



Full wwPDB EM Validation Report ⓘ

Apr 18, 2024 – 04:30 pm BST

PDB ID : 8PW5
EMDB ID : EMD-17989
Title : CS respirasome from murine liver
Authors : Vercellino, I.; Sazanov, L.A.
Deposited on : 2023-07-19
Resolution : 3.60 Å(reported)
Based on initial models : 7o3c, 6g2j

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.60 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.



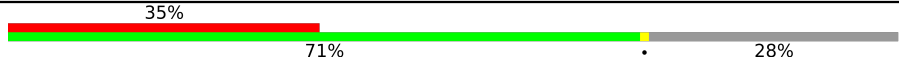

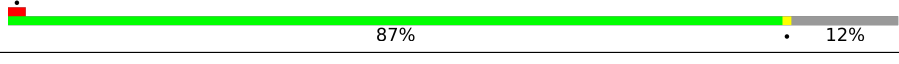
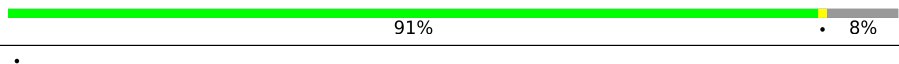
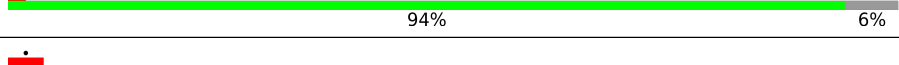
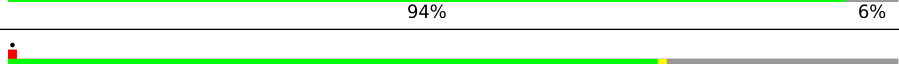
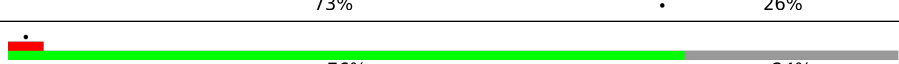
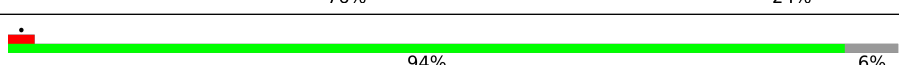
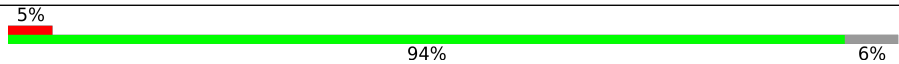
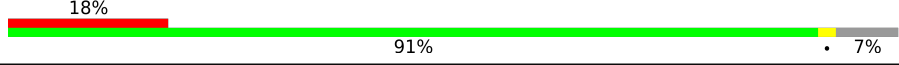
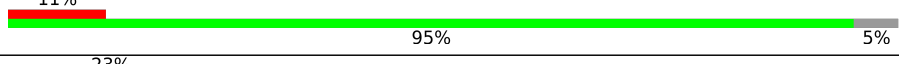
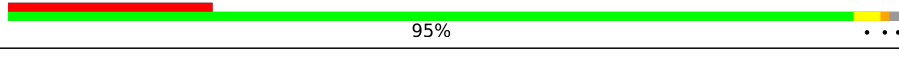
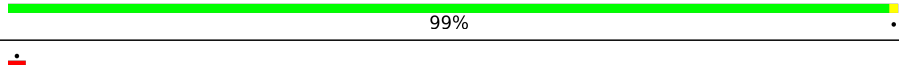
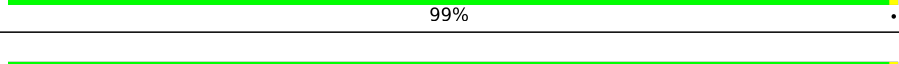
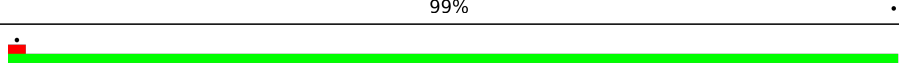
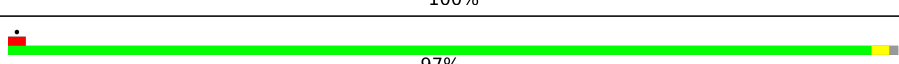
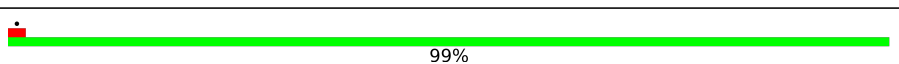








Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	480	92% 7%
1	L	480	93% 7%
2	B	453	93% 7%
2	M	453	93% 7%
3	C	381	100%
3	N	381	99%
4	D	325	74% 26%
4	O	325	74% 26%
5	E	274	32% 72% 28%

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Mol	Chain	Length	Quality of chain
5	P	274	
5	T	274	
6	F	111	
6	Q	111	
7	G	82	
7	R	82	
8	H	89	
8	S	89	
9	J	64	
9	U	64	
10	K	56	
10	V	56	
11	I	113	
12	a	514	
12	n	514	
13	b	227	
13	o	227	
14	c	261	
14	p	261	
15	d	169	
15	q	169	
16	e	146	
16	r	146	
17	f	128	
17	s	128	

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Mol	Chain	Length	Quality of chain
18	g	97	76% 23%
18	t	97	8% 77% 23%
19	h	86	90% 8%
19	u	86	91% 8%
20	i	76	93% 5%
20	v	76	5% 92% 7%
21	k	80	58% 40%
21	x	80	61% 39%
22	l	63	73% 27%
22	y	63	75% 25%
23	m	70	61% 39%
23	z	70	60% 39%
24	w	83	67% 31%
25	6	224	69% 30%
26	C1	263	79% 21%
27	D1	463	6% 92% 7%
28	2	248	86% 14%
29	1	464	93% 7%
30	3	727	95% 5%
31	9	212	83% 16%
32	P1	377	90% 9%
33	Q1	175	72% 28%
34	7	116	82% 17%
35	S1	99	83% 15%
36	T1	156	50% 49%

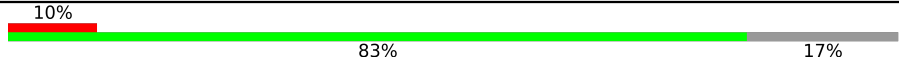
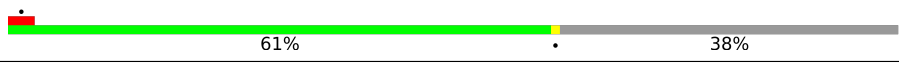


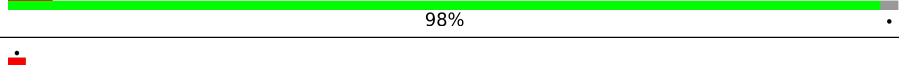
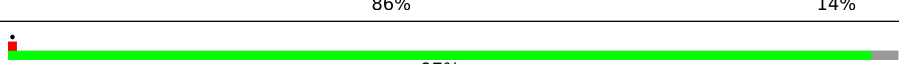
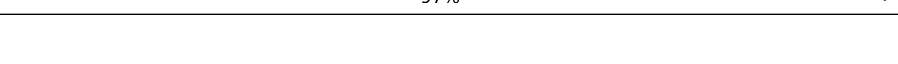
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Mol	Chain	Length	Quality of chain
36	U1	156	56% 44%
37	V1	116	97%
38	W1	131	87% 13%
39	q1	145	100%
40	r1	113	87% 12%
41	s1	104	40% 60%
42	A1	115	6% 99%
43	H1	318	99%
44	J1	172	19% 99%
45	K1	98	99%
46	L1	607	100%
47	M1	459	100%
48	N1	345	99%
49	O1	355	90% 10%
50	X1	172	99%
51	Y1	141	99%
52	Z1	144	98%
53	a1	70	100%
54	b1	84	98%
55	c1	76	63% 37%
56	d1	120	100%
57	e1	106	99%
58	f1	57	11% 93% 7%
59	g1	151	5% 66% 33%
60	h1	189	74% 26%

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Mol	Chain	Length	Quality of chain
61	i1	128	 10% 83% 17%
62	j1	105	 61% 38%
63	k1	104	 74% 26%
64	l1	186	 84% 16%
65	m1	129	 5% 98%
66	n1	179	 99%
67	o1	137	 86% 14%
68	p1	176	 97%

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 130520 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	445	Total	C	N	O	S	0	0
			3459	2163	610	669	17		
1	L	445	Total	C	N	O	S	0	0
			3460	2163	610	670	17		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		
2	M	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		
3	N	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		
4	O	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	196	Total	C	N	O	S	0	0
			1167	705	219	237	6		
5	P	196	Total	C	N	O	S	0	0
			1164	702	219	237	6		
5	T	78	Total	C	N	O	S	0	0
			554	352	103	97	2		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	98	Total	C	N	O	S	0	0
			865	552	154	156	3		
6	Q	102	Total	C	N	O	S	0	0
			900	575	160	162	3		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	77	Total	C	N	O	S	0	0
			654	424	120	109	1		
7	R	77	Total	C	N	O	S	0	0
			654	424	120	109	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	66	Total	C	N	O	S	0	0
			545	333	101	106	5		
8	S	68	Total	C	N	O	S	0	0
			563	343	103	112	5		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	60	Total	C	N	O	0	0
			495	323	86	86		
9	U	60	Total	C	N	O	0	0
			495	323	86	86		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	52	Total	C	N	O	S	0	0
			430	287	76	66	1		
10	V	53	Total	C	N	O	S	0	0
			438	292	77	67	2		

- Molecule 11 is a protein called Cox7a2l protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	111	Total	C	N	O	S	0	0
			807	520	138	144	5		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	n	514	Total	C	N	O	S	0	0
			4021	2691	623	675	32		
12	a	514	Total	C	N	O	S	0	0
			4021	2691	623	675	32		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	o	227	Total	C	N	O	S	0	0
			1817	1180	282	336	19		
13	b	227	Total	C	N	O	S	0	0
			1817	1180	282	336	19		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	p	260	Total	C	N	O	S	0	0
			2118	1418	339	351	10		
14	c	259	Total	C	N	O	S	0	0
			2111	1414	338	349	10		

- Molecule 15 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	q	139	Total	C	N	O	S	0	0
			1156	745	192	212	7		
15	d	139	Total	C	N	O	S	0	0
			1156	745	192	212	7		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	r	104	Total	C	N	O	S	0	0
			842	538	141	161	2		
16	e	103	Total	C	N	O	S	0	0
			833	533	140	158	2		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	s	94	Total	C	N	O	S	0	0
			721	449	126	138	8		
17	f	93	Total	C	N	O	S	0	0
			717	447	125	137	8		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	t	75	Total	C	N	O	S	0	0
			605	392	114	96	3		
18	g	75	Total	C	N	O	S	0	0
			605	392	114	96	3		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	u	79	Total	C	N	O	S	0	0
			654	416	116	117	5		
19	h	79	Total	C	N	O	S	0	0
			654	416	116	117	5		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	v	71	Total	C	N	O	S	0	0
			567	369	102	93	3		
20	i	72	Total	C	N	O	S	0	0
			572	372	103	94	3		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	x	49	Total	C	N	O	S	0	0
			383	248	65	68	2		
21	k	48	Total	C	N	O	S	0	0
			378	245	64	67	2		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	y	47	Total	C	N	O	S	0	0
			386	256	65	63	2		
22	l	46	Total	C	N	O	S	0	0
			380	253	64	61	2		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	z	43	Total	C	N	O	S	0	0
			311	203	51	56	1		
23	m	43	Total	C	N	O	S	0	0
			311	203	51	56	1		

- Molecule 24 is a protein called Cytochrome c oxidase subunit 7A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	w	57	Total	C	N	O	S	0	0
			435	283	71	78	3		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	157	Total	C	N	O	S	0	0
			1258	802	227	215	14		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C1	208	Total	C	N	O	S	0	0
			1730	1116	297	314	3		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	D1	430	3464	2215	595	630	24	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	2	214	1660	1056	279	314	11	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	1	430	3321	2092	596	611	22	0	0

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	3	690	5305	3326	921	1017	41	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	9	178	1431	898	245	276	12	0	0

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	P1	342	2748	1777	483	481	7	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Q1	126	1022	646	180	192	4	0	0

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	7	96	758	470	141	144	3	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	S1	84	671	421	127	120	3	0	0

- Molecule 36 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	T1	79	637	410	95	127	5	0	0
36	U1	88	706	453	104	144	5	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	V1	113	923	602	153	165	3	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	W1	114	970	619	180	165	6	0	0

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	q1	145	1209	777	215	212	5	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	r1	99	796	504	148	141	3	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	s1	42	351	219	62	70	0	0

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	A1	115	932	633	132	160	7	0	0

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	H1	318	2540	1706	384	428	22	0	0

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	J1	172	1308	878	186	229	15	0	0

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	K1	98	737	477	112	137	11	0	0

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	L1	606	4800	3182	746	827	45	0	0

- Molecule 47 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	M1	459	3632	2408	567	617	40	0	0

- Molecule 48 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	N1	345	2703	1795	417	454	37	0	0

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	O1	320	2607	1674	431	492	10	0	0

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	X1	171	1396	889	250	247	10	0	0

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Y1	140	1037	662	175	192	8	0	0

- Molecule 52 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	Z1	141	1167	750	207	202	8	0	0

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	a1	70	572	370	101	97	4	0	0

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	b1	83	651	427	105	115	4	0	0

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	c1	48	398	261	69	67	1	0	0

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	d1	120	996	651	171	165	9	0	0

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	e1	105	877	555	162	152	8	0	0

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	f1	53	456	295	82	77	2	0	0

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	g1	101	850	549	136	161	4	0	0

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	h1	139	1166	764	195	204	3	0	0

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	i1	106	897	584	157	152	4	0	0

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	j1	65	562	370	93	98	1	0	0

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	k1	77	626	414	106	104	2	0	0

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	l1	157	1323	855	220	237	11	0	0

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
65	m1	126	1050	676	189	185	0	0

- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	n1	178	1541	985	276	269	11	0	0

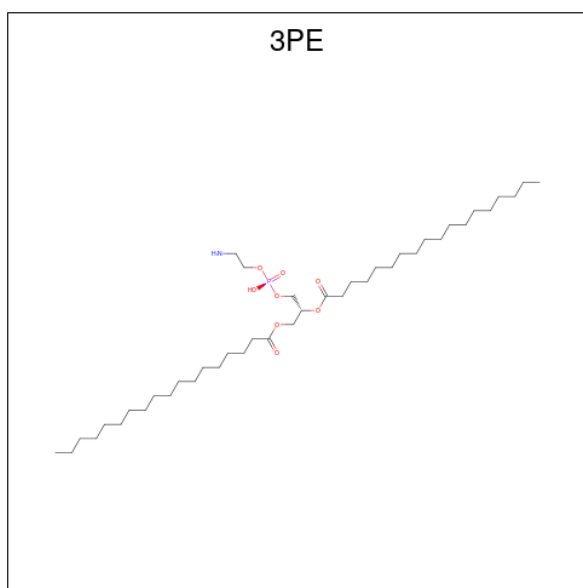
- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	o1	118	1014	639	190	177	8	0	0

- Molecule 68 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	p1	170	1438	903	258	269	8	0	0

- Molecule 69 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



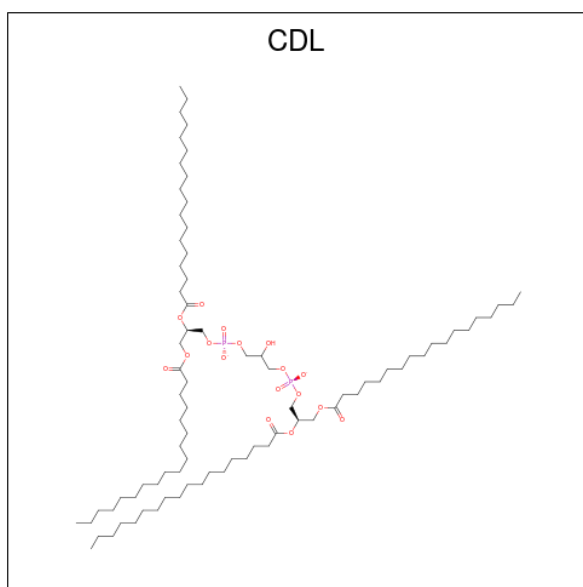
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	A	1	23	13	1	8	1	0
69	C	1	35	25	1	8	1	0
69	C	1	31	21	1	8	1	0
69	E	1	32	22	1	8	1	0
69	E	1	34	24	1	8	1	0
69	G	1	51	41	1	8	1	0
69	L	1	23	13	1	8	1	0
69	N	1	37	27	1	8	1	0
69	O	1	33	23	1	8	1	0
69	R	1	30	20	1	8	1	0
69	n	1	34	24	1	8	1	0
69	n	1	28	18	1	8	1	0
69	n	1	27	17	1	8	1	0
69	o	1	29	19	1	8	1	0
69	p	1	45	35	1	8	1	0
69	t	1	25	15	1	8	1	0
69	v	1	28	18	1	8	1	0
69	z	1	26	16	1	8	1	0
69	6	1	32	22	1	8	1	0
69	r1	1	46	36	1	8	1	0
69	H1	1	51	41	1	8	1	0
69	K1	1	41	31	1	8	1	0

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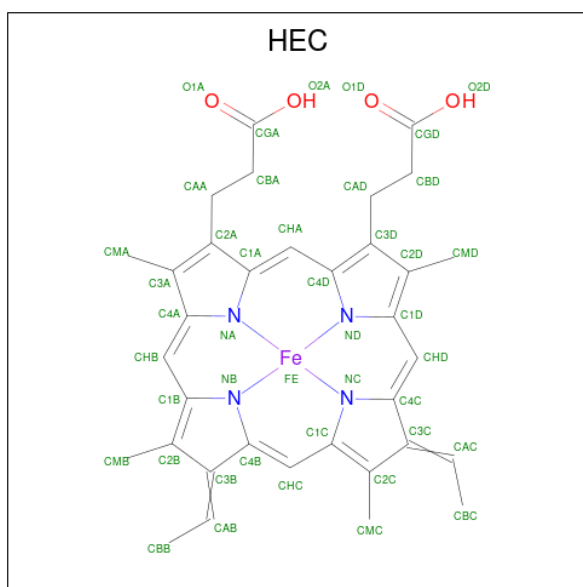
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
69	L1	1	51	41	1	8	1	0
69	L1	1	51	41	1	8	1	0
69	M1	1	51	41	1	8	1	0
69	M1	1	51	41	1	8	1	0
69	N1	1	38	28	1	8	1	0
69	Y1	1	28	18	1	8	1	0
69	Y1	1	42	32	1	8	1	0
69	b1	1	43	33	1	8	1	0
69	d1	1	31	21	1	8	1	0
69	d1	1	32	22	1	8	1	0
69	i1	1	42	32	1	8	1	0
69	m1	1	36	26	1	8	1	0
69	a	1	28	18	1	8	1	0
69	a	1	27	17	1	8	1	0
69	b	1	29	19	1	8	1	0
69	c	1	45	35	1	8	1	0
69	d	1	34	24	1	8	1	0
69	g	1	25	15	1	8	1	0
69	i	1	28	18	1	8	1	0

- Molecule 70 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



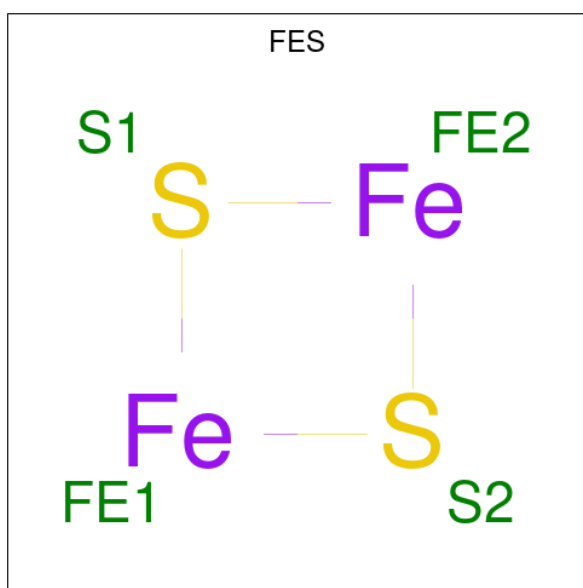
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
70	A	1	46	27	17	2	0
70	D	1	56	37	17	2	0
70	G	1	42	23	17	2	0
70	L	1	46	27	17	2	0
70	O	1	57	38	17	2	0
70	R	1	41	22	17	2	0
70	R	1	57	38	17	2	0
70	R	1	72	53	17	2	0
70	V	1	50	31	17	2	0
70	r1	1	57	38	17	2	0
70	H1	1	51	33	16	2	0
70	L1	1	78	59	17	2	0
70	L1	1	46	27	17	2	0
70	N1	1	90	71	17	2	0

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Mol	Chain	Residues	Atoms				AltConf	
72	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
72	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 73 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



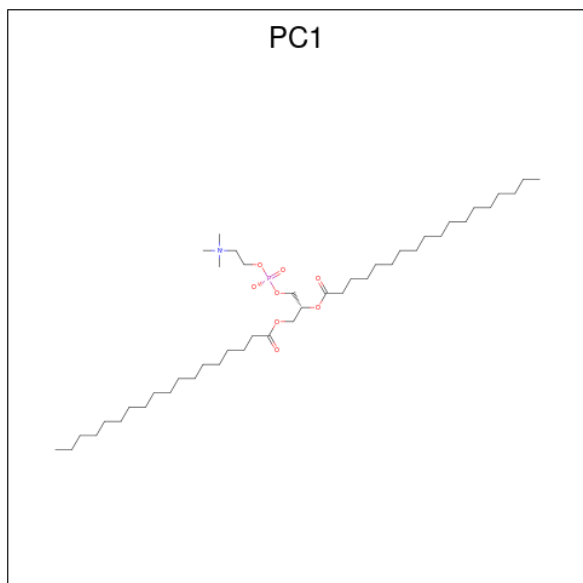
Mol	Chain	Residues	Atoms		AltConf	
73	E	1	Total	Fe	S	0
			4	2	2	
73	P	1	Total	Fe	S	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
73	2	1	4	2	2	0
73	3	1	4	2	2	0

- Molecule 74 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
74	J	1	35	25	1	8	1	0
74	K	1	28	18	1	8	1	0
74	L	1	24	14	1	8	1	0
74	V	1	28	18	1	8	1	0
74	I	1	50	40	1	8	1	0
74	p	1	35	25	1	8	1	0
74	z	1	28	18	1	8	1	0
74	6	1	43	33	1	8	1	0
74	9	1	54	44	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
74	9	1	Total	C	N	O	P	0
			47	37	1	8	1	
74	P1	1	Total	C	N	O	P	0
			31	21	1	8	1	
74	M1	1	Total	C	N	O	P	0
			54	44	1	8	1	
74	g	1	Total	C	N	O	P	0
			50	40	1	8	1	

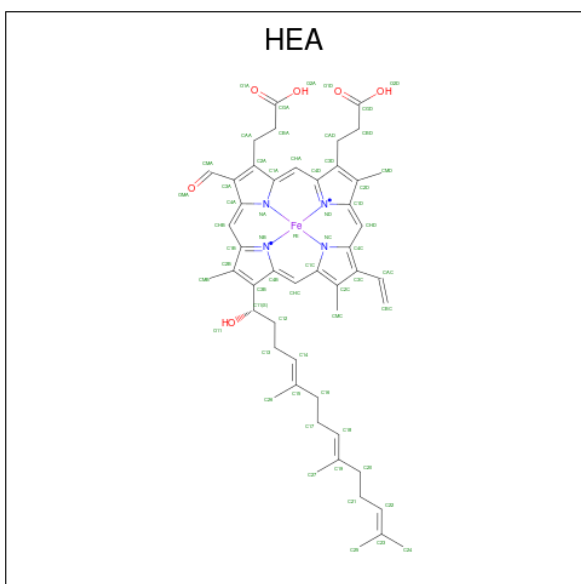
- Molecule 75 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
75	n	1	Total	Cu	0
			1	1	
75	a	1	Total	Cu	0
			1	1	

- Molecule 76 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
76	n	1	Total	Na	0
			1	1	
76	a	1	Total	Na	0
			1	1	

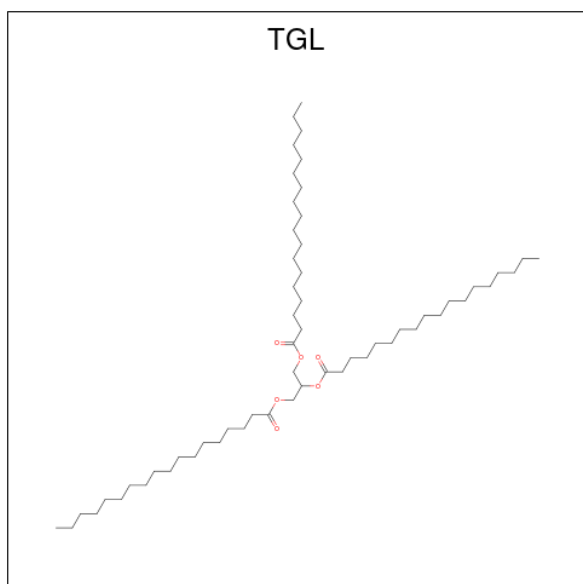
- Molecule 77 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



- Molecule 80 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
80	s	1	Total	Zn	0
			1	1	
80	7	1	Total	Zn	0
			1	1	
80	f	1	Total	Zn	0
			1	1	

- Molecule 81 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



Mol	Chain	Residues	Atoms			AltConf
81	y	1	Total	C	O	0
			37	31	6	
81	l	1	Total	C	O	0
			37	31	6	

- Molecule 82 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
82	6	1	Total	Fe	S	0
			8	4	4	
82	1	1	Total	Fe	S	0
			8	4	4	
82	3	1	Total	Fe	S	0
			8	4	4	
82	3	1	Total	Fe	S	0
			8	4	4	
82	9	1	Total	Fe	S	0
			8	4	4	
82	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 83 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

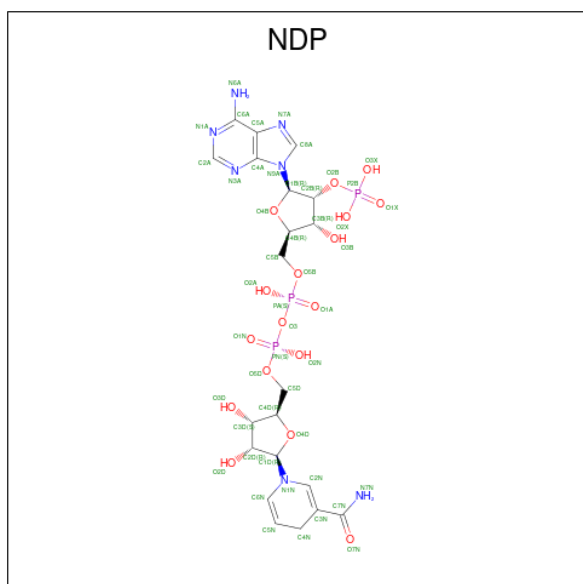


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
83	1	1	31	17	4	9	1	0

- Molecule 84 is POTASSIUM ION (three-letter code: K) (formula: K).

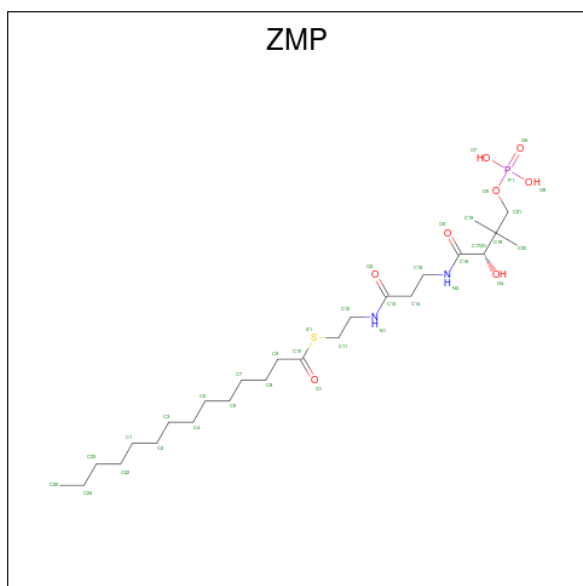
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
84	3	1	1	1	0

- Molecule 85 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
85	P1	1	48	21	7	17	3	0

- Molecule 86 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
86	W1	1	34	23	2	7	1	1	0
86	n1	1	32	21	2	7	1	1	0

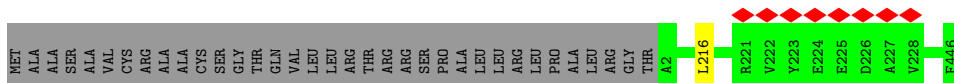
- Molecule 87 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).

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.

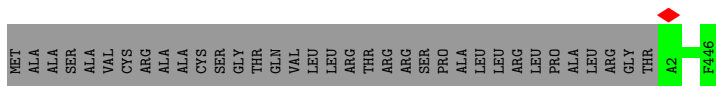
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A:  92% 7%



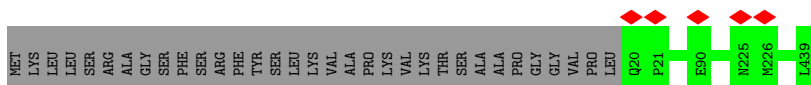
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L:  93% 7%



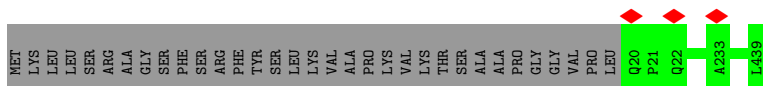
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:  93% 7%



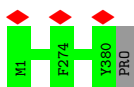
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:  93% 7%



- Molecule 3: Cytochrome b

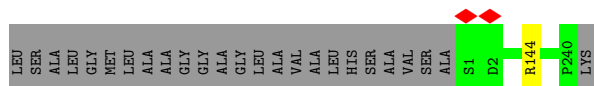
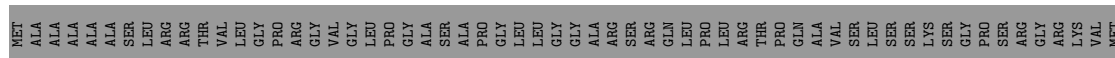
Chain C:  100%



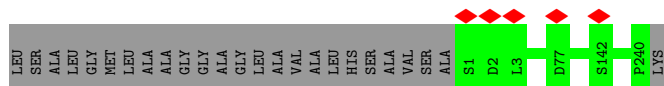
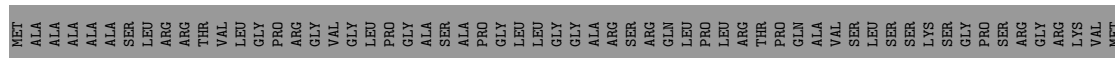
• Molecule 3: Cytochrome b



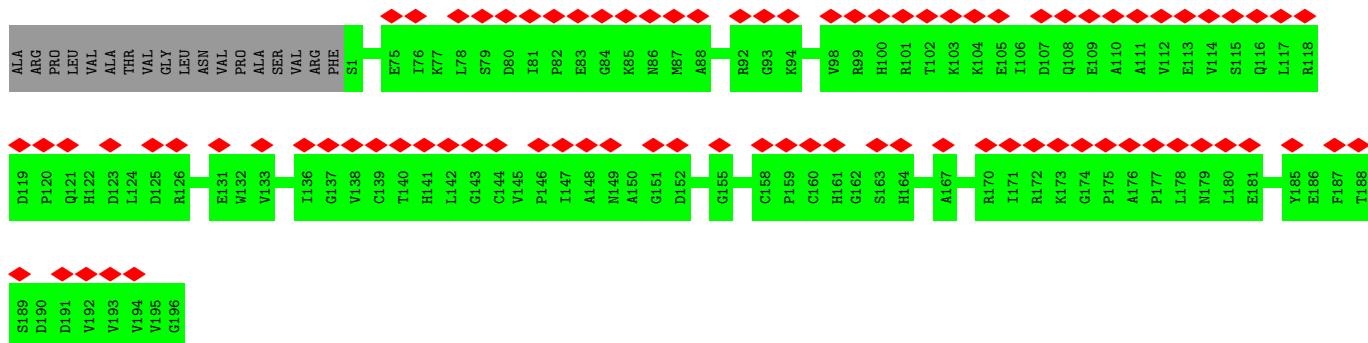
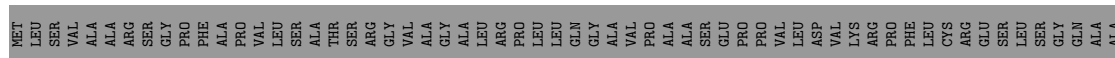
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



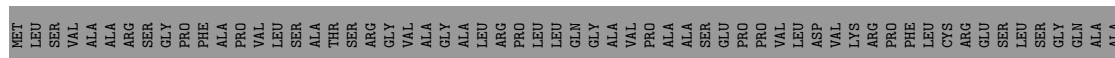
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

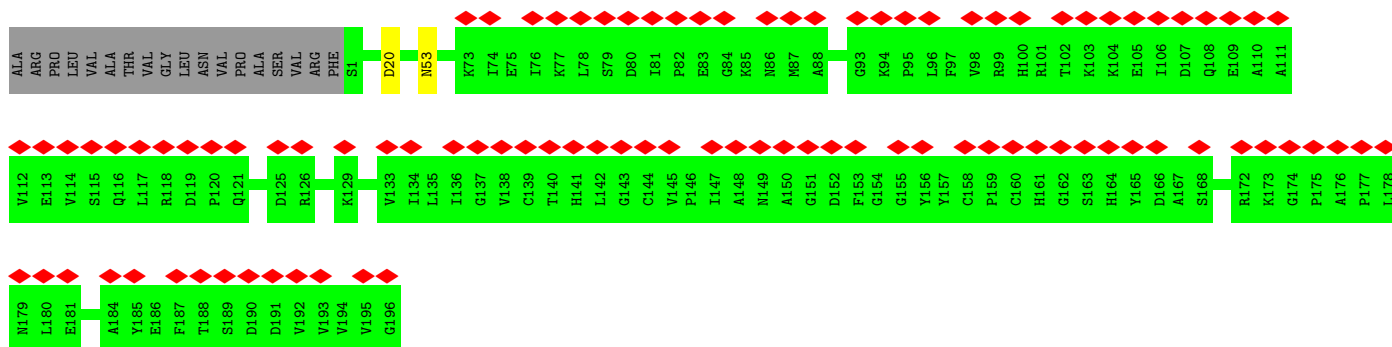


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

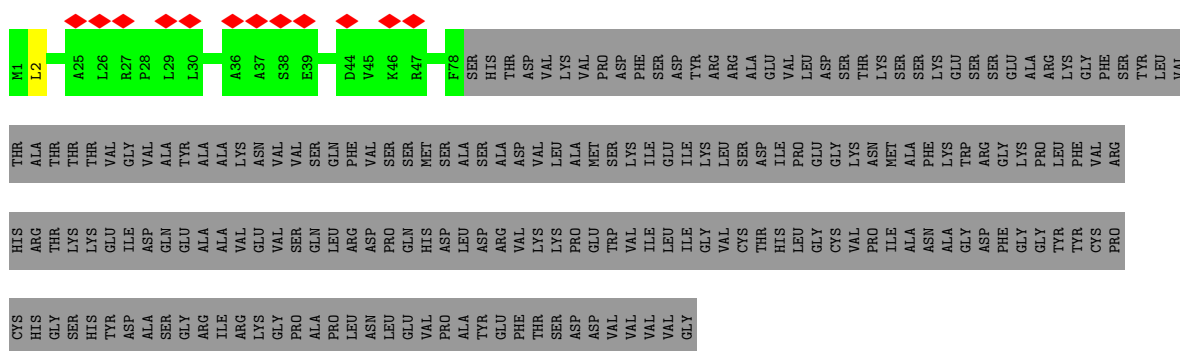


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

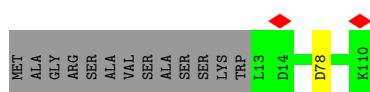
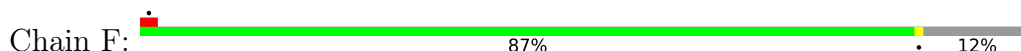




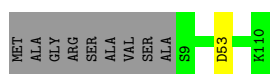
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



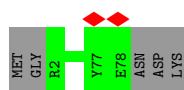
- Molecule 6: Cytochrome b-c1 complex subunit 7



- Molecule 6: Cytochrome b-c1 complex subunit 7



- Molecule 7: Cytochrome b-c1 complex subunit 8



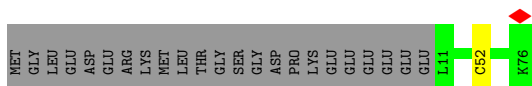
- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain R:  94% 6%




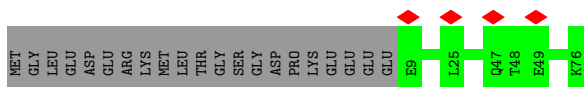
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:  73% 26%



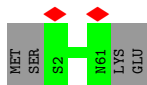
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain S:  76% 24%



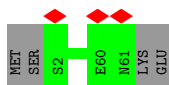
- Molecule 9: Cytochrome b-c1 complex subunit 9

Chain J:  94% 6%

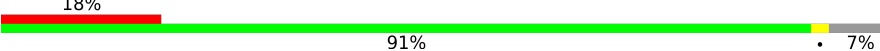


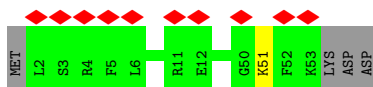
- Molecule 9: Cytochrome b-c1 complex subunit 9

Chain U:  94% 6% 5%



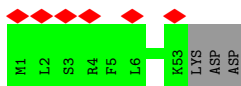
- Molecule 10: Cytochrome b-c1 complex subunit 10

Chain K:  91% 7% 18%

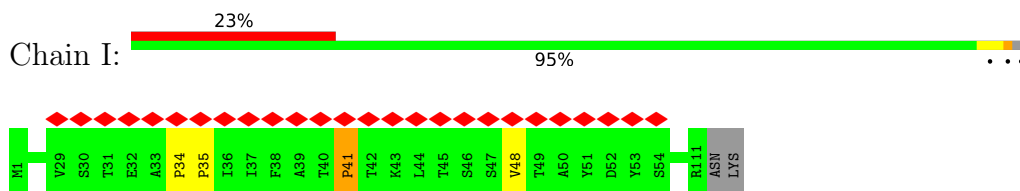


- Molecule 10: Cytochrome b-c1 complex subunit 10

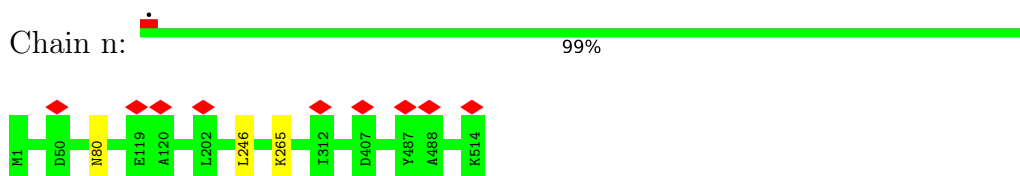
Chain V:  95% 5% 11%



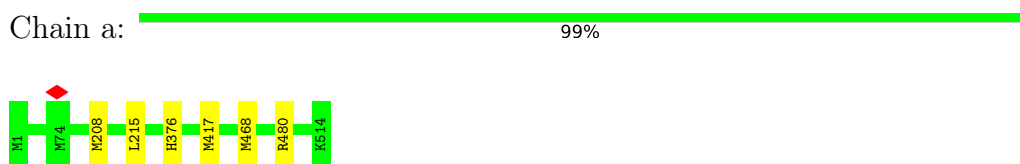
- Molecule 11: Cox7a2l protein



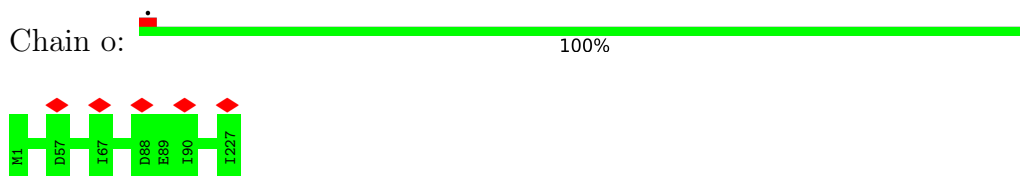
- Molecule 12: Cytochrome c oxidase subunit 1



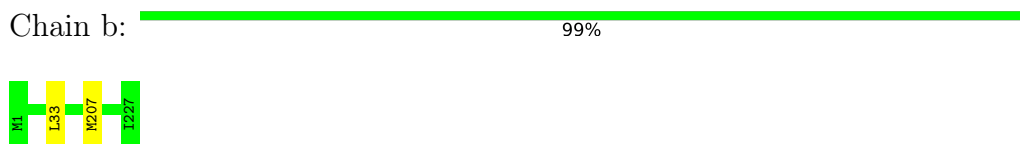
- Molecule 12: Cytochrome c oxidase subunit 1



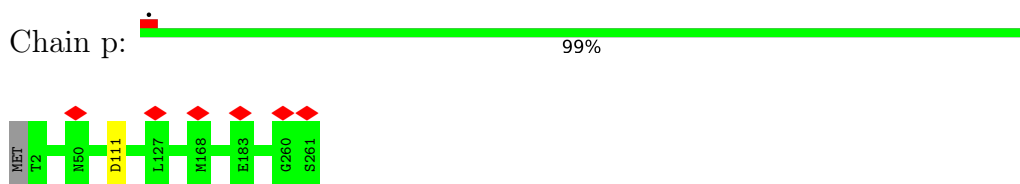
- Molecule 13: Cytochrome c oxidase subunit 2



- Molecule 13: Cytochrome c oxidase subunit 2

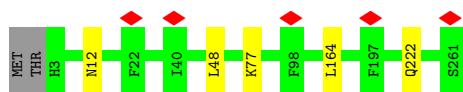


- Molecule 14: Cytochrome c oxidase subunit 3

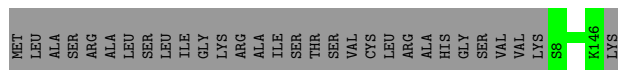
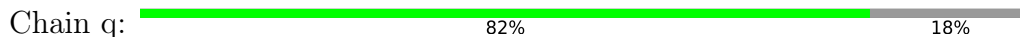


- Molecule 14: Cytochrome c oxidase subunit 3

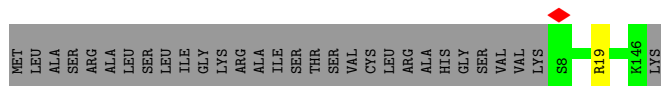
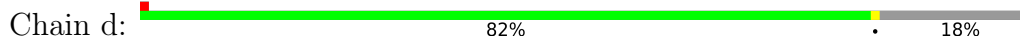




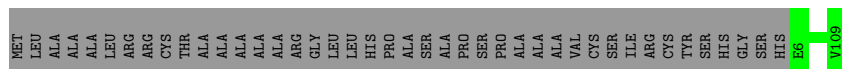
- Molecule 15: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



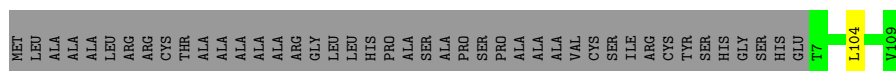
- Molecule 15: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



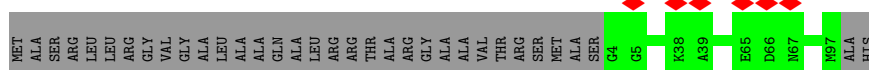
- Molecule 16: Cytochrome c oxidase subunit 5A, mitochondrial



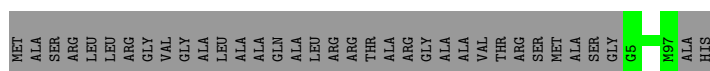
- Molecule 16: Cytochrome c oxidase subunit 5A, mitochondrial



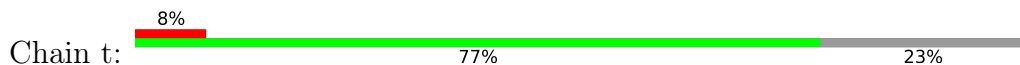
- Molecule 17: Cytochrome c oxidase subunit 5B, mitochondrial

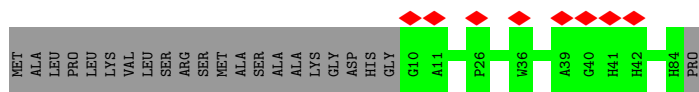


- Molecule 17: Cytochrome c oxidase subunit 5B, mitochondrial

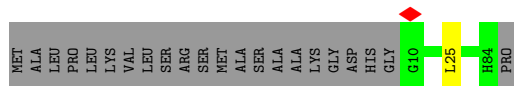
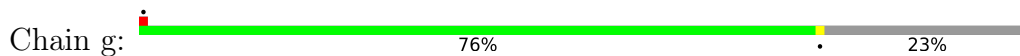


- Molecule 18: Cytochrome c oxidase subunit 6A2, mitochondrial

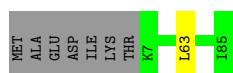




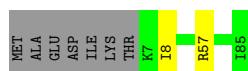
- Molecule 18: Cytochrome c oxidase subunit 6A2, mitochondrial



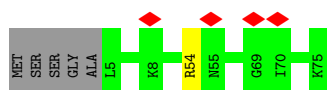
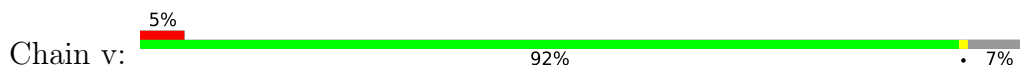
- Molecule 19: Cytochrome c oxidase subunit 6B1



- Molecule 19: Cytochrome c oxidase subunit 6B1



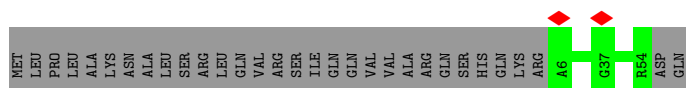
- Molecule 20: Cytochrome c oxidase subunit 6C



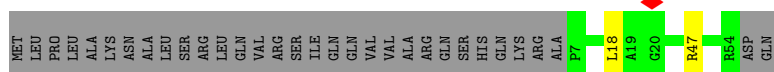
- Molecule 20: Cytochrome c oxidase subunit 6C



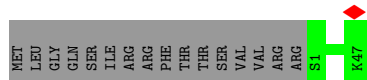
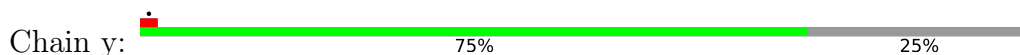
- Molecule 21: Cytochrome c oxidase subunit 7B, mitochondrial



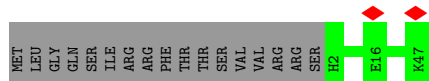
- Molecule 21: Cytochrome c oxidase subunit 7B, mitochondrial



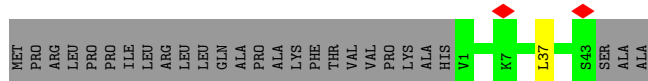
• Molecule 22: Cytochrome c oxidase subunit 7C, mitochondrial



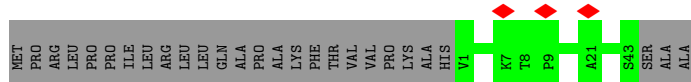
• Molecule 22: Cytochrome c oxidase subunit 7C, mitochondrial



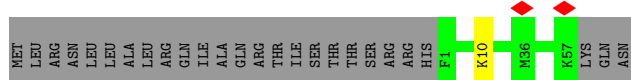
• Molecule 23: Cytochrome c oxidase subunit 8B, mitochondrial



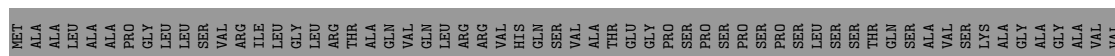
• Molecule 23: Cytochrome c oxidase subunit 8B, mitochondrial

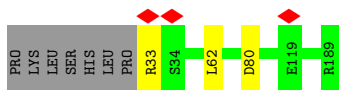


• Molecule 24: Cytochrome c oxidase subunit 7A2, mitochondrial

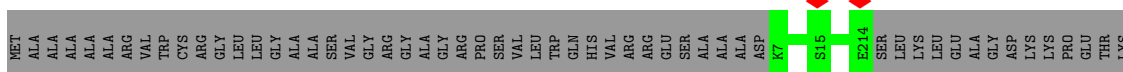
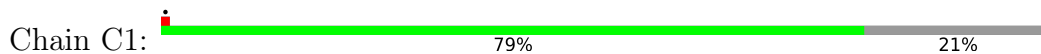


• Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

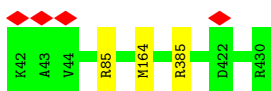
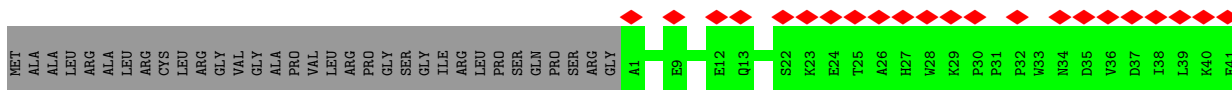




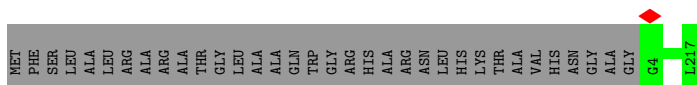
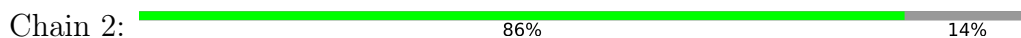
- Molecule 26: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



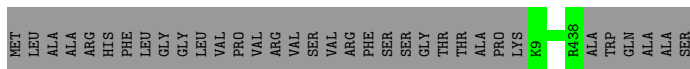
- Molecule 27: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



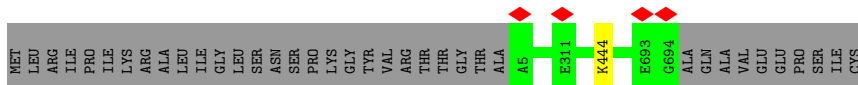
- Molecule 28: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



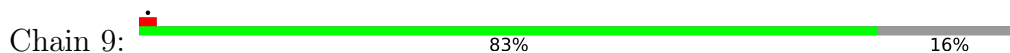
- Molecule 29: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

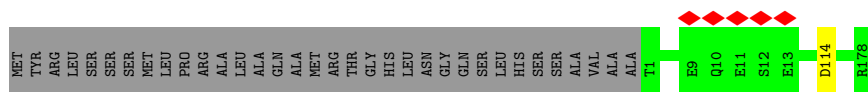


- Molecule 30: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



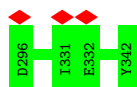
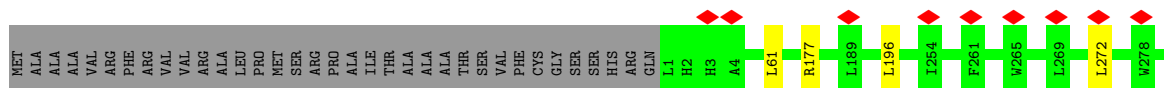
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial





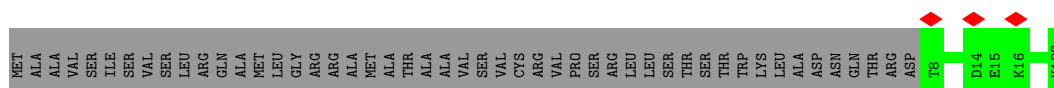
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P1: 90% 9%



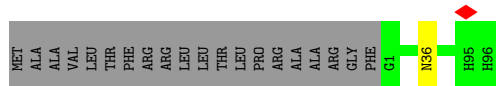
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q1: 72% 28%



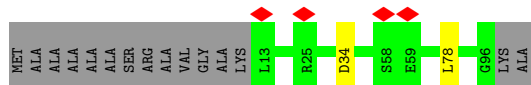
- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 7: 82% 17%



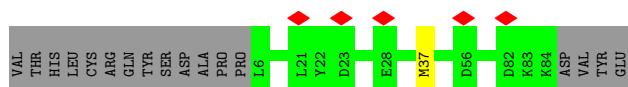
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S1: 83% 15%



- Molecule 36: Acyl carrier protein, mitochondrial

Chain T1: 50% 49%



- Molecule 36: Acyl carrier protein, mitochondrial

Chain U1:  56% 44%

MET ALA SER ARG VAL CYS ALA VAL ARG LEU PRO ALA ALA PHE PRO LEU PRO ARG PRO THR LEU ALA ALA ARG PRO LEU SER THR LEU CYS PRO GLU ILE ARG ARG PRO GLY ALA LEU ALA LEU ALA VAL PRO GLY THR


VAL THR HIS LEU CYS ARG GLN THR S1 D2 A3 E88

- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V1:  97%

MET ALA GLY L3 I115

- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W1:  87% 13%


MET ALA ALA ALA THR GLY LEU ARG GLN ALA ALA ALA ALA ALA ALA SER T17 D65 R116 P130

- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q1:  100%

HI K145

- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r1:  87% 12%

MET VAL A1 A74 L75 V76 SER GLY LYS ALA ALA GLU ALA SER SER ALA MET ALA ALA THR E90 L112

- Molecule 41: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

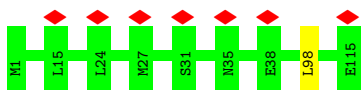
Chain s1:  40% 60%

MET ALA VAL SER LEU LEU ARG ARG GLY ARG ARG ARG ARG LEU LYS ALA VAL LEU LEU LEU GLU ALA ARG VAL PHE PRO GLY LEU VAL VAL VAL ARG LEU THR THR GLU SER GLU LYS ALA LYS GLU LYS GLU LEU HIS PRO LYS THR GLN SER VAL LEU LYS GLU PRO GLU

PRO T27 D28 T29 R68 HIS

- Molecule 42: NADH-ubiquinone oxidoreductase chain 3

Chain A1:  6% 99%



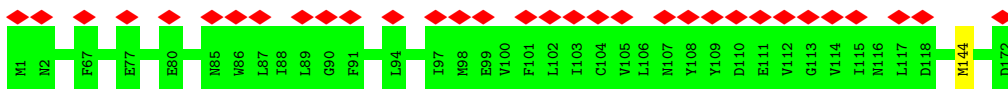
- Molecule 43: NADH-ubiquinone oxidoreductase chain 1

Chain H1:  99%



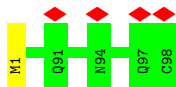
- Molecule 44: NADH-ubiquinone oxidoreductase chain 6

Chain J1:  19% 99%



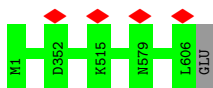
- Molecule 45: NADH-ubiquinone oxidoreductase chain 4L

Chain K1:  99%



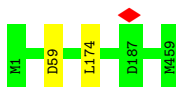
- Molecule 46: NADH-ubiquinone oxidoreductase chain 5

Chain L1:  100%



- Molecule 47: NADH-ubiquinone oxidoreductase chain 4

Chain M1:  100%



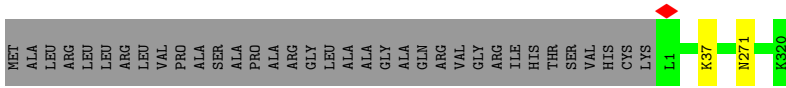
- Molecule 48: NADH-ubiquinone oxidoreductase chain 2

Chain N1:  99%



- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O1:  90% 10%



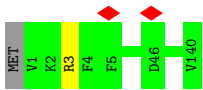
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X1:  99%



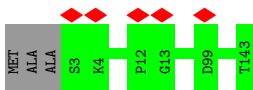
- Molecule 51: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y1:  99%



- Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z1:  98%



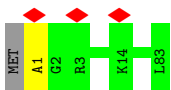
- Molecule 53: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a1:  100%



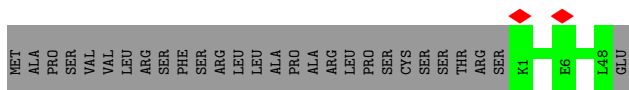
- Molecule 54: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b1:  98%

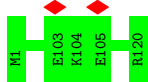


- Molecule 55: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

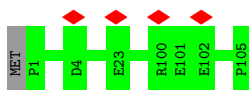
Chain c1:  63% 37%



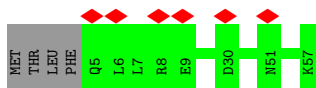
- Molecule 56: NADH dehydrogenase [ubiquinone] 1 subunit C2



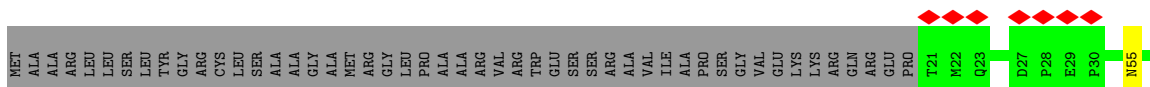
- Molecule 57: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



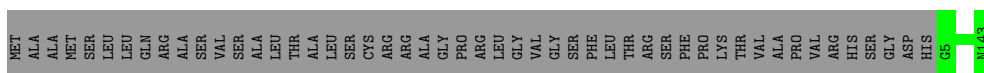
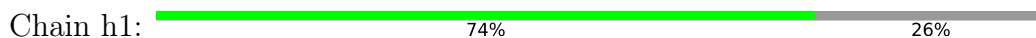
- Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



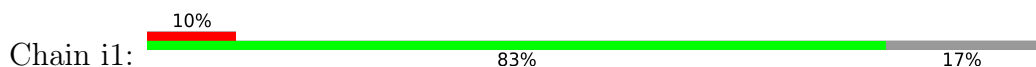
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

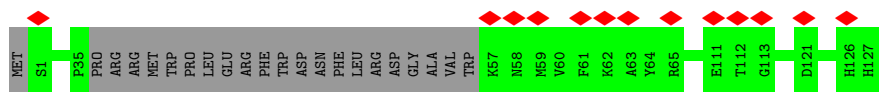


- Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

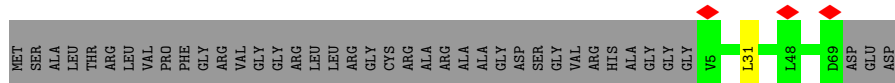


- Molecule 61: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

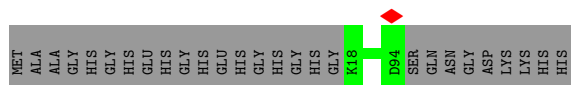
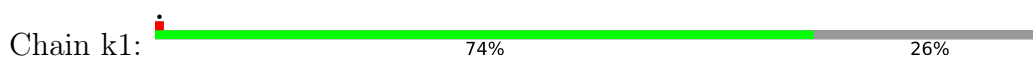




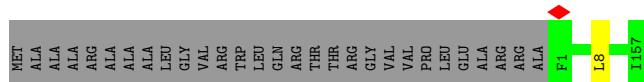
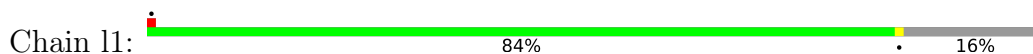
- Molecule 62: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



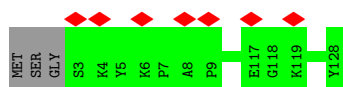
- Molecule 63: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 64: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



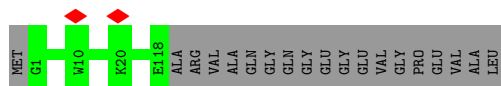
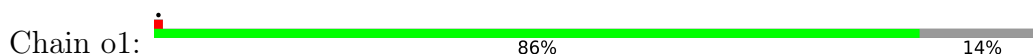
- Molecule 65: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 66: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

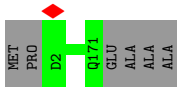


- Molecule 67: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 68: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p1:  97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51488	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	299.97998, 218.35999, 262.87997	wwPDB
Map dimensions	283, 206, 248	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SAC, NA, CDL, 3PE, HEC, NDP, PC1, FES, HEM, SF4, CU, FMN, AYA, K, 2MR, HEA, FME, TGL, MG, DGT, ZN, CUA, ZMP

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	0.27	0/3529	0.56	1/4793 (0.0%)
1	L	0.28	0/3530	0.53	0/4793
2	B	0.27	0/3205	0.50	0/4332
2	M	0.27	0/3205	0.50	0/4332
3	C	0.29	0/3147	0.52	0/4297
3	N	0.30	0/3147	0.55	3/4297 (0.1%)
4	D	0.27	0/1968	0.53	0/2674
4	O	0.28	0/1968	0.53	0/2674
5	E	0.27	0/1176	0.49	0/1609
5	P	0.27	0/1173	0.52	1/1605 (0.1%)
5	T	0.28	0/565	0.66	1/772 (0.1%)
6	F	0.28	0/885	0.65	1/1184 (0.1%)
6	Q	0.29	0/922	0.60	1/1234 (0.1%)
7	G	0.31	0/673	0.63	0/909
7	R	0.32	0/673	0.63	0/909
8	H	0.35	0/552	0.76	1/739 (0.1%)
8	S	0.34	0/570	0.70	0/763
9	J	0.28	0/509	0.54	0/687
9	U	0.31	0/509	0.58	0/687
10	K	0.29	0/446	0.62	0/609
10	V	0.27	0/454	0.64	0/619
11	I	0.28	0/825	0.70	3/1119 (0.3%)
12	a	0.33	0/4162	0.68	5/5686 (0.1%)
12	n	0.33	0/4162	0.59	1/5686 (0.0%)
13	b	0.31	0/1863	0.73	2/2542 (0.1%)
13	o	0.30	0/1863	0.64	0/2542
14	c	0.29	0/2195	0.59	2/3000 (0.1%)
14	p	0.30	0/2202	0.58	1/3010 (0.0%)
15	d	0.29	0/1190	0.68	0/1609
15	q	0.31	0/1190	0.64	0/1609
16	e	0.30	0/851	0.70	1/1155 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	r	0.28	0/860	0.65	0/1167
17	f	0.30	0/734	0.64	0/996
17	s	0.30	0/738	0.60	0/1001
18	g	0.27	0/632	0.65	1/866 (0.1%)
18	t	0.28	0/632	0.57	0/866
19	h	0.32	0/674	0.74	0/910
19	u	0.34	0/674	0.69	1/910 (0.1%)
20	i	0.38	0/584	0.85	1/778 (0.1%)
20	v	0.34	0/579	0.71	0/771
21	k	0.26	0/391	0.54	1/533 (0.2%)
21	x	0.32	0/396	0.61	0/541
22	l	0.30	0/393	0.62	0/527
22	y	0.35	0/399	0.61	0/535
23	m	0.32	0/318	0.71	0/433
23	z	0.31	0/318	0.69	1/433 (0.2%)
24	w	0.28	0/444	0.55	0/598
25	6	0.34	0/1289	0.69	2/1744 (0.1%)
26	C1	0.28	0/1780	0.56	0/2424
27	D1	0.31	0/3540	0.56	0/4795
28	2	0.29	0/1700	0.51	0/2316
29	1	0.29	0/3396	0.55	0/4586
30	3	0.28	0/5392	0.54	0/7305
31	9	0.35	0/1461	0.58	1/1974 (0.1%)
32	P1	0.28	0/2823	0.60	3/3828 (0.1%)
33	Q1	0.27	0/1045	0.52	0/1411
34	7	0.28	0/773	0.52	0/1041
35	S1	0.30	0/682	0.68	2/920 (0.2%)
36	T1	0.27	0/646	0.59	0/869
36	U1	0.32	0/718	0.56	0/970
37	V1	0.25	0/945	0.41	0/1281
38	W1	0.28	0/993	0.57	0/1335
39	q1	0.28	0/1251	0.53	0/1702
40	r1	0.27	0/806	0.55	0/1090
41	s1	0.27	0/360	0.67	0/489
42	A1	0.30	0/948	0.60	1/1295 (0.1%)
43	H1	0.35	0/2607	0.63	2/3564 (0.1%)
44	J1	0.32	0/1330	0.59	1/1810 (0.1%)
45	K1	0.31	0/738	0.57	0/1002
46	L1	0.31	0/4913	0.56	0/6686
47	M1	0.30	0/3709	0.60	2/5052 (0.0%)
48	N1	0.29	0/2755	0.57	1/3751 (0.0%)
49	O1	0.28	0/2674	0.51	0/3626
50	X1	0.27	0/1434	0.55	0/1937

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
51	Y1	0.28	0/1061	0.56	0/1439
52	Z1	0.27	0/1198	0.56	0/1616
53	a1	0.32	0/585	0.61	0/788
54	b1	0.28	0/666	0.55	0/914
55	c1	0.27	0/409	0.53	0/555
56	d1	0.29	0/1028	0.55	0/1387
57	e1	0.29	0/900	0.54	0/1199
58	f1	0.28	0/468	0.65	0/630
59	g1	0.28	0/878	0.51	0/1196
60	h1	0.29	0/1201	0.55	0/1626
61	i1	0.27	0/917	0.54	0/1243
62	j1	0.30	0/587	0.64	1/804 (0.1%)
63	k1	0.30	0/646	0.60	0/873
64	l1	0.29	0/1379	0.55	1/1882 (0.1%)
65	m1	0.33	0/1079	0.64	0/1463
66	n1	0.28	0/1596	0.53	0/2162
67	o1	0.29	0/1039	0.59	0/1394
68	p1	0.28	0/1471	0.52	0/1988
All	All	0.30	0/129891	0.58	46/176303 (0.0%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	468	MET	CG-SD-CE	9.76	115.81	100.20
32	P1	196	LEU	CA-CB-CG	7.44	132.41	115.30
25	6	80	ASP	CB-CG-OD1	6.95	124.55	118.30
6	Q	53	ASP	CB-CG-OD1	6.53	124.18	118.30
32	P1	272	LEU	CA-CB-CG	6.49	130.22	115.30
35	S1	34	ASP	CB-CG-OD1	6.48	124.13	118.30
6	F	78	ASP	CB-CG-OD1	6.41	124.07	118.30
47	M1	59	ASP	CB-CG-OD1	6.40	124.06	118.30
5	P	20	ASP	CB-CG-OD1	6.39	124.05	118.30
12	a	208	MET	CA-CB-CG	6.38	124.14	113.30
18	g	25	LEU	CA-CB-CG	6.30	129.80	115.30
44	J1	144	MET	CA-CB-CG	6.25	123.93	113.30
12	a	417	MET	CB-CG-SD	-6.12	94.05	112.40
11	I	41	PRO	N-CA-CB	6.11	110.63	103.30
23	z	37	LEU	CA-CB-CG	6.05	129.21	115.30
11	I	34	PRO	N-CA-CB	6.02	110.53	103.30
11	I	35	PRO	N-CA-CB	5.96	110.46	103.30
3	N	149	LEU	CB-CG-CD2	-5.88	101.01	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	M1	174	LEU	CA-CB-CG	5.81	128.66	115.30
43	H1	233	LEU	CB-CG-CD1	-5.79	101.16	111.00
31	9	114	ASP	CB-CG-OD1	5.77	123.49	118.30
12	a	417	MET	CA-CB-CG	5.72	123.03	113.30
32	P1	61	LEU	CA-CB-CG	5.70	128.40	115.30
1	A	216	LEU	CA-CB-CG	5.68	128.37	115.30
14	c	164	LEU	CA-CB-CG	5.62	128.23	115.30
16	e	104	LEU	CA-CB-CG	5.62	128.23	115.30
42	A1	98	LEU	CA-CB-CG	5.53	128.02	115.30
64	l1	8	LEU	CA-CB-CG	5.53	128.02	115.30
12	a	215	LEU	CA-CB-CG	5.50	127.94	115.30
5	T	2	LEU	CA-CB-CG	5.48	127.91	115.30
3	N	58	ASP	CB-CG-OD1	5.43	123.18	118.30
14	p	111	ASP	CB-CG-OD1	5.40	123.16	118.30
3	N	149	LEU	CB-CG-CD1	5.38	120.15	111.00
8	H	52	CYS	CA-CB-SG	5.38	123.68	114.00
48	N1	232	LEU	CA-CB-CG	5.30	127.49	115.30
12	n	246	LEU	CB-CG-CD1	5.26	119.94	111.00
13	b	207	MET	CA-CB-CG	5.19	122.12	113.30
20	i	65	MET	CA-CB-CG	5.18	122.11	113.30
13	b	33	LEU	CA-CB-CG	5.14	127.12	115.30
14	c	48	LEU	CA-CB-CG	5.09	127.00	115.30
25	6	62	LEU	CA-CB-CG	5.07	126.96	115.30
19	u	63	LEU	C-N-CA	-5.07	109.04	121.70
62	j1	31	LEU	CA-CB-CG	5.06	126.95	115.30
43	H1	285	LEU	CA-CB-CG	5.05	126.92	115.30
35	S1	78	LEU	CA-CB-CG	5.01	126.82	115.30
21	k	18	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	443/480 (92%)	426 (96%)	17 (4%)	0	100	100
1	L	443/480 (92%)	429 (97%)	14 (3%)	0	100	100
2	B	418/453 (92%)	409 (98%)	9 (2%)	0	100	100
2	M	418/453 (92%)	403 (96%)	15 (4%)	0	100	100
3	C	378/381 (99%)	366 (97%)	12 (3%)	0	100	100
3	N	378/381 (99%)	366 (97%)	12 (3%)	0	100	100
4	D	238/325 (73%)	233 (98%)	5 (2%)	0	100	100
4	O	238/325 (73%)	231 (97%)	7 (3%)	0	100	100
5	E	194/274 (71%)	186 (96%)	8 (4%)	0	100	100
5	P	194/274 (71%)	186 (96%)	8 (4%)	0	100	100
5	T	76/274 (28%)	72 (95%)	4 (5%)	0	100	100
6	F	96/111 (86%)	96 (100%)	0	0	100	100
6	Q	100/111 (90%)	100 (100%)	0	0	100	100
7	G	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
7	R	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
8	H	64/89 (72%)	64 (100%)	0	0	100	100
8	S	66/89 (74%)	63 (96%)	3 (4%)	0	100	100
9	J	58/64 (91%)	57 (98%)	1 (2%)	0	100	100
9	U	58/64 (91%)	56 (97%)	2 (3%)	0	100	100
10	K	50/56 (89%)	49 (98%)	1 (2%)	0	100	100
10	V	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
11	I	109/113 (96%)	100 (92%)	7 (6%)	2 (2%)	8	43
12	a	512/514 (100%)	491 (96%)	20 (4%)	1 (0%)	47	79
12	n	512/514 (100%)	489 (96%)	23 (4%)	0	100	100
13	b	225/227 (99%)	212 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	225/227 (99%)	211 (94%)	14 (6%)	0	100	100
14	c	257/261 (98%)	249 (97%)	8 (3%)	0	100	100
14	p	258/261 (99%)	251 (97%)	7 (3%)	0	100	100
15	d	137/169 (81%)	128 (93%)	9 (7%)	0	100	100
15	q	137/169 (81%)	127 (93%)	10 (7%)	0	100	100
16	e	101/146 (69%)	100 (99%)	1 (1%)	0	100	100
16	r	102/146 (70%)	99 (97%)	3 (3%)	0	100	100
17	f	91/128 (71%)	84 (92%)	7 (8%)	0	100	100
17	s	92/128 (72%)	86 (94%)	6 (6%)	0	100	100
18	g	73/97 (75%)	66 (90%)	7 (10%)	0	100	100
18	t	73/97 (75%)	68 (93%)	5 (7%)	0	100	100
19	h	77/86 (90%)	73 (95%)	3 (4%)	1 (1%)	12	50
19	u	77/86 (90%)	74 (96%)	3 (4%)	0	100	100
20	i	70/76 (92%)	66 (94%)	4 (6%)	0	100	100
20	v	69/76 (91%)	63 (91%)	6 (9%)	0	100	100
21	k	46/80 (58%)	44 (96%)	2 (4%)	0	100	100
21	x	47/80 (59%)	45 (96%)	2 (4%)	0	100	100
22	l	44/63 (70%)	41 (93%)	3 (7%)	0	100	100
22	y	45/63 (71%)	45 (100%)	0	0	100	100
23	m	41/70 (59%)	37 (90%)	4 (10%)	0	100	100
23	z	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
24	w	55/83 (66%)	55 (100%)	0	0	100	100
25	6	155/224 (69%)	148 (96%)	7 (4%)	0	100	100
26	C1	206/263 (78%)	200 (97%)	6 (3%)	0	100	100
27	D1	427/463 (92%)	412 (96%)	15 (4%)	0	100	100
28	2	212/248 (86%)	201 (95%)	11 (5%)	0	100	100
29	1	428/464 (92%)	409 (96%)	19 (4%)	0	100	100
30	3	688/727 (95%)	666 (97%)	22 (3%)	0	100	100
31	9	176/212 (83%)	172 (98%)	4 (2%)	0	100	100
32	P1	340/377 (90%)	326 (96%)	14 (4%)	0	100	100
33	Q1	124/175 (71%)	120 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	7	94/116 (81%)	92 (98%)	2 (2%)	0	100	100
35	S1	82/99 (83%)	75 (92%)	7 (8%)	0	100	100
36	T1	77/156 (49%)	76 (99%)	1 (1%)	0	100	100
36	U1	86/156 (55%)	85 (99%)	1 (1%)	0	100	100
37	V1	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
38	W1	112/131 (86%)	107 (96%)	5 (4%)	0	100	100
39	q1	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
40	r1	95/113 (84%)	92 (97%)	3 (3%)	0	100	100
41	s1	40/104 (38%)	38 (95%)	2 (5%)	0	100	100
42	A1	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
43	H1	316/318 (99%)	296 (94%)	20 (6%)	0	100	100
44	J1	170/172 (99%)	158 (93%)	12 (7%)	0	100	100
45	K1	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
46	L1	604/607 (100%)	567 (94%)	37 (6%)	0	100	100
47	M1	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
48	N1	343/345 (99%)	332 (97%)	11 (3%)	0	100	100
49	O1	318/355 (90%)	300 (94%)	18 (6%)	0	100	100
50	X1	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
51	Y1	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
52	Z1	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
53	a1	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
54	b1	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
55	c1	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
56	d1	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
57	e1	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
58	f1	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
59	g1	99/151 (66%)	95 (96%)	4 (4%)	0	100	100
60	h1	137/189 (72%)	132 (96%)	5 (4%)	0	100	100
61	i1	102/128 (80%)	96 (94%)	6 (6%)	0	100	100
62	j1	63/105 (60%)	61 (97%)	2 (3%)	0	100	100
63	k1	75/104 (72%)	73 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	l1	155/186 (83%)	152 (98%)	3 (2%)	0	100	100
65	m1	124/129 (96%)	120 (97%)	4 (3%)	0	100	100
66	n1	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
67	o1	116/137 (85%)	109 (94%)	7 (6%)	0	100	100
68	p1	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
All	All	15768/18146 (87%)	15159 (96%)	605 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	h	8	ILE
12	a	376	HIS
11	I	48	VAL
11	I	41	PRO

5.3.2 Protein sidechains [i](#)

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	372/398 (94%)	372 (100%)	0	100	100
1	L	372/398 (94%)	372 (100%)	0	100	100
2	B	330/356 (93%)	330 (100%)	0	100	100
2	M	330/356 (93%)	330 (100%)	0	100	100
3	C	332/333 (100%)	332 (100%)	0	100	100
3	N	332/333 (100%)	332 (100%)	0	100	100
4	D	205/260 (79%)	204 (100%)	1 (0%)	88	95
4	O	205/260 (79%)	205 (100%)	0	100	100
5	E	69/224 (31%)	69 (100%)	0	100	100
5	P	68/224 (30%)	67 (98%)	1 (2%)	65	84
5	T	58/224 (26%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	90/99 (91%)	90 (100%)	0	100	100
6	Q	94/99 (95%)	94 (100%)	0	100	100
7	G	70/74 (95%)	70 (100%)	0	100	100
7	R	70/74 (95%)	70 (100%)	0	100	100
8	H	63/83 (76%)	63 (100%)	0	100	100
8	S	65/83 (78%)	65 (100%)	0	100	100
9	J	51/55 (93%)	51 (100%)	0	100	100
9	U	51/55 (93%)	51 (100%)	0	100	100
10	K	42/46 (91%)	41 (98%)	1 (2%)	49	75
10	V	43/46 (94%)	43 (100%)	0	100	100
11	I	73/95 (77%)	73 (100%)	0	100	100
12	a	425/425 (100%)	424 (100%)	1 (0%)	93	98
12	n	425/425 (100%)	423 (100%)	2 (0%)	88	95
13	b	210/210 (100%)	210 (100%)	0	100	100
13	o	210/210 (100%)	210 (100%)	0	100	100
14	c	225/227 (99%)	222 (99%)	3 (1%)	69	86
14	p	226/227 (100%)	226 (100%)	0	100	100
15	d	122/146 (84%)	121 (99%)	1 (1%)	81	91
15	q	122/146 (84%)	122 (100%)	0	100	100
16	e	90/118 (76%)	90 (100%)	0	100	100
16	r	91/118 (77%)	91 (100%)	0	100	100
17	f	80/101 (79%)	80 (100%)	0	100	100
17	s	80/101 (79%)	80 (100%)	0	100	100
18	g	62/78 (80%)	62 (100%)	0	100	100
18	t	62/78 (80%)	62 (100%)	0	100	100
19	h	70/76 (92%)	69 (99%)	1 (1%)	67	85
19	u	70/76 (92%)	70 (100%)	0	100	100
20	i	54/57 (95%)	54 (100%)	0	100	100
20	v	54/57 (95%)	53 (98%)	1 (2%)	57	80
21	k	39/67 (58%)	38 (97%)	1 (3%)	46	74
21	x	39/67 (58%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	l	39/55 (71%)	39 (100%)	0	100	100
22	y	40/55 (73%)	40 (100%)	0	100	100
23	m	33/55 (60%)	33 (100%)	0	100	100
23	z	33/55 (60%)	33 (100%)	0	100	100
24	w	43/67 (64%)	42 (98%)	1 (2%)	50	76
25	6	133/185 (72%)	132 (99%)	1 (1%)	81	91
26	C1	190/227 (84%)	190 (100%)	0	100	100
27	D1	370/394 (94%)	368 (100%)	2 (0%)	88	95
28	2	184/206 (89%)	184 (100%)	0	100	100
29	1	345/370 (93%)	345 (100%)	0	100	100
30	3	580/610 (95%)	579 (100%)	1 (0%)	93	98
31	9	152/178 (85%)	152 (100%)	0	100	100
32	P1	299/325 (92%)	298 (100%)	1 (0%)	92	97
33	Q1	113/153 (74%)	113 (100%)	0	100	100
34	7	81/96 (84%)	80 (99%)	1 (1%)	71	87
35	S1	74/80 (92%)	74 (100%)	0	100	100
36	T1	73/135 (54%)	72 (99%)	1 (1%)	67	85
36	U1	81/135 (60%)	81 (100%)	0	100	100
37	V1	101/102 (99%)	101 (100%)	0	100	100
38	W1	108/114 (95%)	108 (100%)	0	100	100
39	q1	131/131 (100%)	131 (100%)	0	100	100
40	r1	88/96 (92%)	88 (100%)	0	100	100
41	s1	41/95 (43%)	41 (100%)	0	100	100
42	A1	103/103 (100%)	103 (100%)	0	100	100
43	H1	279/279 (100%)	279 (100%)	0	100	100
44	J1	137/137 (100%)	137 (100%)	0	100	100
45	K1	87/87 (100%)	87 (100%)	0	100	100
46	L1	548/549 (100%)	548 (100%)	0	100	100
47	M1	414/414 (100%)	414 (100%)	0	100	100
48	N1	307/307 (100%)	307 (100%)	0	100	100
49	O1	284/309 (92%)	282 (99%)	2 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	X1	153/154 (99%)	153 (100%)	0	100	100
51	Y1	105/106 (99%)	104 (99%)	1 (1%)	76	88
52	Z1	122/123 (99%)	122 (100%)	0	100	100
53	a1	60/60 (100%)	60 (100%)	0	100	100
54	b1	72/73 (99%)	72 (100%)	0	100	100
55	c1	42/67 (63%)	42 (100%)	0	100	100
56	d1	107/107 (100%)	107 (100%)	0	100	100
57	e1	93/94 (99%)	93 (100%)	0	100	100
58	f1	49/53 (92%)	49 (100%)	0	100	100
59	g1	92/129 (71%)	91 (99%)	1 (1%)	73	88
60	h1	123/162 (76%)	123 (100%)	0	100	100
61	i1	99/119 (83%)	99 (100%)	0	100	100
62	j1	61/87 (70%)	61 (100%)	0	100	100
63	k1	60/78 (77%)	60 (100%)	0	100	100
64	l1	142/161 (88%)	142 (100%)	0	100	100
65	m1	112/114 (98%)	112 (100%)	0	100	100
66	n1	163/164 (99%)	163 (100%)	0	100	100
67	o1	109/121 (90%)	109 (100%)	0	100	100
68	p1	155/158 (98%)	155 (100%)	0	100	100
All	All	13551/15419 (88%)	13526 (100%)	25 (0%)	93	98

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	144	ARG
10	K	51	LYS
5	P	53	ASN
12	n	80	ASN
12	n	265	LYS
20	v	54	ARG
24	w	10	LYS
25	6	33	ARG
27	D1	164	MET
27	D1	385	ARG
30	3	444	LYS

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Mol	Chain	Res	Type
32	P1	177	ARG
34	7	36	ASN
36	T1	37	MET
49	O1	37	LYS
49	O1	271	ASN
51	Y1	3	ARG
59	g1	55	ASN
12	a	480	ARG
14	c	12	ASN
14	c	77	LYS
14	c	222	GLN
15	d	19	ARG
19	h	57	ARG
21	k	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	339	GLN
3	C	16	HIS
1	L	53	ASN
1	L	323	HIS
1	L	363	ASN
11	I	24	GLN
11	I	63	GLN
12	n	151	HIS
21	x	41	ASN
43	H1	138	GLN
46	L1	170	GLN
50	X1	98	HIS
66	n1	12	GLN
12	a	98	ASN
12	a	135	ASN
12	a	429	HIS
14	c	160	ASN
14	c	161	GLN
14	c	222	GLN
14	c	231	HIS
18	g	76	ASN
22	l	10	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

11 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
43	FME	H1	1	43	8,9,10	0.96	0	7,9,11	0.89	0
40	AYA	r1	1	40	6,7,8	1.28	1 (16%)	5,8,10	1.28	1 (20%)
47	FME	M1	1	47	8,9,10	0.96	0	7,9,11	0.76	0
54	AYA	b1	1	54	6,7,8	1.25	1 (16%)	5,8,10	1.28	1 (20%)
61	SAC	i1	1	61	7,8,9	1.02	0	8,9,11	0.81	0
44	FME	J1	1	44	8,9,10	0.95	0	7,9,11	0.85	0
46	FME	L1	1	46	8,9,10	0.92	0	7,9,11	0.91	0
45	FME	K1	1	45	8,9,10	0.94	0	7,9,11	1.66	2 (28%)
27	2MR	D1	85	27	10,12,13	2.58	2 (20%)	5,13,15	2.84	2 (40%)
42	FME	A1	1	42	8,9,10	0.94	0	7,9,11	0.79	0
48	FME	N1	1	48	8,9,10	0.96	0	7,9,11	1.04	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	FME	H1	1	43	-	3/7/9/11	-
40	AYA	r1	1	40	-	0/4/6/8	-
47	FME	M1	1	47	-	2/7/9/11	-
54	AYA	b1	1	54	-	0/4/6/8	-
61	SAC	i1	1	61	-	2/7/8/10	-
44	FME	J1	1	44	-	4/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	FME	L1	1	46	-	4/7/9/11	-
45	FME	K1	1	45	-	3/7/9/11	-
27	2MR	D1	85	27	-	4/10/13/15	-
42	FME	A1	1	42	-	1/7/9/11	-
48	FME	N1	1	48	-	2/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D1	85	2MR	CZ-NE	5.89	1.46	1.34
27	D1	85	2MR	CZ-NH2	5.11	1.44	1.33
40	r1	1	AYA	CA-N	-2.49	1.43	1.46
54	b1	1	AYA	CA-N	-2.30	1.44	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D1	85	2MR	CD-NE-CZ	4.86	132.50	123.41
27	D1	85	2MR	NE-CZ-NH2	-3.72	116.07	119.48
45	K1	1	FME	C-CA-N	3.51	116.06	109.73
40	r1	1	AYA	CB-CA-N	2.70	112.61	109.61
54	b1	1	AYA	CB-CA-N	2.57	112.47	109.61
45	K1	1	FME	O-C-CA	-2.14	119.18	124.78
48	N1	1	FME	C-CA-N	2.12	113.56	109.73

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	D1	85	2MR	O-C-CA-CB
43	H1	1	FME	N-CA-CB-CG
44	J1	1	FME	C-CA-CB-CG
44	J1	1	FME	O-C-CA-CB
45	K1	1	FME	O1-CN-N-CA
46	L1	1	FME	CB-CA-N-CN
46	L1	1	FME	N-CA-CB-CG
47	M1	1	FME	N-CA-CB-CG
48	N1	1	FME	C-CA-CB-CG
27	D1	85	2MR	NE-CD-CG-CB
44	J1	1	FME	CB-CG-SD-CE

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Mol	Chain	Res	Type	Atoms
45	K1	1	FME	CA-CB-CG-SD
27	D1	85	2MR	CA-CB-CG-CD
48	N1	1	FME	CA-CB-CG-SD
42	A1	1	FME	N-CA-CB-CG
44	J1	1	FME	N-CA-CB-CG
45	K1	1	FME	N-CA-CB-CG
46	L1	1	FME	CB-CG-SD-CE
43	H1	1	FME	CB-CA-N-CN
47	M1	1	FME	CB-CA-N-CN
43	H1	1	FME	C-CA-CB-CG
46	L1	1	FME	C-CA-CB-CG
27	D1	85	2MR	CG-CD-NE-CZ
61	i1	1	SAC	C-CA-CB-OG
61	i1	1	SAC	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 112 ligands modelled in this entry, 11 are monoatomic - leaving 101 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
69	3PE	z	102	-	25,25,50	0.41	0	28,30,55	0.39	0
86	ZMP	W1	201	-	27,33,36	0.68	1 (3%)	32,40,45	0.93	1 (3%)
70	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.33	0
69	3PE	c	301	-	44,44,50	0.32	0	47,49,55	0.32	0
69	3PE	n	606	-	27,27,50	0.40	0	30,32,55	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	3PE	n	605	-	33,33,50	0.38	0	36,38,55	0.55	1 (2%)
73	FES	3	803	30	0,4,4	-	-	-		
69	3PE	b1	101	-	42,42,50	0.33	0	45,47,55	0.35	0
69	3PE	m1	601	-	35,35,50	0.36	0	38,40,55	0.30	0
82	SF4	9	202	31	0,12,12	-	-	-		
87	DGT	O1	401	78	26,33,33	0.79	1 (3%)	32,52,52	0.46	0
69	3PE	K1	201	-	40,40,50	0.33	0	43,45,55	0.30	0
81	TGL	l	601	-	36,36,62	0.23	0	39,39,65	0.17	0
69	3PE	r1	201	-	45,45,50	0.32	0	48,50,55	0.29	0
70	CDL	R	102	-	56,56,99	0.39	0	62,68,111	0.47	1 (1%)
74	PC1	z	101	-	27,27,53	0.40	0	33,35,61	0.35	0
69	3PE	L	501	-	22,22,50	0.43	0	25,27,55	0.39	0
73	FES	2	301	28	0,4,4	-	-	-		
70	CDL	A	502	-	45,45,99	0.43	0	51,57,111	0.36	0
73	FES	P	201	5	0,4,4	-	-	-		
85	NDP	P1	501	-	45,52,52	0.52	0	53,80,80	0.60	1 (1%)
69	3PE	E	203	-	33,33,50	0.36	0	36,38,55	0.33	0
82	SF4	3	801	30	0,12,12	-	-	-		
69	3PE	g	303	-	24,24,50	0.43	0	27,29,55	0.63	0
69	3PE	b	301	-	28,28,50	0.40	0	31,33,55	0.37	0
77	HEA	a	603	12	57,67,67	1.49	7 (12%)	61,103,103	2.43	23 (37%)
74	PC1	L	503	-	23,23,53	0.44	0	29,31,61	0.61	0
69	3PE	N	403	-	36,36,50	0.35	0	39,41,55	0.31	0
74	PC1	K	101	-	27,27,53	0.39	0	33,35,61	0.47	0
77	HEA	n	604	12	57,67,67	1.44	8 (14%)	61,103,103	2.48	23 (37%)
69	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.33	0
69	3PE	a	605	-	27,27,50	0.40	0	30,32,55	0.46	0
81	TGL	y	601	-	36,36,62	0.24	0	39,39,65	0.18	0
74	PC1	J	101	-	34,34,53	0.35	0	40,42,61	0.34	0
69	3PE	N1	402	-	37,37,50	0.35	0	40,42,55	0.33	0
74	PC1	9	204	-	46,46,53	0.32	0	52,54,61	0.30	0
70	CDL	r1	202	-	56,56,99	0.40	0	62,68,111	0.47	1 (1%)
73	FES	E	201	5	0,4,4	-	-	-		
69	3PE	C	404	-	30,30,50	0.38	0	33,35,55	0.34	0
69	3PE	M1	502	-	50,50,50	0.30	0	53,55,55	0.30	0
70	CDL	D	302	-	55,55,99	0.39	0	61,67,111	0.33	0
71	HEM	C	402	3	41,50,50	1.43	5 (12%)	45,82,82	1.41	6 (13%)
69	3PE	d1	203	-	31,31,50	0.37	0	34,36,55	0.37	0
71	HEM	N	401	3	41,50,50	1.46	3 (7%)	45,82,82	1.74	9 (20%)
69	3PE	A	501	-	22,22,50	0.45	0	25,27,55	0.66	0
74	PC1	g	302	-	49,49,53	0.30	0	55,57,61	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	3PE	Y1	402	-	27,27,50	0.39	0	30,32,55	0.37	0
77	HEA	a	604	12	57,67,67	1.41	8 (14%)	61,103,103	2.39	23 (37%)
69	3PE	i	101	-	27,27,50	0.39	0	30,32,55	0.33	0
69	3PE	p	301	-	44,44,50	0.32	0	47,49,55	0.30	0
69	3PE	E	202	-	31,31,50	0.37	0	34,36,55	0.32	0
79	CUA	b	302	13	0,1,1	-	-	-		
69	3PE	M1	503	-	50,50,50	0.30	0	53,55,55	0.27	0
70	CDL	h1	201	-	69,69,99	0.36	0	75,81,111	0.42	0
69	3PE	t	101	-	24,24,50	0.43	0	27,29,55	0.60	1 (3%)
70	CDL	L	502	-	45,45,99	0.44	0	51,57,111	0.51	0
70	CDL	G	101	-	41,41,99	0.44	0	47,53,111	0.36	0
70	CDL	L1	703	-	45,45,99	0.43	0	51,57,111	0.34	0
69	3PE	L1	704	-	50,50,50	0.31	0	53,55,55	0.28	0
74	PC1	6	203	-	42,42,53	0.34	0	48,50,61	0.47	0
69	3PE	n	607	-	26,26,50	0.40	0	29,31,55	0.36	0
74	PC1	9	203	-	53,53,53	0.30	0	59,61,61	0.44	0
70	CDL	L1	702	-	77,77,99	0.33	0	83,89,111	0.28	0
71	HEM	N	402	3	41,50,50	1.45	4 (9%)	45,82,82	1.58	10 (22%)
70	CDL	g	301	-	34,37,99	0.37	0	37,47,111	0.53	0
77	HEA	n	603	12	57,67,67	1.40	7 (12%)	61,103,103	2.47	22 (36%)
69	3PE	a	606	-	26,26,50	0.40	0	29,31,55	0.36	0
74	PC1	p	302	-	34,34,53	0.36	0	40,42,61	0.33	0
69	3PE	H1	401	-	50,50,50	0.31	0	53,55,55	0.47	1 (1%)
69	3PE	d	201	-	33,33,50	0.37	0	36,38,55	0.53	0
70	CDL	Y1	401	-	93,93,99	0.31	0	99,105,111	0.28	0
82	SF4	6	201	25	0,12,12	-	-	-		
71	HEM	C	401	3	41,50,50	1.44	3 (7%)	45,82,82	1.59	7 (15%)
74	PC1	P1	502	-	30,30,53	0.40	0	36,38,61	0.58	0
82	SF4	9	201	31	0,12,12	-	-	-		
69	3PE	v	101	-	27,27,50	0.40	0	30,32,55	0.33	0
69	3PE	o	302	-	28,28,50	0.39	0	31,33,55	0.37	0
70	CDL	H1	402	-	50,50,99	0.42	0	55,61,111	0.36	0
82	SF4	1	502	29	0,12,12	-	-	-		
74	PC1	V	101	-	27,27,53	0.40	0	33,35,61	0.35	0
70	CDL	d1	201	-	66,66,99	0.36	0	72,78,111	0.31	0
86	ZMP	n1	201	-	25,31,36	0.73	1 (4%)	30,38,45	0.93	1 (3%)
69	3PE	L1	701	-	50,50,50	0.31	0	53,55,55	0.47	0
74	PC1	I	201	-	49,49,53	0.32	0	55,57,61	0.52	1 (1%)
69	3PE	R	104	-	29,29,50	0.38	0	32,34,55	0.34	0
69	3PE	i1	201	-	41,41,50	0.32	0	44,46,55	0.30	0
72	HEC	O	303	4	32,50,50	2.17	4 (12%)	24,82,82	1.60	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	PC1	M1	501	-	53,53,53	0.29	0	59,61,61	0.36	0
69	3PE	O	302	-	32,32,50	0.37	0	35,37,55	0.34	0
69	3PE	G	102	-	50,50,50	0.31	0	53,55,55	0.28	0
69	3PE	Y1	403	-	41,41,50	0.33	0	44,46,55	0.32	0
70	CDL	V	102	-	49,49,99	0.42	0	55,61,111	0.50	1 (1%)
70	CDL	R	101	-	40,40,99	0.45	0	46,52,111	0.53	0
72	HEC	D	301	4	32,50,50	2.23	3 (9%)	24,82,82	1.63	5 (20%)
83	FMN	1	501	-	33,33,33	0.26	0	48,50,50	0.47	1 (2%)
70	CDL	N1	401	-	89,89,99	0.32	0	95,101,111	0.38	0
69	3PE	d1	202	-	30,30,50	0.37	0	33,35,55	0.34	0
79	CUA	o	303	13	0,1,1	-	-	-	-	-
82	SF4	3	802	30	0,12,12	-	-	-	-	-
69	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.33	0
70	CDL	R	103	-	71,71,99	0.36	0	77,83,111	0.43	1 (1%)

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
69	3PE	z	102	-	-	1/29/29/54	-
86	ZMP	W1	201	-	-	5/38/40/43	-
70	CDL	O	301	-	-	15/67/67/110	-
69	3PE	c	301	-	-	10/48/48/54	-
69	3PE	n	606	-	-	9/31/31/54	-
69	3PE	n	605	-	-	10/37/37/54	-
73	FES	3	803	30	-	-	0/1/1/1
69	3PE	b1	101	-	-	10/46/46/54	-
69	3PE	m1	601	-	-	13/39/39/54	-
82	SF4	9	202	31	-	-	0/6/5/5
87	DGT	O1	401	78	-	1/18/34/34	0/3/3/3
69	3PE	K1	201	-	-	12/44/44/54	-
81	TGL	l	601	-	-	0/39/39/65	-
69	3PE	r1	201	-	-	8/49/49/54	-
70	CDL	R	102	-	-	17/67/67/110	-
74	PC1	z	101	-	-	6/31/31/57	-
69	3PE	L	501	-	-	6/26/26/54	-
73	FES	2	301	28	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	CDL	A	502	-	-	13/56/56/110	-
73	FES	P	201	5	-	-	0/1/1/1
85	NDP	P1	501	-	-	5/30/77/77	0/5/5/5
69	3PE	E	203	-	-	9/37/37/54	-
82	SF4	3	801	30	-	-	0/6/5/5
69	3PE	g	303	-	-	9/28/28/54	-
69	3PE	b	301	-	-	9/32/32/54	-
77	HEA	a	603	12	-	13/32/76/76	-
74	PC1	L	503	-	-	9/27/27/57	-
69	3PE	N	403	-	-	7/40/40/54	-
74	PC1	K	101	-	-	4/31/31/57	-
77	HEA	n	604	12	-	7/32/76/76	-
69	3PE	6	202	-	-	4/35/35/54	-
69	3PE	a	605	-	-	6/31/31/54	-
81	TGL	y	601	-	-	3/39/39/65	-
74	PC1	J	101	-	-	7/38/38/57	-
69	3PE	N1	402	-	-	6/41/41/54	-
74	PC1	9	204	-	-	10/50/50/57	-
70	CDL	r1	202	-	-	13/67/67/110	-
73	FES	E	201	5	-	-	0/1/1/1
69	3PE	C	404	-	-	4/34/34/54	-
69	3PE	M1	502	-	-	17/54/54/54	-
70	CDL	D	302	-	-	19/66/66/110	-
71	HEM	C	402	3	-	1/12/54/54	-
69	3PE	d1	203	-	-	7/35/35/54	-
71	HEM	N	401	3	-	3/12/54/54	-
69	3PE	A	501	-	-	9/26/26/54	-
74	PC1	g	302	-	-	8/53/53/57	-
69	3PE	Y1	402	-	-	4/31/31/54	-
77	HEA	a	604	12	-	11/32/76/76	-
69	3PE	i	101	-	-	8/31/31/54	-
69	3PE	p	301	-	-	12/48/48/54	-
69	3PE	E	202	-	-	9/35/35/54	-
69	3PE	M1	503	-	-	14/54/54/54	-
70	CDL	h1	201	-	-	20/80/80/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	t	101	-	-	7/28/28/54	-
70	CDL	L	502	-	-	9/56/56/110	-
70	CDL	G	101	-	-	13/52/52/110	-
70	CDL	L1	703	-	-	15/56/56/110	-
69	3PE	L1	704	-	-	7/54/54/54	-
74	PC1	6	203	-	-	12/46/46/57	-
69	3PE	n	607	-	-	8/30/30/54	-
74	PC1	9	203	-	-	12/57/57/57	-
70	CDL	L1	702	-	-	15/88/88/110	-
71	HEM	N	402	3	-	4/12/54/54	-
70	CDL	g	301	-	-	9/41/45/110	-
77	HEA	n	603	12	-	9/32/76/76	-
69	3PE	a	606	-	-	9/30/30/54	-
74	PC1	p	302	-	-	10/38/38/57	-
69	3PE	H1	401	-	-	9/54/54/54	-
69	3PE	d	201	-	-	6/37/37/54	-
70	CDL	Y1	401	-	-	11/104/104/110	-
82	SF4	6	201	25	-	-	0/6/5/5
71	HEM	C	401	3	-	1/12/54/54	-
74	PC1	P1	502	-	-	15/34/34/57	-
82	SF4	9	201	31	-	-	0/6/5/5
69	3PE	v	101	-	-	7/31/31/54	-
69	3PE	o	302	-	-	10/32/32/54	-
70	CDL	H1	402	-	-	12/59/59/110	-
82	SF4	1	502	29	-	-	0/6/5/5
74	PC1	V	101	-	-	4/31/31/57	-
70	CDL	d1	201	-	-	16/77/77/110	-
86	ZMP	n1	201	-	-	20/36/38/43	-
69	3PE	L1	701	-	-	9/54/54/54	-
74	PC1	I	201	-	-	9/53/53/57	-
69	3PE	R	104	-	-	5/33/33/54	-
69	3PE	i1	201	-	-	6/45/45/54	-
72	HEC	O	303	4	-	4/10/54/54	-
74	PC1	M1	501	-	-	9/57/57/57	-
69	3PE	O	302	-	-	9/36/36/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	G	102	-	-	11/54/54/54	-
69	3PE	Y1	403	-	-	7/45/45/54	-
70	CDL	V	102	-	-	18/60/60/110	-
70	CDL	R	101	-	-	15/51/51/110	-
72	HEC	D	301	4	-	2/10/54/54	-
83	FMN	1	501	-	-	5/18/18/18	0/3/3/3
70	CDL	N1	401	-	-	21/100/100/110	-
69	3PE	d1	202	-	-	7/34/34/54	-
82	SF4	3	802	30	-	-	0/6/5/5
69	3PE	C	403	-	-	9/38/38/54	-
70	CDL	R	103	-	-	19/82/82/110	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	D	301	HEC	C2B-C3B	-6.73	1.33	1.40
72	D	301	HEC	C3C-C2C	-6.41	1.34	1.40
72	O	303	HEC	C2B-C3B	-6.33	1.34	1.40
72	O	303	HEC	C3C-C2C	-6.09	1.34	1.40
72	D	301	HEC	C3D-C2D	5.45	1.53	1.37
72	O	303	HEC	C3D-C2D	5.35	1.53	1.37
77	a	603	HEA	C3B-C2B	4.57	1.45	1.34
77	n	604	HEA	C3D-C2D	4.46	1.46	1.36
77	n	604	HEA	C3B-C2B	4.32	1.44	1.34
77	n	603	HEA	C3B-C2B	4.17	1.44	1.34
77	a	604	HEA	C3B-C2B	4.14	1.44	1.34
77	a	603	HEA	C3D-C2D	4.10	1.45	1.36
77	a	603	HEA	C3A-C2A	4.06	1.46	1.40
71	C	402	HEM	C3C-CAC	3.94	1.55	1.47
71	N	401	HEM	C3C-CAC	3.93	1.55	1.47
71	C	401	HEM	C3C-C2C	-3.91	1.34	1.40
71	N	401	HEM	C3C-C2C	-3.90	1.35	1.40
71	N	402	HEM	C3C-CAC	3.87	1.55	1.47
71	C	401	HEM	C3C-CAC	3.86	1.55	1.47
77	n	603	HEA	C3D-C2D	3.84	1.44	1.36
77	a	604	HEA	C3D-C2D	3.69	1.44	1.36
77	a	604	HEA	C3A-C2A	3.69	1.45	1.40
71	N	402	HEM	C3C-C2C	-3.64	1.35	1.40
71	C	402	HEM	C3C-C2C	-3.49	1.35	1.40
77	a	604	HEA	C3C-C2C	3.45	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	a	603	HEA	C3C-C2C	3.43	1.45	1.40
77	n	603	HEA	C3C-C2C	3.38	1.45	1.40
77	n	604	HEA	C3C-C2C	3.34	1.45	1.40
77	n	603	HEA	C3A-C2A	3.33	1.45	1.40
77	n	604	HEA	C3A-C2A	3.19	1.44	1.40
71	C	401	HEM	CAB-C3B	3.15	1.56	1.47
71	C	402	HEM	CAB-C3B	3.11	1.55	1.47
77	a	603	HEA	C4B-C3B	3.06	1.49	1.44
71	N	401	HEM	CAB-C3B	3.04	1.55	1.47
77	n	604	HEA	C4B-C3B	3.01	1.49	1.44
77	n	603	HEA	C4B-C3B	2.97	1.49	1.44
71	N	402	HEM	CAB-C3B	2.95	1.55	1.47
77	a	604	HEA	C4B-C3B	2.84	1.49	1.44
77	a	603	HEA	C2A-C1A	2.65	1.48	1.42
77	n	604	HEA	C1D-ND	-2.46	1.36	1.40
86	n1	201	ZMP	C9-C10	2.44	1.53	1.50
77	n	604	HEA	C2A-C1A	2.43	1.48	1.42
77	n	603	HEA	C1D-ND	-2.41	1.36	1.40
86	W1	201	ZMP	C9-C10	2.40	1.53	1.50
77	a	603	HEA	C1D-ND	-2.40	1.36	1.40
77	a	604	HEA	C2A-C1A	2.32	1.47	1.42
77	a	604	HEA	C1D-C2D	2.32	1.49	1.44
71	N	402	HEM	FE-NB	2.27	2.08	1.96
87	O1	401	DGT	C5-C6	-2.20	1.42	1.47
77	n	603	HEA	C2A-C1A	2.16	1.47	1.42
77	a	604	HEA	C1D-ND	-2.15	1.36	1.40
71	C	402	HEM	FE-NB	2.08	2.07	1.96
71	C	402	HEM	CMB-C2B	2.07	1.55	1.50
77	n	604	HEA	C4D-C3D	2.03	1.48	1.45
72	O	303	HEC	CAD-C3D	2.03	1.55	1.52

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	a	604	HEA	CMC-C2C-C3C	7.88	139.42	124.68
77	a	603	HEA	CMC-C2C-C3C	7.77	139.22	124.68
77	n	604	HEA	CMC-C2C-C3C	7.59	138.87	124.68
77	n	603	HEA	CMC-C2C-C3C	7.42	138.56	124.68
77	a	604	HEA	CMC-C2C-C1C	-6.87	117.91	128.46
77	n	604	HEA	CMC-C2C-C1C	-6.75	118.09	128.46
77	n	603	HEA	CMC-C2C-C1C	-6.73	118.11	128.46
77	a	603	HEA	CMC-C2C-C1C	-6.68	118.20	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	n	603	HEA	C13-C12-C11	-5.79	105.64	114.35
77	n	604	HEA	CMD-C2D-C1D	-5.25	117.05	125.04
77	n	604	HEA	C3D-C4D-ND	5.14	115.33	110.36
77	n	603	HEA	C3D-C4D-ND	4.97	115.17	110.36
77	a	604	HEA	C3D-C4D-ND	4.96	115.16	110.36
71	N	401	HEM	C3B-C2B-C1B	4.88	110.11	106.49
77	a	603	HEA	CMD-C2D-C1D	-4.59	118.05	125.04
77	a	603	HEA	C3D-C4D-ND	4.59	114.80	110.36
71	C	401	HEM	C3B-C2B-C1B	4.56	109.87	106.49
77	a	603	HEA	CMB-C2B-C1B	-4.35	118.41	125.04
77	n	604	HEA	C13-C12-C11	-4.29	107.91	114.35
77	n	603	HEA	CHA-C4D-C3D	-4.24	118.60	124.84
77	a	603	HEA	C13-C12-C11	-4.05	108.27	114.35
77	n	604	HEA	CMD-C2D-C3D	4.04	137.08	126.12
77	n	603	HEA	C4D-C3D-C2D	-4.00	101.07	106.90
77	a	604	HEA	CHA-C4D-C3D	-3.98	118.99	124.84
77	n	604	HEA	CHA-C4D-C3D	-3.95	119.03	124.84
72	O	303	HEC	CMC-C2C-C1C	-3.91	122.46	128.46
77	n	604	HEA	CMB-C2B-C1B	-3.86	119.16	125.04
77	n	603	HEA	CMB-C2B-C1B	-3.85	119.17	125.04
77	a	603	HEA	C4D-C3D-C2D	-3.84	101.31	106.90
77	n	604	HEA	C4D-C3D-C2D	-3.80	101.36	106.90
77	a	604	HEA	CAD-CBD-CGD	-3.73	105.57	113.60
71	N	401	HEM	CHB-C1B-NB	3.72	128.98	124.38
77	n	603	HEA	CMD-C2D-C1D	-3.71	119.39	125.04
72	D	301	HEC	CMC-C2C-C1C	-3.66	122.83	128.46
71	C	401	HEM	CMC-C2C-C3C	3.66	131.52	124.68
77	a	604	HEA	C4D-C3D-C2D	-3.64	101.59	106.90
77	n	603	HEA	CAA-CBA-CGA	-3.59	103.70	113.76
77	a	603	HEA	CHA-C4D-C3D	-3.58	119.58	124.84
77	n	603	HEA	C13-C14-C15	-3.57	119.07	127.66
77	a	604	HEA	C13-C12-C11	-3.49	109.11	114.35
71	N	401	HEM	CMC-C2C-C3C	3.40	131.05	124.68
71	N	401	HEM	C4C-CHD-C1D	3.35	126.98	122.56
77	a	603	HEA	CMD-C2D-C3D	3.33	135.15	126.12
71	C	402	HEM	C4D-ND-C1D	3.31	108.50	105.07
77	a	604	HEA	CMB-C2B-C1B	-3.25	120.09	125.04
77	a	604	HEA	C26-C15-C16	3.23	120.70	115.27
77	a	604	HEA	CAD-C3D-C4D	3.17	130.20	124.66
71	N	401	HEM	CMB-C2B-C1B	-3.16	120.23	125.04
77	a	603	HEA	CMB-C2B-C3B	3.15	136.34	130.34
77	a	604	HEA	CAA-CBA-CGA	-3.12	105.02	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	n	604	HEA	C26-C15-C16	3.11	120.50	115.27
77	n	603	HEA	CHB-C1B-C2B	-3.07	120.18	124.98
71	N	402	HEM	C4D-ND-C1D	3.07	108.24	105.07
71	N	402	HEM	C3B-C2B-C1B	3.06	108.76	106.49
77	a	603	HEA	C26-C15-C16	3.04	120.38	115.27
77	n	604	HEA	OMA-CMA-C3A	-2.89	118.60	124.91
71	N	402	HEM	CBA-CAA-C2A	-2.89	107.69	112.62
77	n	603	HEA	CMB-C2B-C3B	2.86	135.80	130.34
77	a	604	HEA	C13-C14-C15	-2.86	120.77	127.66
72	O	303	HEC	CMB-C2B-C1B	-2.83	124.12	128.46
71	N	402	HEM	C1B-NB-C4B	2.79	107.96	105.07
77	n	604	HEA	CAA-CBA-CGA	-2.79	105.94	113.76
71	C	401	HEM	C4D-ND-C1D	2.78	107.95	105.07
71	N	402	HEM	CMC-C2C-C3C	2.78	129.88	124.68
77	a	604	HEA	C27-C19-C20	2.77	119.93	115.27
71	C	402	HEM	CMC-C2C-C3C	2.77	129.85	124.68
72	D	301	HEC	CBD-CAD-C3D	-2.72	107.98	112.62
71	C	402	HEM	CBA-CAA-C2A	-2.71	107.99	112.62
77	n	604	HEA	C25-C23-C24	2.70	120.58	114.60
77	n	603	HEA	CMD-C2D-C3D	2.68	133.40	126.12
77	a	603	HEA	CAA-C2A-C3A	2.68	133.46	126.86
77	n	604	HEA	C17-C18-C19	-2.67	121.24	127.66
77	a	603	HEA	CHB-C1B-C2B	-2.66	120.82	124.98
72	O	303	HEC	CAA-CBA-CGA	-2.66	106.31	113.76
71	N	402	HEM	C4B-CHC-C1C	2.66	126.06	122.56
71	C	401	HEM	C4C-CHD-C1D	2.64	126.05	122.56
77	a	603	HEA	C13-C14-C15	-2.64	121.30	127.66
71	N	402	HEM	CHC-C4B-C3B	2.64	128.61	124.57
71	N	401	HEM	C4D-ND-C1D	2.64	107.80	105.07
77	n	604	HEA	C13-C14-C15	-2.61	121.38	127.66
77	n	604	HEA	CAD-C3D-C2D	2.61	132.73	127.88
86	W1	201	ZMP	O1-C10-C9	-2.60	120.91	123.99
77	n	603	HEA	C26-C15-C16	2.60	119.65	115.27
86	n1	201	ZMP	O1-C10-C9	-2.57	120.95	123.99
77	a	604	HEA	C17-C18-C19	-2.57	121.47	127.66
77	n	603	HEA	CHB-C1B-NB	2.56	127.22	124.43
77	a	604	HEA	C25-C23-C24	2.56	120.27	114.60
77	a	603	HEA	C17-C18-C19	-2.56	121.50	127.66
77	n	603	HEA	CAD-C3D-C4D	2.54	129.10	124.66
77	a	603	HEA	CAA-CBA-CGA	-2.54	106.64	113.76
71	C	402	HEM	C3D-C4D-ND	-2.53	107.35	110.17
77	n	604	HEA	C4B-C3B-C2B	-2.52	103.10	107.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	a	604	HEA	CAA-C2A-C3A	2.52	133.07	126.86
77	a	603	HEA	C3B-C4B-NB	2.44	112.73	109.84
77	a	603	HEA	C27-C19-C20	2.43	119.35	115.27
77	n	603	HEA	C27-C19-C20	2.43	119.35	115.27
77	n	603	HEA	C17-C18-C19	-2.42	121.83	127.66
77	a	603	HEA	CAD-C3D-C4D	2.40	128.85	124.66
77	a	604	HEA	C4B-C3B-C2B	-2.39	103.33	107.41
71	C	401	HEM	CAD-CBD-CGD	-2.39	108.46	113.60
77	n	604	HEA	CMB-C2B-C3B	2.38	134.89	130.34
77	n	604	HEA	C3B-C4B-NB	2.38	112.66	109.84
71	N	401	HEM	CAD-CBD-CGD	-2.38	108.48	113.60
77	a	604	HEA	C3B-C4B-NB	2.37	112.65	109.84
77	n	603	HEA	C25-C23-C24	2.36	119.81	114.60
77	a	603	HEA	C4B-C3B-C2B	-2.35	103.39	107.41
77	a	603	HEA	C2B-C1B-NB	2.34	112.69	109.88
71	N	402	HEM	C3D-C4D-ND	-2.31	107.59	110.17
77	a	604	HEA	CMD-C2D-C1D	-2.31	121.52	125.04
77	n	604	HEA	CHB-C1B-C2B	-2.31	121.37	124.98
77	n	604	HEA	CAD-CBD-CGD	-2.31	108.64	113.60
77	a	603	HEA	C25-C23-C24	2.29	119.66	114.60
77	n	604	HEA	C27-C19-C20	2.28	119.11	115.27
85	P1	501	NDP	C5A-C6A-N6A	2.28	123.82	120.35
77	n	603	HEA	C2B-C1B-NB	2.27	112.60	109.88
71	N	401	HEM	CMA-C3A-C4A	-2.26	124.98	128.46
77	n	604	HEA	C2D-C1D-ND	2.25	112.50	109.84
71	C	402	HEM	C1B-NB-C4B	2.19	107.34	105.07
83	1	501	FMN	P-O5'-C5'	2.18	124.31	118.30
71	C	402	HEM	C4B-CHC-C1C	2.17	125.42	122.56
77	n	603	HEA	CAD-CBD-CGD	-2.17	108.94	113.60
71	C	401	HEM	C2B-C1B-NB	-2.16	107.27	109.84
74	I	201	PC1	C2-O21-C21	2.16	123.11	117.79
72	D	301	HEC	C1D-C2D-C3D	-2.16	105.49	107.00
77	a	604	HEA	CBA-CAA-C2A	2.14	116.21	112.60
72	D	301	HEC	CMB-C2B-C1B	-2.13	125.19	128.46
77	a	603	HEA	CAD-CBD-CGD	-2.13	109.03	113.60
77	a	604	HEA	CHB-C1B-C2B	-2.12	121.67	124.98
77	n	603	HEA	CAA-C2A-C3A	2.11	132.07	126.86
71	C	401	HEM	C3D-C4D-ND	-2.11	107.82	110.17
77	a	604	HEA	CMD-C2D-C3D	2.10	131.82	126.12
71	N	402	HEM	CAD-CBD-CGD	-2.09	109.10	113.60
70	R	103	CDL	CA4-OA6-CA5	2.05	122.83	117.79
71	N	401	HEM	CHD-C1D-ND	2.04	126.64	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	r1	202	CDL	CA4-OA6-CA5	2.03	122.79	117.79
69	H1	401	3PE	C2-O21-C21	2.02	122.78	117.79
70	V	102	CDL	CA4-OA6-CA5	2.02	122.77	117.79
70	R	102	CDL	CA4-OA6-CA5	2.02	122.76	117.79
72	D	301	HEC	C2B-C3B-C4B	2.02	108.53	106.35
77	a	604	HEA	CHB-C1B-NB	2.02	126.62	124.43
71	N	402	HEM	CAB-C3B-C2B	-2.01	121.97	128.60
69	n	605	3PE	C2-O21-C21	2.01	122.75	117.79
69	t	101	3PE	C2-O21-C21	2.01	122.73	117.79

There are no chirality outliers.

All (818) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	A	501	3PE	C1-O11-P-O12
69	A	501	3PE	C1-O11-P-O13
69	A	501	3PE	C1-O11-P-O14
69	A	501	3PE	C11-O13-P-O11
69	A	501	3PE	C11-O13-P-O12
69	A	501	3PE	C11-O13-P-O14
69	A	501	3PE	O13-C11-C12-N
69	C	403	3PE	C1-O11-P-O12
69	C	403	3PE	C1-O11-P-O14
69	C	403	3PE	C11-O13-P-O12
69	C	403	3PE	C11-O13-P-O14
69	E	202	3PE	C11-O13-P-O14
69	E	202	3PE	O13-C11-C12-N
69	E	203	3PE	C1-O11-P-O12
69	E	203	3PE	O13-C11-C12-N
69	G	102	3PE	C1-O11-P-O14
69	G	102	3PE	C11-O13-P-O14
69	L	501	3PE	C11-O13-P-O12
69	L	501	3PE	O13-C11-C12-N
69	N	403	3PE	C11-O13-P-O11
69	N	403	3PE	C11-O13-P-O12
69	N	403	3PE	C11-O13-P-O14
69	N	403	3PE	O13-C11-C12-N
69	O	302	3PE	C1-O11-P-O14
69	O	302	3PE	C11-O13-P-O11
69	O	302	3PE	C11-O13-P-O14
69	O	302	3PE	O13-C11-C12-N
69	R	104	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
69	n	605	3PE	C1-O11-P-O12
69	n	605	3PE	C1-O11-P-O14
69	n	605	3PE	C11-O13-P-O11
69	n	605	3PE	C11-O13-P-O12
69	n	605	3PE	C11-O13-P-O14
69	n	605	3PE	O13-C11-C12-N
69	n	606	3PE	C1-O11-P-O12
69	n	606	3PE	C1-O11-P-O14
69	n	606	3PE	O11-C1-C2-O21
69	n	607	3PE	C11-O13-P-O14
69	n	607	3PE	C2-C1-O11-P
69	n	607	3PE	O13-C11-C12-N
69	o	302	3PE	C12-C11-O13-P
69	p	301	3PE	C1-O11-P-O12
69	p	301	3PE	C1-O11-P-O13
69	p	301	3PE	C1-O11-P-O14
69	p	301	3PE	C11-O13-P-O14
69	p	301	3PE	O13-C11-C12-N
69	t	101	3PE	C11-O13-P-O12
69	t	101	3PE	C11-O13-P-O14
69	t	101	3PE	O13-C11-C12-N
69	v	101	3PE	C1-O11-P-O12
69	v	101	3PE	O13-C11-C12-N
69	z	102	3PE	O13-C11-C12-N
69	6	202	3PE	C11-O13-P-O11
69	6	202	3PE	C11-O13-P-O14
69	6	202	3PE	O13-C11-C12-N
69	r1	201	3PE	C1-O11-P-O14
69	r1	201	3PE	C11-O13-P-O11
69	r1	201	3PE	C11-O13-P-O12
69	r1	201	3PE	C11-O13-P-O14
69	r1	201	3PE	O13-C11-C12-N
69	K1	201	3PE	C1-O11-P-O12
69	K1	201	3PE	C1-O11-P-O13
69	K1	201	3PE	C1-O11-P-O14
69	L1	701	3PE	C1-O11-P-O14
69	L1	701	3PE	C11-O13-P-O14
69	L1	704	3PE	C1-O11-P-O12
69	L1	704	3PE	O13-C11-C12-N
69	M1	502	3PE	C1-O11-P-O12
69	M1	502	3PE	C11-O13-P-O11
69	M1	502	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	M1	502	3PE	C11-O13-P-O14
69	M1	502	3PE	O13-C11-C12-N
69	M1	503	3PE	C11-O13-P-O11
69	M1	503	3PE	C11-O13-P-O12
69	M1	503	3PE	C11-O13-P-O14
69	M1	503	3PE	O13-C11-C12-N
69	N1	402	3PE	O13-C11-C12-N
69	Y1	402	3PE	C1-O11-P-O12
69	Y1	402	3PE	C1-O11-P-O13
69	Y1	402	3PE	C1-O11-P-O14
69	Y1	402	3PE	O13-C11-C12-N
69	Y1	403	3PE	C11-O13-P-O11
69	Y1	403	3PE	C11-O13-P-O14
69	d1	202	3PE	C11-O13-P-O12
69	d1	202	3PE	C11-O13-P-O14
69	d1	202	3PE	O13-C11-C12-N
69	d1	203	3PE	C1-O11-P-O12
69	d1	203	3PE	C1-O11-P-O14
69	m1	601	3PE	C1-O11-P-O14
69	m1	601	3PE	C11-O13-P-O12
69	m1	601	3PE	C11-O13-P-O14
69	a	605	3PE	C1-O11-P-O12
69	a	606	3PE	C11-O13-P-O14
69	a	606	3PE	O13-C11-C12-N
69	c	301	3PE	O13-C11-C12-N
69	d	201	3PE	C11-O13-P-O14
69	d	201	3PE	O13-C11-C12-N
69	g	303	3PE	C11-O13-P-O12
69	g	303	3PE	C11-O13-P-O14
69	g	303	3PE	O13-C11-C12-N
69	i	101	3PE	C11-O13-P-O12
69	i	101	3PE	O13-C11-C12-N
70	A	502	CDL	CB2-OB2-PB2-OB3
70	A	502	CDL	CB2-OB2-PB2-OB4
70	A	502	CDL	CB2-OB2-PB2-OB5
70	D	302	CDL	CA3-OA5-PA1-OA3
70	D	302	CDL	CB2-OB2-PB2-OB5
70	D	302	CDL	CB3-OB5-PB2-OB4
70	G	101	CDL	CA2-OA2-PA1-OA4
70	G	101	CDL	CB2-OB2-PB2-OB3
70	G	101	CDL	CB2-OB2-PB2-OB4
70	G	101	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
70	L	502	CDL	CA3-OA5-PA1-OA3
70	O	301	CDL	CB2-OB2-PB2-OB3
70	O	301	CDL	CB3-OB5-PB2-OB4
70	R	101	CDL	CA2-OA2-PA1-OA3
70	R	101	CDL	CA2-OA2-PA1-OA4
70	R	101	CDL	CB2-OB2-PB2-OB3
70	R	102	CDL	CA3-OA5-PA1-OA2
70	R	102	CDL	CA3-OA5-PA1-OA3
70	R	102	CDL	CA3-OA5-PA1-OA4
70	R	102	CDL	CB3-OB5-PB2-OB4
70	R	103	CDL	CA3-OA5-PA1-OA2
70	R	103	CDL	CA3-OA5-PA1-OA3
70	R	103	CDL	CA3-OA5-PA1-OA4
70	R	103	CDL	CB2-OB2-PB2-OB3
70	R	103	CDL	CB2-OB2-PB2-OB4
70	R	103	CDL	CB3-OB5-PB2-OB2
70	R	103	CDL	CB3-OB5-PB2-OB3
70	R	103	CDL	CB3-OB5-PB2-OB4
70	V	102	CDL	CA3-OA5-PA1-OA2
70	V	102	CDL	CA3-OA5-PA1-OA3
70	V	102	CDL	CA3-OA5-PA1-OA4
70	r1	202	CDL	CA2-OA2-PA1-OA3
70	r1	202	CDL	CA2-OA2-PA1-OA4
70	r1	202	CDL	CA2-OA2-PA1-OA5
70	H1	402	CDL	CA2-OA2-PA1-OA3
70	H1	402	CDL	CA2-OA2-PA1-OA4
70	H1	402	CDL	CA2-OA2-PA1-OA5
70	H1	402	CDL	CB2-OB2-PB2-OB3
70	H1	402	CDL	CB2-OB2-PB2-OB4
70	L1	702	CDL	CB2-OB2-PB2-OB3
70	L1	702	CDL	CB2-OB2-PB2-OB4
70	L1	702	CDL	CB3-OB5-PB2-OB2
70	L1	702	CDL	CB3-OB5-PB2-OB4
70	L1	703	CDL	CA2-OA2-PA1-OA3
70	L1	703	CDL	CA2-OA2-PA1-OA4
70	L1	703	CDL	CA3-OA5-PA1-OA3
70	N1	401	CDL	CA2-OA2-PA1-OA4
70	N1	401	CDL	OA6-CA4-CA6-OA8
70	N1	401	CDL	CB2-OB2-PB2-OB3
70	N1	401	CDL	CB2-OB2-PB2-OB4
70	Y1	401	CDL	CA2-OA2-PA1-OA3
70	Y1	401	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
70	d1	201	CDL	CA2-OA2-PA1-OA3
70	d1	201	CDL	CA2-OA2-PA1-OA4
70	d1	201	CDL	OB5-CB3-CB4-OB6
70	h1	201	CDL	CA2-OA2-PA1-OA3
70	h1	201	CDL	CB2-OB2-PB2-OB4
70	h1	201	CDL	CB3-OB5-PB2-OB3
70	g	301	CDL	CA2-OA2-PA1-OA3
70	g	301	CDL	CA2-OA2-PA1-OA4
70	g	301	CDL	CA2-OA2-PA1-OA5
71	N	402	HEM	C2A-CAA-CBA-CGA
74	J	101	PC1	C1-O11-P-O12
74	J	101	PC1	C1-O11-P-O14
74	J	101	PC1	C1-O11-P-O13
74	K	101	PC1	C11-O13-P-O14
74	L	503	PC1	C11-O13-P-O12
74	L	503	PC1	C11-O13-P-O14
74	L	503	PC1	C11-O13-P-O11
74	L	503	PC1	C1-O11-P-O12
74	L	503	PC1	C1-O11-P-O13
74	I	201	PC1	C11-O13-P-O12
74	I	201	PC1	C1-O11-P-O13
74	p	302	PC1	C11-O13-P-O12
74	p	302	PC1	C11-O13-P-O14
74	p	302	PC1	C1-O11-P-O14
74	6	203	PC1	C1-O11-P-O12
74	6	203	PC1	C1-O11-P-O14
74	9	203	PC1	C11-O13-P-O11
74	9	203	PC1	C1-O11-P-O12
74	9	203	PC1	C1-O11-P-O14
74	9	204	PC1	C1-O11-P-O14
74	P1	502	PC1	C11-O13-P-O12
74	P1	502	PC1	C11-O13-P-O14
74	P1	502	PC1	C1-O11-P-O12
74	P1	502	PC1	C1-O11-P-O14
74	M1	501	PC1	C11-O13-P-O12
74	g	302	PC1	C1-O11-P-O14
77	n	603	HEA	C11-C12-C13-C14
77	n	603	HEA	C15-C16-C17-C18
77	n	603	HEA	C19-C20-C21-C22
77	n	604	HEA	C2D-C3D-CAD-CBD
77	n	604	HEA	C4D-C3D-CAD-CBD
77	n	604	HEA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
77	a	603	HEA	C1A-C2A-CAA-CBA
77	a	603	HEA	C3A-C2A-CAA-CBA
77	a	603	HEA	C11-C12-C13-C14
77	a	603	HEA	C14-C15-C16-C17
77	a	603	HEA	C26-C15-C16-C17
77	a	604	HEA	C1A-C2A-CAA-CBA
77	a	604	HEA	C3A-C2A-CAA-CBA
77	a	604	HEA	C14-C15-C16-C17
77	a	604	HEA	C26-C15-C16-C17
83	1	501	FMN	N10-C1'-C2'-O2'
83	1	501	FMN	N10-C1'-C2'-C3'
83	1	501	FMN	C5'-O5'-P-O1P
83	1	501	FMN	C5'-O5'-P-O2P
86	W1	201	ZMP	S1-C11-C12-N1
86	n1	201	ZMP	C17-C18-C21-O5
86	n1	201	ZMP	O4-C17-C18-C21
86	n1	201	ZMP	C16-C17-C18-C21
86	n1	201	ZMP	O4-C17-C18-C19
86	n1	201	ZMP	C16-C17-C18-C20
86	n1	201	ZMP	O3-C16-C17-O4
86	n1	201	ZMP	C17-C16-N2-C15
86	n1	201	ZMP	C13-C14-C15-N2
86	n1	201	ZMP	O1-C10-S1-C11
86	n1	201	ZMP	C9-C10-S1-C11
86	n1	201	ZMP	C7-C8-C9-C10
86	n1	201	ZMP	O3-C16-N2-C15
77	a	604	HEA	C15-C16-C17-C18
70	O	301	CDL	OB5-CB3-CB4-OB6
70	R	103	CDL	OB5-CB3-CB4-OB6
69	M1	502	3PE	C31-C32-C33-C34
71	C	401	HEM	C2A-CAA-CBA-CGA
71	C	402	HEM	C2A-CAA-CBA-CGA
71	N	401	HEM	C2A-CAA-CBA-CGA
74	M1	501	PC1	C21-C22-C23-C24
74	V	101	PC1	C11-C12-N-C13
74	p	302	PC1	C11-C12-N-C13
74	6	203	PC1	C11-C12-N-C14
74	9	204	PC1	C11-C12-N-C15
74	P1	502	PC1	C11-C12-N-C15
77	a	603	HEA	C15-C16-C17-C18
69	C	403	3PE	C1-O11-P-O13
69	C	403	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
69	E	203	3PE	C1-O11-P-O13
69	E	203	3PE	C11-O13-P-O11
69	G	102	3PE	C1-O11-P-O13
69	R	104	3PE	C11-O13-P-O11
69	n	605	3PE	C1-O11-P-O13
69	n	606	3PE	C1-O11-P-O13
69	n	607	3PE	C1-O11-P-O13
69	o	302	3PE	C1-O11-P-O13
69	o	302	3PE	C11-O13-P-O11
69	p	301	3PE	C11-O13-P-O11
69	t	101	3PE	C11-O13-P-O11
69	v	101	3PE	C1-O11-P-O13
69	v	101	3PE	C11-O13-P-O11
69	r1	201	3PE	C1-O11-P-O13
69	K1	201	3PE	C11-O13-P-O11
69	L1	701	3PE	C1-O11-P-O13
69	L1	704	3PE	C1-O11-P-O13
69	M1	502	3PE	C1-O11-P-O13
69	b1	101	3PE	C11-O13-P-O11
69	d1	202	3PE	C1-O11-P-O13
69	d1	202	3PE	C11-O13-P-O11
69	d1	203	3PE	C1-O11-P-O13
69	i1	201	3PE	C11-O13-P-O11
69	m1	601	3PE	C1-O11-P-O13
69	m1	601	3PE	C11-O13-P-O11
69	a	606	3PE	C11-O13-P-O11
69	b	301	3PE	C11-O13-P-O11
69	c	301	3PE	C11-O13-P-O11
69	g	303	3PE	C11-O13-P-O11
69	i	101	3PE	C1-O11-P-O13
69	i	101	3PE	C11-O13-P-O11
70	A	502	CDL	CB3-OB5-PB2-OB2
70	D	302	CDL	CA2-OA2-PA1-OA5
70	D	302	CDL	CA3-OA5-PA1-OA2
70	D	302	CDL	CB3-OB5-PB2-OB2
70	G	101	CDL	CB2-OB2-PB2-OB5
70	O	301	CDL	CB3-OB5-PB2-OB2
70	R	101	CDL	CA2-OA2-PA1-OA5
70	R	102	CDL	CB2-OB2-PB2-OB5
70	R	102	CDL	CB3-OB5-PB2-OB2
70	R	103	CDL	CB2-OB2-PB2-OB5
70	V	102	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
70	r1	202	CDL	CB2-OB2-PB2-OB5
70	H1	402	CDL	CB2-OB2-PB2-OB5
70	L1	702	CDL	CA2-OA2-PA1-OA5
70	L1	702	CDL	CB2-OB2-PB2-OB5
70	L1	703	CDL	CA2-OA2-PA1-OA5
70	L1	703	CDL	CA3-OA5-PA1-OA2
70	L1	703	CDL	CB2-OB2-PB2-OB5
70	N1	401	CDL	CA2-OA2-PA1-OA5
70	N1	401	CDL	CB2-OB2-PB2-OB5
70	N1	401	CDL	CB3-OB5-PB2-OB2
70	Y1	401	CDL	CA2-OA2-PA1-OA5
70	Y1	401	CDL	CB3-OB5-PB2-OB2
70	d1	201	CDL	CA2-OA2-PA1-OA5
70	d1	201	CDL	CA3-OA5-PA1-OA2
70	h1	201	CDL	CA2-OA2-PA1-OA5
70	h1	201	CDL	CB2-OB2-PB2-OB5
70	h1	201	CDL	CB3-OB5-PB2-OB2
74	J	101	PC1	C11-O13-P-O11
74	I	201	PC1	C11-O13-P-O11
74	p	302	PC1	C11-O13-P-O11
74	p	302	PC1	C1-O11-P-O13
74	6	203	PC1	C11-O13-P-O11
74	6	203	PC1	C1-O11-P-O13
74	9	203	PC1	C1-O11-P-O13
74	P1	502	PC1	C11-O13-P-O11
74	P1	502	PC1	C1-O11-P-O13
74	M1	501	PC1	C11-O13-P-O11
70	N1	401	CDL	C81-C82-C83-C84
69	L1	704	3PE	C38-C39-C3A-C3B
70	H1	402	CDL	C13-C14-C15-C16
69	M1	503	3PE	C28-C29-C2A-C2B
69	G	102	3PE	C37-C38-C39-C3A
69	b1	101	3PE	C3A-C3B-C3C-C3D
69	M1	502	3PE	C36-C37-C38-C39
69	H1	401	3PE	C31-C32-C33-C34
70	Y1	401	CDL	C82-C83-C84-C85
74	z	101	PC1	C11-C12-N-C13
69	L1	701	3PE	O13-C11-C12-N
69	b1	101	3PE	O13-C11-C12-N
69	b	301	3PE	O13-C11-C12-N
69	L1	701	3PE	C21-C22-C23-C24
74	9	204	PC1	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
74	M1	501	PC1	C37-C38-C39-C3A
69	M1	502	3PE	C23-C24-C25-C26
69	N1	402	3PE	C36-C37-C38-C39
70	d1	201	CDL	C55-C56-C57-C58
86	n1	201	ZMP	C6-C7-C8-C9
69	N1	402	3PE	C1-C2-C3-O31
70	Y1	401	CDL	C73-C74-C75-C76
70	R	103	CDL	CA5-C11-C12-C13
69	c	301	3PE	C23-C24-C25-C26
74	V	101	PC1	C11-C12-N-C14
74	p	302	PC1	C11-C12-N-C14
74	p	302	PC1	C11-C12-N-C15
74	6	203	PC1	C11-C12-N-C15
74	9	204	PC1	C11-C12-N-C14
69	p	301	3PE	C23-C24-C25-C26
74	I	201	PC1	C25-C26-C27-C28
74	9	204	PC1	C34-C35-C36-C37
70	D	302	CDL	C74-C75-C76-C77
69	L1	704	3PE	C32-C33-C34-C35
69	n	607	3PE	O21-C2-C3-O31
74	V	101	PC1	C11-C12-N-C15
74	z	101	PC1	C11-C12-N-C15
74	6	203	PC1	C11-C12-N-C13
74	9	204	PC1	C11-C12-N-C13
74	P1	502	PC1	C11-C12-N-C13
74	P1	502	PC1	C11-C12-N-C14
77	n	604	HEA	C26-C15-C16-C17
69	L	501	3PE	C11-O13-P-O11
69	O	302	3PE	C1-O11-P-O13
70	G	101	CDL	CB3-OB5-PB2-OB2
70	O	301	CDL	CA2-OA2-PA1-OA5
70	r1	202	CDL	CA3-OA5-PA1-OA2
77	a	603	HEA	O11-C11-C12-C13
69	G	102	3PE	C32-C33-C34-C35
70	d1	201	CDL	C63-C64-C65-C66
69	C	404	3PE	C1-C2-C3-O31
86	W1	201	ZMP	C19-C18-C21-O5
86	W1	201	ZMP	C20-C18-C21-O5
86	n1	201	ZMP	C5-C6-C7-C8
70	D	302	CDL	C1-CB2-OB2-PB2
74	z	101	PC1	C11-C12-N-C14
69	o	302	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
69	N1	402	3PE	O21-C2-C3-O31
86	n1	201	ZMP	O4-C17-C18-C20
69	n	606	3PE	O11-C1-C2-C3
70	O	301	CDL	OB5-CB3-CB4-CB6
70	R	103	CDL	OB5-CB3-CB4-CB6
70	L1	703	CDL	OB5-CB3-CB4-CB6
70	d1	201	CDL	OB5-CB3-CB4-CB6
69	L	501	3PE	C31-C32-C33-C34
69	G	102	3PE	O13-C11-C12-N
69	K1	201	3PE	O13-C11-C12-N
69	i1	201	3PE	O13-C11-C12-N
69	g	303	3PE	O31-C31-C32-C33
69	p	301	3PE	C2-C1-O11-P
69	a	606	3PE	C2-C1-O11-P
69	g	303	3PE	C2-C1-O11-P
74	J	101	PC1	C2-C1-O11-P
70	R	103	CDL	CB3-CB4-CB6-OB8
70	Y1	401	CDL	CB3-CB4-CB6-OB8
69	d1	203	3PE	C21-C22-C23-C24
70	L1	702	CDL	OB5-CB3-CB4-OB6
74	P1	502	PC1	O11-C1-C2-O21
69	C	404	3PE	O21-C2-C3-O31
69	n	606	3PE	O21-C2-C3-O31
70	R	103	CDL	OB6-CB4-CB6-OB8
70	Y1	401	CDL	OB6-CB4-CB6-OB8
69	m1	601	3PE	C2-C1-O11-P
69	c	301	3PE	C2-C1-O11-P
70	D	302	CDL	C1-CA2-OA2-PA1
70	G	101	CDL	C1-CA2-OA2-PA1
70	O	301	CDL	CB4-CB3-OB5-PB2
70	R	101	CDL	CA4-CA3-OA5-PA1
70	R	103	CDL	C1-CB2-OB2-PB2
70	H1	402	CDL	C1-CB2-OB2-PB2
70	h1	201	CDL	C1-CA2-OA2-PA1
74	P1	502	PC1	O21-C21-C22-C23
86	W1	201	ZMP	O1-C10-S1-C11
70	R	101	CDL	OB5-CB3-CB4-CB6
70	D	302	CDL	C52-C51-CB5-OB6
70	L1	702	CDL	CA5-C11-C12-C13
69	b1	101	3PE	C21-C22-C23-C24
86	W1	201	ZMP	C9-C10-S1-C11
69	E	202	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
69	n	607	3PE	C1-C2-C3-O31
69	K1	201	3PE	C2-C1-O11-P
70	H1	402	CDL	C1-CA2-OA2-PA1
70	N1	401	CDL	CA3-CA4-CA6-OA8
70	d1	201	CDL	C1-CB2-OB2-PB2
70	h1	201	CDL	CA4-CA3-OA5-PA1
69	b	301	3PE	O11-C1-C2-O21
70	R	101	CDL	OB5-CB3-CB4-OB6
70	V	102	CDL	OA5-CA3-CA4-OA6
69	N	403	3PE	C25-C26-C27-C28
71	N	402	HEM	C4B-C3B-CAB-CBB
86	n1	201	ZMP	C16-C17-C18-C19
69	b1	101	3PE	C23-C24-C25-C26
69	c	301	3PE	C32-C33-C34-C35
77	n	604	HEA	C14-C15-C16-C17
70	L	502	CDL	C31-C32-C33-C34
69	G	102	3PE	C11-O13-P-O11
69	n	607	3PE	C11-O13-P-O11
69	d	201	3PE	C11-O13-P-O11
70	G	101	CDL	CA2-OA2-PA1-OA5
70	L	502	CDL	CA3-OA5-PA1-OA2
70	R	101	CDL	CB2-OB2-PB2-OB5
70	g	301	CDL	CA3-OA5-PA1-OA2
74	g	302	PC1	C1-O11-P-O13
70	N1	401	CDL	C78-C79-C80-C81
69	t	101	3PE	C2-C1-O11-P
69	a	605	3PE	C2-C1-O11-P
70	D	302	CDL	CB4-CB3-OB5-PB2
70	L	502	CDL	CB4-CB3-OB5-PB2
70	O	301	CDL	C1-CA2-OA2-PA1
70	g	301	CDL	CA4-CA3-OA5-PA1
69	E	203	3PE	C11-O13-P-O12
69	E	203	3PE	C11-O13-P-O14
69	G	102	3PE	C1-O11-P-O12
69	L	501	3PE	C11-O13-P-O14
69	O	302	3PE	C1-O11-P-O12
69	R	104	3PE	C11-O13-P-O14
69	n	607	3PE	C1-O11-P-O14
69	o	302	3PE	C1-O11-P-O14
69	o	302	3PE	C11-O13-P-O14
69	p	301	3PE	C11-O13-P-O12
69	v	101	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
69	v	101	3PE	C11-O13-P-O12
69	v	101	3PE	C11-O13-P-O14
69	r1	201	3PE	C1-O11-P-O12
69	K1	201	3PE	C11-O13-P-O14
69	L1	701	3PE	C1-O11-P-O12
69	M1	502	3PE	C1-O11-P-O14
69	b1	101	3PE	C11-O13-P-O14
69	d1	202	3PE	C1-O11-P-O12
69	d1	202	3PE	C1-O11-P-O14
69	i1	201	3PE	C11-O13-P-O12
69	m1	601	3PE	C1-O11-P-O12
69	a	606	3PE	C11-O13-P-O12
69	b	301	3PE	C11-O13-P-O14
69	c	301	3PE	C11-O13-P-O12
69	i	101	3PE	C1-O11-P-O14
69	i	101	3PE	C11-O13-P-O14
70	A	502	CDL	CB3-OB5-PB2-OB3
70	A	502	CDL	CB3-OB5-PB2-OB4
70	D	302	CDL	CA2-OA2-PA1-OA3
70	D	302	CDL	CA3-OA5-PA1-OA4
70	D	302	CDL	CB2-OB2-PB2-OB4
70	G	101	CDL	CA2-OA2-PA1-OA3
70	G	101	CDL	CB3-OB5-PB2-OB4
70	O	301	CDL	CA2-OA2-PA1-OA3
70	O	301	CDL	CA2-OA2-PA1-OA4
70	O	301	CDL	CB2-OB2-PB2-OB4
70	R	102	CDL	CB2-OB2-PB2-OB3
70	V	102	CDL	CB2-OB2-PB2-OB3
70	r1	202	CDL	CA3-OA5-PA1-OA3
70	r1	202	CDL	CA3-OA5-PA1-OA4
70	r1	202	CDL	CB2-OB2-PB2-OB3
70	L1	702	CDL	CA2-OA2-PA1-OA3
70	L1	702	CDL	CB3-OB5-PB2-OB3
70	L1	703	CDL	CA3-OA5-PA1-OA4
70	L1	703	CDL	CB2-OB2-PB2-OB3
70	N1	401	CDL	CA2-OA2-PA1-OA3
70	N1	401	CDL	CB3-OB5-PB2-OB3
70	N1	401	CDL	CB3-OB5-PB2-OB4
70	Y1	401	CDL	CB3-OB5-PB2-OB3
70	d1	201	CDL	CA3-OA5-PA1-OA3
70	h1	201	CDL	CA2-OA2-PA1-OA4
70	h1	201	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
74	J	101	PC1	C11-O13-P-O14
74	L	503	PC1	C1-O11-P-O14
74	I	201	PC1	C1-O11-P-O12
74	p	302	PC1	C1-O11-P-O12
74	6	203	PC1	C11-O13-P-O12
74	6	203	PC1	C11-O13-P-O14
74	9	203	PC1	C11-O13-P-O12
74	g	302	PC1	C1-O11-P-O12
70	L1	702	CDL	OB5-CB3-CB4-CB6
70	h1	201	CDL	OB5-CB3-CB4-CB6
77	a	604	HEA	O11-C11-C12-C13
69	M1	502	3PE	C12-C11-O13-P
69	b	301	3PE	C12-C11-O13-P
69	c	301	3PE	C12-C11-O13-P
69	g	303	3PE	C12-C11-O13-P
69	i	101	3PE	C12-C11-O13-P
70	g	301	CDL	CB4-CB3-OB5-PB2
70	L1	703	CDL	OB5-CB3-CB4-OB6
70	N1	401	CDL	OB5-CB3-CB4-OB6
70	h1	201	CDL	OB5-CB3-CB4-OB6
74	K	101	PC1	O11-C1-C2-O21
77	a	603	HEA	C2A-CAA-CBA-CGA
70	G	101	CDL	C72-C71-CB7-OB8
70	L	502	CDL	C52-C51-CB5-OB6
74	p	302	PC1	C21-C22-C23-C24
69	n	606	3PE	C1-C2-C3-O31
69	o	302	3PE	C1-C2-C3-O31
69	c	301	3PE	C25-C26-C27-C28
74	J	101	PC1	O13-C11-C12-N
74	L	503	PC1	O13-C11-C12-N
74	I	201	PC1	O13-C11-C12-N
74	9	203	PC1	O13-C11-C12-N
74	M1	501	PC1	O13-C11-C12-N
74	g	302	PC1	O13-C11-C12-N
77	n	603	HEA	C1A-C2A-CAA-CBA
70	N1	401	CDL	C80-C81-C82-C83
69	H1	401	3PE	C2-C1-O11-P
69	i1	201	3PE	C2-C1-O11-P
69	b1	101	3PE	C38-C39-C3A-C3B
70	D	302	CDL	C72-C73-C74-C75
69	H1	401	3PE	O31-C31-C32-C33
69	M1	502	3PE	C3D-C3E-C3F-C3G

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Mol	Chain	Res	Type	Atoms
70	R	102	CDL	C31-C32-C33-C34
69	6	202	3PE	C32-C33-C34-C35
86	n1	201	ZMP	C19-C18-C21-O5
86	n1	201	ZMP	C20-C18-C21-O5
69	t	101	3PE	C3-C2-O21-C21
74	9	203	PC1	C3-C2-O21-C21
70	V	102	CDL	OB5-CB3-CB4-CB6
69	r1	201	3PE	O31-C31-C32-C33
70	L1	702	CDL	C12-C11-CA5-OA6
69	E	202	3PE	O21-C2-C3-O31
69	E	202	3PE	C11-O13-P-O11
69	n	606	3PE	C11-O13-P-O11
69	L1	701	3PE	C11-O13-P-O11
69	M1	503	3PE	C1-O11-P-O13
69	N1	402	3PE	C11-O13-P-O11
69	a	605	3PE	C11-O13-P-O11
69	a	606	3PE	C1-O11-P-O13
69	b	301	3PE	C1-O11-P-O13
70	A	502	CDL	CA2-OA2-PA1-OA5
70	L	502	CDL	CA2-OA2-PA1-OA5
70	O	301	CDL	CA3-OA5-PA1-OA2
70	O	301	CDL	CB2-OB2-PB2-OB5
70	R	103	CDL	CA2-OA2-PA1-OA5
70	V	102	CDL	CA2-OA2-PA1-OA5
70	V	102	CDL	CB3-OB5-PB2-OB2
70	r1	202	CDL	CB3-OB5-PB2-OB2
70	H1	402	CDL	CA3-OA5-PA1-OA2
70	H1	402	CDL	CB3-OB5-PB2-OB2
70	N1	401	CDL	CA3-OA5-PA1-OA2
70	d1	201	CDL	CB2-OB2-PB2-OB5
74	z	101	PC1	C11-O13-P-O11
74	g	302	PC1	C11-O13-P-O11
85	P1	501	NDP	O4D-C1D-N1N-C6N
70	G	101	CDL	C72-C71-CB7-OB9
69	H1	401	3PE	C21-C22-C23-C24
85	P1	501	NDP	PN-O3-PA-O2A
69	M1	502	3PE	C37-C38-C39-C3A
69	n	606	3PE	C2-C1-O11-P
70	N1	401	CDL	C1-CA2-OA2-PA1
69	O	302	3PE	C34-C35-C36-C37
69	H1	401	3PE	C2A-C2B-C2C-C2D
69	L1	704	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
74	I	201	PC1	C36-C37-C38-C39
70	D	302	CDL	OB5-CB3-CB4-CB6
74	6	203	PC1	O11-C1-C2-C3
69	m1	601	3PE	O13-C11-C12-N
77	n	604	HEA	CAA-CBA-CGA-O2A
77	a	604	HEA	CAA-CBA-CGA-O2A
69	M1	503	3PE	O11-C1-C2-O21
70	D	302	CDL	OB5-CB3-CB4-OB6
69	N1	402	3PE	C2-C1-O11-P
74	V	101	PC1	C2-C1-O11-P
85	P1	501	NDP	C2D-C1D-N1N-C6N
69	d1	203	3PE	O21-C21-C22-C23
77	a	603	HEA	CAD-CBD-CGD-O1D
77	a	604	HEA	CAA-CBA-CGA-O1A
69	p	301	3PE	C22-C23-C24-C25
70	g	301	CDL	CA3-CA4-CA6-OA8
69	c	301	3PE	C28-C29-C2A-C2B
77	a	604	HEA	C19-C20-C21-C22
77	a	604	HEA	CAD-CBD-CGD-O1D
69	H1	401	3PE	C3-C2-O21-C21
69	d	201	3PE	C3-C2-O21-C21
69	g	303	3PE	C3-C2-O21-C21
70	h1	201	CDL	CB6-CB4-OB6-CB5
77	a	603	HEA	CAD-CBD-CGD-O2D
70	R	101	CDL	C72-C71-CB7-OB8
70	O	301	CDL	C1-CB2-OB2-PB2
70	V	102	CDL	OB5-CB3-CB4-OB6
70	r1	202	CDL	C52-C51-CB5-OB6
74	9	204	PC1	C35-C36-C37-C38
69	H1	401	3PE	O11-C1-C2-C3
70	r1	202	CDL	OB5-CB3-CB4-CB6
77	n	603	HEA	O11-C11-C12-C13
86	n1	201	ZMP	C12-C11-S1-C10
74	M1	501	PC1	O21-C2-C3-O31
72	O	303	HEC	CAD-CBD-CGD-O2D
70	N1	401	CDL	C79-C80-C81-C82
69	M1	503	3PE	C27-C28-C29-C2A
71	N	402	HEM	CAD-CBD-CGD-O2D
77	n	604	HEA	CAA-CBA-CGA-O1A
74	I	201	PC1	O21-C21-C22-C23
77	a	604	HEA	CAD-CBD-CGD-O2D
70	D	302	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
69	M1	502	3PE	C33-C34-C35-C36
77	n	603	HEA	CAD-CBD-CGD-O1D
70	R	103	CDL	C75-C76-C77-C78
70	d1	201	CDL	CA3-CA4-CA6-OA8
70	r1	202	CDL	OB5-CB3-CB4-OB6
74	9	203	PC1	C37-C38-C39-C3A
72	O	303	HEC	CAD-CBD-CGD-O1D
69	M1	503	3PE	O11-C1-C2-C3
69	c	301	3PE	O11-C1-C2-C3
70	h1	201	CDL	C12-C11-CA5-OA6
69	b1	101	3PE	C34-C35-C36-C37
69	g	303	3PE	O32-C31-C32-C33
71	N	402	HEM	CAD-CBD-CGD-O1D
70	G	101	CDL	C32-C31-CA7-OA8
69	G	102	3PE	C35-C36-C37-C38
83	1	501	FMN	C5'-O5'-P-O3P
86	n1	201	ZMP	N2-C16-C17-O4
69	K1	201	3PE	O21-C21-C22-C23
69	d	201	3PE	O21-C21-C22-C23
77	n	603	HEA	C27-C19-C20-C21
69	E	202	3PE	O31-C31-C32-C33
69	C	403	3PE	O31-C31-C32-C33
69	N	403	3PE	O31-C31-C32-C33
70	A	502	CDL	C12-C11-CA5-OA6
74	K	101	PC1	O21-C21-C22-C23
70	N1	401	CDL	C51-C52-C53-C54
69	L1	701	3PE	C3-C2-O21-C21
74	I	201	PC1	C1-C2-O21-C21
74	6	203	PC1	C3-C2-O21-C21
70	A	502	CDL	C32-C31-CA7-OA8
74	9	204	PC1	O31-C31-C32-C33
74	P1	502	PC1	O31-C31-C32-C33
69	C	404	3PE	O21-C21-C22-C23
69	i1	201	3PE	O31-C31-C32-C33
70	R	102	CDL	C32-C31-CA7-OA8
70	V	102	CDL	C52-C51-CB5-OB6
70	g	301	CDL	C12-C11-CA5-OA6
74	9	204	PC1	C21-C22-C23-C24
69	Y1	403	3PE	C1-C2-C3-O31
69	b	301	3PE	C1-C2-C3-O31
70	R	102	CDL	OA5-CA3-CA4-OA6
70	d1	201	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
70	h1	201	CDL	C52-C51-CB5-OB6
69	E	203	3PE	O31-C31-C32-C33
69	o	302	3PE	O21-C21-C22-C23
69	K1	201	3PE	O31-C31-C32-C33
70	R	102	CDL	C52-C51-CB5-OB6
74	9	203	PC1	C29-C2A-C2B-C2C
70	O	301	CDL	O1-C1-CA2-OA2
70	R	101	CDL	C32-C31-CA7-OA8
69	L	501	3PE	O11-C1-C2-C3
70	A	502	CDL	OB5-CB3-CB4-CB6
69	O	302	3PE	O21-C21-C22-C23
69	M1	502	3PE	O21-C21-C22-C23
69	a	606	3PE	O31-C31-C32-C33
70	L1	702	CDL	C72-C71-CB7-OB8
69	E	203	3PE	O21-C2-C3-O31
69	M1	503	3PE	O21-C2-C3-O31
69	m1	601	3PE	O21-C2-C3-O31
70	R	101	CDL	C12-C11-CA5-OA7
81	y	601	TGL	CC1-CC2-CC3-CC4
77	a	603	HEA	CAA-CBA-CGA-O1A
69	o	302	3PE	C22-C23-C24-C25
70	V	102	CDL	C75-C76-C77-C78
69	b1	101	3PE	O31-C31-C32-C33
70	V	102	CDL	C72-C71-CB7-OB8
70	L1	703	CDL	C32-C31-CA7-OA8
70	h1	201	CDL	C32-C31-CA7-OA8
77	n	603	HEA	CAD-CBD-CGD-O2D
85	P1	501	NDP	C5B-O5B-PA-O3
70	R	102	CDL	C72-C71-CB7-OB8
69	C	403	3PE	C2A-C2B-C2C-C2D
69	M1	503	3PE	C2-C1-O11-P
69	R	104	3PE	O31-C31-C32-C33
70	h1	201	CDL	C72-C71-CB7-OB8
81	y	601	TGL	OG1-CA1-CA2-CA3
69	K1	201	3PE	C25-C26-C27-C28
69	i	101	3PE	O31-C31-C32-C33
70	R	101	CDL	C52-C51-CB5-OB6
69	K1	201	3PE	O22-C21-C22-C23
69	Y1	403	3PE	C23-C24-C25-C26
69	E	202	3PE	O21-C21-C22-C23
69	M1	503	3PE	O31-C31-C32-C33
85	P1	501	NDP	PN-O3-PA-O1A

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Mol	Chain	Res	Type	Atoms
87	O1	401	DGT	PB-O3A-PA-O1A
70	R	102	CDL	C32-C31-CA7-OA9
70	g	301	CDL	C12-C11-CA5-OA7
72	O	303	HEC	CAA-CBA-CGA-O2A
69	C	403	3PE	O32-C31-C32-C33
70	V	102	CDL	C52-C51-CB5-OB7
74	K	101	PC1	O22-C21-C22-C23
69	G	102	3PE	O21-C21-C22-C23
69	m1	601	3PE	O21-C21-C22-C23
69	C	404	3PE	O22-C21-C22-C23
69	N	403	3PE	O32-C31-C32-C33
69	i1	201	3PE	O32-C31-C32-C33
74	P1	502	PC1	O22-C21-C22-C23
70	r1	202	CDL	C17-C18-C19-C20
70	L1	702	CDL	C12-C13-C14-C15
69	d	201	3PE	O22-C21-C22-C23
72	D	301	HEC	CAD-CBD-CGD-O2D
69	p	301	3PE	C25-C26-C27-C28
69	K1	201	3PE	O32-C31-C32-C33
70	h1	201	CDL	C52-C51-CB5-OB7
69	O	302	3PE	O22-C21-C22-C23
69	a	606	3PE	O32-C31-C32-C33
70	A	502	CDL	C12-C11-CA5-OA7
70	R	101	CDL	C32-C31-CA7-OA9
69	Y1	403	3PE	O31-C31-C32-C33
69	E	202	3PE	O32-C31-C32-C33
74	9	204	PC1	O32-C31-C32-C33
74	P1	502	PC1	O32-C31-C32-C33
81	y	601	TGL	OA1-CA1-CA2-CA3
77	n	603	HEA	CAA-CBA-CGA-O2A
69	m1	601	3PE	C32-C33-C34-C35
69	H1	401	3PE	C1-O11-P-O14
69	L1	701	3PE	C11-O13-P-O12
69	a	605	3PE	C1-O11-P-O14
69	a	605	3PE	C11-O13-P-O14
69	a	606	3PE	C1-O11-P-O14
69	b	301	3PE	C1-O11-P-O14
70	L	502	CDL	CA3-OA5-PA1-OA4
70	V	102	CDL	CA2-OA2-PA1-OA3
70	V	102	CDL	CB3-OB5-PB2-OB3
70	L1	703	CDL	CB3-OB5-PB2-OB3
70	N1	401	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
70	d1	201	CDL	CB2-OB2-PB2-OB3
74	z	101	PC1	C1-O11-P-O14
74	g	302	PC1	C11-O13-P-O14
69	o	302	3PE	O22-C21-C22-C23
70	D	302	CDL	C52-C51-CB5-OB7
69	b	301	3PE	O11-C1-C2-C3
74	M1	501	PC1	O11-C1-C2-C3
70	R	102	CDL	C52-C51-CB5-OB7
70	V	102	CDL	C72-C71-CB7-OB9
70	h1	201	CDL	C72-C71-CB7-OB9
69	M1	502	3PE	O31-C31-C32-C33
70	Y1	401	CDL	C32-C31-CA7-OA8
69	E	203	3PE	O32-C31-C32-C33
69	M1	502	3PE	O22-C21-C22-C23
70	h1	201	CDL	C32-C31-CA7-OA9
70	d1	201	CDL	C62-C63-C64-C65
70	A	502	CDL	C32-C31-CA7-OA9
77	a	603	HEA	CAA-CBA-CGA-O2A
69	A	501	3PE	C1-C2-O21-C21
69	n	605	3PE	C1-C2-O21-C21
69	t	101	3PE	C12-C11-O13-P
69	Y1	403	3PE	C12-C11-O13-P
69	d1	203	3PE	C12-C11-O13-P
69	m1	601	3PE	C12-C11-O13-P
69	a	605	3PE	C12-C11-O13-P
70	R	101	CDL	CA6-CA4-OA6-CA5
70	R	102	CDL	CA3-CA4-OA6-CA5
70	R	103	CDL	CA6-CA4-OA6-CA5
70	V	102	CDL	CA6-CA4-OA6-CA5
70	N1	401	CDL	CB6-CB4-OB6-CB5
74	L	503	PC1	C1-C2-O21-C21
74	9	203	PC1	C12-C11-O13-P
74	P1	502	PC1	C3-C2-O21-C21
74	M1	501	PC1	C12-C11-O13-P
77	a	603	HEA	C3B-C11-C12-C13
69	M1	503	3PE	O32-C31-C32-C33
70	L1	703	CDL	C32-C31-CA7-OA9
70	d1	201	CDL	C72-C71-CB7-OB9
70	R	103	CDL	C81-C82-C83-C84
74	M1	501	PC1	C3B-C3C-C3D-C3E
69	d1	203	3PE	C31-C32-C33-C34
69	n	605	3PE	O21-C21-C22-C23

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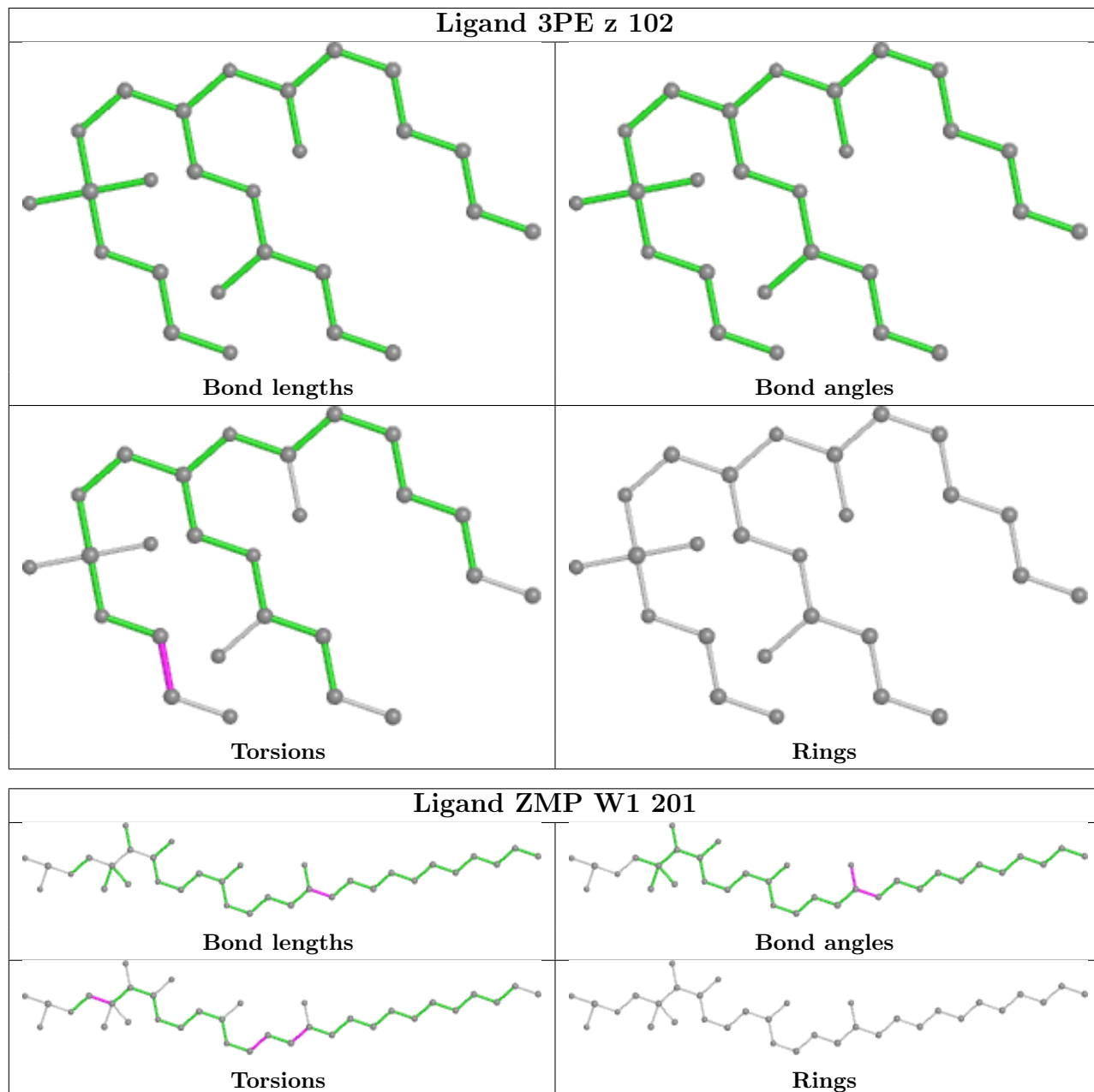
Mol	Chain	Res	Type	Atoms
70	L	502	CDL	C12-C11-CA5-OA6
74	g	302	PC1	O31-C31-C32-C33
71	N	401	HEM	CAA-CBA-CGA-O1A
72	O	303	HEC	CAA-CBA-CGA-O1A
69	b1	101	3PE	O32-C31-C32-C33
69	H1	401	3PE	C23-C24-C25-C26
69	A	501	3PE	O31-C31-C32-C33
69	p	301	3PE	O31-C31-C32-C33
70	L1	703	CDL	C52-C51-CB5-OB6
74	9	203	PC1	O21-C21-C22-C23
69	L1	704	3PE	C39-C3A-C3B-C3C
69	M1	503	3PE	C29-C2A-C2B-C2C
70	L1	702	CDL	C72-C71-CB7-OB9
74	6	203	PC1	C3A-C3B-C3C-C3D
69	R	104	3PE	O32-C31-C32-C33
69	m1	601	3PE	O22-C21-C22-C23
72	D	301	HEC	CAD-CBD-CGD-O1D
70	A	502	CDL	C52-C51-CB5-OB6
70	R	101	CDL	C12-C11-CA5-OA6
74	L	503	PC1	O21-C21-C22-C23
69	E	202	3PE	O22-C21-C22-C23
69	G	102	3PE	O22-C21-C22-C23
70	H1	402	CDL	C17-C18-C19-C20
69	n	605	3PE	O22-C21-C22-C23
70	L	502	CDL	C12-C11-CA5-OA7
70	R	102	CDL	C72-C71-CB7-OB9
70	L1	703	CDL	C52-C51-CB5-OB7
74	9	203	PC1	O22-C21-C22-C23
70	Y1	401	CDL	C32-C31-CA7-OA9
74	g	302	PC1	O32-C31-C32-C33
71	N	401	HEM	CAA-CBA-CGA-O2A
69	Y1	403	3PE	O32-C31-C32-C33
70	R	102	CDL	C12-C11-CA5-OA6
74	z	101	PC1	O21-C21-C22-C23

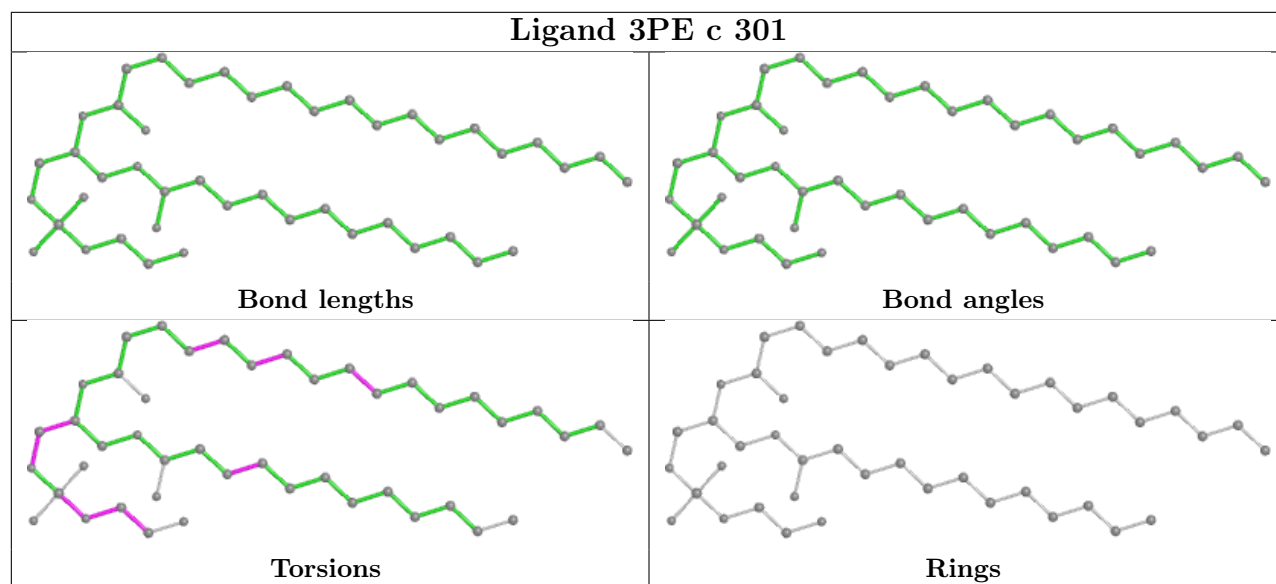
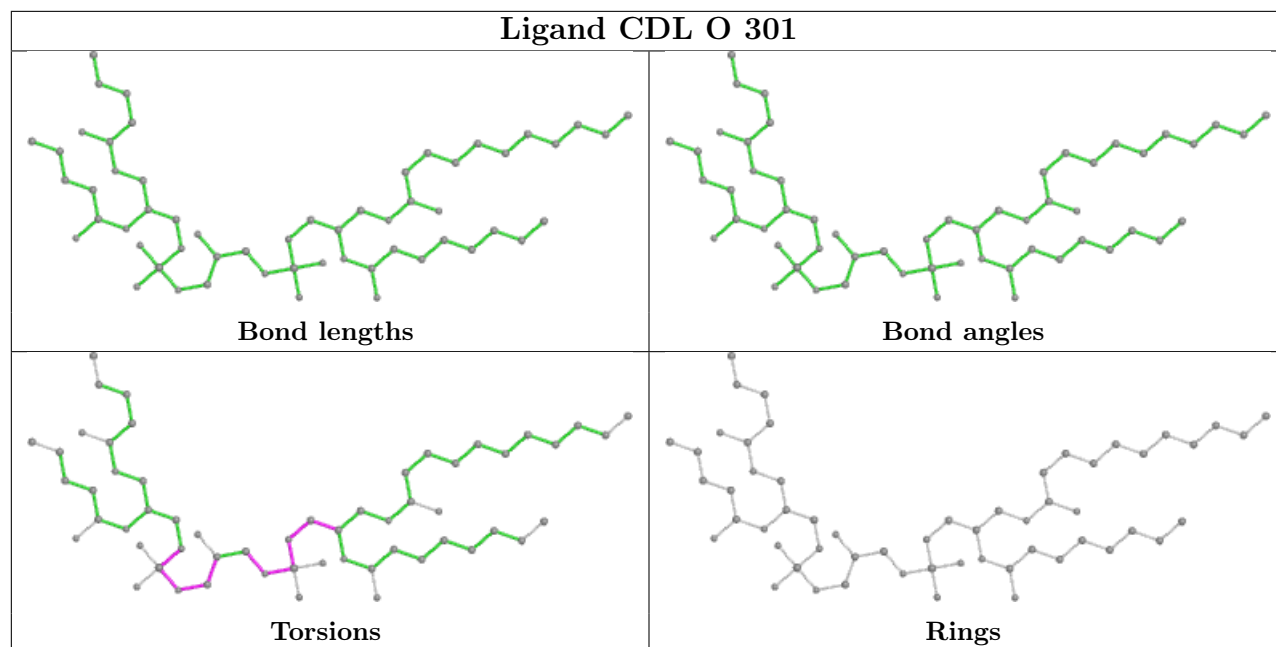
There are no ring outliers.

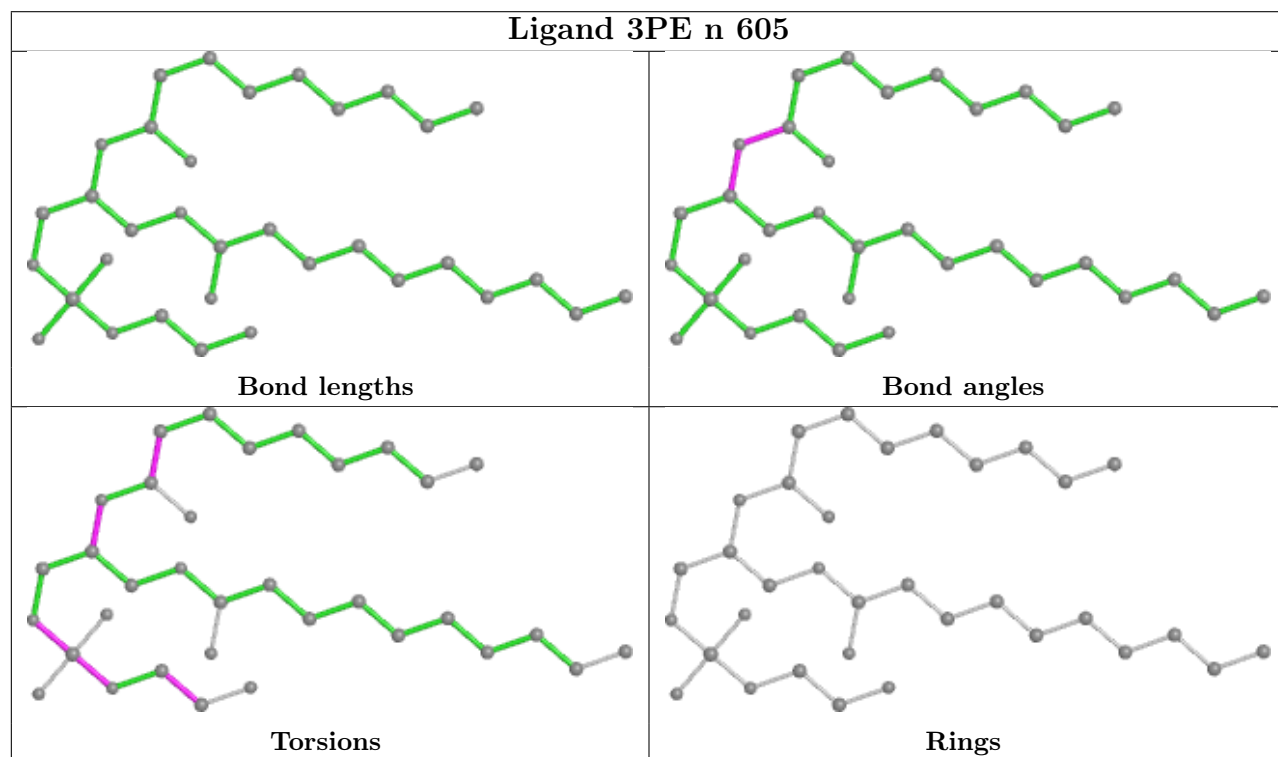
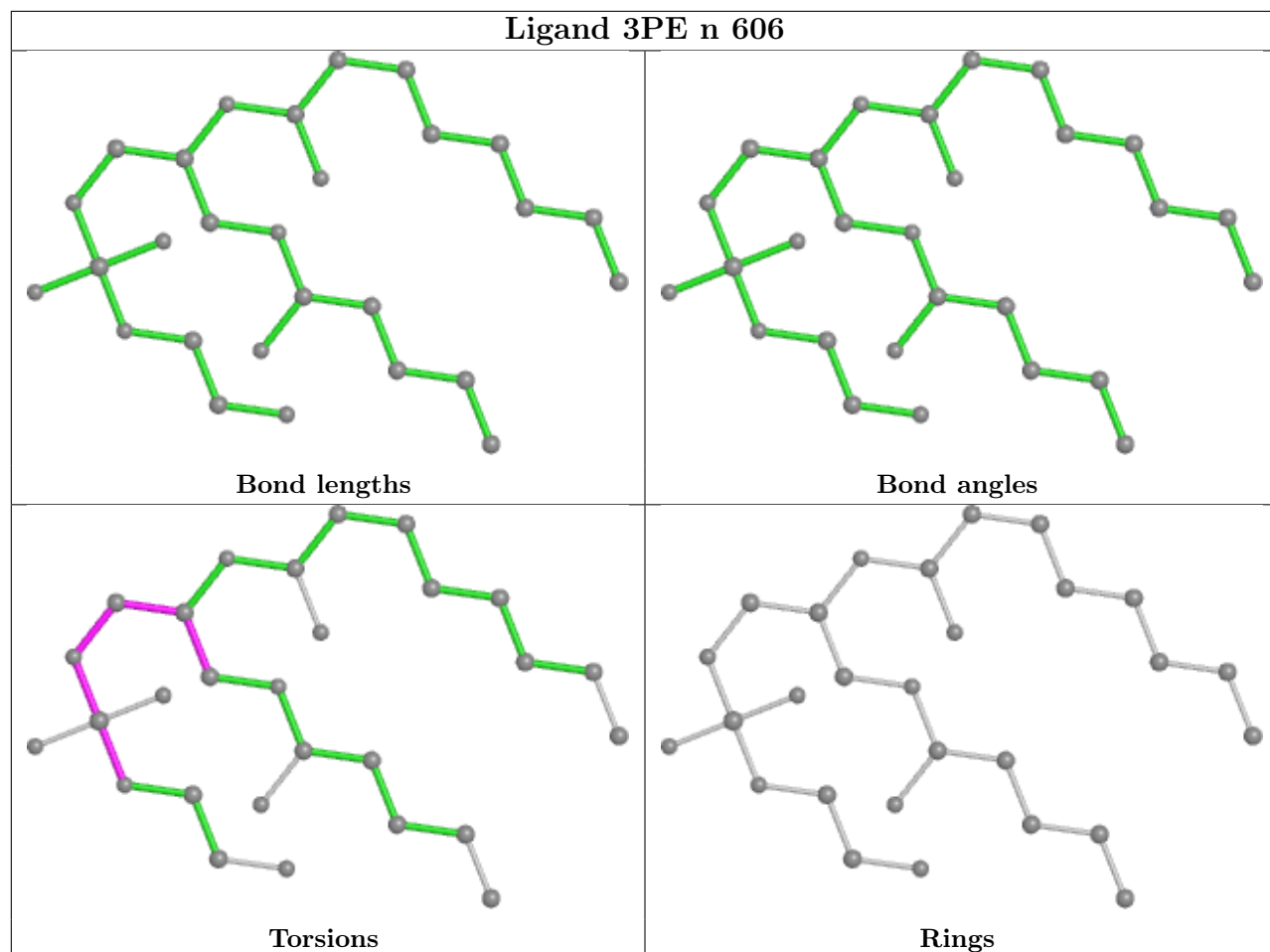
No monomer is involved in short contacts.

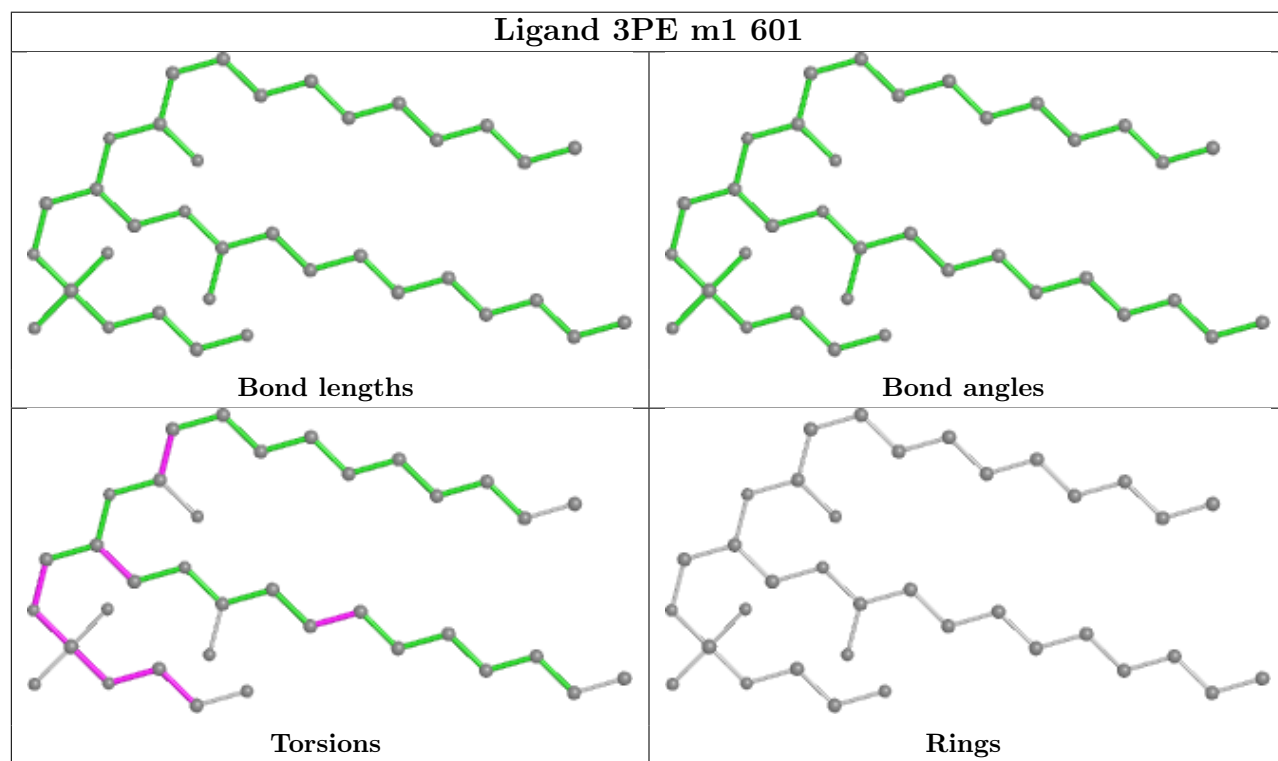
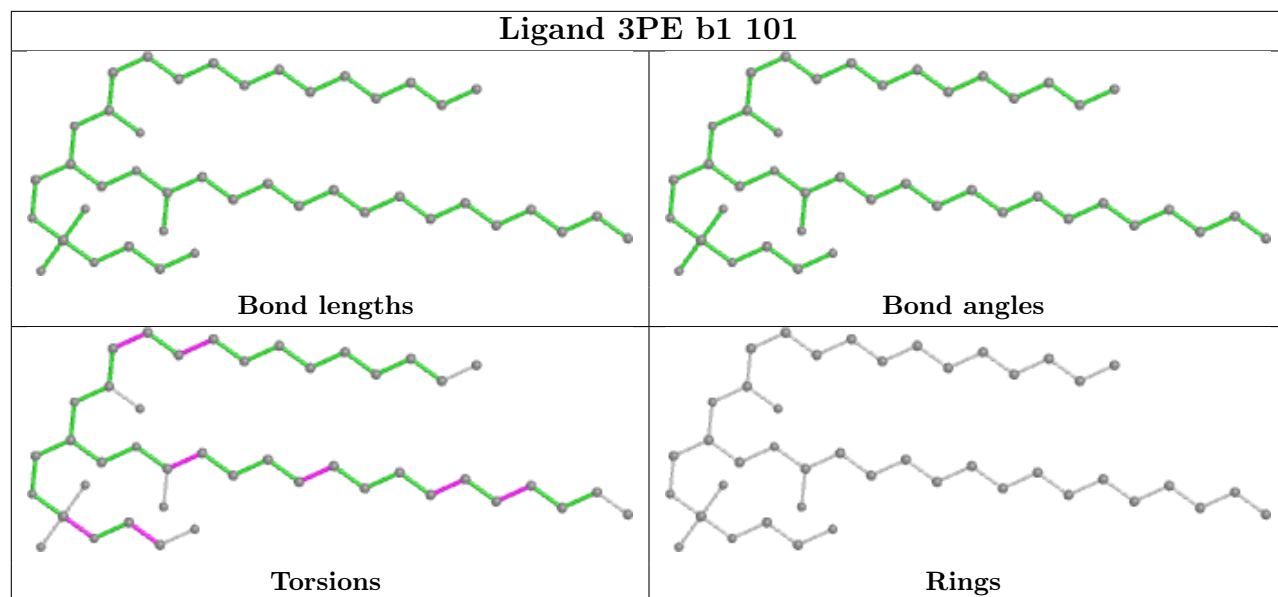
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

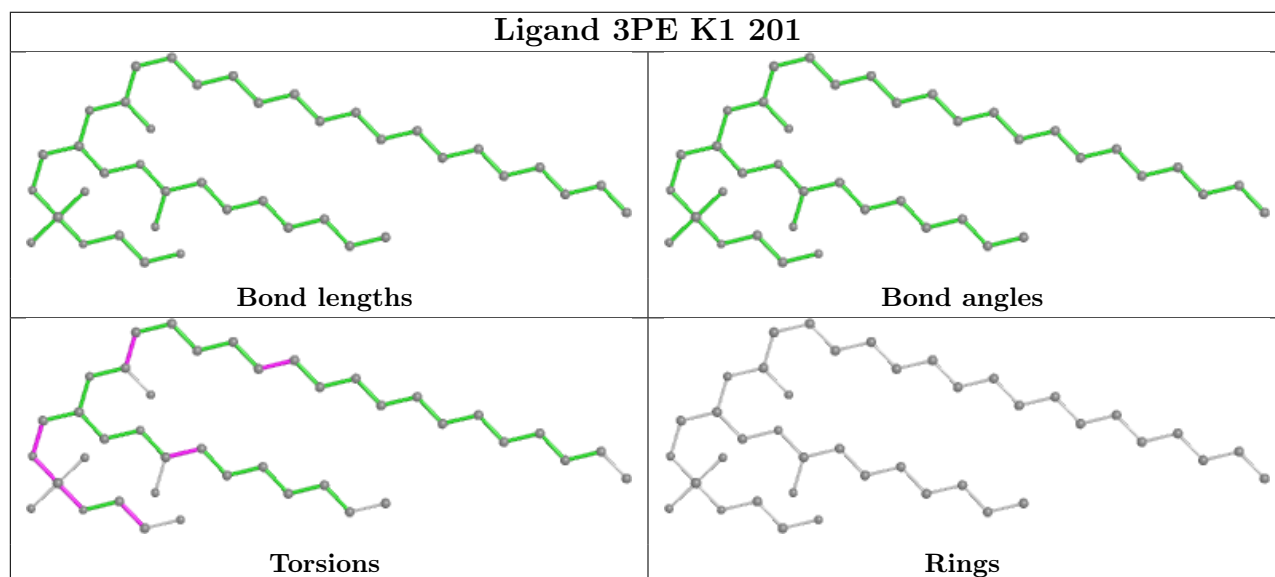
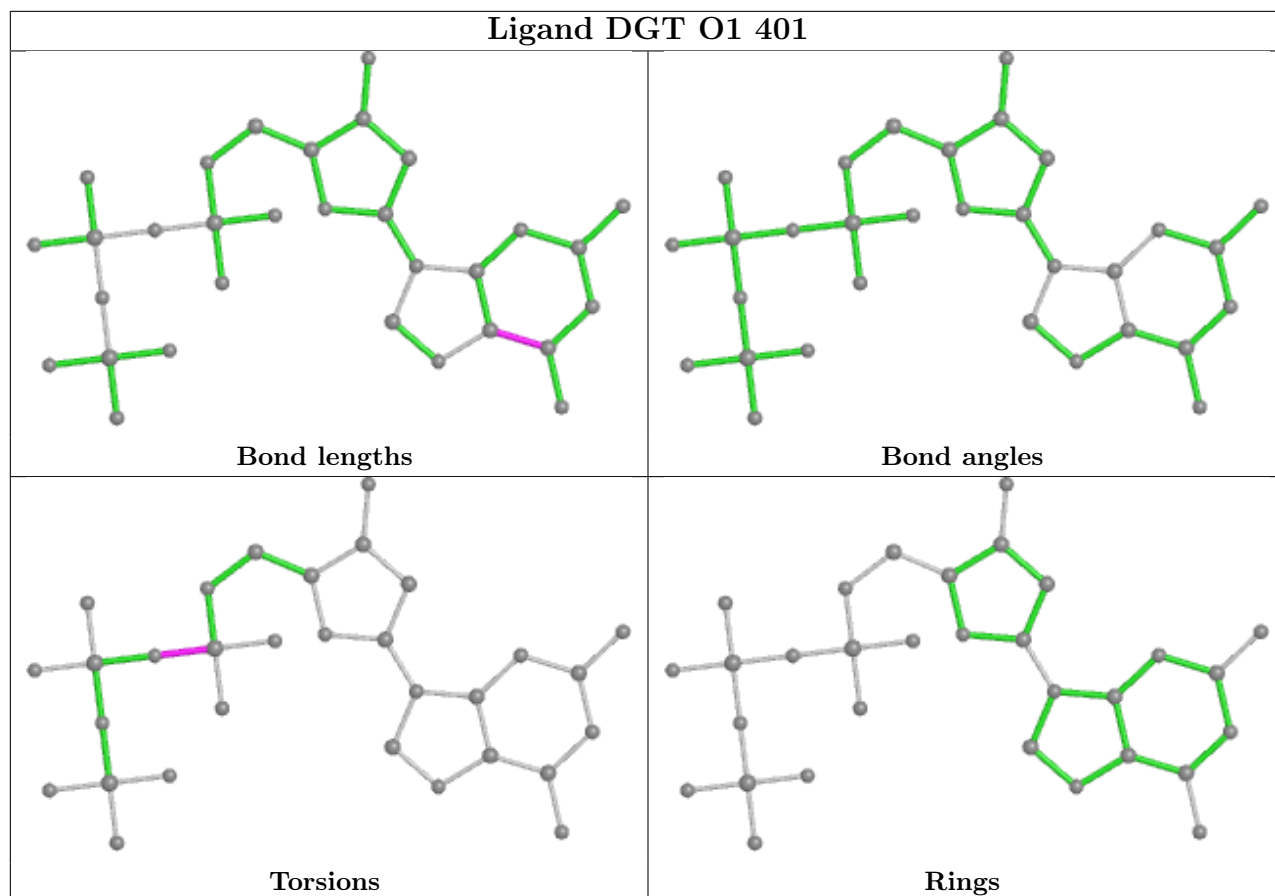
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

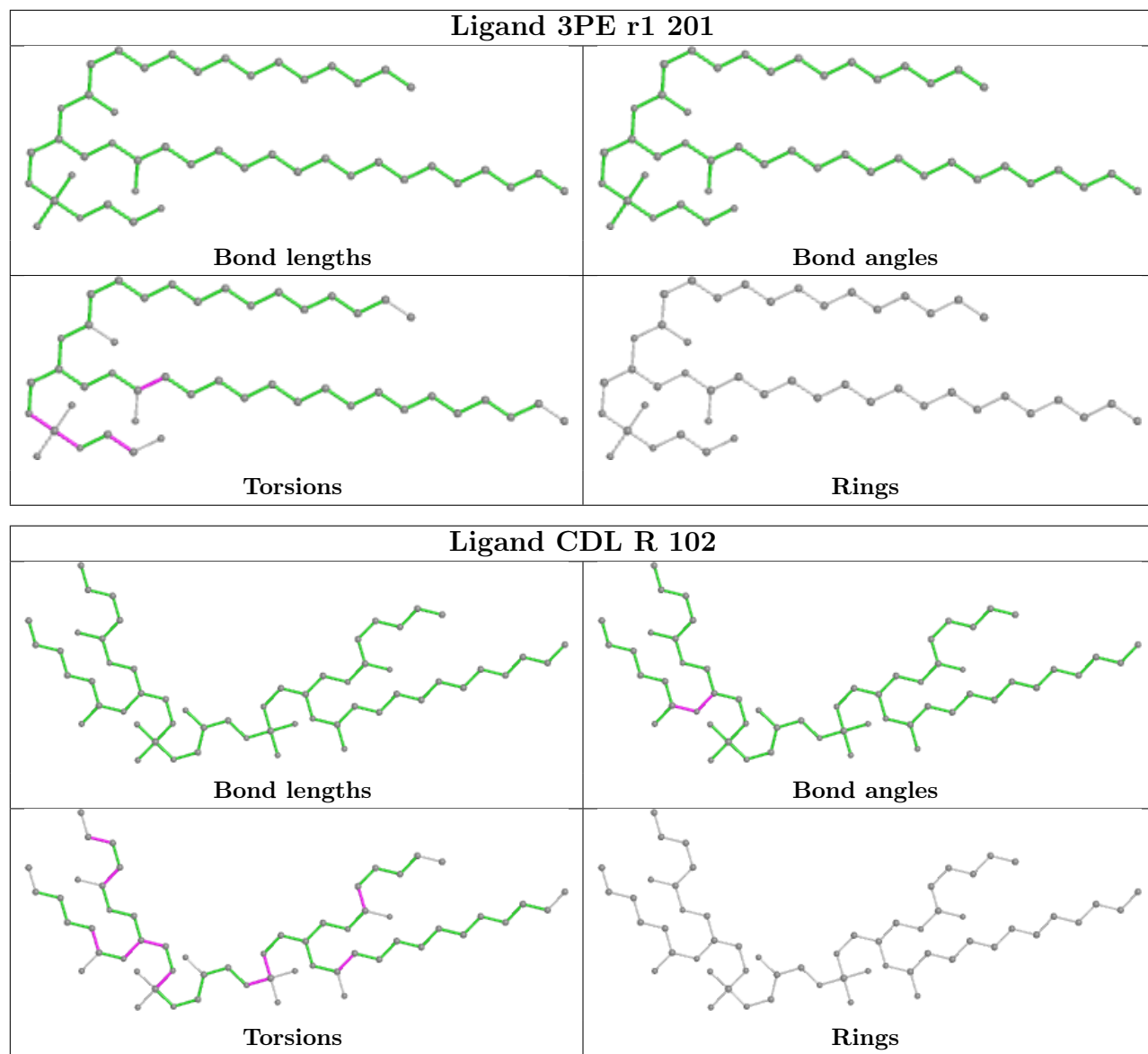


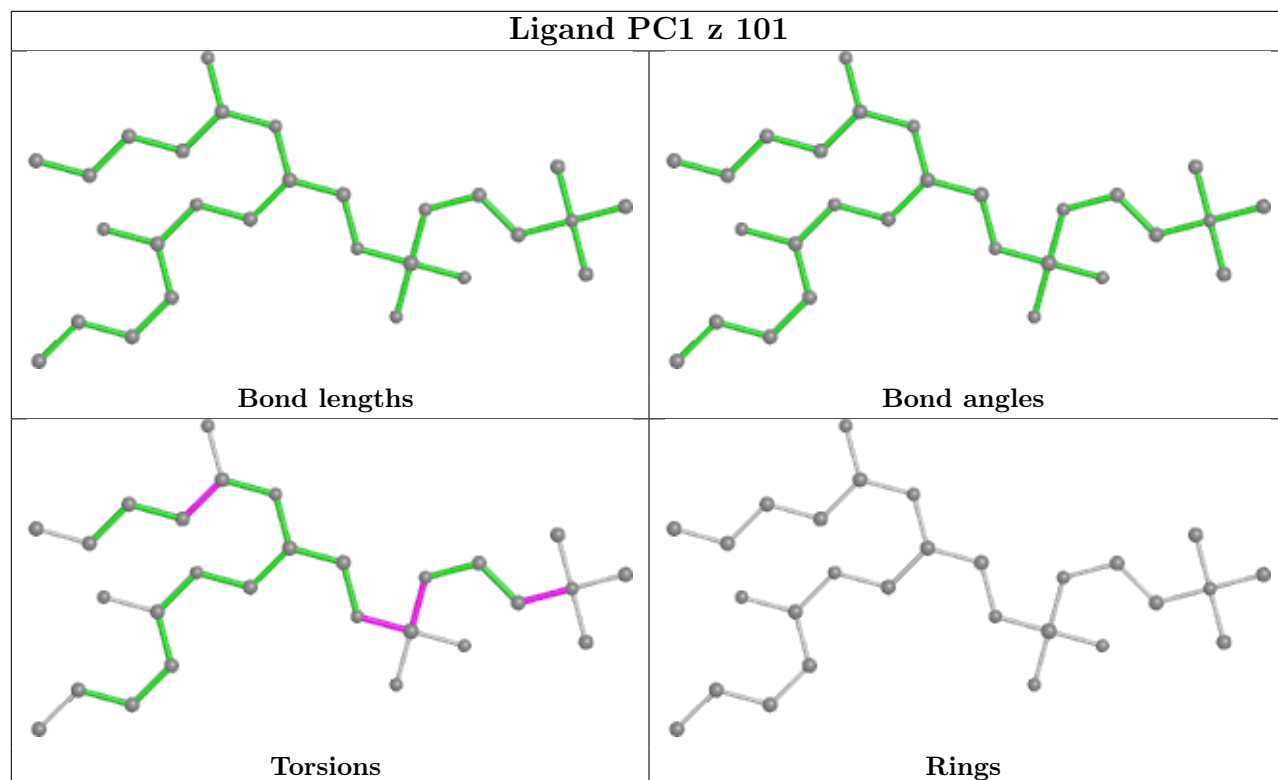


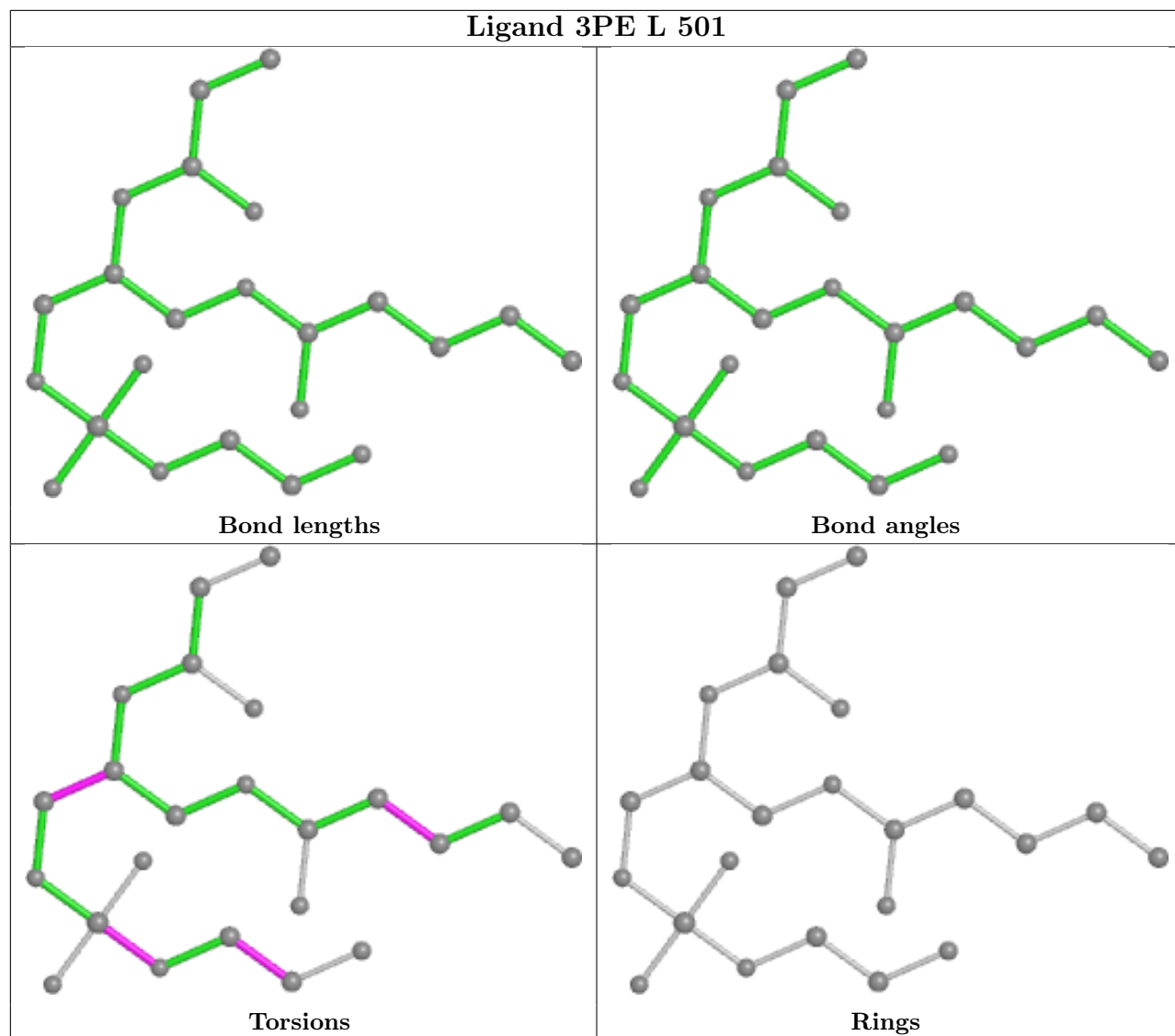


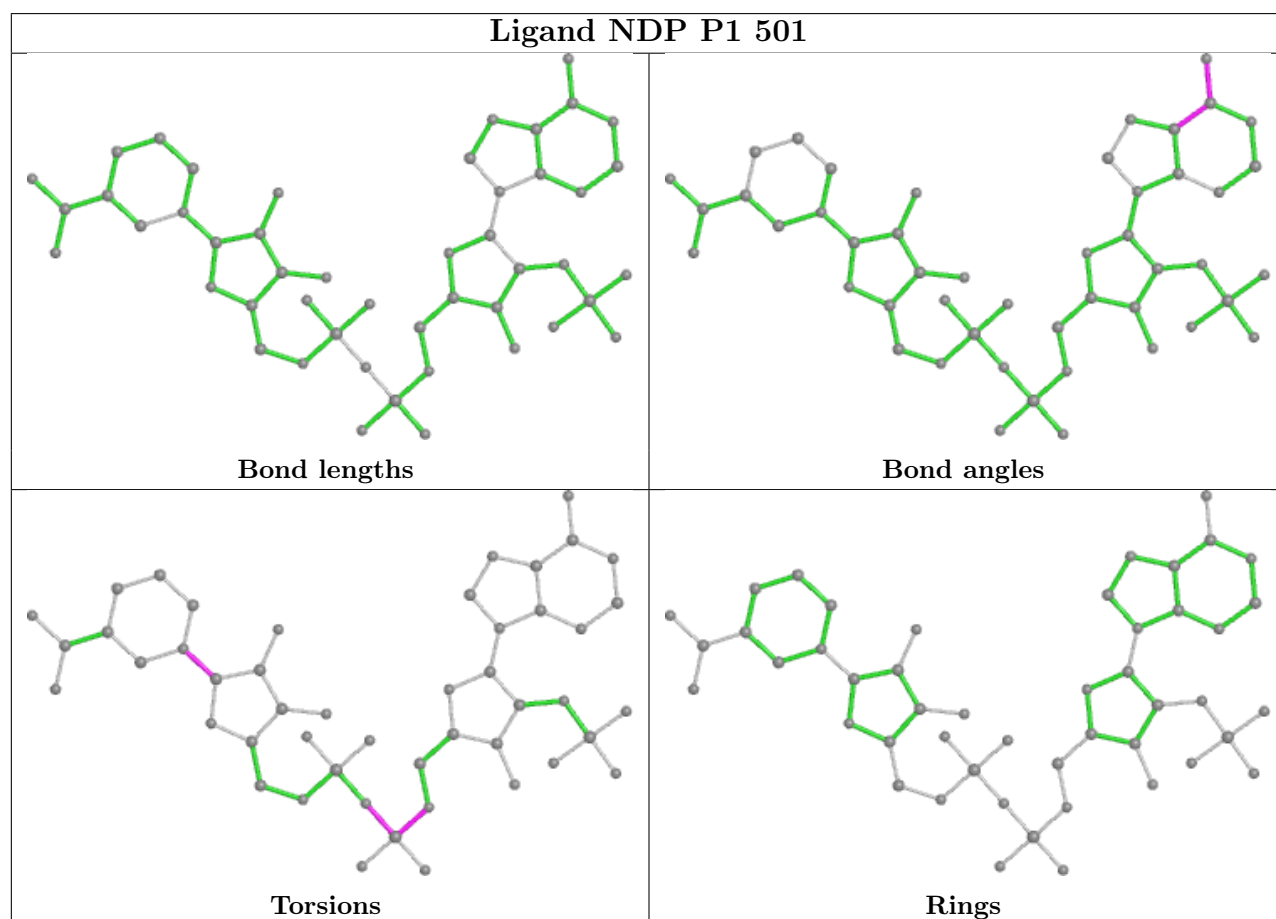
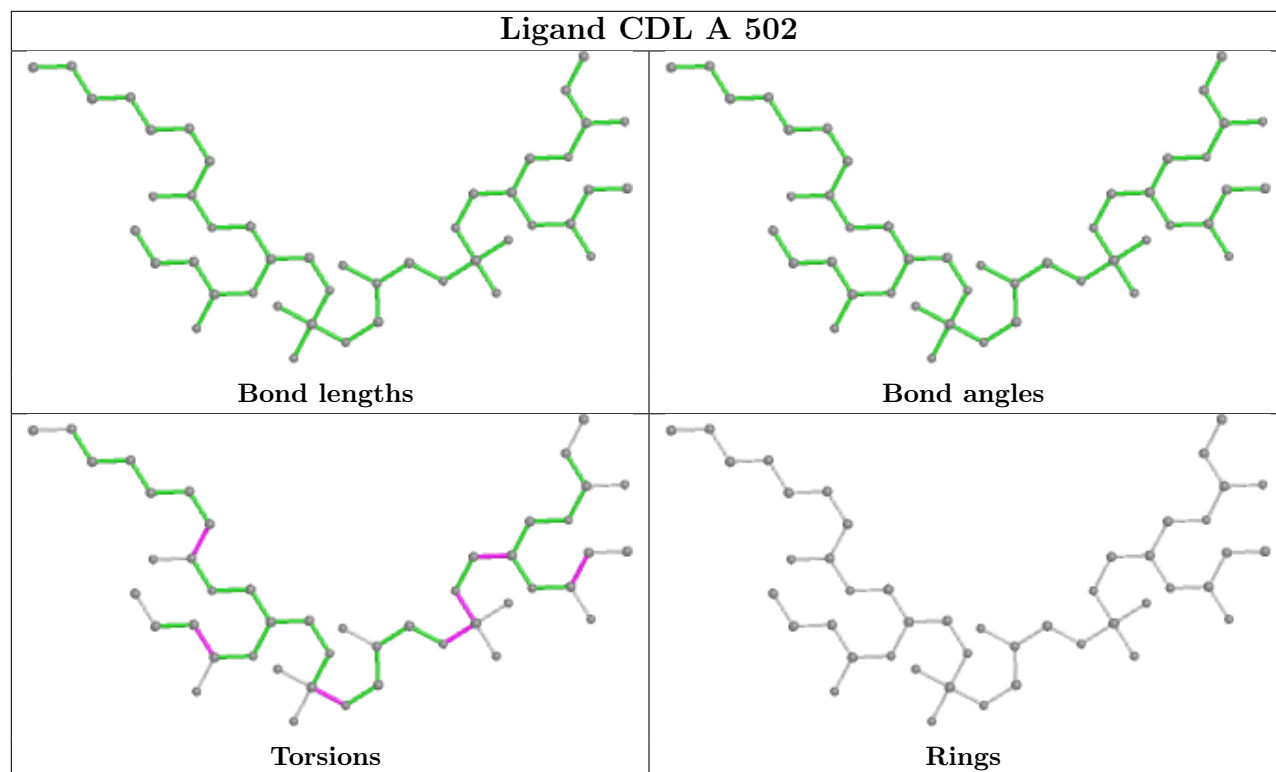


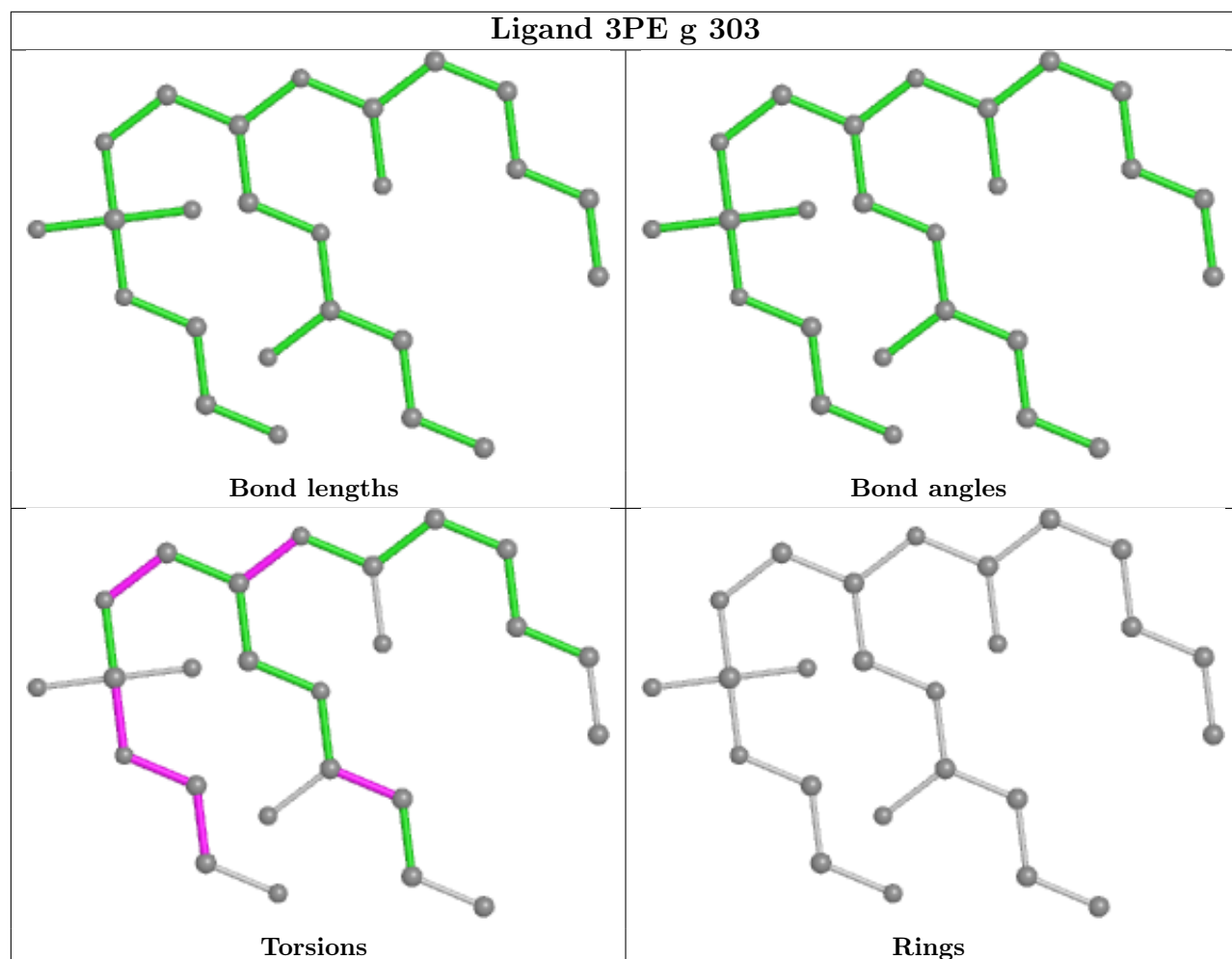
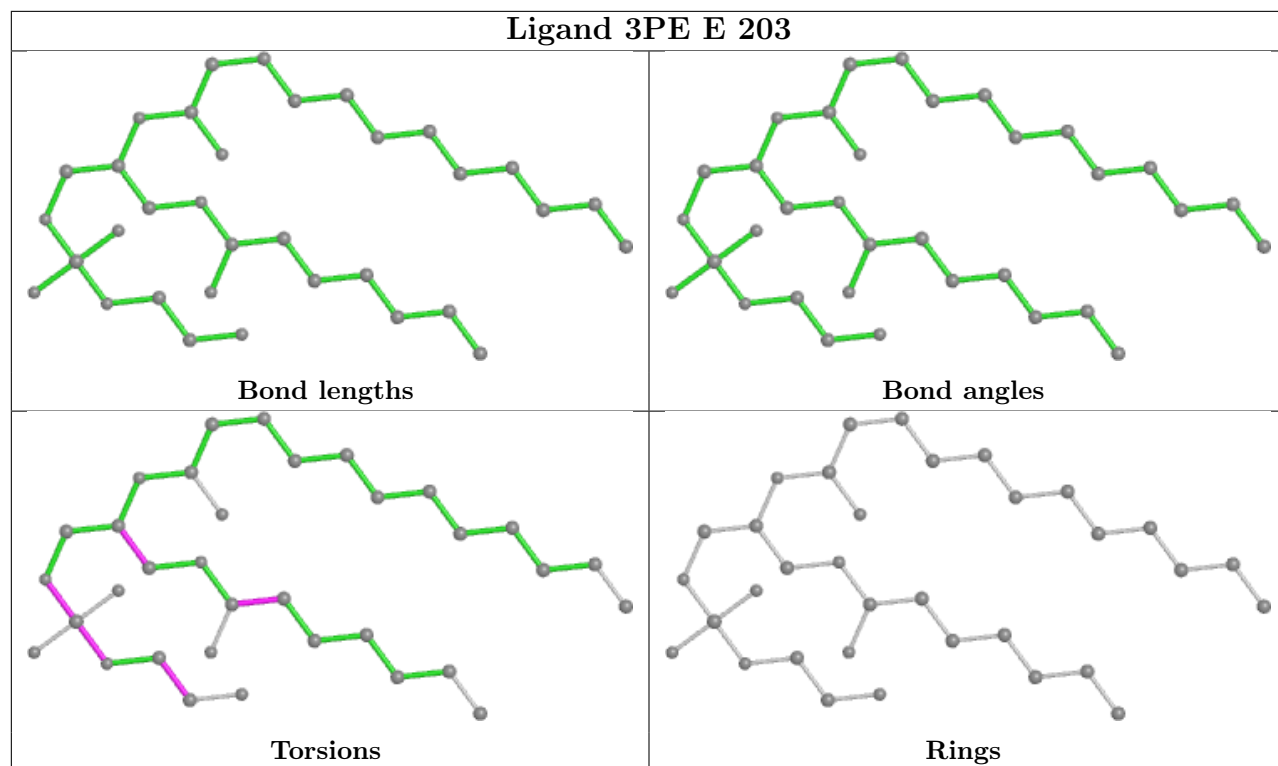


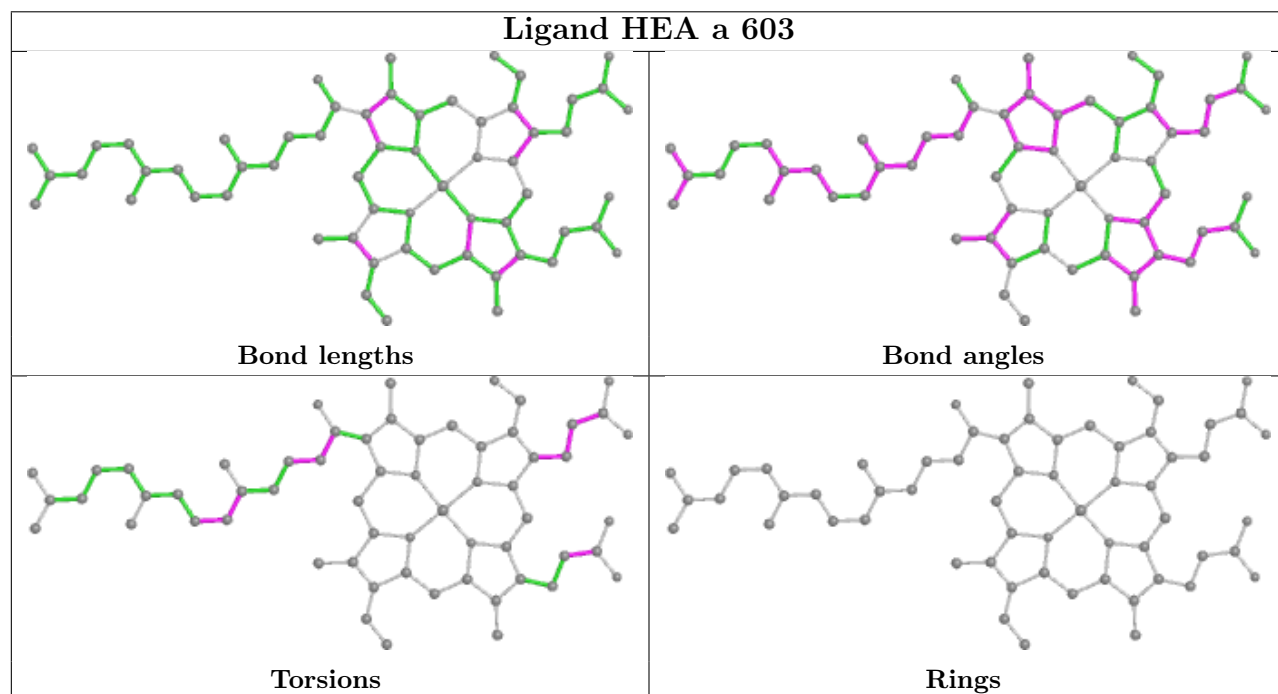
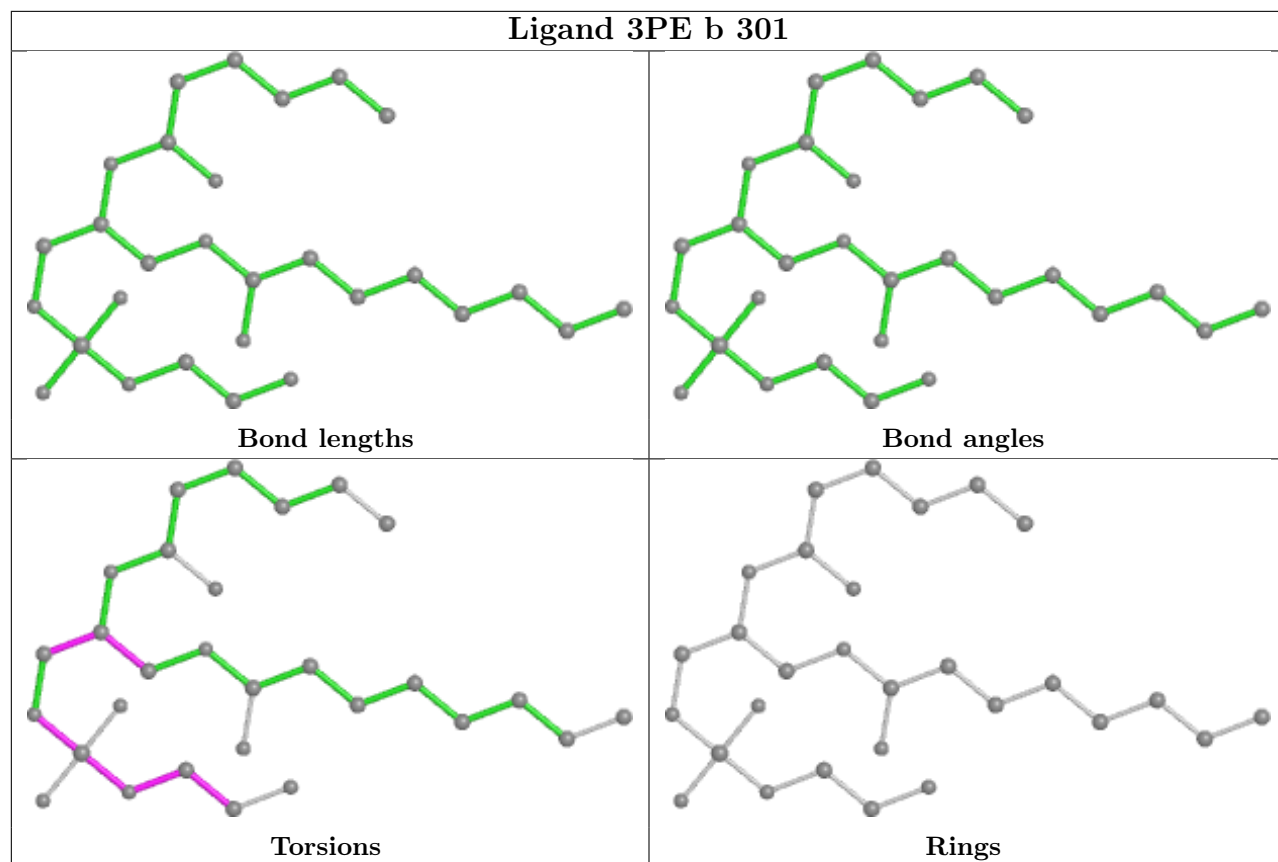


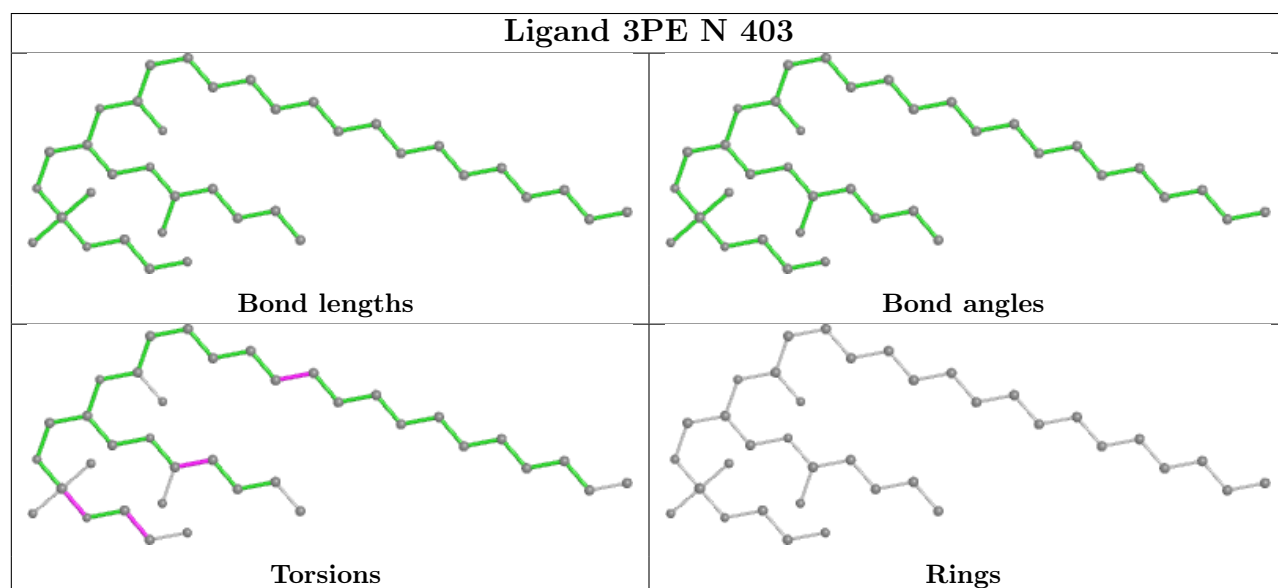
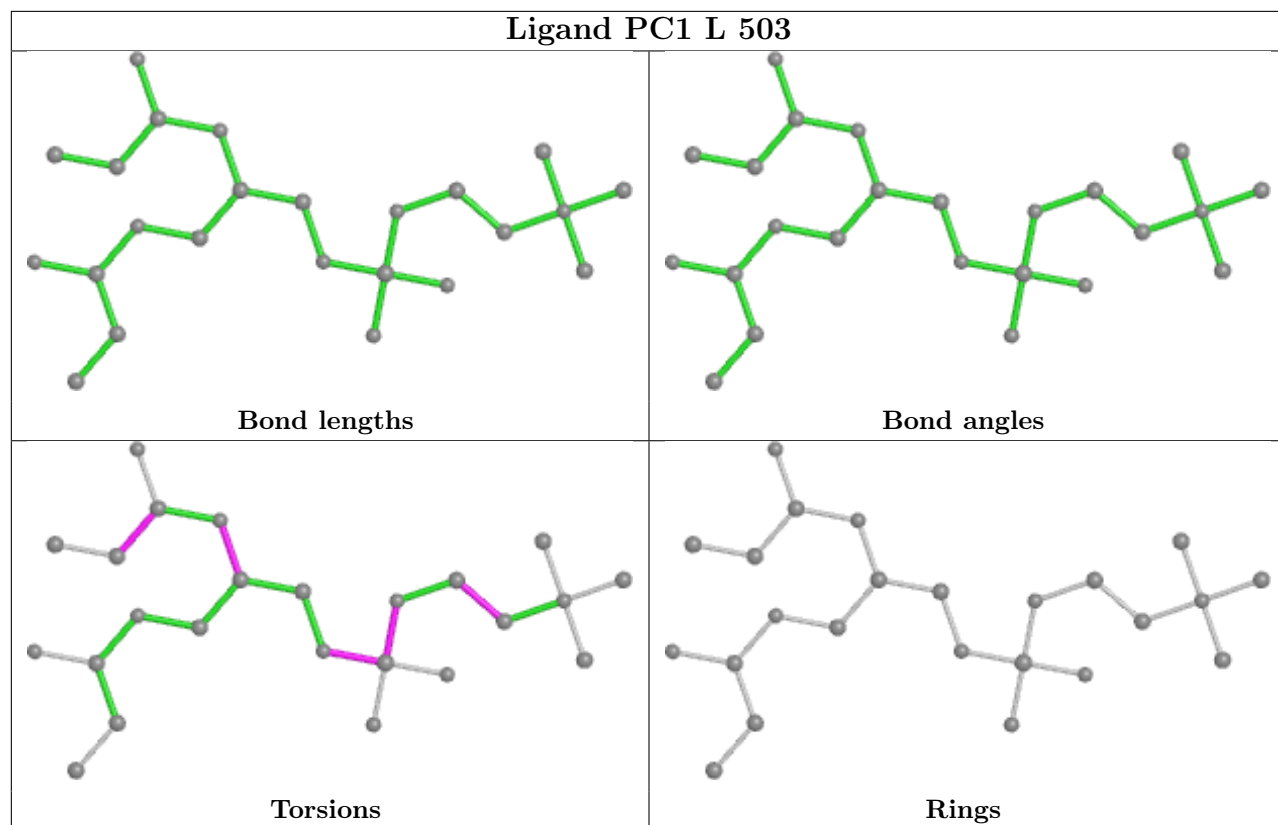


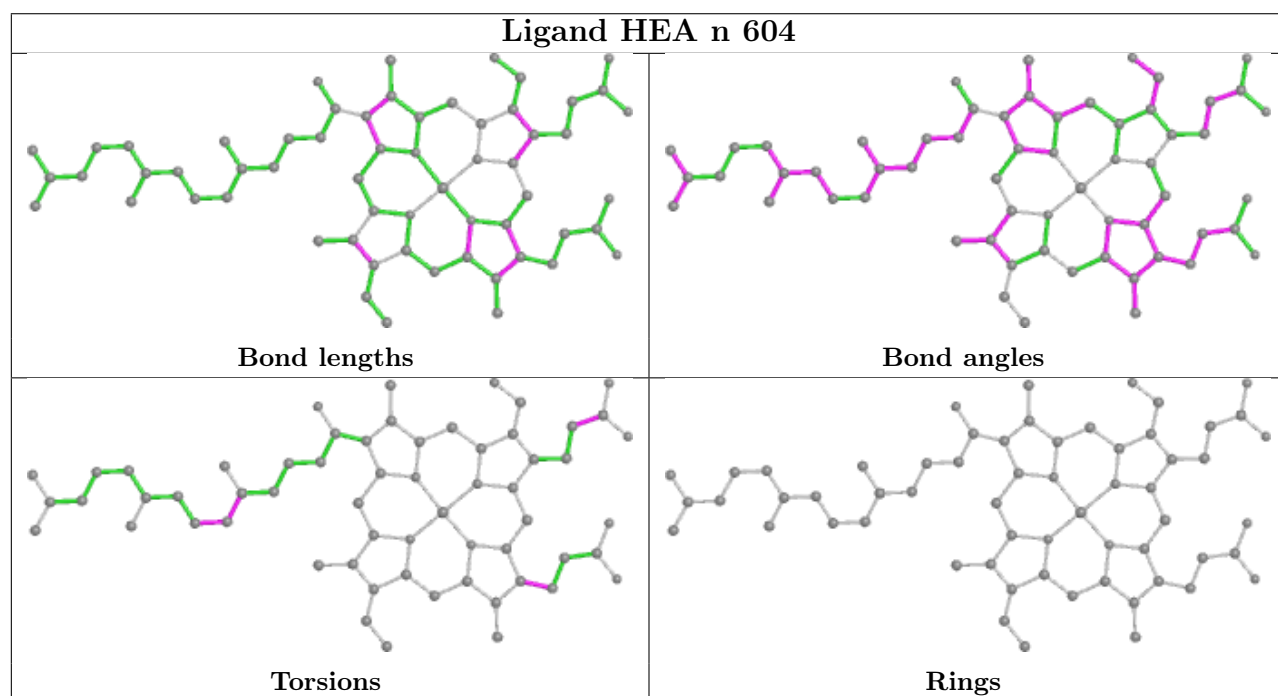
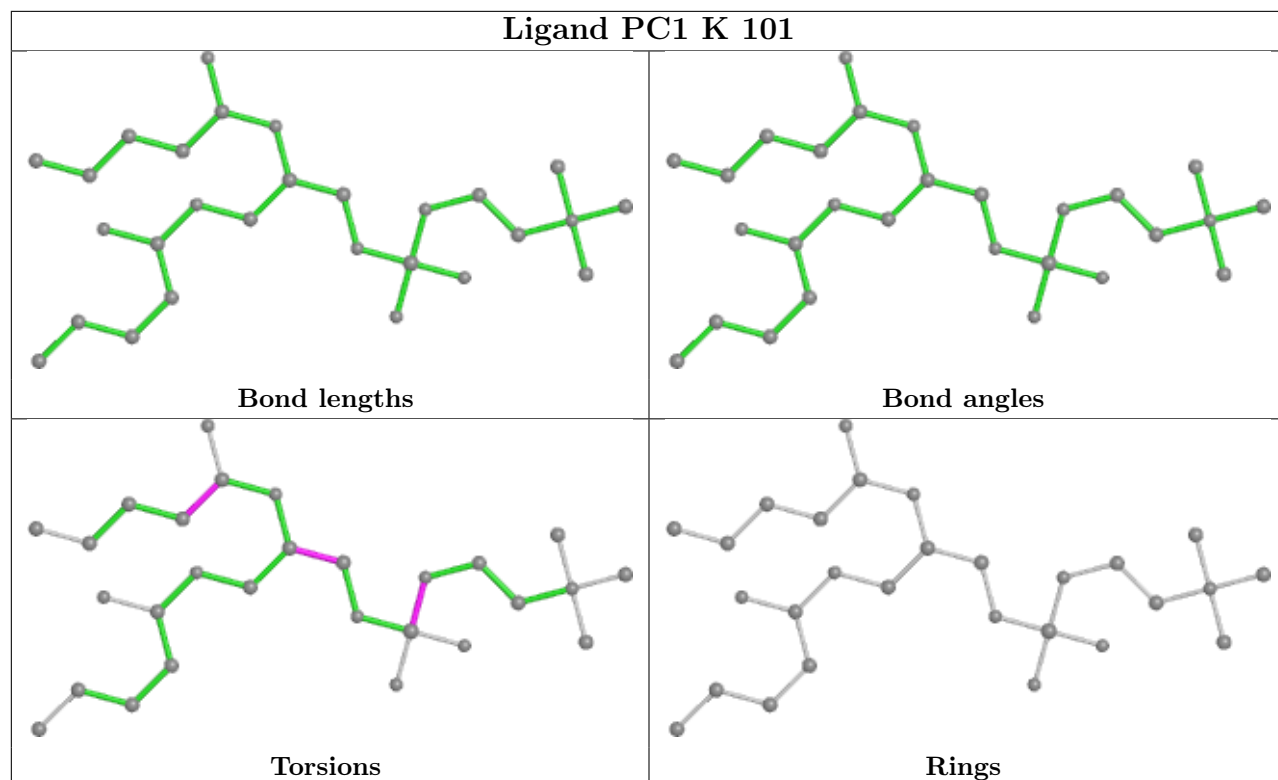


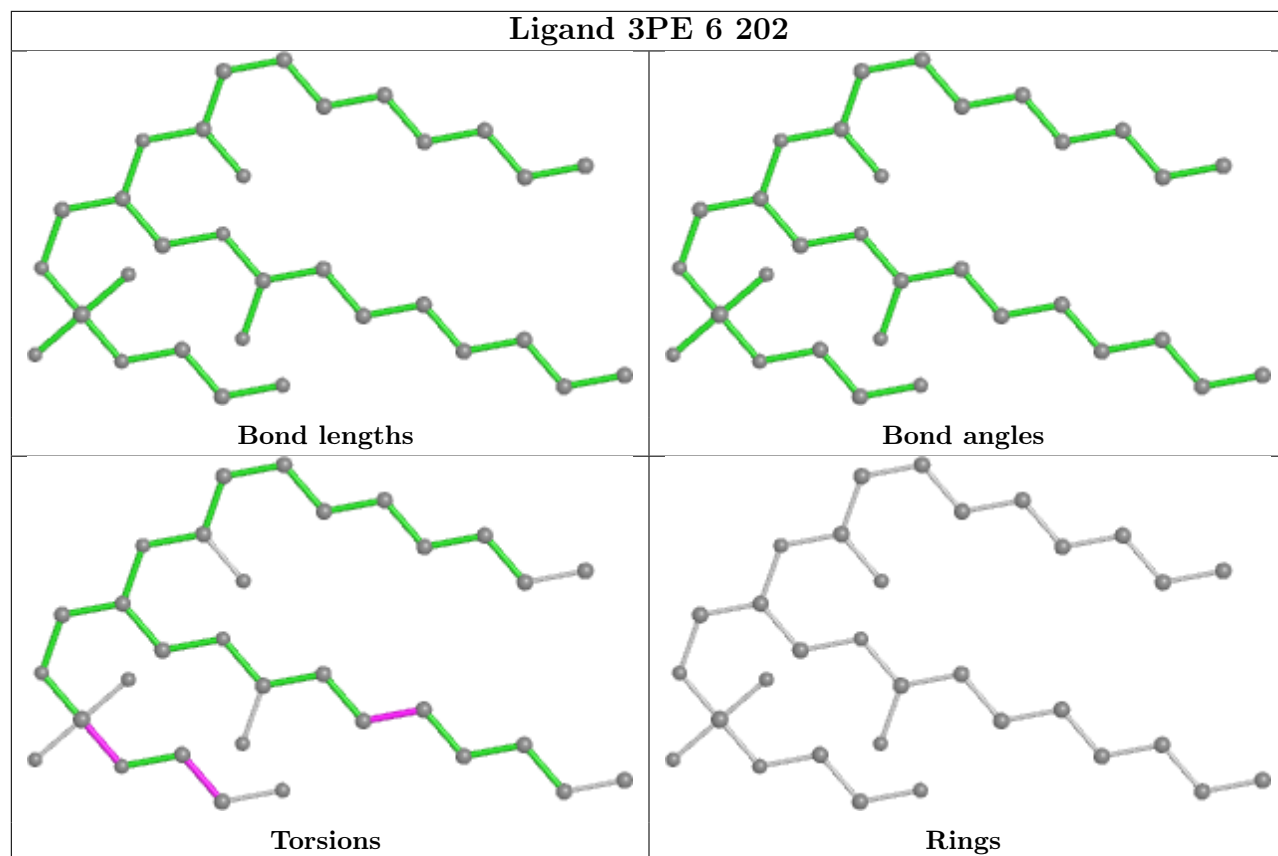


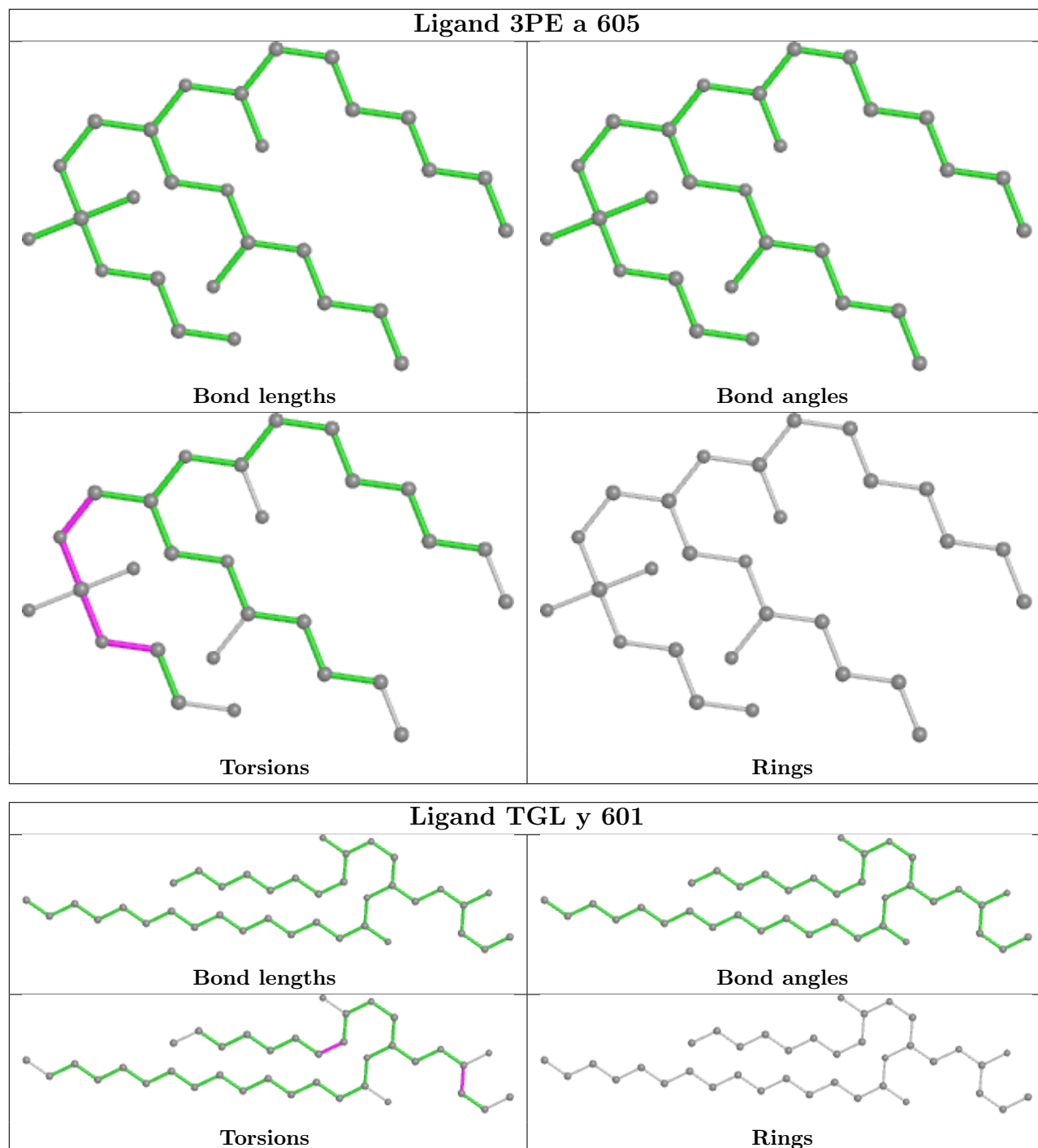


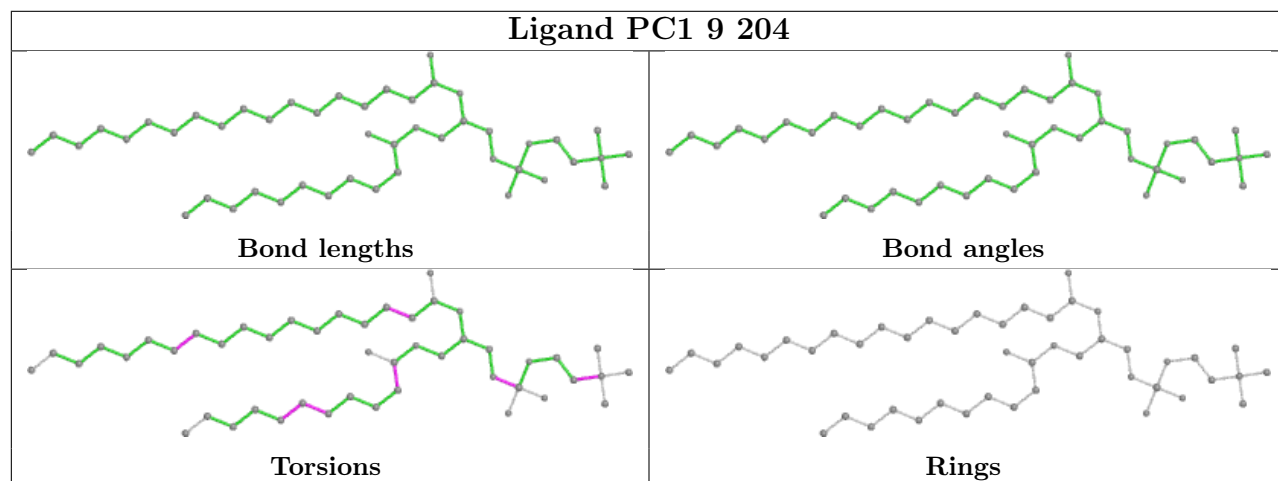
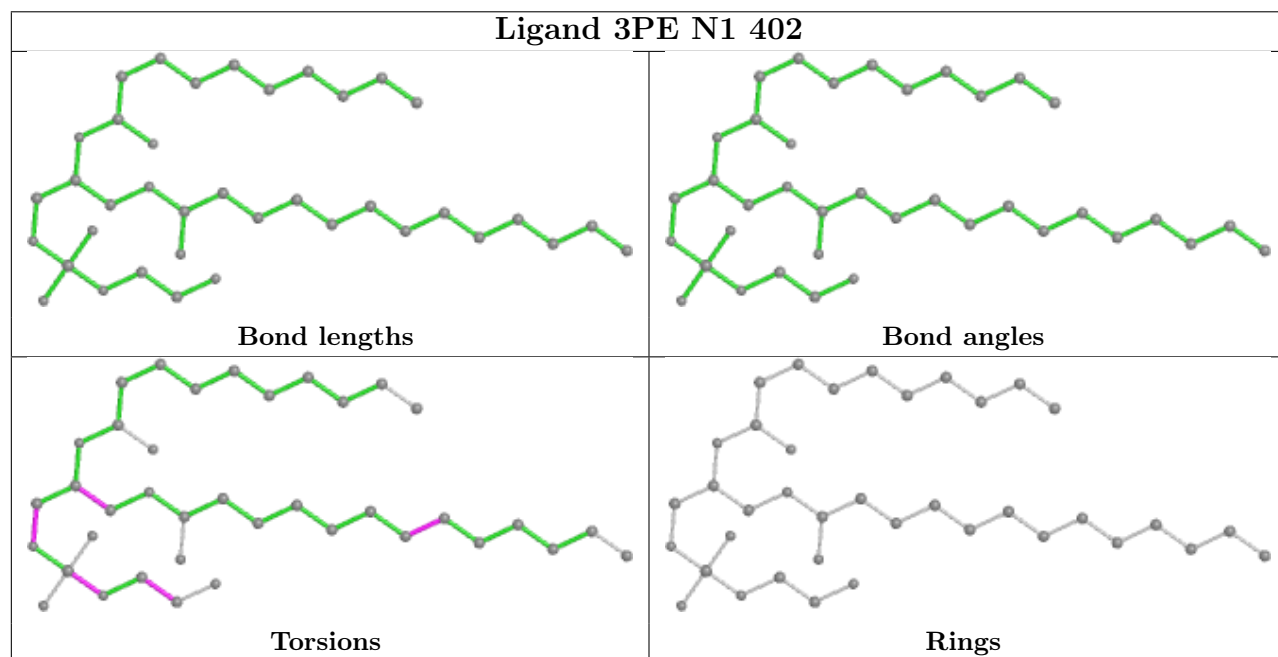
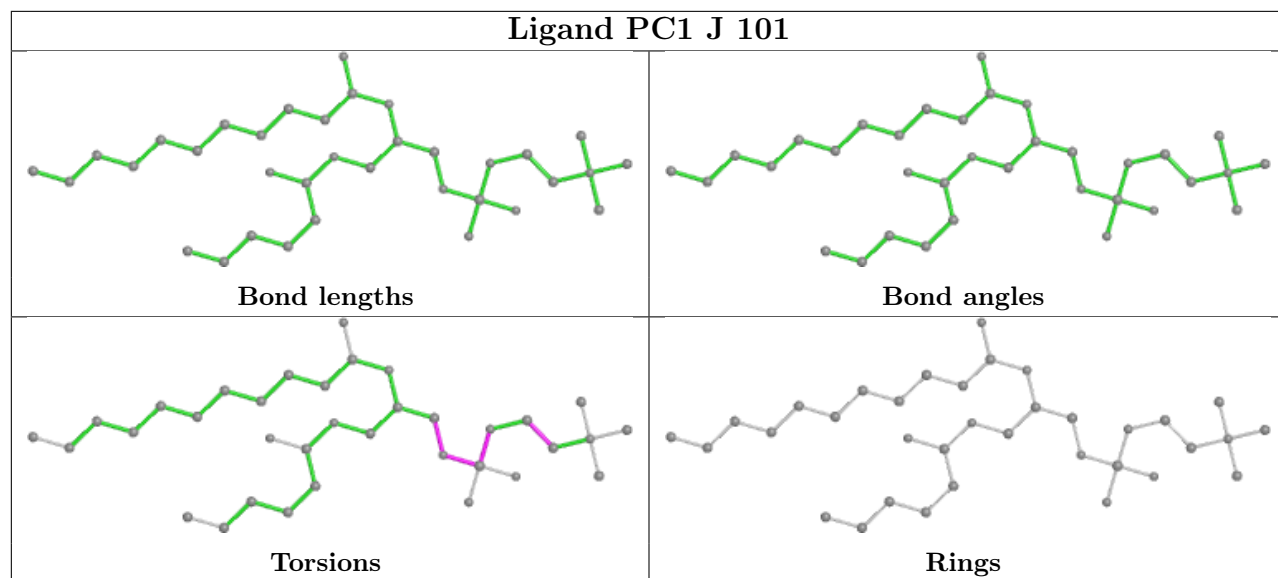


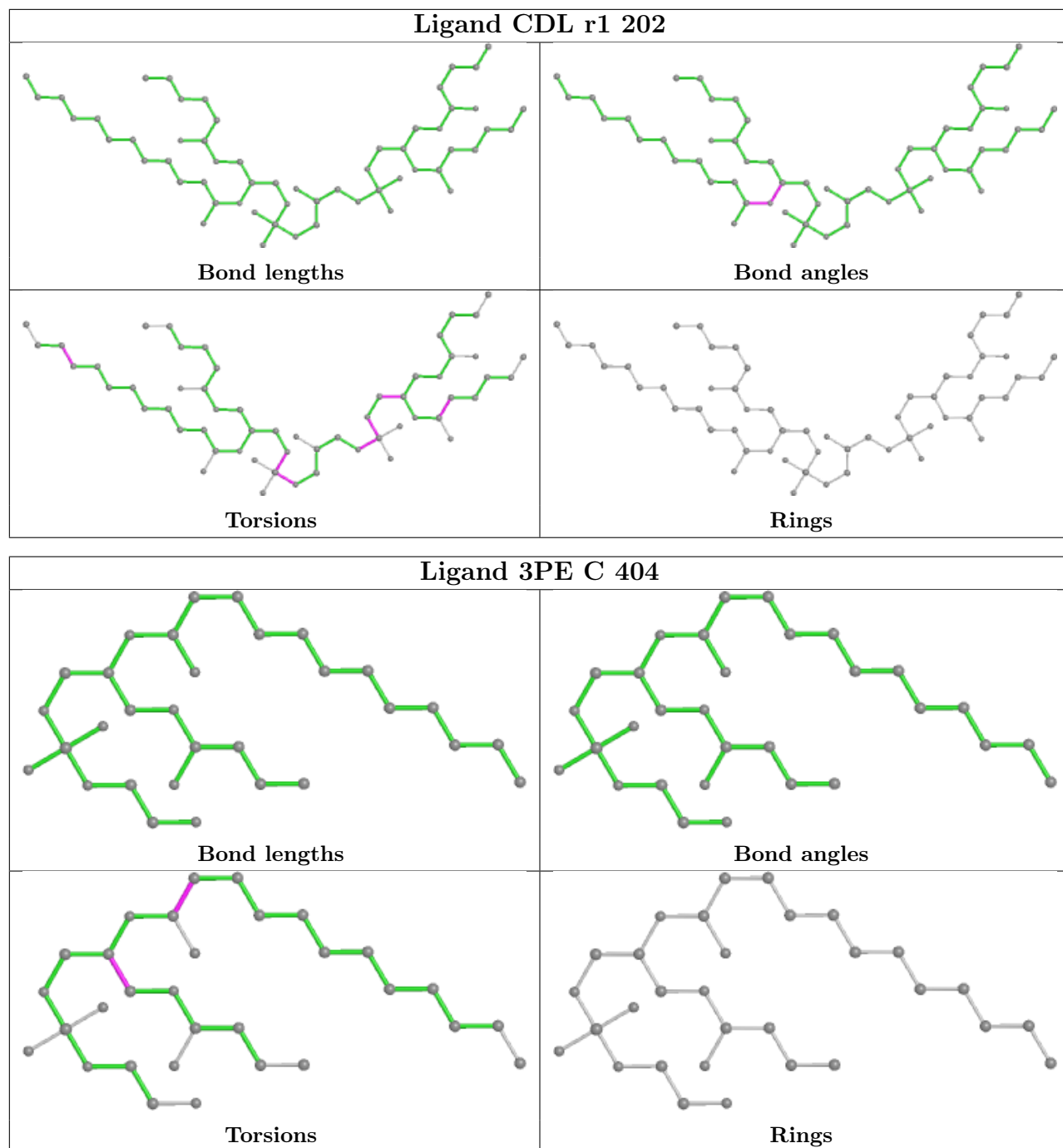


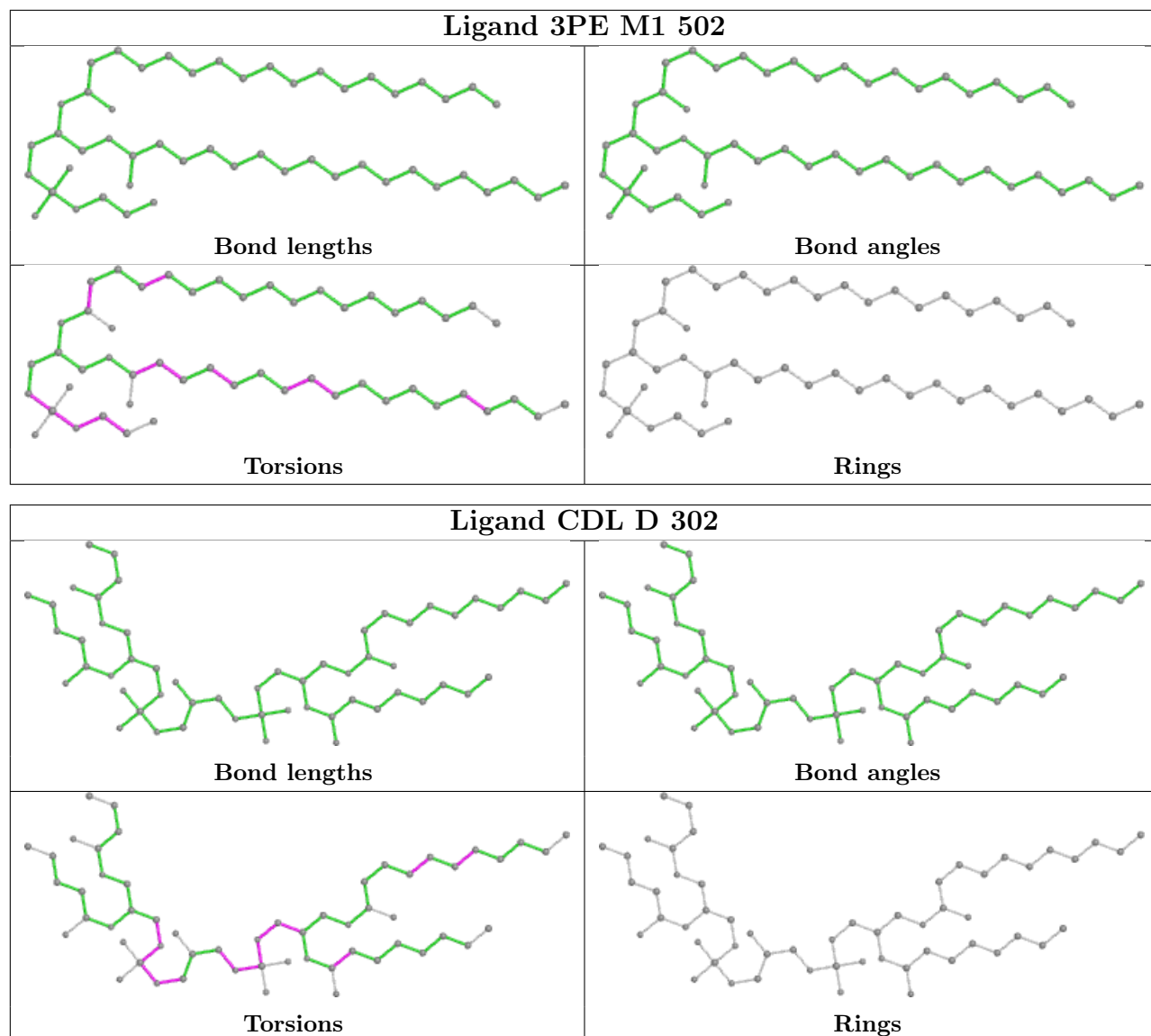


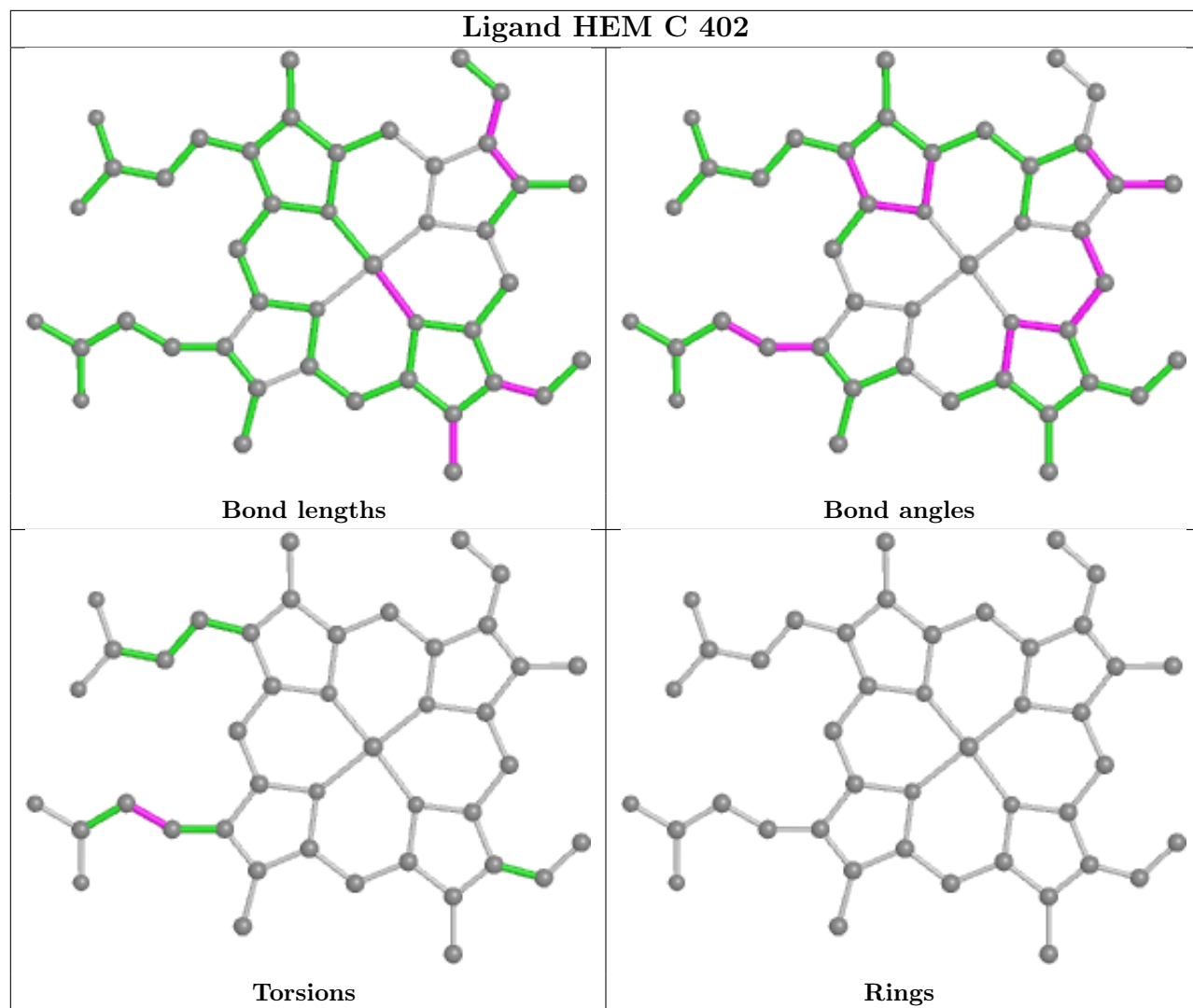


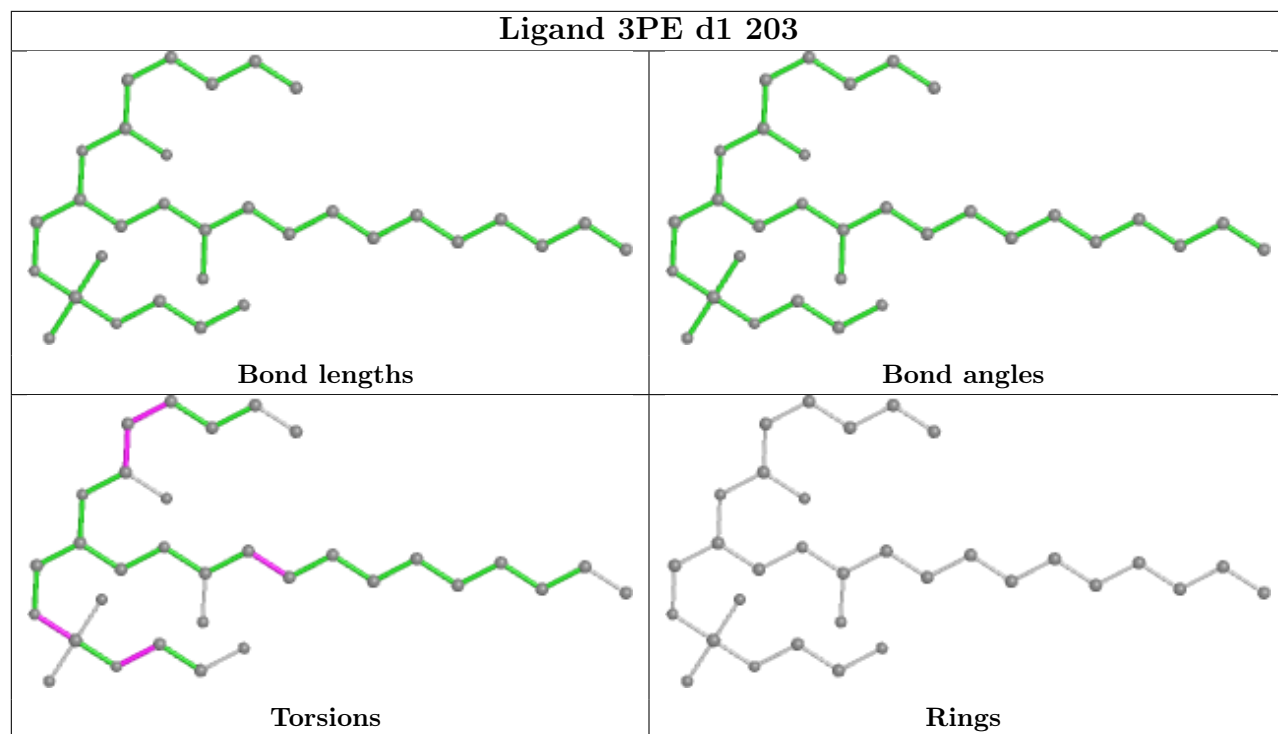


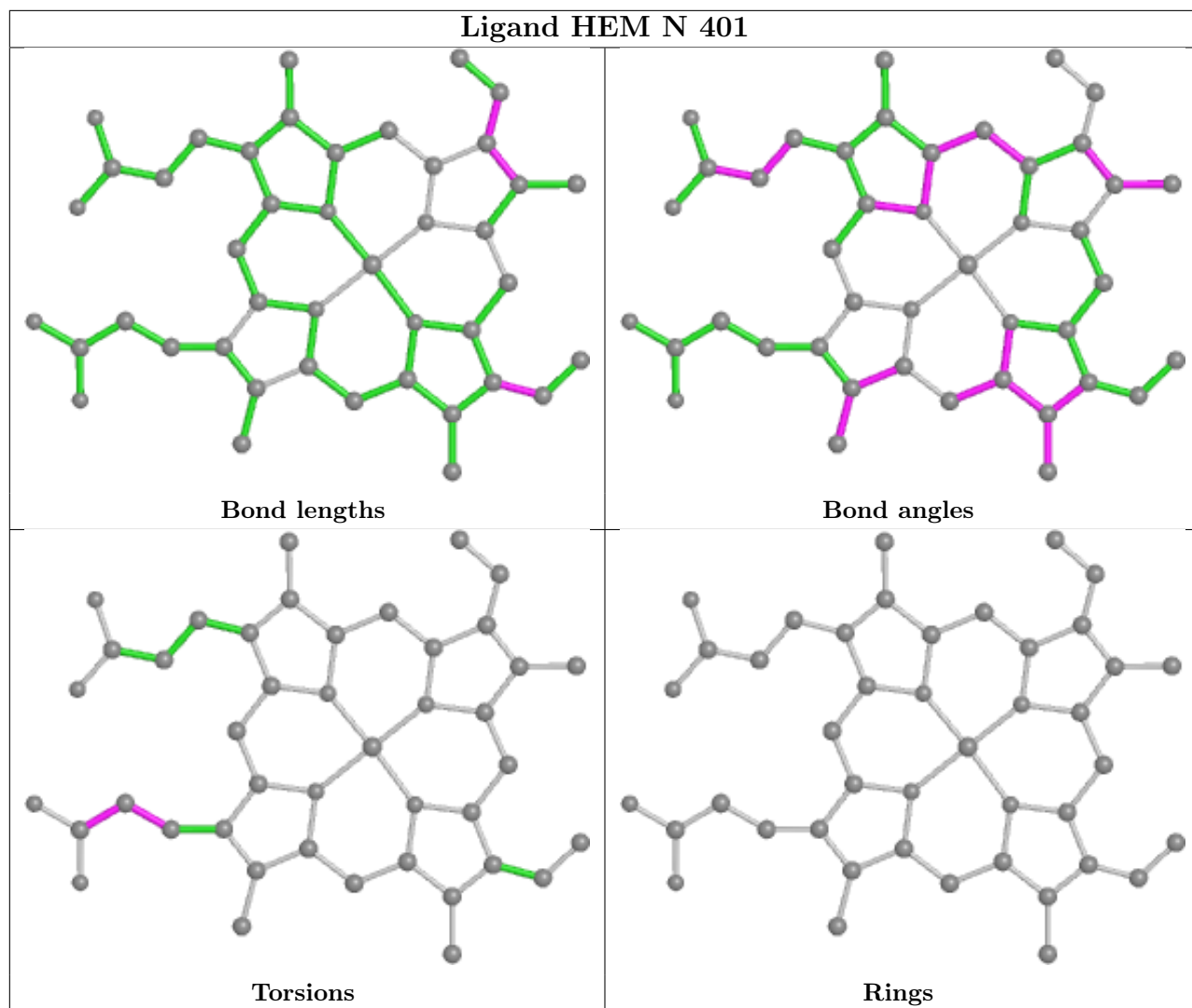


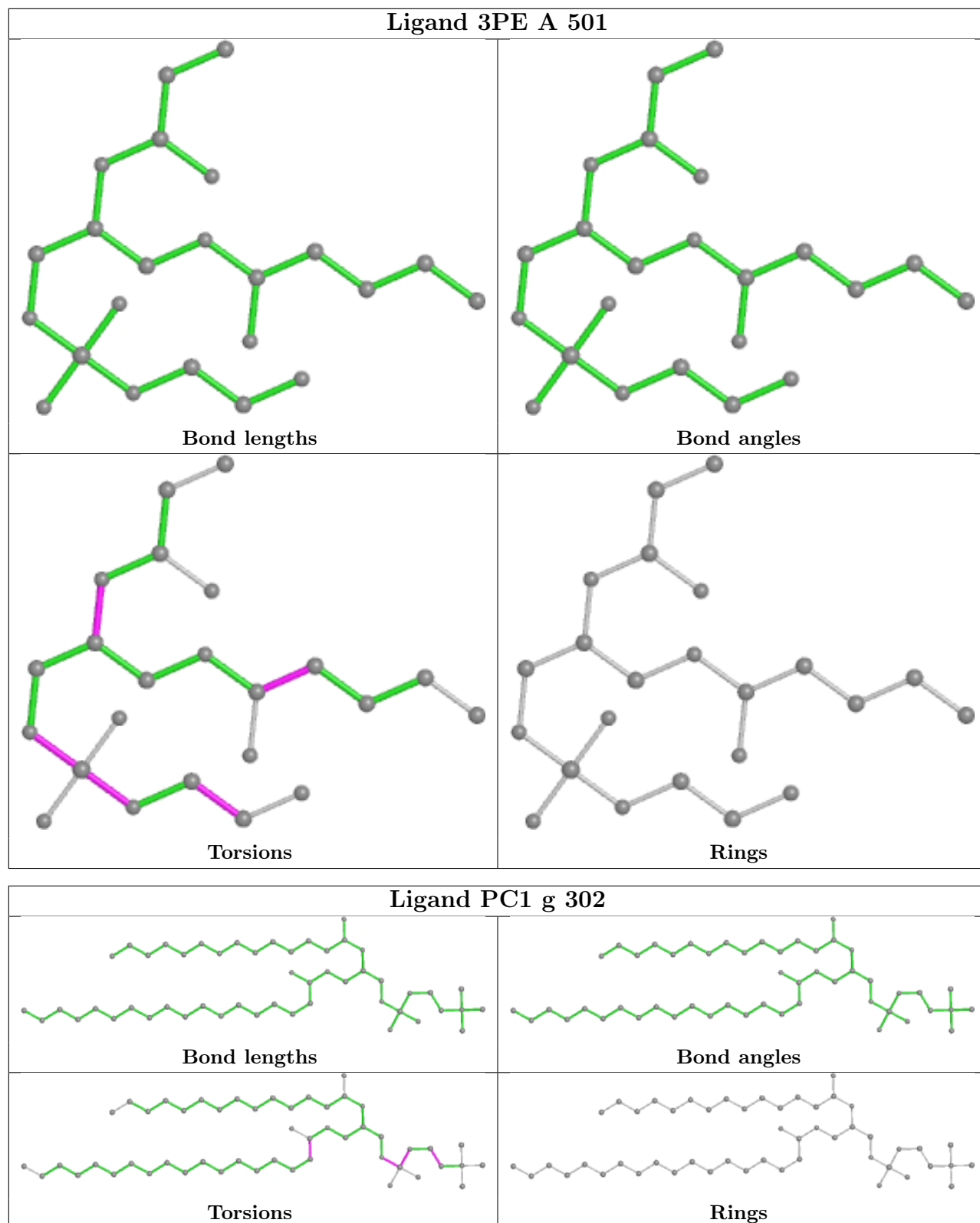


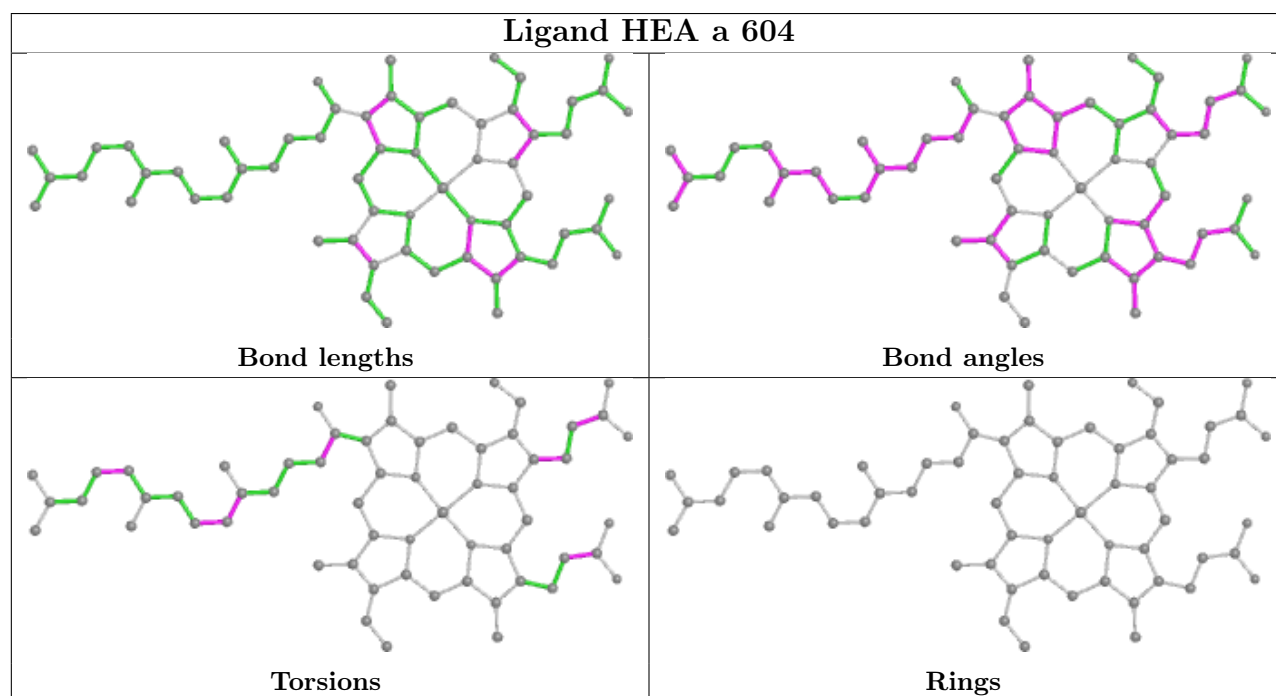
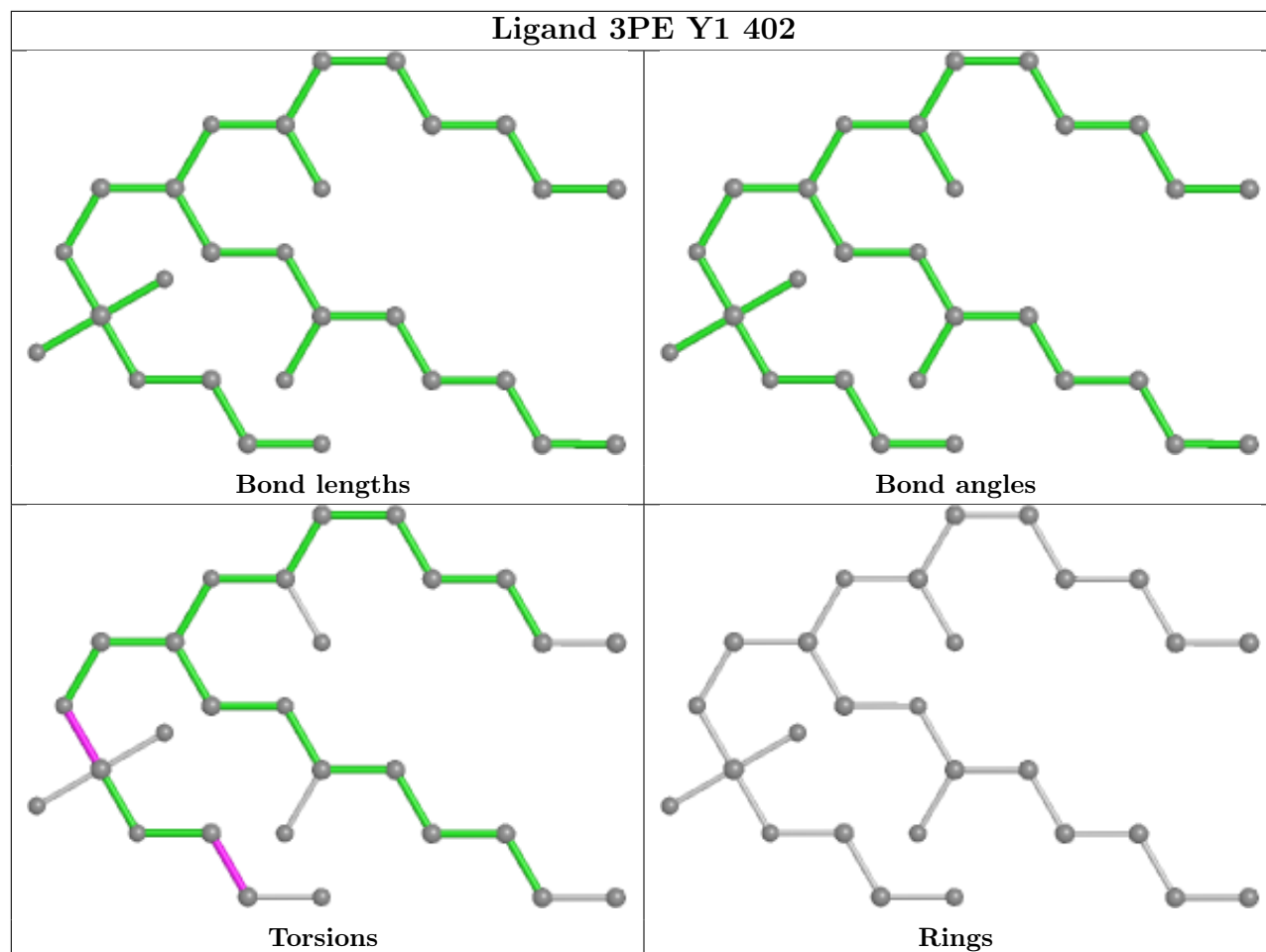


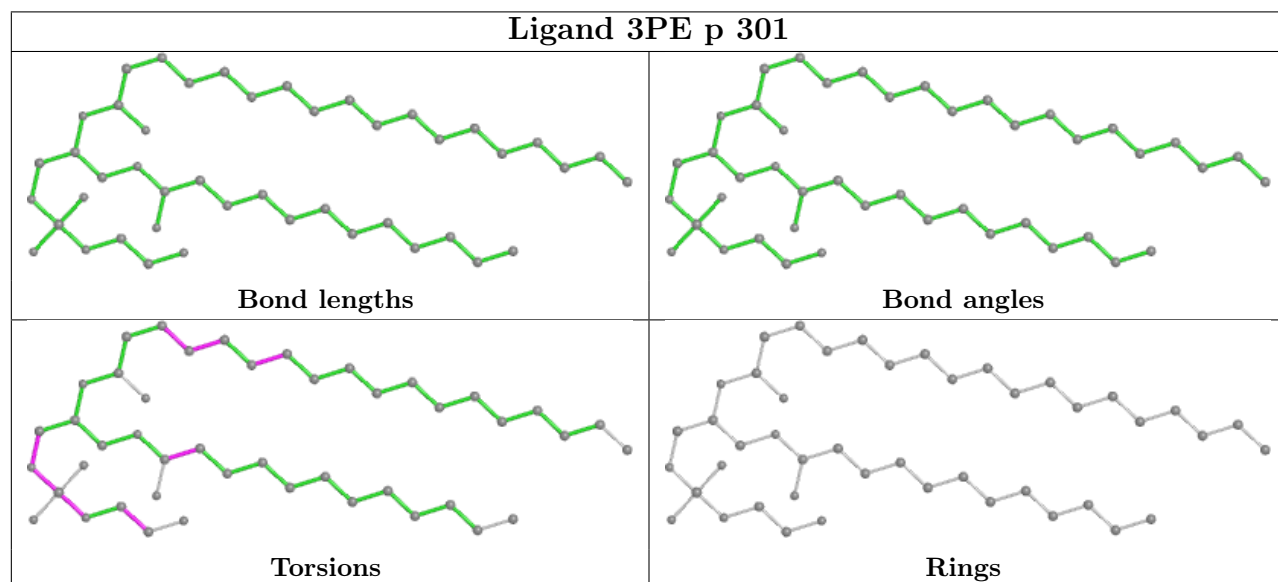
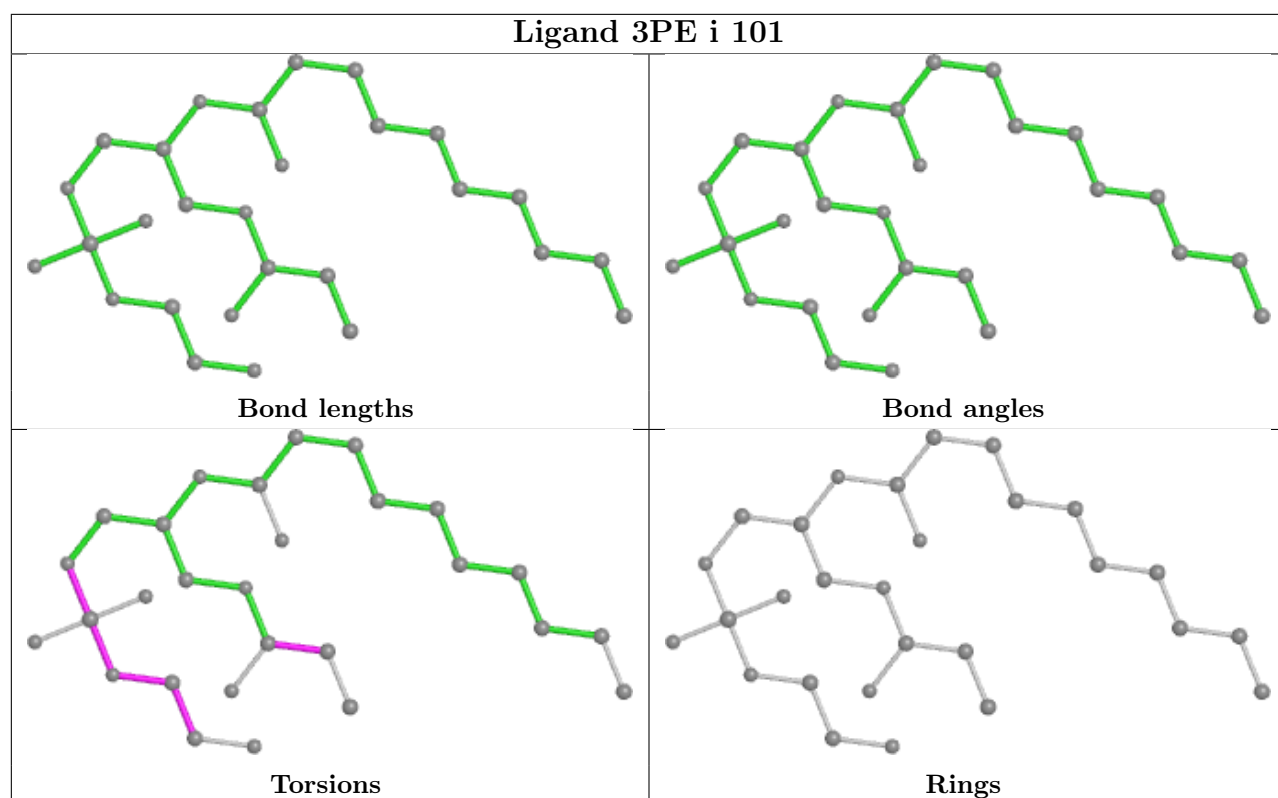


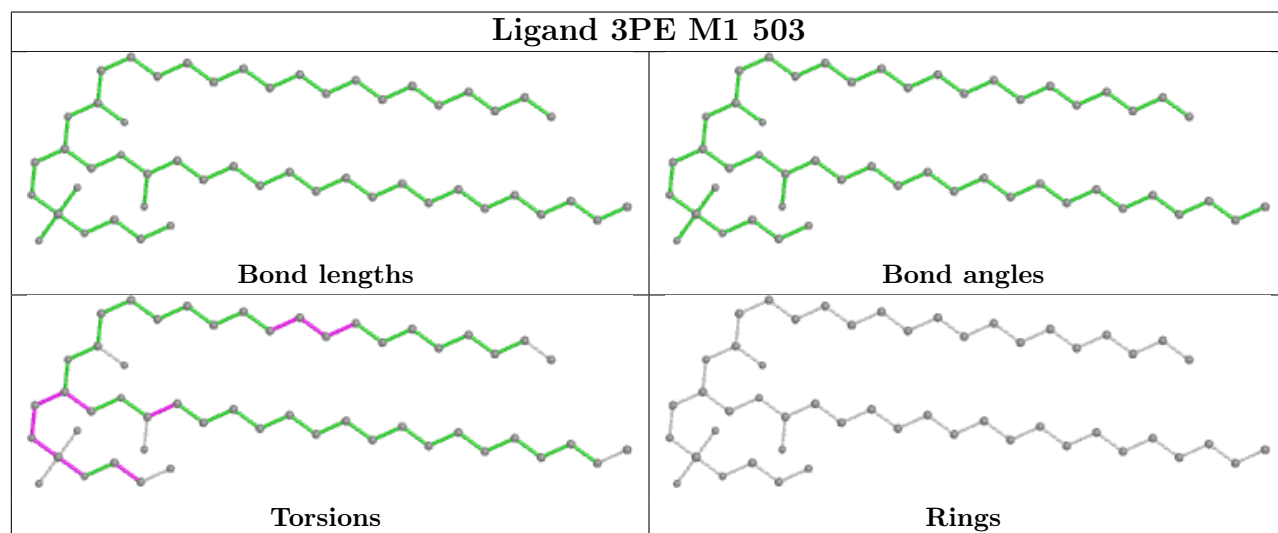
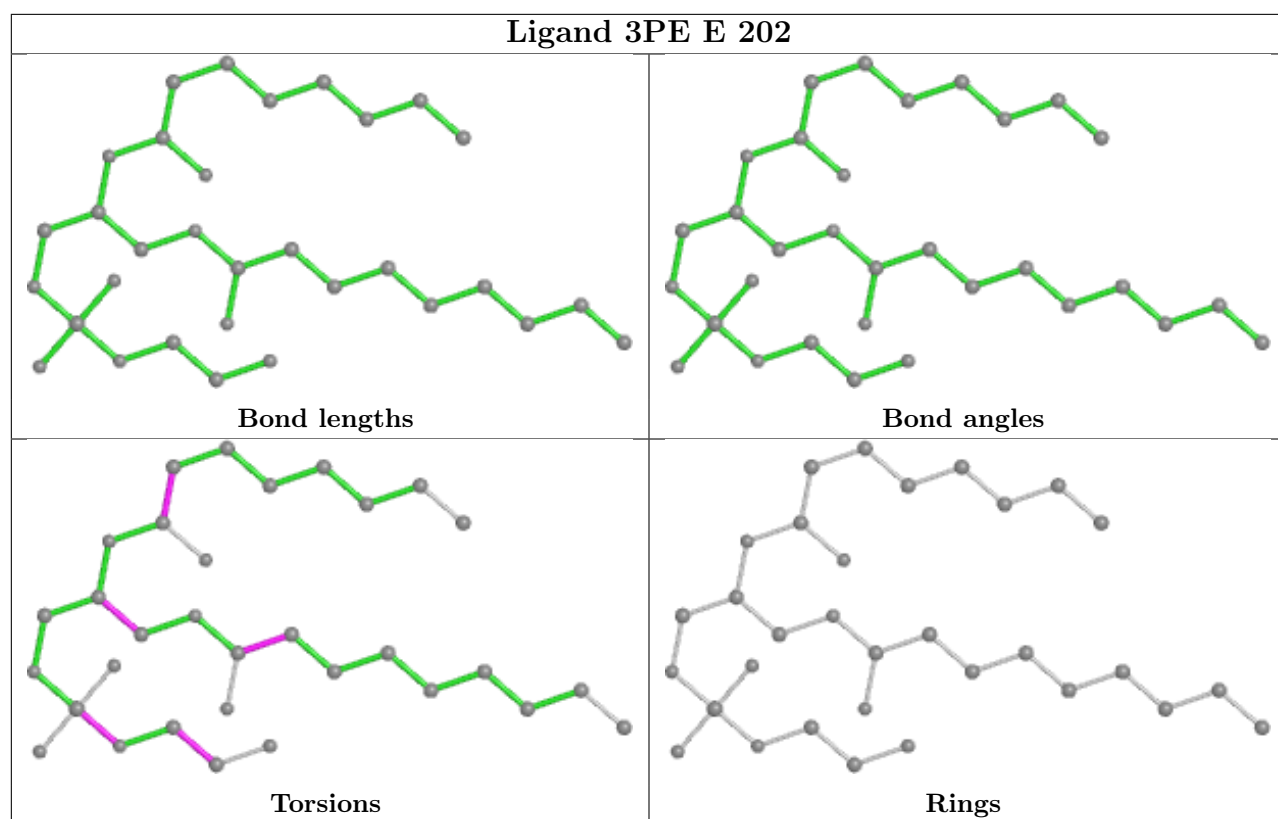


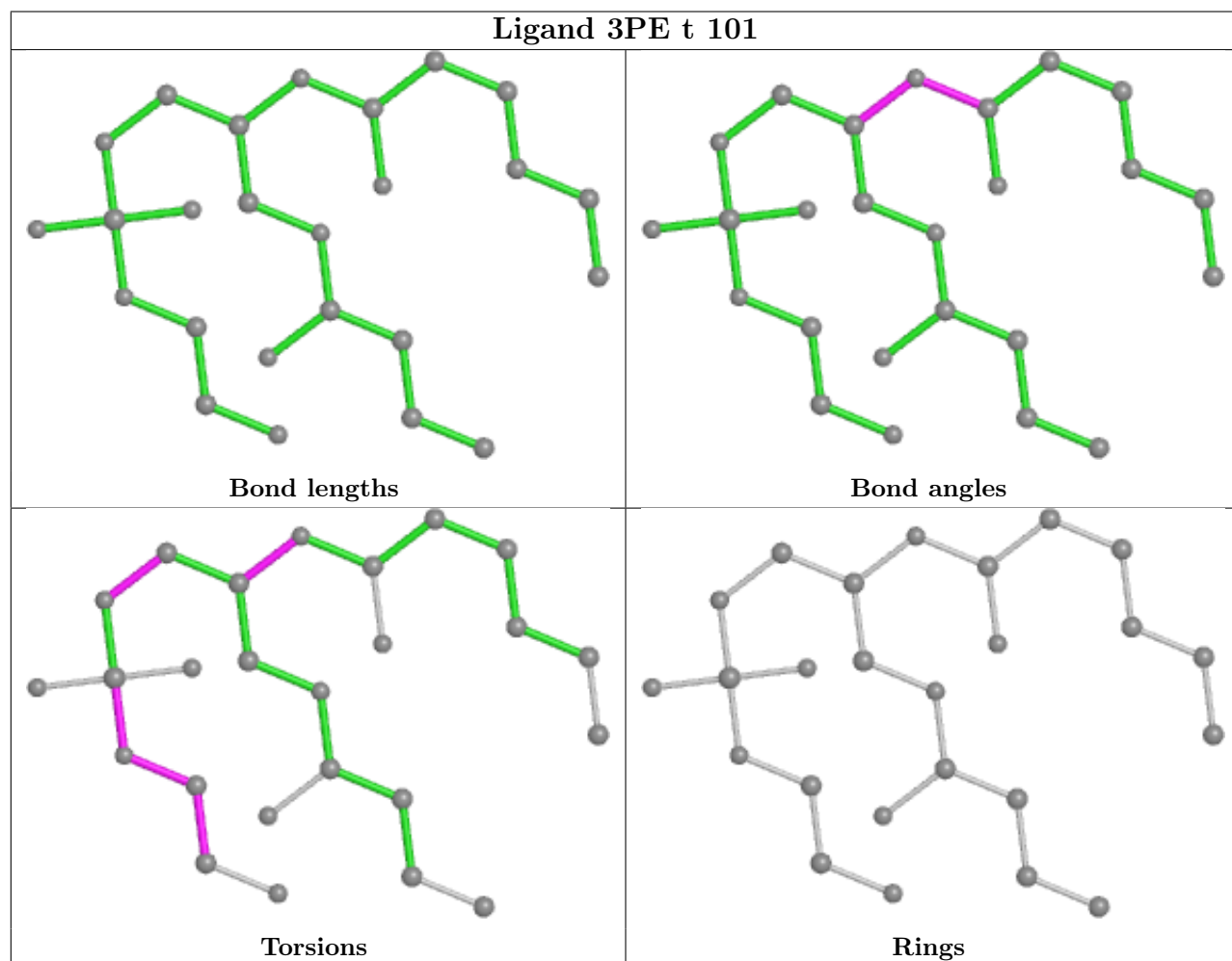
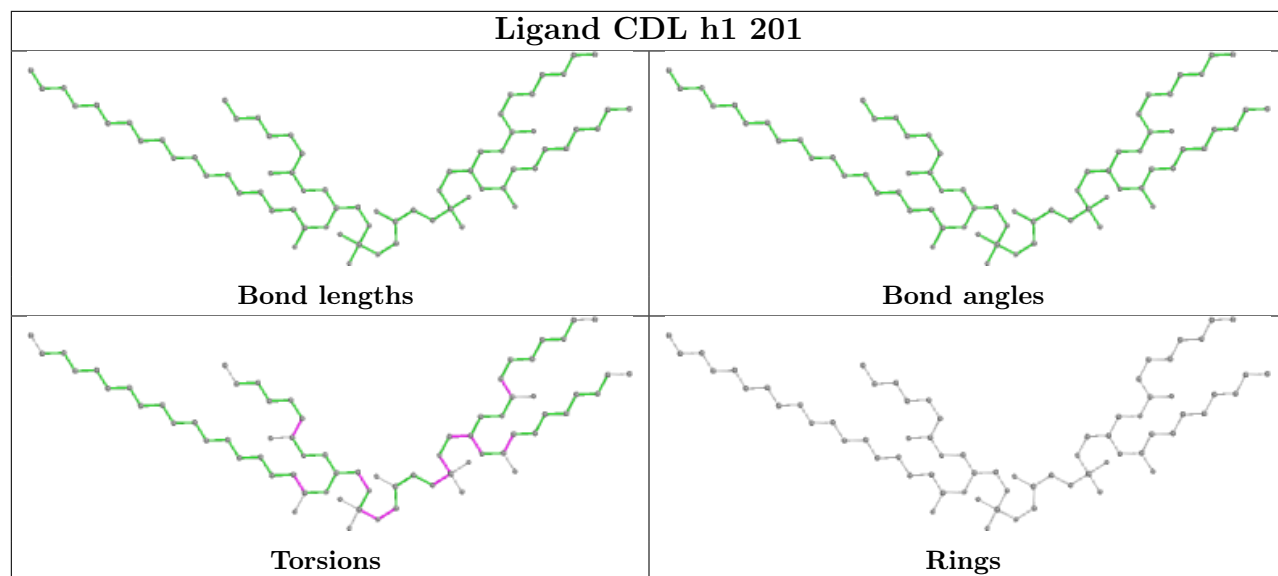


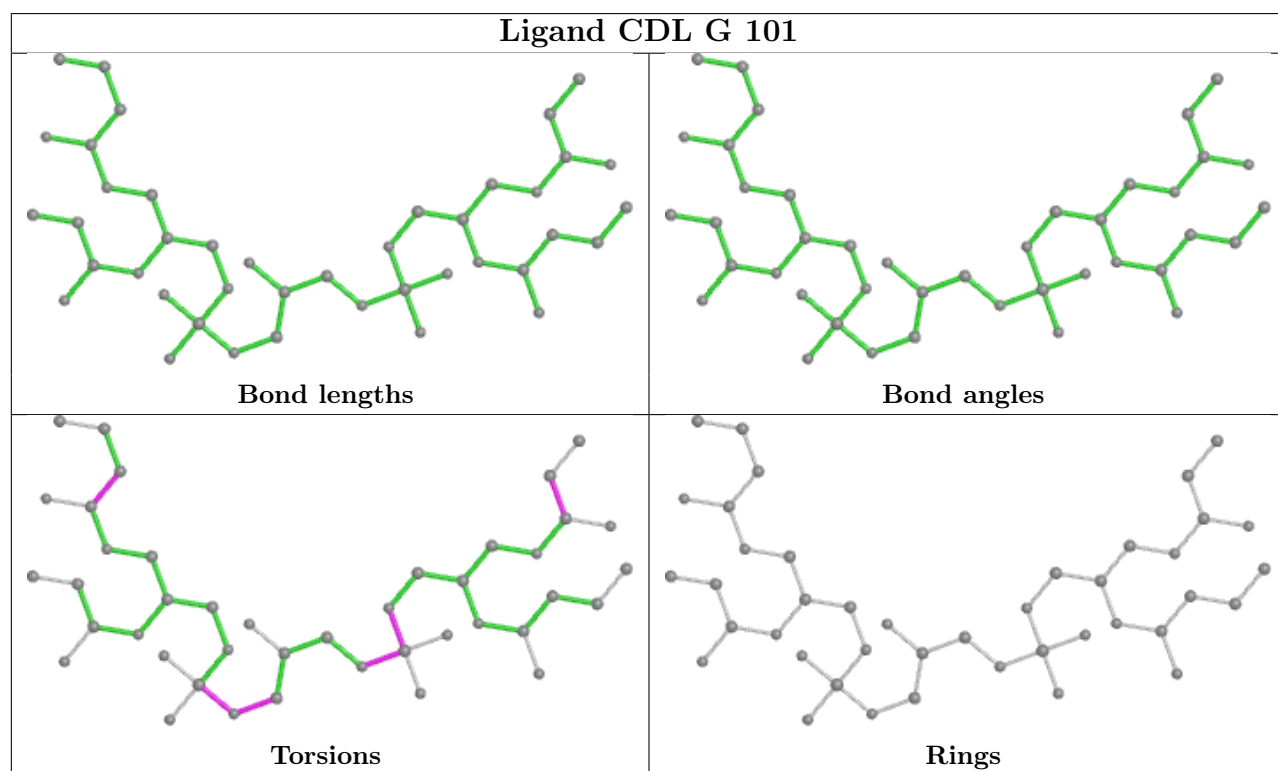
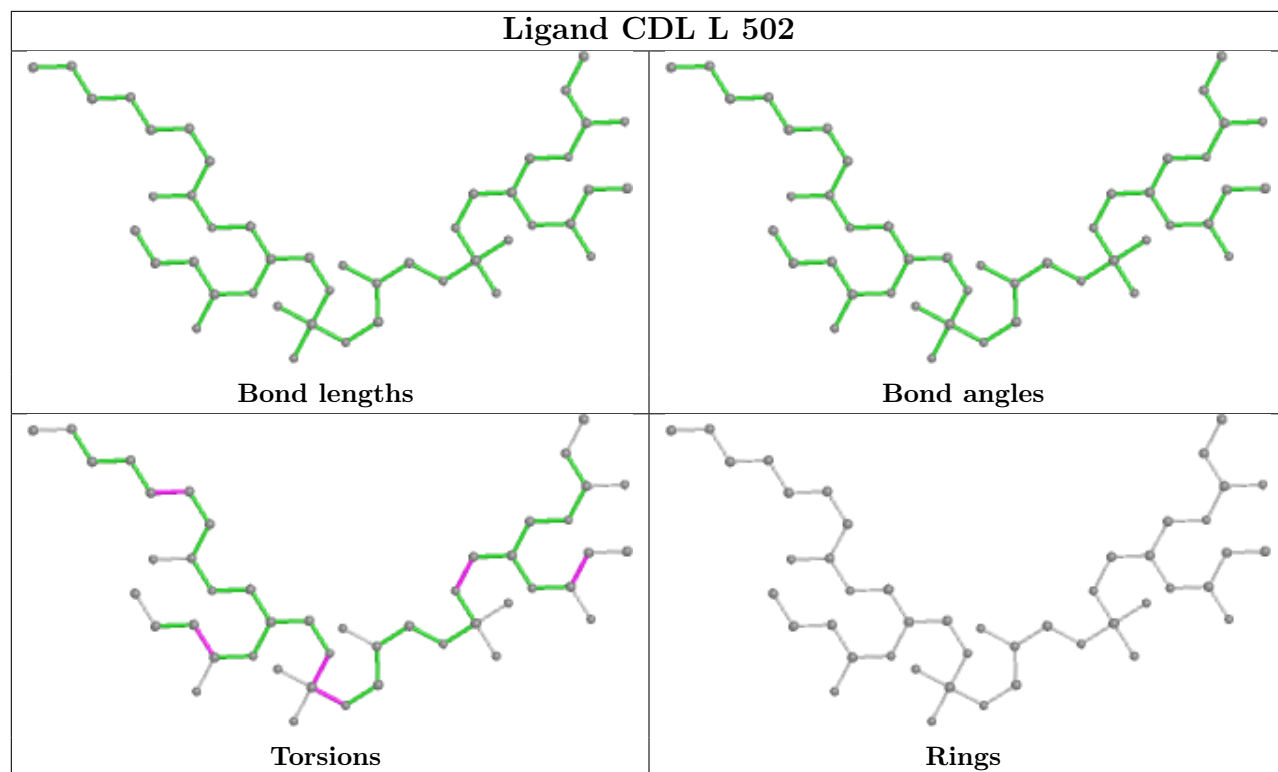


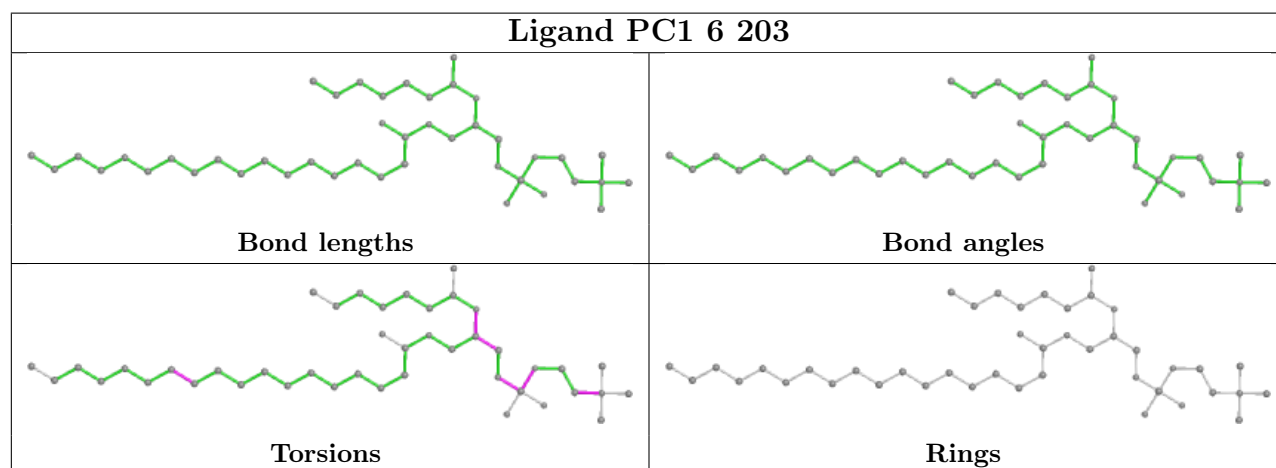
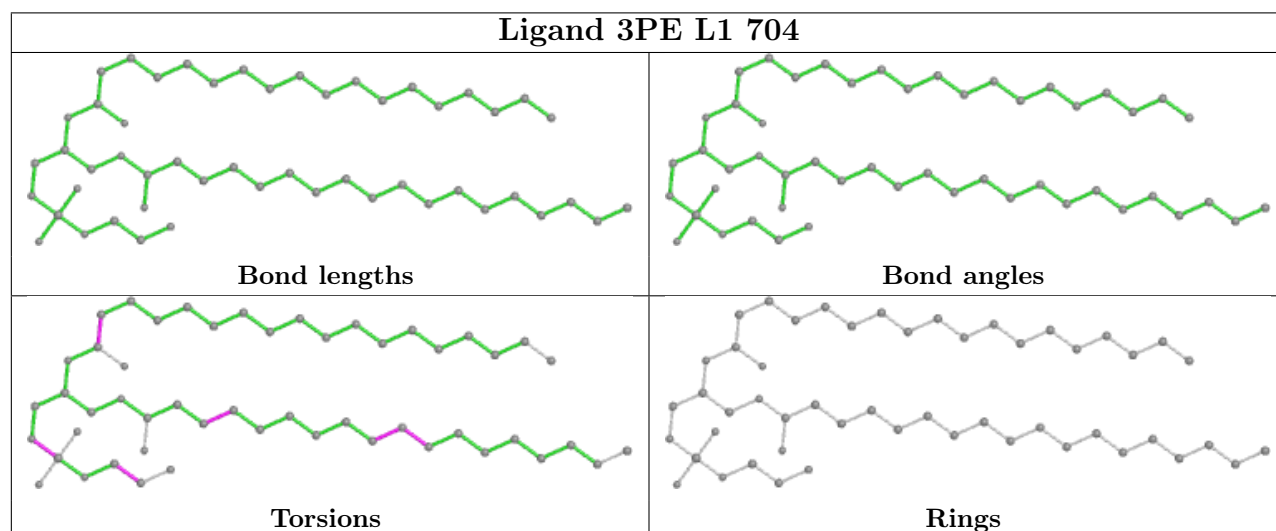
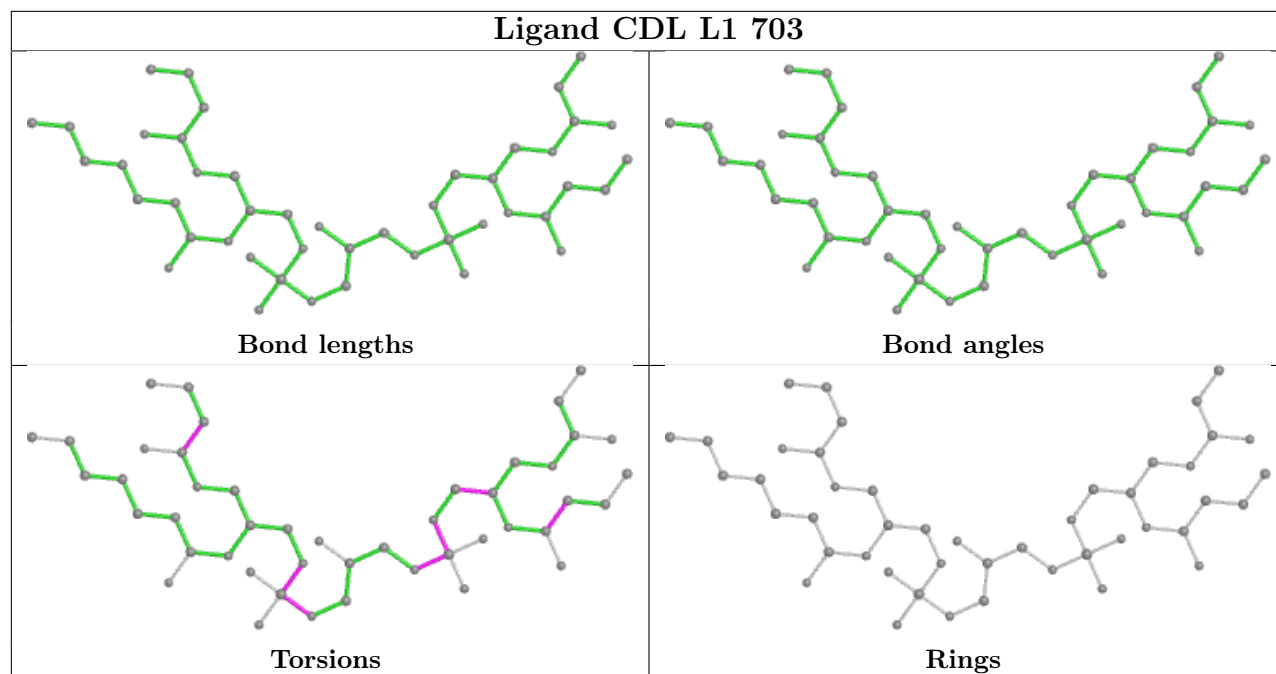


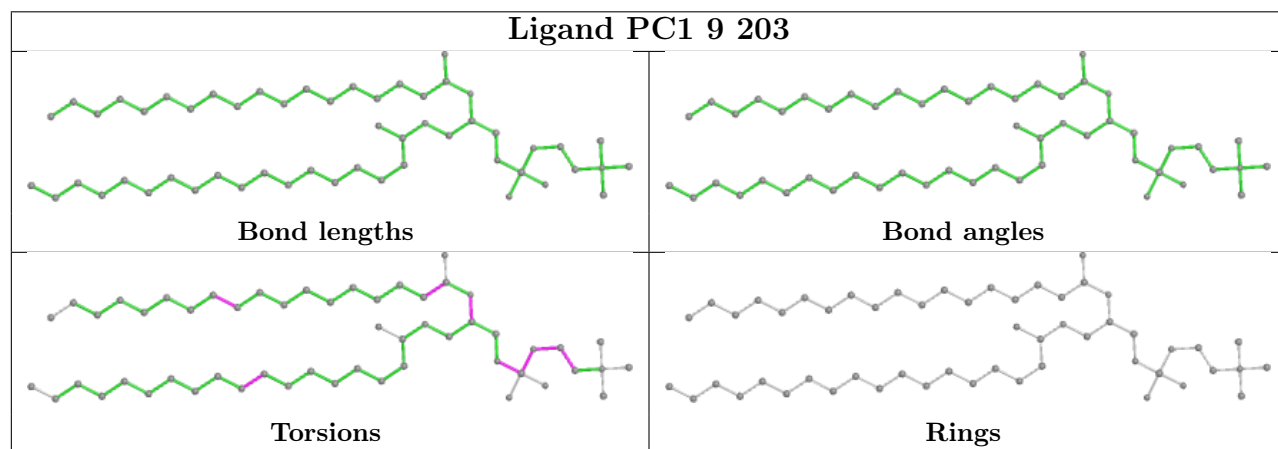
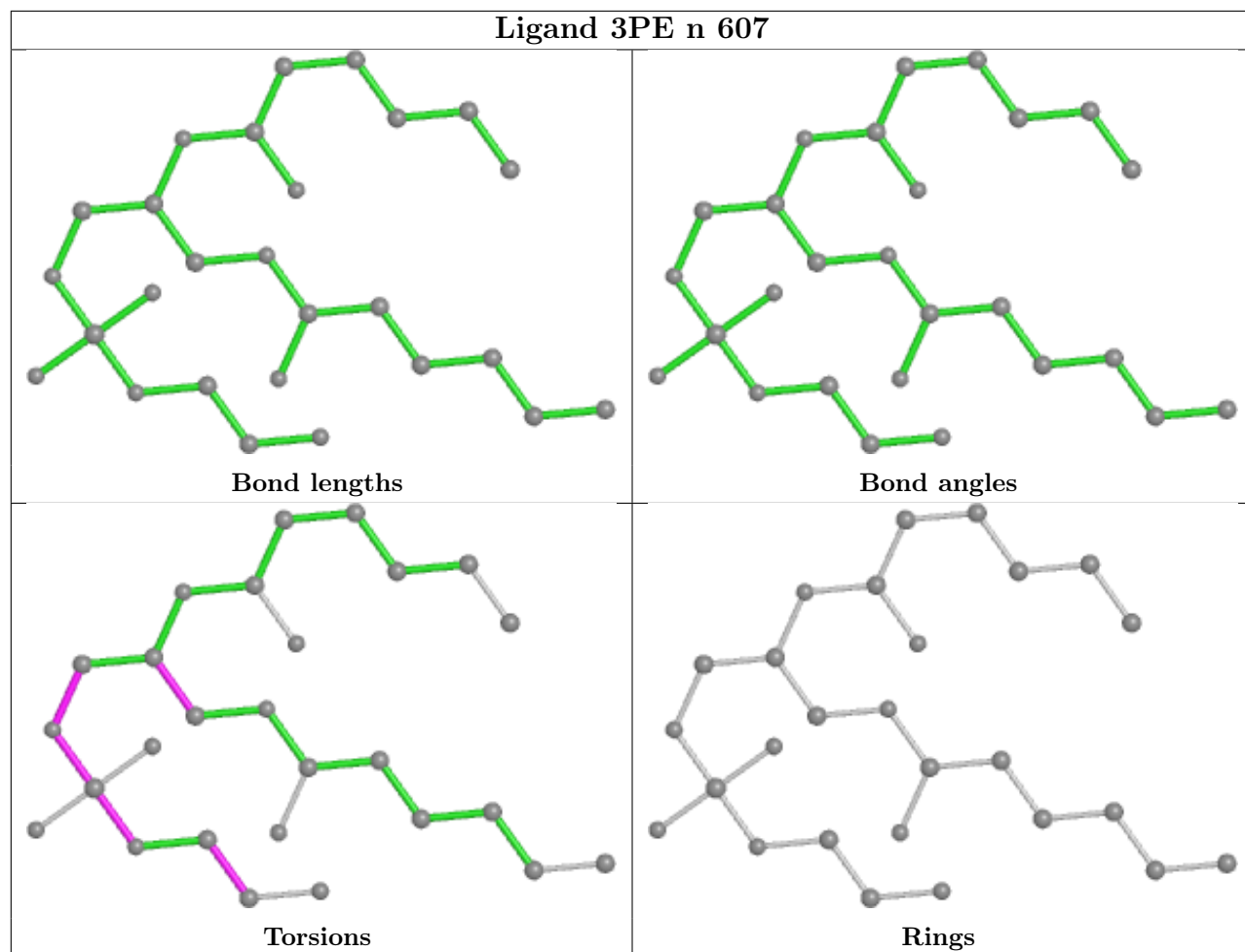


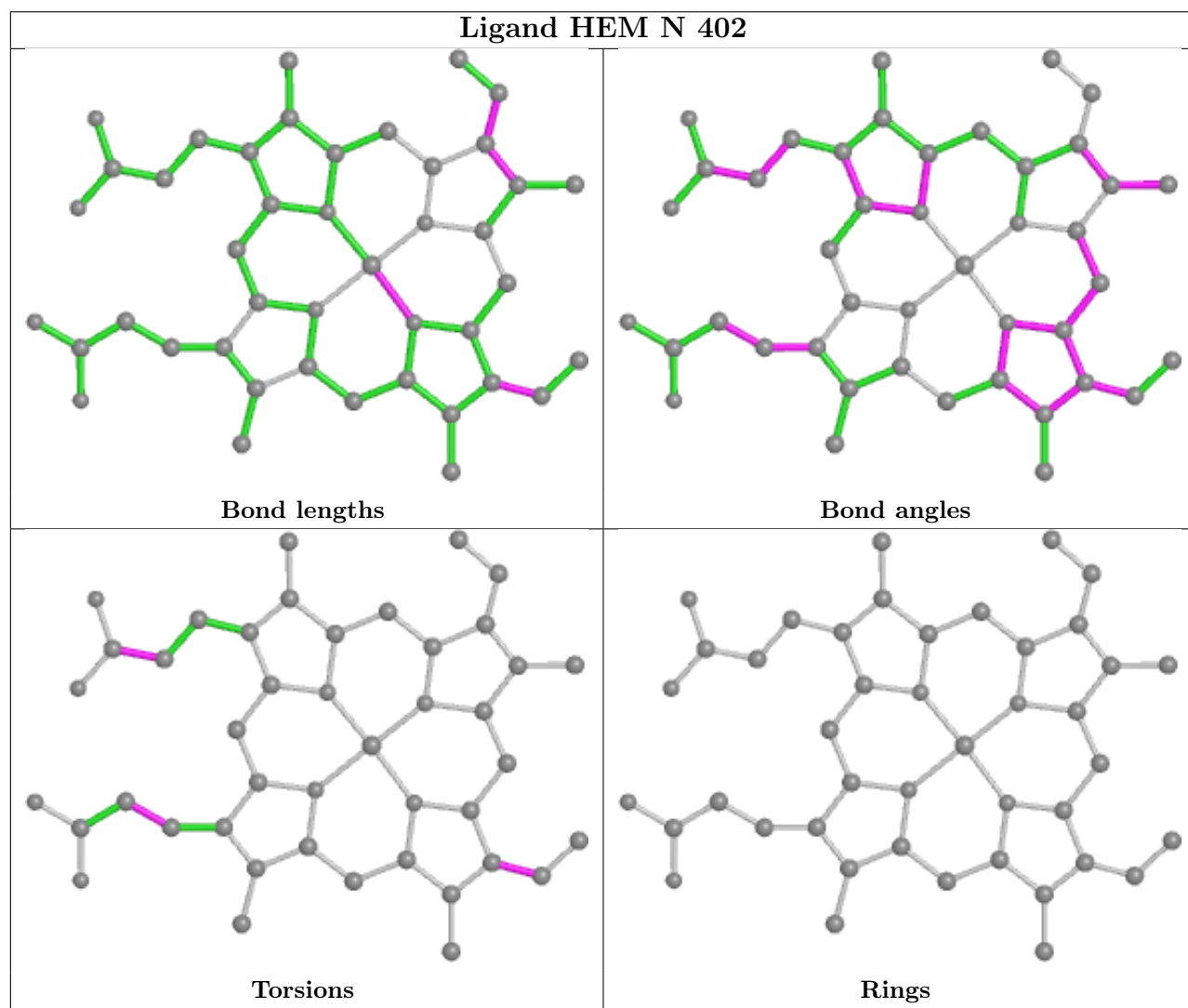
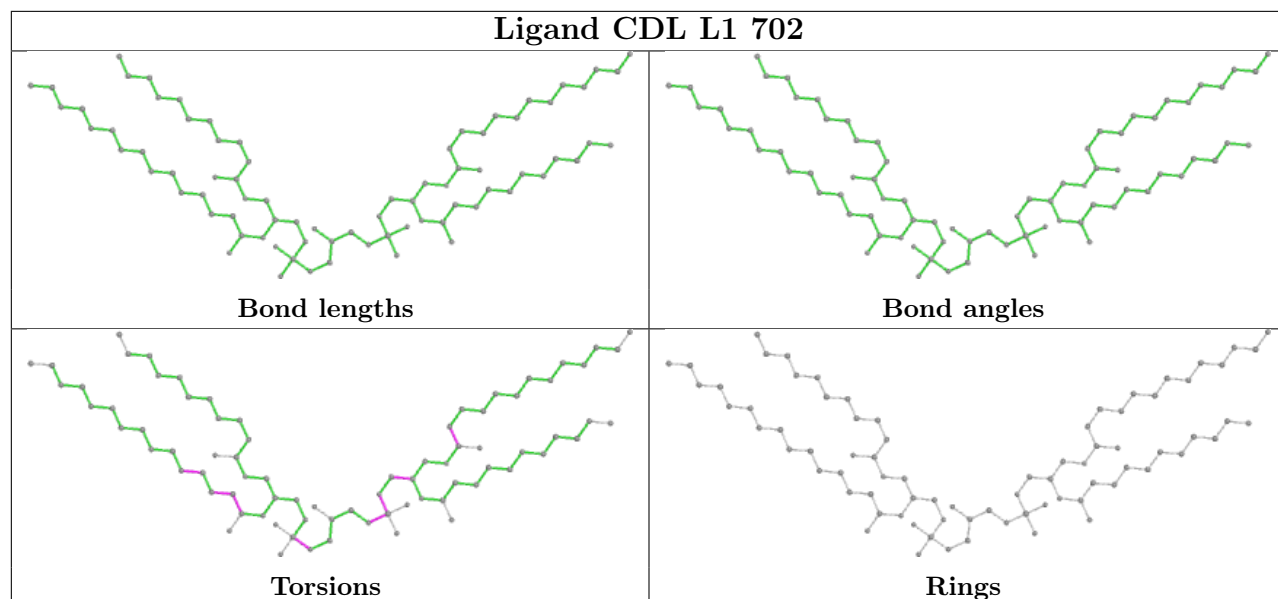


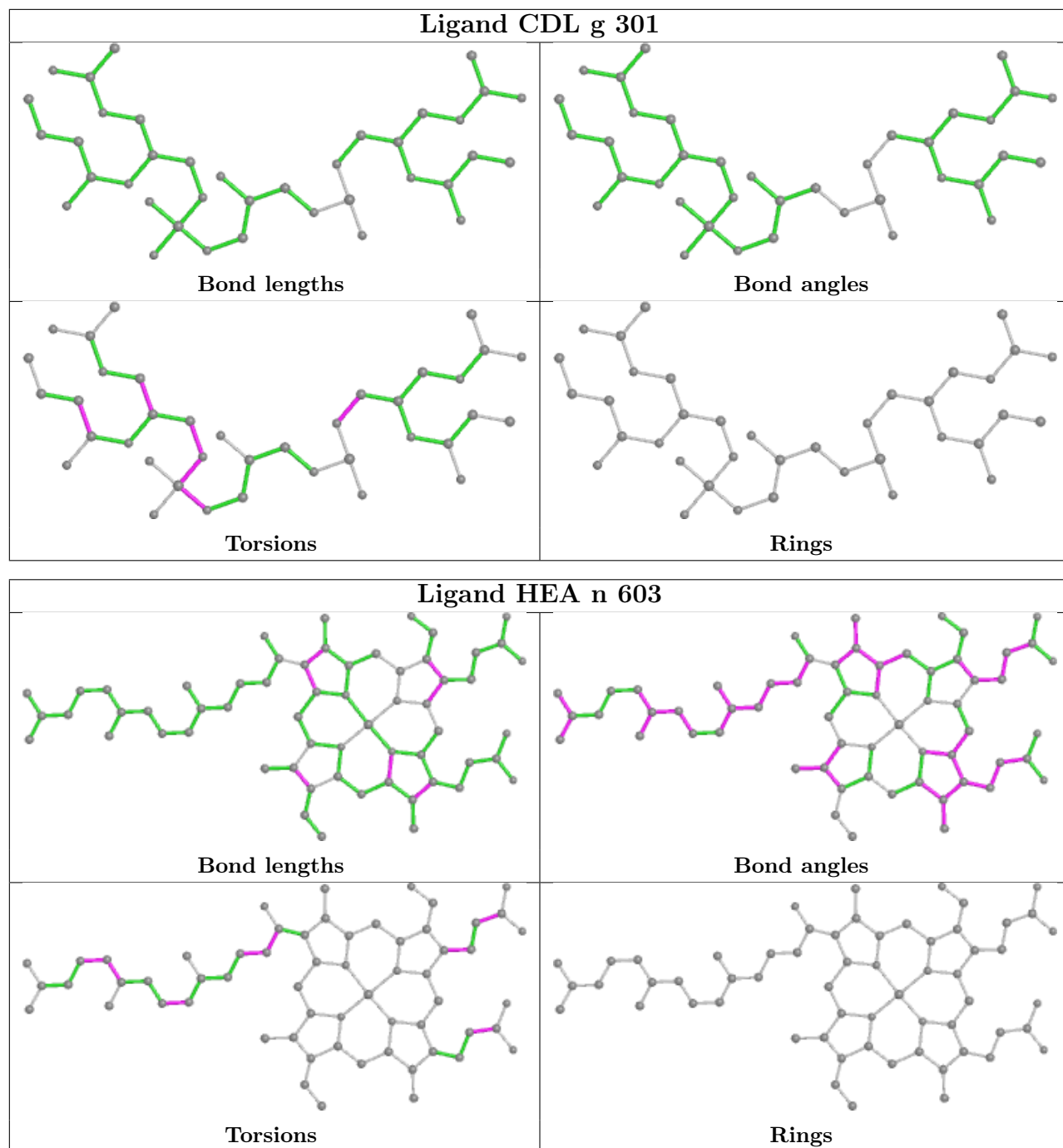


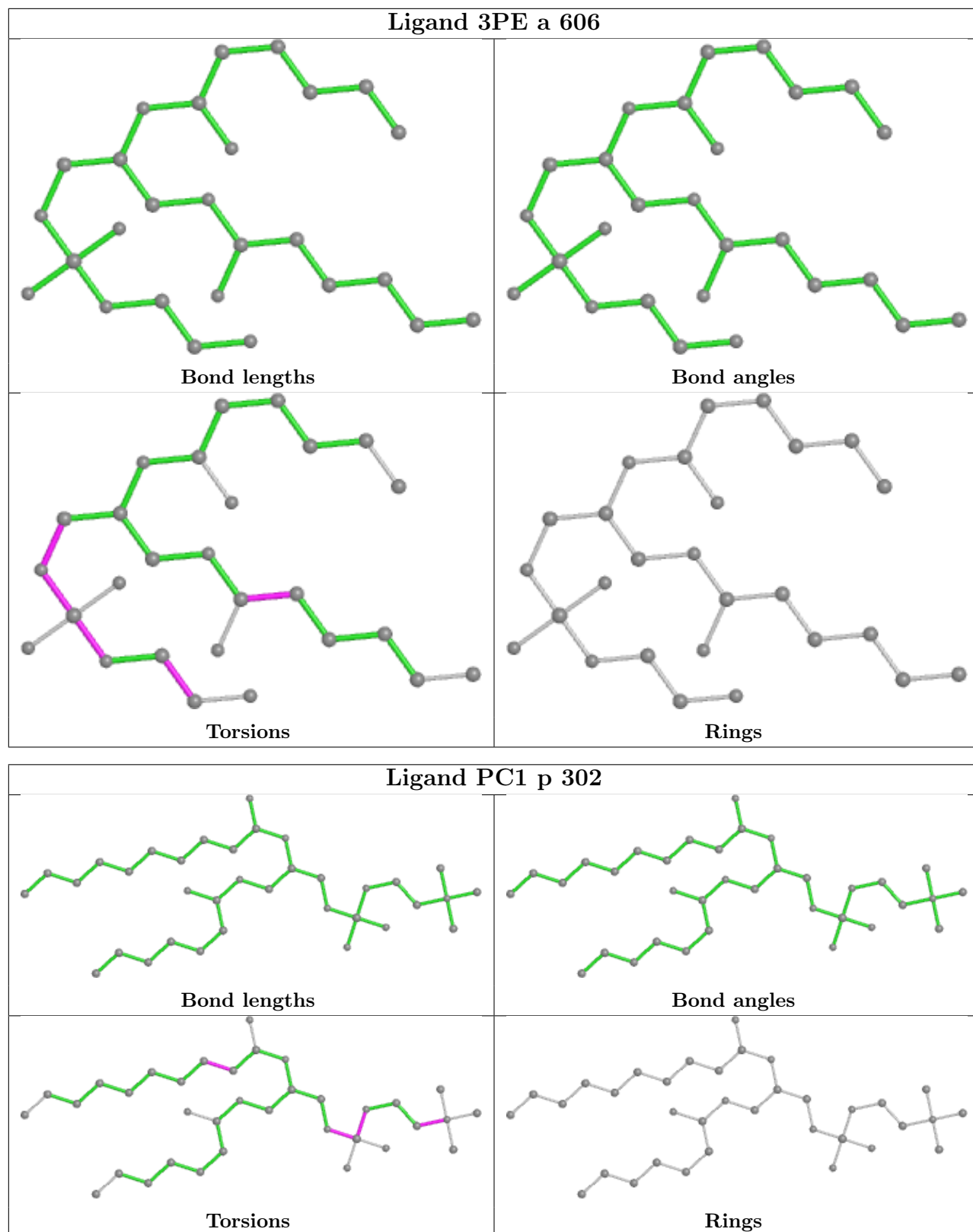


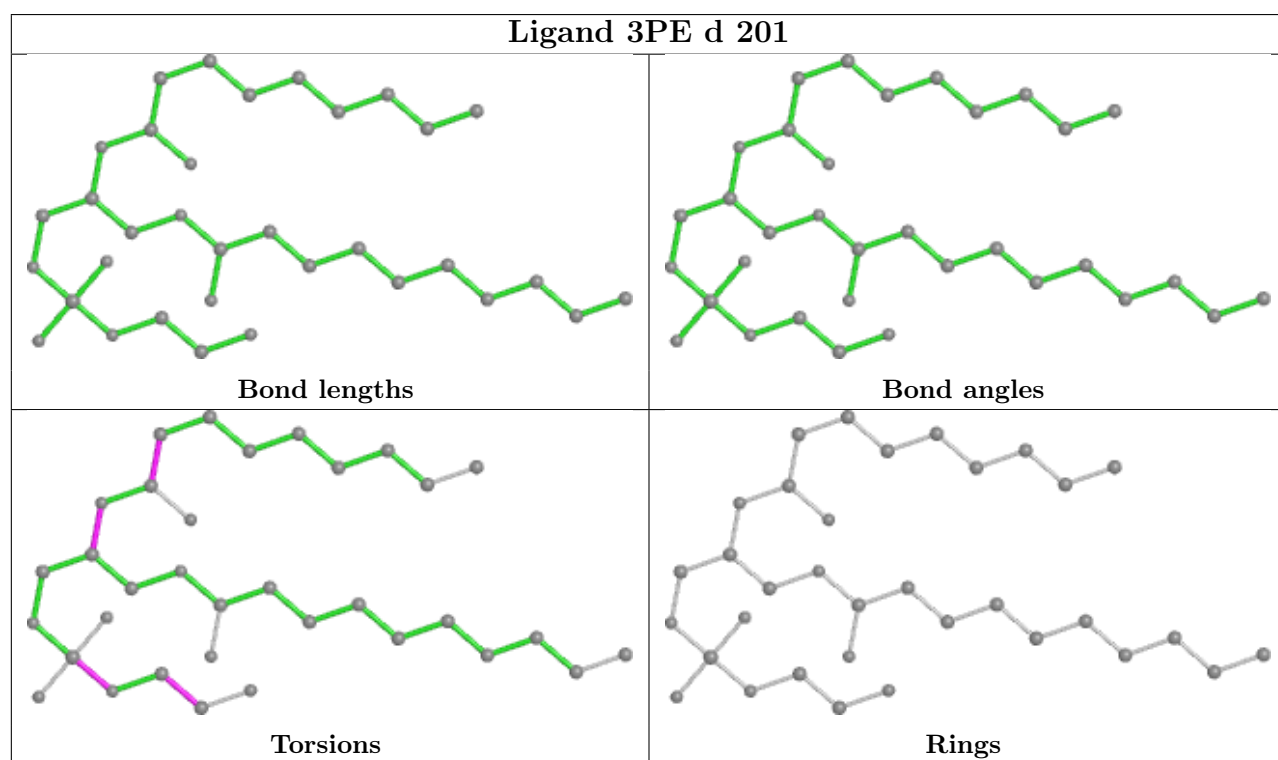
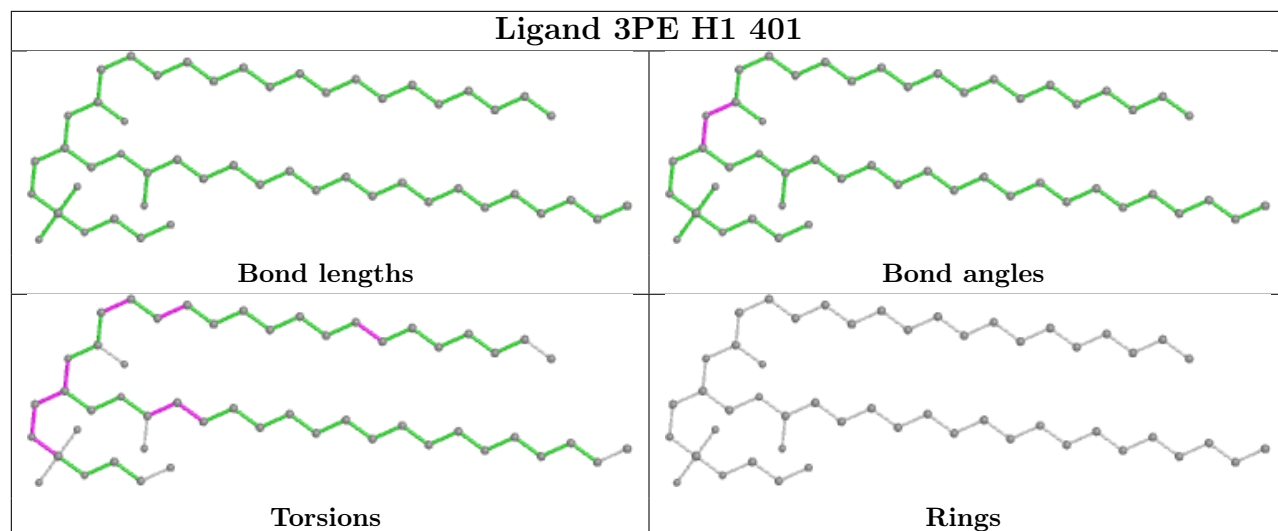


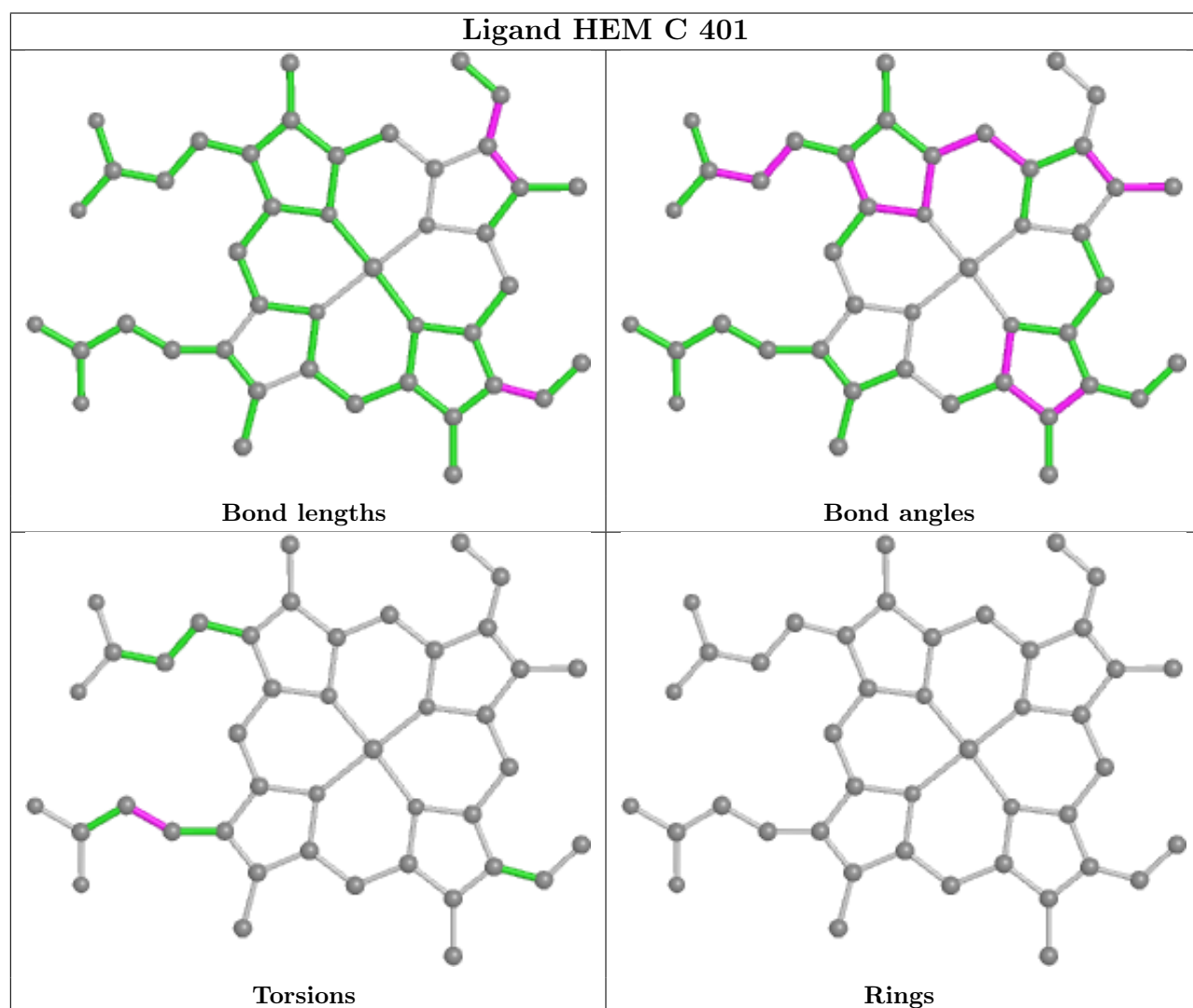
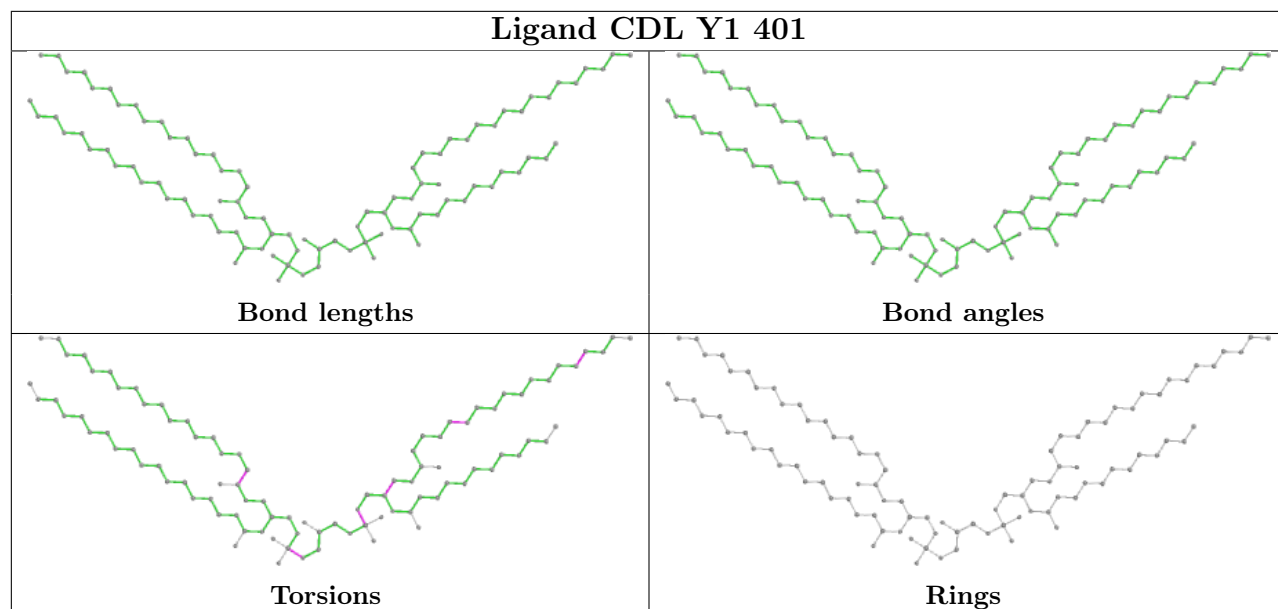


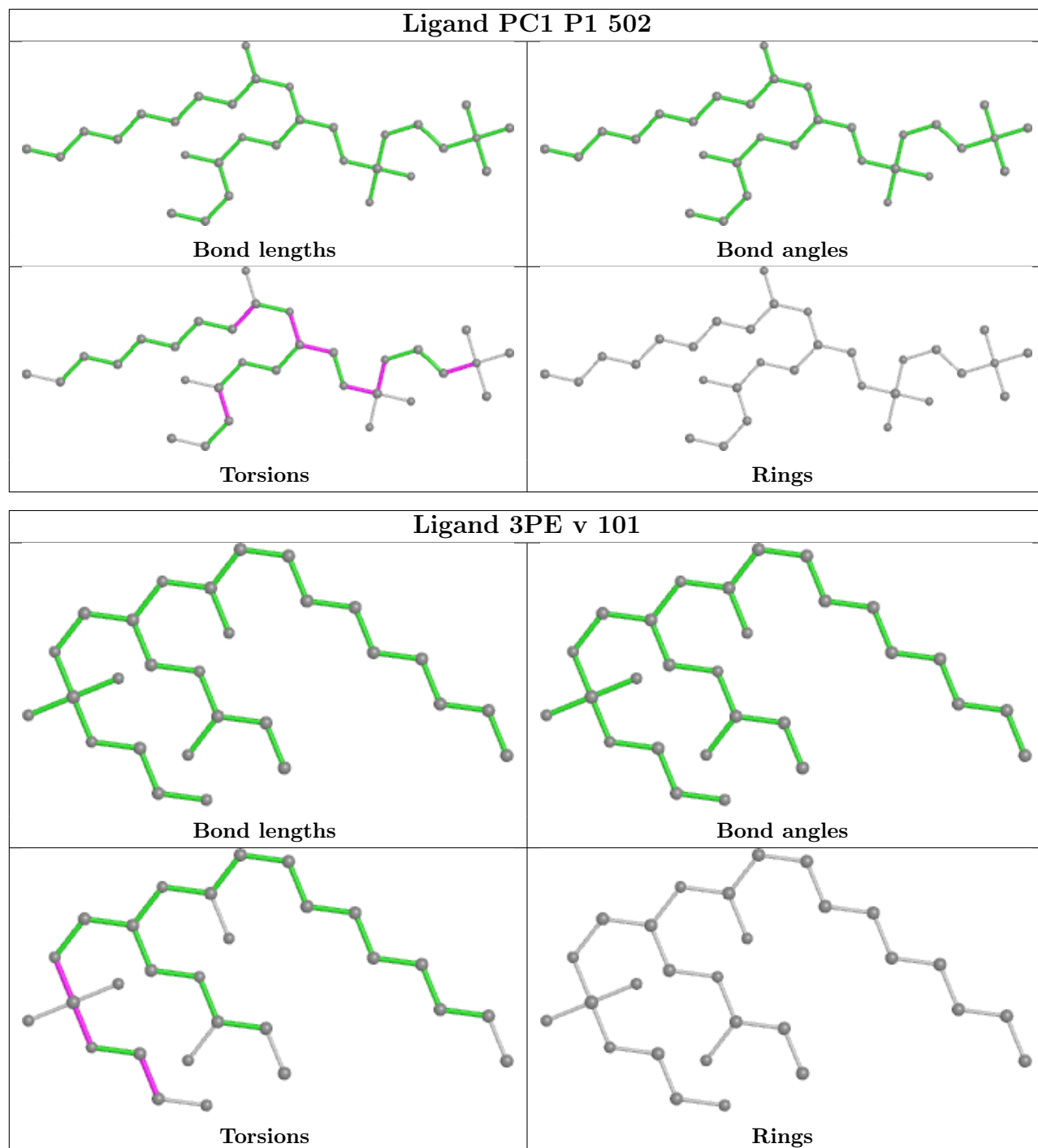


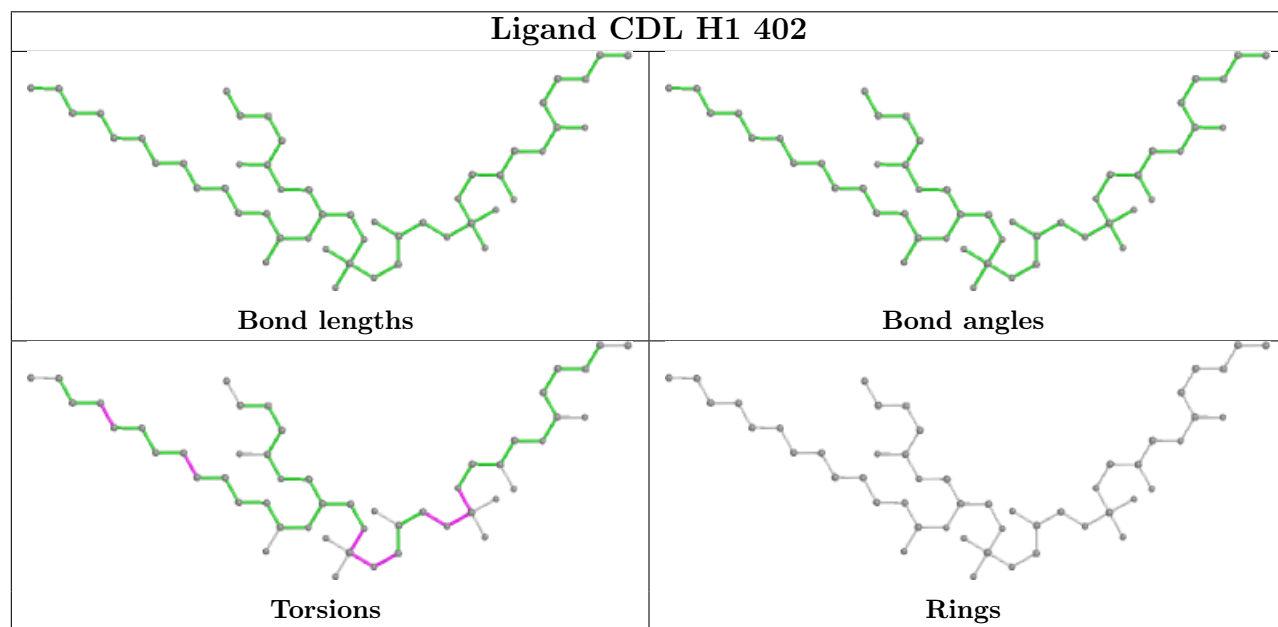
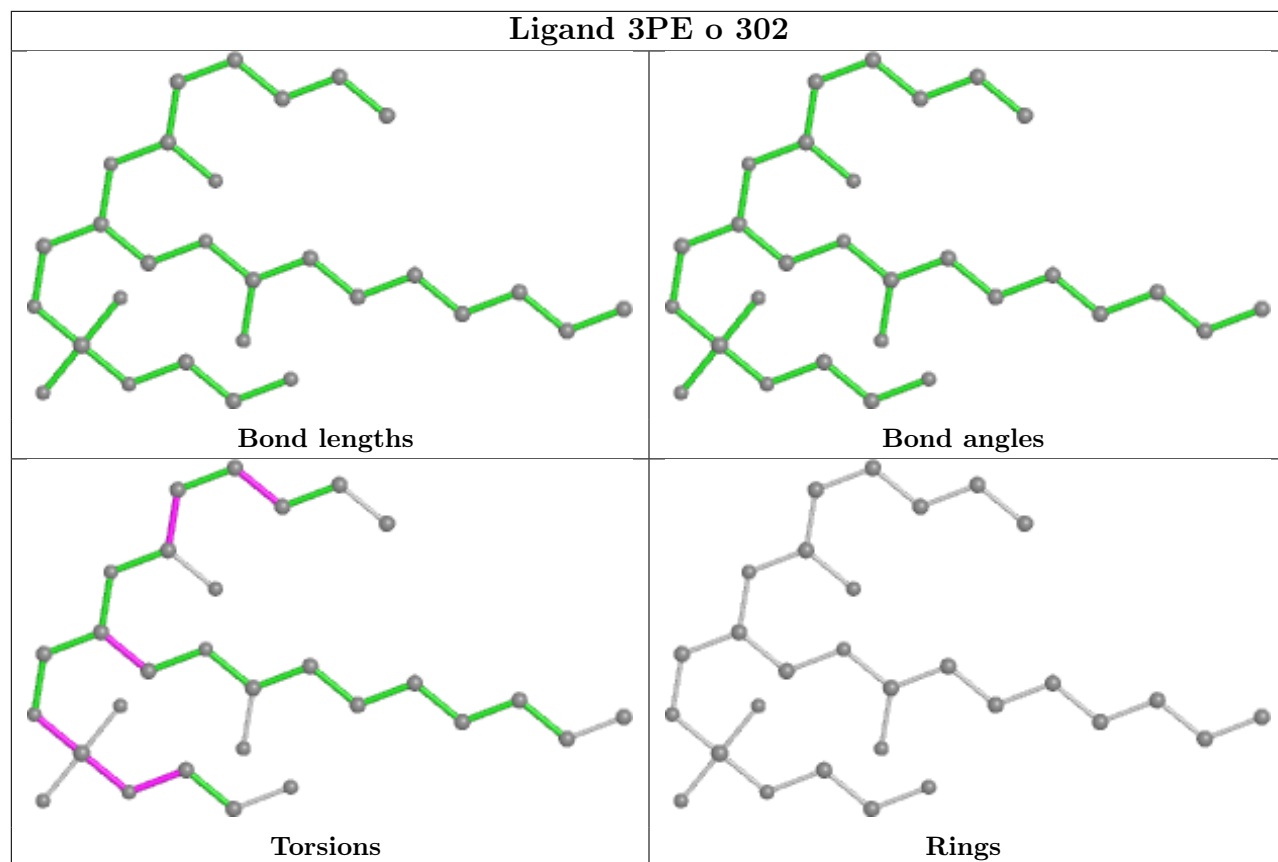


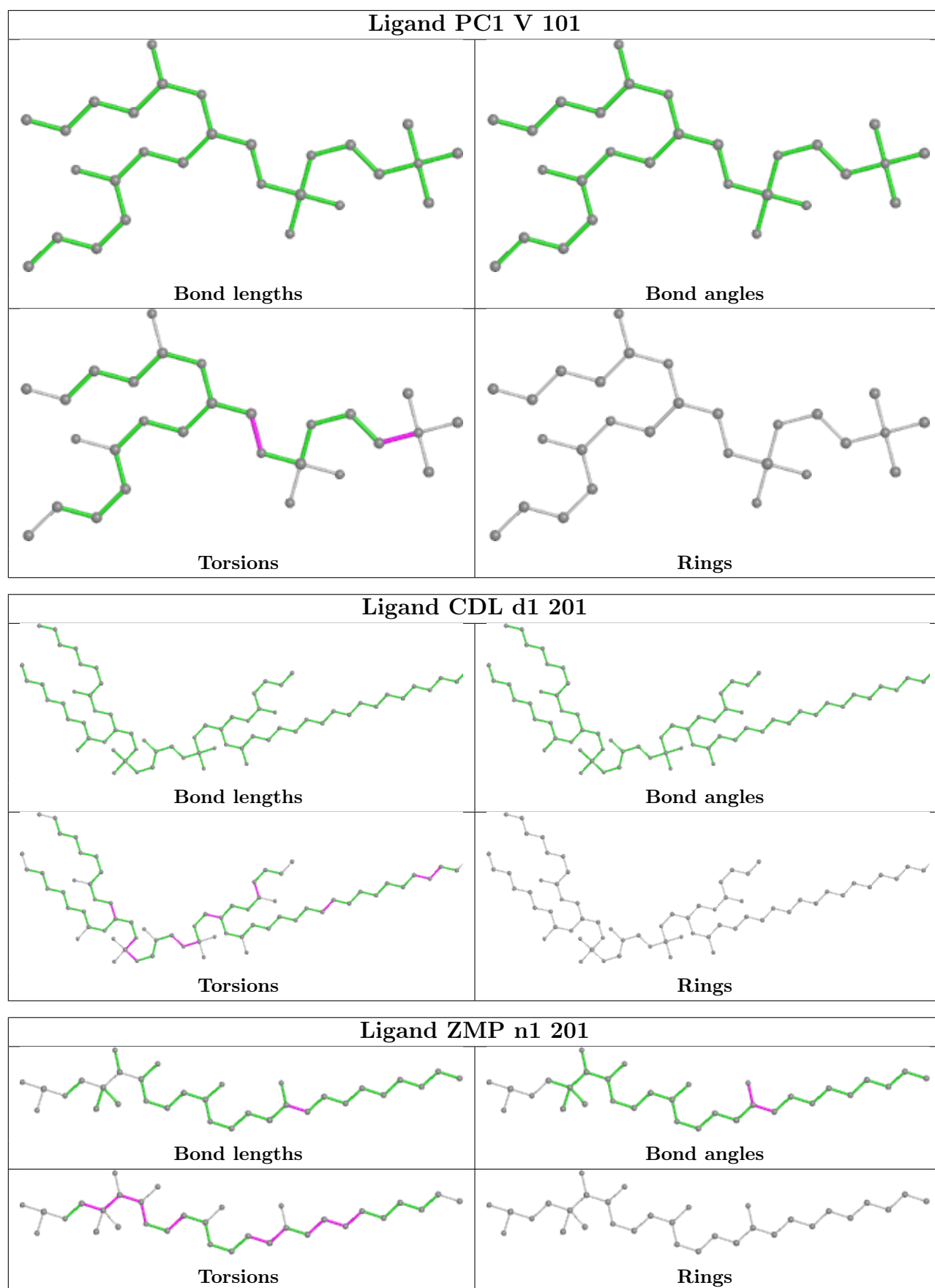


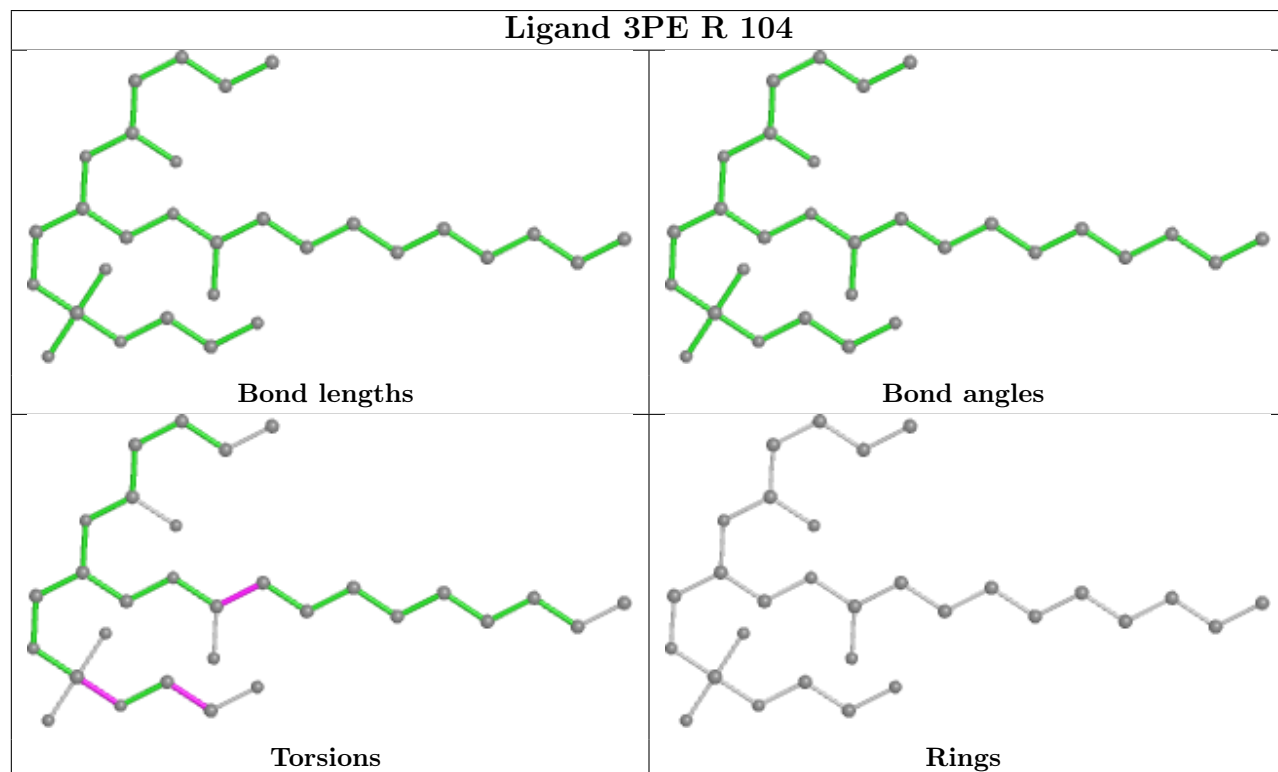
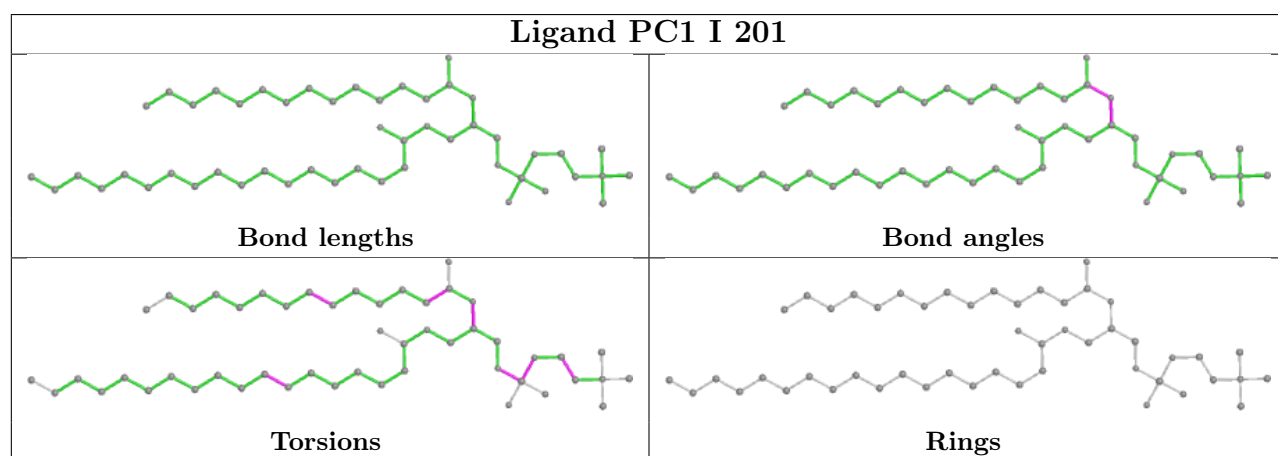
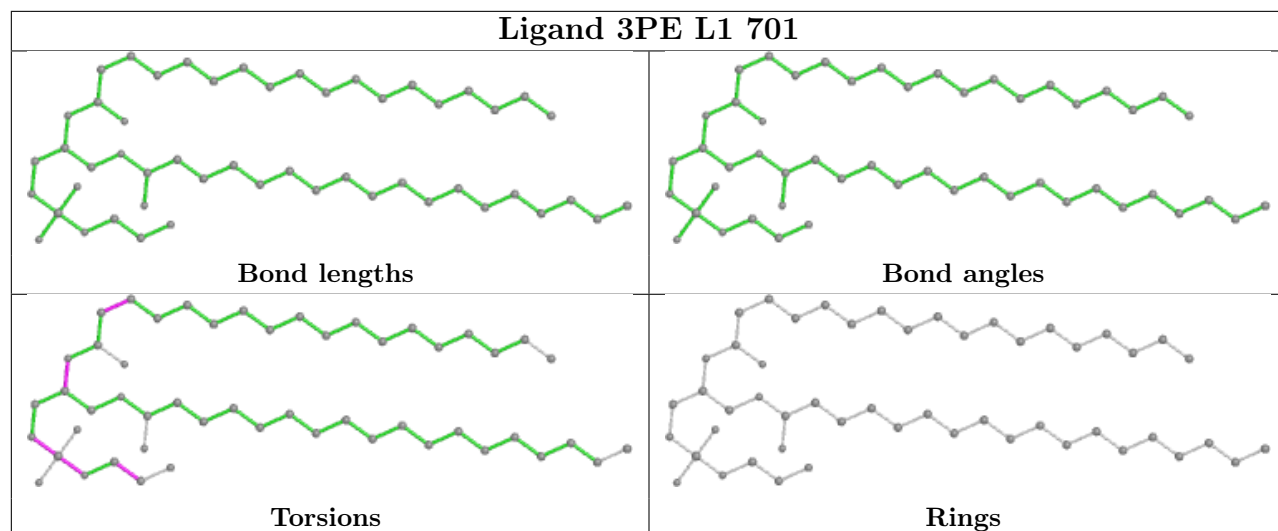


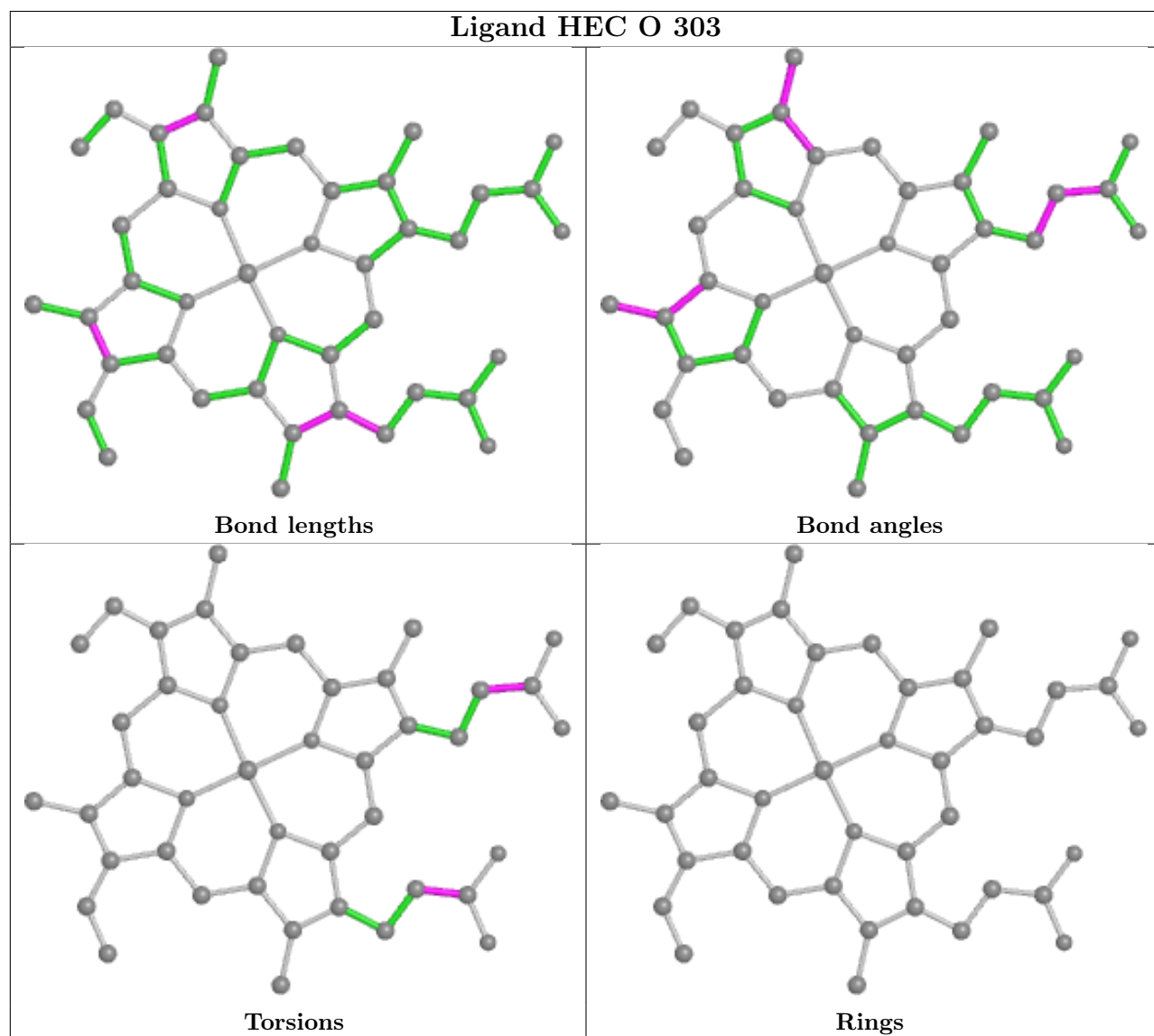
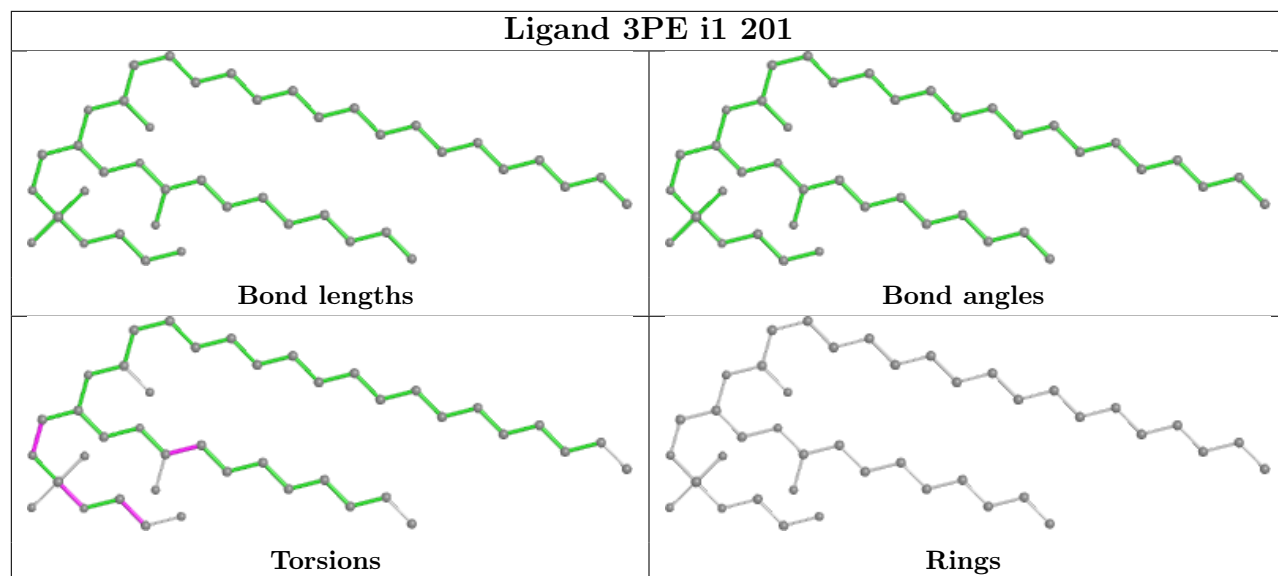


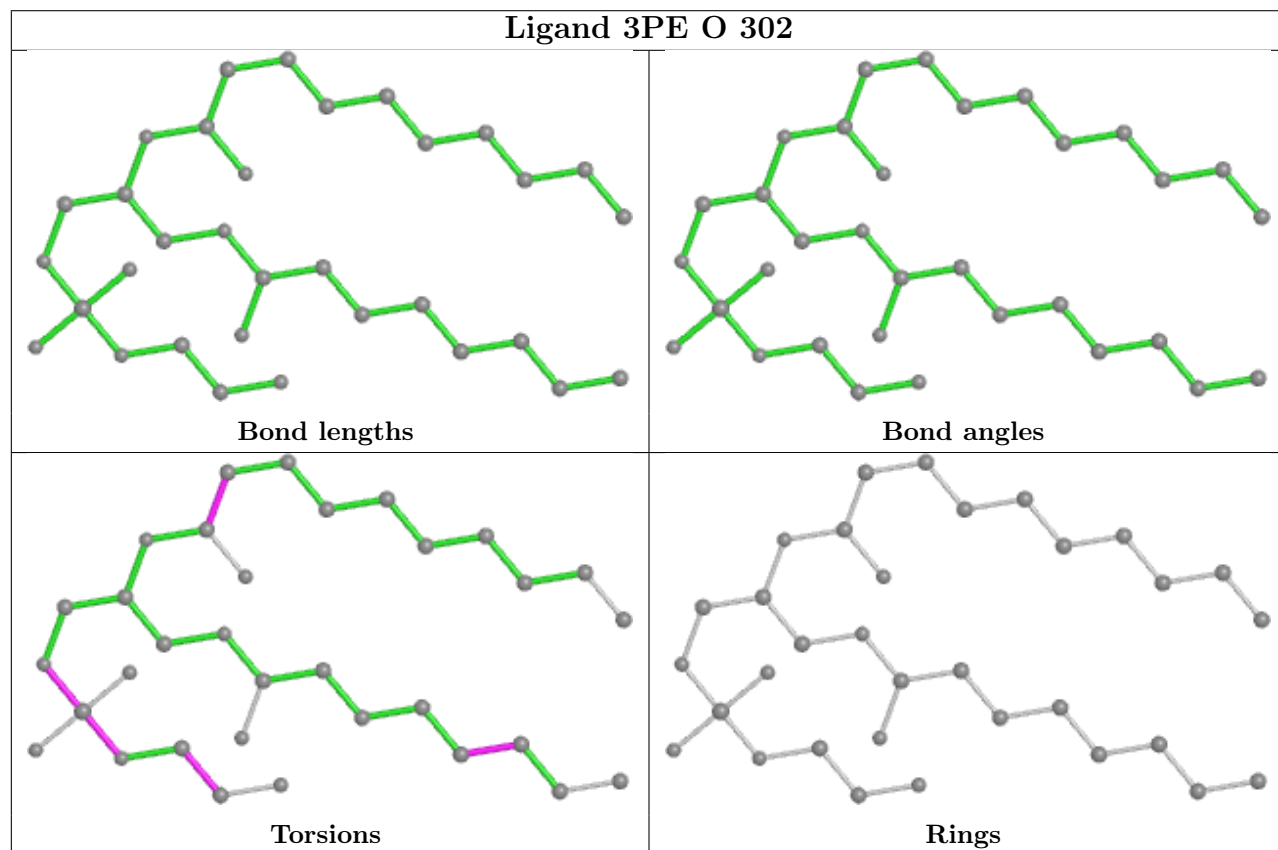
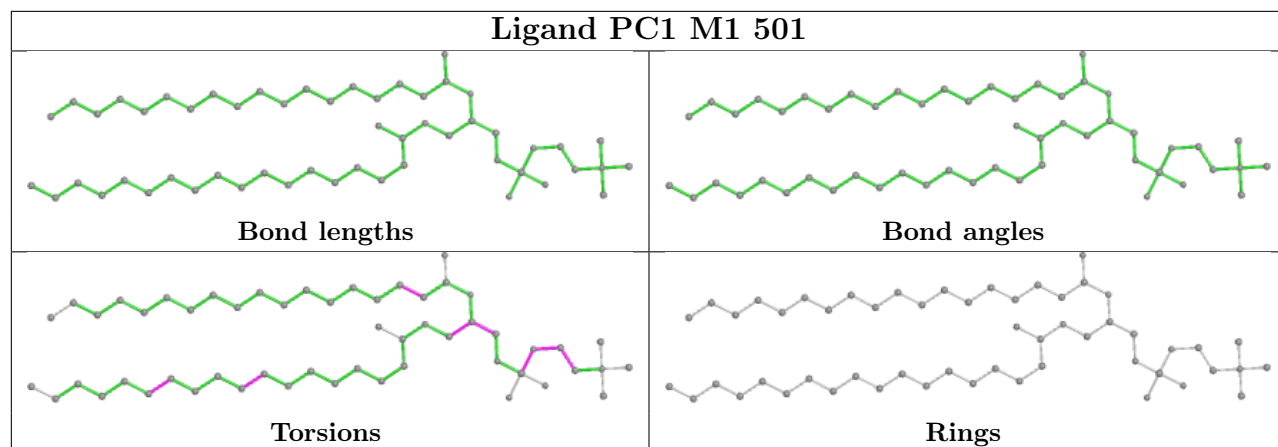


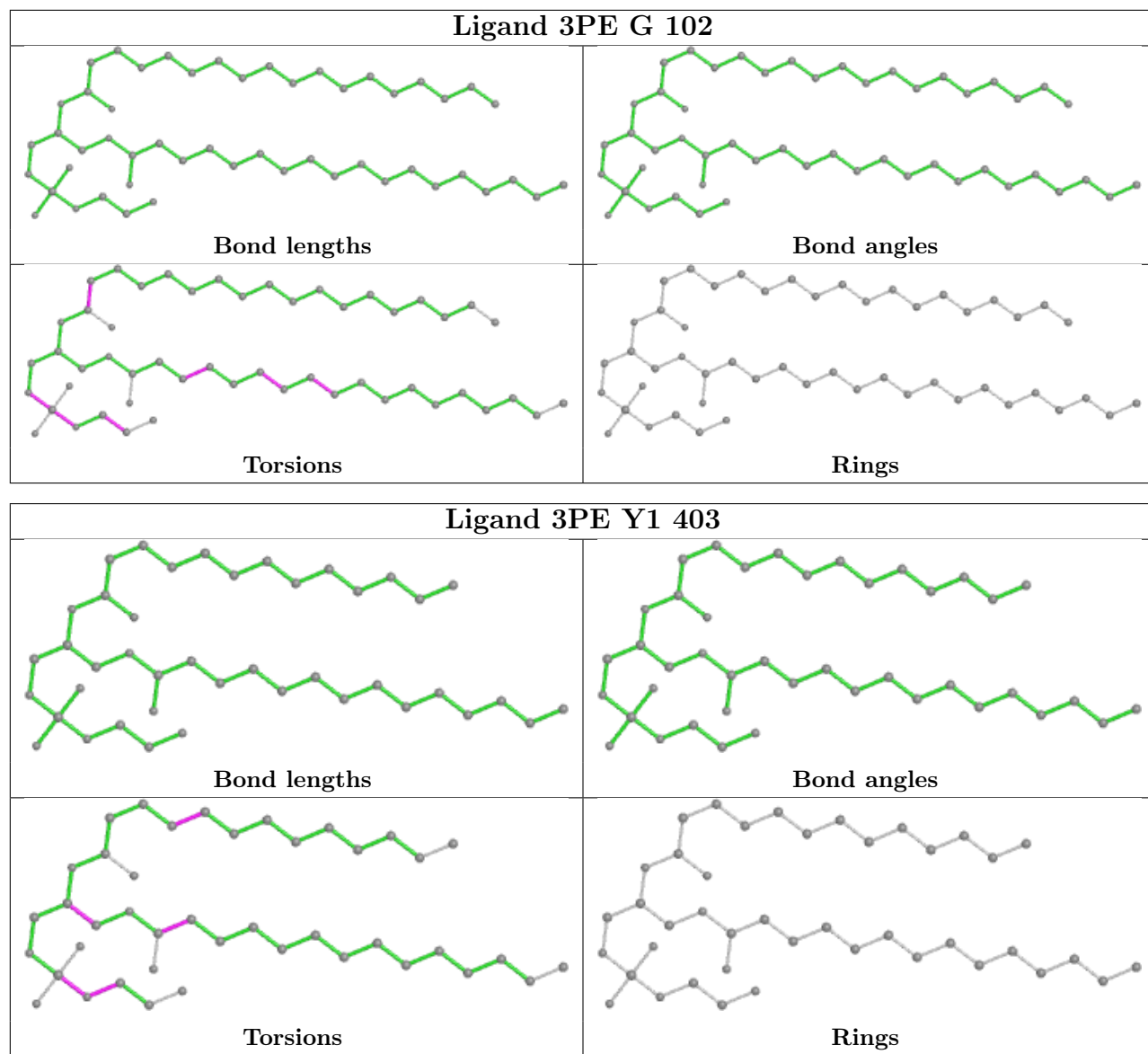


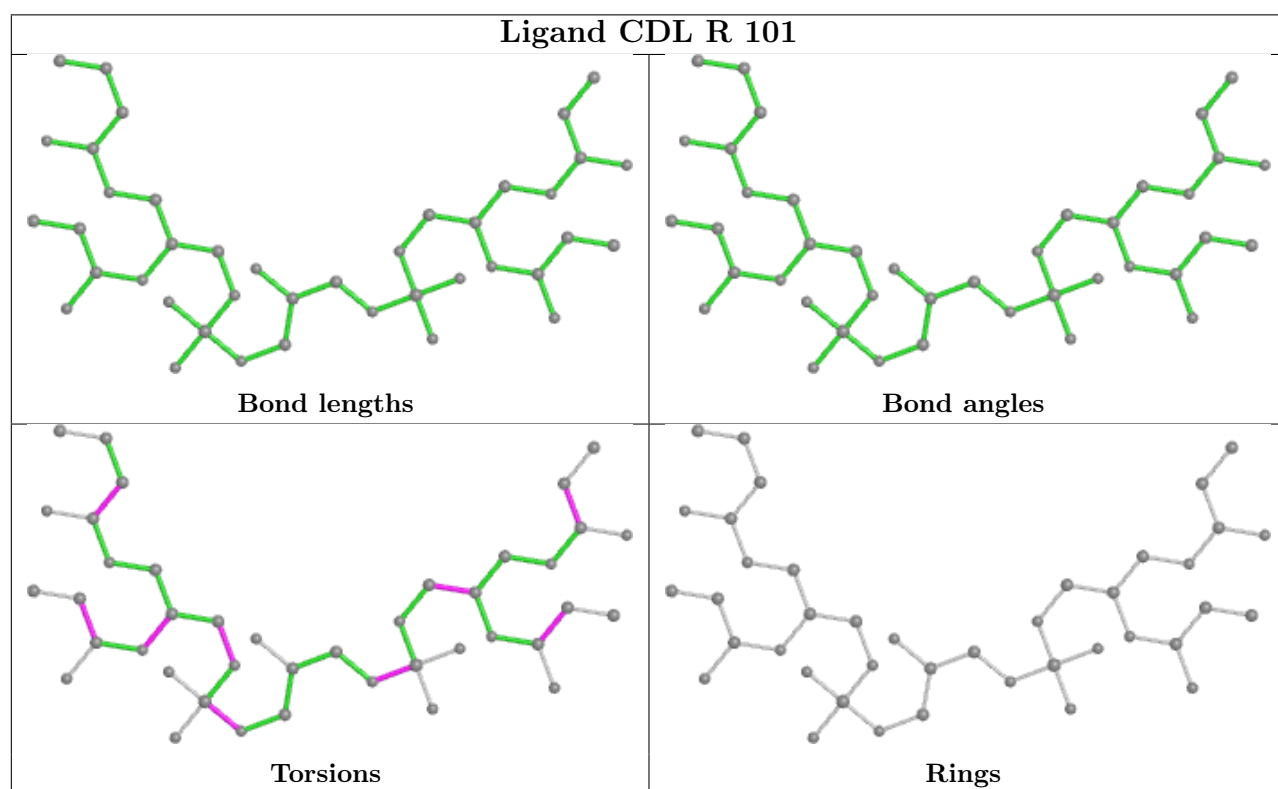
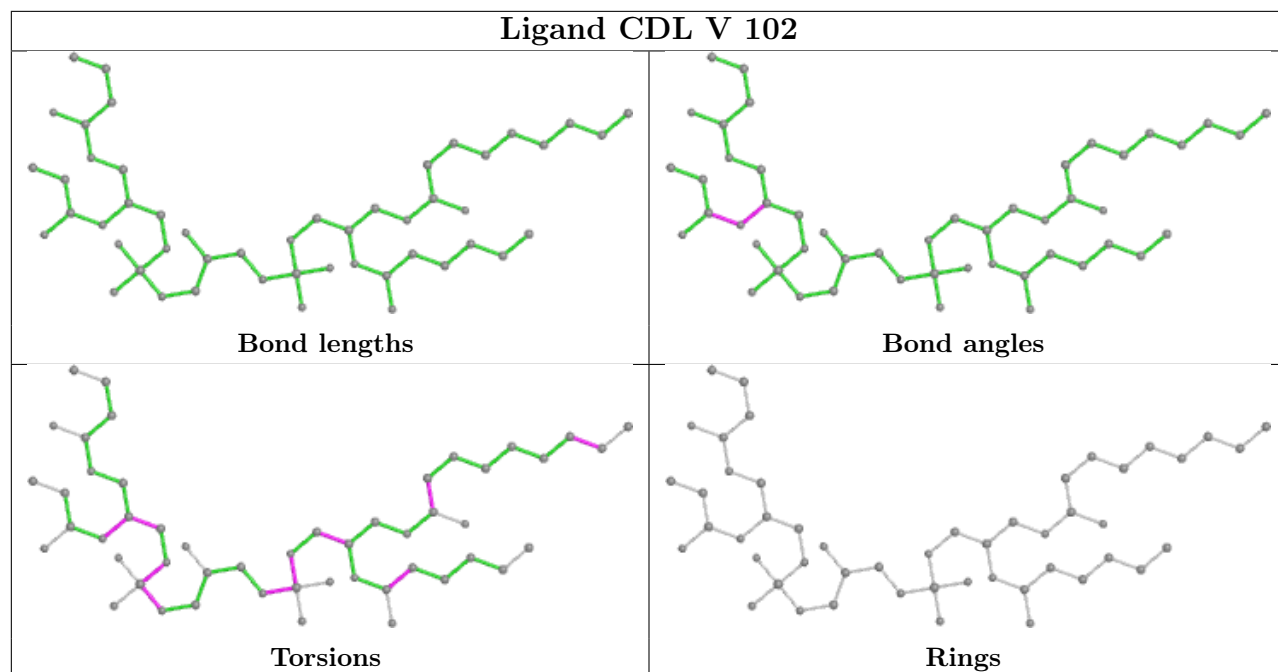


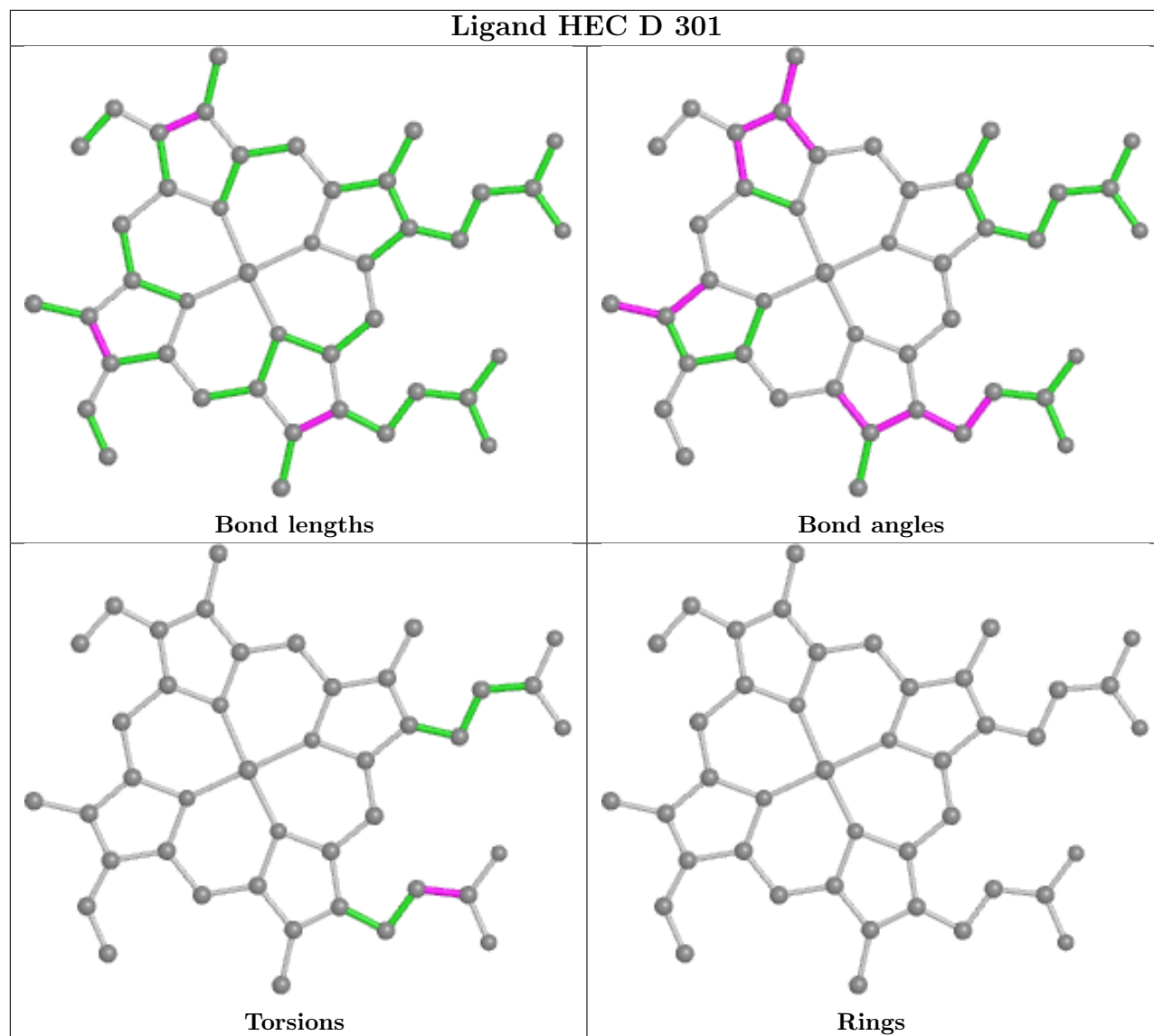


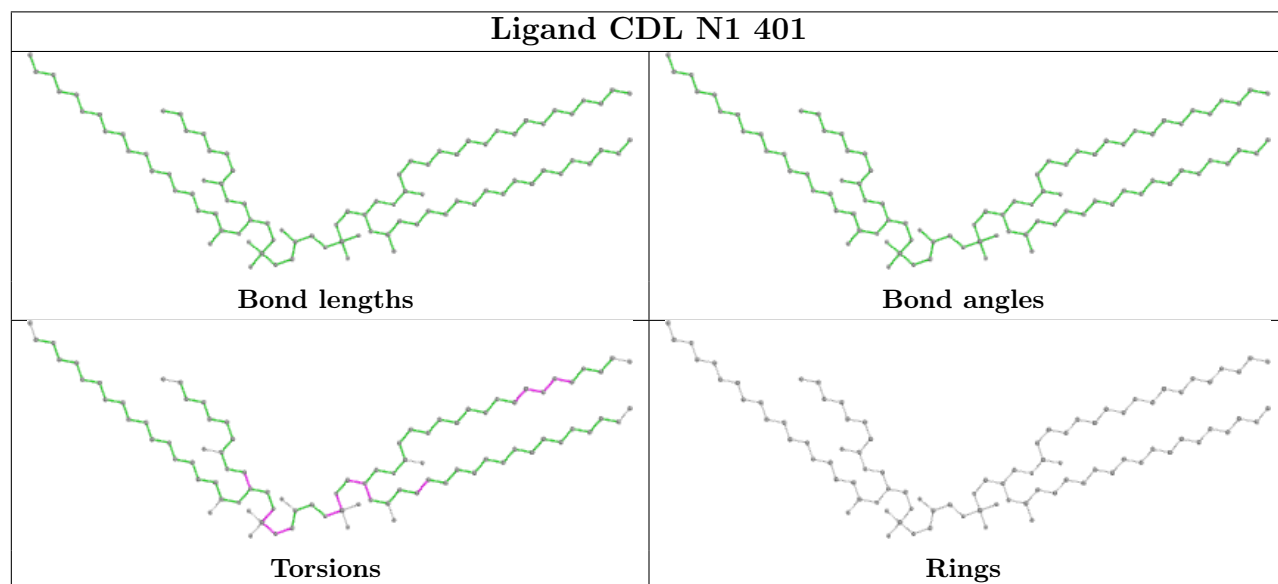
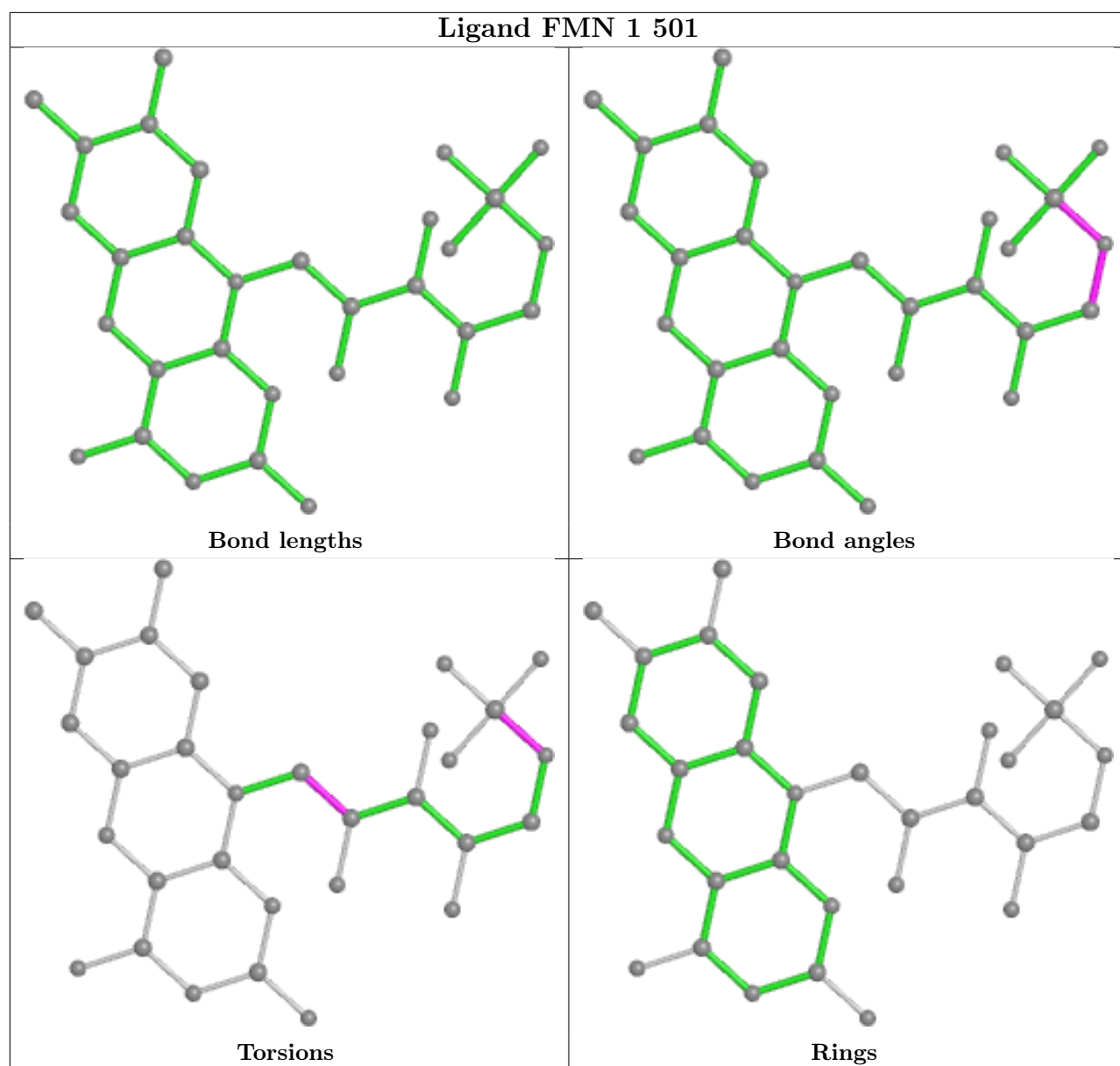


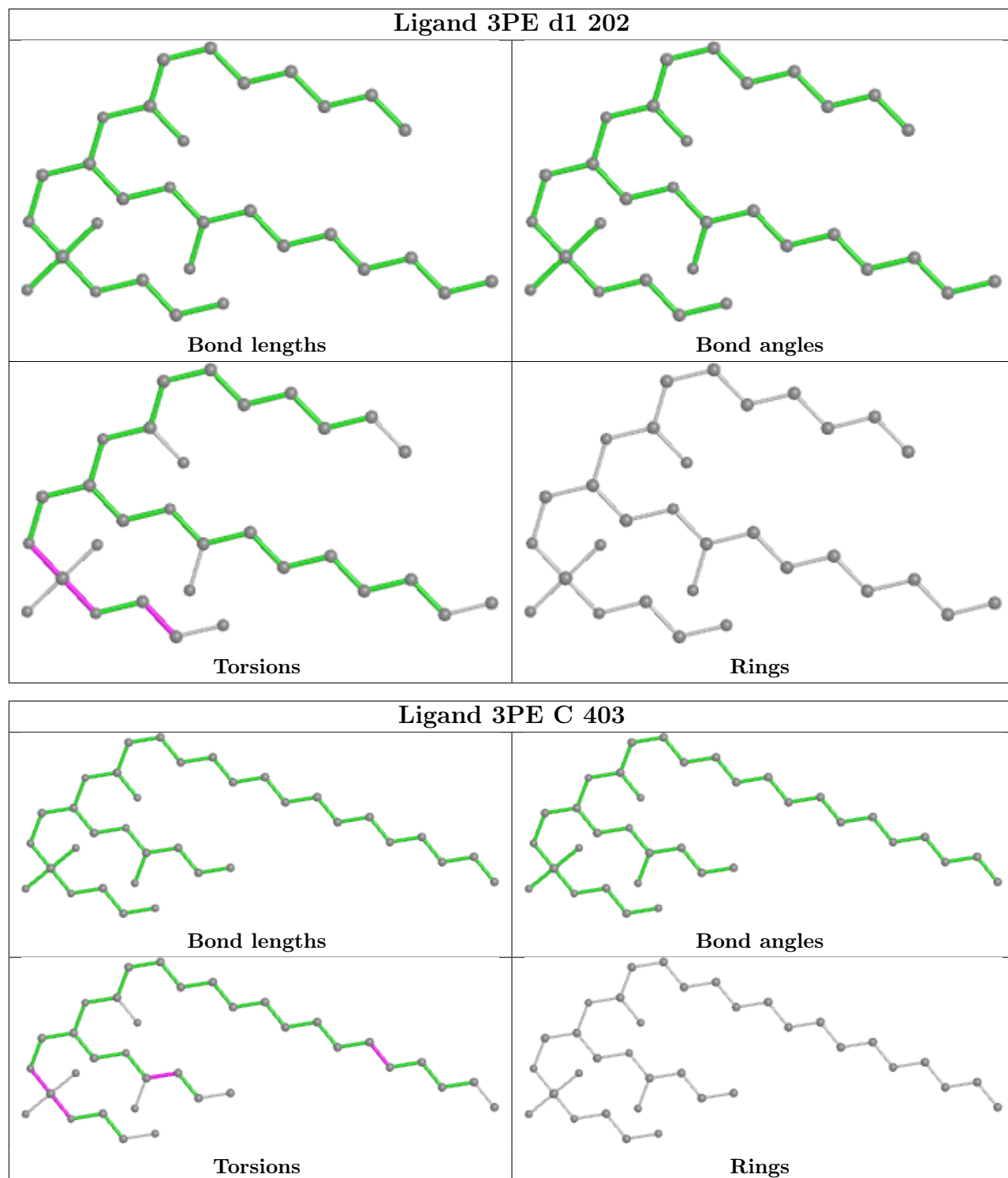


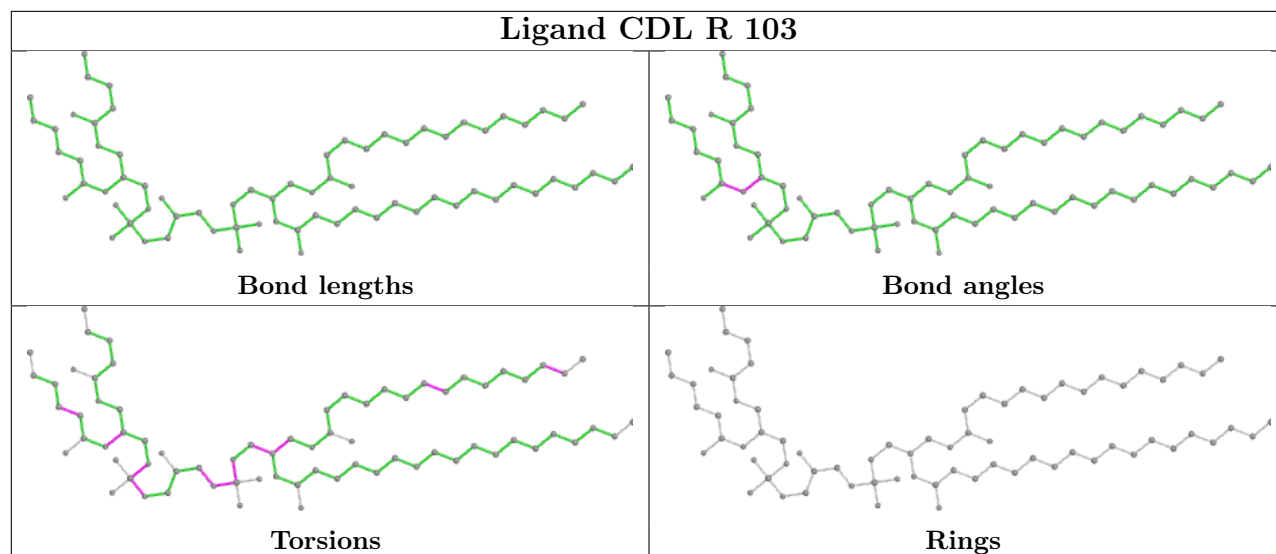












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

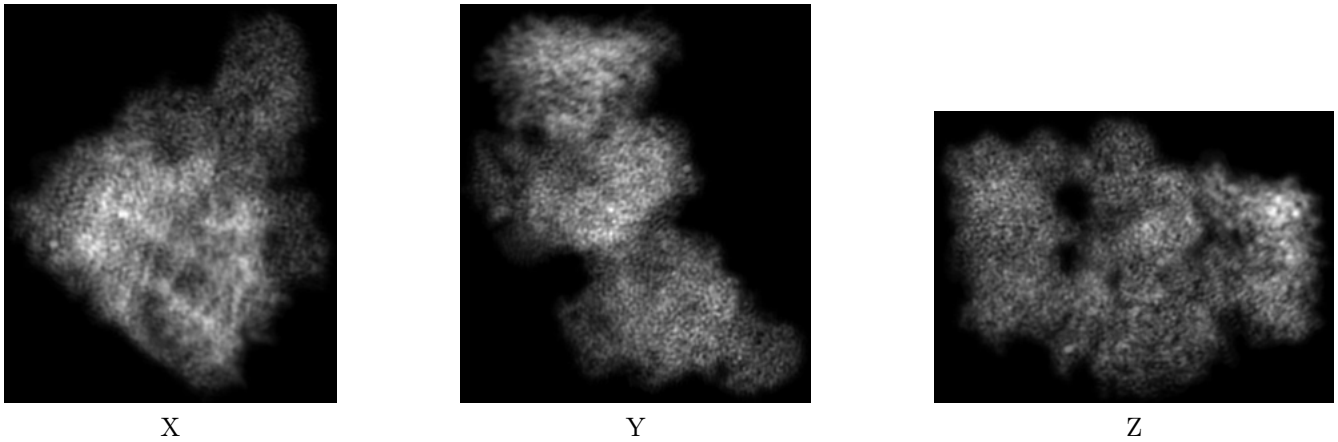
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17989. 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](#)

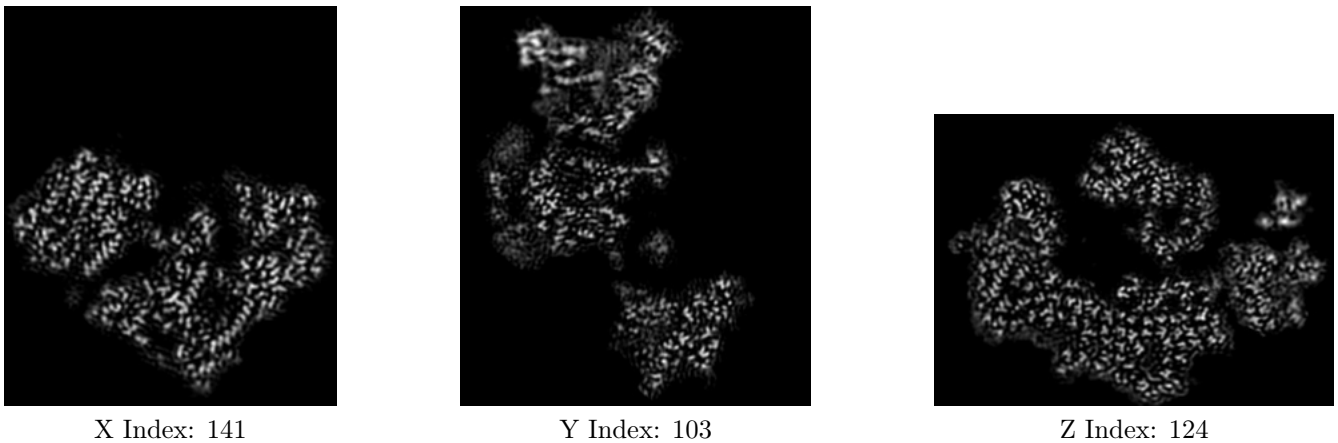
6.1.1 Primary map



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

6.2 Central slices [i](#)

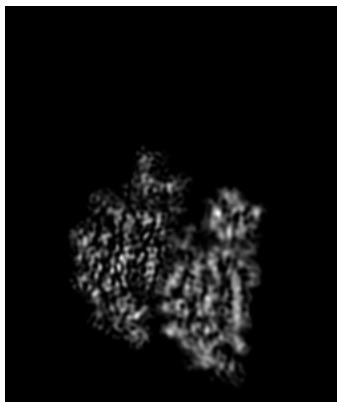
6.2.1 Primary map



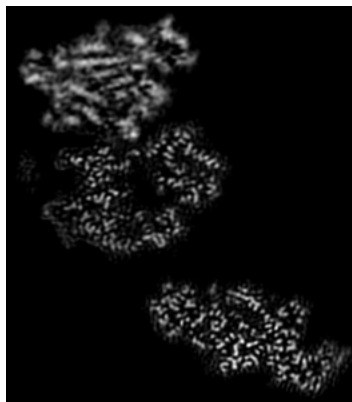
The images above show central slices of the map in three orthogonal directions.

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

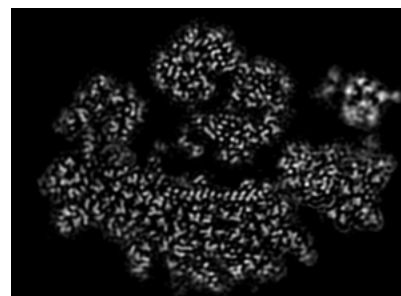
6.3.1 Primary map



X Index: 243



Y Index: 143

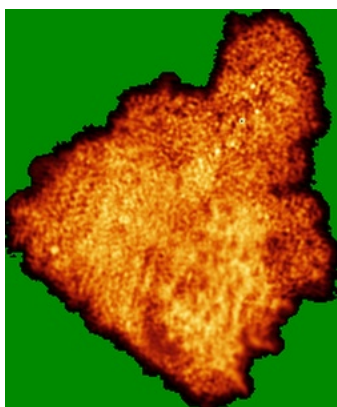


Z Index: 115

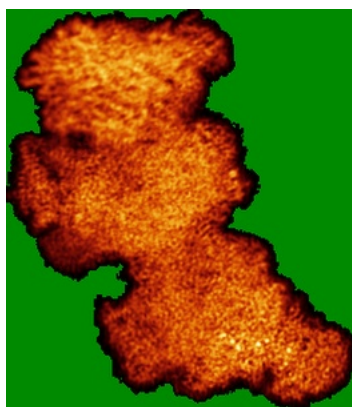
The images above show the largest variance slices of the map in three orthogonal directions.

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

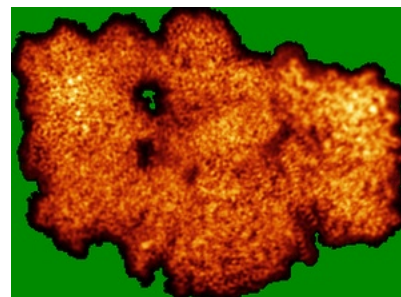
6.4.1 Primary map



X



Y

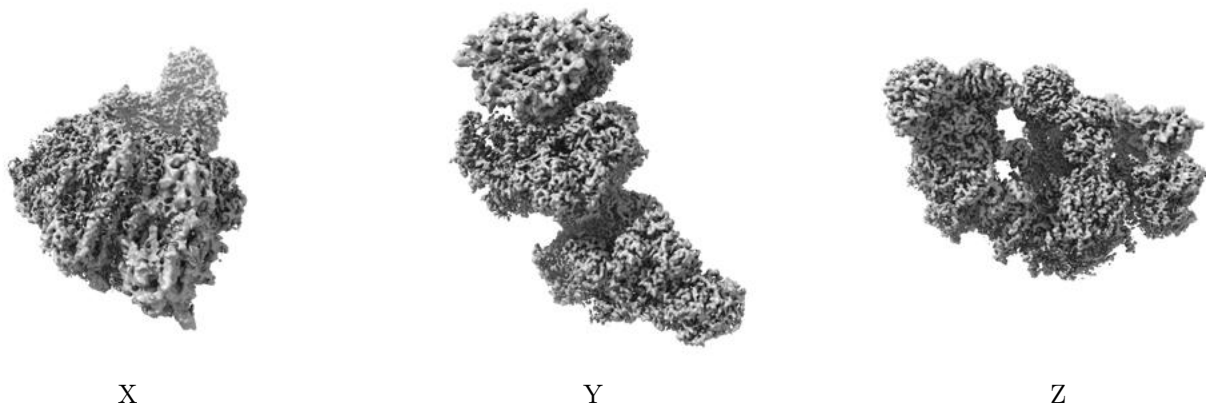


Z

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

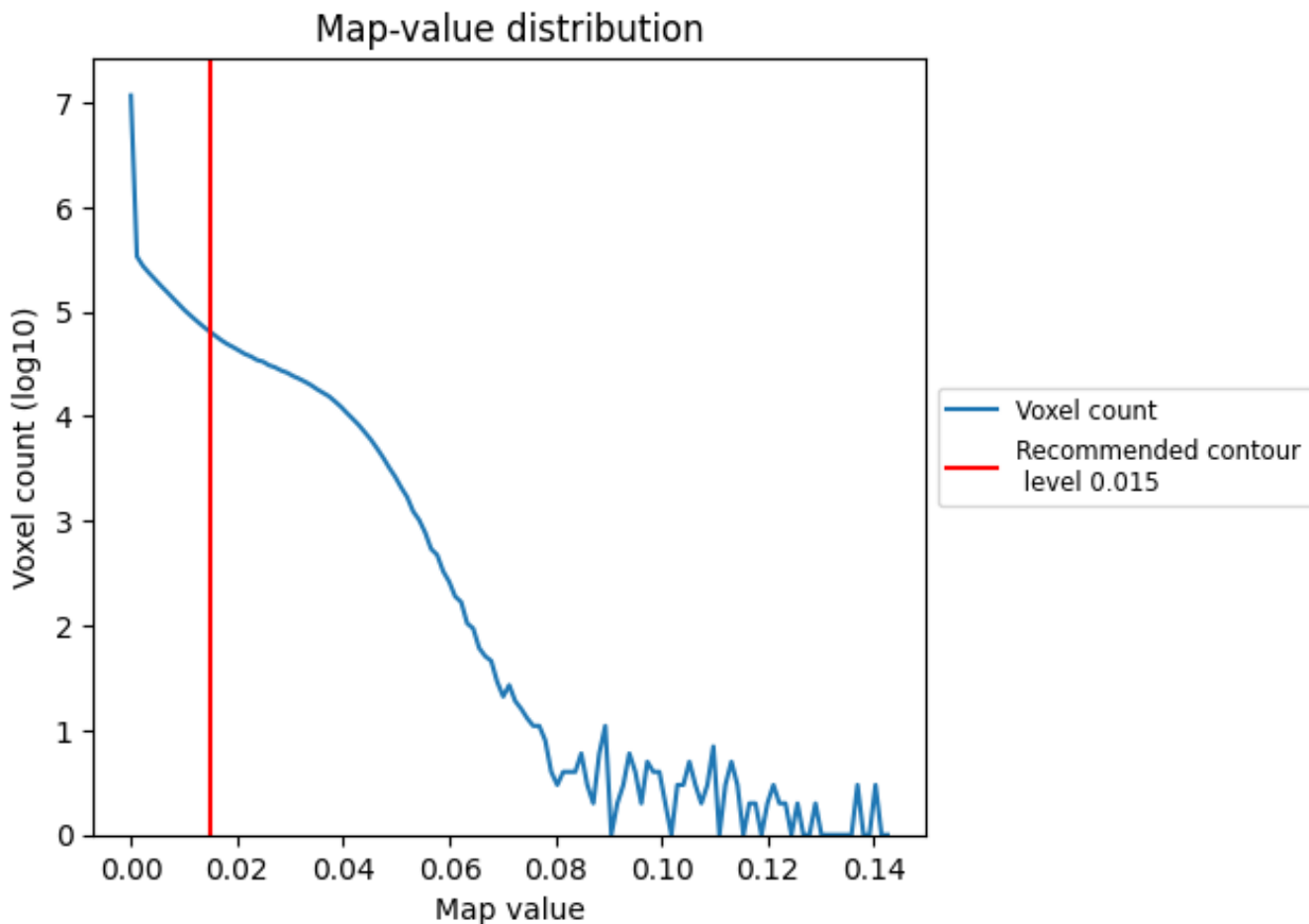
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

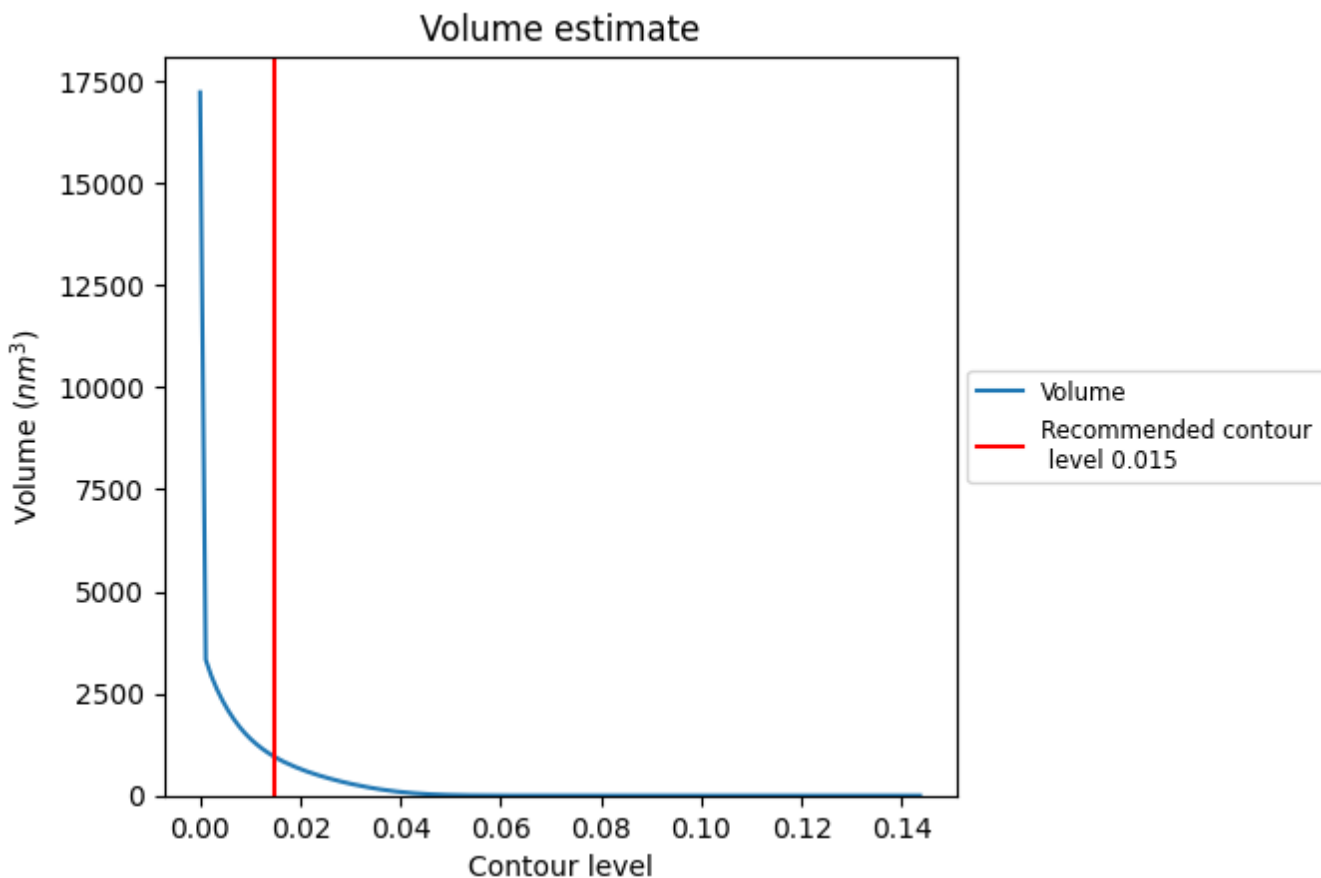
This section contains the results of statistical analysis of the map.

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 940 nm³; this corresponds to an approximate mass of 849 kDa.

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

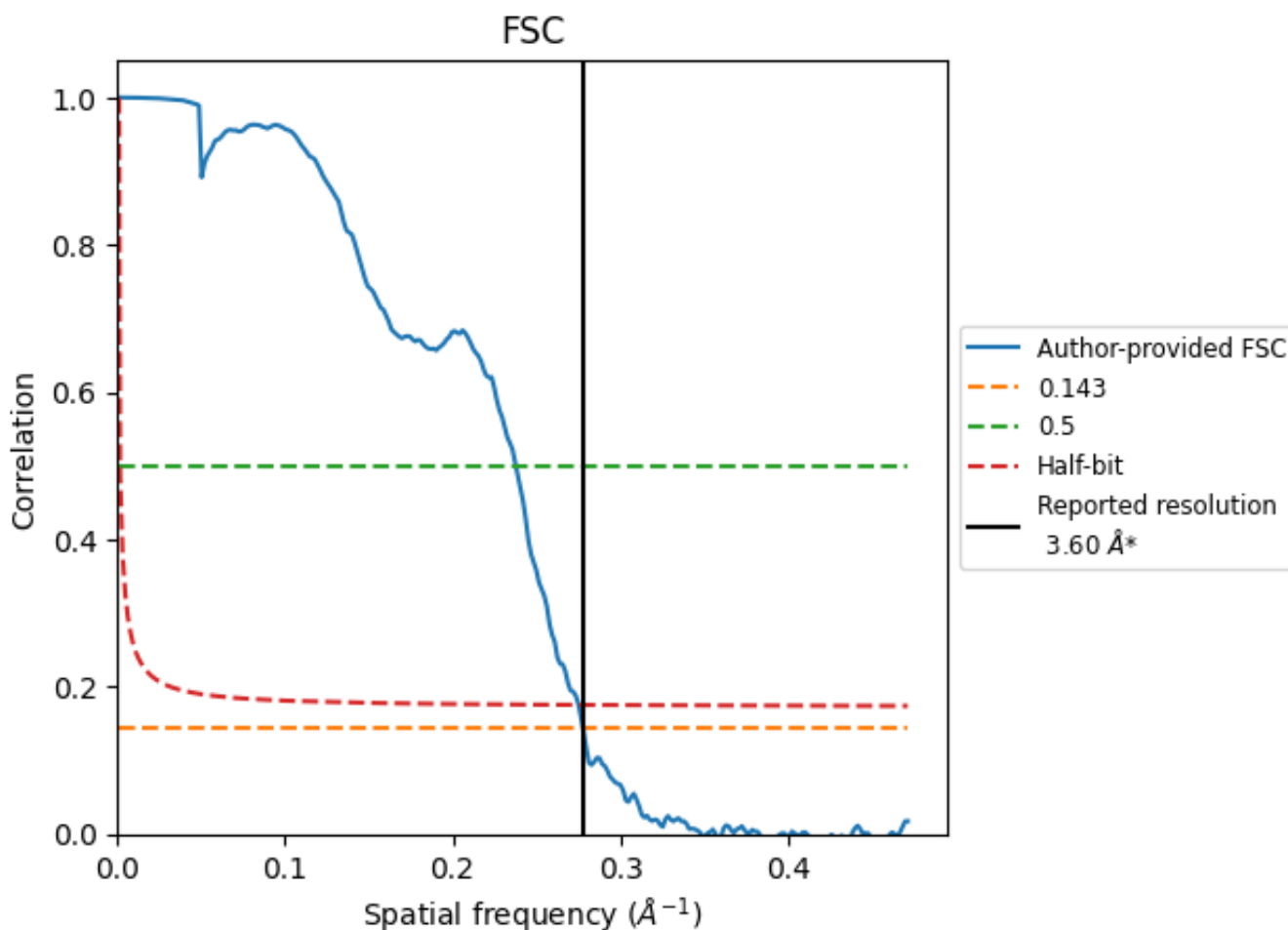
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

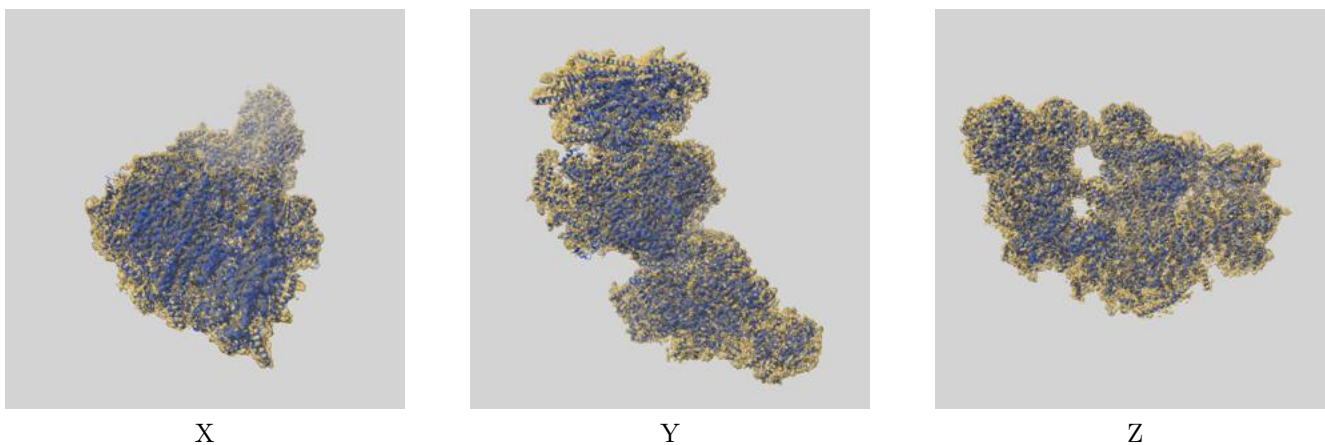
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.21	3.63
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

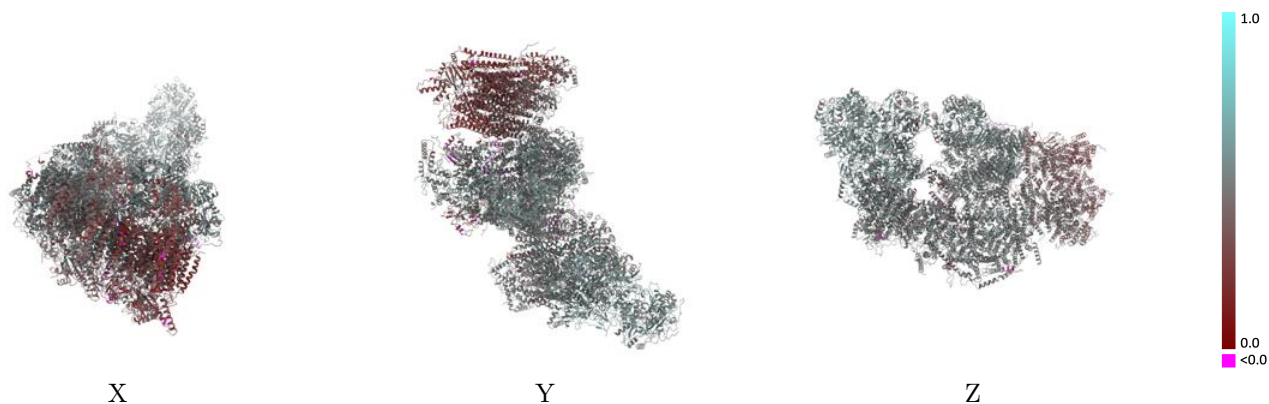
This section contains information regarding the fit between EMDB map EMD-17989 and PDB model 8PW5. Per-residue inclusion information can be found in section 3 on page 32.

9.1 Map-model overlay [i](#)



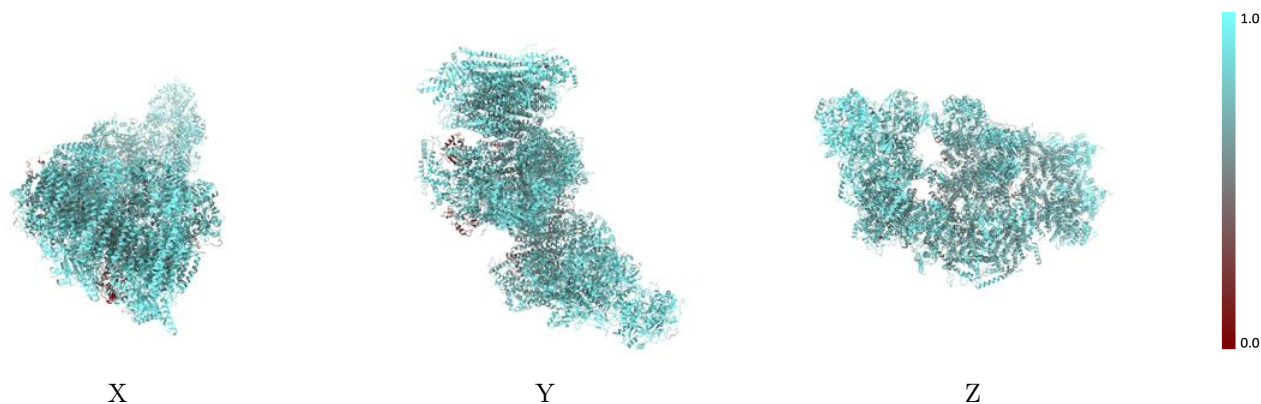
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



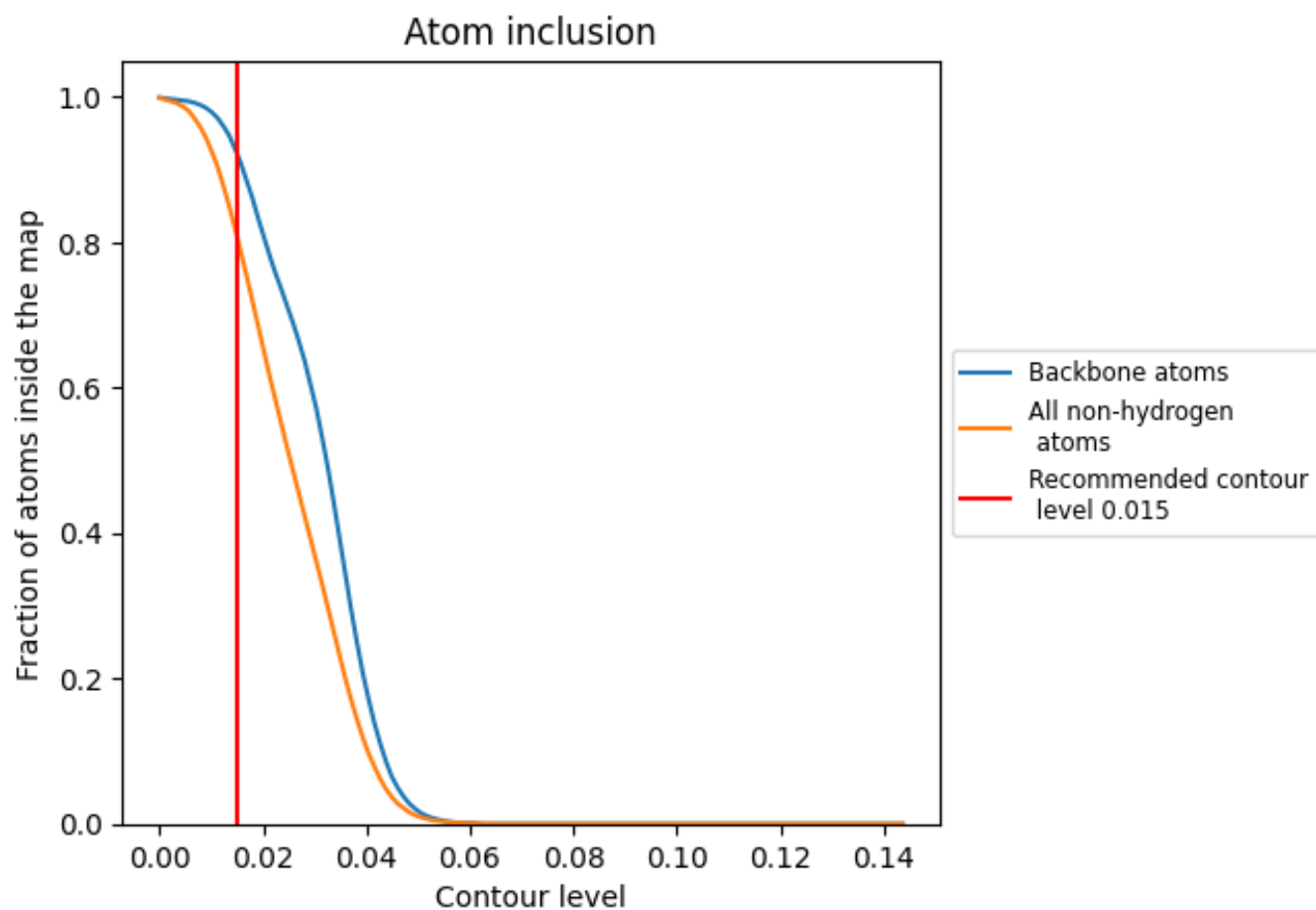
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8080	 0.4650
1	 0.8980	 0.5360
2	 0.8890	 0.5310
3	 0.8580	 0.5280
6	 0.8540	 0.5200
7	 0.8730	 0.5440
9	 0.8630	 0.5330
A	 0.8270	 0.5110
A1	 0.7140	 0.4720
B	 0.8420	 0.5200
C	 0.7850	 0.4980
C1	 0.8800	 0.5470
D	 0.8520	 0.5090
D1	 0.8130	 0.5020
E	 0.5370	 0.3570
F	 0.8000	 0.5020
G	 0.7650	 0.4990
H	 0.7730	 0.4440
H1	 0.7390	 0.4660
I	 0.6620	 0.3060
J	 0.7720	 0.5000
J1	 0.6380	 0.4250
K	 0.6100	 0.4630
K1	 0.7170	 0.4750
L	 0.8180	 0.5060
L1	 0.7810	 0.4900
M	 0.8460	 0.5150
M1	 0.7950	 0.5010
N	 0.8000	 0.5010
N1	 0.7660	 0.4930
O	 0.8200	 0.5070
O1	 0.8260	 0.4900
P	 0.4970	 0.3440
P1	 0.7980	 0.5010
Q	 0.7900	 0.5140



































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Chain	Atom inclusion	Q-score
Q1	0.8470	0.5420
R	0.6750	0.4690
S	0.7460	0.4470
S1	0.8470	0.4820
T	0.7060	0.4930
T1	0.7500	0.4280
U	0.7500	0.5020
U1	0.8090	0.4890
V	0.6510	0.4630
V1	0.8620	0.5210
W1	0.8470	0.5290
X1	0.8360	0.4840
Y1	0.6780	0.4530
Z1	0.8260	0.4950
a	0.8350	0.3120
a1	0.8170	0.4920
b	0.9150	0.3000
b1	0.7670	0.4650
c	0.8060	0.2880
c1	0.7670	0.4680
d	0.9240	0.3070
d1	0.7590	0.4940
e	0.9290	0.3000
e1	0.7840	0.4850
f	0.8860	0.3030
f1	0.7310	0.4540
g	0.8440	0.2980
g1	0.7600	0.4690
h	0.9070	0.2810
h1	0.8220	0.4900
i	0.8940	0.2620
i1	0.7470	0.4570
j1	0.7900	0.4620
k	0.9290	0.2960
k1	0.7960	0.4800
l	0.7370	0.2750
l1	0.8240	0.5090
m	0.7830	0.2450
m1	0.7540	0.4750
n	0.8070	0.4290
n1	0.8350	0.5020
o	0.8340	0.4170

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Chain	Atom inclusion	Q-score
o1	 0.7940	 0.4630
p	 0.7830	 0.4190
p1	 0.8270	 0.4910
q	 0.8680	 0.4120
q1	 0.8950	 0.5450
r	 0.8580	 0.3740
r1	 0.8280	 0.5340
s	 0.8090	 0.4010
s1	 0.8040	 0.4860
t	 0.7470	 0.3770
u	 0.8840	 0.3990
v	 0.7940	 0.3500
w	 0.7670	 0.4310
x	 0.8420	 0.3890
y	 0.8030	 0.4430
z	 0.7580	 0.3910