g	0.23	0/4483	0.54	0/6118
22	k	0.20	0/4483	0.53	0/6118
23	h	0.19	0/2033	0.51	0/2787
23	l	0.18	0/2033	0.51	0/2787
24	i	0.22	0/2270	0.49	0/3107
24	m	0.19	0/2270	0.49	0/3107
25	j	0.16	0/339	0.43	0/457

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
25	n	0.20	0/339	0.49	0/457
26	o	0.17	0/330	0.45	0/448
26	p	0.22	0/336	0.52	0/456
27	q	0.22	0/1049	0.51	0/1434
All	All	0.23	0/76487	0.52	0/104113

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
2	B	0	1
4	D	0	2
7	G	0	3
14	N	0	2
16	Q	0	3
19	a	0	1
22	g	0	1
22	k	0	1
All	All	0	14

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	134	ARG	Sidechain
4	D	163	ARG	Sidechain
4	D	250	ARG	Sidechain
7	G	223	ARG	Sidechain
7	G	280	ARG	Sidechain

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	969	0	970	6	0
2	B	1270	0	1268	4	0
3	C	1586	0	1562	2	0
4	D	3277	0	3217	9	0
5	E	1822	0	1796	6	0
6	F	3241	0	3188	16	0
7	G	5068	0	5037	8	0
8	H	2722	0	2744	7	0
9	I	1319	0	1259	2	0
10	J	1528	0	1612	6	0
11	K	764	0	817	5	0
12	L	5215	0	5174	7	0
13	M	3915	0	4024	20	0
14	N	3556	0	3656	9	0
15	P	2468	0	2498	3	0
16	Q	849	0	812	2	0
17	R	488	0	450	0	0
18	Z	1642	0	1643	2	0
19	a	3504	0	3483	8	0
19	d	3513	0	3489	11	0
20	b	1855	0	1773	3	0
20	e	1855	0	1773	3	0
21	c	1353	0	1297	6	0
21	f	1361	0	1301	4	0
22	g	4322	0	4225	16	0
22	k	4322	0	4225	23	0
23	h	1976	0	1960	3	0
23	l	1976	0	1960	3	0
24	i	2183	0	2144	7	0
24	m	2183	0	2144	9	0
25	j	332	0	331	1	0
25	n	332	0	331	0	0
26	o	324	0	330	0	0
26	p	330	0	335	2	0
27	q	1018	0	942	0	0
28	A	51	0	82	1	0
28	H	204	0	328	0	0
28	L	204	0	328	0	0
28	P	51	0	82	1	0
28	a	204	0	328	0	0
28	c	51	0	82	0	0
28	d	153	0	246	0	0
28	e	102	0	164	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	g	153	0	246	0	0
28	h	102	0	164	0	0
28	i	255	0	410	0	0
28	k	51	0	82	0	0
28	m	306	0	492	2	0
28	n	51	0	82	0	0
28	p	51	0	82	0	0
29	A	51	0	78	0	0
29	H	51	0	78	1	0
29	J	102	0	156	1	0
29	K	51	0	78	0	0
29	L	51	0	78	0	0
29	M	51	0	78	0	0
29	N	51	0	78	0	0
29	P	51	0	78	0	0
29	a	51	0	78	0	0
29	g	51	0	78	0	0
29	q	51	0	78	0	0
30	A	37	0	0	0	0
30	H	37	0	0	0	0
30	J	74	0	0	0	0
30	M	74	0	0	0	0
30	a	37	0	0	0	0
30	c	74	0	0	2	0
30	d	111	0	0	0	0
30	e	37	0	0	0	0
30	f	37	0	0	0	0
30	g	148	0	0	0	0
30	h	111	0	0	0	0
30	i	148	0	0	0	0
30	j	37	0	0	0	0
30	k	37	0	0	0	0
30	m	74	0	0	0	0
31	B	8	0	0	0	0
31	F	8	0	0	1	0
31	G	16	0	0	0	0
31	I	16	0	0	0	0
32	B	63	0	90	3	0
32	a	126	0	180	4	0
32	d	126	0	180	10	0
33	D	54	0	88	2	0
33	H	108	0	176	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	L	54	0	88	0	0
33	M	162	0	264	0	0
33	N	162	0	264	0	0
33	a	162	0	264	0	0
33	b	108	0	176	1	0
33	c	54	0	88	0	0
33	d	108	0	176	0	0
33	f	54	0	88	0	0
33	g	54	0	88	0	0
33	h	54	0	88	0	0
33	i	162	0	264	1	0
33	j	54	0	88	0	0
33	k	108	0	176	1	0
33	l	162	0	264	1	0
33	m	216	0	352	4	0
33	n	54	0	88	0	0
34	D	1	0	0	0	0
34	b	1	0	0	0	0
34	e	1	0	0	0	0
34	g	1	0	0	0	0
34	k	1	0	0	0	0
35	E	4	0	0	0	0
35	G	4	0	0	0	0
35	c	4	0	0	0	0
35	f	4	0	0	0	0
36	F	31	0	19	1	0
37	H	48	0	75	0	0
37	L	192	0	300	2	0
37	M	192	0	300	2	0
37	N	48	0	75	0	0
37	P	48	0	75	1	0
37	a	144	0	225	0	0
37	c	48	0	75	0	0
37	d	144	0	225	0	0
37	f	96	0	150	1	0
37	g	96	0	150	0	0
37	i	240	0	375	1	0
37	j	48	0	75	0	0
37	k	96	0	150	0	0
37	m	96	0	150	0	0
37	o	48	0	75	0	0
38	I	54	0	80	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	L	54	0	80	0	0
38	a	54	0	80	0	0
39	J	61	0	0	0	0
39	g	61	0	0	0	0
40	R	1	0	0	0	0
40	i	1	0	0	0	0
40	m	1	0	0	0	0
41	a	86	0	60	0	0
41	d	86	0	60	0	0
42	b	43	0	30	1	0
42	e	43	0	30	2	0
43	d	100	0	156	0	0
44	g	120	0	108	3	0
44	k	120	0	108	6	0
45	g	1	0	0	0	0
45	k	1	0	0	0	0
46	g	1	0	0	0	0
46	k	1	0	0	0	0
47	h	2	0	0	0	0
47	l	2	0	0	0	0
All	All	82894	0	84720	214	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 1.

The worst 5 of 214 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HD11	11:K:71:ALA:HB3	1.58	0.84
19:d:144:PHE:HB2	32:d:506:U10:H1M3	1.70	0.74
22:k:308:MET:HE3	22:k:357:SER:HB2	1.73	0.70
5:E:98:THR:HG22	5:E:99:THR:H	1.56	0.69
4:D:42:LEU:HB2	4:D:407:PHE:CZ	2.33	0.64

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	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
2	B	160/175 (91%)	153 (96%)	6 (4%)	1 (1%)	21	56
3	C	192/208 (92%)	188 (98%)	4 (2%)	0	100	100
4	D	408/412 (99%)	397 (97%)	11 (3%)	0	100	100
5	E	235/239 (98%)	225 (96%)	9 (4%)	1 (0%)	30	65
6	F	420/431 (97%)	404 (96%)	16 (4%)	0	100	100
7	G	663/674 (98%)	639 (96%)	23 (4%)	1 (0%)	43	76
8	H	339/345 (98%)	330 (97%)	9 (3%)	0	100	100
9	I	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
10	J	197/199 (99%)	192 (98%)	5 (2%)	0	100	100
11	K	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	45
12	L	657/703 (94%)	626 (95%)	31 (5%)	0	100	100
13	M	501/513 (98%)	493 (98%)	7 (1%)	1 (0%)	43	76
14	N	478/499 (96%)	468 (98%)	10 (2%)	0	100	100
15	P	326/330 (99%)	318 (98%)	8 (2%)	0	100	100
16	Q	101/103 (98%)	101 (100%)	0	0	100	100
17	R	59/62 (95%)	54 (92%)	5 (8%)	0	100	100
18	Z	214/217 (99%)	208 (97%)	6 (3%)	0	100	100
19	a	431/440 (98%)	424 (98%)	7 (2%)	0	100	100
19	d	432/440 (98%)	422 (98%)	10 (2%)	0	100	100
20	b	237/450 (53%)	235 (99%)	1 (0%)	1 (0%)	30	65
20	e	237/450 (53%)	231 (98%)	6 (2%)	0	100	100
21	c	178/195 (91%)	172 (97%)	6 (3%)	0	100	100
21	f	179/195 (92%)	175 (98%)	4 (2%)	0	100	100
22	g	542/558 (97%)	528 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	k	542/558 (97%)	526 (97%)	16 (3%)	0	100	100
23	h	250/298 (84%)	240 (96%)	10 (4%)	0	100	100
23	l	250/298 (84%)	239 (96%)	11 (4%)	0	100	100
24	i	271/274 (99%)	262 (97%)	9 (3%)	0	100	100
24	m	271/274 (99%)	259 (96%)	12 (4%)	0	100	100
25	j	41/66 (62%)	39 (95%)	2 (5%)	0	100	100
25	n	41/66 (62%)	40 (98%)	1 (2%)	0	100	100
26	o	40/176 (23%)	38 (95%)	2 (5%)	0	100	100
26	p	41/176 (23%)	41 (100%)	0	0	100	100
27	q	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
All	All	9432/10533 (90%)	9151 (97%)	275 (3%)	6 (0%)	49	80

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	137	CYS
13	M	238	VAL
20	b	369	ASN
7	G	263	VAL
2	B	122	GLY

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	97/97 (100%)	97 (100%)	0	100	100
2	B	136/145 (94%)	133 (98%)	3 (2%)	45	74
3	C	172/183 (94%)	172 (100%)	0	100	100
4	D	341/342 (100%)	341 (100%)	0	100	100
5	E	189/190 (100%)	189 (100%)	0	100	100
6	F	331/335 (99%)	330 (100%)	1 (0%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	530/535 (99%)	527 (99%)	3 (1%)	78	88
8	H	277/279 (99%)	277 (100%)	0	100	100
9	I	136/137 (99%)	136 (100%)	0	100	100
10	J	158/158 (100%)	158 (100%)	0	100	100
11	K	81/81 (100%)	80 (99%)	1 (1%)	63	82
12	L	520/543 (96%)	520 (100%)	0	100	100
13	M	410/416 (99%)	408 (100%)	2 (0%)	81	89
14	N	357/369 (97%)	356 (100%)	1 (0%)	86	91
15	P	248/250 (99%)	248 (100%)	0	100	100
16	Q	87/87 (100%)	87 (100%)	0	100	100
17	R	51/52 (98%)	51 (100%)	0	100	100
18	Z	167/168 (99%)	167 (100%)	0	100	100
19	a	360/366 (98%)	359 (100%)	1 (0%)	86	91
19	d	361/366 (99%)	361 (100%)	0	100	100
20	b	192/319 (60%)	192 (100%)	0	100	100
20	e	192/319 (60%)	192 (100%)	0	100	100
21	c	139/151 (92%)	138 (99%)	1 (1%)	76	86
21	f	140/151 (93%)	140 (100%)	0	100	100
22	g	447/454 (98%)	446 (100%)	1 (0%)	87	92
22	k	447/454 (98%)	447 (100%)	0	100	100
23	h	211/243 (87%)	210 (100%)	1 (0%)	81	89
23	l	211/243 (87%)	210 (100%)	1 (0%)	81	89
24	i	220/221 (100%)	220 (100%)	0	100	100
24	m	220/221 (100%)	219 (100%)	1 (0%)	81	89
25	j	34/53 (64%)	34 (100%)	0	100	100
25	n	34/53 (64%)	34 (100%)	0	100	100
26	o	33/126 (26%)	33 (100%)	0	100	100
26	p	34/126 (27%)	34 (100%)	0	100	100
27	q	103/104 (99%)	103 (100%)	0	100	100
All	All	7666/8337 (92%)	7649 (100%)	17 (0%)	85	92

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	h	102	HIS
24	m	258	VAL
11	K	25	ASN
13	M	365	HIS
13	M	471	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
19	a	192	ASN
22	k	457	ASN
20	e	372	GLN
22	k	269	HIS
23	l	252	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	FME	J	1	10	8,9,10	1.01	0	8,9,11	0.76	0
27	FME	q	1	27	8,9,10	0.95	0	8,9,11	0.98	1 (12%)
4	2MR	D	65	4	10,12,13	2.33	3 (30%)	5,13,15	0.85	0
13	FME	M	1	13	8,9,10	0.92	0	8,9,11	0.95	0
12	FME	L	1	12	8,9,10	0.99	0	8,9,11	0.80	0
1	FME	A	1	1	8,9,10	0.97	0	8,9,11	0.94	1 (12%)

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
10	FME	J	1	10	-	1/7/9/11	-
27	FME	q	1	27	-	0/7/9/11	-
4	2MR	D	65	4	-	0/10/13/15	-
13	FME	M	1	13	-	2/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	65	2MR	CZ-NH2	4.94	1.43	1.33
4	D	65	2MR	CZ-NE	4.35	1.43	1.34
4	D	65	2MR	CQ1-NH1	-2.20	1.42	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	C-CA-N	2.02	113.40	109.50
27	q	1	FME	C-CA-N	2.01	113.38	109.50

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
10	J	1	FME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
12	L	1	FME	C-CA-CB-CG
1	A	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 194 ligands modelled in this entry, 12 are monoatomic - leaving 182 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
28	3PE	i	309	-	50,50,50	0.95	4 (8%)	53,55,55	0.95	3 (5%)
37	3PH	d	502	-	47,47,47	1.37	5 (10%)	50,52,52	1.06	4 (8%)
44	HEA	k	605	22	67,67,67	1.30	5 (7%)	81,103,103	2.20	28 (34%)
28	3PE	a	502	-	50,50,50	0.97	4 (8%)	53,55,55	1.09	4 (7%)
28	3PE	P	403	-	50,50,50	0.98	4 (8%)	53,55,55	1.03	2 (3%)
29	PGT	N	505	-	50,50,50	0.93	4 (8%)	53,56,56	0.93	3 (5%)
33	PC1	H	403	-	53,53,53	0.96	3 (5%)	59,61,61	0.83	1 (1%)
33	PC1	i	308	-	53,53,53	0.96	3 (5%)	59,61,61	0.93	3 (5%)
28	3PE	m	310	-	50,50,50	0.97	4 (8%)	53,55,55	1.06	4 (7%)
29	PGT	K	201	-	50,50,50	0.91	4 (8%)	53,56,56	0.84	2 (3%)
37	3PH	m	309	-	47,47,47	1.38	5 (10%)	50,52,52	1.03	6 (12%)
33	PC1	l	301	-	53,53,53	0.99	3 (5%)	59,61,61	0.87	2 (3%)
37	3PH	k	607	-	47,47,47	1.37	5 (10%)	50,52,52	1.05	4 (8%)
38	P5S	L	809	-	52,53,53	0.94	3 (5%)	54,60,60	0.80	3 (5%)
31	SF4	I	202	9	0,12,12	-	-	-	-	-
37	3PH	L	807	-	47,47,47	1.35	5 (10%)	50,52,52	1.10	5 (10%)
30	DU0	m	313	-	42,42,42	0.64	0	64,66,66	0.95	1 (1%)
29	PGT	M	602	-	50,50,50	0.94	4 (8%)	53,56,56	0.87	4 (7%)
30	DU0	i	316	-	42,42,42	0.61	0	64,66,66	0.85	1 (1%)
31	SF4	B	1001	2	0,12,12	-	-	-	-	-
33	PC1	N	501	-	53,53,53	0.97	3 (5%)	59,61,61	0.88	3 (5%)
33	PC1	d	516	-	53,53,53	0.95	3 (5%)	59,61,61	0.88	3 (5%)
42	HEC	e	504	20	46,50,50	1.86	4 (8%)	58,82,82	1.55	7 (12%)
30	DU0	a	516	-	42,42,42	0.66	0	64,66,66	0.92	3 (4%)
30	DU0	c	202	-	42,42,42	0.66	0	64,66,66	0.85	2 (3%)
29	PGT	J	205	-	50,50,50	0.93	4 (8%)	53,56,56	0.80	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DU0	g	617	-	42,42,42	0.66	0	64,66,66	1.13	5 (7%)
30	DU0	M	607	-	42,42,42	0.66	0	64,66,66	0.81	1 (1%)
28	3PE	p	1001	-	50,50,50	0.98	4 (8%)	53,55,55	0.99	3 (5%)
28	3PE	A	201	-	50,50,50	0.97	4 (8%)	53,55,55	1.04	4 (7%)
28	3PE	m	304	-	50,50,50	0.98	4 (8%)	53,55,55	0.98	2 (3%)
30	DU0	e	503	-	42,42,42	0.62	0	64,66,66	0.70	1 (1%)
30	DU0	h	306	-	42,42,42	0.63	0	64,66,66	0.68	0
30	DU0	d	512	-	42,42,42	0.63	0	64,66,66	0.75	1 (1%)
37	3PH	f	203	-	47,47,47	1.39	6 (12%)	50,52,52	0.98	4 (8%)
37	3PH	d	508	-	47,47,47	1.38	5 (10%)	50,52,52	1.02	5 (10%)
37	3PH	i	303	-	47,47,47	1.38	5 (10%)	50,52,52	0.98	4 (8%)
30	DU0	g	604	-	42,42,42	0.72	1 (2%)	64,66,66	0.91	4 (6%)
37	3PH	i	314	-	47,47,47	1.38	6 (12%)	50,52,52	1.06	5 (10%)
41	HEM	a	515	19	50,50,50	1.29	6 (12%)	67,82,82	1.07	3 (4%)
37	3PH	f	205	-	47,47,47	1.38	5 (10%)	50,52,52	1.08	4 (8%)
37	3PH	g	611	-	47,47,47	1.37	5 (10%)	50,52,52	1.05	4 (8%)
33	PC1	m	303	-	53,53,53	0.94	3 (5%)	59,61,61	0.98	2 (3%)
37	3PH	M	605	-	47,47,47	1.39	5 (10%)	50,52,52	0.97	5 (10%)
28	3PE	H	405	-	50,50,50	0.96	4 (8%)	53,55,55	1.03	4 (7%)
28	3PE	L	806	-	50,50,50	0.96	4 (8%)	53,55,55	1.03	4 (7%)
33	PC1	a	507	-	53,53,53	0.96	3 (5%)	59,61,61	0.88	3 (5%)
33	PC1	k	606	-	53,53,53	0.96	3 (5%)	59,61,61	0.86	2 (3%)
33	PC1	m	312	-	53,53,53	0.96	3 (5%)	59,61,61	0.86	3 (5%)
42	HEC	b	502	20	46,50,50	1.84	3 (6%)	58,82,82	1.66	6 (10%)
29	PGT	g	602	-	50,50,50	0.94	4 (8%)	53,56,56	1.12	5 (9%)
38	P5S	a	513	-	52,53,53	0.93	3 (5%)	54,60,60	0.88	3 (5%)
30	DU0	H	401	-	42,42,42	0.64	0	64,66,66	0.77	1 (1%)
28	3PE	L	802	-	50,50,50	0.95	4 (8%)	53,55,55	0.99	3 (5%)
29	PGT	H	406	-	50,50,50	0.91	4 (8%)	53,56,56	1.16	4 (7%)
33	PC1	d	509	-	53,53,53	0.96	3 (5%)	59,61,61	0.81	1 (1%)
28	3PE	m	305	-	50,50,50	0.96	4 (8%)	53,55,55	0.98	3 (5%)
37	3PH	o	201	-	47,47,47	1.37	5 (10%)	50,52,52	1.01	5 (10%)
28	3PE	a	508	-	50,50,50	0.97	4 (8%)	53,55,55	1.01	2 (3%)
30	DU0	h	304	-	42,42,42	0.69	1 (2%)	64,66,66	1.49	12 (18%)
28	3PE	g	613	-	50,50,50	0.98	4 (8%)	53,55,55	1.09	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DU0	m	302	-	42,42,42	0.67	0	64,66,66	0.88	2 (3%)
33	PC1	n	1001	-	53,53,53	0.96	3 (5%)	59,61,61	0.88	2 (3%)
28	3PE	h	307	-	50,50,50	0.95	4 (8%)	53,55,55	0.97	3 (5%)
33	PC1	a	501	-	53,53,53	0.98	3 (5%)	59,61,61	0.81	1 (1%)
35	FES	c	204	21	0,4,4	-	-	-		
41	HEM	a	505	19	50,50,50	1.30	6 (12%)	67,82,82	1.12	5 (7%)
28	3PE	n	1002	-	50,50,50	0.97	4 (8%)	53,55,55	0.92	2 (3%)
37	3PH	i	318	-	47,47,47	1.36	5 (10%)	50,52,52	1.05	6 (12%)
30	DU0	J	204	-	42,42,42	0.66	0	64,66,66	0.95	3 (4%)
28	3PE	i	311	-	50,50,50	0.98	4 (8%)	53,55,55	1.01	2 (3%)
28	3PE	H	407	-	50,50,50	0.98	4 (8%)	53,55,55	0.91	3 (5%)
37	3PH	m	301	-	47,47,47	1.38	5 (10%)	50,52,52	1.04	4 (8%)
37	3PH	H	409	-	47,47,47	1.37	5 (10%)	50,52,52	1.01	5 (10%)
47	CUA	h	305	23	0,1,1	-	-	-		
28	3PE	d	510	-	50,50,50	0.97	4 (8%)	53,55,55	1.01	2 (3%)
30	DU0	k	608	-	42,42,42	0.64	0	64,66,66	0.88	1 (1%)
33	PC1	H	402	-	53,53,53	0.97	3 (5%)	59,61,61	0.90	2 (3%)
35	FES	f	204	21	0,4,4	-	-	-		
32	U10	a	512	-	63,63,63	0.68	0	78,79,79	0.99	2 (2%)
41	HEM	d	514	19	50,50,50	1.29	7 (14%)	67,82,82	1.17	5 (7%)
37	3PH	j	1003	-	47,47,47	1.37	5 (10%)	50,52,52	1.12	5 (10%)
39	T7X	g	615	-	61,61,61	0.94	4 (6%)	70,73,73	0.83	2 (2%)
33	PC1	f	201	-	53,53,53	0.94	3 (5%)	59,61,61	0.94	3 (5%)
32	U10	d	506	-	63,63,63	0.71	1 (1%)	78,79,79	1.21	2 (2%)
37	3PH	i	301	-	47,47,47	1.38	5 (10%)	50,52,52	1.01	5 (10%)
30	DU0	i	305	-	42,42,42	0.61	0	64,66,66	0.78	2 (3%)
33	PC1	M	608	-	53,53,53	0.96	3 (5%)	59,61,61	0.88	3 (5%)
37	3PH	g	603	-	47,47,47	1.39	6 (12%)	50,52,52	1.08	5 (10%)
28	3PE	H	404	-	50,50,50	0.96	4 (8%)	53,55,55	0.97	2 (3%)
29	PGT	A	202	-	50,50,50	0.95	4 (8%)	53,56,56	0.82	1 (1%)
33	PC1	D	1001	-	53,53,53	0.96	3 (5%)	59,61,61	0.91	3 (5%)
30	DU0	d	505	-	42,42,42	0.66	0	64,66,66	0.75	1 (1%)
28	3PE	c	201	-	50,50,50	0.97	4 (8%)	53,55,55	1.09	3 (5%)
28	3PE	g	601	-	50,50,50	0.96	4 (8%)	53,55,55	0.99	3 (5%)
28	3PE	m	306	-	50,50,50	0.97	4 (8%)	53,55,55	1.02	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	3PE	e	505	-	50,50,50	0.96	4 (8%)	53,55,55	0.97	2 (3%)
30	DU0	h	303	-	42,42,42	0.60	0	64,66,66	0.75	0
28	3PE	m	315	-	50,50,50	0.96	4 (8%)	53,55,55	0.99	1 (1%)
28	3PE	a	509	-	50,50,50	0.97	4 (8%)	53,55,55	0.93	1 (1%)
30	DU0	i	315	-	42,42,42	0.64	0	64,66,66	0.88	3 (4%)
33	PC1	b	501	-	53,53,53	0.96	3 (5%)	59,61,61	0.86	2 (3%)
30	DU0	c	205	-	42,42,42	0.67	0	64,66,66	1.16	7 (10%)
37	3PH	M	604	-	47,47,47	1.39	5 (10%)	50,52,52	1.06	5 (10%)
31	SF4	F	501	6	0,12,12	-	-	-	-	-
33	PC1	m	314	-	53,53,53	0.96	3 (5%)	59,61,61	0.87	1 (1%)
37	3PH	L	801	-	47,47,47	1.38	5 (10%)	50,52,52	1.01	4 (8%)
30	DU0	d	511	-	42,42,42	0.60	0	64,66,66	0.79	1 (1%)
31	SF4	G	703	7	0,12,12	-	-	-	-	-
30	DU0	j	1002	-	42,42,42	0.64	0	64,66,66	0.88	2 (3%)
37	3PH	L	810	-	47,47,47	1.38	5 (10%)	50,52,52	1.05	4 (8%)
37	3PH	a	506	-	47,47,47	1.37	5 (10%)	50,52,52	1.02	4 (8%)
30	DU0	f	202	-	42,42,42	0.68	0	64,66,66	0.87	2 (3%)
31	SF4	I	203	9	0,12,12	-	-	-	-	-
28	3PE	L	808	-	50,50,50	0.99	4 (8%)	53,55,55	0.97	3 (5%)
33	PC1	b	504	-	53,53,53	0.96	3 (5%)	59,61,61	0.87	3 (5%)
28	3PE	h	301	-	50,50,50	0.97	4 (8%)	53,55,55	0.94	3 (5%)
30	DU0	A	203	-	42,42,42	0.63	0	64,66,66	0.89	4 (6%)
32	U10	a	511	-	63,63,63	0.68	0	78,79,79	0.96	4 (5%)
38	P5S	I	201	-	52,53,53	0.94	3 (5%)	54,60,60	0.94	4 (7%)
44	HEA	g	610	22	67,67,67	1.29	7 (10%)	81,103,103	2.22	27 (33%)
37	3PH	c	206	-	47,47,47	1.38	5 (10%)	50,52,52	1.06	6 (12%)
43	CDL	d	501	-	99,99,99	0.92	7 (7%)	105,111,111	0.96	5 (4%)
29	PGT	a	514	-	50,50,50	0.91	4 (8%)	53,56,56	0.86	2 (3%)
44	HEA	g	606	22	67,67,67	1.32	9 (13%)	81,103,103	2.26	29 (35%)
28	3PE	i	306	-	50,50,50	0.98	4 (8%)	53,55,55	0.98	4 (7%)
37	3PH	a	510	-	47,47,47	1.38	5 (10%)	50,52,52	1.01	4 (8%)
30	DU0	g	616	-	42,42,42	0.62	0	64,66,66	1.13	5 (7%)
44	HEA	k	604	22	67,67,67	1.33	7 (10%)	81,103,103	2.22	27 (33%)
32	U10	d	504	-	63,63,63	0.66	0	78,79,79	0.94	2 (2%)
35	FES	E	401	5	0,4,4	-	-	-	-	-
28	3PE	d	503	-	50,50,50	0.95	4 (8%)	53,55,55	0.98	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	T7X	J	202	-	61,61,61	0.96	4 (6%)	70,73,73	0.96	5 (7%)
35	FES	G	701	7	0,4,4	-	-	-		
33	PC1	c	203	-	53,53,53	0.97	3 (5%)	59,61,61	0.86	2 (3%)
33	PC1	M	609	-	53,53,53	0.96	3 (5%)	59,61,61	0.88	3 (5%)
33	PC1	i	313	-	53,53,53	0.96	3 (5%)	59,61,61	0.98	4 (6%)
28	3PE	L	805	-	50,50,50	0.95	4 (8%)	53,55,55	1.03	2 (3%)
30	DU0	J	203	-	42,42,42	0.66	0	64,66,66	0.68	0
37	3PH	M	603	-	47,47,47	1.38	5 (10%)	50,52,52	1.00	4 (8%)
28	3PE	H	408	-	50,50,50	0.96	4 (8%)	53,55,55	0.97	3 (5%)
36	FMN	F	502	-	33,33,33	1.06	2 (6%)	48,50,50	1.29	8 (16%)
33	PC1	M	601	-	53,53,53	0.98	3 (5%)	59,61,61	0.85	1 (1%)
37	3PH	i	304	-	47,47,47	1.37	5 (10%)	50,52,52	1.00	3 (6%)
30	DU0	M	610	-	42,42,42	0.65	0	64,66,66	0.82	2 (3%)
29	PGT	q	1000	-	50,50,50	0.94	4 (8%)	53,56,56	0.84	2 (3%)
33	PC1	l	303	-	53,53,53	0.96	3 (5%)	59,61,61	0.89	2 (3%)
28	3PE	i	317	-	50,50,50	0.97	4 (8%)	53,55,55	0.98	3 (5%)
30	DU0	g	605	-	42,42,42	0.62	0	64,66,66	0.89	3 (4%)
33	PC1	j	1001	-	53,53,53	0.96	3 (5%)	59,61,61	0.92	4 (6%)
37	3PH	L	811	-	47,47,47	1.37	5 (10%)	50,52,52	1.09	6 (12%)
37	3PH	N	503	-	47,47,47	1.39	6 (12%)	50,52,52	1.02	4 (8%)
33	PC1	l	304	-	53,53,53	0.97	3 (5%)	59,61,61	0.95	3 (5%)
29	PGT	J	201	-	50,50,50	0.93	4 (8%)	53,56,56	0.91	4 (7%)
28	3PE	i	307	-	50,50,50	0.97	4 (8%)	53,55,55	1.18	4 (7%)
29	PGT	P	401	-	50,50,50	0.94	4 (8%)	53,56,56	0.82	2 (3%)
28	3PE	g	607	-	50,50,50	0.97	4 (8%)	53,55,55	0.96	1 (1%)
28	3PE	k	603	-	50,50,50	0.97	4 (8%)	53,55,55	0.97	2 (3%)
33	PC1	k	609	-	53,53,53	0.96	3 (5%)	59,61,61	0.84	2 (3%)
33	PC1	L	803	-	53,53,53	0.97	3 (5%)	59,61,61	0.95	3 (5%)
37	3PH	a	504	-	47,47,47	1.38	5 (10%)	50,52,52	1.10	6 (12%)
32	U10	B	1002	-	63,63,63	0.69	0	78,79,79	1.14	4 (5%)
33	PC1	m	311	-	53,53,53	0.96	3 (5%)	59,61,61	0.86	2 (3%)
33	PC1	N	504	-	53,53,53	0.98	3 (5%)	59,61,61	0.88	2 (3%)
28	3PE	e	502	-	50,50,50	0.97	4 (8%)	53,55,55	0.98	2 (3%)
30	DU0	i	302	-	42,42,42	0.67	0	64,66,66	0.87	2 (3%)
31	SF4	G	702	7	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	PC1	h	302	-	53,53,53	0.98	3 (5%)	59,61,61	0.93	3 (5%)
41	HEM	d	507	19	50,50,50	1.31	6 (12%)	67,82,82	1.06	3 (4%)
33	PC1	g	612	-	53,53,53	0.96	3 (5%)	59,61,61	0.89	4 (6%)
33	PC1	a	517	-	53,53,53	0.98	3 (5%)	59,61,61	0.88	2 (3%)
37	3PH	P	402	-	47,47,47	1.38	5 (10%)	50,52,52	1.11	5 (10%)
28	3PE	d	515	-	50,50,50	0.98	4 (8%)	53,55,55	0.94	4 (7%)
37	3PH	M	606	-	47,47,47	1.37	5 (10%)	50,52,52	0.99	3 (6%)
37	3PH	k	601	-	47,47,47	1.41	5 (10%)	50,52,52	1.01	3 (6%)
33	PC1	i	310	-	53,53,53	0.96	3 (5%)	59,61,61	0.90	1 (1%)
29	PGT	L	804	-	50,50,50	0.94	4 (8%)	53,56,56	1.13	5 (9%)
37	3PH	d	513	-	47,47,47	1.37	5 (10%)	50,52,52	1.03	4 (8%)
47	CUA	l	302	23	0,1,1	-	-	-	-	-
28	3PE	m	307	-	50,50,50	0.97	4 (8%)	53,55,55	0.97	2 (3%)
33	PC1	N	502	-	53,53,53	0.96	3 (5%)	59,61,61	0.84	2 (3%)
28	3PE	a	503	-	50,50,50	0.97	4 (8%)	53,55,55	0.94	4 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	3PE	i	309	-	-	15/54/54/54	-
37	3PH	d	502	-	-	6/49/49/49	-
44	HEA	k	605	22	-	6/36/76/76	-
28	3PE	a	502	-	-	10/54/54/54	-
28	3PE	P	403	-	-	10/54/54/54	-
29	PGT	N	505	-	-	11/55/55/55	-
33	PC1	H	403	-	-	6/57/57/57	-
33	PC1	i	308	-	-	11/57/57/57	-
28	3PE	m	310	-	-	9/54/54/54	-
29	PGT	K	201	-	-	9/55/55/55	-
37	3PH	m	309	-	-	7/49/49/49	-
33	PC1	l	301	-	-	11/57/57/57	-
37	3PH	k	607	-	-	8/49/49/49	-
38	P5S	L	809	-	-	5/59/59/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SF4	I	202	9	-	-	0/6/5/5
37	3PH	L	807	-	-	4/49/49/49	-
30	DU0	m	313	-	-	1/10/98/98	0/6/6/6
29	PGT	M	602	-	-	10/55/55/55	-
30	DU0	i	316	-	-	0/10/98/98	0/6/6/6
33	PC1	N	501	-	-	11/57/57/57	-
31	SF4	B	1001	2	-	-	0/6/5/5
33	PC1	d	516	-	-	7/57/57/57	-
42	HEC	e	504	20	-	8/14/54/54	-
30	DU0	a	516	-	-	2/10/98/98	0/6/6/6
30	DU0	c	202	-	-	2/10/98/98	0/6/6/6
29	PGT	J	205	-	-	13/55/55/55	-
30	DU0	g	617	-	-	5/10/98/98	0/6/6/6
30	DU0	M	607	-	-	0/10/98/98	0/6/6/6
28	3PE	p	1001	-	-	8/54/54/54	-
28	3PE	A	201	-	-	17/54/54/54	-
28	3PE	m	304	-	-	5/54/54/54	-
30	DU0	e	503	-	-	0/10/98/98	0/6/6/6
30	DU0	h	306	-	-	2/10/98/98	0/6/6/6
30	DU0	d	512	-	-	0/10/98/98	0/6/6/6
37	3PH	f	203	-	-	9/49/49/49	-
37	3PH	d	508	-	-	7/49/49/49	-
37	3PH	i	303	-	-	7/49/49/49	-
30	DU0	g	604	-	-	0/10/98/98	0/6/6/6
37	3PH	i	314	-	-	10/49/49/49	-
41	HEM	a	515	19	-	6/14/54/54	-
37	3PH	f	205	-	-	12/49/49/49	-
37	3PH	g	611	-	-	8/49/49/49	-
33	PC1	m	303	-	-	11/57/57/57	-
37	3PH	M	605	-	-	5/49/49/49	-
28	3PE	H	405	-	-	14/54/54/54	-
28	3PE	L	806	-	-	10/54/54/54	-
33	PC1	a	507	-	-	16/57/57/57	-
33	PC1	k	606	-	-	10/57/57/57	-
33	PC1	m	312	-	-	12/57/57/57	-
42	HEC	b	502	20	-	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PGT	g	602	-	-	13/55/55/55	-
38	P5S	a	513	-	-	7/59/59/59	-
30	DU0	H	401	-	-	1/10/98/98	0/6/6/6
28	3PE	L	802	-	-	9/54/54/54	-
29	PGT	H	406	-	-	10/55/55/55	-
33	PC1	d	509	-	-	7/57/57/57	-
28	3PE	m	305	-	-	10/54/54/54	-
37	3PH	o	201	-	-	6/49/49/49	-
28	3PE	a	508	-	-	13/54/54/54	-
30	DU0	h	304	-	-	0/10/98/98	0/6/6/6
28	3PE	g	613	-	-	13/54/54/54	-
30	DU0	m	302	-	-	1/10/98/98	0/6/6/6
33	PC1	n	1001	-	-	15/57/57/57	-
28	3PE	h	307	-	-	13/54/54/54	-
33	PC1	a	501	-	-	11/57/57/57	-
35	FES	c	204	21	-	-	0/1/1/1
41	HEM	a	505	19	-	6/14/54/54	-
28	3PE	n	1002	-	-	9/54/54/54	-
37	3PH	i	318	-	-	9/49/49/49	-
30	DU0	J	204	-	-	2/10/98/98	0/6/6/6
28	3PE	i	311	-	-	6/54/54/54	-
28	3PE	H	407	-	-	12/54/54/54	-
37	3PH	m	301	-	-	5/49/49/49	-
37	3PH	H	409	-	-	4/49/49/49	-
28	3PE	d	510	-	-	10/54/54/54	-
30	DU0	k	608	-	-	1/10/98/98	0/6/6/6
33	PC1	H	402	-	-	13/57/57/57	-
35	FES	f	204	21	-	-	0/1/1/1
32	U10	a	512	-	-	8/63/87/87	0/1/1/1
41	HEM	d	514	19	-	8/14/54/54	-
37	3PH	j	1003	-	-	6/49/49/49	-
39	T7X	g	615	-	-	12/56/80/80	0/1/1/1
33	PC1	f	201	-	-	19/57/57/57	-
32	U10	d	506	-	-	6/63/87/87	0/1/1/1
37	3PH	i	301	-	-	12/49/49/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DU0	i	305	-	-	1/10/98/98	0/6/6/6
33	PC1	M	608	-	-	11/57/57/57	-
37	3PH	g	603	-	-	12/49/49/49	-
28	3PE	H	404	-	-	8/54/54/54	-
29	PGT	A	202	-	-	12/55/55/55	-
33	PC1	D	1001	-	-	9/57/57/57	-
30	DU0	d	505	-	-	1/10/98/98	0/6/6/6
28	3PE	c	201	-	-	14/54/54/54	-
28	3PE	g	601	-	-	12/54/54/54	-
28	3PE	m	306	-	-	11/54/54/54	-
28	3PE	e	505	-	-	15/54/54/54	-
30	DU0	h	303	-	-	0/10/98/98	0/6/6/6
28	3PE	m	315	-	-	12/54/54/54	-
28	3PE	a	509	-	-	9/54/54/54	-
30	DU0	i	315	-	-	0/10/98/98	0/6/6/6
33	PC1	b	501	-	-	12/57/57/57	-
30	DU0	c	205	-	-	2/10/98/98	0/6/6/6
37	3PH	M	604	-	-	13/49/49/49	-
33	PC1	m	314	-	-	12/57/57/57	-
31	SF4	F	501	6	-	-	0/6/5/5
37	3PH	L	801	-	-	8/49/49/49	-
30	DU0	d	511	-	-	1/10/98/98	0/6/6/6
37	3PH	L	810	-	-	13/49/49/49	-
30	DU0	j	1002	-	-	0/10/98/98	0/6/6/6
31	SF4	G	703	7	-	-	0/6/5/5
37	3PH	a	506	-	-	9/49/49/49	-
30	DU0	f	202	-	-	1/10/98/98	0/6/6/6
31	SF4	I	203	9	-	-	0/6/5/5
28	3PE	L	808	-	-	15/54/54/54	-
33	PC1	b	504	-	-	11/57/57/57	-
28	3PE	h	301	-	-	15/54/54/54	-
30	DU0	A	203	-	-	0/10/98/98	0/6/6/6
32	U10	a	511	-	-	10/63/87/87	0/1/1/1
38	P5S	I	201	-	-	18/59/59/59	-
44	HEA	g	610	22	-	7/36/76/76	-
37	3PH	c	206	-	-	7/49/49/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	CDL	d	501	-	-	28/110/110/110	-
29	PGT	a	514	-	-	5/55/55/55	-
44	HEA	g	606	22	-	5/36/76/76	-
28	3PE	i	306	-	-	14/54/54/54	-
37	3PH	a	510	-	-	6/49/49/49	-
30	DU0	g	616	-	-	1/10/98/98	0/6/6/6
44	HEA	k	604	22	-	6/36/76/76	-
32	U10	d	504	-	-	8/63/87/87	0/1/1/1
35	FES	E	401	5	-	-	0/1/1/1
28	3PE	d	503	-	-	15/54/54/54	-
39	T7X	J	202	-	-	9/56/80/80	0/1/1/1
35	FES	G	701	7	-	-	0/1/1/1
33	PC1	c	203	-	-	13/57/57/57	-
33	PC1	M	609	-	-	9/57/57/57	-
33	PC1	i	313	-	-	17/57/57/57	-
28	3PE	L	805	-	-	12/54/54/54	-
30	DU0	J	203	-	-	0/10/98/98	0/6/6/6
37	3PH	M	603	-	-	7/49/49/49	-
28	3PE	H	408	-	-	7/54/54/54	-
36	FMN	F	502	-	-	1/18/18/18	0/3/3/3
33	PC1	M	601	-	-	6/57/57/57	-
37	3PH	i	304	-	-	7/49/49/49	-
30	DU0	M	610	-	-	0/10/98/98	0/6/6/6
29	PGT	q	1000	-	-	12/55/55/55	-
33	PC1	l	303	-	-	10/57/57/57	-
28	3PE	i	317	-	-	19/54/54/54	-
30	DU0	g	605	-	-	0/10/98/98	0/6/6/6
33	PC1	j	1001	-	-	10/57/57/57	-
37	3PH	L	811	-	-	9/49/49/49	-
37	3PH	N	503	-	-	6/49/49/49	-
33	PC1	l	304	-	-	16/57/57/57	-
29	PGT	J	201	-	-	10/55/55/55	-
28	3PE	i	307	-	-	16/54/54/54	-
29	PGT	P	401	-	-	17/55/55/55	-
28	3PE	g	607	-	-	7/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	3PE	k	603	-	-	9/54/54/54	-
33	PC1	k	609	-	-	15/57/57/57	-
33	PC1	L	803	-	-	18/57/57/57	-
37	3PH	a	504	-	-	7/49/49/49	-
32	U10	B	1002	-	-	13/63/87/87	0/1/1/1
33	PC1	m	311	-	-	11/57/57/57	-
33	PC1	N	504	-	-	10/57/57/57	-
28	3PE	e	502	-	-	8/54/54/54	-
30	DU0	i	302	-	-	0/10/98/98	0/6/6/6
31	SF4	G	702	7	-	-	0/6/5/5
33	PC1	h	302	-	-	15/57/57/57	-
41	HEM	d	507	19	-	7/14/54/54	-
33	PC1	g	612	-	-	9/57/57/57	-
33	PC1	a	517	-	-	16/57/57/57	-
37	3PH	P	402	-	-	14/49/49/49	-
28	3PE	d	515	-	-	8/54/54/54	-
37	3PH	M	606	-	-	10/49/49/49	-
37	3PH	k	601	-	-	11/49/49/49	-
33	PC1	i	310	-	-	13/57/57/57	-
29	PGT	L	804	-	-	13/55/55/55	-
37	3PH	d	513	-	-	11/49/49/49	-
28	3PE	m	307	-	-	17/54/54/54	-
33	PC1	N	502	-	-	13/57/57/57	-
28	3PE	a	503	-	-	13/54/54/54	-

The worst 5 of 567 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	k	601	3PH	P-O11	7.68	1.84	1.60
37	M	605	3PH	P-O11	7.50	1.84	1.60
37	i	301	3PH	P-O11	7.46	1.83	1.60
37	M	604	3PH	P-O11	7.45	1.83	1.60
37	f	203	3PH	P-O11	7.45	1.83	1.60

The worst 5 of 632 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	506	U10	C6-C1-C2	7.42	125.02	119.17
42	b	502	HEC	CBC-CAC-C3C	-6.38	114.68	127.43
44	k	604	HEA	C3A-C2A-C1A	-6.28	101.10	107.05
44	g	606	HEA	C3A-C2A-C1A	-6.23	101.15	107.05
42	e	504	HEC	CBB-CAB-C3B	-6.00	115.45	127.43

There are no chirality outliers.

5 of 1491 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	201	3PE	C1-O11-P-O14
28	A	201	3PE	C11-O13-P-O12
28	H	404	3PE	C1-O11-P-O12
28	H	404	3PE	C11-O13-P-O14
28	H	404	3PE	C2-C1-O11-P

There are no ring outliers.

33 monomers are involved in 53 short contacts:

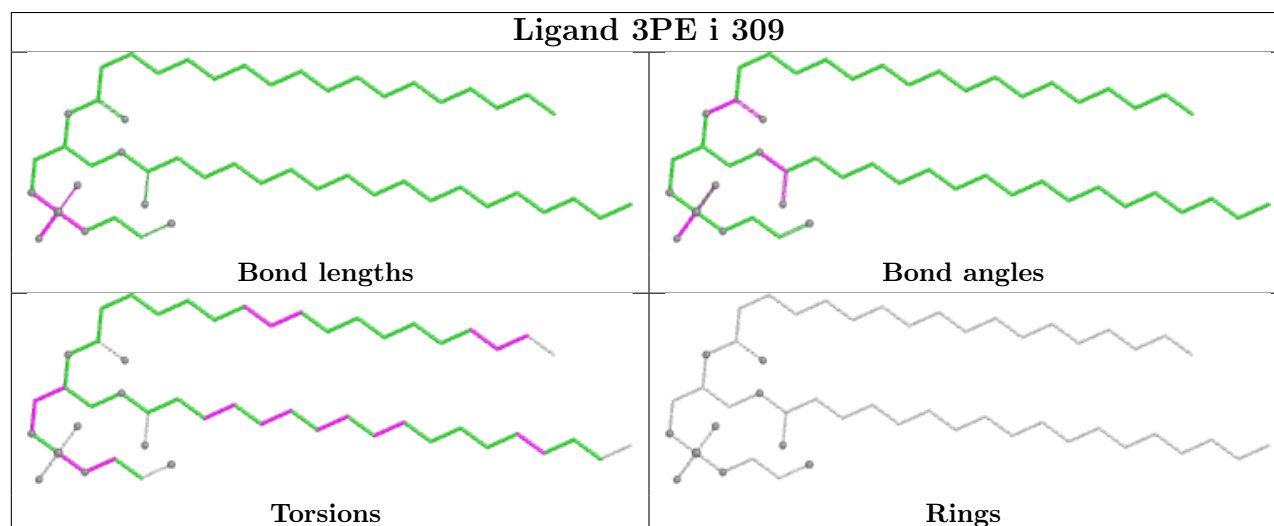
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	k	605	HEA	1	0
28	P	403	3PE	1	0
28	m	310	3PE	1	0
42	e	504	HEC	2	0
30	c	202	DU0	1	0
28	A	201	3PE	1	0
37	f	205	3PH	1	0
42	b	502	HEC	1	0
29	H	406	PGT	1	0
33	H	402	PC1	2	0
32	a	512	U10	3	0
32	d	506	U10	9	0
37	i	301	3PH	1	0
33	D	1001	PC1	2	0
28	m	315	3PE	1	0
33	b	501	PC1	1	0
30	c	205	DU0	1	0
37	M	604	3PH	2	0
31	F	501	SF4	1	0
32	a	511	U10	1	0
44	g	610	HEA	1	0
44	g	606	HEA	2	0

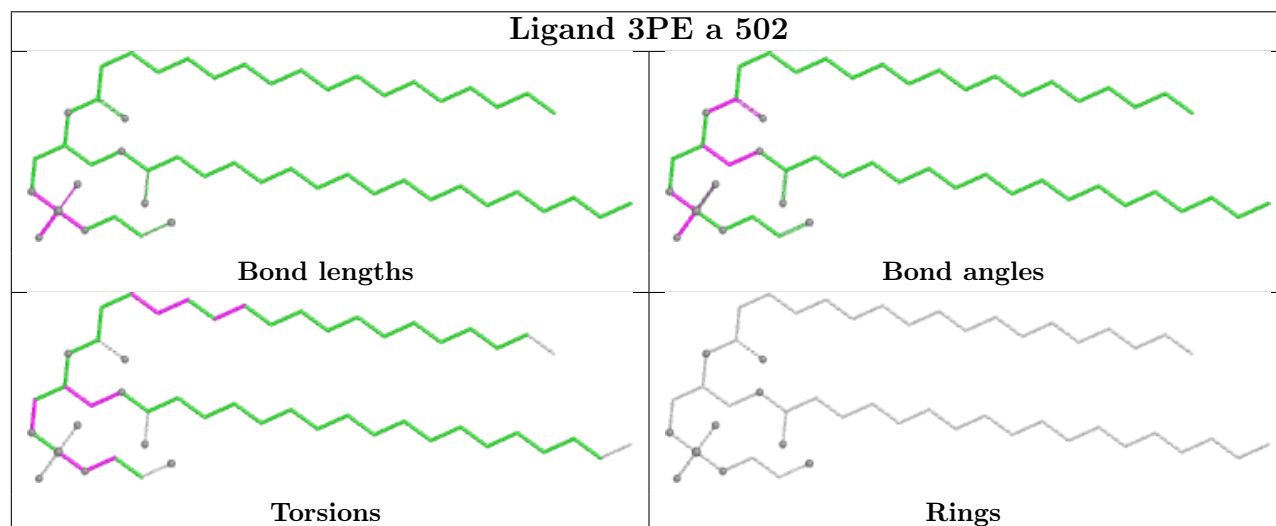
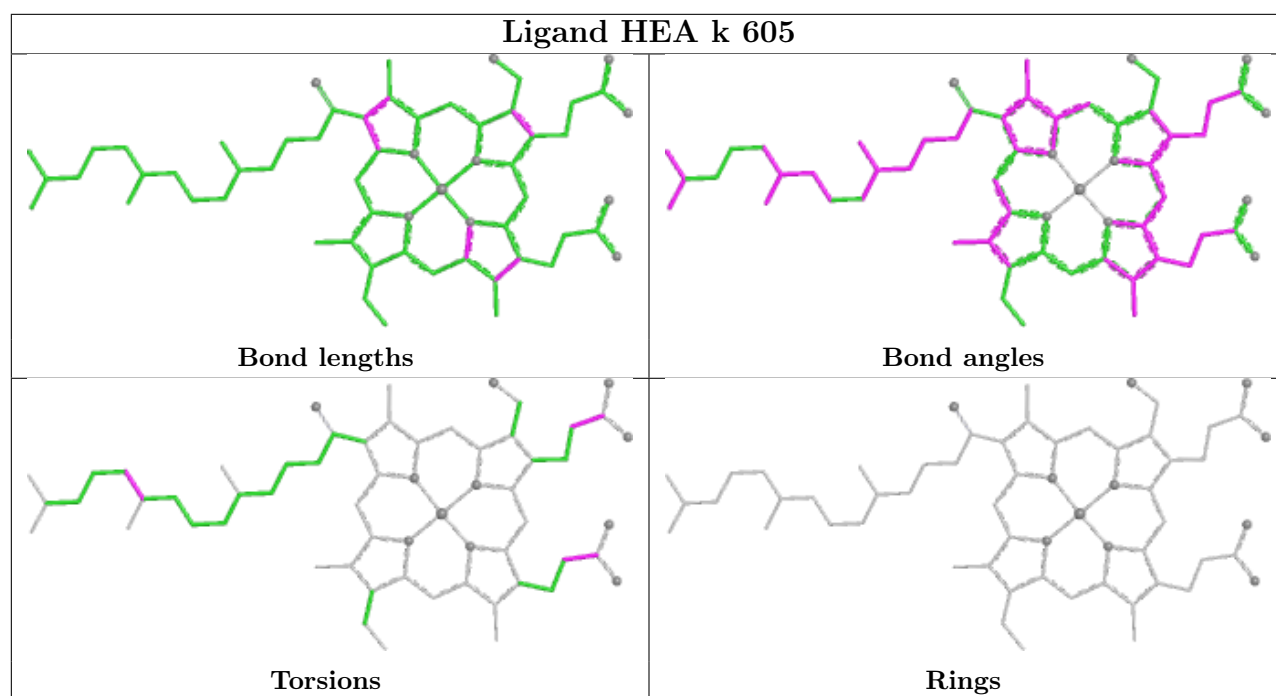
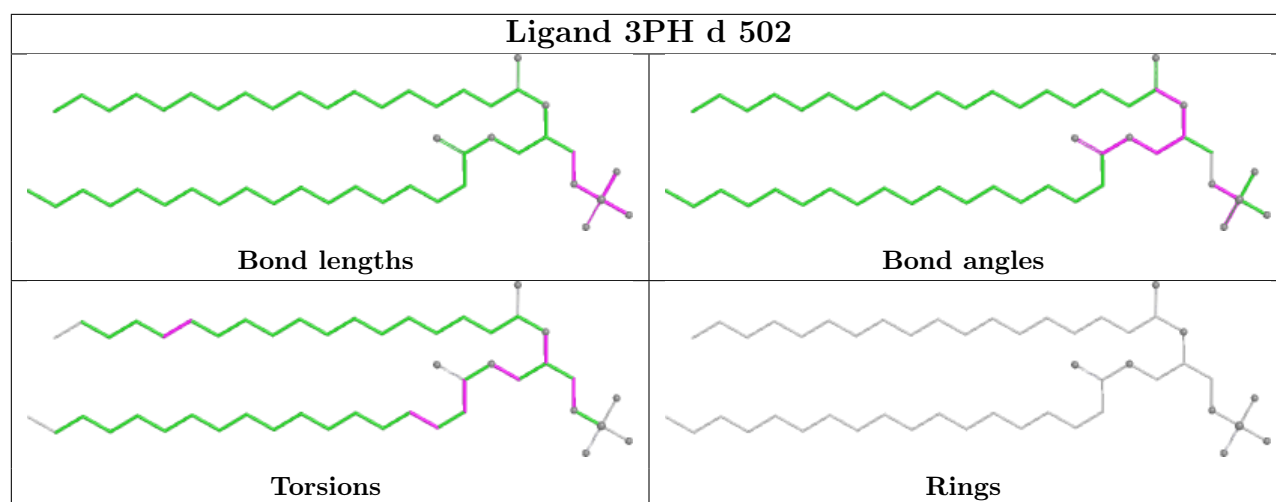
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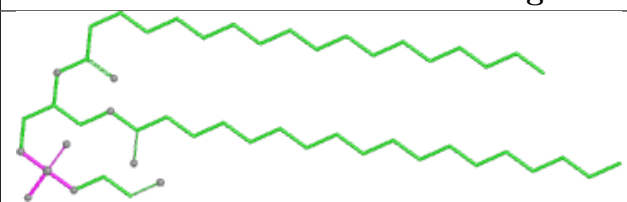
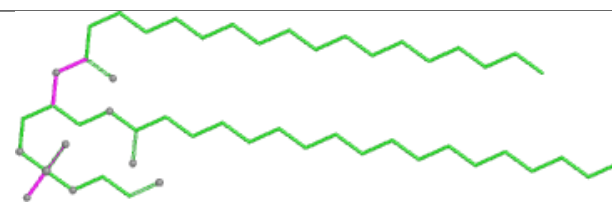
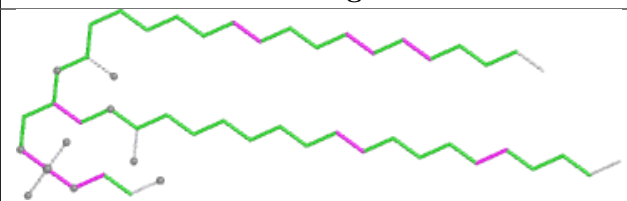
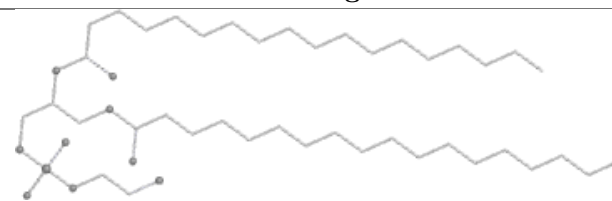
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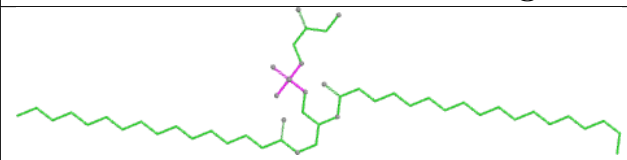
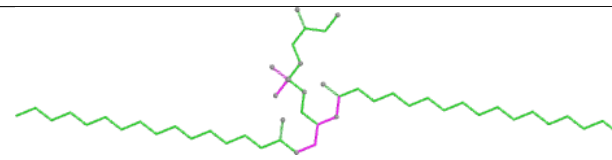
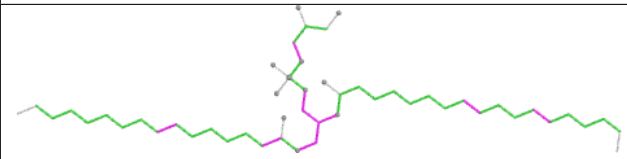
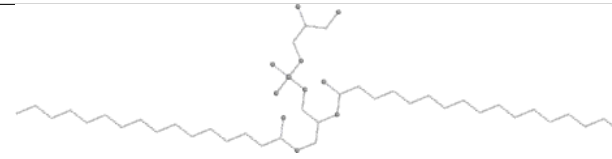
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	k	604	HEA	5	0
32	d	504	U10	1	0
33	i	313	PC1	1	0
36	F	502	FMN	1	0
37	L	811	3PH	2	0
33	l	304	PC1	1	0
29	J	201	PGT	1	0
33	k	609	PC1	1	0
32	B	1002	U10	3	0
33	m	311	PC1	4	0
37	P	402	3PH	1	0

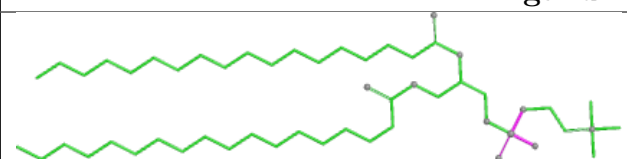
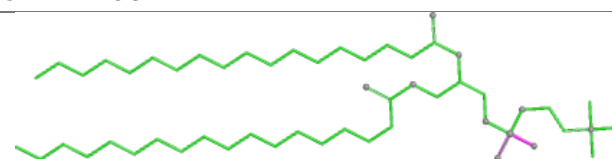
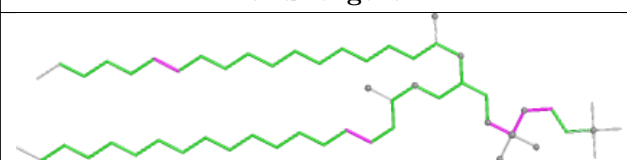
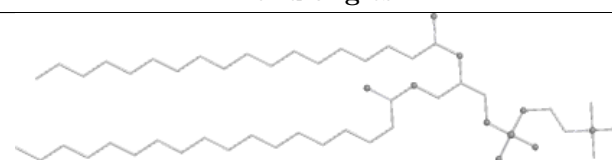
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

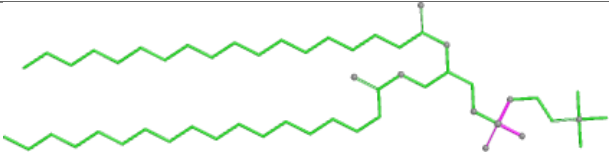
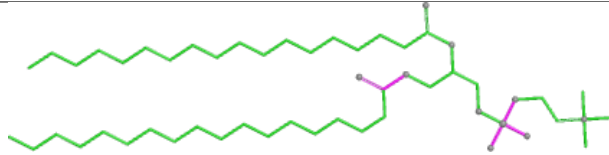
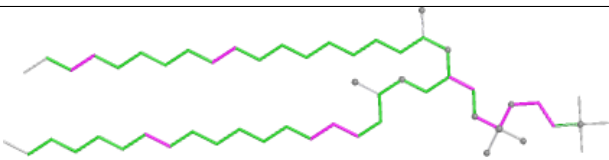
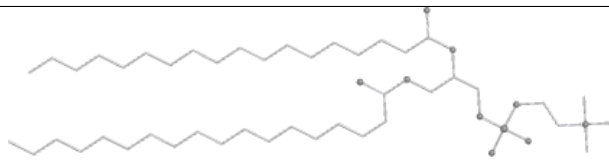
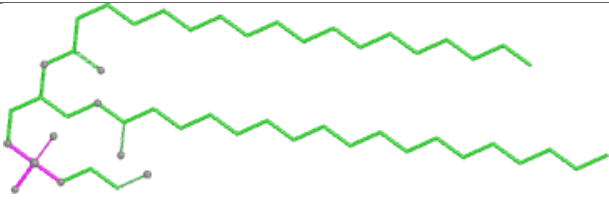
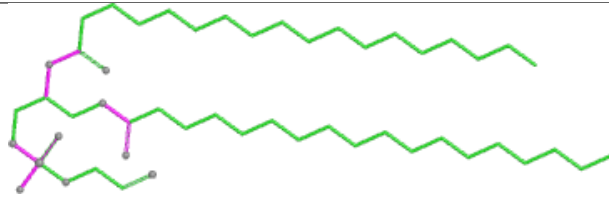
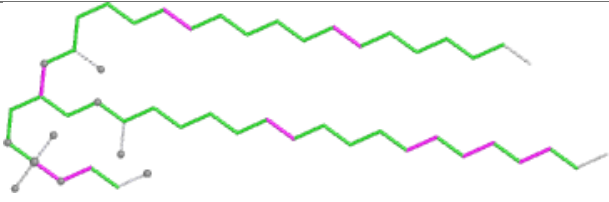
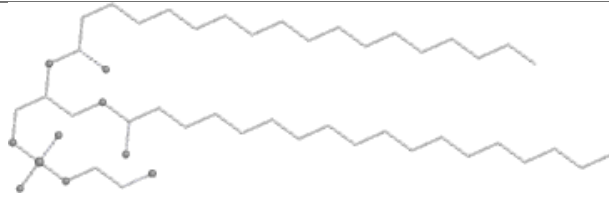
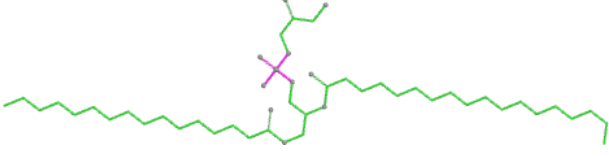
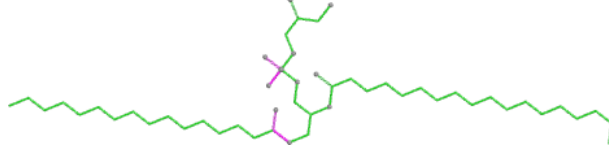
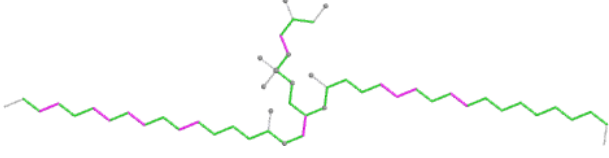
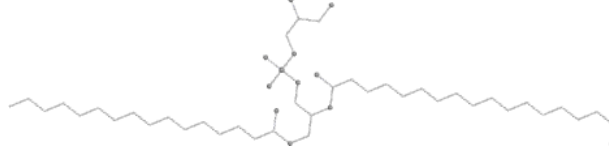


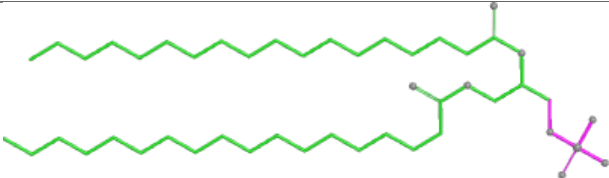

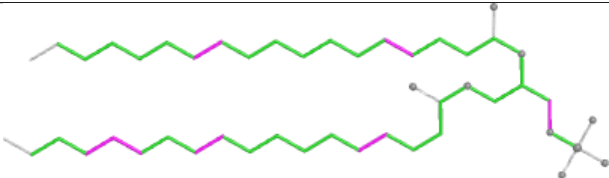
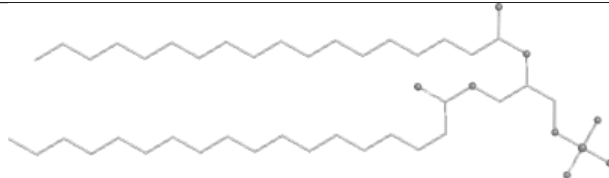


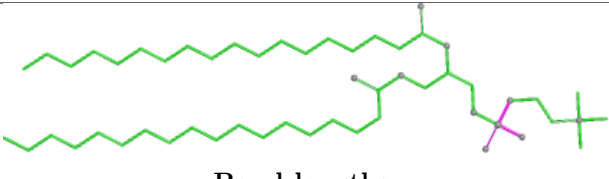
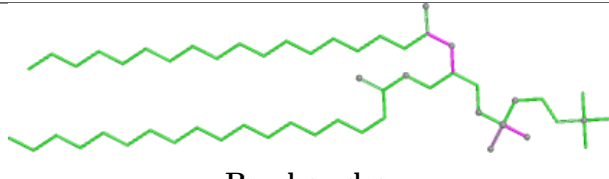
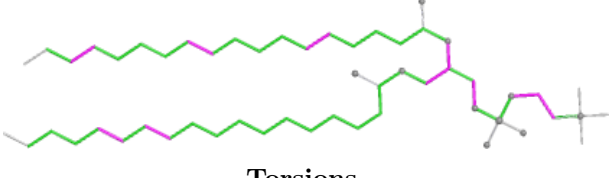
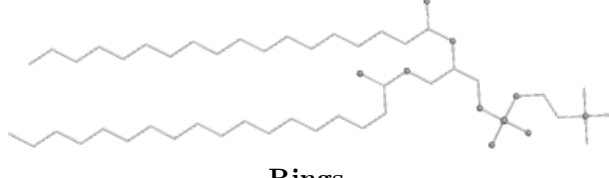
Ligand 3PE P 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

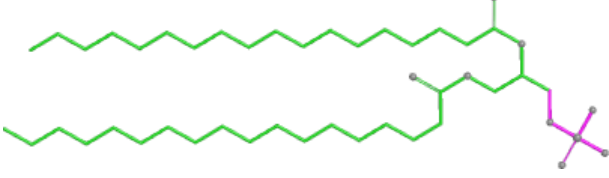
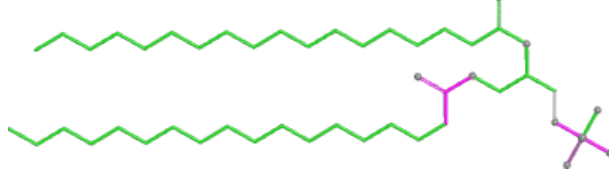

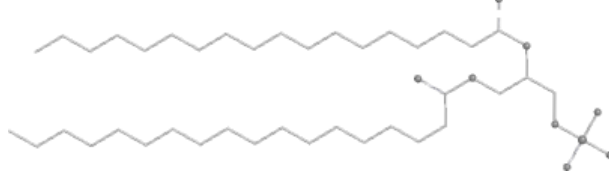
Ligand PGT N 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

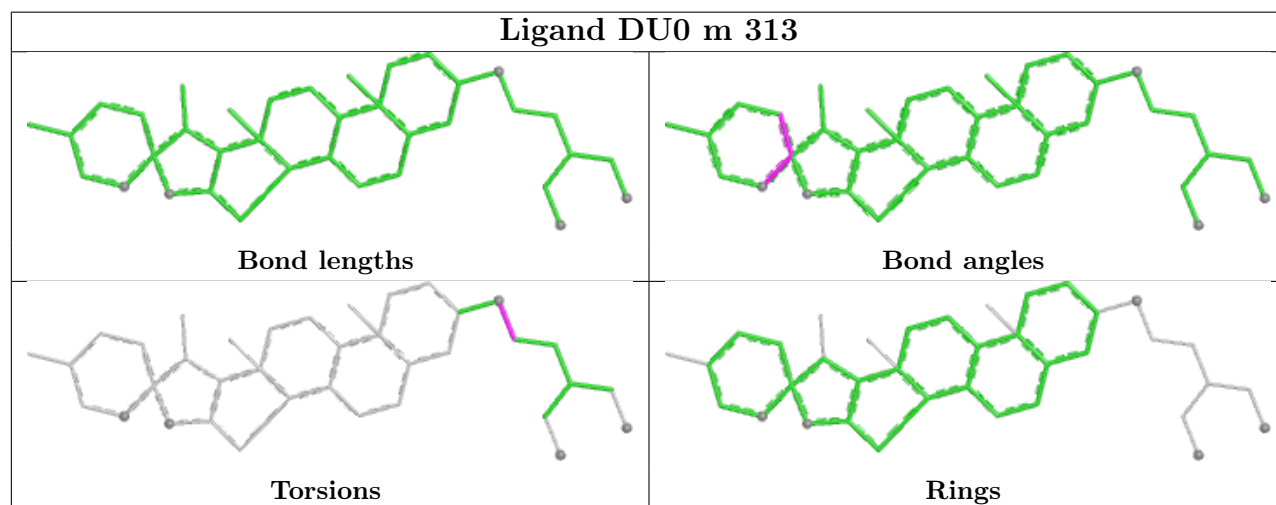
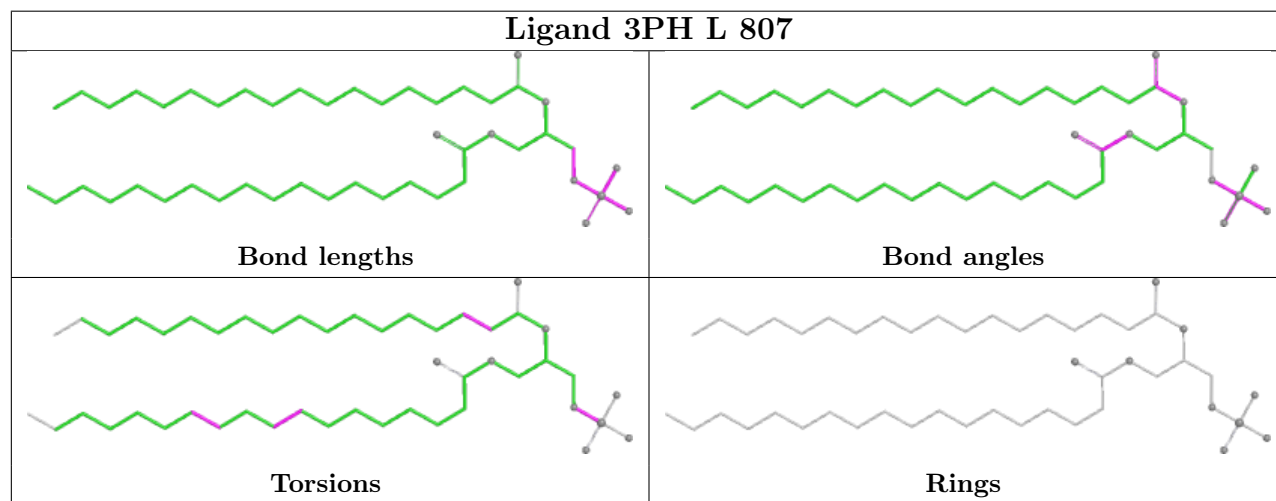
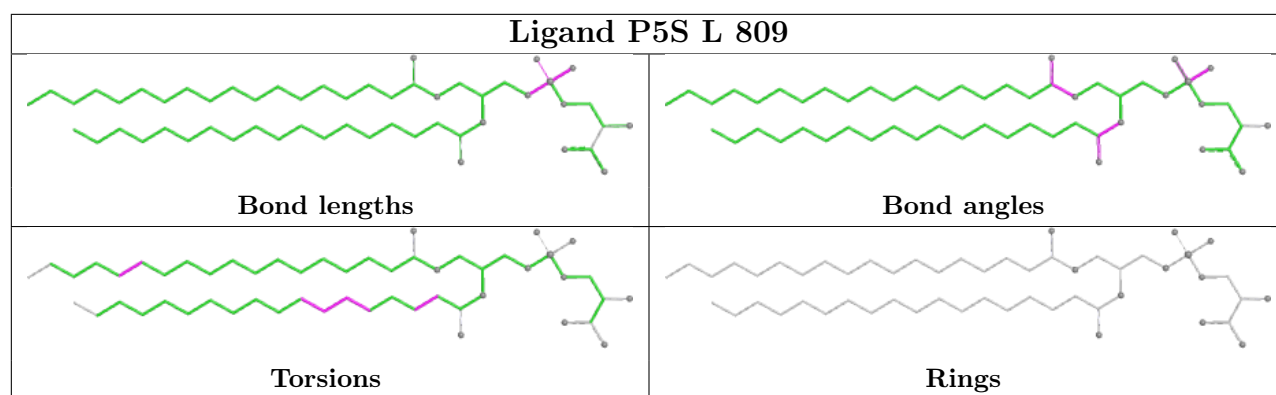
Ligand PC1 H 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

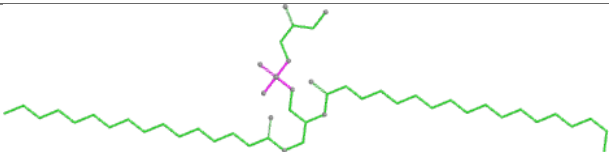
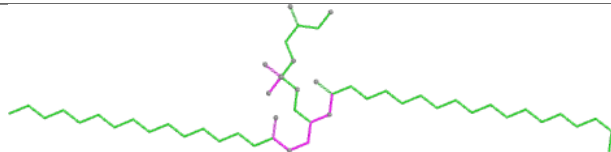
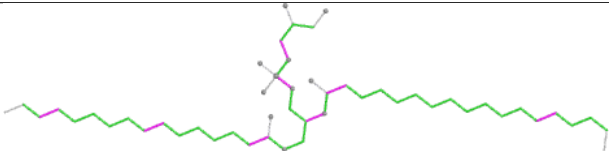
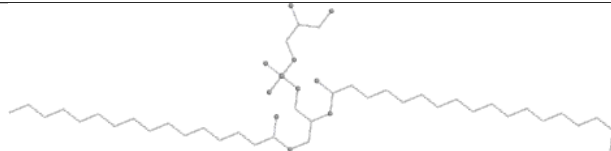
Ligand PC1 i 308	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand 3PE m 310	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PGT K 201	
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 <p>Torsions</p>	 <p>Rings</p>

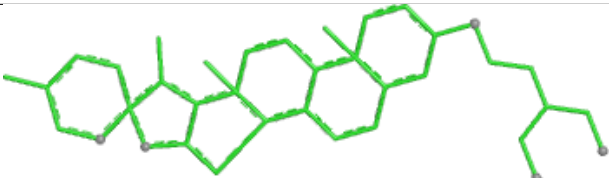
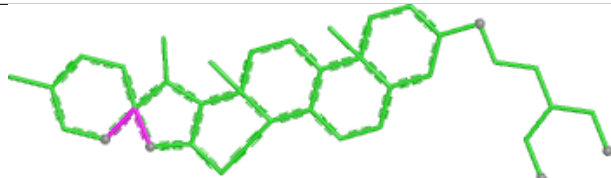
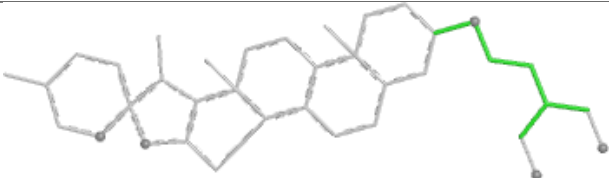
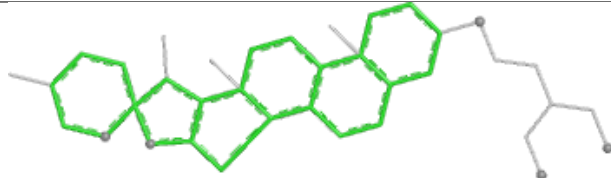
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 <p>Torsions</p>	 <p>Rings</p>

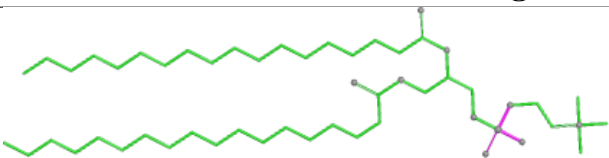
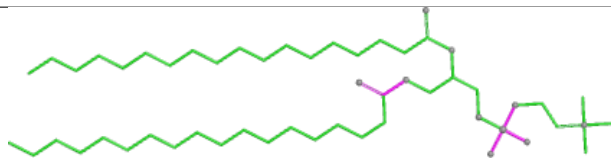
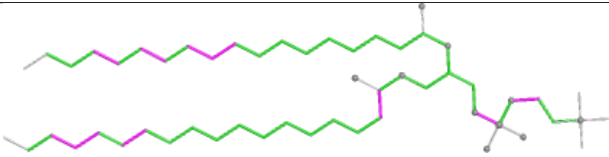
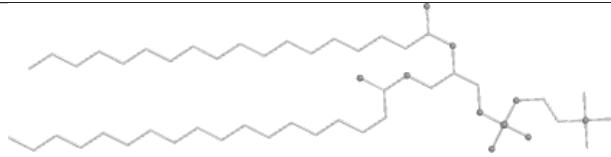
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 <p>Torsions</p>	 <p>Rings</p>

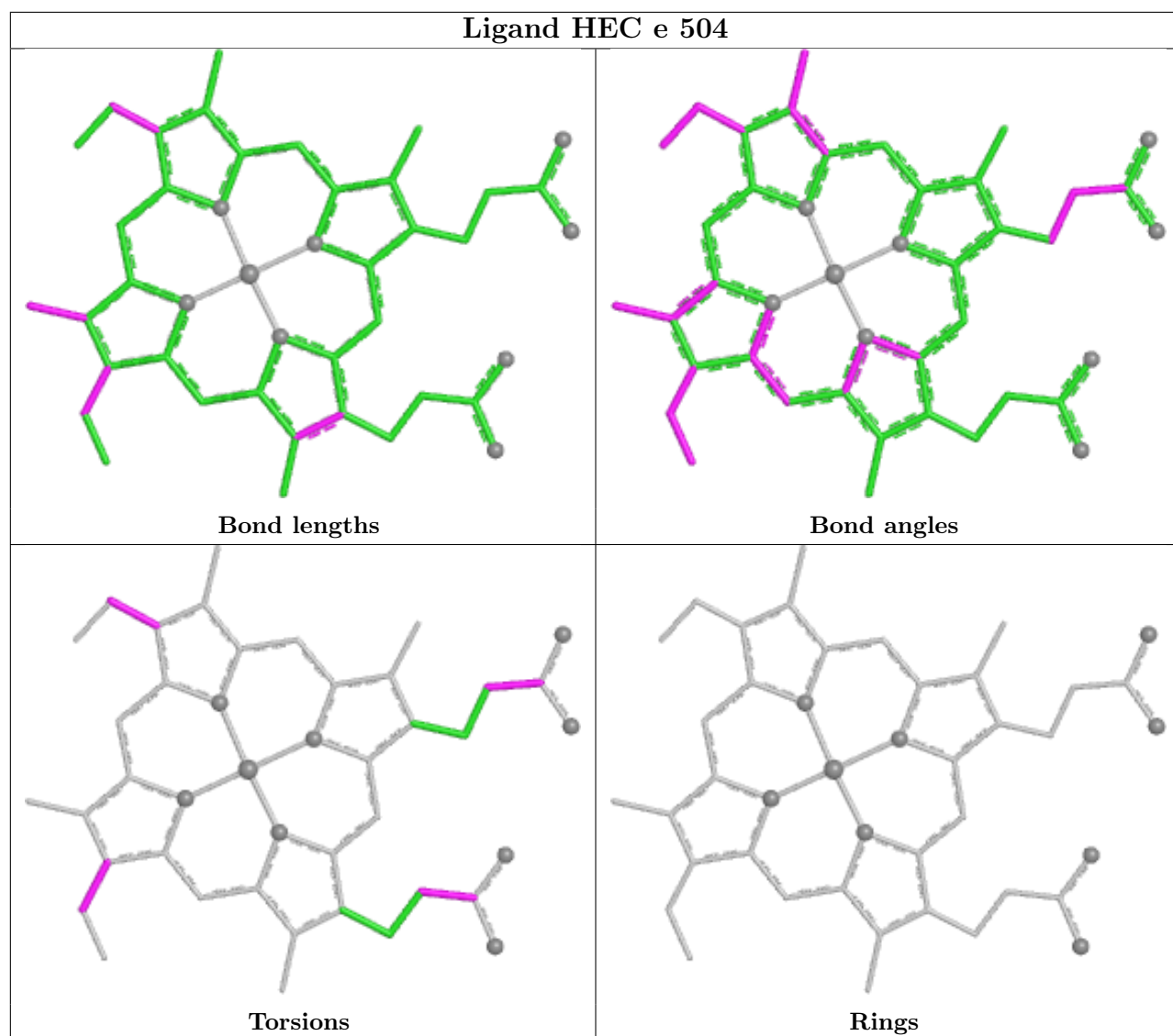
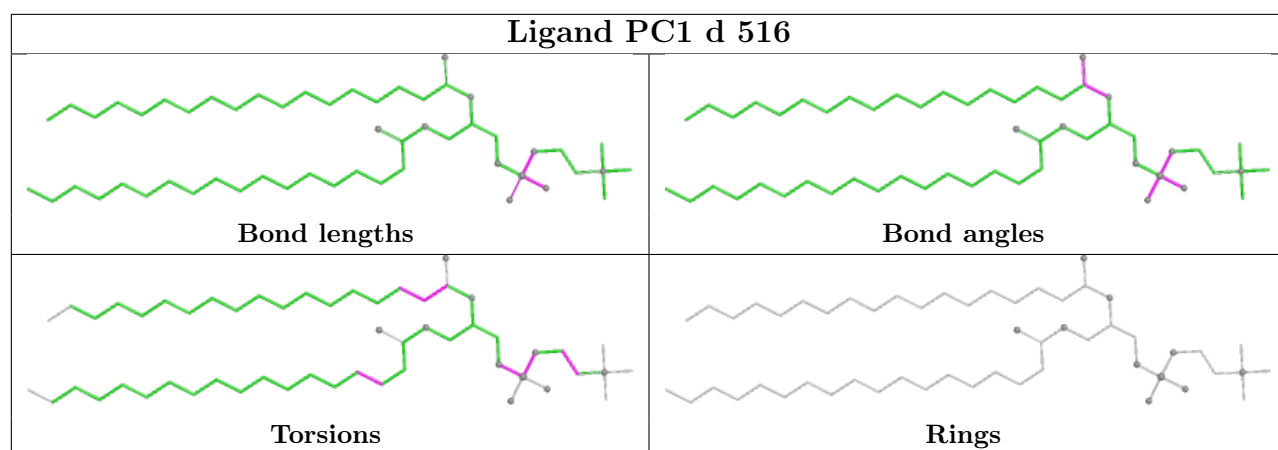
Ligand 3PH k 607	
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 <p>Torsions</p>	 <p>Rings</p>



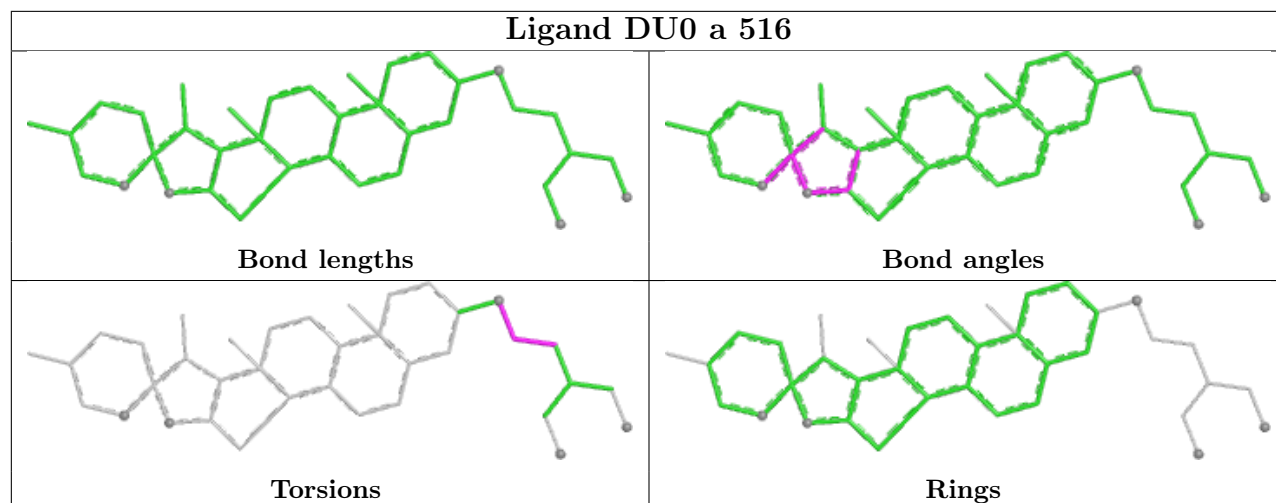
Ligand PGT M 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DU0 i 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

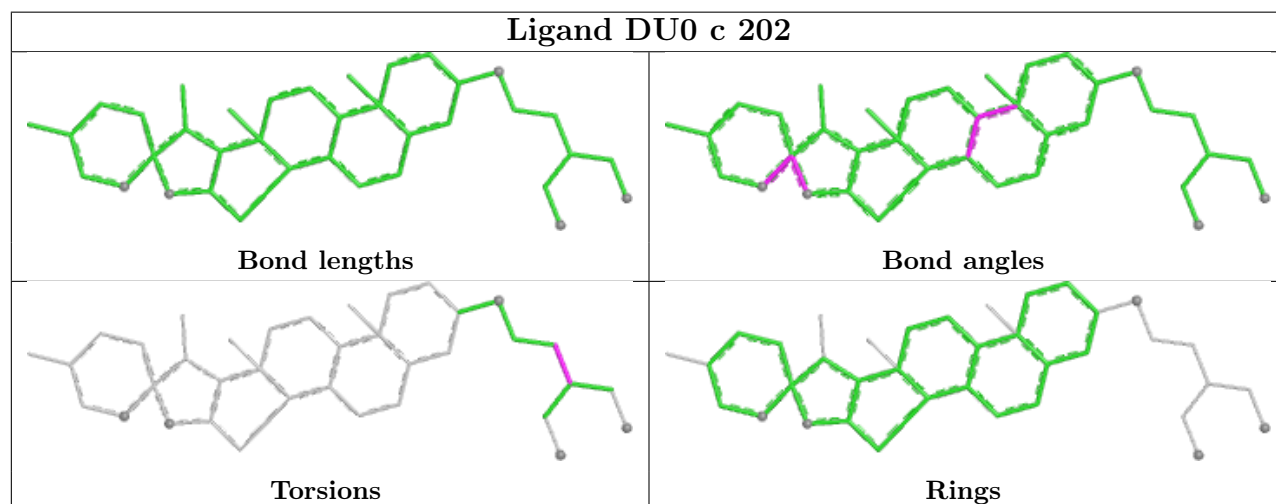
Ligand PC1 N 501	
	
Bond lengths	Bond angles
	
Torsions	Rings



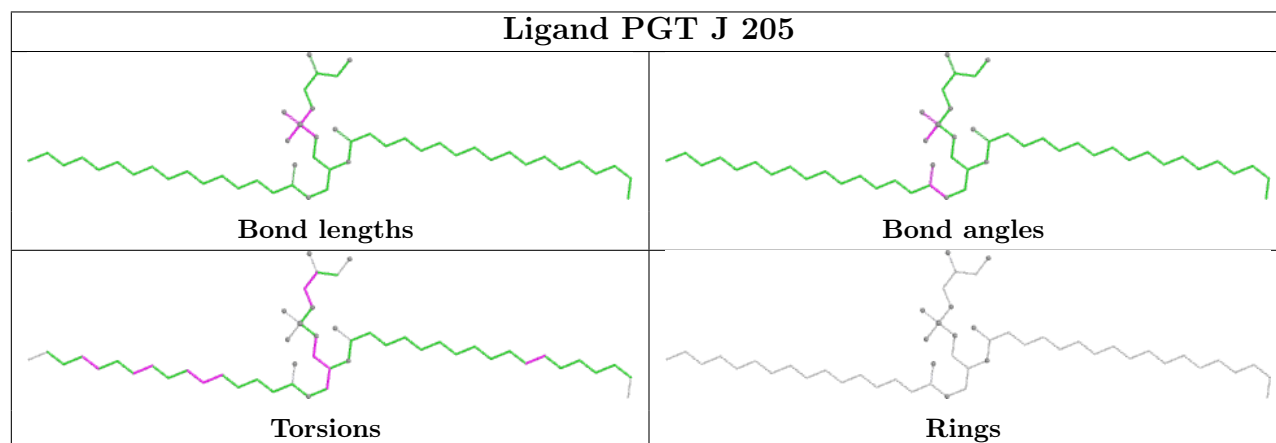
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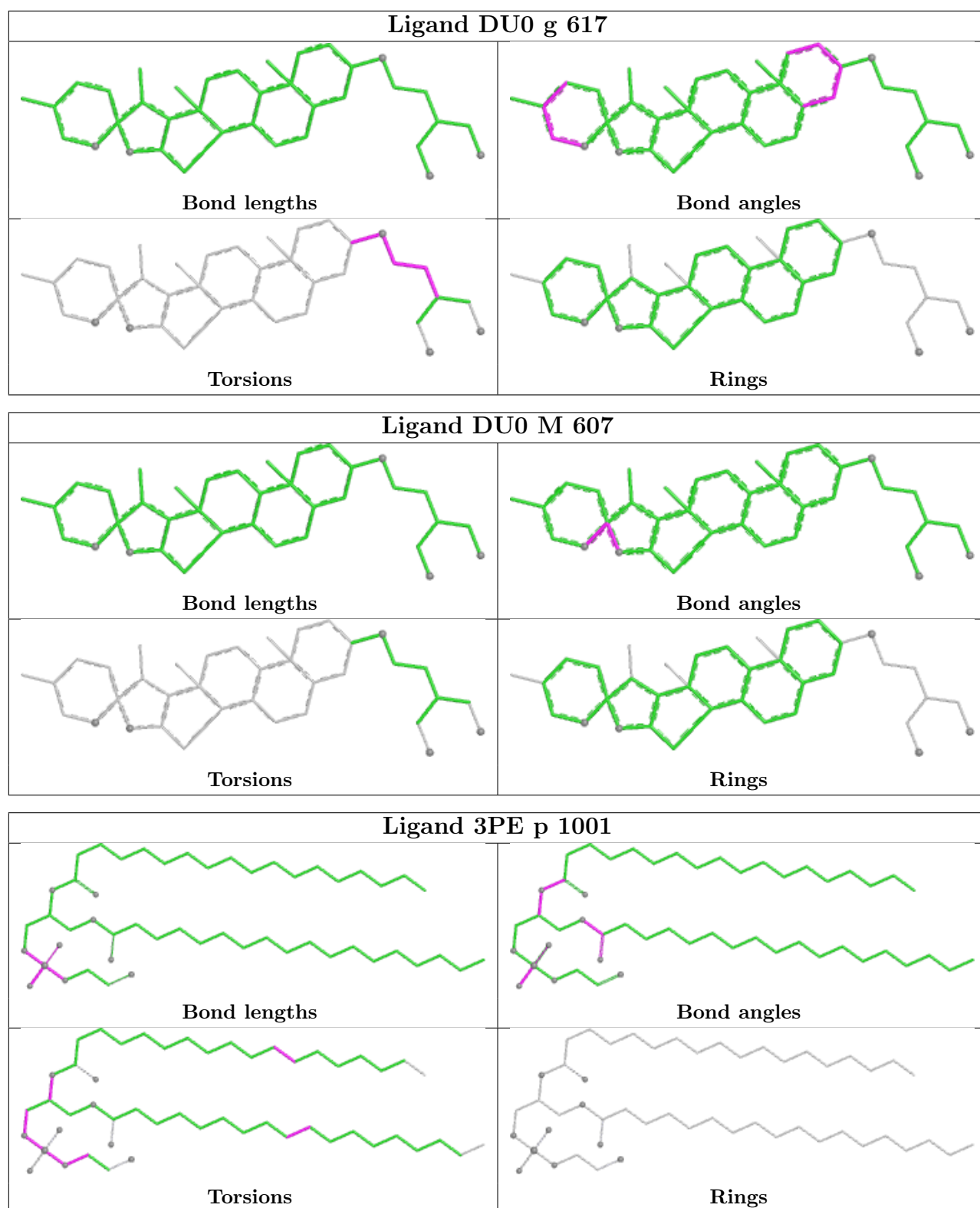


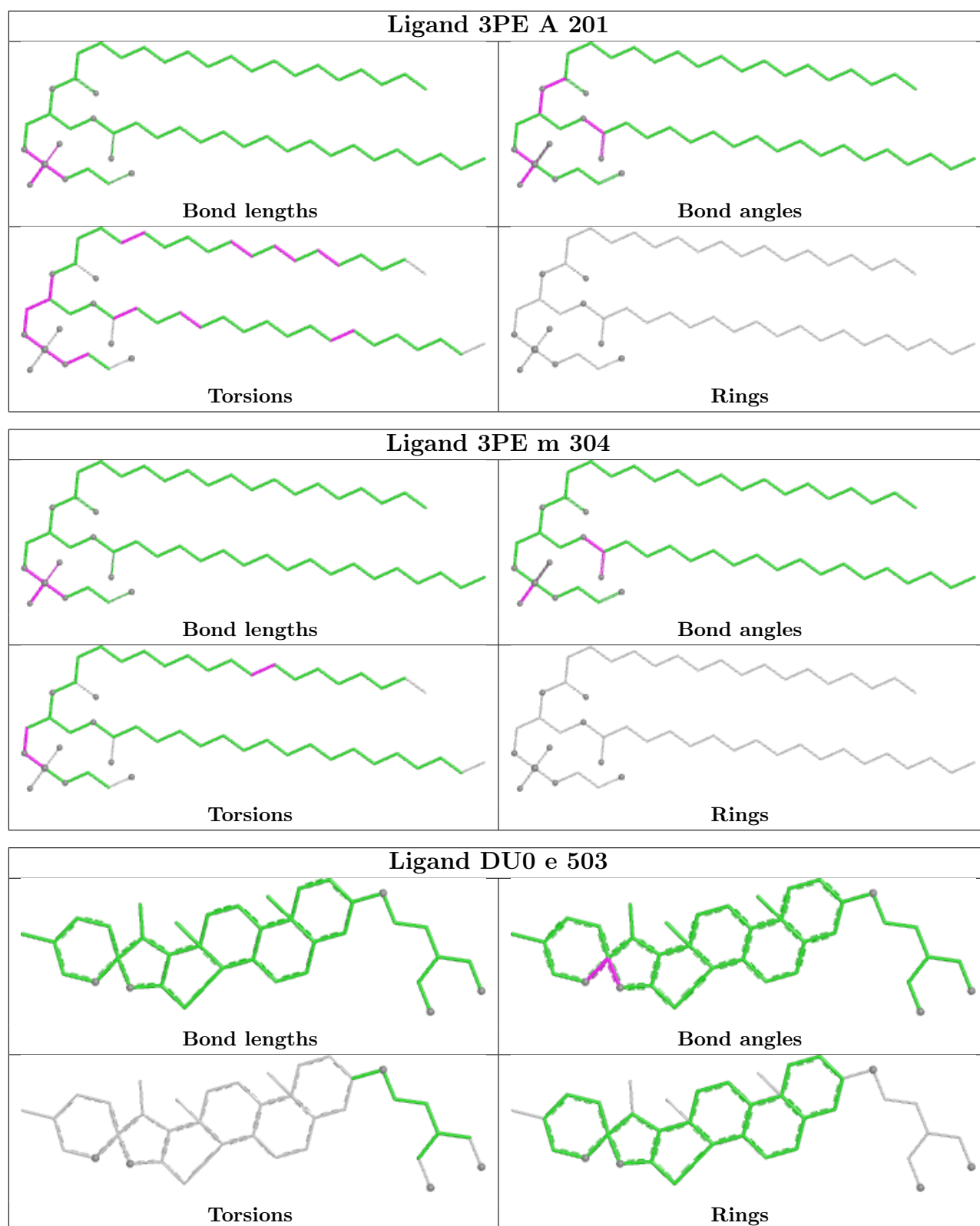
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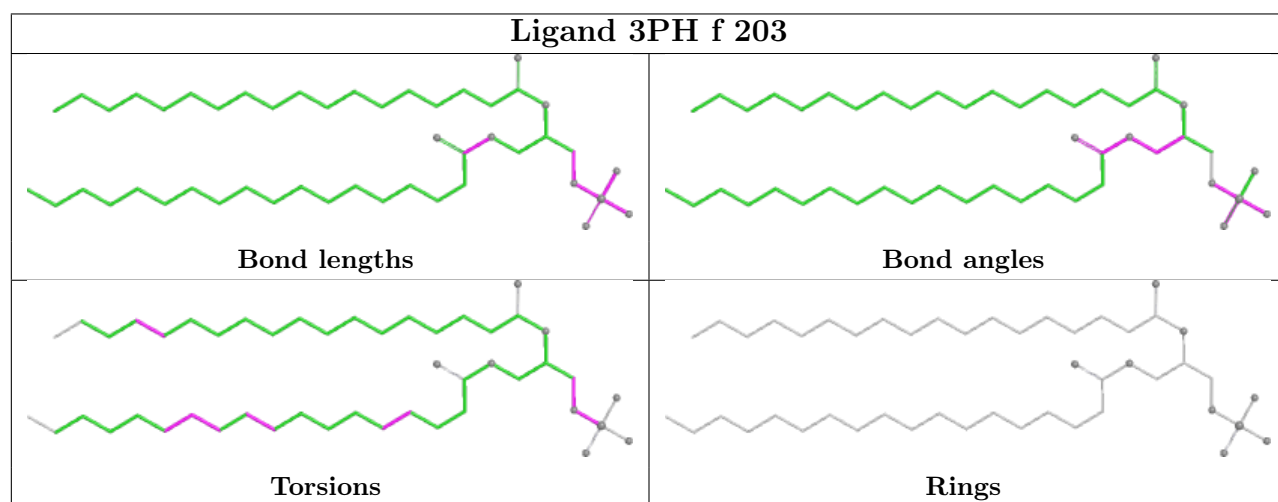
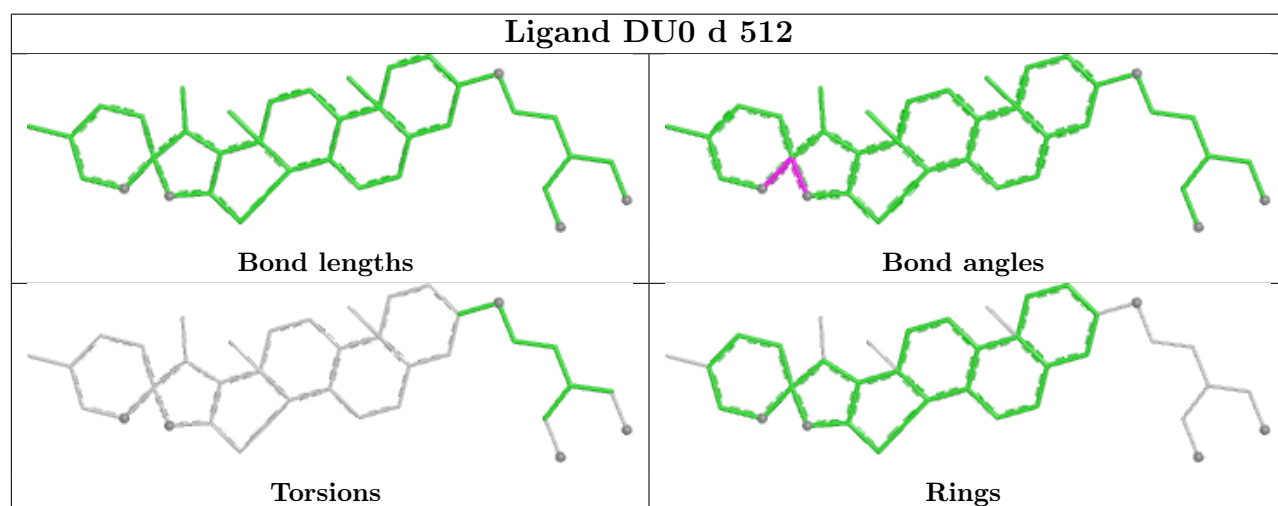
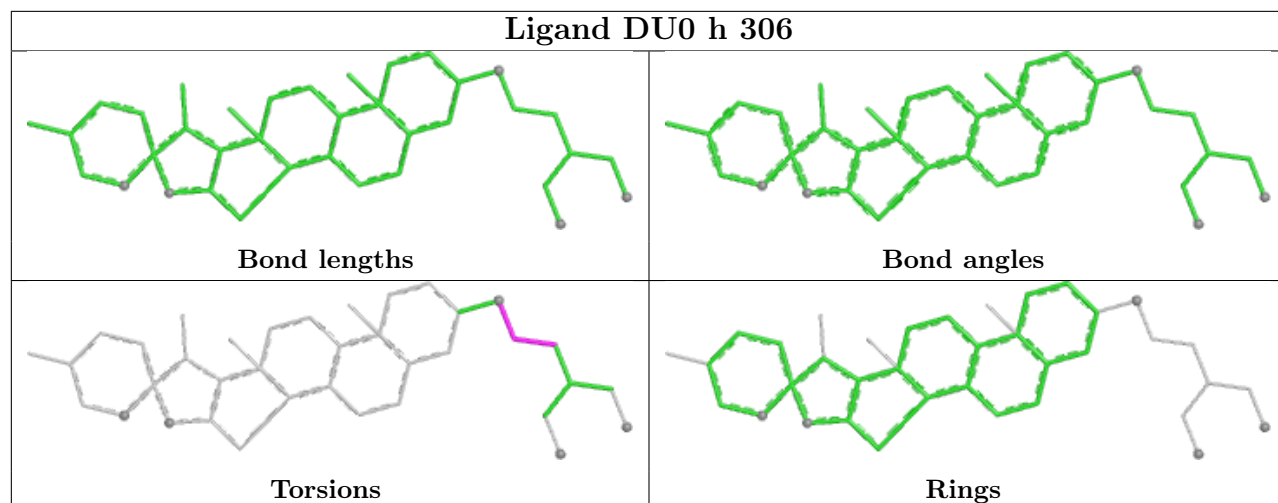


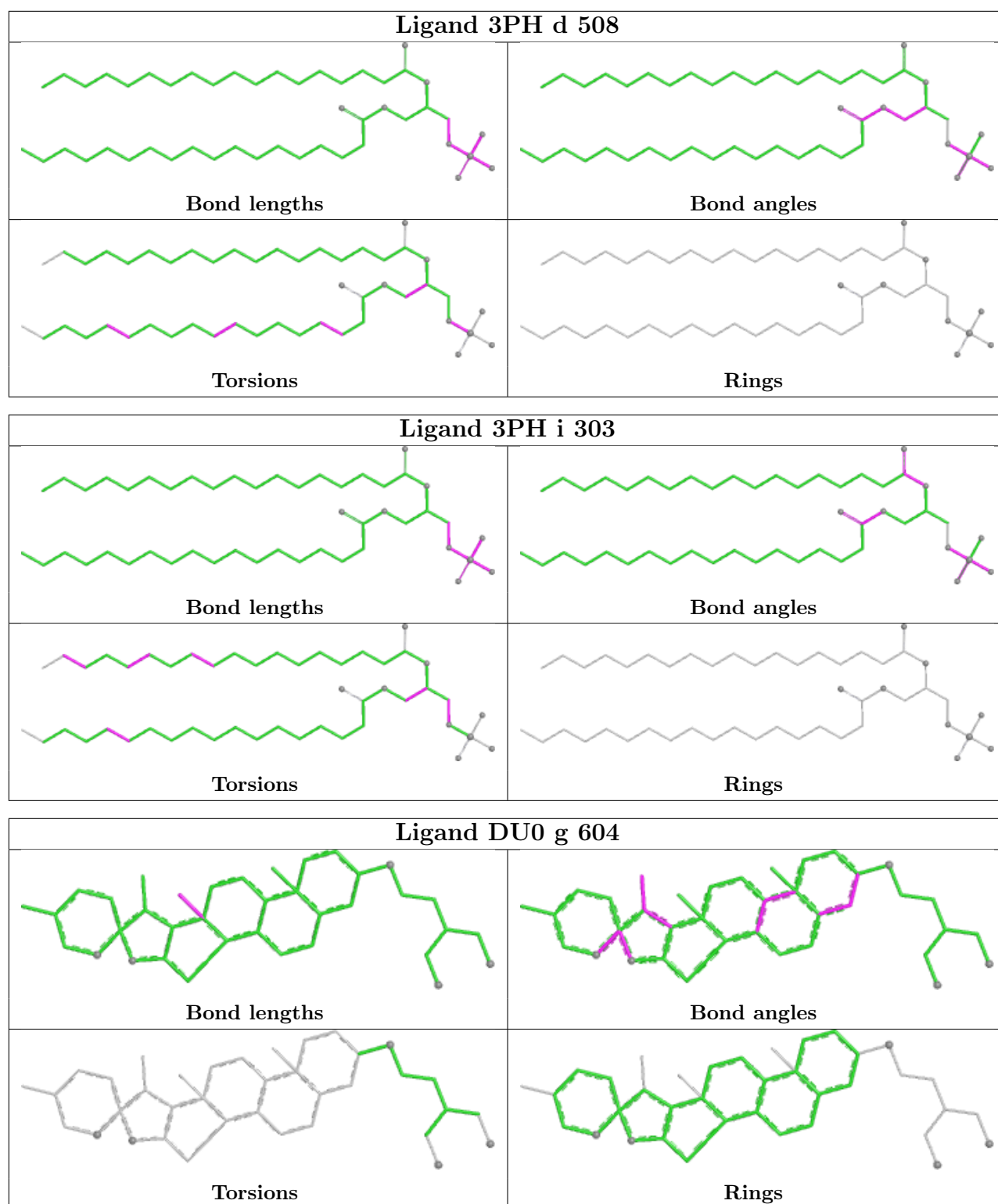
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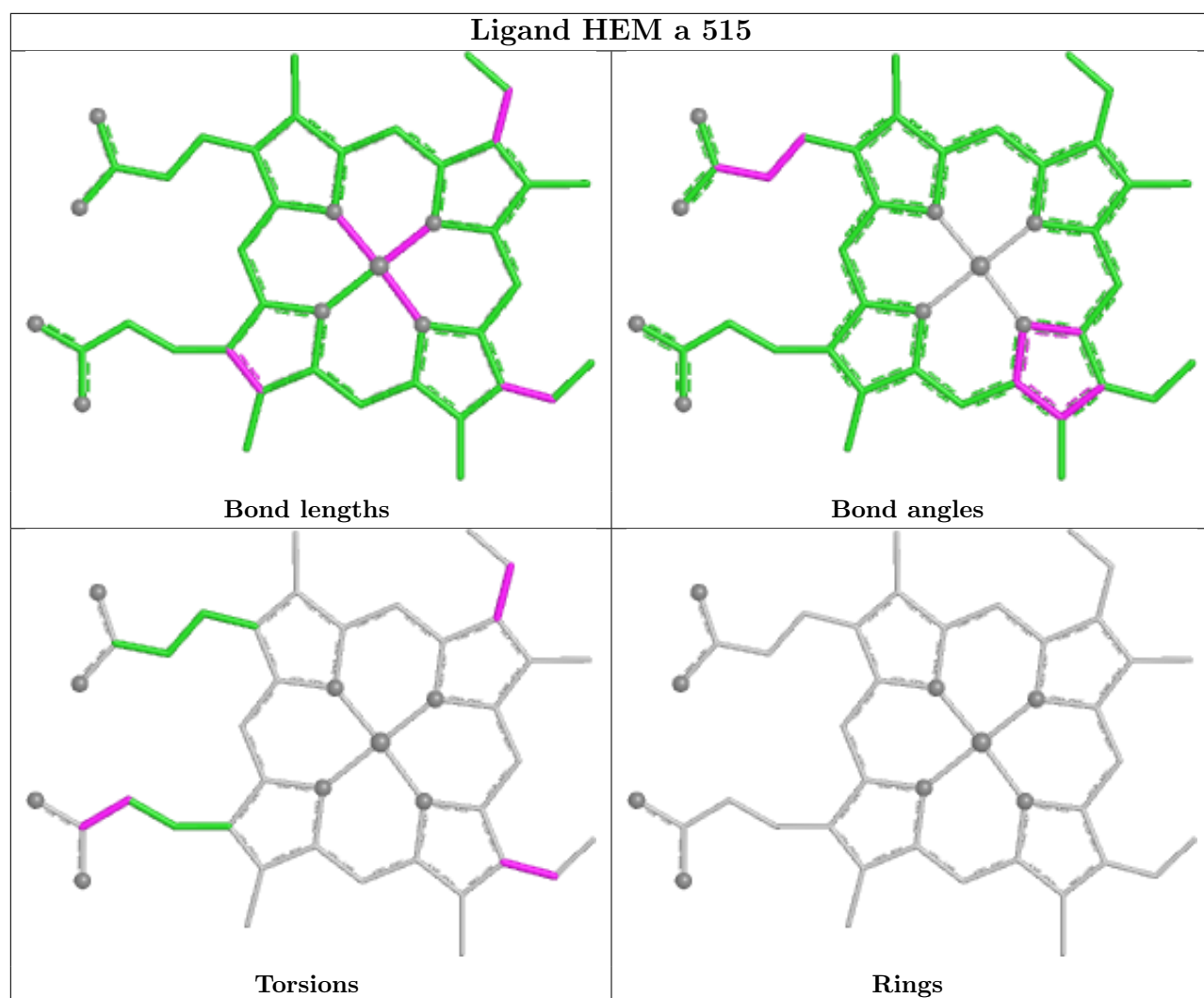
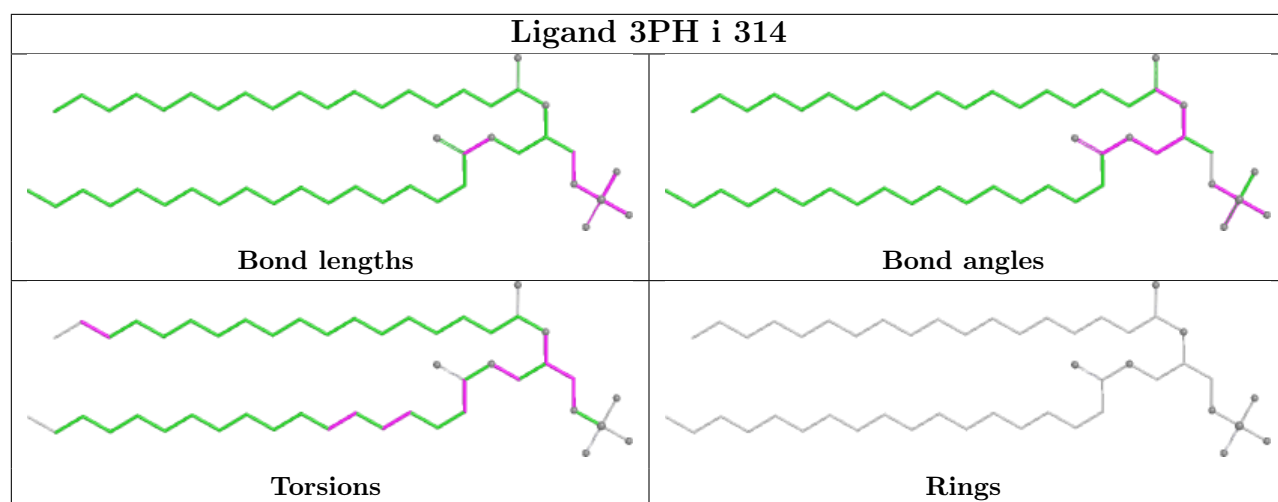


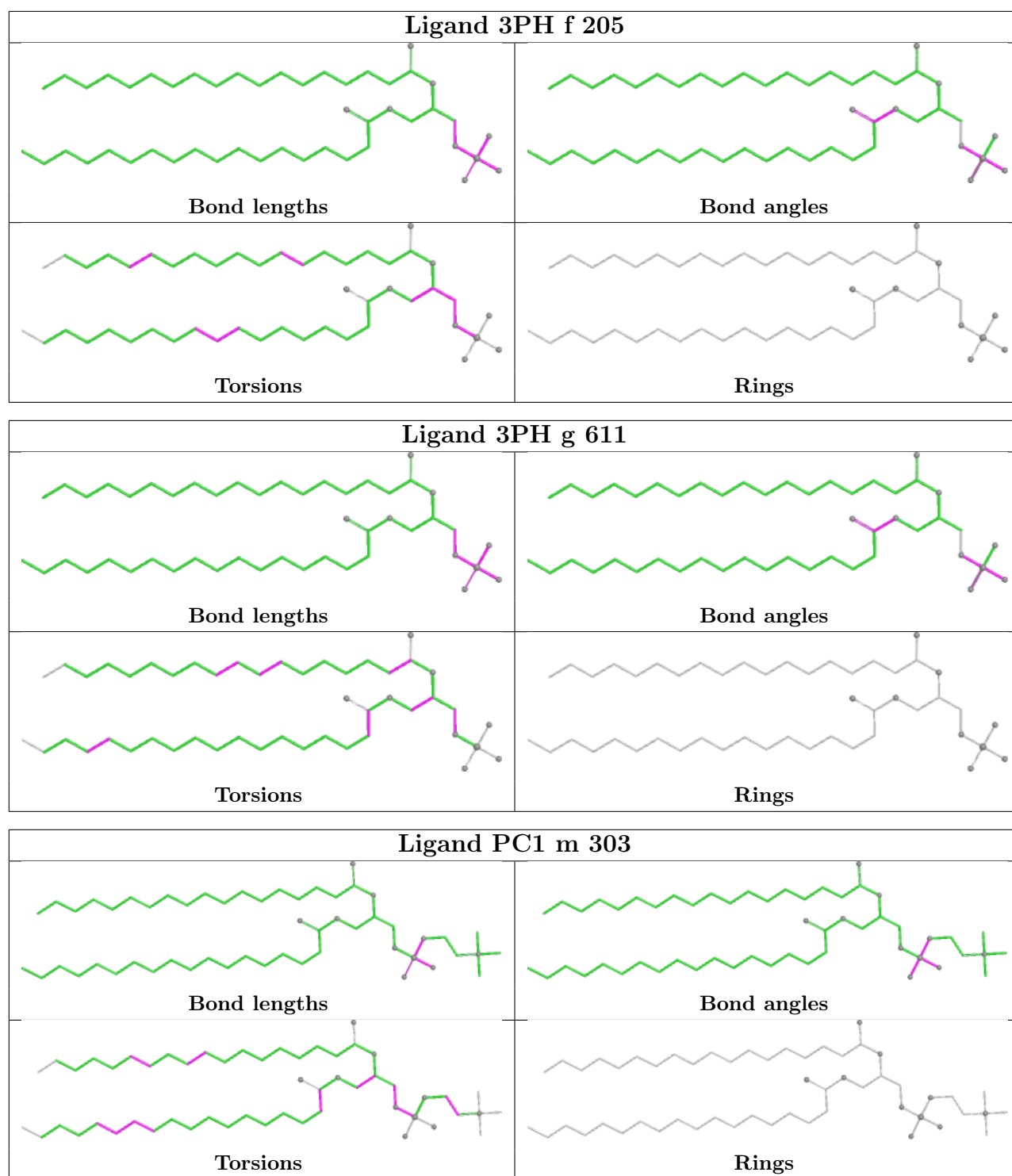


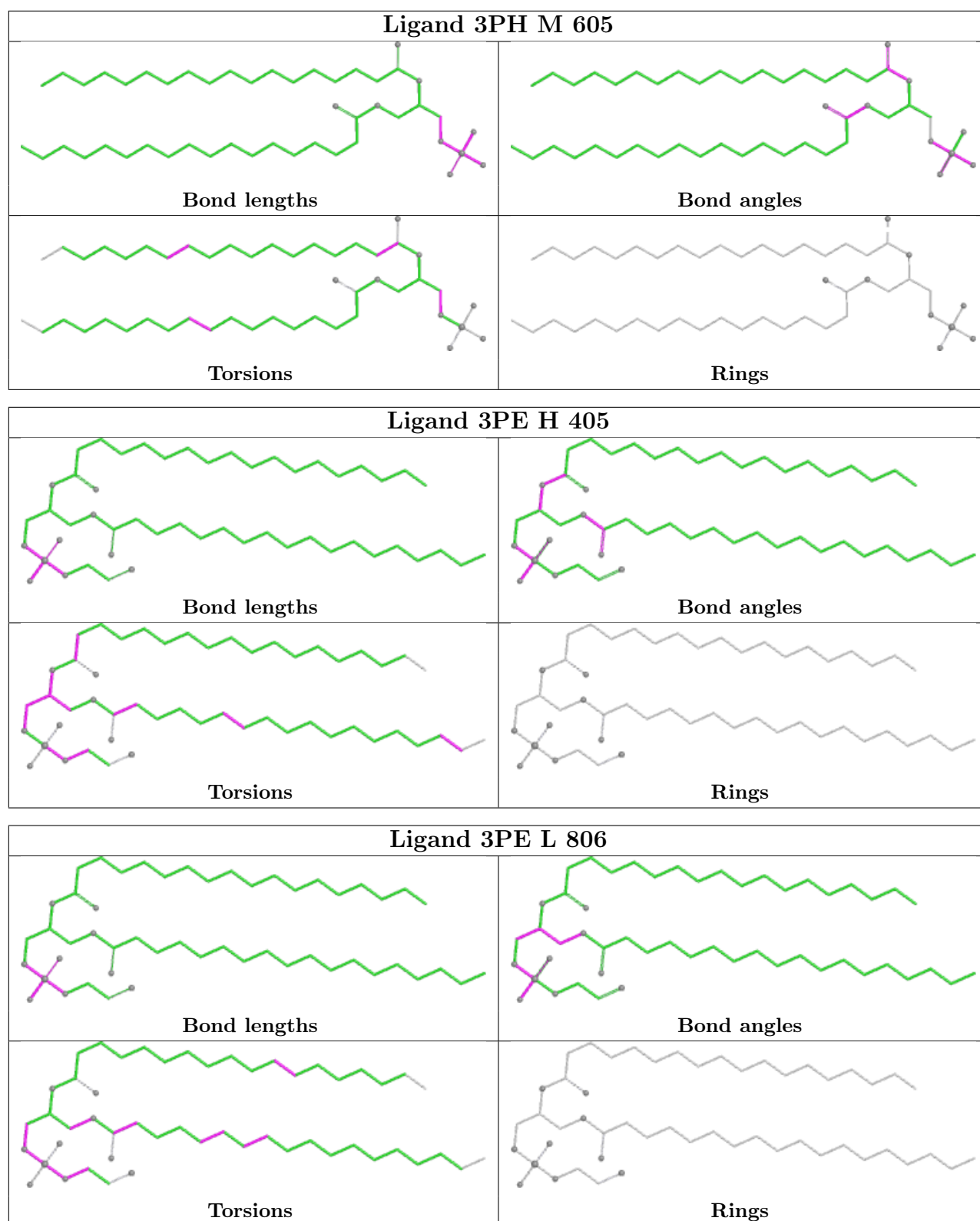


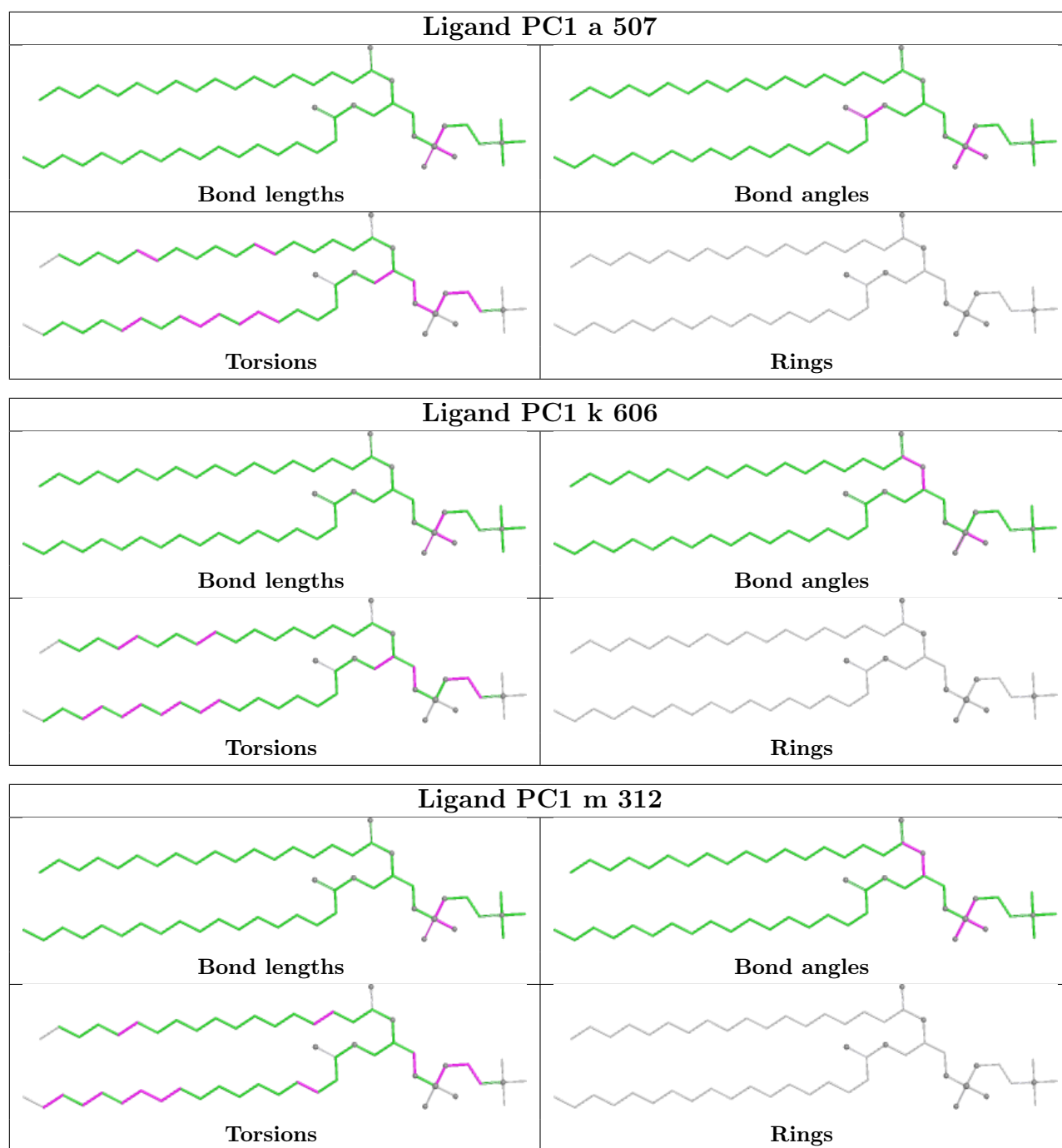




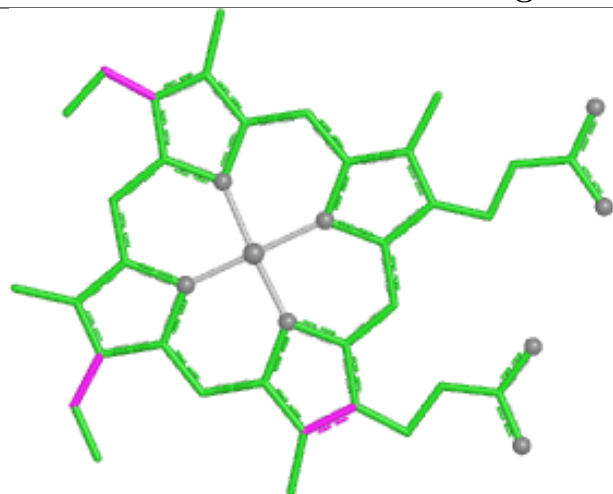




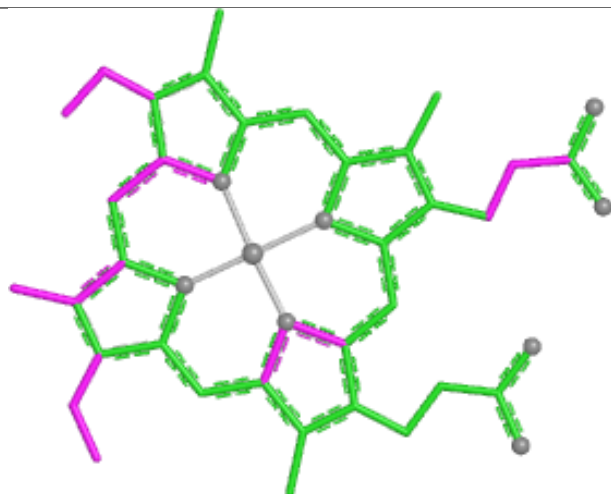




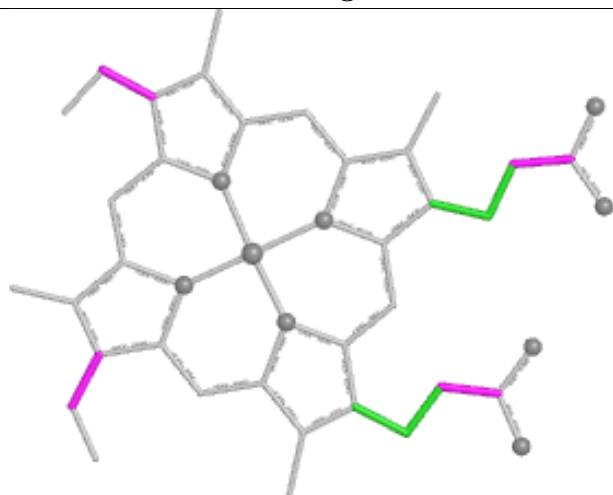
Ligand HEC b 502



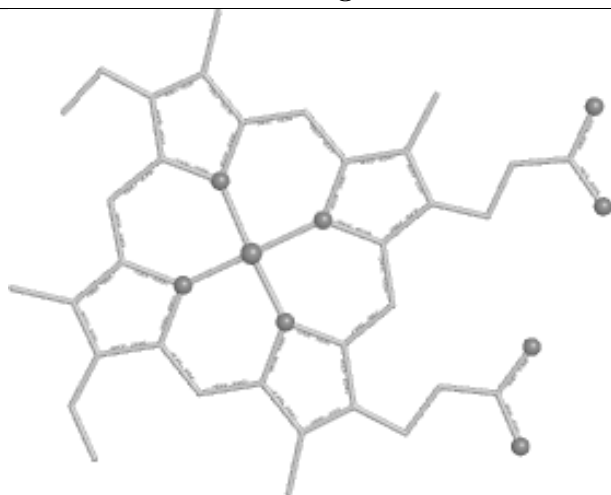
Bond lengths



Bond angles

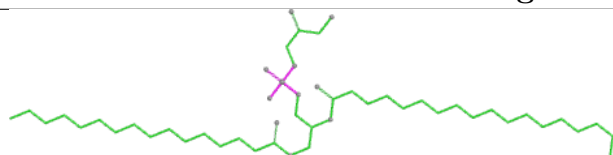


Torsions

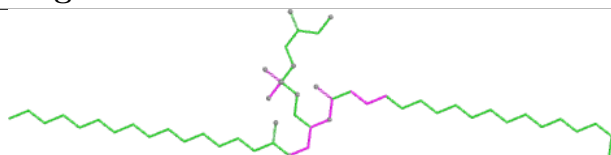


Rings

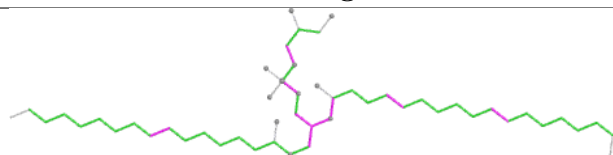
Ligand PGT g 602



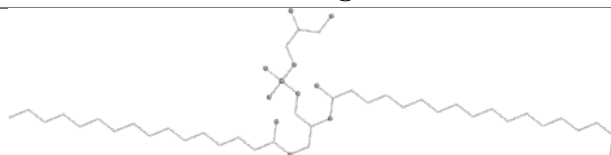
Bond lengths



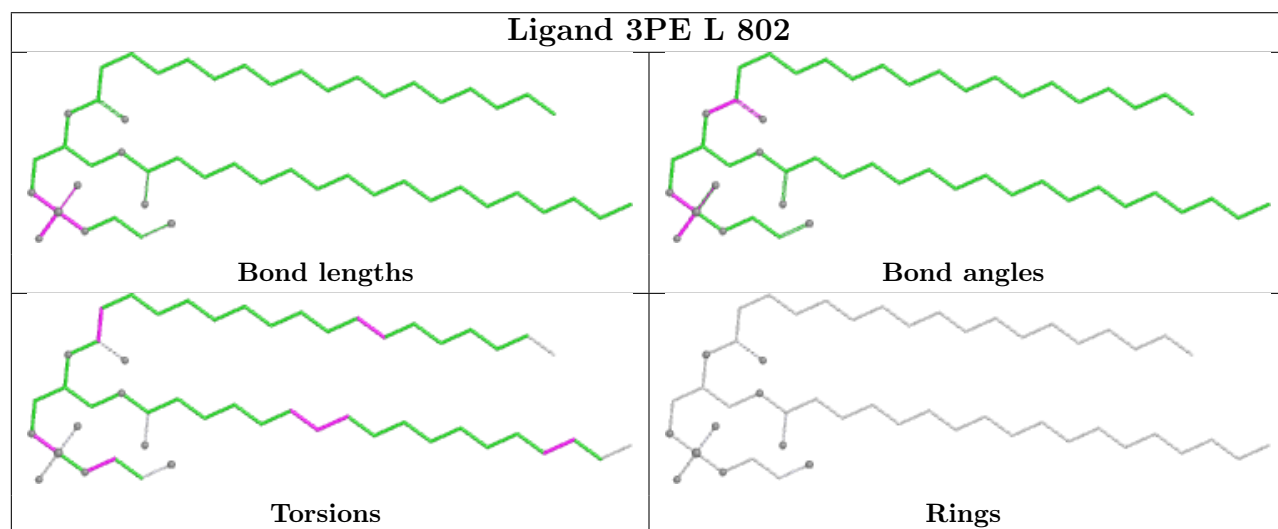
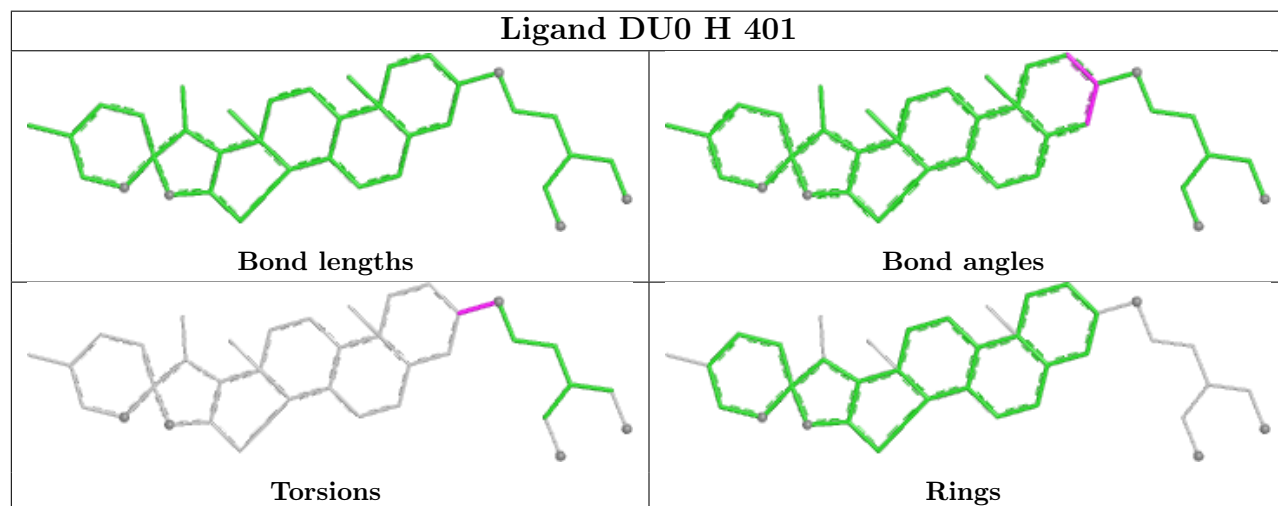
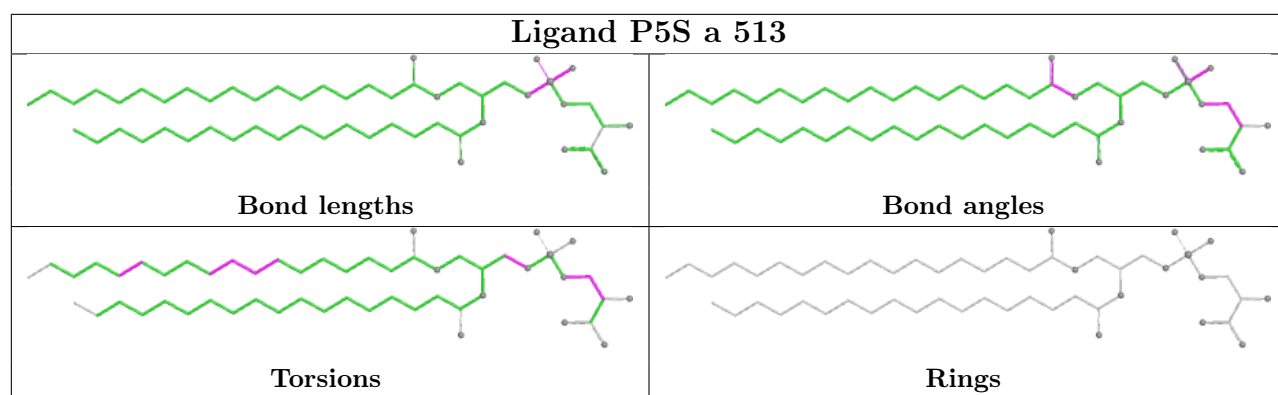
Bond angles

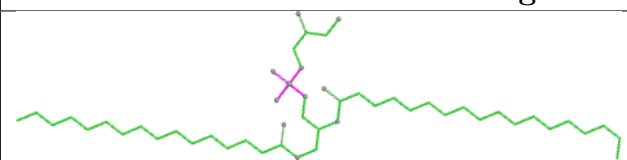
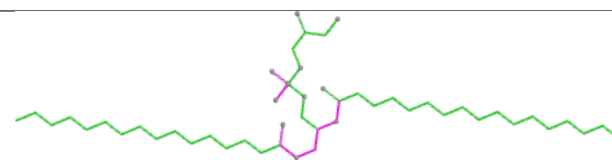
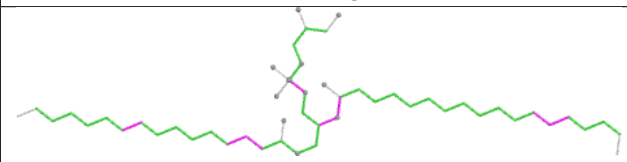
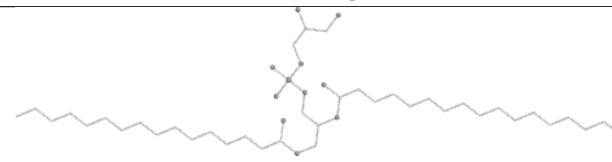


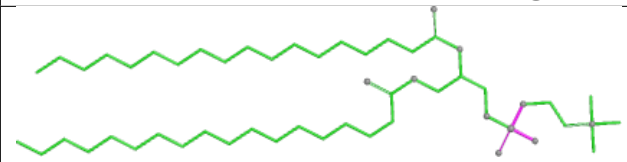
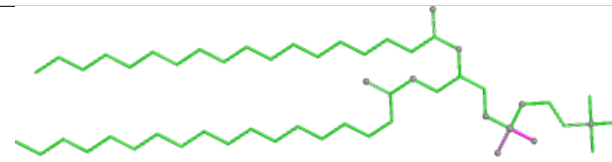
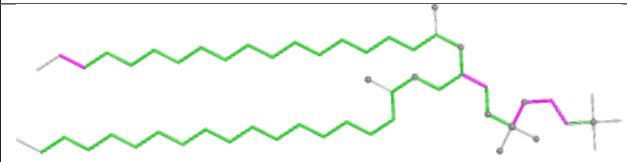
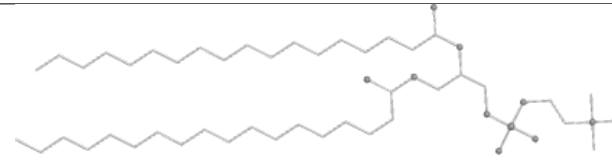
Torsions


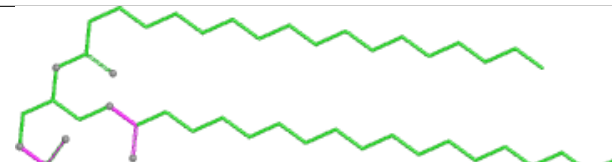

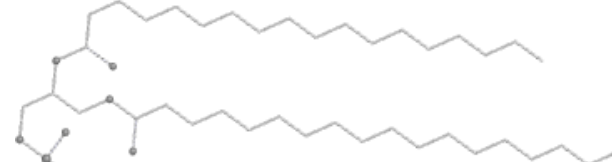


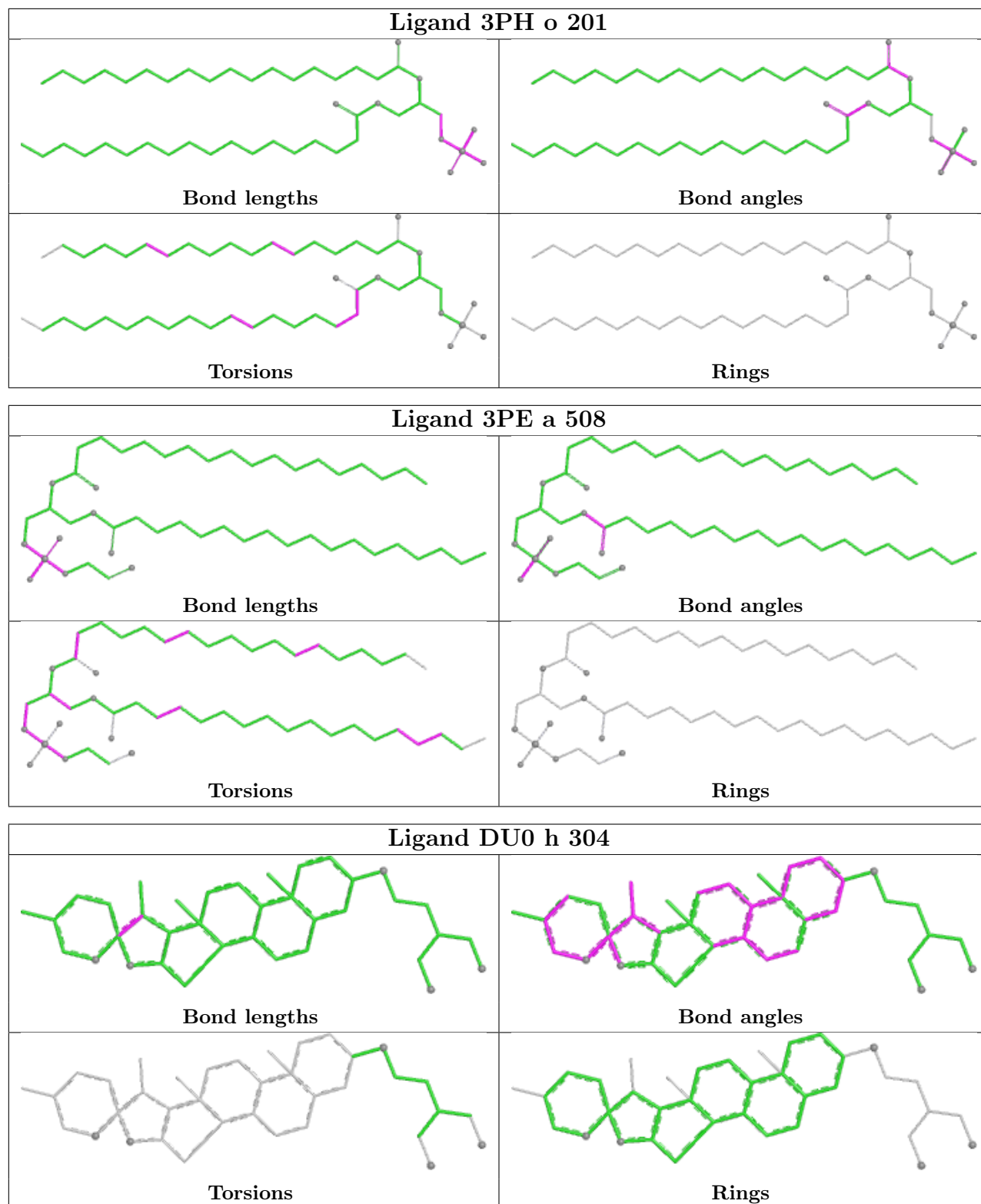
Rings

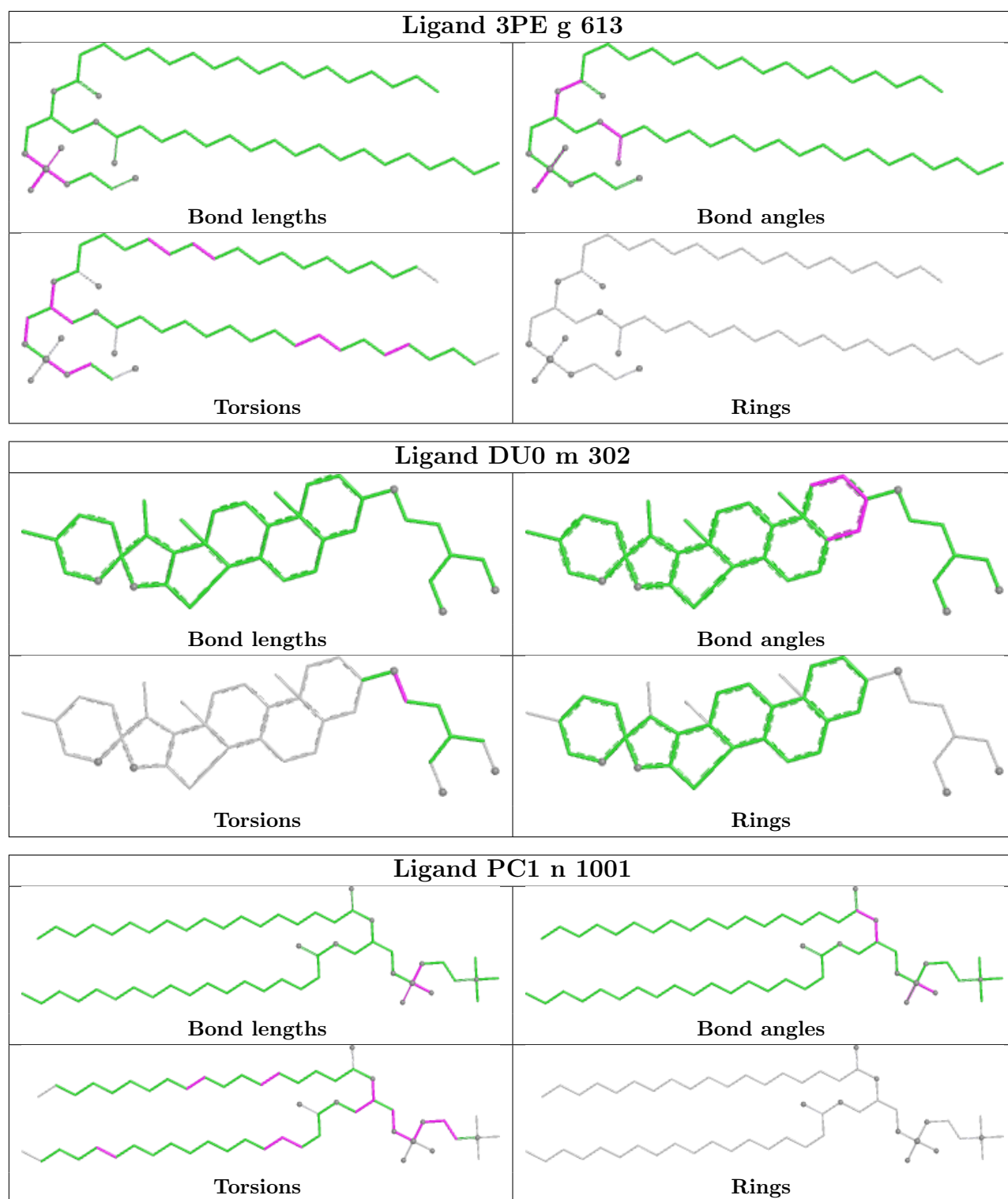


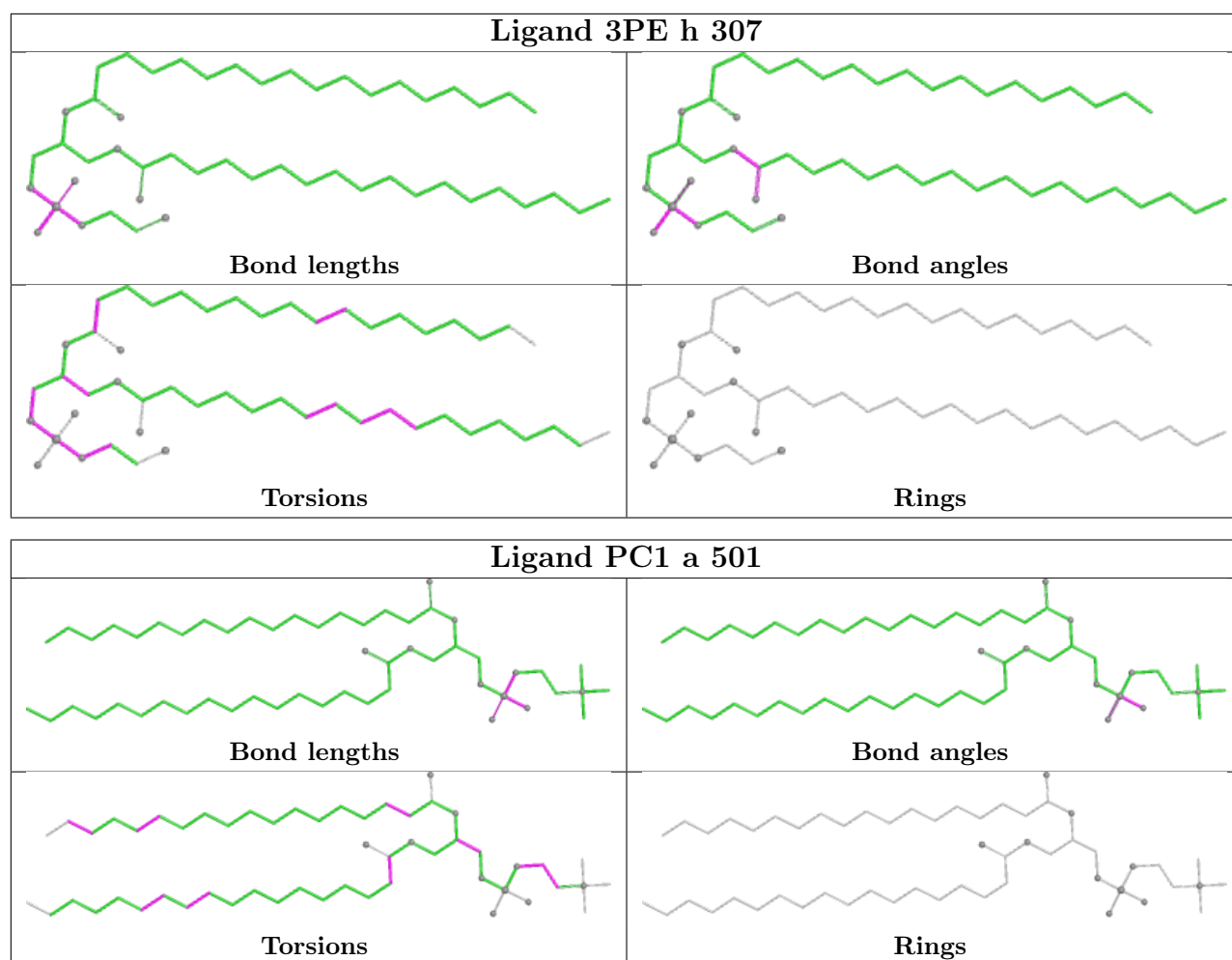
Ligand PGT H 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

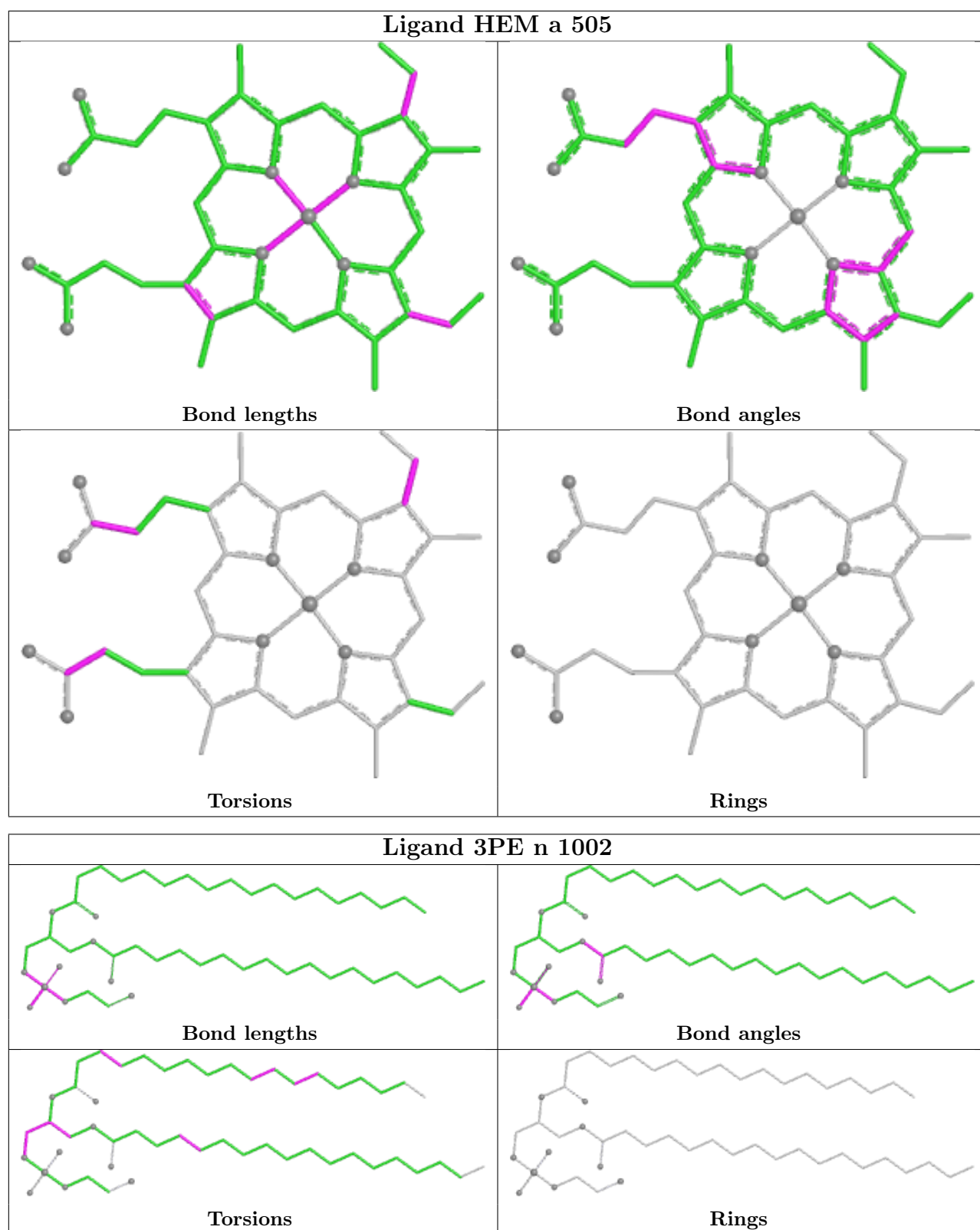
Ligand PC1 d 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

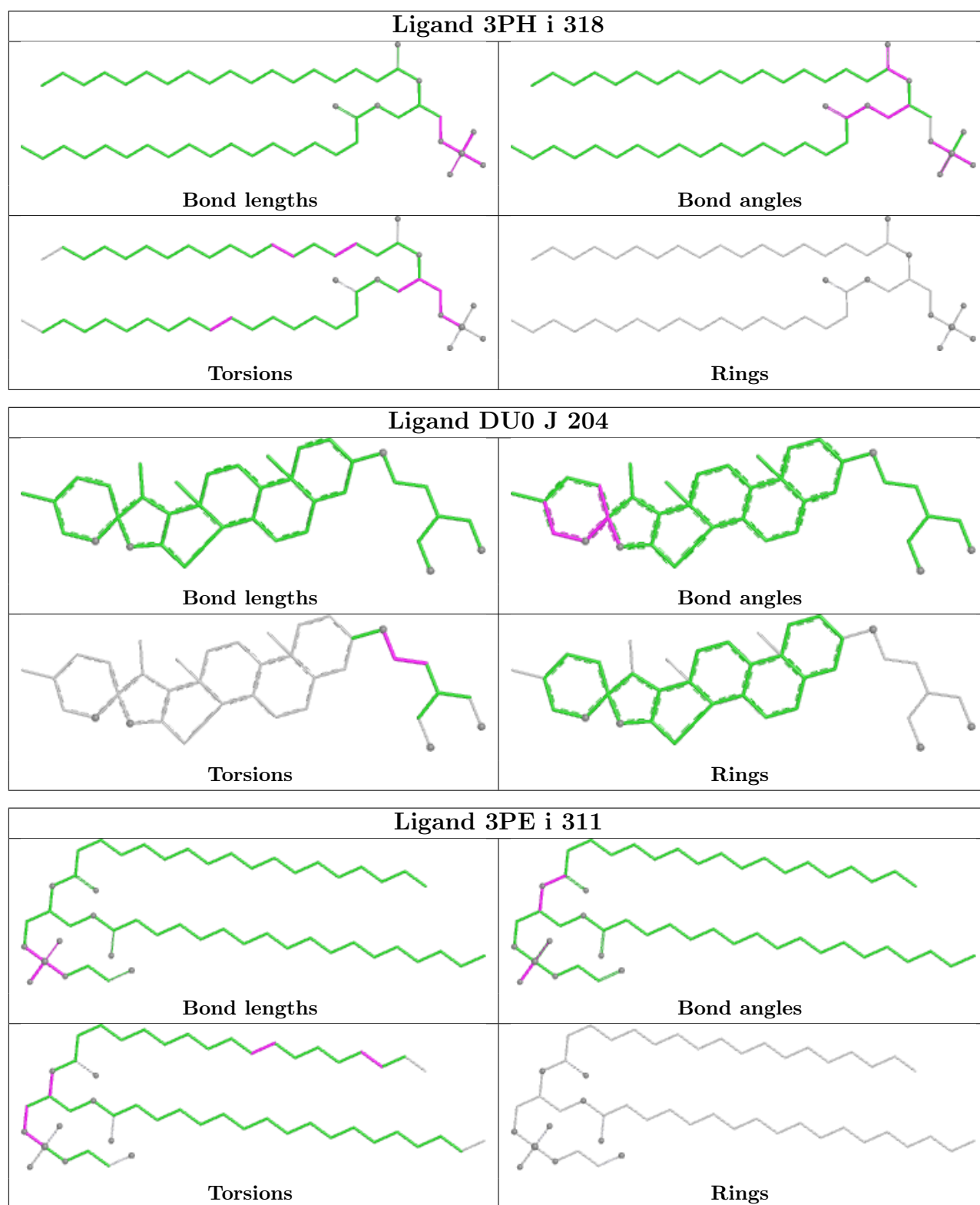
Ligand 3PE m 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

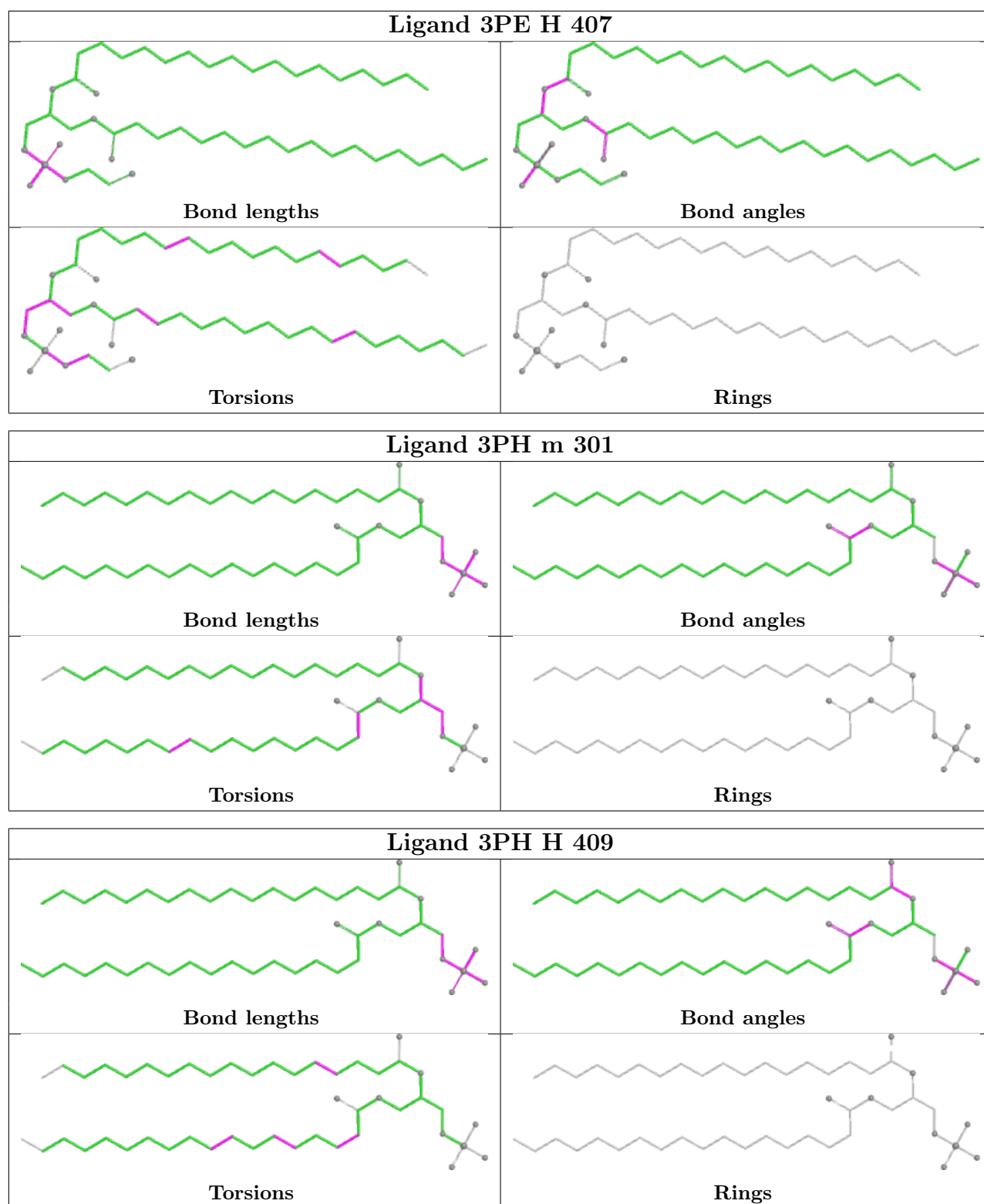


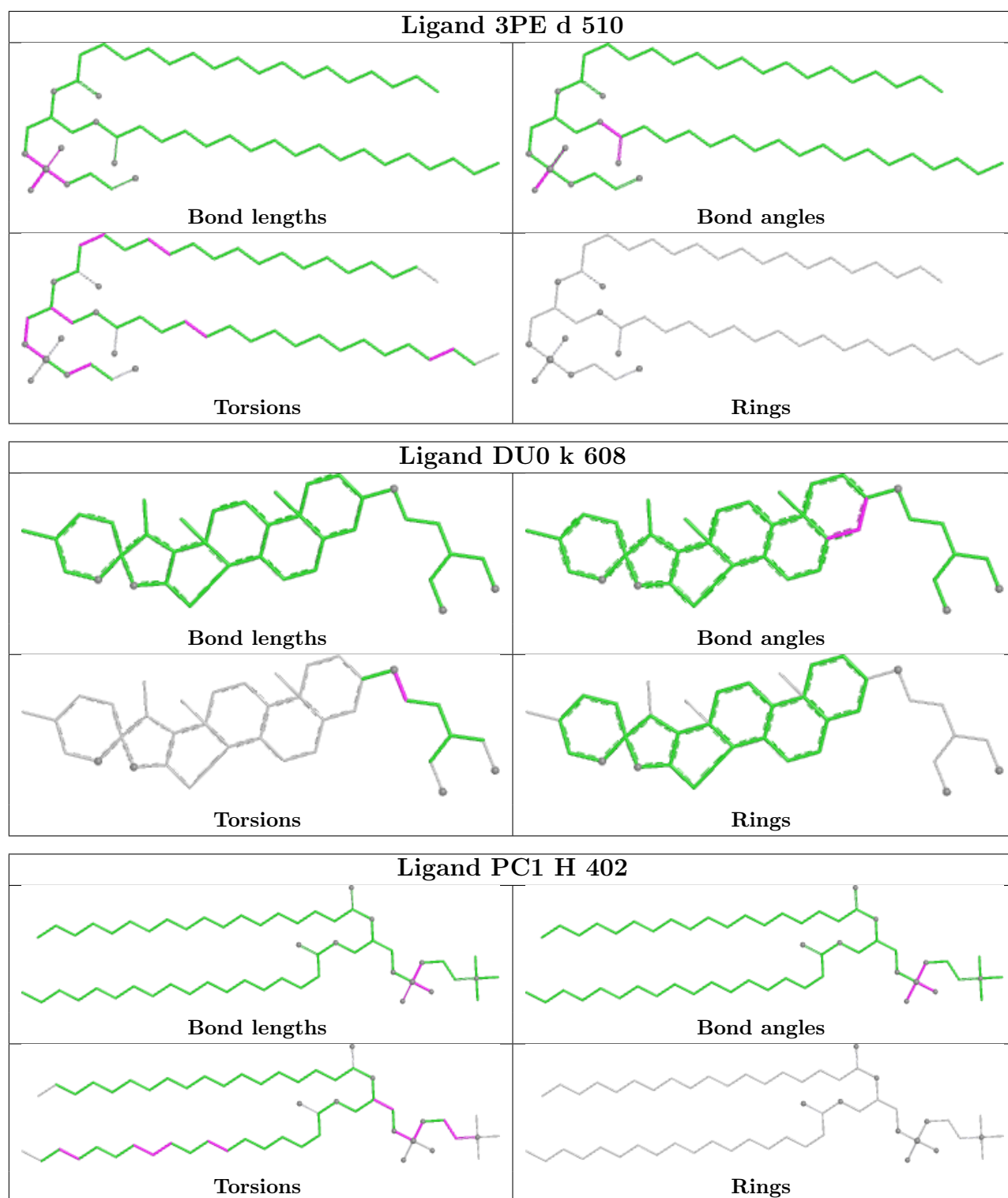


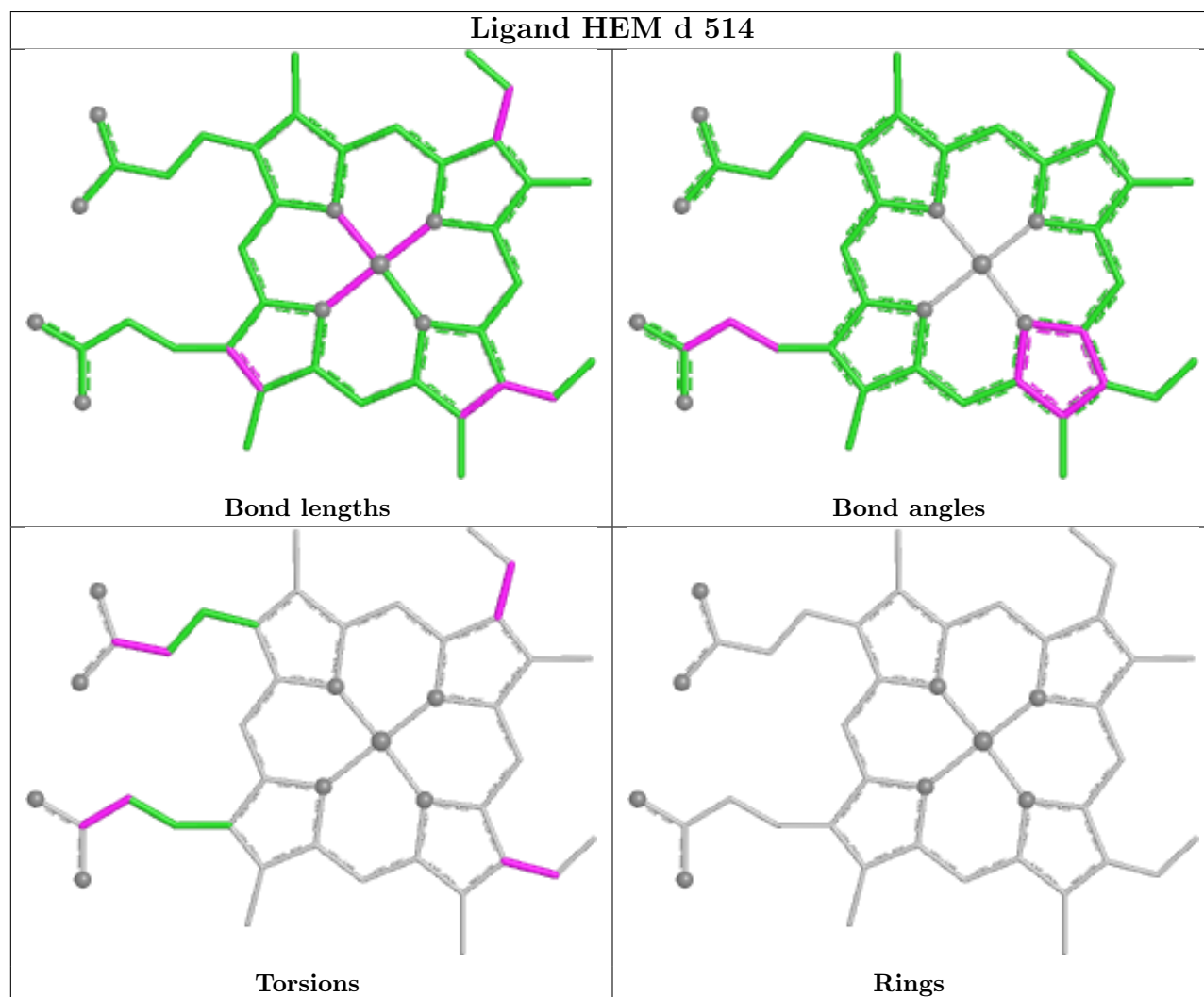
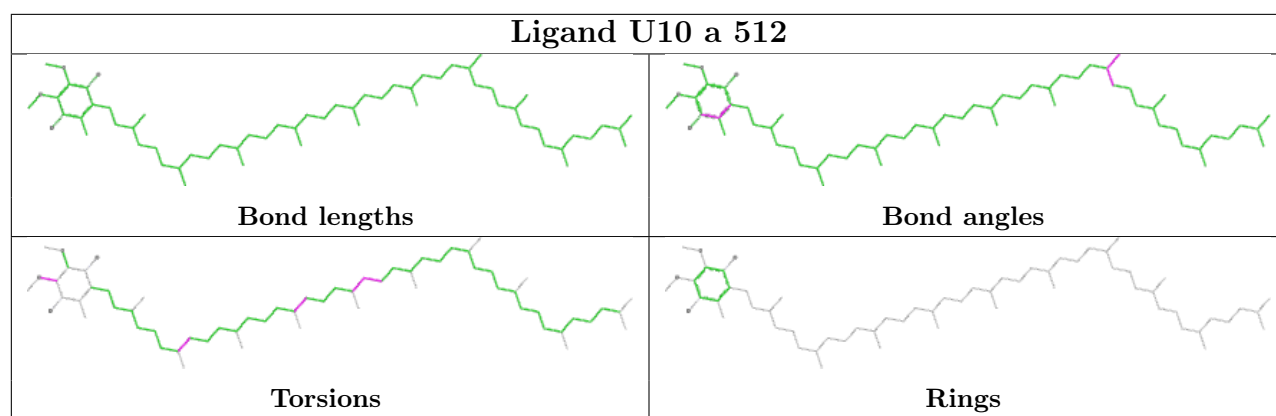


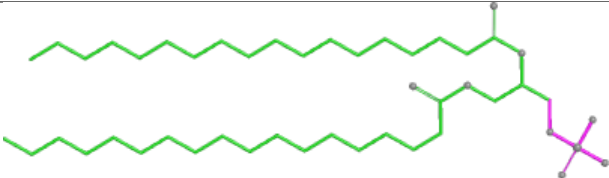

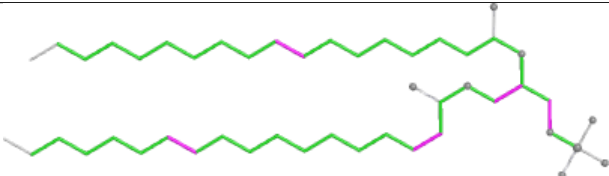
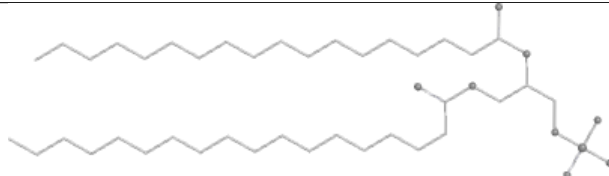


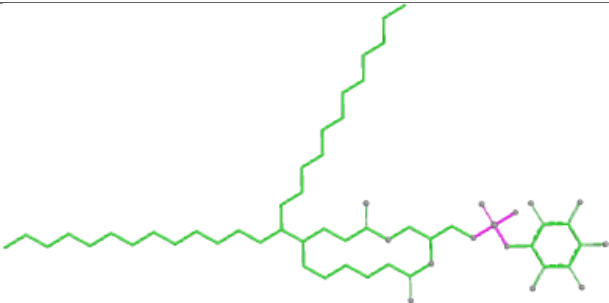
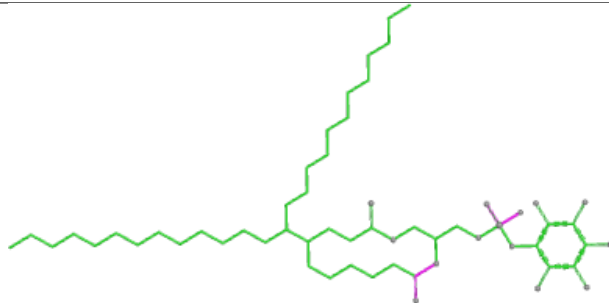
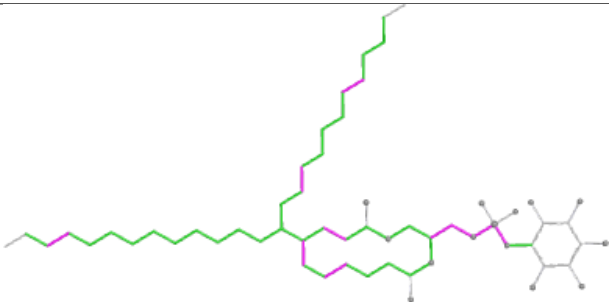
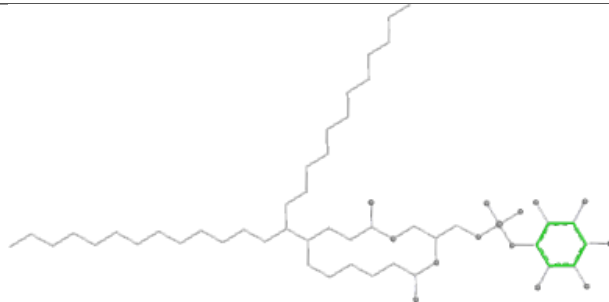


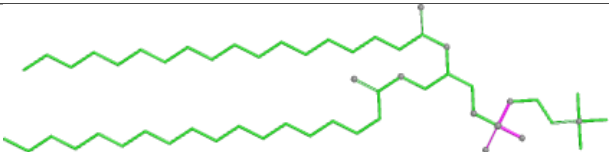
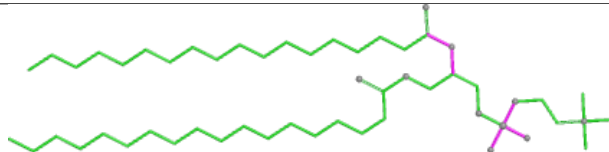
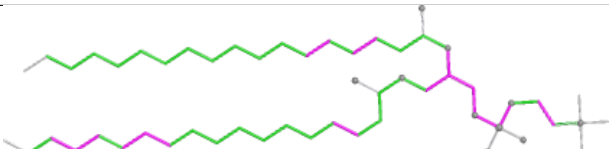
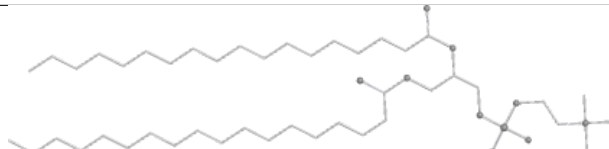


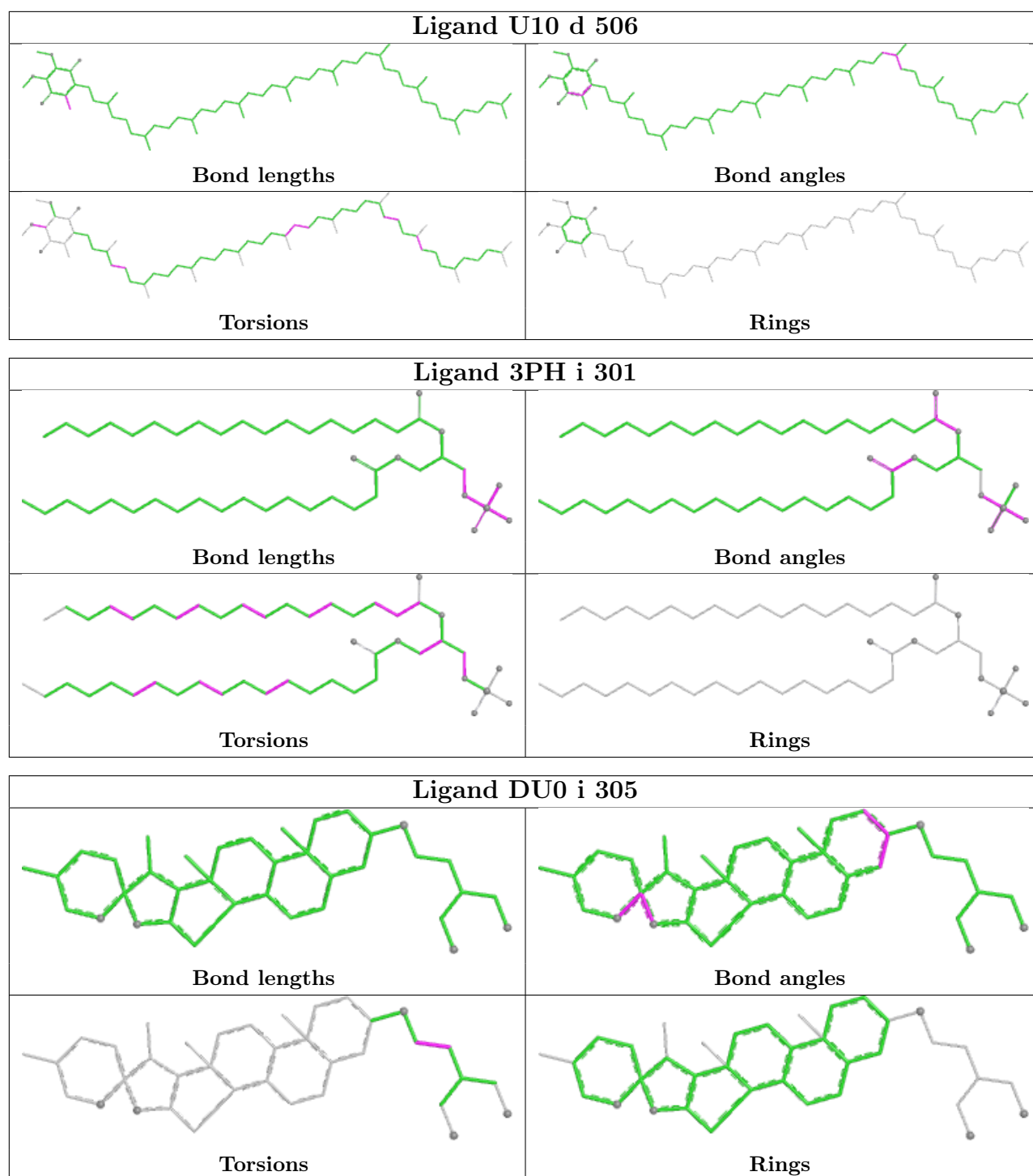


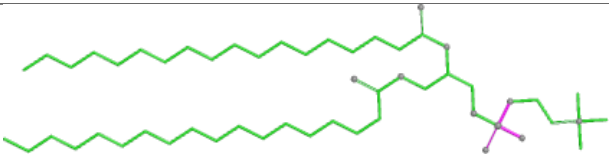
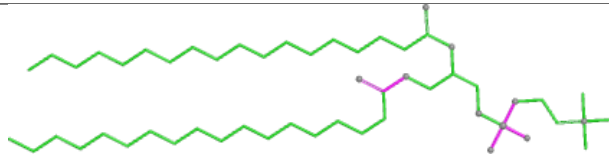
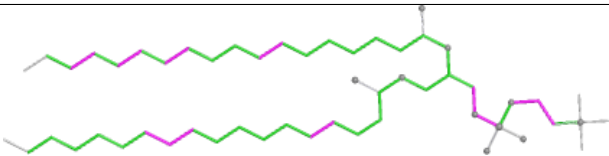
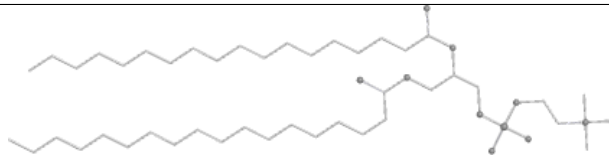


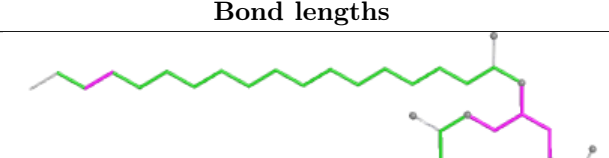
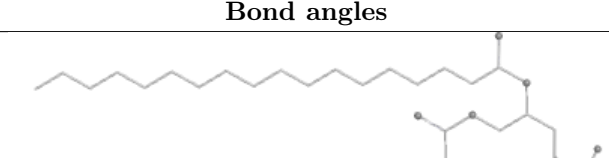
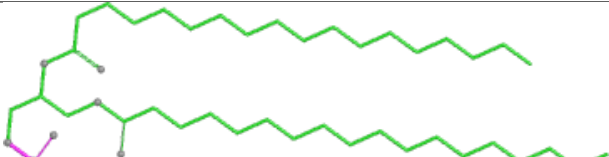
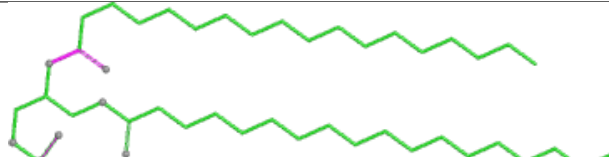
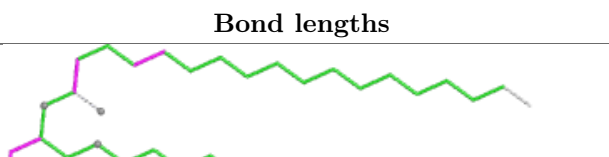
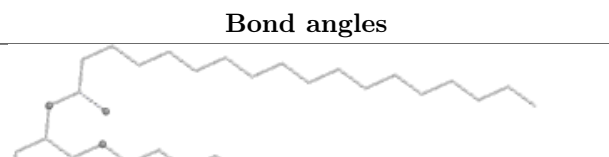


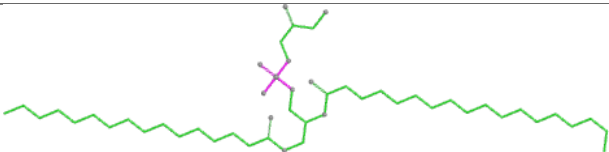
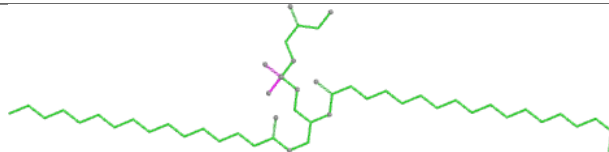
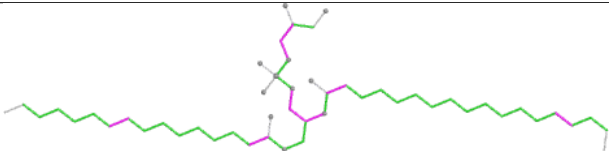
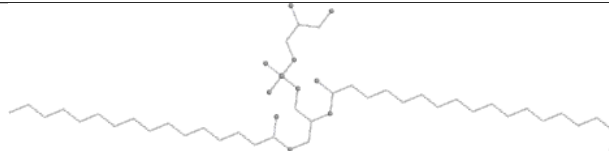
Ligand 3PH j 1003	
	
Bond lengths	Bond angles
	
Torsions	Rings

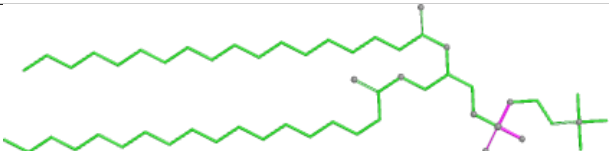
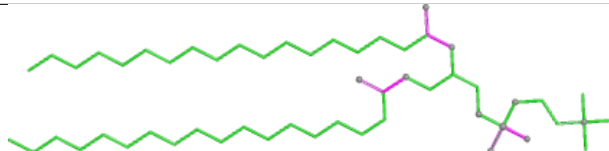
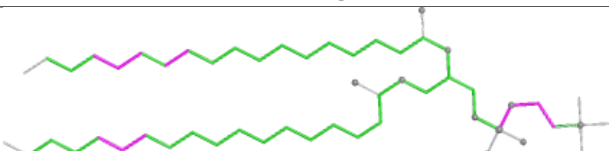
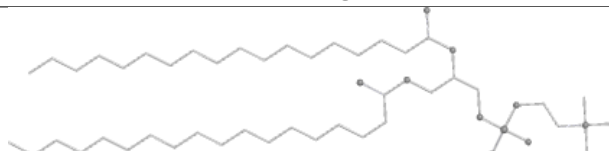
Ligand T7X g 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

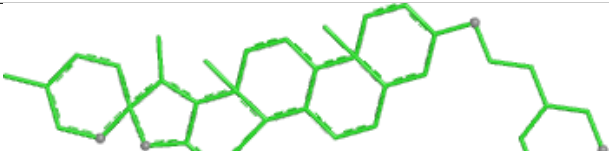
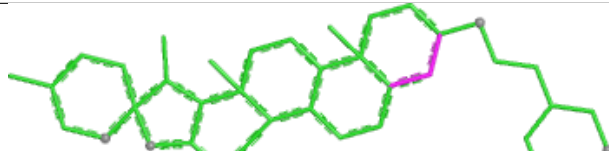
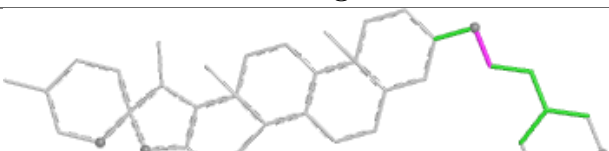
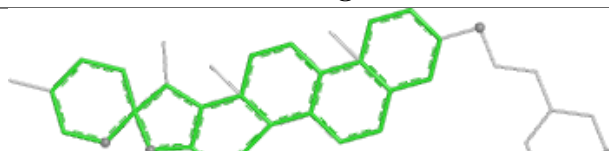
Ligand PC1 f 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

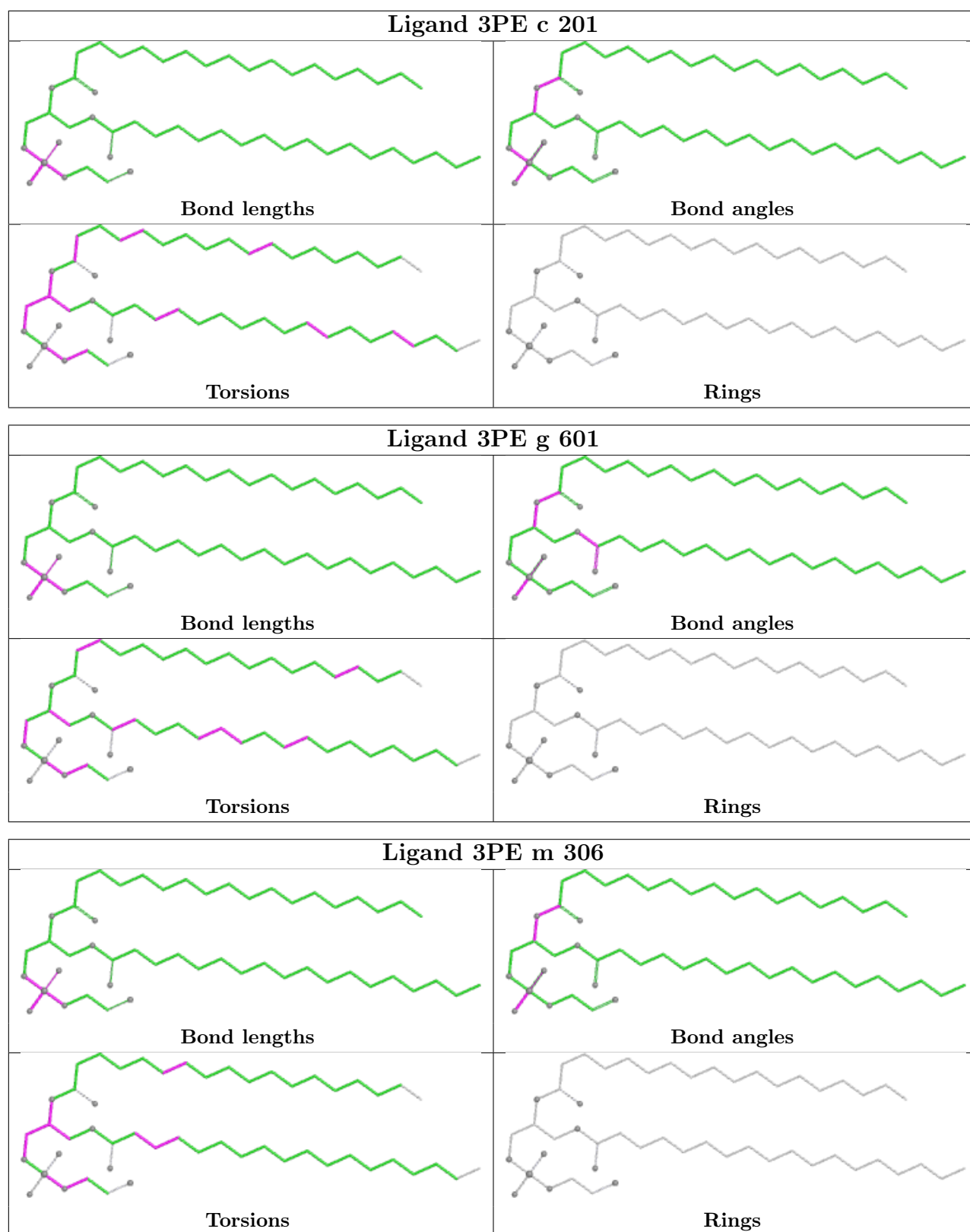


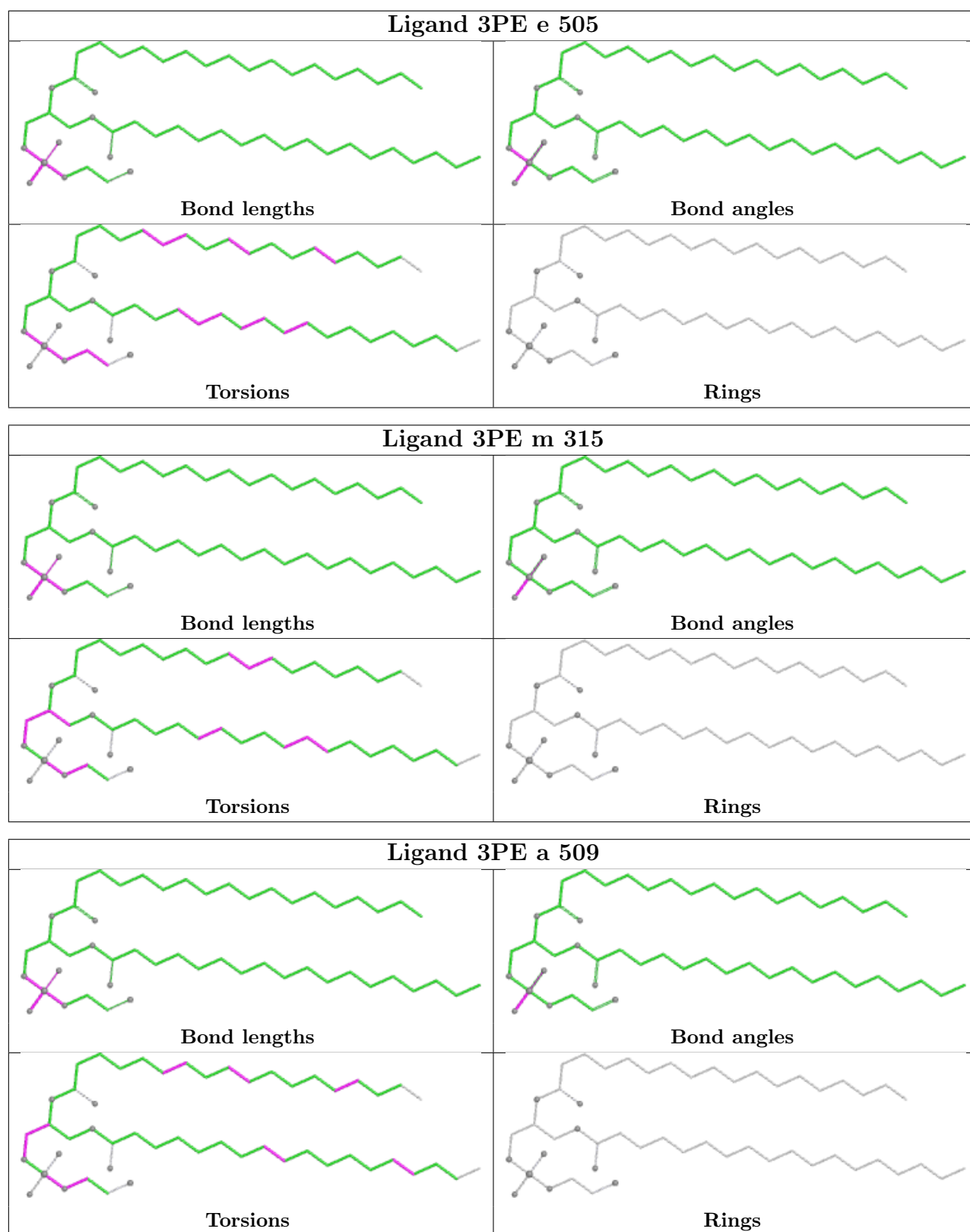
Ligand PC1 M 608	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand 3PH g 603	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand 3PE H 404	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

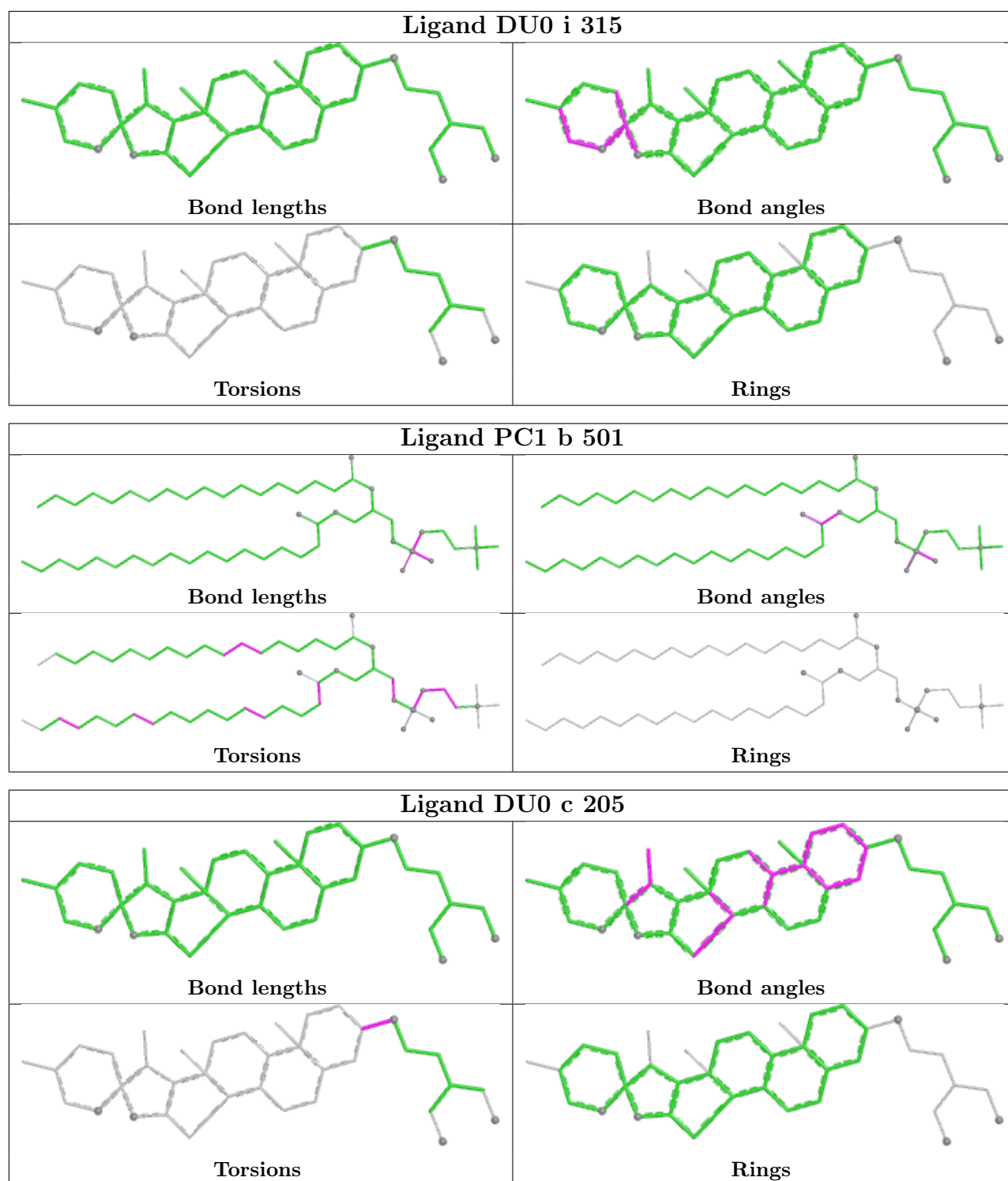
Ligand PGT A 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

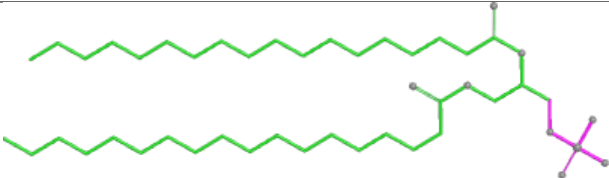
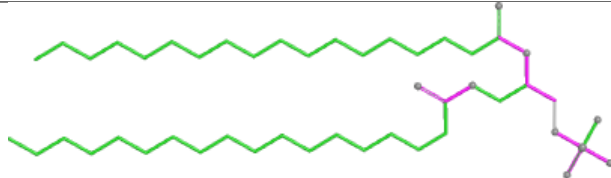
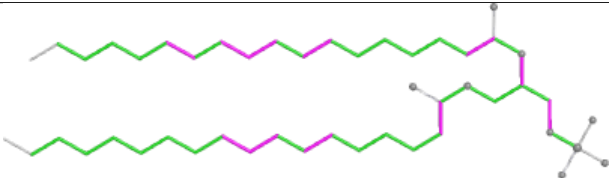
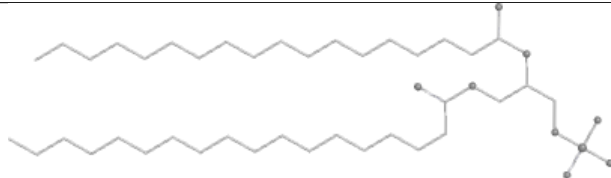
Ligand PC1 D 1001	
	
Bond lengths	Bond angles
	
Torsions	Rings

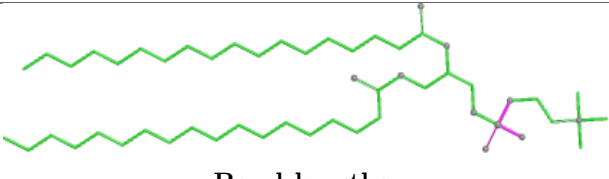
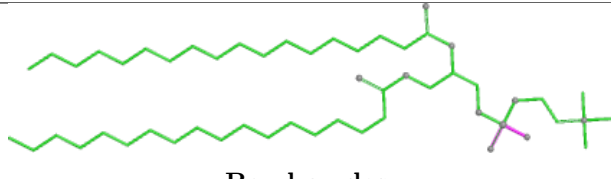
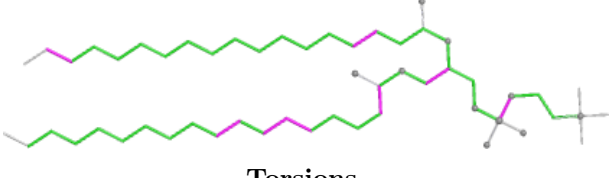
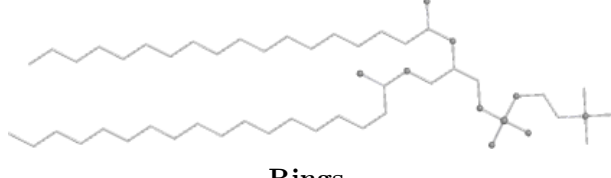
Ligand DU0 d 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

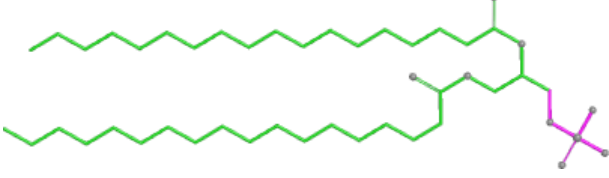
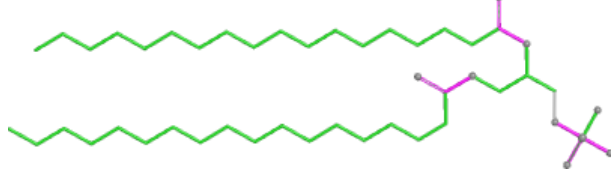
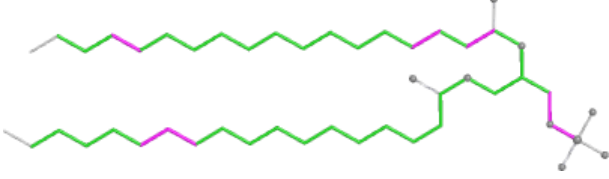
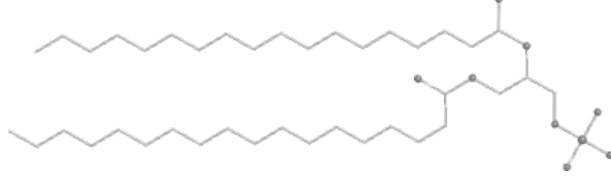


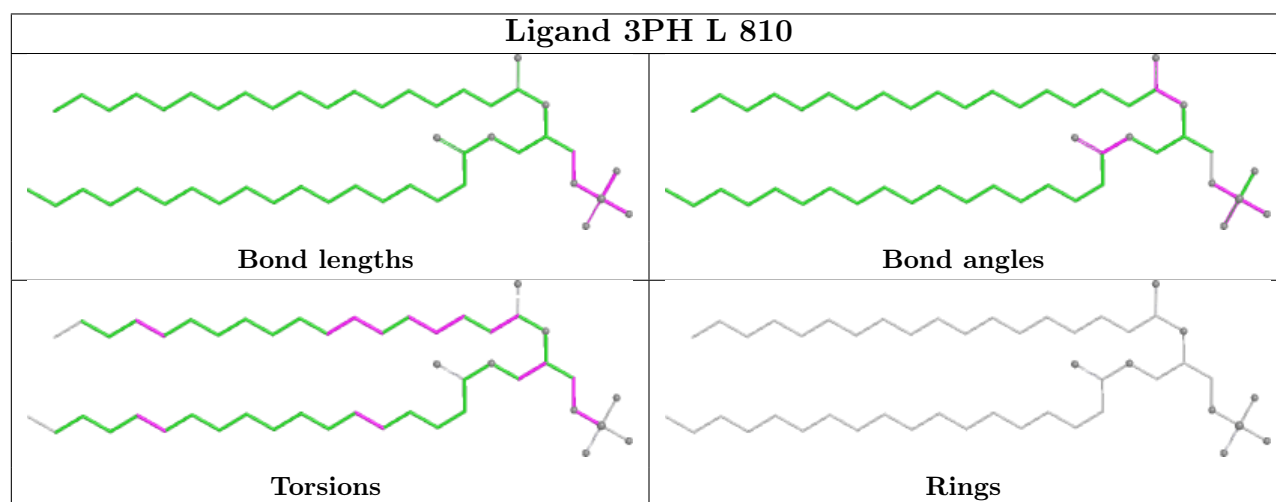
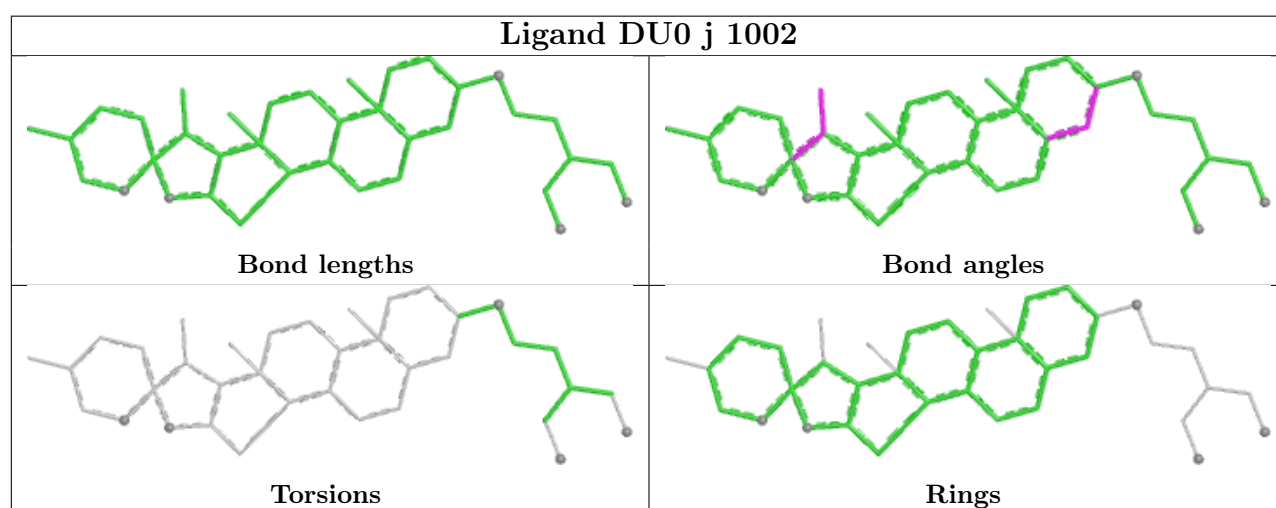
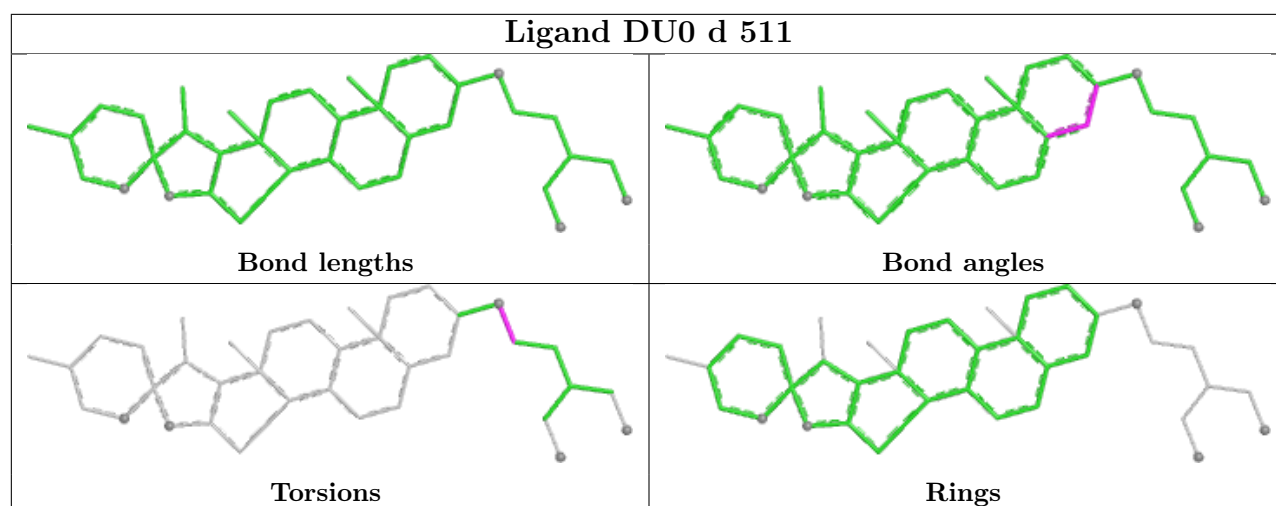


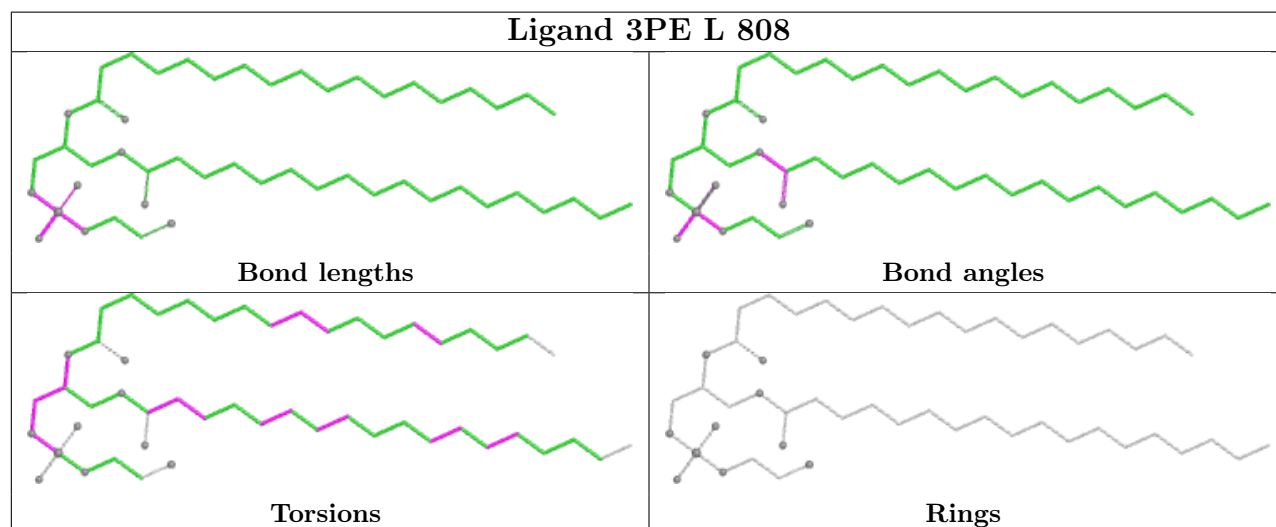
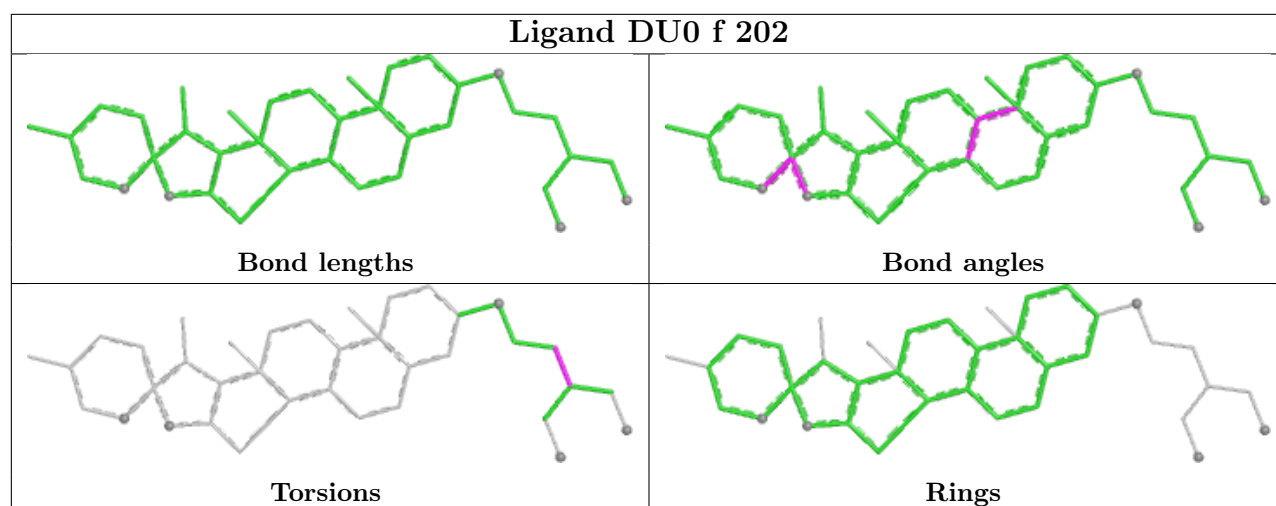
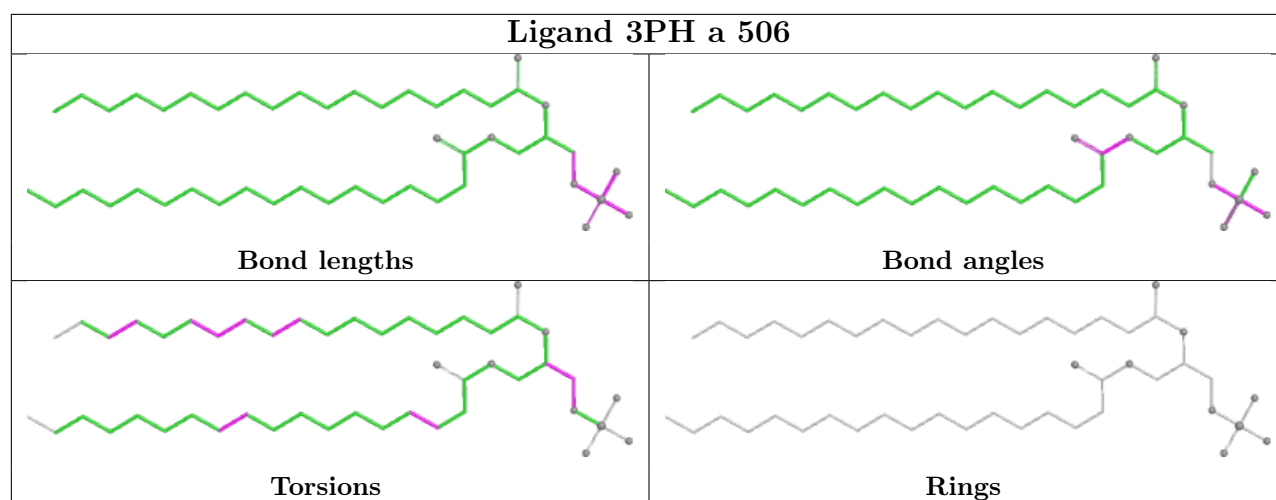


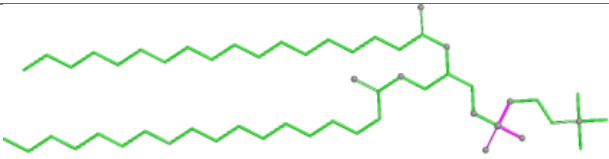
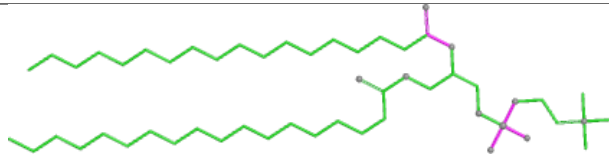
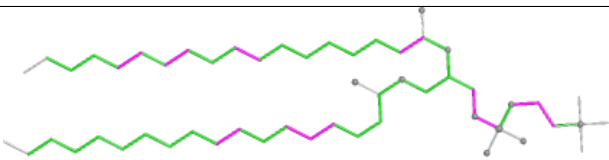
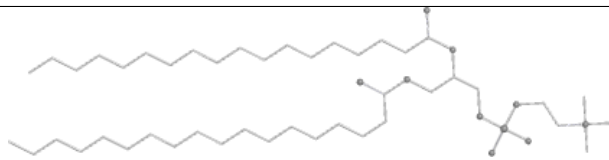
Ligand 3PH M 604	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

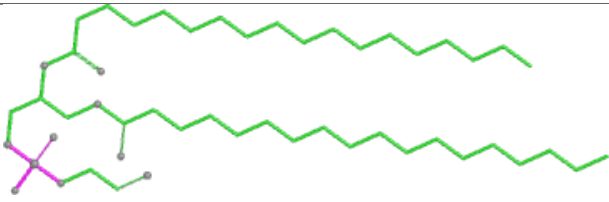
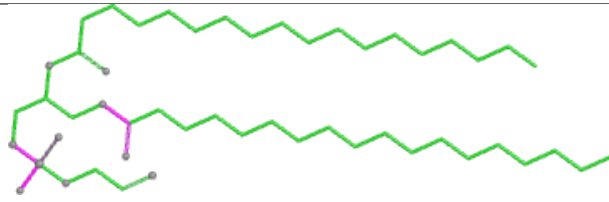
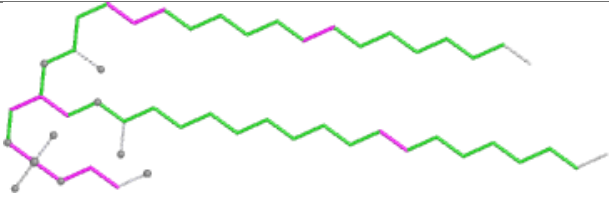
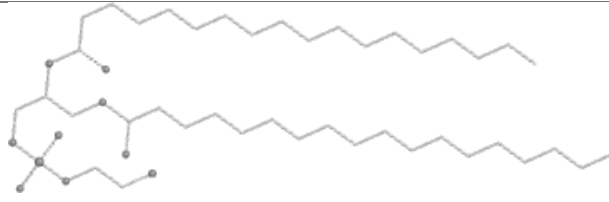
Ligand PC1 m 314	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

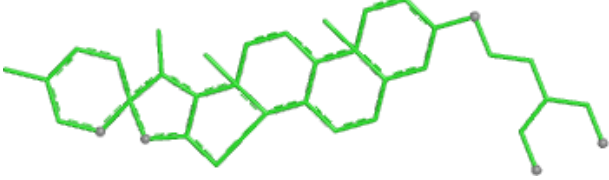
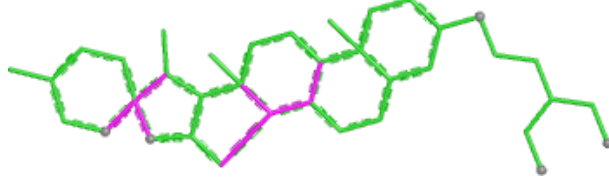
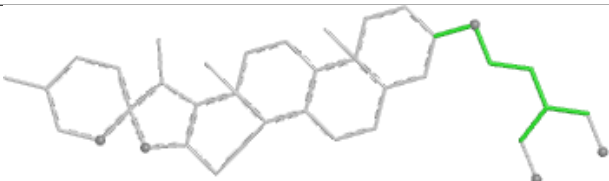
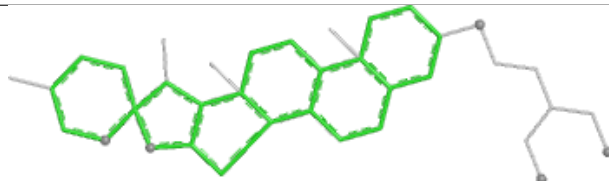
Ligand 3PH L 801	
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 <p>Torsions</p>	 <p>Rings</p>

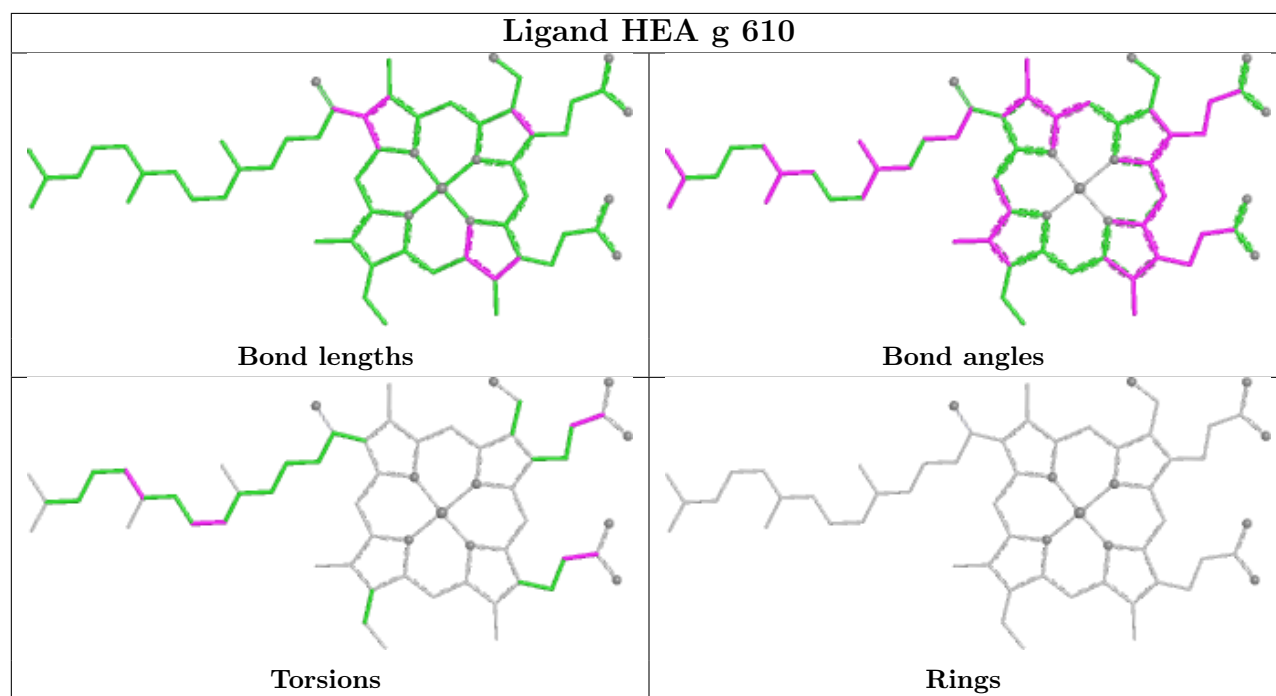
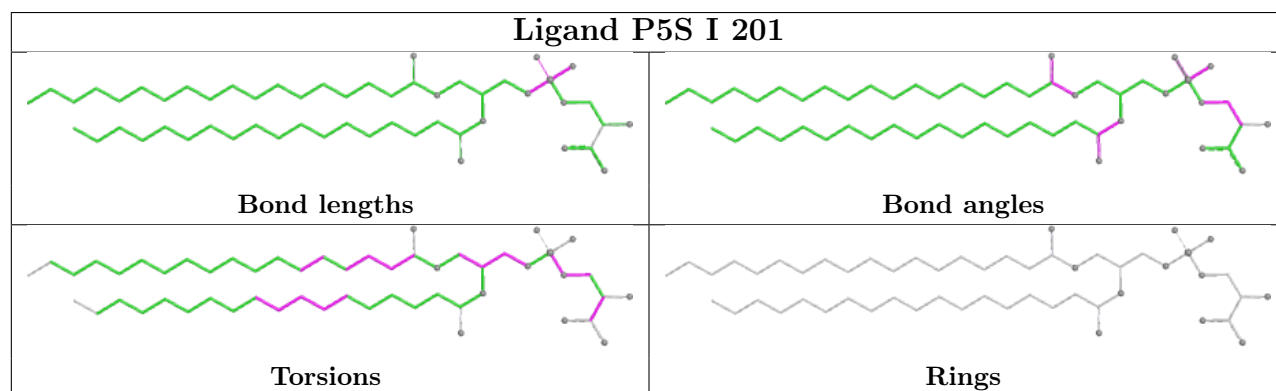
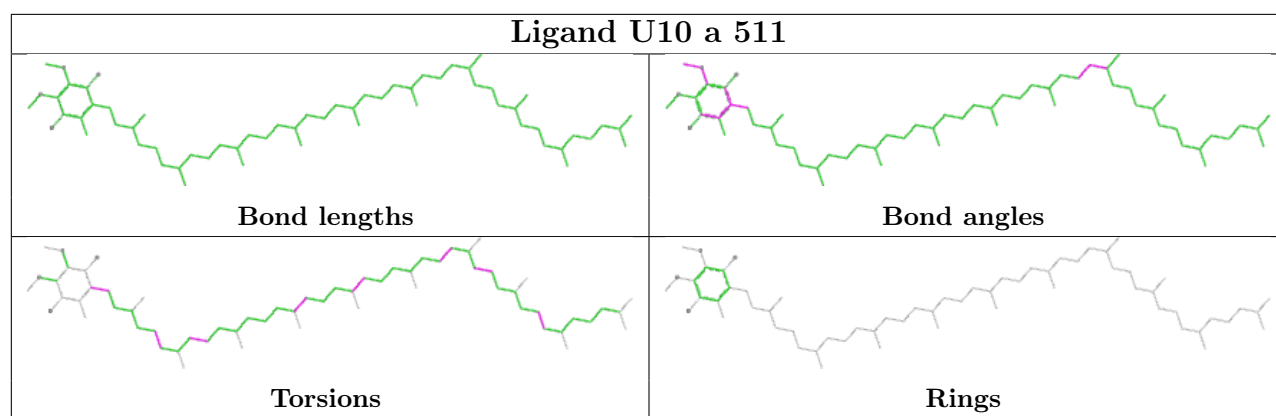


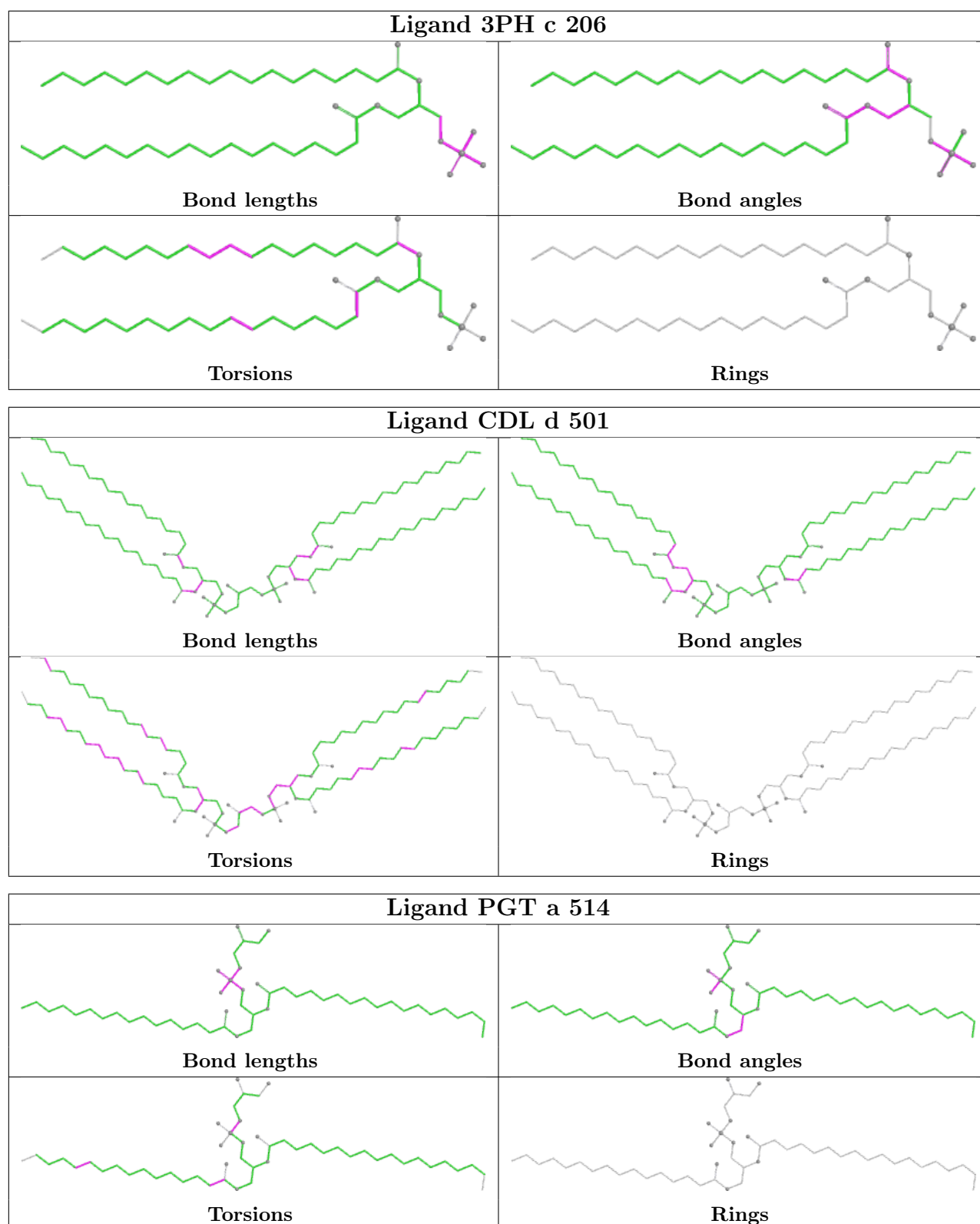


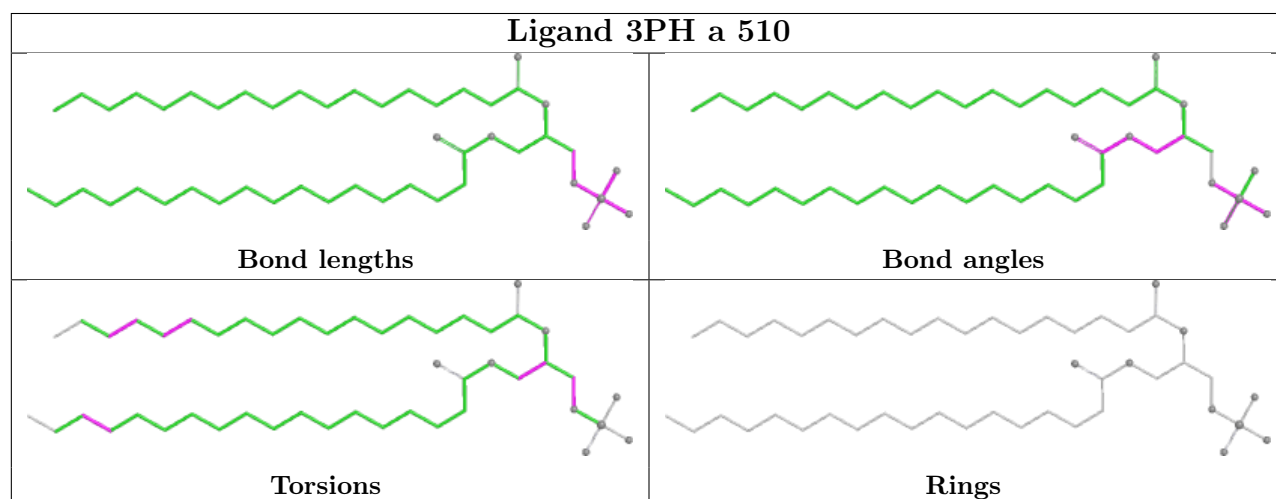
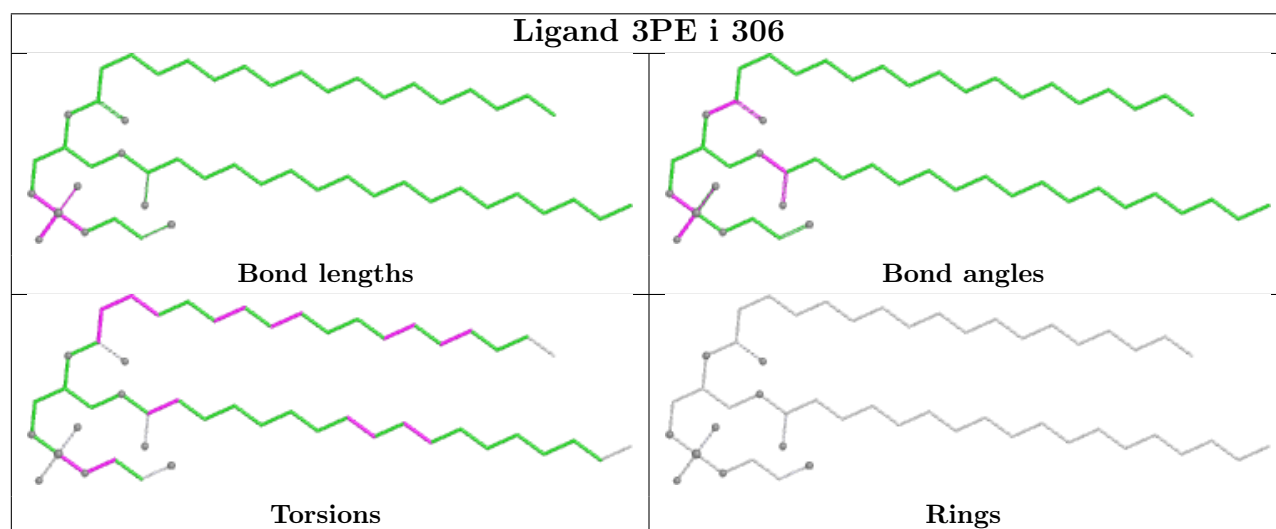
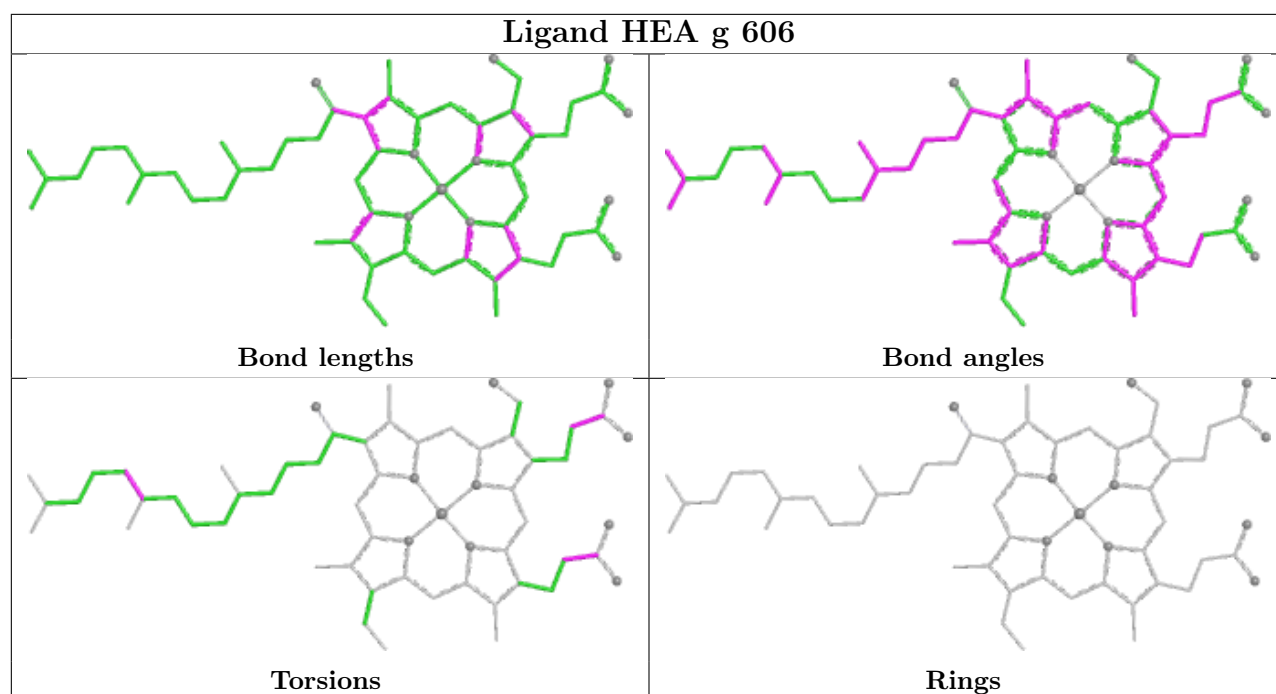
Ligand PC1 b 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

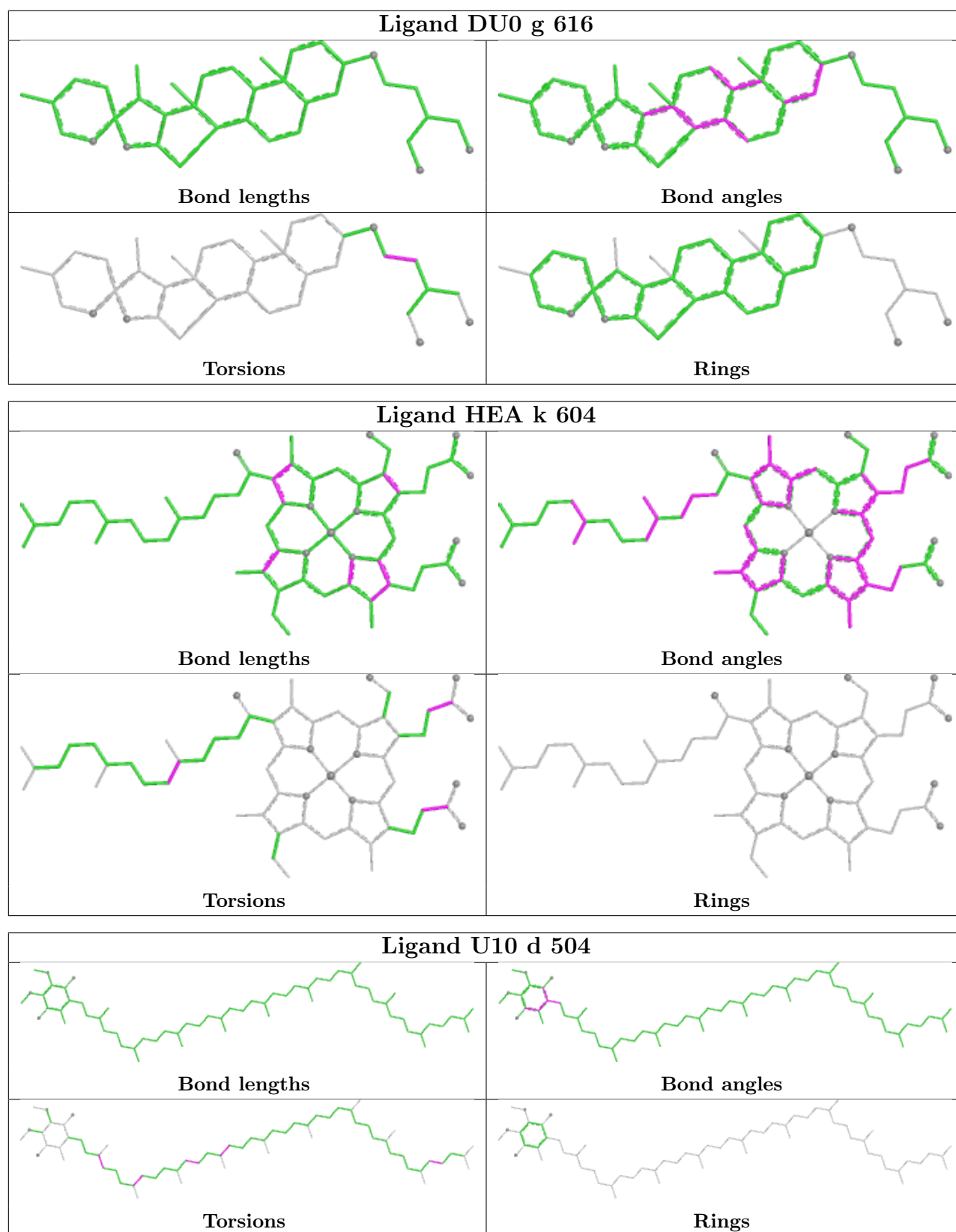
Ligand 3PE h 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

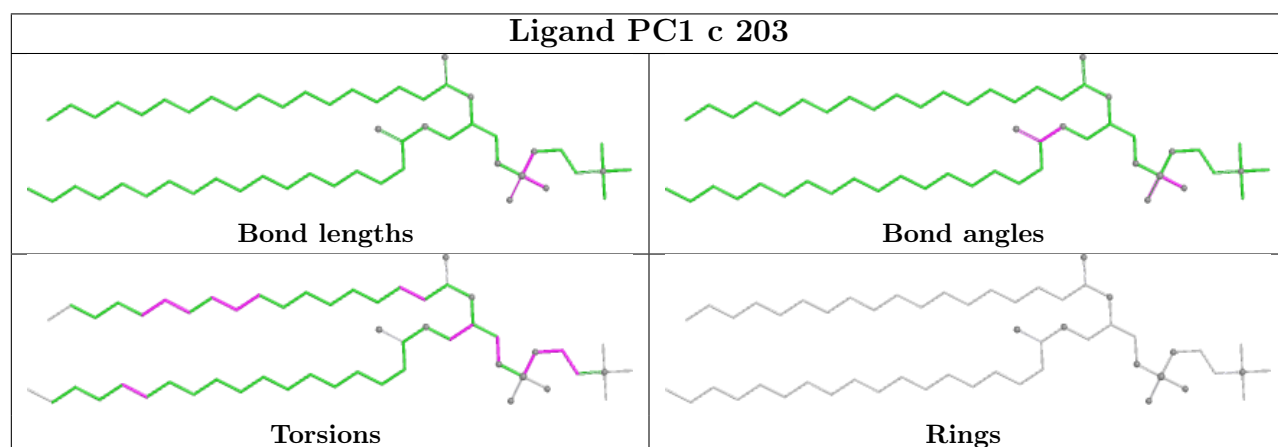
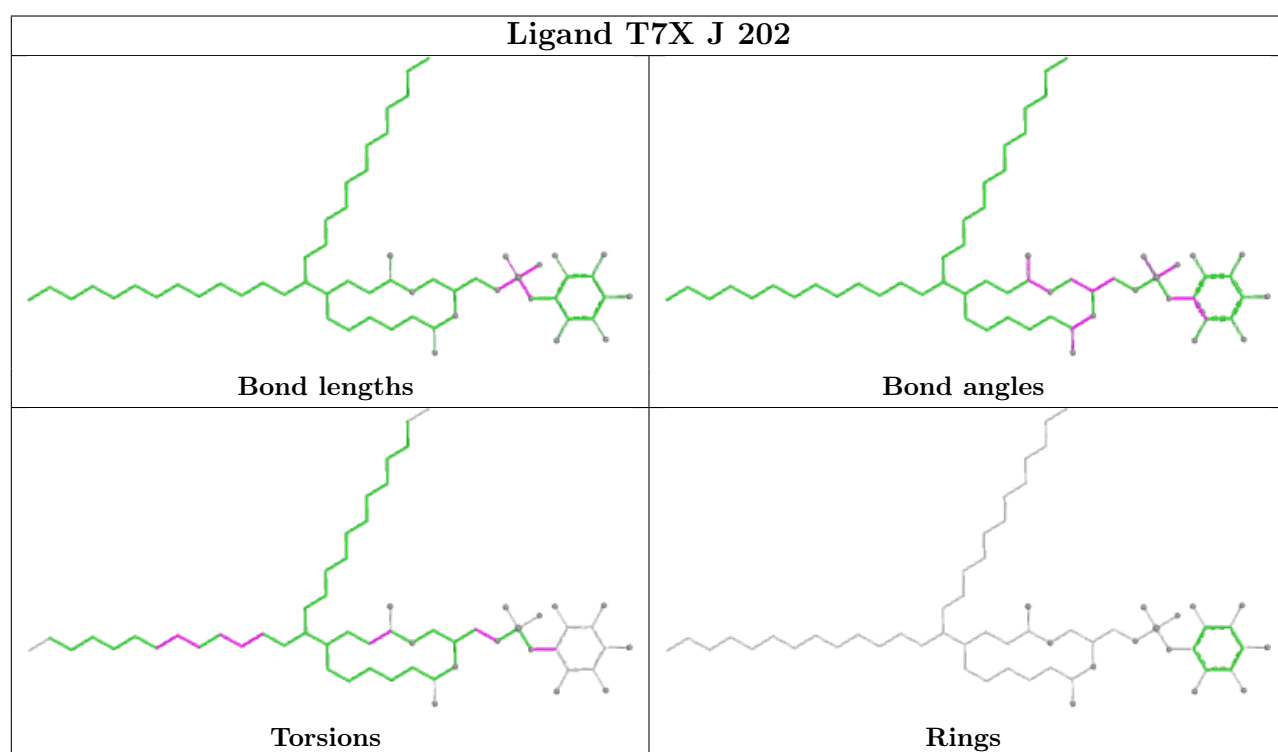
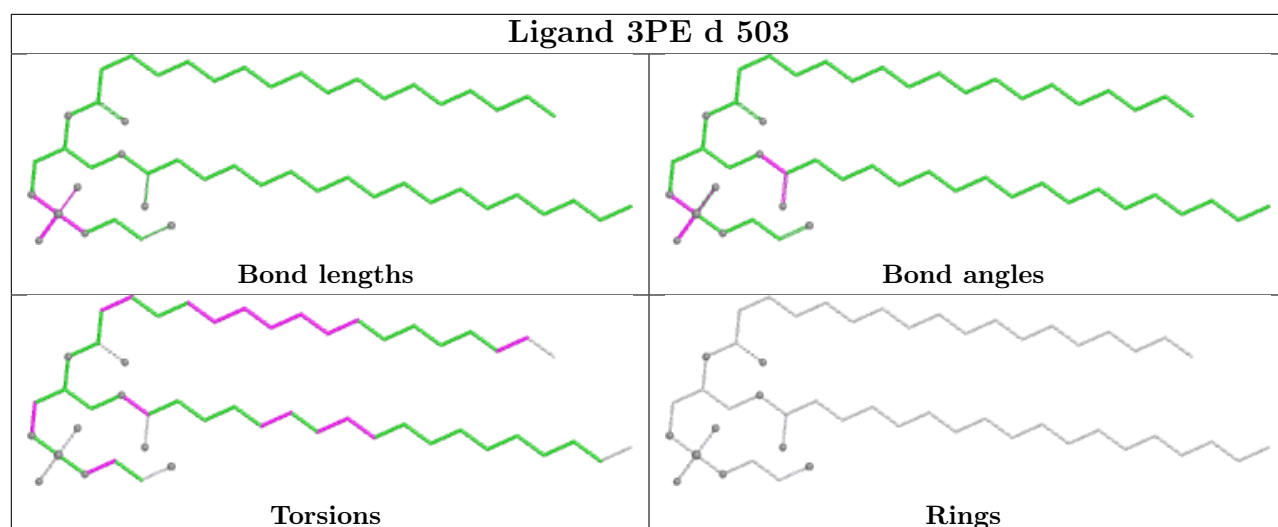
Ligand DU0 A 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

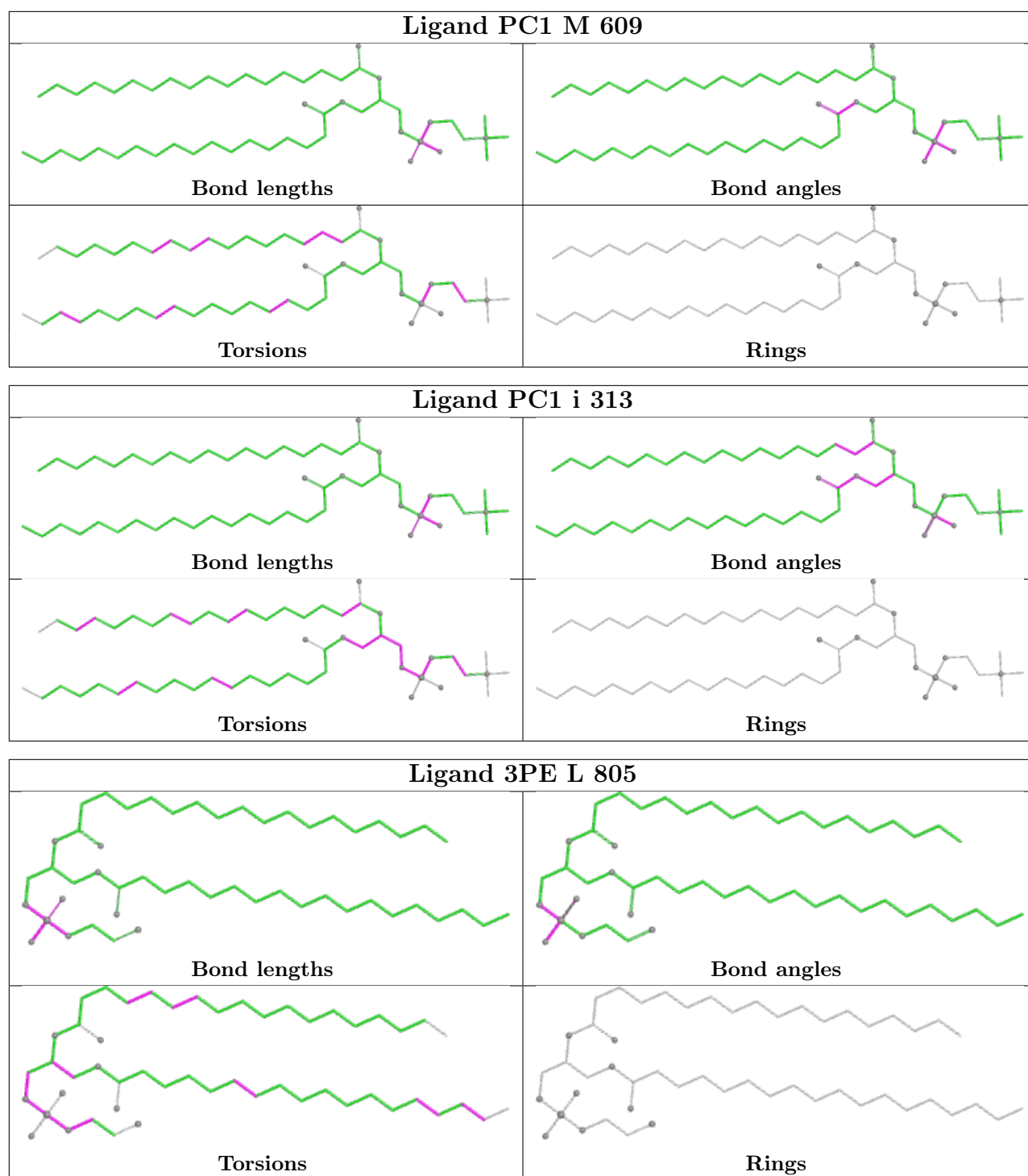


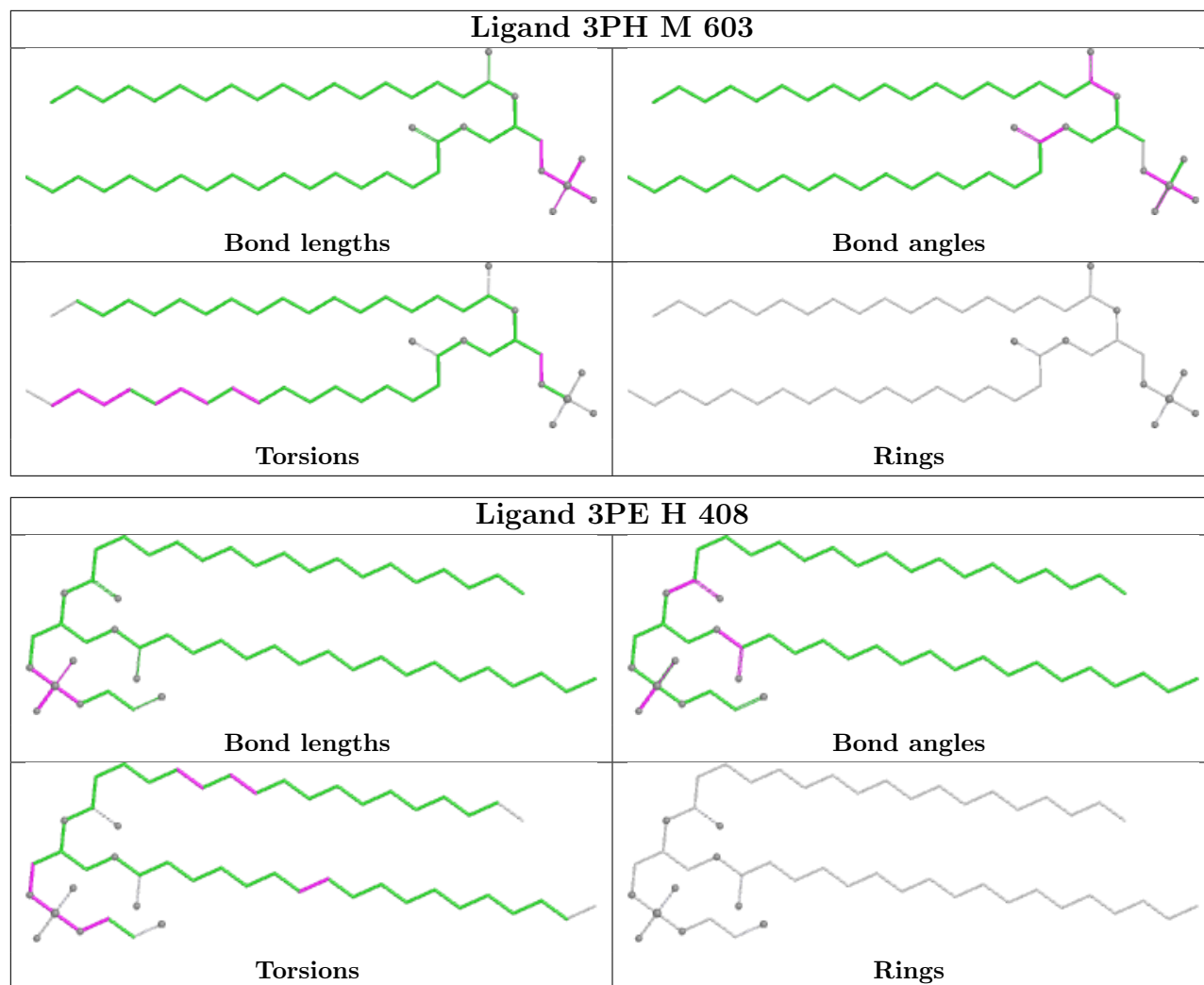


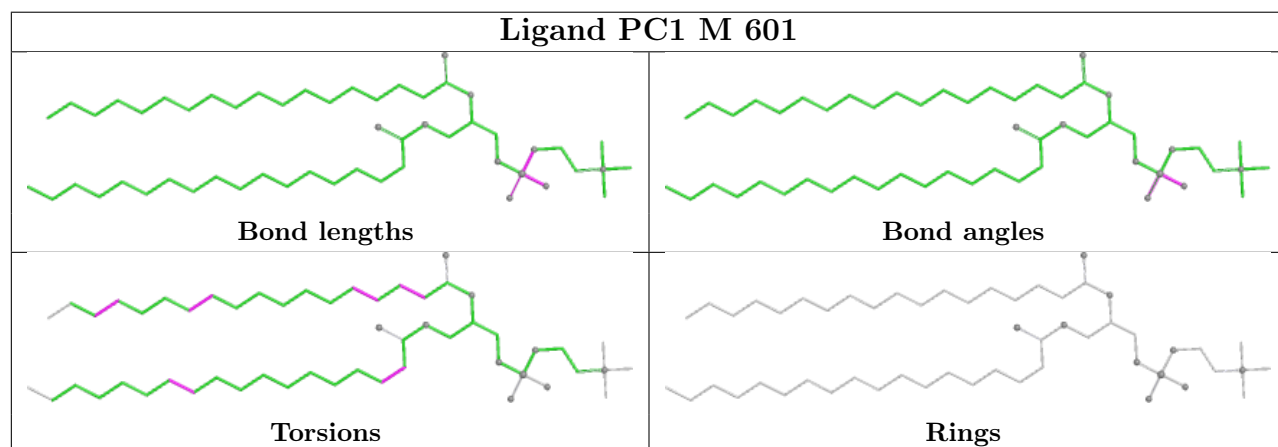
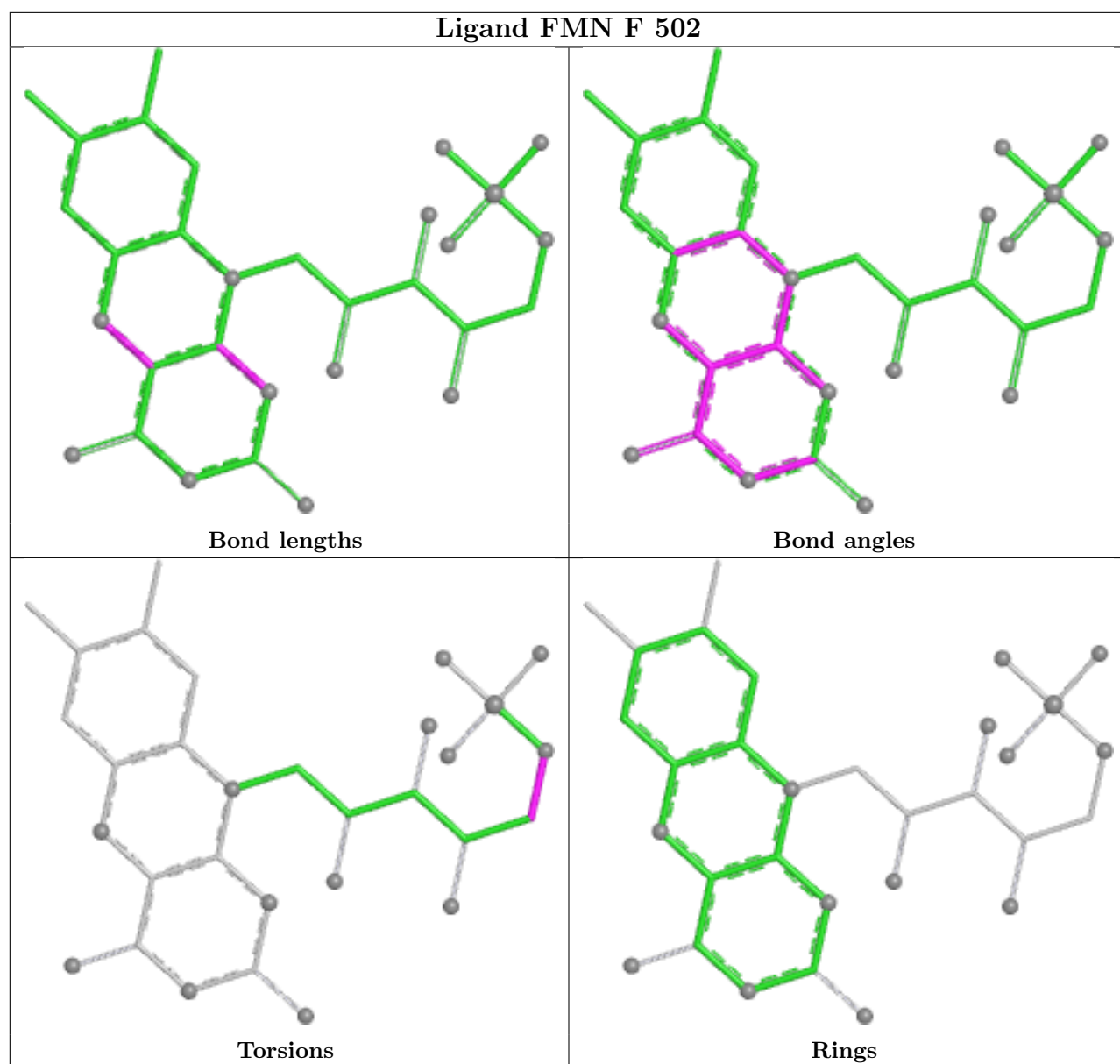


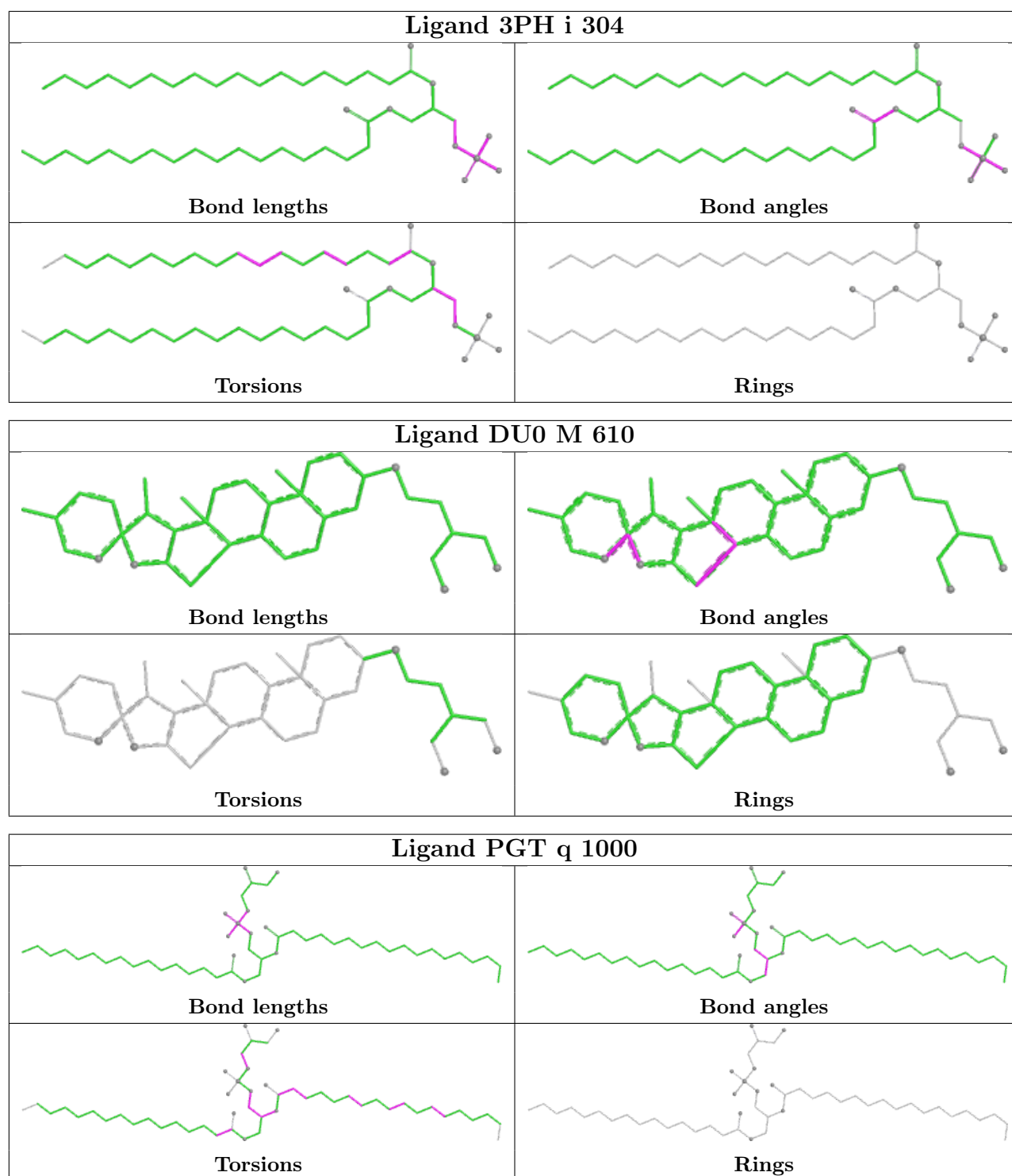


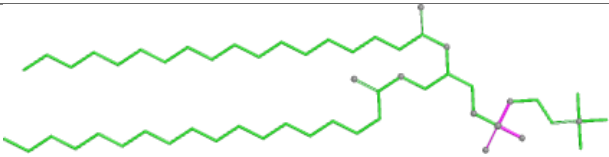
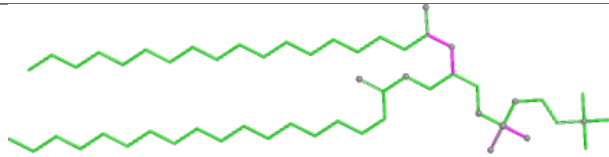
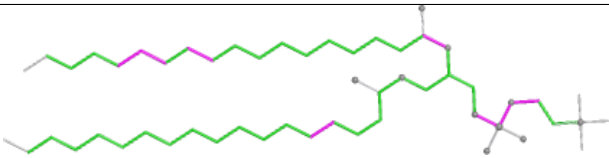
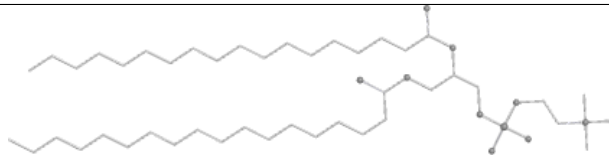


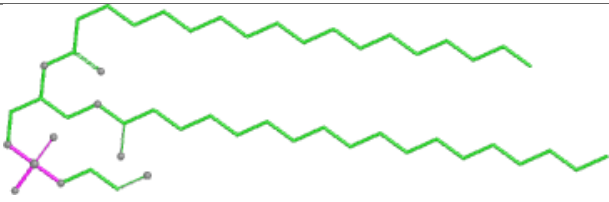
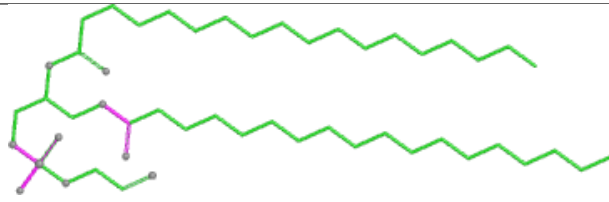
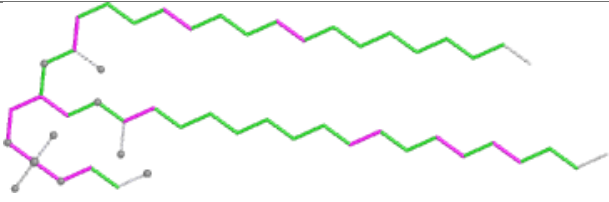
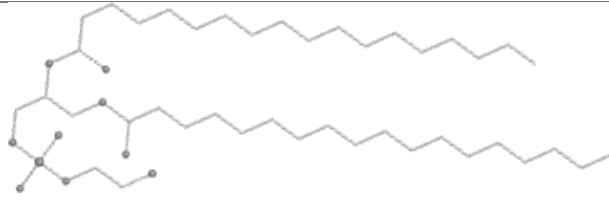


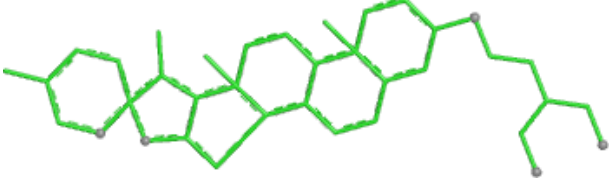
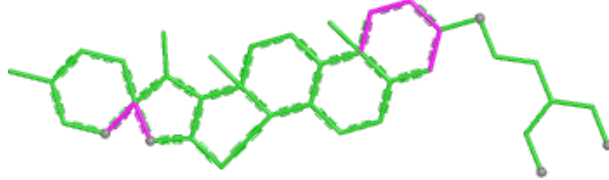
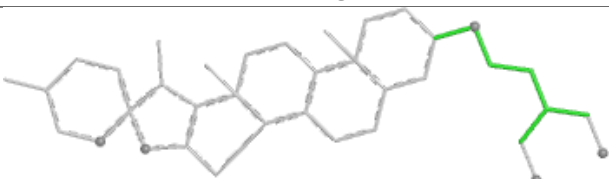
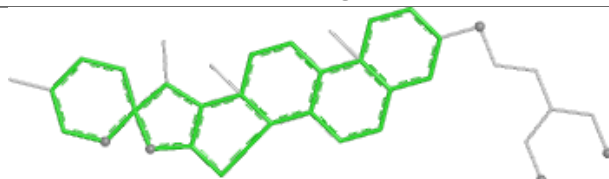


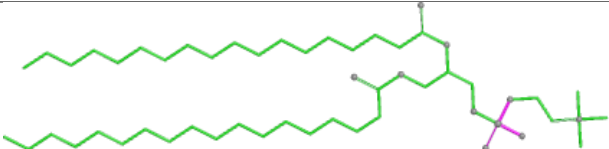
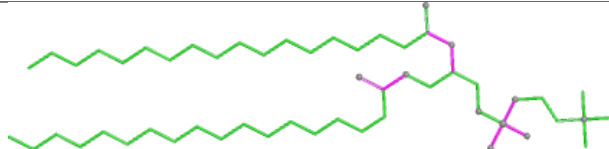
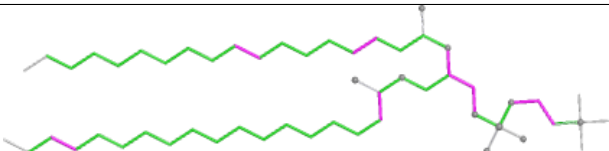
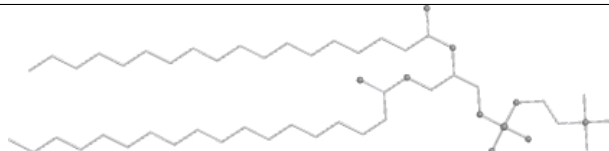


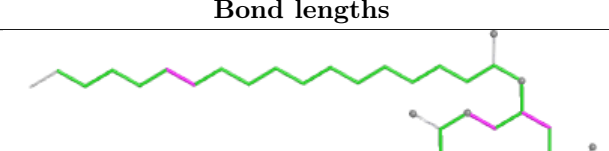
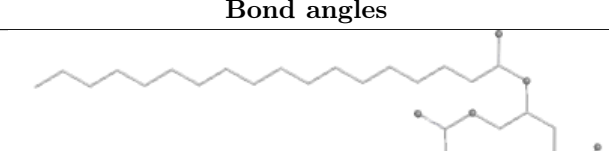
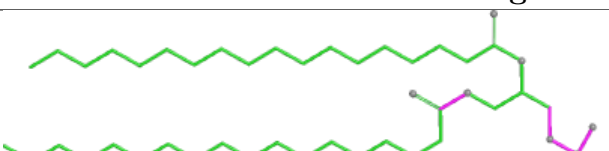

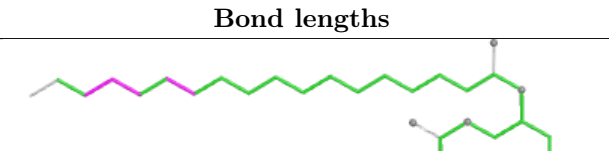
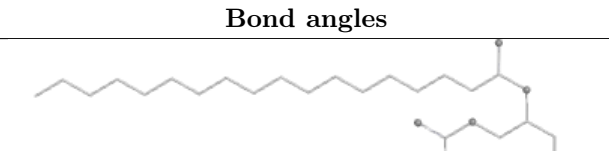


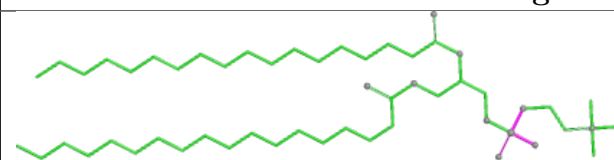
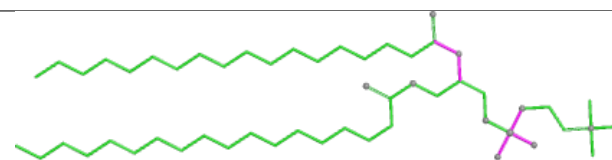
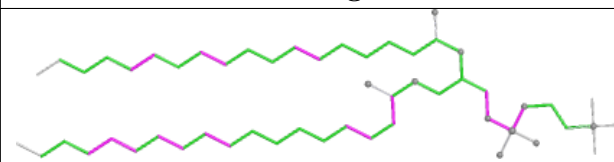
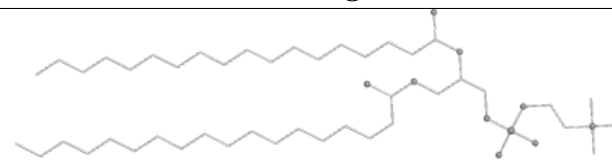


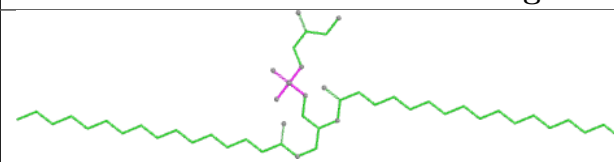
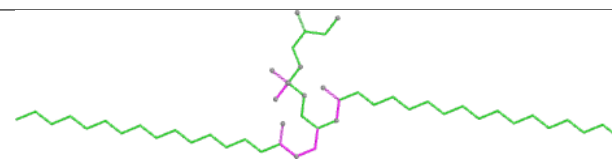
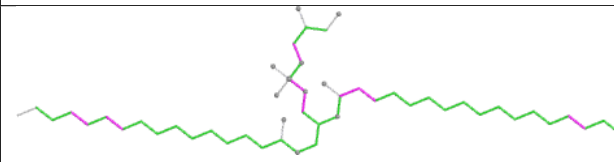
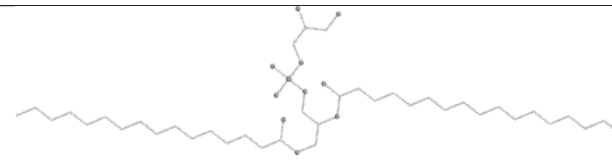
Ligand PC1 l 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

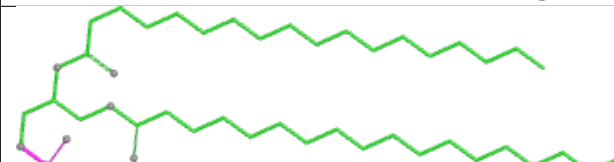
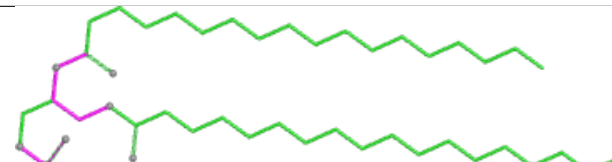

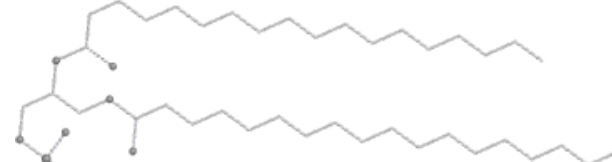
Ligand 3PE i 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

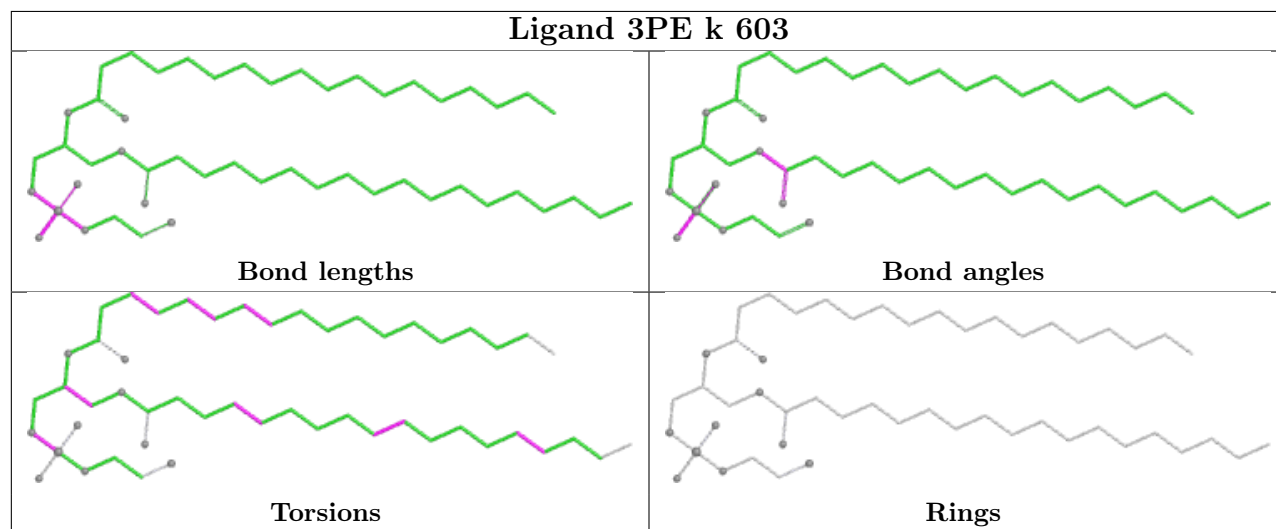
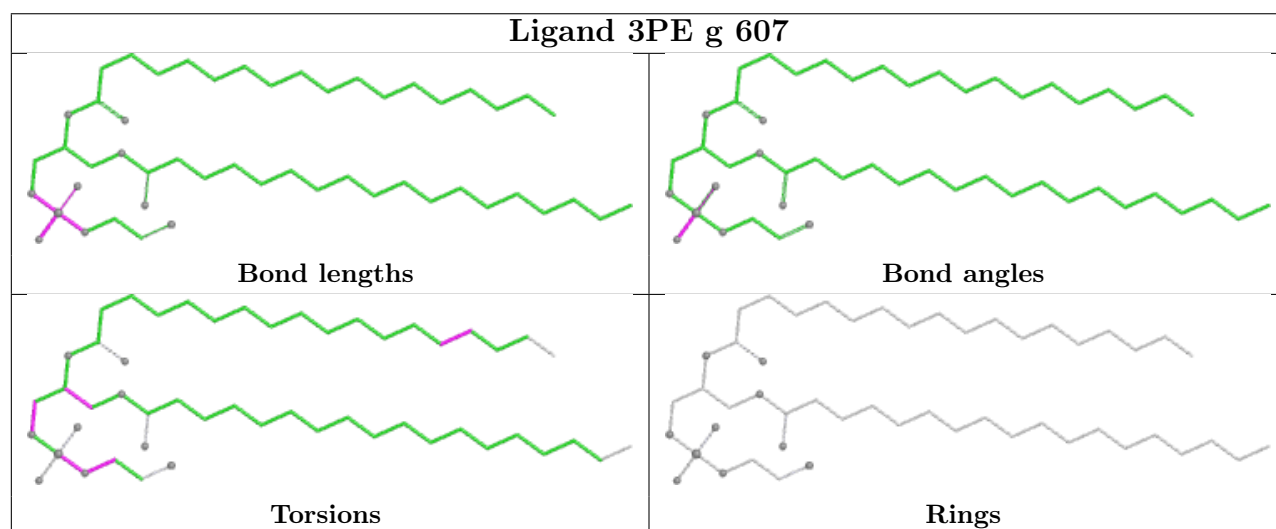
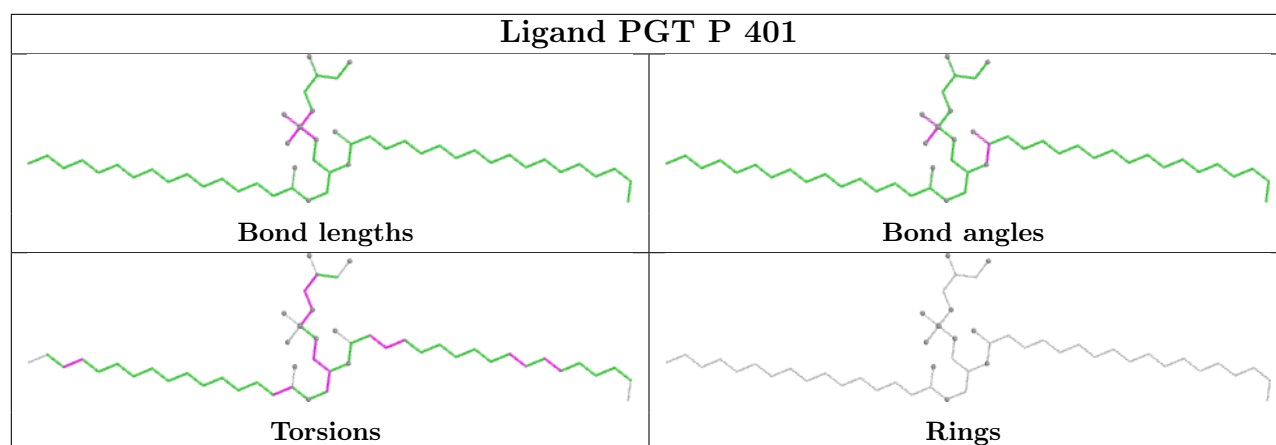
Ligand DU0 g 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

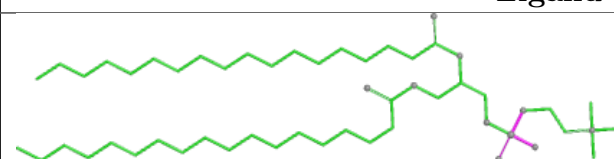
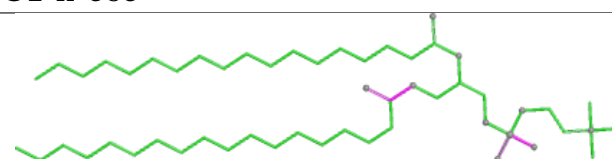
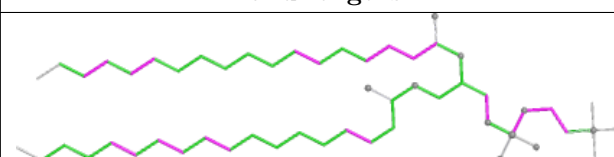
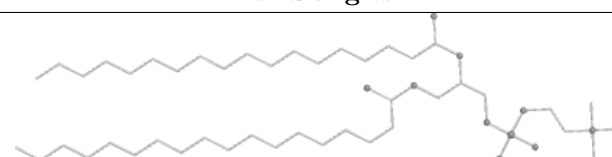
Ligand PC1 j 1001	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand 3PH L 811	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand 3PH N 503	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

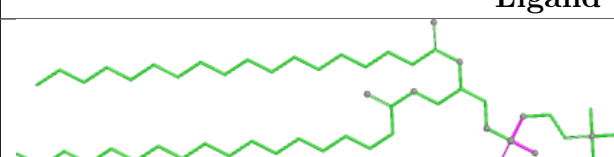
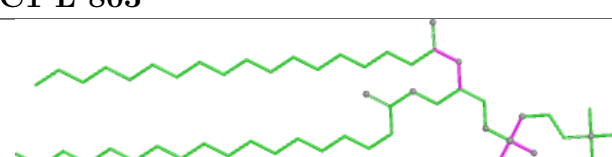
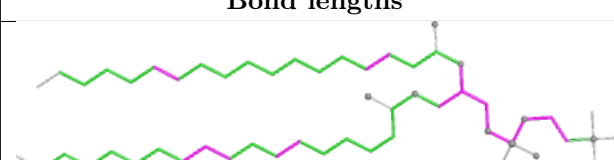
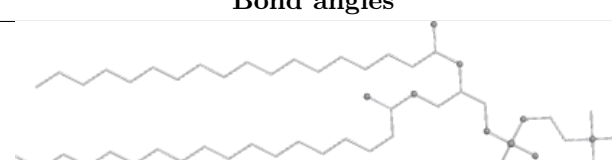
Ligand PC1 l 304	
	
Bond lengths	Bond angles
	
Torsions	Rings



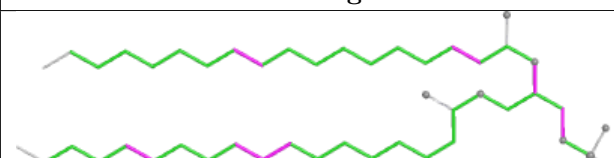
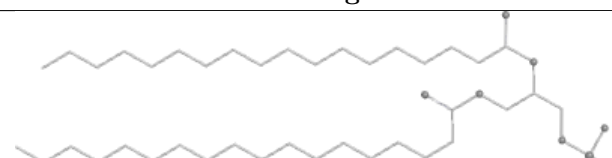
Ligand PGT J 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

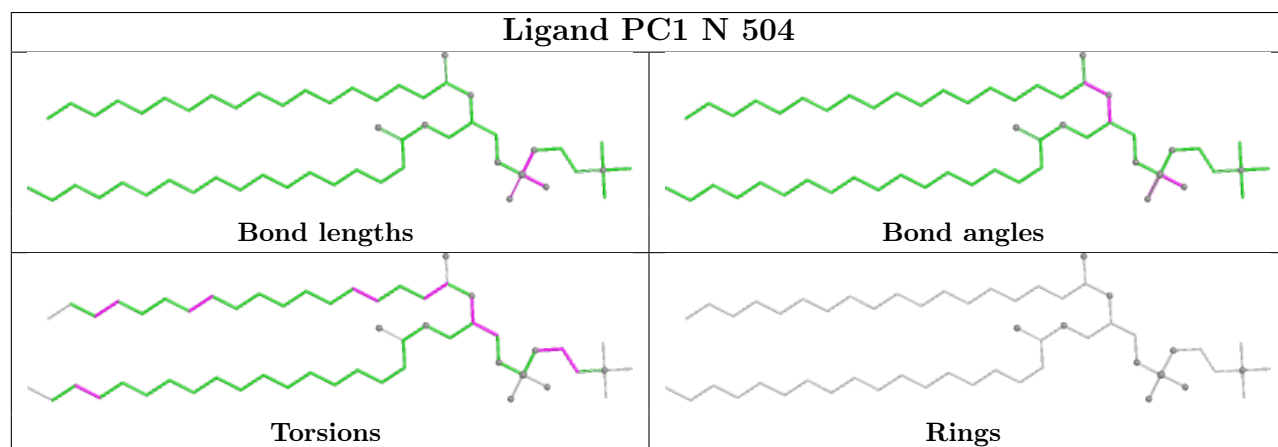
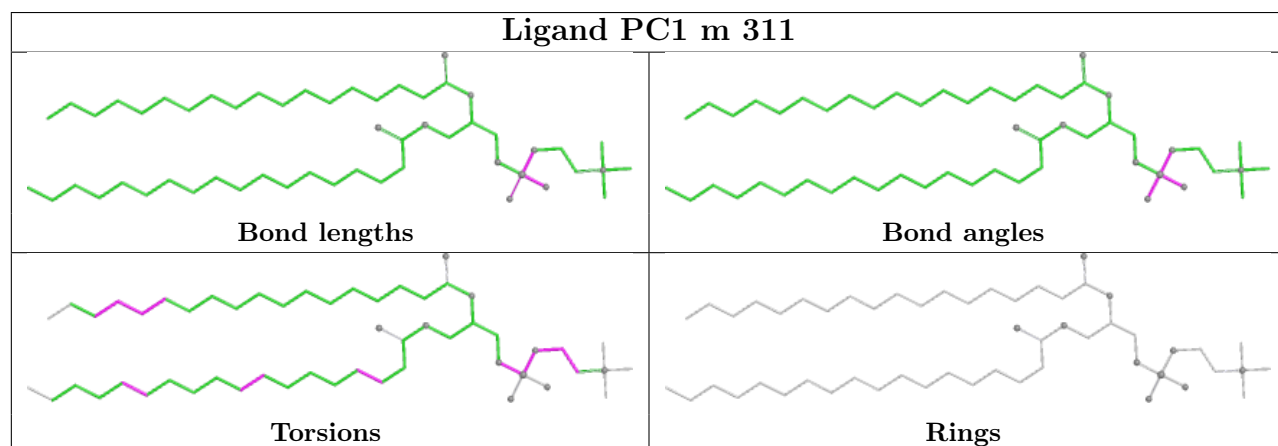
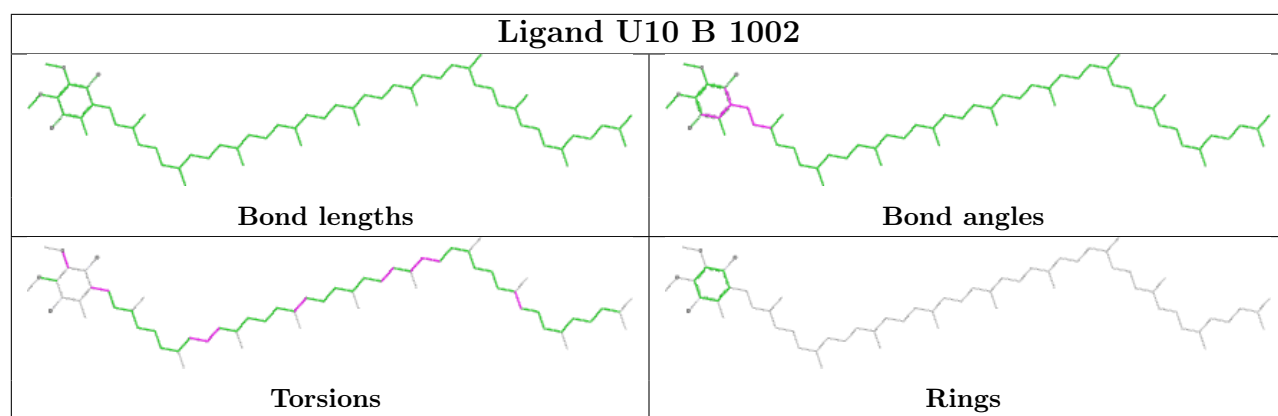
Ligand 3PE i 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

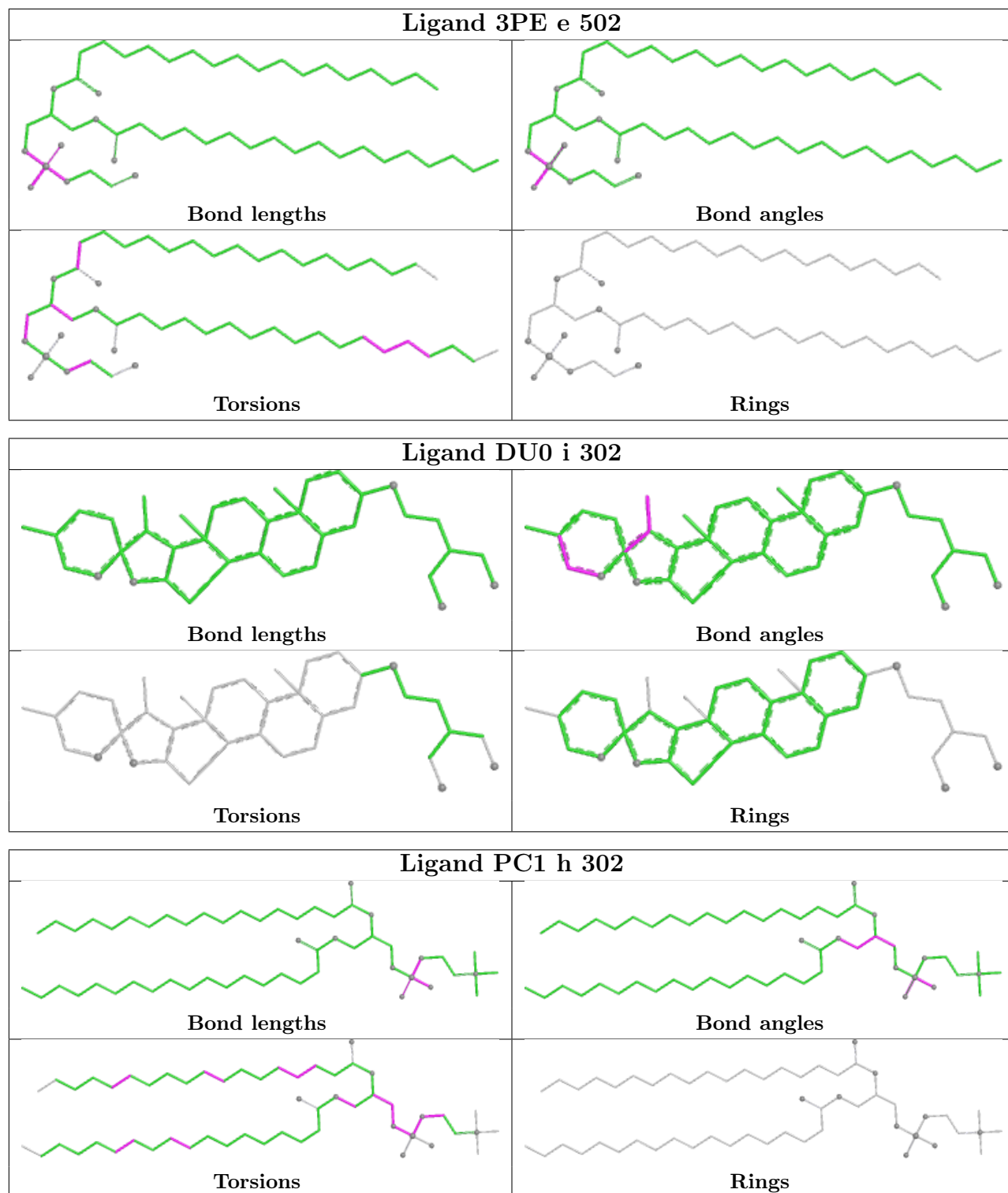


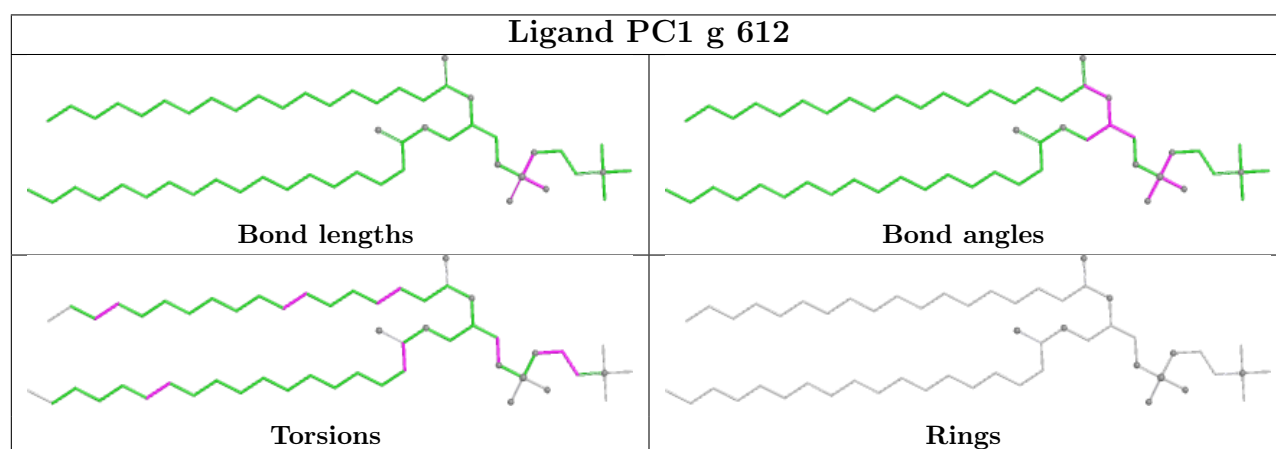
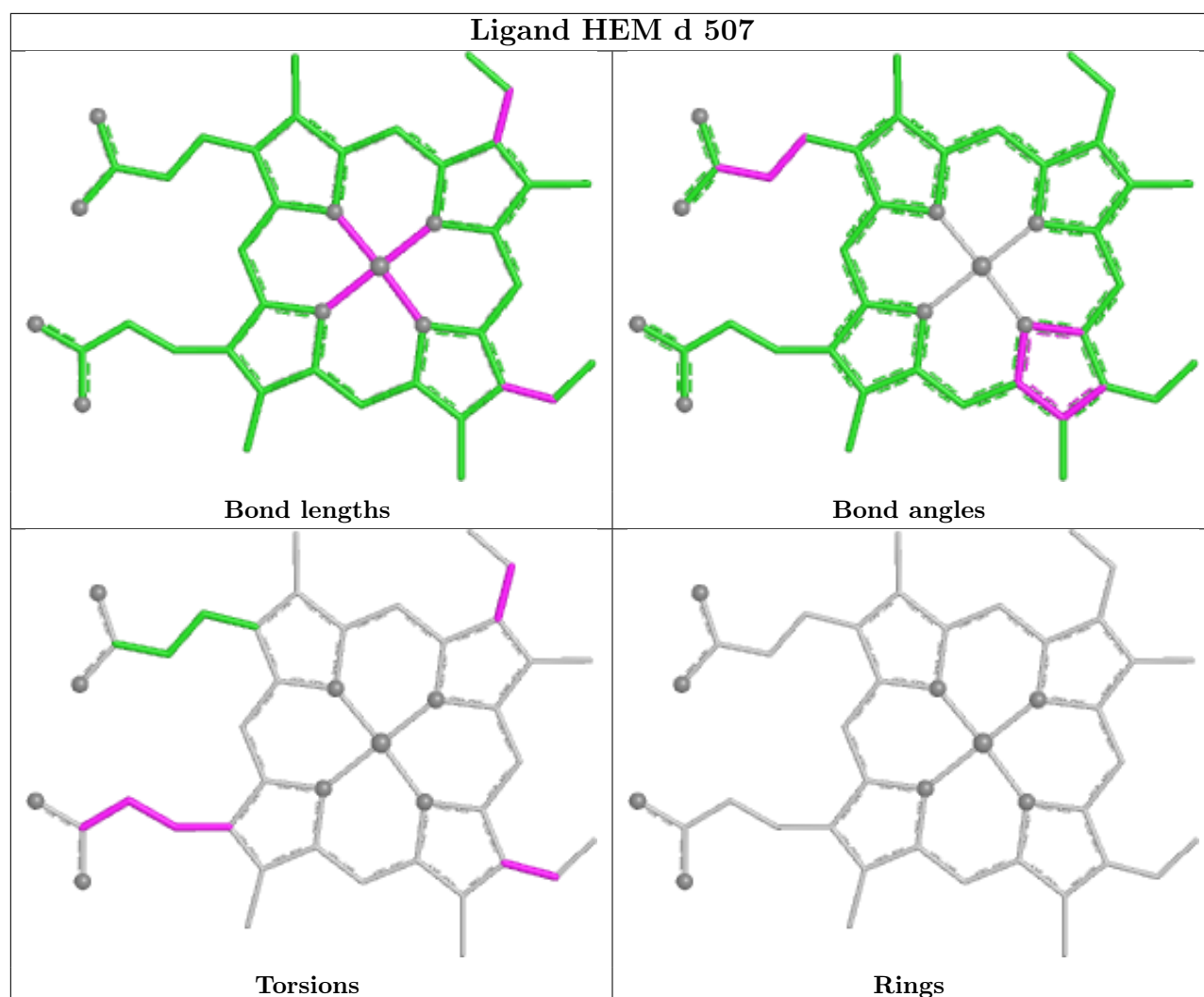
Ligand PC1 k 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

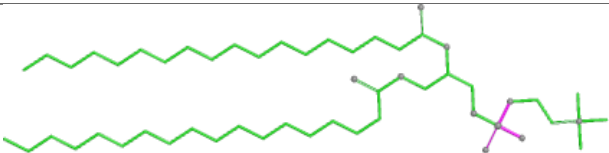
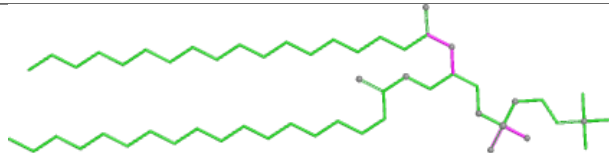
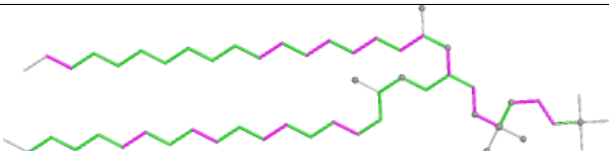
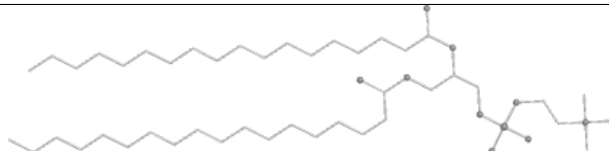


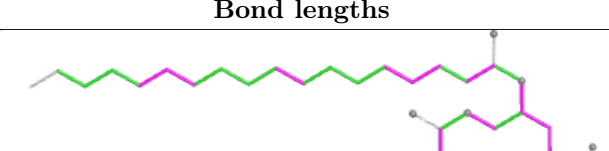
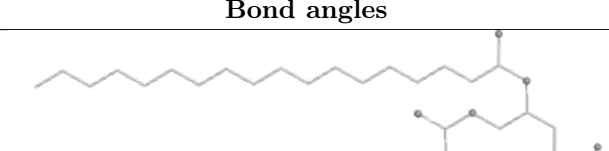
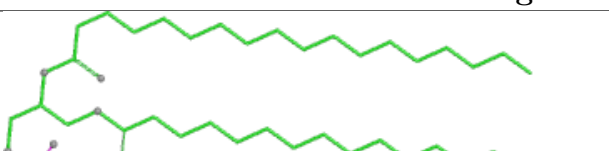
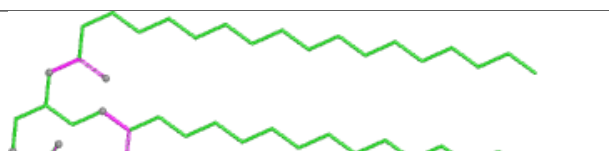
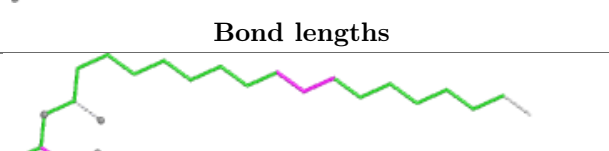
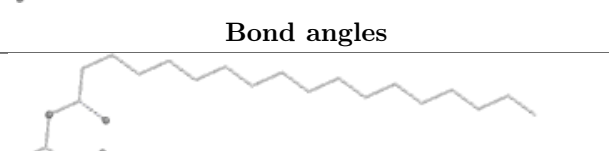
Ligand PC1 L 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

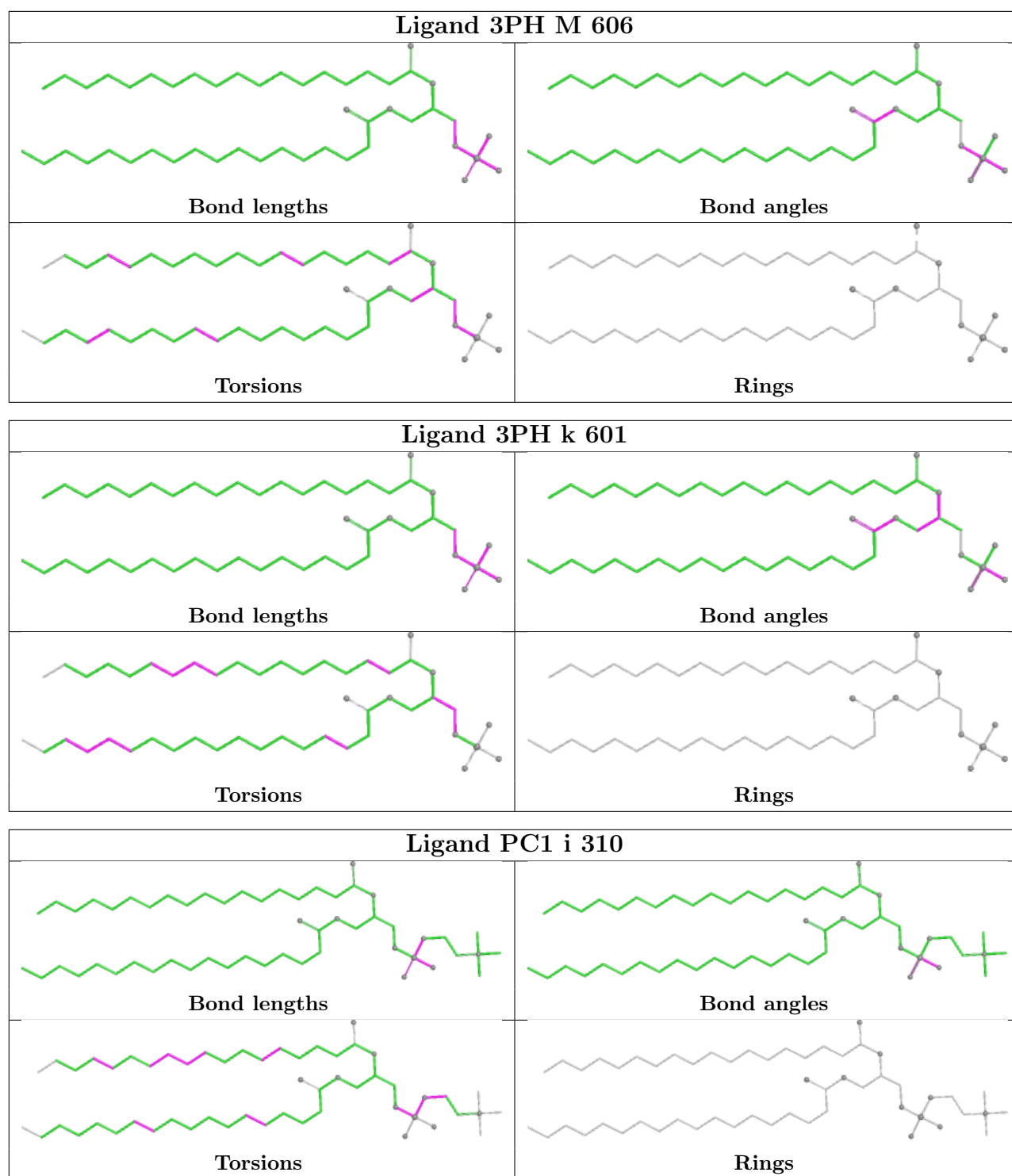
Ligand 3PH a 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

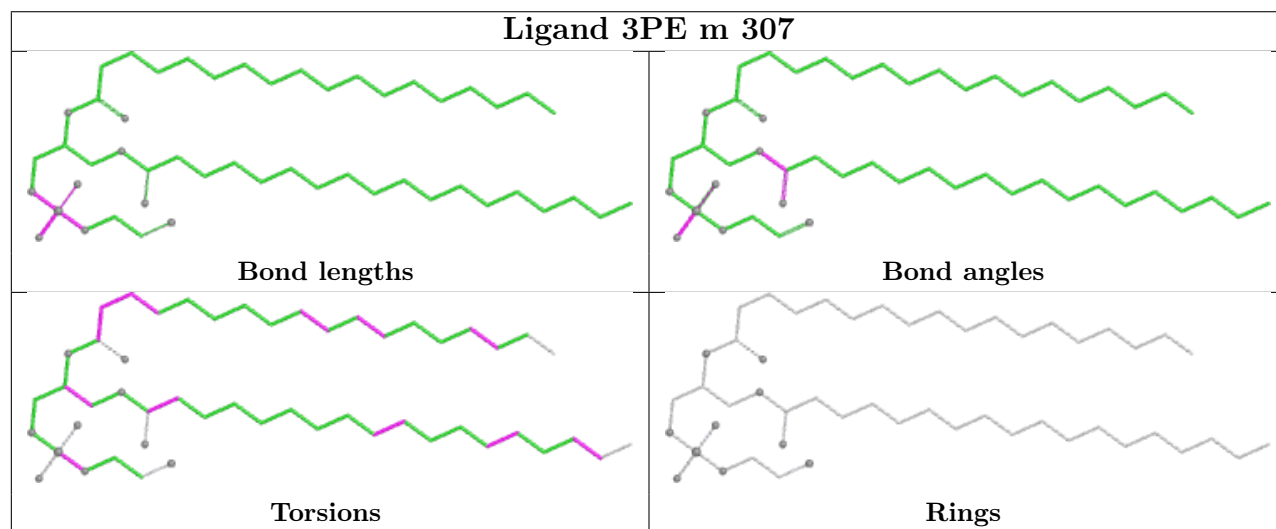
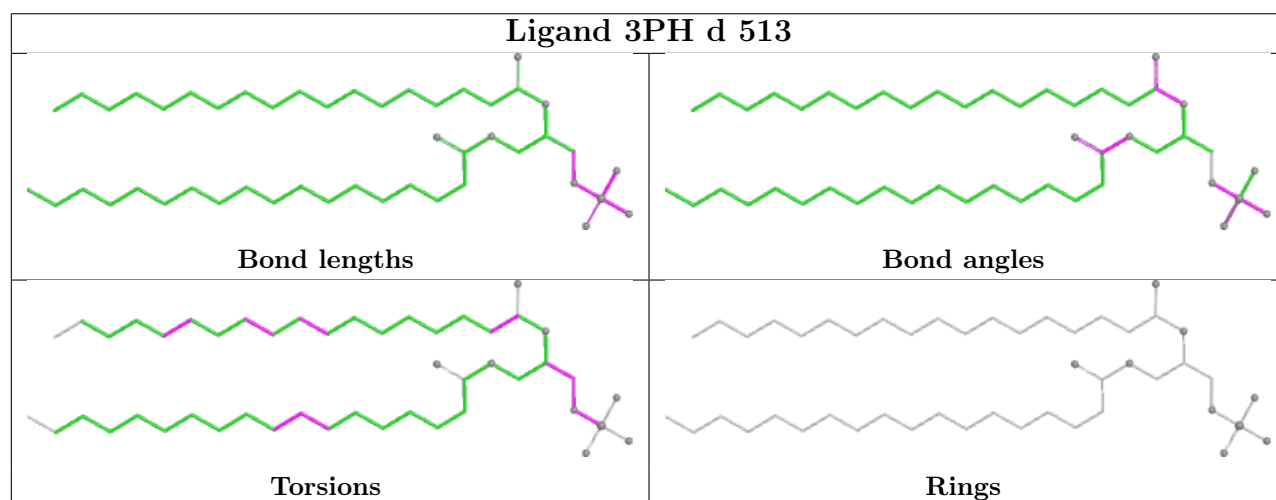
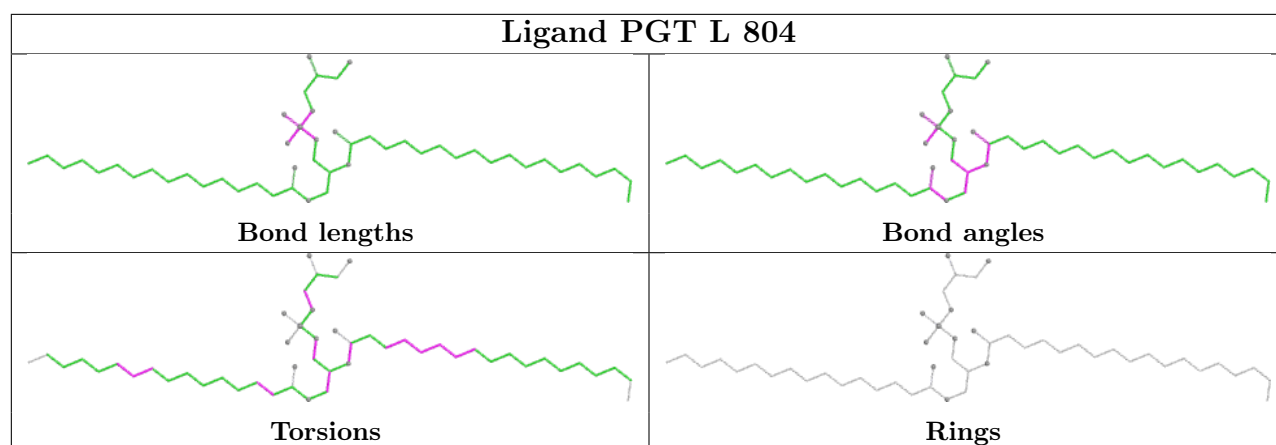


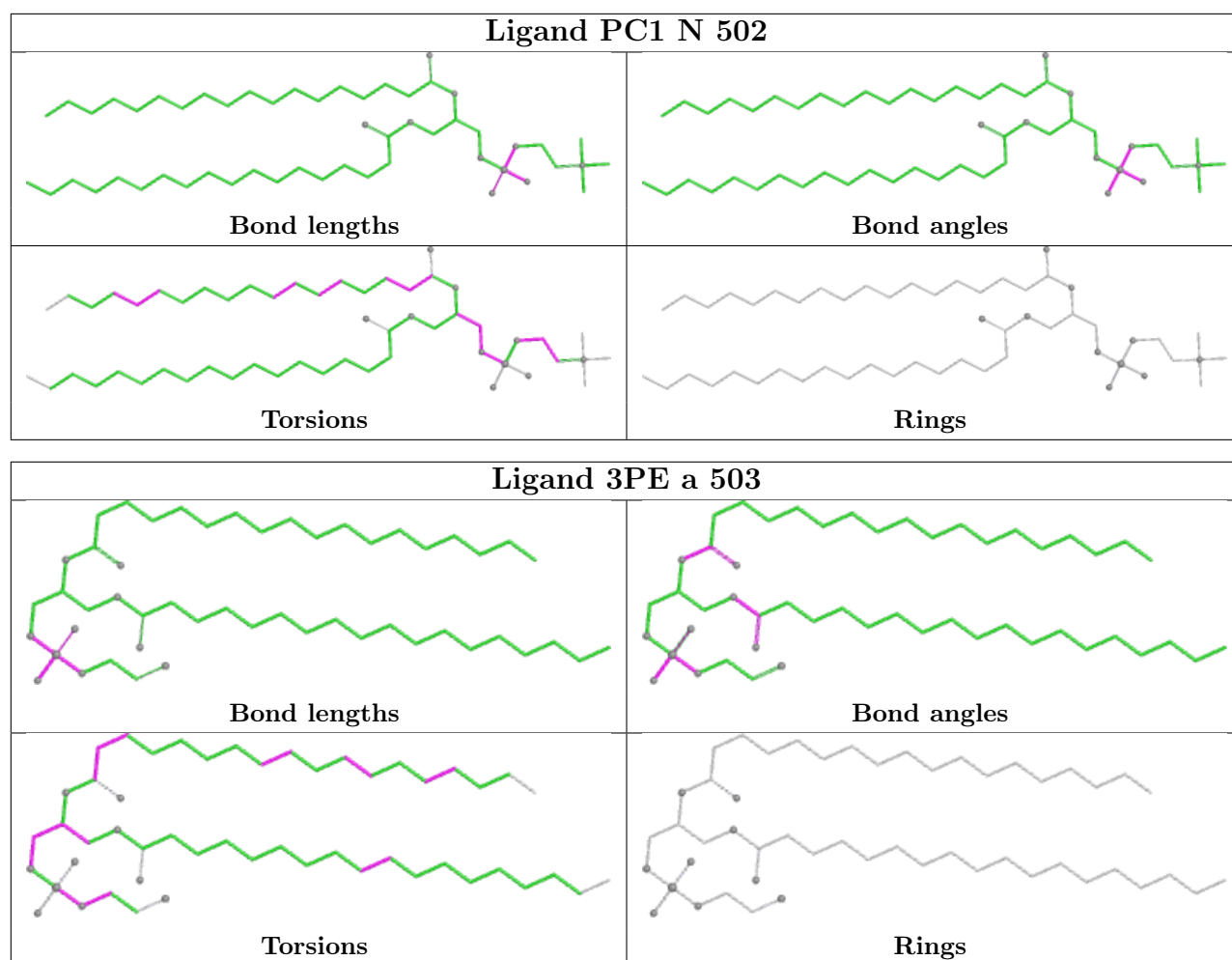




Ligand PC1 a 517	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand 3PH P 402	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand 3PE d 515	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>







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.

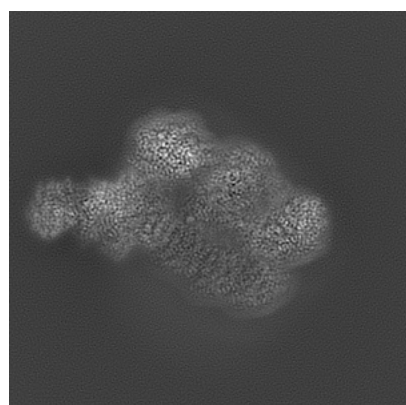
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51181. These allow visual inspection of the internal detail of the map and identification of artifacts.

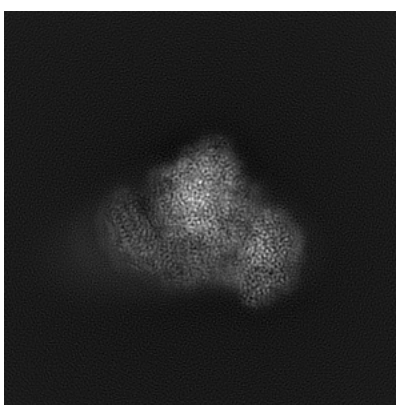
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

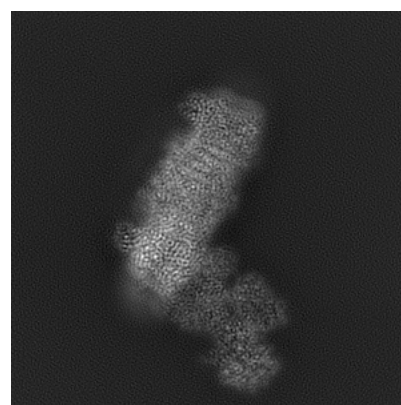
6.1.1 Primary map



X



Y

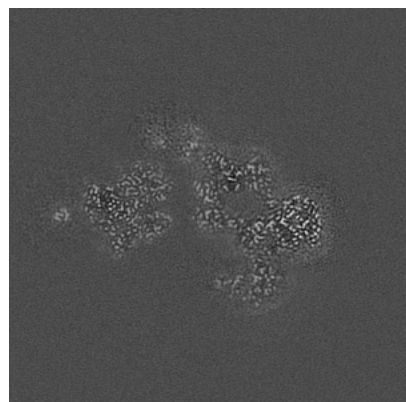


Z

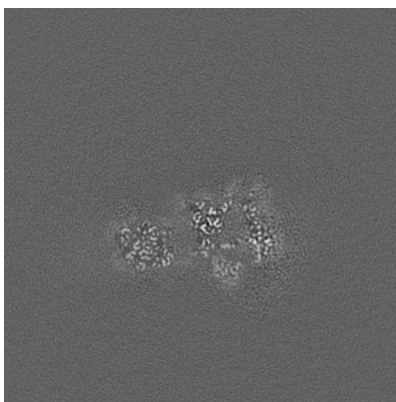
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

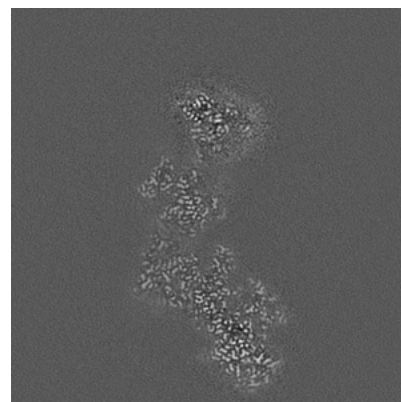
6.2.1 Primary map



X Index: 187



Y Index: 187

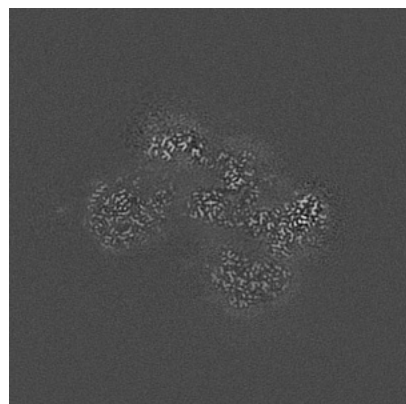


Z Index: 187

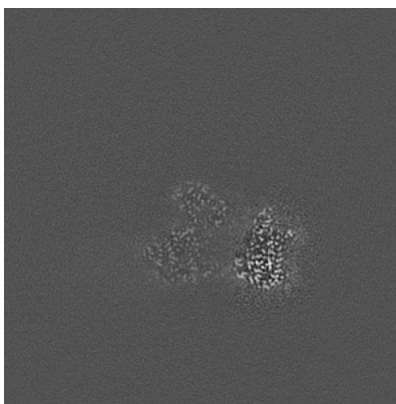
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

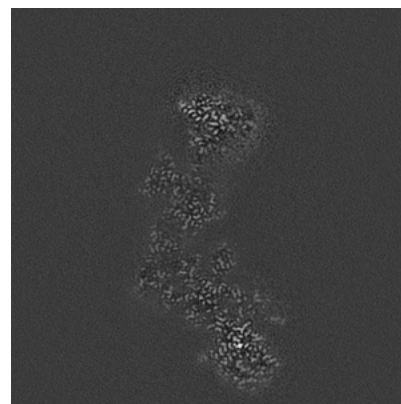
6.3.1 Primary map



X Index: 175



Y Index: 144

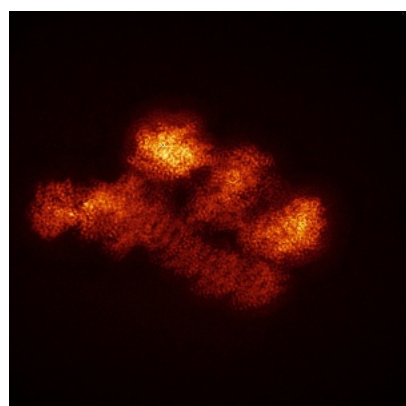


Z Index: 184

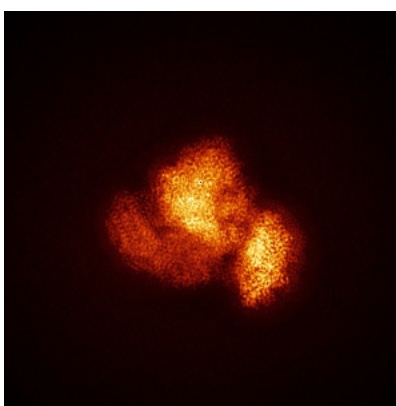
The images above show the largest variance slices of the map in three orthogonal directions.

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

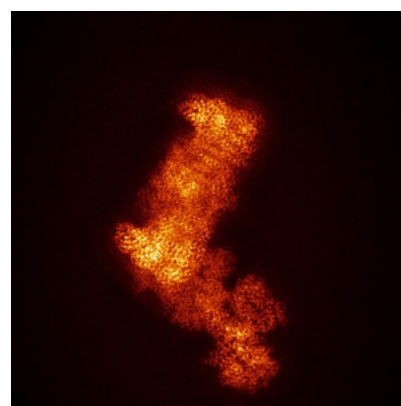
6.4.1 Primary map



X



Y

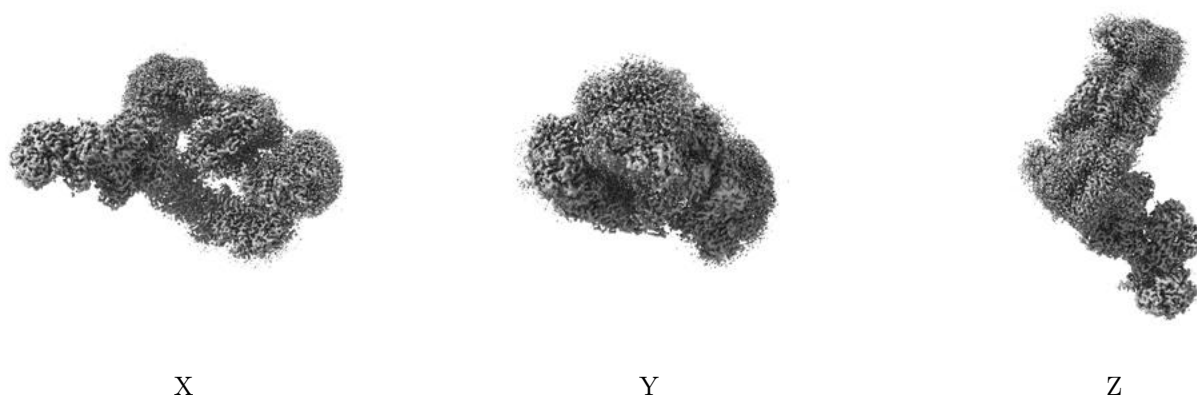


Z

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 5.34. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

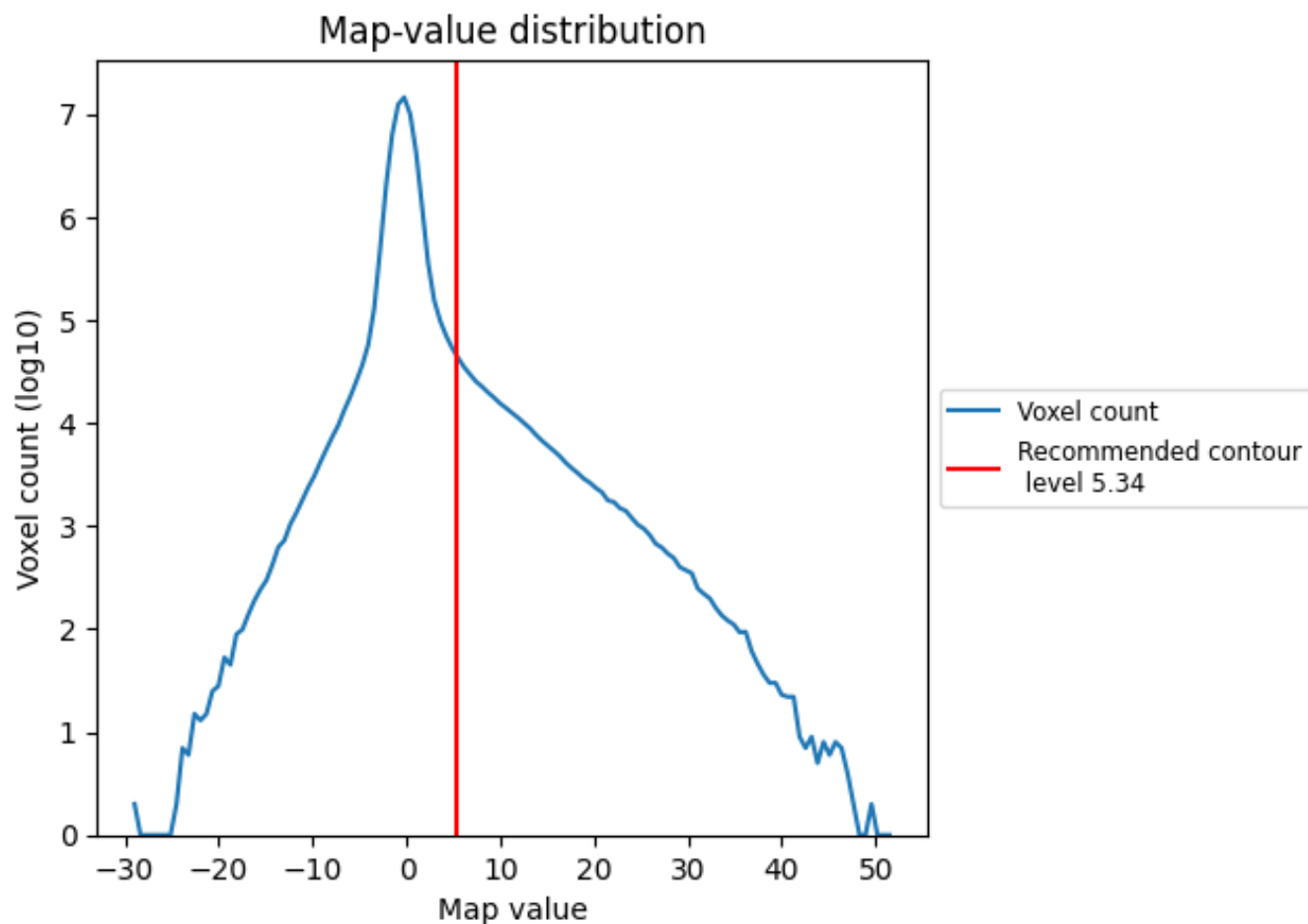
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

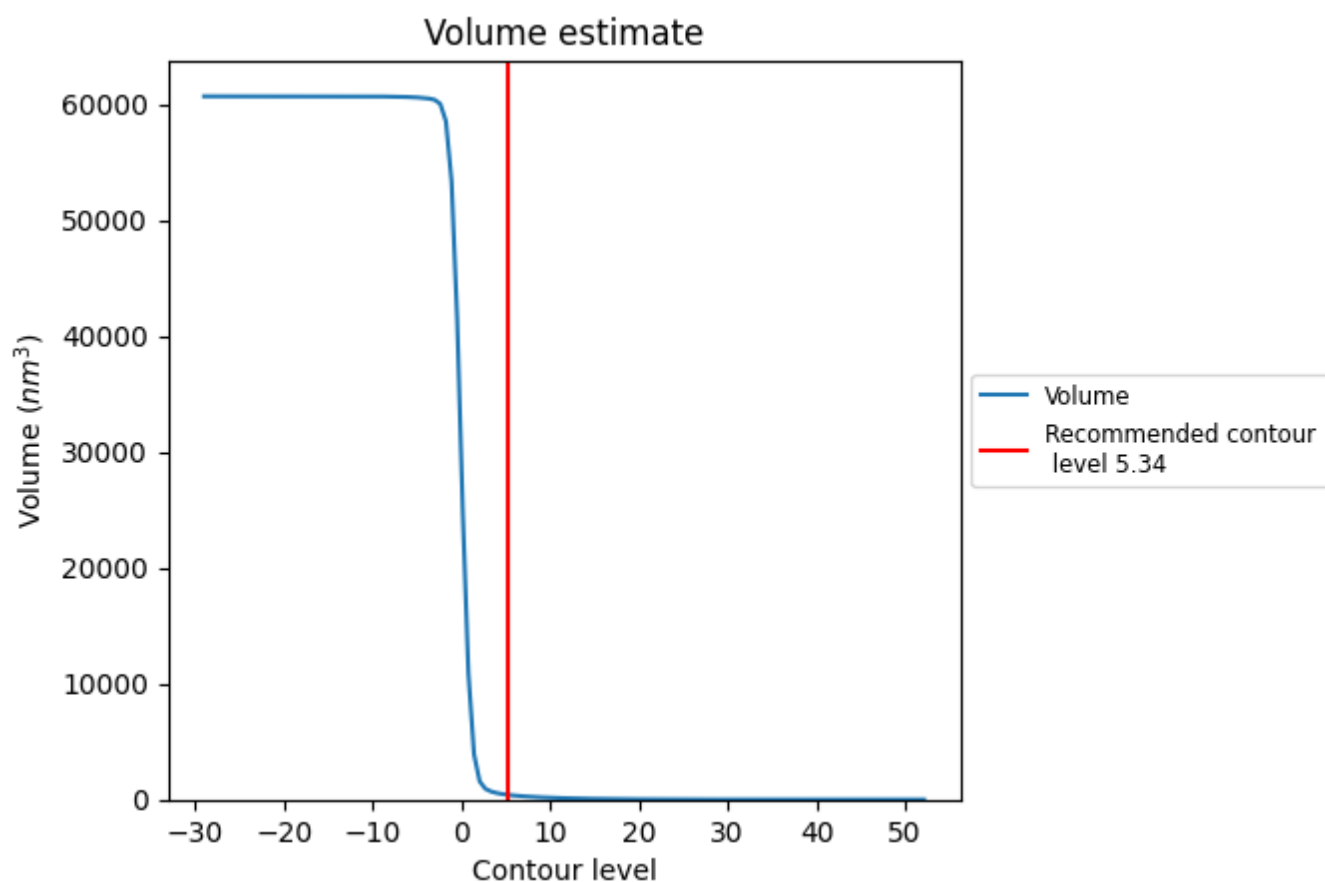
This section contains the results of statistical analysis of the map.

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.

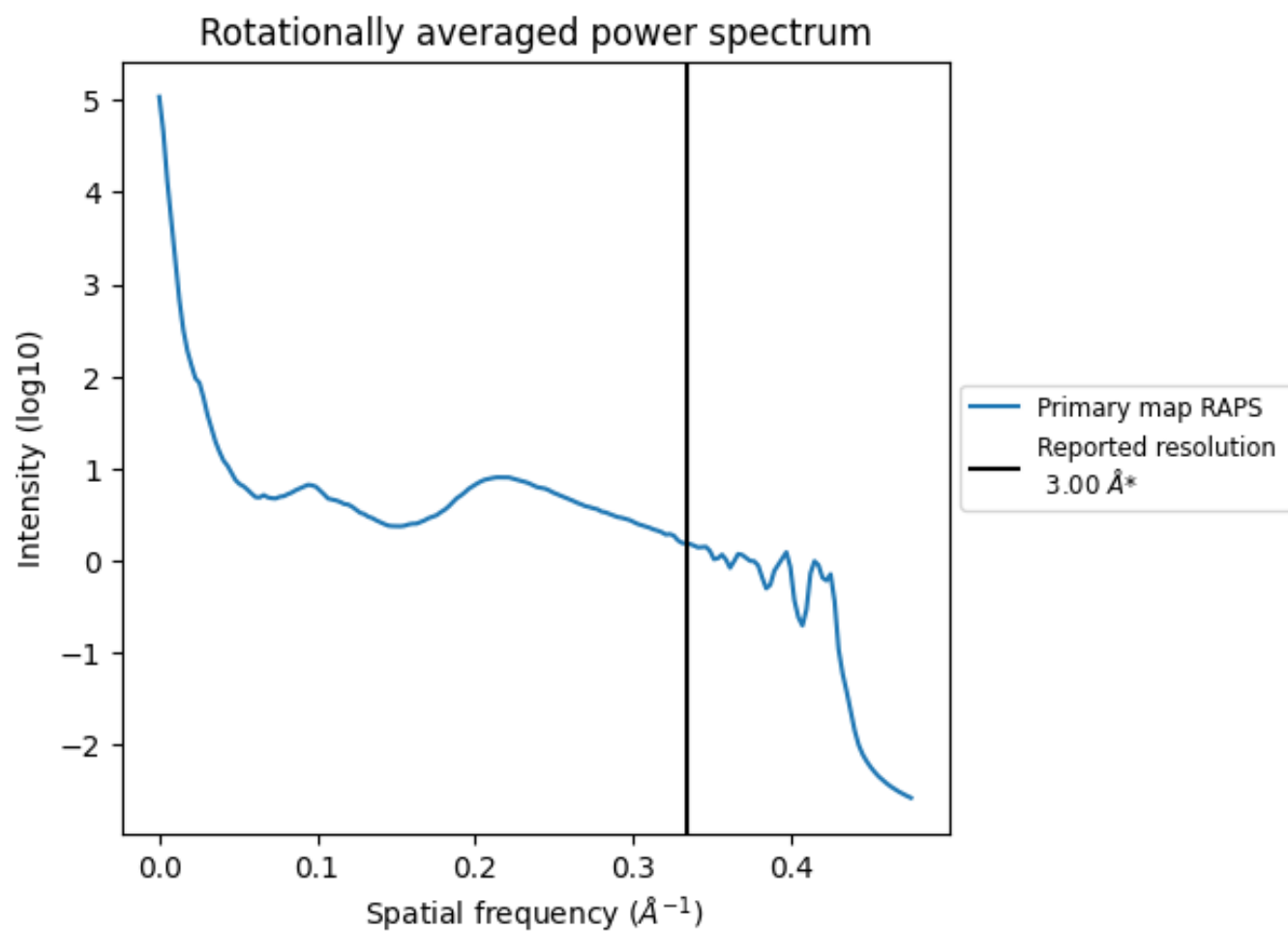
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 399 nm^3 ; this corresponds to an approximate mass of 360 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

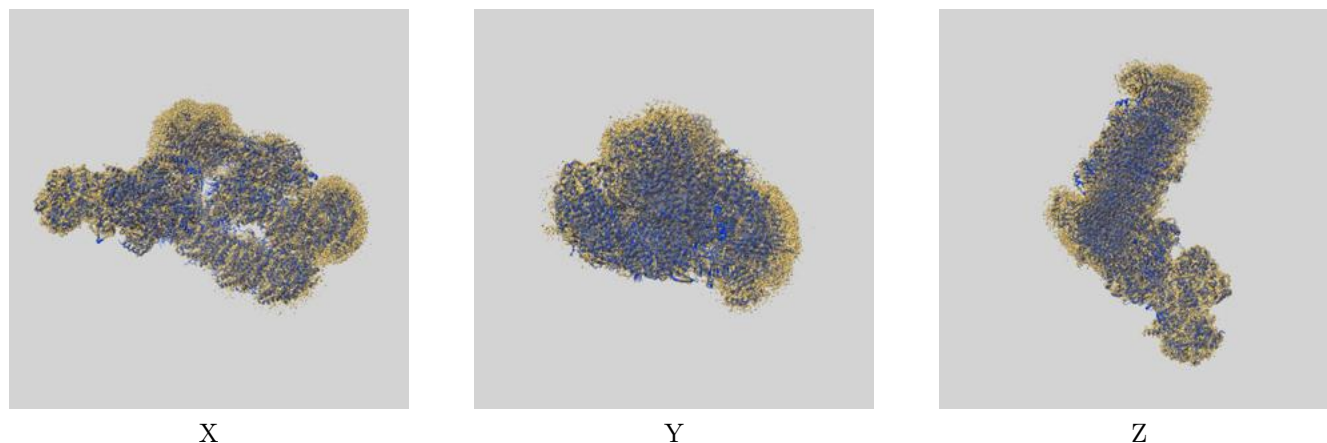
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

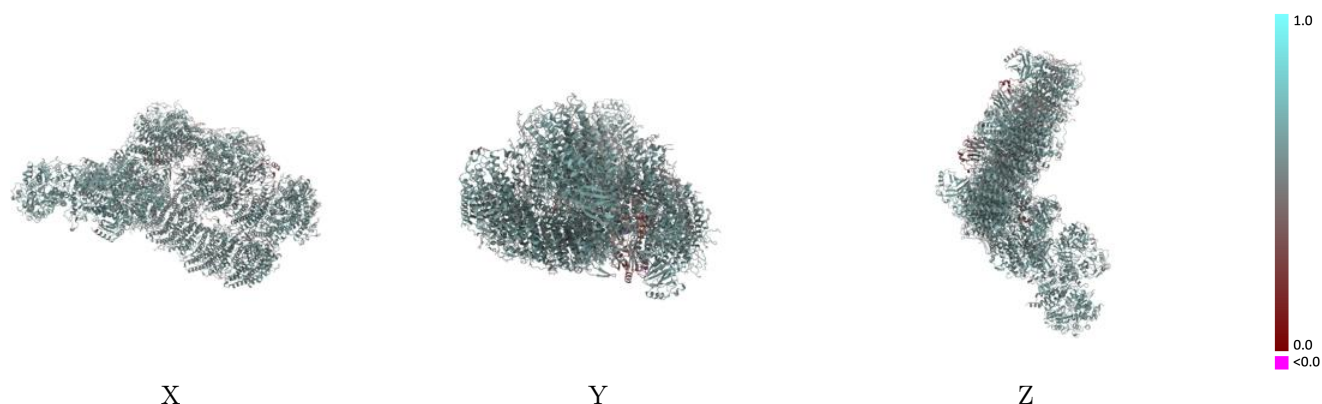
This section contains information regarding the fit between EMDB map EMD-51181 and PDB model 9GAE. Per-residue inclusion information can be found in section [3](#) on page [28](#).

9.1 Map-model overlay [i](#)



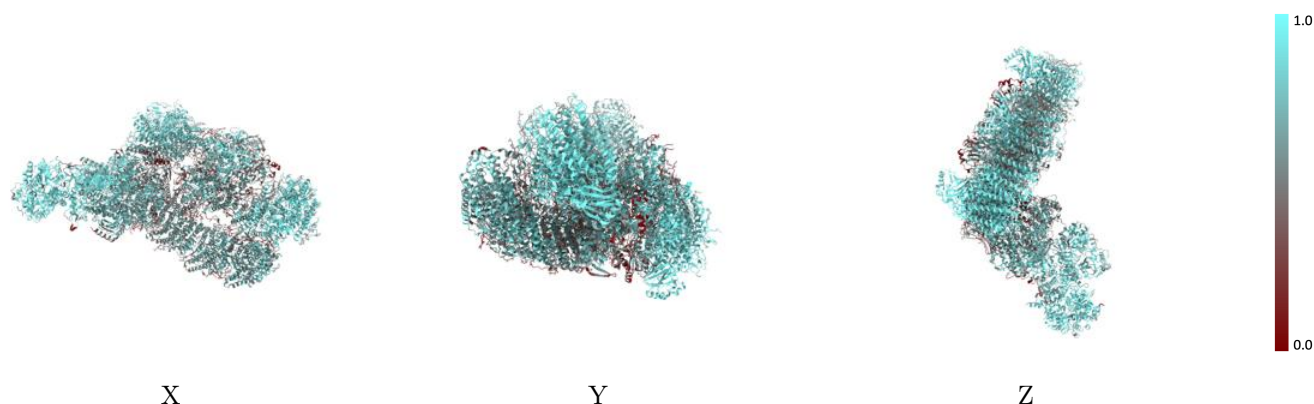
The images above show the 3D surface view of the map at the recommended contour level 5.34 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



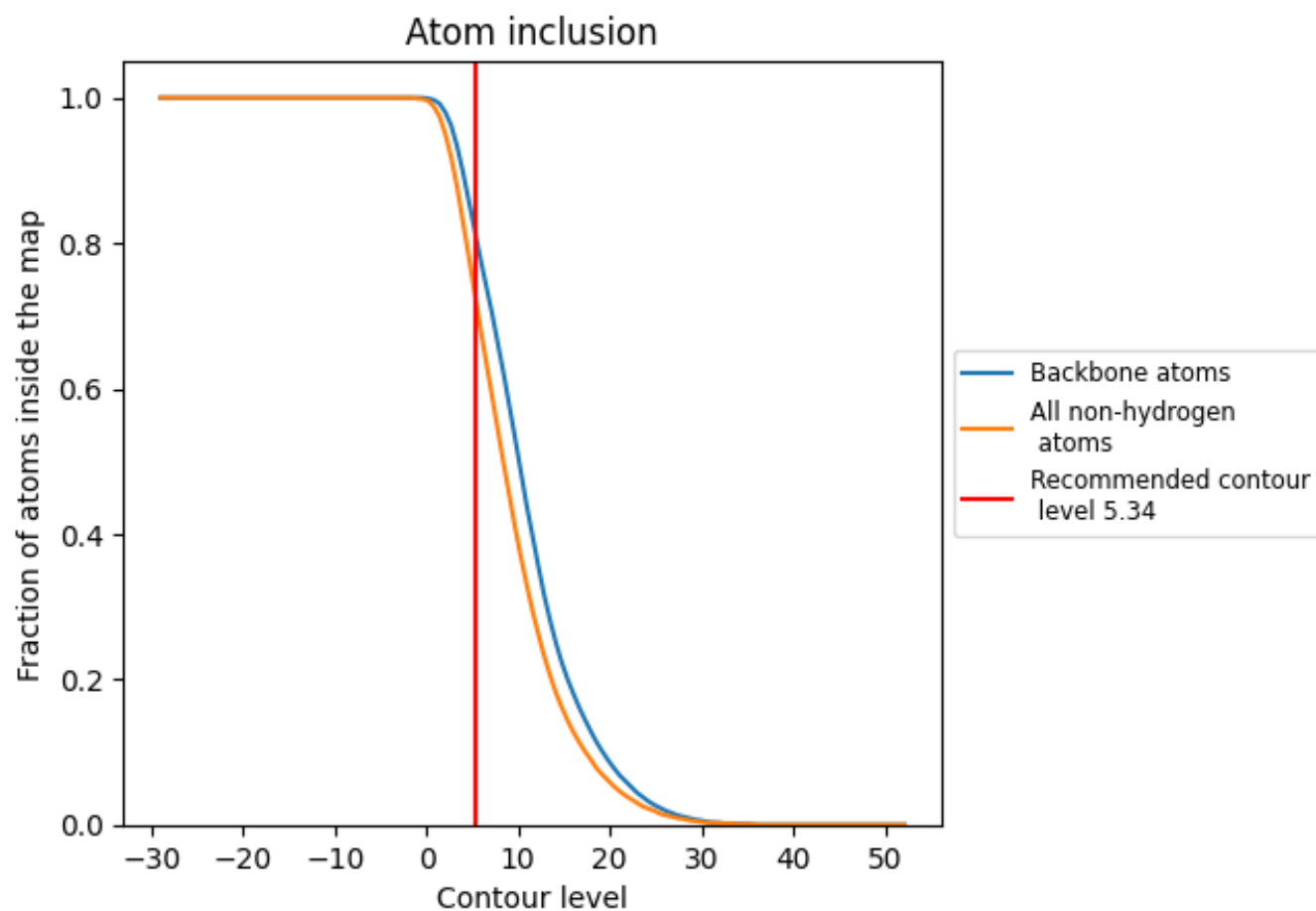
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.34).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% 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 (5.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7260	 0.5710
A	 0.5860	 0.5730
B	 0.7190	 0.5970
C	 0.7180	 0.5980
D	 0.7180	 0.6000
E	 0.8500	 0.5760
F	 0.8560	 0.5780
G	 0.8120	 0.5790
H	 0.6170	 0.5810
I	 0.7650	 0.6040
J	 0.5410	 0.5670
K	 0.6090	 0.5870
L	 0.6790	 0.5710
M	 0.6820	 0.5790
N	 0.6640	 0.5850
P	 0.5080	 0.5420
Q	 0.7720	 0.5830
R	 0.4400	 0.5440
Z	 0.6430	 0.5830
a	 0.6740	 0.5770
b	 0.5890	 0.5600
c	 0.4400	 0.4490
d	 0.7490	 0.5740
e	 0.7720	 0.5730
f	 0.4810	 0.4310
g	 0.8830	 0.5860
h	 0.8580	 0.5630
i	 0.7250	 0.5550
j	 0.7030	 0.5230
k	 0.9260	 0.5870
l	 0.8850	 0.5690
m	 0.8300	 0.5570
n	 0.7510	 0.5280
o	 0.6790	 0.5460
p	 0.5380	 0.5610
q	 0.6180	 0.5750

