



Full wwPDB EM Validation Report ⓘ

Dec 17, 2024 – 03:19 PM EST

PDB ID : 8UGI
EMDB ID : EMD-42226
Title : High resolution in-situ structure of typeA supercomplex in respiratory chain (I1III2IV1,composite)
Authors : Zheng, W.; Zhang, K.; Zhu, J.
Deposited on : 2023-10-05
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

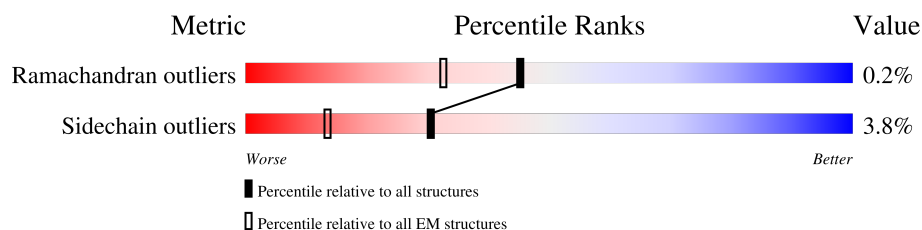
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 2.10 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	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	1A	115	
2	1B	258	
3	1C	264	
4	1D	476	
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	

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Mol	Chain	Length	Quality of chain
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24	1Y	141	
25	1Z	144	
26	1a	70	
27	1b	84	
28	1c	76	
29	1d	122	
30	1e	106	
31	1f	135	
32	1g	154	
33	1h	189	









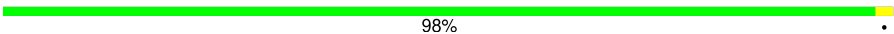
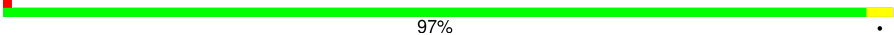
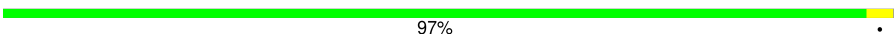










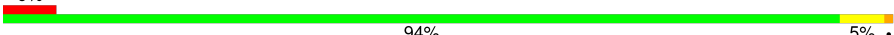
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Mol	Chain	Length	Quality of chain
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	113	
44	1s	471	
45	3A	480	
45	3N	480	
46	3B	453	
46	3O	453	
47	3C	379	
47	3P	379	
48	3D	325	
48	3Q	325	
49	3E	274	
49	3I	274	
49	3R	274	
49	3V	274	
50	3F	111	
50	3S	111	

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Mol	Chain	Length	Quality of chain
51	3G	82	
51	3T	82	
52	3H	91	
52	3U	91	
53	3J	64	
53	3W	64	
54	3X	56	
54	3Y	56	
55	4A	514	
56	4B	227	
57	4C	261	
58	4D	169	
59	4E	152	
60	4F	129	
61	4G	97	
62	4H	86	
63	4I	75	
64	4J	80	
65	4K	80	
66	4L	63	
67	4M	70	
68	4N	82	

2 Entry composition

There are 93 unique types of molecules in this entry. The entry contains 124291 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	115	Total	C	N	O	S	0	0
			916	616	134	159	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	155	Total	C	N	O	S	0	0
			1242	791	226	211	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	209	Total	C	N	O	S	0	0
			1740	1125	297	316	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1C	104	GLN	ARG	conflict	UNP A0A286ZNN4
1C	154	GLY	ASP	conflict	UNP A0A286ZNN4

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1D	429	Total	C	N	O	S	0	0
			3452	2207	593	628	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1D	0	GLY	GLU	conflict	UNP A0A8D0QM68

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	432	Total	C	N	O	S	0	0
			3325	2100	592	613	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1G	699	Total	C	N	O	S	0	0
			5362	3360	933	1029	40		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1H	318	Total	C	N	O	S	0	0
			2504	1673	385	425	21		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	98	Total	C	N	O	S	0	0
			750	494	113	129	14		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1L	606	Total	C	N	O	S	0	0
			4818	3195	746	826	51		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1M	459	Total	C	N	O	S	0	0
			3632	2411	572	610	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1N	347	Total	C	N	O	S	0	0
			2712	1783	420	463	46		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1O	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1P	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1Q	129	Total	C	N	O	S	0	0
			1047	659	186	199	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit AB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	1U	86	Total	C	N	O	S	0	0
			694	448	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1V	115	Total	C	N	O	S	0	0
			927	599	157	168	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1W	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1Z	141	Total	C	N	O	S	0	0
			1168	752	202	205	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1a	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1b	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	1c	49	Total	C	N	O	0	0
			417	276	71	70		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1d	119	Total	C	N	O	S	0	0
			985	641	171	168	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

1 [Sus scrofa].

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1f	-77	MET	-	initiating methionine	UNP A0A8D1IZ33
1f	-76	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-75	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-74	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-73	ILE	-	expression tag	UNP A0A8D1IZ33
1f	-72	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-71	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-70	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-69	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-68	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-67	THR	-	expression tag	UNP A0A8D1IZ33
1f	-66	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-65	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-64	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-63	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-62	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-61	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-60	CYS	-	expression tag	UNP A0A8D1IZ33
1f	-59	ASP	-	expression tag	UNP A0A8D1IZ33
1f	-58	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-57	ASN	-	expression tag	UNP A0A8D1IZ33
1f	-56	GLN	-	expression tag	UNP A0A8D1IZ33
1f	-55	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-54	VAL	-	expression tag	UNP A0A8D1IZ33
1f	-53	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-52	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-51	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-50	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-49	PHE	-	expression tag	UNP A0A8D1IZ33

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1g	100	Total	C	N	O	S	0	0
			835	535	138	158	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1h	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1i	128	Total	C	N	O	S	0	0
			1100	723	194	181	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1i	0	ACE	-	acetylation	UNP A0A4X1UIV8

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1j	71	Total	C	N	O	S	0	0
			601	394	99	107	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1k	81	Total	C	N	O	S	0	0
			649	422	110	116	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1l	156	Total	C	N	O	S	0	0
			1310	847	213	242	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	1m	128	Total	C	N	O	0	0
			1062	691	182	189		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1o	0	MYR	-	insertion	UNP F1SCH1

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1q	145	Total	C	N	O	S	0	0
			1212	775	219	213	5		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	94	Total	C	N	O	S	0	0
			759	478	143	135	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
45	3N	445	Total	C	N	O	S	1	0
			3424	2162	606	637	19		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3B	418	Total	C	N	O	S	0	0
			3138	1965	555	610	8		
46	3O	417	Total	C	N	O	S	0	0
			3124	1960	554	602	8		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
47	3P	379	Total	C	N	O	S	0	0
			3024	2031	471	501	21		

- Molecule 48 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
48	3Q	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
49	3I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
49	3R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	3S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3G	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
51	3T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	3U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		

- Molecule 53 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	3J	56	Total	C	N	O	0	0
			464	305	82	77		
53	3W	56	Total	C	N	O	0	0
			464	305	82	77		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
54	3Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 55 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4A	513	Total	C	N	O	S	1	0
			4025	2692	625	677	31		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4B	227	Total	C	N	O	S	0	0
			1829	1190	281	340	18		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	4C	259	Total	C	N	O	S	0	0
			2096	1399	336	351	10		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	4D	139	Total	C	N	O	S	0	0
			1163	757	190	212	4		

- Molecule 59 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	4E	105	Total	C	N	O	S	0	0
			852	544	144	162	2		

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	4F	97	Total	C	N	O	S	0	0
			734	455	130	143	6		

- Molecule 61 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	4G	75	Total	C	N	O	S	0	0
			617	398	118	100	1		

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	4H	82	Total	C	N	O	S	0	0
			687	434	125	123	5		

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	4I	67	Total	C	N	O	S	0	0
			550	359	97	91	3		

- Molecule 64 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	4J	58	Total	C	N	O	S	0	0
			456	293	78	82	3		

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	4K	49	Total	C	N	O	S	0	0
			383	249	65	68	1		

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	4L	46	Total	C	N	O	S	0	0
			381	254	64	61	2		

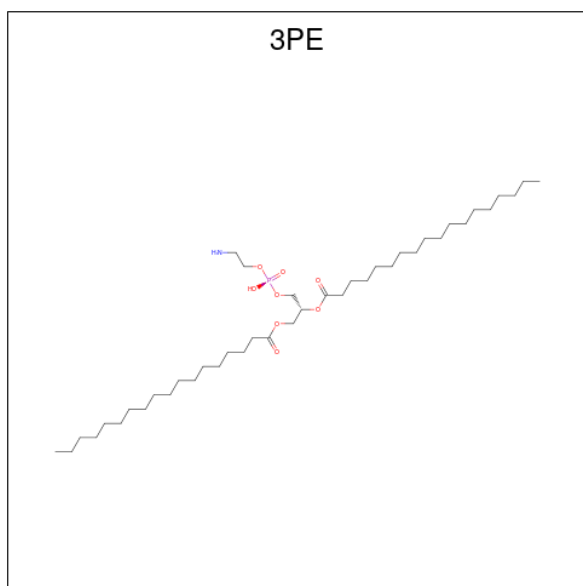
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	4M	43	Total	C	N	O	0	0
			338	222	57	59		

- Molecule 68 is a protein called Cytochrome c oxidase subunit NDUFA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	4N	82	Total	C	N	O	S	0	0
			660	432	112	114	2		

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



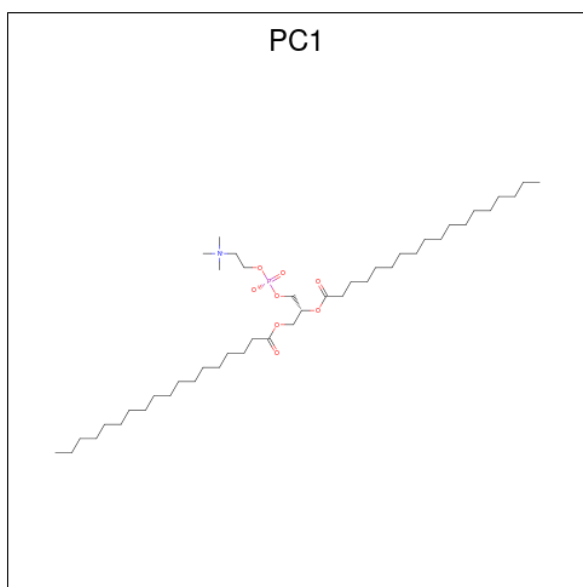
Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1J	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1L	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1L	1	Total	C	N	O	P	0
			31	21	1	8	1	
69	1M	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1M	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1M	1	Total	C	N	O	P	0
			50	40	1	8	1	
69	1N	1	Total	C	N	O	P	0
			49	39	1	8	1	
69	1N	1	Total	C	N	O	P	0
			33	23	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	1Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			30	20	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
69	1d	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1j	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	3A	1	Total	C	N	O	P	0
			27	17	1	8	1	
69	3A	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	3C	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	3C	1	Total	C	N	O	P	0
			34	24	1	8	1	
69	3D	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	3G	1	Total	C	N	O	P	0
			29	19	1	8	1	
69	3N	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	3N	1	Total	C	N	O	P	0
			25	15	1	8	1	
69	3P	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	3R	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	3Y	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



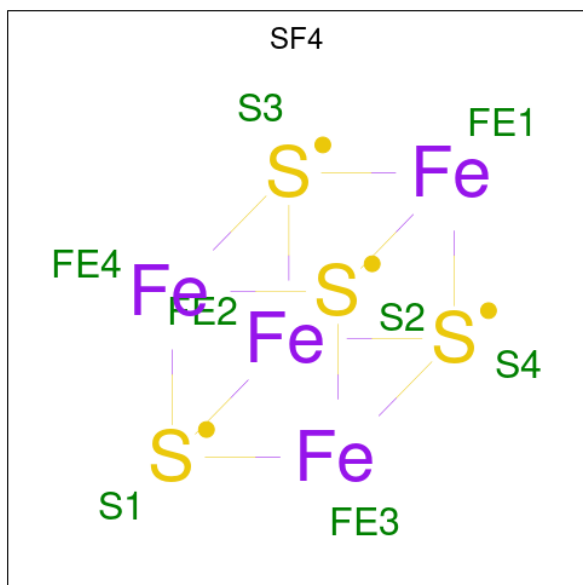
Mol	Chain	Residues	Atoms					AltConf
70	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1B	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1B	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	1M	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	1P	1	Total	C	N	O	P	0
			33	23	1	8	1	
70	1Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1Z	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	
70	1m	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1q	1	Total	C	N	O	P	0
			49	39	1	8	1	
70	3E	1	Total	C	N	O	P	0
			47	37	1	8	1	
70	3R	1	Total	C	N	O	P	0
			45	35	1	8	1	

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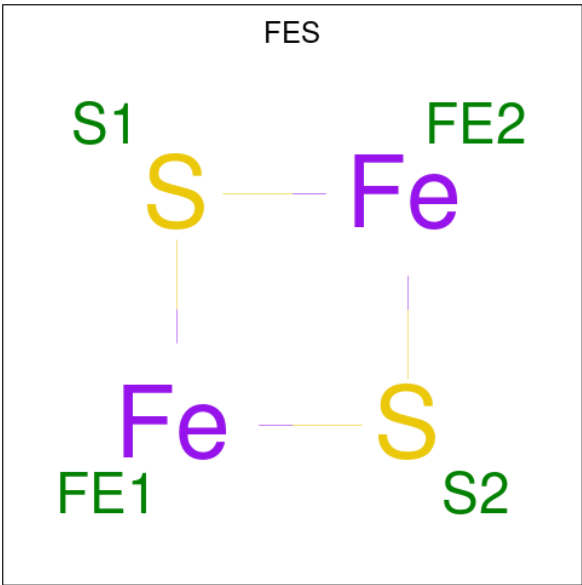
Mol	Chain	Residues	Atoms					AltConf
70	3X	1	Total	C	N	O	P	0
			29	19	1	8	1	

- Molecule 71 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



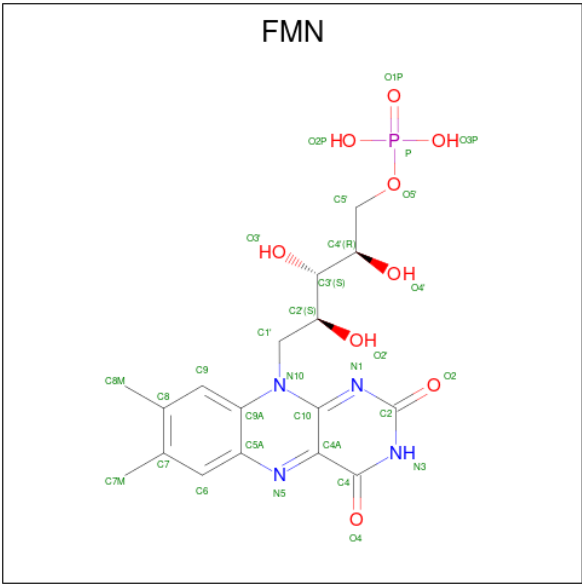
Mol	Chain	Residues	Atoms			AltConf
71	1B	1	Total	Fe	S	0
			8	4	4	
71	1F	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	

- Molecule 72 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 73 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

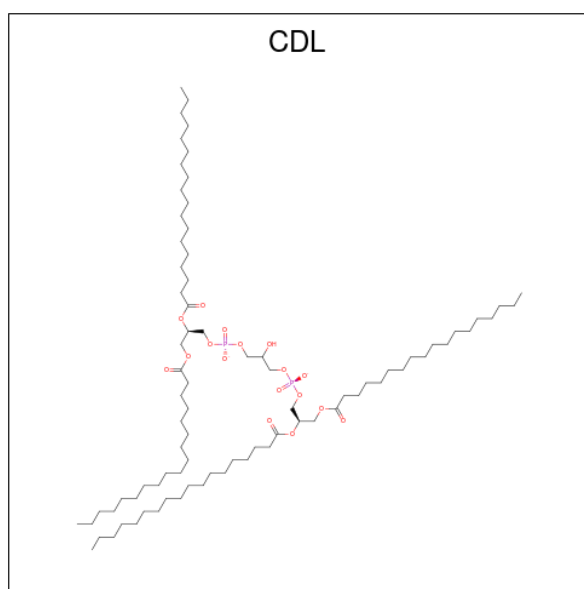


Mol	Chain	Residues	Atoms					AltConf
73	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 74 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
74	1G	1	Total	K	0
			1	1	

- Molecule 75 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



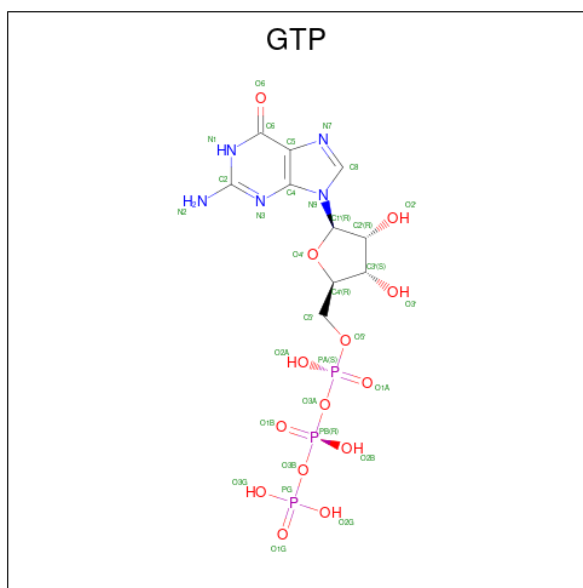
Mol	Chain	Residues	Atoms				AltConf
75	1L	1	Total	C	O	P	0
			76	57	17	2	
75	1N	1	Total	C	O	P	0
			62	43	17	2	
75	1X	1	Total	C	O	P	0
			86	67	17	2	
75	1d	1	Total	C	O	P	0
			65	46	17	2	
75	1h	1	Total	C	O	P	0
			80	61	17	2	
75	1q	1	Total	C	O	P	0
			61	42	17	2	
75	3A	1	Total	C	O	P	0
			58	39	17	2	
75	3G	1	Total	C	O	P	0
			52	33	17	2	

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Mol	Chain	Residues	Atoms				AltConf
75	3G	1	Total	C	O	P	0
			56	37	17	2	
75	3N	1	Total	C	O	P	0
			43	24	17	2	
75	3P	1	Total	C	O	P	0
			56	37	17	2	
75	3T	1	Total	C	O	P	0
			57	38	17	2	
75	4B	1	Total	C	O	P	0
			100	81	17	2	
75	4C	1	Total	C	O	P	0
			100	81	17	2	
75	4D	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 76 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
76	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

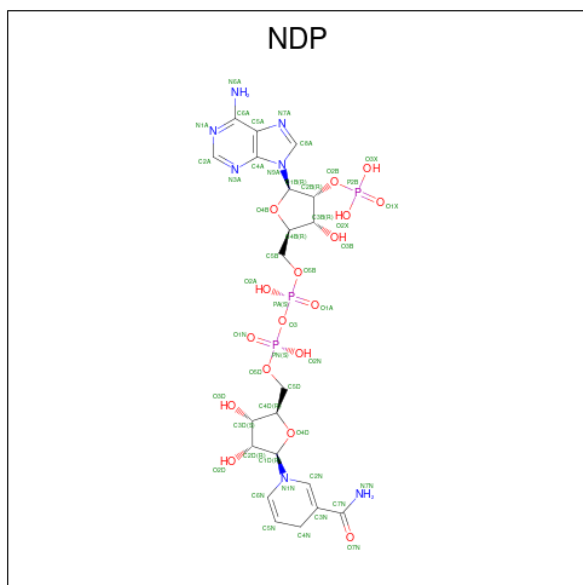
Mol	Chain	Residues	Atoms		AltConf
77	1O	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
77	4A	1	Total	Mg	0
			1	1	

- Molecule 78 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

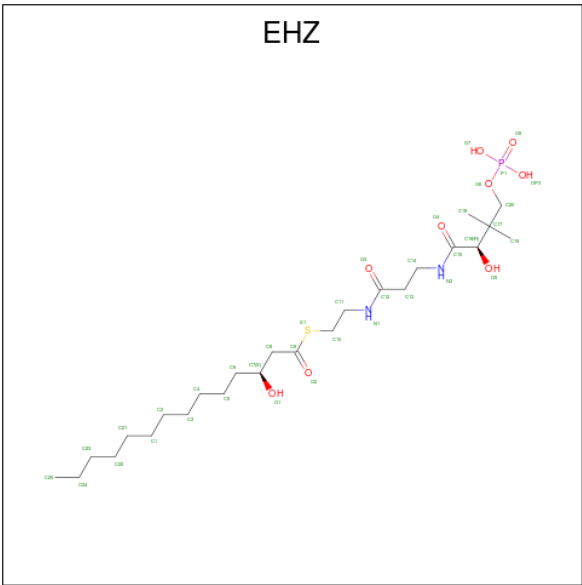


Mol	Chain	Residues	Atoms					AltConf
78	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

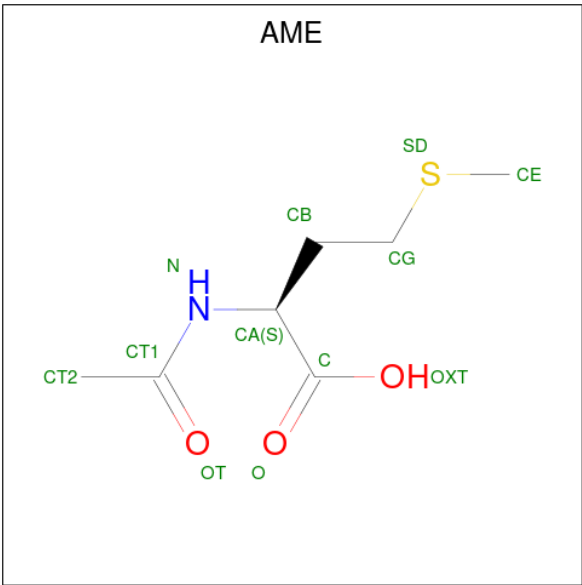
Mol	Chain	Residues	Atoms		AltConf
79	1R	1	Total	Zn	0
			1	1	
79	4F	1	Total	Zn	0
			1	1	

- Molecule 80 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



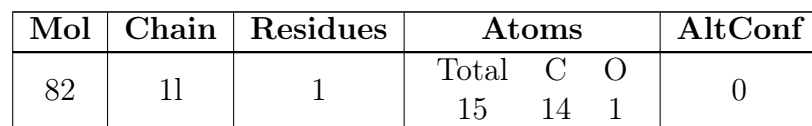
Mol	Chain	Residues	Atoms						AltConf
80	1T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
80	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 81 is N-ACETYLMETHIONINE (three-letter code: AME) (formula: C₇H₁₃NO₃S).



Mol	Chain	Residues	Atoms					AltConf
81	1h	1	Total	C	N	O	S	0
			11	7	1	2	1	

- Molecule 82 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).



- # HEM

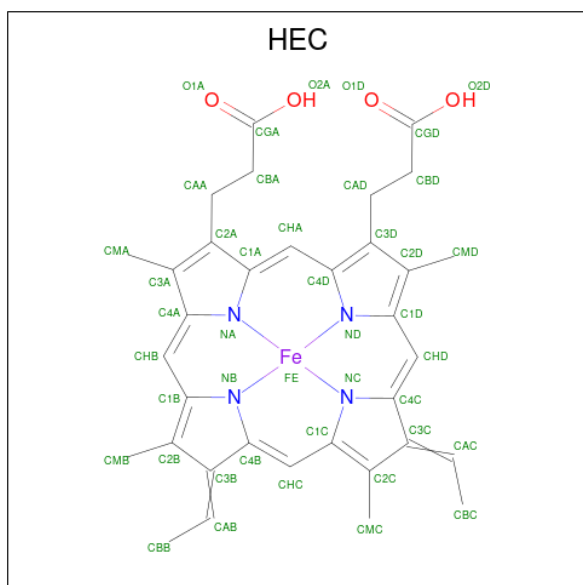
Mol	Chain	Residues	Atoms					AltConf
83	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
83	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0

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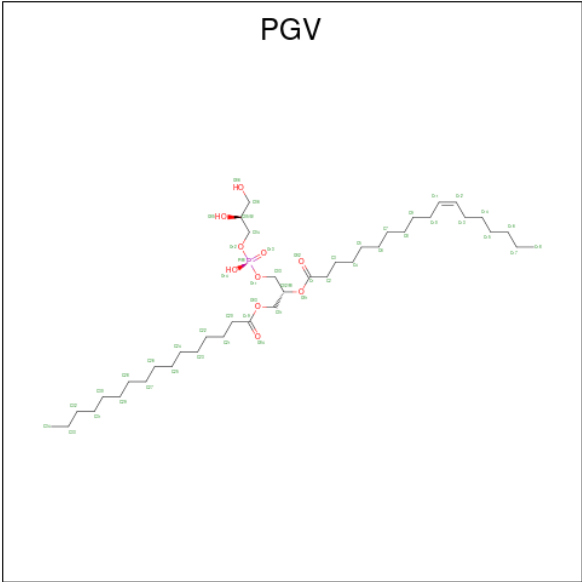
Mol	Chain	Residues	Atoms					AltConf
83	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 84 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
84	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
84	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 85 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



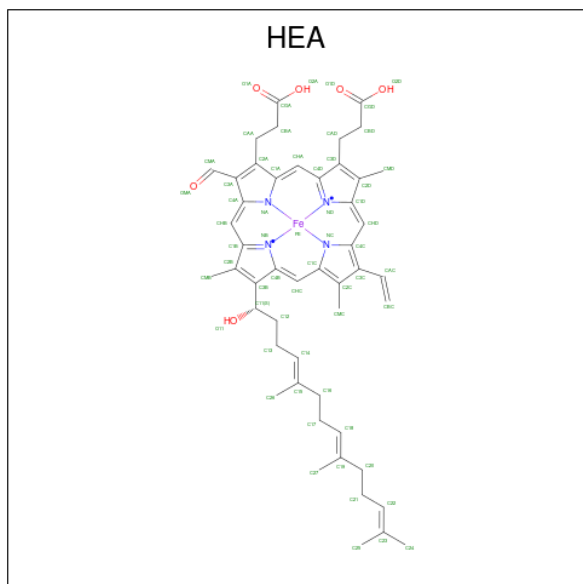
Mol	Chain	Residues	Atoms				AltConf
85	4A	1	Total	C	O	P	0
			51	40	10	1	
85	4A	1	Total	C	O	P	0
			51	40	10	1	
85	4A	1	Total	C	O	P	0
			51	40	10	1	
85	4B	1	Total	C	O	P	0
			51	40	10	1	
85	4C	1	Total	C	O	P	0
			51	40	10	1	
85	4C	1	Total	C	O	P	0
			51	40	10	1	
85	4C	1	Total	C	O	P	0
			51	40	10	1	
85	4C	1	Total	C	O	P	0
			51	40	10	1	
85	4C	1	Total	C	O	P	0
			51	40	10	1	
85	4C	1	Total	C	O	P	0
			51	40	10	1	
85	4G	1	Total	C	O	P	0
			51	40	10	1	
85	4J	1	Total	C	O	P	0
			51	40	10	1	
85	4K	1	Total	C	O	P	0
			51	40	10	1	
85	4L	1	Total	C	O	P	0
			51	40	10	1	

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Mol	Chain	Residues	Atoms				AltConf
85	4M	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 86 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
86	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
86	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

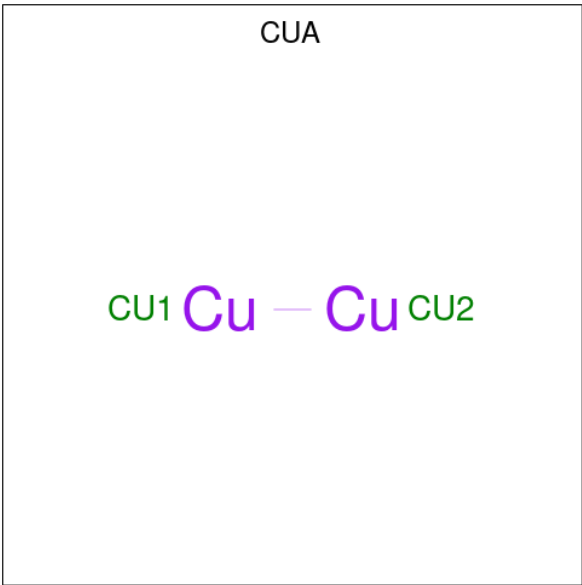
- Molecule 87 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
87	4A	1	Total	Cu	0
			1	1	

- Molecule 88 is SODIUM ION (three-letter code: NA) (formula: Na).

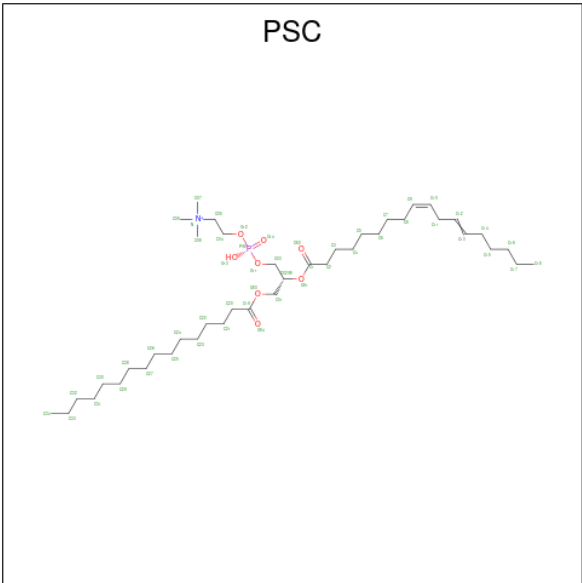
Mol	Chain	Residues	Atoms		AltConf
88	4A	1	Total	Na	0
			1	1	

- Molecule 89 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms		AltConf
89	4B	1	Total	Cu	0
			2	2	

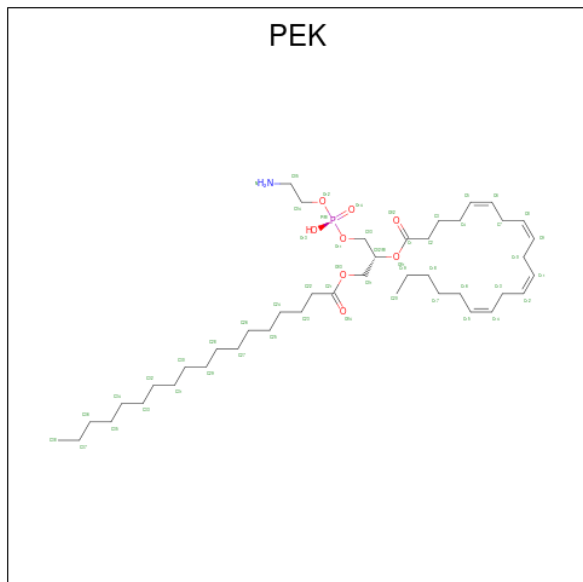
- Molecule 90 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



Mol	Chain	Residues	Atoms					AltConf
90	4B	1	Total	C	N	O	P	0
			52	42	1	8	1	

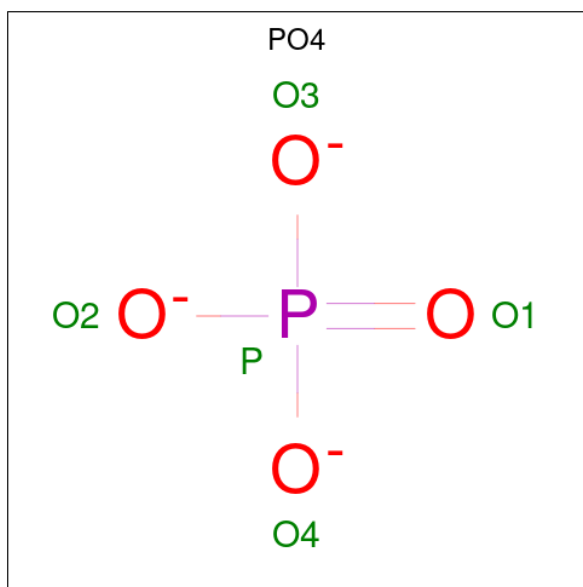
- Molecule 91 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(ST

EAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE
(three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
91	4G	1	Total	C	N	O	P	0
			53	43	1	8	1	
91	4G	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 92 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
92	4H	1	Total	O	P	0
			5	4	1	

- Molecule 93 is water.

Mol	Chain	Residues	Atoms			AltConf
93	1A	21	Total	O		0
			21	21		
93	1B	53	Total	O		0
			53	53		
93	1C	96	Total	O		0
			96	96		
93	1D	138	Total	O		0
			138	138		
93	1E	55	Total	O		0
			55	55		
93	1F	113	Total	O		0
			113	113		
93	1G	255	Total	O		0
			255	255		
93	1H	80	Total	O		0
			80	80		
93	1I	75	Total	O		0
			75	75		
93	1J	56	Total	O		0
			56	56		
93	1K	38	Total	O		0
			38	38		
93	1L	228	Total	O		0
			228	228		
93	1M	201	Total	O		0
			201	201		
93	1N	154	Total	O		0
			154	154		
93	1O	150	Total	O		0
			150	150		
93	1P	118	Total	O		0
			118	118		
93	1Q	63	Total	O		0
			63	63		
93	1R	41	Total	O		0
			41	41		
93	1S	56	Total	O		0
			56	56		

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Mol	Chain	Residues	Atoms		AltConf
93	1T	12	Total 12	O 12	0
93	1U	26	Total 26	O 26	0
93	1V	20	Total 20	O 20	0
93	1W	37	Total 37	O 37	0
93	1X	106	Total 106	O 106	0
93	1Y	39	Total 39	O 39	0
93	1Z	83	Total 83	O 83	0
93	1a	30	Total 30	O 30	0
93	1b	35	Total 35	O 35	0
93	1c	23	Total 23	O 23	0
93	1d	95	Total 95	O 95	0
93	1e	91	Total 91	O 91	0
93	1f	43	Total 43	O 43	0
93	1g	76	Total 76	O 76	0
93	1h	116	Total 116	O 116	0
93	1i	48	Total 48	O 48	0
93	1j	37	Total 37	O 37	0
93	1k	35	Total 35	O 35	0
93	1l	97	Total 97	O 97	0
93	1m	78	Total 78	O 78	0
93	1n	122	Total 122	O 122	0

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Mol	Chain	Residues	Atoms		AltConf
93	1o	101	Total 101	O 101	0
93	1p	141	Total 141	O 141	0
93	1q	47	Total 47	O 47	0
93	1r	25	Total 25	O 25	0
93	1s	15	Total 15	O 15	0
93	3A	184	Total 184	O 184	0
93	3B	110	Total 110	O 110	0
93	3C	222	Total 222	O 222	0
93	3D	131	Total 131	O 131	0
93	3E	45	Total 45	O 45	0
93	3F	115	Total 115	O 115	0
93	3G	78	Total 78	O 78	0
93	3H	26	Total 26	O 26	0
93	3I	5	Total 5	O 5	0
93	3J	27	Total 27	O 27	0
93	3N	231	Total 231	O 231	0
93	3O	184	Total 184	O 184	0
93	3P	152	Total 152	O 152	0
93	3Q	98	Total 98	O 98	0
93	3R	47	Total 47	O 47	0
93	3S	71	Total 71	O 71	0

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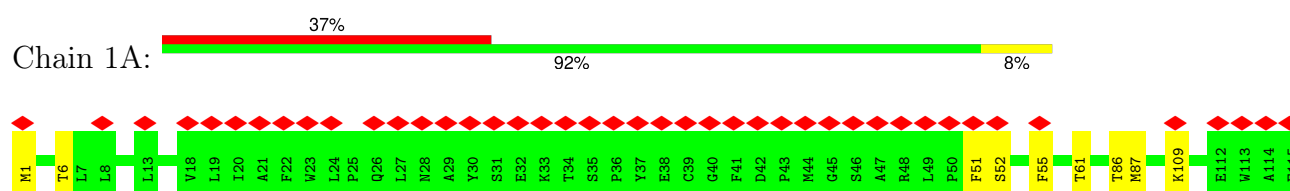
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Mol	Chain	Residues	Atoms		AltConf
93	3T	40	Total 40	O 40	0
93	3U	110	Total 110	O 110	0
93	3V	7	Total 7	O 7	0
93	3W	31	Total 31	O 31	0
93	3X	25	Total 25	O 25	0
93	3Y	16	Total 16	O 16	0
93	4A	110	Total 110	O 110	0
93	4B	115	Total 115	O 115	0
93	4C	103	Total 103	O 103	0
93	4D	81	Total 81	O 81	0
93	4E	55	Total 55	O 55	0
93	4F	67	Total 67	O 67	0
93	4G	39	Total 39	O 39	0
93	4H	43	Total 43	O 43	0
93	4I	25	Total 25	O 25	0
93	4J	34	Total 34	O 34	0
93	4K	27	Total 27	O 27	0
93	4L	23	Total 23	O 23	0
93	4M	28	Total 28	O 28	0
93	4N	53	Total 53	O 53	0

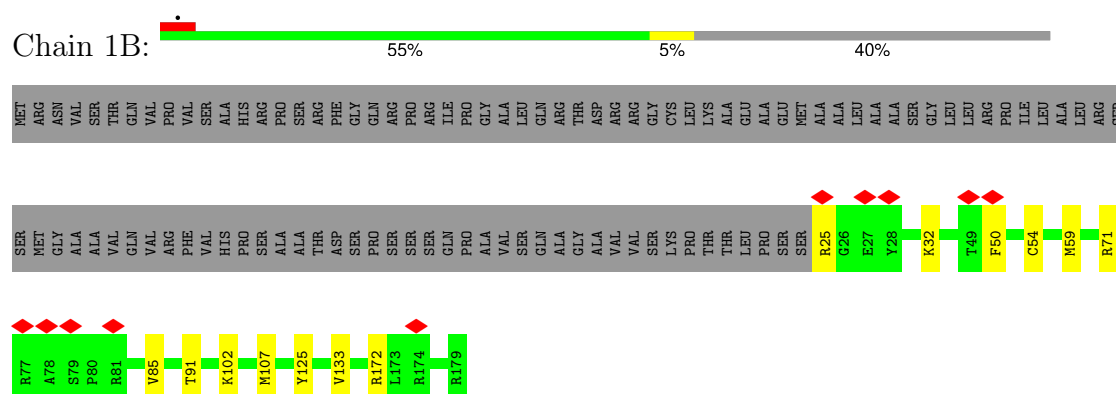
3 Residue-property plots

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

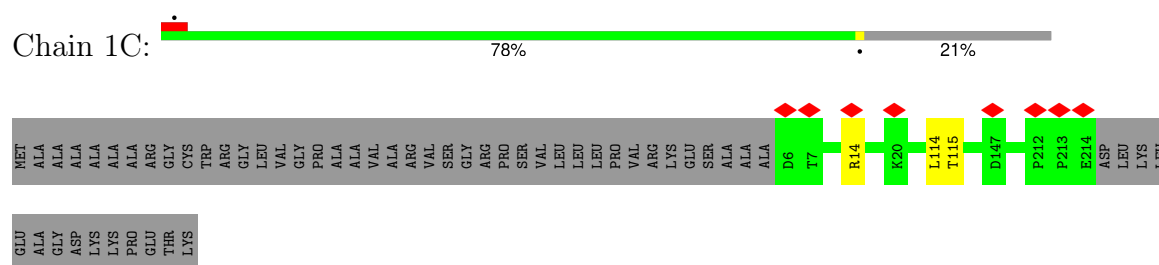
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

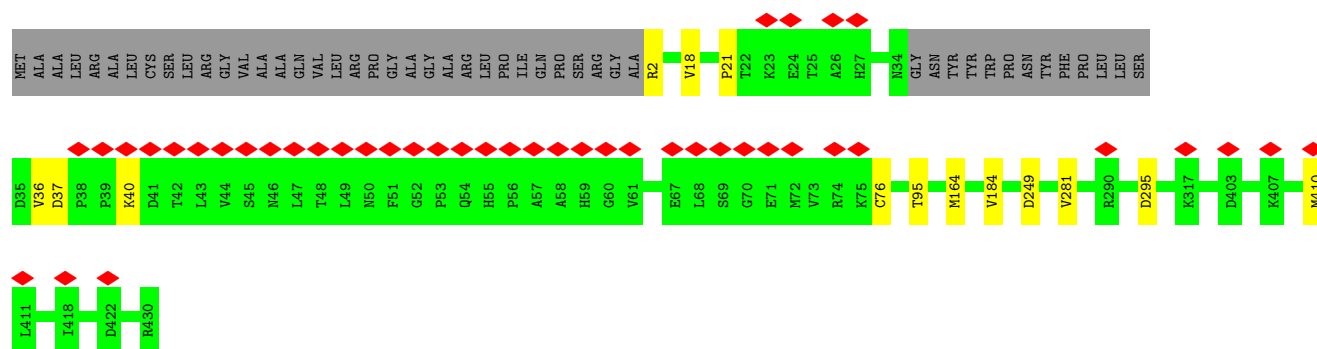


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

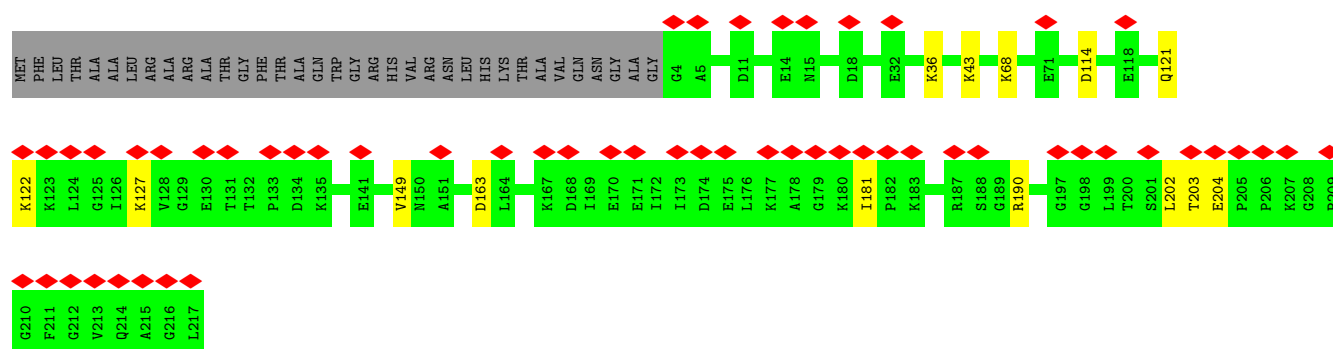
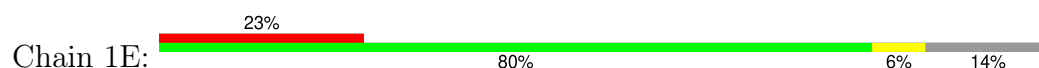


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

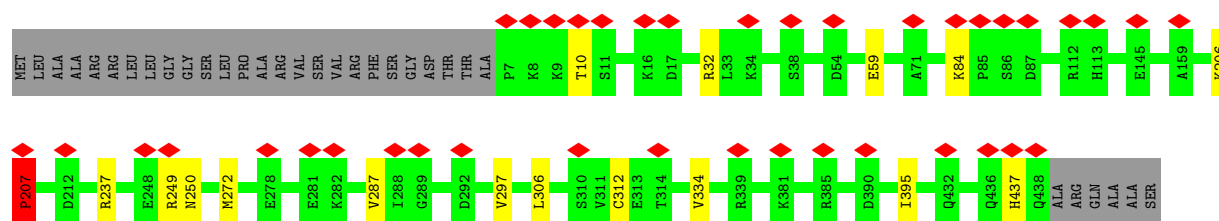
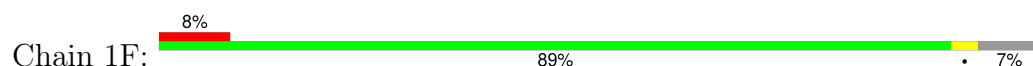




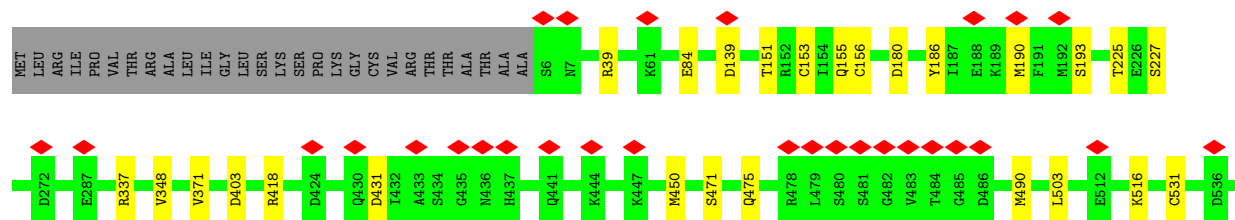
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

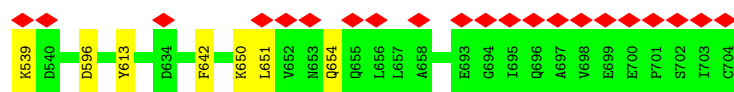


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

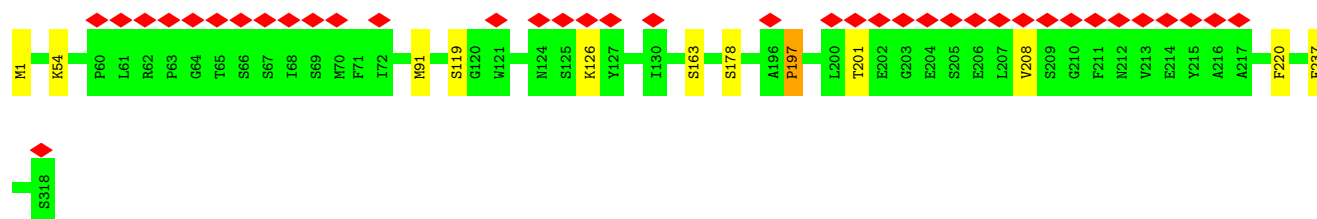


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

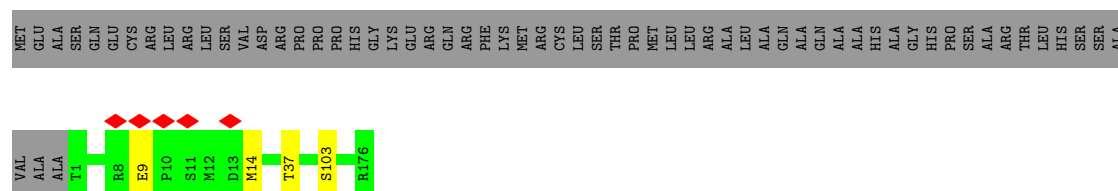




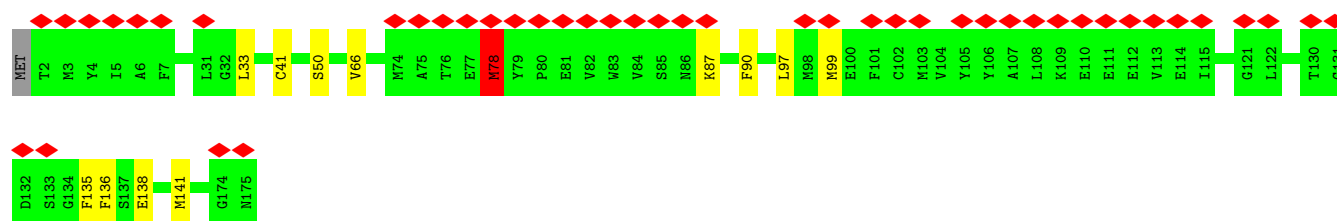
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



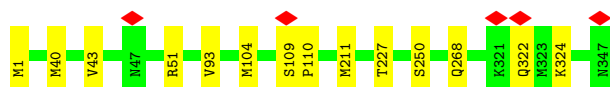
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain 1M:  97%




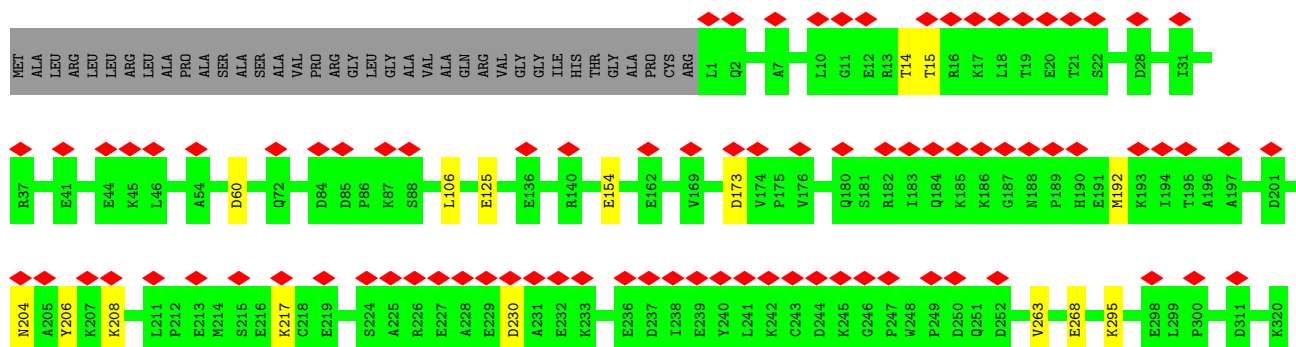
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 1N:  96%




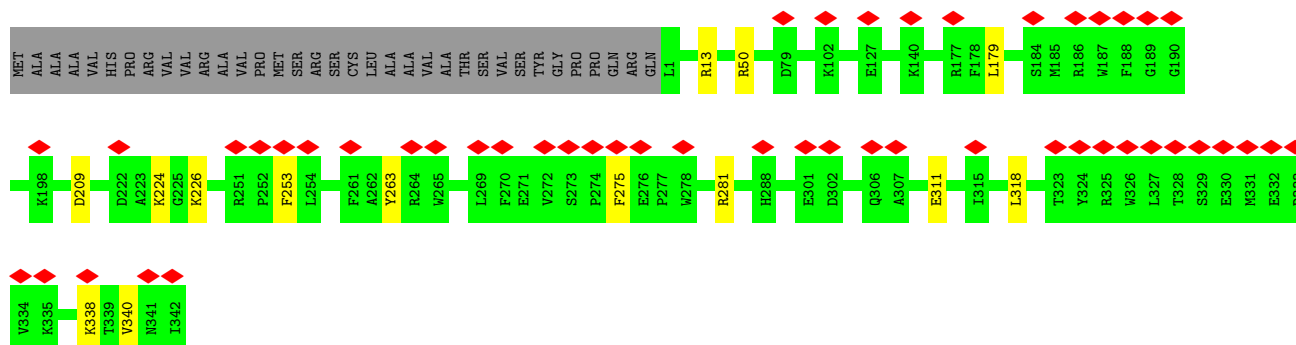
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 1O:  24% 85% 10%



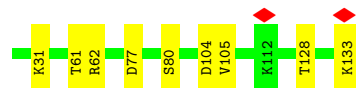
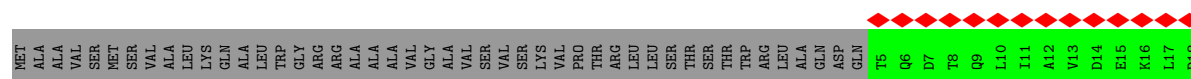
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P:  13% 87% 9%

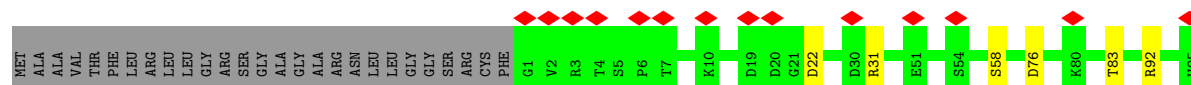
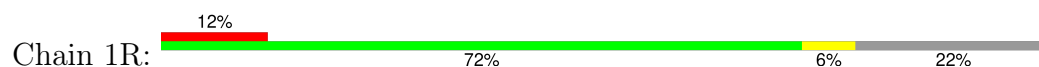


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

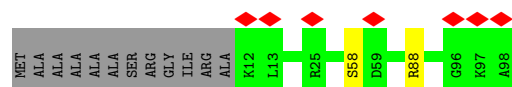
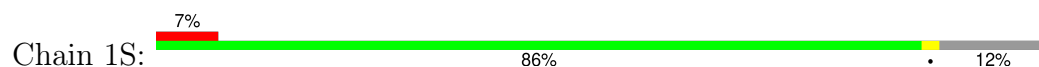
Chain 1Q:  9% 69% 5% 26%



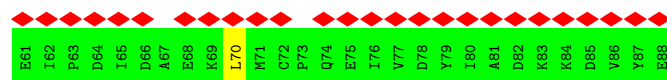
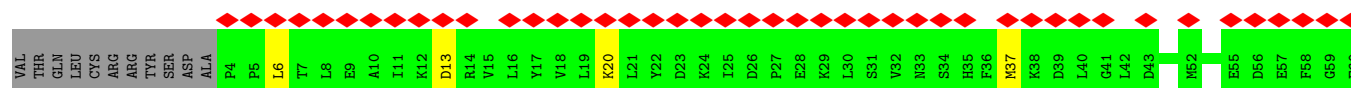
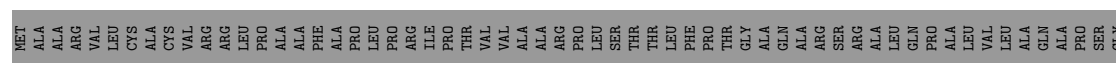
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



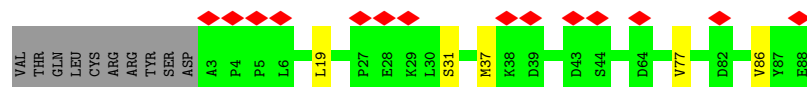
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



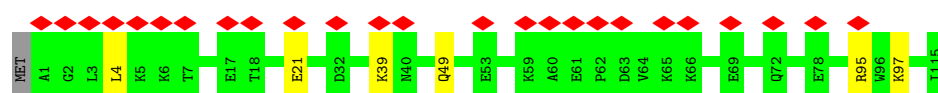
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



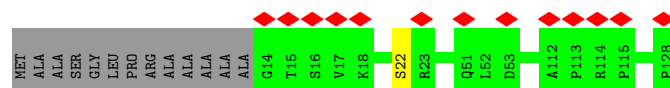
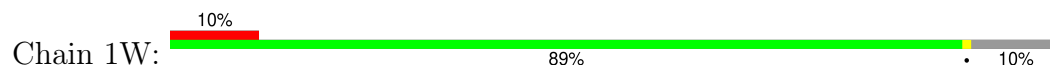
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



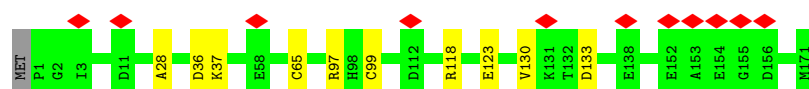
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



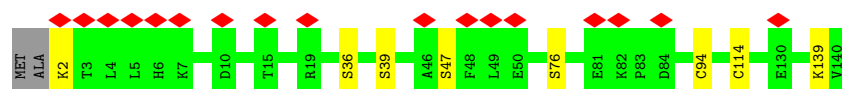
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



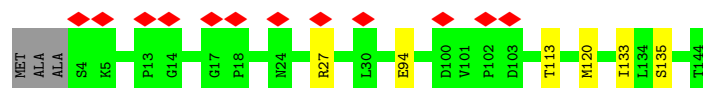
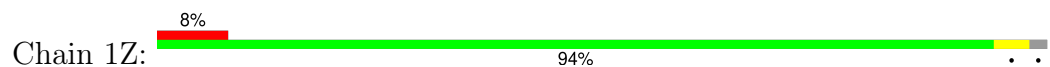
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



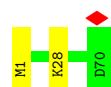
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



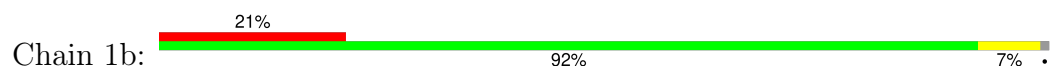
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

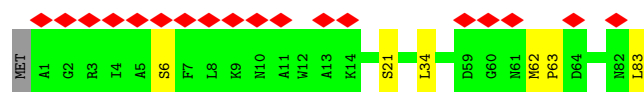


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

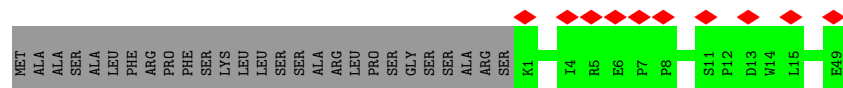


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

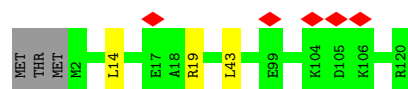




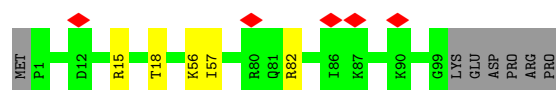
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



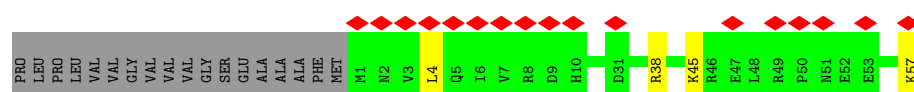
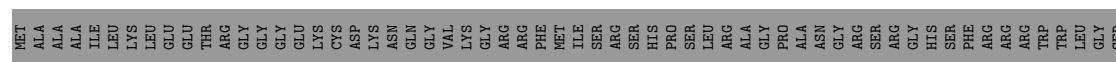
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



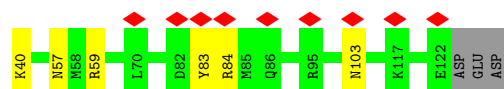
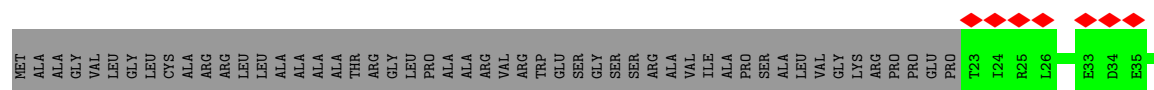
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

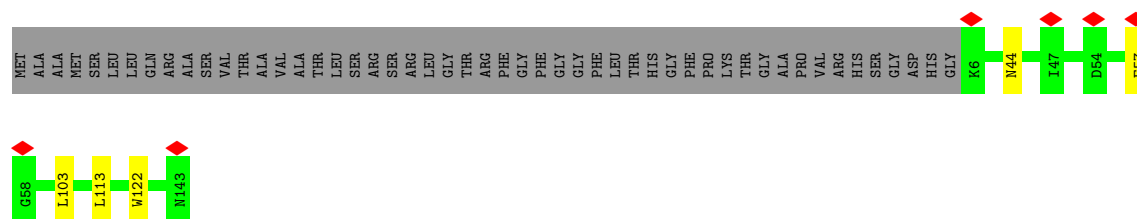


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

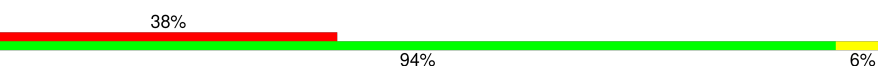


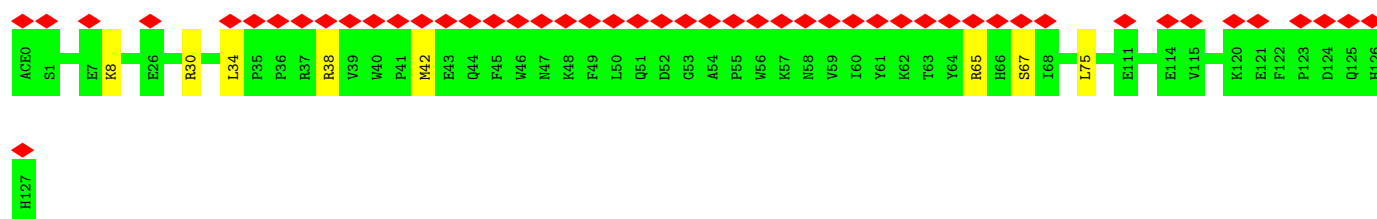
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain 1h: 



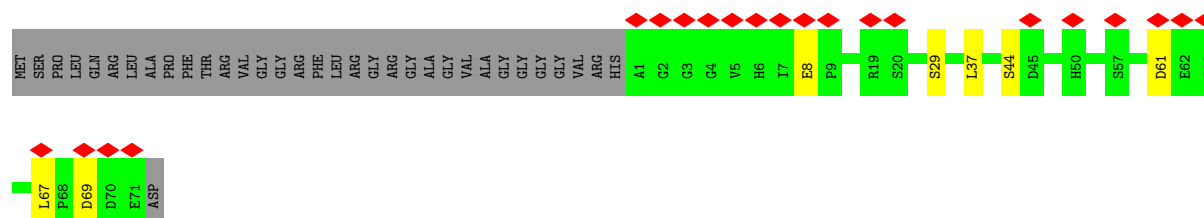
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i: 




- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j: 




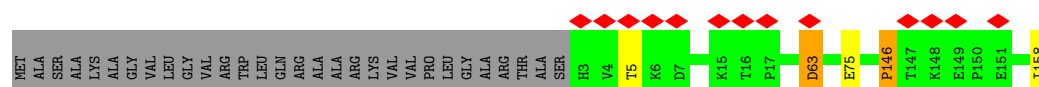
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 1k: 



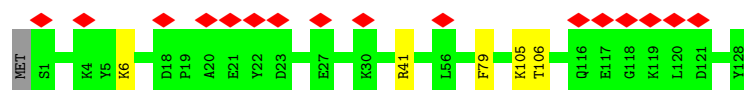
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain 1l: 



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 1m: 




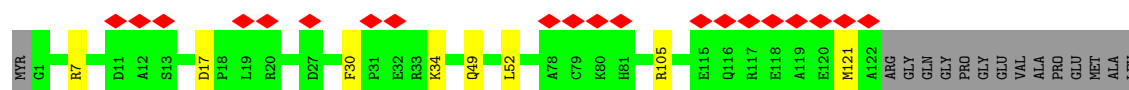
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 1n: 



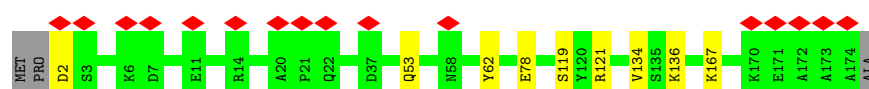
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 1o: 



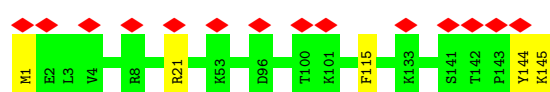
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain 1p: 




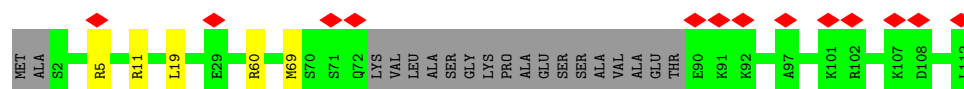
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain 1q: 



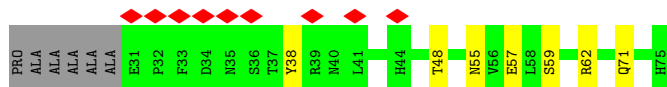
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain 1r: 

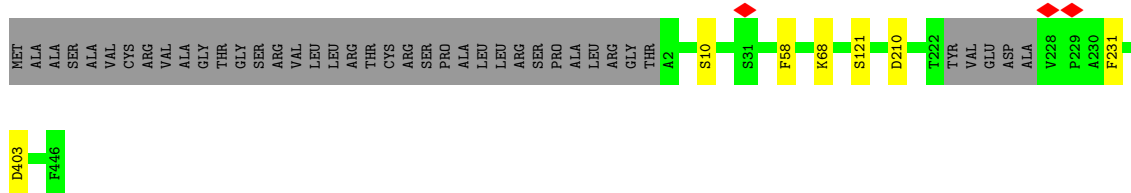


- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

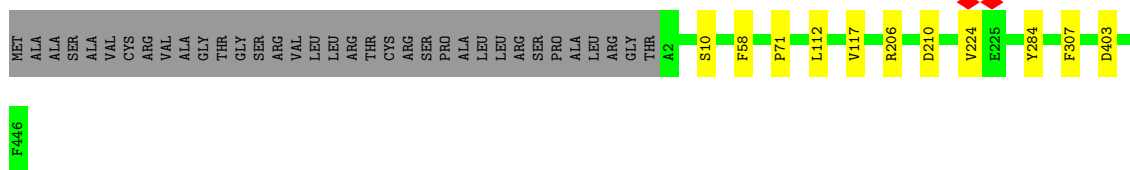
Chain 1s: 



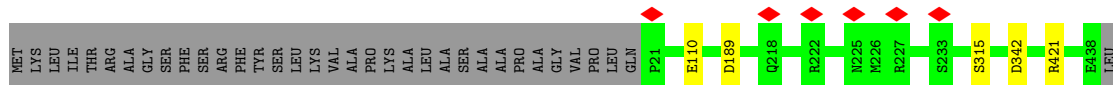
- Chain 3A: 90% 8%



- Chain 3N: 90% • 7%

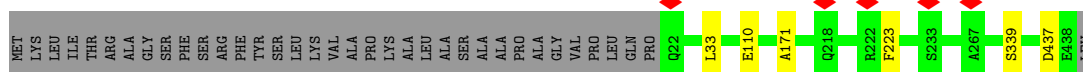


- Chain 3B:  91% • 8%



- 

Chain 3O:  91% 8%



- Molecule 47: Cytochrome b

Chain 3C:  98%



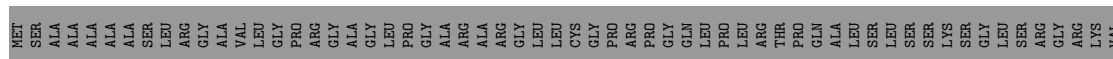
- Molecule 47: Cytochrome b

Chain 3P:  99%



- Molecule 48: Cytochrome c1, heme protein, mitochondrial

Chain 3D:  70% 27%



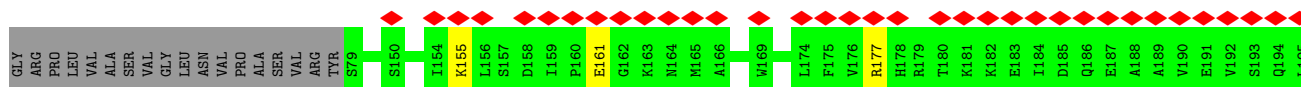
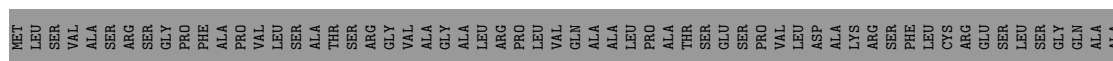
- Molecule 48: Cytochrome c1, heme protein, mitochondrial

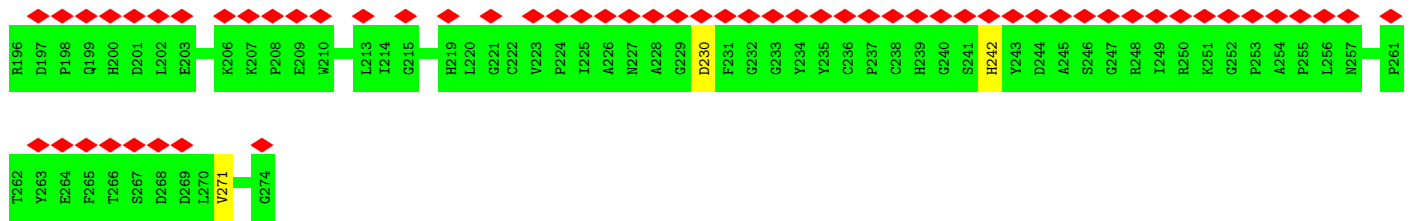
Chain 3Q:  73% 26%



- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

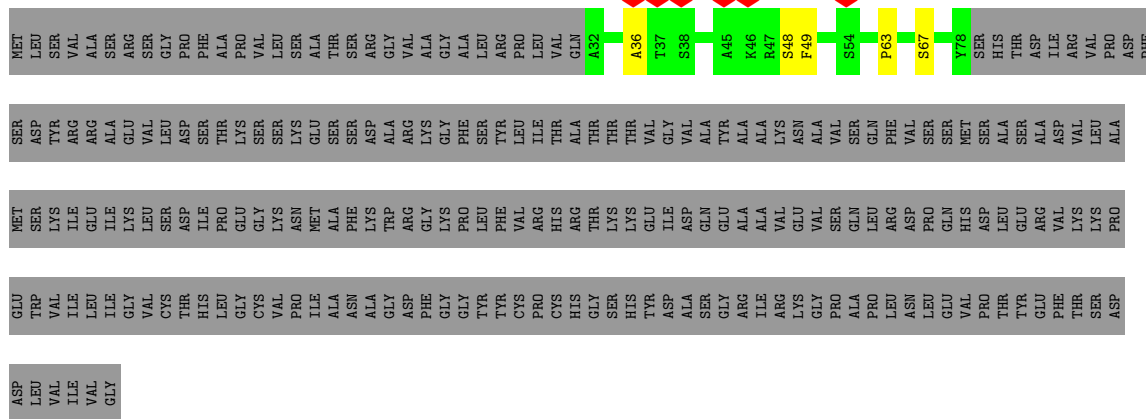
Chain 3E:  35% 69% 28%





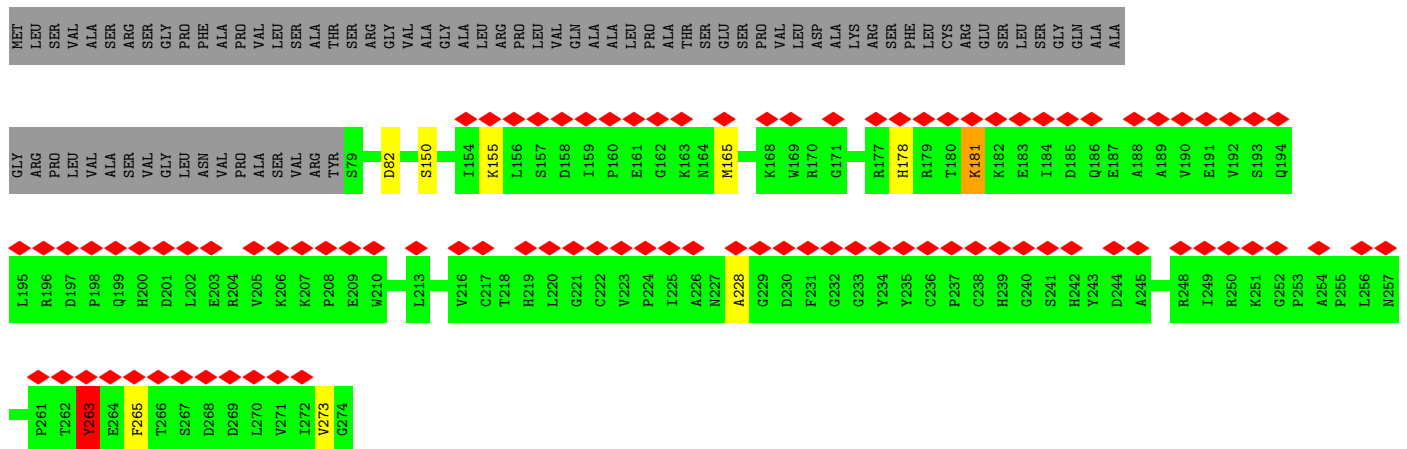
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3I: 15% 83%



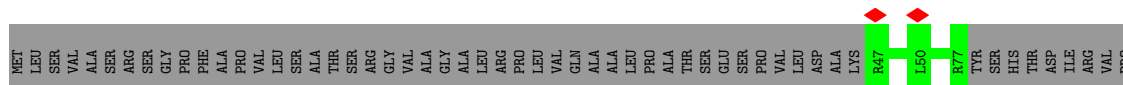
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

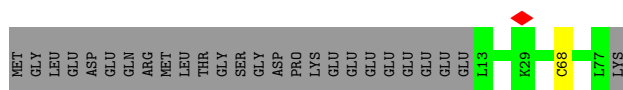
Chain 3R: 34% 68% 28%



- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3V: 11% 89%





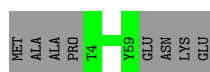
- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3J: 81% 12%



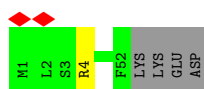
- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3W: 88% 12%



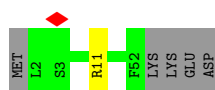
- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3X: 91% 7%



- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3Y: 89% 9%



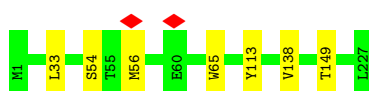
- Molecule 55: Cytochrome c oxidase subunit 1

Chain 4A: 98%



- Molecule 56: Cytochrome c oxidase subunit 2

Chain 4B: 97%




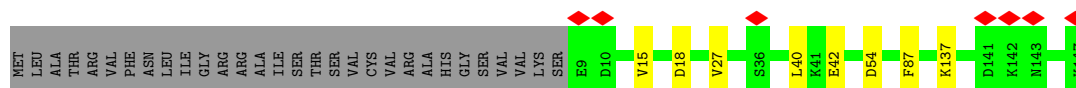
- Molecule 57: Cytochrome c oxidase subunit 3

Chain 4C:  97%



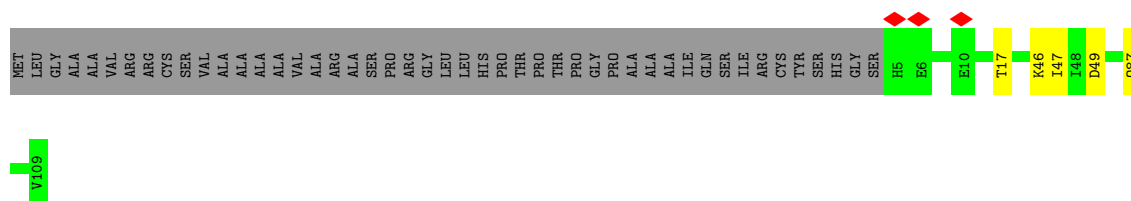
- Molecule 58: Cytochrome c oxidase subunit 4

Chain 4D:  78% 5% 18%



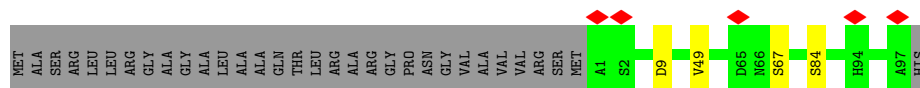
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 4E:  66% 31%



- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 4F:  72% 25%



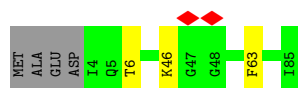
- Molecule 61: Cytochrome c oxidase subunit 6A2

Chain 4G:  8% 68% 9% 23%




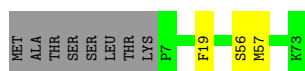
- Molecule 62: Cytochrome c oxidase subunit 6B1

Chain 4H:  92% 5%

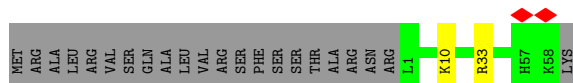


- Molecule 63: Cytochrome c oxidase subunit 6C

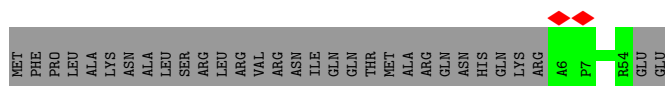
Chain 4I:  85% 11%



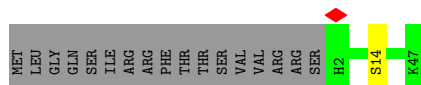
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



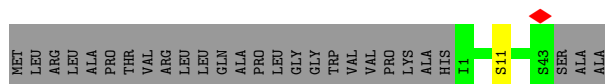
- Molecule 65: Cytochrome c oxidase subunit 7B



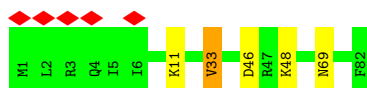
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 67: Cytochrome c oxidase subunit 8



- Molecule 68: Cytochrome c oxidase subunit NDUF4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	400000	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.632	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	370.296, 370.296, 370.296	wwPDB
Map dimensions	888, 888, 888	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.417, 0.417, 0.417	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4, AME, CU, MYR, FES, GTP, HEA, CDL, FME, PEK, HEC, NA, MG, ACE, FMN, NDP, PGV, K, 3PE, CUA, PC1, HEM, PO4, EH2, PSC

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	1A	0.25	0/930	0.49	0/1271
2	1B	0.27	0/1273	0.54	0/1722
3	1C	0.26	0/1791	0.51	0/2439
4	1D	0.36	2/3545 (0.1%)	0.65	4/4806 (0.1%)
5	1E	0.27	0/1698	0.51	1/2311 (0.0%)
6	1F	0.36	1/3401 (0.0%)	0.62	3/4595 (0.1%)
7	1G	0.26	0/5451	0.51	0/7387
8	1H	0.27	0/2566	0.54	3/3509 (0.1%)
9	1I	0.26	0/1443	0.51	0/1952
10	1J	0.28	0/1364	0.56	1/1850 (0.1%)
11	1K	0.26	0/751	0.47	0/1018
12	1L	0.27	0/4939	0.45	0/6718
13	1M	0.26	0/3713	0.47	0/5063
14	1N	0.26	0/2765	0.46	0/3758
15	1O	0.27	0/2650	0.51	0/3588
16	1P	0.26	0/2828	0.50	0/3834
17	1Q	0.26	0/1070	0.51	0/1446
18	1R	0.25	0/755	0.51	0/1018
19	1S	0.27	0/711	0.54	0/956
20	1T	0.26	0/701	0.45	0/946
20	1U	0.26	0/706	0.42	0/954
21	1V	0.25	0/946	0.43	0/1281
22	1W	0.26	0/995	0.51	0/1340
23	1X	0.27	0/1436	0.51	0/1938
24	1Y	0.41	2/1037 (0.2%)	0.55	1/1404 (0.1%)
25	1Z	0.27	0/1199	0.52	0/1617
26	1a	0.26	0/577	0.45	0/777
27	1b	1.12	3/664 (0.5%)	1.23	6/912 (0.7%)
28	1c	0.25	0/430	0.47	0/581
29	1d	0.28	0/1016	0.49	0/1374
30	1e	0.27	0/836	0.52	0/1118

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	1f	0.25	0/499	0.54	0/673
32	1g	0.27	0/858	0.53	0/1165
33	1h	0.27	0/1184	0.52	0/1603
34	1i	0.25	0/1138	0.49	0/1551
35	1j	0.24	0/627	0.46	0/858
36	1k	0.26	0/668	0.44	0/903
37	1l	0.41	1/1365 (0.1%)	0.72	4/1867 (0.2%)
38	1m	0.27	0/1092	0.54	0/1481
39	1n	0.26	0/1549	0.52	0/2098
40	1o	0.26	0/1069	0.52	0/1430
41	1p	0.26	0/1481	0.52	0/1997
42	1q	0.25	0/1253	0.50	0/1704
43	1r	0.27	0/777	0.51	0/1051
44	1s	0.27	0/394	0.51	0/533
45	3A	0.30	0/3481	0.54	0/4722
45	3N	0.31	0/3496	0.55	0/4723
46	3B	0.30	0/3190	0.52	0/4317
46	3O	0.30	0/3175	0.54	1/4292 (0.0%)
47	3C	0.60	4/3123 (0.1%)	0.74	8/4269 (0.2%)
47	3P	0.29	0/3122	0.48	0/4269
48	3D	0.83	6/1946 (0.3%)	1.00	11/2641 (0.4%)
48	3Q	0.60	3/1962 (0.2%)	0.80	4/2663 (0.2%)
49	3E	0.30	0/1551	0.56	0/2098
49	3I	0.79	2/342 (0.6%)	1.38	7/465 (1.5%)
49	3R	0.42	2/1551 (0.1%)	0.59	0/2098
49	3V	0.29	0/225	0.61	0/303
50	3F	0.32	0/888	0.55	0/1193
50	3S	0.30	0/888	0.53	0/1193
51	3G	0.32	0/649	0.57	0/878
51	3T	1.17	4/649 (0.6%)	1.38	7/878 (0.8%)
52	3H	0.32	0/539	0.67	1/724 (0.1%)
52	3U	0.43	1/539 (0.2%)	0.60	0/724
53	3J	0.51	0/476	0.65	0/641
53	3W	0.31	0/476	0.54	0/641
54	3X	0.29	0/445	0.53	0/608
54	3Y	0.29	0/437	0.54	0/598
55	4A	0.33	2/4165 (0.0%)	0.59	4/5691 (0.1%)
56	4B	0.24	0/1866	0.46	0/2544
57	4C	0.24	0/2179	0.39	0/2981
58	4D	0.25	0/1197	0.42	0/1617
59	4E	0.24	0/871	0.48	0/1182
60	4F	0.24	0/749	0.49	0/1016
61	4G	0.24	0/644	0.51	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
62	4H	0.25	0/708	0.48	0/956
63	4I	0.25	0/563	0.46	0/748
64	4J	0.24	0/466	0.42	0/631
65	4K	0.23	0/396	0.42	0/543
66	4L	0.25	0/394	0.41	0/528
67	4M	0.23	0/349	0.42	0/477
68	4N	0.25	0/680	0.44	0/921
All	All	0.35	33/116518 (0.0%)	0.57	66/158051 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	1F	0	2
8	1H	0	1
49	3R	0	2
All	All	0	5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	3D	265	PRO	CG-CD	-22.86	0.75	1.50
51	3T	74	PRO	CG-CD	-21.57	0.79	1.50
27	1b	63	PRO	CB-CG	20.89	2.54	1.50
47	3C	270	PRO	CB-CG	19.83	2.49	1.50
48	3Q	74	PRO	CG-CD	-19.53	0.86	1.50
47	3C	270	PRO	CG-CD	-17.70	0.92	1.50
27	1b	63	PRO	CG-CD	-17.12	0.94	1.50
51	3T	73	ASN	C-N	12.99	1.58	1.34
6	1F	207	PRO	CG-CD	-12.54	1.09	1.50
48	3D	265	PRO	N-CD	12.30	1.65	1.47
4	1D	21	PRO	CG-CD	-11.81	1.11	1.50
48	3D	329	PRO	CG-CD	-11.53	1.12	1.50
48	3D	265	PRO	CB-CG	11.14	2.05	1.50
49	3I	48	SER	C-N	-11.12	1.08	1.34
51	3T	74	PRO	CB-CG	10.88	2.04	1.50
37	1l	146	PRO	CG-CD	-10.52	1.16	1.50
48	3D	329	PRO	CB-CG	-10.27	0.98	1.50
55	4A	501	PRO	CG-CD	-9.75	1.18	1.50
55	4A	501	PRO	CB-CG	-9.18	1.04	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1Y	114	CYS	CB-SG	7.83	1.95	1.82
47	3C	270	PRO	N-CD	7.62	1.58	1.47
47	3C	269	LYS	C-N	7.52	1.48	1.34
27	1b	63	PRO	N-CD	7.04	1.57	1.47
4	1D	21	PRO	CB-CG	-6.96	1.15	1.50
24	1Y	94	CYS	CB-SG	-6.79	1.70	1.82
48	3Q	74	PRO	CB-CG	6.39	1.81	1.50
48	3D	265	PRO	CA-CB	-6.05	1.41	1.53
52	3U	68	CYS	CB-SG	-5.56	1.72	1.81
51	3T	74	PRO	N-CD	5.50	1.55	1.47
49	3R	263	TYR	CZ-OH	-5.45	1.28	1.37
49	3I	49	PHE	C-N	-5.38	1.21	1.34
48	3Q	74	PRO	N-CD	5.11	1.55	1.47
49	3R	263	TYR	CD1-CE1	-5.05	1.31	1.39

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	3C	270	PRO	CB-CG-CD	-25.58	6.74	106.50
27	1b	63	PRO	CB-CG-CD	-25.44	7.28	106.50
48	3Q	74	PRO	N-CD-CG	-23.27	68.30	103.20
51	3T	74	PRO	N-CD-CG	-22.38	69.62	103.20
48	3D	265	PRO	N-CD-CG	-20.79	72.01	103.20
55	4A	501	PRO	N-CD-CG	-19.90	73.36	103.20
4	1D	21	PRO	N-CD-CG	-19.68	73.68	103.20
55	4A	501	PRO	CA-CB-CG	-19.43	67.09	104.00
48	3D	329	PRO	CB-CG-CD	18.84	179.96	106.50
6	1F	207	PRO	N-CD-CG	-17.61	76.78	103.20
4	1D	21	PRO	CA-CB-CG	-17.24	71.24	104.00
48	3D	329	PRO	N-CD-CG	-15.90	79.35	103.20
51	3T	74	PRO	CA-CB-CG	-15.21	75.09	104.00
6	1F	207	PRO	CA-CB-CG	-14.99	75.52	104.00
37	1I	146	PRO	N-CD-CG	-14.82	80.97	103.20
48	3Q	74	PRO	CA-CB-CG	-14.36	76.71	104.00
49	3I	49	PHE	O-C-N	-14.23	99.93	122.70
48	3D	329	PRO	CA-CB-CG	-13.79	77.81	104.00
51	3T	74	PRO	CB-CG-CD	-13.23	54.89	106.50
47	3C	270	PRO	CA-N-CD	-12.99	93.31	111.50
27	1b	63	PRO	N-CA-CB	-12.76	87.99	103.30
48	3D	265	PRO	CA-N-CD	-12.73	93.68	111.50
51	3T	74	PRO	N-CA-CB	-12.68	88.08	103.30
27	1b	63	PRO	CA-N-CD	-12.41	94.12	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	1l	146	PRO	CA-CB-CG	-11.94	81.31	104.00
47	3C	270	PRO	N-CA-CB	-11.34	89.69	103.30
4	1D	21	PRO	CB-CG-CD	11.10	149.78	106.50
55	4A	501	PRO	CB-CG-CD	10.89	148.98	106.50
49	3I	48	SER	O-C-N	-10.70	105.58	122.70
51	3T	74	PRO	CA-N-CD	-10.44	96.89	111.50
47	3C	269	LYS	C-N-CD	10.02	149.45	128.40
48	3D	265	PRO	CA-CB-CG	-9.85	85.28	104.00
49	3I	49	PHE	CA-C-N	9.61	138.33	117.20
52	3H	77	GLU	C-N-CA	9.40	145.19	121.70
24	1Y	94	CYS	CA-CB-SG	9.36	130.84	114.00
48	3D	265	PRO	CB-CG-CD	-9.26	70.39	106.50
27	1b	62	MET	C-N-CD	9.14	147.60	128.40
47	3C	270	PRO	N-CD-CG	-9.09	89.56	103.20
27	1b	63	PRO	CA-CB-CG	-8.69	87.48	104.00
47	3C	270	PRO	CA-CB-CG	-8.57	87.72	104.00
49	3I	48	SER	C-N-CA	8.47	142.88	121.70
8	1H	197	PRO	N-CD-CG	-8.34	90.69	103.20
6	1F	207	PRO	N-CA-CB	-8.24	93.41	103.30
10	1J	78	MET	CA-CB-CG	7.97	126.85	113.30
51	3T	73	ASN	C-N-CD	7.95	145.09	128.40
49	3I	49	PHE	C-N-CA	7.90	141.45	121.70
27	1b	63	PRO	N-CD-CG	-7.82	91.47	103.20
48	3D	264	THR	N-CA-CB	-7.75	95.56	110.30
37	1l	146	PRO	N-CA-CB	-7.71	94.05	103.30
55	4A	501	PRO	CA-N-CD	-7.58	100.89	111.50
48	3D	328	PRO	C-N-CD	7.45	144.05	128.40
51	3T	73	ASN	CA-C-N	7.45	137.95	117.10
48	3Q	74	PRO	N-CA-CB	-7.27	94.58	103.30
8	1H	197	PRO	CA-CB-CG	-7.07	90.57	104.00
49	3I	48	SER	CA-C-N	7.01	132.62	117.20
8	1H	197	PRO	CA-N-CD	-6.87	101.88	111.50
48	3D	329	PRO	CA-N-CD	-6.84	101.92	111.50
37	1l	63	ASP	CB-CG-OD1	6.73	124.36	118.30
48	3D	264	THR	C-N-CD	6.53	142.12	128.40
4	1D	21	PRO	CA-N-CD	-6.17	102.86	111.50
46	3O	33	LEU	CA-CB-CG	5.90	128.87	115.30
5	1E	163	ASP	CB-CG-OD1	5.67	123.40	118.30
47	3C	269	LYS	O-C-N	-5.66	110.35	121.10
48	3Q	74	PRO	CA-N-CD	-5.59	103.67	111.50
49	3I	63	PRO	CA-N-CD	-5.56	103.72	111.50
47	3C	269	LYS	CA-C-N	5.08	131.33	117.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
6	1F	207	PRO	Peptide
8	1H	91	MET	Peptide
49	3R	263	TYR	Sidechain
49	3R	265	PHE	Sidechain

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	1A	113/115 (98%)	105 (93%)	6 (5%)	2 (2%)	7	3
2	1B	153/258 (59%)	145 (95%)	8 (5%)	0	100	100
3	1C	207/264 (78%)	204 (99%)	3 (1%)	0	100	100
4	1D	427/476 (90%)	408 (96%)	19 (4%)	0	100	100
5	1E	212/249 (85%)	198 (93%)	14 (7%)	0	100	100
6	1F	430/464 (93%)	410 (95%)	18 (4%)	2 (0%)	25	23
7	1G	697/727 (96%)	672 (96%)	22 (3%)	3 (0%)	30	29
8	1H	316/318 (99%)	297 (94%)	18 (6%)	1 (0%)	37	37
9	1I	174/239 (73%)	169 (97%)	5 (3%)	0	100	100
10	1J	172/175 (98%)	157 (91%)	13 (8%)	2 (1%)	11	7
11	1K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	1L	604/606 (100%)	572 (95%)	30 (5%)	2 (0%)	37	37
13	1M	457/459 (100%)	450 (98%)	6 (1%)	1 (0%)	44	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1N	345/347 (99%)	334 (97%)	10 (3%)	1 (0%)	37	37
15	1O	318/357 (89%)	308 (97%)	10 (3%)	0	100	100
16	1P	340/377 (90%)	324 (95%)	16 (5%)	0	100	100
17	1Q	127/175 (73%)	120 (94%)	7 (6%)	0	100	100
18	1R	94/123 (76%)	88 (94%)	6 (6%)	0	100	100
19	1S	85/99 (86%)	81 (95%)	4 (5%)	0	100	100
20	1T	83/156 (53%)	83 (100%)	0	0	100	100
20	1U	84/156 (54%)	83 (99%)	1 (1%)	0	100	100
21	1V	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
22	1W	113/128 (88%)	109 (96%)	4 (4%)	0	100	100
23	1X	169/172 (98%)	161 (95%)	7 (4%)	1 (1%)	22	19
24	1Y	137/141 (97%)	136 (99%)	1 (1%)	0	100	100
25	1Z	139/144 (96%)	138 (99%)	1 (1%)	0	100	100
26	1a	68/70 (97%)	68 (100%)	0	0	100	100
27	1b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	1c	47/76 (62%)	47 (100%)	0	0	100	100
29	1d	117/122 (96%)	116 (99%)	1 (1%)	0	100	100
30	1e	97/106 (92%)	93 (96%)	4 (4%)	0	100	100
31	1f	55/135 (41%)	51 (93%)	4 (7%)	0	100	100
32	1g	98/154 (64%)	87 (89%)	11 (11%)	0	100	100
33	1h	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
34	1i	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
35	1j	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
36	1k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	149 (97%)	5 (3%)	0	100	100
38	1m	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
39	1n	170/179 (95%)	163 (96%)	7 (4%)	0	100	100
40	1o	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
41	1p	171/176 (97%)	170 (99%)	1 (1%)	0	100	100
42	1q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	1r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	1s	43/471 (9%)	41 (95%)	2 (5%)	0	100	100
45	3A	436/480 (91%)	423 (97%)	12 (3%)	1 (0%)	44	45
45	3N	444/480 (92%)	424 (96%)	18 (4%)	2 (0%)	25	23
46	3B	414/453 (91%)	397 (96%)	17 (4%)	0	100	100
46	3O	413/453 (91%)	402 (97%)	10 (2%)	1 (0%)	44	45
47	3C	377/379 (100%)	370 (98%)	6 (2%)	1 (0%)	37	37
47	3P	377/379 (100%)	369 (98%)	8 (2%)	0	100	100
48	3D	235/325 (72%)	232 (99%)	3 (1%)	0	100	100
48	3Q	237/325 (73%)	228 (96%)	9 (4%)	0	100	100
49	3E	194/274 (71%)	169 (87%)	24 (12%)	1 (0%)	25	23
49	3I	45/274 (16%)	40 (89%)	4 (9%)	1 (2%)	5	2
49	3R	194/274 (71%)	167 (86%)	23 (12%)	4 (2%)	5	2
49	3V	29/274 (11%)	28 (97%)	1 (3%)	0	100	100
50	3F	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
50	3S	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
51	3G	72/82 (88%)	70 (97%)	2 (3%)	0	100	100
51	3T	72/82 (88%)	71 (99%)	0	1 (1%)	9	5
52	3H	63/91 (69%)	61 (97%)	1 (2%)	1 (2%)	8	4
52	3U	63/91 (69%)	62 (98%)	1 (2%)	0	100	100
53	3J	54/64 (84%)	51 (94%)	1 (2%)	2 (4%)	2	1
53	3W	54/64 (84%)	53 (98%)	1 (2%)	0	100	100
54	3X	50/56 (89%)	47 (94%)	3 (6%)	0	100	100
54	3Y	49/56 (88%)	45 (92%)	4 (8%)	0	100	100
55	4A	512/514 (100%)	500 (98%)	12 (2%)	0	100	100
56	4B	225/227 (99%)	216 (96%)	9 (4%)	0	100	100
57	4C	257/261 (98%)	249 (97%)	8 (3%)	0	100	100
58	4D	137/169 (81%)	130 (95%)	7 (5%)	0	100	100
59	4E	103/152 (68%)	99 (96%)	4 (4%)	0	100	100
60	4F	95/129 (74%)	94 (99%)	1 (1%)	0	100	100
61	4G	73/97 (75%)	69 (94%)	4 (6%)	0	100	100
62	4H	80/86 (93%)	77 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	4I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
64	4J	56/80 (70%)	55 (98%)	1 (2%)	0	100	100
65	4K	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
66	4L	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
67	4M	41/70 (59%)	41 (100%)	0	0	100	100
68	4N	80/82 (98%)	72 (90%)	7 (9%)	1 (1%)	10	6
All	All	14074/17005 (83%)	13535 (96%)	508 (4%)	31 (0%)	45	45

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	1J	66	VAL
13	1M	82	SER
23	1X	28	ALA
47	3C	270	PRO
49	3E	271	VAL
45	3N	224	VAL
49	3R	150	SER
68	4N	33	VAL
7	1G	155	GLN
8	1H	208	VAL
49	3I	36	ALA
53	3J	54	LYS
49	3R	228	ALA
49	3R	273	VAL
1	1A	52	SER
6	1F	249	ARG
6	1F	297	VAL
7	1G	186	TYR
7	1G	654	GLN
10	1J	78	MET
46	3O	171	ALA
49	3R	181	LYS
1	1A	109	LYS
12	1L	208	CYS
12	1L	601	LEU
14	1N	110	PRO
52	3H	78	ASP
53	3J	58	HIS
51	3T	74	PRO

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Mol	Chain	Res	Type
45	3A	231	PHE
45	3N	71	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	99/99 (100%)	93 (94%)	6 (6%)	15	13
2	1B	131/212 (62%)	117 (89%)	14 (11%)	5	3
3	1C	190/227 (84%)	187 (98%)	3 (2%)	58	65
4	1D	371/405 (92%)	358 (96%)	13 (4%)	31	34
5	1E	183/207 (88%)	170 (93%)	13 (7%)	12	10
6	1F	346/368 (94%)	332 (96%)	14 (4%)	27	28
7	1G	588/610 (96%)	558 (95%)	30 (5%)	20	19
8	1H	274/274 (100%)	265 (97%)	9 (3%)	33	36
9	1I	151/201 (75%)	147 (97%)	4 (3%)	41	46
10	1J	140/141 (99%)	128 (91%)	12 (9%)	8	6
11	1K	84/84 (100%)	82 (98%)	2 (2%)	44	49
12	1L	539/539 (100%)	516 (96%)	23 (4%)	25	25
13	1M	408/408 (100%)	394 (97%)	14 (3%)	32	35
14	1N	310/310 (100%)	298 (96%)	12 (4%)	27	29
15	1O	283/307 (92%)	267 (94%)	16 (6%)	17	15
16	1P	296/323 (92%)	282 (95%)	14 (5%)	22	22
17	1Q	117/152 (77%)	108 (92%)	9 (8%)	10	8
18	1R	79/97 (81%)	72 (91%)	7 (9%)	8	5
19	1S	77/82 (94%)	75 (97%)	2 (3%)	41	46
20	1T	79/133 (59%)	74 (94%)	5 (6%)	15	13
20	1U	79/133 (59%)	74 (94%)	5 (6%)	15	13
21	1V	100/101 (99%)	94 (94%)	6 (6%)	16	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	1W	107/112 (96%)	106 (99%)	1 (1%)	75	82
23	1X	153/154 (99%)	144 (94%)	9 (6%)	16	14
24	1Y	101/102 (99%)	95 (94%)	6 (6%)	16	14
25	1Z	123/124 (99%)	117 (95%)	6 (5%)	21	20
26	1a	58/58 (100%)	56 (97%)	2 (3%)	32	35
27	1b	69/70 (99%)	65 (94%)	4 (6%)	17	15
28	1c	45/66 (68%)	45 (100%)	0	100	100
29	1d	106/109 (97%)	103 (97%)	3 (3%)	38	43
30	1e	87/94 (93%)	82 (94%)	5 (6%)	17	15
31	1f	54/113 (48%)	50 (93%)	4 (7%)	11	9
32	1g	92/129 (71%)	86 (94%)	6 (6%)	14	12
33	1h	121/158 (77%)	116 (96%)	5 (4%)	26	27
34	1i	120/120 (100%)	112 (93%)	8 (7%)	13	11
35	1j	62/84 (74%)	55 (89%)	7 (11%)	4	2
36	1k	63/76 (83%)	62 (98%)	1 (2%)	58	65
37	1l	141/161 (88%)	136 (96%)	5 (4%)	31	34
38	1m	113/114 (99%)	108 (96%)	5 (4%)	24	24
39	1n	156/160 (98%)	151 (97%)	5 (3%)	34	37
40	1o	110/119 (92%)	102 (93%)	8 (7%)	11	9
41	1p	154/156 (99%)	145 (94%)	9 (6%)	17	15
42	1q	131/131 (100%)	126 (96%)	5 (4%)	28	30
43	1r	85/98 (87%)	80 (94%)	5 (6%)	16	14
44	1s	44/351 (12%)	37 (84%)	7 (16%)	2	1
45	3A	367/397 (92%)	361 (98%)	6 (2%)	58	65
45	3N	372/397 (94%)	363 (98%)	9 (2%)	44	49
46	3B	328/355 (92%)	323 (98%)	5 (2%)	60	67
46	3O	327/355 (92%)	323 (99%)	4 (1%)	67	74
47	3C	332/332 (100%)	328 (99%)	4 (1%)	67	74
47	3P	332/332 (100%)	328 (99%)	4 (1%)	67	74
48	3D	202/258 (78%)	197 (98%)	5 (2%)	42	47
48	3Q	204/258 (79%)	204 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	3E	166/225 (74%)	161 (97%)	5 (3%)	36	40
49	3I	36/225 (16%)	35 (97%)	1 (3%)	38	43
49	3R	166/225 (74%)	160 (96%)	6 (4%)	30	32
49	3V	24/225 (11%)	24 (100%)	0	100	100
50	3F	90/99 (91%)	89 (99%)	1 (1%)	70	77
50	3S	90/99 (91%)	89 (99%)	1 (1%)	70	77
51	3G	67/73 (92%)	67 (100%)	0	100	100
51	3T	67/73 (92%)	67 (100%)	0	100	100
52	3H	62/85 (73%)	62 (100%)	0	100	100
52	3U	62/85 (73%)	62 (100%)	0	100	100
53	3J	46/52 (88%)	42 (91%)	4 (9%)	8	6
53	3W	46/52 (88%)	46 (100%)	0	100	100
54	3X	42/46 (91%)	41 (98%)	1 (2%)	44	49
54	3Y	41/46 (89%)	40 (98%)	1 (2%)	44	49
55	4A	425/425 (100%)	418 (98%)	7 (2%)	58	65
56	4B	210/210 (100%)	203 (97%)	7 (3%)	33	36
57	4C	223/225 (99%)	216 (97%)	7 (3%)	35	39
58	4D	124/149 (83%)	116 (94%)	8 (6%)	14	12
59	4E	92/124 (74%)	87 (95%)	5 (5%)	18	17
60	4F	80/101 (79%)	76 (95%)	4 (5%)	20	20
61	4G	65/80 (81%)	56 (86%)	9 (14%)	3	1
62	4H	73/76 (96%)	70 (96%)	3 (4%)	26	27
63	4I	54/61 (88%)	51 (94%)	3 (6%)	17	16
64	4J	49/68 (72%)	47 (96%)	2 (4%)	26	27
65	4K	38/66 (58%)	38 (100%)	0	100	100
66	4L	39/55 (71%)	38 (97%)	1 (3%)	41	46
67	4M	37/57 (65%)	36 (97%)	1 (3%)	40	44
68	4N	70/70 (100%)	65 (93%)	5 (7%)	12	10
All	All	12267/14333 (86%)	11799 (96%)	468 (4%)	30	30

All (468) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	6	THR
1	1A	51	PHE
1	1A	55	PHE
1	1A	61	THR
1	1A	86	THR
1	1A	87	MET
2	1B	25	ARG
2	1B	32	LYS
2	1B	50	PHE
2	1B	54	CYS
2	1B	59	MET
2	1B	71	ARG
2	1B	76	PHE
2	1B	85	VAL
2	1B	91	THR
2	1B	102	LYS
2	1B	107	MET
2	1B	125	TYR
2	1B	133	VAL
2	1B	172	ARG
3	1C	14	ARG
3	1C	114	LEU
3	1C	115	THR
4	1D	2	ARG
4	1D	18	VAL
4	1D	36	VAL
4	1D	37	ASP
4	1D	40	LYS
4	1D	76	CYS
4	1D	95	THR
4	1D	164	MET
4	1D	184	VAL
4	1D	249	ASP
4	1D	281	VAL
4	1D	295	ASP
4	1D	410	MET
5	1E	36	LYS
5	1E	43	LYS
5	1E	68	LYS
5	1E	114	ASP
5	1E	121	GLN
5	1E	122	LYS
5	1E	127	LYS

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Mol	Chain	Res	Type
5	1E	149	VAL
5	1E	181	ILE
5	1E	190	ARG
5	1E	202	LEU
5	1E	203	THR
5	1E	204	GLU
6	1F	10	THR
6	1F	32	ARG
6	1F	59	GLU
6	1F	84	LYS
6	1F	207	PRO
6	1F	237	ARG
6	1F	250	ASN
6	1F	272	MET
6	1F	287	VAL
6	1F	306	LEU
6	1F	312	CYS
6	1F	334	VAL
6	1F	395	ILE
6	1F	437	HIS
7	1G	39	ARG
7	1G	84	GLU
7	1G	139	ASP
7	1G	151	THR
7	1G	153	CYS
7	1G	156	CYS
7	1G	180	ASP
7	1G	190	MET
7	1G	193	SER
7	1G	225	THR
7	1G	227	SER
7	1G	337	ARG
7	1G	348	VAL
7	1G	371	VAL
7	1G	403	ASP
7	1G	418	ARG
7	1G	431	ASP
7	1G	450	MET
7	1G	471	SER
7	1G	475	GLN
7	1G	490	MET
7	1G	503	LEU

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Mol	Chain	Res	Type
7	1G	516	LYS
7	1G	531	CYS
7	1G	539	LYS
7	1G	596	ASP
7	1G	613	TYR
7	1G	642	PHE
7	1G	650	LYS
7	1G	651	LEU
8	1H	54	LYS
8	1H	119	SER
8	1H	126	LYS
8	1H	163	SER
8	1H	178	SER
8	1H	197	PRO
8	1H	201	THR
8	1H	220	PHE
8	1H	237	PHE
9	1I	9	GLU
9	1I	14	MET
9	1I	37	THR
9	1I	103	SER
10	1J	33	LEU
10	1J	41	CYS
10	1J	50	SER
10	1J	78	MET
10	1J	87	LYS
10	1J	90	PHE
10	1J	97	LEU
10	1J	99	MET
10	1J	135	PHE
10	1J	136	PHE
10	1J	138	GLU
10	1J	141	MET
11	1K	53	PHE
11	1K	59	MET
12	1L	25	ASN
12	1L	47	SER
12	1L	77	SER
12	1L	140	LEU
12	1L	163	ASP
12	1L	206	ASN
12	1L	207	GLU

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Mol	Chain	Res	Type
12	1L	208	CYS
12	1L	336	LYS
12	1L	340	PHE
12	1L	351	ASN
12	1L	355	ASP
12	1L	364	LYS
12	1L	419	THR
12	1L	440	LEU
12	1L	491	LEU
12	1L	498	PHE
12	1L	517	SER
12	1L	526	LEU
12	1L	531	SER
12	1L	543	SER
12	1L	544	MET
12	1L	554	ASP
13	1M	57	PHE
13	1M	83	HIS
13	1M	94	LEU
13	1M	104	LEU
13	1M	116	ILE
13	1M	122	PHE
13	1M	168	GLN
13	1M	206	LYS
13	1M	220	HIS
13	1M	265	SER
13	1M	303	ILE
13	1M	305	THR
13	1M	350	THR
13	1M	365	THR
14	1N	40	MET
14	1N	43	VAL
14	1N	51	ARG
14	1N	93	VAL
14	1N	104	MET
14	1N	109	SER
14	1N	211	MET
14	1N	227	THR
14	1N	250	SER
14	1N	268	GLN
14	1N	322	GLN
14	1N	324	LYS

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Mol	Chain	Res	Type
15	1O	14	THR
15	1O	15	THR
15	1O	60	ASP
15	1O	106	LEU
15	1O	125	GLU
15	1O	154	GLU
15	1O	173	ASP
15	1O	192	MET
15	1O	204	ASN
15	1O	206	TYR
15	1O	208	LYS
15	1O	217	LYS
15	1O	230	ASP
15	1O	263	VAL
15	1O	268	GLU
15	1O	295	LYS
16	1P	13	ARG
16	1P	50	ARG
16	1P	179	LEU
16	1P	209	ASP
16	1P	224	LYS
16	1P	226	LYS
16	1P	253	PHE
16	1P	263	TYR
16	1P	275	PHE
16	1P	281	ARG
16	1P	311	GLU
16	1P	318	LEU
16	1P	338	LYS
16	1P	340	VAL
17	1Q	31	LYS
17	1Q	61	THR
17	1Q	62	ARG
17	1Q	77	ASP
17	1Q	80	SER
17	1Q	104	ASP
17	1Q	105	VAL
17	1Q	128	THR
17	1Q	133	LYS
18	1R	22	ASP
18	1R	31	ARG
18	1R	58	SER

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Mol	Chain	Res	Type
18	1R	76	ASP
18	1R	83	THR
18	1R	92	ARG
18	1R	96	HIS
19	1S	58	SER
19	1S	88	ARG
20	1T	6	LEU
20	1T	13	ASP
20	1T	20	LYS
20	1T	37	MET
20	1T	70	LEU
20	1U	19	LEU
20	1U	31	SER
20	1U	37	MET
20	1U	77	VAL
20	1U	86	VAL
21	1V	4	LEU
21	1V	21	GLU
21	1V	39	LYS
21	1V	49	GLN
21	1V	95	ARG
21	1V	97	LYS
22	1W	22	SER
23	1X	36	ASP
23	1X	37	LYS
23	1X	65	CYS
23	1X	97	ARG
23	1X	99	CYS
23	1X	118	ARG
23	1X	123	GLU
23	1X	130	VAL
23	1X	133	ASP
24	1Y	2	LYS
24	1Y	36	SER
24	1Y	39	SER
24	1Y	47	SER
24	1Y	76	SER
24	1Y	139	LYS
25	1Z	27	ARG
25	1Z	94	GLU
25	1Z	113	THR
25	1Z	120	MET

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Mol	Chain	Res	Type
25	1Z	133	ILE
25	1Z	135	SER
26	1a	1	MET
26	1a	28	LYS
27	1b	6	SER
27	1b	21	SER
27	1b	34	LEU
27	1b	83	LEU
29	1d	14	LEU
29	1d	19	ARG
29	1d	43	LEU
30	1e	15	ARG
30	1e	18	THR
30	1e	56	LYS
30	1e	57	ILE
30	1e	82	ARG
31	1f	4	LEU
31	1f	38	ARG
31	1f	45	LYS
31	1f	57	LYS
32	1g	40	LYS
32	1g	57	ASN
32	1g	59	ARG
32	1g	83	TYR
32	1g	84	ARG
32	1g	103	ASN
33	1h	44	ASN
33	1h	57	GLU
33	1h	103	LEU
33	1h	113	LEU
33	1h	122	TRP
34	1i	8	LYS
34	1i	30	ARG
34	1i	34	LEU
34	1i	38	ARG
34	1i	42	MET
34	1i	65	ARG
34	1i	67	SER
34	1i	75	LEU
35	1j	8	GLU
35	1j	29	SER
35	1j	37	LEU

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Mol	Chain	Res	Type
35	1j	44	SER
35	1j	61	ASP
35	1j	67	LEU
35	1j	69	ASP
36	1k	18	TYR
37	1l	5	THR
37	1l	63	ASP
37	1l	75	GLU
37	1l	146	PRO
37	1l	158	ILE
38	1m	6	LYS
38	1m	41	ARG
38	1m	79	PHE
38	1m	105	LYS
38	1m	106	THR
39	1n	52	ASN
39	1n	58	LYS
39	1n	84	SER
39	1n	122	GLU
39	1n	131	SER
40	1o	7	ARG
40	1o	17	ASP
40	1o	30	PHE
40	1o	34	LYS
40	1o	49	GLN
40	1o	52	LEU
40	1o	105	ARG
40	1o	121	MET
41	1p	2	ASP
41	1p	53	GLN
41	1p	62	TYR
41	1p	78	GLU
41	1p	119	SER
41	1p	121	ARG
41	1p	134	VAL
41	1p	136	LYS
41	1p	167	LYS
42	1q	1	MET
42	1q	21	ARG
42	1q	115	PHE
42	1q	144	TYR
42	1q	145	LYS

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Mol	Chain	Res	Type
43	1r	5	ARG
43	1r	11	ARG
43	1r	19	LEU
43	1r	60	ARG
43	1r	69	MET
44	1s	38	TYR
44	1s	48	THR
44	1s	55	ASN
44	1s	57	GLU
44	1s	59	SER
44	1s	62	ARG
44	1s	71	GLN
45	3A	10	SER
45	3A	58	PHE
45	3A	68	LYS
45	3A	121	SER
45	3A	210	ASP
45	3A	403	ASP
46	3B	110	GLU
46	3B	189	ASP
46	3B	315	SER
46	3B	342	ASP
46	3B	421	ARG
47	3C	80	ARG
47	3C	90	PHE
47	3C	183	PHE
47	3C	379	TRP
48	3D	109	LEU
48	3D	113	SER
48	3D	232	ARG
48	3D	249	MET
48	3D	258	LEU
49	3E	155	LYS
49	3E	161	GLU
49	3E	177	ARG
49	3E	230	ASP
49	3E	242	HIS
50	3F	118	GLU
49	3I	67	SER
53	3J	54	LYS
53	3J	56	ILE
53	3J	57	LYS

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Mol	Chain	Res	Type
53	3J	58	HIS
45	3N	10	SER
45	3N	58	PHE
45	3N	112	LEU
45	3N	117	VAL
45	3N	206	ARG
45	3N	210	ASP
45	3N	284	TYR
45	3N	307	PHE
45	3N	403	ASP
46	3O	110	GLU
46	3O	223	PHE
46	3O	339	SER
46	3O	437	ASP
47	3P	1	MET
47	3P	80	ARG
47	3P	90	PHE
47	3P	379	TRP
49	3R	82	ASP
49	3R	155	LYS
49	3R	165	MET
49	3R	178	HIS
49	3R	181	LYS
49	3R	263	TYR
50	3S	39	GLU
54	3X	4	ARG
54	3Y	11	ARG
55	4A	38	ARG
55	4A	109	PHE
55	4A	212	ASP
55	4A	238	PHE
55	4A	316	THR
55	4A	468	MET
55	4A	513	LEU
56	4B	33	LEU
56	4B	54	SER
56	4B	56	MET
56	4B	65	TRP
56	4B	113	TYR
56	4B	138	VAL
56	4B	149	THR
57	4C	41	LEU

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Mol	Chain	Res	Type
57	4C	44	SER
57	4C	129	VAL
57	4C	143	SER
57	4C	192	VAL
57	4C	214	PHE
57	4C	244	PHE
58	4D	15	VAL
58	4D	18	ASP
58	4D	27	VAL
58	4D	40	LEU
58	4D	42	GLU
58	4D	54	ASP
58	4D	87	PHE
58	4D	137	LYS
59	4E	17	THR
59	4E	46	LYS
59	4E	47	ILE
59	4E	49	ASP
59	4E	87	GLN
60	4F	9	ASP
60	4F	49	VAL
60	4F	67	SER
60	4F	84	SER
61	4G	15	THR
61	4G	18	PHE
61	4G	25	LEU
61	4G	30	LEU
61	4G	33	LEU
61	4G	37	LEU
61	4G	54	ARG
61	4G	64	ASP
61	4G	75	VAL
62	4H	6	THR
62	4H	46	LYS
62	4H	63	PHE
63	4I	19	PHE
63	4I	56	SER
63	4I	57	MET
64	4J	10	LYS
64	4J	33	ARG
66	4L	14	SER
67	4M	11	SER

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Mol	Chain	Res	Type
68	4N	11	LYS
68	4N	33	VAL
68	4N	46	ASP
68	4N	48	LYS
68	4N	69	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
6	1F	373	ASN
11	1K	83	ASN
12	1L	296	ASN
12	1L	524	ASN
13	1M	220	HIS
14	1N	322	GLN
15	1O	200	GLN
15	1O	204	ASN
29	1d	12	GLN
29	1d	46	ASN
29	1d	59	HIS
29	1d	61	GLN
29	1d	97	HIS
33	1h	44	ASN
37	1l	99	ASN
39	1n	77	GLN
40	1o	49	GLN
41	1p	130	GLN
43	1r	50	ASN
44	1s	43	HIS
45	3A	21	ASN
45	3A	207	GLN
45	3A	215	HIS
47	3C	54	HIS
53	3J	49	GLN
45	3N	9	GLN
45	3N	215	HIS
47	3P	16	ASN
47	3P	221	HIS
48	3Q	105	ASN
49	3R	219	HIS
49	3R	257	ASN
51	3T	64	GLN

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Mol	Chain	Res	Type
57	4C	243	HIS
62	4H	22	ASN
67	4M	39	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

7 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	$\# Z > 2$
56	FME	4B	1	56	8,9,10	0.95	0	8,9,11	0.91	0
8	FME	1H	1	8	8,9,10	0.55	0	8,9,11	1.04	1 (12%)
1	FME	1A	1	1	8,9,10	0.55	0	8,9,11	1.02	1 (12%)
12	FME	1L	1	12	8,9,10	0.55	0	8,9,11	0.91	1 (12%)
11	FME	1K	1	11	8,9,10	0.53	0	8,9,11	0.98	1 (12%)
14	FME	1N	1	14	8,9,10	0.56	0	8,9,11	0.96	1 (12%)
13	FME	1M	1	13	8,9,10	0.54	0	8,9,11	1.08	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	FME	4B	1	56	-	4/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
1	FME	1A	1	1	-	1/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FME	1K	1	11	-	2/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-
13	FME	1M	1	13	-	1/7/9/11	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1K	1	FME	O-C-CA	-2.67	117.91	124.77
8	1H	1	FME	O-C-CA	-2.66	117.93	124.77
13	1M	1	FME	O-C-CA	-2.65	117.94	124.77
14	1N	1	FME	O-C-CA	-2.62	118.04	124.77
1	1A	1	FME	O-C-CA	-2.46	118.44	124.77
12	1L	1	FME	O-C-CA	-2.41	118.57	124.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	1H	1	FME	O1-CN-N-CA
56	4B	1	FME	O1-CN-N-CA
56	4B	1	FME	C-CA-CB-CG
11	1K	1	FME	N-CA-CB-CG
56	4B	1	FME	N-CA-CB-CG
56	4B	1	FME	CB-CG-SD-CE
11	1K	1	FME	C-CA-CB-CG
13	1M	1	FME	C-CA-CB-CG
1	1A	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 109 ligands modelled in this entry, 7 are monoatomic - leaving 102 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	$\# Z > 2$
70	PC1	3X	101	-	28,28,53	0.37	0	34,36,61	0.64	1 (2%)
85	PGV	4K	101	-	50,50,50	0.30	0	53,56,56	0.33	0
83	HEM	3P	502	47	42,50,50	1.31	6 (14%)	46,82,82	1.80	12 (26%)
70	PC1	1m	201	-	45,45,53	0.30	0	51,53,61	1.10	3 (5%)
85	PGV	4A	601	-	50,50,50	0.27	0	53,56,56	0.32	0
73	FMN	1F	501	-	33,33,33	0.62	0	48,50,50	0.66	1 (2%)
71	SF4	1G	802	7	0,12,12	-	-	-		
72	FES	1E	301	5	0,4,4	-	-	-		
70	PC1	1Z	201	-	43,43,53	0.28	0	49,51,61	0.33	0
70	PC1	1B	202	-	45,45,53	0.28	0	51,53,61	0.33	0
69	3PE	1Y	202	-	39,39,50	0.29	0	42,44,55	0.40	0
69	3PE	3D	502	-	32,32,50	0.36	0	35,37,55	0.52	0
69	3PE	1d	201	-	47,47,50	0.29	0	50,52,55	0.44	0
85	PGV	4G	101	-	50,50,50	0.29	0	53,56,56	0.46	1 (1%)
69	3PE	1L	701	-	45,45,50	0.31	0	48,50,55	0.47	0
75	CDL	4D	201	-	99,99,99	0.27	0	105,111,111	0.38	0
75	CDL	3A	501	-	57,57,99	0.34	0	63,69,111	0.55	0
75	CDL	3G	102	-	51,51,99	0.36	0	57,63,111	0.66	1 (1%)
76	GTP	1O	401	77	29,34,34	1.00	2 (6%)	35,54,54	1.06	1 (2%)
69	3PE	1Y	203	-	29,29,50	0.34	0	32,34,55	0.71	1 (3%)
80	EHZ	1n	201	-	31,36,37	0.18	0	36,44,47	1.12	1 (2%)
75	CDL	1d	202	-	64,64,99	0.33	0	70,76,111	0.41	0
80	EHZ	1T	101	20	31,36,37	0.20	0	36,44,47	1.10	1 (2%)
69	3PE	3N	501	-	31,31,50	0.35	0	34,36,55	0.74	1 (2%)
69	3PE	1M	504	-	49,49,50	0.27	0	52,54,55	0.36	0
70	PC1	3R	303	-	44,44,53	0.30	0	50,52,61	0.42	0
85	PGV	4C	301	-	50,50,50	0.28	0	53,56,56	0.32	0
69	3PE	1L	703	-	44,44,50	0.28	0	47,49,55	0.48	0
69	3PE	3C	504	-	33,33,50	0.36	0	36,38,55	0.53	0
75	CDL	4B	302	-	99,99,99	0.27	0	105,111,111	0.31	0
69	3PE	1J	201	-	43,43,50	0.29	0	46,48,55	0.39	0
69	3PE	1j	101	-	43,43,50	0.29	0	46,48,55	0.45	0
85	PGV	4C	304	-	50,50,50	0.30	0	53,56,56	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	PGV	4L	101	-	50,50,50	0.30	0	53,56,56	0.38	0
71	SF4	1I	203	9	0,12,12	-	-	-		
75	CDL	1L	702	-	75,75,99	0.29	0	81,87,111	0.39	0
85	PGV	4M	101	-	50,50,50	0.29	0	53,56,56	0.31	0
75	CDL	1q	202	-	60,60,99	0.34	0	66,72,111	0.43	0
85	PGV	4C	302	-	50,50,50	0.30	0	53,56,56	0.68	1 (1%)
69	3PE	1Y	205	-	40,40,50	0.30	0	43,45,55	0.68	1 (2%)
75	CDL	1X	201	-	85,85,99	0.28	0	91,97,111	0.40	0
70	PC1	1h	203	-	46,46,53	0.28	0	52,54,61	0.31	0
70	PC1	1Y	201	-	34,34,53	0.33	0	40,42,61	0.43	0
69	3PE	1N	901	-	48,48,50	0.32	0	51,53,55	0.41	0
69	3PE	3A	502	-	26,26,50	0.37	0	29,31,55	0.68	1 (3%)
85	PGV	4B	301	-	50,50,50	0.28	0	53,56,56	0.34	0
71	SF4	1G	801	7	0,12,12	-	-	-		
69	3PE	3P	503	-	32,32,50	0.33	0	35,37,55	0.56	0
81	AME	1h	201	-	9,10,11	0.52	0	9,11,13	1.10	1 (11%)
71	SF4	1I	202	9	0,12,12	-	-	-		
85	PGV	4A	603	-	50,50,50	0.30	0	53,56,56	0.35	0
69	3PE	1N	903	-	32,32,50	0.33	0	35,37,55	0.44	0
69	3PE	3Y	101	-	29,29,50	0.36	0	32,34,55	0.46	0
69	3PE	3A	503	-	31,31,50	0.35	0	34,36,55	0.42	0
70	PC1	1B	203	-	47,47,53	0.28	0	53,55,61	0.45	0
69	3PE	3N	503	-	24,24,50	0.37	0	27,29,55	0.54	0
71	SF4	1B	201	2	0,12,12	-	-	-		
85	PGV	4C	303	-	50,50,50	0.29	0	53,56,56	0.33	0
85	PGV	4J	101	-	50,50,50	0.29	0	53,56,56	0.36	0
75	CDL	3N	502	-	42,42,99	0.40	0	48,54,111	0.62	0
83	HEM	3C	502	47	42,50,50	1.30	6 (14%)	46,82,82	1.72	9 (19%)
85	PGV	4C	307	-	50,50,50	0.29	0	53,56,56	0.36	0
69	3PE	1M	502	-	50,50,50	0.28	0	53,55,55	0.40	0
69	3PE	3R	302	-	46,46,50	0.29	0	49,51,55	0.34	0
82	MYR	1l	201	-	13,14,15	0.31	0	12,13,15	0.29	0
85	PGV	4A	602	-	50,50,50	0.28	0	53,56,56	0.36	0
75	CDL	4C	306	-	99,99,99	0.27	0	105,111,111	0.41	1 (0%)
72	FES	1G	803	7	0,4,4	-	-	-		
70	PC1	1A	202	-	34,34,53	0.32	0	40,42,61	0.40	0
75	CDL	1N	902	-	61,61,99	0.31	0	67,73,111	0.58	1 (1%)
69	3PE	1Y	204	-	26,26,50	0.36	0	29,31,55	0.43	0
91	PEK	4G	102	-	52,52,52	0.47	0	55,57,57	0.46	0
75	CDL	1h	202	-	79,79,99	0.30	0	85,91,111	0.45	0
71	SF4	1F	502	6	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
72	FES	3E	301	49	0,4,4	-	-	-		
70	PC1	1P	401	-	32,32,53	0.33	0	38,40,61	0.47	0
85	PGV	4C	305	-	50,50,50	0.30	0	53,56,56	0.57	1 (1%)
84	HEC	3Q	501	48	32,50,50	2.31	12 (37%)	30,82,82	2.45	6 (20%)
75	CDL	3G	103	-	55,55,99	0.35	0	61,67,111	0.48	0
69	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.34	0
92	PO4	4H	101	-	4,4,4	0.97	0	6,6,6	0.44	0
84	HEC	3D	501	48	30,49,50	2.33	12 (40%)	28,80,82	2.41	5 (17%)
70	PC1	1M	503	-	43,43,53	0.32	0	49,51,61	0.37	0
75	CDL	3T	101	-	56,56,99	0.36	0	62,68,111	0.71	2 (3%)
90	PSC	4B	304	-	51,51,51	0.48	0	57,59,59	0.44	0
72	FES	3R	301	49	0,4,4	-	-	-		
89	CUA	4B	303	56	0,1,1	-	-	-		
69	3PE	3G	101	-	28,28,50	0.35	0	31,33,55	0.44	0
75	CDL	3P	504	-	55,55,99	0.37	0	61,67,111	0.61	1 (1%)
91	PEK	4G	103	-	51,51,52	0.48	0	54,56,57	0.46	0
78	NDP	1P	402	-	47,52,52	0.66	0	61,80,80	0.92	3 (4%)
83	HEM	3C	501	47	42,50,50	1.30	6 (14%)	46,82,82	1.80	9 (19%)
70	PC1	1q	201	-	48,48,53	0.28	0	54,56,61	0.55	1 (1%)
69	3PE	1L	704	-	30,30,50	0.34	0	33,35,55	0.69	1 (3%)
86	HEA	4A	604	55	58,67,67	2.20	20 (34%)	63,103,103	2.48	25 (39%)
70	PC1	3E	302	-	46,46,53	0.28	0	52,54,61	0.39	0
83	HEM	3P	501	47	42,50,50	1.29	5 (11%)	46,82,82	1.82	9 (19%)
69	3PE	1M	501	-	44,44,50	0.29	0	47,49,55	0.37	0
69	3PE	3C	503	-	34,34,50	0.36	0	37,39,55	0.55	0
70	PC1	1I	201	-	53,53,53	0.27	0	59,61,61	0.38	0
70	PC1	1H	401	-	47,47,53	0.29	0	53,55,61	0.38	0
86	HEA	4A	605	55	58,67,67	2.20	20 (34%)	63,103,103	2.41	27 (42%)

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
70	PC1	3X	101	-	-	4/32/32/57	-
85	PGV	4K	101	-	-	14/55/55/55	-
83	HEM	3P	502	47	-	6/12/54/54	-
70	PC1	1m	201	-	-	11/49/49/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	PGV	4A	601	-	-	10/55/55/55	-
73	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
71	SF4	1G	802	7	-	-	0/6/5/5
72	FES	1E	301	5	-	-	0/1/1/1
70	PC1	1Z	201	-	-	1/47/47/57	-
70	PC1	1B	202	-	-	8/49/49/57	-
69	3PE	1Y	202	-	-	9/43/43/54	-
69	3PE	3D	502	-	-	4/36/36/54	-
69	3PE	1d	201	-	-	16/51/51/54	-
85	PGV	4G	101	-	-	8/55/55/55	-
69	3PE	1L	701	-	-	5/49/49/54	-
75	CDL	4D	201	-	-	16/110/110/110	-
75	CDL	3A	501	-	-	5/68/68/110	-
75	CDL	3G	102	-	-	10/62/62/110	-
76	GTP	1O	401	77	-	4/18/38/38	0/3/3/3
69	3PE	1Y	203	-	-	13/33/33/54	-
80	EHZ	1n	201	-	-	3/42/44/45	-
75	CDL	1d	202	-	-	22/75/75/110	-
80	EHZ	1T	101	20	-	14/42/44/45	-
69	3PE	3N	501	-	-	10/35/35/54	-
69	3PE	1M	504	-	-	5/53/53/54	-
70	PC1	3R	303	-	-	5/48/48/57	-
85	PGV	4C	301	-	-	1/55/55/55	-
69	3PE	1L	703	-	-	9/48/48/54	-
69	3PE	3C	504	-	-	9/37/37/54	-
75	CDL	4B	302	-	-	15/110/110/110	-
69	3PE	1J	201	-	-	10/47/47/54	-
69	3PE	1j	101	-	-	3/47/47/54	-
85	PGV	4C	304	-	-	15/55/55/55	-
85	PGV	4L	101	-	-	7/55/55/55	-
71	SF4	1I	203	9	-	-	0/6/5/5
75	CDL	1L	702	-	-	11/86/86/110	-
85	PGV	4M	101	-	-	8/55/55/55	-
75	CDL	1q	202	-	-	7/71/71/110	-
85	PGV	4C	302	-	-	6/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	1Y	205	-	-	15/44/44/54	-
75	CDL	1X	201	-	-	18/96/96/110	-
70	PC1	1h	203	-	-	12/50/50/57	-
70	PC1	1Y	201	-	-	8/38/38/57	-
69	3PE	1N	901	-	-	13/52/52/54	-
69	3PE	3A	502	-	-	7/30/30/54	-
85	PGV	4B	301	-	-	11/55/55/55	-
71	SF4	1G	801	7	-	-	0/6/5/5
69	3PE	3P	503	-	-	10/36/36/54	-
81	AME	1h	201	-	-	2/9/10/12	-
71	SF4	1I	202	9	-	-	0/6/5/5
85	PGV	4A	603	-	-	11/55/55/55	-
69	3PE	1N	903	-	-	3/36/36/54	-
69	3PE	3Y	101	-	-	2/33/33/54	-
69	3PE	3A	503	-	-	6/35/35/54	-
70	PC1	1B	203	-	-	12/51/51/57	-
69	3PE	3N	503	-	-	7/28/28/54	-
85	PGV	4C	303	-	-	10/55/55/55	-
71	SF4	1B	201	2	-	-	0/6/5/5
85	PGV	4J	101	-	-	10/55/55/55	-
75	CDL	3N	502	-	-	8/53/53/110	-
83	HEM	3C	502	47	-	4/12/54/54	-
85	PGV	4C	307	-	-	4/55/55/55	-
69	3PE	1M	502	-	-	10/54/54/54	-
69	3PE	3R	302	-	-	9/50/50/54	-
82	MYR	1I	201	-	-	2/12/12/13	-
85	PGV	4A	602	-	-	6/55/55/55	-
75	CDL	4C	306	-	-	24/110/110/110	-
72	FES	1G	803	7	-	-	0/1/1/1
70	PC1	1A	202	-	-	3/38/38/57	-
75	CDL	1N	902	-	-	10/71/71/110	-
69	3PE	1Y	204	-	-	5/30/30/54	-
91	PEK	4G	102	-	-	10/56/56/56	-
75	CDL	1h	202	-	-	10/90/90/110	-
71	SF4	1F	502	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	FES	3E	301	49	-	-	0/1/1/1
70	PC1	1P	401	-	-	10/36/36/57	-
85	PGV	4C	305	-	-	16/55/55/55	-
84	HEC	3Q	501	48	-	4/10/54/54	-
75	CDL	3G	103	-	-	11/66/66/110	-
69	3PE	1A	201	-	-	9/50/50/54	-
84	HEC	3D	501	48	-	3/9/53/54	-
70	PC1	1M	503	-	-	8/47/47/57	-
75	CDL	3T	101	-	-	13/67/67/110	-
90	PSC	4B	304	-	-	17/55/55/55	-
72	FES	3R	301	49	-	-	0/1/1/1
69	3PE	3G	101	-	-	10/32/32/54	-
75	CDL	3P	504	-	-	13/66/66/110	-
91	PEK	4G	103	-	-	9/55/55/56	-
78	NDP	1P	402	-	-	2/30/77/77	0/5/5/5
83	HEM	3C	501	47	-	5/12/54/54	-
70	PC1	1q	201	-	-	7/52/52/57	-
69	3PE	1L	704	-	-	8/34/34/54	-
86	HEA	4A	604	55	-	8/32/76/76	-
70	PC1	3E	302	-	-	2/50/50/57	-
83	HEM	3P	501	47	-	6/12/54/54	-
69	3PE	1M	501	-	-	7/48/48/54	-
69	3PE	3C	503	-	-	11/38/38/54	-
70	PC1	1I	201	-	-	9/57/57/57	-
70	PC1	1H	401	-	-	13/51/51/57	-
86	HEA	4A	605	55	-	7/32/76/76	-

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	3Q	501	HEC	C3C-C2C	6.60	1.48	1.40
84	3Q	501	HEC	C2B-C3B	6.45	1.48	1.40
84	3D	501	HEC	C3C-C2C	6.42	1.47	1.40
84	3D	501	HEC	C2B-C3B	6.23	1.47	1.40
86	4A	604	HEA	C3B-C2B	5.48	1.47	1.34
86	4A	605	HEA	C3B-C2B	5.46	1.47	1.34
86	4A	604	HEA	C3A-C2A	5.43	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	4A	605	HEA	C3A-C2A	5.39	1.47	1.40
86	4A	605	HEA	CHD-C1D	5.25	1.47	1.34
86	4A	604	HEA	CHD-C1D	5.24	1.47	1.34
86	4A	605	HEA	CHC-C4B	5.19	1.47	1.34
86	4A	604	HEA	CHC-C4B	5.12	1.47	1.34
86	4A	605	HEA	C3D-C2D	4.96	1.47	1.36
86	4A	605	HEA	C3A-C4A	4.94	1.48	1.41
86	4A	604	HEA	C3A-C4A	4.94	1.48	1.41
86	4A	605	HEA	C3C-C2C	4.87	1.47	1.40
86	4A	604	HEA	C3D-C2D	4.82	1.47	1.36
86	4A	604	HEA	C3C-C2C	4.73	1.46	1.40
83	3P	502	HEM	C1B-NB	-3.36	1.34	1.40
83	3C	502	HEM	C1B-NB	-3.30	1.34	1.40
83	3P	502	HEM	C4D-ND	-3.28	1.34	1.40
84	3D	501	HEC	C3D-C2D	3.27	1.47	1.37
84	3Q	501	HEC	C3D-C2D	3.26	1.47	1.37
83	3C	501	HEM	C1B-NB	-3.21	1.34	1.40
84	3D	501	HEC	C2A-C3A	3.20	1.47	1.37
83	3C	502	HEM	C4D-ND	-3.16	1.34	1.40
83	3P	501	HEM	C4D-ND	-3.16	1.34	1.40
83	3C	501	HEM	C4D-ND	-3.14	1.34	1.40
84	3Q	501	HEC	C2A-C3A	3.13	1.47	1.37
83	3P	501	HEM	C1B-NB	-3.12	1.34	1.40
84	3Q	501	HEC	C3C-C4C	3.11	1.48	1.43
84	3D	501	HEC	C3C-C4C	3.07	1.48	1.43
84	3D	501	HEC	C4B-C3B	3.05	1.48	1.43
84	3Q	501	HEC	C4B-C3B	3.01	1.48	1.43
86	4A	604	HEA	C2A-C1A	2.89	1.49	1.42
86	4A	605	HEA	C2A-C1A	2.87	1.48	1.42
86	4A	604	HEA	C4B-C3B	2.74	1.49	1.44
86	4A	605	HEA	C4B-C3B	2.74	1.49	1.44
76	1O	401	GTP	C5-C6	-2.71	1.42	1.47
84	3Q	501	HEC	C3A-C4A	2.68	1.48	1.42
84	3D	501	HEC	C3A-C4A	2.67	1.48	1.42
86	4A	604	HEA	C1D-ND	-2.64	1.35	1.40
84	3D	501	HEC	C2A-C1A	2.62	1.48	1.42
84	3Q	501	HEC	C2A-C1A	2.61	1.48	1.42
86	4A	604	HEA	FE-ND	2.58	2.12	1.98
86	4A	604	HEA	C4B-NB	-2.57	1.35	1.40
86	4A	605	HEA	C1D-ND	-2.56	1.35	1.40
84	3Q	501	HEC	C1D-CHD	2.56	1.48	1.41
86	4A	605	HEA	FE-NB	2.54	2.12	1.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	4A	605	HEA	FE-ND	2.53	2.12	1.98
86	4A	604	HEA	FE-NB	2.51	2.12	1.98
84	3D	501	HEC	C1D-CHD	2.48	1.47	1.41
83	3P	501	HEM	FE-NB	2.48	2.11	1.98
86	4A	604	HEA	C4D-C3D	2.48	1.49	1.45
84	3D	501	HEC	C4D-CHA	2.47	1.47	1.41
83	3C	501	HEM	CHB-C1B	2.45	1.40	1.34
83	3P	501	HEM	CHB-C1B	2.44	1.40	1.34
83	3C	501	HEM	FE-NB	2.43	2.11	1.98
86	4A	605	HEA	C4B-NB	-2.43	1.36	1.40
83	3C	502	HEM	FE-NB	2.39	2.11	1.98
84	3Q	501	HEC	C1C-CHC	2.39	1.47	1.41
84	3Q	501	HEC	C4D-CHA	2.38	1.47	1.41
86	4A	605	HEA	C1D-C2D	2.33	1.49	1.44
86	4A	605	HEA	C4C-CHD	2.31	1.47	1.41
84	3D	501	HEC	C1C-CHC	2.30	1.47	1.41
86	4A	604	HEA	C4C-CHD	2.29	1.47	1.41
83	3P	502	HEM	C4B-NB	-2.27	1.34	1.38
83	3P	502	HEM	FE-NB	2.27	2.10	1.98
86	4A	605	HEA	C1C-CHC	2.24	1.47	1.41
83	3C	502	HEM	CHB-C1B	2.24	1.40	1.34
84	3D	501	HEC	C1B-CHB	2.19	1.47	1.41
86	4A	604	HEA	C1C-CHC	2.19	1.47	1.41
83	3C	501	HEM	C1D-ND	-2.19	1.34	1.38
84	3Q	501	HEC	C1B-CHB	2.18	1.47	1.41
83	3C	502	HEM	C1D-ND	-2.18	1.34	1.38
83	3C	501	HEM	C4B-NB	-2.15	1.34	1.38
86	4A	604	HEA	C1D-C2D	2.15	1.48	1.44
83	3P	502	HEM	C1D-ND	-2.13	1.34	1.38
83	3P	502	HEM	CHB-C1B	2.13	1.39	1.34
76	1O	401	GTP	C8-N7	-2.12	1.31	1.34
86	4A	604	HEA	CHA-C4D	2.11	1.46	1.40
83	3C	502	HEM	C4B-NB	-2.09	1.34	1.38
86	4A	604	HEA	CHB-C1B	2.08	1.46	1.40
83	3P	501	HEM	C1D-ND	-2.07	1.34	1.38
86	4A	604	HEA	C1B-C2B	2.06	1.48	1.44
86	4A	605	HEA	CHB-C1B	2.05	1.46	1.40
86	4A	605	HEA	C1B-C2B	2.05	1.48	1.44
86	4A	605	HEA	CHA-C4D	2.04	1.46	1.40
86	4A	605	HEA	C4D-C3D	2.01	1.48	1.45

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	4A	605	HEA	C3D-C4D-ND	6.71	116.84	110.35
86	4A	604	HEA	C3D-C4D-ND	6.51	116.64	110.35
84	3Q	501	HEC	C1D-C2D-C3D	-6.38	102.56	107.00
84	3D	501	HEC	C1D-C2D-C3D	-6.22	102.67	107.00
80	1n	201	EHZ	C10-S1-C9	6.21	120.20	101.84
70	1m	201	PC1	O21-C21-C22	5.92	124.29	111.48
80	1T	101	EHZ	C10-S1-C9	5.91	119.31	101.84
84	3Q	501	HEC	CMC-C2C-C3C	5.82	132.66	125.82
86	4A	605	HEA	C2B-C1B-NB	5.80	116.61	109.90
84	3D	501	HEC	CMC-C2C-C3C	5.78	132.61	125.82
86	4A	604	HEA	C2B-C1B-NB	5.71	116.50	109.90
84	3D	501	HEC	CMB-C2B-C3B	5.64	132.46	125.82
86	4A	604	HEA	C3B-C4B-NB	5.64	116.32	109.84
86	4A	605	HEA	C3B-C4B-NB	5.57	116.24	109.84
84	3Q	501	HEC	CMB-C2B-C3B	5.56	132.35	125.82
86	4A	605	HEA	C2D-C1D-ND	5.54	116.21	109.84
83	3C	501	HEM	CHC-C4B-NB	5.46	130.31	124.44
86	4A	604	HEA	C2D-C1D-ND	5.43	116.08	109.84
83	3P	501	HEM	CHC-C4B-NB	5.21	130.04	124.44
86	4A	604	HEA	CBA-CAA-C2A	-4.71	104.79	112.55
83	3P	502	HEM	CHC-C4B-NB	4.69	129.49	124.44
83	3P	501	HEM	CHD-C1D-ND	4.57	129.35	124.44
83	3C	501	HEM	CHD-C1D-ND	4.57	129.35	124.44
83	3C	502	HEM	CHC-C4B-NB	4.56	129.34	124.44
78	1P	402	NDP	P2B-O2B-C2B	-4.47	111.48	123.43
76	1O	401	GTP	C4'-O4'-C1'	-4.47	105.83	109.92
86	4A	605	HEA	C1D-C2D-C3D	-4.31	102.45	106.98
83	3C	502	HEM	CHD-C1D-ND	4.29	129.05	124.44
84	3Q	501	HEC	CAA-CBA-CGA	-4.25	102.37	113.83
83	3P	502	HEM	CHD-C1D-ND	4.21	128.96	124.44
84	3D	501	HEC	CAA-CBA-CGA	-4.17	102.59	113.83
83	3P	501	HEM	CBA-CAA-C2A	-4.11	105.62	112.54
86	4A	604	HEA	CHA-C4D-ND	-4.06	120.06	124.44
83	3P	502	HEM	CHA-C4D-ND	4.03	129.37	124.37
86	4A	605	HEA	C3C-C4C-NC	3.86	114.20	109.21
86	4A	604	HEA	C3C-C4C-NC	3.84	114.18	109.21
86	4A	604	HEA	C1D-C2D-C3D	-3.83	102.95	106.98
86	4A	605	HEA	CBA-CAA-C2A	-3.78	106.32	112.55
86	4A	604	HEA	C13-C14-C15	-3.62	119.35	127.62
86	4A	605	HEA	C1B-C2B-C3B	-3.59	102.64	106.80
84	3Q	501	HEC	CBD-CAD-C3D	-3.58	106.52	112.54
83	3P	502	HEM	CHB-C1B-NB	3.51	128.73	124.37
86	4A	604	HEA	C1B-C2B-C3B	-3.51	102.73	106.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	4A	604	HEA	CAD-C3D-C4D	3.48	130.76	124.70
83	3P	502	HEM	C1B-NB-C4B	3.46	109.31	105.21
86	4A	604	HEA	C4D-C3D-C2D	-3.42	101.91	106.89
83	3C	502	HEM	CHA-C4D-ND	3.41	128.60	124.37
83	3C	502	HEM	C1B-NB-C4B	3.32	109.14	105.21
83	3C	502	HEM	CHB-C1B-NB	3.32	128.49	124.37
85	4C	302	PGV	O01-C1-C2	3.28	118.58	111.48
83	3C	501	HEM	CHA-C4D-ND	3.25	128.40	124.37
75	1N	902	CDL	OB6-CB5-C51	3.22	116.82	111.09
86	4A	604	HEA	C4B-C3B-C2B	-3.22	102.03	107.44
86	4A	605	HEA	C4D-C3D-C2D	-3.18	102.27	106.89
69	1Y	205	3PE	O21-C21-C22	3.16	118.31	111.48
83	3C	501	HEM	C1B-NB-C4B	3.12	108.91	105.21
86	4A	605	HEA	C4B-C3B-C2B	-3.09	102.25	107.44
83	3P	501	HEM	C1B-NB-C4B	3.05	108.82	105.21
83	3P	501	HEM	CHA-C4D-ND	3.05	128.15	124.37
81	1h	201	AME	O-C-CA	-3.05	116.94	124.77
83	3P	501	HEM	CHD-C1D-C2D	-3.00	120.29	125.03
83	3C	501	HEM	CHD-C1D-C2D	-2.97	120.34	125.03
86	4A	604	HEA	C13-C12-C11	-2.96	109.67	114.39
83	3P	501	HEM	CHB-C1B-NB	2.92	127.99	124.37
86	4A	604	HEA	CMC-C2C-C3C	2.90	130.48	124.68
69	1Y	203	3PE	O21-C21-C22	2.88	117.72	111.48
83	3C	501	HEM	CHB-C1B-NB	2.87	127.93	124.37
86	4A	605	HEA	CMC-C2C-C3C	2.85	130.38	124.68
86	4A	605	HEA	C13-C14-C15	-2.85	121.11	127.62
78	1P	402	NDP	O4D-C1D-C2D	-2.80	100.61	106.62
70	1m	201	PC1	O21-C21-O22	-2.79	117.19	123.70
83	3C	502	HEM	C3B-C4B-NB	-2.78	107.47	109.47
86	4A	605	HEA	C26-C15-C16	2.74	119.98	115.23
86	4A	605	HEA	C13-C12-C11	-2.72	110.04	114.39
86	4A	604	HEA	C17-C18-C19	-2.71	121.42	127.62
83	3P	502	HEM	C3B-C4B-NB	-2.70	107.53	109.47
83	3C	502	HEM	CHD-C1D-C2D	-2.68	120.80	125.03
86	4A	605	HEA	C27-C19-C20	2.67	119.86	115.23
86	4A	605	HEA	C17-C18-C19	-2.67	121.52	127.62
85	4C	305	PGV	O01-C1-C2	2.66	117.24	111.48
86	4A	604	HEA	CHB-C1B-NB	-2.66	121.58	124.44
70	1q	201	PC1	O21-C21-C22	2.65	117.22	111.48
69	1L	704	3PE	O21-C21-C22	2.63	117.17	111.48
86	4A	605	HEA	CHA-C4D-ND	-2.63	121.61	124.44
86	4A	604	HEA	C26-C15-C16	2.62	119.78	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	4A	605	HEA	CHB-C1B-NB	-2.61	121.63	124.44
86	4A	604	HEA	C27-C19-C20	2.56	119.67	115.23
86	4A	605	HEA	C1D-ND-C4D	-2.50	102.24	105.21
83	3C	501	HEM	CBA-CAA-C2A	-2.50	108.33	112.54
86	4A	605	HEA	C4B-NB-C1B	-2.48	102.27	105.21
70	1m	201	PC1	C2-O21-C21	2.46	123.69	117.80
86	4A	604	HEA	CMD-C2D-C1D	2.41	128.81	125.03
83	3P	502	HEM	CHA-C4D-C3D	-2.37	120.85	125.23
86	4A	604	HEA	C1D-ND-C4D	-2.37	102.41	105.21
86	4A	604	HEA	C4B-NB-C1B	-2.36	102.41	105.21
75	3G	102	CDL	OA6-CA4-CA3	2.35	116.79	108.34
86	4A	605	HEA	CMB-C2B-C1B	2.35	128.71	125.03
86	4A	605	HEA	C25-C23-C24	2.31	119.90	114.59
70	3X	101	PC1	O21-C21-C22	2.28	116.41	111.48
83	3P	502	HEM	C4D-ND-C1D	2.27	107.90	105.21
83	3P	502	HEM	O2D-CGD-CBD	2.27	121.17	114.00
86	4A	605	HEA	CMD-C2D-C1D	2.26	128.57	125.03
84	3D	501	HEC	CMA-C3A-C2A	2.26	129.20	124.94
69	3N	501	3PE	O21-C2-C1	2.26	116.44	108.34
78	1P	402	NDP	C5A-C6A-N6A	2.25	123.75	120.31
86	4A	604	HEA	C25-C23-C24	2.24	119.75	114.59
83	3P	502	HEM	CHD-C1D-C2D	-2.22	121.53	125.03
86	4A	605	HEA	CHA-C4D-C3D	-2.21	121.55	124.77
86	4A	604	HEA	CMB-C2B-C1B	2.20	128.47	125.03
83	3C	502	HEM	O2A-CGA-CBA	2.20	120.94	114.00
86	4A	604	HEA	CHD-C1D-C2D	-2.19	120.73	126.94
85	4G	101	PGV	O01-C1-C2	2.17	116.18	111.48
86	4A	605	HEA	CHD-C1D-C2D	-2.15	120.87	126.94
69	3A	502	3PE	O21-C21-C22	2.14	116.12	111.48
84	3Q	501	HEC	CMA-C3A-C2A	2.11	128.92	124.94
75	3T	101	CDL	OA8-CA6-CA4	2.09	114.42	108.40
75	3T	101	CDL	OA6-CA4-CA3	2.08	115.82	108.34
73	1F	501	FMN	C4-N3-C2	-2.08	121.95	125.64
83	3P	502	HEM	CHB-C1B-C2B	-2.08	121.05	126.94
75	3P	504	CDL	OB6-CB4-CB6	-2.08	100.88	108.34
86	4A	605	HEA	CHB-C1B-C2B	-2.07	121.76	125.03
83	3P	502	HEM	O2A-CGA-CBA	2.06	120.50	114.00
75	4C	306	CDL	OB6-CB5-C51	2.05	115.92	111.48
83	3C	502	HEM	CHB-C1B-C2B	-2.04	121.17	126.94
83	3P	501	HEM	O2A-CGA-CBA	2.04	120.43	114.00
83	3C	501	HEM	O2A-CGA-CBA	2.03	120.42	114.00
83	3P	501	HEM	CAD-C3D-C4D	2.02	128.22	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	4A	605	HEA	C21-C22-C23	-2.01	120.92	127.64
83	3C	501	HEM	CMC-C2C-C3C	2.01	128.70	124.68

There are no chirality outliers.

All (775) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1A	201	3PE	C1-O11-P-O13
69	1A	201	3PE	C1-O11-P-O14
69	1J	201	3PE	C1-O11-P-O13
69	1J	201	3PE	C1-O11-P-O14
69	1J	201	3PE	C11-O13-P-O12
69	1J	201	3PE	C12-C11-O13-P
69	1L	701	3PE	O32-C31-O31-C3
69	1L	701	3PE	C32-C31-O31-C3
69	1L	704	3PE	O22-C21-O21-C2
69	1L	704	3PE	C22-C21-O21-C2
69	1M	501	3PE	C1-O11-P-O14
69	1M	502	3PE	C2-C1-O11-P
69	1N	901	3PE	C11-O13-P-O14
69	1N	903	3PE	O21-C2-C3-O31
69	1Y	202	3PE	C1-O11-P-O12
69	1Y	202	3PE	C1-O11-P-O13
69	1Y	202	3PE	C2-C1-O11-P
69	1Y	203	3PE	O22-C21-O21-C2
69	1Y	203	3PE	C22-C21-O21-C2
69	1Y	204	3PE	C11-O13-P-O14
69	1Y	204	3PE	C12-C11-O13-P
69	1Y	204	3PE	O32-C31-O31-C3
69	1Y	204	3PE	C32-C31-O31-C3
69	1Y	205	3PE	C1-O11-P-O13
69	1Y	205	3PE	C11-O13-P-O11
69	1Y	205	3PE	C11-O13-P-O12
69	1Y	205	3PE	O32-C31-O31-C3
69	1Y	205	3PE	C32-C31-O31-C3
69	1Y	205	3PE	O22-C21-O21-C2
69	1Y	205	3PE	C22-C21-O21-C2
69	1d	201	3PE	C11-O13-P-O11
69	1d	201	3PE	C11-O13-P-O14
69	1d	201	3PE	C2-C1-O11-P
69	1d	201	3PE	O32-C31-O31-C3
69	1d	201	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
69	1j	101	3PE	O22-C21-O21-C2
69	1j	101	3PE	C22-C21-O21-C2
69	3A	502	3PE	O32-C31-O31-C3
69	3A	502	3PE	C32-C31-O31-C3
69	3A	502	3PE	O22-C21-O21-C2
69	3A	502	3PE	C22-C21-O21-C2
69	3A	503	3PE	C1-O11-P-O14
69	3A	503	3PE	C2-C1-O11-P
69	3C	503	3PE	C1-O11-P-O14
69	3C	503	3PE	C11-O13-P-O11
69	3C	503	3PE	C11-O13-P-O14
69	3C	504	3PE	C1-O11-P-O12
69	3C	504	3PE	C2-C1-O11-P
69	3C	504	3PE	O13-C11-C12-N
69	3G	101	3PE	C1-O11-P-O12
69	3G	101	3PE	C1-O11-P-O13
69	3G	101	3PE	C1-O11-P-O14
69	3G	101	3PE	O32-C31-O31-C3
69	3G	101	3PE	C32-C31-O31-C3
69	3N	501	3PE	C1-O11-P-O13
69	3N	501	3PE	C1-O11-P-O14
69	3N	503	3PE	O22-C21-O21-C2
69	3N	503	3PE	C22-C21-O21-C2
69	3P	503	3PE	C11-O13-P-O11
69	3P	503	3PE	C11-O13-P-O12
69	3P	503	3PE	C11-O13-P-O14
70	1A	202	PC1	C1-O11-P-O14
70	1A	202	PC1	O13-C11-C12-N
70	1B	203	PC1	O13-C11-C12-N
70	1H	401	PC1	C11-O13-P-O11
70	1H	401	PC1	C1-O11-P-O14
70	1H	401	PC1	C1-O11-P-O13
70	1H	401	PC1	C12-C11-O13-P
70	1H	401	PC1	O13-C11-C12-N
70	1I	201	PC1	C11-O13-P-O14
70	1P	401	PC1	O32-C31-O31-C3
70	1P	401	PC1	C32-C31-O31-C3
70	1Y	201	PC1	C1-O11-P-O14
70	1Z	201	PC1	C1-O11-P-O14
70	1h	203	PC1	C11-O13-P-O14
70	1h	203	PC1	O32-C31-O31-C3
70	1h	203	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
70	1m	201	PC1	C11-O13-P-O14
70	1m	201	PC1	O22-C21-O21-C2
70	1m	201	PC1	C22-C21-O21-C2
70	1q	201	PC1	C11-O13-P-O14
70	1q	201	PC1	O22-C21-O21-C2
70	1q	201	PC1	C22-C21-O21-C2
70	1q	201	PC1	O32-C31-O31-C3
70	1q	201	PC1	C32-C31-O31-C3
70	3R	303	PC1	C1-O11-P-O14
70	3R	303	PC1	O32-C31-O31-C3
70	3R	303	PC1	C32-C31-O31-C3
70	3X	101	PC1	C1-O11-P-O14
70	3X	101	PC1	O13-C11-C12-N
75	1L	702	CDL	CB2-OB2-PB2-OB4
75	1L	702	CDL	CB2-OB2-PB2-OB5
75	1N	902	CDL	CA3-OA5-PA1-OA3
75	1X	201	CDL	C1-CA2-OA2-PA1
75	1X	201	CDL	CA2-OA2-PA1-OA4
75	1X	201	CDL	CA2-OA2-PA1-OA5
75	1d	202	CDL	CA2-OA2-PA1-OA4
75	1d	202	CDL	CA2-OA2-PA1-OA5
75	1d	202	CDL	CA3-OA5-PA1-OA2
75	1d	202	CDL	CA3-OA5-PA1-OA4
75	1d	202	CDL	CB3-OB5-PB2-OB2
75	1d	202	CDL	CB3-OB5-PB2-OB3
75	1d	202	CDL	CB3-OB5-PB2-OB4
75	1d	202	CDL	OB5-CB3-CB4-OB6
75	1h	202	CDL	CA2-OA2-PA1-OA4
75	1h	202	CDL	CA2-OA2-PA1-OA5
75	1h	202	CDL	CB3-OB5-PB2-OB4
75	1h	202	CDL	OB7-CB5-OB6-CB4
75	1h	202	CDL	C51-CB5-OB6-CB4
75	1h	202	CDL	OB9-CB7-OB8-CB6
75	1h	202	CDL	C71-CB7-OB8-CB6
75	3A	501	CDL	CB2-OB2-PB2-OB4
75	3A	501	CDL	CB2-OB2-PB2-OB5
75	3G	102	CDL	CA3-OA5-PA1-OA2
75	3G	102	CDL	CA3-OA5-PA1-OA3
75	3G	102	CDL	CB2-OB2-PB2-OB4
75	3G	102	CDL	CB2-OB2-PB2-OB5
75	3G	103	CDL	CB2-OB2-PB2-OB4
75	3G	103	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
75	3G	103	CDL	CB3-OB5-PB2-OB2
75	3G	103	CDL	CB3-OB5-PB2-OB3
75	3P	504	CDL	OB5-CB3-CB4-OB6
75	3P	504	CDL	OB9-CB7-OB8-CB6
75	3P	504	CDL	C71-CB7-OB8-CB6
75	3T	101	CDL	OB9-CB7-OB8-CB6
75	3T	101	CDL	C71-CB7-OB8-CB6
75	4B	302	CDL	CA3-OA5-PA1-OA3
75	4B	302	CDL	OA9-CA7-OA8-CA6
75	4B	302	CDL	C31-CA7-OA8-CA6
75	4B	302	CDL	CB3-OB5-PB2-OB2
75	4B	302	CDL	CB3-OB5-PB2-OB3
75	4C	306	CDL	C1-CA2-OA2-PA1
75	4C	306	CDL	OB7-CB5-OB6-CB4
75	4C	306	CDL	C51-CB5-OB6-CB4
75	4C	306	CDL	OB9-CB7-OB8-CB6
75	4C	306	CDL	C71-CB7-OB8-CB6
75	4D	201	CDL	C1-CA2-OA2-PA1
75	4D	201	CDL	CB3-OB5-PB2-OB3
75	4D	201	CDL	OB7-CB5-OB6-CB4
75	4D	201	CDL	C51-CB5-OB6-CB4
75	4D	201	CDL	OB9-CB7-OB8-CB6
75	4D	201	CDL	C71-CB7-OB8-CB6
76	1O	401	GTP	PB-O3A-PA-O5'
80	1T	101	EHZ	N2-C15-C16-O5
82	1I	201	MYR	O1-C1-C2-C3
83	3C	501	HEM	C2B-C3B-CAB-CBB
83	3C	502	HEM	C2B-C3B-CAB-CBB
83	3P	502	HEM	C2B-C3B-CAB-CBB
85	4A	601	PGV	C03-O11-P-O12
85	4A	601	PGV	C03-O11-P-O13
85	4A	601	PGV	O04-C19-O03-C01
85	4A	601	PGV	C20-C19-O03-C01
85	4A	602	PGV	C02-C03-O11-P
85	4A	603	PGV	O03-C01-C02-O01
85	4B	301	PGV	C04-O12-P-O11
85	4C	302	PGV	C03-O11-P-O13
85	4C	302	PGV	O02-C1-O01-C02
85	4C	302	PGV	C2-C1-O01-C02
85	4C	303	PGV	C04-O12-P-O11
85	4C	303	PGV	C04-O12-P-O14
85	4C	303	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
85	4C	303	PGV	C20-C19-O03-C01
85	4C	304	PGV	C03-O11-P-O12
85	4C	304	PGV	C03-O11-P-O14
85	4C	304	PGV	C02-C03-O11-P
85	4C	305	PGV	C03-O11-P-O12
85	4C	305	PGV	C03-O11-P-O14
85	4C	305	PGV	C02-C03-O11-P
85	4C	305	PGV	O02-C1-O01-C02
85	4C	305	PGV	C2-C1-O01-C02
85	4G	101	PGV	O02-C1-O01-C02
85	4G	101	PGV	C2-C1-O01-C02
85	4G	101	PGV	O04-C19-O03-C01
85	4G	101	PGV	C20-C19-O03-C01
85	4K	101	PGV	C03-O11-P-O12
85	4K	101	PGV	C03-O11-P-O14
85	4K	101	PGV	O04-C19-O03-C01
85	4K	101	PGV	C20-C19-O03-C01
86	4A	604	HEA	C3B-C11-C12-C13
86	4A	604	HEA	O11-C11-C12-C13
90	4B	304	PSC	C03-O11-P-O12
90	4B	304	PSC	C03-O11-P-O13
90	4B	304	PSC	O02-C1-O01-C02
91	4G	102	PEK	C04-O12-P-O11
91	4G	102	PEK	C04-O12-P-O13
91	4G	103	PEK	O12-C04-C05-N
90	4B	304	PSC	C2-C1-O01-C02
80	1T	101	EHZ	C13-C12-N1-C11
75	3G	102	CDL	O1-C1-CB2-OB2
75	1N	902	CDL	OB7-CB5-OB6-CB4
75	1N	902	CDL	C51-CB5-OB6-CB4
76	1O	401	GTP	C3'-C4'-C5'-O5'
69	3Y	101	3PE	C2-C1-O11-P
85	4C	305	PGV	C05-C04-O12-P
80	1T	101	EHZ	O3-C12-N1-C11
75	3N	502	CDL	OA6-CA4-CA6-OA8
76	1O	401	GTP	O4'-C4'-C5'-O5'
75	3P	504	CDL	CB5-C51-C52-C53
90	4B	304	PSC	C19-C20-C21-C22
70	1P	401	PC1	C21-C22-C23-C24
85	4J	101	PGV	C19-C20-C21-C22
85	4A	603	PGV	C05-C04-O12-P
69	3C	503	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
85	4G	101	PGV	C1-C2-C3-C4
70	1H	401	PC1	C22-C23-C24-C25
85	4L	101	PGV	C1-C2-C3-C4
75	1q	202	CDL	CA5-C11-C12-C13
85	4B	301	PGV	C4-C5-C6-C7
69	3G	101	3PE	C31-C32-C33-C34
75	4C	306	CDL	O1-C1-CA2-OA2
75	1d	202	CDL	C32-C33-C34-C35
69	3N	501	3PE	C2-C1-O11-P
70	1H	401	PC1	C2-C1-O11-P
70	1h	203	PC1	C2-C1-O11-P
75	3T	101	CDL	CA4-CA3-OA5-PA1
69	3C	504	3PE	C31-C32-C33-C34
69	3R	302	3PE	C35-C36-C37-C38
75	1L	702	CDL	C37-C38-C39-C40
75	4D	201	CDL	C75-C76-C77-C78
85	4J	101	PGV	C22-C23-C24-C25
69	1L	703	3PE	C33-C34-C35-C36
75	1d	202	CDL	C42-C43-C44-C45
75	1q	202	CDL	C14-C15-C16-C17
85	4L	101	PGV	C2-C3-C4-C5
78	1P	402	NDP	O4D-C1D-N1N-C6N
75	4D	201	CDL	O1-C1-CB2-OB2
70	1I	201	PC1	C31-C32-C33-C34
75	4B	302	CDL	C59-C60-C61-C62
69	1L	703	3PE	C39-C3A-C3B-C3C
69	1d	201	3PE	C32-C33-C34-C35
69	1d	201	3PE	C23-C24-C25-C26
70	1Y	201	PC1	C32-C33-C34-C35
91	4G	102	PEK	C26-C27-C28-C29
69	1Y	205	3PE	C2D-C2E-C2F-C2G
90	4B	304	PSC	C27-C28-C29-C30
69	3A	503	3PE	C32-C33-C34-C35
69	3A	503	3PE	C36-C37-C38-C39
90	4B	304	PSC	C22-C23-C24-C25
69	3R	302	3PE	C21-C22-C23-C24
85	4C	307	PGV	C02-C03-O11-P
85	4C	304	PGV	C24-C25-C26-C27
70	1q	201	PC1	C2A-C2B-C2C-C2D
75	3G	103	CDL	CA5-C11-C12-C13
70	1h	203	PC1	C32-C33-C34-C35
90	4B	304	PSC	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
69	1N	901	3PE	C31-C32-C33-C34
80	1T	101	EHZ	C21-C22-C23-C24
69	1M	504	3PE	C2B-C2C-C2D-C2E
70	1M	503	PC1	C21-C22-C23-C24
75	1L	702	CDL	C33-C34-C35-C36
90	4B	304	PSC	C20-C21-C22-C23
69	1N	901	3PE	O11-C1-C2-O21
69	3A	502	3PE	O11-C1-C2-O21
83	3C	501	HEM	C4B-C3B-CAB-CBB
83	3C	502	HEM	C4B-C3B-CAB-CBB
83	3P	502	HEM	C4B-C3B-CAB-CBB
75	4D	201	CDL	C38-C39-C40-C41
69	3P	503	3PE	C21-C22-C23-C24
70	1A	202	PC1	C21-C22-C23-C24
91	4G	103	PEK	C21-C22-C23-C24
70	1M	503	PC1	C32-C33-C34-C35
69	1Y	202	3PE	O21-C2-C3-O31
75	1N	902	CDL	OA6-CA4-CA6-OA8
85	4C	305	PGV	O03-C01-C02-O01
70	1B	202	PC1	C38-C39-C3A-C3B
70	3R	303	PC1	C26-C27-C28-C29
85	4B	301	PGV	C27-C28-C29-C30
70	1m	201	PC1	C22-C23-C24-C25
69	1L	703	3PE	C2-C1-O11-P
69	1Y	203	3PE	C2-C1-O11-P
75	1h	202	CDL	C1-CB2-OB2-PB2
85	4C	303	PGV	C05-C04-O12-P
75	3G	102	CDL	CA2-C1-CB2-OB2
75	4C	306	CDL	CB2-C1-CA2-OA2
70	1B	203	PC1	C32-C33-C34-C35
70	1M	503	PC1	C2A-C2B-C2C-C2D
69	1M	502	3PE	C2D-C2E-C2F-C2G
69	3N	501	3PE	C33-C34-C35-C36
75	1X	201	CDL	C19-C20-C21-C22
80	1T	101	EHZ	O4-C15-C16-O5
69	1Y	203	3PE	O11-C1-C2-C3
69	3A	503	3PE	O11-C1-C2-C3
70	1P	401	PC1	O11-C1-C2-C3
85	4B	301	PGV	C6-C7-C8-C9
91	4G	102	PEK	C22-C23-C24-C25
69	1Y	205	3PE	C29-C2A-C2B-C2C
69	3Y	101	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
69	1d	201	3PE	C26-C27-C28-C29
75	3P	504	CDL	CA5-C11-C12-C13
69	1Y	203	3PE	C1-C2-C3-O31
69	3P	503	3PE	C1-C2-C3-O31
70	1P	401	PC1	C1-C2-C3-O31
70	1h	203	PC1	C1-C2-C3-O31
75	1X	201	CDL	CB3-CB4-CB6-OB8
75	1d	202	CDL	CA3-CA4-CA6-OA8
85	4C	305	PGV	O03-C01-C02-C03
85	4J	101	PGV	O03-C01-C02-C03
75	1X	201	CDL	C58-C59-C60-C61
75	3T	101	CDL	C31-CA7-OA8-CA6
69	1N	901	3PE	C28-C29-C2A-C2B
69	3R	302	3PE	C27-C28-C29-C2A
75	4C	306	CDL	C81-C82-C83-C84
75	4D	201	CDL	C62-C63-C64-C65
85	4L	101	PGV	C5-C6-C7-C8
69	1M	504	3PE	C27-C28-C29-C2A
85	4C	303	PGV	C5-C6-C7-C8
75	4C	306	CDL	C75-C76-C77-C78
69	1L	701	3PE	C28-C29-C2A-C2B
91	4G	102	PEK	C21-C22-C23-C24
75	4D	201	CDL	C14-C15-C16-C17
69	3P	503	3PE	C27-C28-C29-C2A
70	1I	201	PC1	C2B-C2C-C2D-C2E
70	1M	503	PC1	C23-C24-C25-C26
70	1Y	201	PC1	O21-C2-C3-O31
69	3R	302	3PE	C23-C24-C25-C26
69	1N	901	3PE	C32-C33-C34-C35
69	1M	504	3PE	C26-C27-C28-C29
69	1N	903	3PE	C35-C36-C37-C38
86	4A	605	HEA	C3B-C11-C12-C13
80	1T	101	EHZ	O4-C15-C16-C17
70	1h	203	PC1	C2A-C2B-C2C-C2D
85	4K	101	PGV	C22-C23-C24-C25
75	3T	101	CDL	C52-C53-C54-C55
73	1F	501	FMN	C4'-C5'-O5'-P
75	1X	201	CDL	C1-CB2-OB2-PB2
75	1d	202	CDL	C1-CA2-OA2-PA1
75	1d	202	CDL	CA4-CA3-OA5-PA1
85	4A	603	PGV	C02-C03-O11-P
85	4B	301	PGV	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
85	4K	101	PGV	C02-C03-O11-P
83	3C	501	HEM	C3D-CAD-CBD-CGD
70	1m	201	PC1	C23-C24-C25-C26
69	1J	201	3PE	C34-C35-C36-C37
69	1N	901	3PE	O11-C1-C2-C3
75	1d	202	CDL	OB5-CB3-CB4-CB6
75	3P	504	CDL	OB5-CB3-CB4-CB6
75	1N	902	CDL	C32-C31-CA7-OA8
90	4B	304	PSC	C1-C2-C3-C4
69	1Y	203	3PE	O31-C31-C32-C33
75	1d	202	CDL	C12-C11-CA5-OA6
75	3G	102	CDL	C72-C71-CB7-OB8
75	1X	201	CDL	C18-C19-C20-C21
91	4G	103	PEK	C23-C24-C25-C26
69	1L	703	3PE	C1-C2-C3-O31
75	1N	902	CDL	CA3-CA4-CA6-OA8
75	3N	502	CDL	CA3-CA4-CA6-OA8
85	4A	603	PGV	O03-C01-C02-C03
90	4B	304	PSC	O03-C01-C02-C03
75	1X	201	CDL	C61-C62-C63-C64
75	4C	306	CDL	C59-C60-C61-C62
69	1Y	203	3PE	O11-C1-C2-O21
75	3P	504	CDL	C51-CB5-OB6-CB4
75	4B	302	CDL	C1-CA2-OA2-PA1
76	1O	401	GTP	C4'-C5'-O5'-PA
85	4C	304	PGV	C05-C04-O12-P
85	4K	101	PGV	C05-C04-O12-P
69	3P	503	3PE	C22-C23-C24-C25
69	1A	201	3PE	O31-C31-C32-C33
69	1A	201	3PE	O21-C21-C22-C23
75	1q	202	CDL	C52-C51-CB5-OB6
75	1X	201	CDL	CA7-C31-C32-C33
69	1L	703	3PE	O21-C2-C3-O31
69	1Y	203	3PE	O21-C2-C3-O31
69	1d	201	3PE	O21-C2-C3-O31
69	3G	101	3PE	O21-C2-C3-O31
75	1X	201	CDL	OB6-CB4-CB6-OB8
75	3G	103	CDL	OA6-CA4-CA6-OA8
90	4B	304	PSC	O03-C01-C02-O01
69	1J	201	3PE	C3A-C3B-C3C-C3D
75	4C	306	CDL	C36-C37-C38-C39
69	1L	703	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
85	4B	301	PGV	C2-C3-C4-C5
85	4A	603	PGV	C1-C2-C3-C4
69	3C	504	3PE	C29-C2A-C2B-C2C
75	1N	902	CDL	C12-C13-C14-C15
69	1d	201	3PE	O21-C21-C22-C23
70	1B	202	PC1	O31-C31-C32-C33
75	3N	502	CDL	CA2-C1-CB2-OB2
75	1X	201	CDL	C36-C37-C38-C39
85	4C	305	PGV	C26-C27-C28-C29
69	1Y	202	3PE	O11-C1-C2-C3
85	4B	301	PGV	C01-C02-C03-O11
75	4C	306	CDL	C51-C52-C53-C54
69	1Y	202	3PE	C23-C24-C25-C26
69	1d	201	3PE	C2C-C2D-C2E-C2F
85	4C	304	PGV	C23-C24-C25-C26
83	3P	501	HEM	C2B-C3B-CAB-CBB
85	4C	302	PGV	C22-C23-C24-C25
75	4C	306	CDL	C16-C17-C18-C19
75	1L	702	CDL	C11-C12-C13-C14
81	1h	201	AME	CB-CA-N-CT1
69	3A	503	3PE	O11-C1-C2-O21
70	1B	203	PC1	O11-C1-C2-O21
75	4B	302	CDL	OA5-CA3-CA4-OA6
85	4B	301	PGV	O01-C02-C03-O11
69	1N	903	3PE	C1-C2-C3-O31
69	3N	503	3PE	C1-C2-C3-O31
70	1B	203	PC1	C1-C2-C3-O31
75	4B	302	CDL	CB3-CB4-CB6-OB8
69	3C	504	3PE	O31-C31-C32-C33
75	3G	103	CDL	C52-C53-C54-C55
69	1L	704	3PE	C12-C11-O13-P
69	1M	502	3PE	C12-C11-O13-P
69	1M	504	3PE	C12-C11-O13-P
69	1j	101	3PE	C12-C11-O13-P
69	3C	503	3PE	C12-C11-O13-P
69	3C	504	3PE	C12-C11-O13-P
70	1B	203	PC1	C12-C11-O13-P
70	1m	201	PC1	C12-C11-O13-P
80	1T	101	EHZ	C15-C16-C17-C19
69	1M	502	3PE	O21-C2-C3-O31
69	3A	502	3PE	O21-C2-C3-O31
69	3N	501	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
70	1B	203	PC1	O21-C2-C3-O31
75	1d	202	CDL	OA6-CA4-CA6-OA8
75	4B	302	CDL	OB6-CB4-CB6-OB8
85	4C	303	PGV	C02-C03-O11-P
75	4C	306	CDL	C71-C72-C73-C74
70	1h	203	PC1	O13-C11-C12-N
70	1m	201	PC1	O13-C11-C12-N
69	1M	502	3PE	C24-C25-C26-C27
86	4A	605	HEA	C2A-CAA-CBA-CGA
70	1B	203	PC1	C24-C25-C26-C27
70	1I	201	PC1	C32-C33-C34-C35
69	3P	503	3PE	C25-C26-C27-C28
70	1h	203	PC1	C2B-C2C-C2D-C2E
75	4C	306	CDL	C79-C80-C81-C82
86	4A	604	HEA	C4D-C3D-CAD-CBD
69	3A	502	3PE	O11-C1-C2-C3
75	4B	302	CDL	OA5-CA3-CA4-CA6
69	1M	502	3PE	C3F-C3G-C3H-C3I
80	1T	101	EHZ	C15-C16-C17-C20
69	1Y	203	3PE	C23-C24-C25-C26
69	1A	201	3PE	C36-C37-C38-C39
70	1B	202	PC1	C23-C24-C25-C26
85	4K	101	PGV	C3-C4-C5-C6
75	3A	501	CDL	C52-C53-C54-C55
80	1n	201	EHZ	C11-C10-S1-C9
69	1Y	202	3PE	O11-C1-C2-O21
70	1P	401	PC1	O11-C1-C2-O21
75	4C	306	CDL	C52-C53-C54-C55
85	4C	301	PGV	C11-C12-C13-C14
85	4M	101	PGV	C9-C10-C11-C12
75	1X	201	CDL	C31-C32-C33-C34
69	3N	503	3PE	O21-C2-C3-O31
69	3P	503	3PE	O21-C2-C3-O31
70	1P	401	PC1	O21-C2-C3-O31
70	1h	203	PC1	O21-C2-C3-O31
85	4C	304	PGV	O03-C01-C02-O01
85	4J	101	PGV	O03-C01-C02-O01
69	1M	502	3PE	C1-C2-C3-O31
69	1Y	202	3PE	C1-C2-C3-O31
70	1Y	201	PC1	C1-C2-C3-O31
75	1X	201	CDL	C12-C11-CA5-OA6
69	1A	201	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
75	3A	501	CDL	O1-C1-CA2-OA2
69	1d	201	3PE	C3C-C3D-C3E-C3F
75	1h	202	CDL	C34-C35-C36-C37
69	1N	901	3PE	C2B-C2C-C2D-C2E
69	3G	101	3PE	C36-C37-C38-C39
69	1J	201	3PE	C1-O11-P-O12
69	1L	701	3PE	C11-O13-P-O14
69	1L	704	3PE	C11-O13-P-O14
69	1M	501	3PE	C1-O11-P-O13
69	1N	901	3PE	C11-O13-P-O12
69	1Y	205	3PE	C1-O11-P-O14
69	3C	503	3PE	C11-O13-P-O12
69	3C	504	3PE	C1-O11-P-O13
69	3C	504	3PE	C1-O11-P-O14
69	3G	101	3PE	C11-O13-P-O14
69	3N	501	3PE	C1-O11-P-O12
69	3N	501	3PE	C11-O13-P-O14
69	3N	503	3PE	C11-O13-P-O14
70	1B	203	PC1	C1-O11-P-O14
70	1H	401	PC1	C11-O13-P-O14
70	1H	401	PC1	C1-O11-P-O12
70	1I	201	PC1	C11-O13-P-O11
70	1P	401	PC1	C11-O13-P-O11
70	1m	201	PC1	C11-O13-P-O11
75	1L	702	CDL	CA2-OA2-PA1-OA4
75	1d	202	CDL	CA2-OA2-PA1-OA3
75	1d	202	CDL	CA3-OA5-PA1-OA3
75	1d	202	CDL	CB2-OB2-PB2-OB3
75	1h	202	CDL	CB3-OB5-PB2-OB2
75	1q	202	CDL	CA3-OA5-PA1-OA3
75	3G	102	CDL	CA3-OA5-PA1-OA4
75	3G	103	CDL	CA2-OA2-PA1-OA3
75	3N	502	CDL	CB3-OB5-PB2-OB3
75	3P	504	CDL	CA3-OA5-PA1-OA3
75	3P	504	CDL	CB3-OB5-PB2-OB3
75	3T	101	CDL	CA3-OA5-PA1-OA2
75	3T	101	CDL	CA3-OA5-PA1-OA3
75	3T	101	CDL	CA3-OA5-PA1-OA4
75	4B	302	CDL	CB3-OB5-PB2-OB4
75	4C	306	CDL	CB2-OB2-PB2-OB3
75	4C	306	CDL	CB3-OB5-PB2-OB3
75	4D	201	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
75	4D	201	CDL	CB2-OB2-PB2-OB3
85	4A	601	PGV	C03-O11-P-O14
85	4A	603	PGV	C03-O11-P-O13
85	4B	301	PGV	C04-O12-P-O13
85	4C	305	PGV	C04-O12-P-O13
85	4G	101	PGV	C04-O12-P-O14
85	4K	101	PGV	C04-O12-P-O13
85	4L	101	PGV	C03-O11-P-O13
69	3R	302	3PE	C26-C27-C28-C29
70	1H	401	PC1	C37-C38-C39-C3A
75	4C	306	CDL	C11-C12-C13-C14
69	1A	201	3PE	C2-C1-O11-P
69	1Y	204	3PE	C2-C1-O11-P
75	1d	202	CDL	CB4-CB3-OB5-PB2
75	3N	502	CDL	CB4-CB3-OB5-PB2
85	4A	603	PGV	C2-C3-C4-C5
85	4C	305	PGV	C24-C25-C26-C27
69	1M	501	3PE	C23-C24-C25-C26
69	3C	503	3PE	C29-C2A-C2B-C2C
75	1X	201	CDL	C55-C56-C57-C58
85	4K	101	PGV	C9-C10-C11-C12
85	4B	301	PGV	C1-C2-C3-C4
69	3R	302	3PE	C32-C33-C34-C35
69	3N	501	3PE	C1-C2-O21-C21
69	3N	501	3PE	C3-C2-O21-C21
75	4B	302	CDL	C38-C39-C40-C41
75	1d	202	CDL	OA5-CA3-CA4-CA6
75	3G	103	CDL	C11-C12-C13-C14
86	4A	604	HEA	C2D-C3D-CAD-CBD
85	4C	304	PGV	C11-C12-C13-C14
85	4G	101	PGV	C11-C12-C13-C14
85	4J	101	PGV	C11-C12-C13-C14
70	1H	401	PC1	C21-C22-C23-C24
69	1L	701	3PE	C25-C26-C27-C28
70	1I	201	PC1	C38-C39-C3A-C3B
69	1Y	205	3PE	C2-C1-O11-P
69	3C	503	3PE	C2C-C2D-C2E-C2F
85	4C	304	PGV	O03-C19-C20-C21
85	4A	601	PGV	C11-C10-C9-C8
69	3N	501	3PE	C1-C2-C3-O31
69	1L	704	3PE	C23-C24-C25-C26
70	3X	101	PC1	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
69	1N	901	3PE	C2D-C2E-C2F-C2G
80	1n	201	EHZ	C7-C8-C9-O2
80	1T	101	EHZ	C1-C2-C3-C4
85	4M	101	PGV	C11-C12-C13-C14
69	1Y	205	3PE	C2A-C2B-C2C-C2D
85	4C	304	PGV	C3-C4-C5-C6
75	3G	102	CDL	C72-C71-CB7-OB9
69	1Y	203	3PE	C21-C22-C23-C24
75	1X	201	CDL	C35-C36-C37-C38
84	3D	501	HEC	C3D-CAD-CBD-CGD
85	4C	303	PGV	C11-C12-C13-C14
85	4M	101	PGV	C3-C4-C5-C6
85	4M	101	PGV	C22-C23-C24-C25
75	4D	201	CDL	OB6-CB4-CB6-OB8
75	3A	501	CDL	CA7-C31-C32-C33
69	3C	503	3PE	C23-C24-C25-C26
85	4C	302	PGV	C21-C22-C23-C24
70	1B	202	PC1	C35-C36-C37-C38
91	4G	103	PEK	C02-C03-O11-P
69	1M	502	3PE	C21-C22-C23-C24
85	4K	101	PGV	C1-C2-C3-C4
83	3P	501	HEM	CAA-CBA-CGA-O1A
83	3C	501	HEM	CAA-CBA-CGA-O2A
83	3P	502	HEM	CAA-CBA-CGA-O1A
80	1T	101	EHZ	C10-C11-N1-C12
80	1n	201	EHZ	C10-C11-N1-C12
85	4A	601	PGV	O03-C01-C02-C03
69	3C	503	3PE	C1-C2-O21-C21
86	4A	604	HEA	CAD-CBD-CGD-O2D
69	1M	501	3PE	C21-C22-C23-C24
83	3P	501	HEM	CAD-CBD-CGD-O1D
69	1A	201	3PE	O32-C31-C32-C33
83	3P	502	HEM	CAA-CBA-CGA-O2A
86	4A	605	HEA	CAD-CBD-CGD-O1D
90	4B	304	PSC	C5-C6-C7-C8
69	3C	503	3PE	O11-C1-C2-O21
85	4L	101	PGV	C21-C22-C23-C24
85	4A	602	PGV	C11-C12-C13-C14
75	1X	201	CDL	C12-C13-C14-C15
75	4C	306	CDL	C38-C39-C40-C41
69	1M	501	3PE	C2-C1-O11-P
70	1Y	201	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
85	4J	101	PGV	C5-C6-C7-C8
81	1h	201	AME	C-CA-N-CT1
69	1J	201	3PE	C3D-C3E-C3F-C3G
70	1B	203	PC1	O11-C1-C2-C3
85	4M	101	PGV	C01-C02-C03-O11
83	3C	502	HEM	CAA-CBA-CGA-O2A
83	3P	501	HEM	CAD-CBD-CGD-O2D
69	1Y	202	3PE	C2D-C2E-C2F-C2G
85	4C	305	PGV	C9-C10-C11-C12
91	4G	102	PEK	O03-C01-C02-O01
83	3P	501	HEM	CAA-CBA-CGA-O2A
69	1L	704	3PE	C22-C23-C24-C25
78	1P	402	NDP	C2N-C3N-C7N-N7N
91	4G	102	PEK	C6-C7-C8-C9
91	4G	102	PEK	C9-C10-C11-C12
91	4G	103	PEK	C11-C12-C13-C14
69	1J	201	3PE	C23-C24-C25-C26
83	3C	502	HEM	CAA-CBA-CGA-O1A
86	4A	604	HEA	CAD-CBD-CGD-O1D
86	4A	605	HEA	CAD-CBD-CGD-O2D
85	4J	101	PGV	C2-C3-C4-C5
69	1d	201	3PE	O22-C21-C22-C23
85	4K	101	PGV	C5-C6-C7-C8
70	1h	203	PC1	C22-C23-C24-C25
86	4A	605	HEA	C26-C15-C16-C17
83	3C	501	HEM	CAA-CBA-CGA-O1A
75	1L	702	CDL	CA4-CA3-OA5-PA1
75	3N	502	CDL	C1-CB2-OB2-PB2
75	3T	101	CDL	C53-C54-C55-C56
75	4D	201	CDL	C12-C13-C14-C15
69	3D	502	3PE	C35-C36-C37-C38
85	4A	603	PGV	C5-C6-C7-C8
86	4A	604	HEA	C19-C20-C21-C22
69	1M	502	3PE	C38-C39-C3A-C3B
75	4C	306	CDL	C72-C73-C74-C75
69	1M	501	3PE	C36-C37-C38-C39
80	1T	101	EHZ	C1-C21-C22-C23
91	4G	103	PEK	O01-C02-C03-O11
75	1q	202	CDL	C52-C51-CB5-OB7
80	1T	101	EHZ	C12-C13-C14-N2
85	4C	304	PGV	C9-C10-C11-C12
85	4K	101	PGV	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
70	1I	201	PC1	C34-C35-C36-C37
75	4B	302	CDL	C12-C11-CA5-OA6
69	3R	302	3PE	C22-C23-C24-C25
75	4D	201	CDL	C73-C74-C75-C76
75	3T	101	CDL	OA5-CA3-CA4-CA6
91	4G	103	PEK	C01-C02-C03-O11
70	1M	503	PC1	C2-C1-O11-P
75	1X	201	CDL	C63-C64-C65-C66
75	4C	306	CDL	C18-C19-C20-C21
70	1B	202	PC1	O32-C31-C32-C33
90	4B	304	PSC	C2-C3-C4-C5
84	3Q	501	HEC	CAA-CBA-CGA-O2A
69	1J	201	3PE	C28-C29-C2A-C2B
70	1H	401	PC1	C38-C39-C3A-C3B
86	4A	604	HEA	C26-C15-C16-C17
91	4G	103	PEK	O03-C21-C22-C23
70	1Y	201	PC1	C2-C3-O31-C31
69	1d	201	3PE	C36-C37-C38-C39
85	4C	303	PGV	C14-C15-C16-C17
69	1Y	203	3PE	O32-C31-C32-C33
69	1L	703	3PE	C29-C2A-C2B-C2C
75	3N	502	CDL	CB6-CB4-OB6-CB5
75	3G	102	CDL	C12-C13-C14-C15
84	3D	501	HEC	CAA-CBA-CGA-O2A
70	1B	202	PC1	C33-C34-C35-C36
85	4C	305	PGV	C6-C7-C8-C9
70	1M	503	PC1	C28-C29-C2A-C2B
69	1L	703	3PE	C34-C35-C36-C37
70	1B	203	PC1	C22-C23-C24-C25
84	3Q	501	HEC	CAA-CBA-CGA-O1A
69	1d	201	3PE	C1-C2-C3-O31
83	3P	501	HEM	C4B-C3B-CAB-CBB
70	1B	202	PC1	C3D-C3E-C3F-C3G
84	3D	501	HEC	CAA-CBA-CGA-O1A
70	3X	101	PC1	C21-C22-C23-C24
85	4A	603	PGV	C24-C25-C26-C27
85	4J	101	PGV	C9-C10-C11-C12
69	1Y	205	3PE	C12-C11-O13-P
80	1T	101	EHZ	C15-C16-C17-C18
70	1I	201	PC1	C22-C23-C24-C25
85	4C	304	PGV	C29-C30-C31-C32
85	4C	305	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
75	1N	902	CDL	C32-C31-CA7-OA9
70	1I	201	PC1	O21-C2-C3-O31
75	1N	902	CDL	OB6-CB4-CB6-OB8
75	3T	101	CDL	OB6-CB4-CB6-OB8
75	4B	302	CDL	C60-C61-C62-C63
85	4A	601	PGV	C9-C10-C11-C12
85	4C	307	PGV	C11-C12-C13-C14
85	4L	101	PGV	C9-C10-C11-C12
75	1L	702	CDL	C72-C71-CB7-OB8
69	1M	504	3PE	C3A-C3B-C3C-C3D
85	4A	602	PGV	C6-C7-C8-C9
85	4C	302	PGV	C24-C25-C26-C27
75	4C	306	CDL	C22-C23-C24-C25
85	4L	101	PGV	C24-C25-C26-C27
85	4M	101	PGV	C27-C28-C29-C30
90	4B	304	PSC	O03-C19-C20-C21
75	1d	202	CDL	C12-C11-CA5-OA7
69	1Y	205	3PE	C26-C27-C28-C29
75	3P	504	CDL	C32-C31-CA7-OA8
85	4A	602	PGV	C14-C15-C16-C17
91	4G	103	PEK	C22-C23-C24-C25
91	4G	102	PEK	C14-C15-C16-C17
85	4C	304	PGV	C02-C01-O03-C19
69	1L	703	3PE	C25-C26-C27-C28
85	4C	307	PGV	C5-C6-C7-C8
70	1q	201	PC1	C34-C35-C36-C37
75	3G	103	CDL	C72-C73-C74-C75
90	4B	304	PSC	C24-C25-C26-C27
85	4A	602	PGV	C28-C29-C30-C31
69	3R	302	3PE	C37-C38-C39-C3A
85	4A	603	PGV	C20-C21-C22-C23
69	1A	201	3PE	O22-C21-C22-C23
83	3P	502	HEM	CAD-CBD-CGD-O2D
70	3R	303	PC1	C39-C3A-C3B-C3C
70	1P	401	PC1	O21-C21-C22-C23
85	4A	601	PGV	O03-C19-C20-C21
70	1B	203	PC1	C23-C24-C25-C26
69	3G	101	3PE	C1-C2-C3-O31
75	1N	902	CDL	CB3-CB4-CB6-OB8
83	3P	502	HEM	CAD-CBD-CGD-O1D
69	1Y	203	3PE	O21-C21-C22-C23
75	3T	101	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
85	4C	305	PGV	O03-C19-C20-C21
75	3G	103	CDL	OB6-CB4-CB6-OB8
85	4M	101	PGV	C20-C21-C22-C23
69	1N	901	3PE	O31-C31-C32-C33
70	1m	201	PC1	O21-C21-C22-C23
85	4A	602	PGV	C2-C3-C4-C5
91	4G	102	PEK	C23-C24-C25-C26
69	1L	704	3PE	O21-C21-C22-C23
75	1q	202	CDL	C53-C54-C55-C56
75	4C	306	CDL	CA2-C1-CB2-OB2
69	3D	502	3PE	C24-C25-C26-C27
85	4J	101	PGV	C6-C7-C8-C9
69	1M	502	3PE	C3-C2-O21-C21
70	1m	201	PC1	C3-C2-O21-C21
85	4C	304	PGV	C01-C02-O01-C1
85	4C	304	PGV	C21-C22-C23-C24
70	1B	202	PC1	C37-C38-C39-C3A
85	4A	603	PGV	C26-C27-C28-C29
80	1T	101	EHZ	N2-C15-C16-C17
75	3N	502	CDL	C52-C51-CB5-OB6
85	4C	303	PGV	C2-C3-C4-C5
85	4C	307	PGV	C14-C15-C16-C17
69	1M	501	3PE	C3A-C3B-C3C-C3D
70	3E	302	PC1	C3B-C3C-C3D-C3E
70	3E	302	PC1	C36-C37-C38-C39
69	1N	901	3PE	C23-C24-C25-C26
85	4B	301	PGV	C23-C24-C25-C26
69	1L	704	3PE	O22-C21-C22-C23
75	3P	504	CDL	C32-C31-CA7-OA9
69	3P	503	3PE	C24-C25-C26-C27
70	1H	401	PC1	C2C-C2D-C2E-C2F
69	1N	901	3PE	C34-C35-C36-C37
85	4J	101	PGV	C26-C27-C28-C29
69	1Y	205	3PE	C23-C24-C25-C26
69	3R	302	3PE	C34-C35-C36-C37
75	1L	702	CDL	C36-C37-C38-C39
70	1P	401	PC1	O22-C21-C22-C23
75	3P	504	CDL	C72-C71-CB7-OB9
69	3N	503	3PE	C31-C32-C33-C34
69	1Y	203	3PE	O22-C21-C22-C23
70	1M	503	PC1	O22-C21-C22-C23
90	4B	304	PSC	O04-C19-C20-C21

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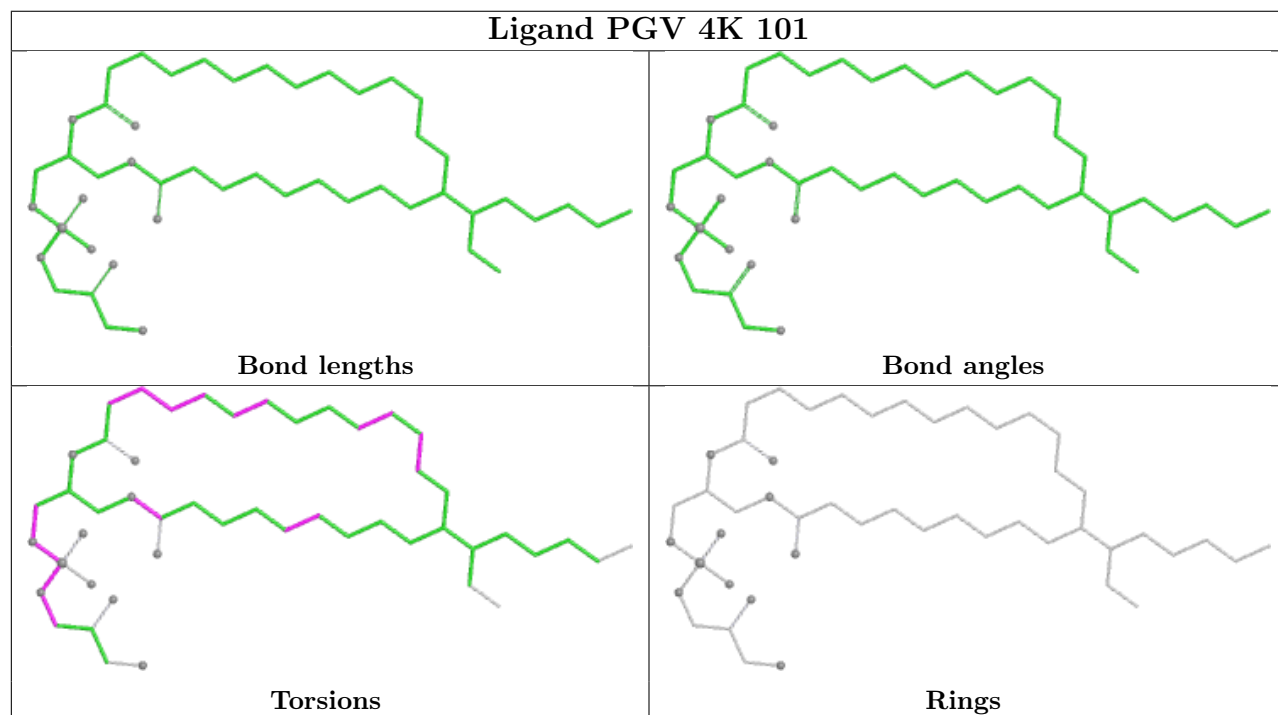
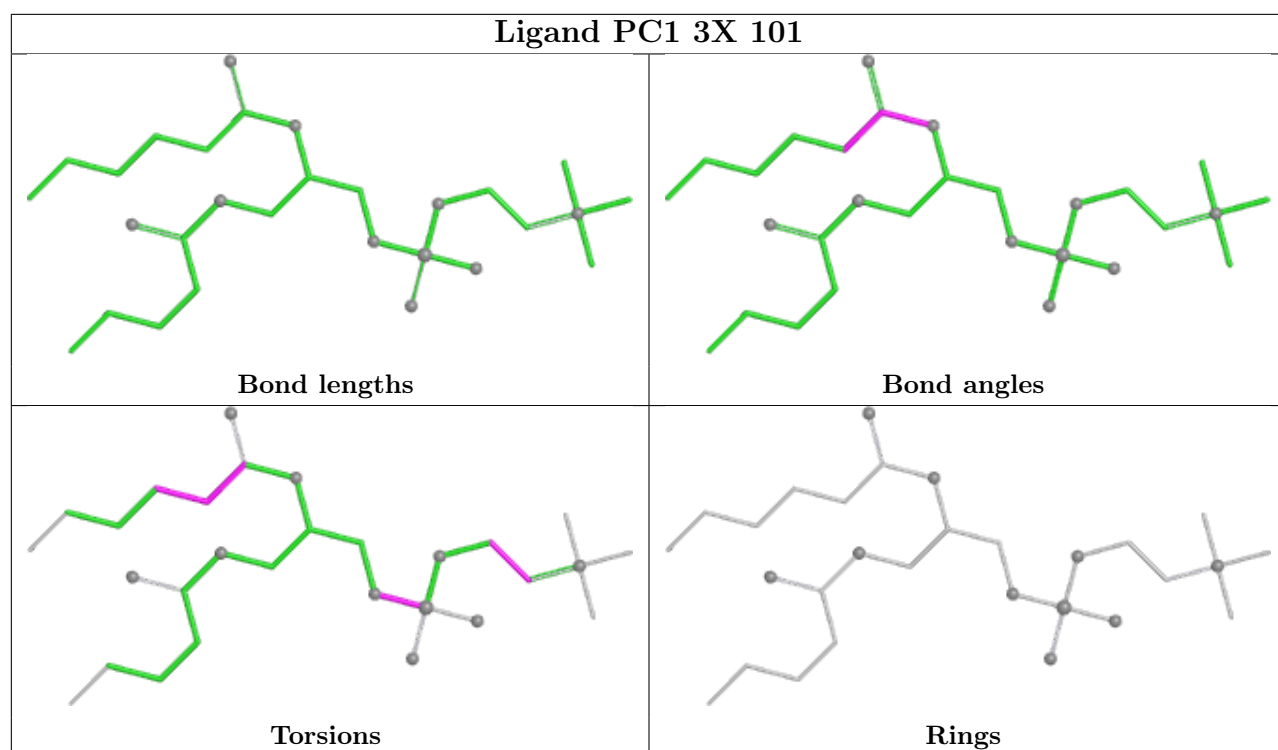
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Mol	Chain	Res	Type	Atoms
70	1Y	201	PC1	O22-C21-C22-C23
75	1L	702	CDL	C72-C71-CB7-OB9
69	3D	502	3PE	C31-C32-C33-C34
82	1l	201	MYR	C3-C4-C5-C6
69	1N	901	3PE	O32-C31-C32-C33
75	3P	504	CDL	C72-C71-CB7-OB8
84	3Q	501	HEC	CAD-CBD-CGD-O2D
86	4A	605	HEA	CAA-CBA-CGA-O2A
70	1m	201	PC1	O22-C21-C22-C23
70	1M	503	PC1	O21-C21-C22-C23
84	3Q	501	HEC	CAD-CBD-CGD-O1D
85	4C	305	PGV	O04-C19-C20-C21
70	1B	203	PC1	C2A-C2B-C2C-C2D
85	4K	101	PGV	C2-C3-C4-C5
69	3N	503	3PE	O31-C31-C32-C33
70	1Y	201	PC1	O21-C21-C22-C23
70	1h	203	PC1	O31-C31-C32-C33
75	1L	702	CDL	C32-C31-CA7-OA8
75	1q	202	CDL	C12-C11-CA5-OA6
85	4M	101	PGV	O01-C1-C2-C3
86	4A	605	HEA	CAA-CBA-CGA-O1A
75	3T	101	CDL	C52-C51-CB5-OB7
69	1d	201	3PE	O31-C31-C32-C33
69	3D	502	3PE	C34-C35-C36-C37
85	4G	101	PGV	C2-C3-C4-C5
85	4A	601	PGV	O04-C19-C20-C21

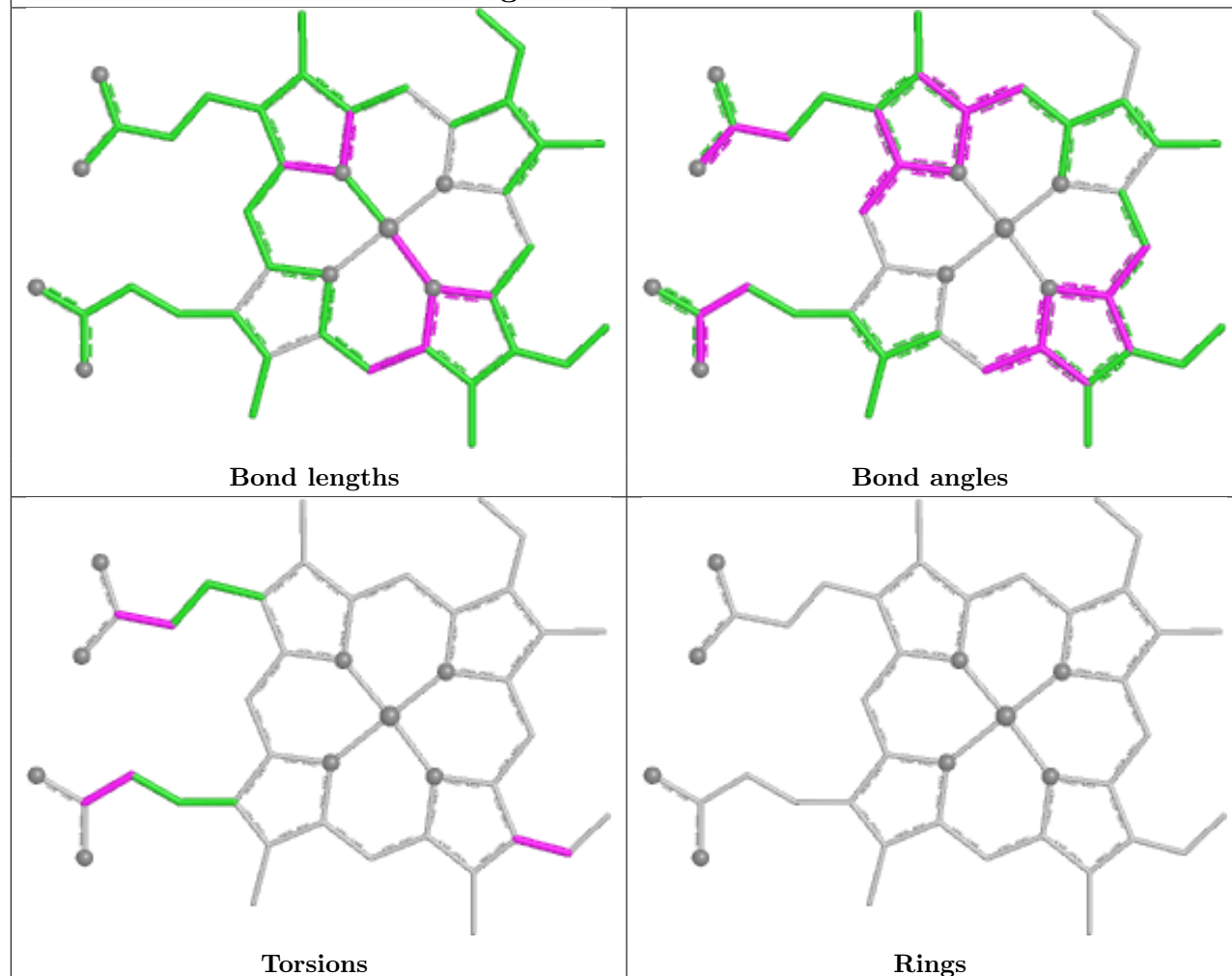
There are no ring outliers.

No monomer is involved in short contacts.

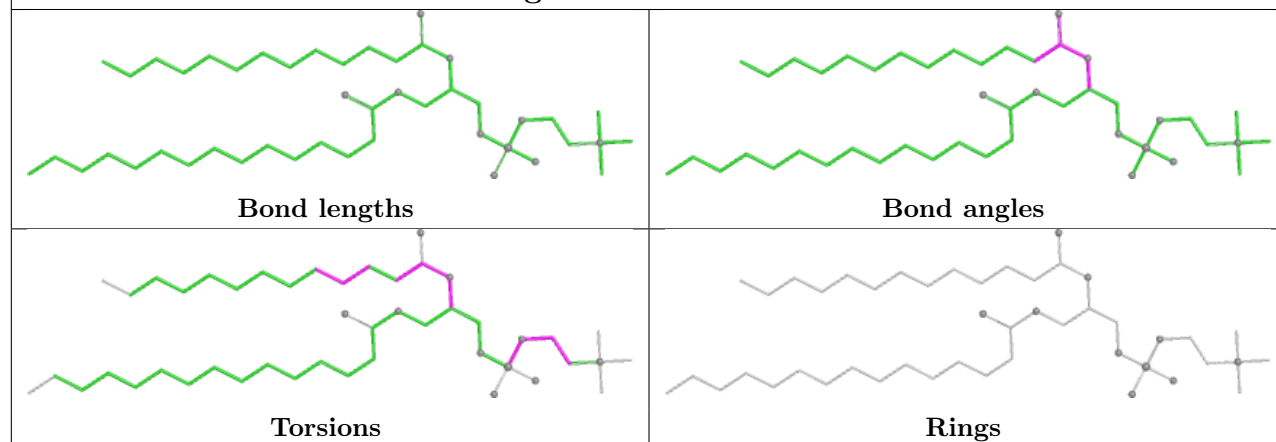
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

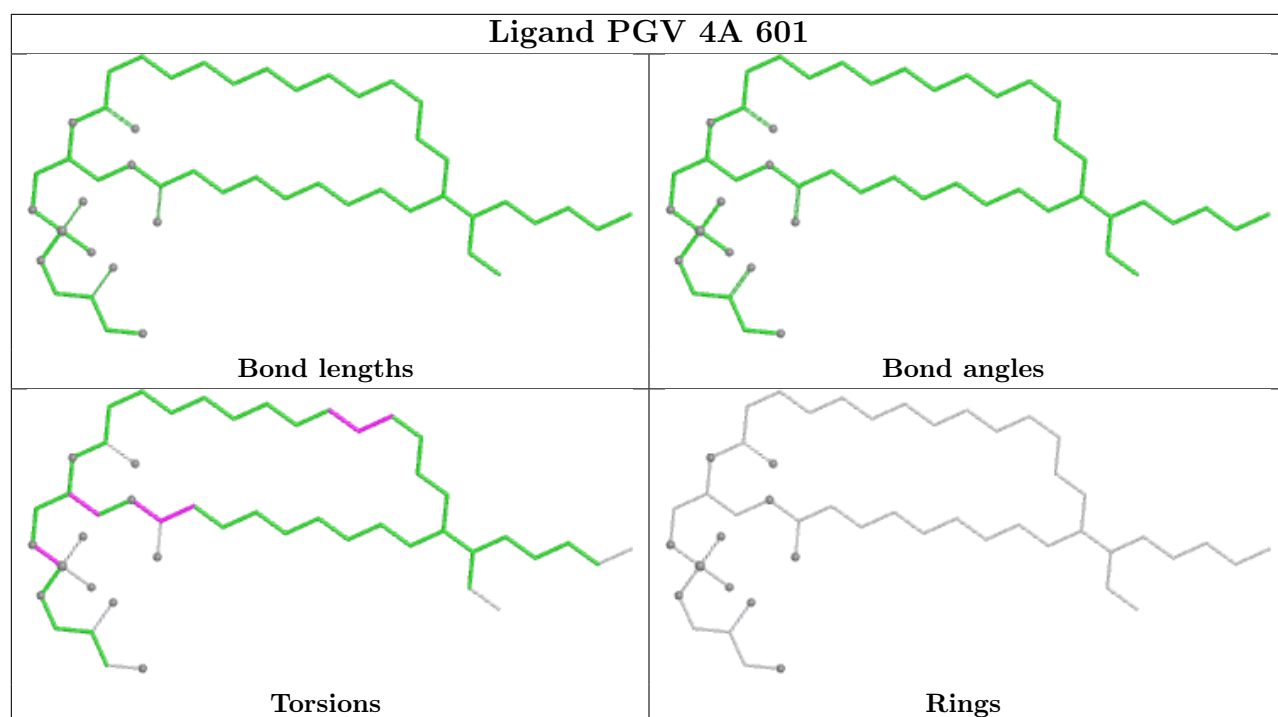


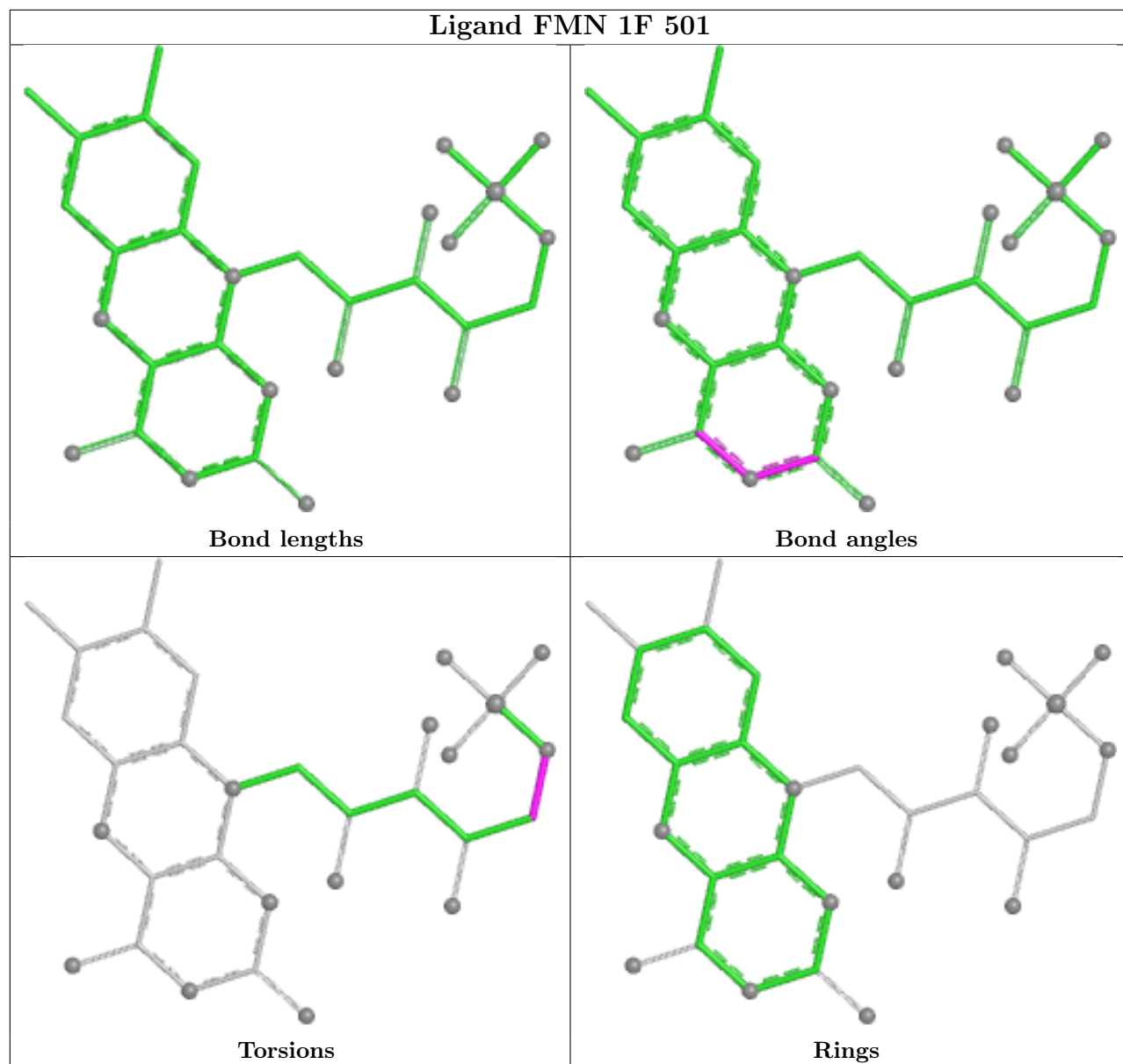
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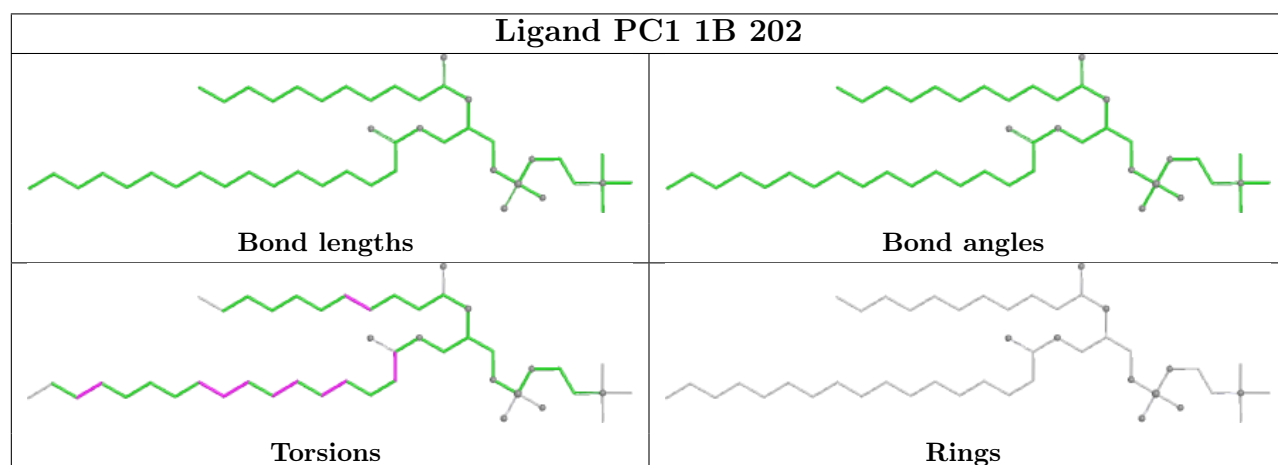
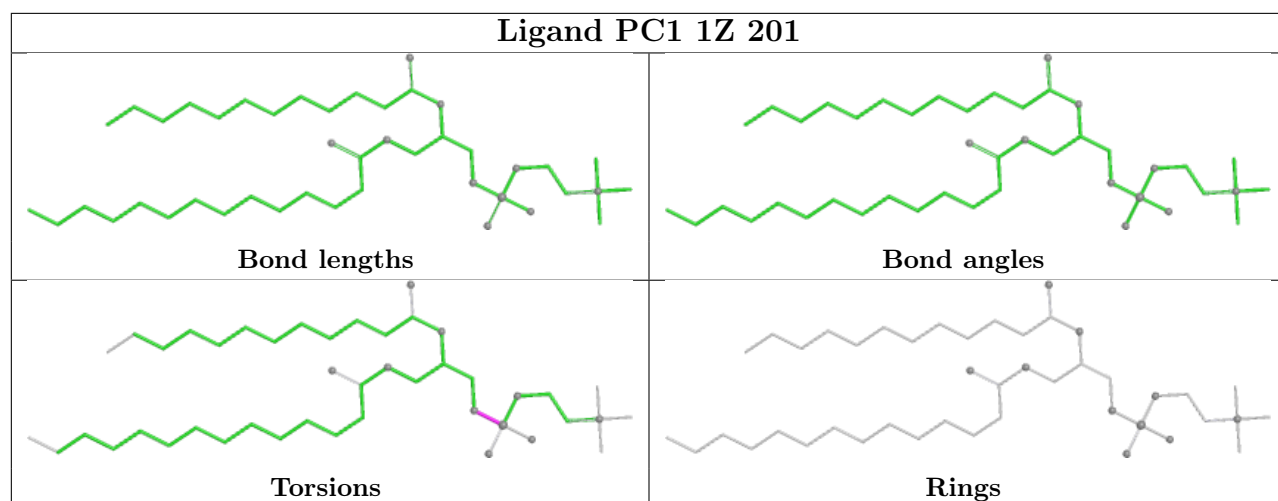
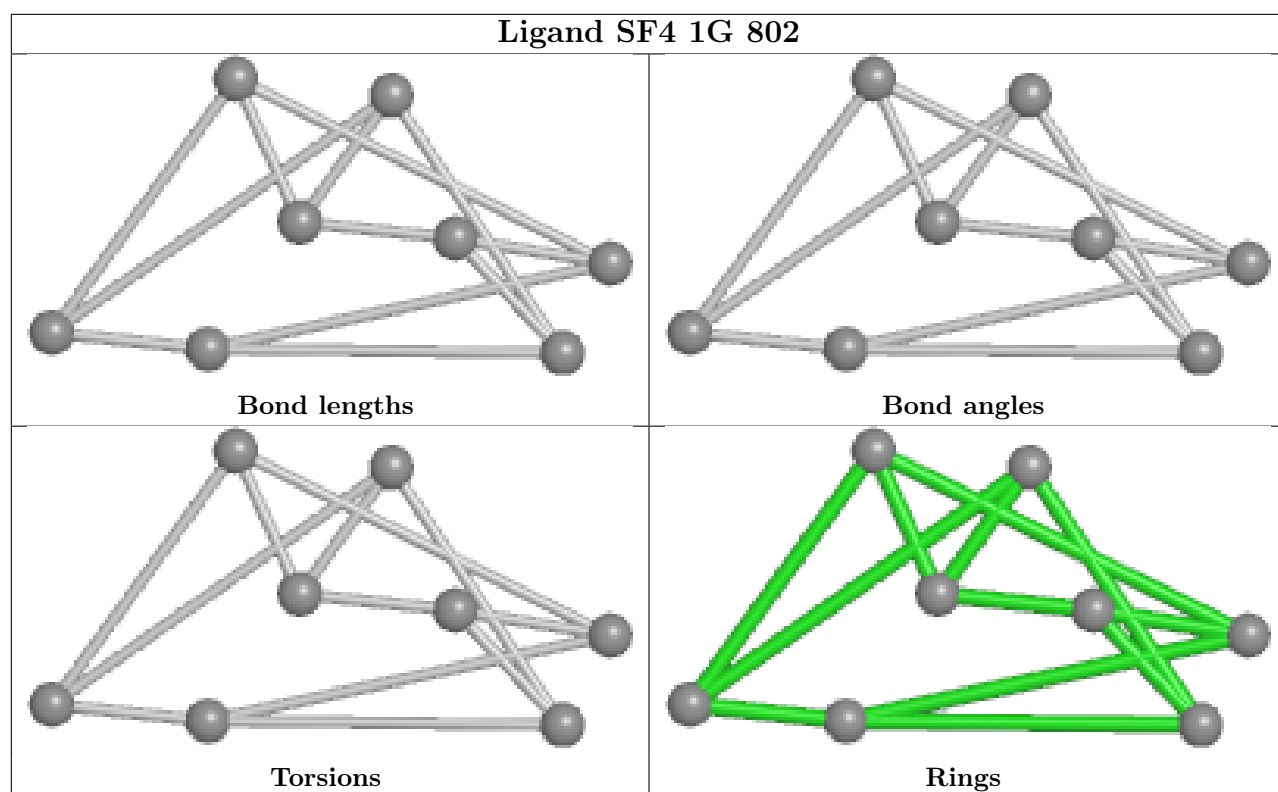


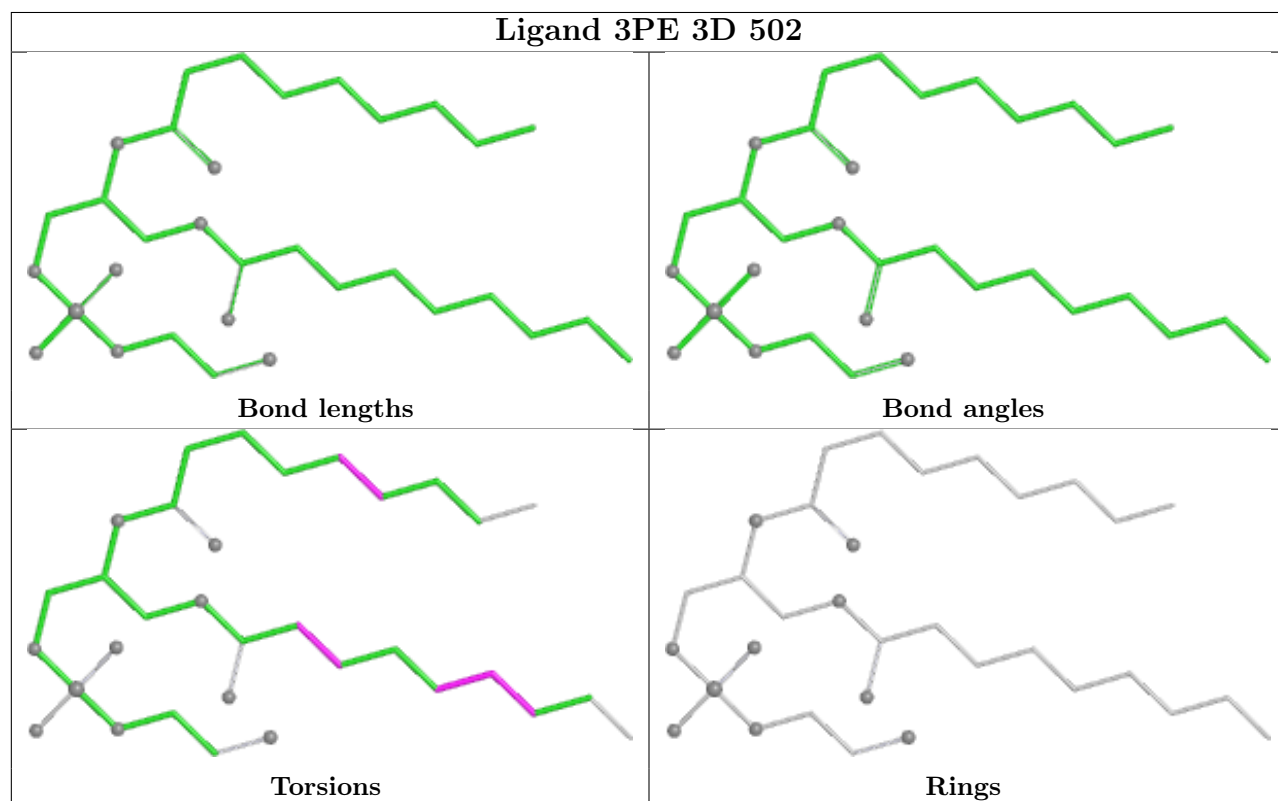
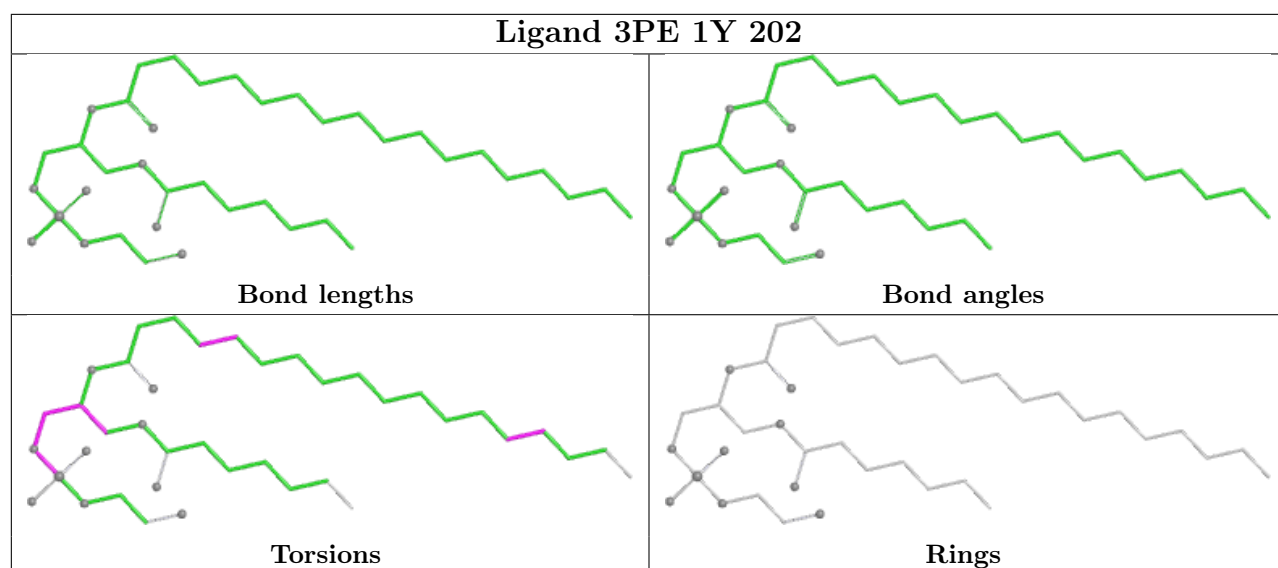
Ligand PC1 1m 201

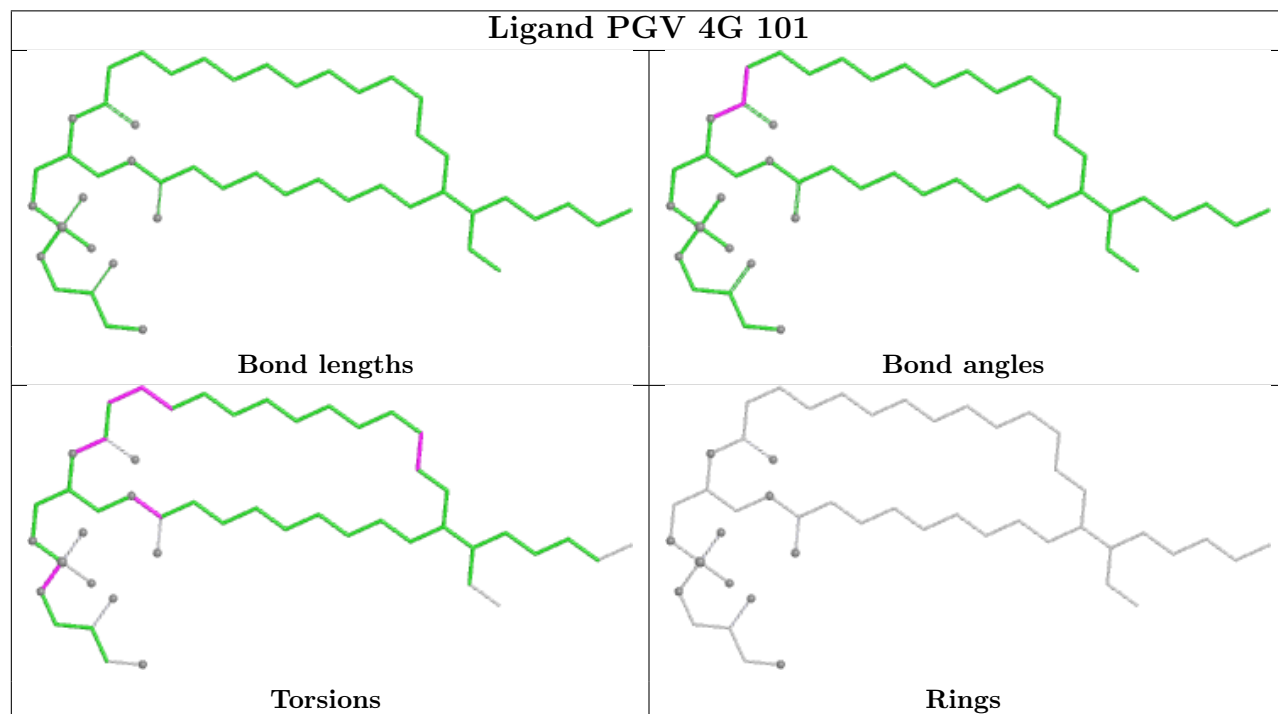
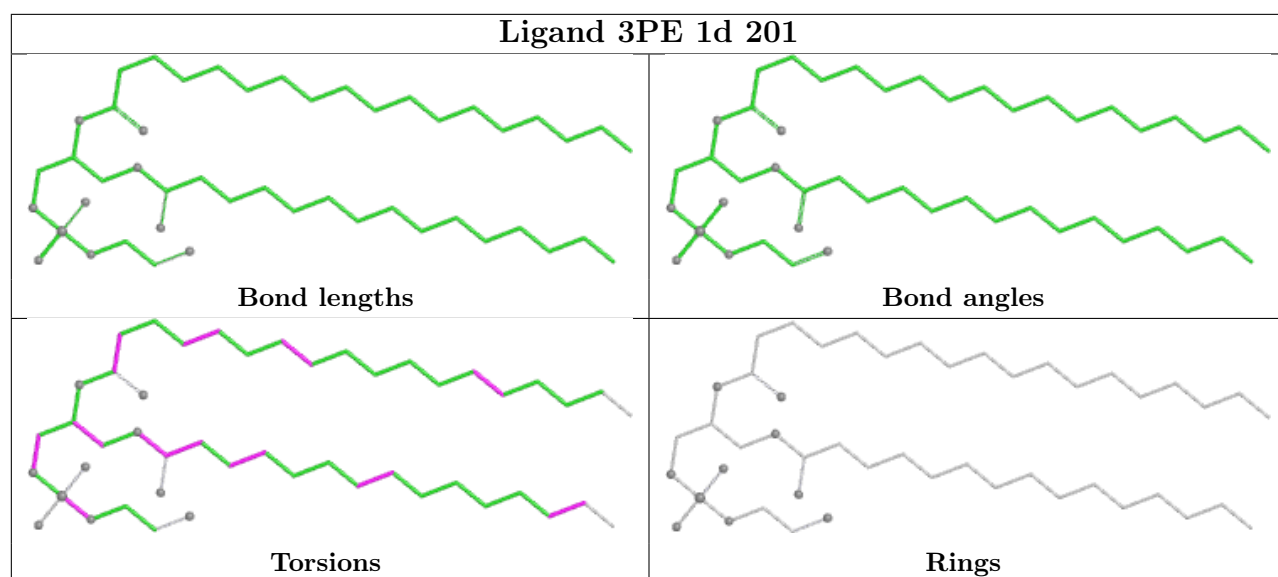


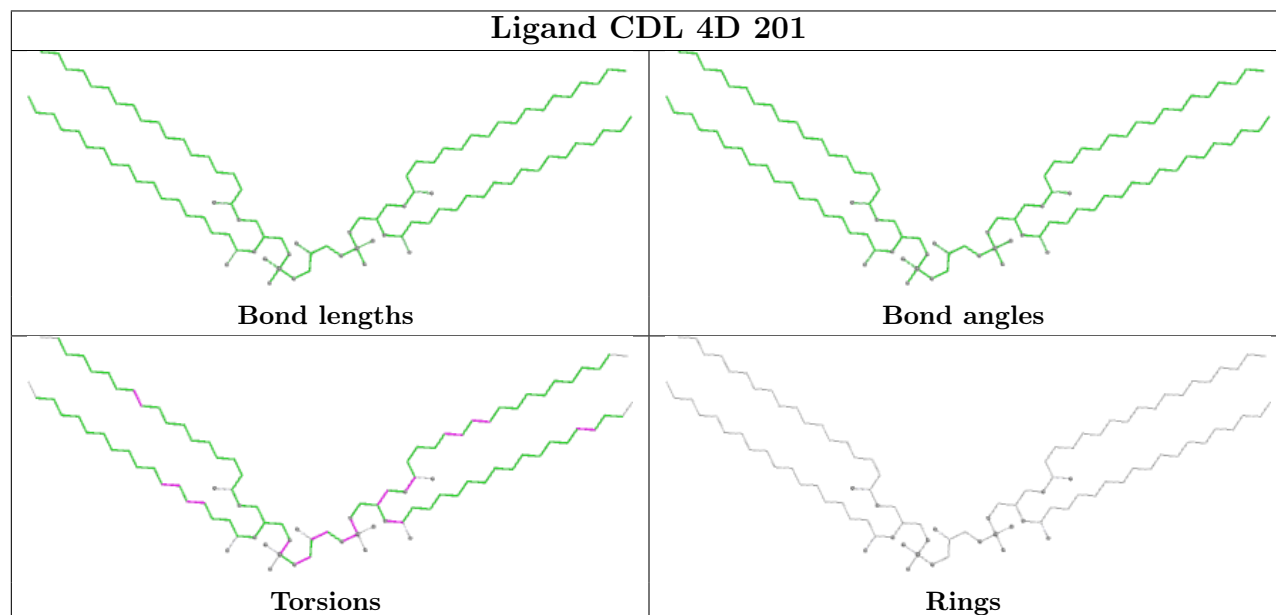
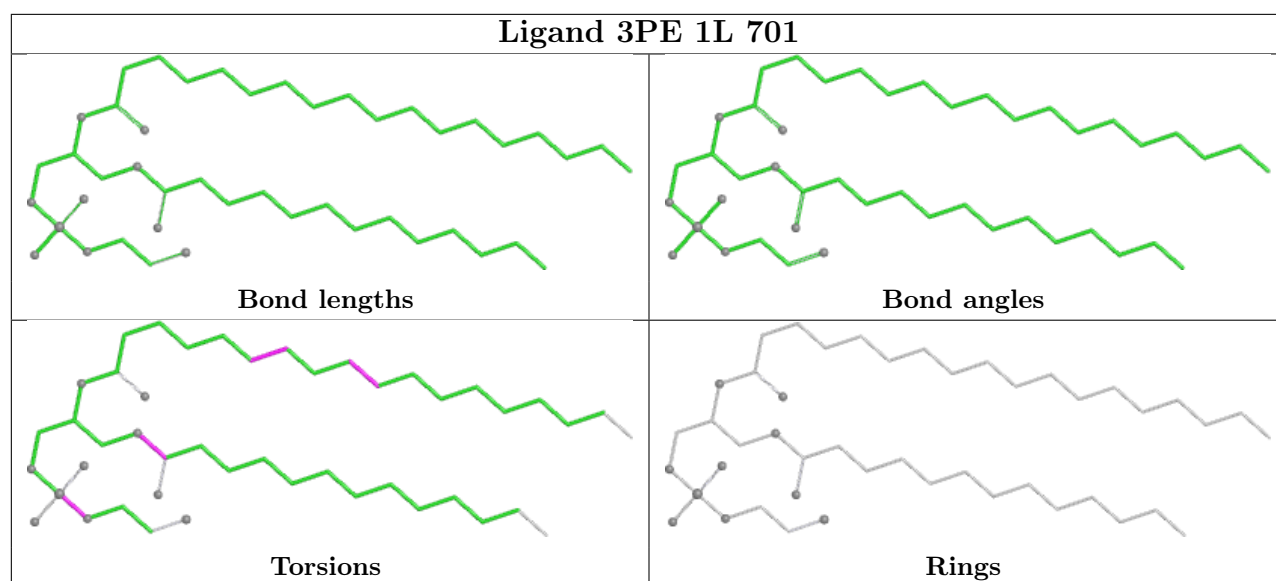


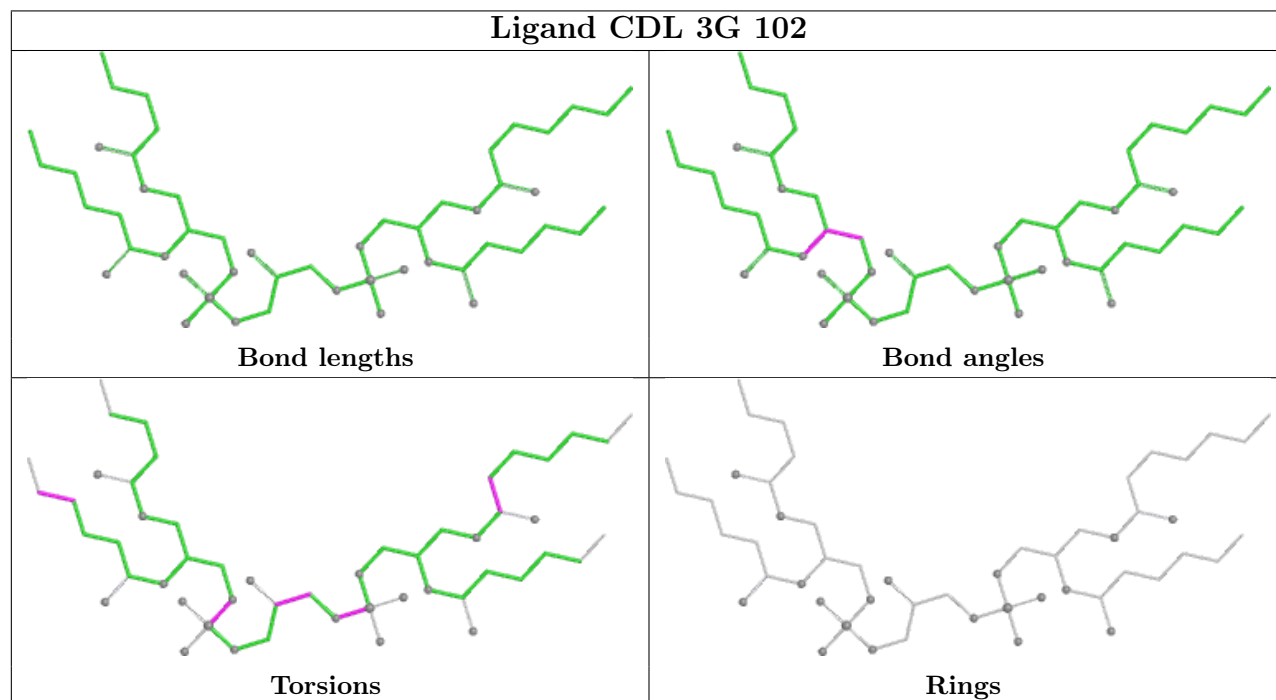
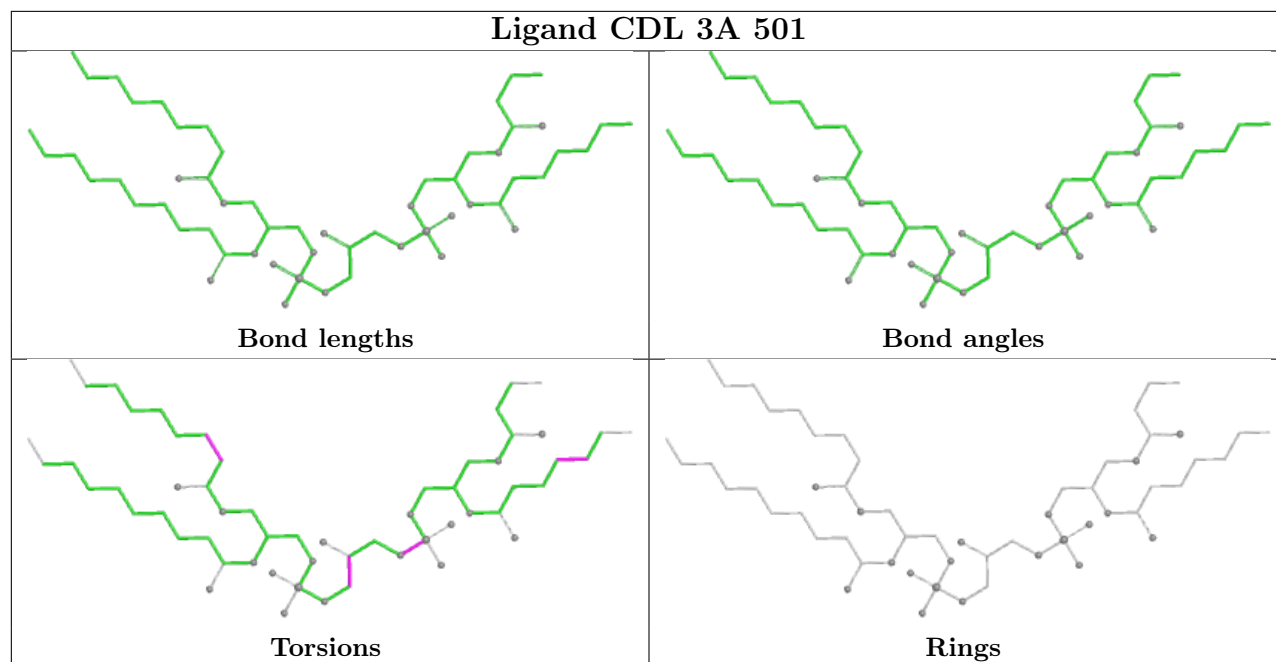




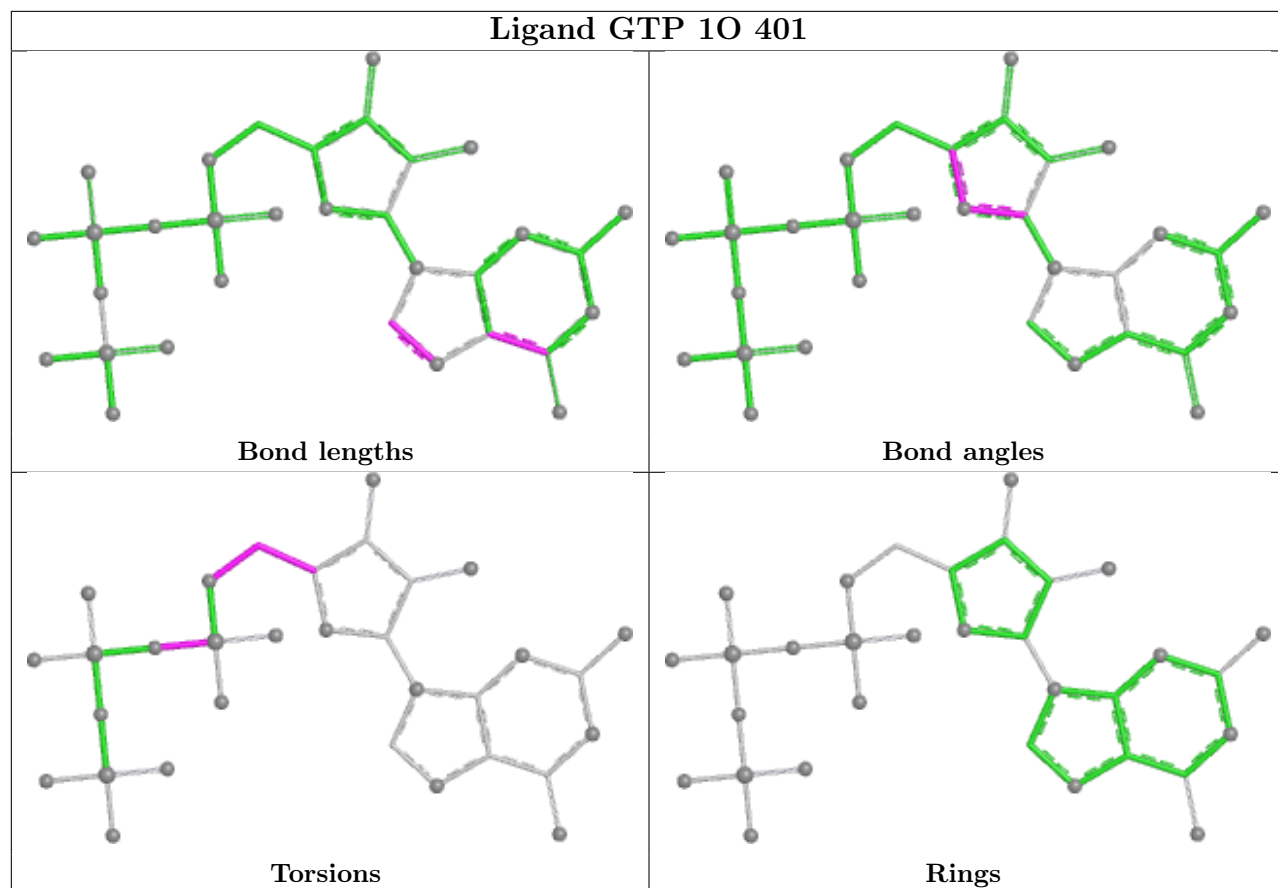




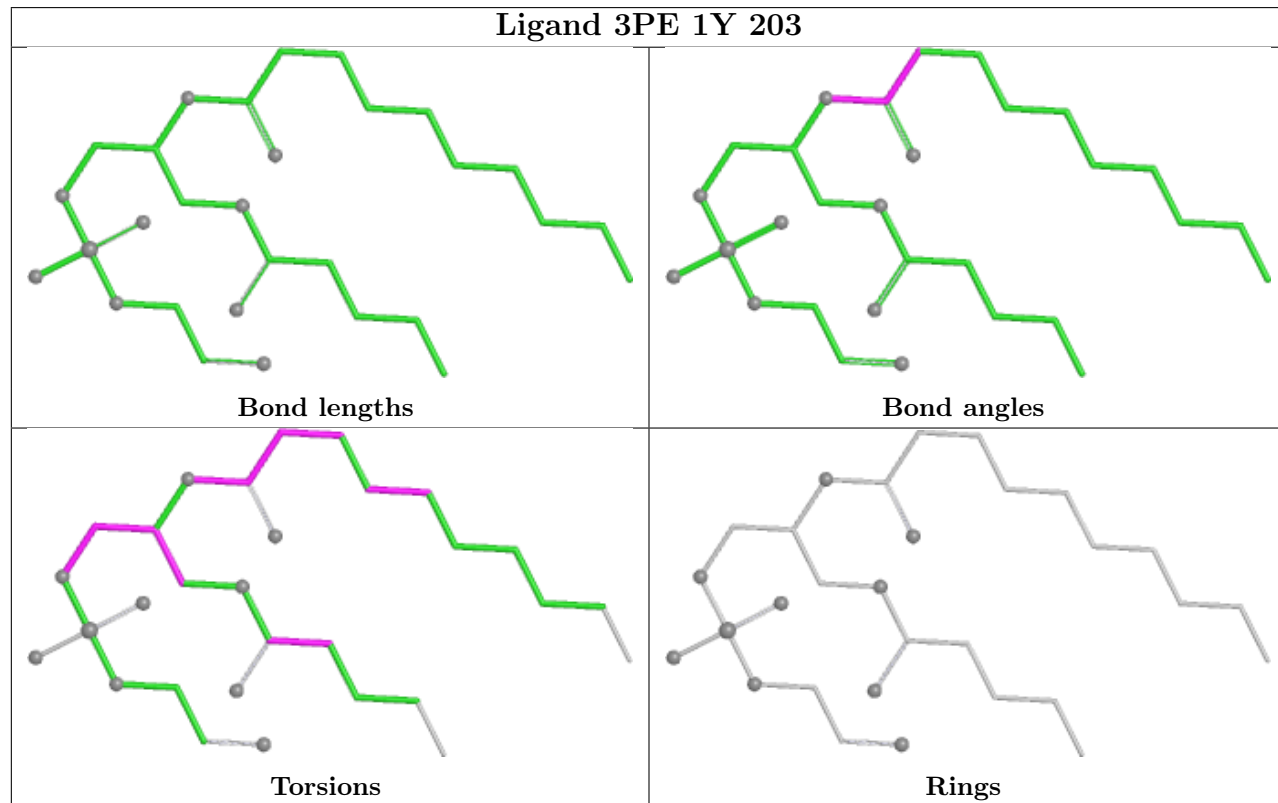


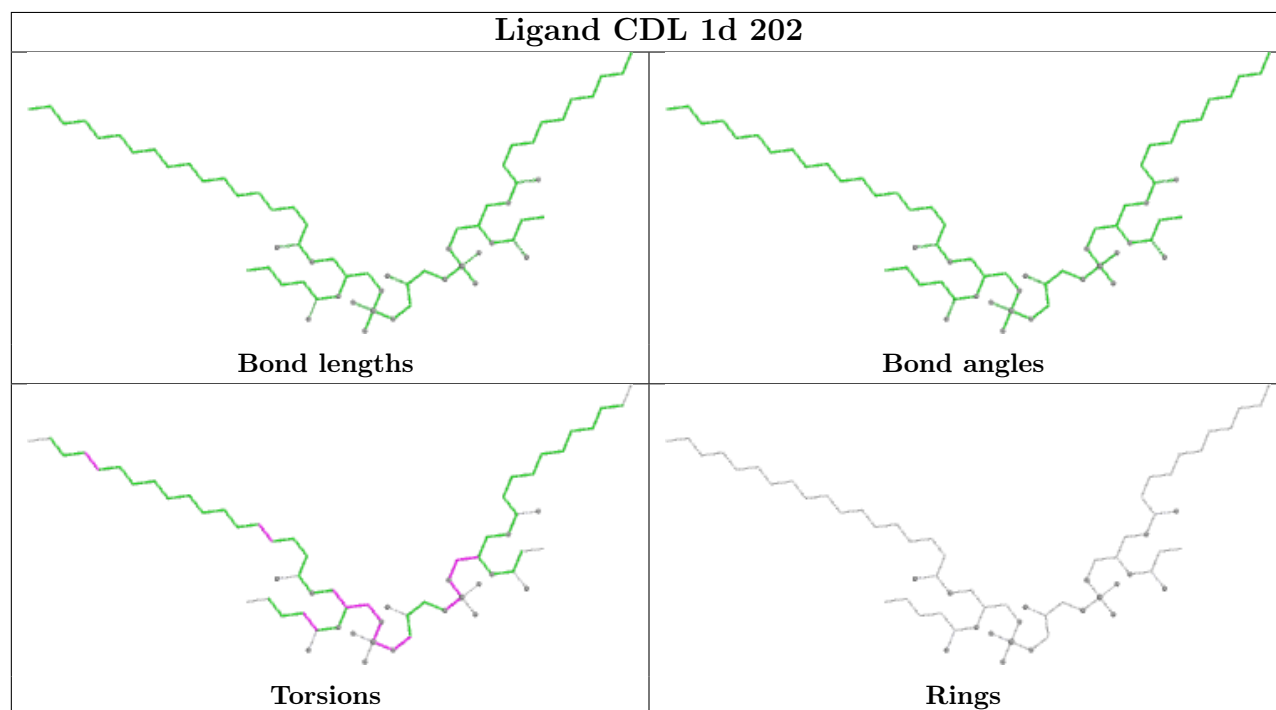
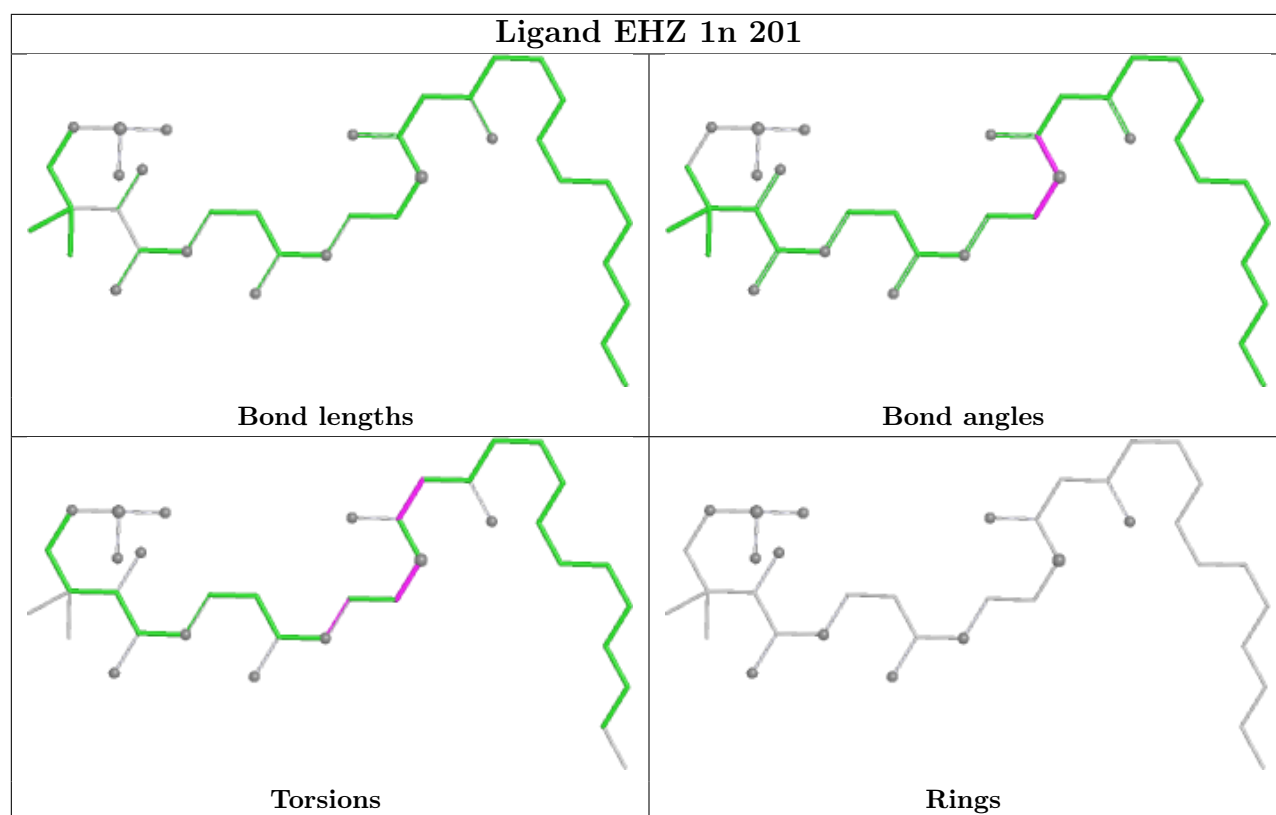


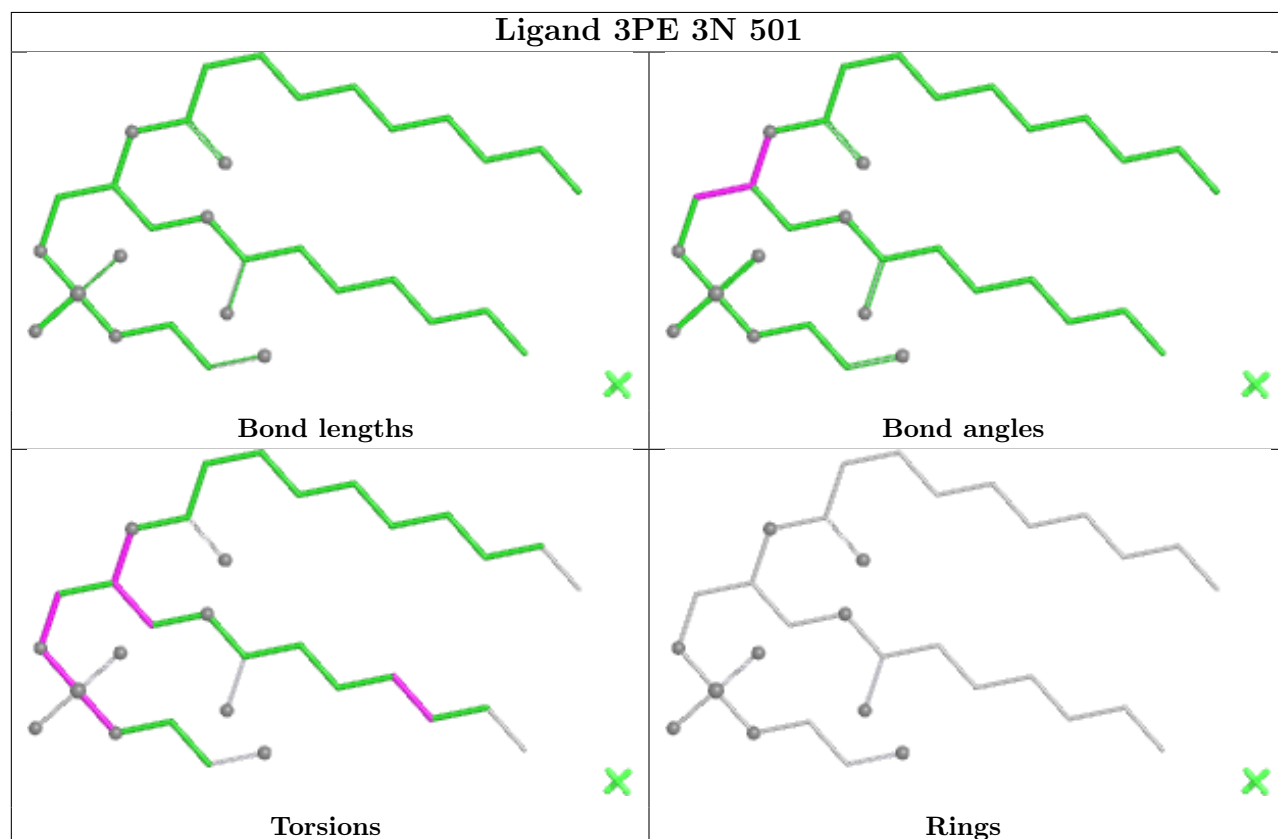
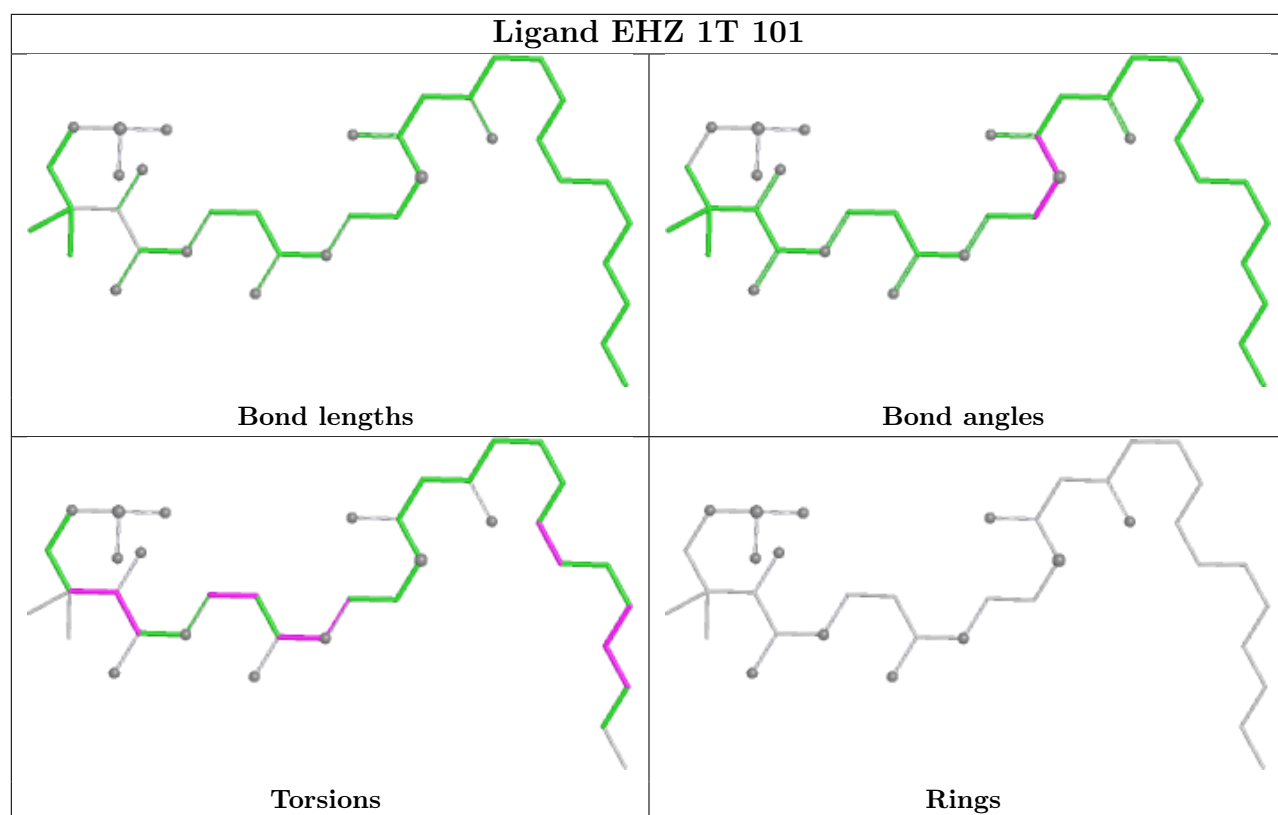
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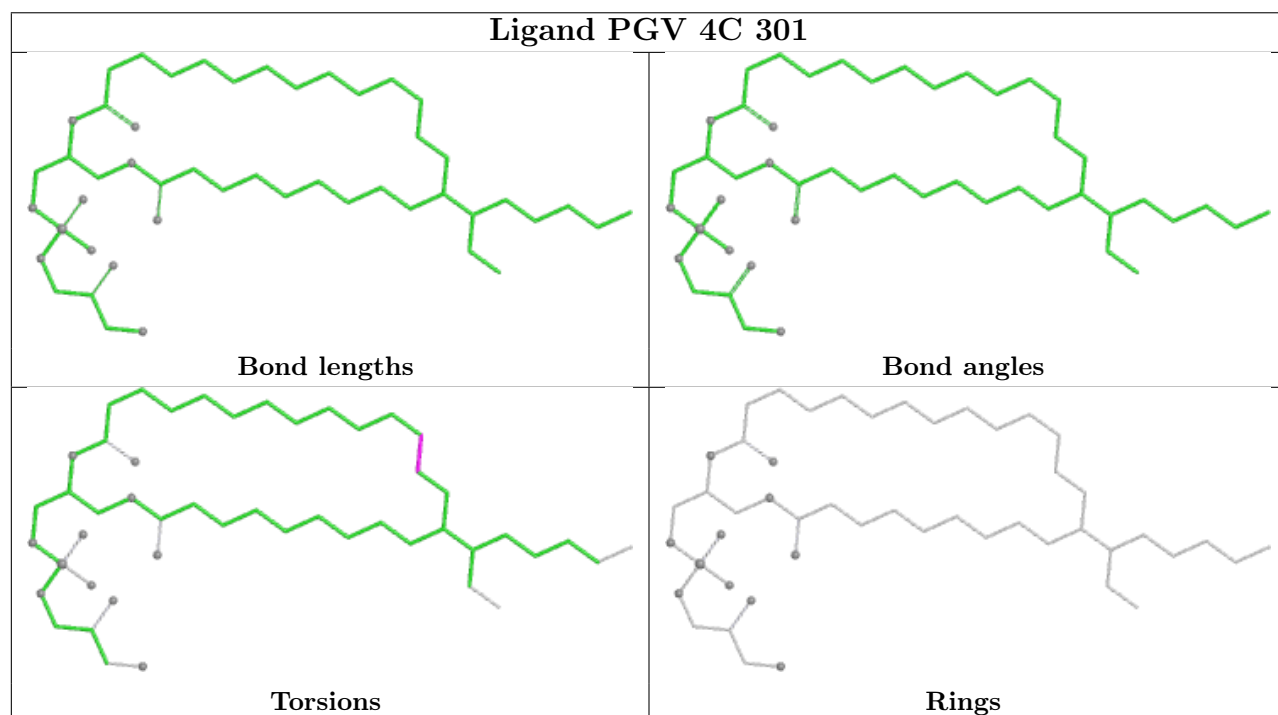
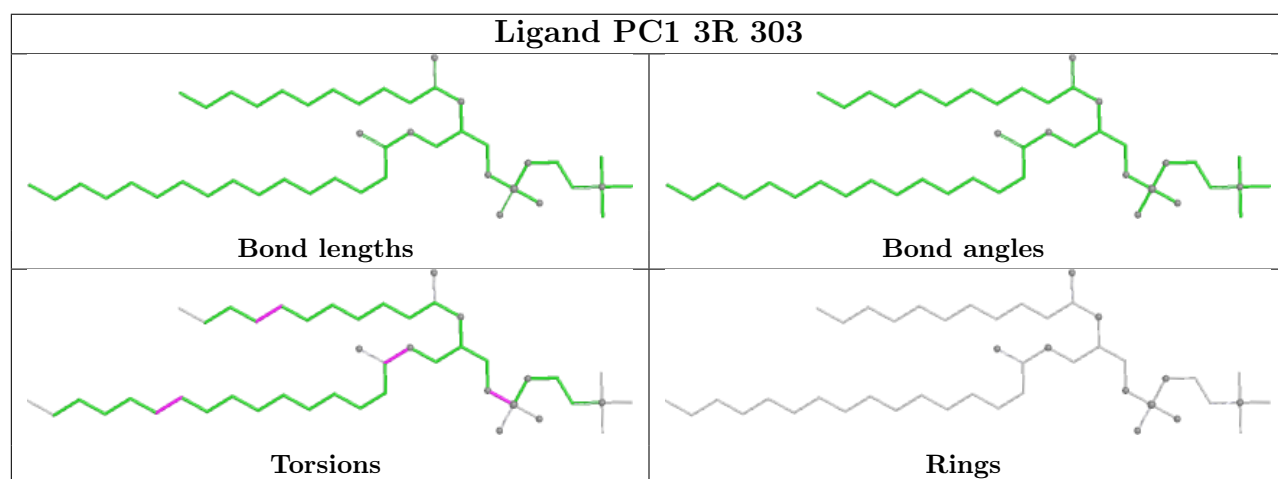
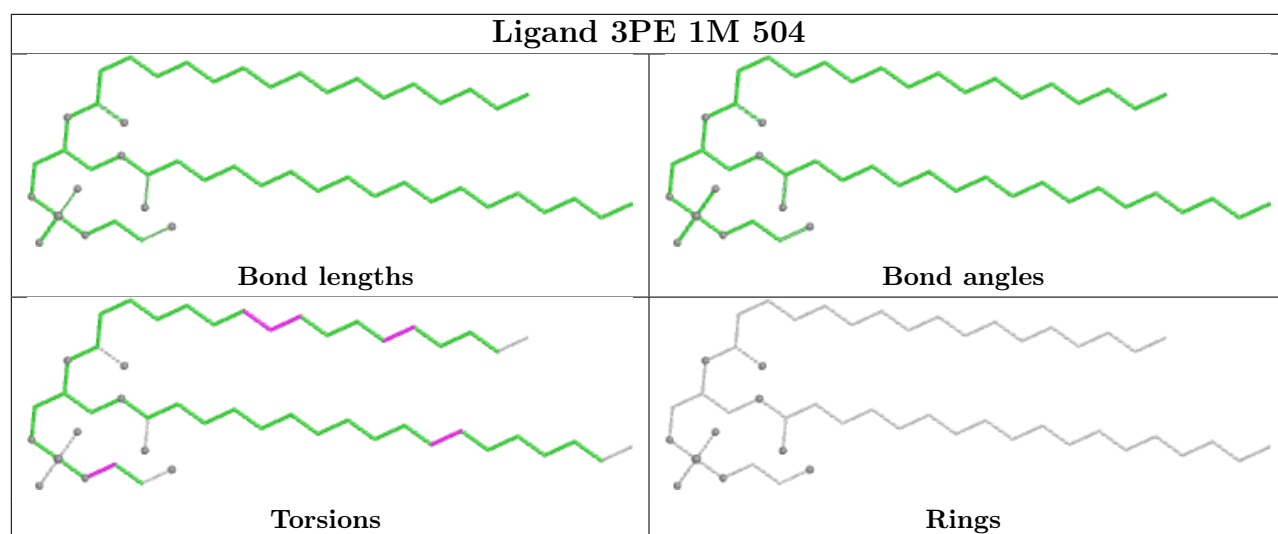


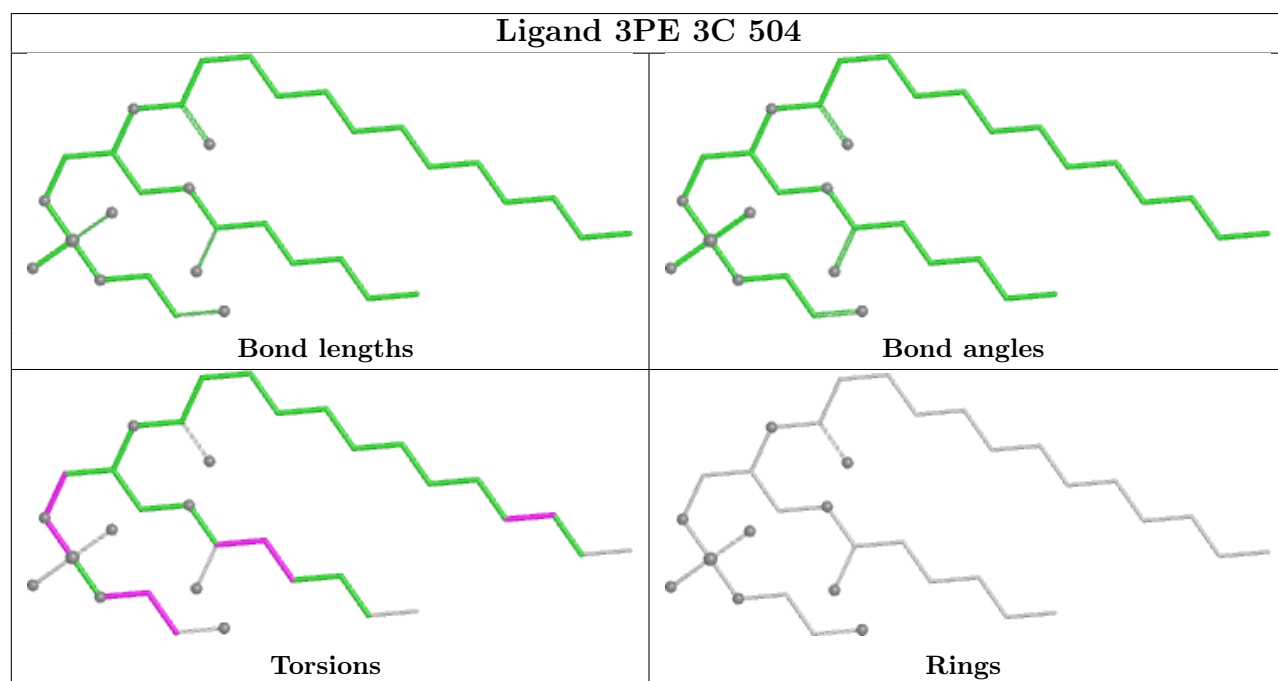
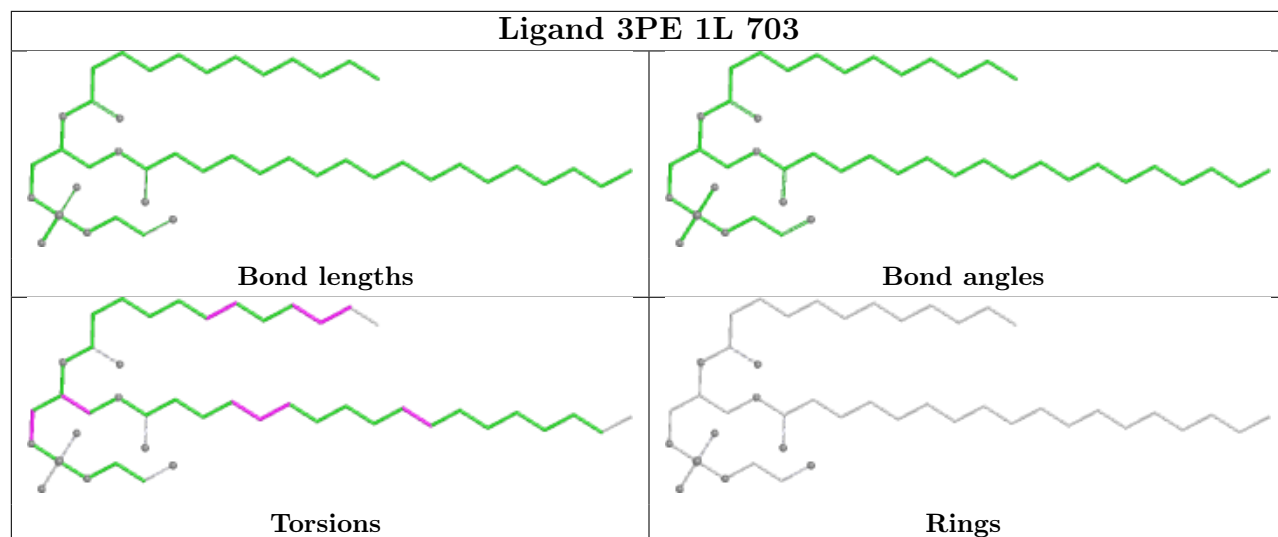
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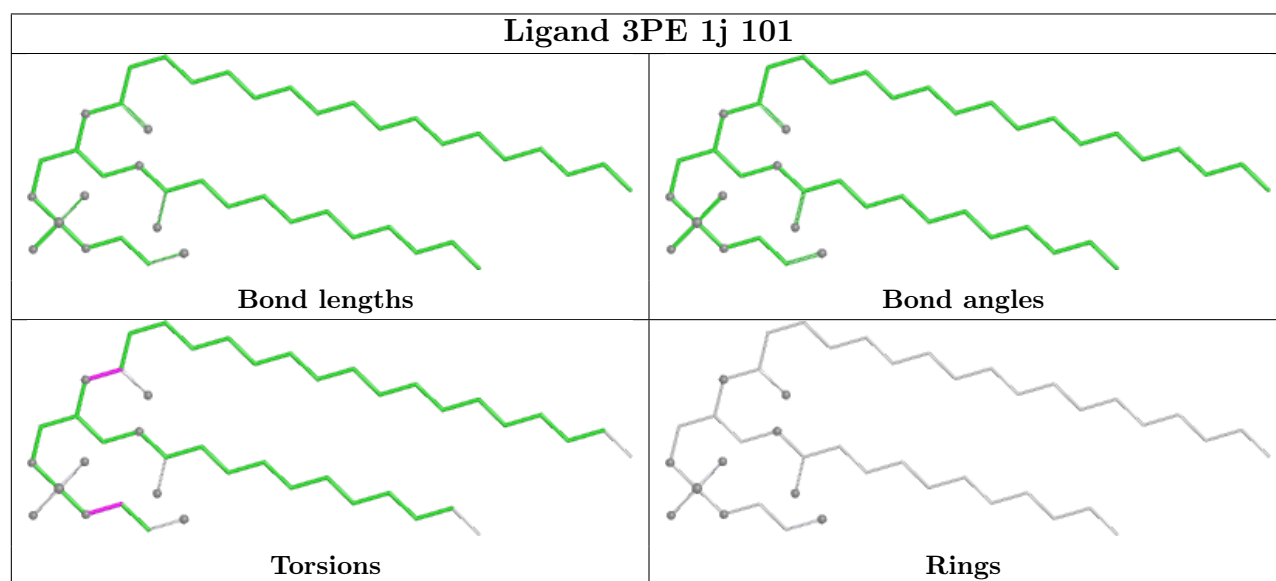
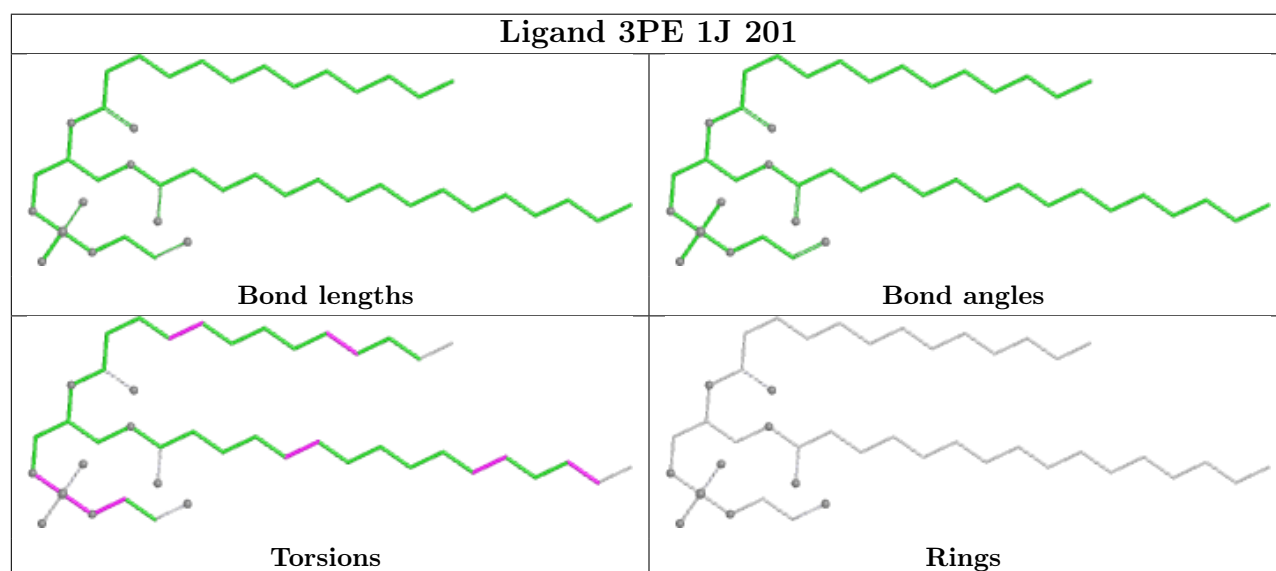
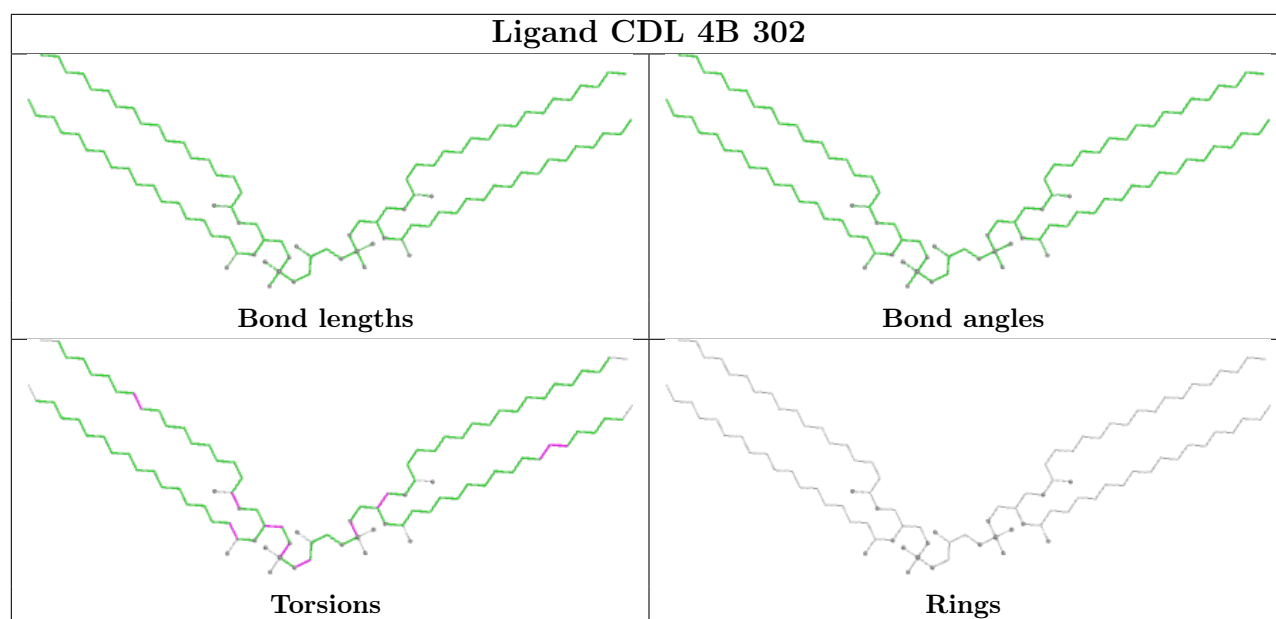


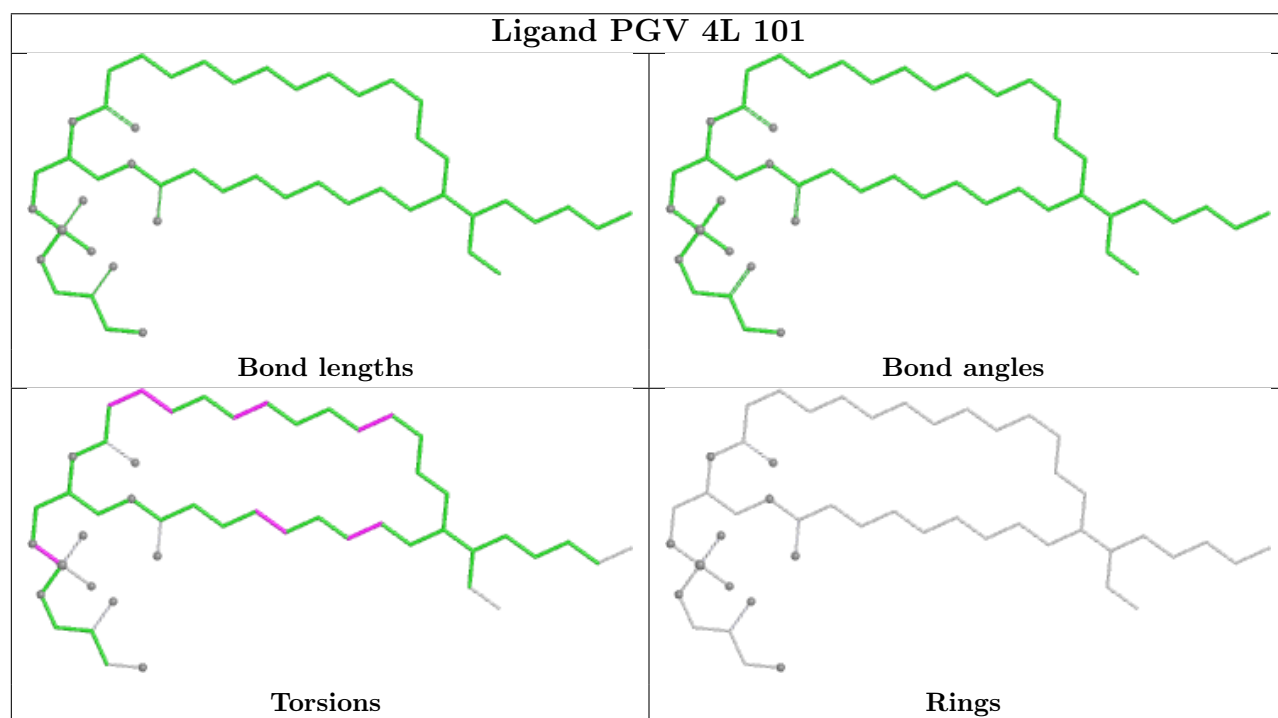
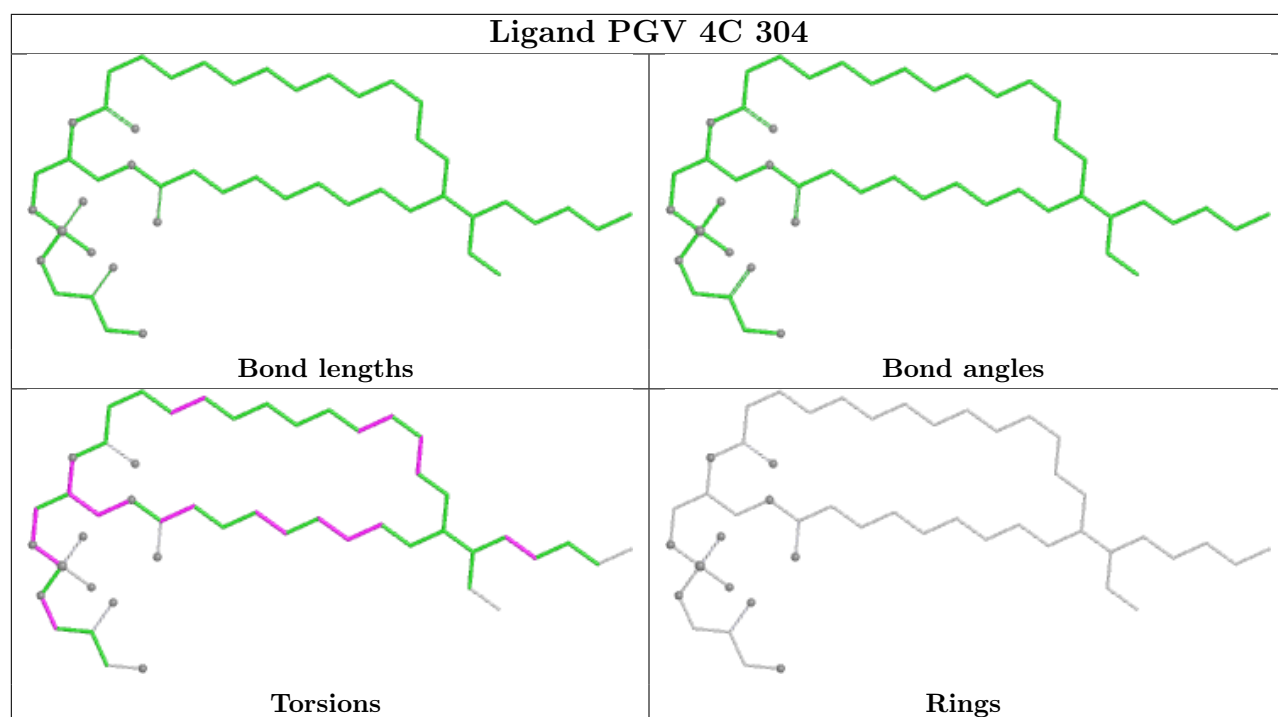


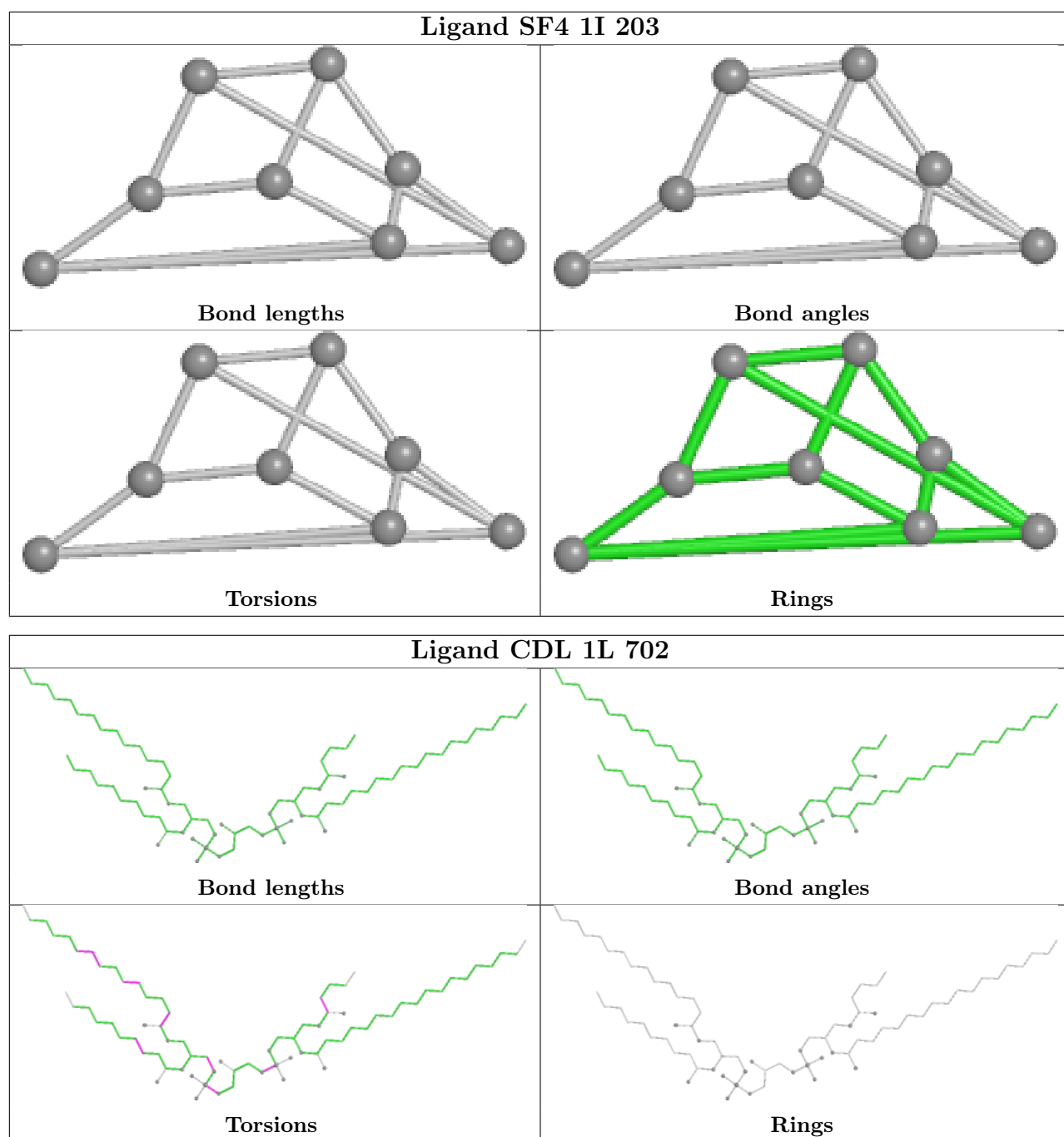


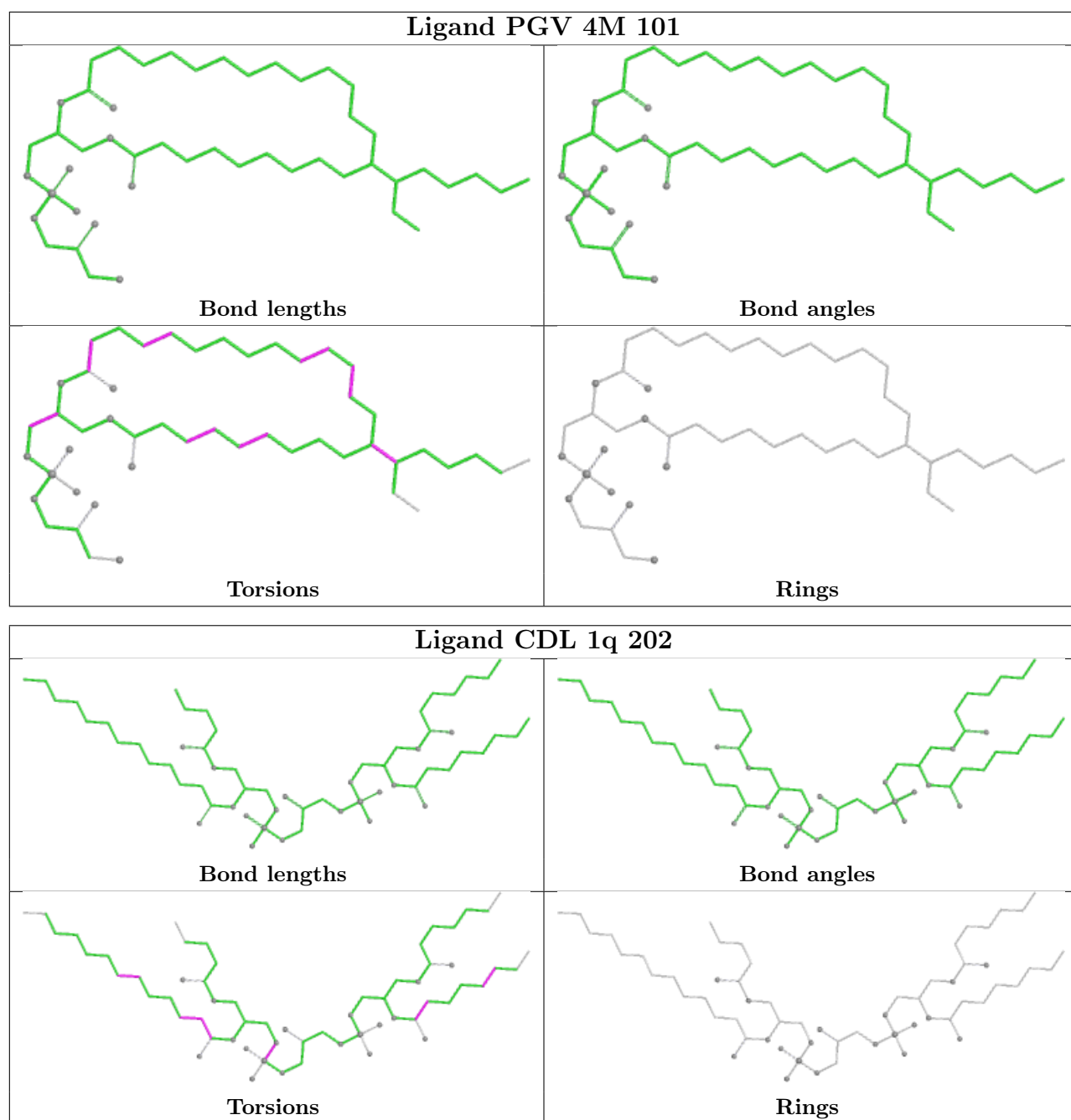


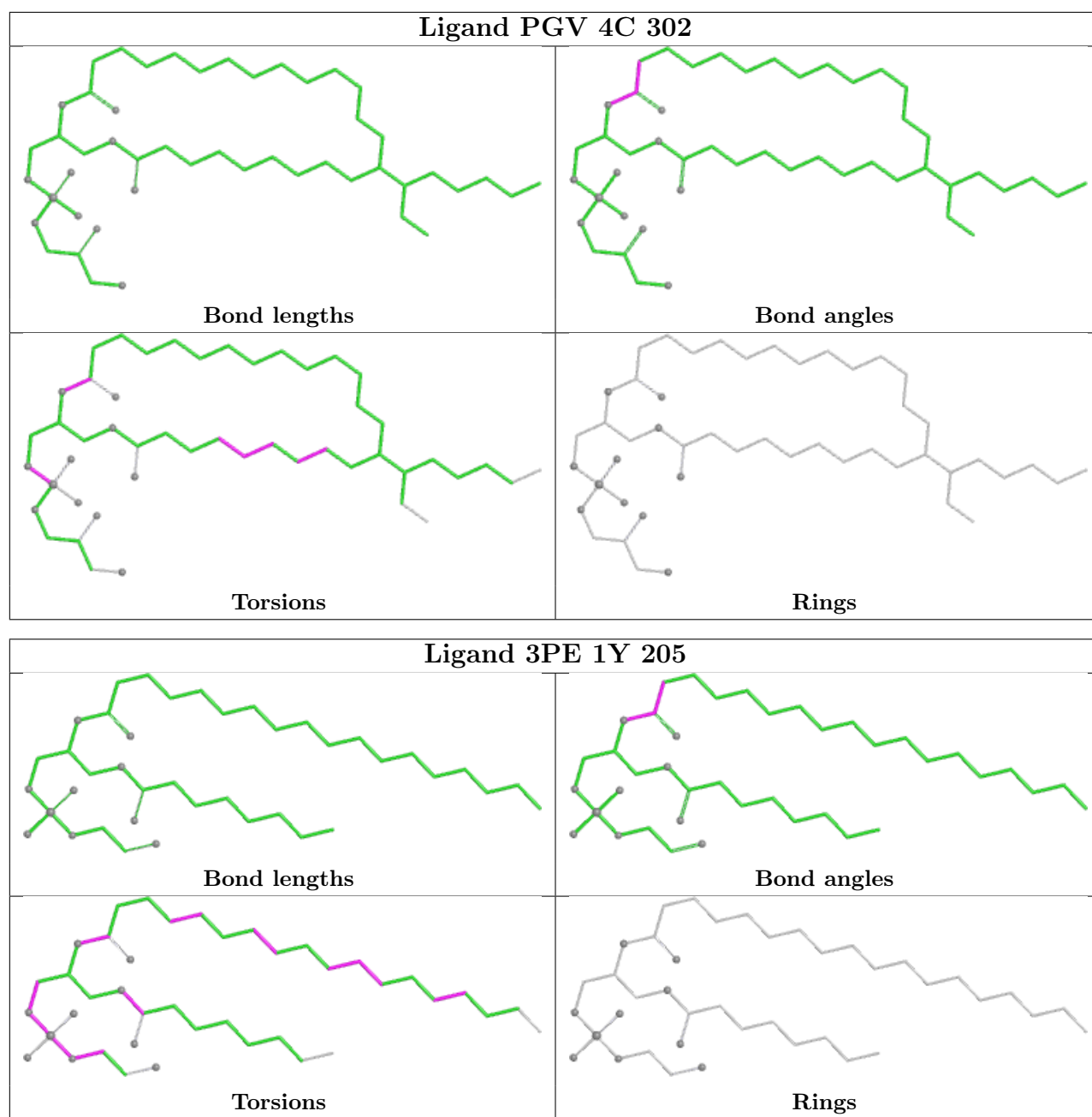


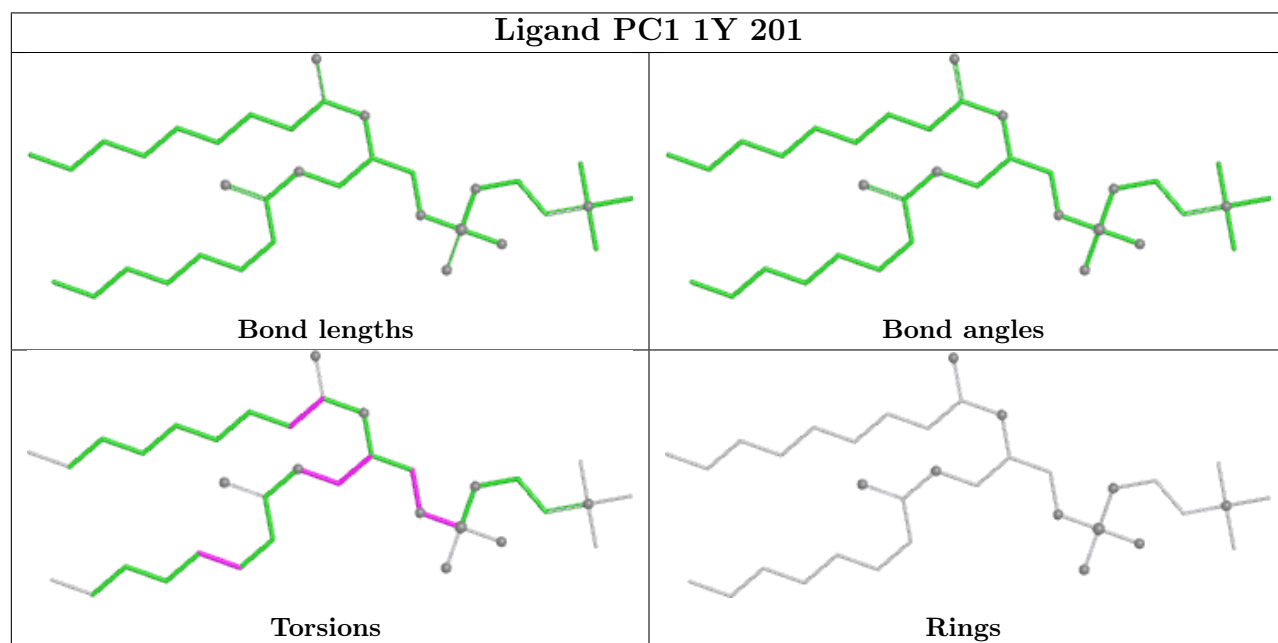
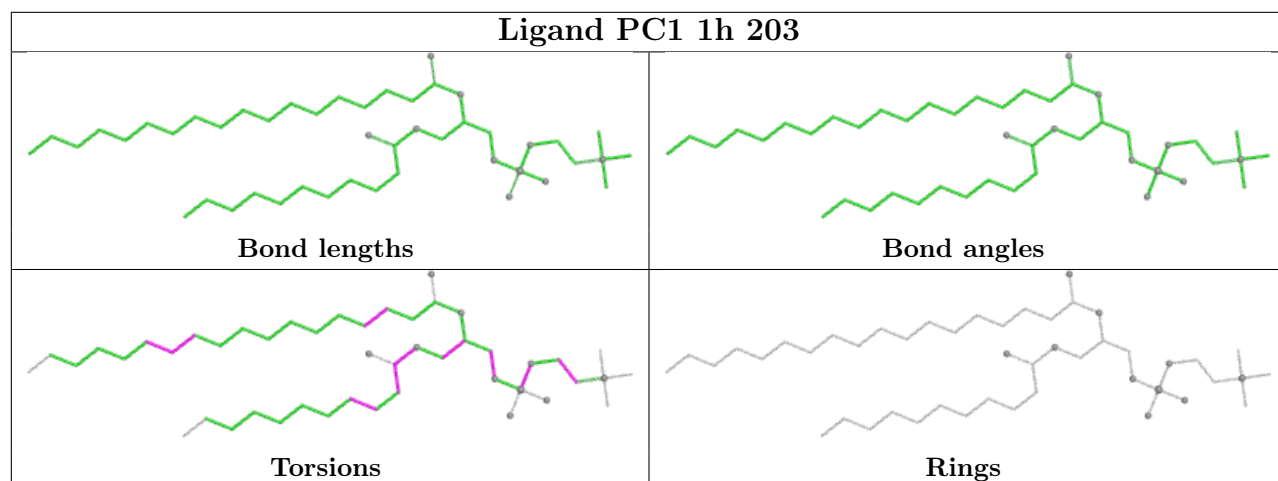
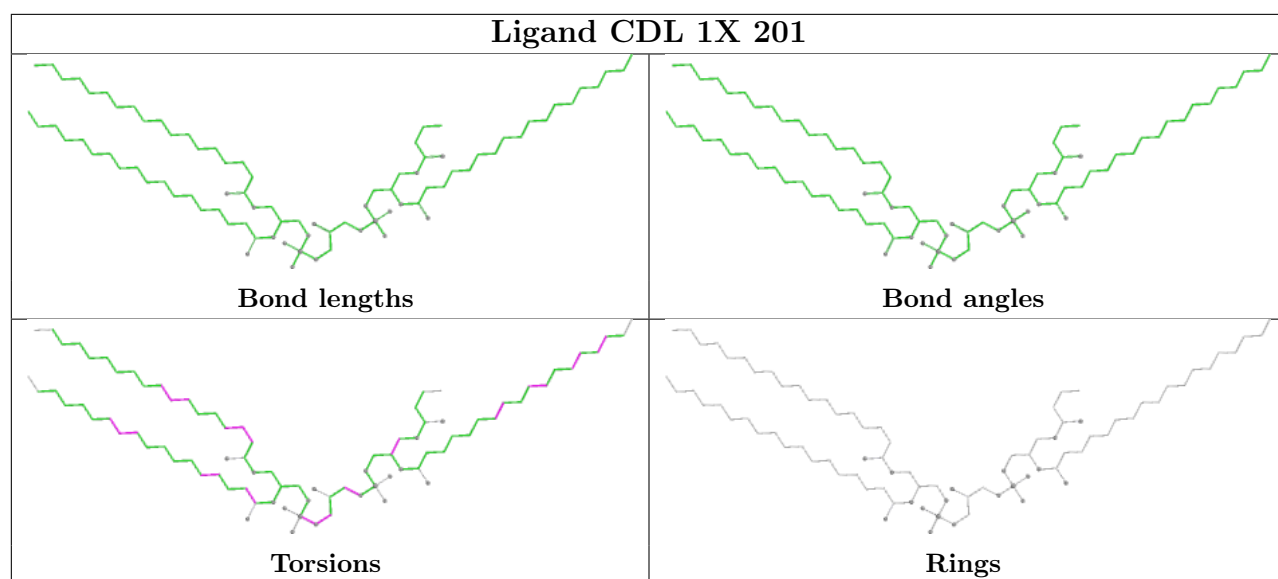


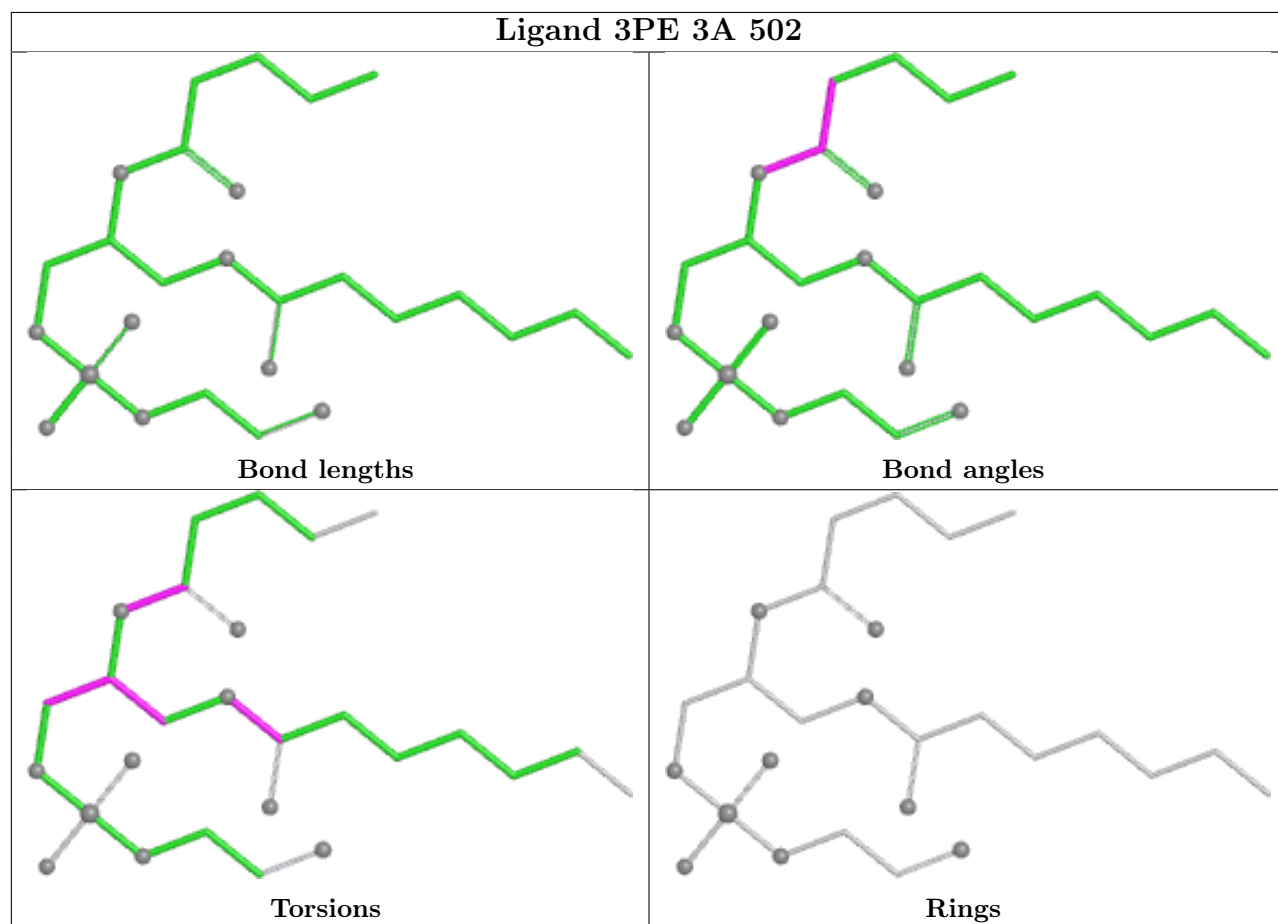
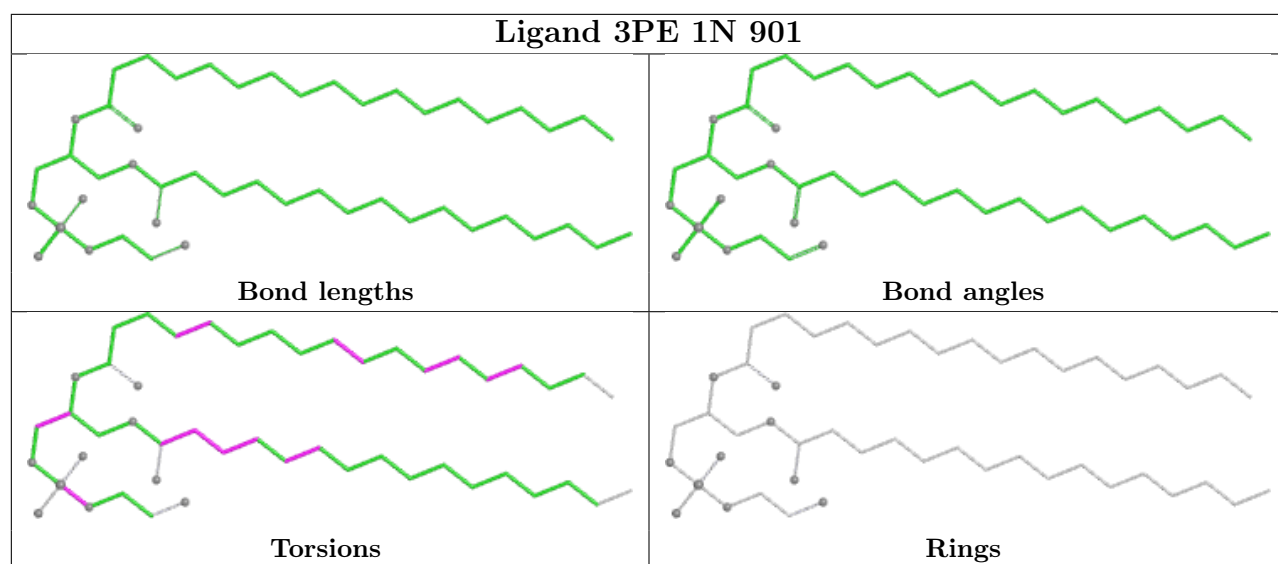


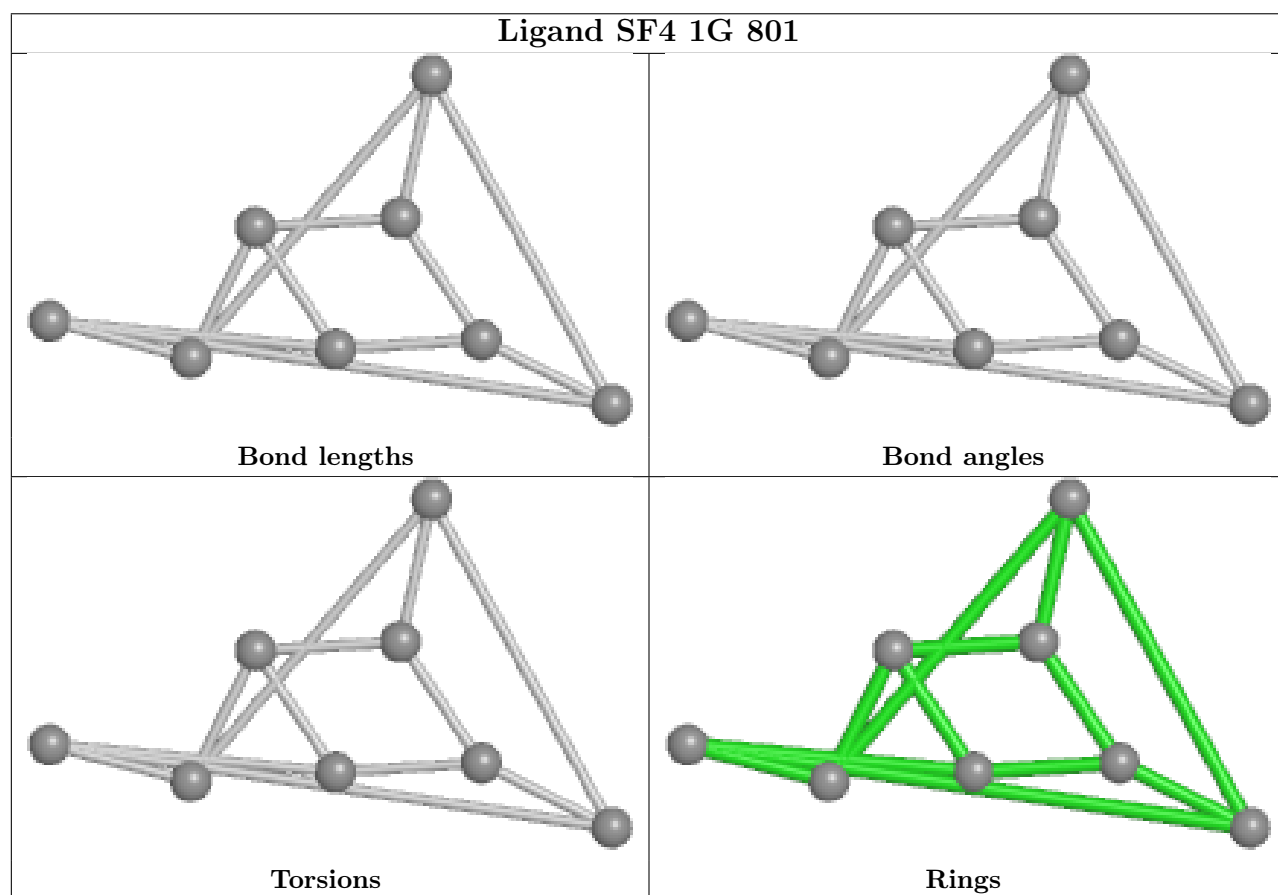
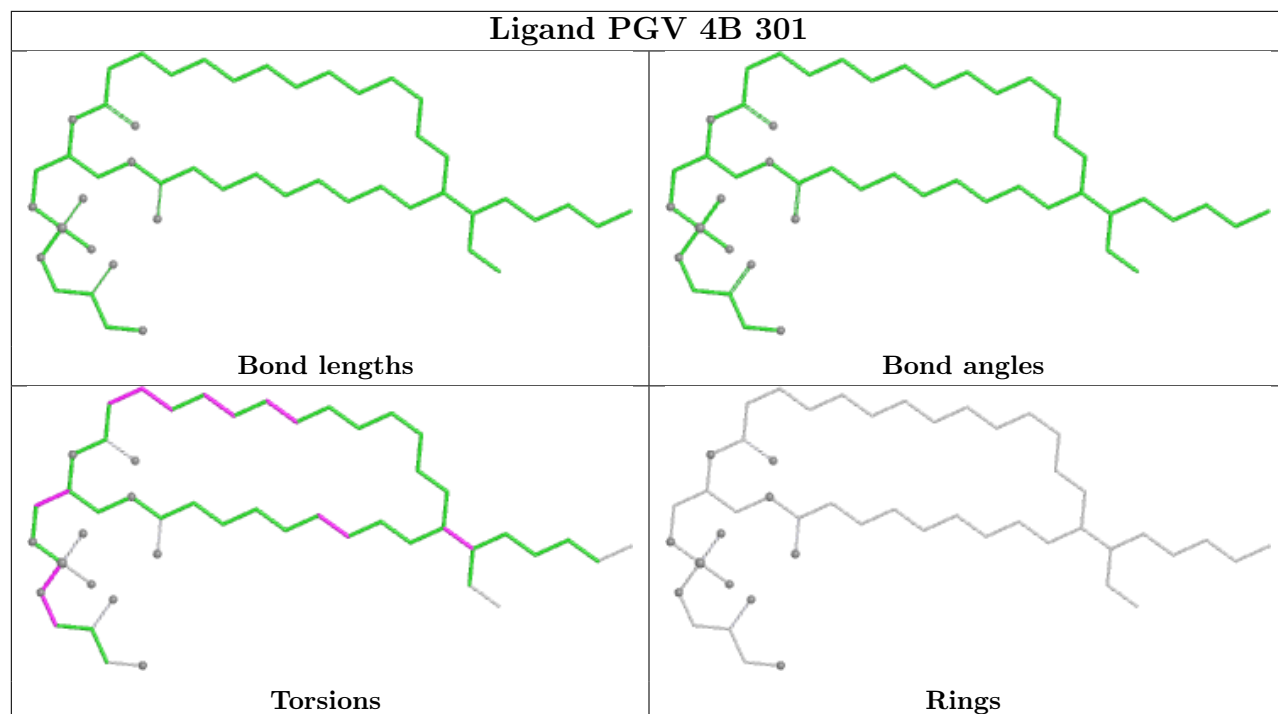


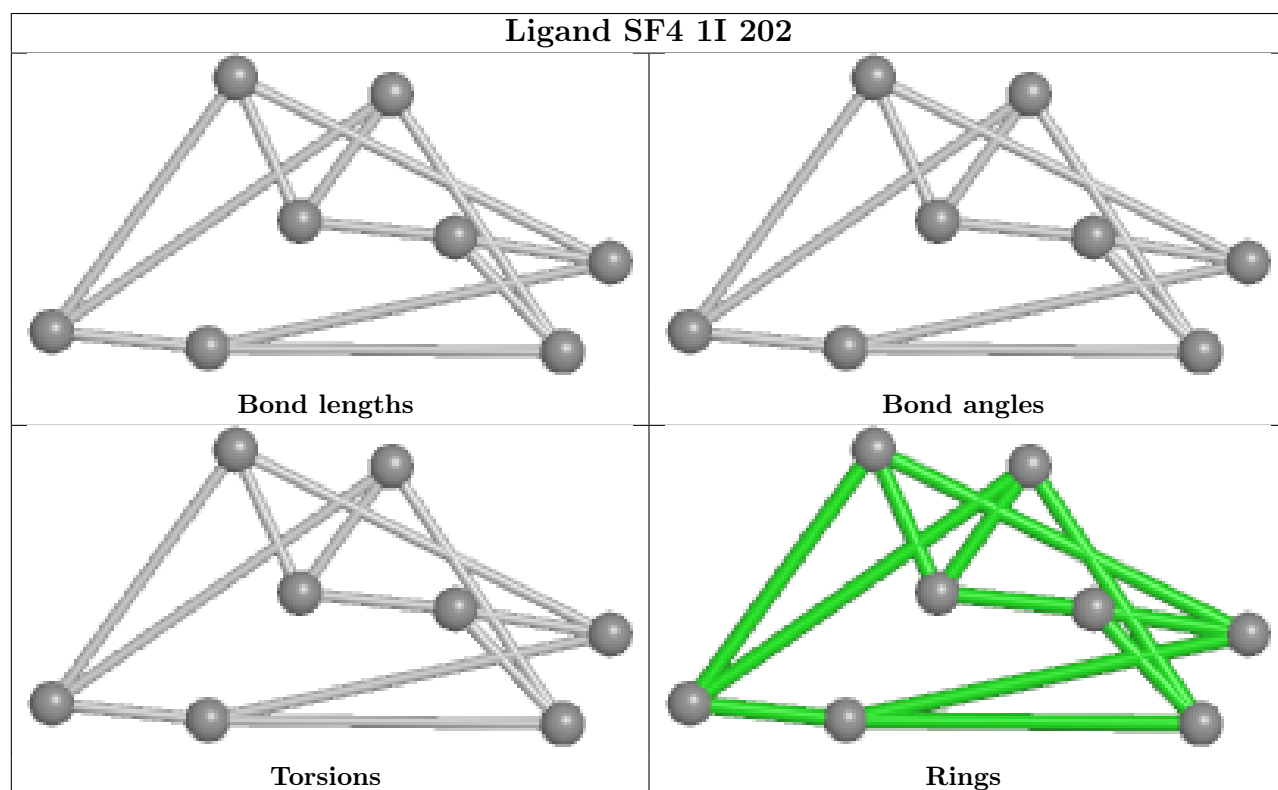
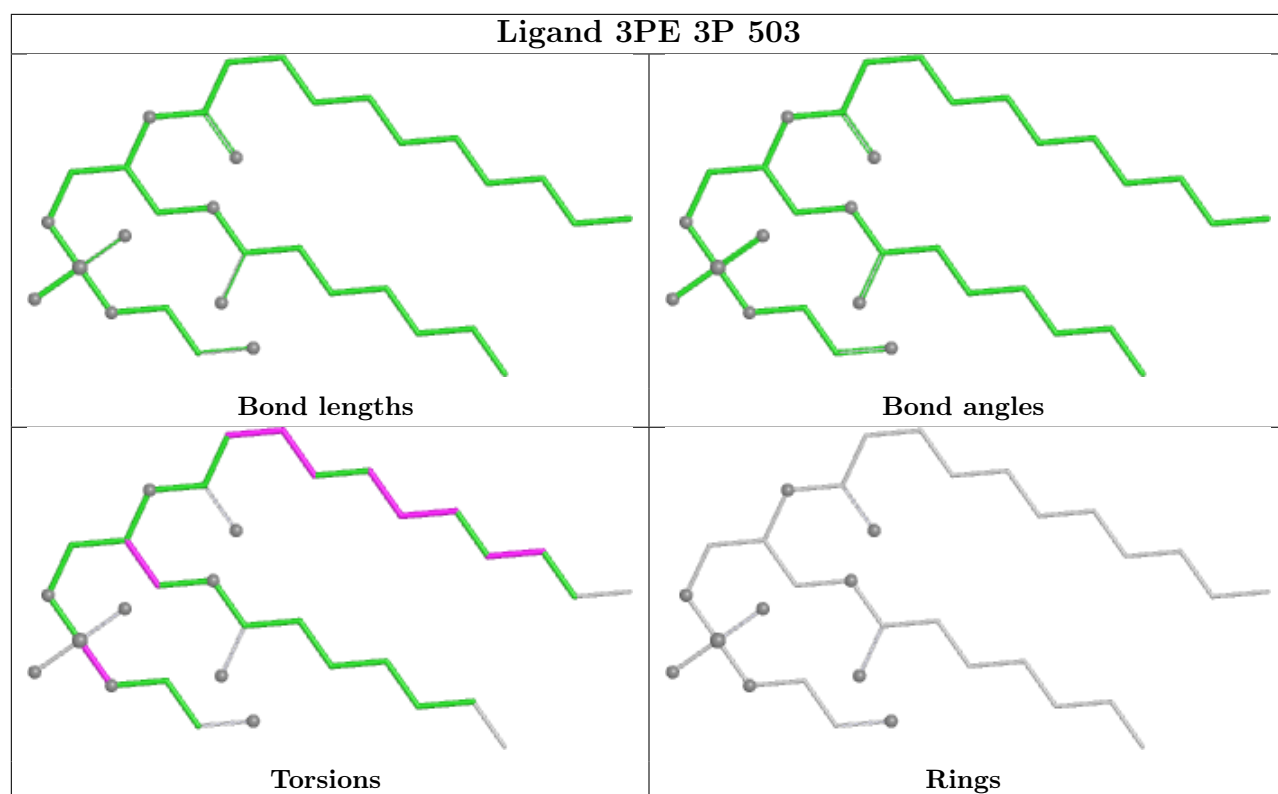


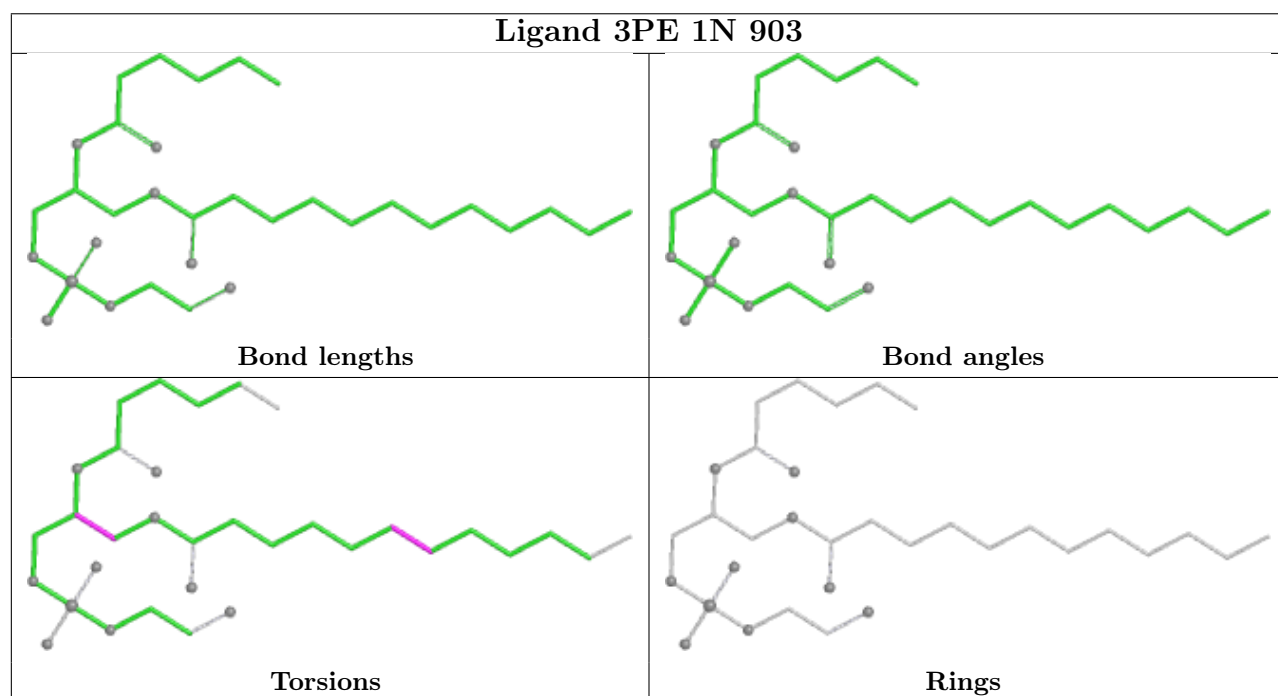
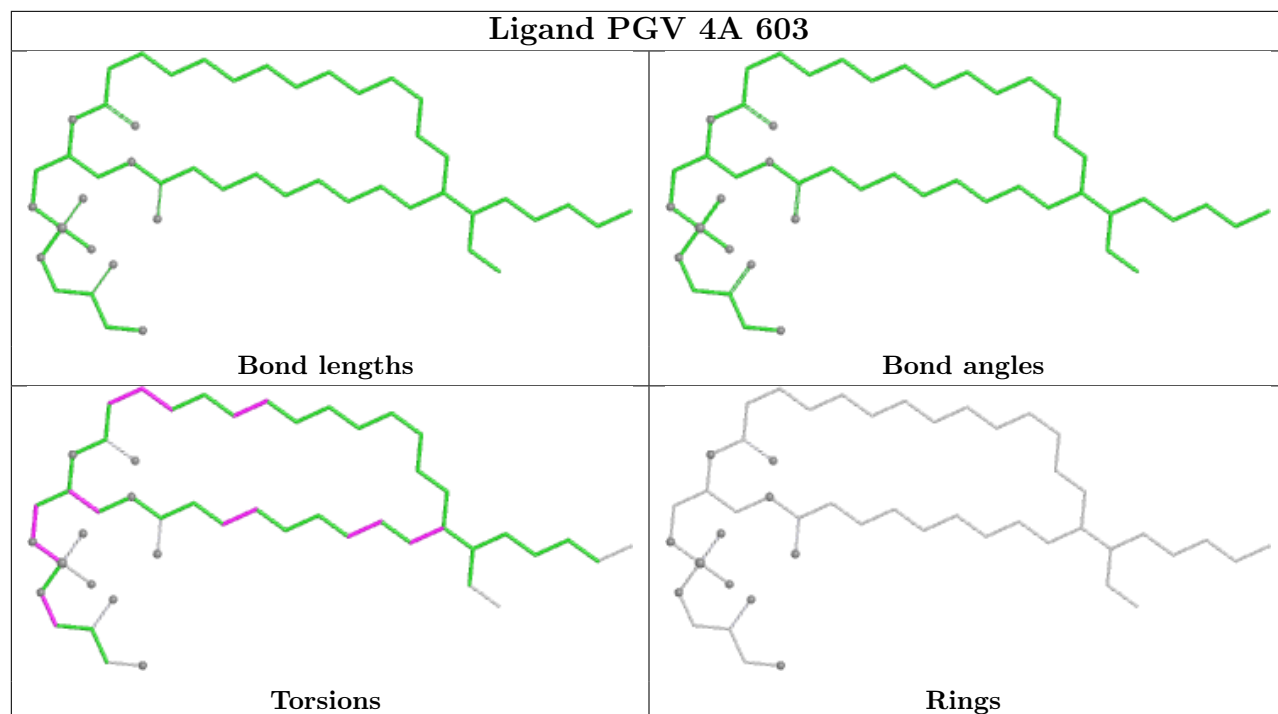


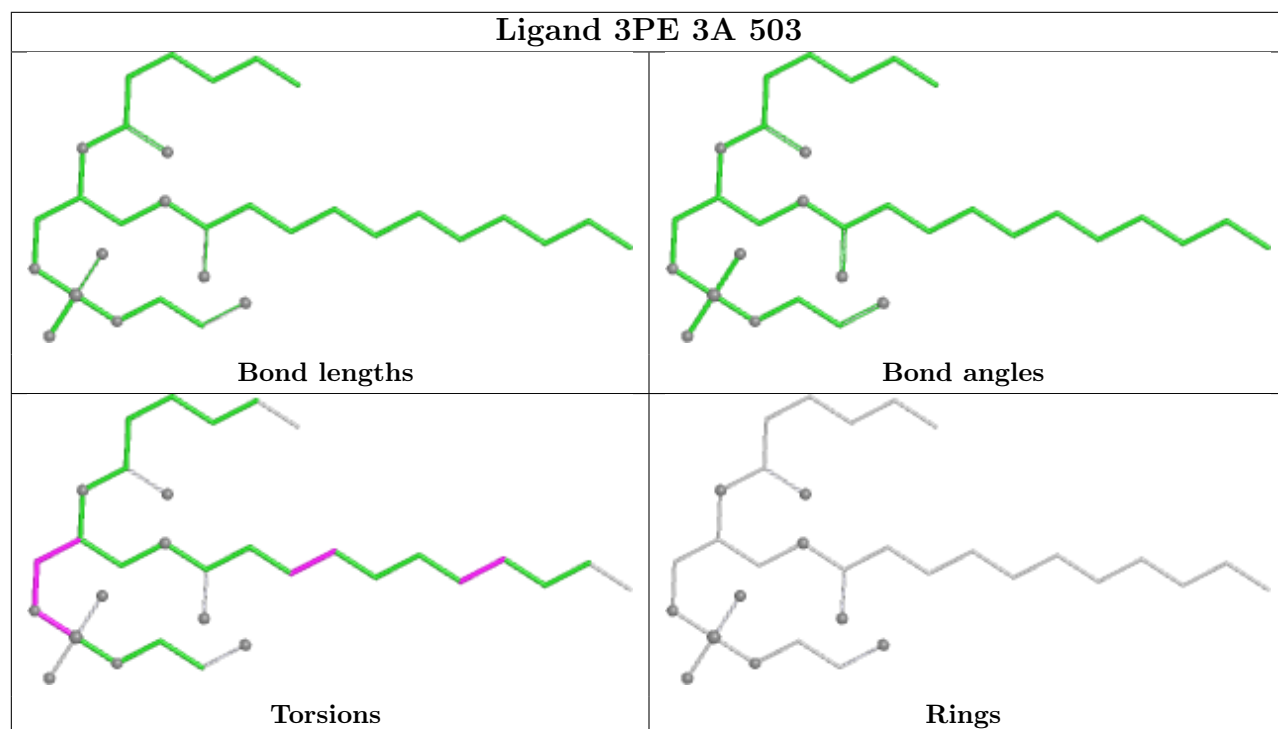
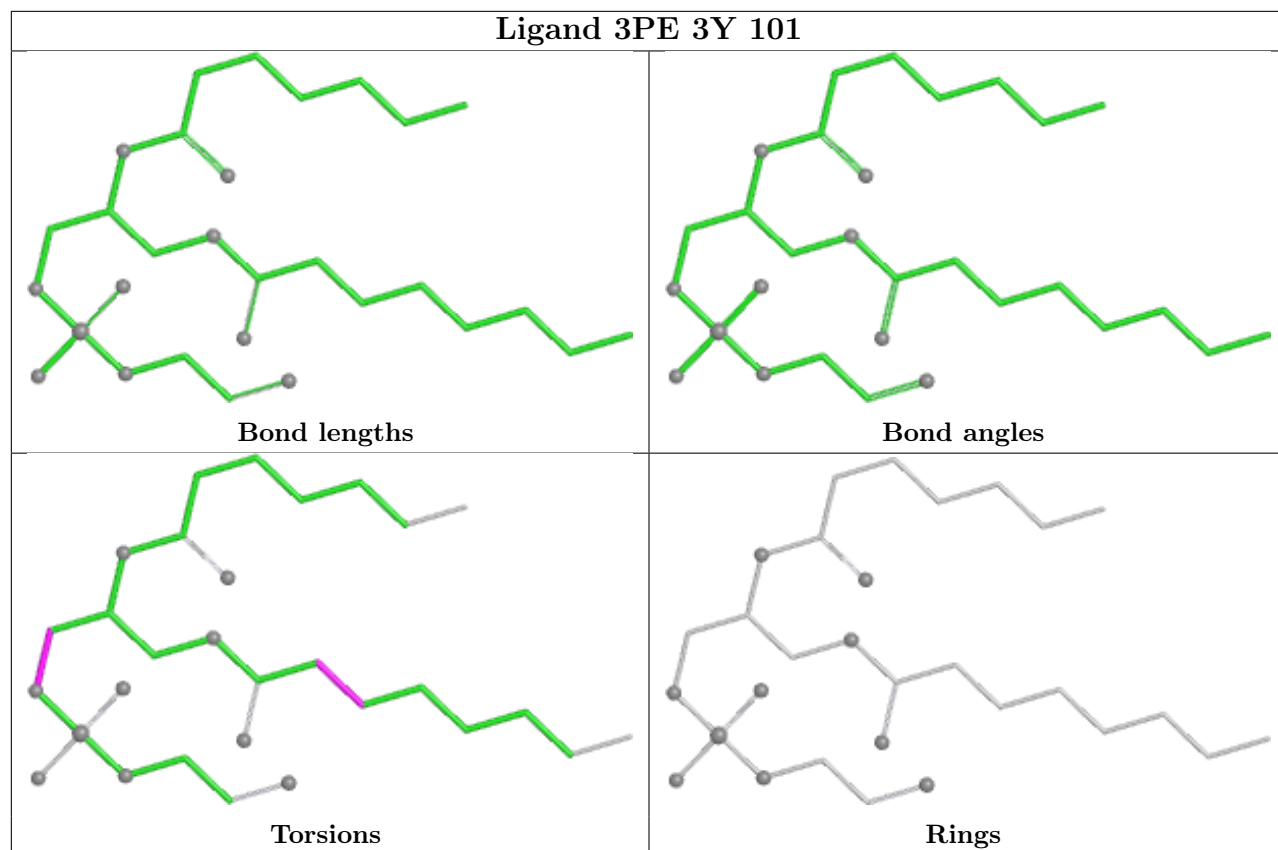


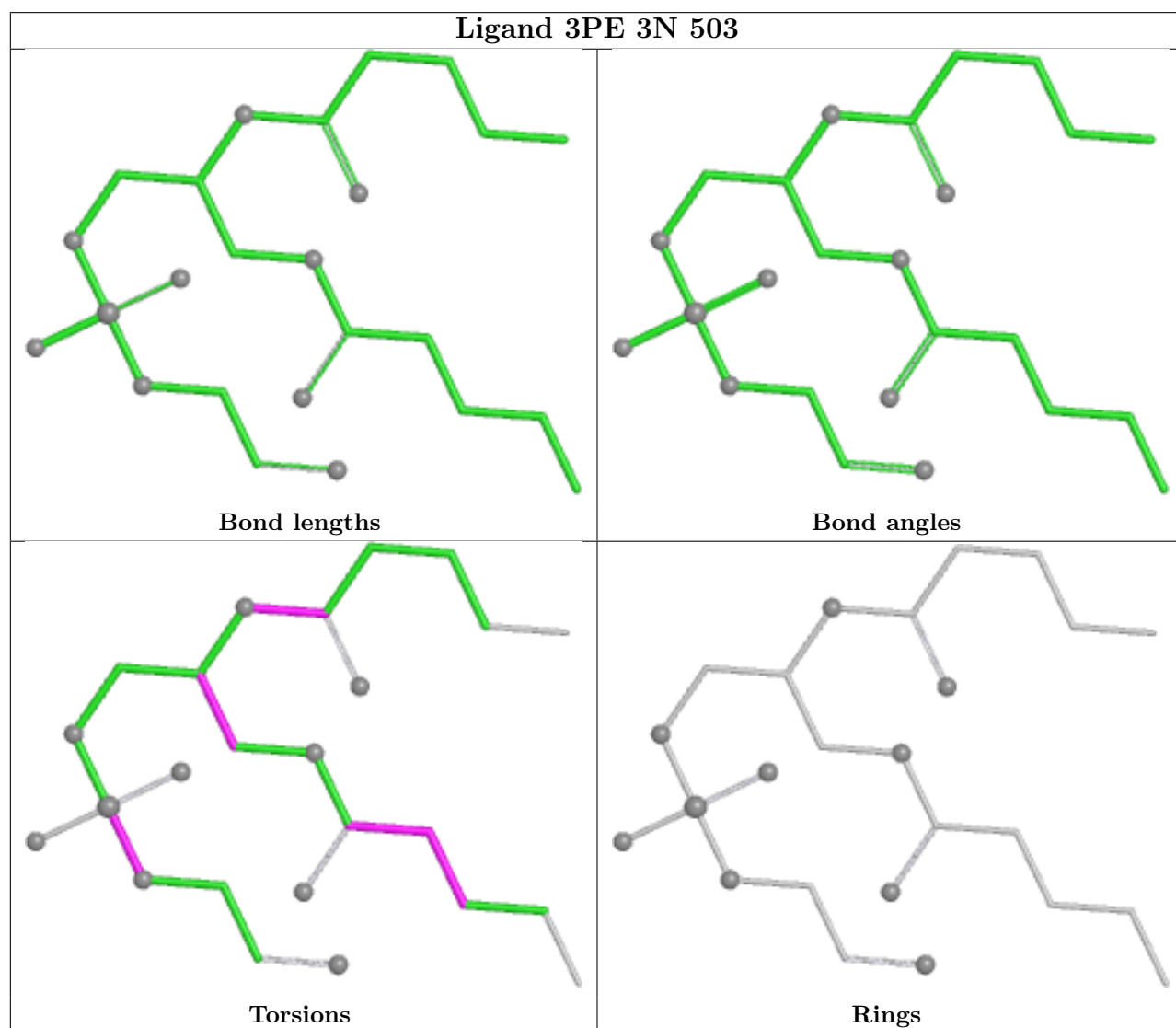
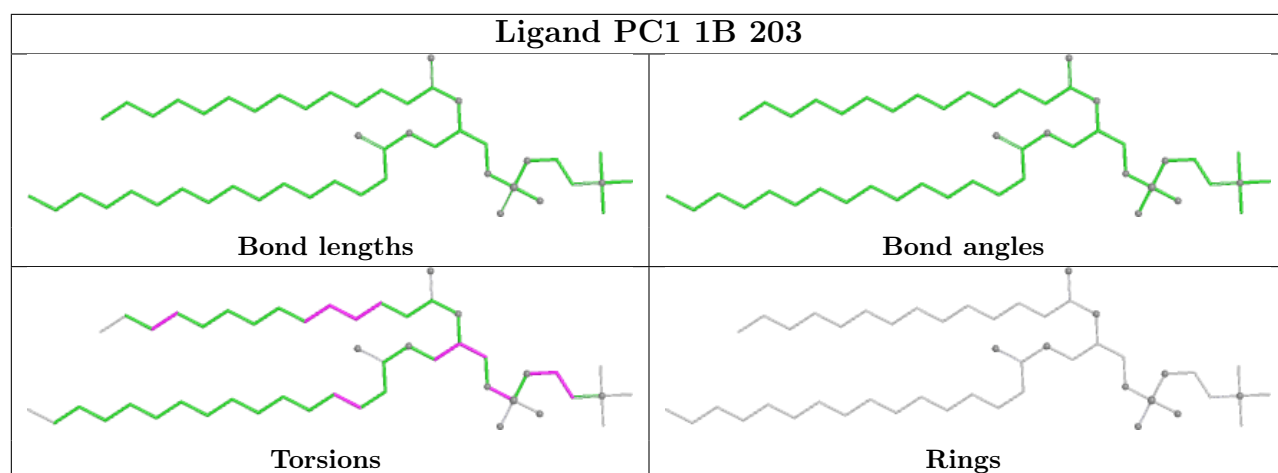


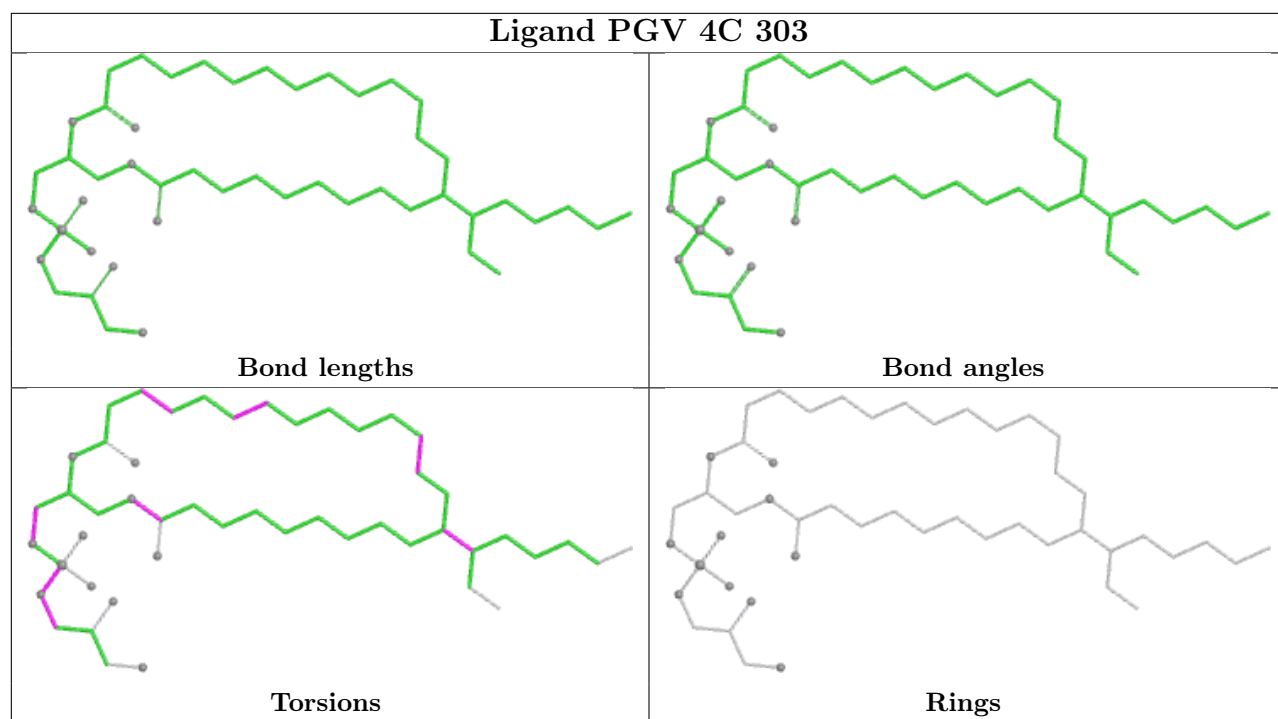
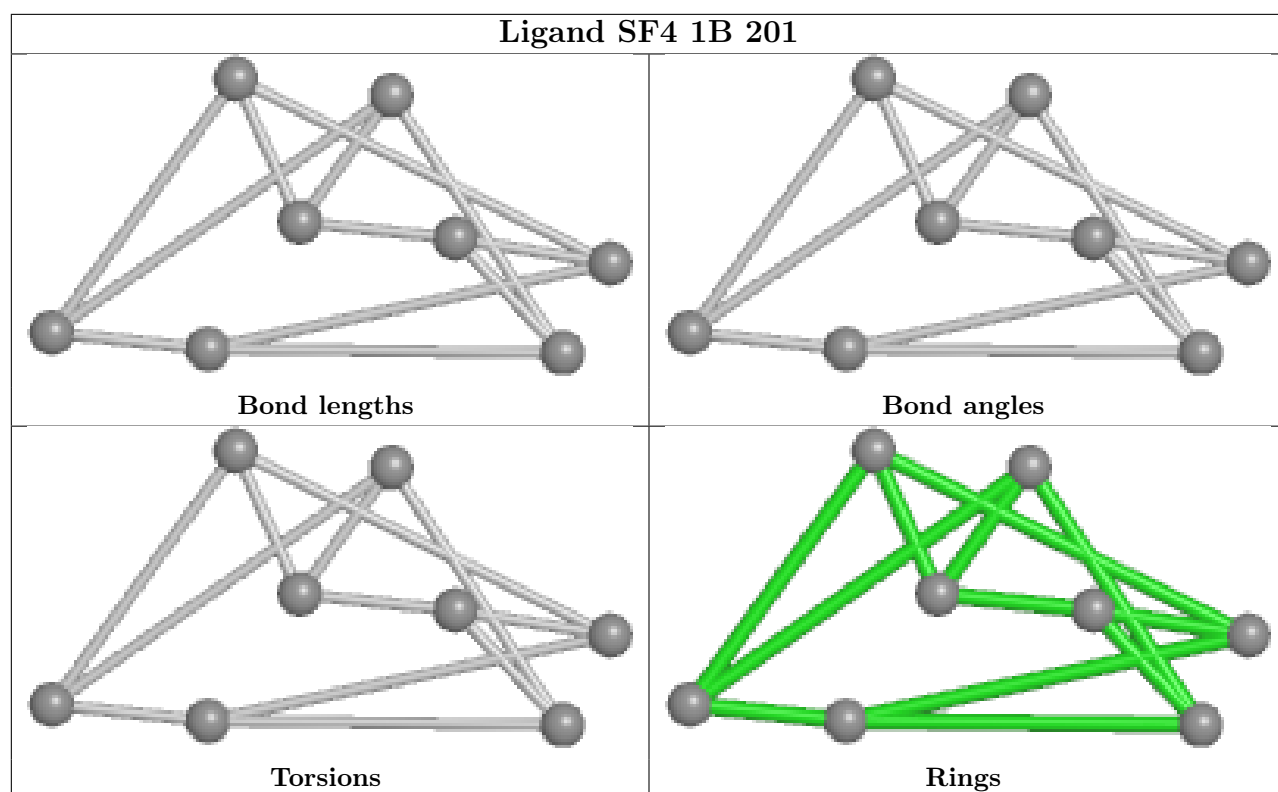


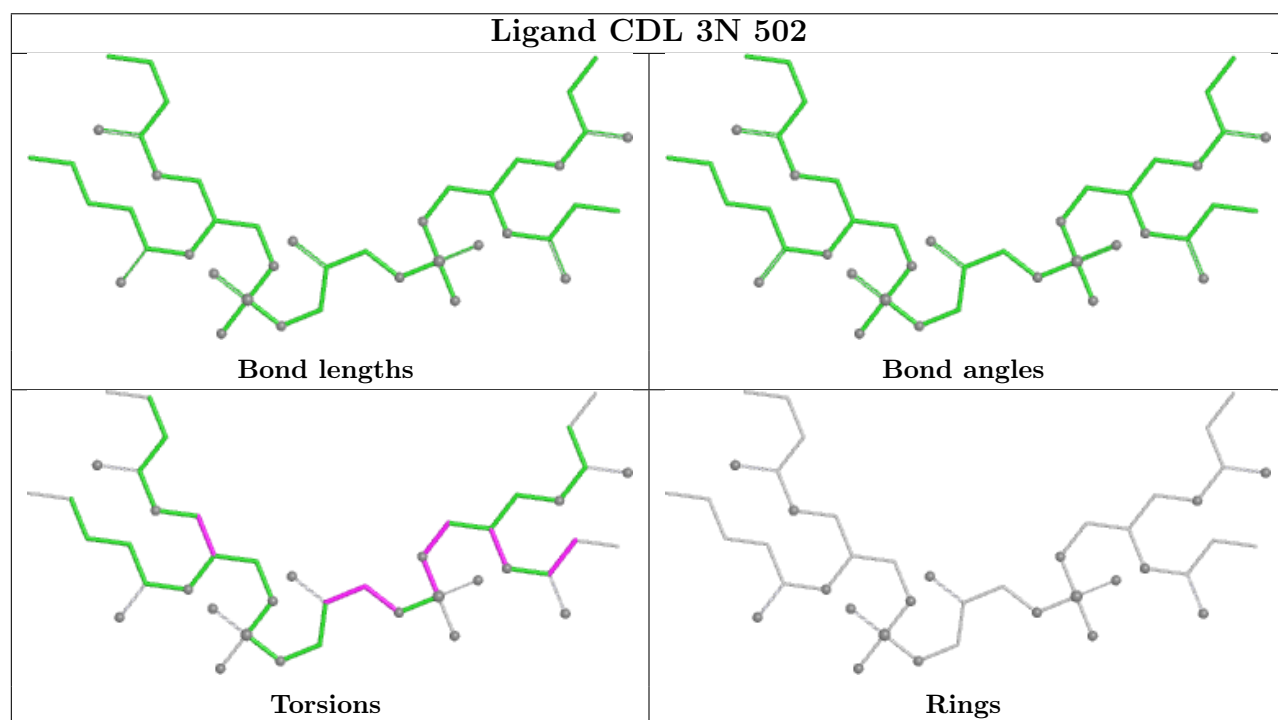
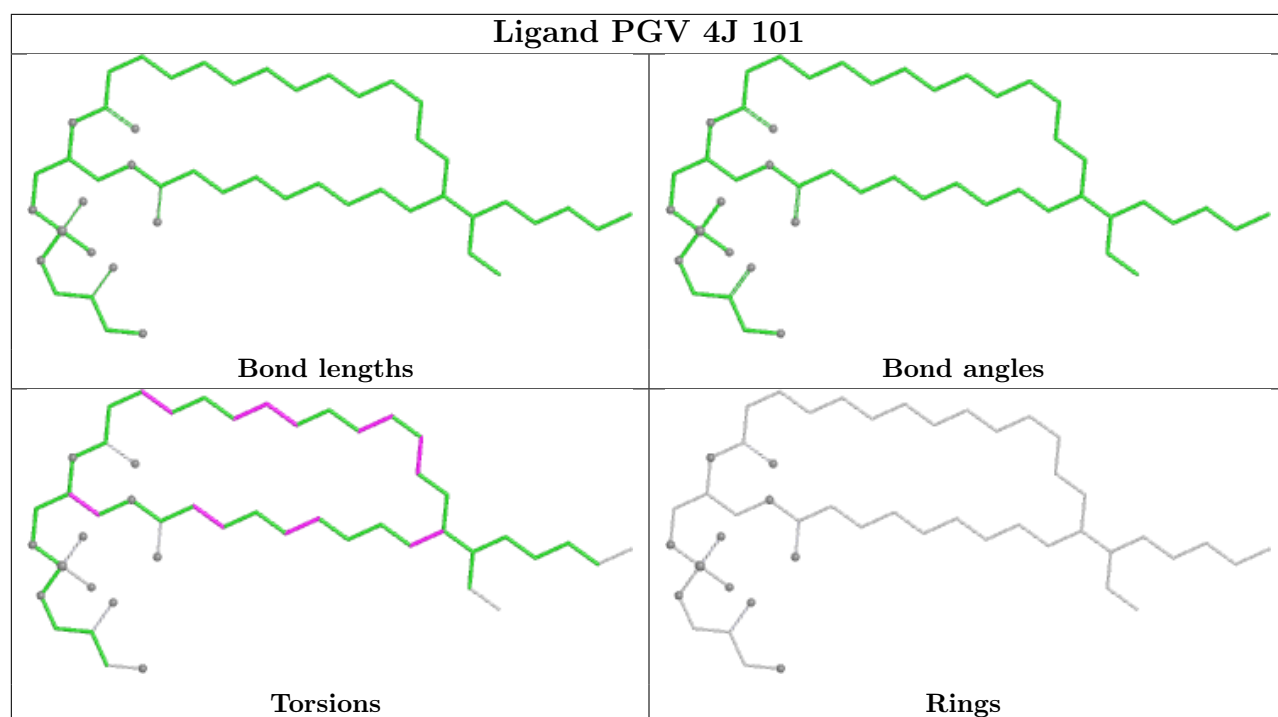




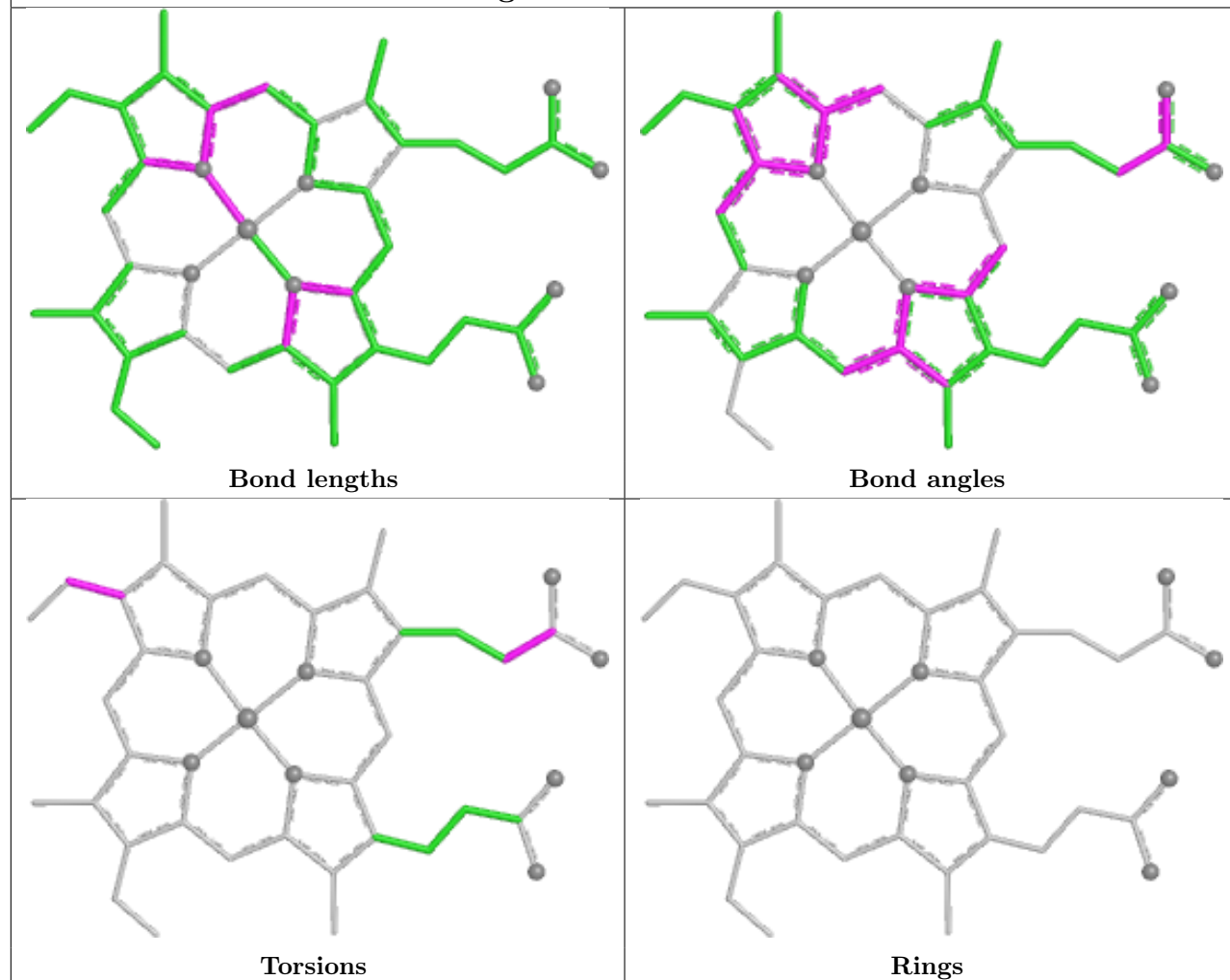




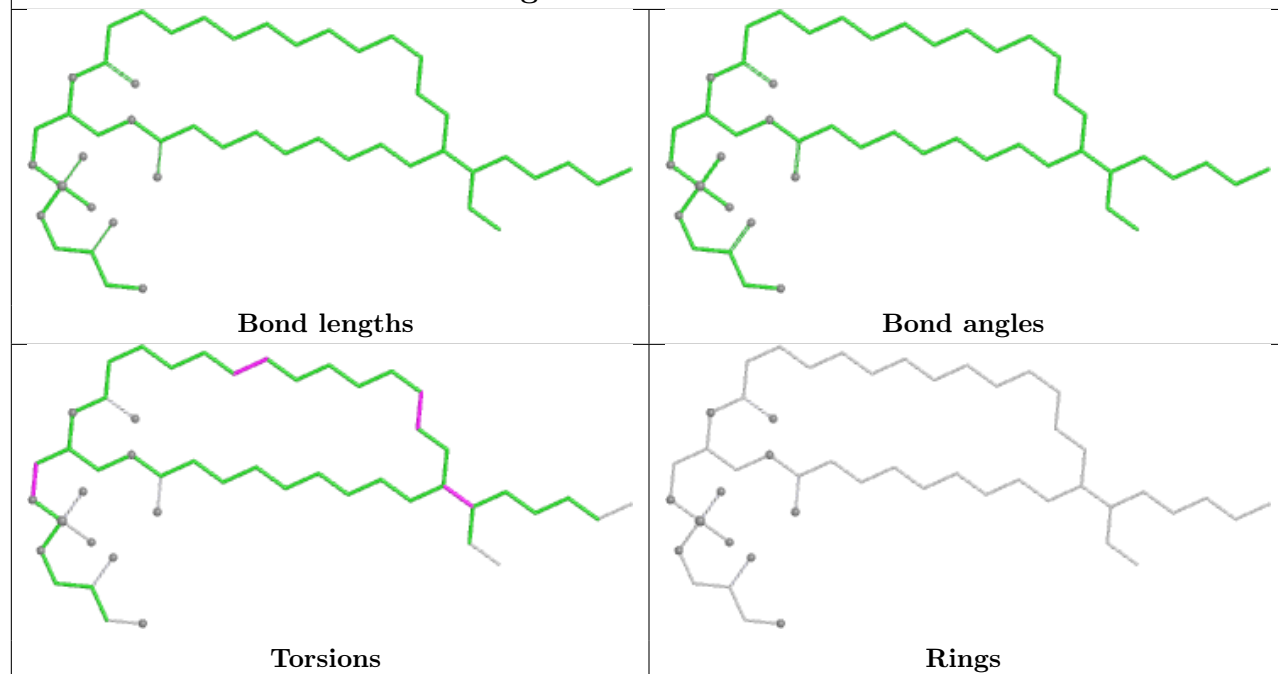


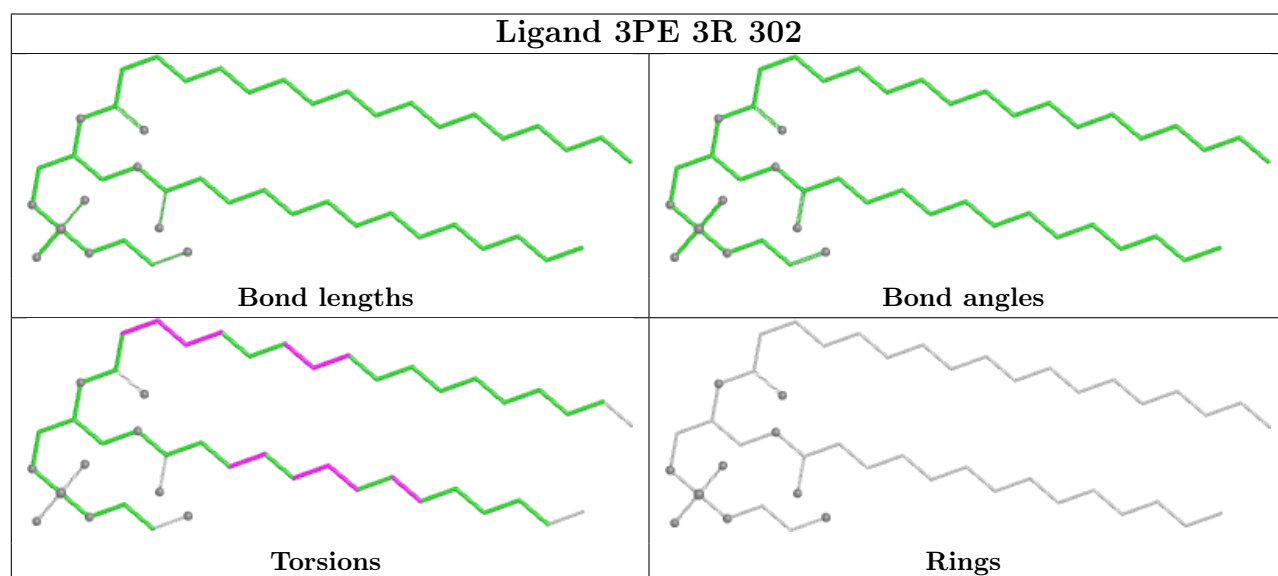
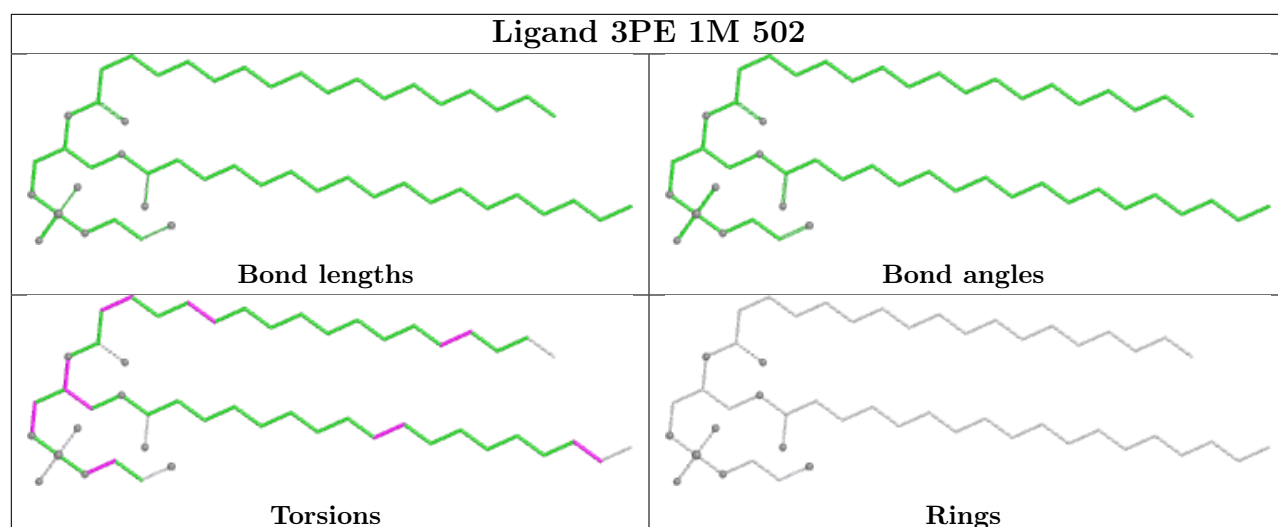


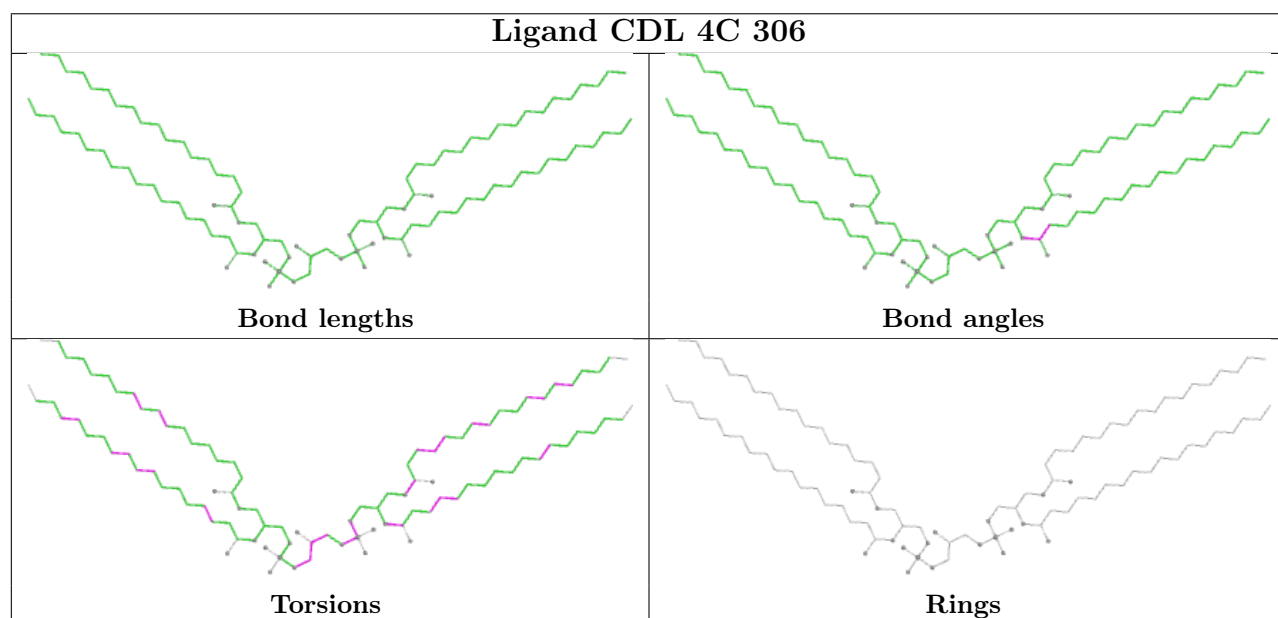
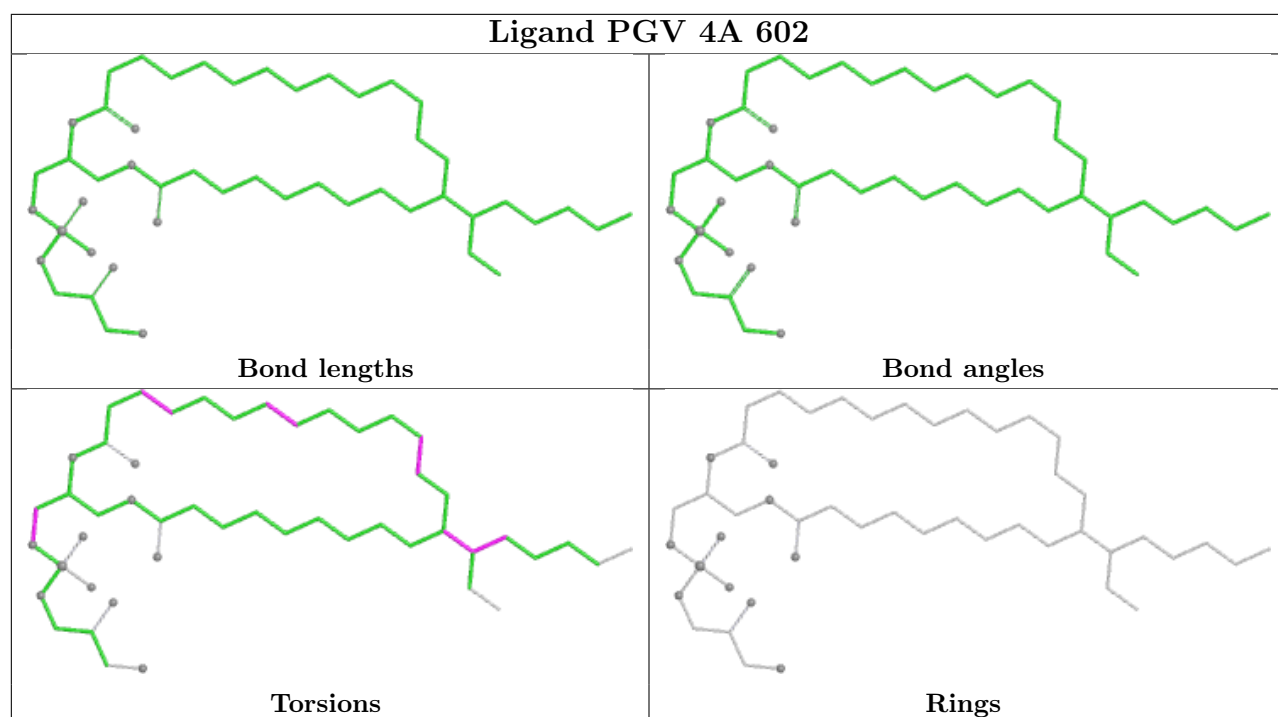
Ligand HEM 3C 502

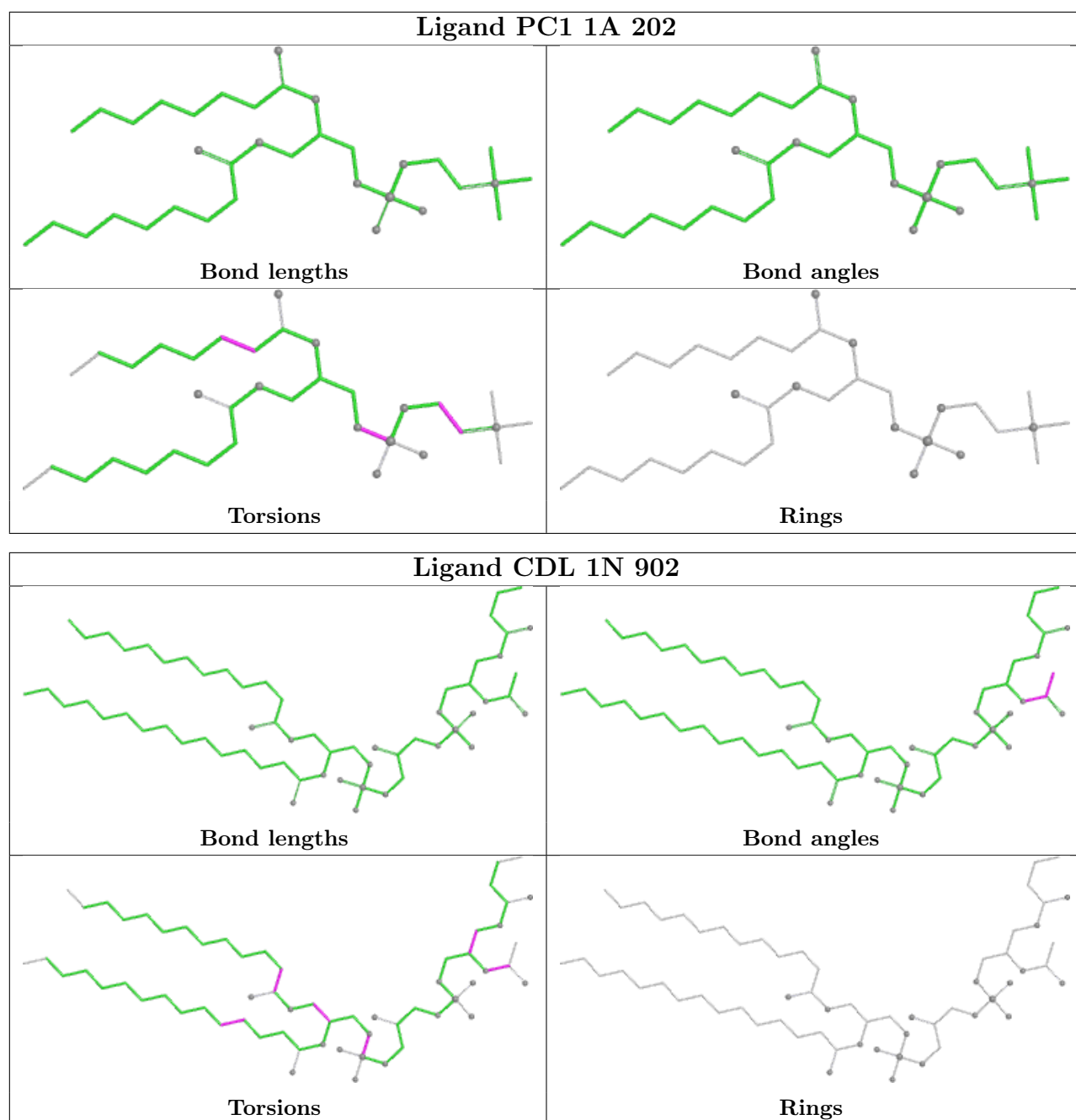


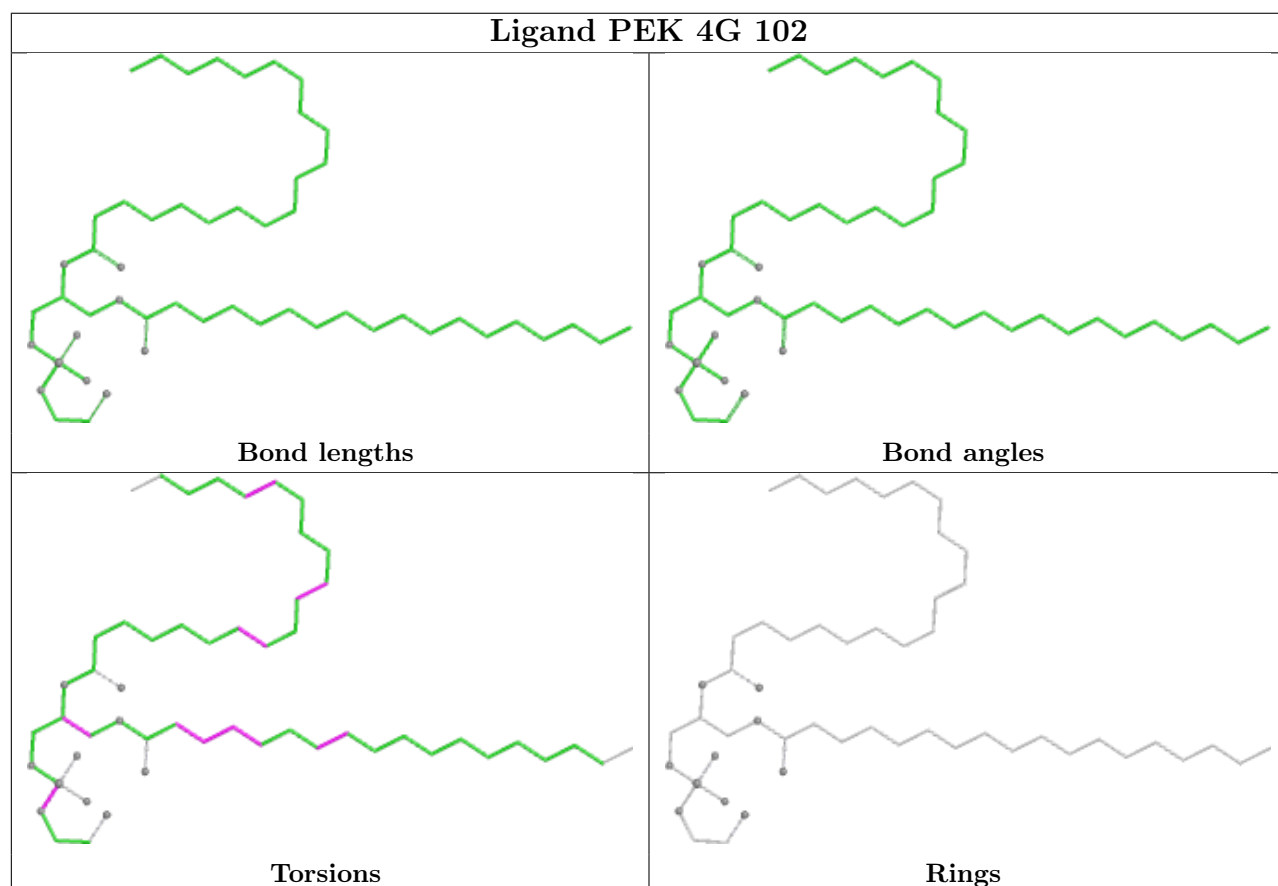
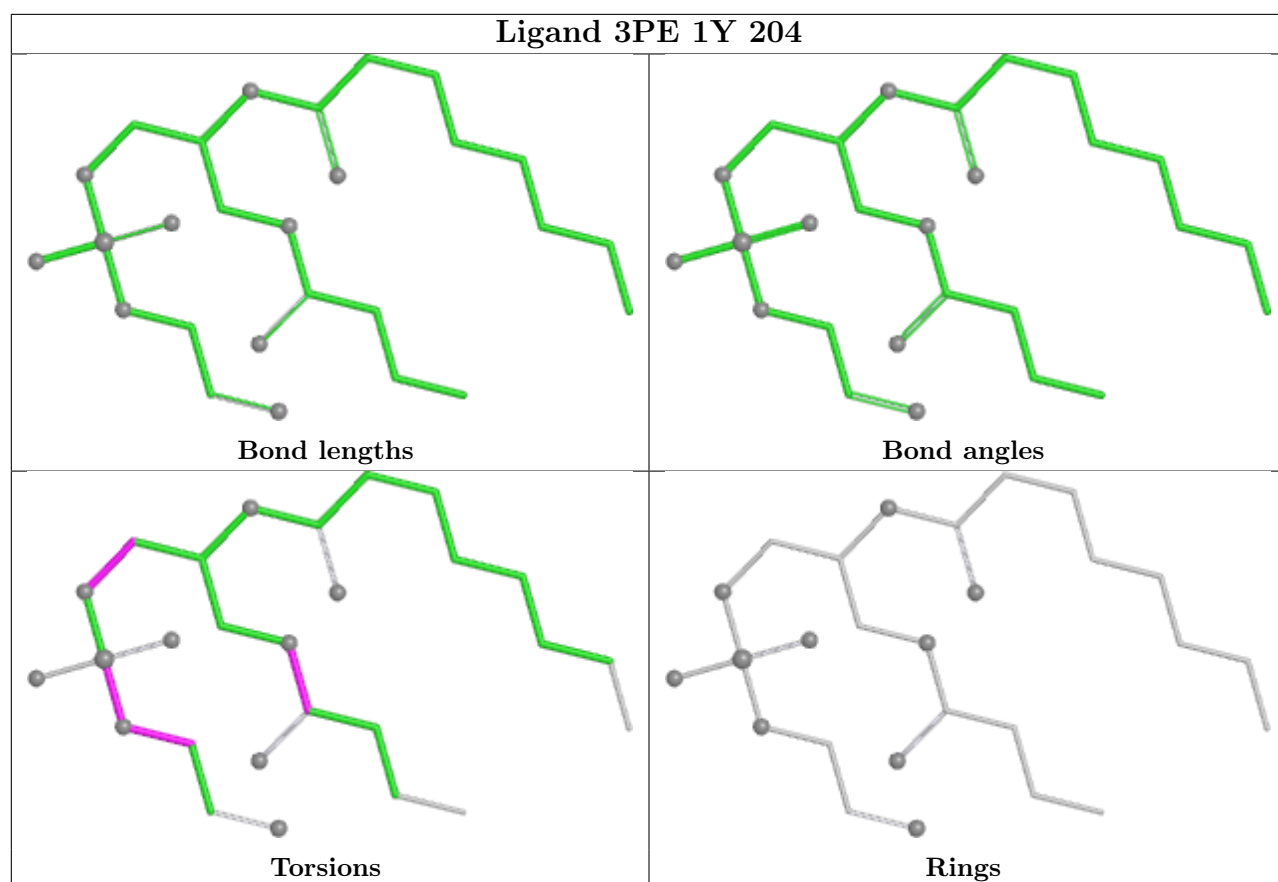
Ligand PGV 4C 307

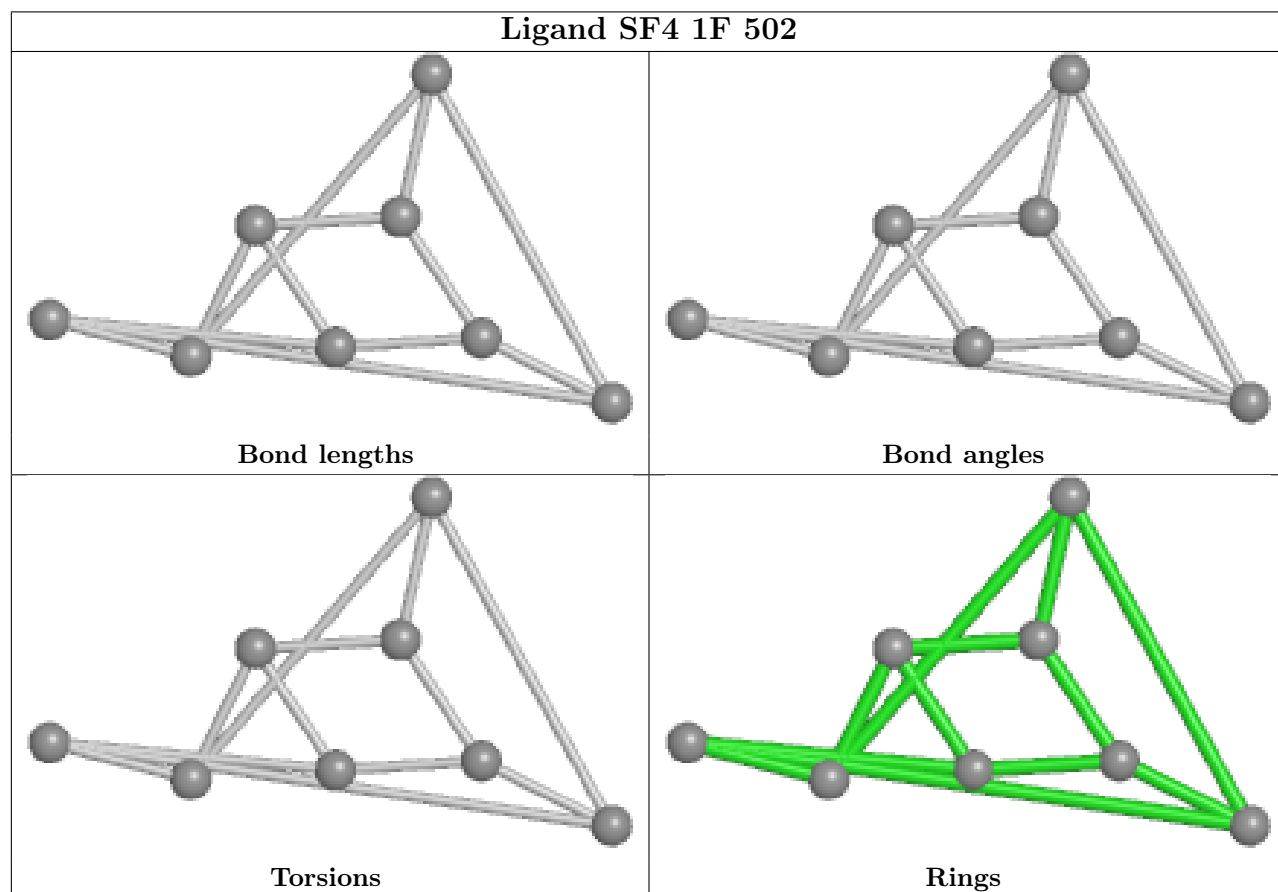
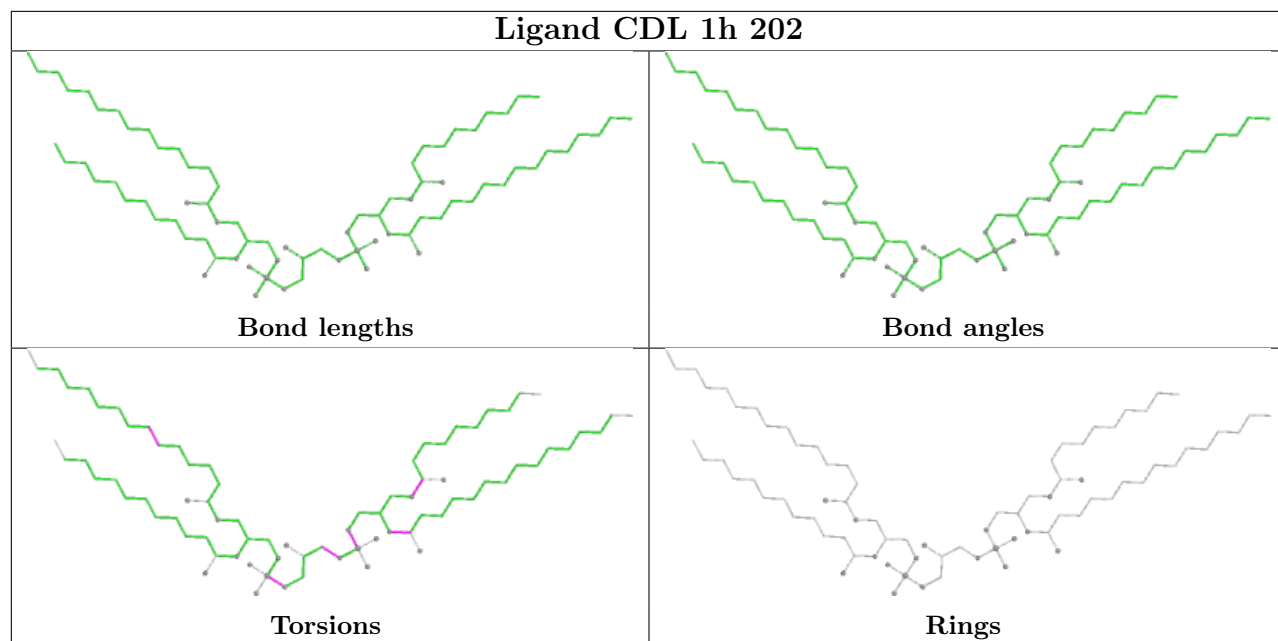


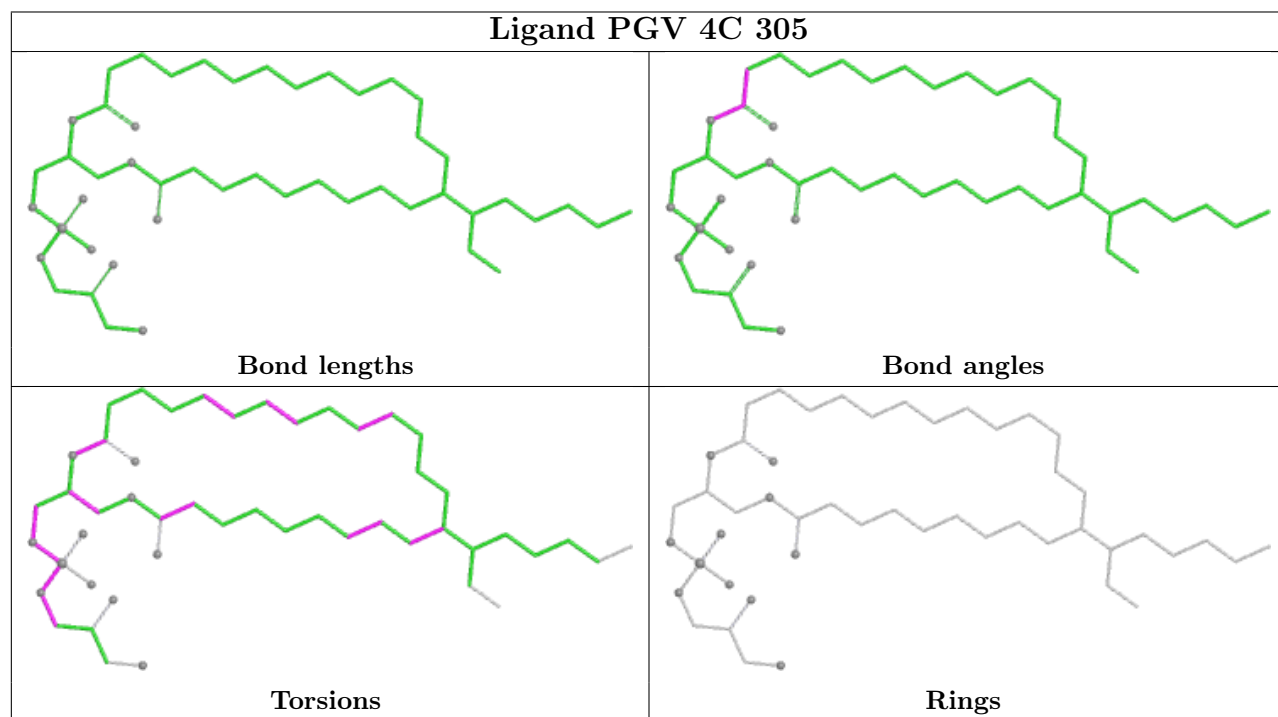
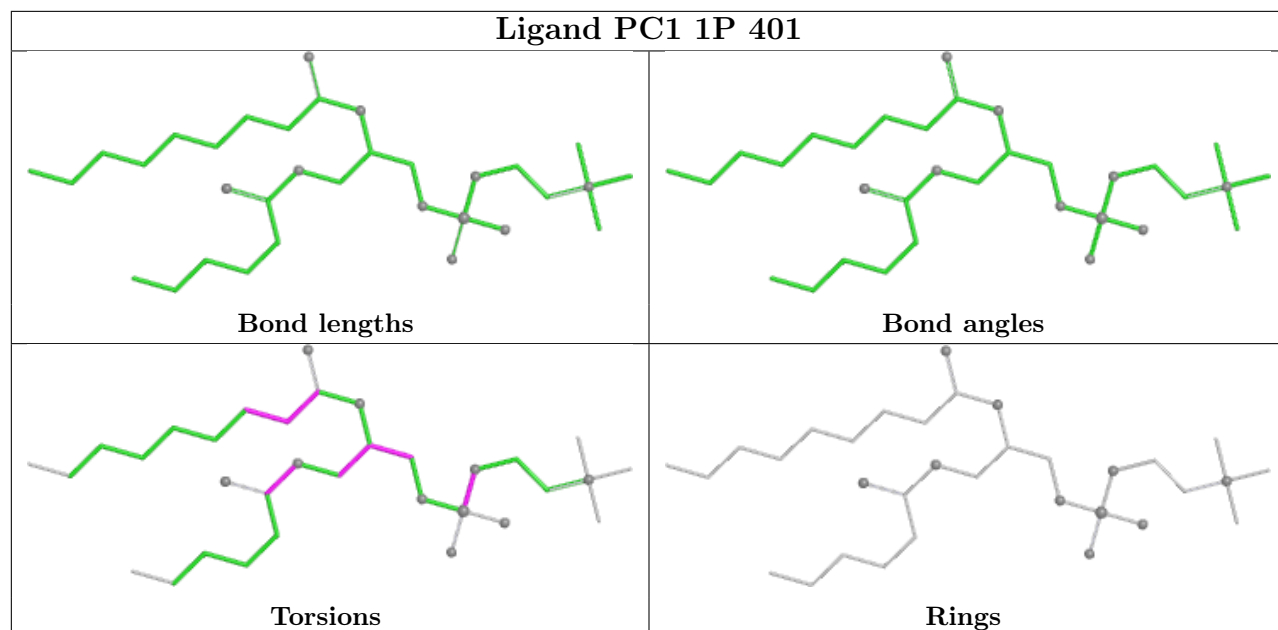




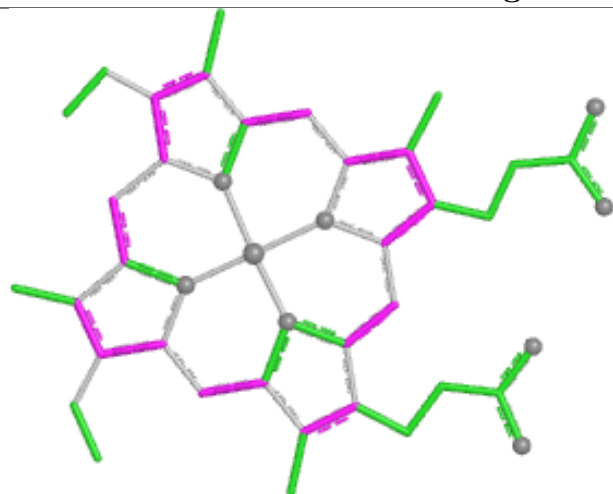




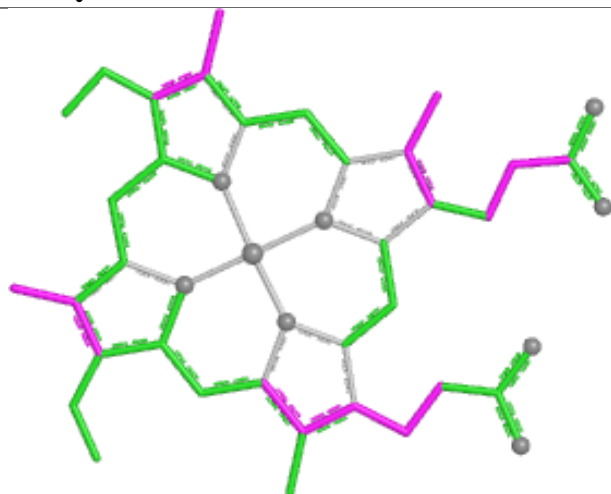




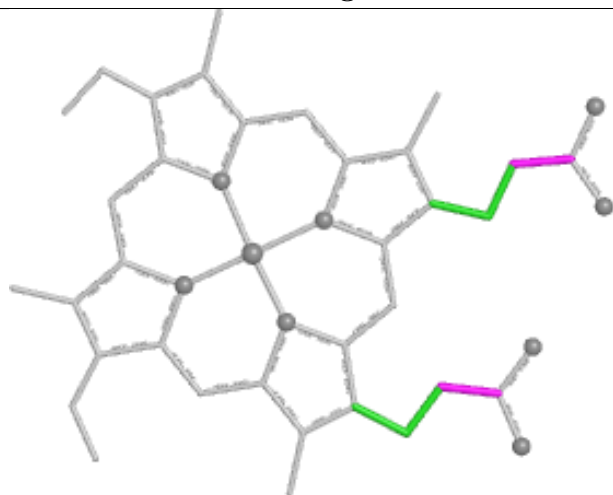
Ligand HEC 3Q 501



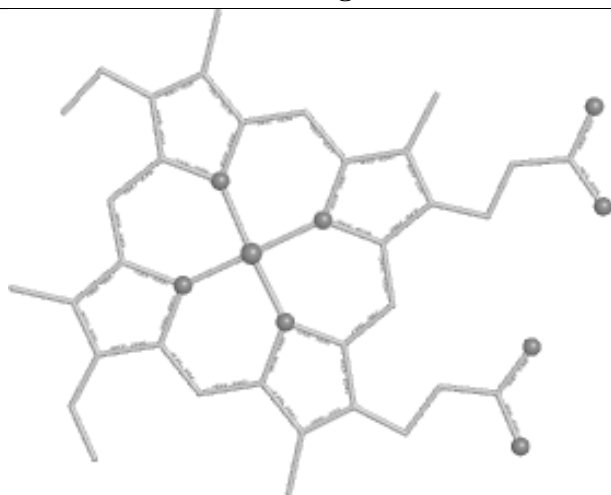
Bond lengths



Bond angles

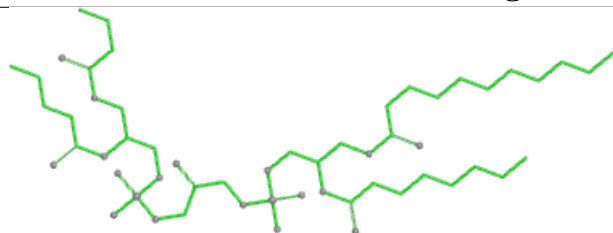


Torsions

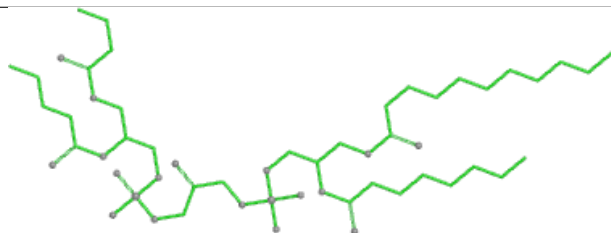


Rings

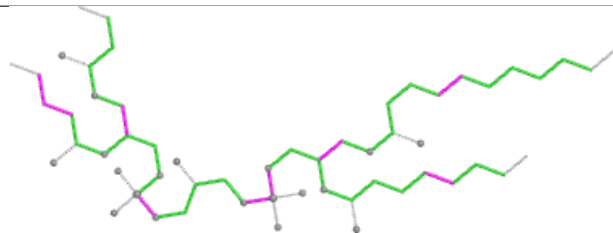
Ligand CDL 3G 103



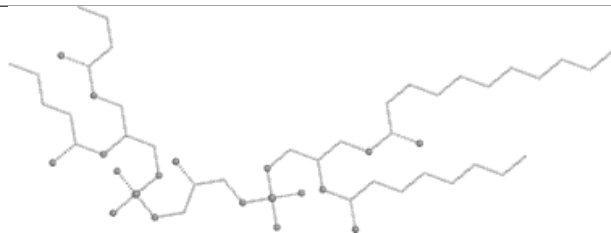
Bond lengths



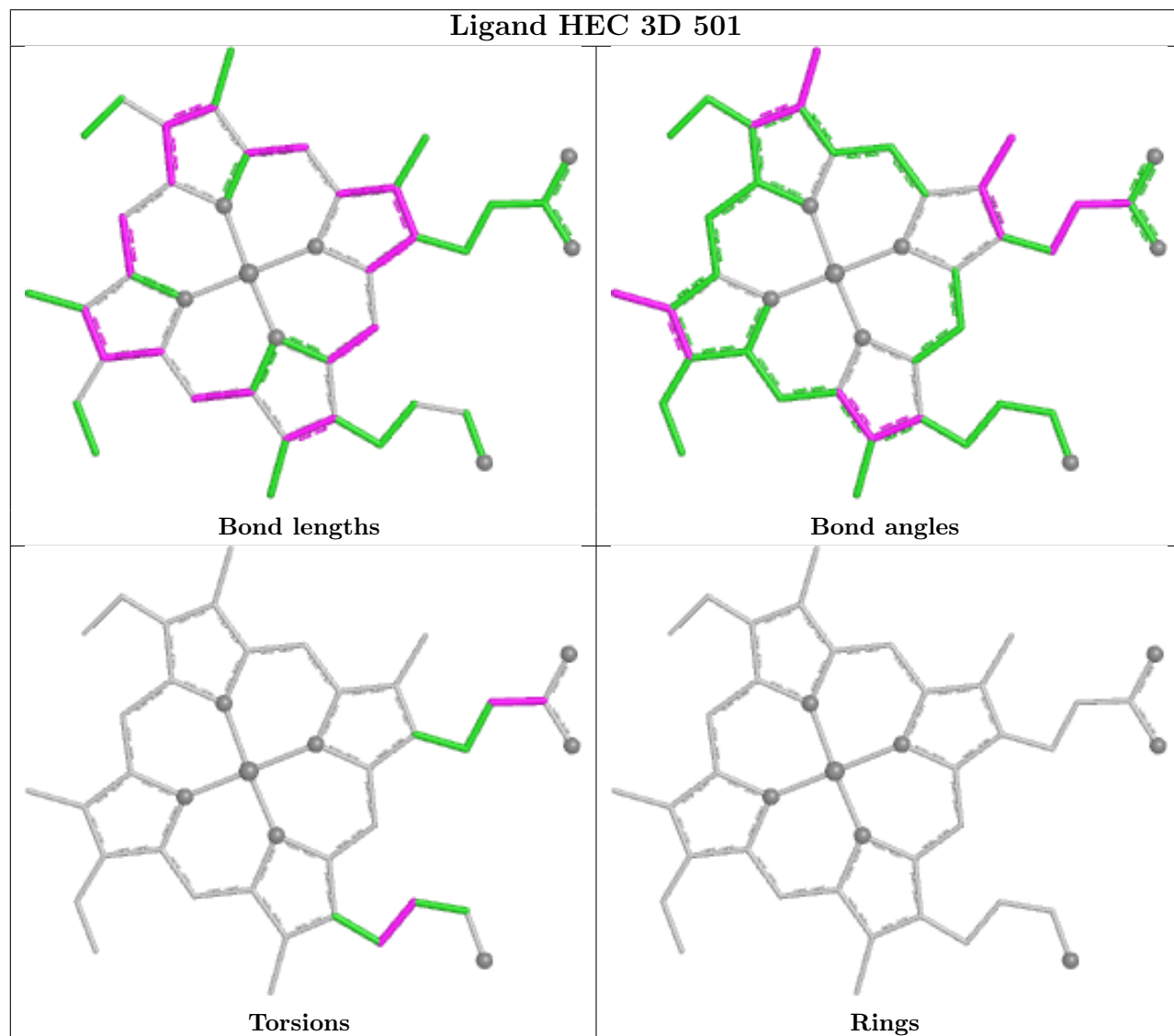
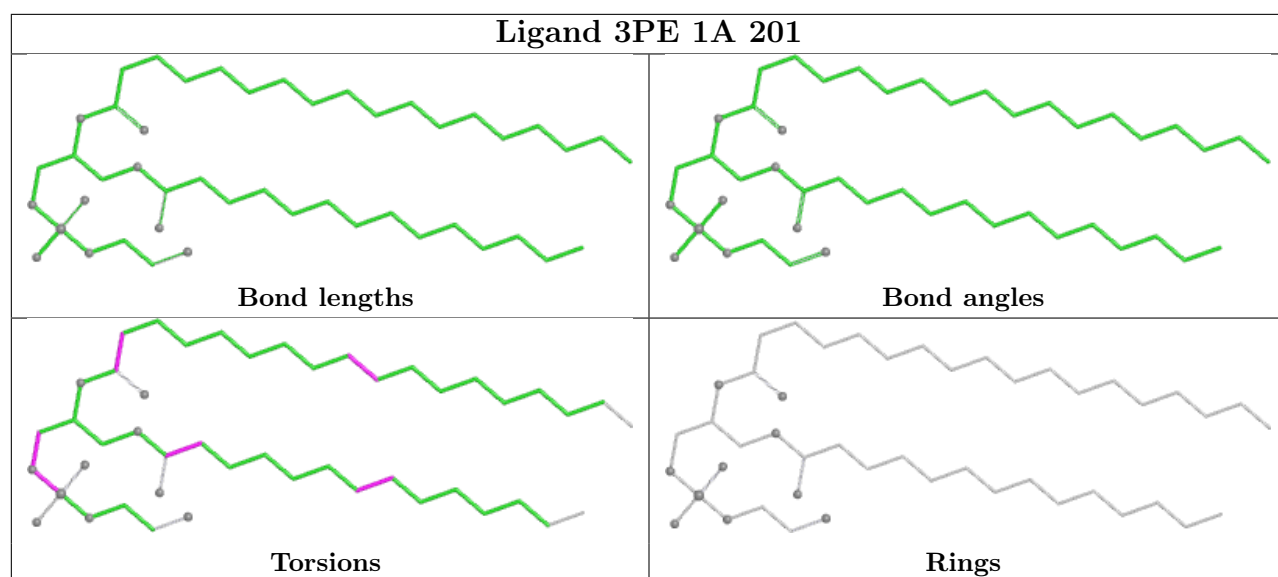
Bond angles

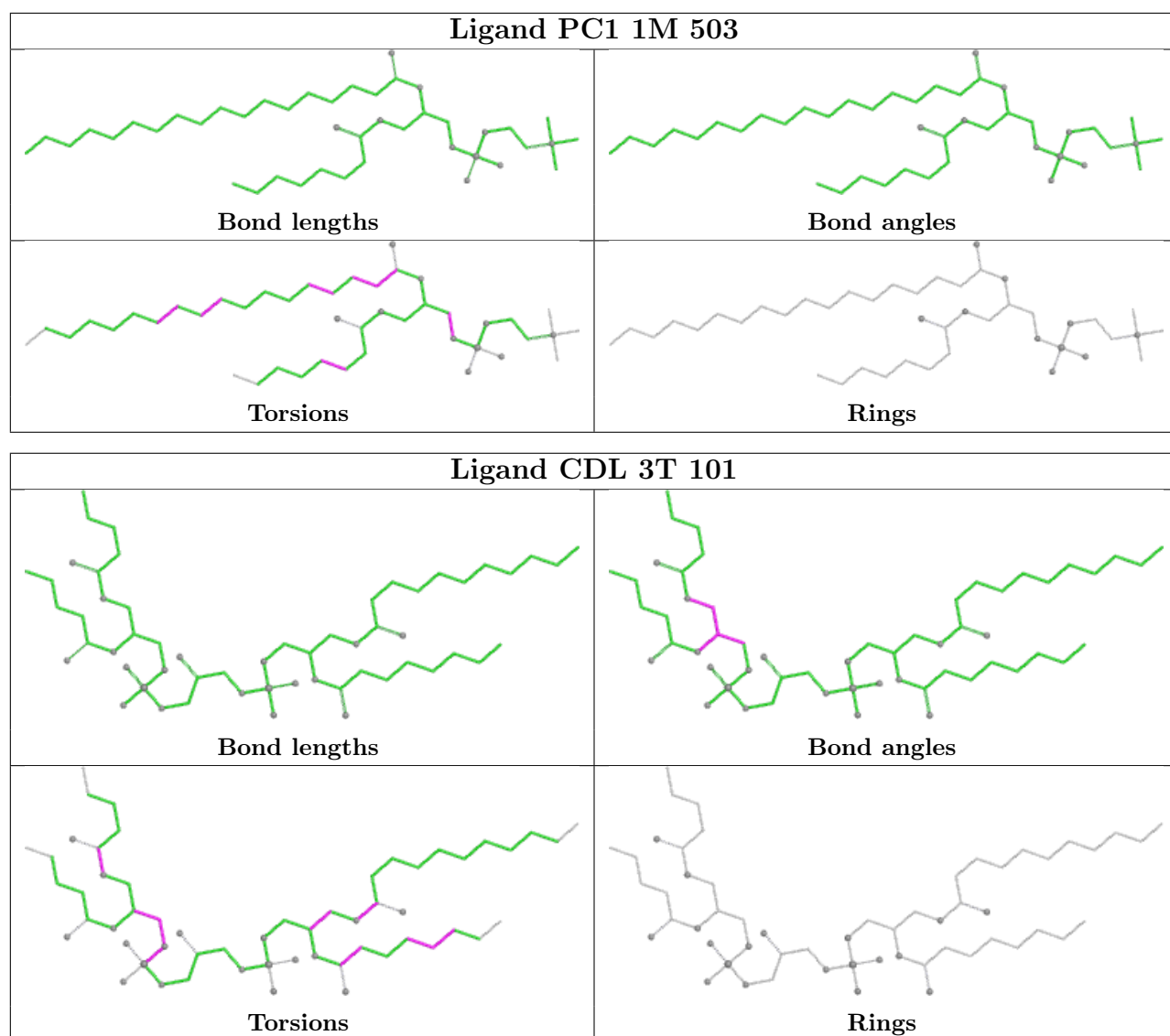


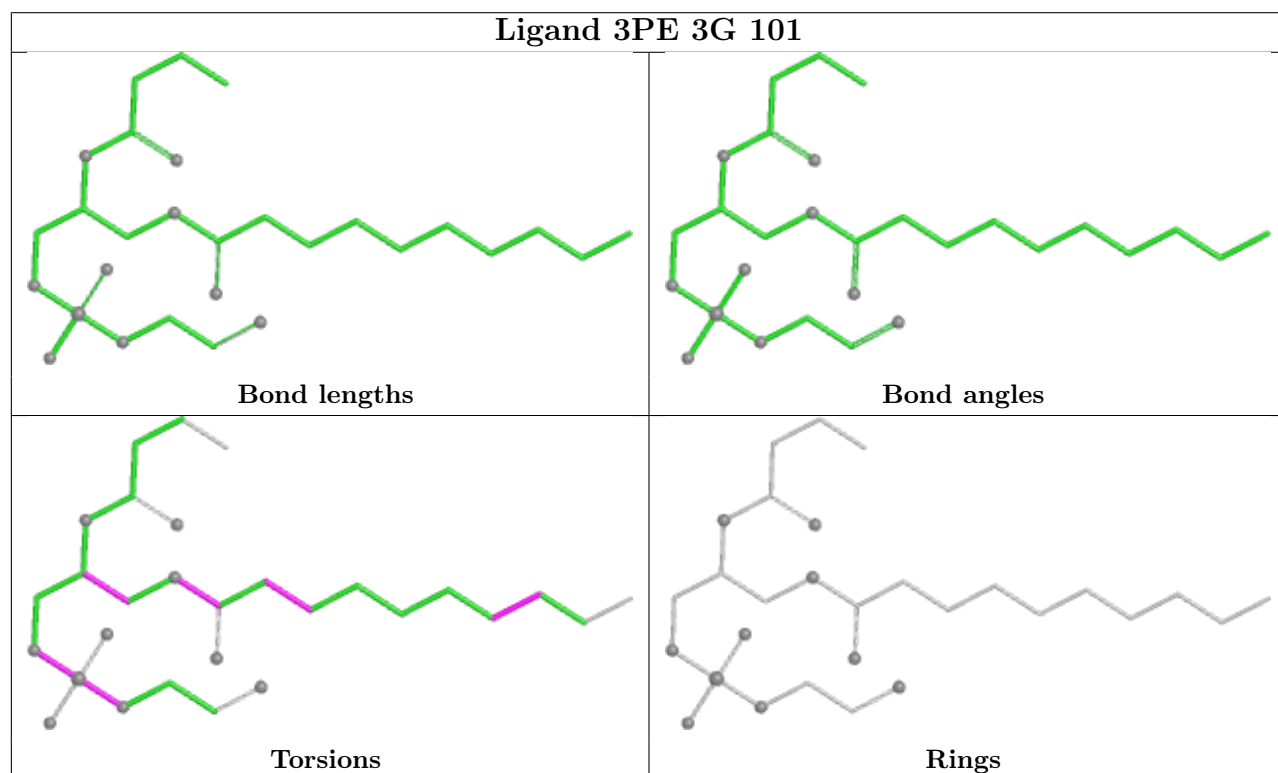
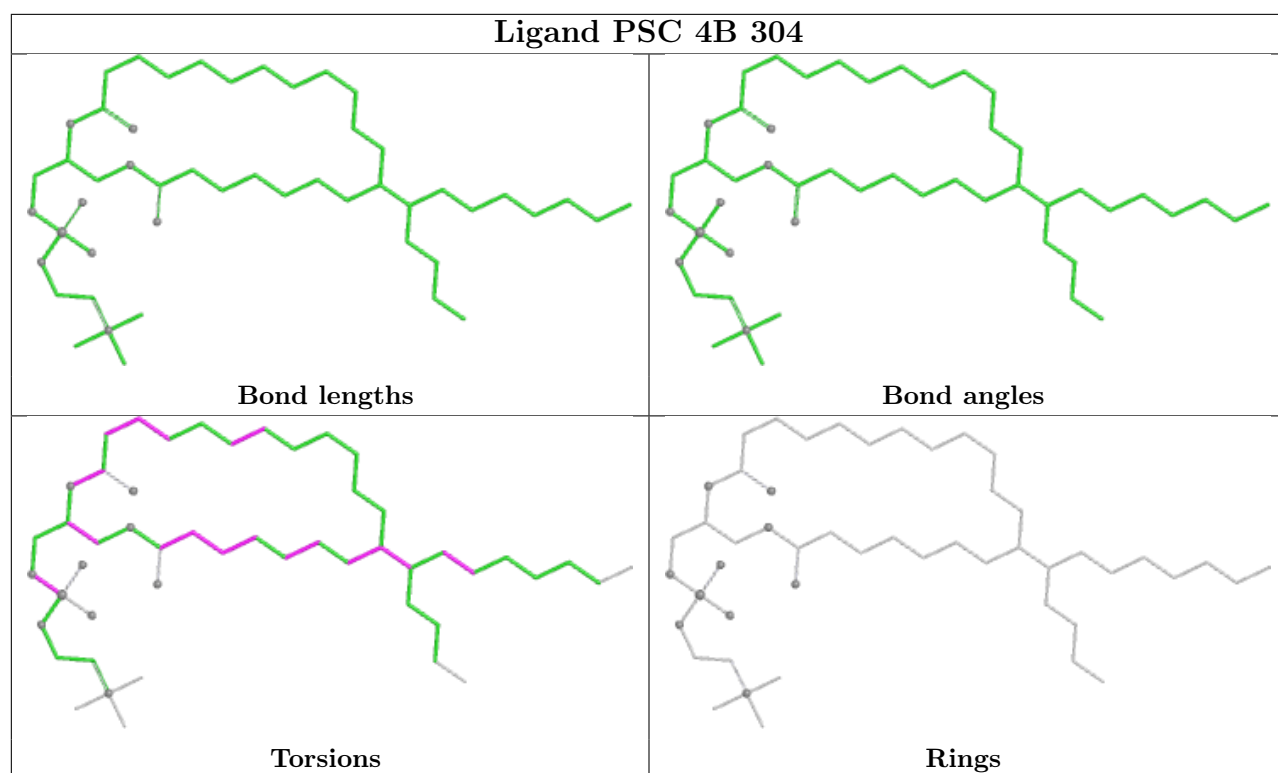
Torsions

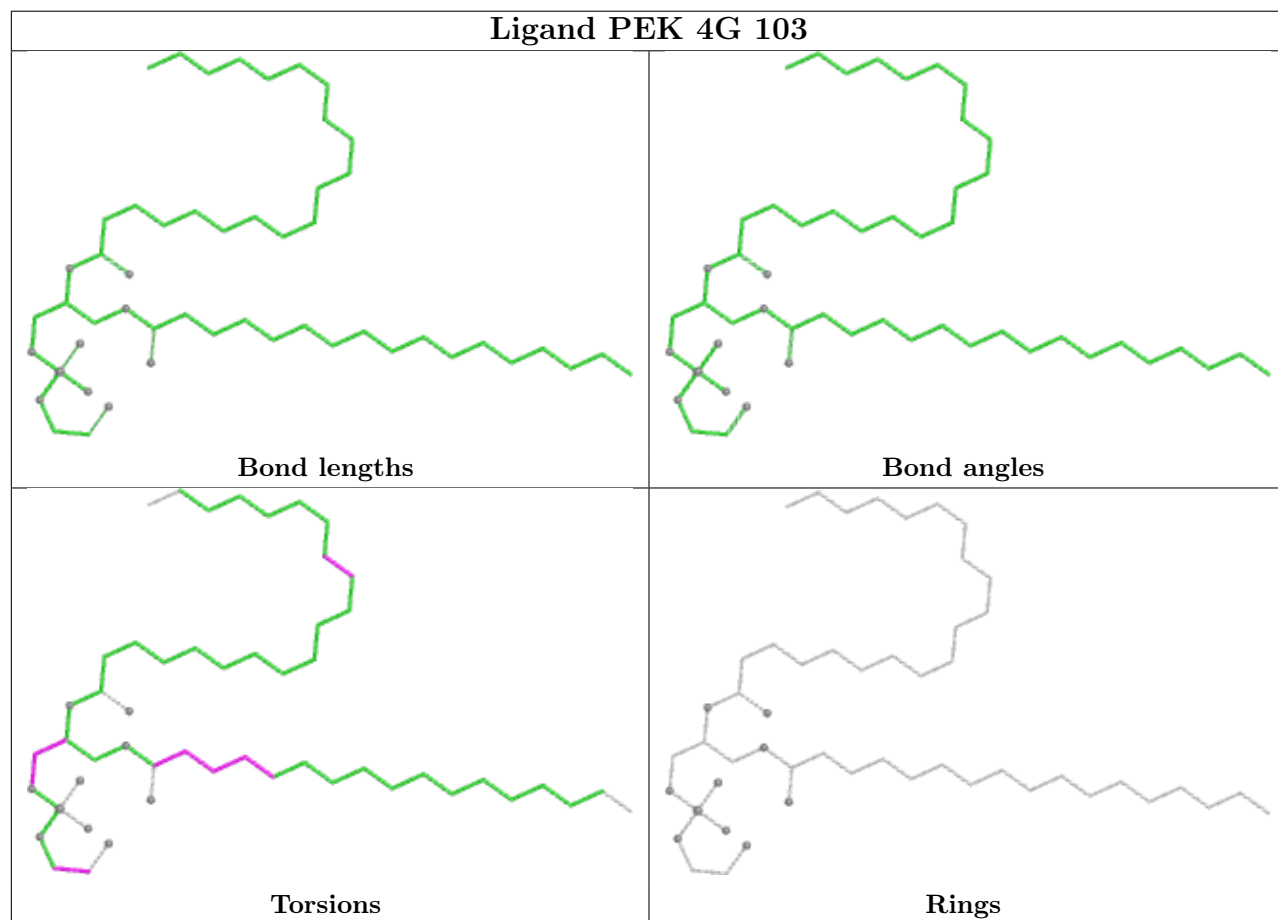
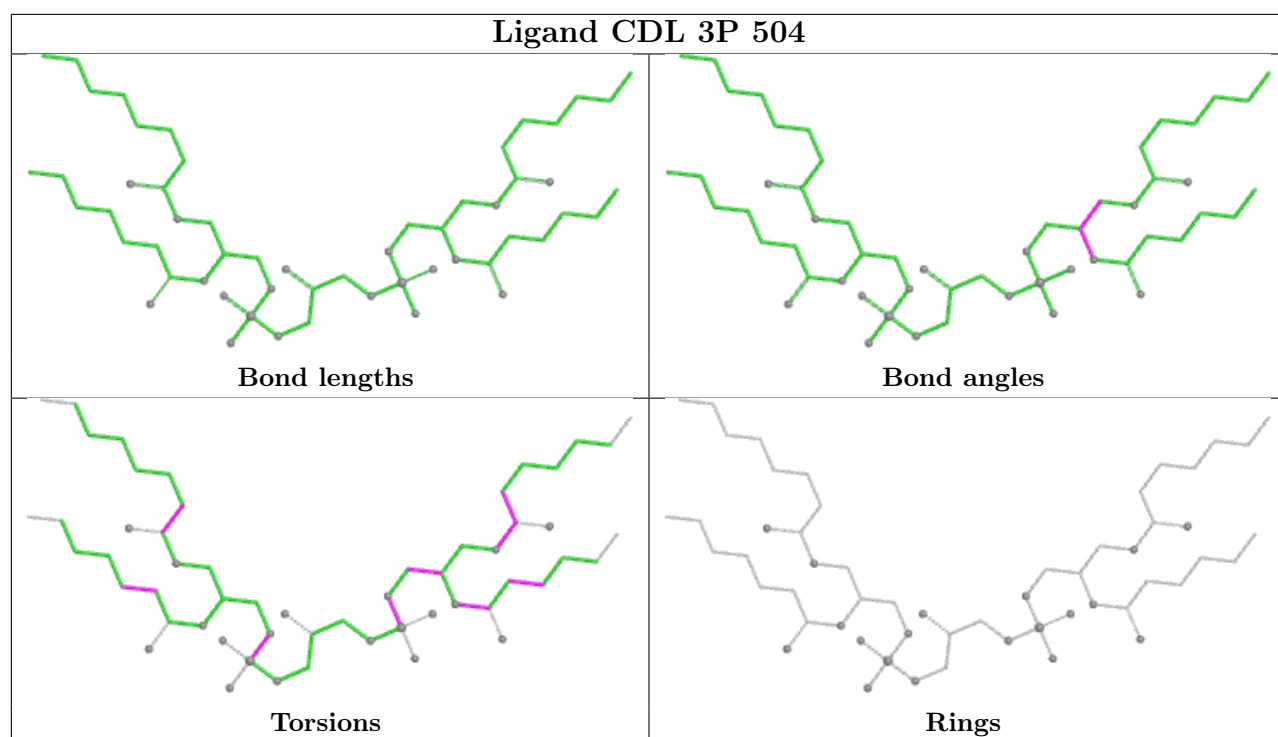


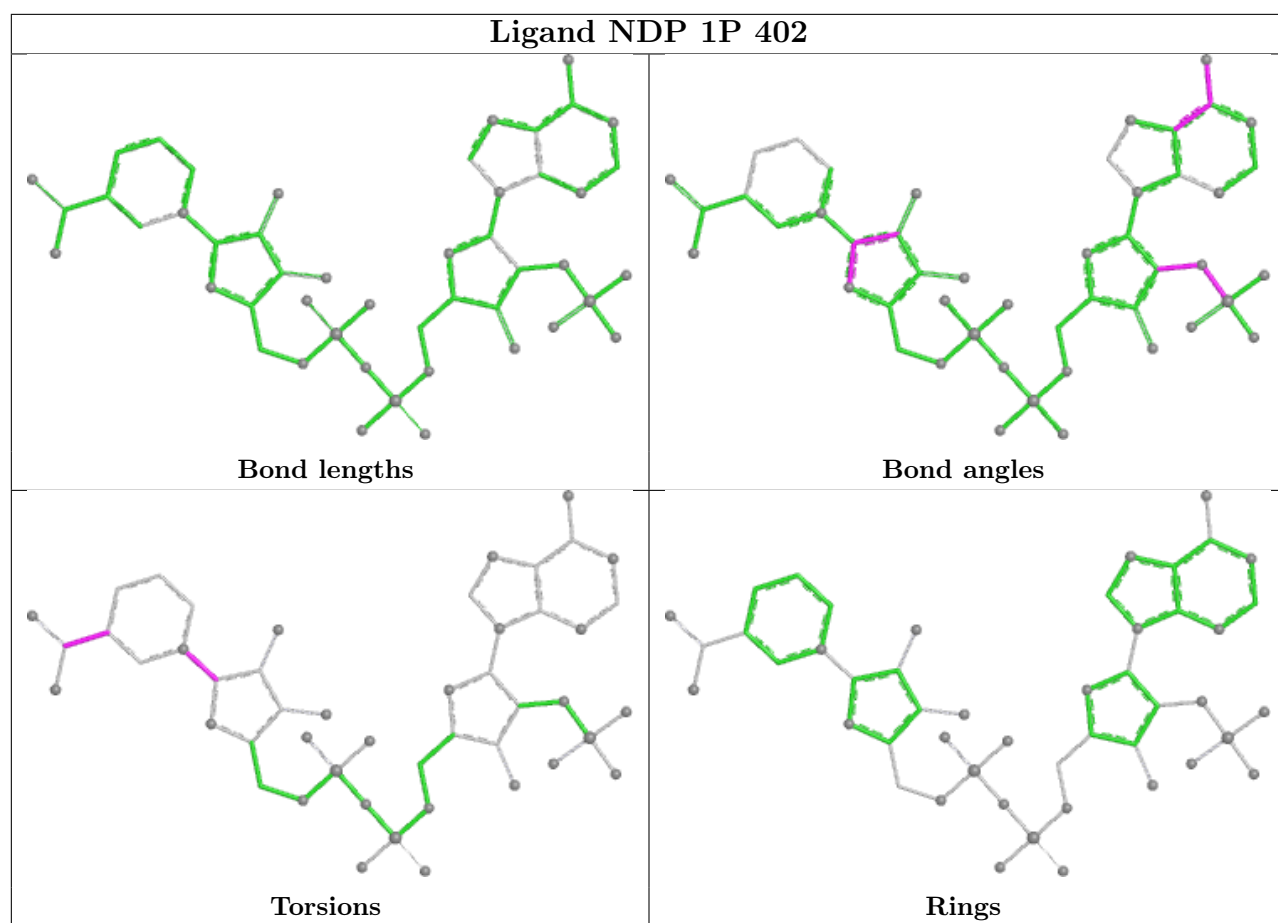
Rings



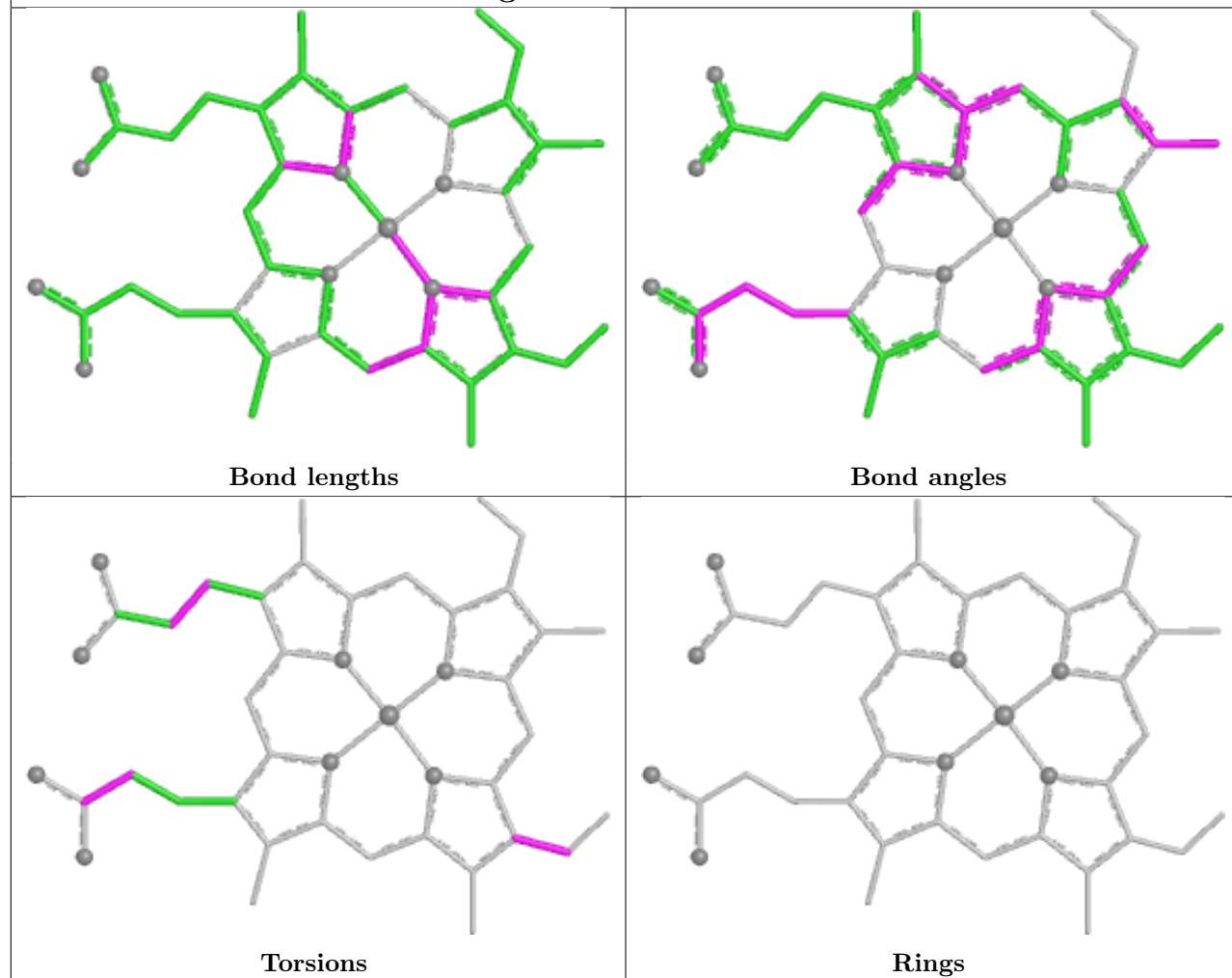




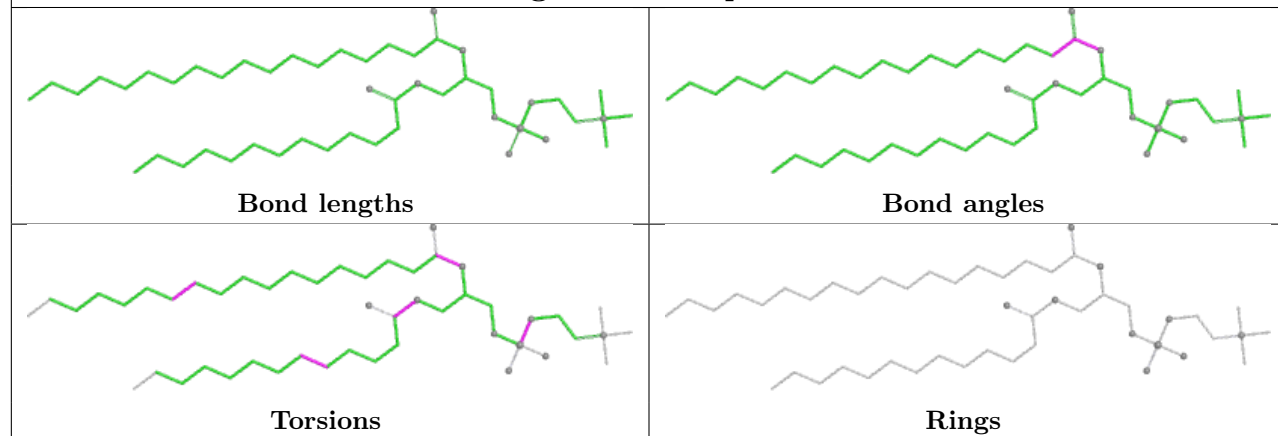


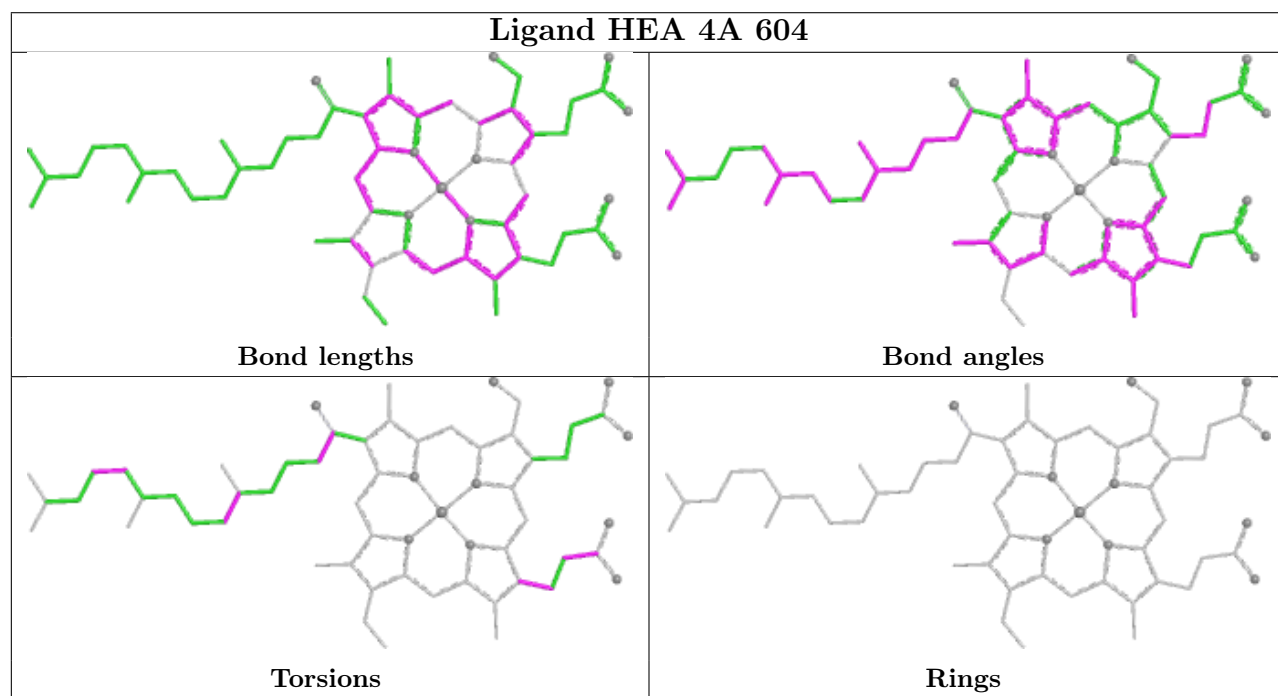
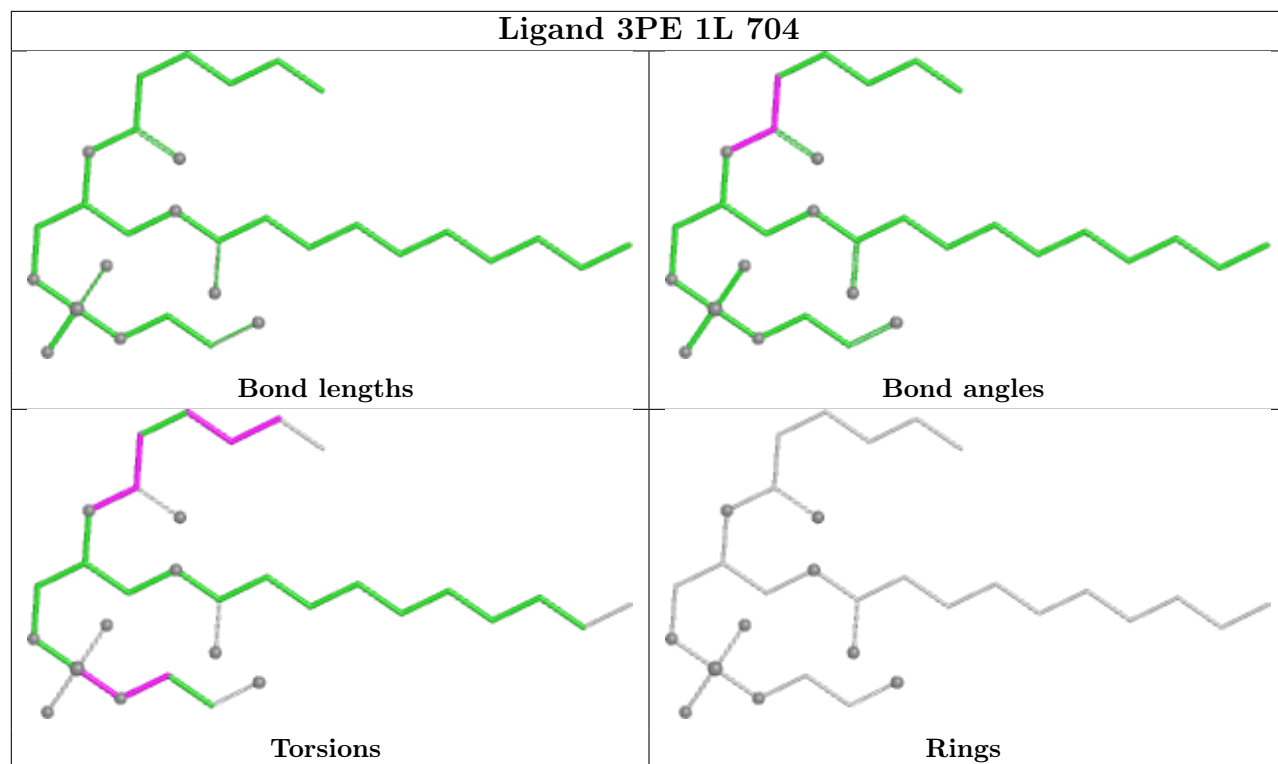


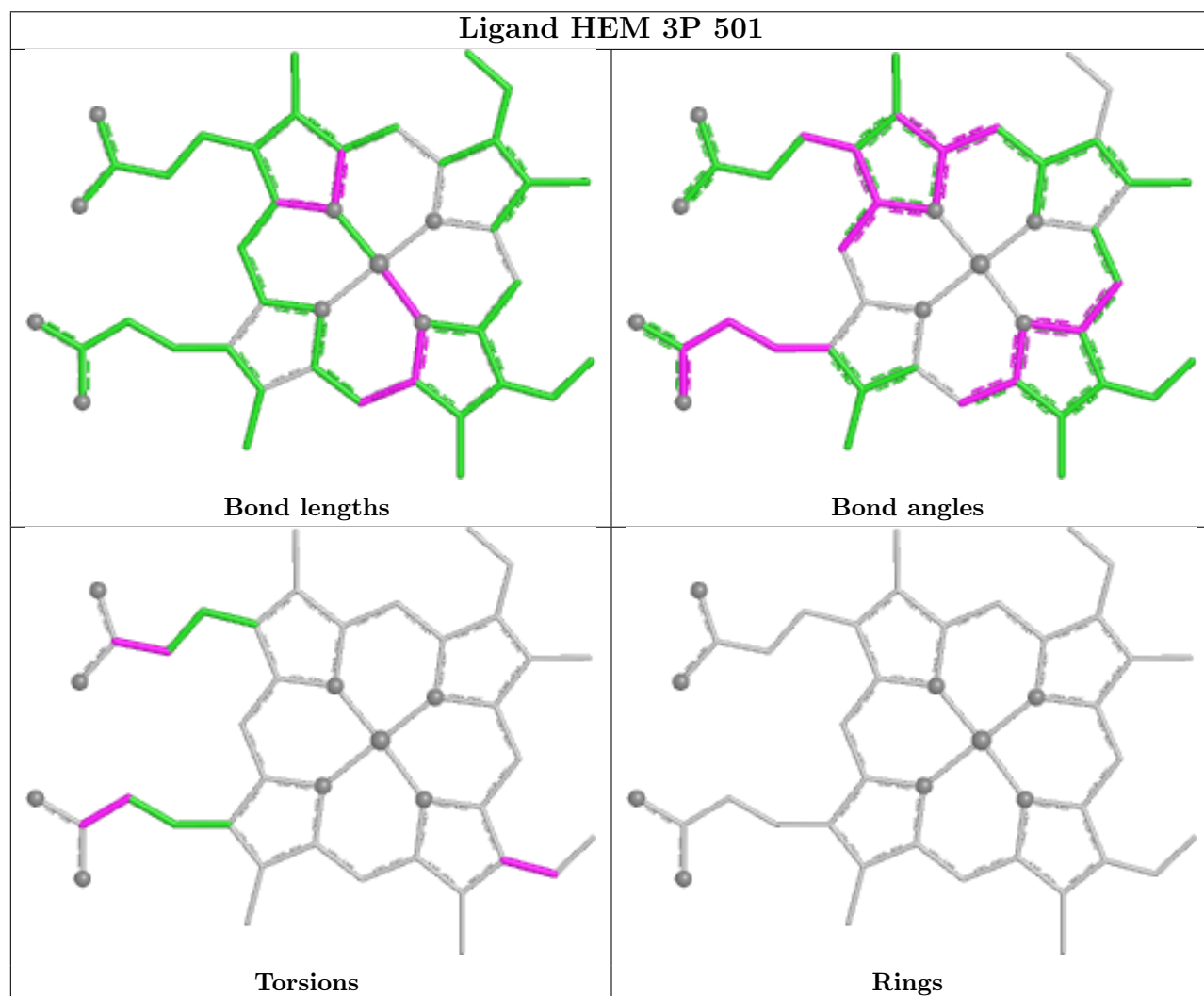
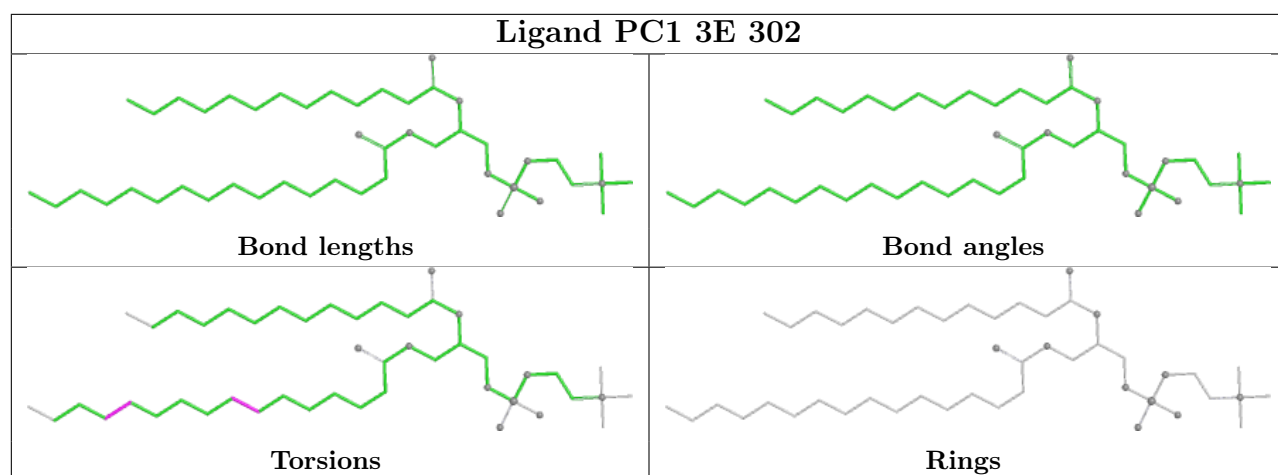
Ligand HEM 3C 501

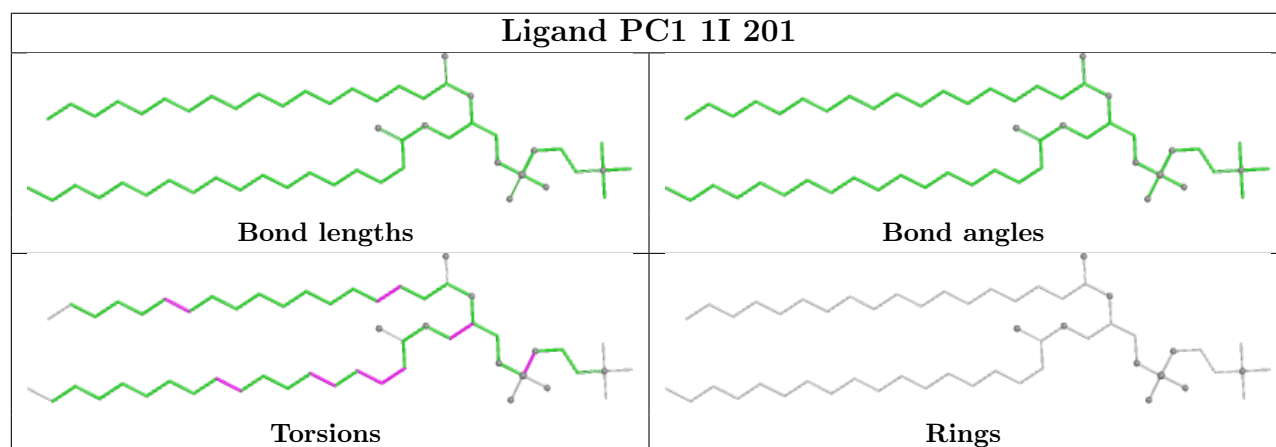
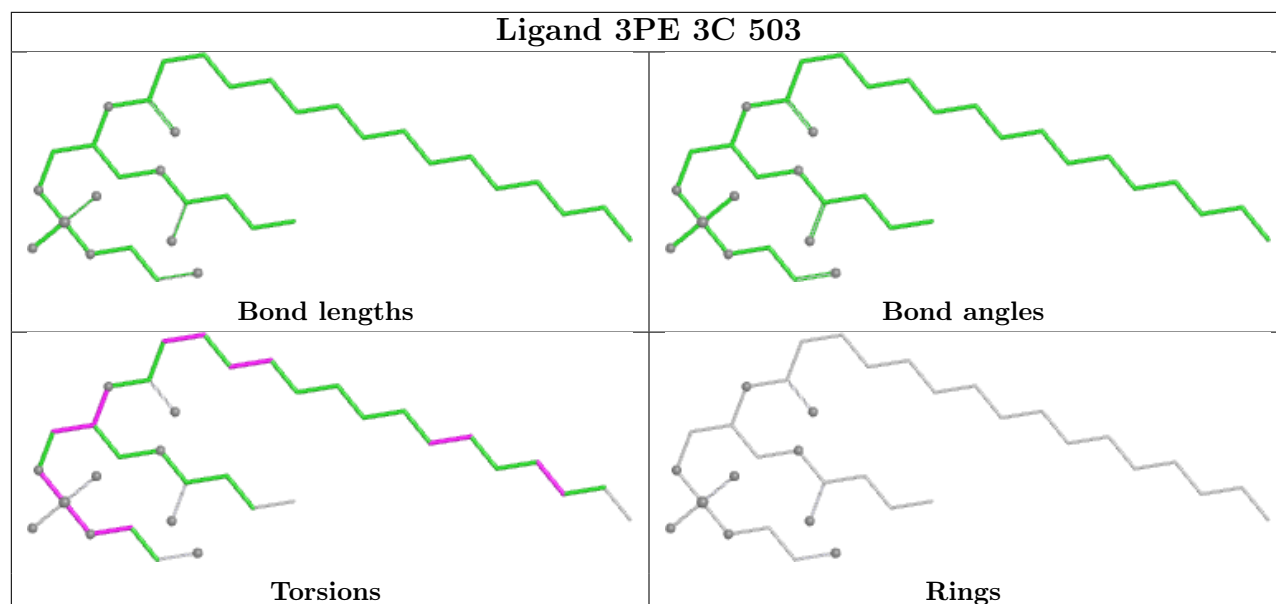
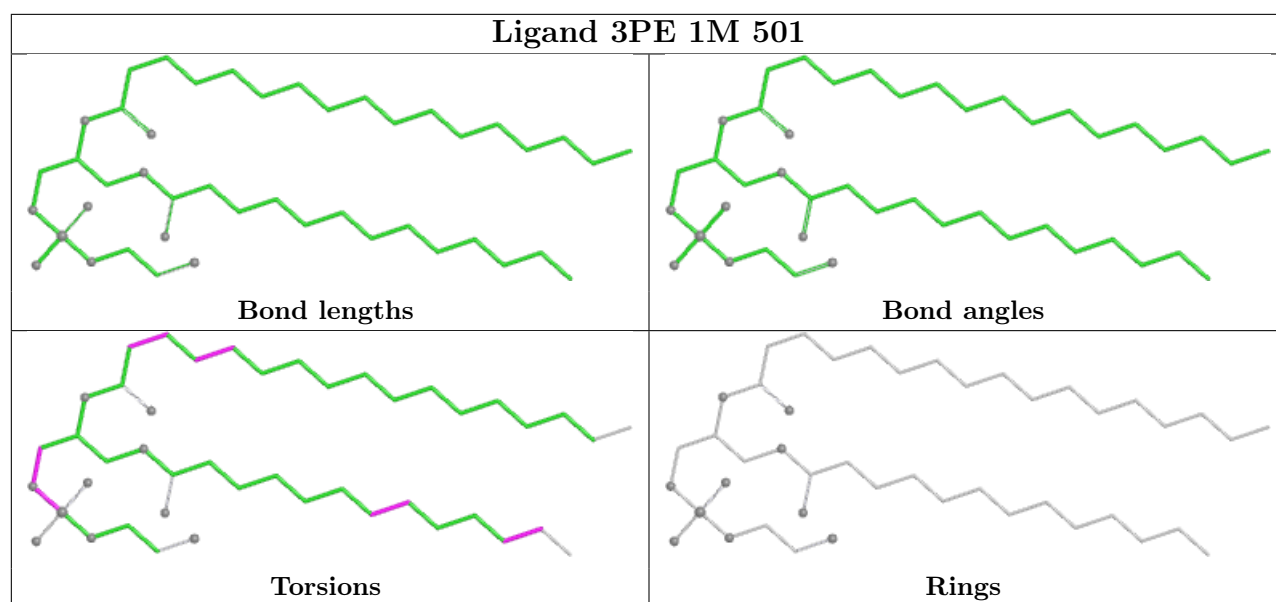


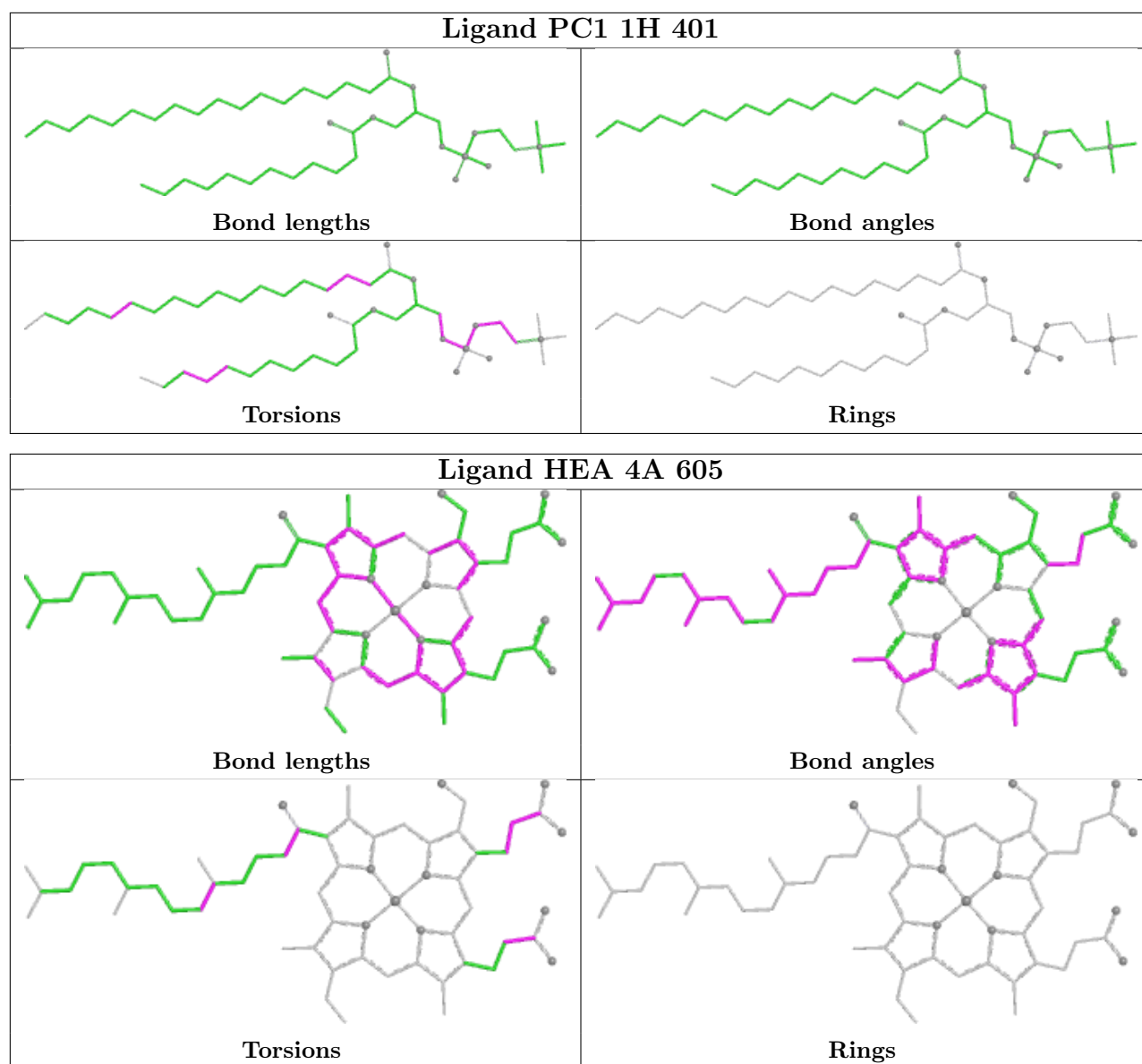
Ligand PC1 1q 201











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
49	3I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3I	48:SER	C	49:PHE	N	1.08

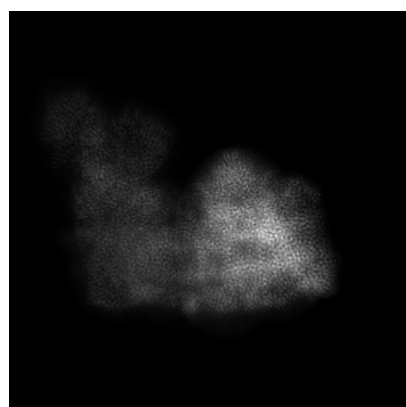
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42226. These allow visual inspection of the internal detail of the map and identification of artifacts.

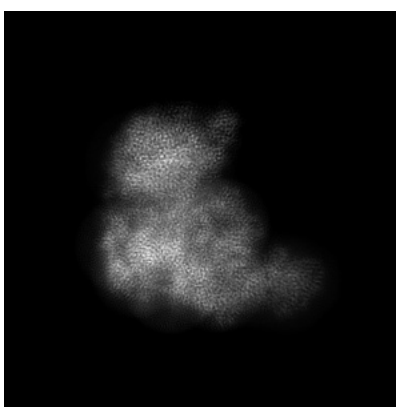
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

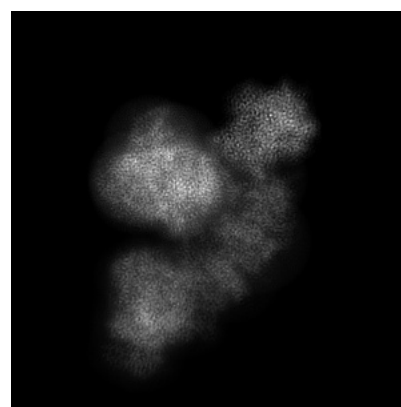
6.1.1 Primary map



X



Y

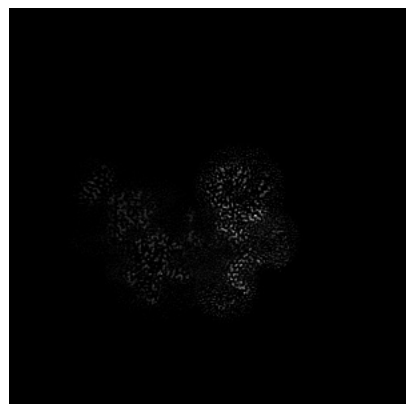


Z

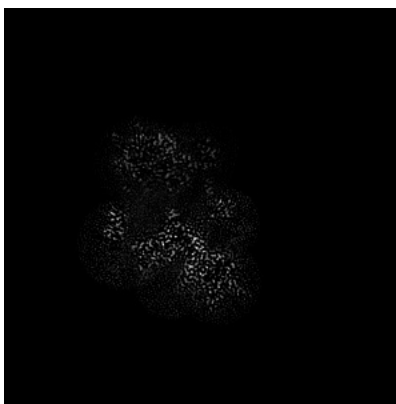
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

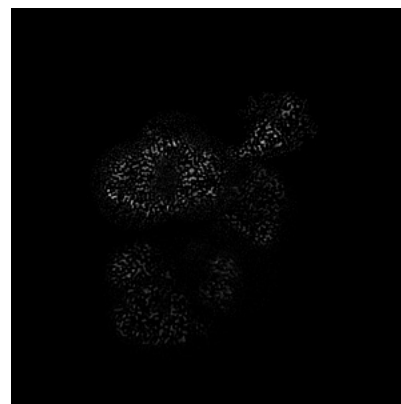
6.2.1 Primary map



X Index: 444



Y Index: 444

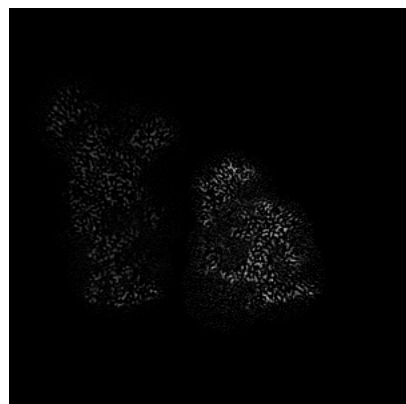


Z Index: 444

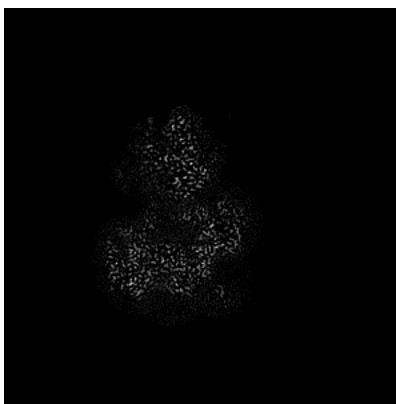
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

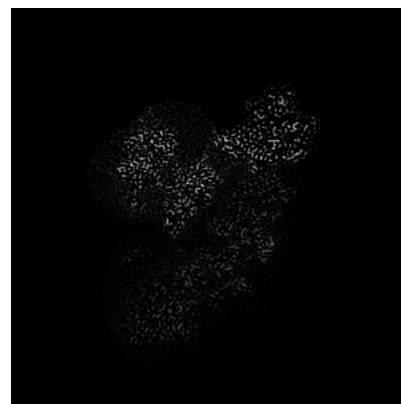
6.3.1 Primary map



X Index: 322



Y Index: 568

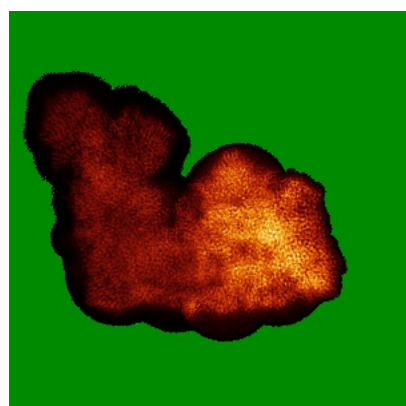


Z Index: 387

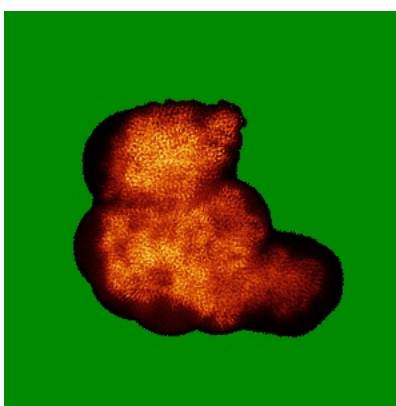
The images above show the largest variance slices of the map in three orthogonal directions.

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

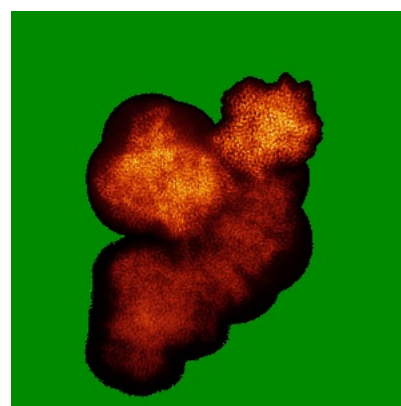
6.4.1 Primary map



X



Y

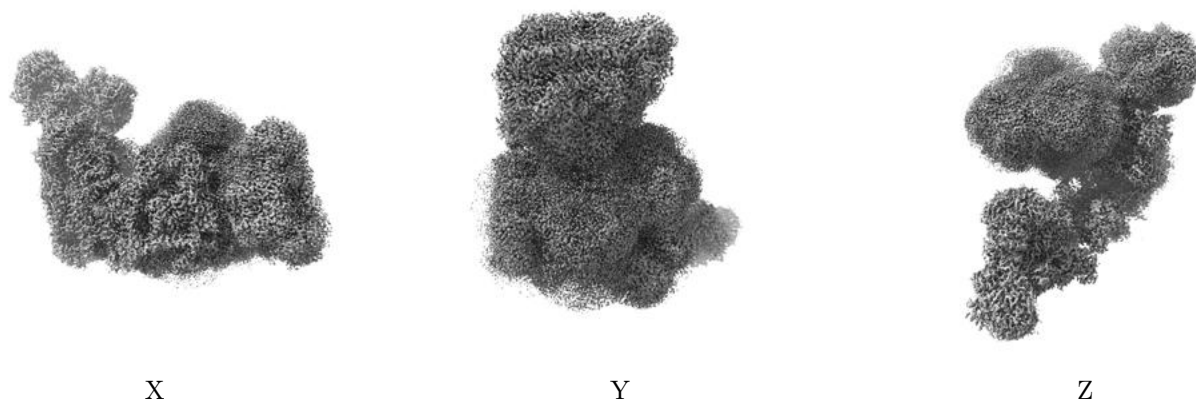


Z

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

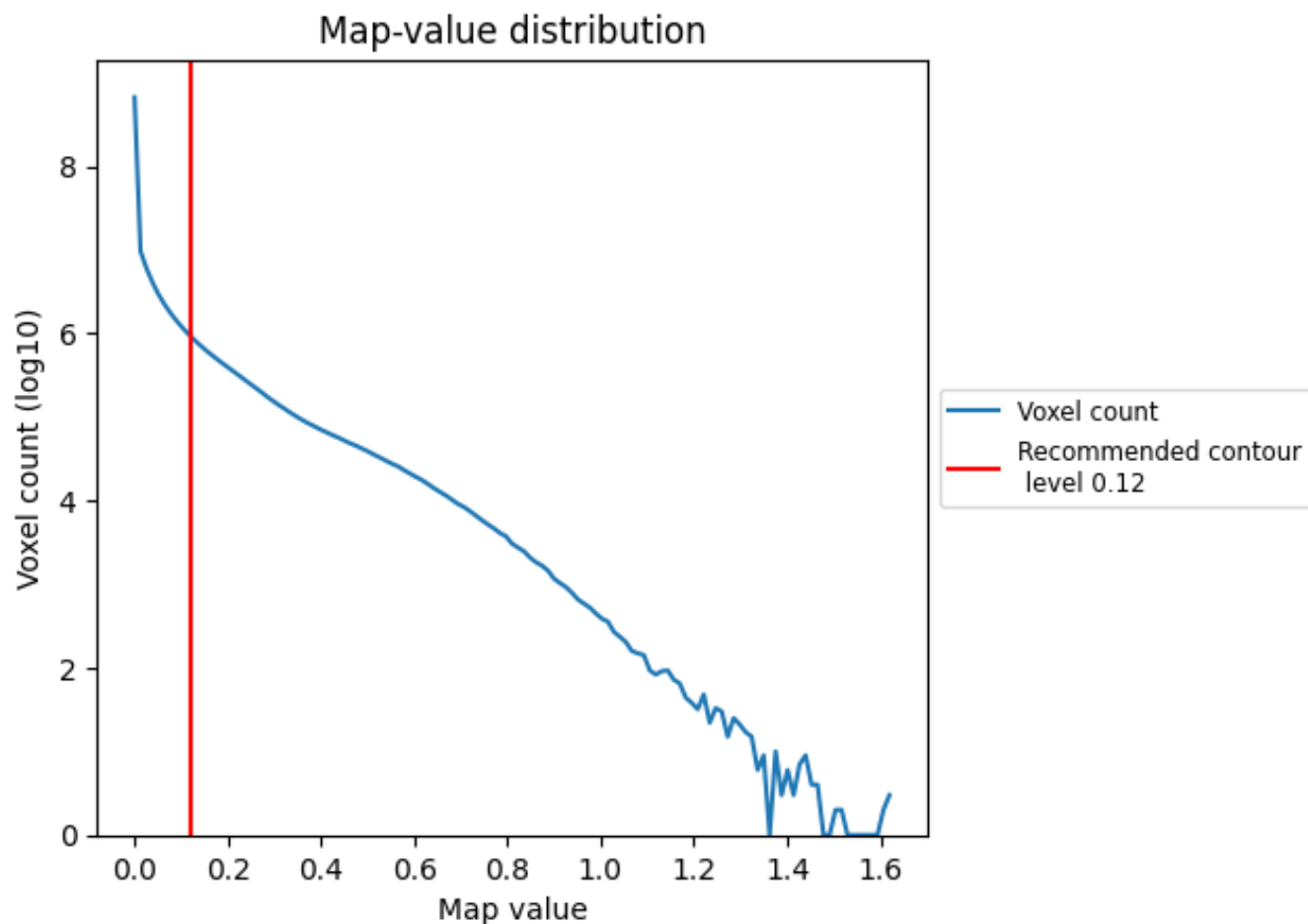
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

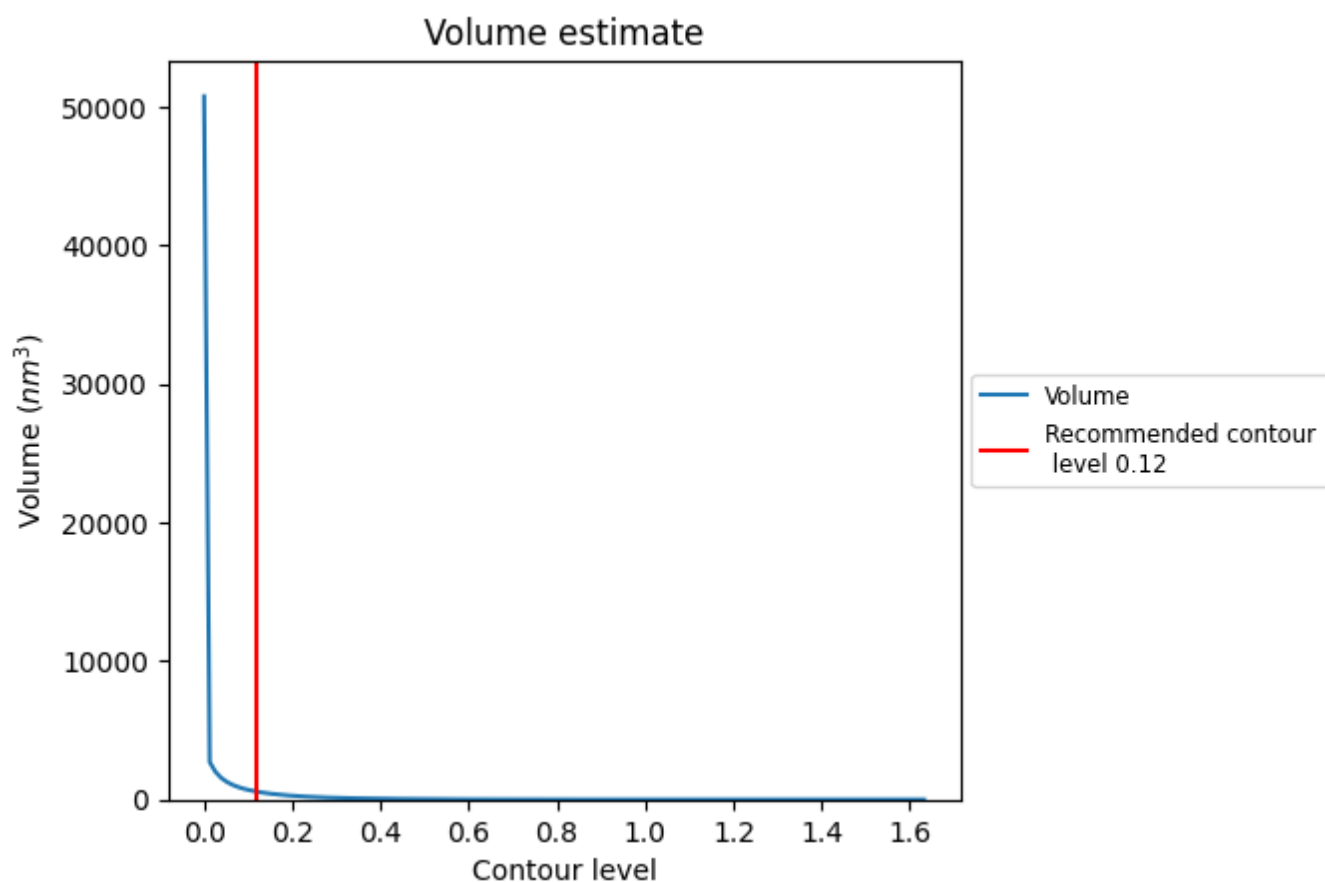
This section contains the results of statistical analysis of the map.

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.

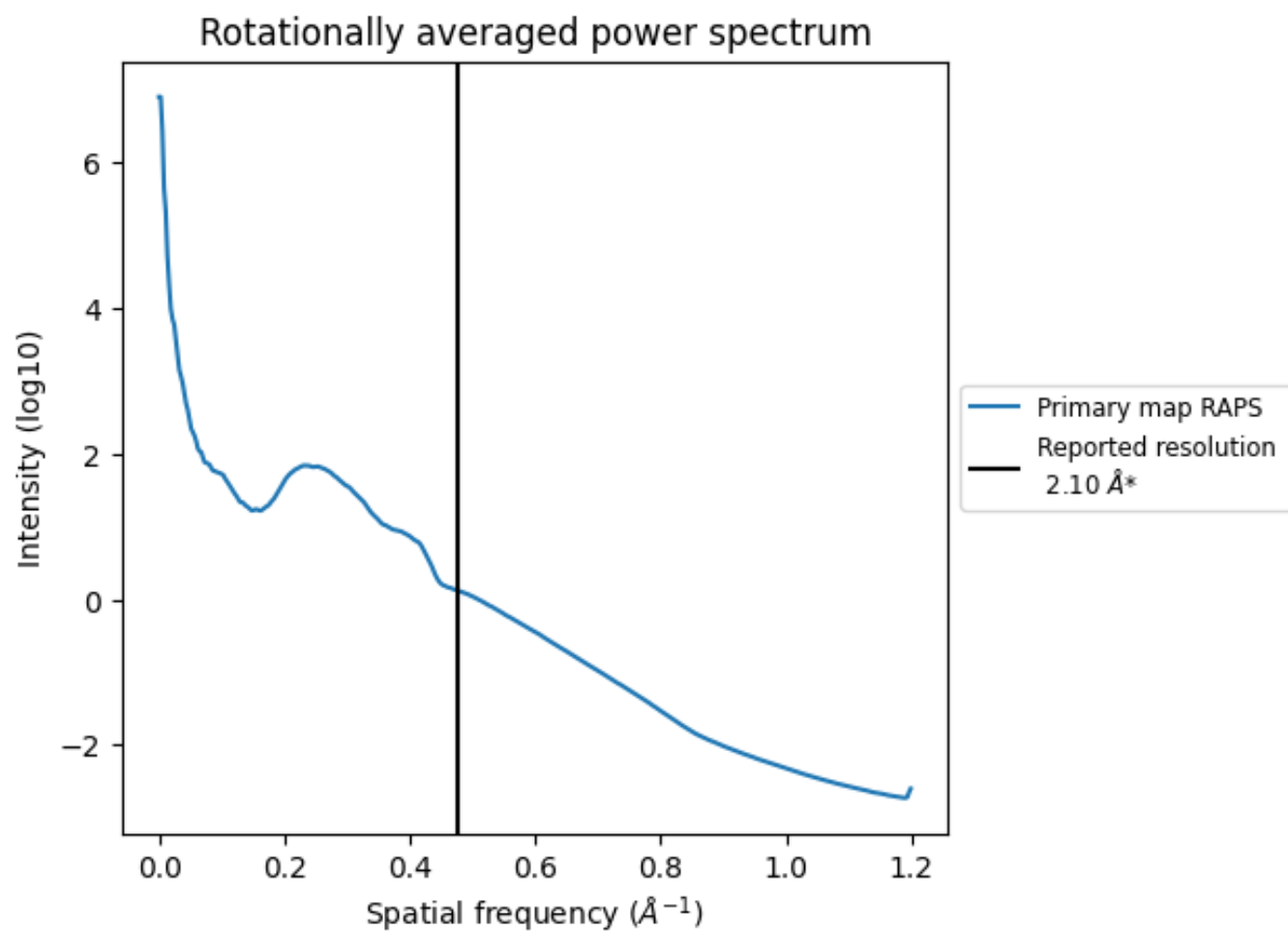
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 569 nm³; this corresponds to an approximate mass of 514 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

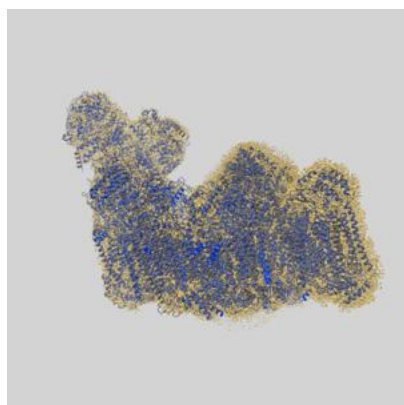
8 Fourier-Shell correlation

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

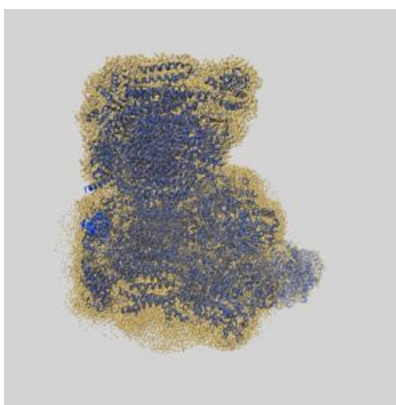
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42226 and PDB model 8UGI. Per-residue inclusion information can be found in section [3](#) on page [37](#).

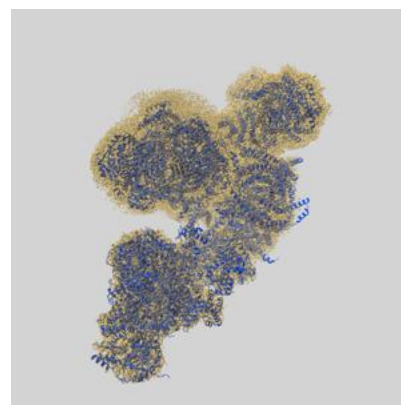
9.1 Map-model overlay [i](#)



X



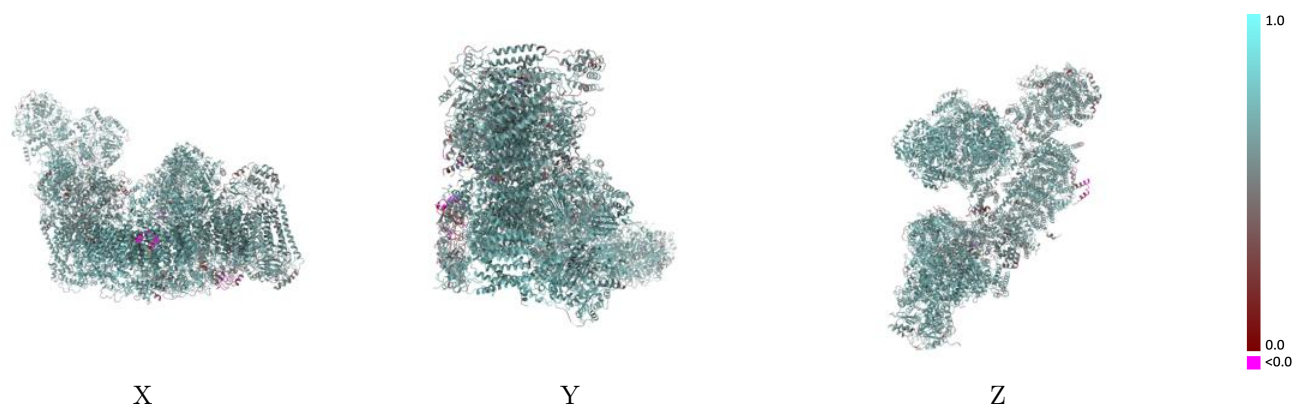
Y



Z

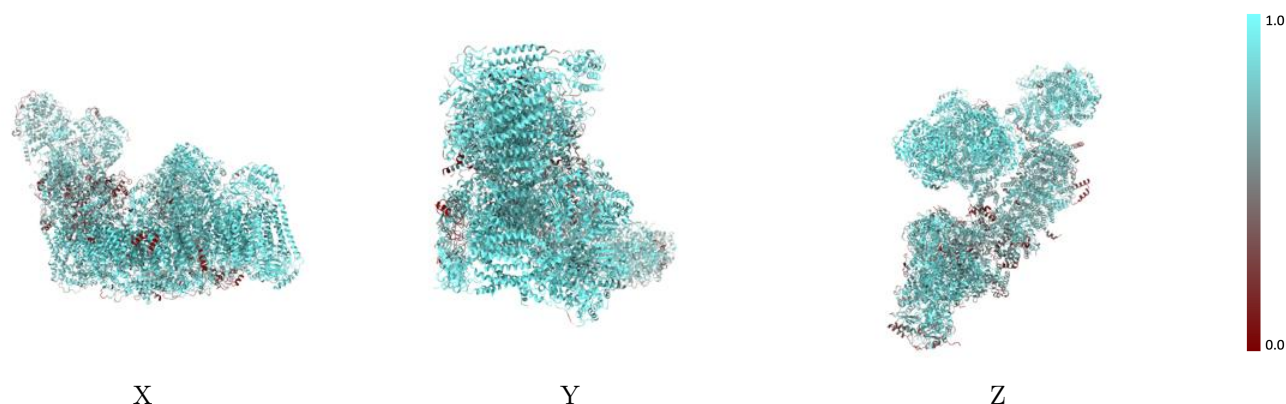
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



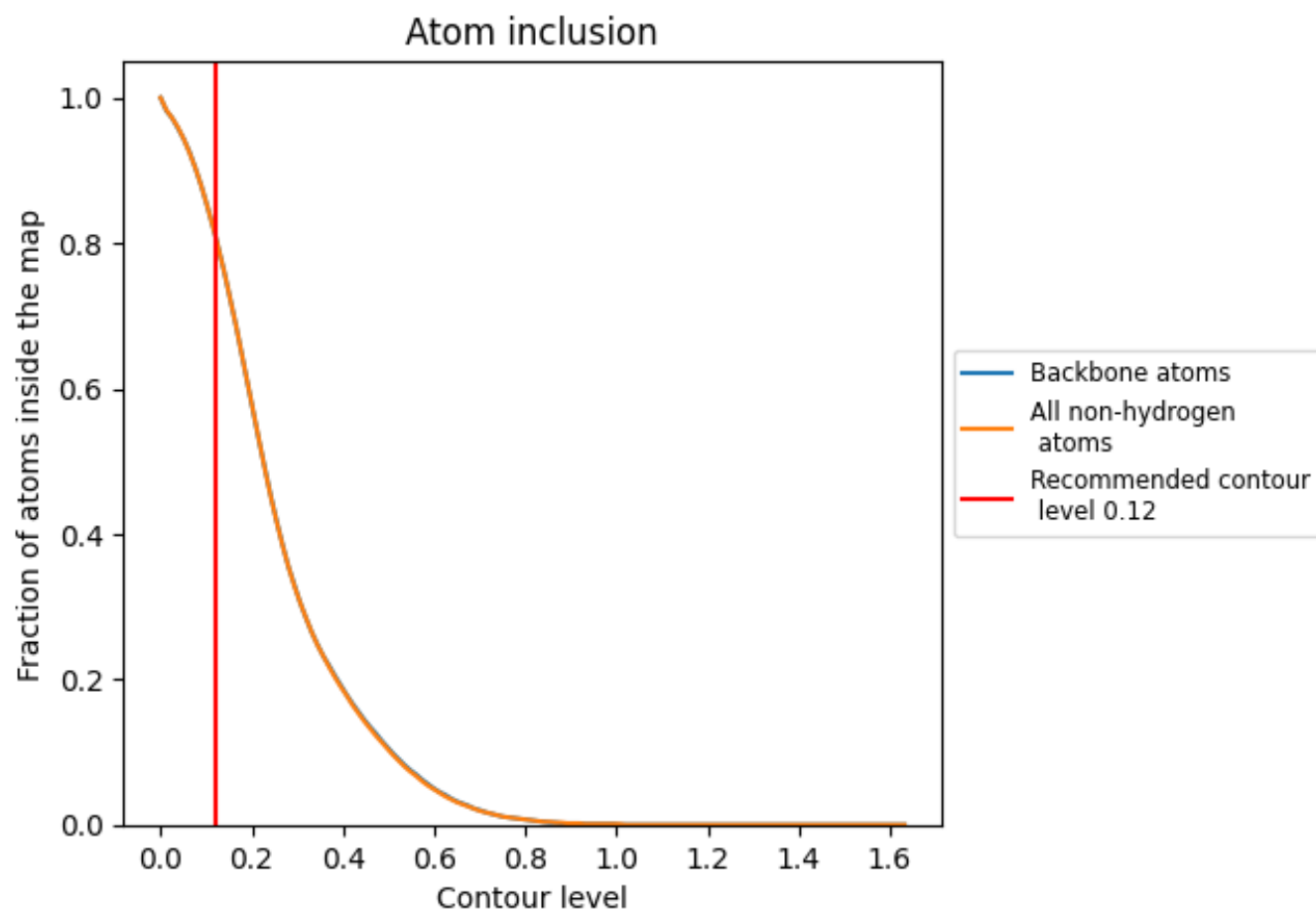
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).







































































9.4 Atom inclusion ⓘ



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

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8110	 0.6290
1A	 0.5190	 0.5330
1B	 0.7830	 0.6630
1C	 0.8480	 0.6870
1D	 0.7960	 0.6680
1E	 0.6080	 0.5860
1F	 0.7220	 0.6170
1G	 0.8100	 0.6560
1H	 0.7760	 0.6240
1I	 0.8700	 0.6900
1J	 0.6170	 0.5640
1K	 0.9020	 0.6730
1L	 0.8600	 0.6620
1M	 0.9120	 0.6880
1N	 0.9020	 0.6860
1O	 0.6060	 0.5640
1P	 0.7150	 0.6230
1Q	 0.7540	 0.6250
1R	 0.7400	 0.6380
1S	 0.7690	 0.6130
1T	 0.2250	 0.4150
1U	 0.6450	 0.6190
1V	 0.5750	 0.6070
1W	 0.7400	 0.6490
1X	 0.7720	 0.6300
1Y	 0.6240	 0.5950
1Z	 0.7610	 0.6400
1a	 0.8560	 0.6560
1b	 0.6820	 0.6010
1c	 0.5860	 0.5910
1d	 0.7900	 0.6610
1e	 0.8390	 0.6470
1f	 0.6250	 0.5700
1g	 0.7350	 0.6110
1h	 0.7890	 0.6540













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Chain	Atom inclusion	Q-score
1i	0.5040	0.4740
1j	0.5840	0.5440
1k	0.5970	0.5710
1l	0.7700	0.6440
1m	0.7570	0.6210
1n	0.7920	0.6340
1o	0.6910	0.5950
1p	0.7720	0.6270
1q	0.7100	0.6630
1r	0.6990	0.6480
1s	0.5900	0.5740
3A	0.9450	0.6800
3B	0.9270	0.6670
3C	0.9880	0.7070
3D	0.9560	0.6770
3E	0.5280	0.4410
3F	0.9730	0.6820
3G	0.9560	0.6510
3H	0.8620	0.5730
3I	0.7010	0.5410
3J	0.9620	0.6820
3N	0.9370	0.6780
3O	0.9260	0.6560
3P	0.9800	0.7090
3Q	0.9540	0.6850
3R	0.5250	0.3980
3S	0.9570	0.6990
3T	0.9270	0.6610
3U	0.8700	0.5800
3V	0.7210	0.5630
3W	0.9820	0.6920
3X	0.9090	0.6210
3Y	0.9190	0.6390
4A	0.9490	0.6290
4B	0.8690	0.5720
4C	0.8990	0.5850
4D	0.8030	0.5190
4E	0.8260	0.5190
4F	0.8400	0.5430
4G	0.7930	0.5020
4H	0.8580	0.5360
4I	0.8670	0.5790

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Chain	Atom inclusion	Q-score
4J	 0.8620	 0.5620
4K	 0.7910	 0.5190
4L	 0.8730	 0.5580
4M	 0.8250	 0.5480
4N	 0.8070	 0.5330