



Full wwPDB EM Validation Report ⓘ

Apr 18, 2024 – 08:18 pm BST

PDB ID : 8PW6
EMDB ID : EMD-17990
Title : C respirasome from murine liver
Authors : Vercellino, I.; Sazanov, L.A.
Deposited on : 2023-07-19
Resolution : 3.30 Å (reported)
Based on initial models : 6g2j, 7o3c

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 i

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

The reported resolution of this entry is 3.30 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.



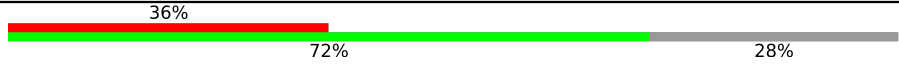

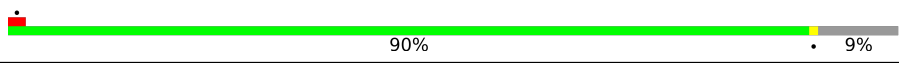
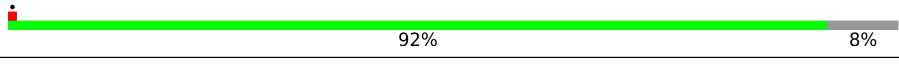
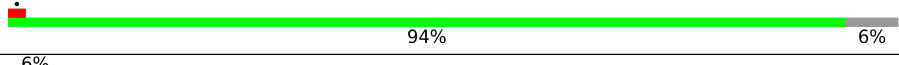
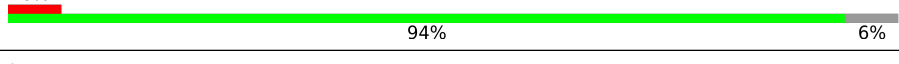
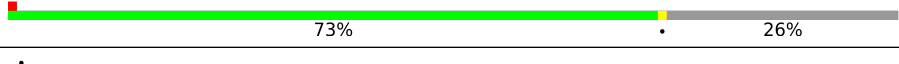

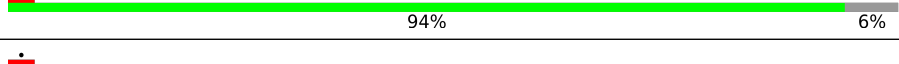
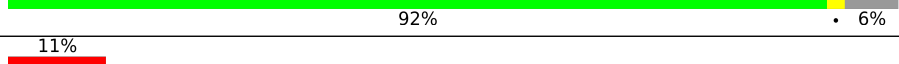
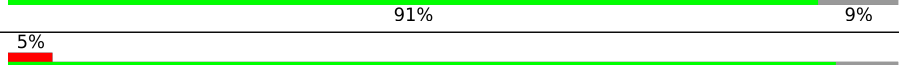
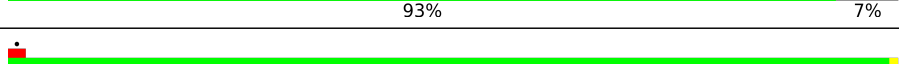
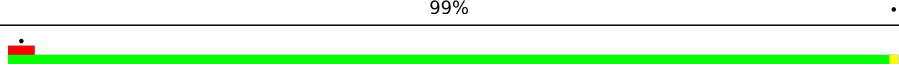
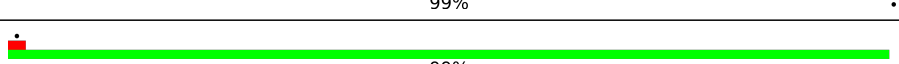
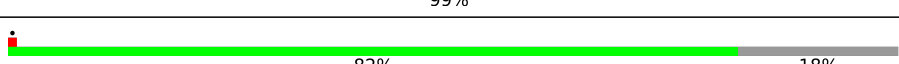
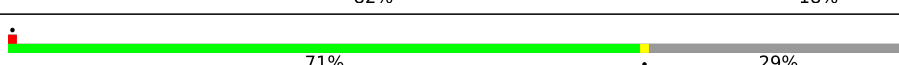
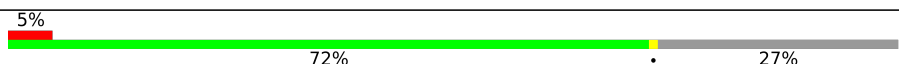
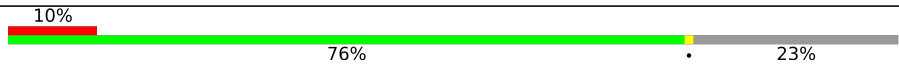
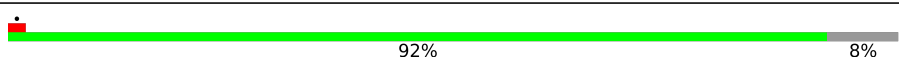
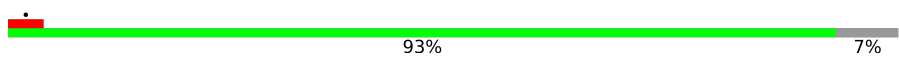

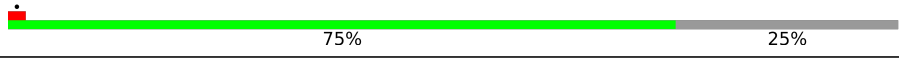
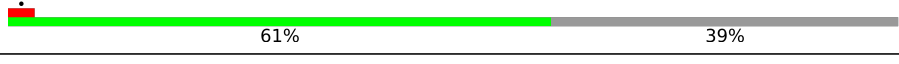


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	93% 7%
1	L	480	92% 7%
2	B	453	92% 8%
2	M	453	93% 7%
3	C	381	99%
3	N	381	99%
4	D	325	74% 26%
4	O	325	74% 26%
5	E	274	38% 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	n	514	
12	o	227	
13	p	261	
14	q	169	
15	r	146	
16	s	128	
17	t	97	
18	u	86	
19	v	76	
20	x	80	
21	y	63	
22	z	70	
23	w	83	

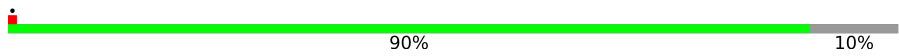
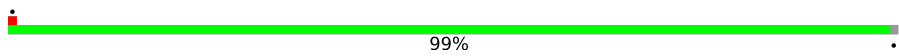
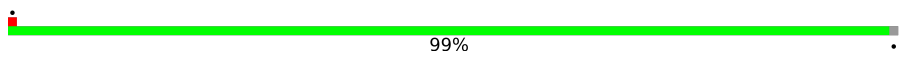
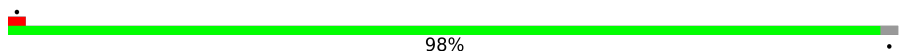
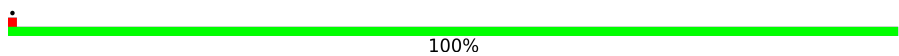
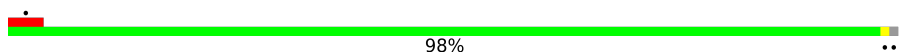

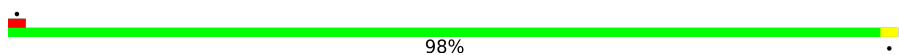
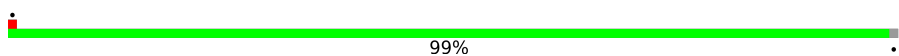
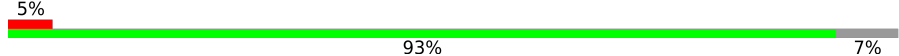

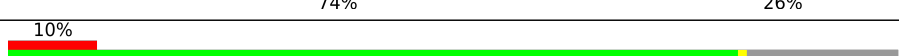
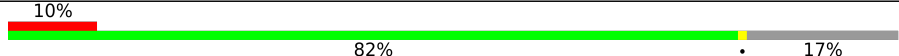

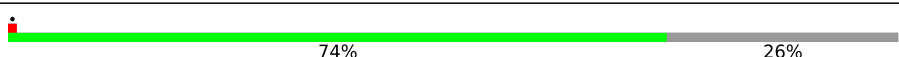

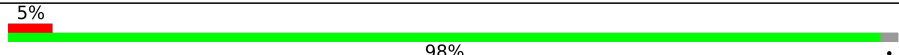
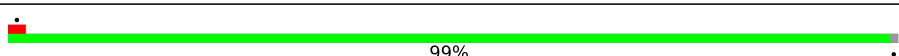
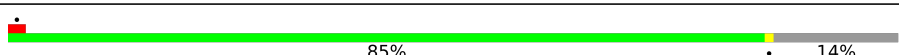
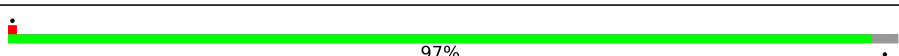
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Mol	Chain	Length	Quality of chain
24	6	224	69% 30%
25	C1	263	79% 21%
26	D1	463	5% 92% 7%
27	2	248	85% 14%
28	1	464	92% 7%
29	3	727	95% 5%
30	9	212	84% 16%
31	P1	377	90% 9%
32	Q1	175	72% 28%
33	7	116	82% 17%
34	S1	99	84% 15%
35	T1	156	51% 49%
35	U1	156	56% 44%
36	V1	116	97%
37	W1	131	87% 13%
38	q1	145	100%
39	r1	113	86% 12%
40	s1	104	38% 60%
41	A1	115	100%
42	H1	318	99%
43	J1	172	17% 100%
44	K1	98	99%
45	L1	607	100%
46	M1	459	100%
47	N1	345	100%

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Mol	Chain	Length	Quality of chain
48	O1	355	 90% 10%
49	X1	172	 99%
50	Y1	141	 99%
51	Z1	144	 98%
52	a1	70	 100%
53	b1	84	 98%
54	c1	76	 63% 37%
55	d1	120	 98%
56	e1	106	 99%
57	f1	57	 5% 93% 7%
58	g1	151	 5% 67% 33%
59	h1	189	 74% 26%
60	i1	128	 10% 82% 17%
61	j1	105	 61% 38%
62	k1	104	 74% 26%
63	l1	186	 84% 16%
64	m1	129	 5% 98%
65	n1	179	 99%
66	o1	137	 85% 14%
67	p1	176	 97%

2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 115643 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	418	Total	C	N	O	S	0	0
			3138	1970	552	607	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
			1167	705	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	101	Total	C	N	O	S	0	0
			894	572	159	160	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	51	Total	C	N	O	S	0	0
			422	281	75	65	1		
10	V	52	Total	C	N	O	S	0	0
			430	287	76	66	1		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

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

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	p	260	Total	C	N	O	S	0	0
			2118	1418	339	351	10		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

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

- Molecule 15 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	104	Total	C	N	O	S	0	0
			842	538	141	161	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	s	93	Total	C	N	O	S	0	0
			717	447	125	137	8		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

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

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6B1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	v	71	Total	C	N	O	S	0	0
			567	369	102	93	3		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	x	49	Total	C	N	O	S	0	0
			383	248	65	68	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	y	47	Total	C	N	O	S	0	0
			386	256	65	63	2		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

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

- Molecule 23 is a protein called Cytochrome c oxidase subunit 7A2, mitochondrial.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	6	157	1258	802	227	215	14	0	0

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	2	214	1660	1056	279	314	11	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	1	430	3321	2092	596	611	22	0	0

- Molecule 29 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	3	690	5305	3326	921	1017	41	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	9	178	1431	898	245	276	12	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

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

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	7	96	758	470	141	144	3	0	0

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 35 is a protein called Acyl carrier protein, mitochondrial.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 3.

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

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 1.

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

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 47 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 48 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 49 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 50 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 51 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

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

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

- Molecule 53 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 54 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 55 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 56 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 57 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

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

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

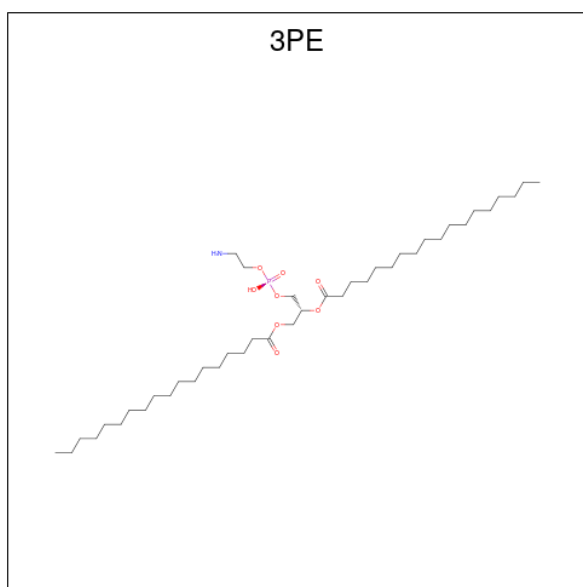
- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 68 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



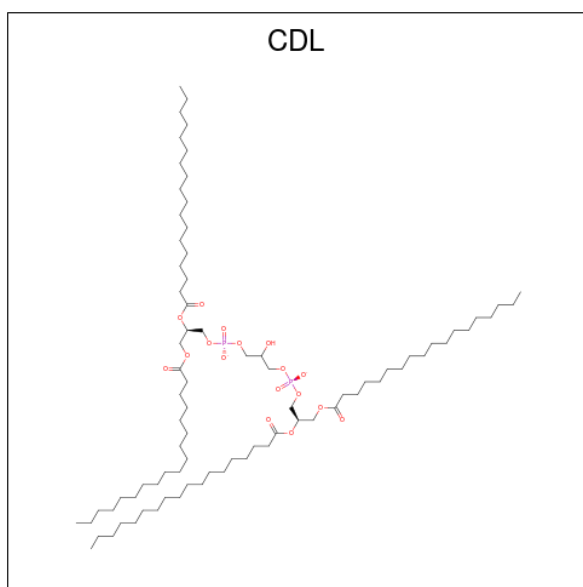
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
68	A	1	23	13	1	8	1	0
68	C	1	35	25	1	8	1	0
68	C	1	51	41	1	8	1	0
68	C	1	31	21	1	8	1	0
68	L	1	23	13	1	8	1	0
68	N	1	34	24	1	8	1	0
68	N	1	37	27	1	8	1	0
68	P	1	33	23	1	8	1	0
68	R	1	30	20	1	8	1	0
68	n	1	34	24	1	8	1	0
68	n	1	28	18	1	8	1	0
68	o	1	29	19	1	8	1	0
68	p	1	45	35	1	8	1	0
68	q	1	26	16	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
68	t	1	Total 25	C 15	N 1	O 8	P 1	0
68	v	1	Total 28	C 18	N 1	O 8	P 1	0
68	x	1	Total 27	C 17	N 1	O 8	P 1	0
68	6	1	Total 32	C 22	N 1	O 8	P 1	0
68	D1	1	Total 51	C 41	N 1	O 8	P 1	0
68	A1	1	Total 43	C 33	N 1	O 8	P 1	0
68	H1	1	Total 46	C 36	N 1	O 8	P 1	0
68	K1	1	Total 41	C 31	N 1	O 8	P 1	0
68	L1	1	Total 51	C 41	N 1	O 8	P 1	0
68	L1	1	Total 51	C 41	N 1	O 8	P 1	0
68	M1	1	Total 51	C 41	N 1	O 8	P 1	0
68	M1	1	Total 36	C 26	N 1	O 8	P 1	0
68	N1	1	Total 38	C 28	N 1	O 8	P 1	0
68	Y1	1	Total 28	C 18	N 1	O 8	P 1	0
68	Y1	1	Total 42	C 32	N 1	O 8	P 1	0
68	Z1	1	Total 51	C 41	N 1	O 8	P 1	0
68	d1	1	Total 31	C 21	N 1	O 8	P 1	0
68	d1	1	Total 32	C 22	N 1	O 8	P 1	0
68	i1	1	Total 42	C 32	N 1	O 8	P 1	0

- Molecule 69 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



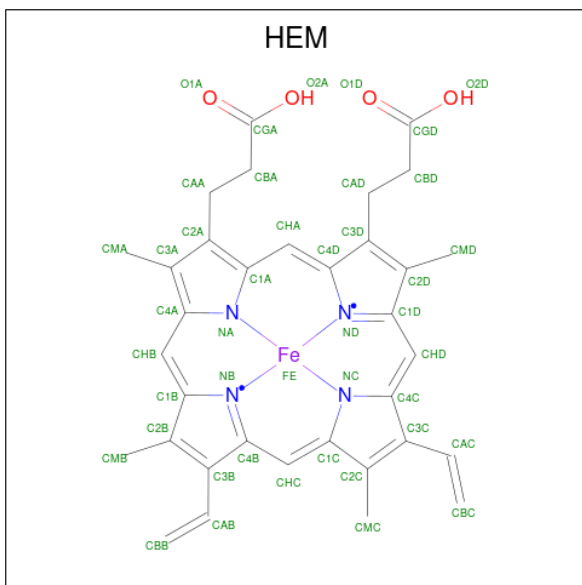
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
69	A	1	46	27	17	2	0
69	C	1	42	23	17	2	0
69	D	1	56	37	17	2	0
69	L	1	46	27	17	2	0
69	R	1	57	38	17	2	0
69	R	1	41	22	17	2	0
69	R	1	57	38	17	2	0
69	V	1	38	20	16	2	0
69	H1	1	51	33	16	2	0
69	L1	1	78	59	17	2	0
69	L1	1	46	27	17	2	0
69	N1	1	90	71	17	2	0
69	Y1	1	94	75	17	2	0
69	Y1	1	72	53	17	2	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
69	a1	1	Total	C	O	P	0
			57	38	17	2	
69	d1	1	Total	C	O	P	0
			67	48	17	2	
69	h1	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 70 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



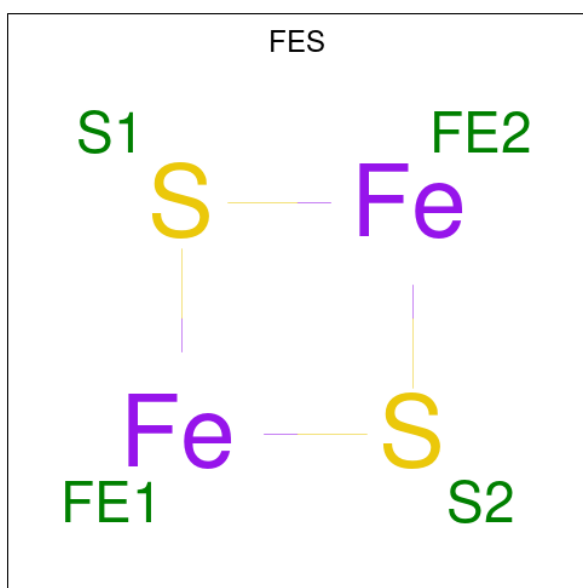
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
70	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
70	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 71 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 72 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



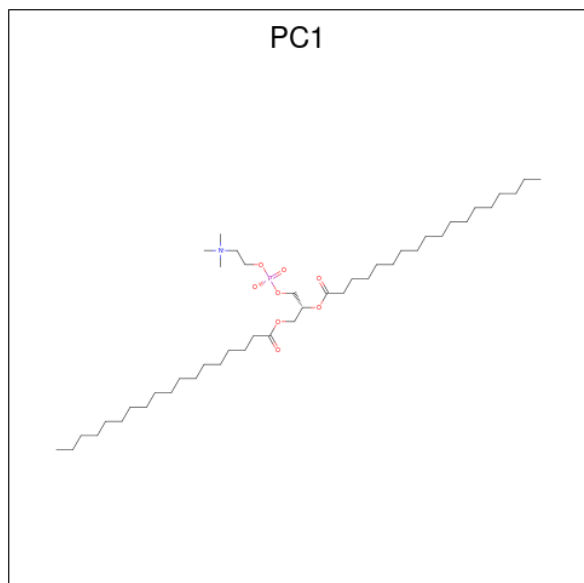
Mol	Chain	Residues	Atoms		AltConf
72	E	1	Total	Fe S	0
			4	2 2	
72	P	1	Total	Fe S	0
			4	2 2	

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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
72	2	1	4	2	2	0
72	3	1	4	2	2	0

- Molecule 73 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	
73	E	1	35	25	1	8	1	0
73	K	1	28	18	1	8	1	0
73	L	1	24	14	1	8	1	0
73	V	1	28	18	1	8	1	0
73	p	1	35	25	1	8	1	0
73	p	1	50	40	1	8	1	0
73	z	1	28	18	1	8	1	0
73	6	1	43	33	1	8	1	0
73	9	1	54	44	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
73	9	1	Total	C	N	O	P	0
			47	37	1	8	1	
73	A1	1	Total	C	N	O	P	0
			31	21	1	8	1	
73	M1	1	Total	C	N	O	P	0
			54	44	1	8	1	

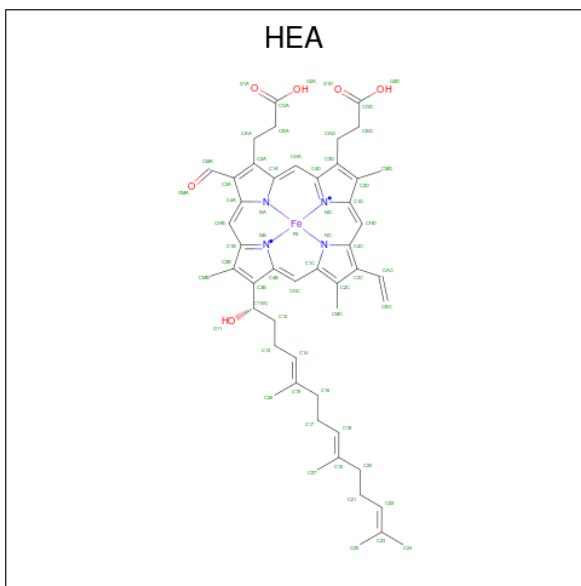
- Molecule 74 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
74	n	1	Total	Cu	0
			1	1	

- Molecule 75 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
75	n	1	Total	Na	0
			1	1	

- Molecule 76 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).

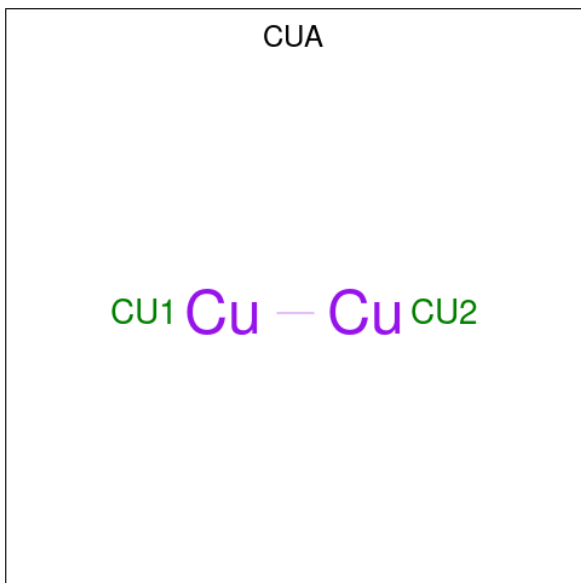


Mol	Chain	Residues	Atoms					AltConf
76	n	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
76	n	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 77 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
77	o	1	Total	Mg	0
			1	1	
77	O1	1	Total	Mg	0
			1	1	

- Molecule 78 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).

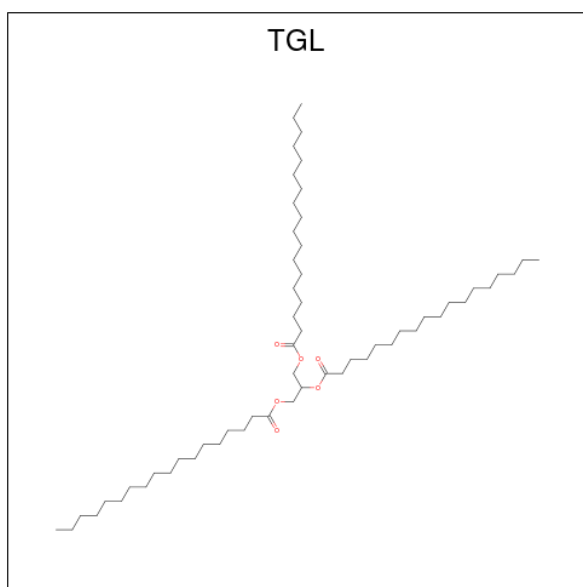


Mol	Chain	Residues	Atoms		AltConf
78	o	1	Total	Cu	0
			2	2	

- Molecule 79 is ZINC ION (three-letter code: ZN) (formula: Zn).

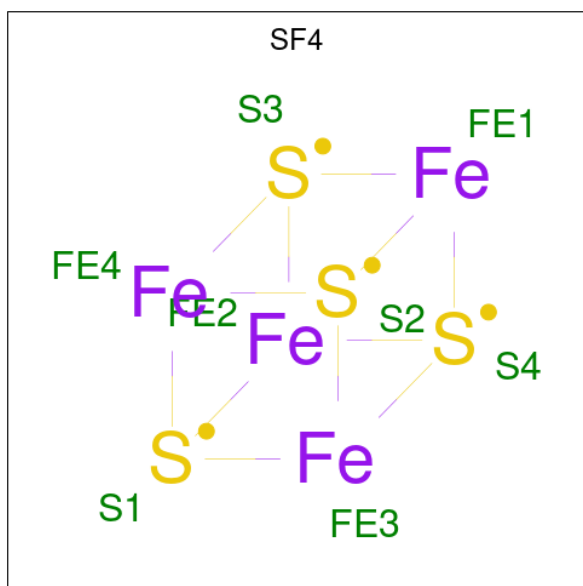
Mol	Chain	Residues	Atoms		AltConf
79	s	1	Total	Zn	0
			1	1	
79	7	1	Total	Zn	0
			1	1	

- Molecule 80 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



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

- Molecule 81 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



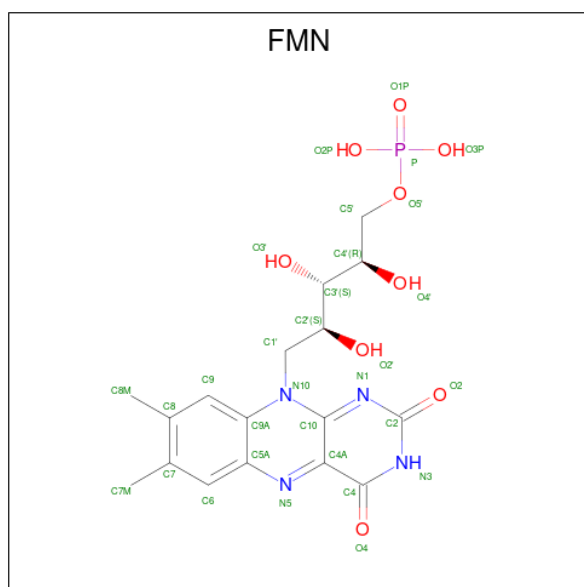
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
81	6	1	8	4	4	0
81	1	1	8	4	4	0
81	3	1	8	4	4	0

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Mol	Chain	Residues	Atoms			AltConf
81	3	1	Total	Fe	S	0
			8	4	4	
81	9	1	Total	Fe	S	0
			8	4	4	
81	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 82 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

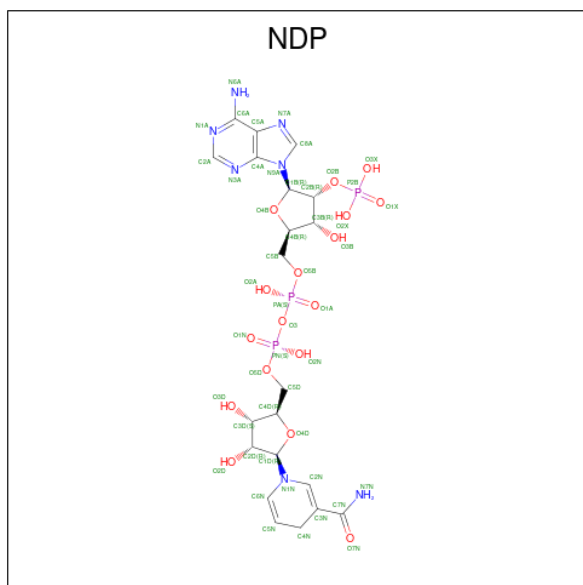


Mol	Chain	Residues	Atoms					AltConf
82	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 83 is POTASSIUM ION (three-letter code: K) (formula: K).

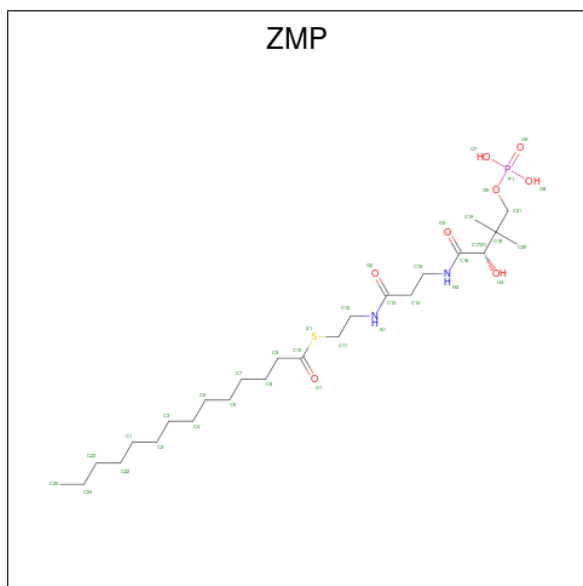
Mol	Chain	Residues	Atoms		AltConf
83	3	1	Total	K	0
			1	1	

- Molecule 84 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



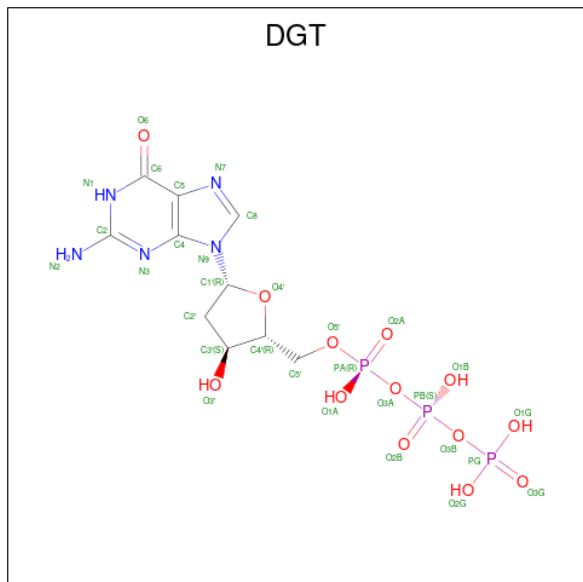
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
84	P1	1	48	21	7	17	3	0

- Molecule 85 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
85	W1	1	34	23	2	7	1	1	0
85	n1	1	32	21	2	7	1	1	0

- Molecule 86 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

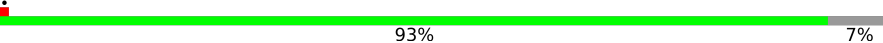


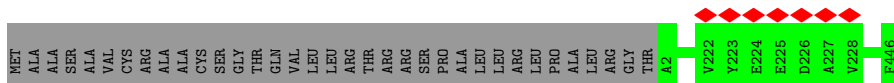
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
86	O1	1	31	10	5	13	3	0

3 Residue-property plots [i](#)

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

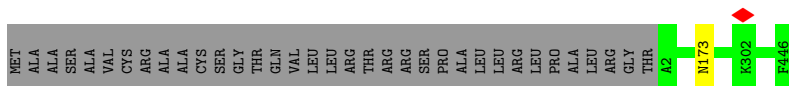
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A:  93% 7%



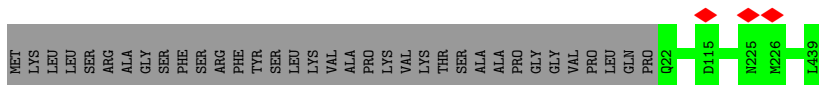
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L:  92% 7%



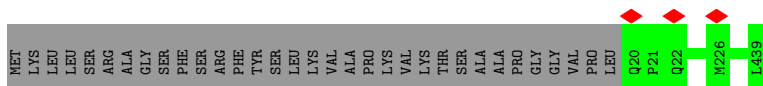
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:  92% 8%



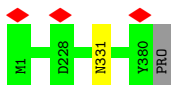
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:  93% 7%

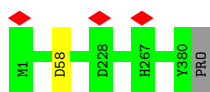


- Molecule 3: Cytochrome b

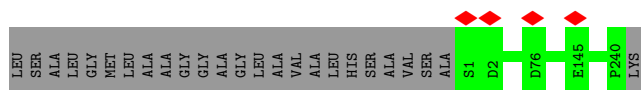
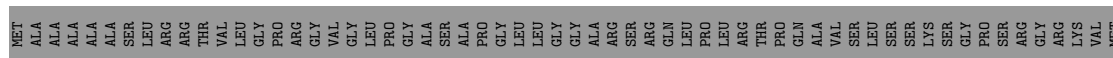
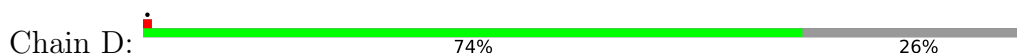
Chain C:  99%



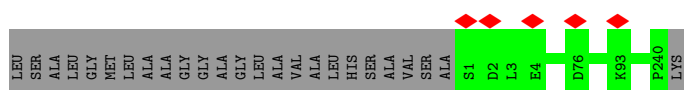
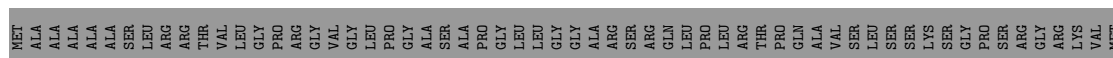
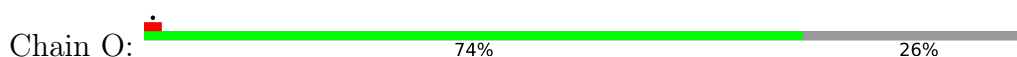
• Molecule 3: Cytochrome b



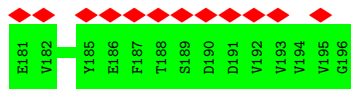
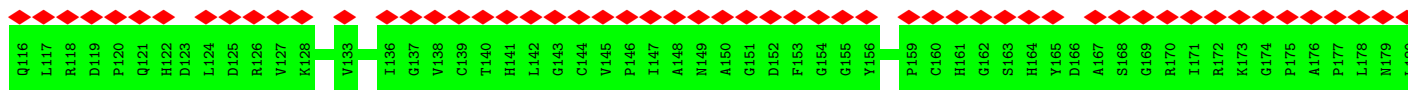
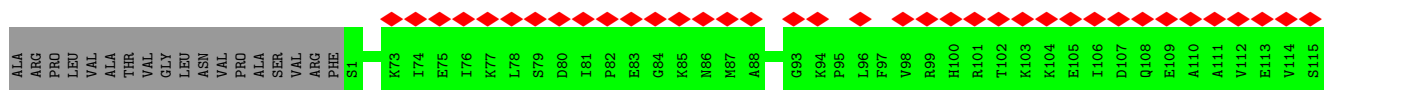
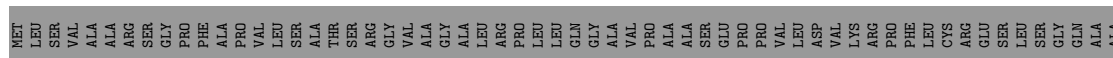
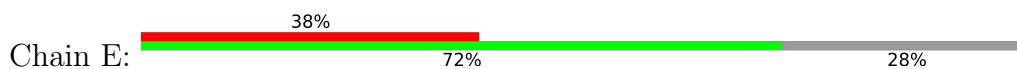
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



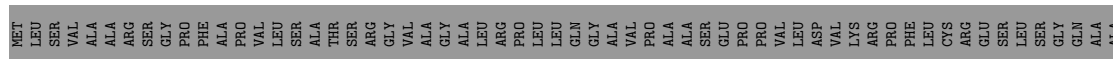
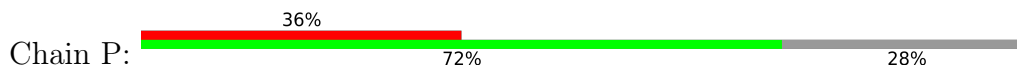
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

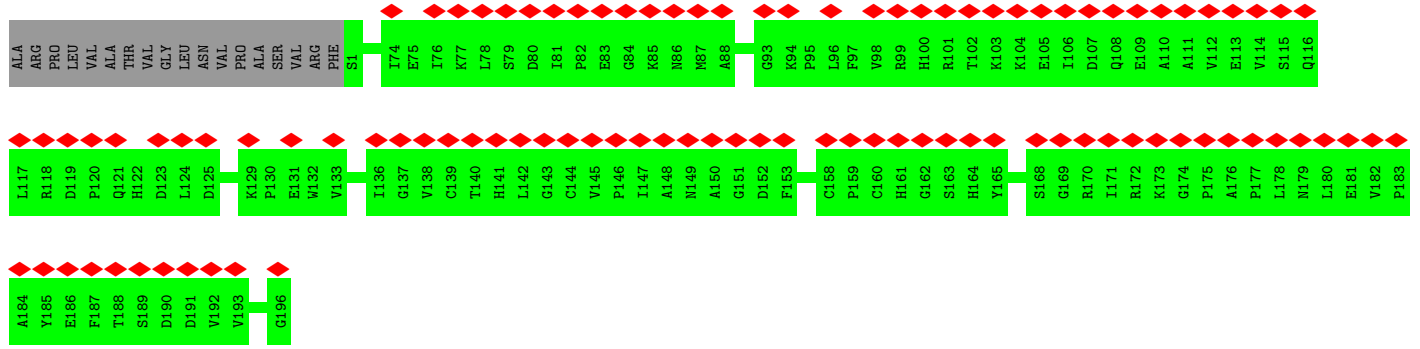


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

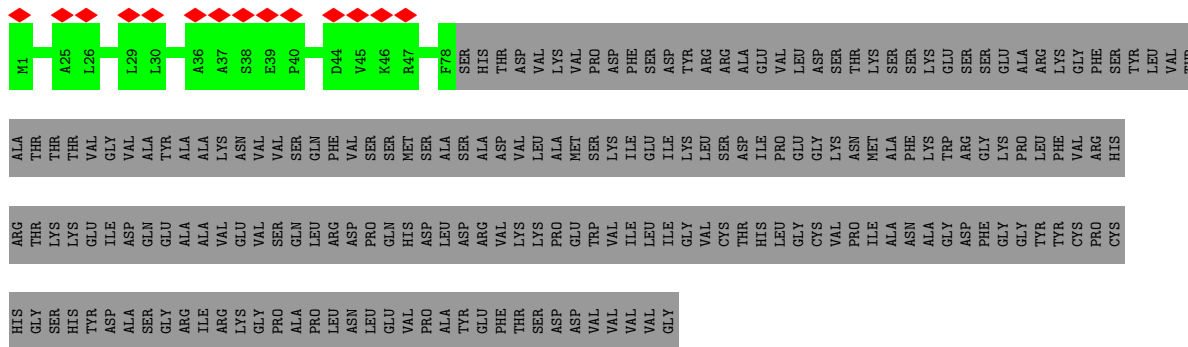


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

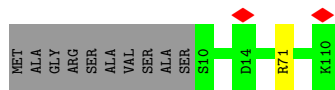
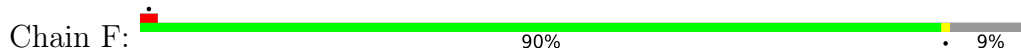




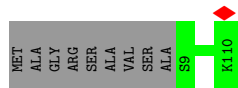
● Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



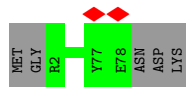
● Molecule 6: Cytochrome b-c1 complex subunit 7



● Molecule 6: Cytochrome b-c1 complex subunit 7



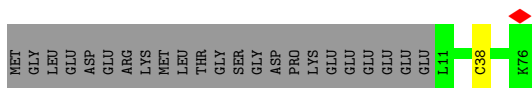
● Molecule 7: Cytochrome b-c1 complex subunit 8



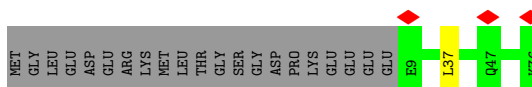
● Molecule 7: Cytochrome b-c1 complex subunit 8



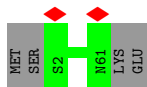
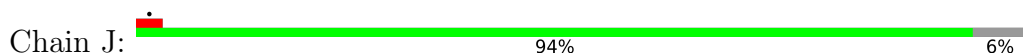
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



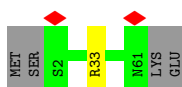
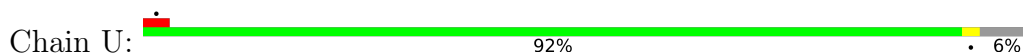
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



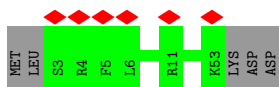
- Molecule 9: Cytochrome b-c1 complex subunit 9



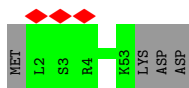
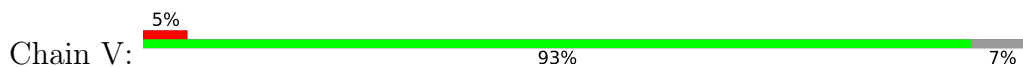
- Molecule 9: Cytochrome b-c1 complex subunit 9



- Molecule 10: Cytochrome b-c1 complex subunit 10

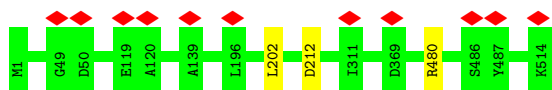


- Molecule 10: Cytochrome b-c1 complex subunit 10



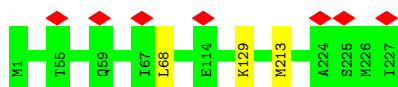
- Molecule 11: Cytochrome c oxidase subunit 1

Chain n:  99%



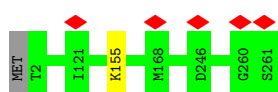
- Molecule 12: Cytochrome c oxidase subunit 2

Chain o:  99%




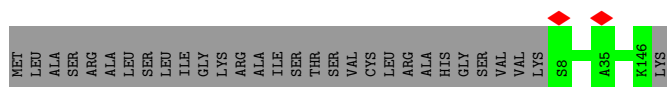
- Molecule 13: Cytochrome c oxidase subunit 3

Chain p:  99%



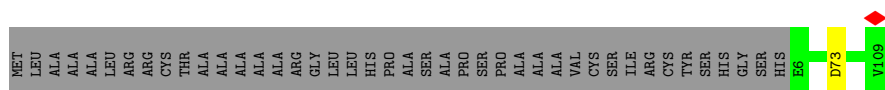
- Molecule 14: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain q:  82% 18%



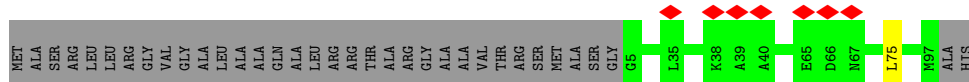
- Molecule 15: Cytochrome c oxidase subunit 5A, mitochondrial

Chain r:  71% 29%



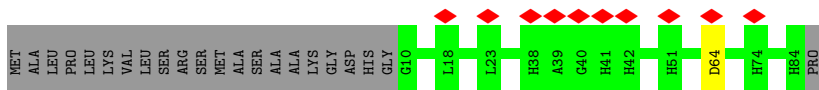
- Molecule 16: Cytochrome c oxidase subunit 5B, mitochondrial

Chain s:  5% 72% 27%

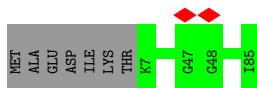
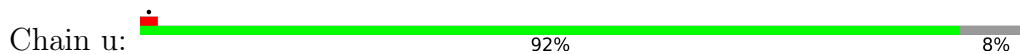


- Molecule 17: Cytochrome c oxidase subunit 6A2, mitochondrial

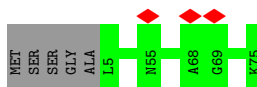
Chain t:  10% 76% 23%



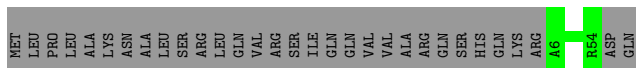
- Molecule 18: Cytochrome c oxidase subunit 6B1



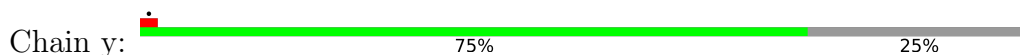
- Molecule 19: Cytochrome c oxidase subunit 6C



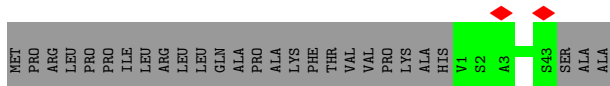
- Molecule 20: Cytochrome c oxidase subunit 7B, mitochondrial



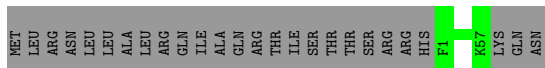
- Molecule 21: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 22: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 23: Cytochrome c oxidase subunit 7A2, mitochondrial



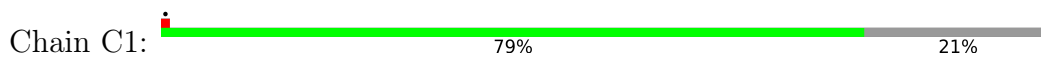
- Molecule 24: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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

PRO LYS LEU SER HIS LEU PRO R33 R34 D44 E119 D147 R189

- Molecule 25: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



MET ALA ALA ALA ALA ARG VAL TRP CYS ARG ARG GLY LEU LEU ALA ALA ALA VAL ARG GLY ARG GLY ILE ARG PRO SER VAL GLN TRP TRP GLN HIS VAL ARG ARG GLU SER ALA ALA ASP K7 D16 E214 SER LEU LYS LEU LEU GLU ALA GLY ASP LYS LYS PRO GLU THR LYS

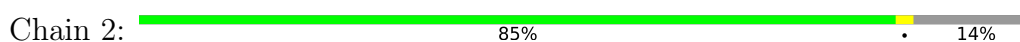
- Molecule 26: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



MET ALA ALA LEU LEU ALA ARG ARG CYS ARG ARG GLY VAL GLY ALA PRO VAL VAL ARG PRO GLY SER ARG ILE LEU PRO GLN SER ARG GLY A1 R2 E9 E12 Q13 S22 K23 E24 T26 A26 H27 W28 K29 P30 P31 P32 D37 I38 L39 K40 E41 K42 A43

V44 T45 R85 M170 L208 D422 R430

- Molecule 27: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



MET PHE SER LEU ALA ARG ALA ARG THR LEU LEU ALA ALA GLN TRP GLY ARG HIS ALA ARG ASN LEU HIS LYS THR ALA VAL HIS GLN ASN GLY ALA G4 N37 D112 D114 K183 L217

- Molecule 28: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



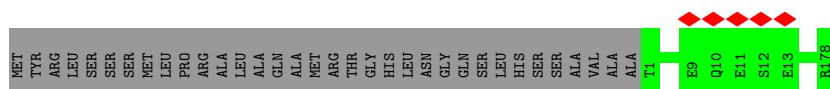
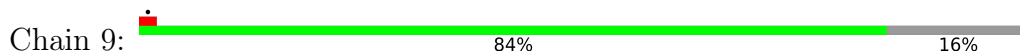
MET LEU ALA ARG PRO HIS PHE LEU LEU VAL PRO VAL VAL SER PRO VAL ARG PHE VAL SER SER THR THR THR THR ALA PRO LYS K9 K96 R438 ALA TRP GLN ALA SER

- Molecule 29: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

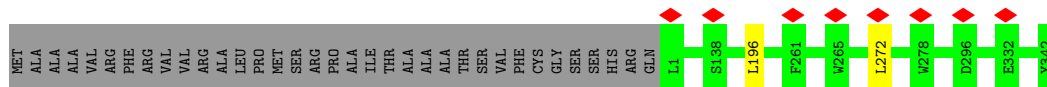
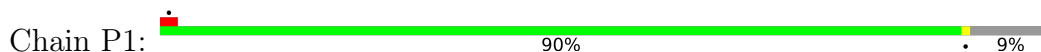


MET LEU ARG ILE PRO ILE LYS ARG ALA LEU LEU ILE GLY LEU SER ASN SER PRO LYS GLY TYR VAL THR THR THR THR THR ALA A5 M74 E311 K444 D540 N653 A658 D659 E693 G694 ALA GLN ALA VAL VAL GLU PRO PRO SER ILE CYS

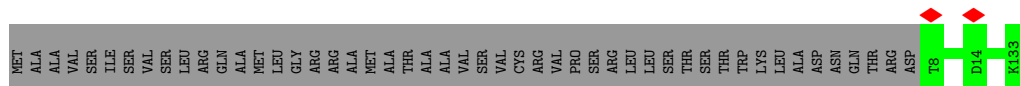
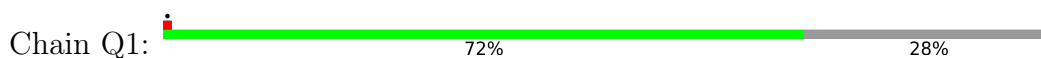
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



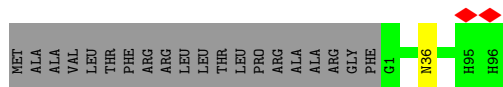
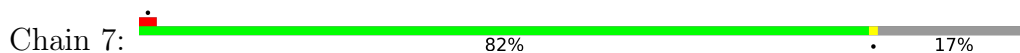
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



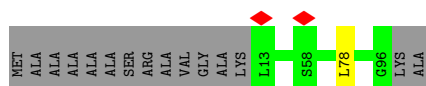
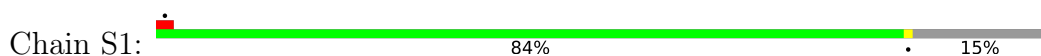
- Molecule 32: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



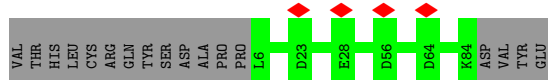
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 34: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



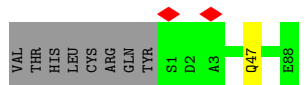
- Molecule 35: Acyl carrier protein, mitochondrial



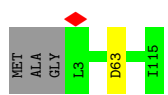
- Molecule 35: Acyl carrier protein, mitochondrial



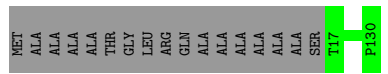
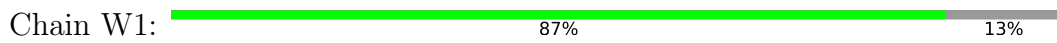
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- Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



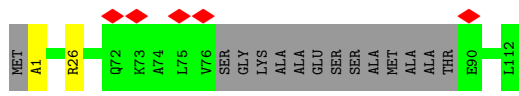
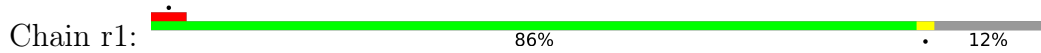
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



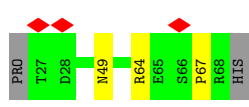
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 40: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

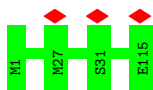


MET ALA VAL SER LEU LEU ARG GLY GLY ARG ARG TLE ARG ALA LEU LYS ALA ALA VAL VAL LEU LEU GLU ALA ARG VAL PHE PRO GLY LEU VAL VAL VAL VAL ARG SER THR SER SER LYS ALA LYS GLU LEU LEU HIS PRO LYS GLN SER VAL VAL LYS GLU PRO GLU

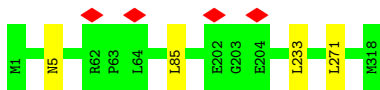


- Molecule 41: NADH-ubiquinone oxidoreductase chain 3

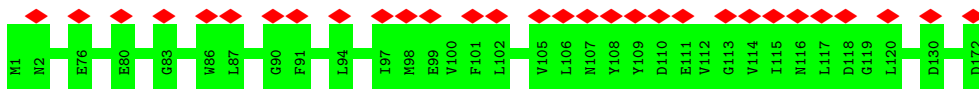




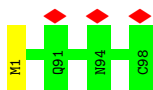
- Molecule 42: NADH-ubiquinone oxidoreductase chain 1



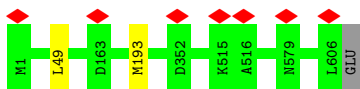
- Molecule 43: NADH-ubiquinone oxidoreductase chain 6



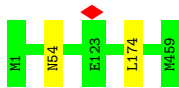
- Molecule 44: NADH-ubiquinone oxidoreductase chain 4L



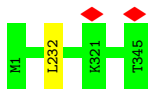
- Molecule 45: NADH-ubiquinone oxidoreductase chain 5



- Molecule 46: NADH-ubiquinone oxidoreductase chain 4

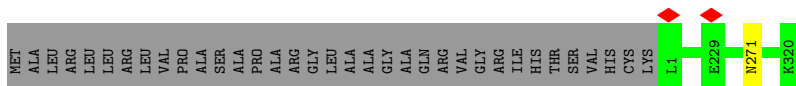


- Molecule 47: NADH-ubiquinone oxidoreductase chain 2



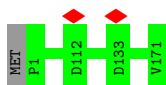
- Molecule 48: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O1:  90% 10%



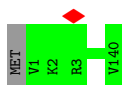
- Molecule 49: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X1:  99%



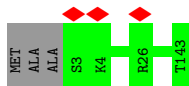
- Molecule 50: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y1:  99%



- Molecule 51: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z1:  98%



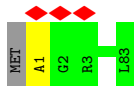
- Molecule 52: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a1:  100%



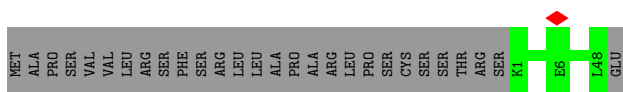
- Molecule 53: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b1:  98%



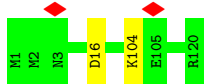
- Molecule 54: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c1:  63% 37%



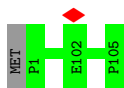
- Molecule 55: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d1: 98%



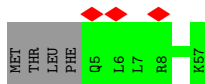
- Molecule 56: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e1: 99%



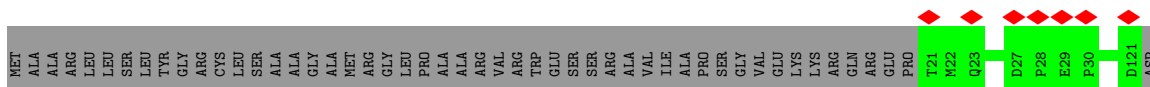
- Molecule 57: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f1: 5% 93% 7%



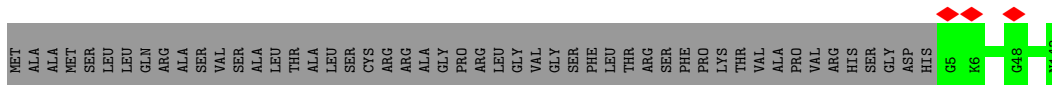
- Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g1: 5% 67% 33%



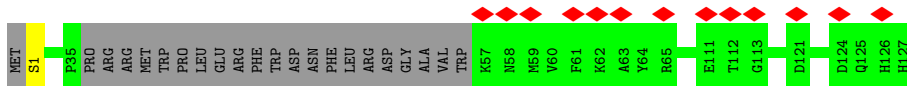
- Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h1: 5% 74% 26%

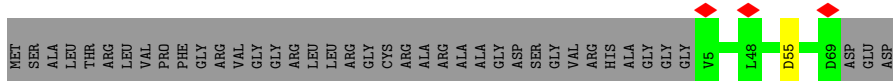


- Molecule 60: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

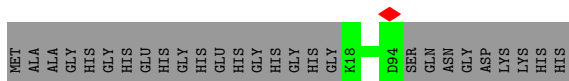
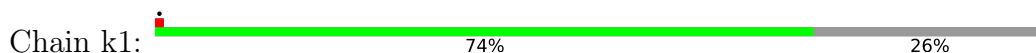
Chain i1: 10% 82% 17%



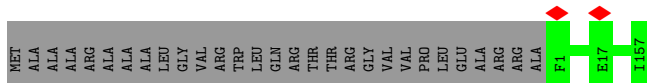
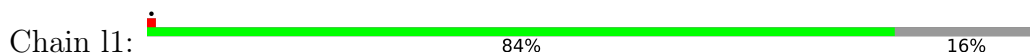
- Molecule 61: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



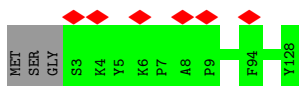
- Molecule 62: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 63: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



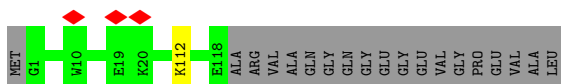
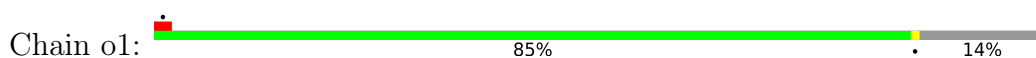
- Molecule 64: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



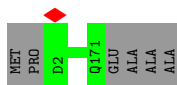
- Molecule 65: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 66: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 67: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103207	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	0.154	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	297.86, 218.35999, 261.81998	wwPDB
Map dimensions	281, 206, 247	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, 2MR, AYA, MG, SAC, FME, K, DGT, SF4, TGL, CUA, FES, HEC, NDP, HEA, FMN, HEM, NA, ZN, PC1, 3PE, CDL, 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	0.28	0/3529	0.56	0/4793
1	L	0.28	0/3530	0.55	0/4793
2	B	0.27	0/3188	0.51	0/4308
2	M	0.28	0/3205	0.53	0/4332
3	C	0.30	0/3147	0.52	0/4297
3	N	0.29	0/3147	0.52	1/4297 (0.0%)
4	D	0.29	0/1968	0.52	0/2674
4	O	0.27	0/1968	0.50	0/2674
5	E	0.27	0/1176	0.52	0/1609
5	P	0.27	0/1176	0.49	0/1609
5	T	0.30	0/565	0.65	0/772
6	F	0.27	0/916	0.57	0/1226
6	Q	0.30	0/922	0.56	0/1234
7	G	0.34	0/673	0.62	0/909
7	R	0.36	0/673	0.66	0/909
8	H	0.35	0/552	0.76	1/739 (0.1%)
8	S	0.32	0/570	0.71	1/763 (0.1%)
9	J	0.30	0/509	0.62	0/687
9	U	0.30	0/509	0.53	0/687
10	K	0.27	0/438	0.61	0/598
10	V	0.27	0/446	0.62	0/609
11	n	0.33	0/4162	0.60	2/5686 (0.0%)
12	o	0.31	0/1863	0.67	1/2542 (0.0%)
13	p	0.30	0/2202	0.57	0/3010
14	q	0.30	0/1190	0.57	0/1609
15	r	0.31	0/860	0.67	1/1167 (0.1%)
16	s	0.28	0/734	0.56	1/996 (0.1%)
17	t	0.28	0/632	0.61	1/866 (0.1%)
18	u	0.33	0/674	0.64	0/910
19	v	0.29	0/579	0.61	0/771
20	x	0.31	0/396	0.65	0/541

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	y	0.29	0/399	0.54	0/535
22	z	0.29	0/318	0.57	0/433
23	w	0.28	0/444	0.65	0/598
24	6	0.35	0/1289	0.71	3/1744 (0.2%)
25	C1	0.30	0/1780	0.57	0/2424
26	D1	0.32	0/3540	0.58	3/4795 (0.1%)
27	2	0.33	0/1700	0.64	2/2316 (0.1%)
28	1	0.30	0/3396	0.58	1/4586 (0.0%)
29	3	0.30	0/5392	0.57	0/7305
30	9	0.32	0/1461	0.56	0/1974
31	P1	0.29	0/2823	0.59	2/3828 (0.1%)
32	Q1	0.28	0/1045	0.54	0/1411
33	7	0.29	0/773	0.55	0/1041
34	S1	0.32	0/682	0.66	1/920 (0.1%)
35	T1	0.30	0/646	0.68	0/869
35	U1	0.33	0/718	0.52	0/970
36	V1	0.29	0/945	0.50	1/1281 (0.1%)
37	W1	0.30	0/993	0.58	0/1335
38	q1	0.31	0/1251	0.55	0/1702
39	r1	0.30	0/806	0.56	0/1090
40	s1	0.34	0/360	0.79	2/489 (0.4%)
41	A1	0.30	0/948	0.57	0/1295
42	H1	0.35	0/2607	0.65	3/3564 (0.1%)
43	J1	0.30	0/1330	0.52	0/1810
44	K1	0.29	0/738	0.58	0/1002
45	L1	0.31	0/4913	0.56	2/6686 (0.0%)
46	M1	0.29	0/3709	0.56	1/5052 (0.0%)
47	N1	0.30	0/2755	0.56	1/3751 (0.0%)
48	O1	0.28	0/2674	0.51	0/3626
49	X1	0.27	0/1434	0.51	0/1937
50	Y1	0.28	0/1061	0.49	0/1439
51	Z1	0.29	0/1198	0.56	0/1616
52	a1	0.27	0/585	0.56	0/788
53	b1	0.26	0/666	0.47	0/914
54	c1	0.29	0/409	0.52	0/555
55	d1	0.29	0/1028	0.58	1/1387 (0.1%)
56	e1	0.27	0/900	0.51	0/1199
57	f1	0.29	0/468	0.56	0/630
58	g1	0.29	0/878	0.51	0/1196
59	h1	0.28	0/1201	0.54	0/1626
60	i1	0.28	0/917	0.53	0/1243
61	j1	0.27	0/587	0.57	1/804 (0.1%)
62	k1	0.30	0/646	0.55	0/873

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
63	l1	0.28	0/1379	0.54	0/1882
64	m1	0.30	0/1079	0.57	0/1463
65	n1	0.30	0/1596	0.57	0/2162
66	o1	0.31	0/1039	0.62	0/1394
67	p1	0.29	0/1471	0.52	0/1988
All	All	0.30	0/115076	0.57	33/156145 (0.0%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	s1	67	PRO	CA-N-CD	-9.47	98.24	111.50
24	6	44	ASP	CB-CG-OD1	8.40	125.86	118.30
27	2	114	ASP	CB-CG-OD1	8.10	125.59	118.30
12	o	68	LEU	CA-CB-CG	7.83	133.31	115.30
11	n	212	ASP	CB-CG-OD1	7.34	124.91	118.30
3	N	58	ASP	CB-CG-OD1	6.96	124.56	118.30
42	H1	233	LEU	CB-CG-CD1	-6.70	99.61	111.00
17	t	64	ASP	CB-CG-OD1	6.49	124.14	118.30
31	P1	272	LEU	CA-CB-CG	6.47	130.19	115.30
27	2	112	ASP	CB-CG-OD1	6.37	124.04	118.30
55	d1	16	ASP	CB-CG-OD1	6.25	123.92	118.30
15	r	73	ASP	CB-CG-OD1	6.05	123.74	118.30
36	V1	63	ASP	CB-CG-OD1	6.01	123.71	118.30
61	j1	55	ASP	CB-CG-OD1	5.77	123.50	118.30
31	P1	196	LEU	CA-CB-CG	5.71	128.44	115.30
42	H1	271	LEU	CB-CG-CD2	-5.67	101.36	111.00
42	H1	85	LEU	CA-CB-CG	5.62	128.22	115.30
28	1	96	ASN	N-CA-C	-5.55	96.00	111.00
45	L1	193	MET	CG-SD-CE	-5.52	91.36	100.20
8	H	38	CYS	CA-CB-SG	5.49	123.87	114.00
8	S	37	LEU	CA-CB-CG	5.41	127.73	115.30
26	D1	170	MET	CB-CG-SD	5.39	128.58	112.40
47	N1	232	LEU	CA-CB-CG	5.39	127.69	115.30
24	6	44	ASP	CB-CG-OD2	-5.29	113.54	118.30
46	M1	174	LEU	CA-CB-CG	5.28	127.45	115.30
40	s1	67	PRO	N-CD-CG	-5.24	95.34	103.20
45	L1	49	LEU	CA-CB-CG	5.22	127.31	115.30
34	S1	78	LEU	CA-CB-CG	5.21	127.28	115.30
16	s	75	LEU	CA-CB-CG	5.19	127.23	115.30
24	6	147	ASP	CB-CG-OD1	5.17	122.95	118.30
26	D1	208	LEU	CA-CB-CG	5.15	127.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D1	422	ASP	CB-CG-OD1	5.15	122.93	118.30
11	n	202	LEU	CA-CB-CG	5.04	126.89	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 [i](#)

5.3.1 Protein backbone [i](#)

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%)	427 (96%)	16 (4%)	0	100	100
2	B	416/453 (92%)	410 (99%)	6 (1%)	0	100	100
2	M	418/453 (92%)	400 (96%)	18 (4%)	0	100	100
3	C	378/381 (99%)	368 (97%)	10 (3%)	0	100	100
3	N	378/381 (99%)	364 (96%)	14 (4%)	0	100	100
4	D	238/325 (73%)	228 (96%)	10 (4%)	0	100	100
4	O	238/325 (73%)	231 (97%)	7 (3%)	0	100	100
5	E	194/274 (71%)	188 (97%)	6 (3%)	0	100	100
5	P	194/274 (71%)	187 (96%)	7 (4%)	0	100	100
5	T	76/274 (28%)	72 (95%)	4 (5%)	0	100	100
6	F	99/111 (89%)	99 (100%)	0	0	100	100
6	Q	100/111 (90%)	99 (99%)	1 (1%)	0	100	100
7	G	75/82 (92%)	73 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	R	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
8	H	64/89 (72%)	62 (97%)	2 (3%)	0	100	100
8	S	66/89 (74%)	64 (97%)	2 (3%)	0	100	100
9	J	58/64 (91%)	56 (97%)	2 (3%)	0	100	100
9	U	58/64 (91%)	56 (97%)	2 (3%)	0	100	100
10	K	49/56 (88%)	47 (96%)	2 (4%)	0	100	100
10	V	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
11	n	512/514 (100%)	498 (97%)	14 (3%)	0	100	100
12	o	225/227 (99%)	212 (94%)	13 (6%)	0	100	100
13	p	258/261 (99%)	251 (97%)	7 (3%)	0	100	100
14	q	137/169 (81%)	130 (95%)	7 (5%)	0	100	100
15	r	102/146 (70%)	99 (97%)	3 (3%)	0	100	100
16	s	91/128 (71%)	84 (92%)	7 (8%)	0	100	100
17	t	73/97 (75%)	70 (96%)	3 (4%)	0	100	100
18	u	77/86 (90%)	75 (97%)	2 (3%)	0	100	100
19	v	69/76 (91%)	63 (91%)	6 (9%)	0	100	100
20	x	47/80 (59%)	44 (94%)	3 (6%)	0	100	100
21	y	45/63 (71%)	45 (100%)	0	0	100	100
22	z	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
23	w	55/83 (66%)	55 (100%)	0	0	100	100
24	6	155/224 (69%)	148 (96%)	7 (4%)	0	100	100
25	C1	206/263 (78%)	198 (96%)	8 (4%)	0	100	100
26	D1	427/463 (92%)	410 (96%)	17 (4%)	0	100	100
27	2	212/248 (86%)	202 (95%)	9 (4%)	1 (0%)	29	61
28	1	428/464 (92%)	409 (96%)	19 (4%)	0	100	100
29	3	688/727 (95%)	658 (96%)	30 (4%)	0	100	100
30	9	176/212 (83%)	173 (98%)	3 (2%)	0	100	100
31	P1	340/377 (90%)	324 (95%)	16 (5%)	0	100	100
32	Q1	124/175 (71%)	121 (98%)	3 (2%)	0	100	100
33	7	94/116 (81%)	91 (97%)	3 (3%)	0	100	100
34	S1	82/99 (83%)	77 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	T1	77/156 (49%)	74 (96%)	3 (4%)	0	100	100
35	U1	86/156 (55%)	83 (96%)	3 (4%)	0	100	100
36	V1	111/116 (96%)	109 (98%)	2 (2%)	0	100	100
37	W1	112/131 (86%)	108 (96%)	4 (4%)	0	100	100
38	q1	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
39	r1	95/113 (84%)	91 (96%)	4 (4%)	0	100	100
40	s1	40/104 (38%)	39 (98%)	1 (2%)	0	100	100
41	A1	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
42	H1	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
43	J1	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
44	K1	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
45	L1	604/607 (100%)	575 (95%)	29 (5%)	0	100	100
46	M1	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
47	N1	343/345 (99%)	333 (97%)	10 (3%)	0	100	100
48	O1	318/355 (90%)	297 (93%)	21 (7%)	0	100	100
49	X1	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
50	Y1	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
51	Z1	139/144 (96%)	136 (98%)	3 (2%)	0	100	100
52	a1	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
53	b1	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
54	c1	46/76 (60%)	44 (96%)	2 (4%)	0	100	100
55	d1	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
56	e1	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
57	f1	51/57 (90%)	50 (98%)	1 (2%)	0	100	100
58	g1	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
59	h1	137/189 (72%)	131 (96%)	6 (4%)	0	100	100
60	i1	102/128 (80%)	95 (93%)	7 (7%)	0	100	100
61	j1	63/105 (60%)	58 (92%)	5 (8%)	0	100	100
62	k1	75/104 (72%)	74 (99%)	1 (1%)	0	100	100
63	l1	155/186 (83%)	151 (97%)	4 (3%)	0	100	100
64	m1	124/129 (96%)	121 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
65	n1	176/179 (98%)	170 (97%)	6 (3%)	0	100	100
66	o1	116/137 (85%)	109 (94%)	7 (6%)	0	100	100
67	p1	168/176 (96%)	166 (99%)	2 (1%)	0	100	100
All	All	13983/16116 (87%)	13472 (96%)	510 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	2	183	LYS

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%)	371 (100%)	1 (0%)	92	96
2	B	328/356 (92%)	328 (100%)	0	100	100
2	M	330/356 (93%)	330 (100%)	0	100	100
3	C	332/333 (100%)	331 (100%)	1 (0%)	92	96
3	N	332/333 (100%)	332 (100%)	0	100	100
4	D	205/260 (79%)	205 (100%)	0	100	100
4	O	205/260 (79%)	205 (100%)	0	100	100
5	E	69/224 (31%)	69 (100%)	0	100	100
5	P	69/224 (31%)	69 (100%)	0	100	100
5	T	58/224 (26%)	58 (100%)	0	100	100
6	F	93/99 (94%)	92 (99%)	1 (1%)	73	85
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	50 (98%)	1 (2%)	55	76
10	K	41/46 (89%)	41 (100%)	0	100	100
10	V	42/46 (91%)	42 (100%)	0	100	100
11	n	425/425 (100%)	424 (100%)	1 (0%)	93	97
12	o	210/210 (100%)	208 (99%)	2 (1%)	76	86
13	p	226/227 (100%)	225 (100%)	1 (0%)	91	95
14	q	122/146 (84%)	122 (100%)	0	100	100
15	r	91/118 (77%)	91 (100%)	0	100	100
16	s	80/101 (79%)	80 (100%)	0	100	100
17	t	62/78 (80%)	62 (100%)	0	100	100
18	u	70/76 (92%)	70 (100%)	0	100	100
19	v	54/57 (95%)	54 (100%)	0	100	100
20	x	39/67 (58%)	39 (100%)	0	100	100
21	y	40/55 (73%)	40 (100%)	0	100	100
22	z	33/55 (60%)	33 (100%)	0	100	100
23	w	43/67 (64%)	43 (100%)	0	100	100
24	6	133/185 (72%)	132 (99%)	1 (1%)	81	89
25	C1	190/227 (84%)	190 (100%)	0	100	100
26	D1	370/394 (94%)	370 (100%)	0	100	100
27	2	184/206 (89%)	183 (100%)	1 (0%)	88	93
28	1	345/370 (93%)	345 (100%)	0	100	100
29	3	580/610 (95%)	579 (100%)	1 (0%)	93	97
30	9	152/178 (85%)	152 (100%)	0	100	100
31	P1	299/325 (92%)	299 (100%)	0	100	100
32	Q1	113/153 (74%)	113 (100%)	0	100	100
33	7	81/96 (84%)	80 (99%)	1 (1%)	71	83
34	S1	74/80 (92%)	74 (100%)	0	100	100
35	T1	73/135 (54%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	U1	81/135 (60%)	80 (99%)	1 (1%)	71	83
36	V1	101/102 (99%)	101 (100%)	0	100	100
37	W1	108/114 (95%)	108 (100%)	0	100	100
38	q1	131/131 (100%)	131 (100%)	0	100	100
39	r1	88/96 (92%)	87 (99%)	1 (1%)	73	85
40	s1	41/95 (43%)	39 (95%)	2 (5%)	25	56
41	A1	103/103 (100%)	103 (100%)	0	100	100
42	H1	279/279 (100%)	278 (100%)	1 (0%)	91	95
43	J1	137/137 (100%)	137 (100%)	0	100	100
44	K1	87/87 (100%)	87 (100%)	0	100	100
45	L1	548/549 (100%)	548 (100%)	0	100	100
46	M1	414/414 (100%)	413 (100%)	1 (0%)	93	97
47	N1	307/307 (100%)	307 (100%)	0	100	100
48	O1	284/309 (92%)	283 (100%)	1 (0%)	91	95
49	X1	153/154 (99%)	153 (100%)	0	100	100
50	Y1	105/106 (99%)	105 (100%)	0	100	100
51	Z1	122/123 (99%)	122 (100%)	0	100	100
52	a1	60/60 (100%)	60 (100%)	0	100	100
53	b1	72/73 (99%)	72 (100%)	0	100	100
54	c1	42/67 (63%)	42 (100%)	0	100	100
55	d1	107/107 (100%)	106 (99%)	1 (1%)	78	87
56	e1	93/94 (99%)	93 (100%)	0	100	100
57	f1	49/53 (92%)	49 (100%)	0	100	100
58	g1	92/129 (71%)	92 (100%)	0	100	100
59	h1	123/162 (76%)	123 (100%)	0	100	100
60	i1	99/119 (83%)	99 (100%)	0	100	100
61	j1	61/87 (70%)	61 (100%)	0	100	100
62	k1	60/78 (77%)	60 (100%)	0	100	100
63	l1	142/161 (88%)	142 (100%)	0	100	100
64	m1	112/114 (98%)	112 (100%)	0	100	100
65	n1	163/164 (99%)	163 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	o1	109/121 (90%)	108 (99%)	1 (1%)	78	87
67	p1	155/158 (98%)	155 (100%)	0	100	100
All	All	12029/13709 (88%)	12008 (100%)	21 (0%)	93	97

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	331	ASN
6	F	71	ARG
1	L	173	ASN
9	U	33	ARG
11	n	480	ARG
12	o	129	LYS
12	o	213	MET
13	p	155	LYS
24	6	33	ARG
27	2	37	ASN
29	3	444	LYS
33	7	36	ASN
39	r1	26	ARG
40	s1	49	ASN
40	s1	64	ARG
42	H1	5	ASN
46	M1	54	ASN
48	O1	271	ASN
35	U1	47	GLN
55	d1	104	LYS
66	o1	112	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
1	A	363	ASN
4	D	71	GLN
8	H	65	HIS
8	H	69	HIS
1	L	173	ASN
3	N	207	ASN
11	n	451	ASN

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Mol	Chain	Res	Type
13	p	70	HIS
15	r	94	ASN
27	2	58	ASN
46	M1	366	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
46	FME	M1	1	46	8,9,10	0.97	0	7,9,11	0.79	0
60	SAC	i1	1	60	7,8,9	1.00	0	8,9,11	0.98	1 (12%)
39	AYA	r1	1	39	6,7,8	1.29	1 (16%)	5,8,10	1.29	1 (20%)
45	FME	L1	1	45	8,9,10	0.91	0	7,9,11	0.95	0
47	FME	N1	1	47	8,9,10	0.92	0	7,9,11	0.94	0
41	FME	A1	1	41	8,9,10	0.94	0	7,9,11	0.83	0
53	AYA	b1	1	53	6,7,8	1.26	1 (16%)	5,8,10	1.29	1 (20%)
26	2MR	D1	85	26	10,12,13	2.58	2 (20%)	5,13,15	2.79	2 (40%)
42	FME	H1	1	42	8,9,10	0.97	0	7,9,11	0.77	0
44	FME	K1	1	44	8,9,10	0.90	0	7,9,11	1.83	2 (28%)
43	FME	J1	1	43	8,9,10	0.94	0	7,9,11	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	FME	M1	1	46	-	2/7/9/11	-
60	SAC	i1	1	60	-	0/7/8/10	-
39	AYA	r1	1	39	-	0/4/6/8	-
45	FME	L1	1	45	-	3/7/9/11	-
47	FME	N1	1	47	-	4/7/9/11	-
41	FME	A1	1	41	-	1/7/9/11	-
53	AYA	b1	1	53	-	0/4/6/8	-
26	2MR	D1	85	26	-	3/10/13/15	-
42	FME	H1	1	42	-	3/7/9/11	-
44	FME	K1	1	44	-	5/7/9/11	-
43	FME	J1	1	43	-	3/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D1	85	2MR	CZ-NE	5.89	1.46	1.34
26	D1	85	2MR	CZ-NH2	5.01	1.44	1.33
39	r1	1	AYA	CA-N	-2.55	1.43	1.46
53	b1	1	AYA	CA-N	-2.35	1.44	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D1	85	2MR	CD-NE-CZ	5.27	133.27	123.41
44	K1	1	FME	C-CA-N	4.05	117.05	109.73
26	D1	85	2MR	NE-CZ-NH2	-3.00	116.73	119.48
39	r1	1	AYA	CB-CA-N	2.72	112.63	109.61
53	b1	1	AYA	CB-CA-N	2.61	112.51	109.61
60	i1	1	SAC	OG-CB-CA	-2.35	104.98	110.97
44	K1	1	FME	O-C-CA	-2.20	119.02	124.78

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	H1	1	FME	N-CA-CB-CG
43	J1	1	FME	C-CA-CB-CG
44	K1	1	FME	O1-CN-N-CA
44	K1	1	FME	N-CA-CB-CG
45	L1	1	FME	CB-CA-N-CN
45	L1	1	FME	N-CA-CB-CG

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 94 ligands modelled in this entry, 7 are monoatomic - leaving 87 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	$\# Z > 2$
81	SF4	3	801	29	0,12,12	-	-	-		
68	3PE	M1	502	-	50,50,50	0.30	0	53,55,55	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	3PE	n	605	-	33,33,50	0.38	0	36,38,55	0.56	1 (2%)
73	PC1	z	101	-	27,27,53	0.38	0	33,35,61	0.35	0
81	SF4	6	201	24	0,12,12	-	-	-		
68	3PE	C	405	-	50,50,50	0.31	0	53,55,55	0.28	0
68	3PE	Z1	401	-	50,50,50	0.31	0	53,55,55	0.46	1 (1%)
70	HEM	N	403	3	41,50,50	1.43	4 (9%)	45,82,82	1.38	6 (13%)
68	3PE	R	304	-	29,29,50	0.38	0	32,34,55	0.33	0
73	PC1	6	203	-	42,42,53	0.33	0	48,50,61	0.49	0
68	3PE	L1	701	-	50,50,50	0.31	0	53,55,55	0.47	0
68	3PE	q	201	-	25,25,50	0.41	0	28,30,55	0.40	0
71	HEC	D	301	4	32,50,50	2.18	3 (9%)	24,82,82	1.54	5 (20%)
68	3PE	v	101	-	27,27,50	0.40	0	30,32,55	0.34	0
68	3PE	n	606	-	27,27,50	0.41	0	30,32,55	0.38	0
68	3PE	x	101	-	26,26,50	0.40	0	29,31,55	0.35	0
81	SF4	9	202	30	0,12,12	-	-	-		
73	PC1	9	203	-	53,53,53	0.30	0	59,61,61	0.45	0
73	PC1	p	302	-	34,34,53	0.36	0	40,42,61	0.33	0
70	HEM	N	402	3	41,50,50	1.44	3 (7%)	45,82,82	1.50	9 (20%)
68	3PE	6	202	-	31,31,50	0.37	0	34,36,55	0.32	0
72	FES	P	202	5	0,4,4	-	-	-		
73	PC1	9	204	-	46,46,53	0.32	0	52,54,61	0.28	0
68	3PE	L	501	-	22,22,50	0.43	0	25,27,55	0.38	0
69	CDL	L1	703	-	45,45,99	0.43	0	51,57,111	0.36	0
68	3PE	C	406	-	30,30,50	0.39	0	33,35,55	0.34	0
68	3PE	N1	402	-	37,37,50	0.35	0	40,42,55	0.33	0
68	3PE	A	501	-	22,22,50	0.45	0	25,27,55	0.65	0
69	CDL	H1	402	-	50,50,99	0.42	0	55,61,111	0.36	0
68	3PE	d1	203	-	31,31,50	0.37	0	34,36,55	0.34	0
76	HEA	n	603	11	57,67,67	1.44	7 (12%)	61,103,103	2.45	23 (37%)
68	3PE	D1	501	-	50,50,50	0.31	0	53,55,55	0.29	0
73	PC1	A1	601	-	30,30,53	0.40	0	36,38,61	0.55	0
73	PC1	L	503	-	23,23,53	0.44	0	29,31,61	0.62	0
68	3PE	Y1	403	-	41,41,50	0.33	0	44,46,55	0.31	0
80	TGL	y	601	-	36,36,62	0.23	0	39,39,65	0.17	0
68	3PE	L1	704	-	50,50,50	0.30	0	53,55,55	0.31	0
81	SF4	3	802	29	0,12,12	-	-	-		
85	ZMP	W1	201	-	27,33,36	0.66	1 (3%)	32,40,45	0.98	1 (3%)
70	HEM	C	402	3	41,50,50	1.44	4 (9%)	45,82,82	1.46	8 (17%)
68	3PE	P	201	-	32,32,50	0.37	0	35,37,55	0.34	0
68	3PE	p	301	-	44,44,50	0.32	0	47,49,55	0.31	0
84	NDP	P1	501	-	45,52,52	0.53	0	53,80,80	0.60	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	CDL	Y1	404	-	71,71,99	0.36	0	77,83,111	0.44	1 (1%)
69	CDL	D	302	-	55,55,99	0.39	0	61,67,111	0.34	0
82	FMN	1	501	-	33,33,33	0.27	0	48,50,50	0.47	1 (2%)
68	3PE	H1	401	-	45,45,50	0.32	0	48,50,55	0.29	0
69	CDL	V	102	-	34,37,99	0.35	0	37,47,111	0.31	0
72	FES	E	201	5	0,4,4	-	-	-	-	-
69	CDL	R	301	-	56,56,99	0.38	0	62,68,111	0.33	0
68	3PE	o	302	-	28,28,50	0.39	0	31,33,55	0.37	0
69	CDL	L1	702	-	77,77,99	0.34	0	83,89,111	0.29	0
68	3PE	t	101	-	24,24,50	0.43	0	27,29,55	0.60	1 (3%)
68	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.35	0
86	DGT	O1	401	77	26,33,33	0.77	1 (3%)	32,52,52	0.48	0
76	HEA	n	604	11	57,67,67	1.46	8 (14%)	61,103,103	2.39	22 (36%)
69	CDL	L	502	-	45,45,99	0.44	0	51,57,111	0.50	0
73	PC1	p	303	-	49,49,53	0.33	0	55,57,61	0.57	1 (1%)
71	HEC	O	301	4	32,50,50	2.19	3 (9%)	24,82,82	1.59	4 (16%)
69	CDL	d1	201	-	66,66,99	0.36	0	72,78,111	0.31	0
69	CDL	C	404	-	41,41,99	0.45	0	47,53,111	0.35	0
73	PC1	V	101	-	27,27,53	0.39	0	33,35,61	0.34	0
73	PC1	K	101	-	27,27,53	0.39	0	33,35,61	0.36	0
68	3PE	K1	201	-	40,40,50	0.33	0	43,45,55	0.33	0
68	3PE	Y1	402	-	27,27,50	0.40	0	30,32,55	0.37	0
73	PC1	M1	501	-	53,53,53	0.29	0	59,61,61	0.35	0
69	CDL	h1	201	-	69,69,99	0.36	0	75,81,111	0.43	0
81	SF4	9	201	30	0,12,12	-	-	-	-	-
73	PC1	E	202	-	34,34,53	0.35	0	40,42,61	0.36	0
69	CDL	N1	401	-	89,89,99	0.32	0	95,101,111	0.39	1 (1%)
70	HEM	C	401	3	41,50,50	1.42	3 (7%)	45,82,82	1.49	8 (17%)
72	FES	2	301	27	0,4,4	-	-	-	-	-
78	CUA	o	303	12	0,1,1	-	-	-	-	-
68	3PE	N	401	-	33,33,50	0.36	0	36,38,55	0.34	0
68	3PE	M1	503	-	35,35,50	0.36	0	38,40,55	0.31	0
81	SF4	1	502	28	0,12,12	-	-	-	-	-
68	3PE	N	404	-	36,36,50	0.35	0	39,41,55	0.33	0
68	3PE	d1	202	-	30,30,50	0.38	0	33,35,55	0.33	0
68	3PE	A1	602	-	42,42,50	0.33	0	45,47,55	0.31	0
69	CDL	A	502	-	45,45,99	0.43	0	51,57,111	0.37	0
69	CDL	a1	101	-	56,56,99	0.40	0	62,68,111	0.46	1 (1%)
68	3PE	i1	201	-	41,41,50	0.33	0	44,46,55	0.30	0
69	CDL	R	302	-	40,40,99	0.46	0	46,52,111	0.54	0
72	FES	3	803	29	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	ZMP	n1	201	-	25,31,36	0.76	1 (4%)	30,38,45	0.90	1 (3%)
69	CDL	R	303	-	56,56,99	0.39	0	62,68,111	0.47	1 (1%)
69	CDL	Y1	401	-	93,93,99	0.31	0	99,105,111	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	SF4	3	801	29	-	-	0/6/5/5
68	3PE	M1	502	-	-	14/54/54/54	-
68	3PE	n	605	-	-	11/37/37/54	-
73	PC1	z	101	-	-	3/31/31/57	-
81	SF4	6	201	24	-	-	0/6/5/5
68	3PE	C	405	-	-	8/54/54/54	-
68	3PE	Z1	401	-	-	10/54/54/54	-
70	HEM	N	403	3	-	4/12/54/54	-
68	3PE	R	304	-	-	6/33/33/54	-
73	PC1	6	203	-	-	6/46/46/57	-
68	3PE	L1	701	-	-	8/54/54/54	-
68	3PE	q	201	-	-	10/29/29/54	-
71	HEC	D	301	4	-	0/10/54/54	-
68	3PE	v	101	-	-	5/31/31/54	-
68	3PE	n	606	-	-	13/31/31/54	-
68	3PE	x	101	-	-	9/30/30/54	-
81	SF4	9	202	30	-	-	0/6/5/5
73	PC1	9	203	-	-	10/57/57/57	-
73	PC1	p	302	-	-	8/38/38/57	-
70	HEM	N	402	3	-	2/12/54/54	-
68	3PE	6	202	-	-	4/35/35/54	-
72	FES	P	202	5	-	-	0/1/1/1
73	PC1	9	204	-	-	14/50/50/57	-
68	3PE	L	501	-	-	6/26/26/54	-
69	CDL	L1	703	-	-	12/56/56/110	-
68	3PE	C	406	-	-	5/34/34/54	-
68	3PE	N1	402	-	-	10/41/41/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	3PE	A	501	-	-	10/26/26/54	-
69	CDL	H1	402	-	-	14/59/59/110	-
68	3PE	d1	203	-	-	6/35/35/54	-
76	HEA	n	603	11	-	10/32/76/76	-
68	3PE	D1	501	-	-	8/54/54/54	-
73	PC1	A1	601	-	-	14/34/34/57	-
73	PC1	L	503	-	-	9/27/27/57	-
68	3PE	Y1	403	-	-	11/45/45/54	-
80	TGL	y	601	-	-	1/39/39/65	-
68	3PE	L1	704	-	-	15/54/54/54	-
85	ZMP	W1	201	-	-	5/38/40/43	-
81	SF4	3	802	29	-	-	0/6/5/5
70	HEM	C	402	3	-	1/12/54/54	-
68	3PE	P	201	-	-	5/36/36/54	-
68	3PE	p	301	-	-	9/48/48/54	-
84	NDP	P1	501	-	-	6/30/77/77	0/5/5/5
69	CDL	Y1	404	-	-	18/82/82/110	-
69	CDL	D	302	-	-	17/66/66/110	-
82	FMN	1	501	-	-	6/18/18/18	0/3/3/3
68	3PE	H1	401	-	-	11/49/49/54	-
69	CDL	V	102	-	-	8/41/45/110	-
72	FES	E	201	5	-	-	0/1/1/1
69	CDL	R	301	-	-	19/67/67/110	-
68	3PE	o	302	-	-	9/32/32/54	-
69	CDL	L1	702	-	-	19/88/88/110	-
68	3PE	t	101	-	-	10/28/28/54	-
68	3PE	C	403	-	-	10/38/38/54	-
86	DGT	O1	401	77	-	4/18/34/34	0/3/3/3
76	HEA	n	604	11	-	9/32/76/76	-
69	CDL	L	502	-	-	9/56/56/110	-
73	PC1	p	303	-	-	11/53/53/57	-
71	HEC	O	301	4	-	0/10/54/54	-
69	CDL	d1	201	-	-	16/77/77/110	-
69	CDL	C	404	-	-	12/52/52/110	-
73	PC1	V	101	-	-	6/31/31/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
73	PC1	K	101	-	-	10/31/31/57	-
68	3PE	K1	201	-	-	12/44/44/54	-
68	3PE	Y1	402	-	-	8/31/31/54	-
73	PC1	M1	501	-	-	13/57/57/57	-
69	CDL	h1	201	-	-	20/80/80/110	-
81	SF4	9	201	30	-	-	0/6/5/5
73	PC1	E	202	-	-	7/38/38/57	-
69	CDL	N1	401	-	-	15/100/100/110	-
70	HEM	C	401	3	-	2/12/54/54	-
72	FES	2	301	27	-	-	0/1/1/1
68	3PE	N	401	-	-	5/37/37/54	-
68	3PE	M1	503	-	-	8/39/39/54	-
81	SF4	1	502	28	-	-	0/6/5/5
68	3PE	N	404	-	-	7/40/40/54	-
68	3PE	d1	202	-	-	9/34/34/54	-
68	3PE	A1	602	-	-	9/46/46/54	-
69	CDL	A	502	-	-	14/56/56/110	-
69	CDL	a1	101	-	-	13/67/67/110	-
68	3PE	i1	201	-	-	6/45/45/54	-
69	CDL	R	302	-	-	10/51/51/110	-
72	FES	3	803	29	-	-	0/1/1/1
85	ZMP	n1	201	-	-	19/36/38/43	-
69	CDL	R	303	-	-	16/67/67/110	-
69	CDL	Y1	401	-	-	13/104/104/110	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	O	301	HEC	C2B-C3B	-6.49	1.34	1.40
71	D	301	HEC	C3C-C2C	-6.45	1.34	1.40
71	O	301	HEC	C3C-C2C	-6.39	1.34	1.40
71	D	301	HEC	C2B-C3B	-6.31	1.34	1.40
71	O	301	HEC	C3D-C2D	5.38	1.53	1.37
71	D	301	HEC	C3D-C2D	5.32	1.53	1.37
76	n	604	HEA	C3D-C2D	4.44	1.46	1.36
76	n	603	HEA	C3B-C2B	4.41	1.44	1.34
76	n	604	HEA	C3B-C2B	4.24	1.44	1.34
76	n	603	HEA	C3D-C2D	4.16	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	N	402	HEM	C3C-CAC	3.96	1.55	1.47
70	C	401	HEM	C3C-CAC	3.94	1.55	1.47
70	C	402	HEM	C3C-CAC	3.91	1.55	1.47
76	n	604	HEA	C3A-C2A	3.83	1.45	1.40
70	N	403	HEM	C3C-CAC	3.81	1.55	1.47
70	N	402	HEM	C3C-C2C	-3.63	1.35	1.40
70	C	402	HEM	C3C-C2C	-3.60	1.35	1.40
70	N	403	HEM	C3C-C2C	-3.56	1.35	1.40
70	C	401	HEM	C3C-C2C	-3.52	1.35	1.40
76	n	603	HEA	C3C-C2C	3.43	1.45	1.40
76	n	603	HEA	C3A-C2A	3.39	1.45	1.40
70	N	403	HEM	CAB-C3B	3.13	1.56	1.47
76	n	603	HEA	C4B-C3B	3.11	1.49	1.44
70	N	402	HEM	CAB-C3B	3.11	1.55	1.47
70	C	402	HEM	CAB-C3B	3.08	1.55	1.47
76	n	604	HEA	C3C-C2C	3.08	1.44	1.40
70	C	401	HEM	CAB-C3B	3.04	1.55	1.47
76	n	604	HEA	C4B-C3B	2.95	1.49	1.44
76	n	604	HEA	C2A-C1A	2.74	1.48	1.42
85	n1	201	ZMP	C9-C10	2.57	1.53	1.50
76	n	603	HEA	C2A-C1A	2.54	1.48	1.42
76	n	603	HEA	C1D-ND	-2.49	1.36	1.40
85	W1	201	ZMP	C9-C10	2.28	1.53	1.50
76	n	604	HEA	C1D-ND	-2.27	1.36	1.40
70	C	402	HEM	FE-NB	2.26	2.08	1.96
76	n	604	HEA	C1D-C2D	2.07	1.48	1.44
70	N	403	HEM	CMB-C2B	2.05	1.55	1.50
86	O1	401	DGT	C5-C6	-2.01	1.43	1.47

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	n	603	HEA	CMC-C2C-C3C	7.09	137.95	124.68
76	n	604	HEA	CMC-C2C-C3C	7.06	137.89	124.68
76	n	604	HEA	CMC-C2C-C1C	-6.32	118.76	128.46
76	n	603	HEA	CMC-C2C-C1C	-6.27	118.83	128.46
76	n	604	HEA	CMD-C2D-C1D	-4.94	117.51	125.04
76	n	603	HEA	CMD-C2D-C1D	-4.79	117.74	125.04
76	n	604	HEA	C3D-C4D-ND	4.77	114.98	110.36
76	n	603	HEA	CMB-C2B-C1B	-4.54	118.12	125.04
76	n	603	HEA	C13-C12-C11	-4.47	107.64	114.35
76	n	603	HEA	C3D-C4D-ND	4.42	114.63	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	n	604	HEA	CMB-C2B-C1B	-4.30	118.49	125.04
76	n	604	HEA	CHA-C4D-C3D	-3.98	118.99	124.84
76	n	603	HEA	C26-C15-C16	3.92	121.86	115.27
76	n	604	HEA	CMD-C2D-C3D	3.82	136.49	126.12
76	n	604	HEA	C13-C12-C11	-3.76	108.69	114.35
76	n	603	HEA	C4D-C3D-C2D	-3.74	101.44	106.90
76	n	603	HEA	CHA-C4D-C3D	-3.69	119.41	124.84
76	n	604	HEA	C4D-C3D-C2D	-3.60	101.65	106.90
76	n	604	HEA	C26-C15-C16	3.58	121.29	115.27
76	n	603	HEA	CMD-C2D-C3D	3.53	135.69	126.12
71	O	301	HEC	CMC-C2C-C1C	-3.51	123.08	128.46
71	D	301	HEC	CMC-C2C-C1C	-3.42	123.21	128.46
70	C	402	HEM	C4D-ND-C1D	3.40	108.58	105.07
76	n	603	HEA	CMB-C2B-C3B	3.29	136.61	130.34
70	C	401	HEM	CMC-C2C-C3C	3.21	130.69	124.68
70	N	402	HEM	CMC-C2C-C3C	3.18	130.63	124.68
70	N	403	HEM	C4D-ND-C1D	3.14	108.32	105.07
76	n	603	HEA	C17-C18-C19	-3.10	120.20	127.66
76	n	603	HEA	CAA-CBA-CGA	-3.07	105.16	113.76
76	n	603	HEA	CHB-C1B-C2B	-3.00	120.28	124.98
70	C	402	HEM	CMC-C2C-C3C	3.00	130.29	124.68
76	n	603	HEA	C13-C14-C15	-2.92	120.63	127.66
70	C	401	HEM	C4D-ND-C1D	2.91	108.08	105.07
70	N	403	HEM	CMC-C2C-C3C	2.90	130.10	124.68
70	N	402	HEM	C4D-ND-C1D	2.82	107.99	105.07
70	C	402	HEM	CBA-CAA-C2A	-2.75	107.93	112.62
76	n	604	HEA	CMB-C2B-C3B	2.70	135.50	130.34
70	C	401	HEM	C3B-C2B-C1B	2.64	108.44	106.49
76	n	604	HEA	CHB-C1B-C2B	-2.63	120.86	124.98
70	N	402	HEM	C3B-C2B-C1B	2.63	108.43	106.49
85	W1	201	ZMP	O1-C10-C9	-2.62	120.89	123.99
76	n	604	HEA	CAD-CBD-CGD	-2.60	108.01	113.60
71	D	301	HEC	CMB-C2B-C1B	-2.60	124.47	128.46
71	O	301	HEC	CBD-CAD-C3D	-2.57	108.23	112.62
76	n	604	HEA	C17-C18-C19	-2.56	121.49	127.66
70	N	402	HEM	C4C-CHD-C1D	2.55	125.92	122.56
76	n	604	HEA	C4B-C3B-C2B	-2.52	103.10	107.41
70	C	402	HEM	C3D-C4D-ND	-2.52	107.36	110.17
85	n1	201	ZMP	O1-C10-C9	-2.51	121.03	123.99
76	n	603	HEA	CHB-C1B-NB	2.49	127.14	124.43
71	O	301	HEC	CMB-C2B-C1B	-2.49	124.64	128.46
76	n	603	HEA	C27-C19-C20	2.48	119.44	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
71	O	301	HEC	C1D-C2D-C3D	-2.48	105.27	107.00
76	n	604	HEA	C25-C23-C24	2.41	119.93	114.60
70	C	401	HEM	C4C-CHD-C1D	2.38	125.70	122.56
84	P1	501	NDP	C5A-C6A-N6A	2.38	123.97	120.35
70	C	401	HEM	C1B-NB-C4B	2.38	107.53	105.07
76	n	604	HEA	CHB-C1B-NB	2.38	127.01	124.43
76	n	603	HEA	C25-C23-C24	2.37	119.83	114.60
76	n	604	HEA	CAD-C3D-C2D	2.35	132.25	127.88
70	C	401	HEM	C4B-CHC-C1C	2.33	125.64	122.56
70	N	403	HEM	C3D-C4D-ND	-2.33	107.57	110.17
82	l	501	FMN	P-O5'-C5'	2.33	124.71	118.30
76	n	604	HEA	C3B-C4B-NB	2.31	112.58	109.84
76	n	604	HEA	C13-C14-C15	-2.28	122.17	127.66
70	N	402	HEM	CBA-CAA-C2A	-2.27	108.75	112.62
70	N	402	HEM	C1B-NB-C4B	2.26	107.41	105.07
76	n	604	HEA	CAA-CBA-CGA	-2.25	107.45	113.76
76	n	603	HEA	C2B-C1B-NB	2.25	112.58	109.88
70	N	402	HEM	C4B-CHC-C1C	2.24	125.51	122.56
70	N	403	HEM	C1B-NB-C4B	2.24	107.38	105.07
70	C	402	HEM	CMB-C2B-C1B	-2.23	121.64	125.04
76	n	603	HEA	CAD-CBD-CGD	-2.21	108.84	113.60
71	D	301	HEC	C1D-C2D-C3D	-2.21	105.46	107.00
73	p	303	PC1	C2-O21-C21	2.20	123.20	117.79
76	n	603	HEA	CAD-C3D-C4D	2.18	128.47	124.66
70	N	402	HEM	C3D-C4D-ND	-2.13	107.79	110.17
70	N	403	HEM	CMB-C2B-C1B	-2.12	121.81	125.04
68	t	101	3PE	C2-O21-C21	2.09	122.95	117.79
70	C	401	HEM	C3D-C4D-ND	-2.09	107.84	110.17
76	n	603	HEA	C4B-C3B-C2B	-2.09	103.84	107.41
71	D	301	HEC	CBD-CAD-C3D	-2.09	109.06	112.62
76	n	604	HEA	C27-C19-C20	2.08	118.77	115.27
70	N	402	HEM	CAD-CBD-CGD	-2.08	109.13	113.60
69	Y1	404	CDL	CA4-OA6-CA5	2.08	122.91	117.79
68	n	605	3PE	C2-O21-C21	2.07	122.89	117.79
71	D	301	HEC	CAA-CBA-CGA	-2.06	108.00	113.76
70	N	403	HEM	CMA-C3A-C4A	-2.05	125.31	128.46
70	C	402	HEM	C1B-NB-C4B	2.05	107.19	105.07
76	n	603	HEA	C26-C15-C14	-2.05	118.42	123.68
69	a1	101	CDL	CA4-OA6-CA5	2.04	122.81	117.79
70	C	401	HEM	CAD-CBD-CGD	-2.04	109.22	113.60
70	C	402	HEM	C2D-C1D-ND	-2.04	107.44	109.88
69	R	303	CDL	CA4-OA6-CA5	2.03	122.80	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	Z1	401	3PE	C2-O21-C21	2.03	122.79	117.79
69	N1	401	CDL	CB4-OB6-CB5	2.02	122.77	117.79
70	C	402	HEM	C4B-CHC-C1C	2.01	125.21	122.56

There are no chirality outliers.

All (712) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
68	A	501	3PE	C11-O13-P-O11
68	A	501	3PE	C11-O13-P-O12
68	A	501	3PE	C11-O13-P-O14
68	C	403	3PE	C1-O11-P-O12
68	C	403	3PE	C1-O11-P-O14
68	C	403	3PE	C11-O13-P-O11
68	C	403	3PE	C11-O13-P-O12
68	C	403	3PE	C11-O13-P-O14
68	C	403	3PE	O13-C11-C12-N
68	C	405	3PE	O13-C11-C12-N
68	C	406	3PE	O13-C11-C12-N
68	L	501	3PE	C11-O13-P-O12
68	L	501	3PE	C11-O13-P-O14
68	L	501	3PE	O13-C11-C12-N
68	N	404	3PE	C11-O13-P-O11
68	N	404	3PE	C11-O13-P-O12
68	N	404	3PE	C11-O13-P-O14
68	N	404	3PE	O13-C11-C12-N
68	P	201	3PE	O13-C11-C12-N
68	R	304	3PE	C11-O13-P-O12
68	n	605	3PE	C11-O13-P-O11
68	n	605	3PE	C11-O13-P-O12
68	n	605	3PE	C11-O13-P-O14
68	n	605	3PE	O13-C11-C12-N
68	n	606	3PE	C1-O11-P-O12
68	n	606	3PE	C1-O11-P-O14
68	p	301	3PE	C11-O13-P-O12
68	p	301	3PE	O13-C11-C12-N
68	q	201	3PE	C1-O11-P-O12
68	q	201	3PE	C1-O11-P-O13
68	q	201	3PE	C1-O11-P-O14
68	q	201	3PE	C11-O13-P-O11
68	q	201	3PE	C11-O13-P-O12
68	q	201	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
68	t	101	3PE	C11-O13-P-O12
68	t	101	3PE	C11-O13-P-O14
68	t	101	3PE	O13-C11-C12-N
68	v	101	3PE	C1-O11-P-O12
68	v	101	3PE	C1-O11-P-O14
68	x	101	3PE	C11-O13-P-O11
68	x	101	3PE	C11-O13-P-O12
68	x	101	3PE	C11-O13-P-O14
68	x	101	3PE	O13-C11-C12-N
68	D1	501	3PE	C1-O11-P-O12
68	D1	501	3PE	O13-C11-C12-N
68	A1	602	3PE	C11-O13-P-O11
68	A1	602	3PE	C11-O13-P-O12
68	A1	602	3PE	C11-O13-P-O14
68	H1	401	3PE	C1-O11-P-O12
68	H1	401	3PE	C1-O11-P-O13
68	H1	401	3PE	C1-O11-P-O14
68	K1	201	3PE	C1-O11-P-O12
68	K1	201	3PE	C1-O11-P-O13
68	K1	201	3PE	C1-O11-P-O14
68	K1	201	3PE	C11-O13-P-O14
68	K1	201	3PE	O13-C11-C12-N
68	L1	701	3PE	C1-O11-P-O12
68	L1	701	3PE	C1-O11-P-O13
68	L1	701	3PE	C1-O11-P-O14
68	L1	701	3PE	O13-C11-C12-N
68	L1	704	3PE	C1-O11-P-O12
68	L1	704	3PE	C11-O13-P-O12
68	L1	704	3PE	O13-C11-C12-N
68	M1	502	3PE	C11-O13-P-O11
68	M1	502	3PE	C11-O13-P-O12
68	M1	502	3PE	C11-O13-P-O14
68	M1	502	3PE	O13-C11-C12-N
68	M1	503	3PE	C1-O11-P-O14
68	M1	503	3PE	C11-O13-P-O11
68	M1	503	3PE	C11-O13-P-O12
68	M1	503	3PE	C11-O13-P-O14
68	N1	402	3PE	C1-O11-P-O12
68	N1	402	3PE	C11-O13-P-O11
68	N1	402	3PE	C11-O13-P-O12
68	N1	402	3PE	C11-O13-P-O14
68	N1	402	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
68	Y1	402	3PE	C1-O11-P-O12
68	Y1	402	3PE	C1-O11-P-O13
68	Y1	402	3PE	C1-O11-P-O14
68	Y1	402	3PE	C11-O13-P-O11
68	Y1	402	3PE	C11-O13-P-O12
68	Y1	402	3PE	C11-O13-P-O14
68	Y1	403	3PE	C1-O11-P-O12
68	Y1	403	3PE	C11-O13-P-O12
68	Y1	403	3PE	C11-O13-P-O14
68	d1	202	3PE	C1-O11-P-O12
68	d1	202	3PE	C11-O13-P-O11
68	d1	202	3PE	C11-O13-P-O12
68	d1	202	3PE	C11-O13-P-O14
68	d1	202	3PE	O13-C11-C12-N
68	d1	203	3PE	C1-O11-P-O12
68	d1	203	3PE	C1-O11-P-O13
68	d1	203	3PE	C1-O11-P-O14
68	d1	203	3PE	O13-C11-C12-N
69	A	502	CDL	CB2-OB2-PB2-OB4
69	A	502	CDL	CB3-OB5-PB2-OB3
69	A	502	CDL	CB3-OB5-PB2-OB4
69	C	404	CDL	CA2-OA2-PA1-OA3
69	C	404	CDL	CA2-OA2-PA1-OA4
69	C	404	CDL	CA2-OA2-PA1-OA5
69	C	404	CDL	CB3-OB5-PB2-OB3
69	C	404	CDL	CB3-OB5-PB2-OB4
69	D	302	CDL	CA2-OA2-PA1-OA3
69	D	302	CDL	CA2-OA2-PA1-OA4
69	D	302	CDL	CA2-OA2-PA1-OA5
69	D	302	CDL	CA3-OA5-PA1-OA3
69	D	302	CDL	CA3-OA5-PA1-OA4
69	D	302	CDL	CB3-OB5-PB2-OB2
69	L	502	CDL	CA3-OA5-PA1-OA3
69	R	301	CDL	CB2-OB2-PB2-OB3
69	R	302	CDL	CA2-OA2-PA1-OA3
69	R	302	CDL	CA2-OA2-PA1-OA4
69	R	302	CDL	CA2-OA2-PA1-OA5
69	R	303	CDL	CA2-OA2-PA1-OA4
69	R	303	CDL	CB2-OB2-PB2-OB3
69	V	102	CDL	CA3-OA5-PA1-OA4
69	H1	402	CDL	CA2-OA2-PA1-OA3
69	H1	402	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
69	L1	702	CDL	CA2-OA2-PA1-OA3
69	L1	702	CDL	CA2-OA2-PA1-OA4
69	L1	702	CDL	CA3-OA5-PA1-OA3
69	L1	702	CDL	CB2-OB2-PB2-OB3
69	L1	702	CDL	CB2-OB2-PB2-OB4
69	L1	702	CDL	CB2-OB2-PB2-OB5
69	L1	702	CDL	CB3-OB5-PB2-OB2
69	L1	702	CDL	CB3-OB5-PB2-OB3
69	L1	702	CDL	CB3-OB5-PB2-OB4
69	L1	703	CDL	CA2-OA2-PA1-OA3
69	L1	703	CDL	CA2-OA2-PA1-OA4
69	L1	703	CDL	CA3-OA5-PA1-OA3
69	L1	703	CDL	CB2-OB2-PB2-OB3
69	L1	703	CDL	CB2-OB2-PB2-OB5
69	N1	401	CDL	CB2-OB2-PB2-OB3
69	N1	401	CDL	CB2-OB2-PB2-OB4
69	Y1	401	CDL	CA2-OA2-PA1-OA3
69	Y1	401	CDL	CA2-OA2-PA1-OA4
69	Y1	404	CDL	CA2-OA2-PA1-OA3
69	Y1	404	CDL	CA2-OA2-PA1-OA5
69	Y1	404	CDL	CB2-OB2-PB2-OB3
69	Y1	404	CDL	CB2-OB2-PB2-OB4
69	Y1	404	CDL	CB3-OB5-PB2-OB2
69	Y1	404	CDL	CB3-OB5-PB2-OB3
69	Y1	404	CDL	CB3-OB5-PB2-OB4
69	a1	101	CDL	CA2-OA2-PA1-OA3
69	a1	101	CDL	CA2-OA2-PA1-OA4
69	a1	101	CDL	CB2-OB2-PB2-OB5
69	d1	201	CDL	CA3-OA5-PA1-OA2
69	d1	201	CDL	CA3-OA5-PA1-OA3
69	d1	201	CDL	OB5-CB3-CB4-OB6
69	h1	201	CDL	CA2-OA2-PA1-OA3
69	h1	201	CDL	CB2-OB2-PB2-OB3
69	h1	201	CDL	CB2-OB2-PB2-OB4
69	h1	201	CDL	CB3-OB5-PB2-OB4
70	C	401	HEM	C2A-CAA-CBA-CGA
73	E	202	PC1	C1-O11-P-O12
73	K	101	PC1	C1-O11-P-O12
73	K	101	PC1	C1-O11-P-O14
73	K	101	PC1	C1-O11-P-O13
73	L	503	PC1	C11-O13-P-O12
73	L	503	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
73	L	503	PC1	C11-O13-P-O11
73	L	503	PC1	C1-O11-P-O12
73	L	503	PC1	C1-O11-P-O13
73	V	101	PC1	C11-O13-P-O12
73	p	302	PC1	C1-O11-P-O12
73	p	303	PC1	C1-O11-P-O12
73	p	303	PC1	C1-O11-P-O14
73	6	203	PC1	C1-O11-P-O12
73	6	203	PC1	C1-O11-P-O14
73	9	203	PC1	C1-O11-P-O12
73	9	203	PC1	C1-O11-P-O14
73	9	203	PC1	C1-O11-P-O13
73	9	203	PC1	O13-C11-C12-N
73	A1	601	PC1	C11-O13-P-O12
73	A1	601	PC1	C11-O13-P-O14
73	A1	601	PC1	C11-O13-P-O11
73	M1	501	PC1	C11-O13-P-O12
73	M1	501	PC1	C11-O13-P-O14
73	M1	501	PC1	C11-O13-P-O11
76	n	604	HEA	C1A-C2A-CAA-CBA
76	n	604	HEA	C3A-C2A-CAA-CBA
76	n	604	HEA	C14-C15-C16-C17
76	n	604	HEA	C26-C15-C16-C17
76	n	604	HEA	C15-C16-C17-C18
82	1	501	FMN	N10-C1'-C2'-O2'
82	1	501	FMN	N10-C1'-C2'-C3'
82	1	501	FMN	C5'-O5'-P-O1P
82	1	501	FMN	C5'-O5'-P-O2P
84	P1	501	NDP	C5B-O5B-PA-O3
85	W1	201	ZMP	S1-C11-C12-N1
85	W1	201	ZMP	O1-C10-S1-C11
85	W1	201	ZMP	C9-C10-S1-C11
85	n1	201	ZMP	C17-C18-C21-O5
85	n1	201	ZMP	O4-C17-C18-C21
85	n1	201	ZMP	C16-C17-C18-C21
85	n1	201	ZMP	O4-C17-C18-C19
85	n1	201	ZMP	C16-C17-C18-C20
85	n1	201	ZMP	O3-C16-C17-O4
85	n1	201	ZMP	C17-C16-N2-C15
86	O1	401	DGT	PB-O3B-PG-O1G
76	n	604	HEA	C4D-C3D-CAD-CBD
85	n1	201	ZMP	O3-C16-N2-C15

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Mol	Chain	Res	Type	Atoms
76	n	604	HEA	C2D-C3D-CAD-CBD
69	D	302	CDL	C1-CB2-OB2-PB2
76	n	603	HEA	C19-C20-C21-C22
73	9	204	PC1	C11-C12-N-C15
73	p	303	PC1	C31-C32-C33-C34
69	N1	401	CDL	OA6-CA4-CA6-OA8
70	N	402	HEM	C2A-CAA-CBA-CGA
68	L1	701	3PE	C21-C22-C23-C24
68	L1	704	3PE	C31-C32-C33-C34
69	L1	702	CDL	CA5-C11-C12-C13
68	M1	503	3PE	C2-C1-O11-P
69	H1	402	CDL	C1-CB2-OB2-PB2
76	n	603	HEA	C15-C16-C17-C18
68	M1	502	3PE	C27-C28-C29-C2A
68	A	501	3PE	C1-O11-P-O13
68	C	403	3PE	C1-O11-P-O13
68	C	405	3PE	C11-O13-P-O11
68	L	501	3PE	C11-O13-P-O11
68	N	401	3PE	C11-O13-P-O11
68	P	201	3PE	C11-O13-P-O11
68	R	304	3PE	C11-O13-P-O11
68	n	605	3PE	C1-O11-P-O13
68	n	606	3PE	C1-O11-P-O13
68	n	606	3PE	C11-O13-P-O11
68	o	302	3PE	C1-O11-P-O13
68	o	302	3PE	C11-O13-P-O11
68	p	301	3PE	C11-O13-P-O11
68	t	101	3PE	C11-O13-P-O11
68	v	101	3PE	C1-O11-P-O13
68	x	101	3PE	C1-O11-P-O13
68	D1	501	3PE	C1-O11-P-O13
68	H1	401	3PE	C11-O13-P-O11
68	L1	704	3PE	C11-O13-P-O11
68	Y1	403	3PE	C1-O11-P-O13
68	Y1	403	3PE	C11-O13-P-O11
68	d1	202	3PE	C1-O11-P-O13
69	A	502	CDL	CB2-OB2-PB2-OB5
69	A	502	CDL	CB3-OB5-PB2-OB2
69	C	404	CDL	CB2-OB2-PB2-OB5
69	C	404	CDL	CB3-OB5-PB2-OB2
69	D	302	CDL	CA3-OA5-PA1-OA2
69	D	302	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
69	R	301	CDL	CA2-OA2-PA1-OA5
69	R	301	CDL	CB3-OB5-PB2-OB2
69	R	302	CDL	CB2-OB2-PB2-OB5
69	R	303	CDL	CA3-OA5-PA1-OA2
69	H1	402	CDL	CA2-OA2-PA1-OA5
69	L1	702	CDL	CA2-OA2-PA1-OA5
69	L1	702	CDL	CA3-OA5-PA1-OA2
69	L1	703	CDL	CA2-OA2-PA1-OA5
69	N1	401	CDL	CA2-OA2-PA1-OA5
69	N1	401	CDL	CB2-OB2-PB2-OB5
69	Y1	401	CDL	CA2-OA2-PA1-OA5
69	Y1	401	CDL	CB3-OB5-PB2-OB2
69	Y1	404	CDL	CA3-OA5-PA1-OA2
69	Y1	404	CDL	CB2-OB2-PB2-OB5
69	a1	101	CDL	CA2-OA2-PA1-OA5
69	a1	101	CDL	CA3-OA5-PA1-OA2
69	d1	201	CDL	CB2-OB2-PB2-OB5
69	h1	201	CDL	CA2-OA2-PA1-OA5
69	h1	201	CDL	CB2-OB2-PB2-OB5
69	h1	201	CDL	CB3-OB5-PB2-OB2
73	E	202	PC1	C11-O13-P-O11
73	E	202	PC1	C1-O11-P-O13
73	K	101	PC1	C11-O13-P-O11
73	p	302	PC1	C1-O11-P-O13
73	p	303	PC1	C1-O11-P-O13
73	6	203	PC1	C1-O11-P-O13
73	A1	601	PC1	C1-O11-P-O13
68	C	405	3PE	C32-C33-C34-C35
73	V	101	PC1	C11-C12-N-C13
73	9	204	PC1	C11-C12-N-C13
68	D1	501	3PE	C38-C39-C3A-C3B
85	n1	201	ZMP	C6-C7-C8-C9
68	M1	502	3PE	C28-C29-C2A-C2B
73	9	204	PC1	C2A-C2B-C2C-C2D
68	C	405	3PE	C37-C38-C39-C3A
73	9	204	PC1	C2B-C2C-C2D-C2E
68	L1	704	3PE	C36-C37-C38-C39
73	K	101	PC1	C11-C12-N-C13
68	N1	402	3PE	C36-C37-C38-C39
68	o	302	3PE	O13-C11-C12-N
68	L1	704	3PE	C23-C24-C25-C26
70	C	402	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
68	A1	602	3PE	C3A-C3B-C3C-C3D
69	N1	401	CDL	C81-C82-C83-C84
68	A1	602	3PE	C38-C39-C3A-C3B
73	p	303	PC1	C25-C26-C27-C28
73	p	302	PC1	C11-C12-N-C13
68	Z1	401	3PE	C31-C32-C33-C34
69	d1	201	CDL	C63-C64-C65-C66
68	D1	501	3PE	C32-C33-C34-C35
68	H1	401	3PE	C31-C32-C33-C34
69	D	302	CDL	OB5-CB3-CB4-OB6
69	R	301	CDL	OB5-CB3-CB4-OB6
69	Y1	404	CDL	OB5-CB3-CB4-OB6
69	d1	201	CDL	C55-C56-C57-C58
69	Y1	401	CDL	C82-C83-C84-C85
68	n	606	3PE	O21-C2-C3-O31
73	K	101	PC1	C11-C12-N-C15
73	V	101	PC1	C11-C12-N-C15
73	9	204	PC1	C11-C12-N-C14
68	D1	501	3PE	C31-C32-C33-C34
68	n	606	3PE	C23-C24-C25-C26
85	n1	201	ZMP	C5-C6-C7-C8
68	K1	201	3PE	C11-O13-P-O11
68	M1	503	3PE	C1-O11-P-O13
68	N1	402	3PE	C1-O11-P-O13
69	L	502	CDL	CA3-OA5-PA1-OA2
69	R	303	CDL	CA2-OA2-PA1-OA5
69	V	102	CDL	CA3-OA5-PA1-OA2
69	H1	402	CDL	CB2-OB2-PB2-OB5
73	9	203	PC1	C11-O13-P-O11
84	P1	501	NDP	C2D-C1D-N1N-C6N
69	A	502	CDL	OB5-CB3-CB4-CB6
69	R	301	CDL	OB5-CB3-CB4-CB6
69	d1	201	CDL	OB5-CB3-CB4-CB6
73	M1	501	PC1	C37-C38-C39-C3A
73	K	101	PC1	C11-C12-N-C14
73	V	101	PC1	C11-C12-N-C14
68	N1	402	3PE	C1-C2-C3-O31
69	N1	401	CDL	CA3-CA4-CA6-OA8
69	Y1	401	CDL	CB3-CB4-CB6-OB8
69	Y1	404	CDL	CB3-CB4-CB6-OB8
69	D	302	CDL	C74-C75-C76-C77
69	H1	402	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
85	n1	201	ZMP	C19-C18-C21-O5
73	A1	601	PC1	C21-C22-C23-C24
76	n	603	HEA	C11-C12-C13-C14
68	n	606	3PE	O11-C1-C2-O21
68	M1	502	3PE	O11-C1-C2-O21
69	V	102	CDL	OA5-CA3-CA4-OA6
73	9	204	PC1	C21-C22-C23-C24
68	N	404	3PE	C25-C26-C27-C28
68	Z1	401	3PE	O31-C31-C32-C33
85	n1	201	ZMP	O4-C17-C18-C20
73	9	204	PC1	C34-C35-C36-C37
73	p	302	PC1	C11-C12-N-C14
68	M1	502	3PE	O11-C1-C2-C3
68	Z1	401	3PE	O11-C1-C2-C3
69	D	302	CDL	OB5-CB3-CB4-CB6
69	V	102	CDL	OA5-CA3-CA4-CA6
69	Y1	404	CDL	OB5-CB3-CB4-CB6
69	a1	101	CDL	OB5-CB3-CB4-CB6
68	H1	401	3PE	O13-C11-C12-N
69	H1	402	CDL	C13-C14-C15-C16
69	R	301	CDL	O1-C1-CA2-OA2
68	x	101	3PE	C2-C1-O11-P
69	R	301	CDL	C1-CA2-OA2-PA1
69	h1	201	CDL	CB3-CB4-CB6-OB8
68	L1	704	3PE	C1-O11-P-O13
69	R	301	CDL	CB2-OB2-PB2-OB5
69	R	303	CDL	CB2-OB2-PB2-OB5
68	d1	203	3PE	C21-C22-C23-C24
73	M1	501	PC1	C21-C22-C23-C24
69	A	502	CDL	OB5-CB3-CB4-OB6
68	x	101	3PE	O21-C2-C3-O31
68	N1	402	3PE	O21-C2-C3-O31
69	Y1	401	CDL	OB6-CB4-CB6-OB8
69	Y1	404	CDL	OB6-CB4-CB6-OB8
68	Z1	401	3PE	C2-C1-O11-P
69	D	302	CDL	CB4-CB3-OB5-PB2
69	R	301	CDL	CB4-CB3-OB5-PB2
69	R	302	CDL	CA4-CA3-OA5-PA1
69	R	303	CDL	C1-CB2-OB2-PB2
73	E	202	PC1	C2-C1-O11-P
73	V	101	PC1	C2-C1-O11-P
73	A1	601	PC1	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
85	n1	201	ZMP	O1-C10-S1-C11
68	q	201	3PE	O11-C1-C2-C3
73	6	203	PC1	C35-C36-C37-C38
85	n1	201	ZMP	C20-C18-C21-O5
73	M1	501	PC1	C3B-C3C-C3D-C3E
85	n1	201	ZMP	C9-C10-S1-C11
68	p	301	3PE	C34-C35-C36-C37
85	n1	201	ZMP	C13-C14-C15-N2
68	n	605	3PE	C2-C1-O11-P
68	d1	202	3PE	C1-C2-C3-O31
69	L	502	CDL	CB4-CB3-OB5-PB2
69	H1	402	CDL	C1-CA2-OA2-PA1
69	Y1	404	CDL	C1-CB2-OB2-PB2
69	a1	101	CDL	C1-CB2-OB2-PB2
68	q	201	3PE	O11-C1-C2-O21
69	L1	702	CDL	OB5-CB3-CB4-OB6
84	P1	501	NDP	C2D-C1D-N1N-C2N
85	n1	201	ZMP	C16-C17-C18-C19
73	9	204	PC1	C35-C36-C37-C38
73	p	302	PC1	C11-C12-N-C15
84	P1	501	NDP	PN-O3-PA-O2A
86	O1	401	DGT	PB-O3A-PA-O1A
69	R	303	CDL	CB3-OB5-PB2-OB2
69	L1	703	CDL	CA3-OA5-PA1-OA2
84	P1	501	NDP	O4D-C1D-N1N-C6N
68	t	101	3PE	C2-C1-O11-P
68	K1	201	3PE	C2-C1-O11-P
69	h1	201	CDL	CA4-CA3-OA5-PA1
68	A	501	3PE	C1-O11-P-O12
68	A	501	3PE	C1-O11-P-O14
68	C	405	3PE	C11-O13-P-O14
68	N	401	3PE	C11-O13-P-O12
68	N	401	3PE	C11-O13-P-O14
68	P	201	3PE	C1-O11-P-O14
68	P	201	3PE	C11-O13-P-O14
68	R	304	3PE	C11-O13-P-O14
68	n	605	3PE	C1-O11-P-O12
68	n	605	3PE	C1-O11-P-O14
68	n	606	3PE	C11-O13-P-O14
68	o	302	3PE	C1-O11-P-O14
68	o	302	3PE	C11-O13-P-O14
68	x	101	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
68	H1	401	3PE	C11-O13-P-O14
68	L1	704	3PE	C1-O11-P-O14
68	M1	503	3PE	C1-O11-P-O12
68	N1	402	3PE	C1-O11-P-O14
68	Y1	403	3PE	C1-O11-P-O14
68	d1	202	3PE	C1-O11-P-O14
69	A	502	CDL	CB2-OB2-PB2-OB3
69	C	404	CDL	CB2-OB2-PB2-OB3
69	C	404	CDL	CB2-OB2-PB2-OB4
69	D	302	CDL	CB2-OB2-PB2-OB4
69	D	302	CDL	CB3-OB5-PB2-OB4
69	L	502	CDL	CA3-OA5-PA1-OA4
69	R	301	CDL	CA2-OA2-PA1-OA3
69	R	301	CDL	CA2-OA2-PA1-OA4
69	R	301	CDL	CB2-OB2-PB2-OB4
69	R	301	CDL	CB3-OB5-PB2-OB4
69	R	302	CDL	CB2-OB2-PB2-OB3
69	R	303	CDL	CA2-OA2-PA1-OA3
69	R	303	CDL	CA3-OA5-PA1-OA3
69	V	102	CDL	CA3-OA5-PA1-OA3
69	H1	402	CDL	CA2-OA2-PA1-OA4
69	H1	402	CDL	CB2-OB2-PB2-OB3
69	L1	702	CDL	CA3-OA5-PA1-OA4
69	L1	703	CDL	CA3-OA5-PA1-OA4
69	N1	401	CDL	CA2-OA2-PA1-OA3
69	N1	401	CDL	CA2-OA2-PA1-OA4
69	Y1	401	CDL	CA3-OA5-PA1-OA3
69	Y1	401	CDL	CB3-OB5-PB2-OB3
69	Y1	404	CDL	CA3-OA5-PA1-OA3
69	a1	101	CDL	CA3-OA5-PA1-OA3
69	a1	101	CDL	CA3-OA5-PA1-OA4
69	a1	101	CDL	CB2-OB2-PB2-OB4
69	d1	201	CDL	CB2-OB2-PB2-OB3
69	h1	201	CDL	CA2-OA2-PA1-OA4
73	E	202	PC1	C11-O13-P-O14
73	E	202	PC1	C1-O11-P-O14
73	K	101	PC1	C11-O13-P-O12
73	K	101	PC1	C11-O13-P-O14
73	L	503	PC1	C1-O11-P-O14
73	9	203	PC1	C11-O13-P-O12
73	A1	601	PC1	C1-O11-P-O14
73	A1	601	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
69	L1	702	CDL	OB5-CB3-CB4-CB6
69	h1	201	CDL	OB5-CB3-CB4-CB6
68	Z1	401	3PE	O13-C11-C12-N
76	n	603	HEA	O11-C11-C12-C13
68	p	301	3PE	C32-C33-C34-C35
68	N	401	3PE	C12-C11-O13-P
68	P	201	3PE	C12-C11-O13-P
68	n	606	3PE	C12-C11-O13-P
68	p	301	3PE	C12-C11-O13-P
68	L1	704	3PE	C12-C11-O13-P
69	R	302	CDL	OB5-CB3-CB4-OB6
69	a1	101	CDL	OB5-CB3-CB4-OB6
69	h1	201	CDL	OB5-CB3-CB4-OB6
68	A	501	3PE	O21-C21-C22-C23
68	d1	203	3PE	O21-C21-C22-C23
68	o	302	3PE	C1-C2-C3-O31
73	E	202	PC1	O13-C11-C12-N
73	L	503	PC1	O13-C11-C12-N
73	p	303	PC1	O13-C11-C12-N
73	z	101	PC1	O13-C11-C12-N
73	M1	501	PC1	O13-C11-C12-N
68	o	302	3PE	O21-C2-C3-O31
69	h1	201	CDL	OB6-CB4-CB6-OB8
69	H1	402	CDL	C15-C16-C17-C18
69	a1	101	CDL	C52-C51-CB5-OB6
68	L1	701	3PE	C2-C1-O11-P
73	z	101	PC1	O31-C31-C32-C33
73	A1	601	PC1	C11-C12-N-C13
68	C	403	3PE	C2A-C2B-C2C-C2D
68	p	301	3PE	C2C-C2D-C2E-C2F
68	L1	704	3PE	C37-C38-C39-C3A
68	A1	602	3PE	C2-C1-O11-P
68	i1	201	3PE	C2-C1-O11-P
84	P1	501	NDP	O4D-C1D-N1N-C2N
68	N	401	3PE	C1-O11-P-O13
68	6	202	3PE	C11-O13-P-O11
68	M1	502	3PE	C1-O11-P-O13
68	i1	201	3PE	C11-O13-P-O11
69	A	502	CDL	CA2-OA2-PA1-OA5
69	L	502	CDL	CA2-OA2-PA1-OA5
69	R	301	CDL	CA3-OA5-PA1-OA2
69	V	102	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
69	H1	402	CDL	CB3-OB5-PB2-OB2
69	N1	401	CDL	CA3-OA5-PA1-OA2
69	Y1	401	CDL	C73-C74-C75-C76
68	n	606	3PE	C1-C2-C3-O31
69	d1	201	CDL	CA3-CA4-CA6-OA8
69	C	404	CDL	C72-C71-CB7-OB8
69	N1	401	CDL	C51-C52-C53-C54
73	M1	501	PC1	C28-C29-C2A-C2B
68	Y1	403	3PE	C23-C24-C25-C26
69	Y1	404	CDL	C72-C73-C74-C75
68	p	301	3PE	C2-C1-O11-P
69	D	302	CDL	C1-CA2-OA2-PA1
69	R	301	CDL	C1-CB2-OB2-PB2
68	Z1	401	3PE	C21-C22-C23-C24
68	H1	401	3PE	O31-C31-C32-C33
68	L1	704	3PE	C3D-C3E-C3F-C3G
73	6	203	PC1	C37-C38-C39-C3A
73	A1	601	PC1	O21-C21-C22-C23
68	n	606	3PE	O11-C1-C2-C3
68	A	501	3PE	O13-C11-C12-N
68	Z1	401	3PE	O11-C1-C2-O21
68	D1	501	3PE	O21-C21-C22-C23
69	L1	702	CDL	O1-C1-CB2-OB2
69	d1	201	CDL	O1-C1-CB2-OB2
68	A1	602	3PE	C35-C36-C37-C38
69	C	404	CDL	C72-C71-CB7-OB9
73	M1	501	PC1	O21-C2-C3-O31
73	9	204	PC1	C23-C24-C25-C26
68	M1	502	3PE	C2-C1-O11-P
73	z	101	PC1	C2-C1-O11-P
69	H1	402	CDL	C72-C71-CB7-OB9
76	n	604	HEA	CAA-CBA-CGA-O1A
69	d1	201	CDL	C54-C55-C56-C57
69	L1	703	CDL	CB3-CB4-CB6-OB8
73	p	303	PC1	C23-C24-C25-C26
76	n	603	HEA	CAD-CBD-CGD-O1D
68	t	101	3PE	C3-C2-O21-C21
73	p	303	PC1	C1-C2-O21-C21
73	6	203	PC1	C3-C2-O21-C21
73	9	203	PC1	C3-C2-O21-C21
76	n	603	HEA	C27-C19-C20-C21
69	L	502	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
69	R	302	CDL	C72-C71-CB7-OB8
73	p	302	PC1	O11-C1-C2-C3
76	n	604	HEA	CAA-CBA-CGA-O2A
68	H1	401	3PE	C22-C23-C24-C25
85	n1	201	ZMP	C12-C11-S1-C10
68	M1	502	3PE	O21-C2-C3-O31
69	N1	401	CDL	OB6-CB4-CB6-OB8
69	d1	201	CDL	OA6-CA4-CA6-OA8
69	d1	201	CDL	OB6-CB4-CB6-OB8
73	9	204	PC1	C29-C2A-C2B-C2C
70	N	403	HEM	CAD-CBD-CGD-O2D
68	i1	201	3PE	C24-C25-C26-C27
69	h1	201	CDL	C12-C11-CA5-OA6
68	Y1	403	3PE	C1-C2-C3-O31
69	Y1	401	CDL	C72-C71-CB7-OB8
68	R	304	3PE	O11-C1-C2-O21
73	p	302	PC1	O11-C1-C2-O21
76	n	603	HEA	CAD-CBD-CGD-O2D
73	9	203	PC1	C37-C38-C39-C3A
69	Y1	401	CDL	C17-C18-C19-C20
69	H1	402	CDL	C17-C18-C19-C20
69	Y1	404	CDL	CA5-C11-C12-C13
73	M1	501	PC1	C3A-C3B-C3C-C3D
68	v	101	3PE	O31-C31-C32-C33
69	R	302	CDL	C12-C11-CA5-OA6
69	L1	703	CDL	OB6-CB4-CB6-OB8
68	Z1	401	3PE	O32-C31-C32-C33
68	A	501	3PE	O31-C31-C32-C33
69	R	301	CDL	C52-C51-CB5-OB6
73	A1	601	PC1	O31-C31-C32-C33
82	1	501	FMN	C5'-O5'-P-O3P
85	W1	201	ZMP	C2-C1-C22-C23
85	n1	201	ZMP	N2-C16-C17-O4
69	h1	201	CDL	C32-C31-CA7-OA8
68	C	405	3PE	C35-C36-C37-C38
69	R	303	CDL	C31-C32-C33-C34
70	N	403	HEM	CAD-CBD-CGD-O1D
69	d1	201	CDL	CA2-OA2-PA1-OA5
76	n	603	HEA	C18-C19-C20-C21
73	p	303	PC1	C22-C23-C24-C25
68	A1	602	3PE	O31-C31-C32-C33
69	Y1	401	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
73	9	203	PC1	C35-C36-C37-C38
68	D1	501	3PE	C39-C3A-C3B-C3C
68	p	301	3PE	C23-C24-C25-C26
68	L	501	3PE	O31-C31-C32-C33
69	R	303	CDL	C72-C71-CB7-OB8
69	h1	201	CDL	C72-C71-CB7-OB8
68	Z1	401	3PE	C3-C2-O21-C21
73	A1	601	PC1	C3-C2-O21-C21
70	N	403	HEM	CAA-CBA-CGA-O2A
68	N	404	3PE	O31-C31-C32-C33
69	L1	702	CDL	C72-C71-CB7-OB8
69	A	502	CDL	C12-C11-CA5-OA6
69	C	404	CDL	C32-C31-CA7-OA8
73	9	204	PC1	O31-C31-C32-C33
68	M1	502	3PE	C2C-C2D-C2E-C2F
69	h1	201	CDL	C1-CA2-OA2-PA1
69	V	102	CDL	OB5-CB3-CB4-OB6
73	A1	601	PC1	O11-C1-C2-O21
68	K1	201	3PE	O31-C31-C32-C33
68	C	406	3PE	O31-C31-C32-C33
70	N	403	HEM	CAA-CBA-CGA-O1A
69	A	502	CDL	C32-C31-CA7-OA8
73	9	204	PC1	C2F-C2G-C2H-C2I
68	R	304	3PE	O11-C1-C2-C3
68	t	101	3PE	O11-C1-C2-C3
69	R	302	CDL	OB5-CB3-CB4-CB6
73	M1	501	PC1	O11-C1-C2-C3
68	H1	401	3PE	C3B-C3C-C3D-C3E
68	n	606	3PE	O21-C21-C22-C23
69	R	303	CDL	C52-C51-CB5-OB6
68	t	101	3PE	O21-C2-C3-O31
68	d1	202	3PE	O21-C2-C3-O31
76	n	603	HEA	CAA-CBA-CGA-O1A
86	O1	401	DGT	C5'-O5'-PA-O3A
68	C	403	3PE	O31-C31-C32-C33
68	K1	201	3PE	O21-C21-C22-C23
68	i1	201	3PE	O31-C31-C32-C33
68	o	302	3PE	C21-C22-C23-C24
73	M1	501	PC1	C29-C2A-C2B-C2C
69	L1	702	CDL	C1-CB2-OB2-PB2
68	t	101	3PE	O31-C31-C32-C33
68	L1	704	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
69	V	102	CDL	C12-C11-CA5-OA6
68	K1	201	3PE	C25-C26-C27-C28
68	i1	201	3PE	C2B-C2C-C2D-C2E
68	N	404	3PE	O32-C31-C32-C33
73	9	204	PC1	O32-C31-C32-C33
68	6	202	3PE	O21-C21-C22-C23
69	R	301	CDL	C52-C51-CB5-OB7
73	9	203	PC1	C29-C2A-C2B-C2C
68	q	201	3PE	O21-C21-C22-C23
69	A	502	CDL	C12-C11-CA5-OA7
69	A	502	CDL	C32-C31-CA7-OA9
69	L1	702	CDL	C72-C71-CB7-OB9
69	h1	201	CDL	C32-C31-CA7-OA9
68	6	202	3PE	O22-C21-C22-C23
68	A1	602	3PE	O32-C31-C32-C33
68	K1	201	3PE	O32-C31-C32-C33
69	R	303	CDL	C72-C71-CB7-OB9
69	h1	201	CDL	C72-C71-CB7-OB9
68	Z1	401	3PE	C2A-C2B-C2C-C2D
85	W1	201	ZMP	C22-C1-C2-C3
68	M1	503	3PE	C21-C22-C23-C24
73	p	303	PC1	C2-C1-O11-P
69	R	303	CDL	C52-C51-CB5-OB7
73	A1	601	PC1	O32-C31-C32-C33
68	R	304	3PE	C1-O11-P-O14
68	6	202	3PE	C11-O13-P-O14
69	A	502	CDL	CA2-OA2-PA1-OA3
69	L	502	CDL	CA2-OA2-PA1-OA3
69	L1	703	CDL	CB3-OB5-PB2-OB3
69	N1	401	CDL	CB3-OB5-PB2-OB3
73	V	101	PC1	C11-O13-P-O14
68	C	406	3PE	O32-C31-C32-C33
68	L	501	3PE	O32-C31-C32-C33
68	n	606	3PE	O22-C21-C22-C23
68	v	101	3PE	O13-C11-C12-N
68	Y1	402	3PE	O13-C11-C12-N
68	K1	201	3PE	O22-C21-C22-C23
86	O1	401	DGT	PB-O3B-PG-O3G
68	A	501	3PE	C3-C2-O21-C21
68	n	605	3PE	C1-C2-O21-C21
68	o	302	3PE	C12-C11-O13-P
68	x	101	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
68	L1	701	3PE	C3-C2-O21-C21
68	Y1	403	3PE	C12-C11-O13-P
69	L	502	CDL	CB6-CB4-OB6-CB5
69	N1	401	CDL	CB6-CB4-OB6-CB5
69	Y1	404	CDL	CA3-CA4-OA6-CA5
69	a1	101	CDL	CA3-CA4-OA6-CA5
69	h1	201	CDL	CB6-CB4-OB6-CB5
73	L	503	PC1	C1-C2-O21-C21
73	9	204	PC1	C12-C11-O13-P
68	C	406	3PE	O21-C21-C22-C23
68	L1	704	3PE	O31-C31-C32-C33
69	R	303	CDL	C12-C11-CA5-OA6
68	C	405	3PE	O21-C21-C22-C23
68	n	605	3PE	O21-C21-C22-C23
69	R	303	CDL	C32-C31-CA7-OA8
69	D	302	CDL	C75-C76-C77-C78
68	L1	701	3PE	O31-C31-C32-C33
69	R	301	CDL	C72-C71-CB7-OB8
73	K	101	PC1	O21-C21-C22-C23
68	C	403	3PE	O32-C31-C32-C33
68	C	406	3PE	O22-C21-C22-C23
68	i1	201	3PE	O32-C31-C32-C33
69	d1	201	CDL	C57-C58-C59-C60
70	N	402	HEM	CAD-CBD-CGD-O2D
68	Y1	402	3PE	O31-C31-C32-C33
68	Y1	403	3PE	O31-C31-C32-C33
73	p	302	PC1	O31-C31-C32-C33
69	L	502	CDL	C52-C51-CB5-OB6
73	L	503	PC1	O21-C21-C22-C23
68	q	201	3PE	O22-C21-C22-C23
82	1	501	FMN	O4'-C4'-C5'-O5'
69	N1	401	CDL	C52-C51-CB5-OB6
80	y	601	TGL	OG2-CB1-CB2-CB3
68	M1	502	3PE	C26-C27-C28-C29
68	C	405	3PE	O22-C21-C22-C23
68	n	605	3PE	O22-C21-C22-C23
68	t	101	3PE	O32-C31-C32-C33
68	L1	704	3PE	O22-C21-C22-C23
68	Y1	403	3PE	O32-C31-C32-C33
76	n	603	HEA	CAA-CBA-CGA-O2A
73	p	303	PC1	C26-C27-C28-C29
68	M1	502	3PE	O31-C31-C32-C33

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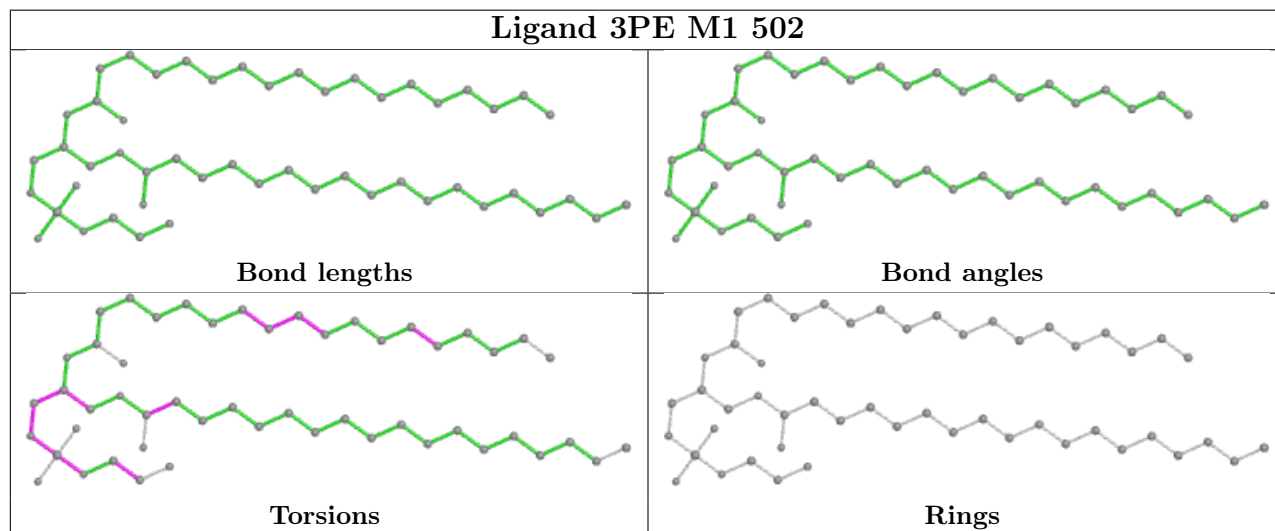
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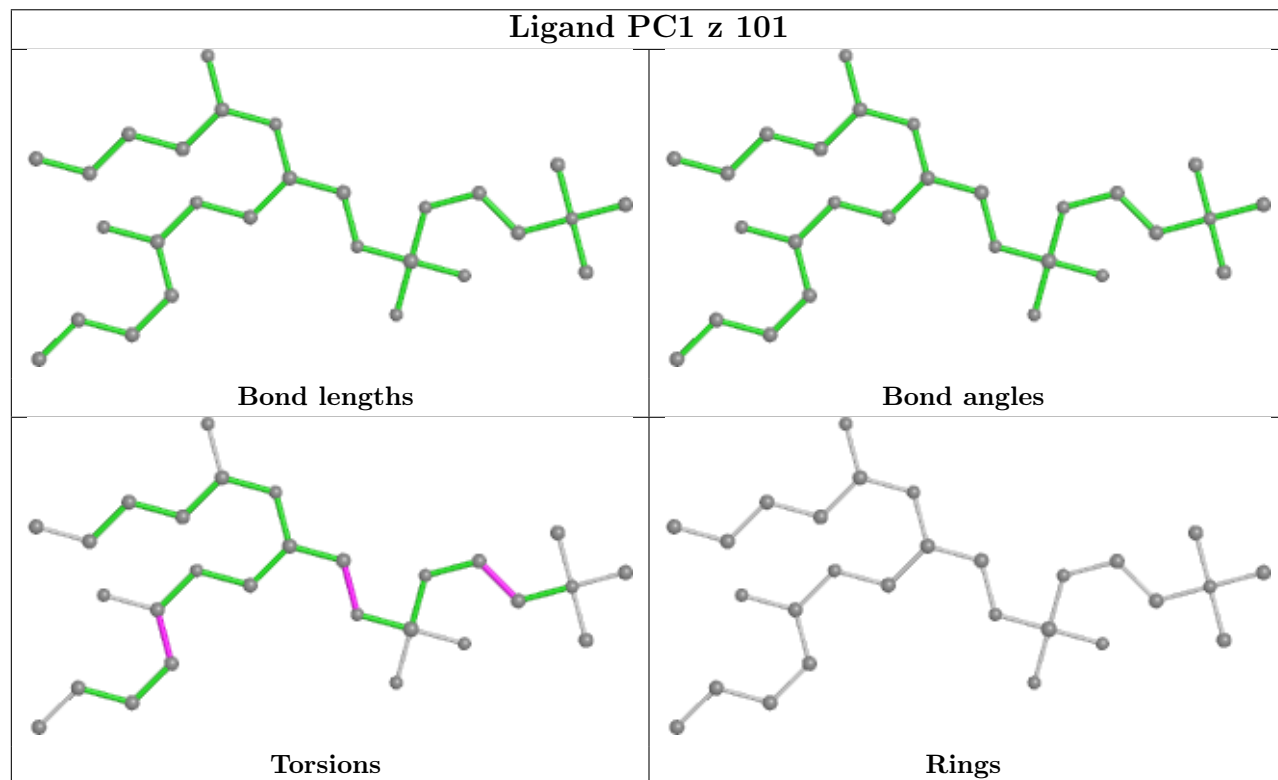
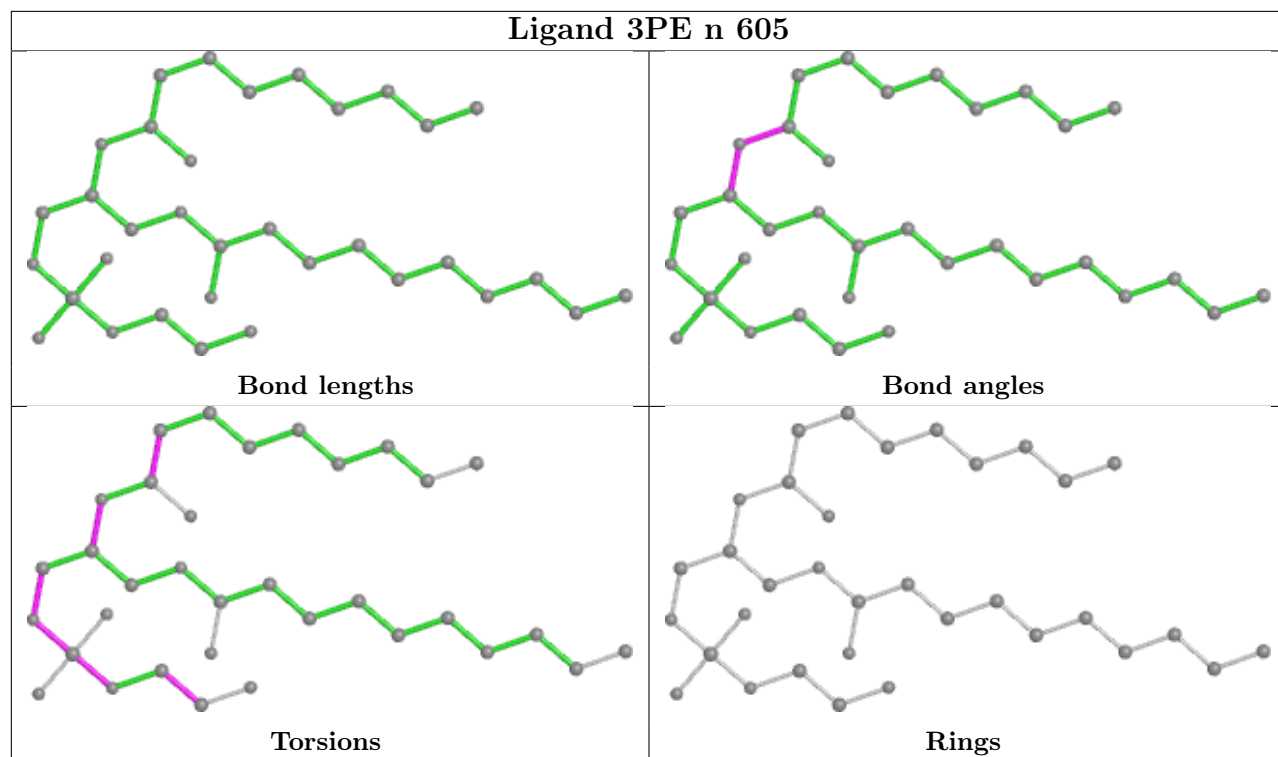
Mol	Chain	Res	Type	Atoms
69	L1	703	CDL	C32-C31-CA7-OA8
69	d1	201	CDL	C72-C71-CB7-OB8
69	R	301	CDL	C72-C71-CB7-OB9
70	C	401	HEM	CAA-CBA-CGA-O1A
73	M1	501	PC1	C23-C24-C25-C26
68	H1	401	3PE	C33-C34-C35-C36

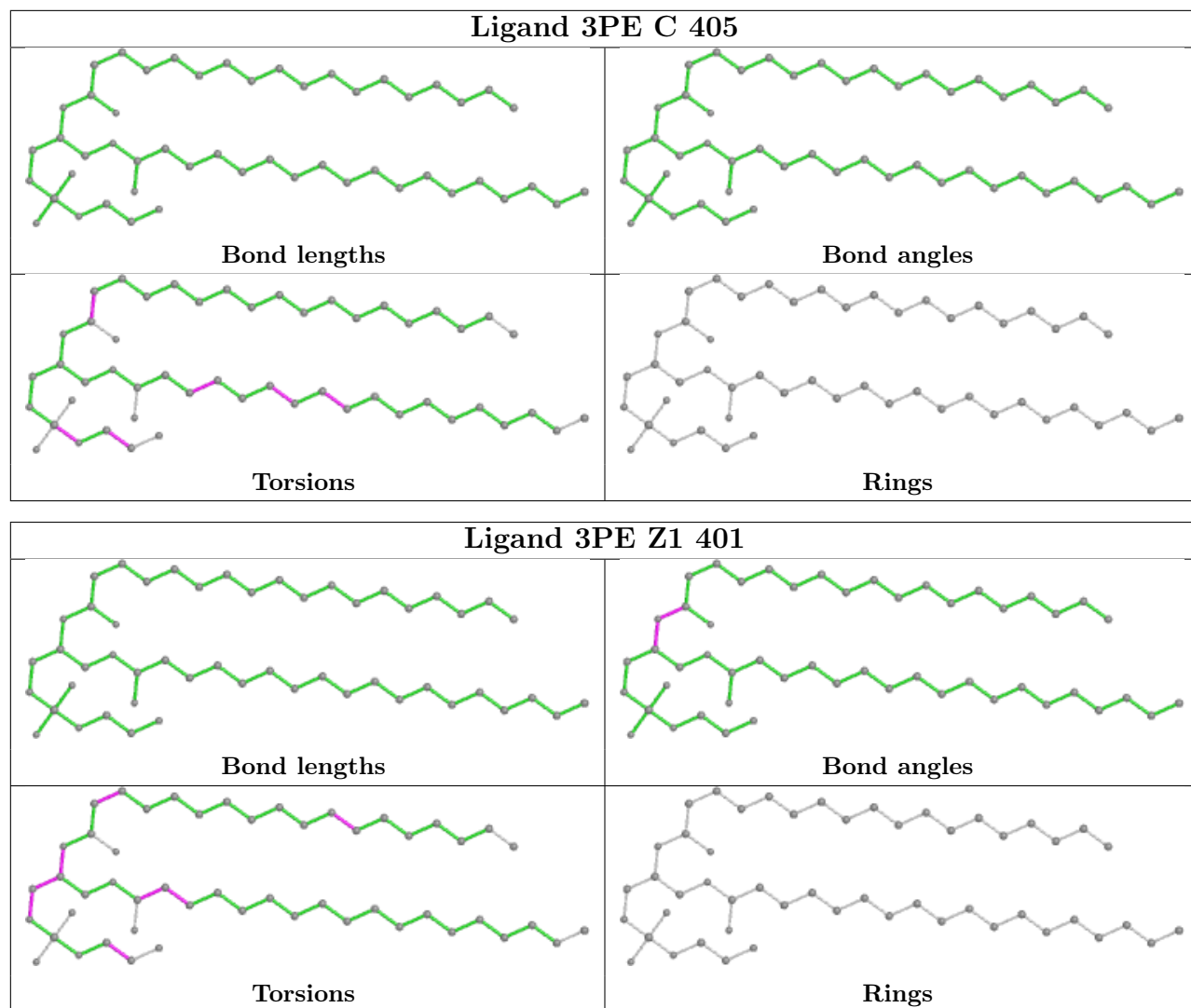
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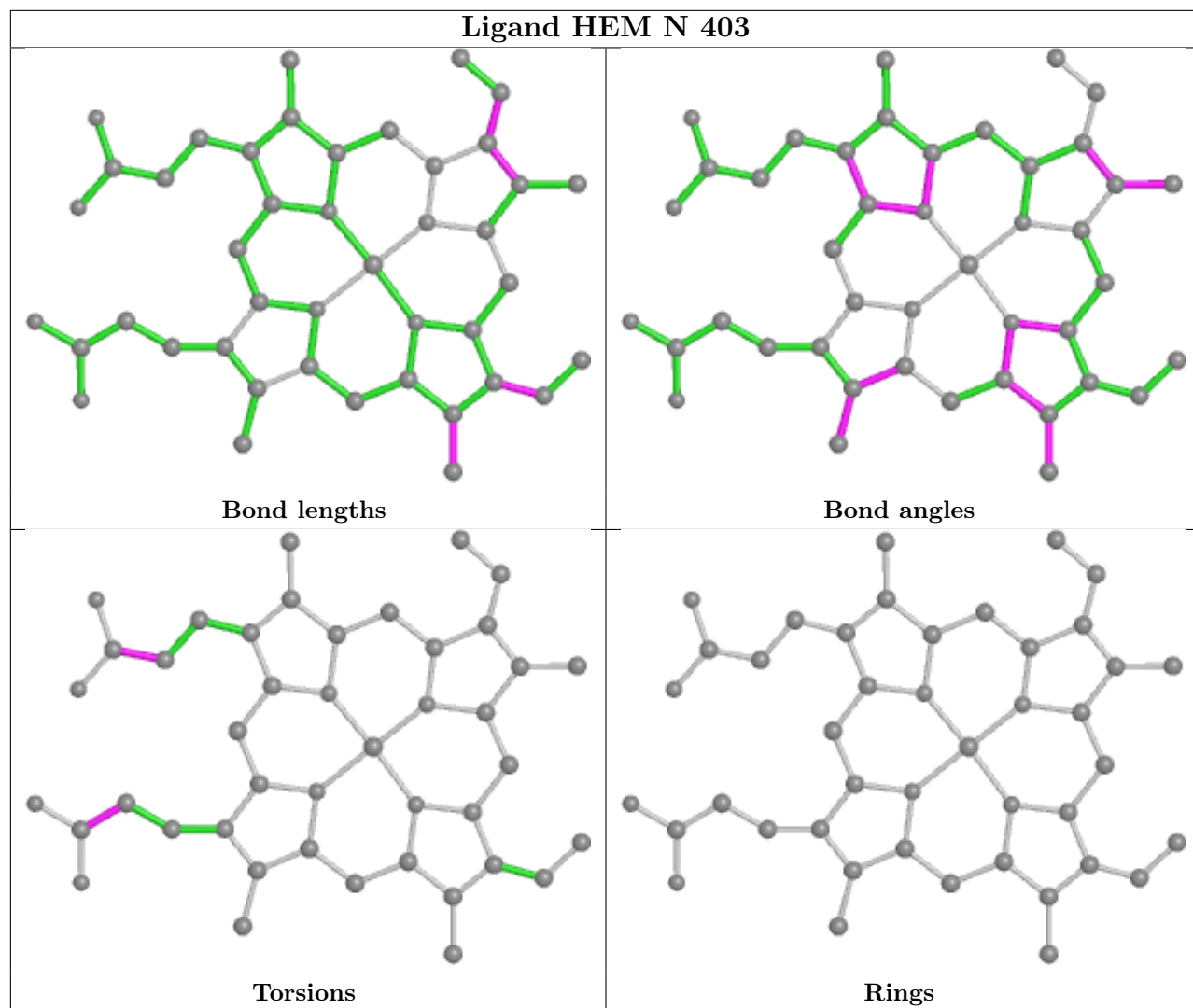
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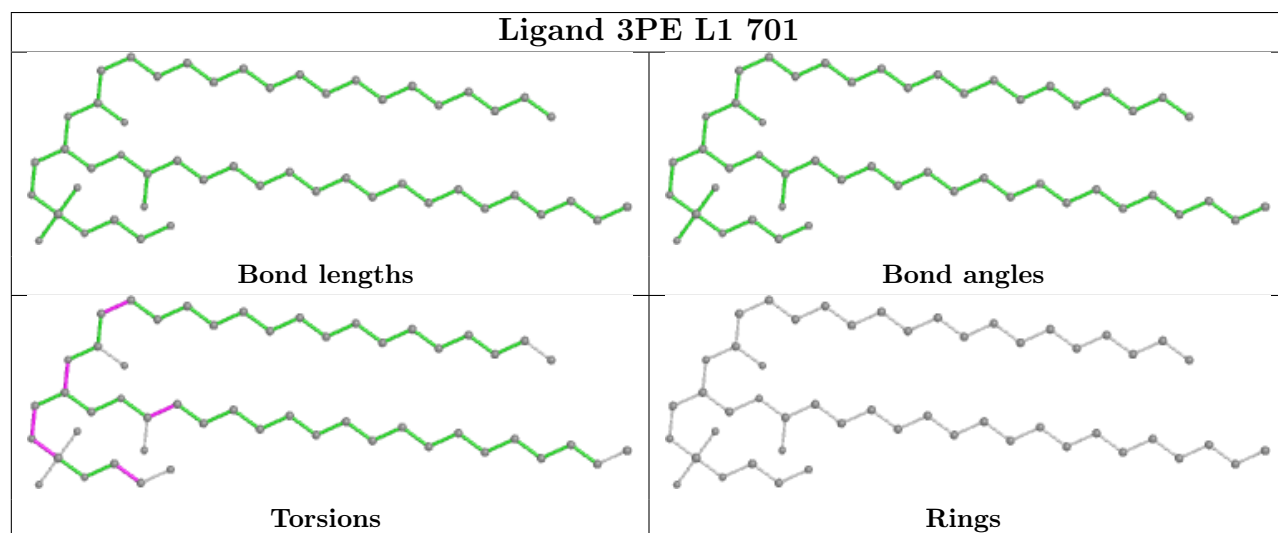
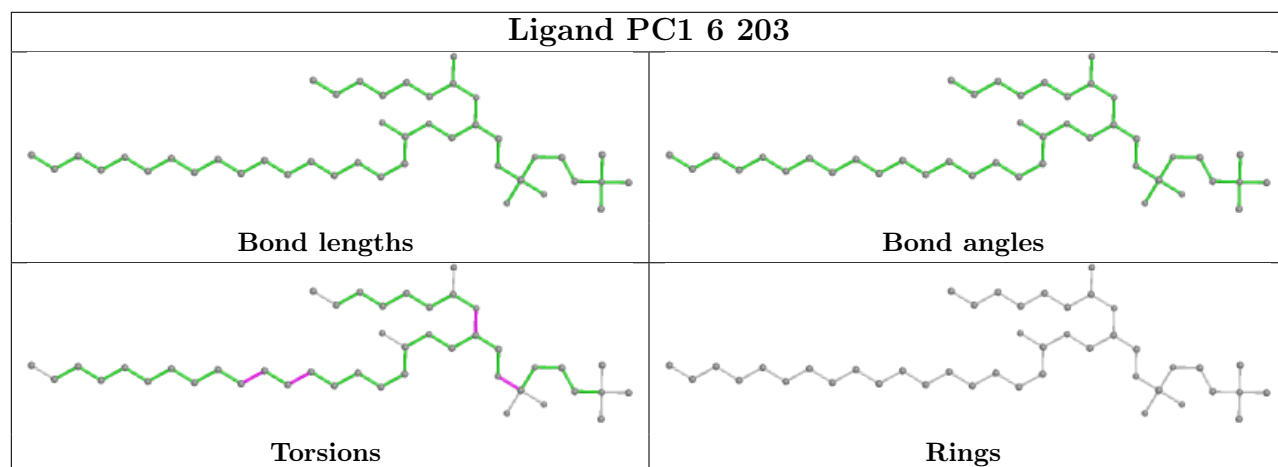
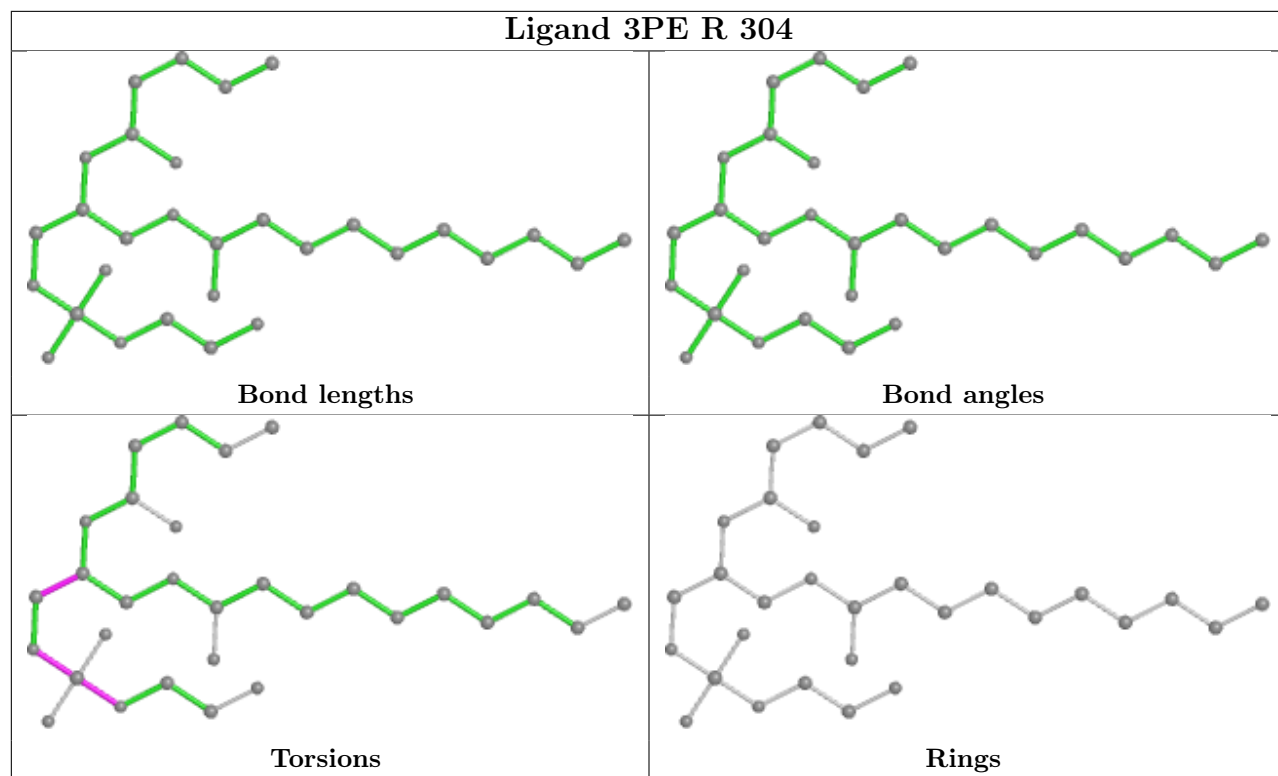
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

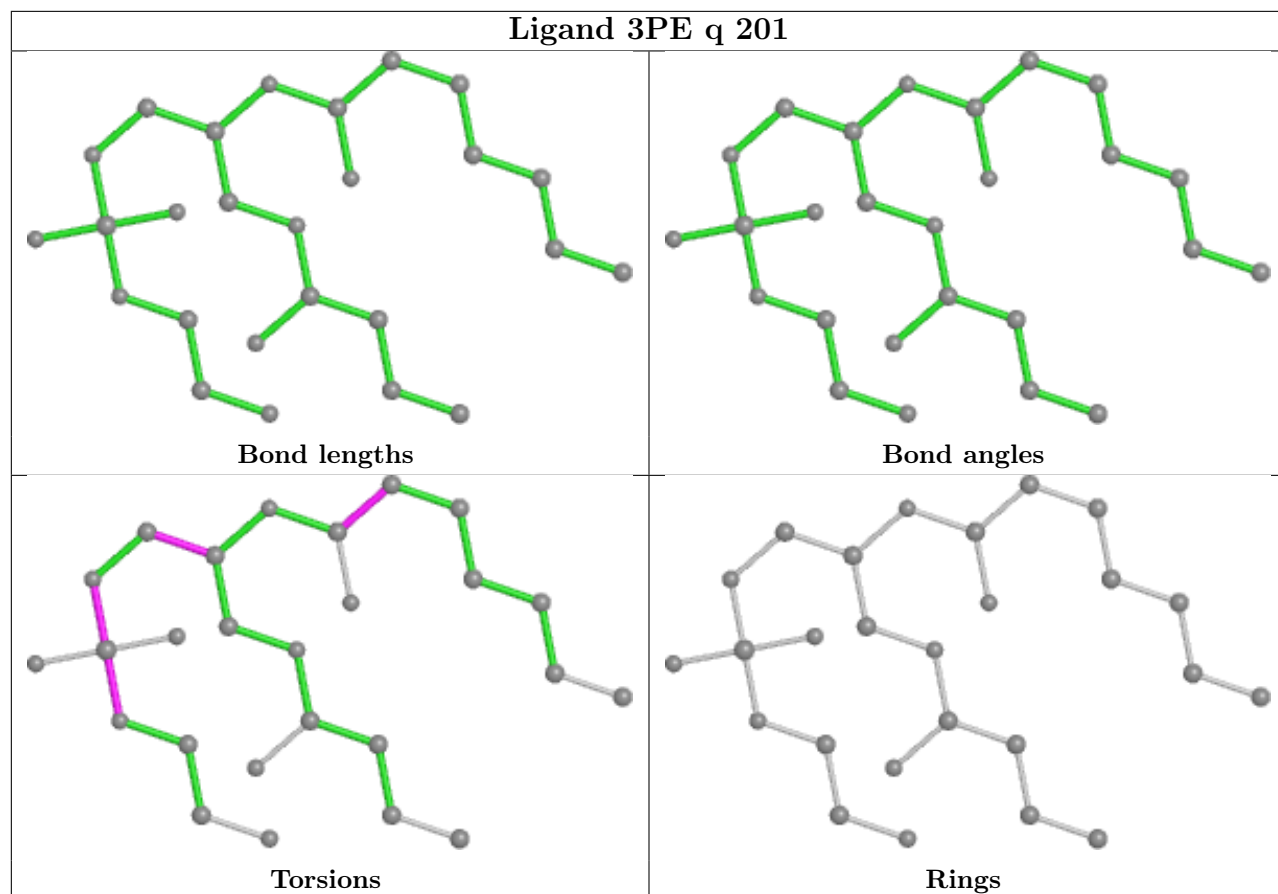


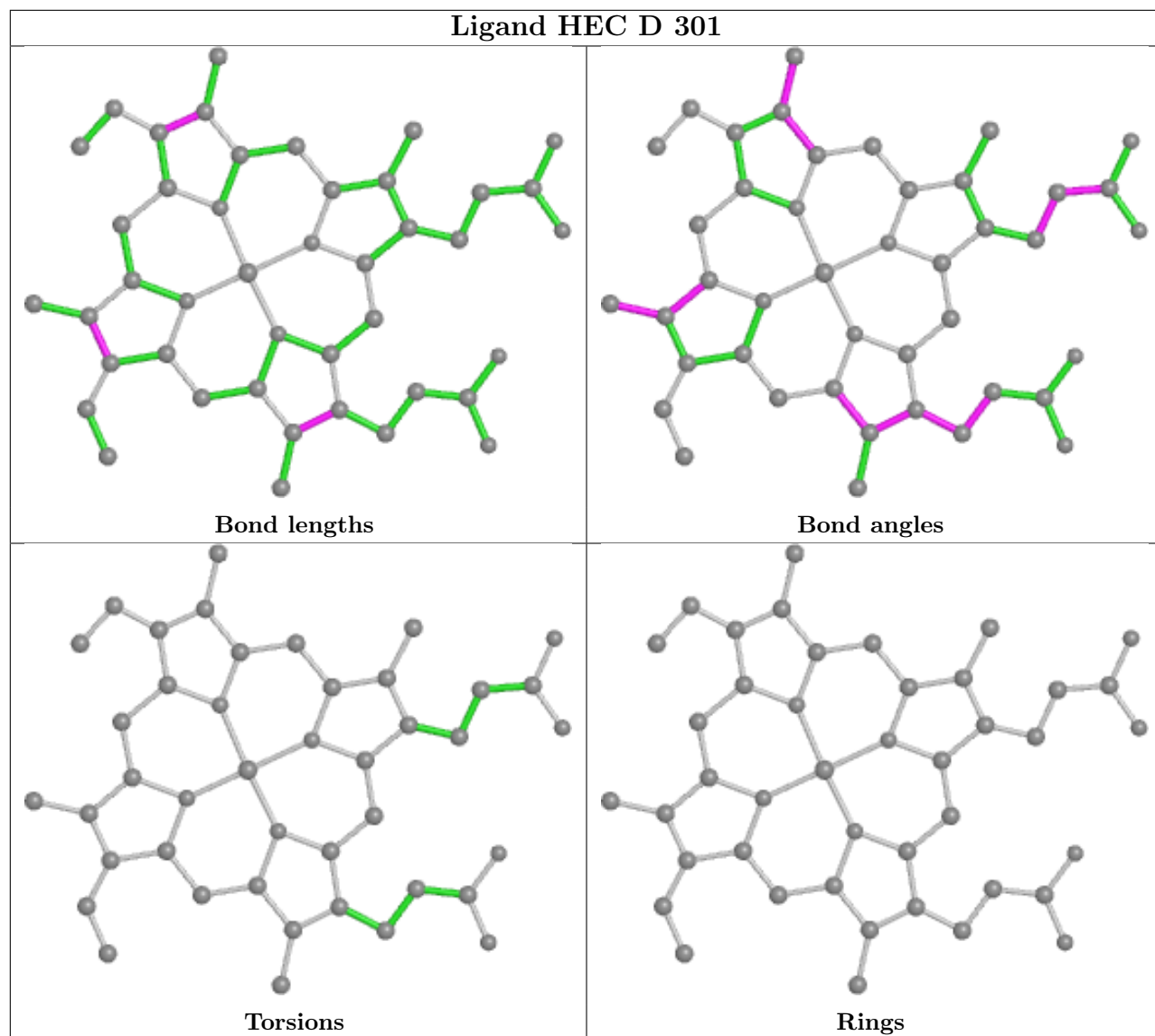


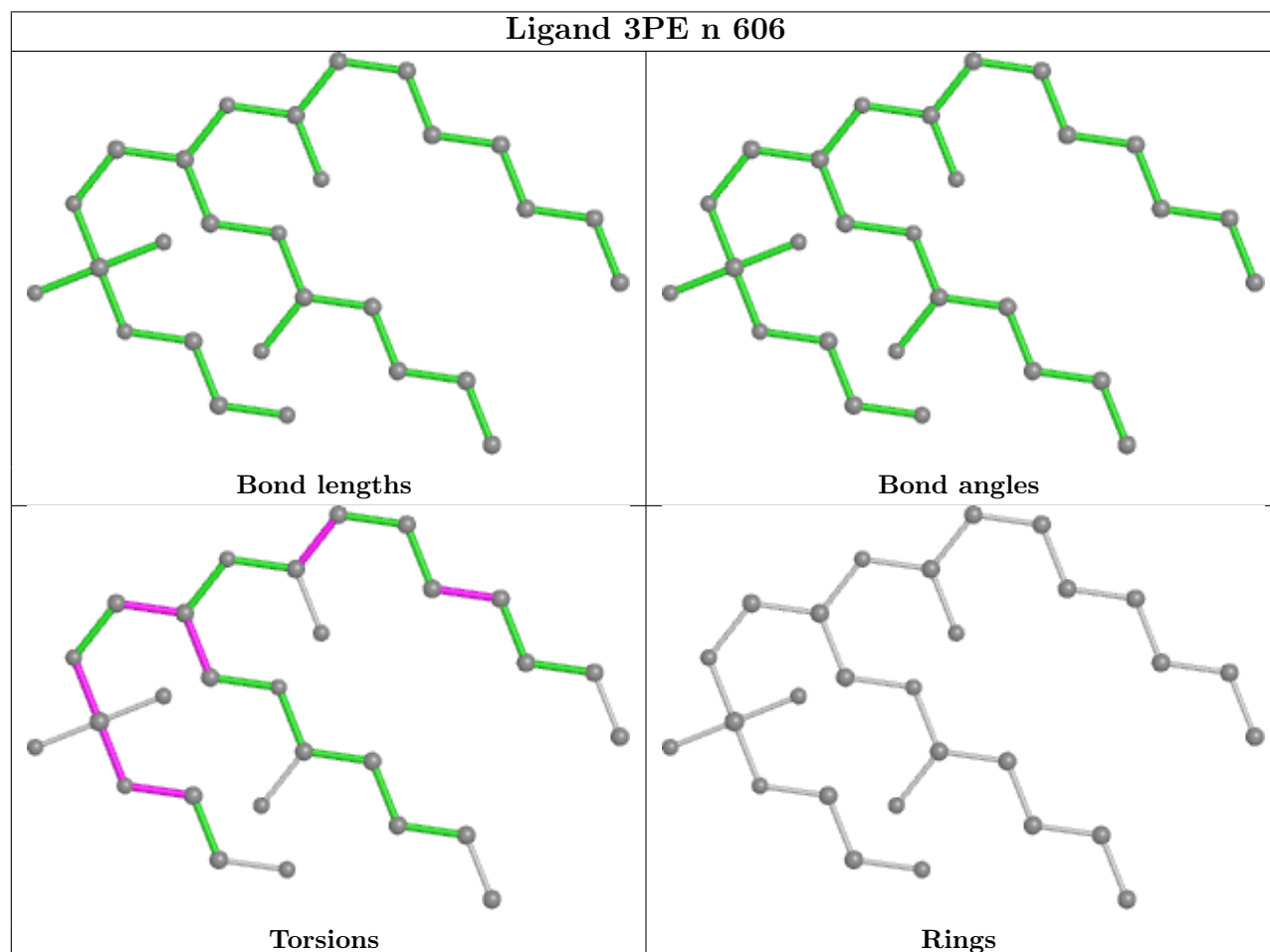
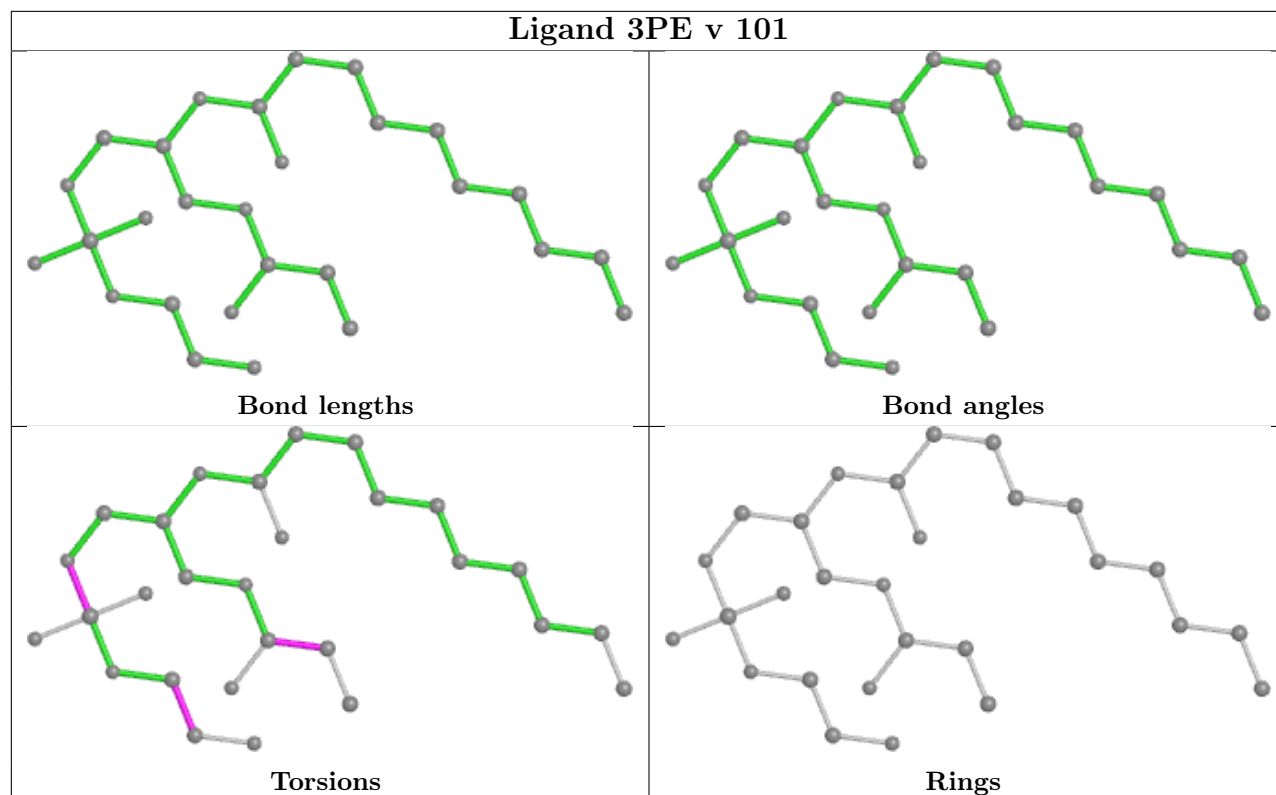


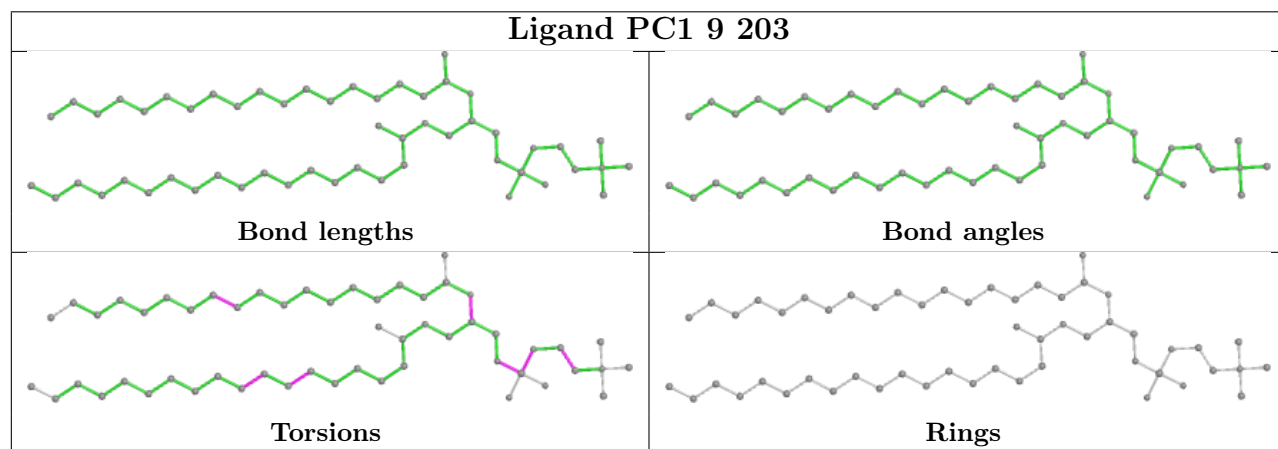
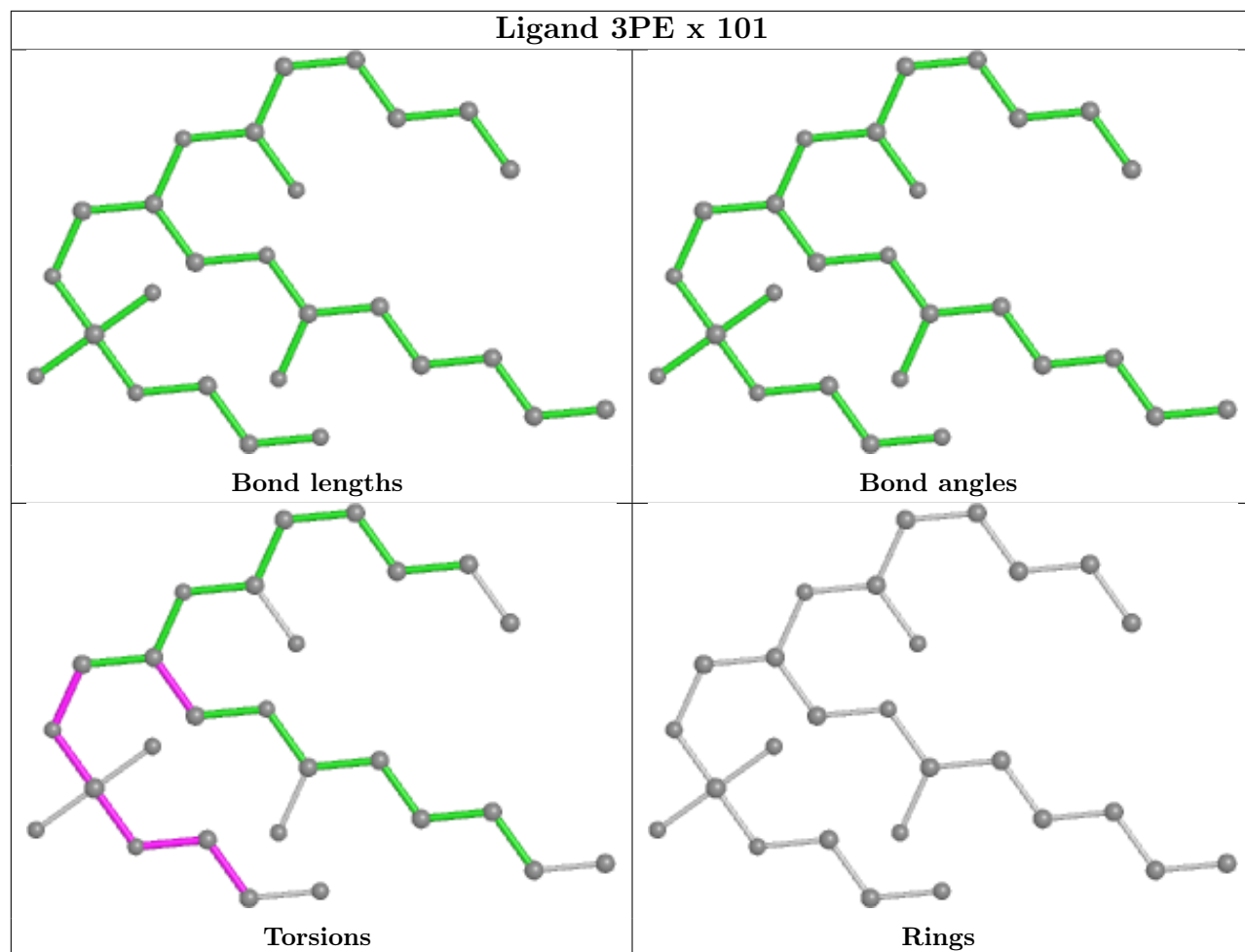


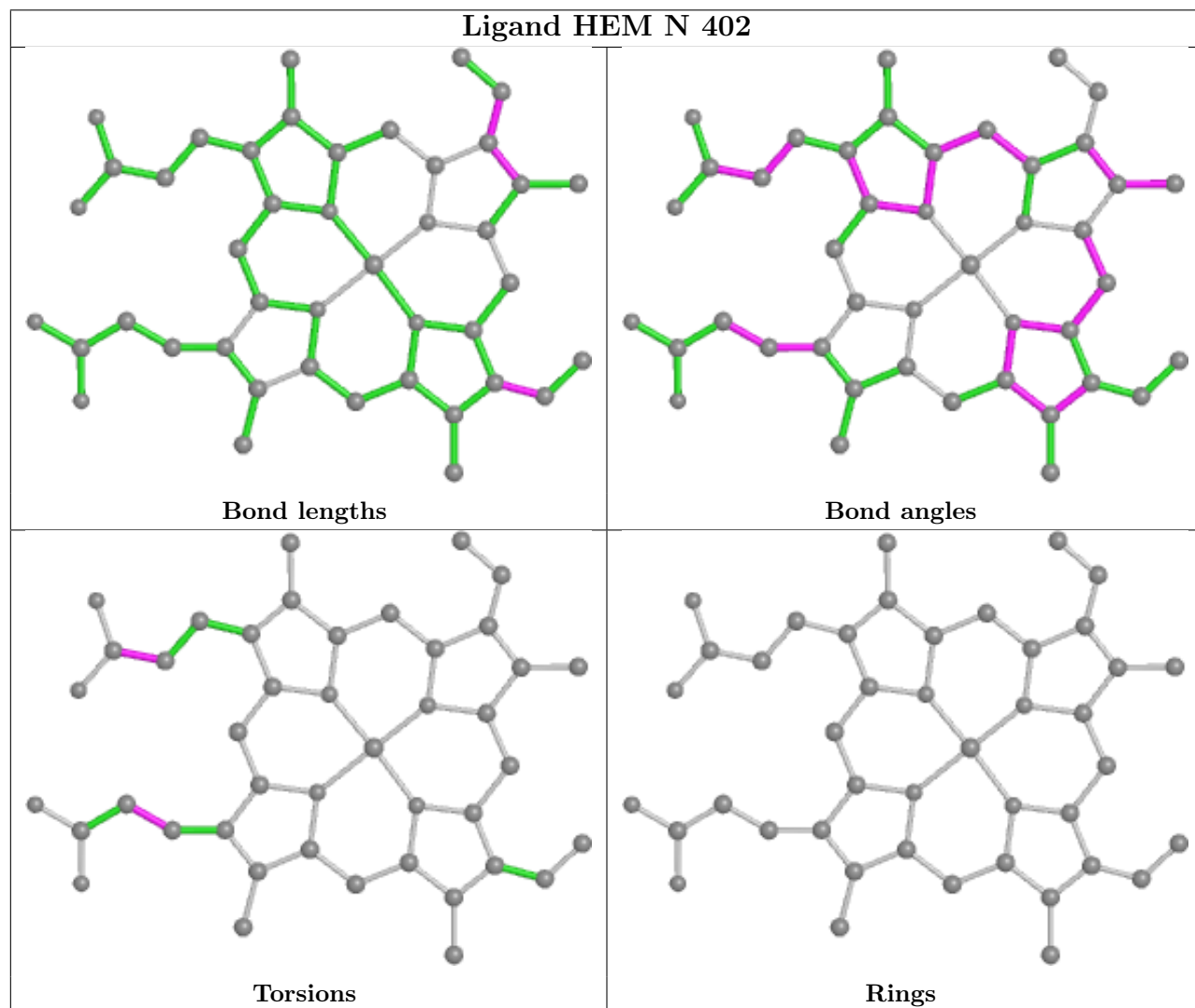
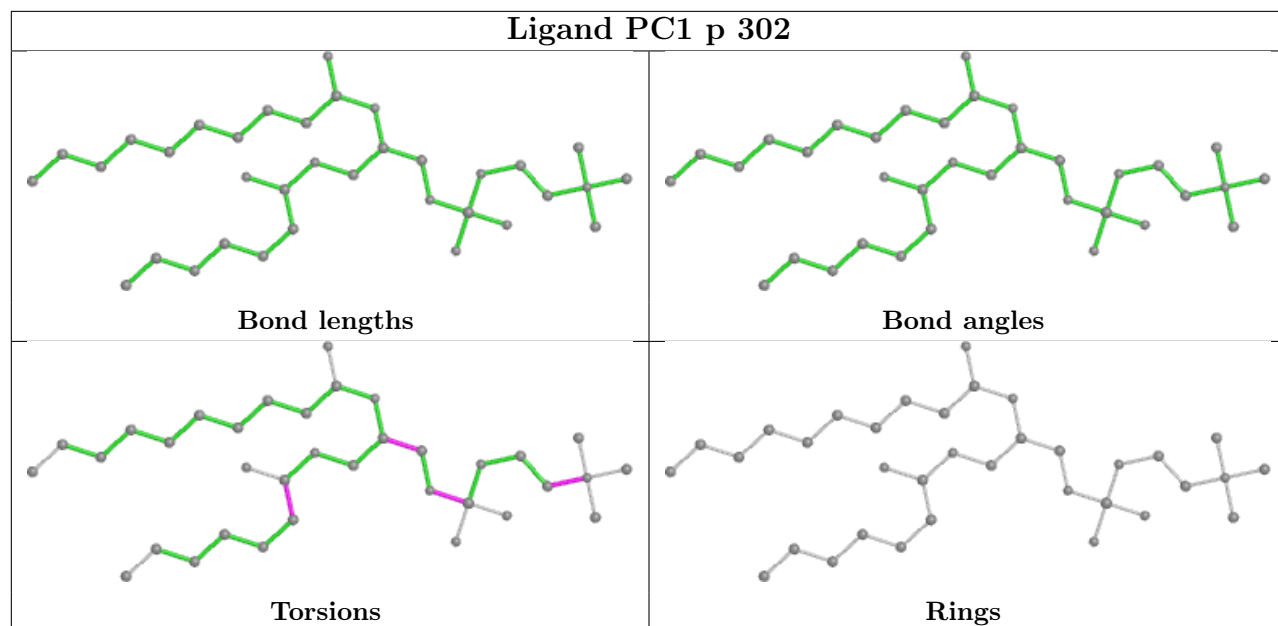


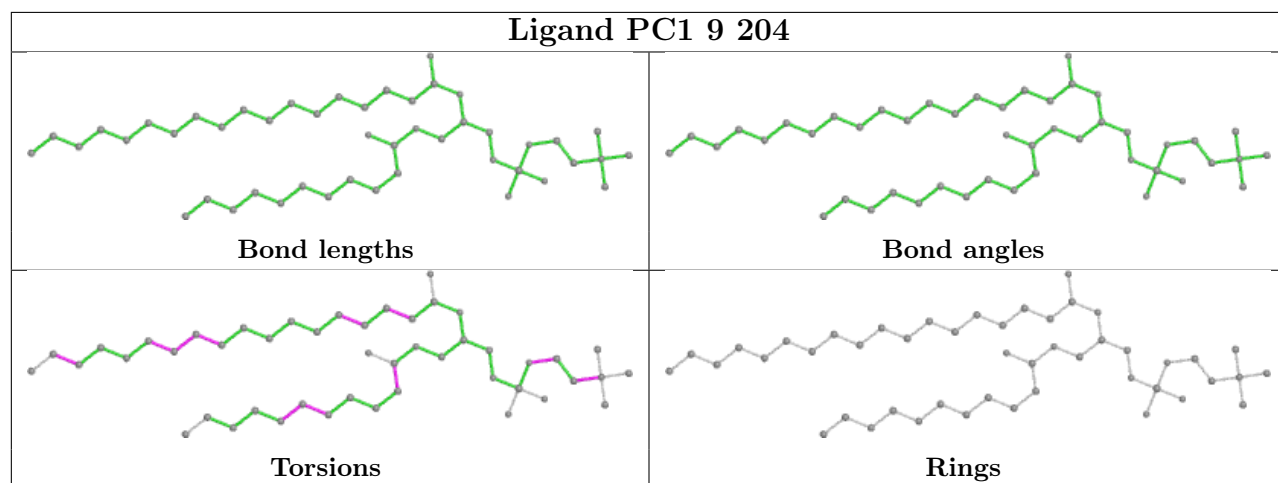
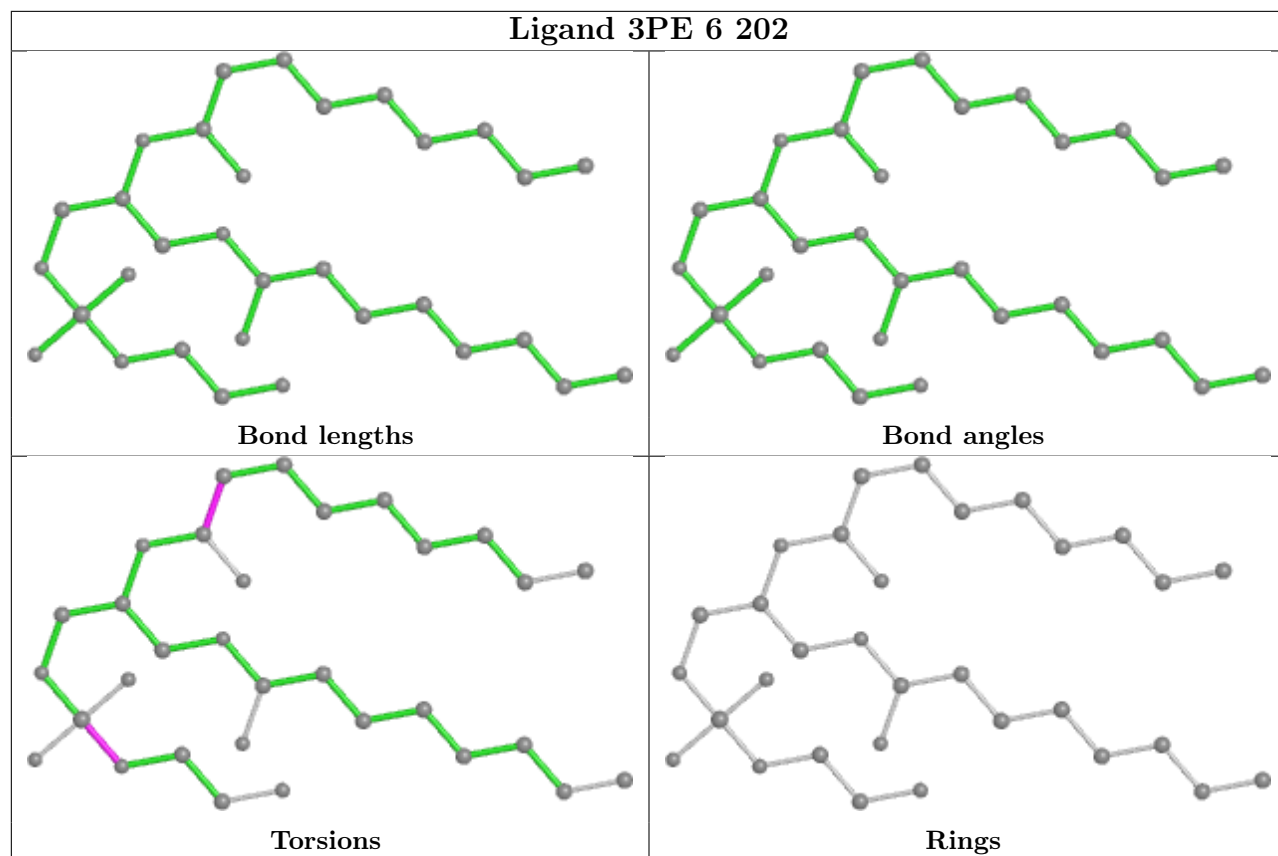


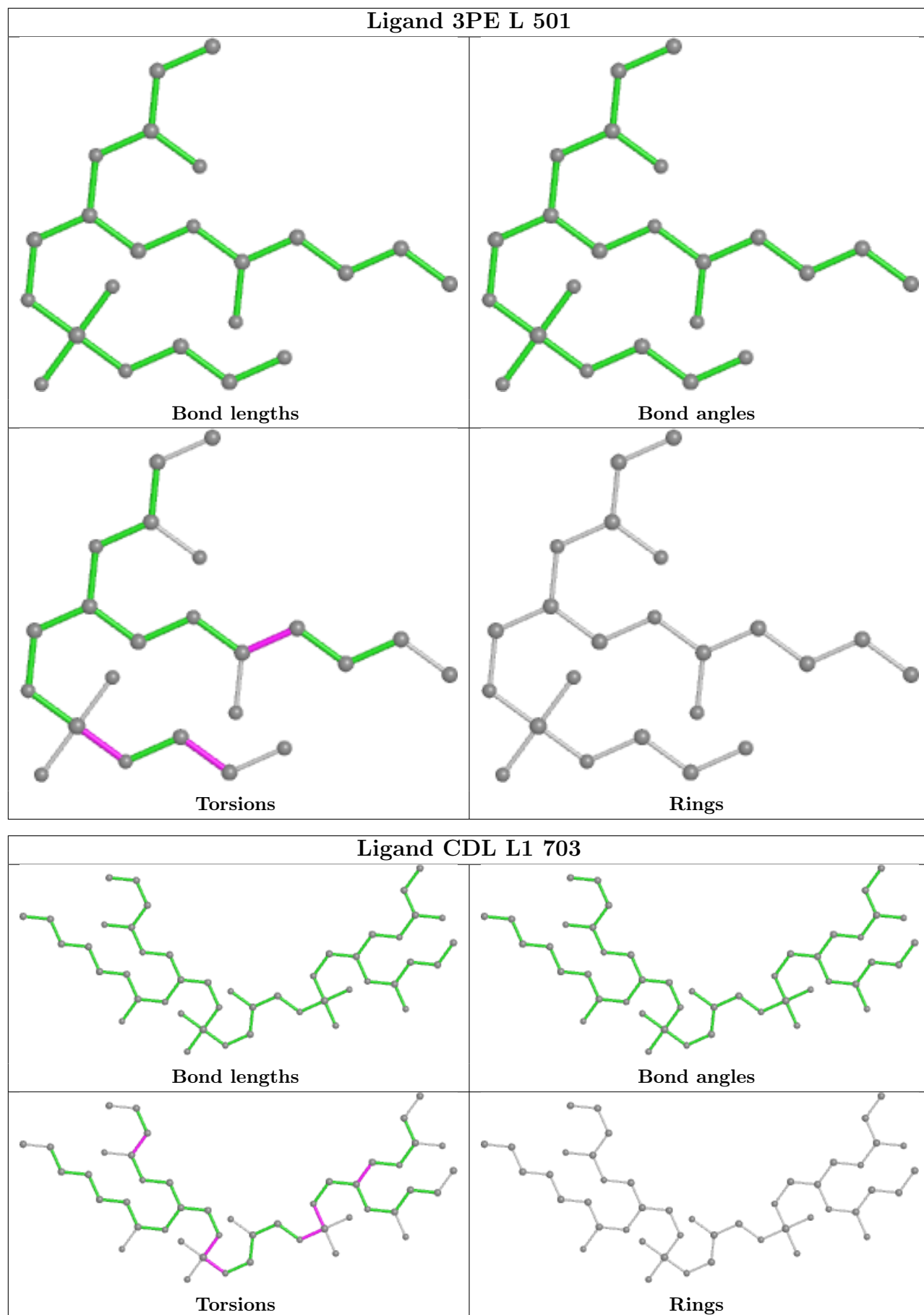


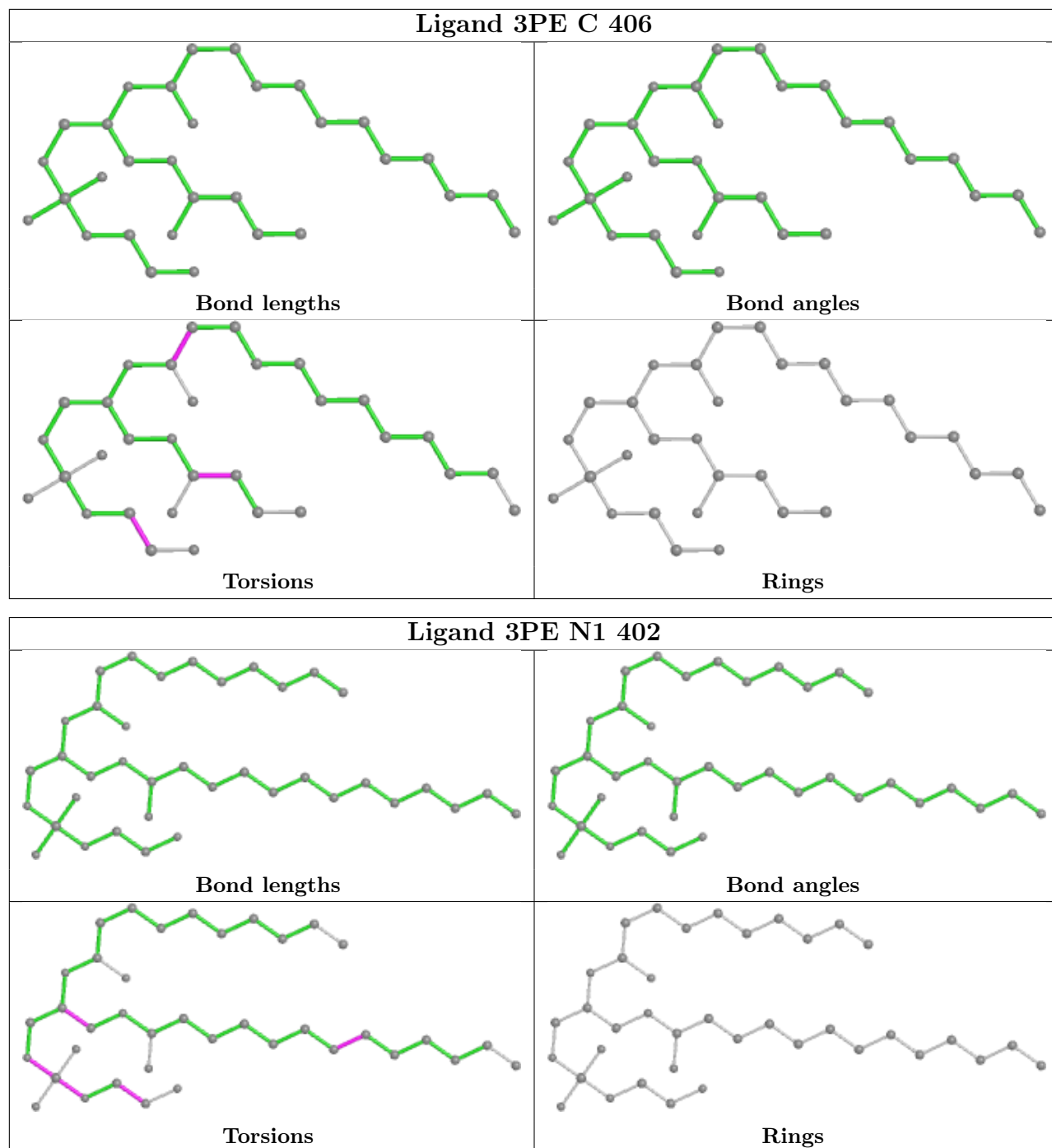


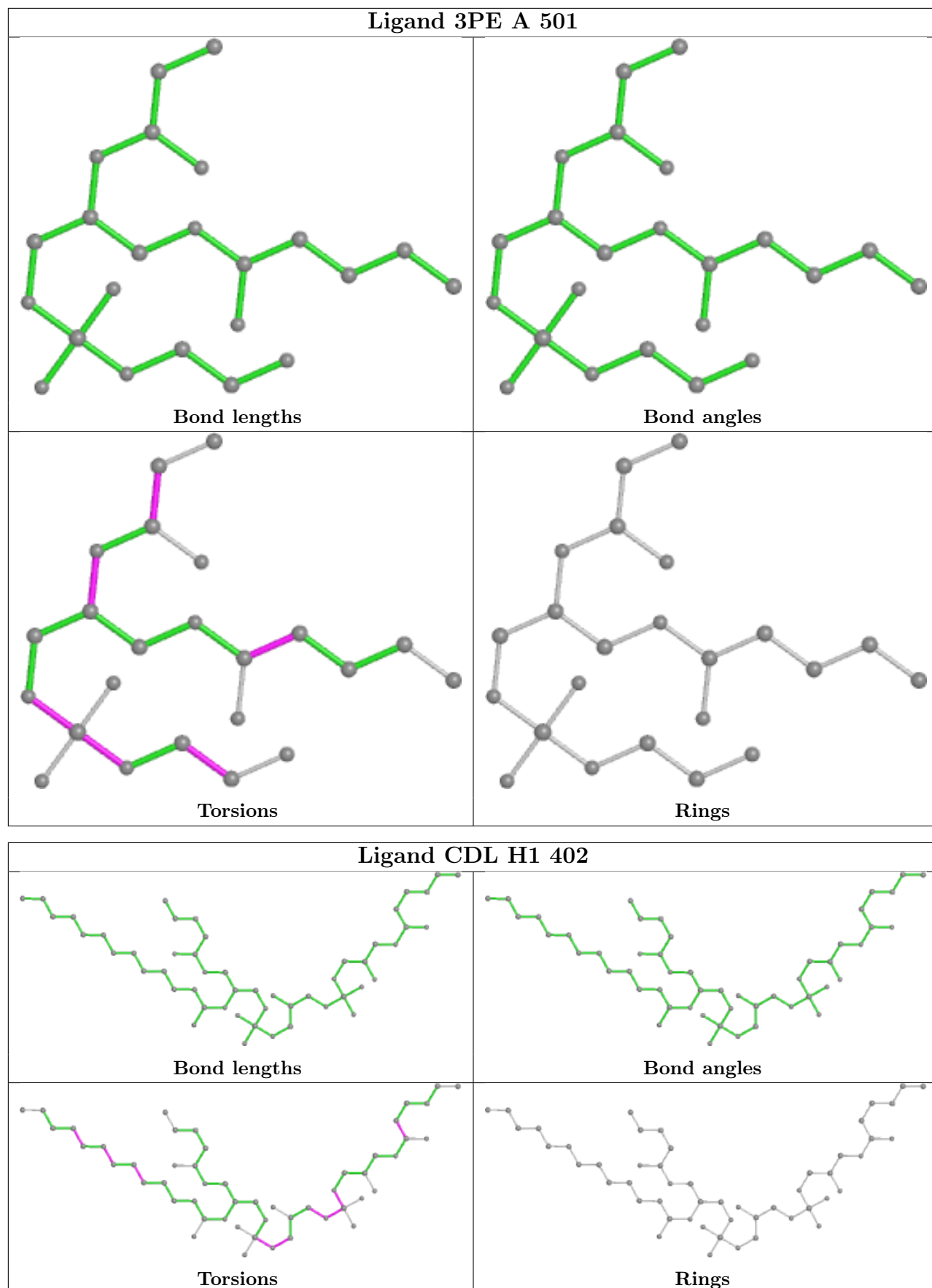


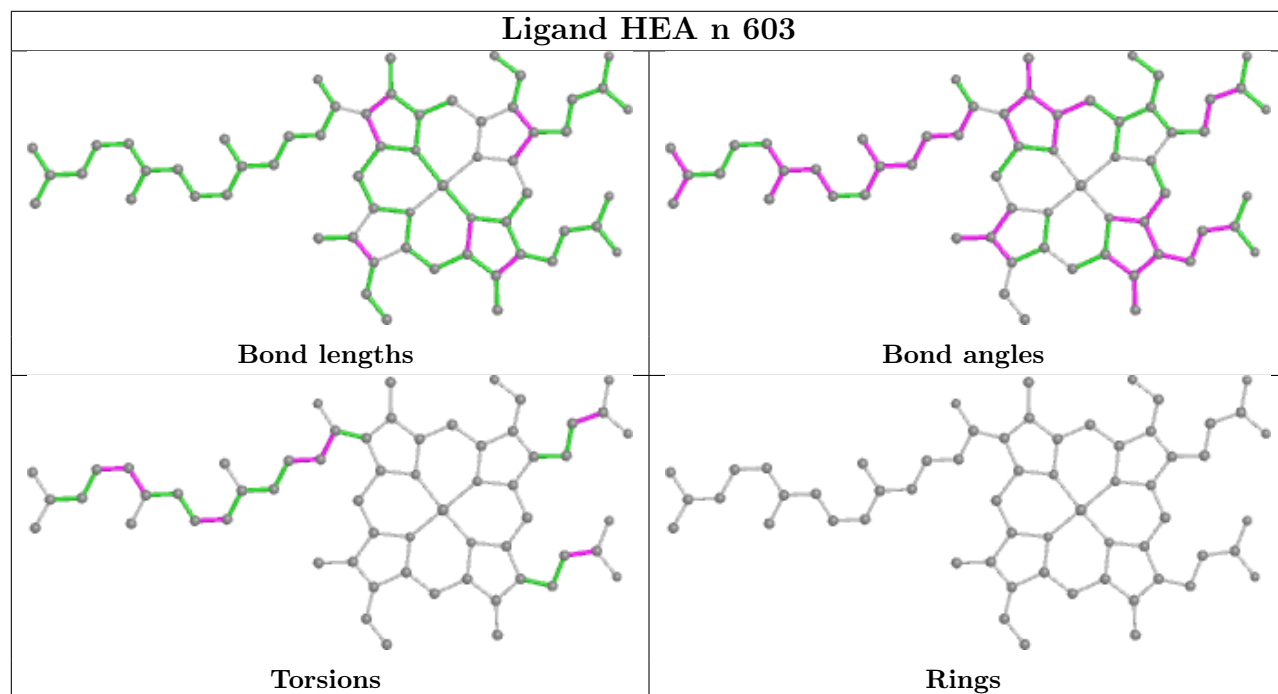
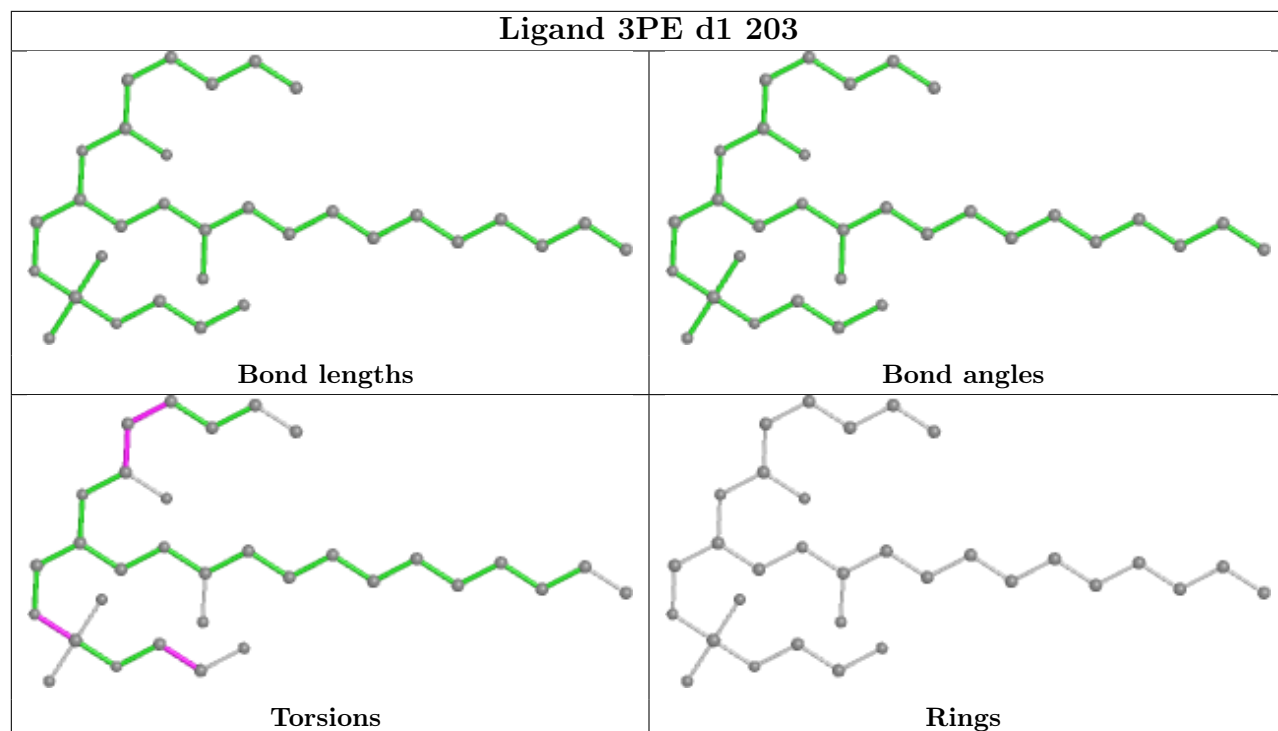


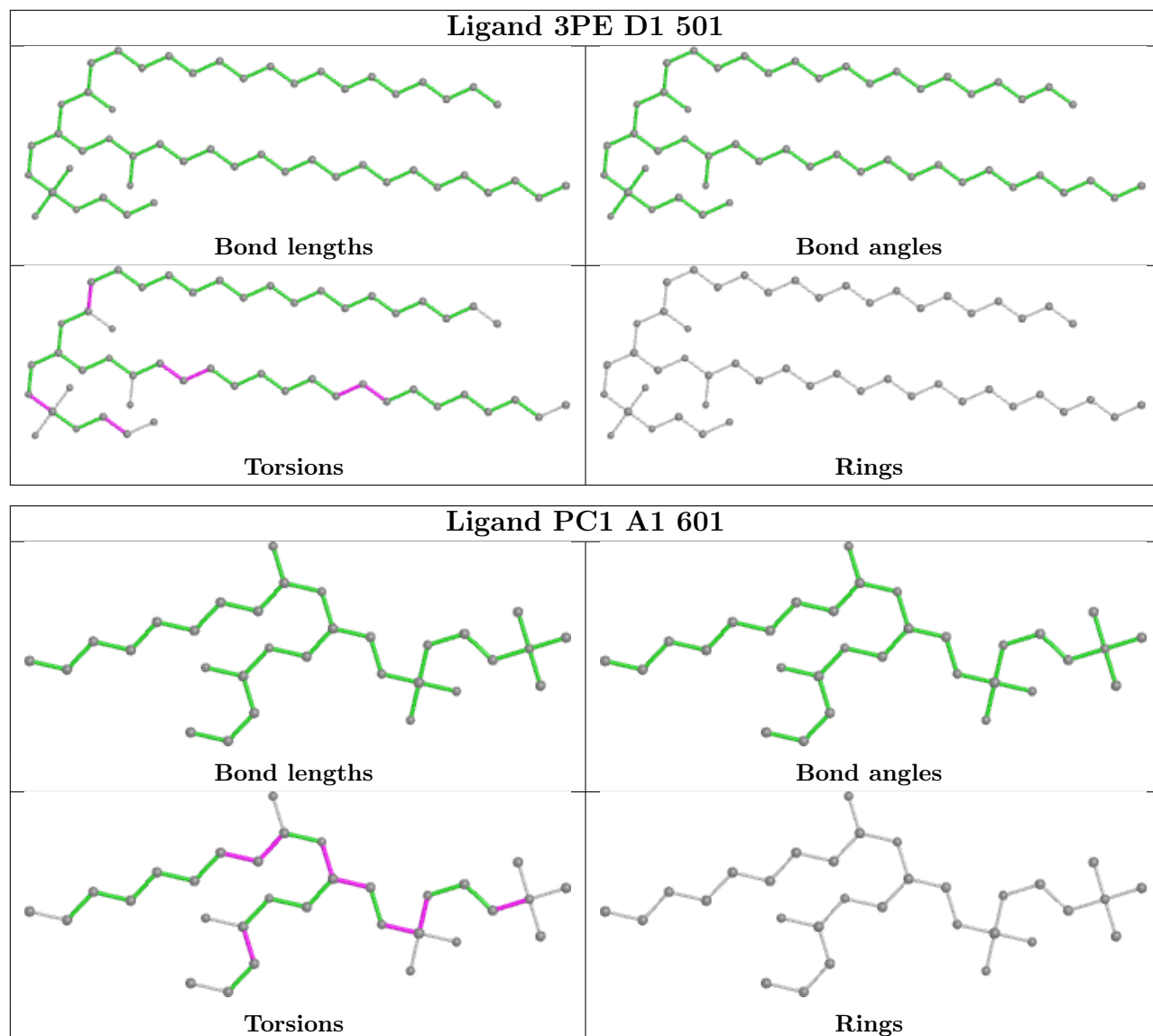


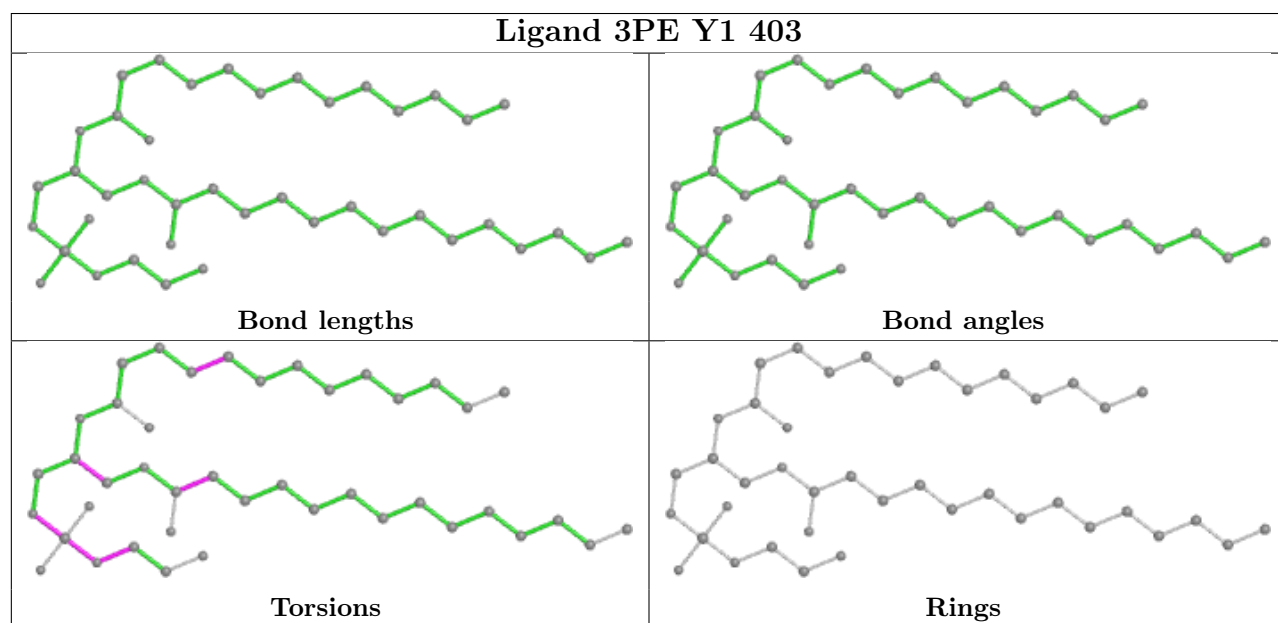
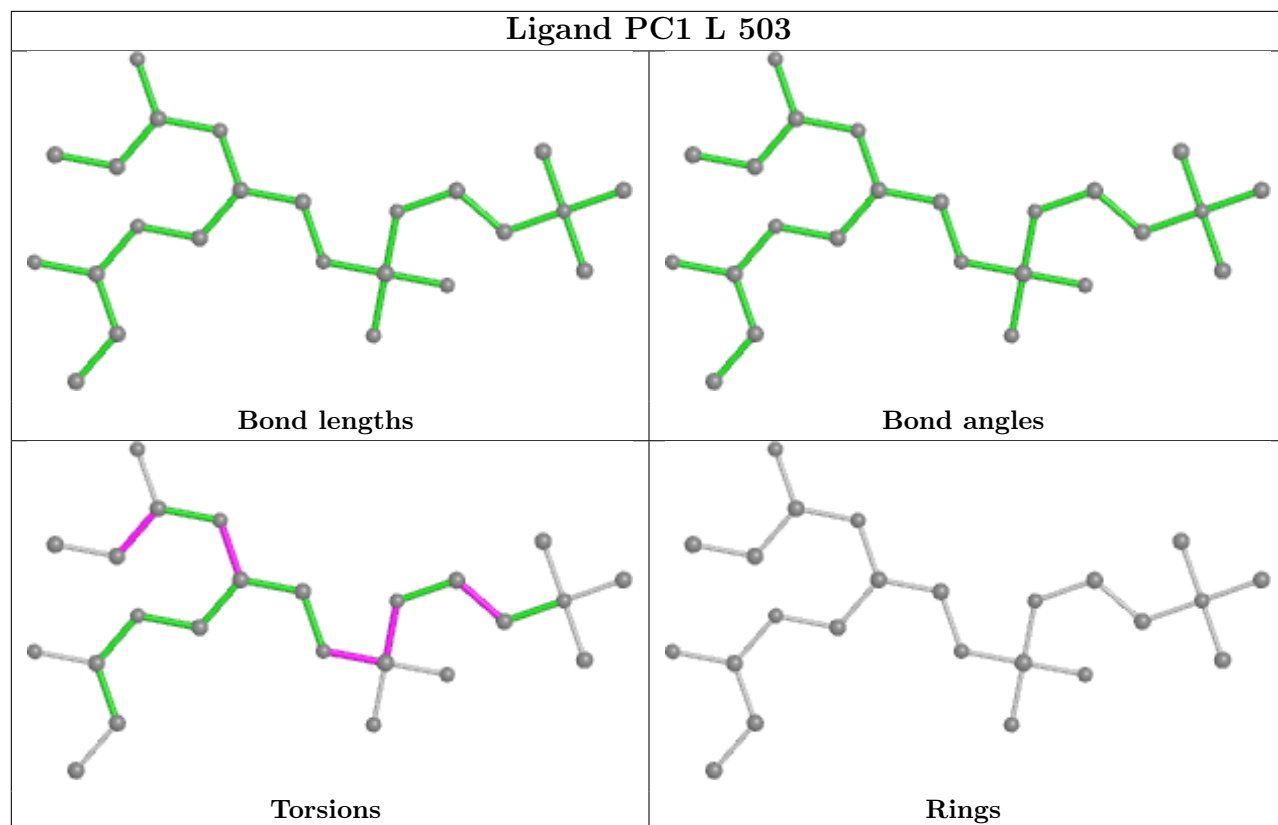


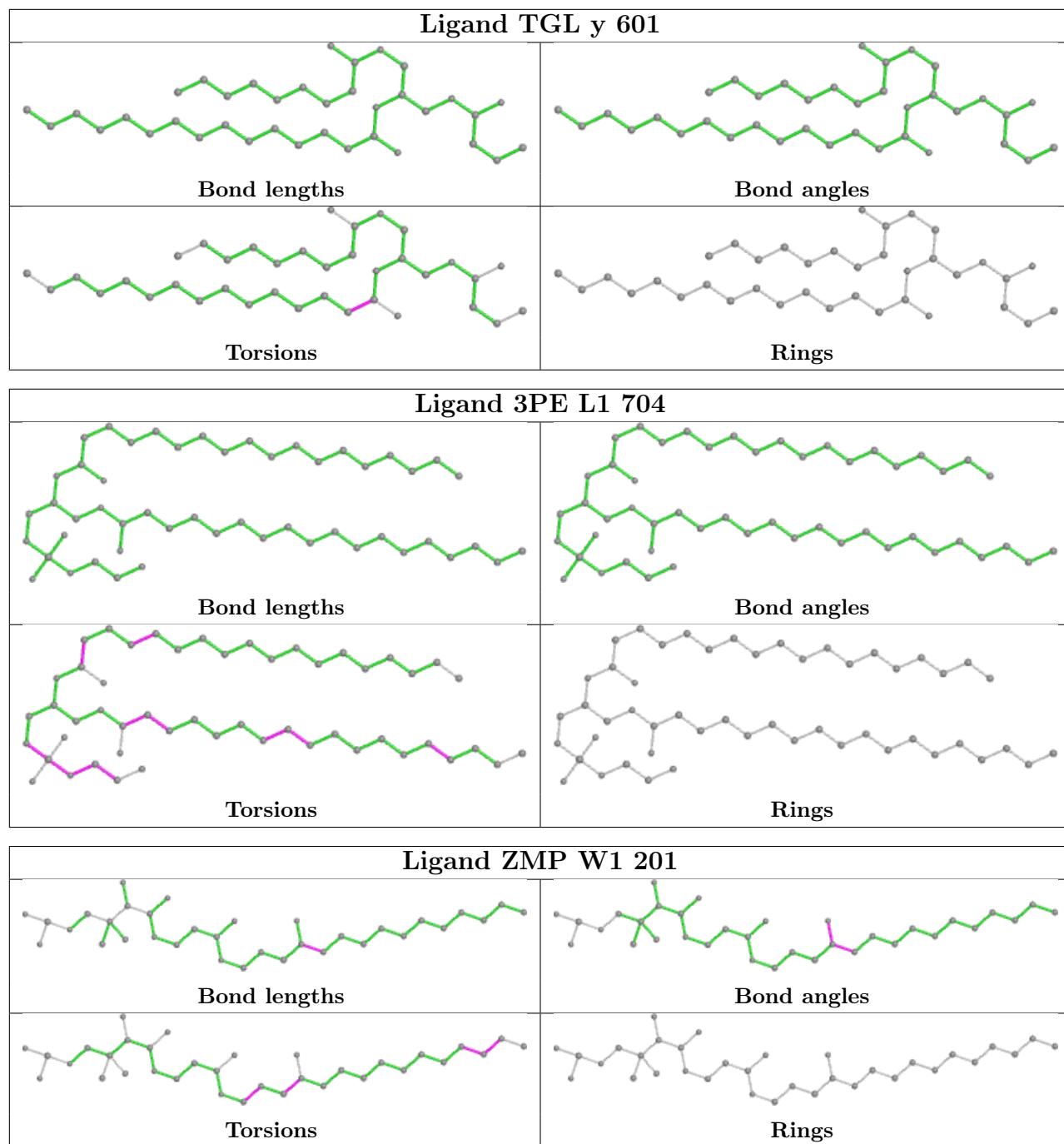


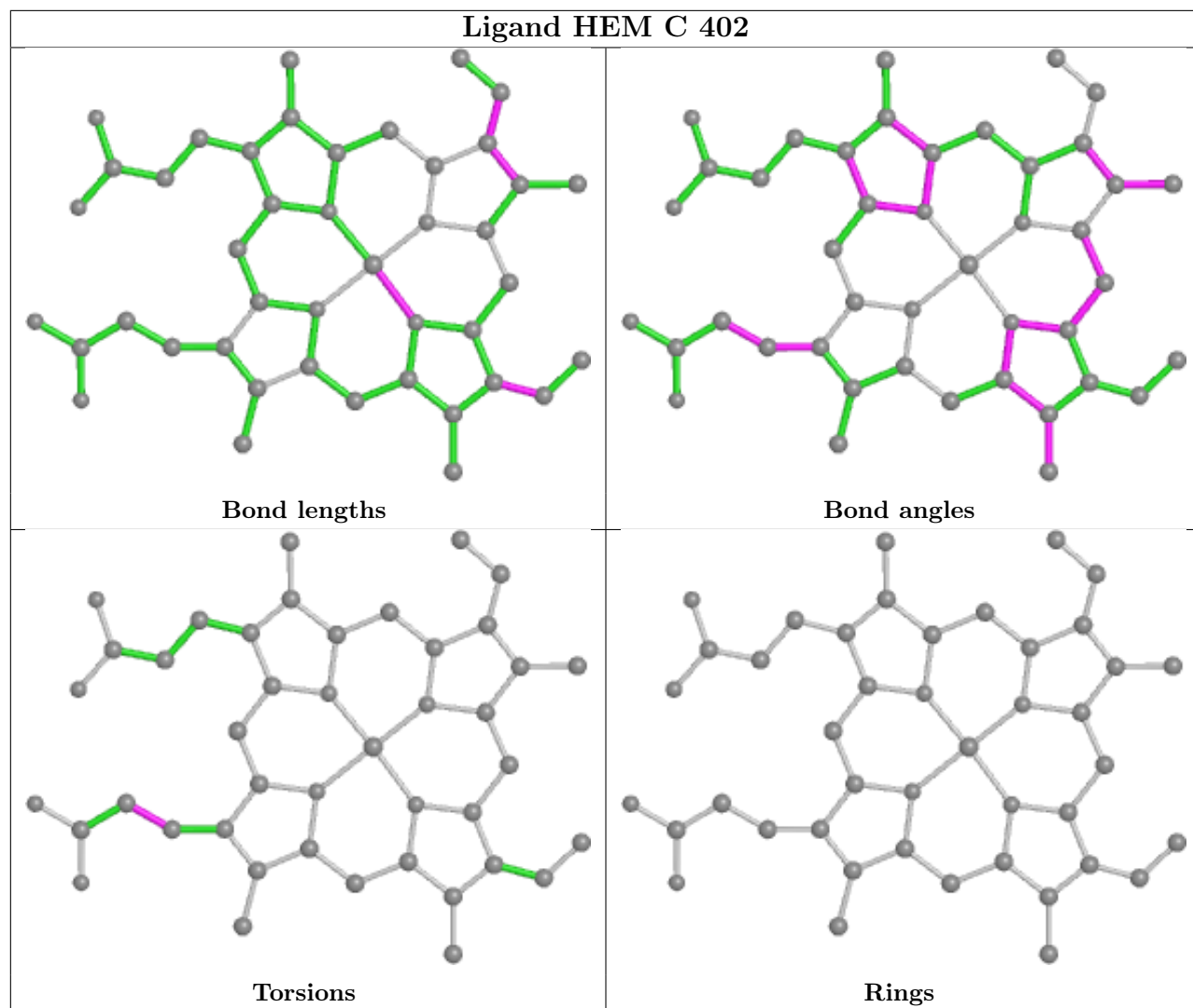


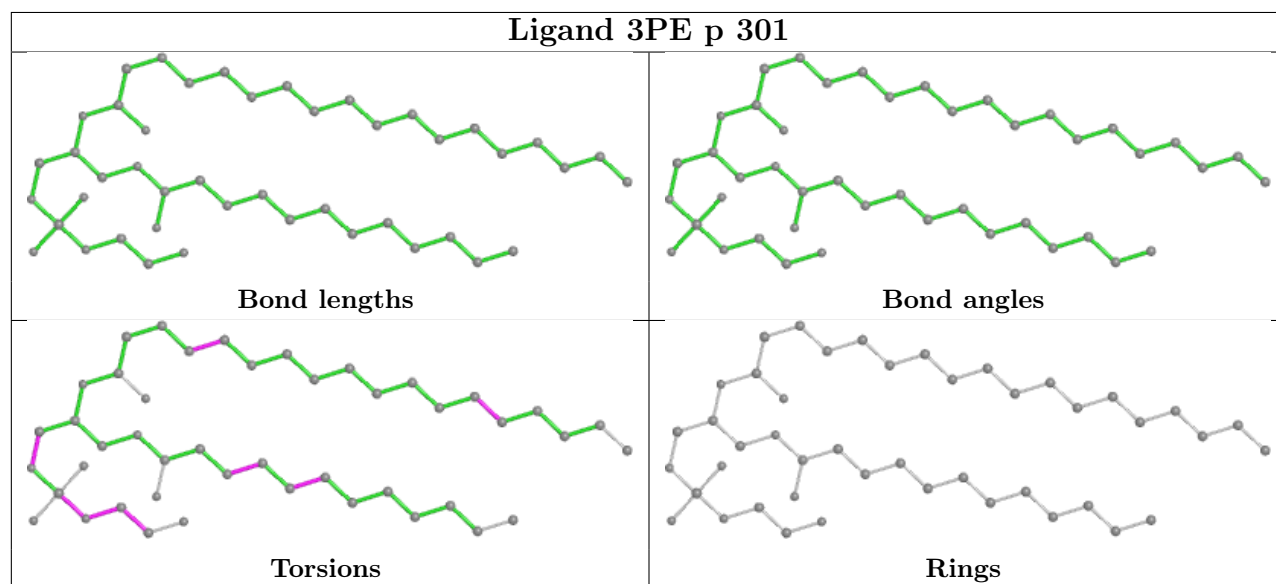
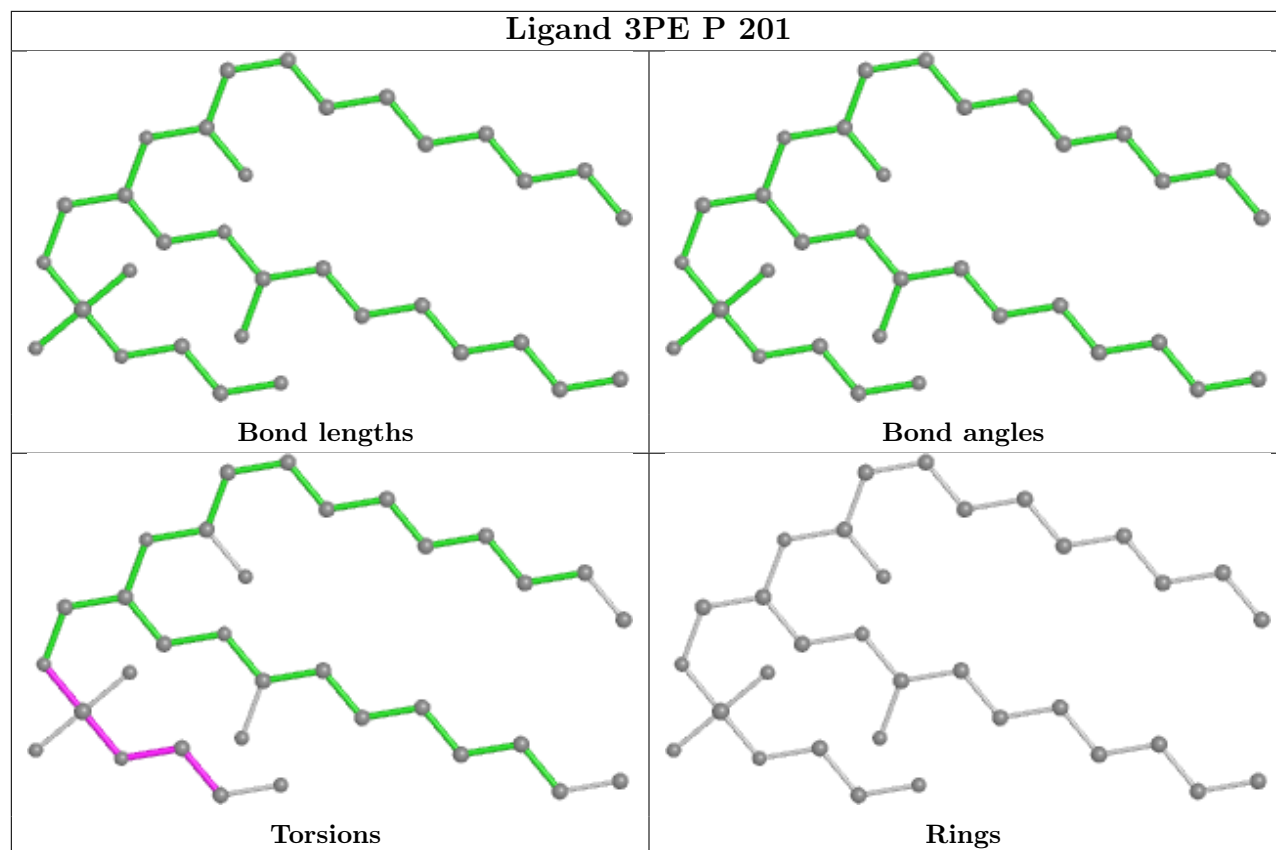


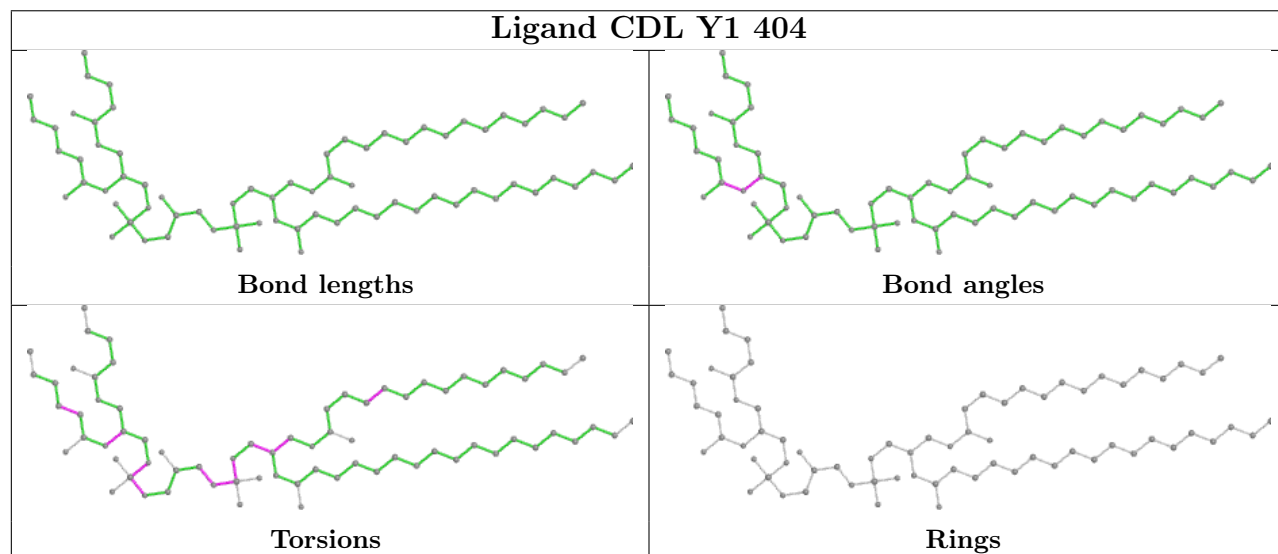
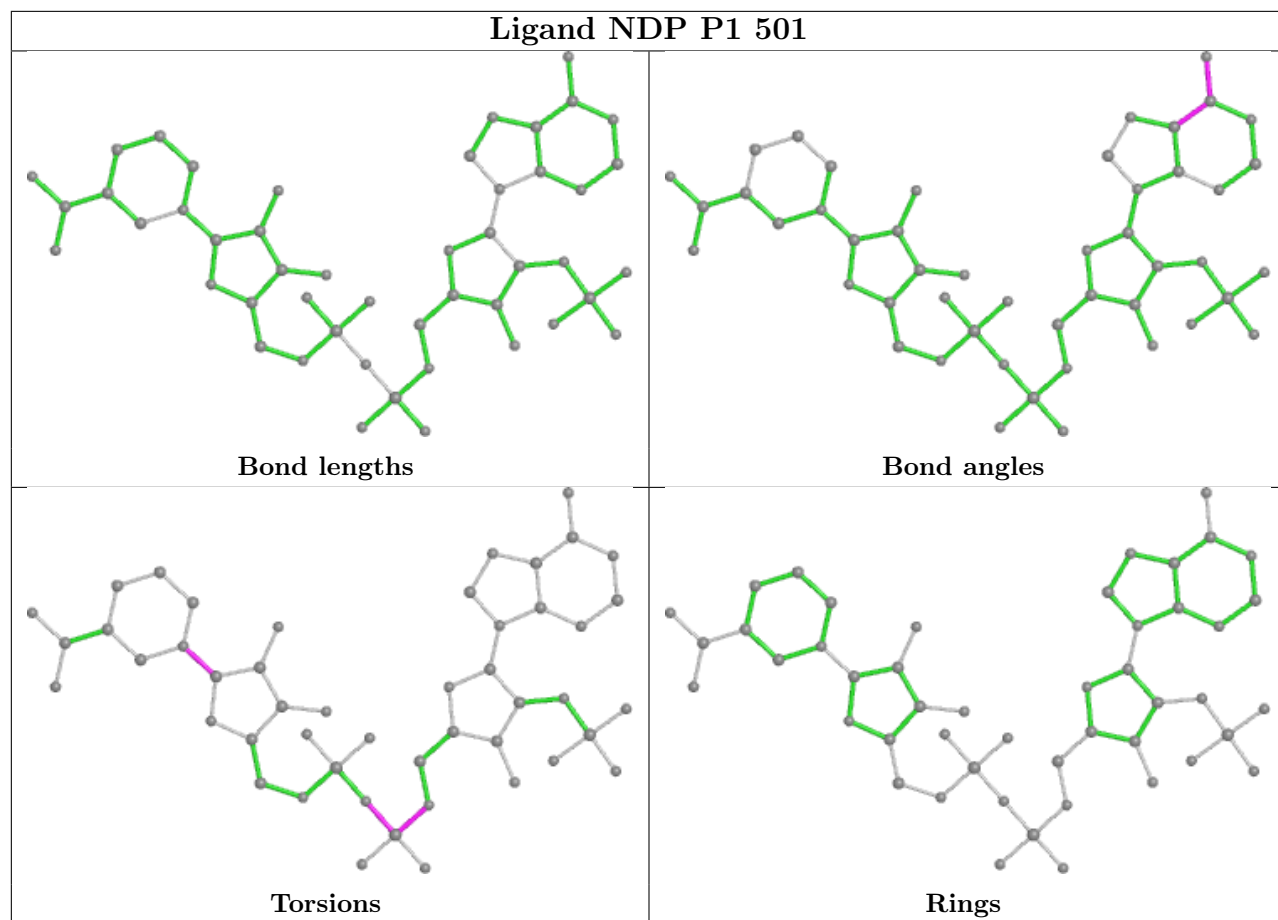


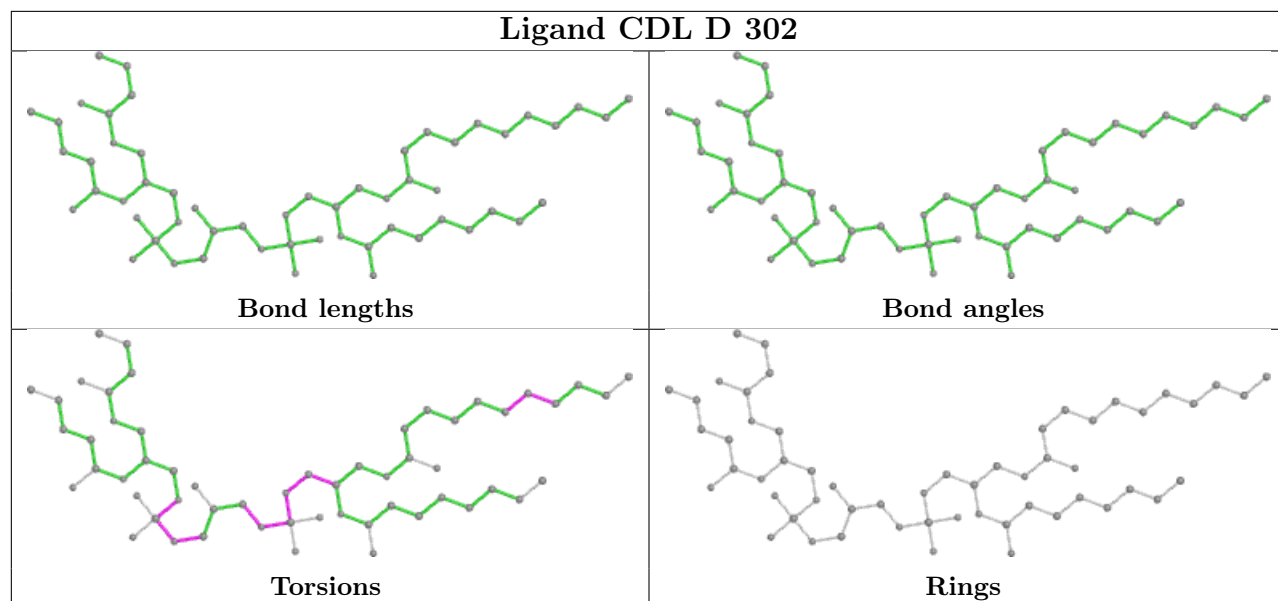


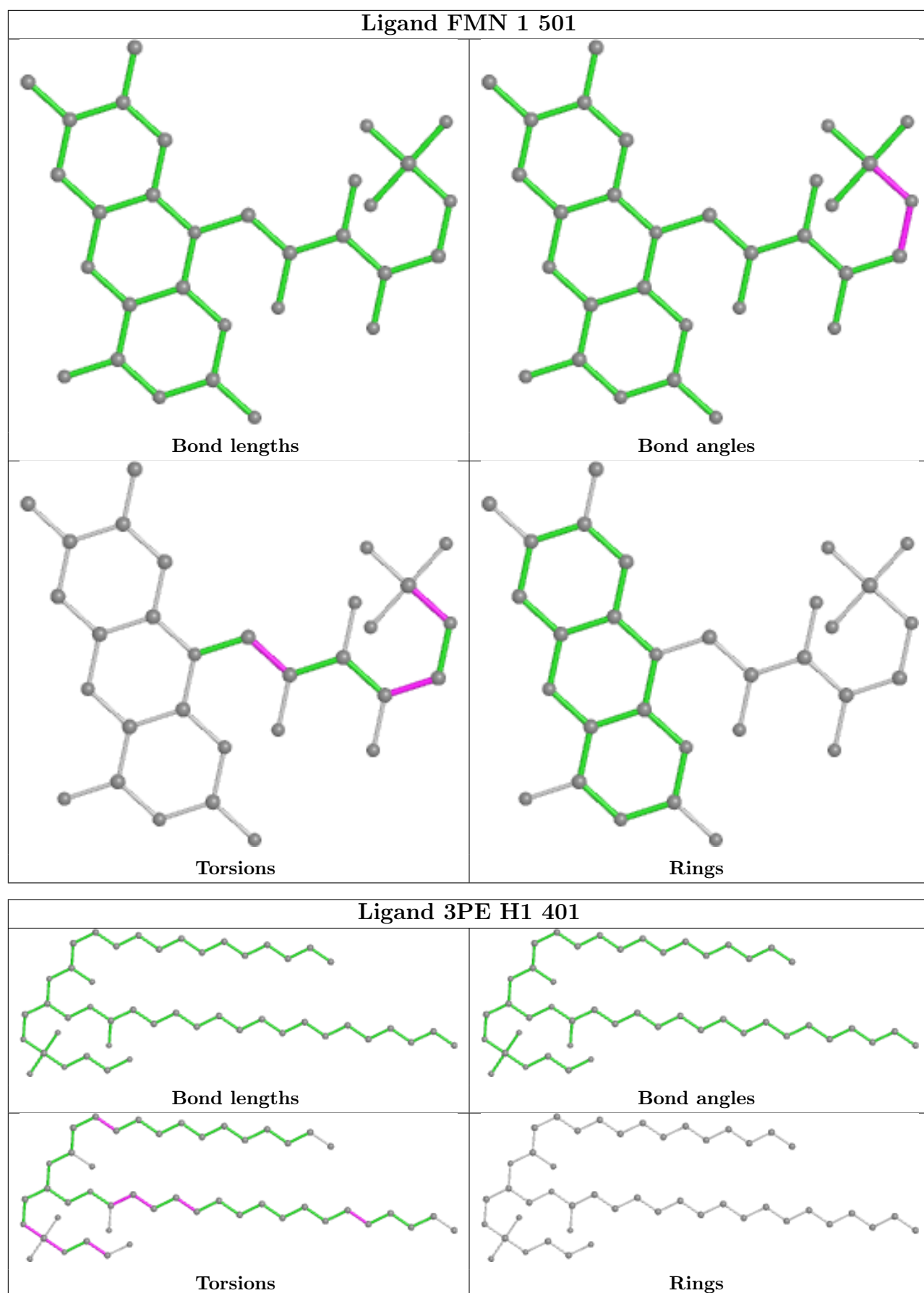


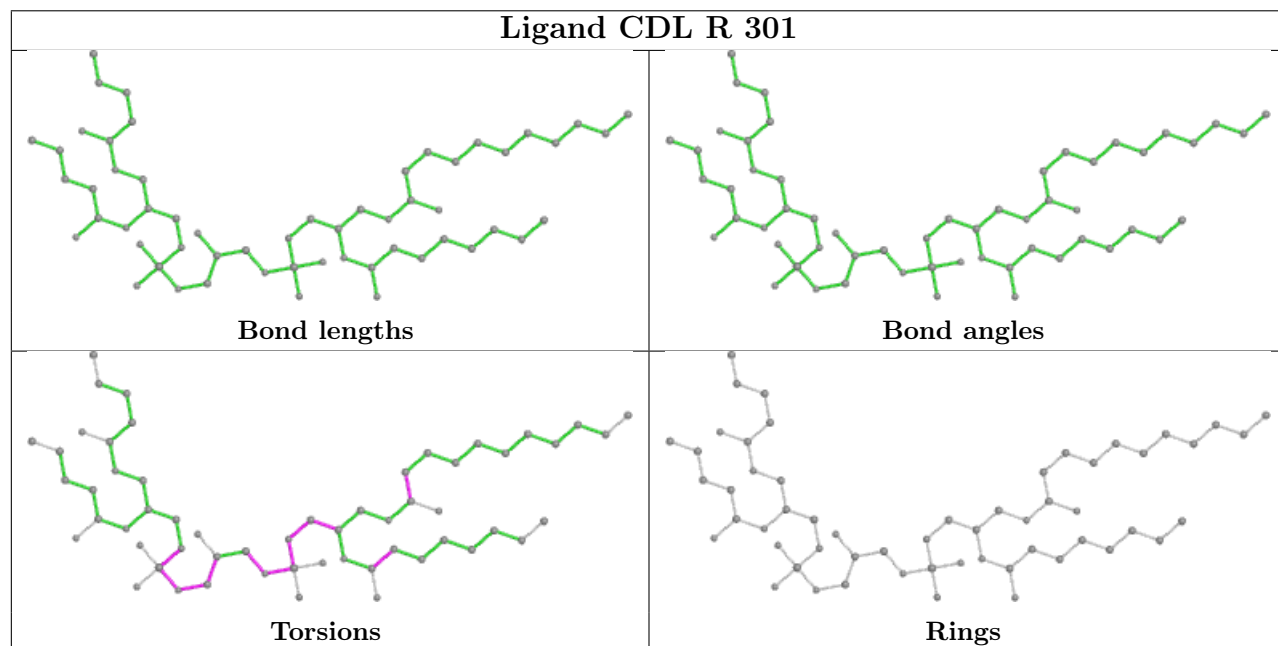
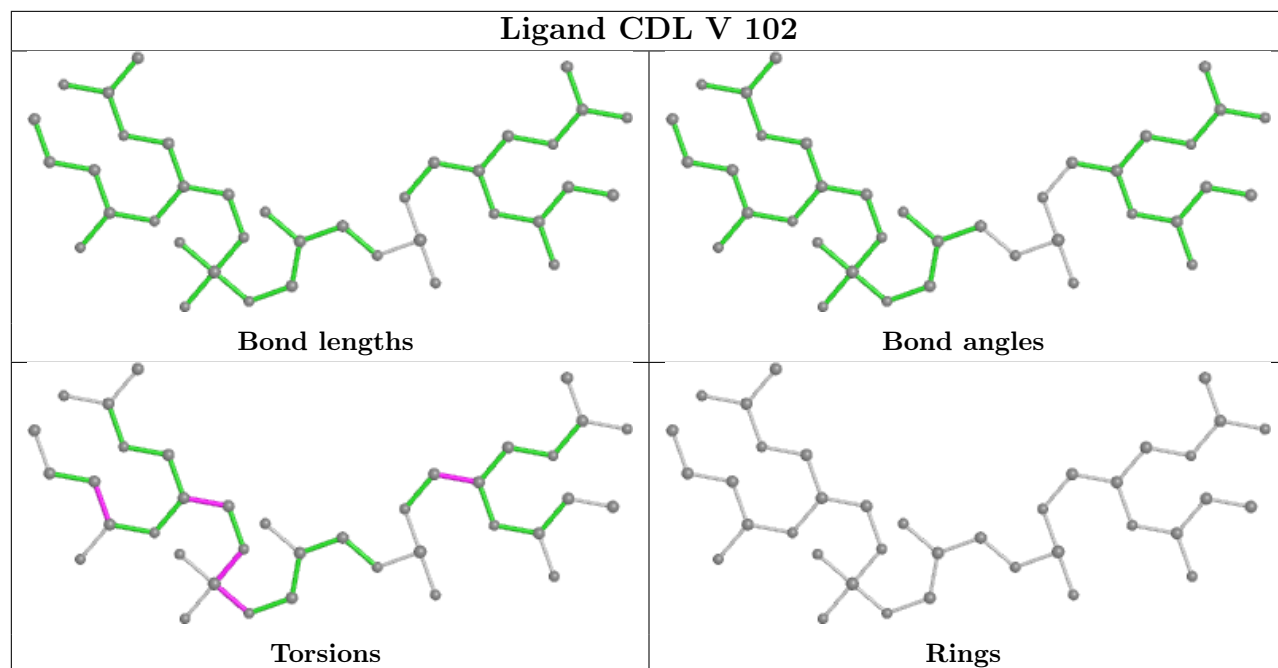


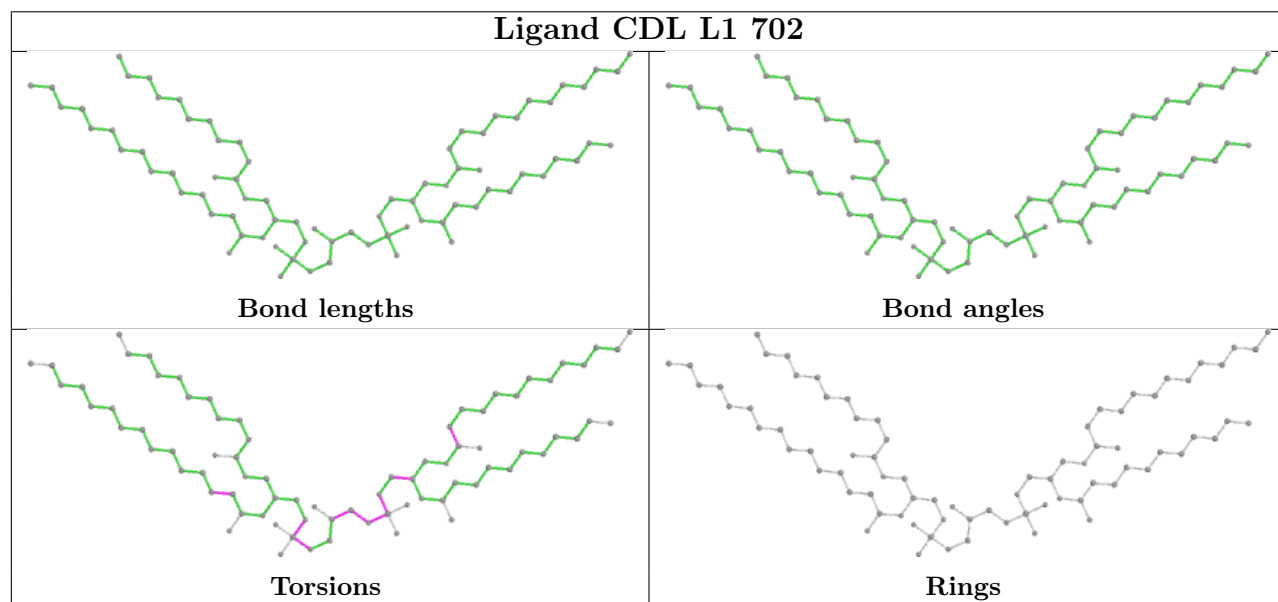
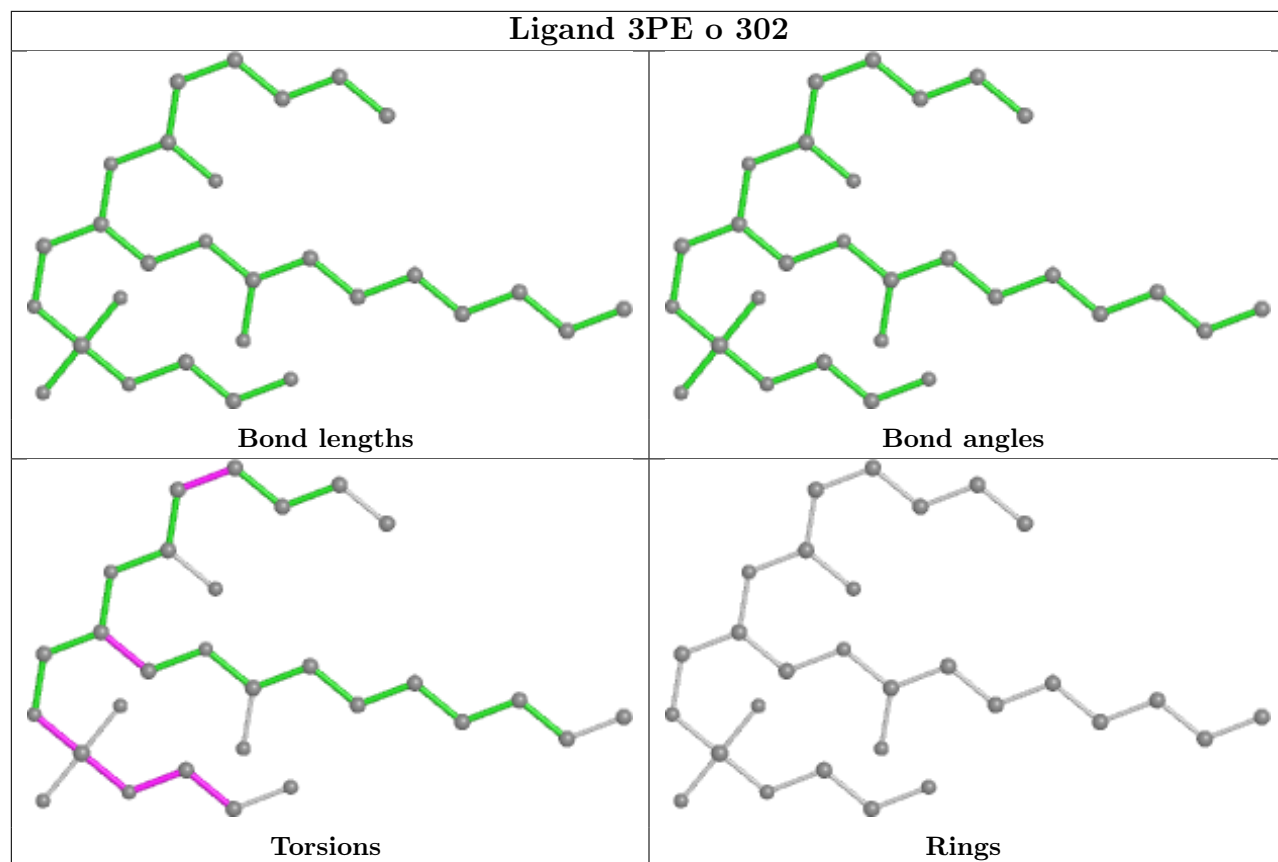


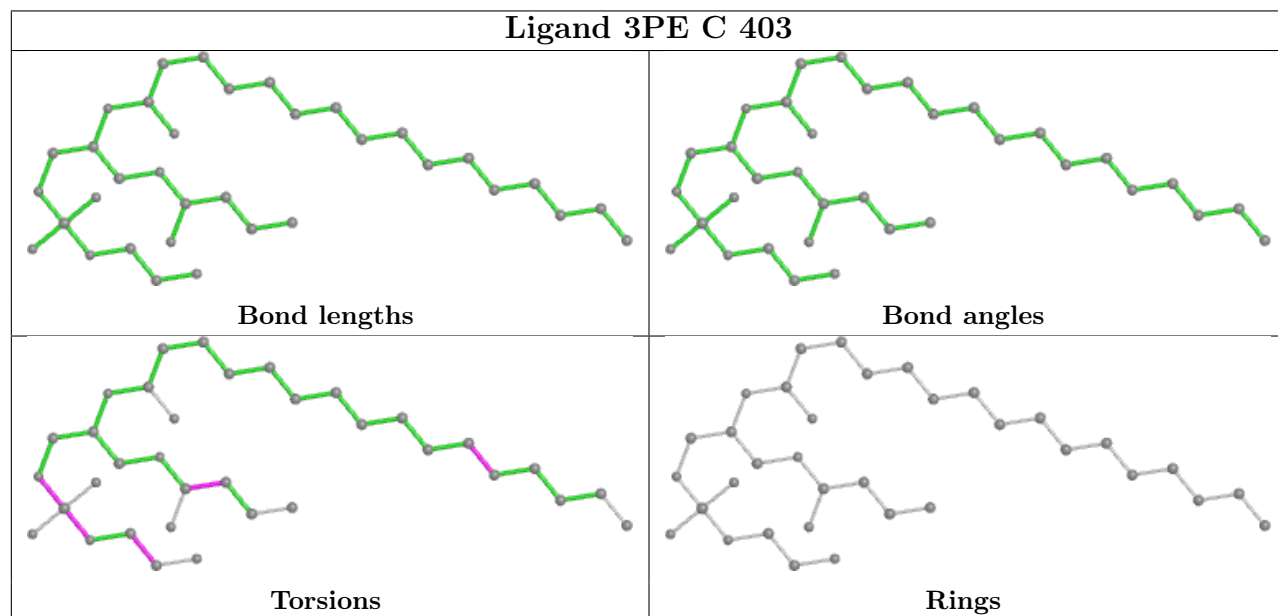
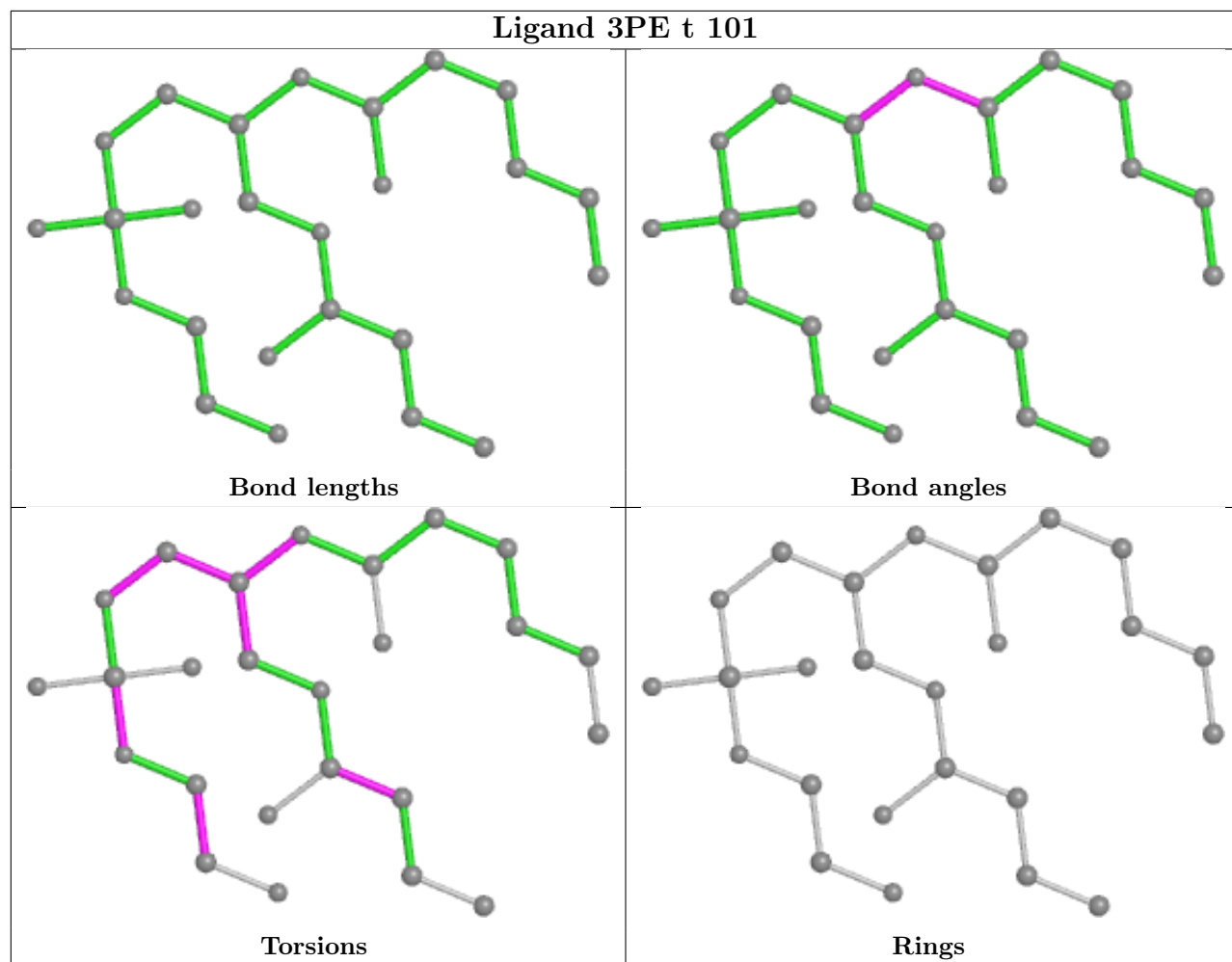


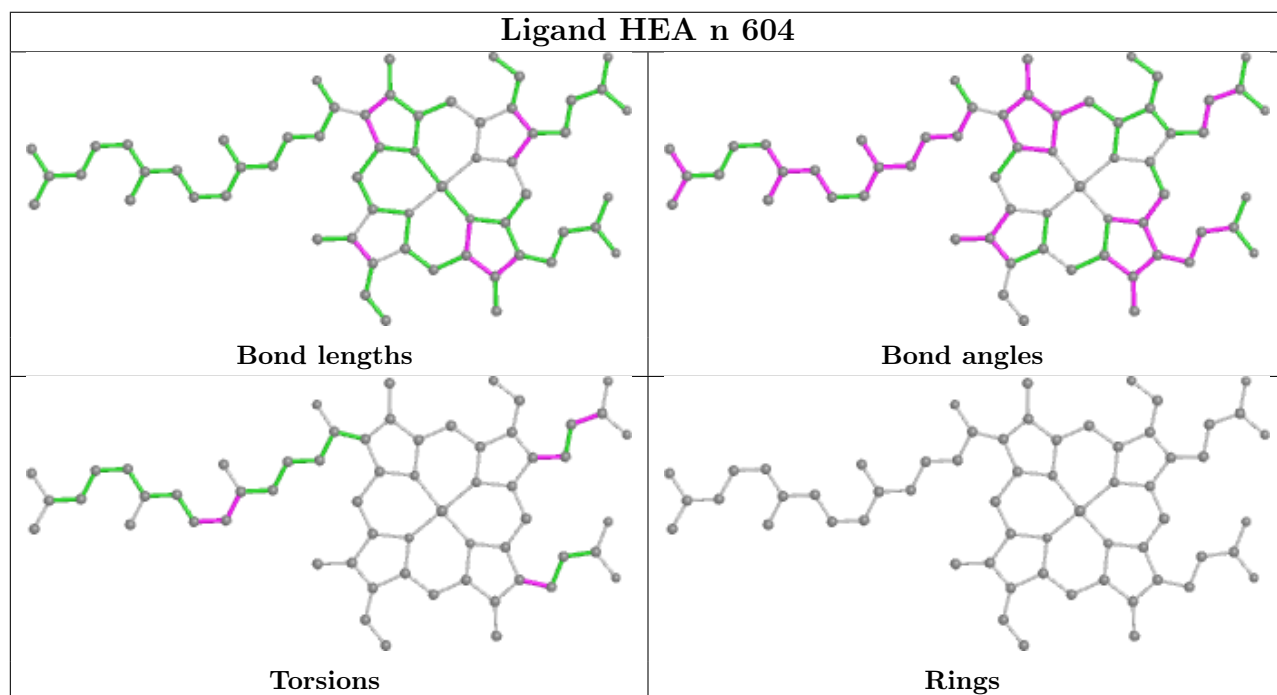
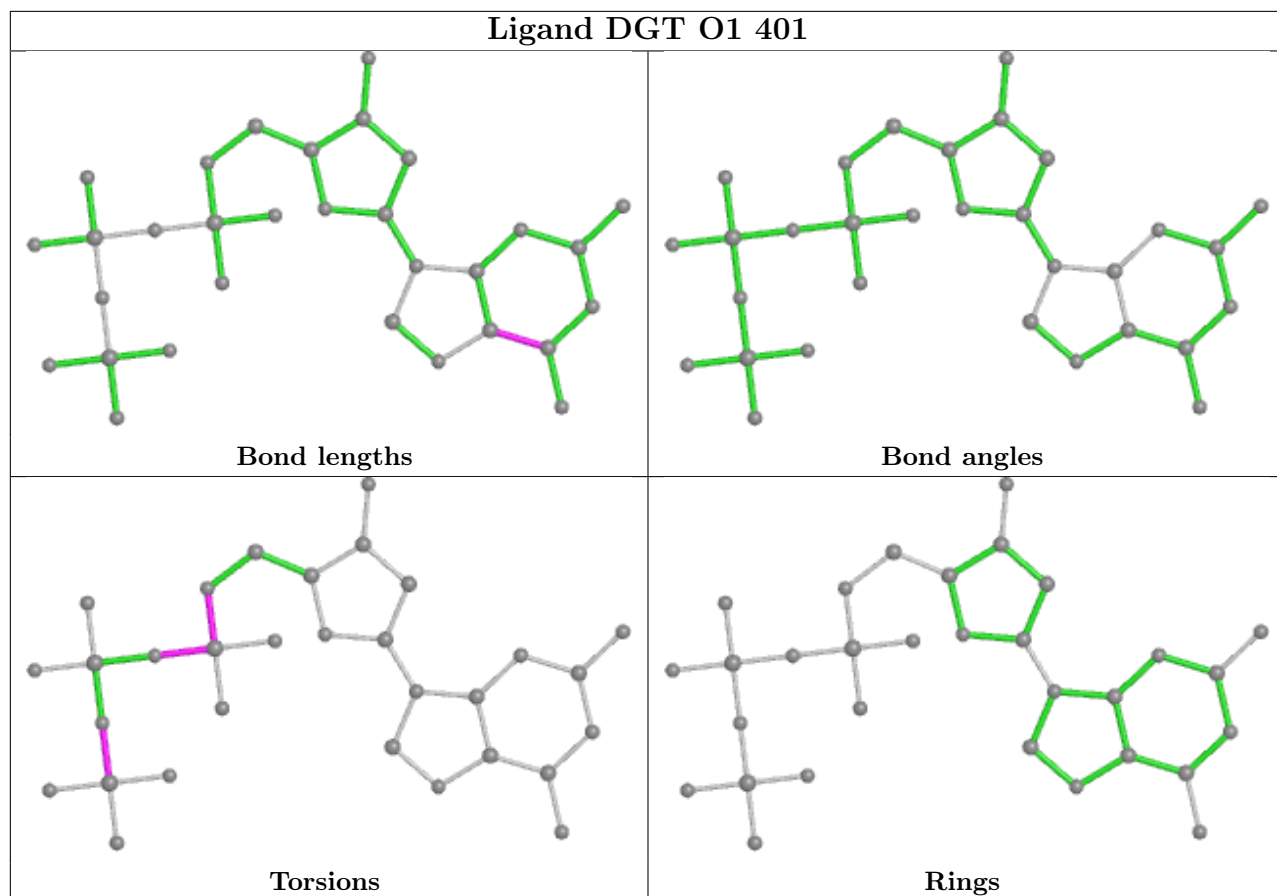


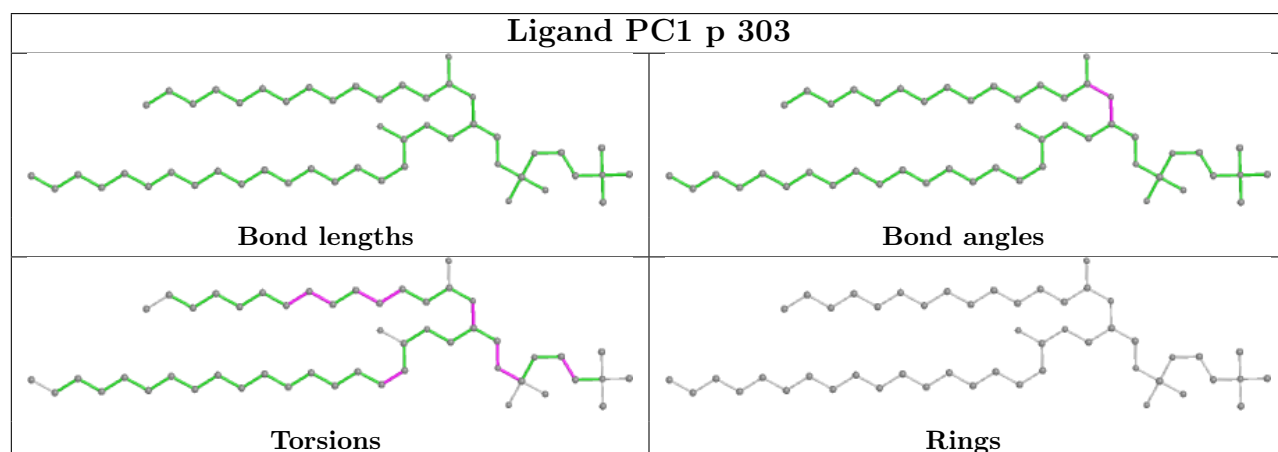
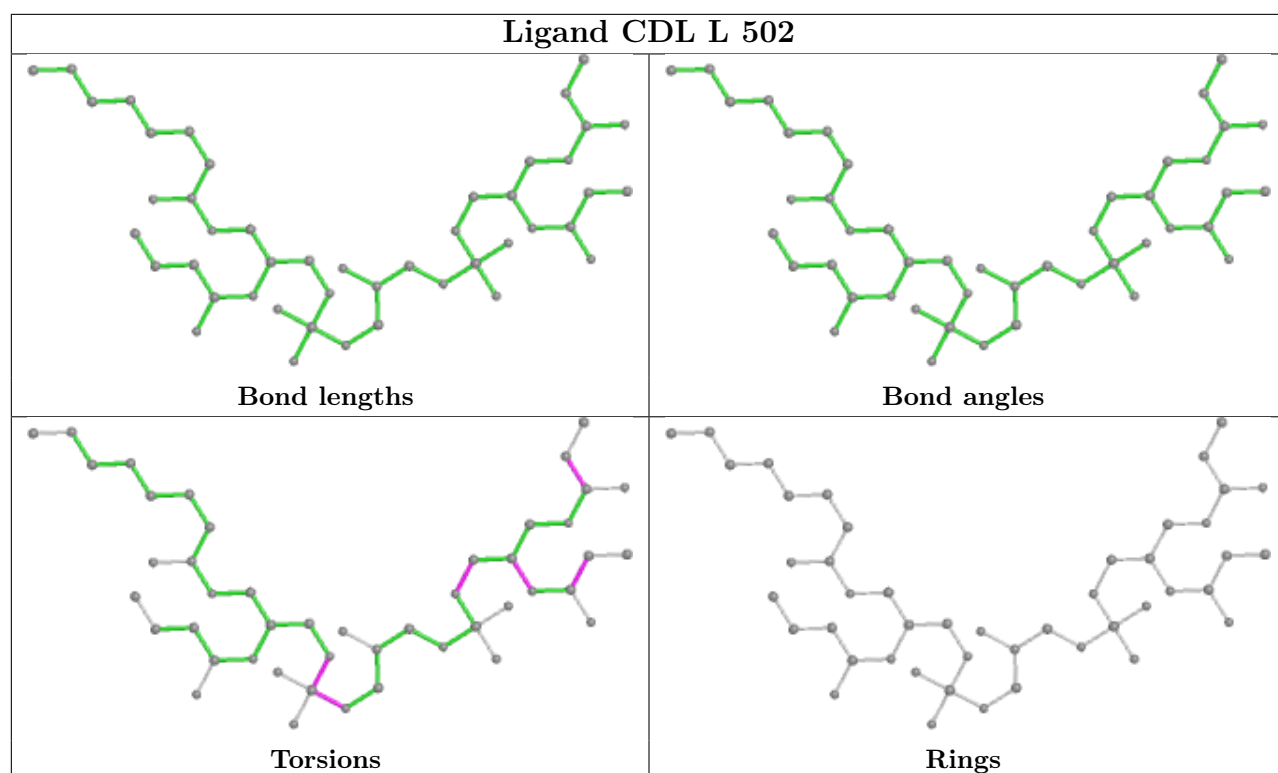


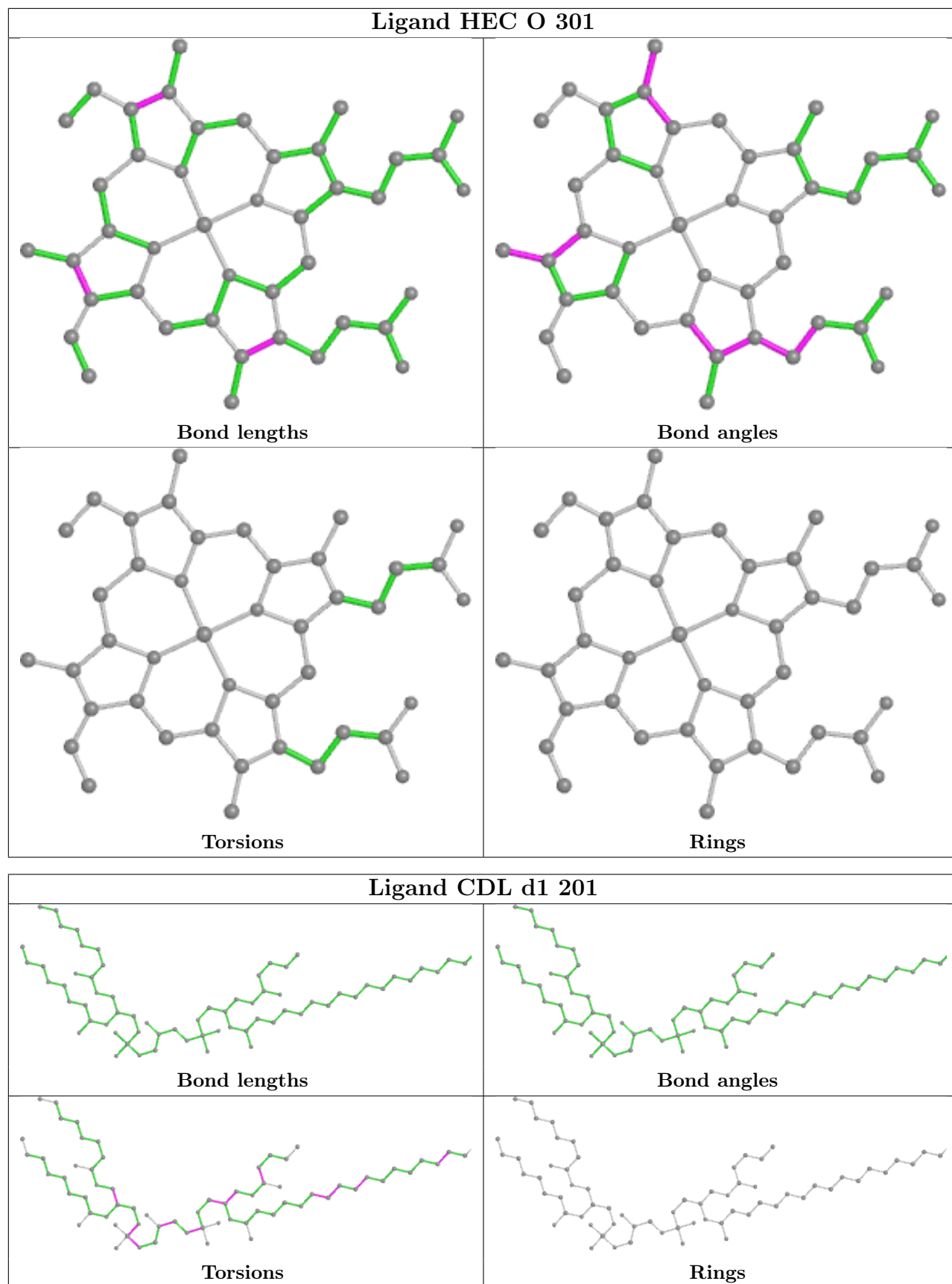


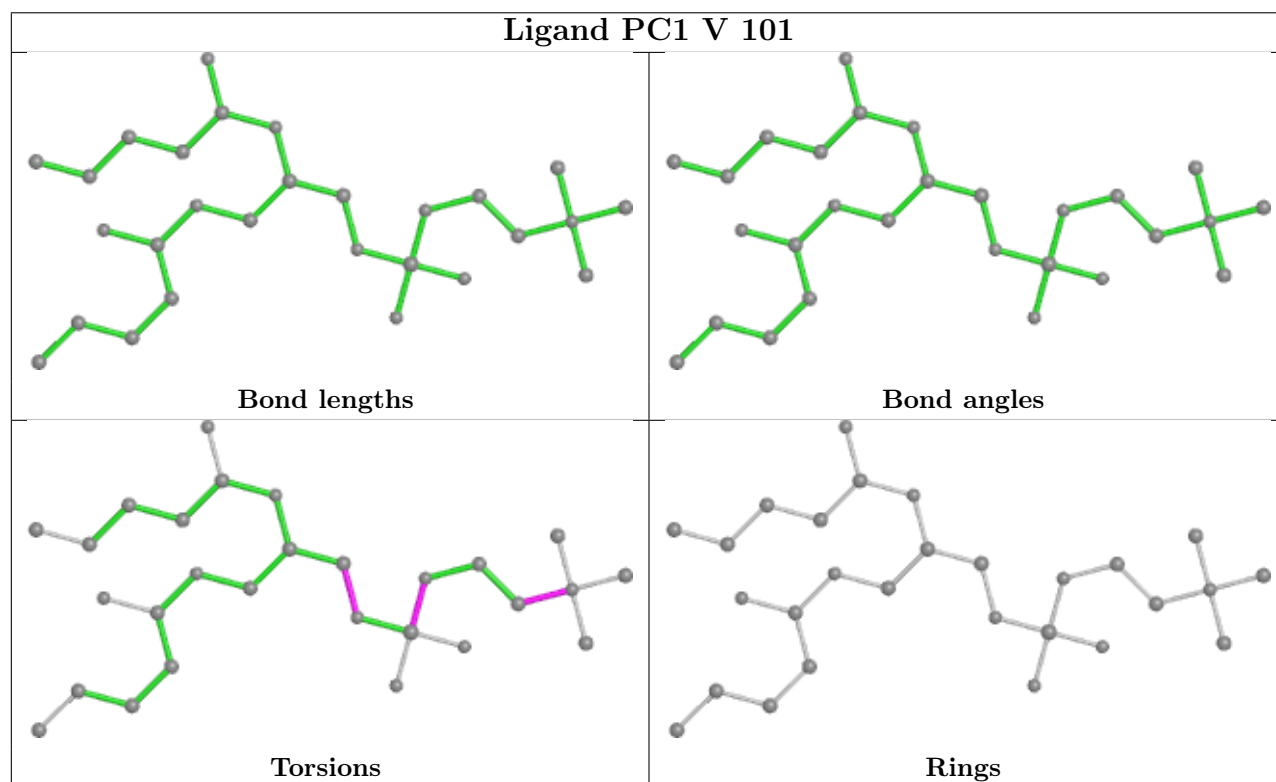
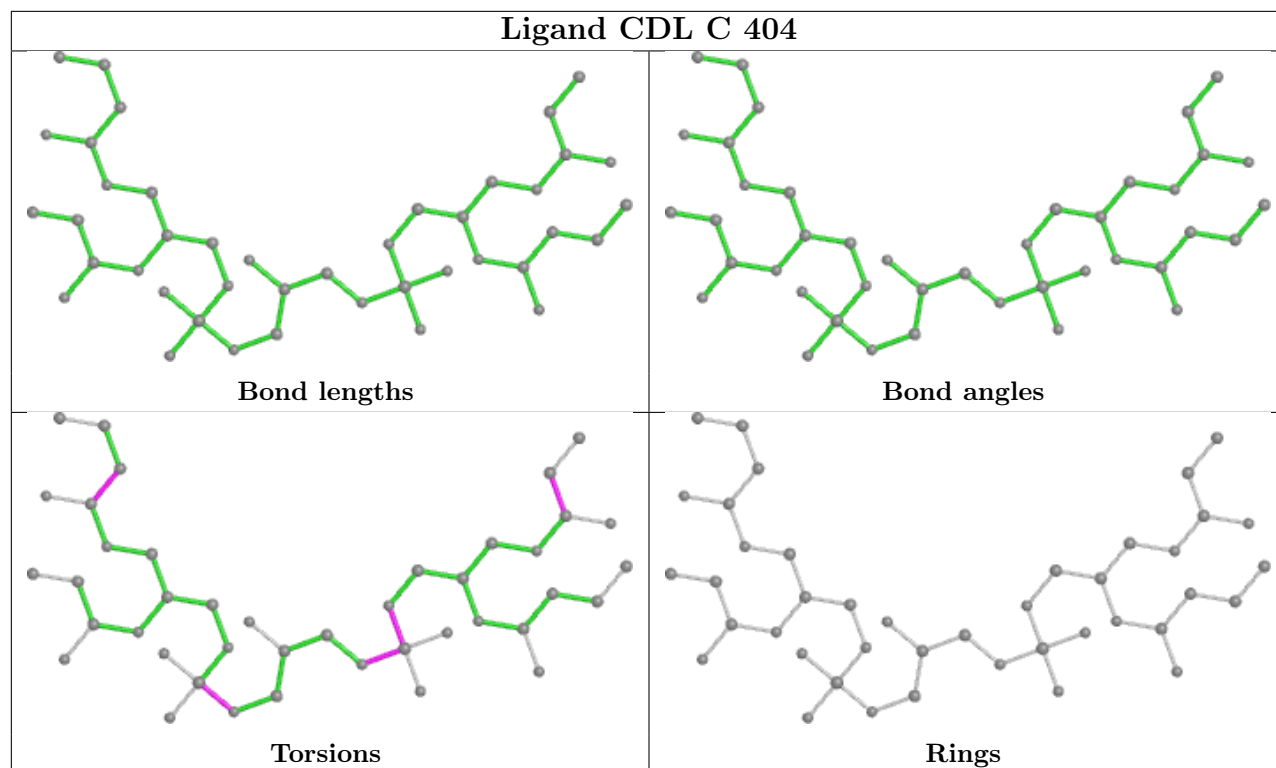


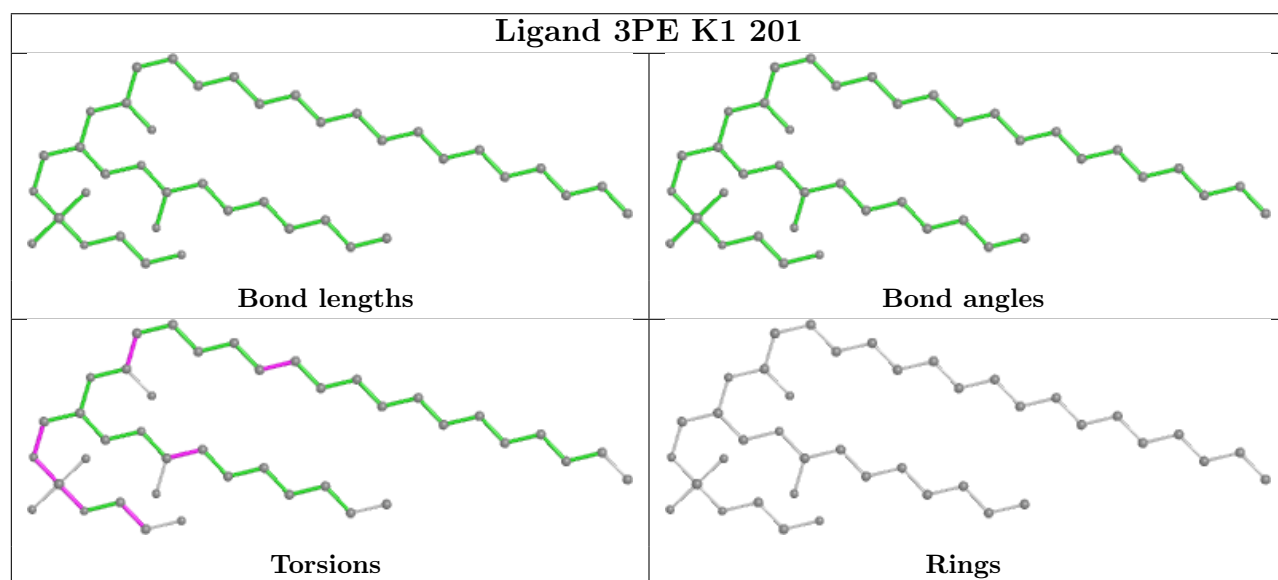
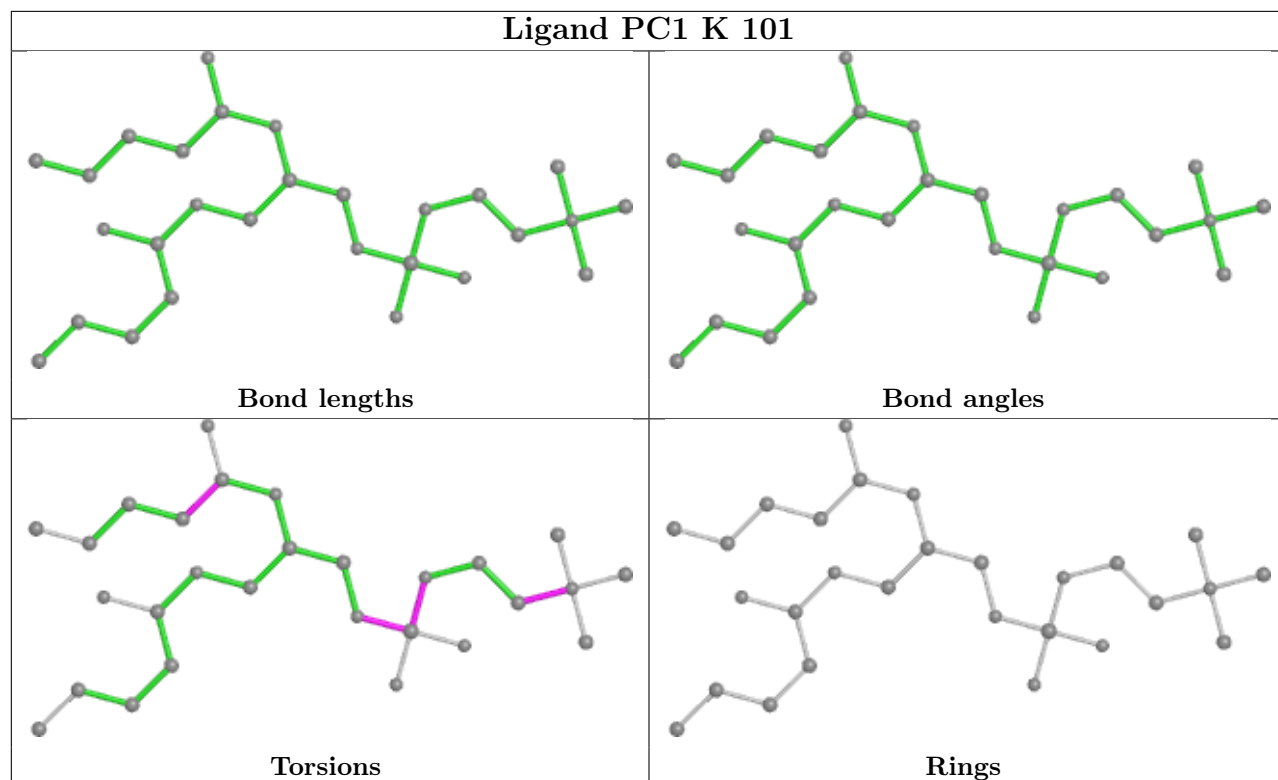


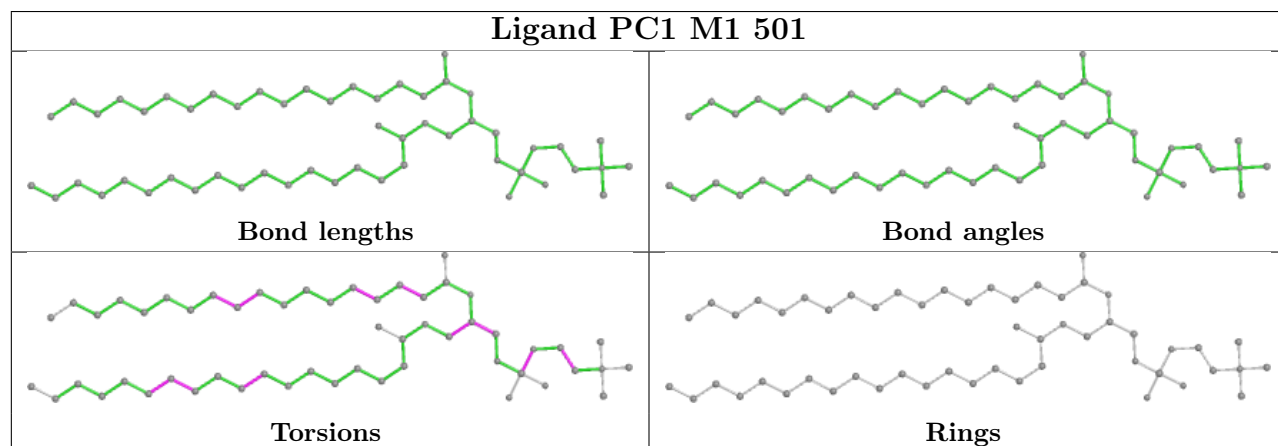
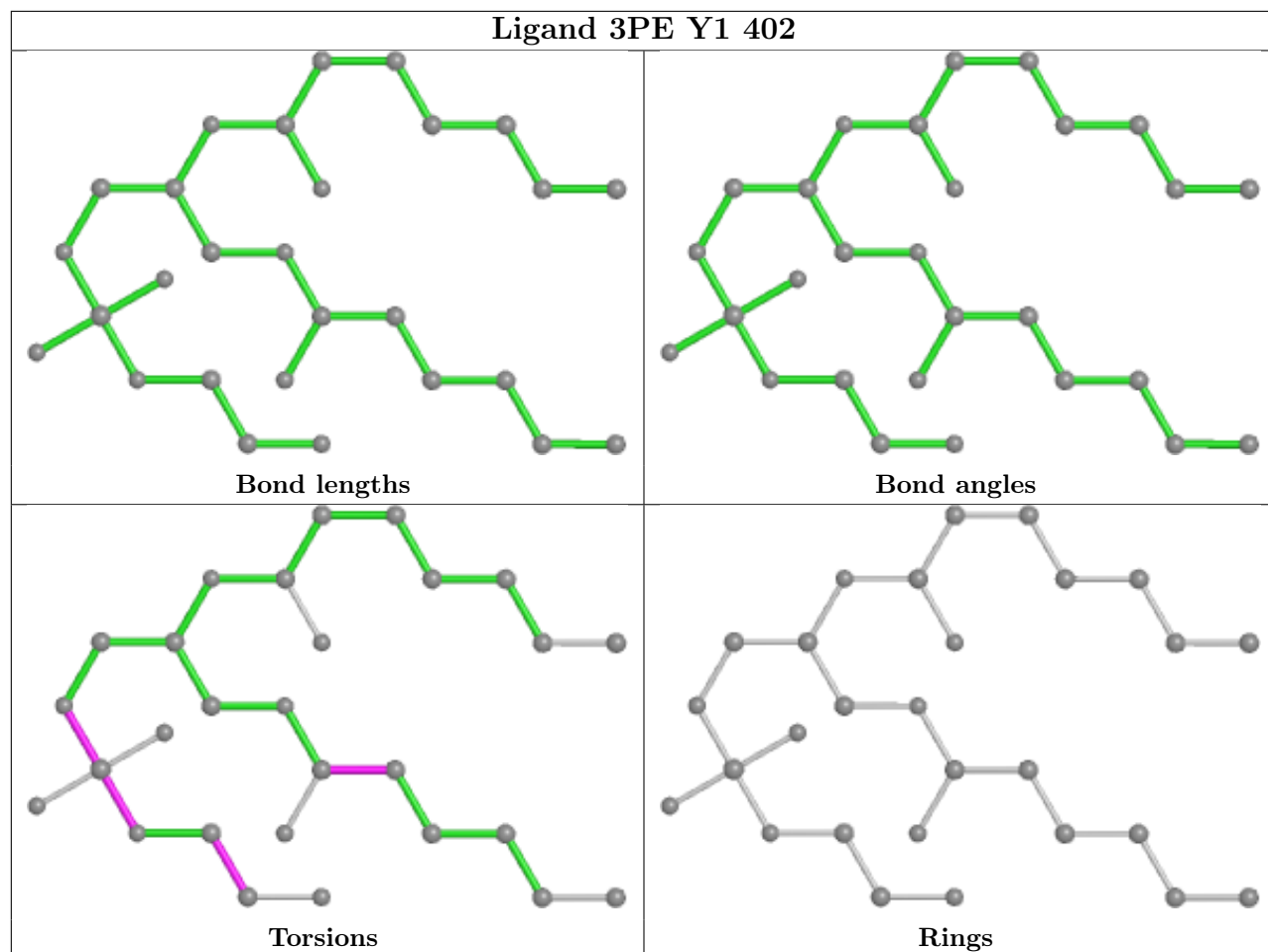


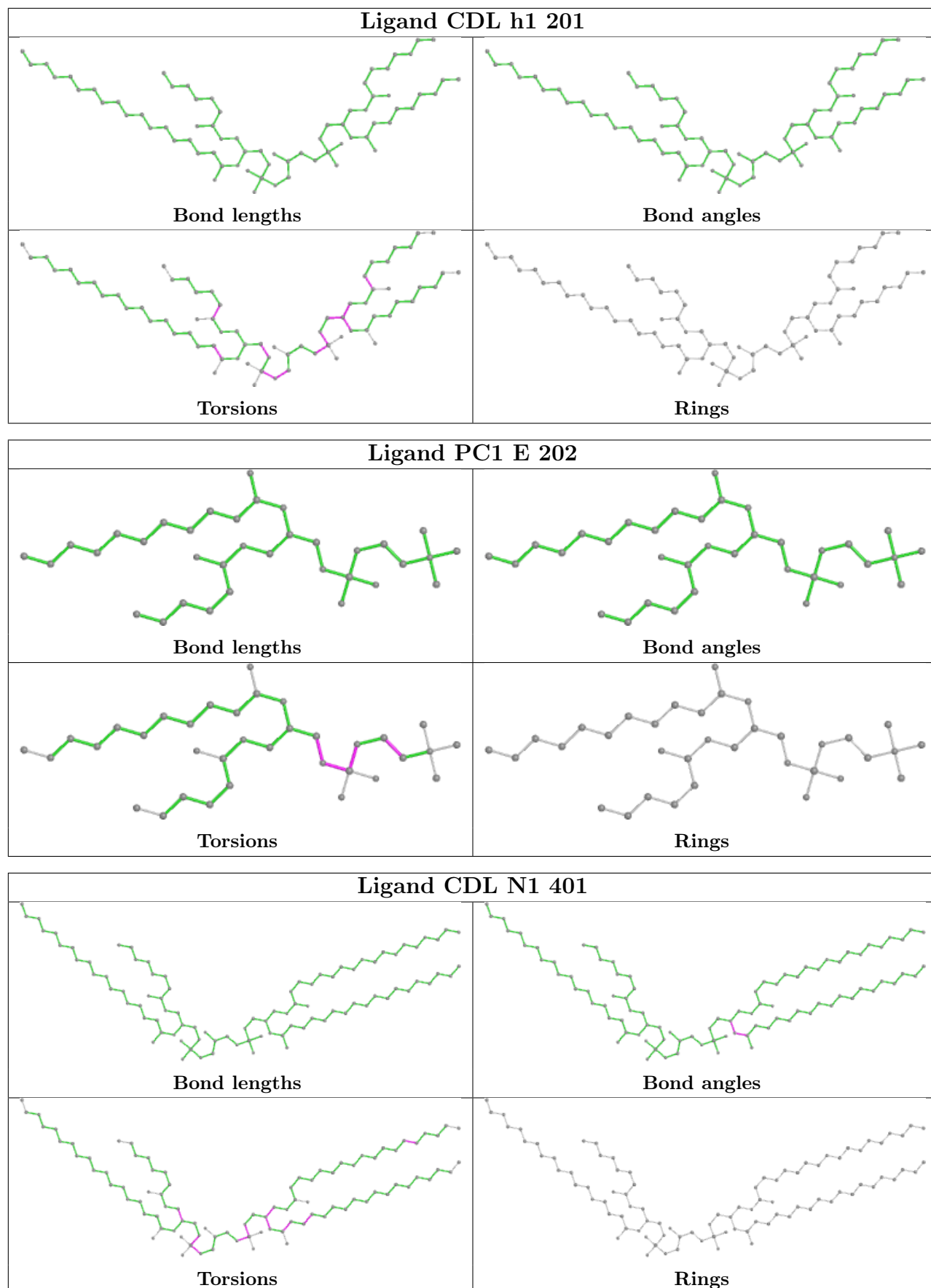


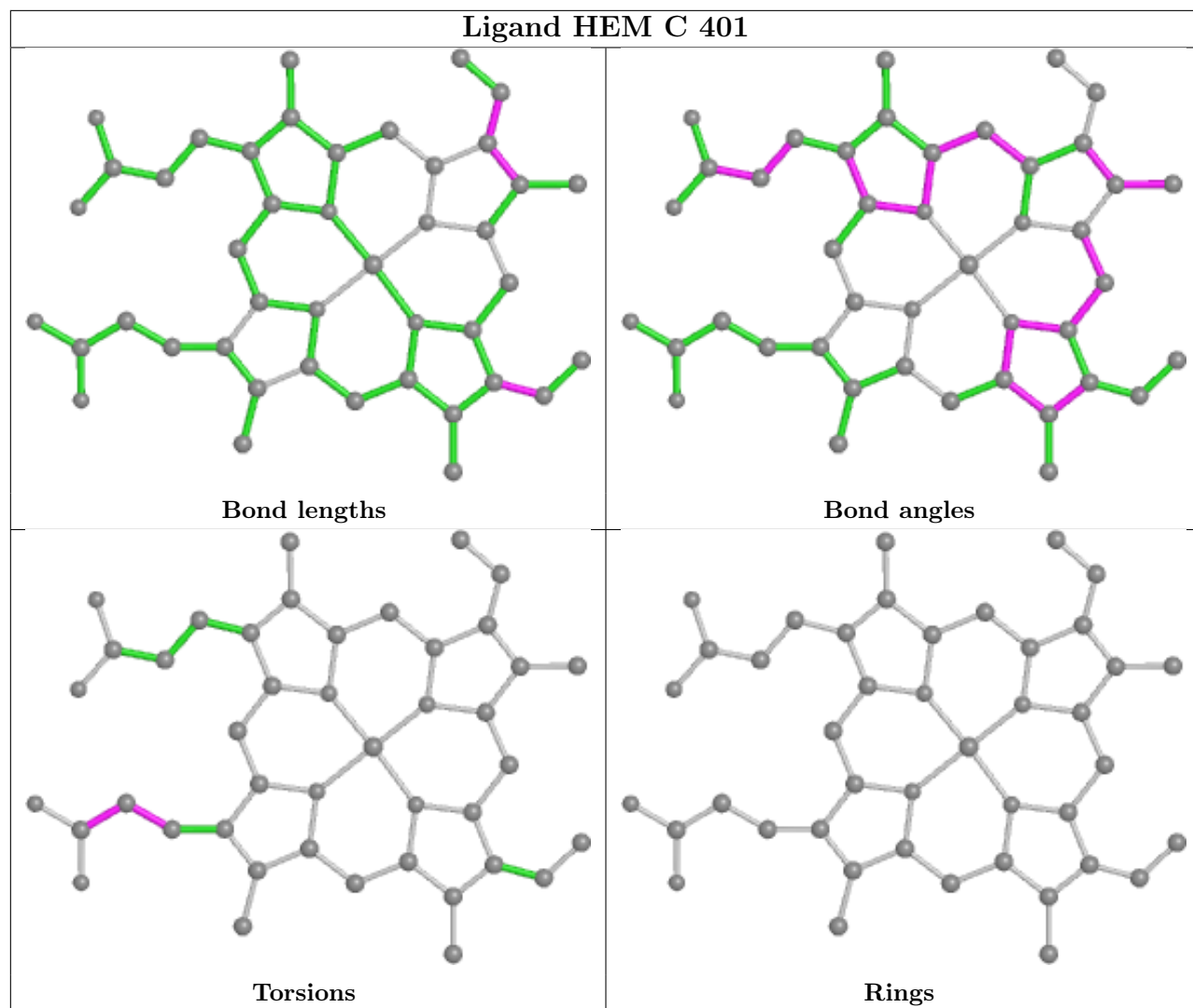


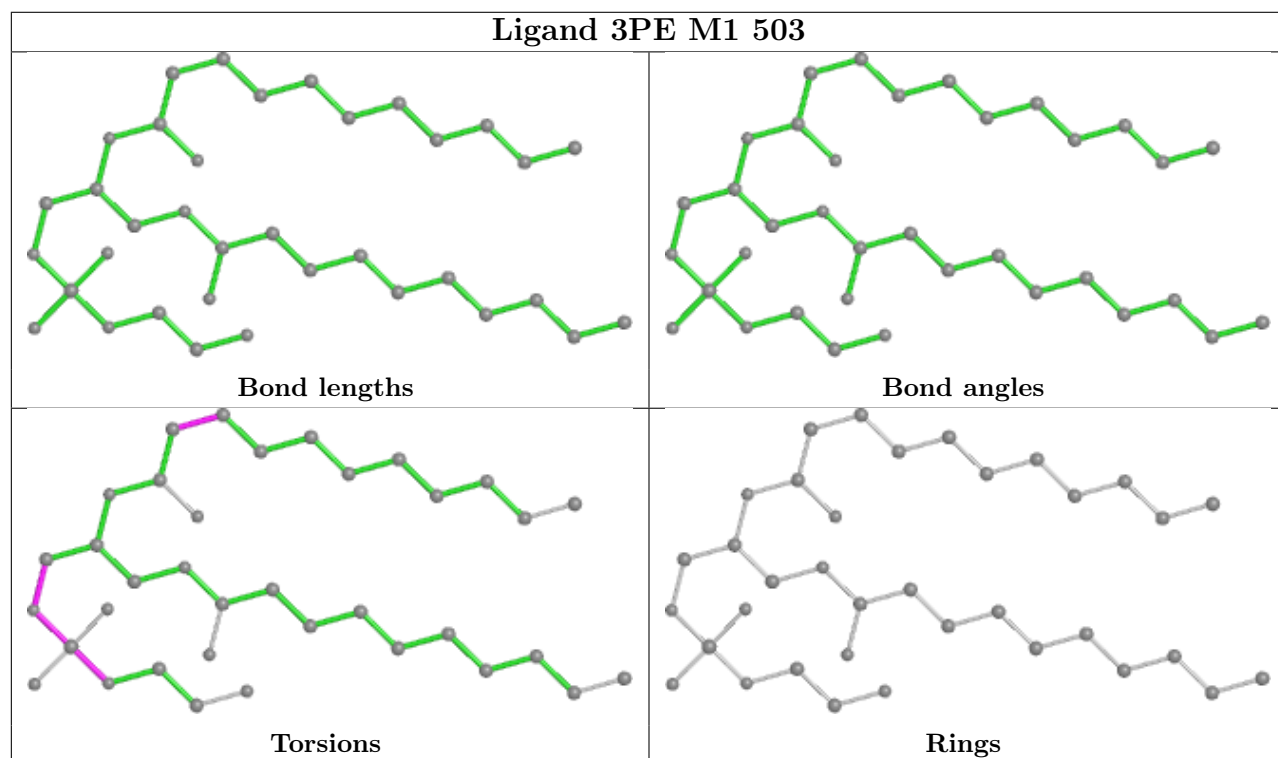
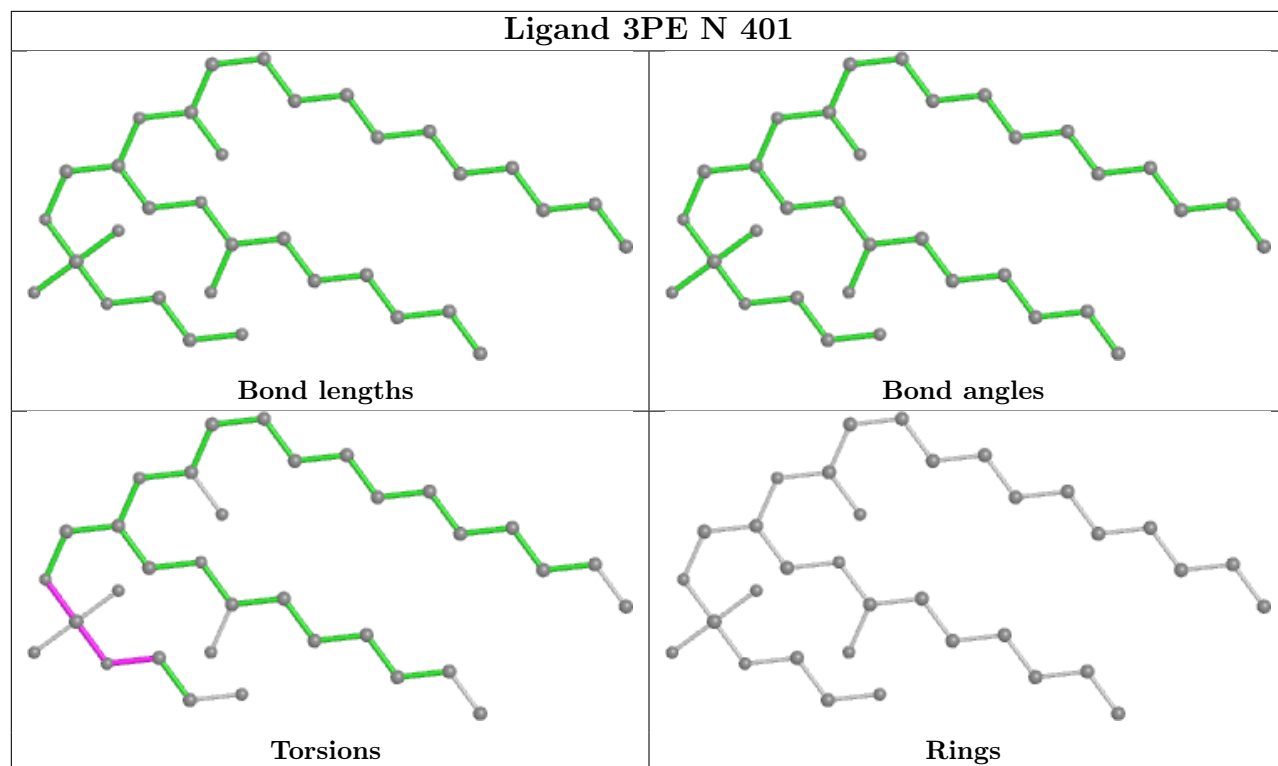


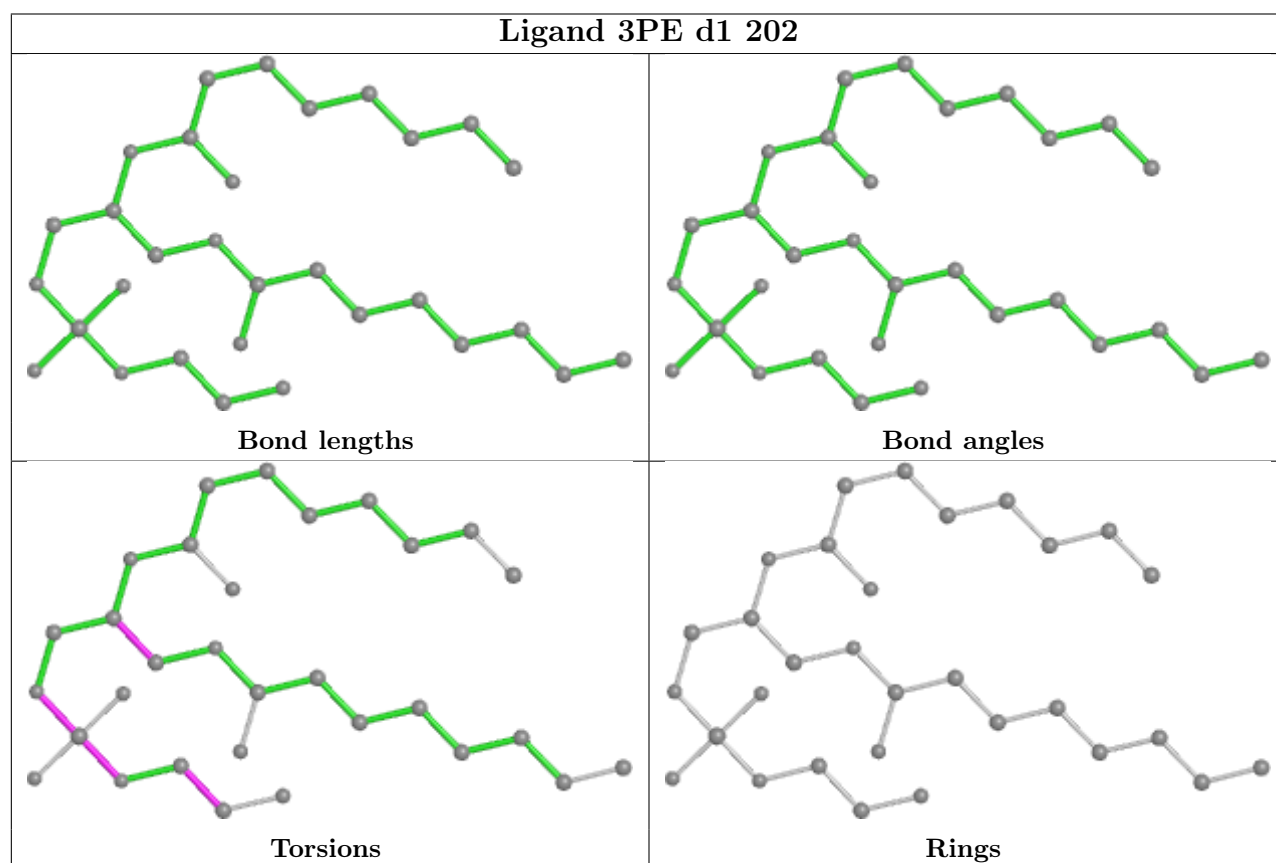
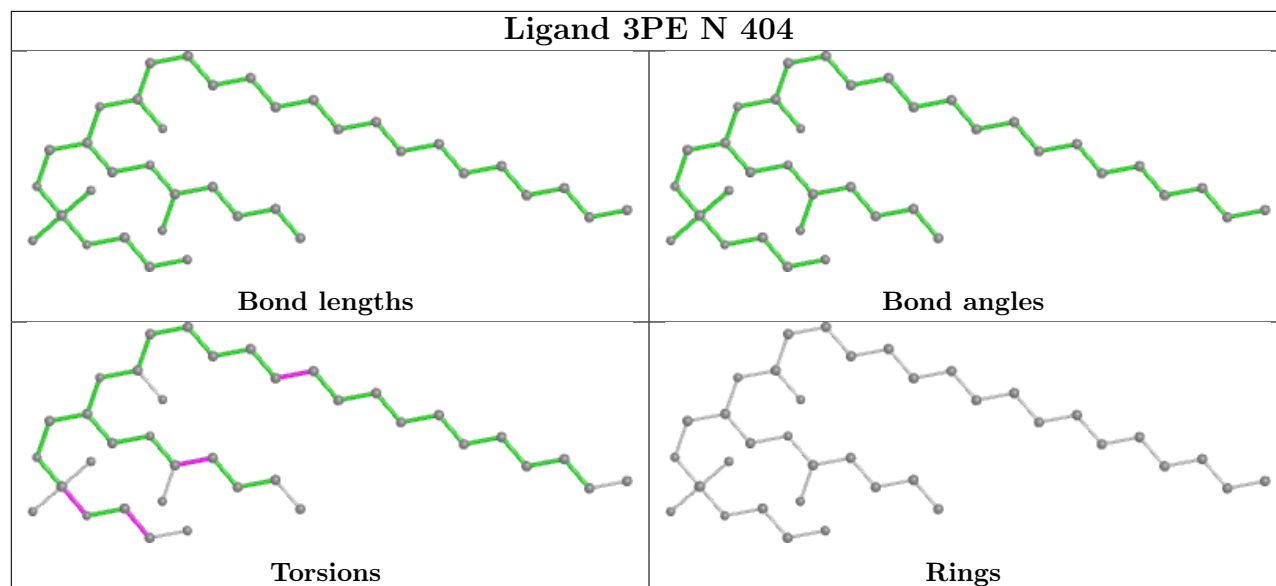


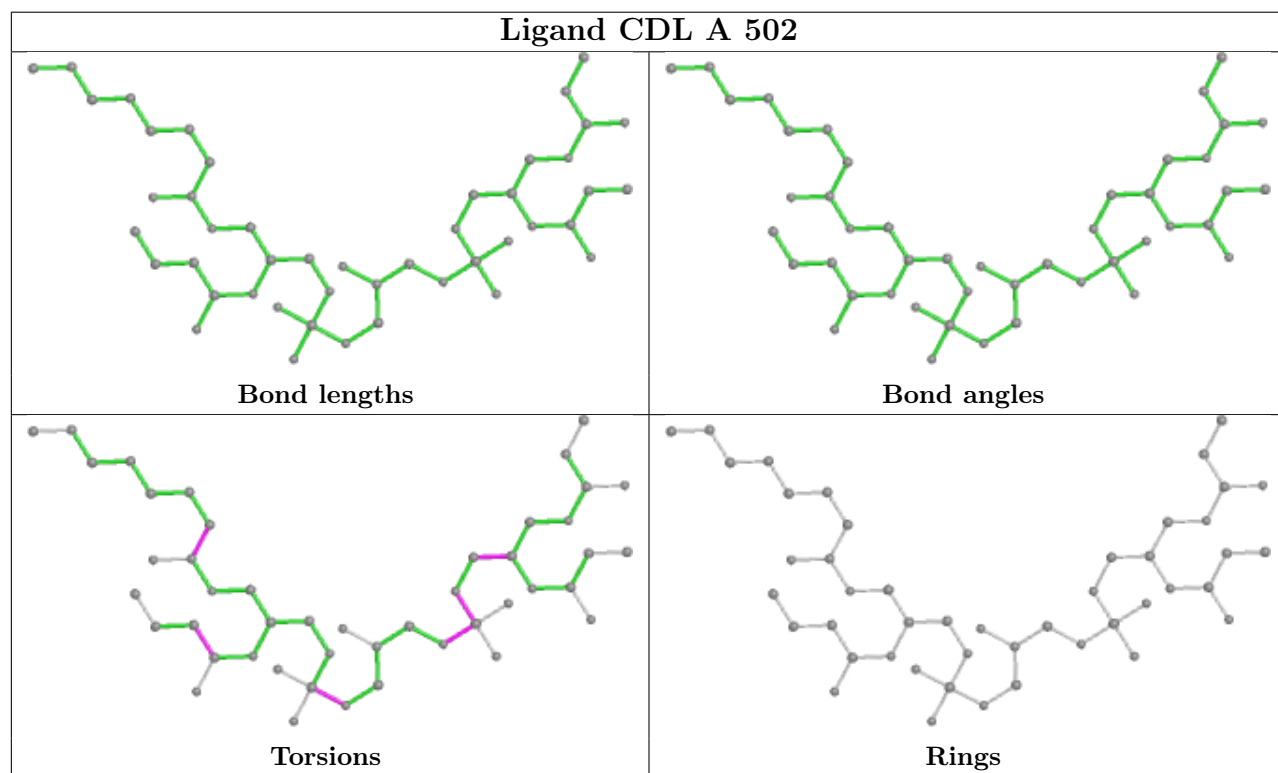
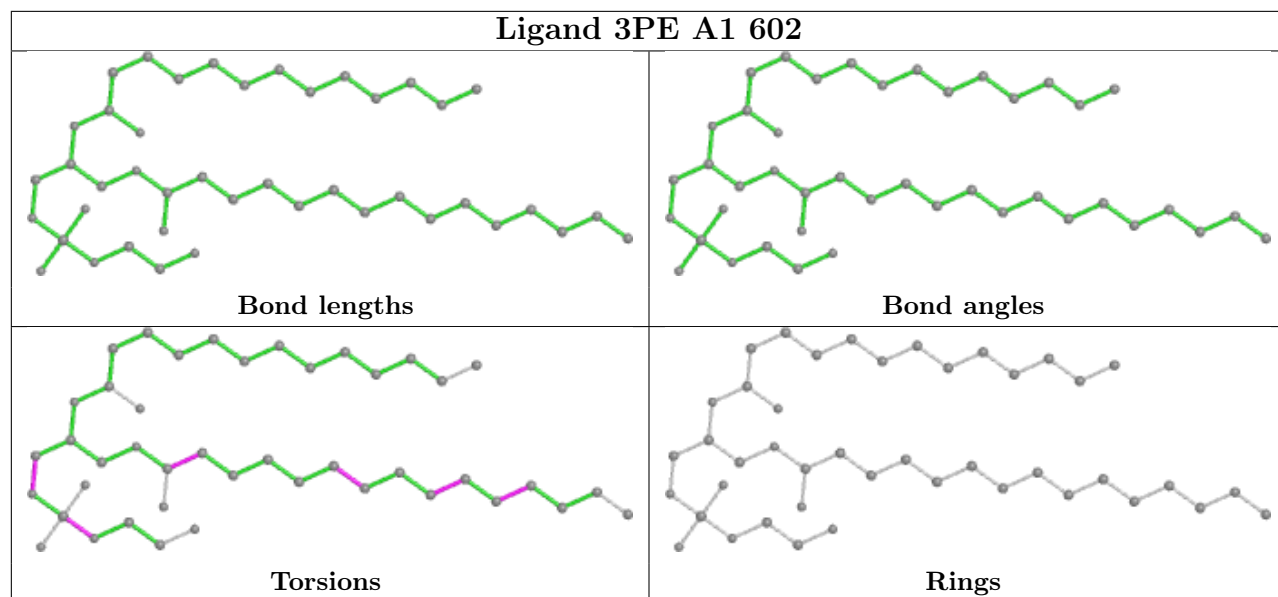


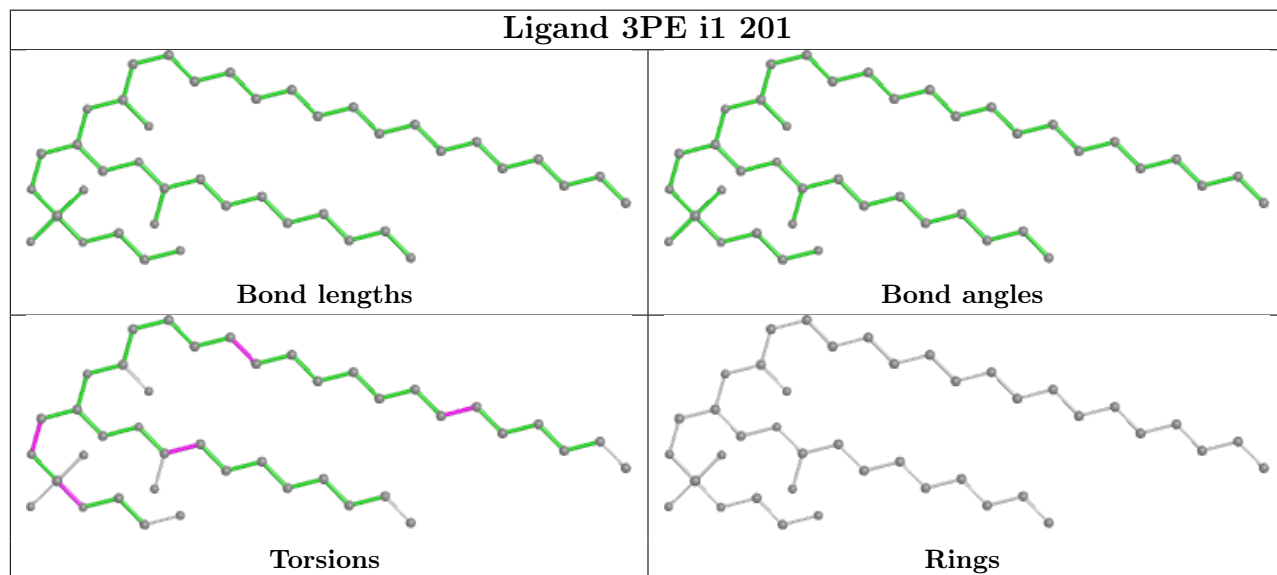
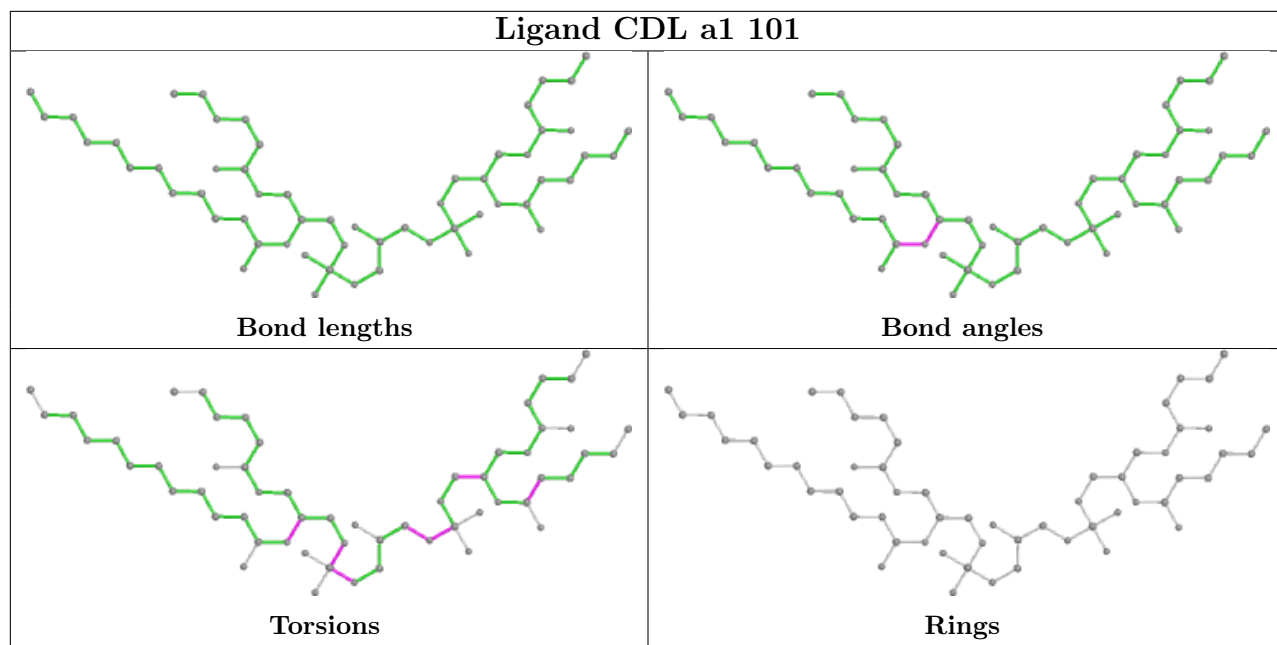


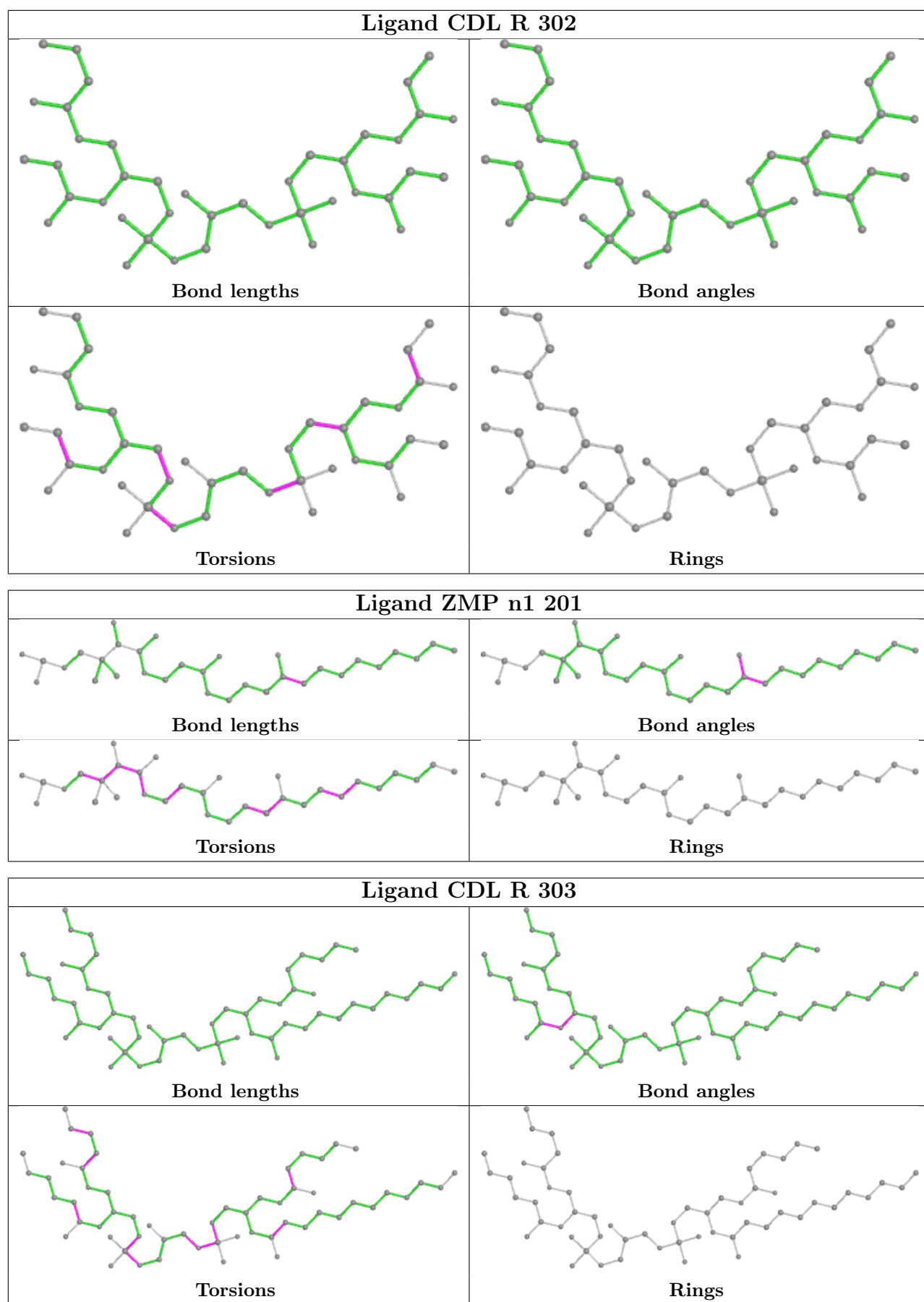


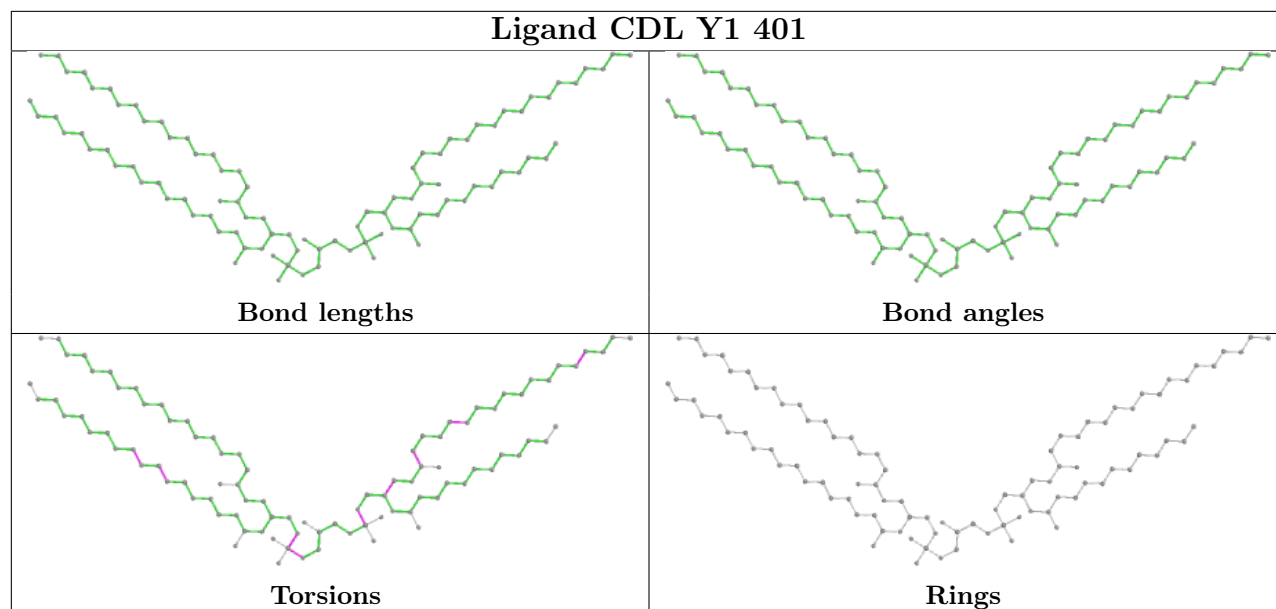












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

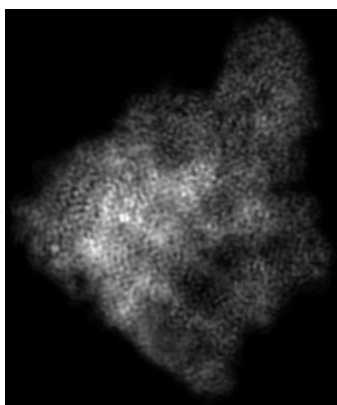
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17990. These allow visual inspection of the internal detail of the map and identification of artifacts.

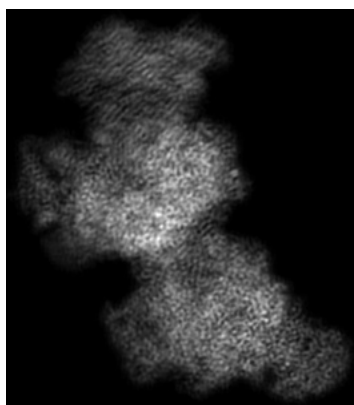
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

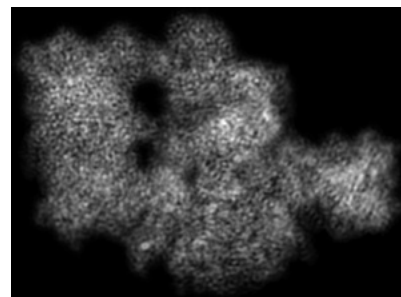
6.1.1 Primary map



X



Y



Z

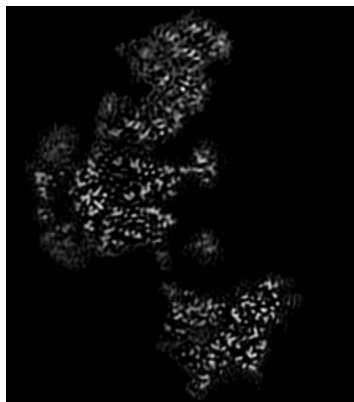
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

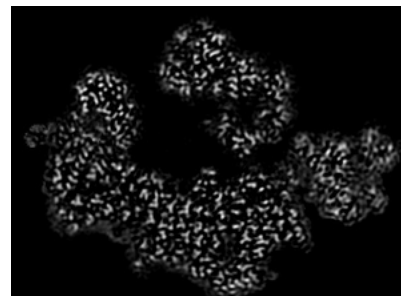
6.2.1 Primary map



X Index: 140



Y Index: 103



Z Index: 123

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: 140



Y Index: 75

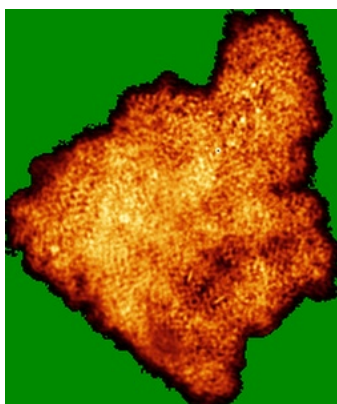


Z Index: 118

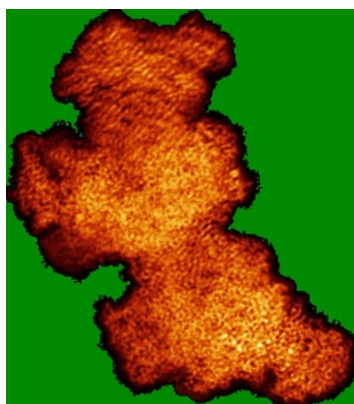
The images above show the largest variance slices of the map in three orthogonal directions.

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

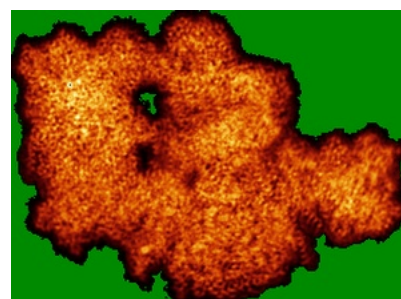
6.4.1 Primary map



X



Y

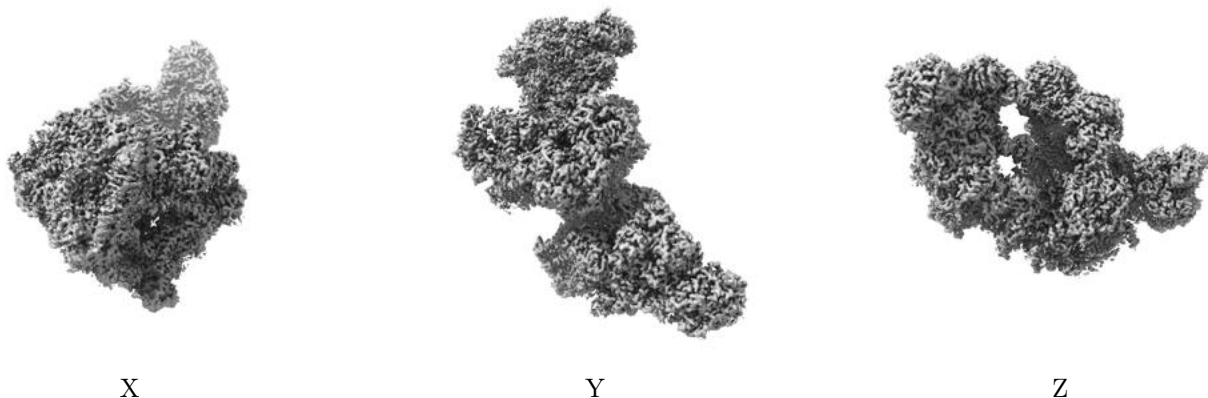


Z

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

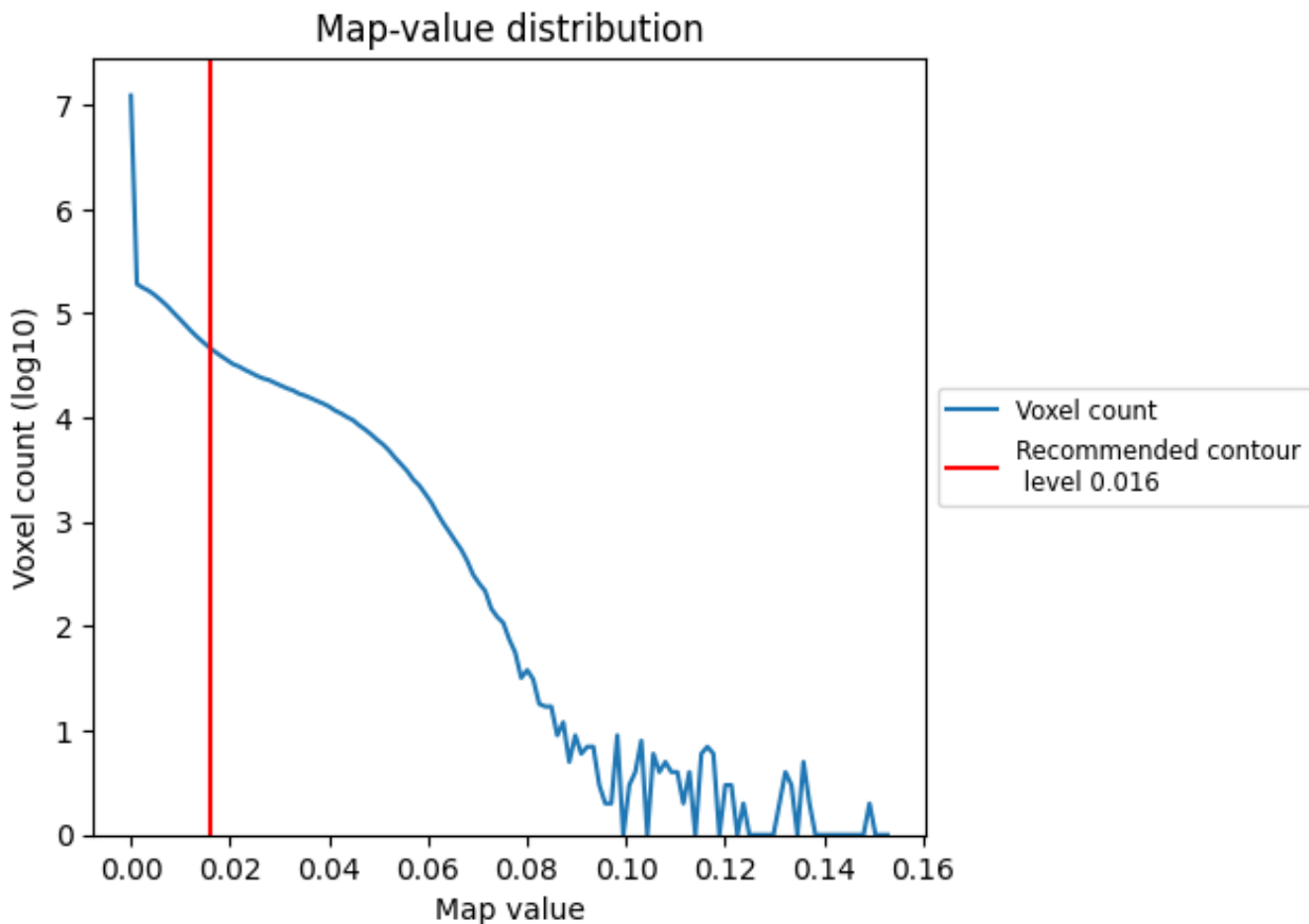
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

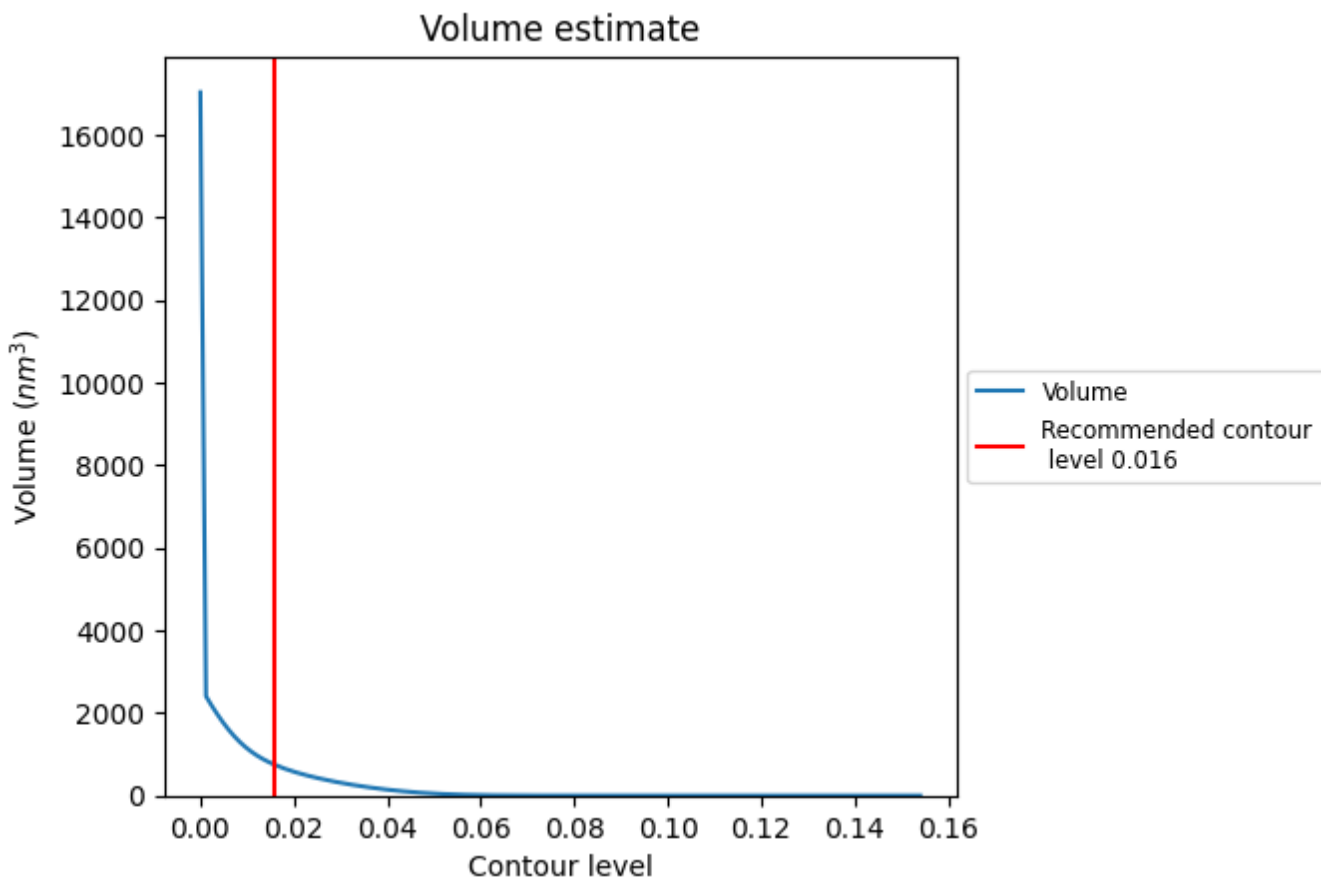
This section contains the results of statistical analysis of the map.

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 743 nm³; this corresponds to an approximate mass of 671 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.

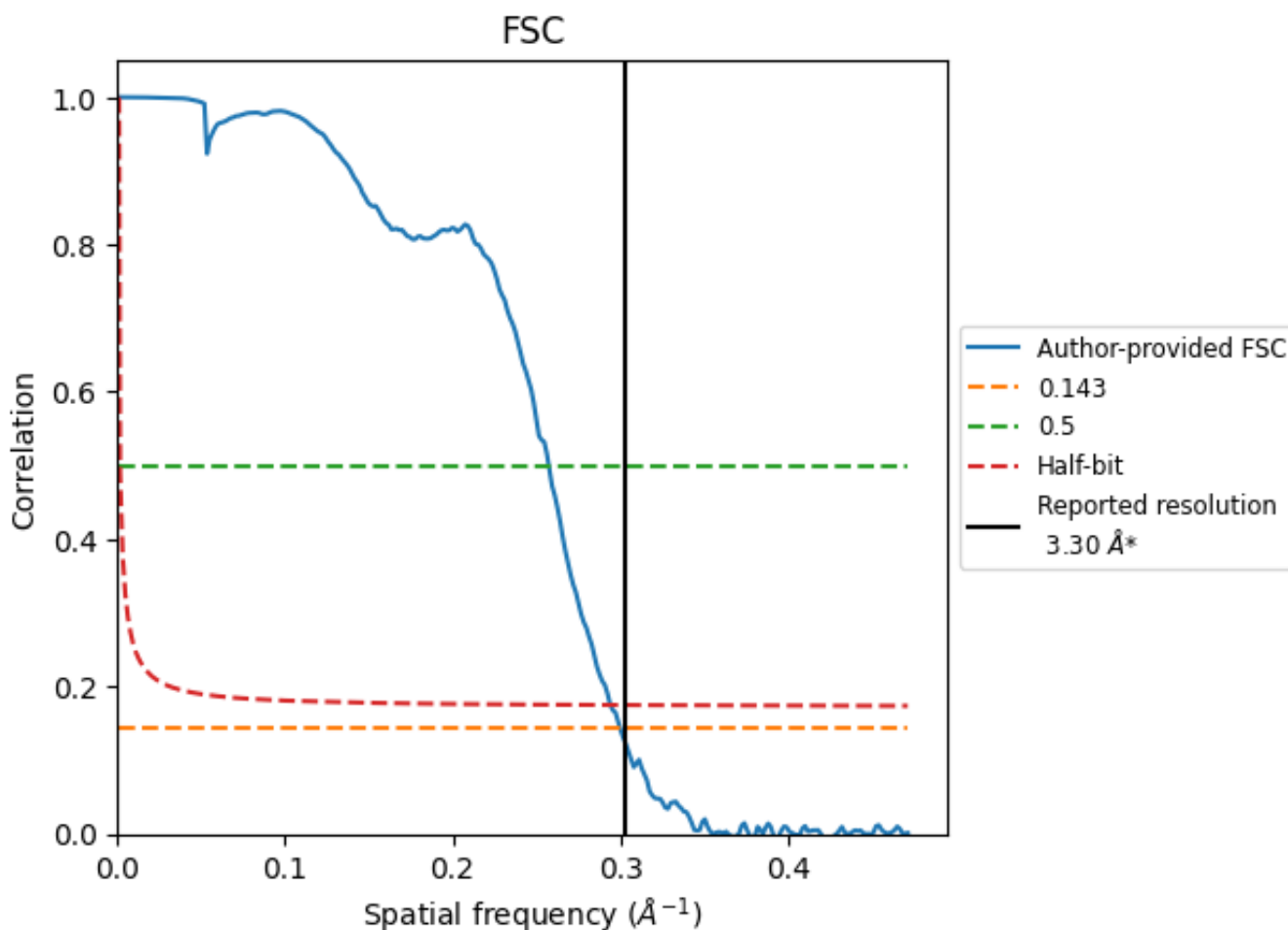
7.3 Rotationally averaged power spectrum [i](#)

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

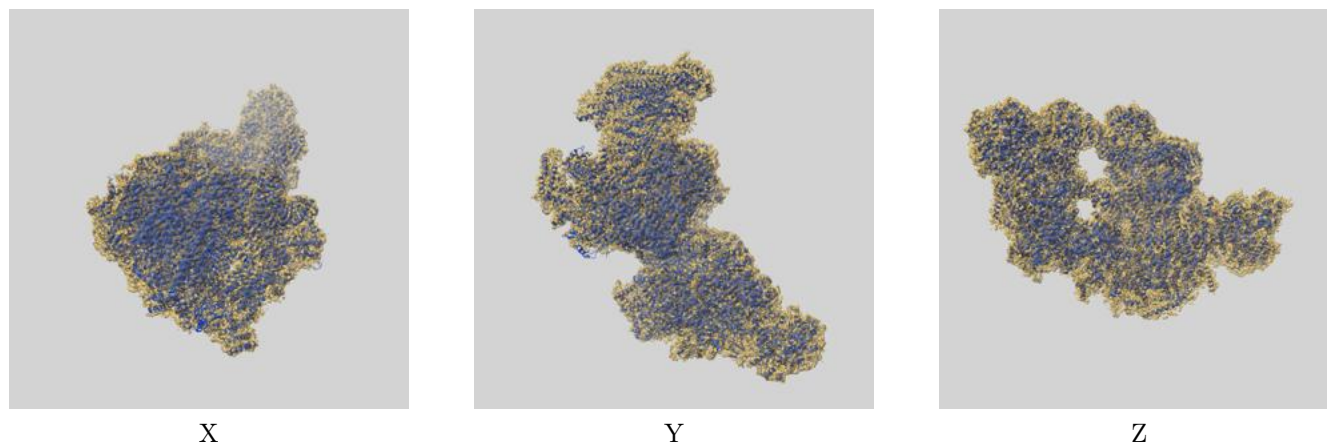
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	3.89	3.40
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

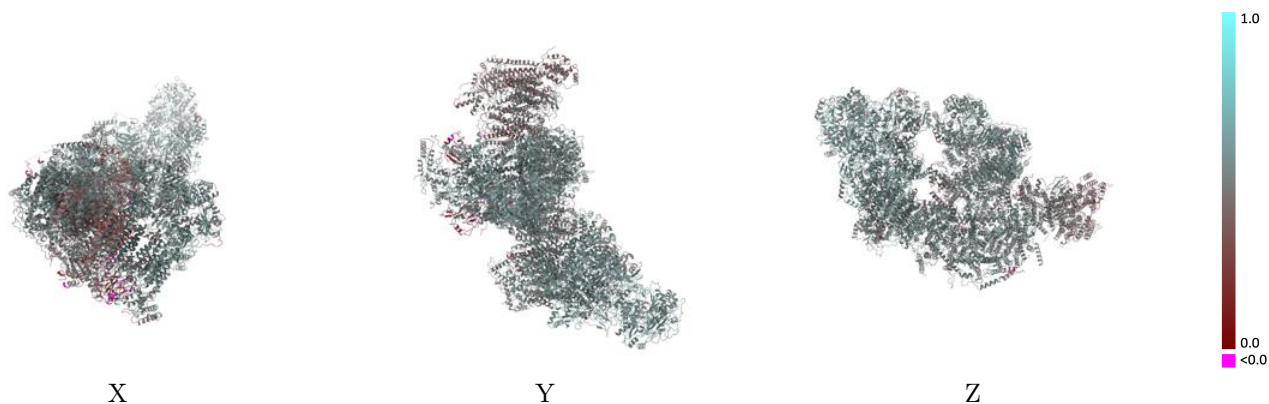
This section contains information regarding the fit between EMDB map EMD-17990 and PDB model 8PW6. Per-residue inclusion information can be found in section 3 on page 29.

9.1 Map-model overlay [i](#)



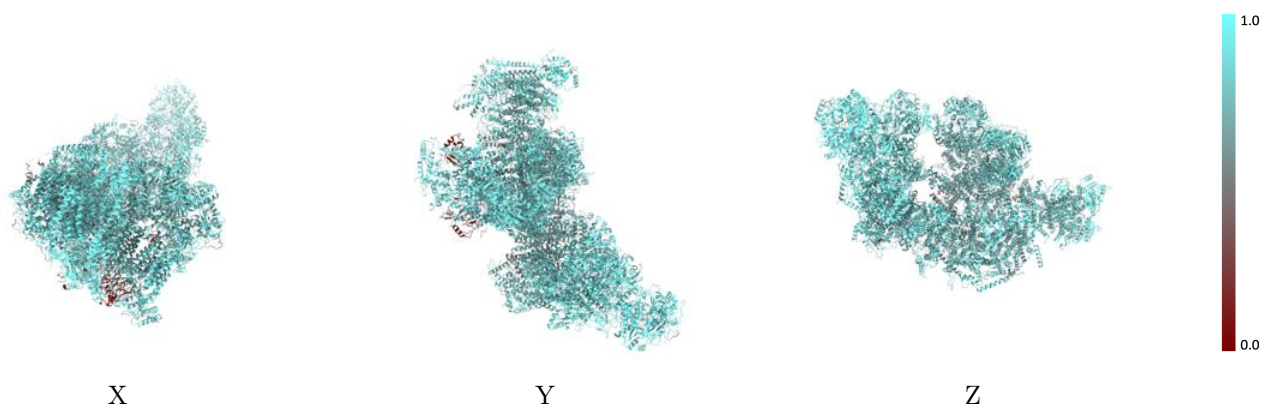
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



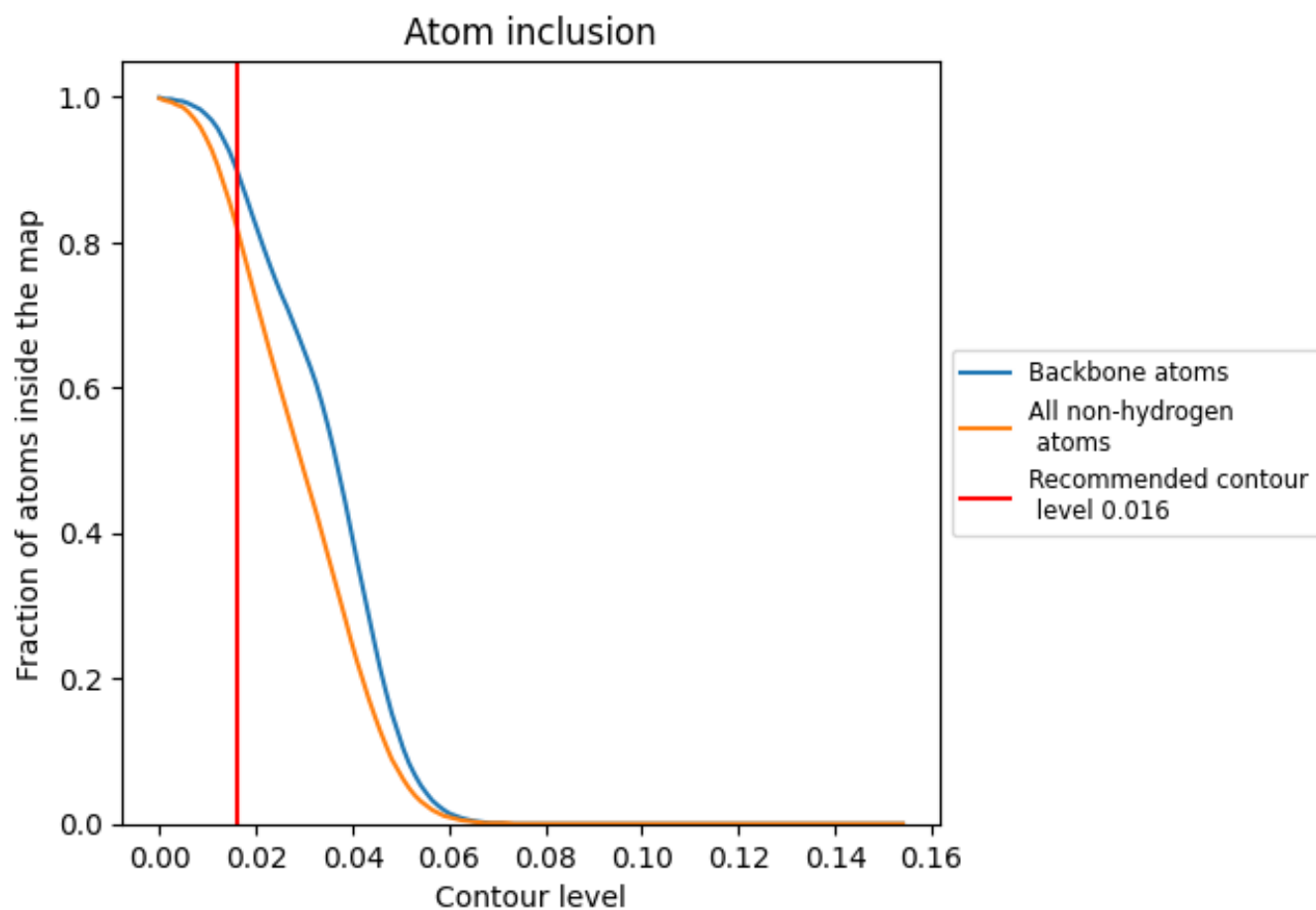
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 82% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8210	 0.5140
1	 0.8940	 0.5550
2	 0.8910	 0.5520
3	 0.8740	 0.5540
6	 0.8800	 0.5540
7	 0.8850	 0.5510
9	 0.8770	 0.5580
A	 0.8440	 0.5370
A1	 0.7500	 0.4950
B	 0.8410	 0.5430
C	 0.8390	 0.5430
C1	 0.9190	 0.5920
D	 0.8550	 0.5290
D1	 0.8470	 0.5410
E	 0.5030	 0.3560
F	 0.8360	 0.5430
G	 0.8380	 0.5250
H	 0.8120	 0.4680
H1	 0.7860	 0.5100
J	 0.8090	 0.5140
J1	 0.6690	 0.4550
K	 0.7000	 0.5130
K1	 0.7480	 0.5110
L	 0.8310	 0.5360
L1	 0.8060	 0.5290
M	 0.8470	 0.5380
M1	 0.8120	 0.5330
N	 0.8160	 0.5330
N1	 0.7890	 0.5270
O	 0.8390	 0.5300
O1	 0.8460	 0.5260
P	 0.5000	 0.3510
P1	 0.8440	 0.5460
Q	 0.7940	 0.5400
Q1	 0.8690	 0.5750






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Chain	Atom inclusion	Q-score
R	0.7370	0.5110
S	0.7310	0.4490
S1	0.8740	0.5240
T	0.6040	0.4810
T1	0.7420	0.4420
U	0.7930	0.5190
U1	0.8370	0.5320
V	0.6930	0.4700
V1	0.8760	0.5540
W1	0.8700	0.5590
X1	0.8280	0.5120
Y1	0.6850	0.4810
Z1	0.8310	0.5220
a1	0.8150	0.5240
b1	0.8030	0.5000
c1	0.7850	0.5030
d1	0.7690	0.5130
e1	0.8050	0.5210
f1	0.7580	0.5040
g1	0.7910	0.5040
h1	0.8240	0.5210
i1	0.7470	0.4790
j1	0.7970	0.4950
k1	0.8290	0.5200
l1	0.8450	0.5400
m1	0.7990	0.5160
n	0.8410	0.4470
n1	0.8520	0.5310
o	0.8260	0.4160
o1	0.8130	0.4980
p	0.8070	0.4350
p1	0.8420	0.5210
q	0.8710	0.4190
q1	0.8950	0.5660
r	0.8690	0.4010
r1	0.8630	0.5580
s	0.8010	0.4170
s1	0.8040	0.5260
t	0.7290	0.3820
u	0.8570	0.4230
v	0.8050	0.3780
w	0.8160	0.4630

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Chain	Atom inclusion	Q-score
x	 0.8680	 0.3990
y	 0.8440	 0.4680
z	 0.8040	 0.3900