



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 05:17 PM UTC

PDB ID : 8UGJ / pdb_00008ugj
EMDB ID : EMD-42227
Title : In-situ structure of typeB supercomplex in respiratory chain (composite)
Authors : Zheng, W.; Zhang, K.; Zhu, J.
Deposited on : 2023-10-05
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

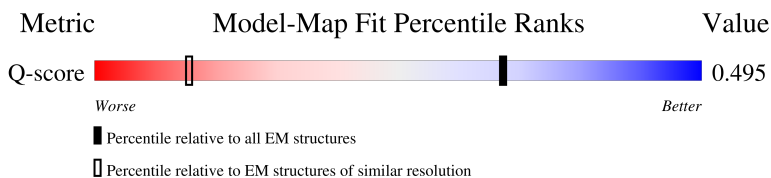
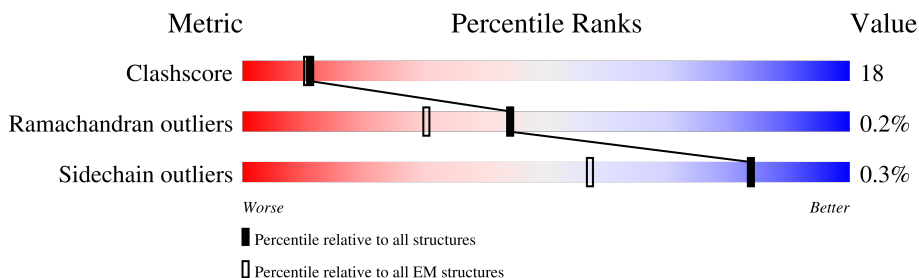
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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	12% 62% 37% .
2	1B	258	37% 23% 40%
3	1C	264	60% 19% 21%
4	1D	476	58% 32% 10%

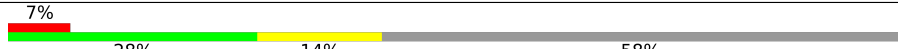
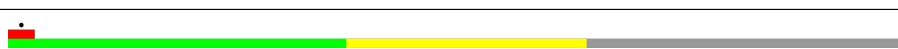
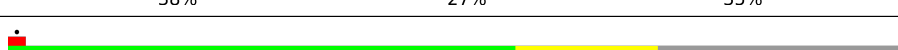
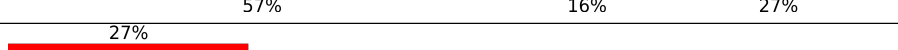
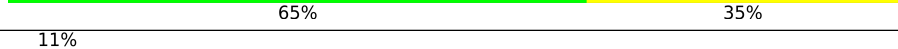
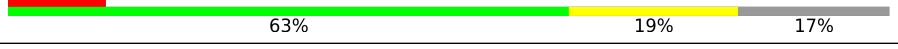
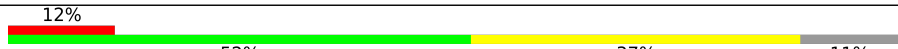
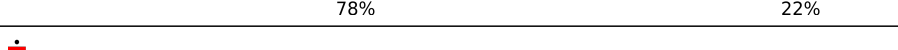
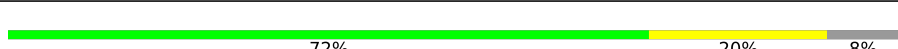
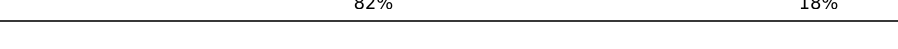
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Mol	Chain	Length	Quality of chain
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24	1Y	141	
25	1Z	144	
26	1a	70	
27	1b	84	
28	1c	76	

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Mol	Chain	Length	Quality of chain
29	1d	122	
30	1e	106	
31	1f	135	
32	1g	154	
33	1h	189	
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	326	
48	3Q	326	
49	3E	274	

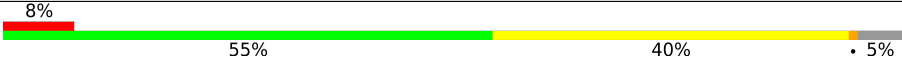
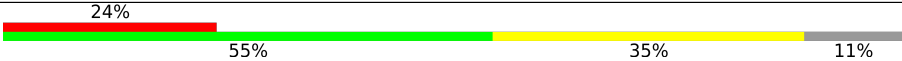
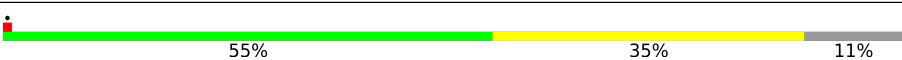
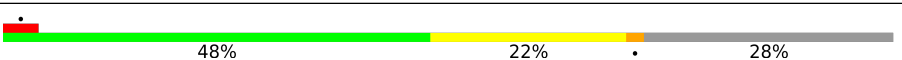
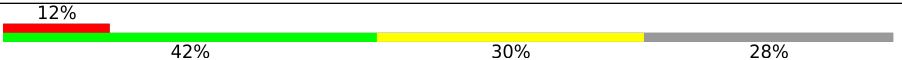
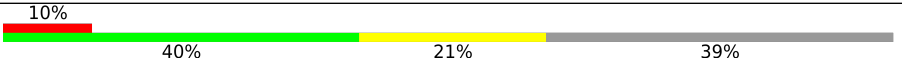
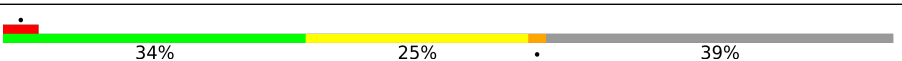
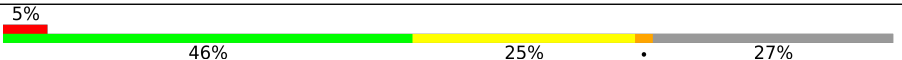
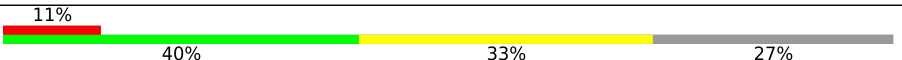
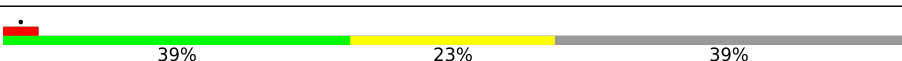
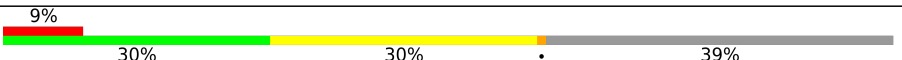
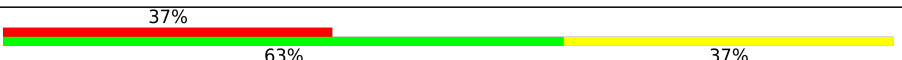
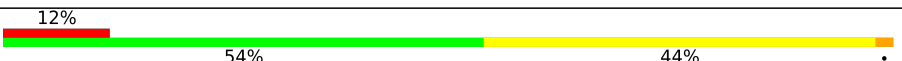
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Mol	Chain	Length	Quality of chain
49	3I	274	
49	3R	274	
49	3V	274	
50	3F	111	
50	3S	111	
51	3G	82	
51	3T	82	
52	3H	91	
52	3U	91	
53	3J	60	
53	3W	60	
54	3X	56	
54	3Y	56	
55	4A	514	
55	8A	514	
56	4B	229	
56	8B	229	
57	4C	261	
57	8C	261	
58	4D	169	
58	8D	169	
59	4E	152	
59	8E	152	
60	4F	128	
60	8F	128	

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Mol	Chain	Length	Quality of chain
61	4G	97	
61	8G	97	
62	4H	86	
62	8H	86	
63	4I	75	
63	8I	75	
64	4J	80	
64	8J	80	
65	4K	80	
65	8K	80	
66	4L	63	
66	8L	63	
67	4M	70	
67	8M	70	
68	4N	82	
68	8N	82	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
71	SF4	1B	201	-	-	X	-
71	SF4	1F	502	-	-	X	-
71	SF4	1G	801	-	-	X	-
72	FES	1G	803	-	-	X	-
72	FES	3E	301	-	-	X	-
72	FES	3R	301	-	-	X	-
91	CUA	4B	304	-	-	X	-
91	CUA	8B	304	-	-	X	-

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 134346 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.

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
			340	211	65	63	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
			224	136	48	39	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3E	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3E	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3E	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3E	56	ARG	SER	conflict	UNP A0A4X1TWD8
3I	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3I	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3I	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3I	56	ARG	SER	conflict	UNP A0A4X1TWD8
3R	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3R	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3R	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3R	56	ARG	SER	conflict	UNP A0A4X1TWD8
3V	34	VAL	LEU	conflict	UNP A0A4X1TWD8
3V	45	LEU	ALA	conflict	UNP A0A4X1TWD8
3V	49	VAL	PHE	conflict	UNP A0A4X1TWD8
3V	56	ARG	SER	conflict	UNP A0A4X1TWD8

- 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 Complex III subunit 9.

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	514	Total	C	N	O	S	0	0
			4026	2693	625	676	32		
55	8A	514	Total	C	N	O	S	0	0
			4026	2693	625	676	32		

- 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
			1828	1190	281	339	18		
56	8B	227	Total	C	N	O	S	0	0
			1828	1190	281	339	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		
57	8C	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		
58	8D	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		
59	8E	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		
60	8F	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		
61	8G	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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
62	8H	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		
63	8I	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		
64	8J	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		
65	8K	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		
66	8L	46	Total	C	N	O	S	0	0
			381	254	64	61	2		

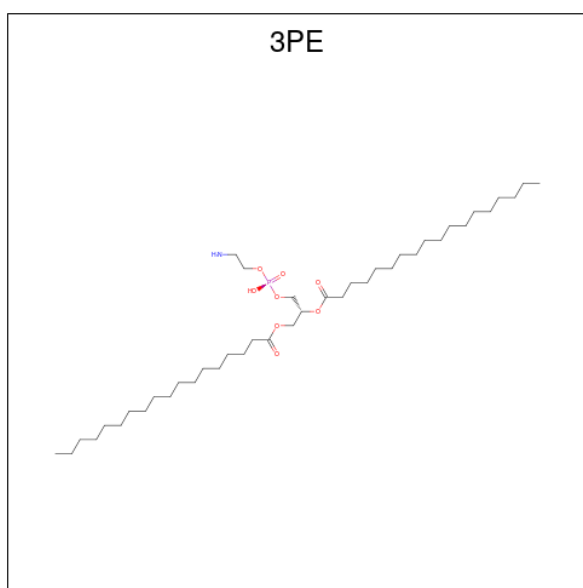
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	4M	43	Total	C	N	O	0	0
			338	222	57	59		
67	8M	43	Total	C	N	O	0	0
			338	222	57	59		

- Molecule 68 is a protein called Cytochrome c oxidase subunit NDUF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	4N	82	Total	C	N	O	S	0	0
			660	432	112	114	2		
68	8N	82	Total	C	N	O	S	0	0
			660	432	112	114	2		

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



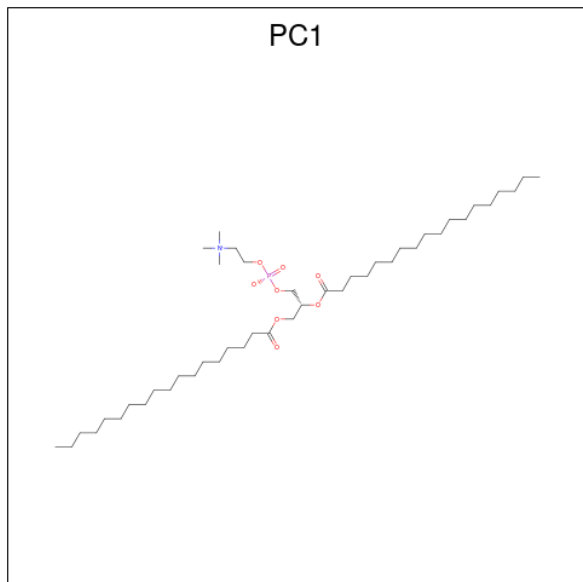
Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1K	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1L	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1M	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1M	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1M	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1M	1	Total	C	N	O	P	0
			50	40	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	1N	1	Total 49	C 39	N 1	O 8	P 1	0
69	1P	1	Total 35	C 25	N 1	O 8	P 1	0
69	1Y	1	Total 31	C 21	N 1	O 8	P 1	0
69	1Y	1	Total 40	C 30	N 1	O 8	P 1	0
69	1Y	1	Total 30	C 20	N 1	O 8	P 1	0
69	1Y	1	Total 33	C 23	N 1	O 8	P 1	0
69	1Y	1	Total 27	C 17	N 1	O 8	P 1	0
69	1d	1	Total 49	C 39	N 1	O 8	P 1	0
69	1j	1	Total 44	C 34	N 1	O 8	P 1	0
69	1m	1	Total 41	C 31	N 1	O 8	P 1	0
69	3A	1	Total 27	C 17	N 1	O 8	P 1	0
69	3A	1	Total 32	C 22	N 1	O 8	P 1	0
69	3C	1	Total 35	C 25	N 1	O 8	P 1	0
69	3C	1	Total 34	C 24	N 1	O 8	P 1	0
69	3D	1	Total 33	C 23	N 1	O 8	P 1	0
69	3G	1	Total 29	C 19	N 1	O 8	P 1	0
69	3N	1	Total 33	C 23	N 1	O 8	P 1	0
69	3N	1	Total 25	C 15	N 1	O 8	P 1	0
69	3P	1	Total 33	C 23	N 1	O 8	P 1	0
69	3R	1	Total 47	C 37	N 1	O 8	P 1	0
69	3Y	1	Total 30	C 20	N 1	O 8	P 1	0

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



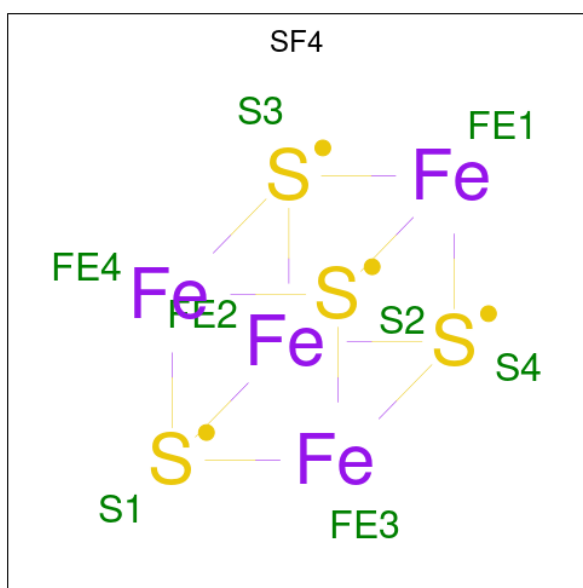
Mol	Chain	Residues	Atoms					AltConf
70	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1B	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1B	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1H	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	1M	1	Total	C	N	O	P	0
			35	25	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
			46	36	1	8	1	
70	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	

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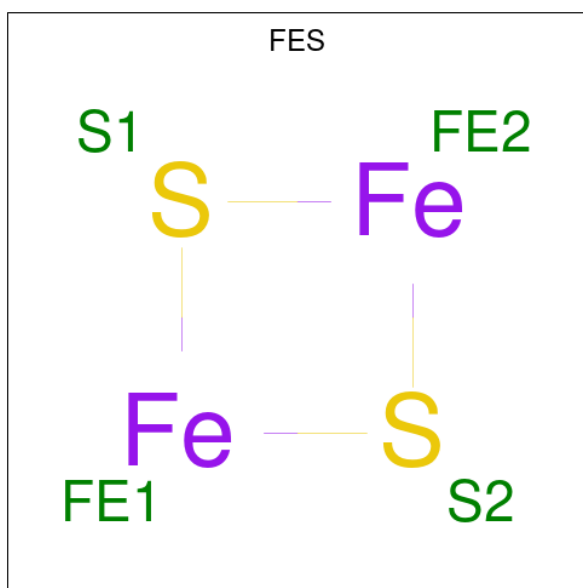
Mol	Chain	Residues	Atoms					AltConf
70	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	
70	1q	1	Total	C	N	O	P	0
			49	39	1	8	1	
70	3J	1	Total	C	N	O	P	0
			47	37	1	8	1	
70	3R	1	Total	C	N	O	P	0
			45	35	1	8	1	
70	3X	1	Total	C	N	O	P	0
			29	19	1	8	1	

- Molecule 71 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



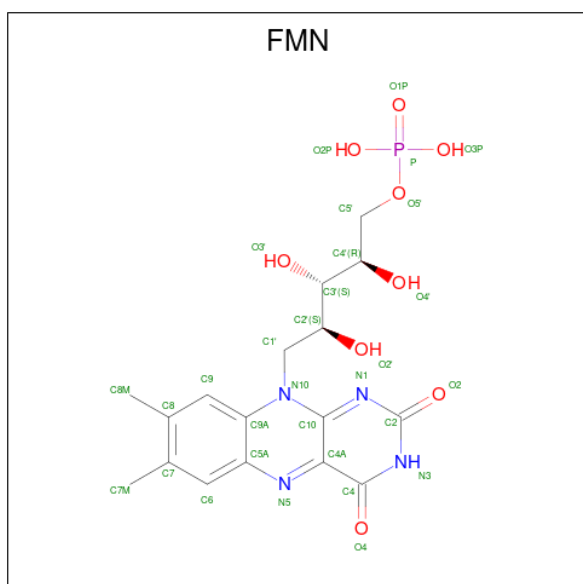
Mol	Chain	Residues	Atoms			AltConf
71	1B	1	Total	Fe	S	0
			8	4	4	
71	1F	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	

- Molecule 72 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: 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 (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

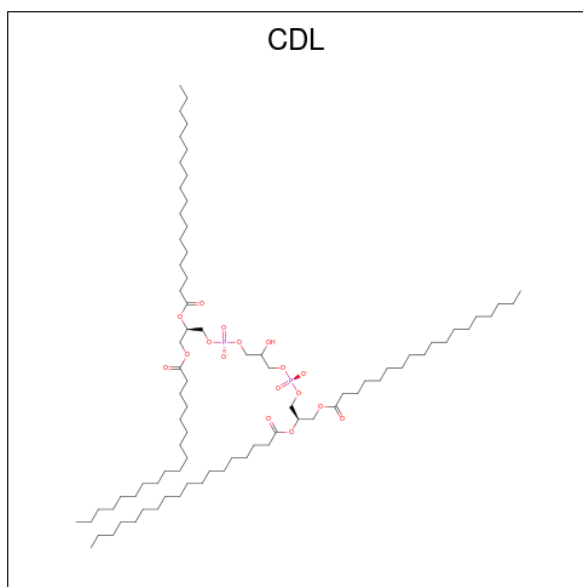


Mol	Chain	Residues	Atoms					AltConf
73	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 74 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 75 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



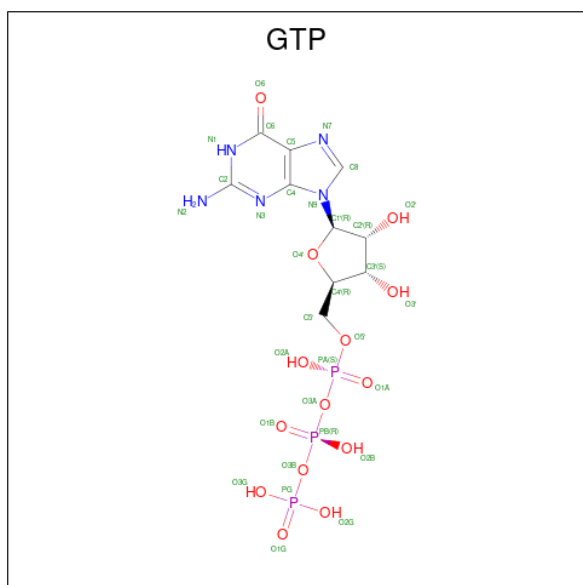
Mol	Chain	Residues	Atoms				AltConf
75	1H	1	Total	C	O	P	0
			51	32	17	2	
75	1L	1	Total	C	O	P	0
			76	57	17	2	
75	1N	1	Total	C	O	P	0
			62	43	17	2	
75	1X	1	Total	C	O	P	0
			86	67	17	2	
75	1d	1	Total	C	O	P	0
			65	46	17	2	
75	1h	1	Total	C	O	P	0
			80	61	17	2	
75	1q	1	Total	C	O	P	0
			61	42	17	2	
75	3A	1	Total	C	O	P	0
			58	39	17	2	

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Mol	Chain	Residues	Atoms				AltConf
75	3G	1	Total	C	O	P	0
			52	33	17	2	
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	
75	8B	1	Total	C	O	P	0
			100	81	17	2	
75	8C	1	Total	C	O	P	0
			100	81	17	2	
75	8D	1	Total	C	O	P	0
			100	81	17	2	

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

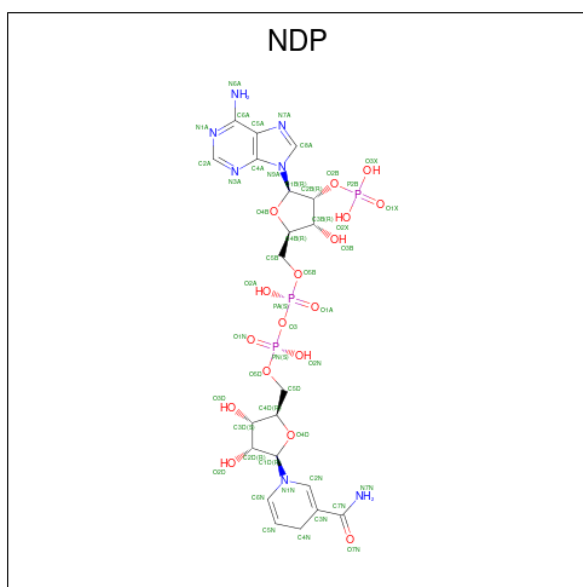


Mol	Chain	Residues	Atoms					AltConf
76	1O	1	Total 32	C 10	N 5	O 14	P 3	0

- Molecule 77 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
77	1O	1	Total Mg 1 1	0
77	4A	1	Total Mg 1 1	0
77	8A	1	Total Mg 1 1	0

- Molecule 78 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



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

- Molecule 79 is ZINC ION (CCD ID: ZN) (formula: Zn).

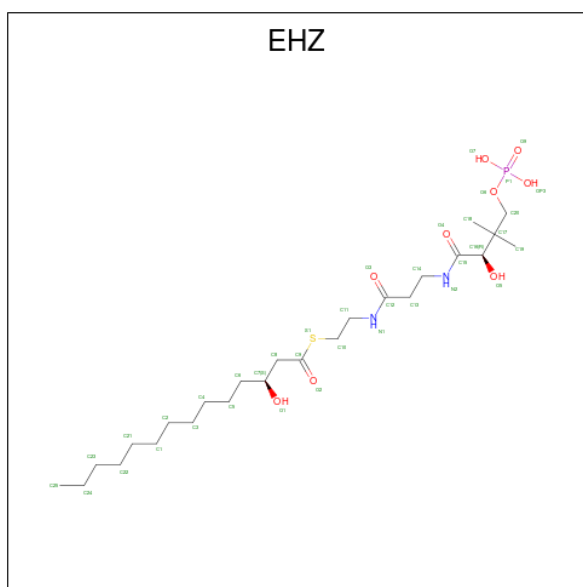
Mol	Chain	Residues	Atoms	AltConf
79	1R	1	Total Zn 1 1	0
79	4F	1	Total Zn 1 1	0

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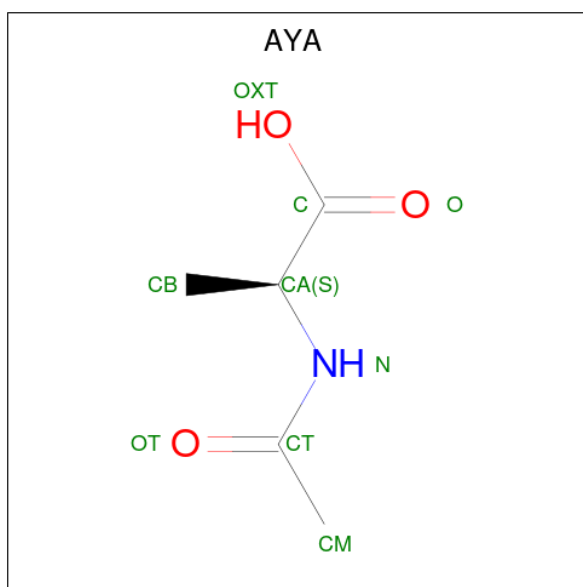
Mol	Chain	Residues	Atoms		AltConf
79	8F	1	Total	Zn	0
			1	1	

- Molecule 80 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



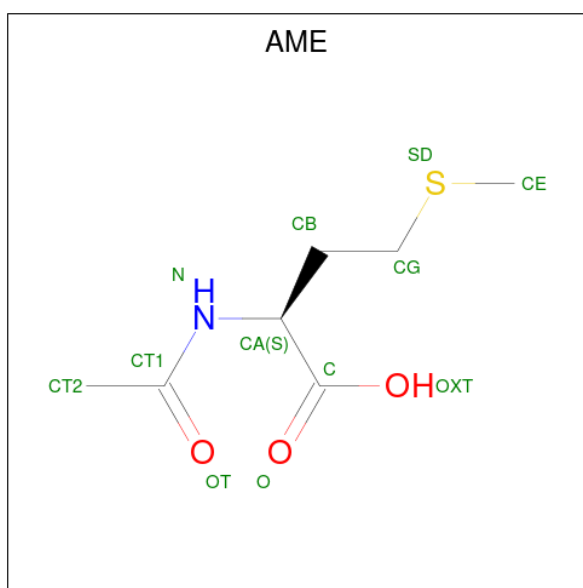
Mol	Chain	Residues	Atoms						AltConf
80	1T	1	Total 37	C 25	N 2	O 8	P 1	S 1	0
80	1n	1	Total 37	C 25	N 2	O 8	P 1	S 1	0

- Molecule 81 is N-ACETYLALANINE (CCD ID: AYA) (formula: C₅H₉NO₃).



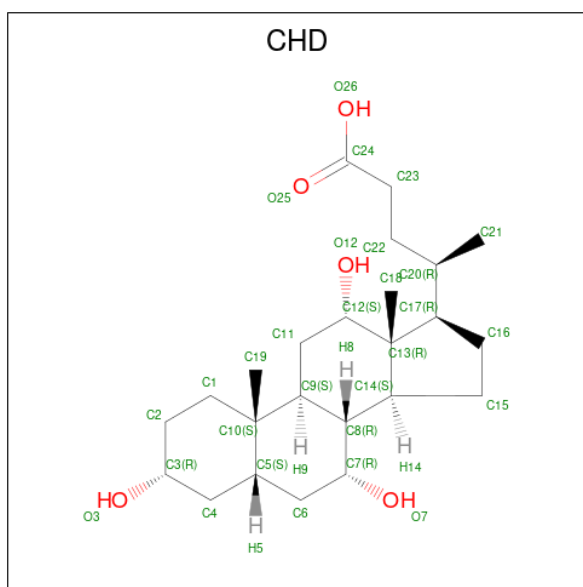
Mol	Chain	Residues	Atoms				AltConf
81	1Y	1	Total	C	N	O	0
			8	5	1	2	
81	1q	1	Total	C	N	O	0
			8	5	1	2	

- Molecule 82 is N-ACETYL METHIONINE (CCD ID: AME) (formula: $C_7H_{13}NO_3S$).



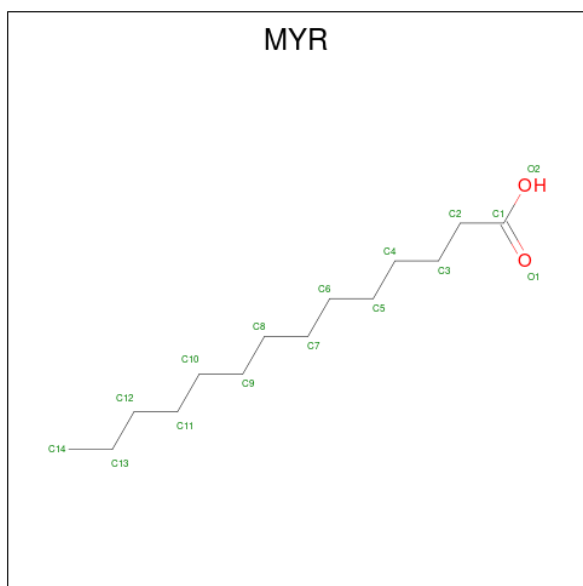
Mol	Chain	Residues	Atoms					AltConf
82	1h	1	Total	C	N	O	S	0
			11	7	1	2	1	

- Molecule 83 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



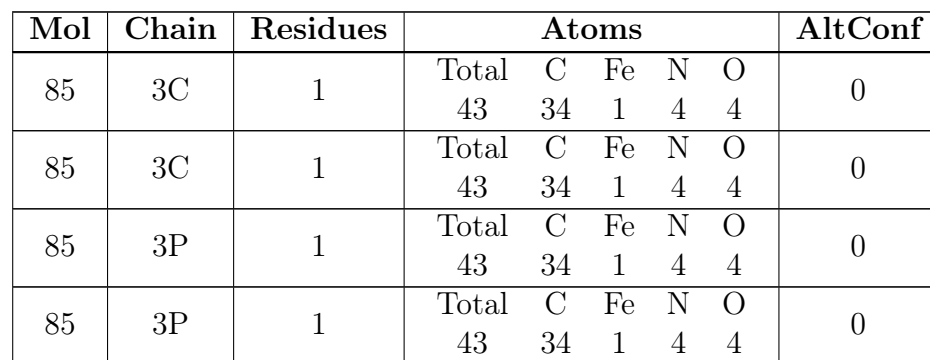
Mol	Chain	Residues	Atoms			AltConf
83	1i	1	Total	C	O	0
			29	24	5	

- Molecule 84 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
84	1l	1	Total	C	O	0
			15	14	1	

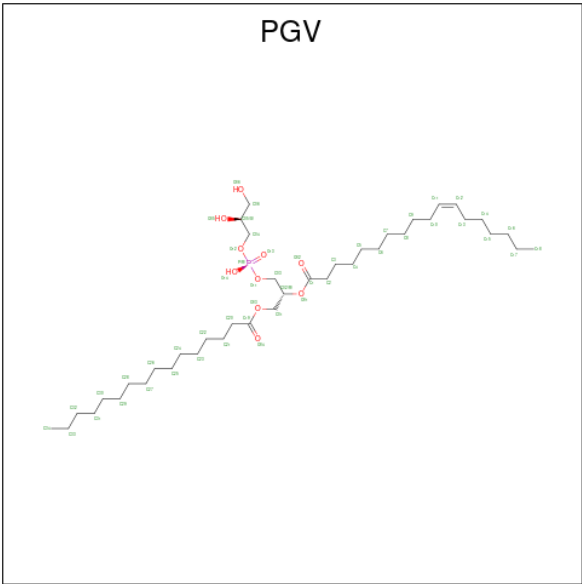
- Molecule 85 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



-
- The chemical structure of HEC (Hydroxyethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure includes various side chains and a central hydroxyl group (OH). The atoms are labeled with codes: O1A, O2A, O1D, O2D, CGA, CGD, CAA, CBA, CAD, CBD, CMA, C3A, C4A, C3B, C4B, CMB, CAB, CBB, C2A, C1A, C2B, C1B, C2C, C1C, C2D, C1D, C2E, C1E, C3C, C4C, C3D, C4D, C3E, C4E, C3F, C4F, C3G, C4G, C3H, C4H, C3I, C4I, C3J, C4J, C3K, C4K, C3L, C4L, C3M, C4M, C3N, C4N, C3O, C4O, C3P, C4P, C3Q, C4Q, C3R, C4R, C3S, C4S, C3T, C4T, C3U, C4U, C3V, C4V, C3W, C4W, C3X, C4X, C3Y, C4Y, C3Z, C4Z, C3AA, C4AA, C3AB, C4AB, C3AC, C4AC, C3AD, C4AD, C3AE, C4AE, C3AF, C4AF, C3AG, C4AG, C3AH, C4AH, C3AI, C4AI, C3AJ, C4AJ, C3AK, C4AK, C3AL, C4AL, C3AM, C4AM, C3AN, C4AN, C3AO, C4AO, C3AP, C4AP, C3AQ, C4AQ, C3AR, C4AR, C3AS, C4AS, C3AT, C4AT, C3AU, C4AU, C3AV, C4AV, C3AW, C4AW, C3AX, C4AX, C3AY, C4AY, C3AZ, C4AZ, C3BA, C4BA, C3BB, C4BB, C3BC, C4BC, C3BD, C4BD, C3BE, C4BE, C3BF, C4BF, C3BG, C4BG, C3BH, C4BH, C3BI, C4BI, C3BJ, C4BJ, C3BK, C4BK, C3BL, C4BL, C3BM, C4BM, C3BN, C4BN, C3BO, C4BO, C3BP, C4BP, C3BQ, C4BQ, C3BR, C4BR, C3BS, C4BS, C3BT, C4BT, C3BU, C4BU, C3BV, C4BV, C3BW, 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Mol	Chain	Residues	Atoms					AltConf
86	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
86	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 87 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



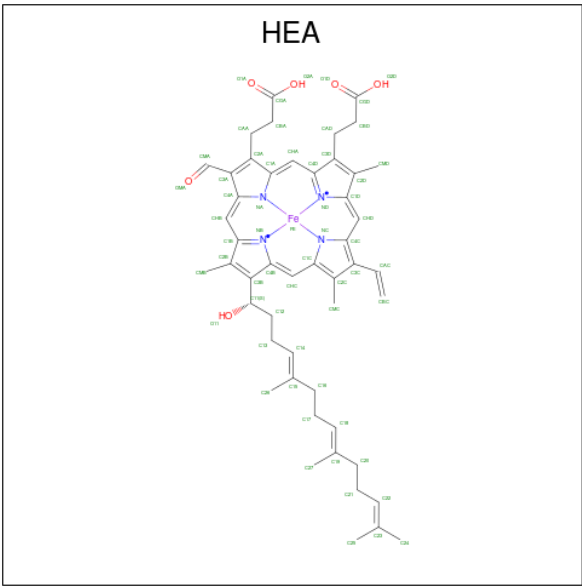
Mol	Chain	Residues	Atoms				AltConf
87	4A	1	Total	C	O	P	0
			51	40	10	1	
87	4A	1	Total	C	O	P	0
			51	40	10	1	
87	4A	1	Total	C	O	P	0
			51	40	10	1	
87	4B	1	Total	C	O	P	0
			51	40	10	1	
87	4B	1	Total	C	O	P	0
			51	40	10	1	
87	4C	1	Total	C	O	P	0
			51	40	10	1	
87	4C	1	Total	C	O	P	0
			51	40	10	1	
87	4C	1	Total	C	O	P	0
			51	40	10	1	
87	4C	1	Total	C	O	P	0
			51	40	10	1	

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Mol	Chain	Residues	Atoms				AltConf
87	4C	1	Total 51	C 40	O 10	P 1	0
87	4G	1	Total 51	C 40	O 10	P 1	0
87	4J	1	Total 51	C 40	O 10	P 1	0
87	4K	1	Total 51	C 40	O 10	P 1	0
87	4L	1	Total 51	C 40	O 10	P 1	0
87	4M	1	Total 51	C 40	O 10	P 1	0
87	8A	1	Total 51	C 40	O 10	P 1	0
87	8A	1	Total 51	C 40	O 10	P 1	0
87	8A	1	Total 51	C 40	O 10	P 1	0
87	8B	1	Total 51	C 40	O 10	P 1	0
87	8B	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8C	1	Total 51	C 40	O 10	P 1	0
87	8G	1	Total 51	C 40	O 10	P 1	0
87	8J	1	Total 51	C 40	O 10	P 1	0
87	8K	1	Total 51	C 40	O 10	P 1	0
87	8L	1	Total 51	C 40	O 10	P 1	0

- Molecule 88 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
88	4A	1	Total 60	C 49	Fe 1	N 4	O 6	0
88	4A	1	Total 60	C 49	Fe 1	N 4	O 6	0
88	8A	1	Total 60	C 49	Fe 1	N 4	O 6	0
88	8A	1	Total 60	C 49	Fe 1	N 4	O 6	0

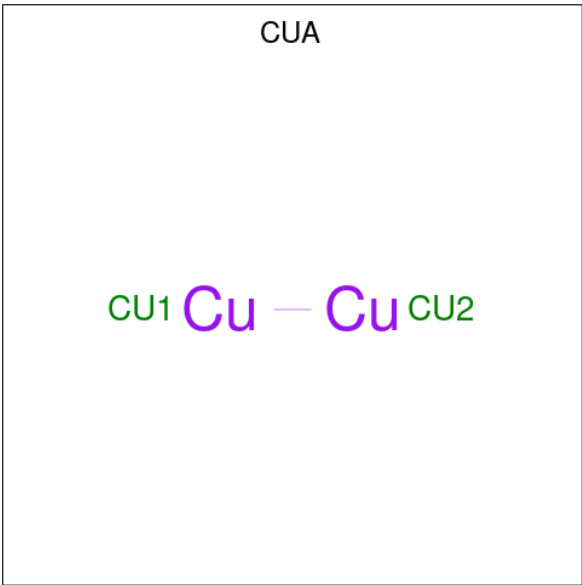
- Molecule 89 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
89	4A	1	Total	Cu	0
			1	1	
89	8A	1	Total	Cu	0
			1	1	

- Molecule 90 is SODIUM ION (CCD ID: NA) (formula: Na).

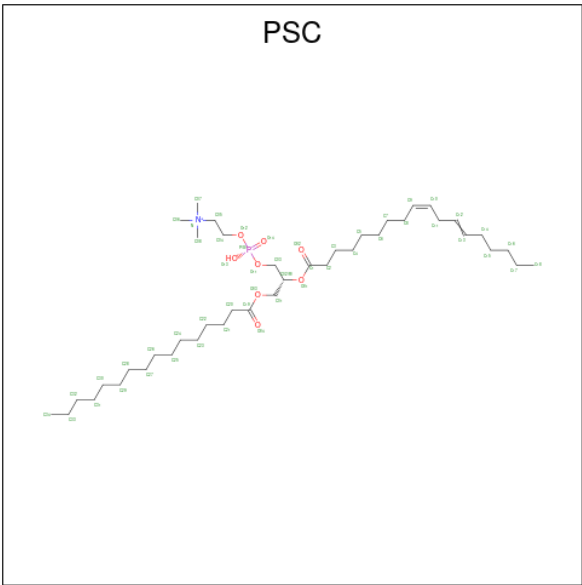
Mol	Chain	Residues	Atoms		AltConf
90	4A	1	Total	Na	0
			1	1	
90	8A	1	Total	Na	0
			1	1	

- Molecule 91 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		AltConf
91	4B	1	Total	Cu	0
			2	2	
91	8B	1	Total	Cu	0
			2	2	

- Molecule 92 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



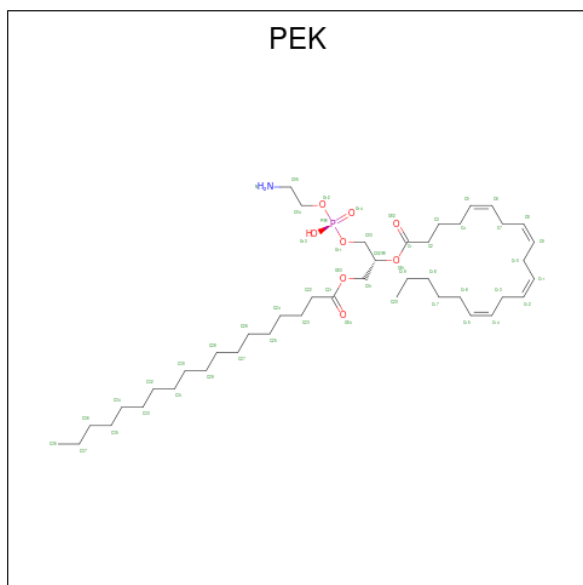
Mol	Chain	Residues	Atoms					AltConf
92	4B	1	Total	C	N	O	P	0
			52	42	1	8	1	

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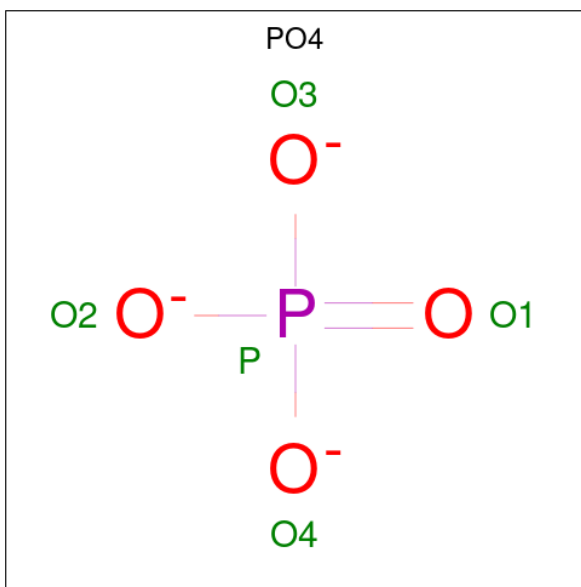
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
92	8B	1	52	42	1	8	1	0

- Molecule 93 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).

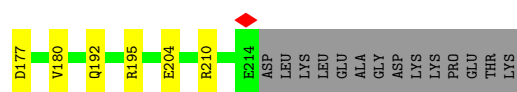


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
93	4C	1	52	42	1	8	1	0
93	4G	1	53	43	1	8	1	0
93	8C	1	52	42	1	8	1	0
93	8G	1	53	43	1	8	1	0

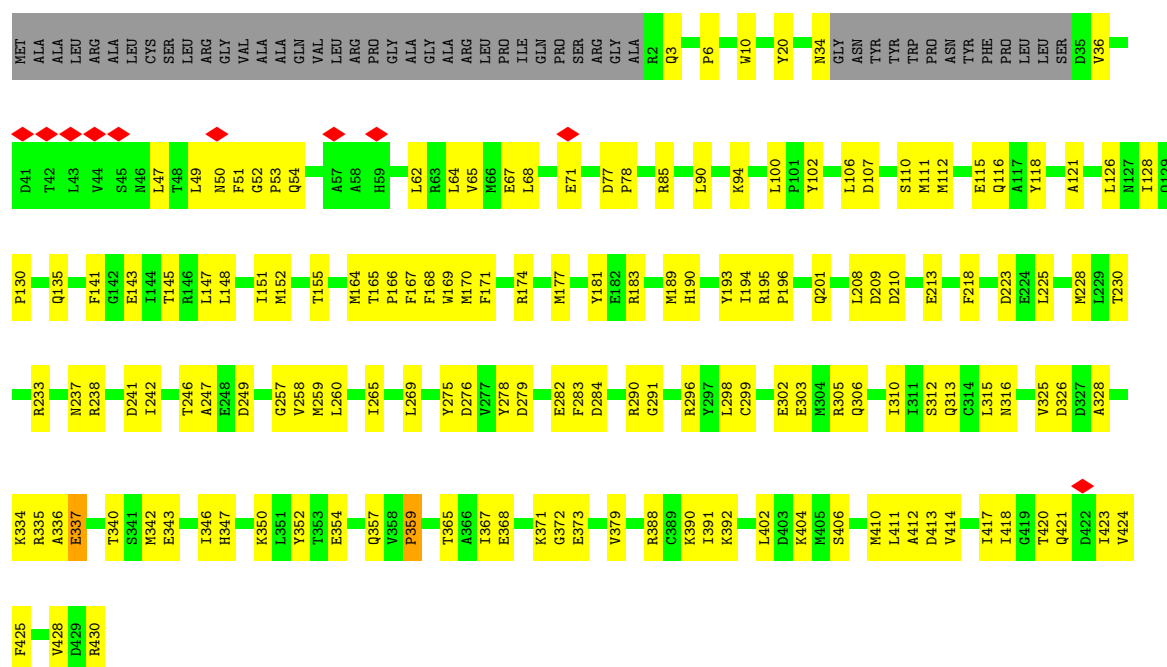
- Molecule 94 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



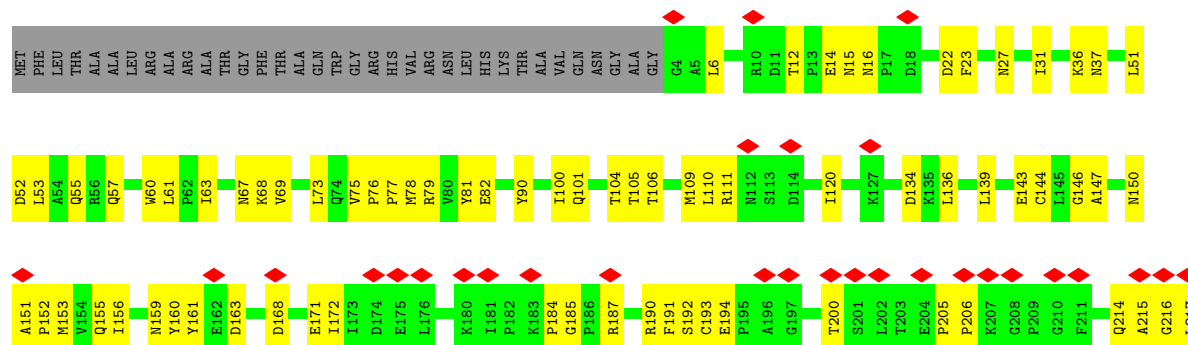
Mol	Chain	Residues	Atoms			AltConf
94	4H	1	Total	O	P	0
			5	4	1	
94	8H	1	Total	O	P	0
			5	4	1	



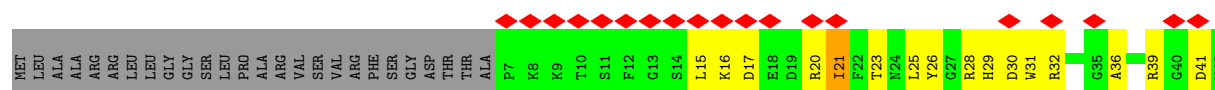
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

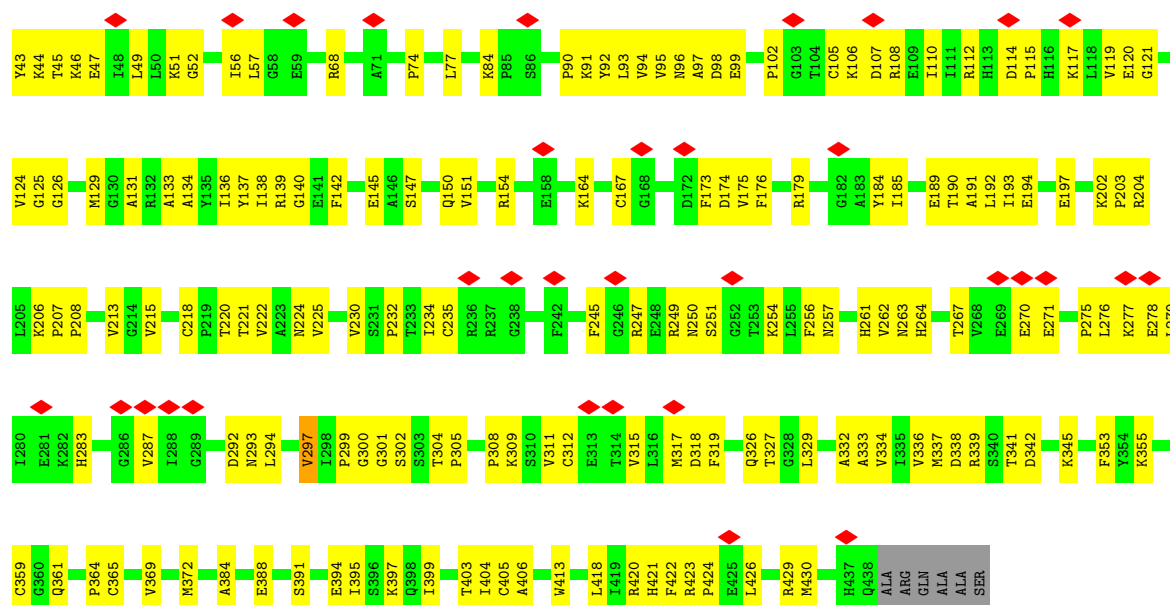


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



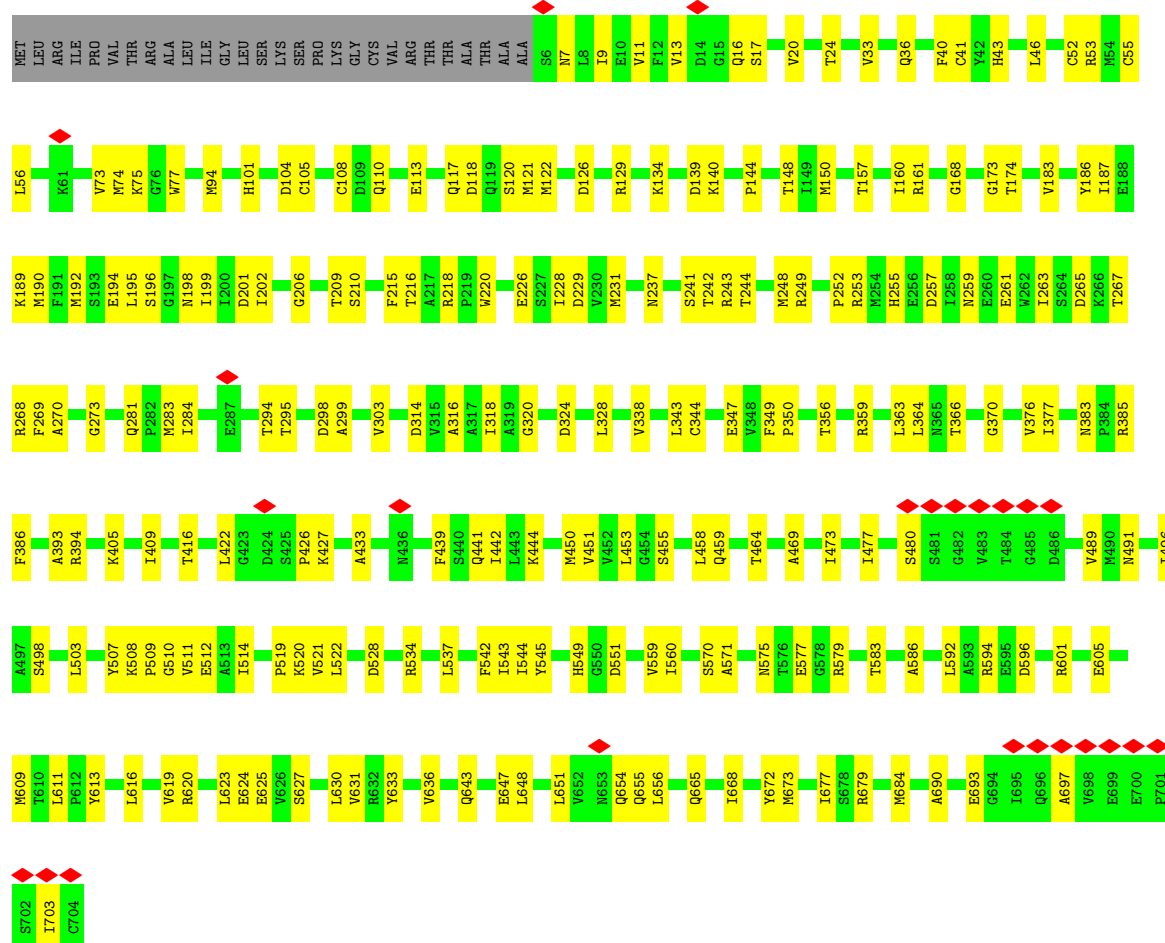
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



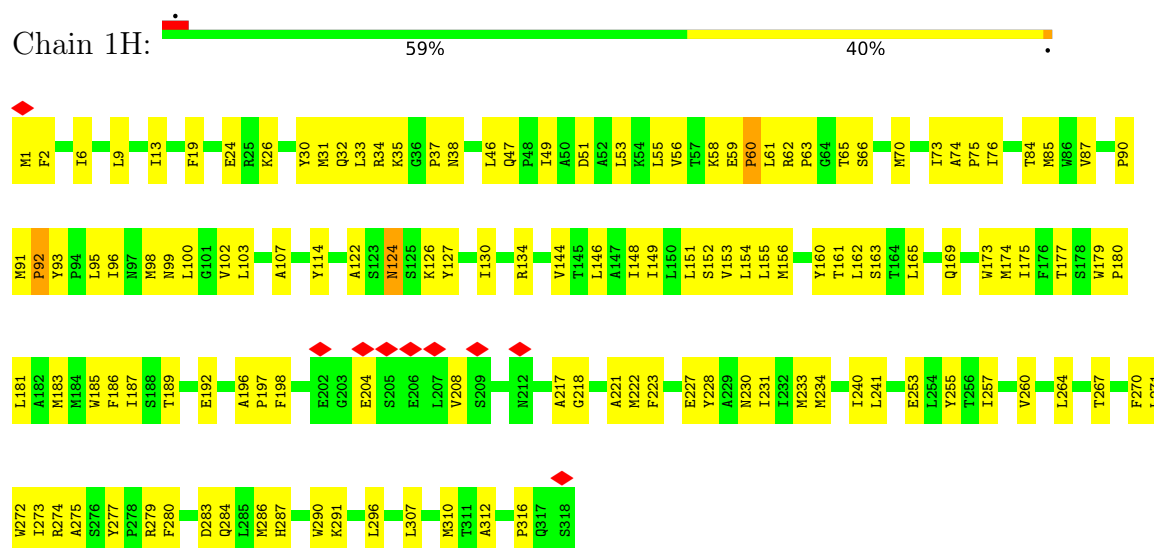


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

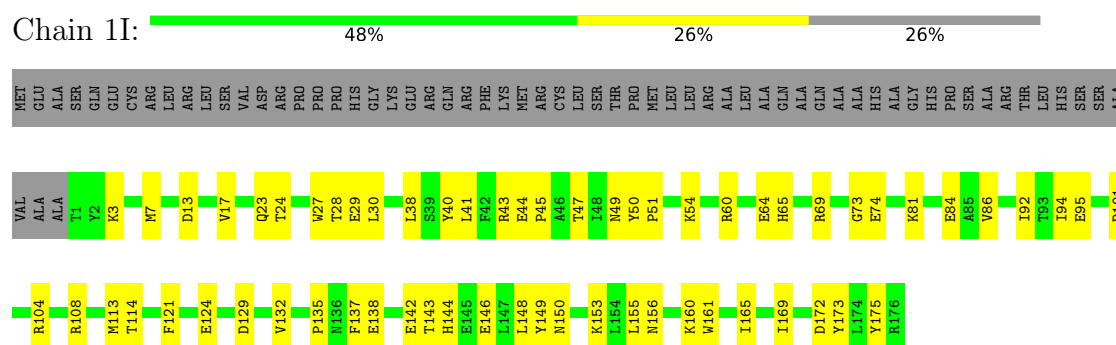
Chain 1G: 66% 30% .



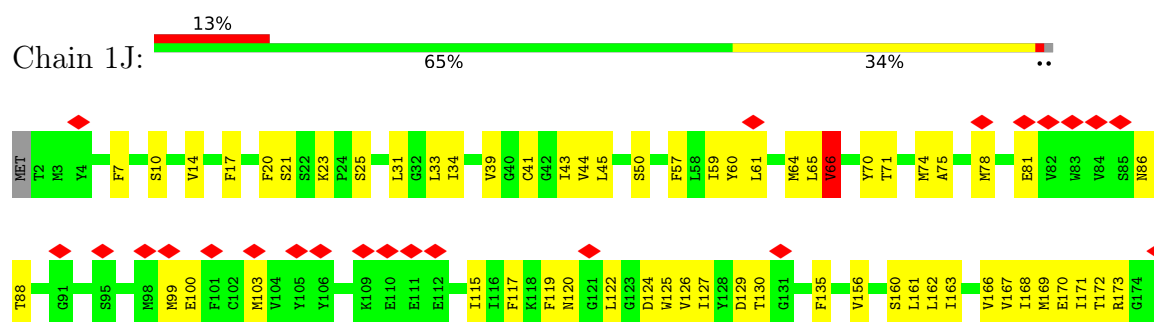
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



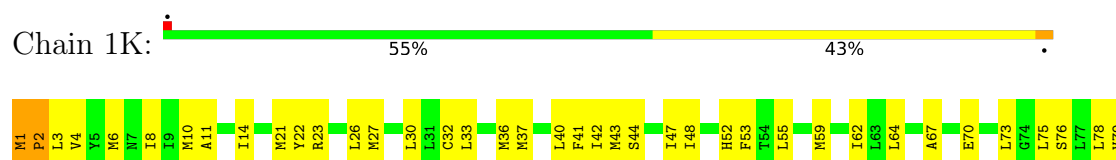
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

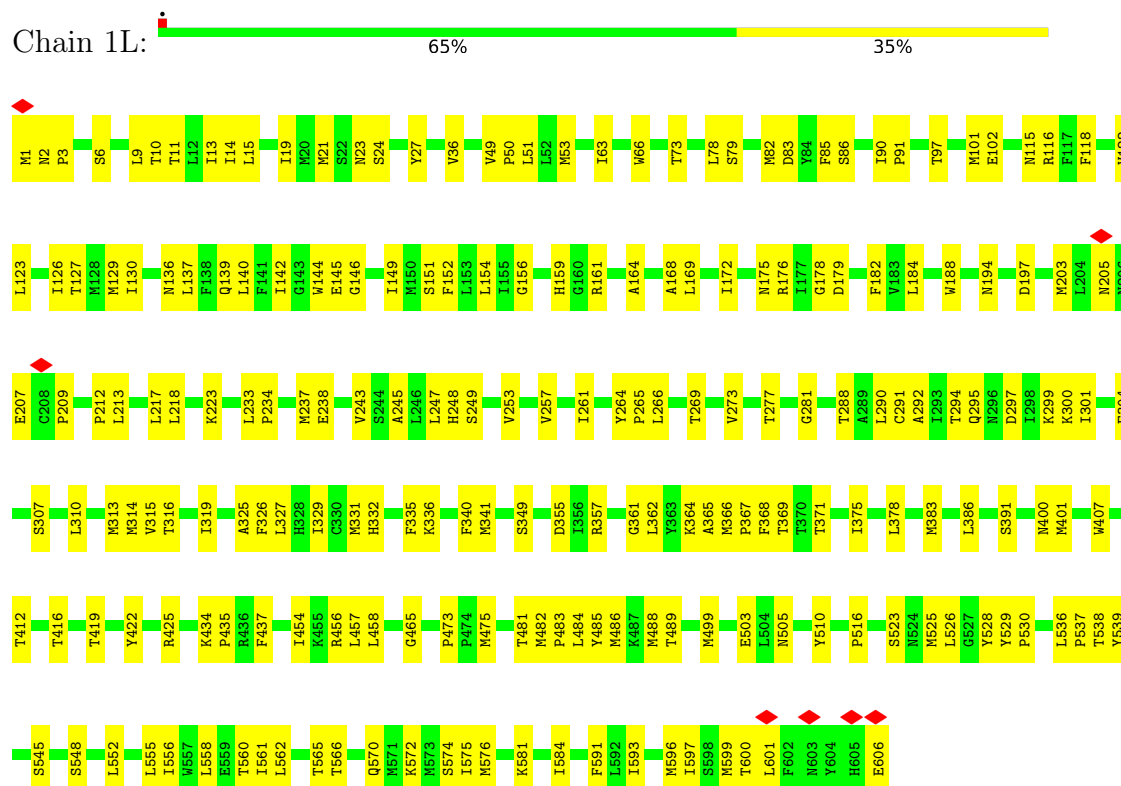


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

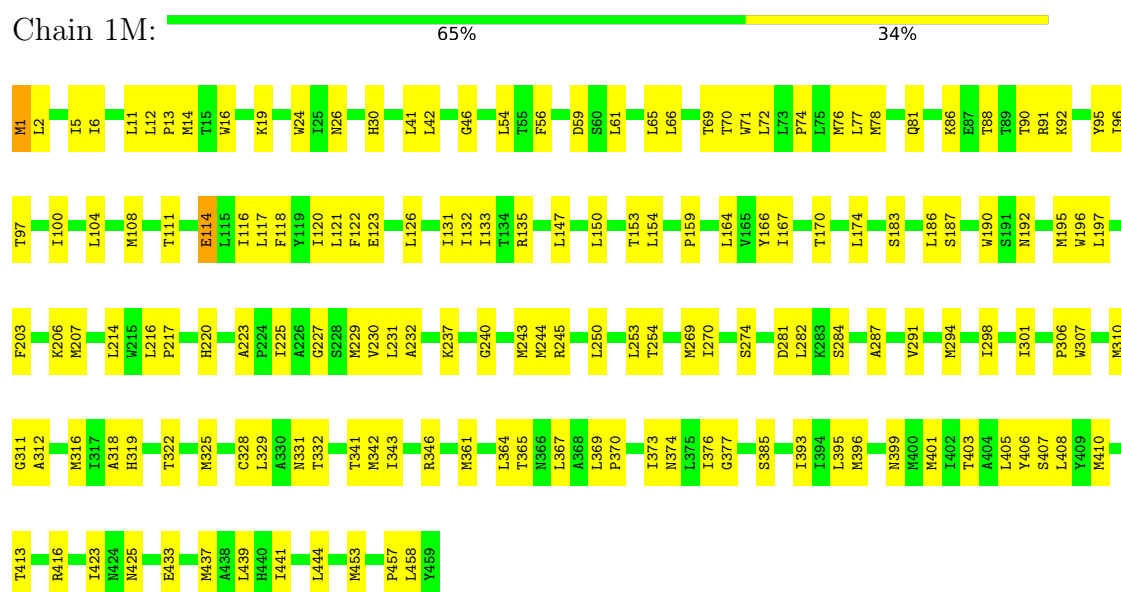




• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

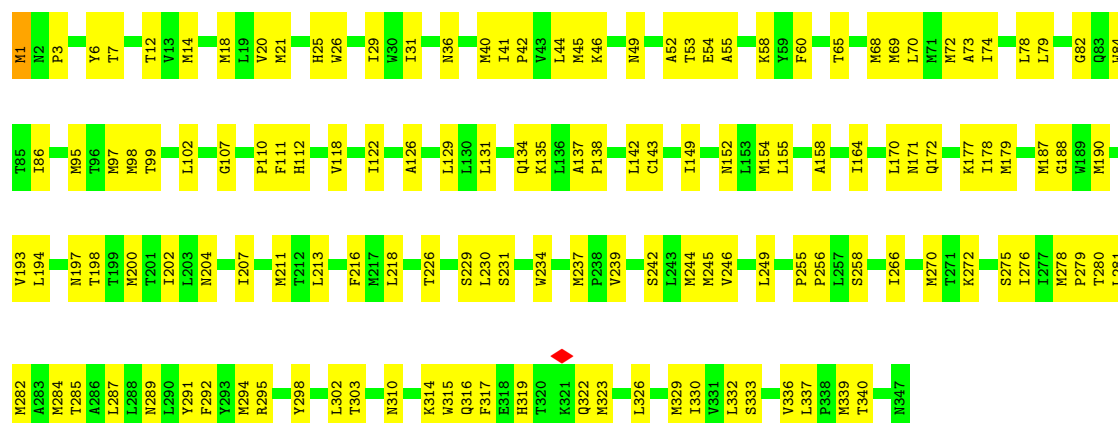


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



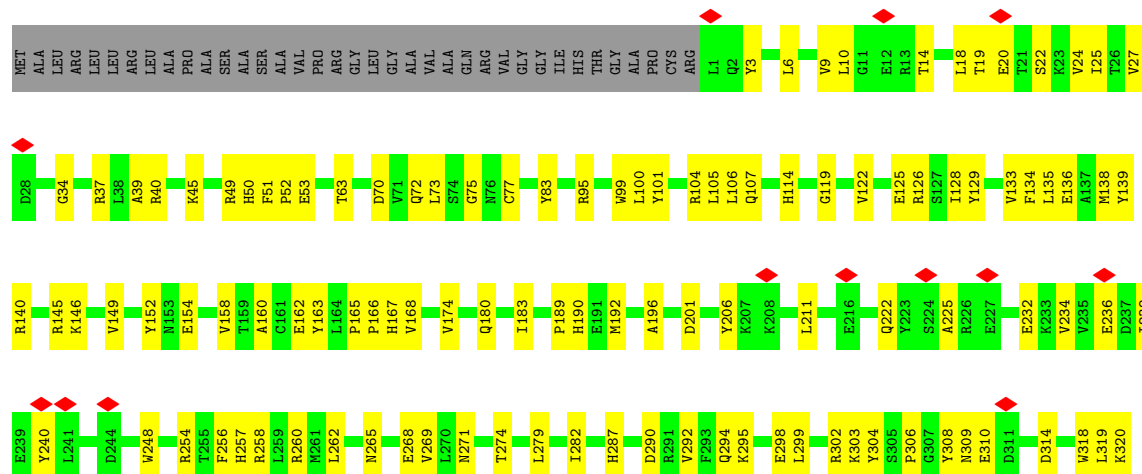
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 1N:  60% 40%



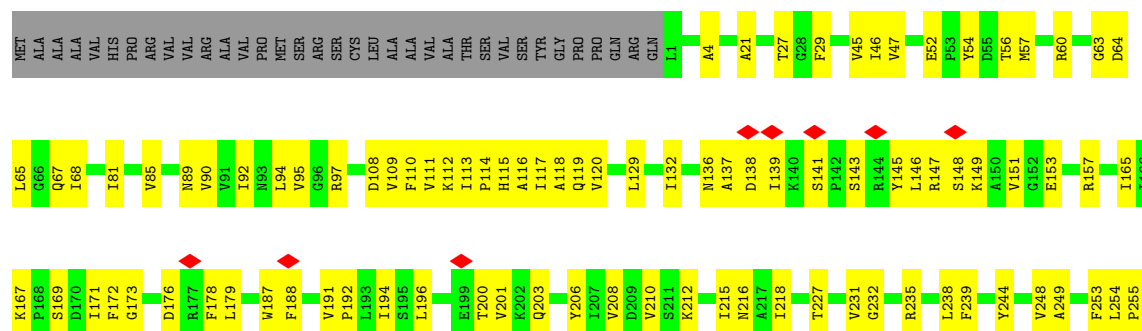
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 1O:  58% 32% 10%



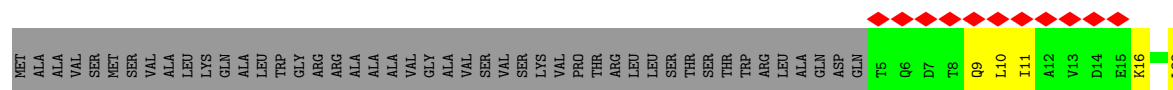
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P:  60% 31% 9%





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



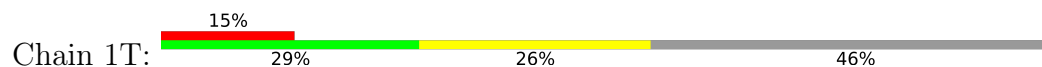
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



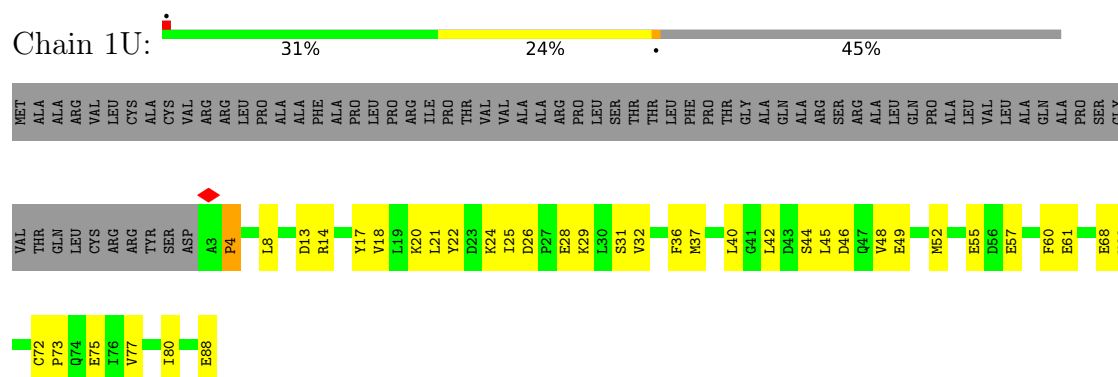
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



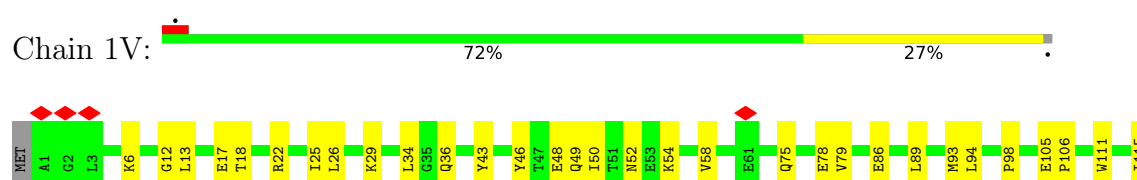
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



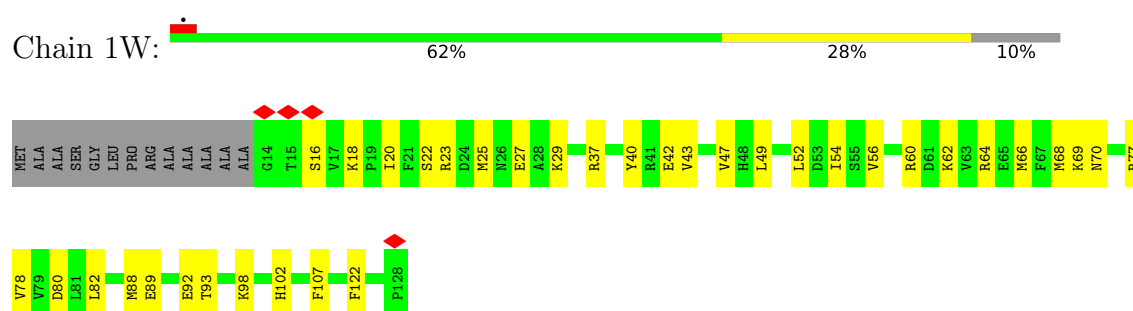
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



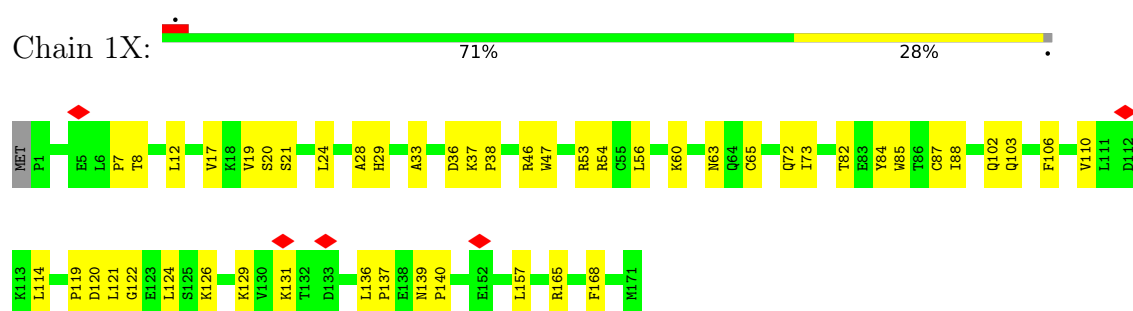
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



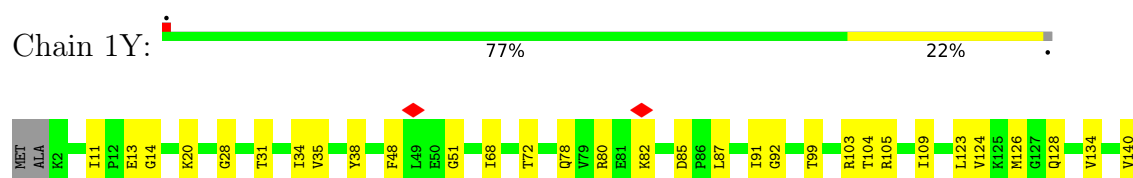
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



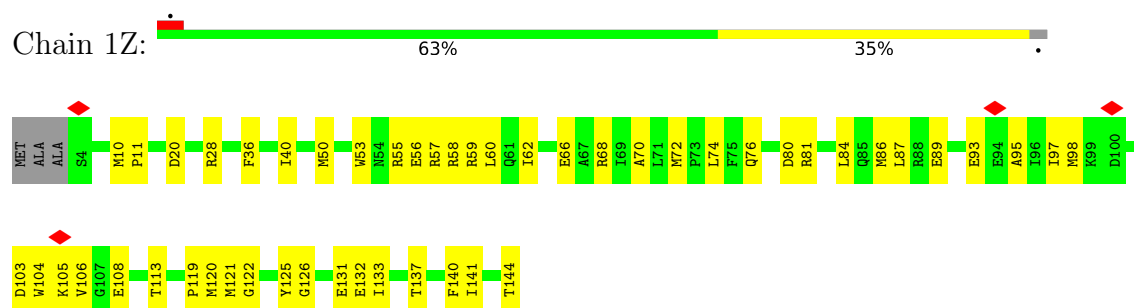
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



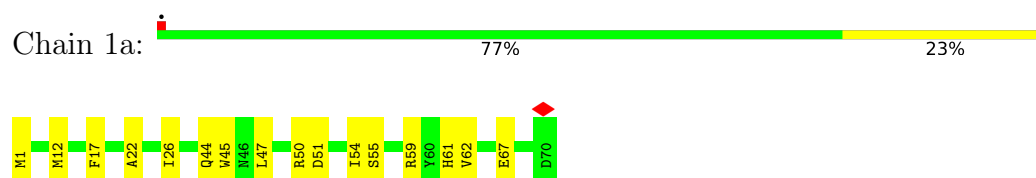
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



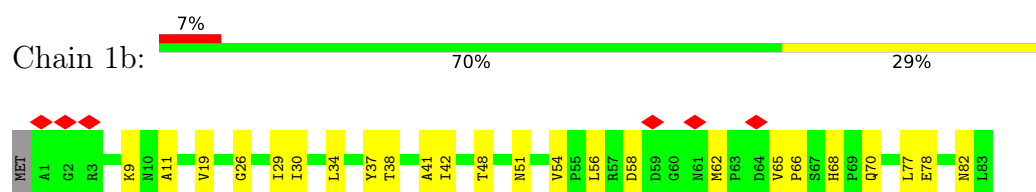
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



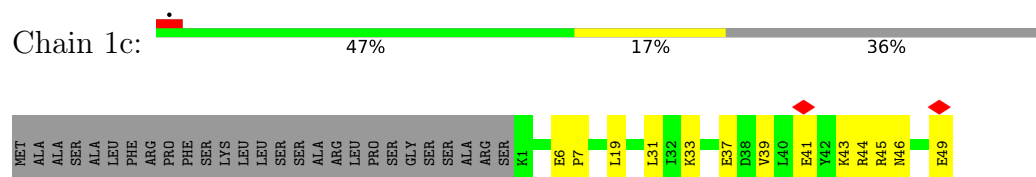
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



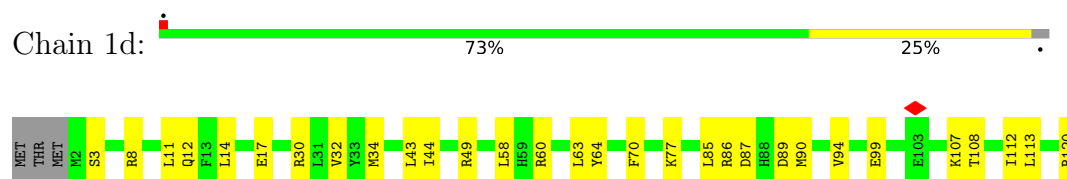
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



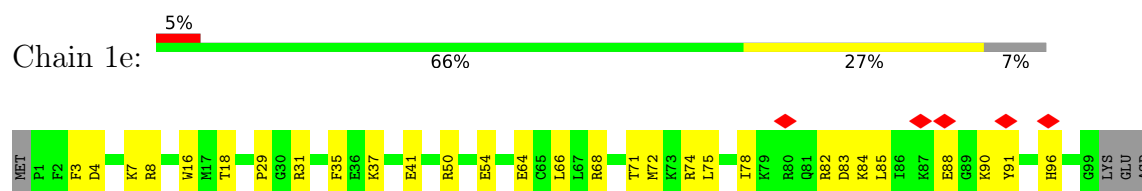
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



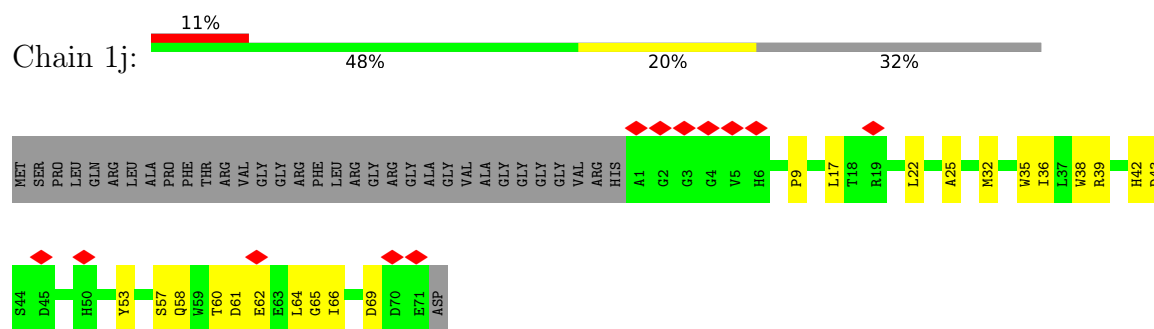
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



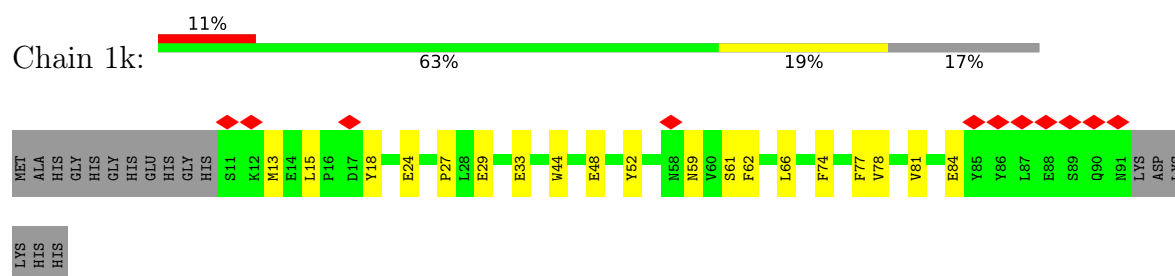
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



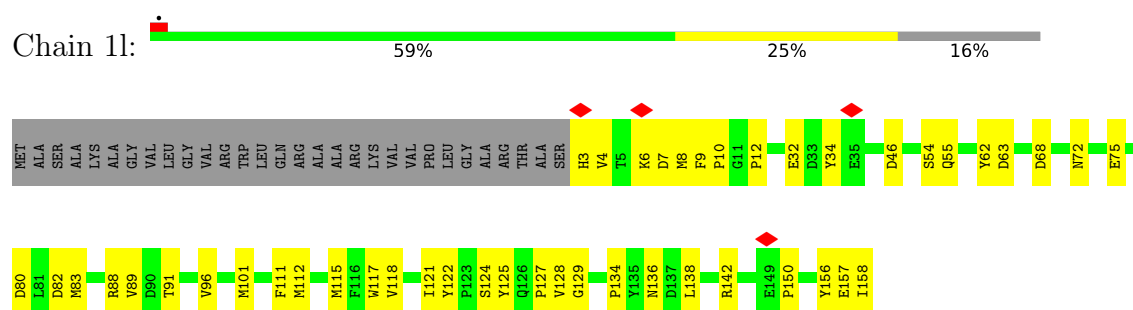
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



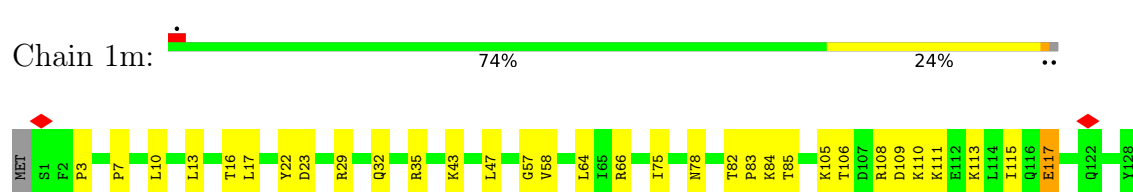
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



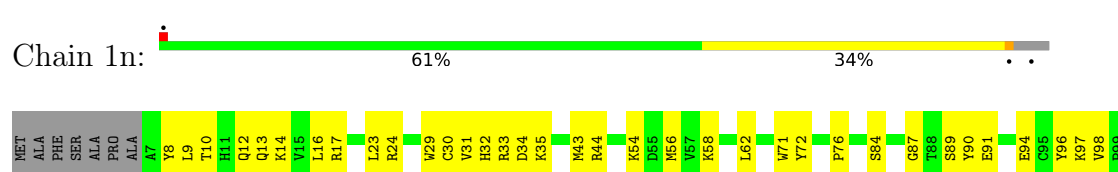
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

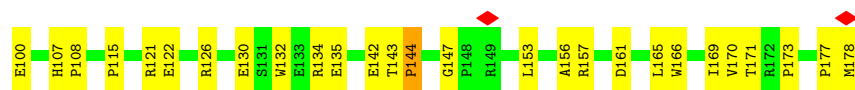


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

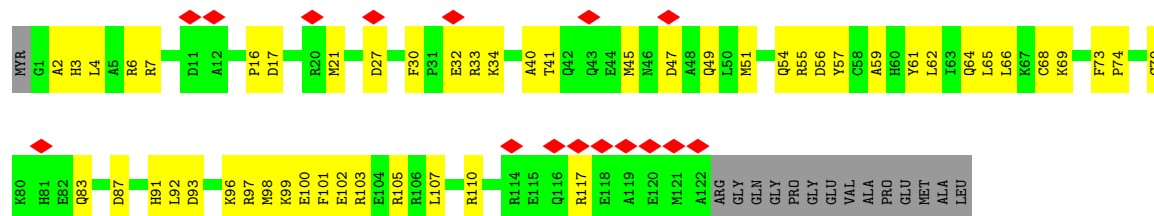


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

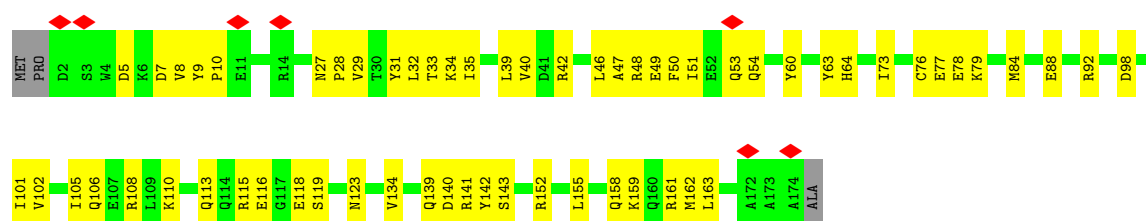




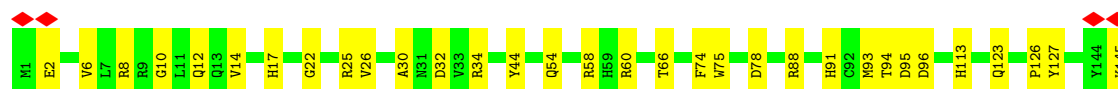
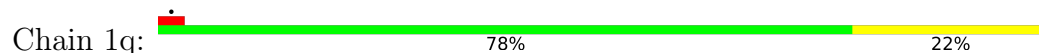
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



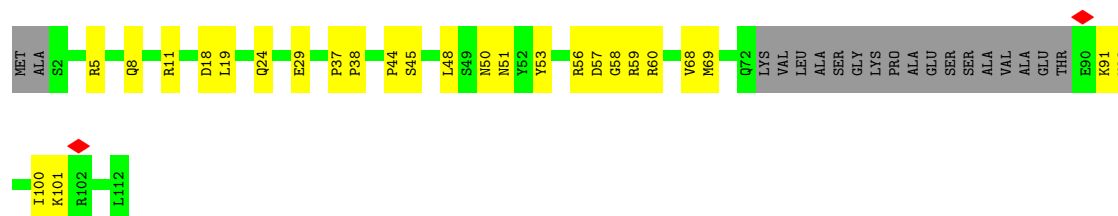
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



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

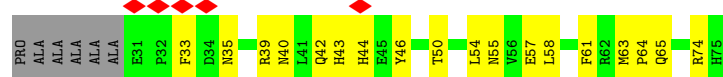


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

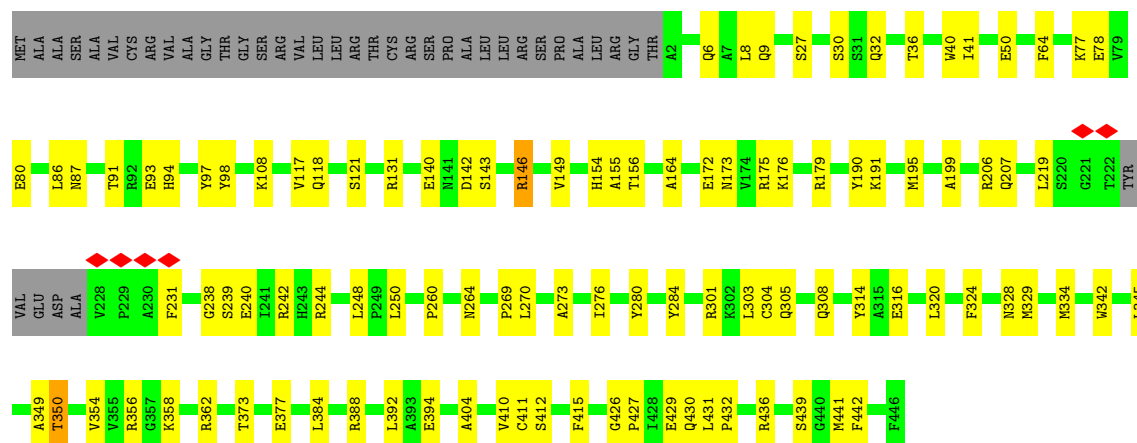


- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

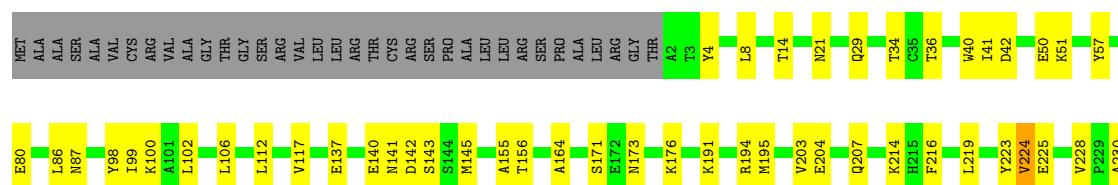


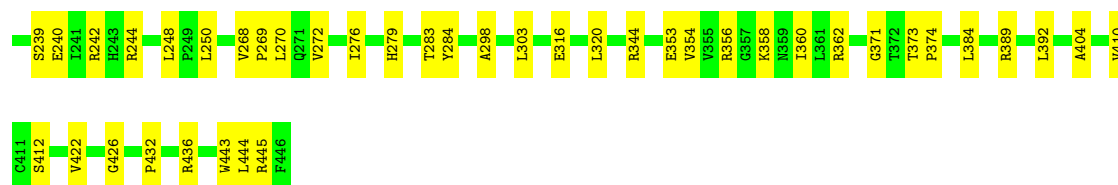


- Chain 3A: 70% 21% 8%



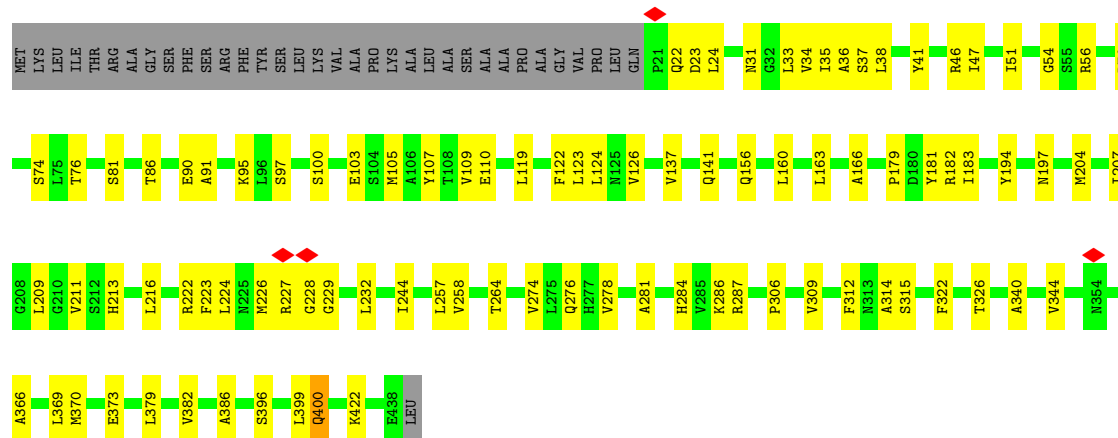
- Chain 3N: 74% 19% 7%





- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3B: 72% 21% 8%



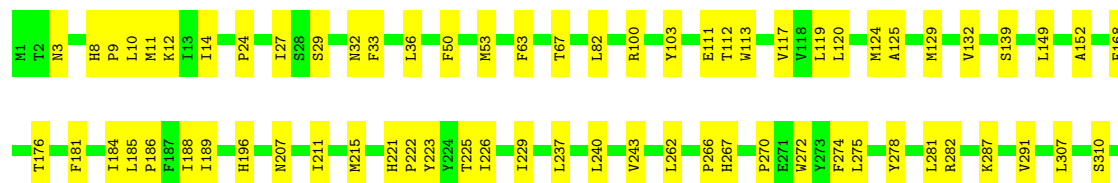
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3O: 72% 20% 8%



- Molecule 47: Cytochrome b

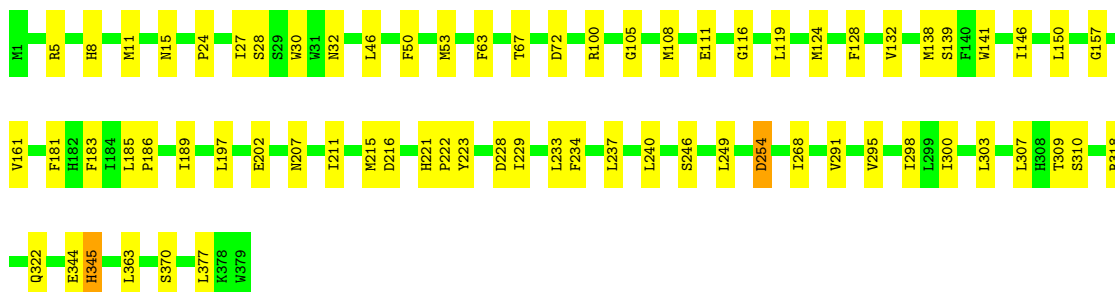
Chain 3C: 79% 21%





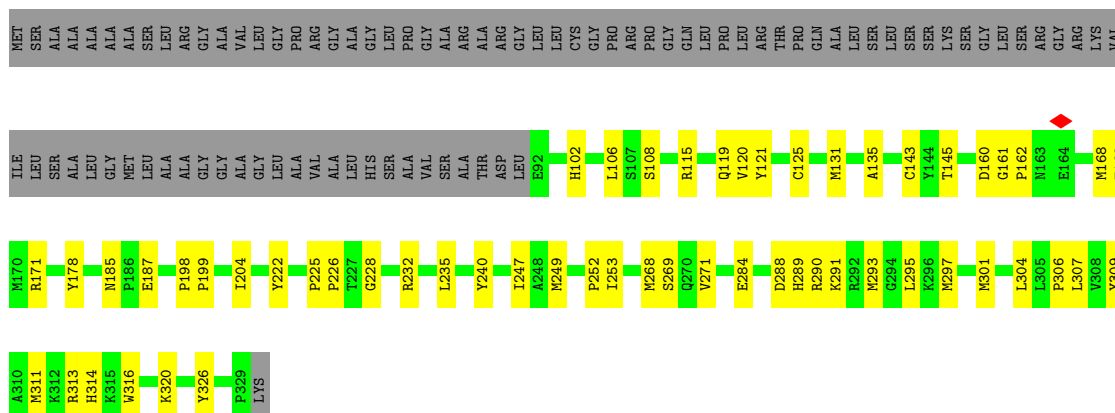
• Molecule 47: Cytochrome b

Chain 3P: 82% 18%



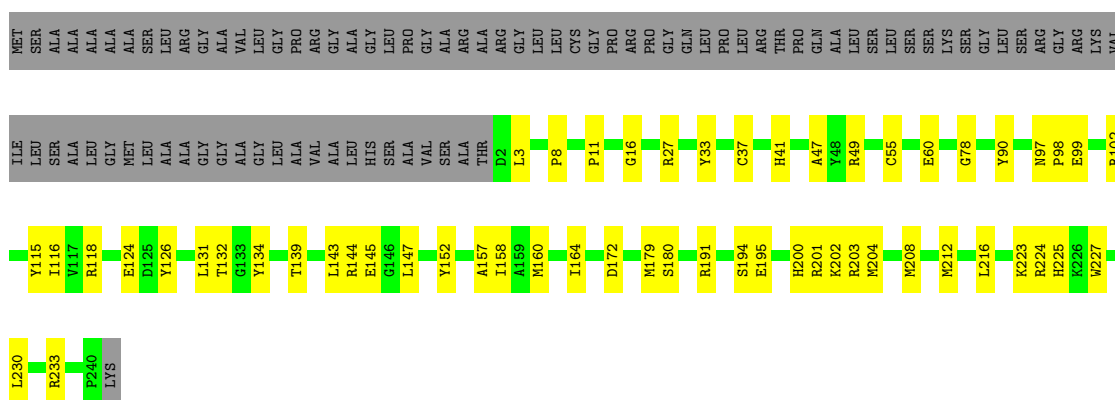
• Molecule 48: Cytochrome c1

Chain 3D: 55% 17% 27%

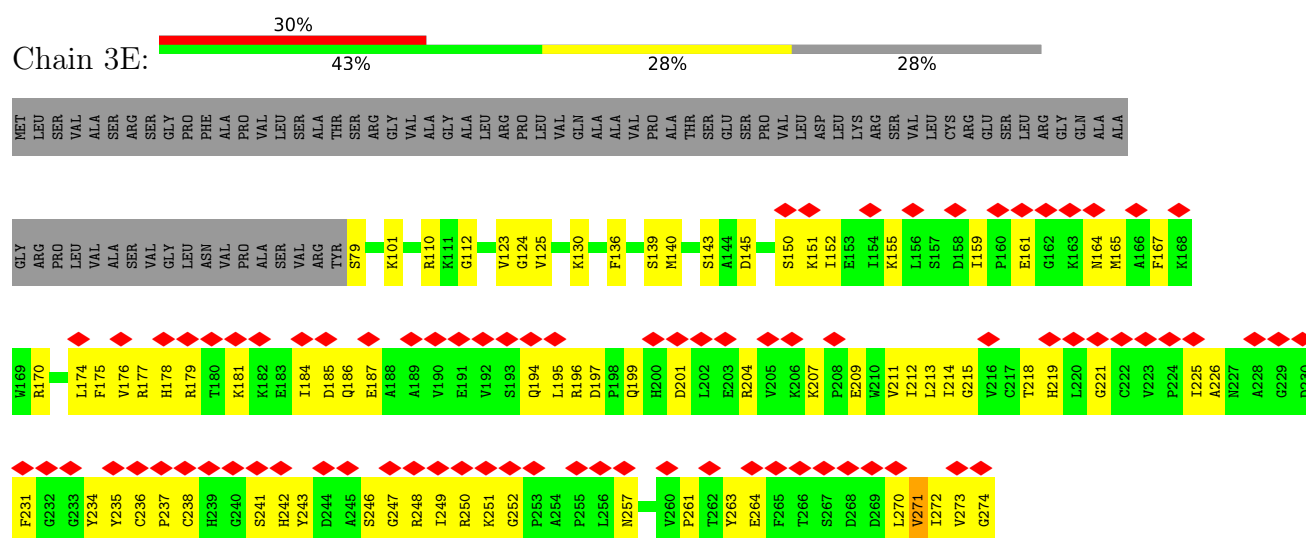


• Molecule 48: Cytochrome c1

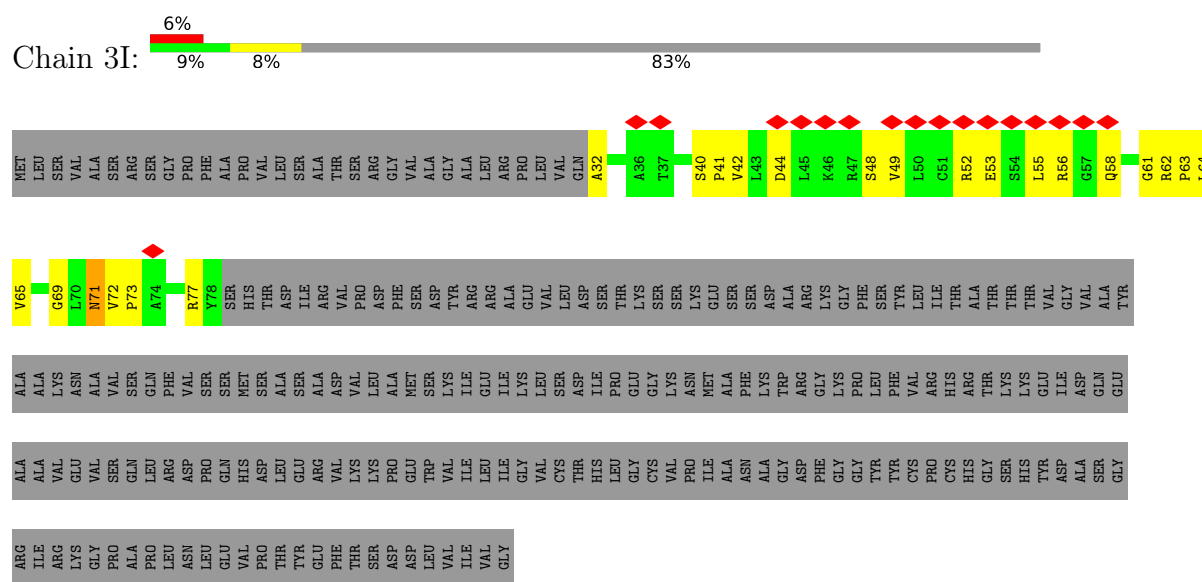
Chain 3Q: 56% 17% 27%

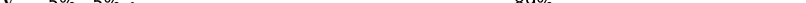


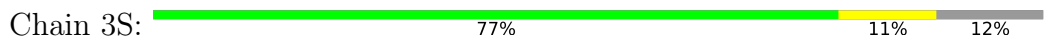
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

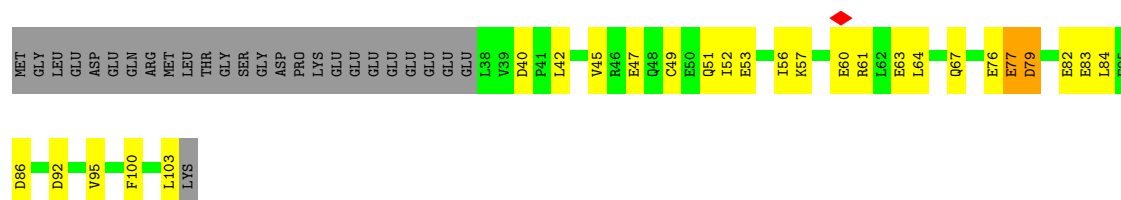


• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

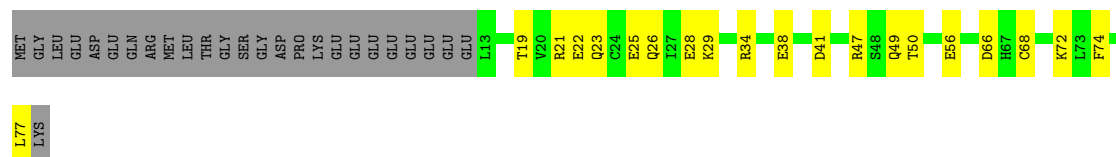


- Chain 3V: 

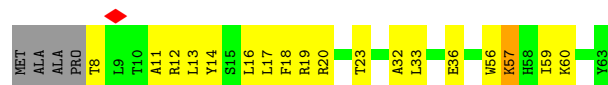




- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



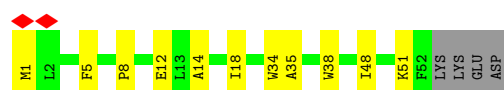
- Molecule 53: Complex III subunit 9



- Molecule 53: Complex III subunit 9



- Molecule 54: Cytochrome b-c1 complex subunit 10

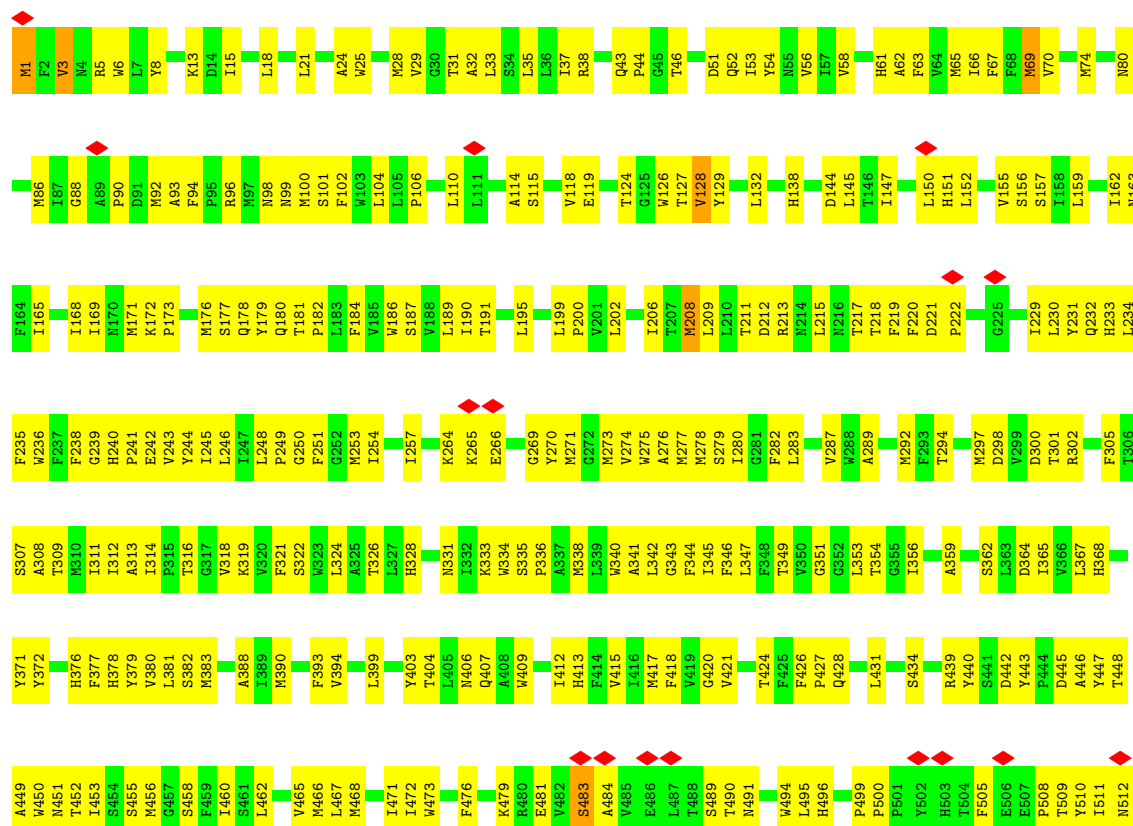


- Molecule 54: Cytochrome b-c1 complex subunit 10



- Molecule 55: Cytochrome c oxidase subunit 1

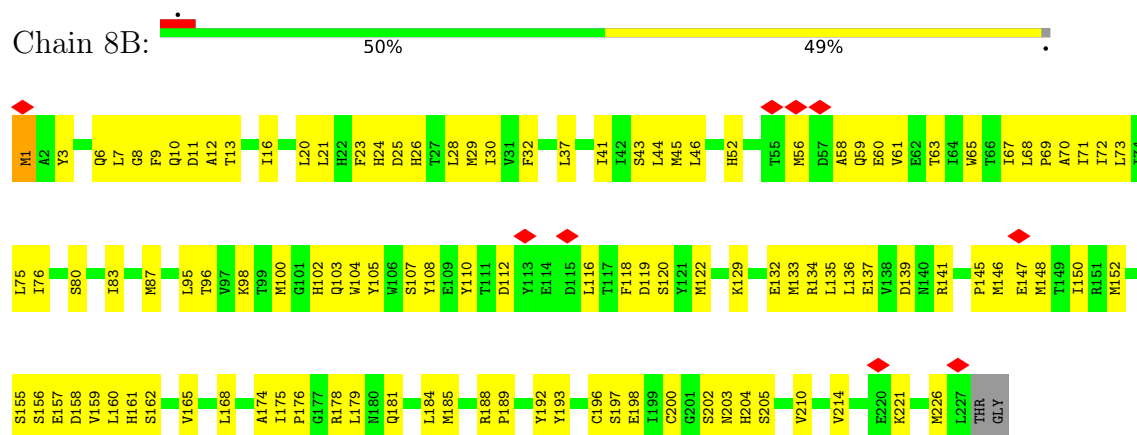


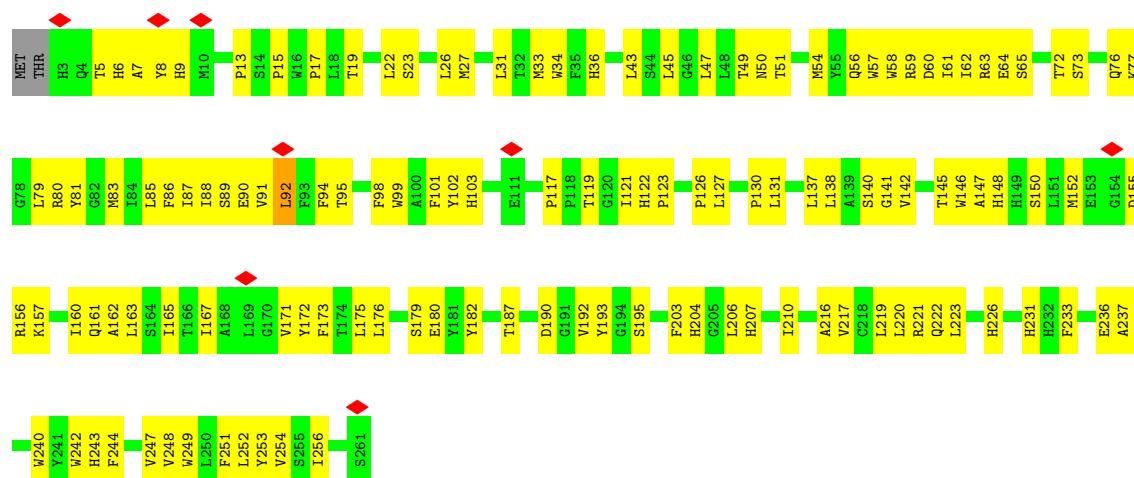


- Molecule 56: Cytochrome c oxidase subunit 2

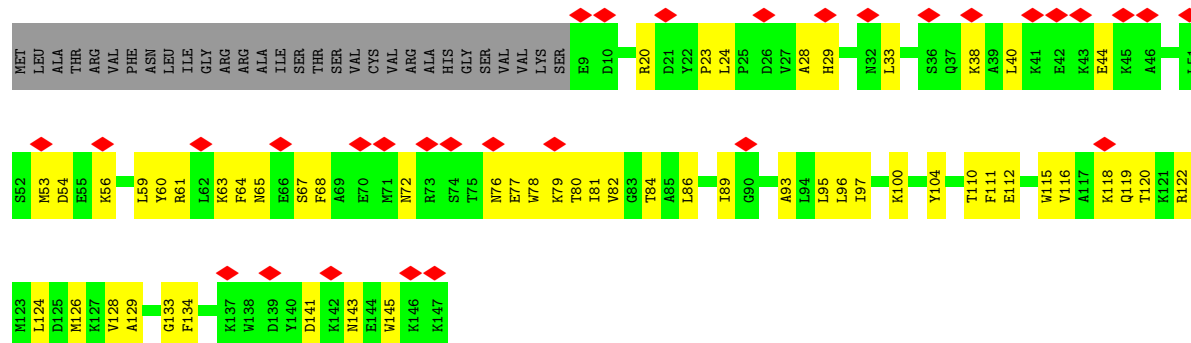


- Molecule 56: Cytochrome c oxidase subunit 2

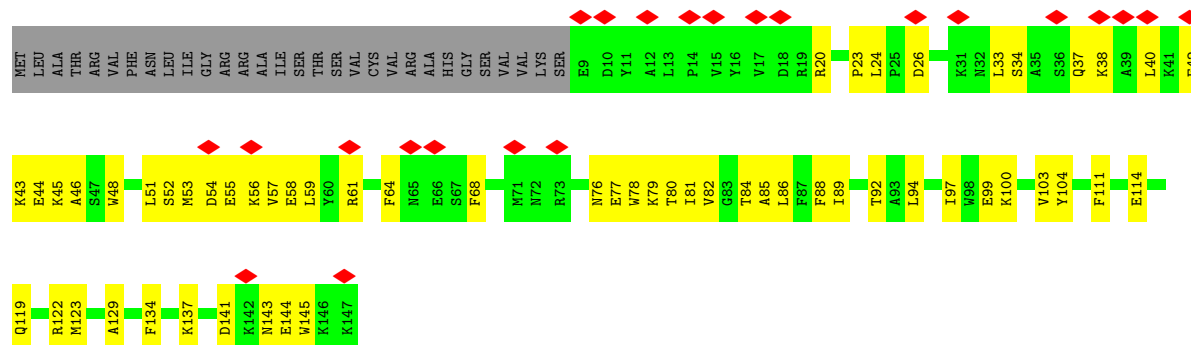




• Molecule 58: Cytochrome c oxidase subunit 4

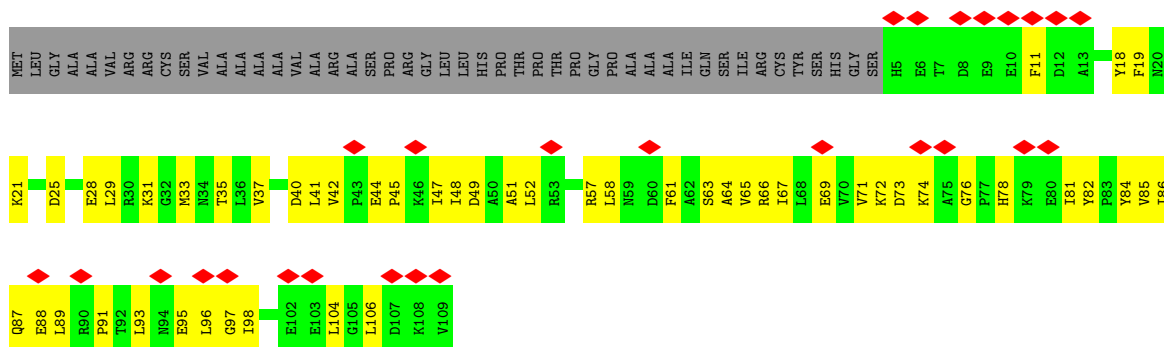


• Molecule 58: Cytochrome c oxidase subunit 4



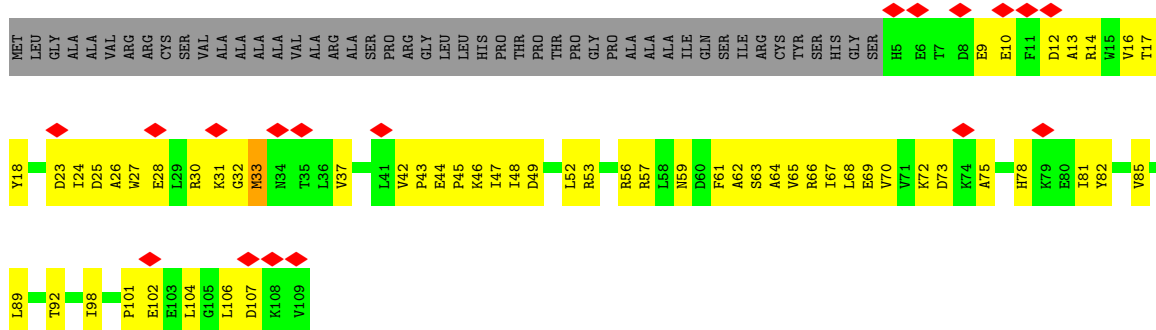
• Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial





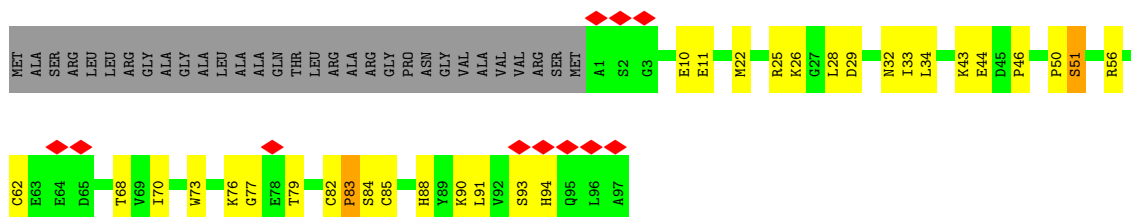
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 8E: 12% 32% 37% 31%



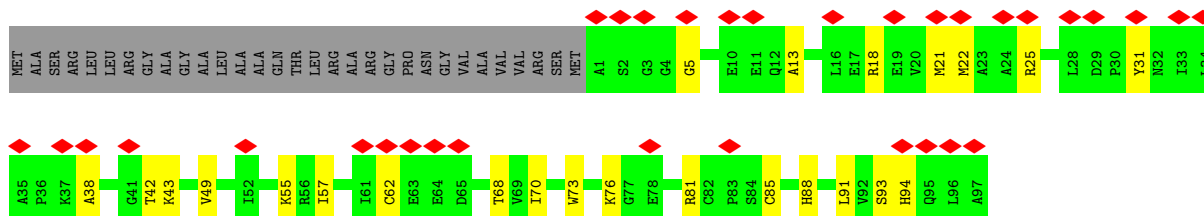
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 4F: 9% 51% 23% 24%

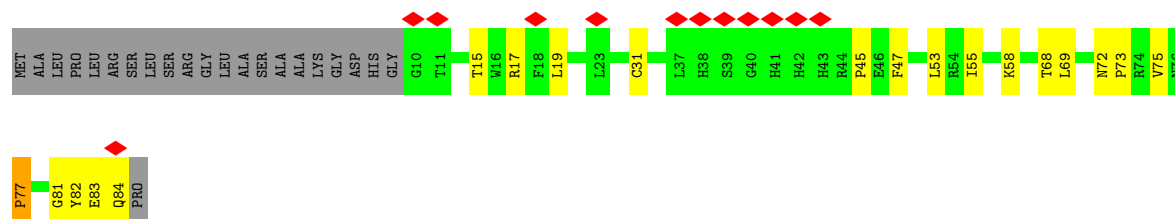


- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial

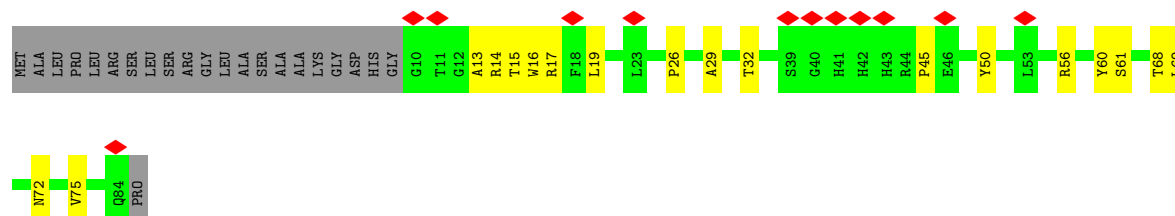
Chain 8F: 26% 57% 19% 24%



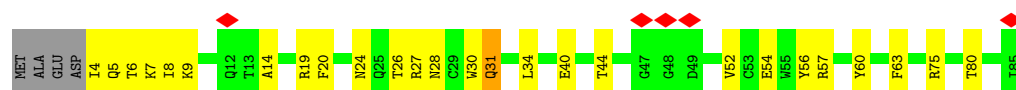
- Molecule 61: Cytochrome c oxidase subunit 6A2



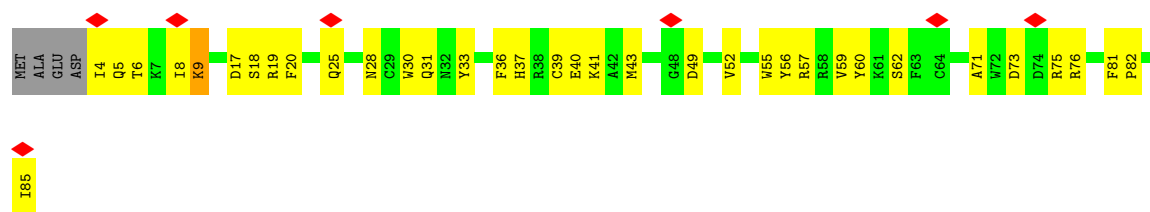
• Molecule 61: Cytochrome c oxidase subunit 6A2



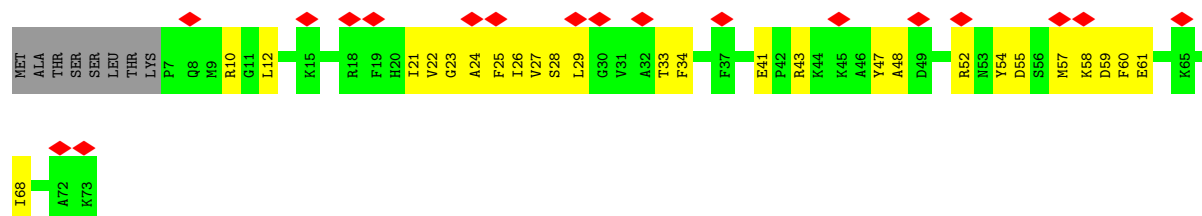
• Molecule 62: Cytochrome c oxidase subunit 6B1



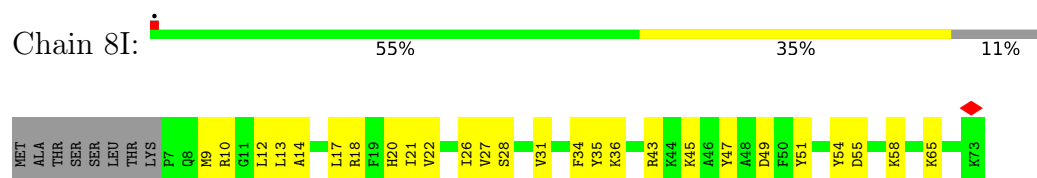
• Molecule 62: Cytochrome c oxidase subunit 6B1



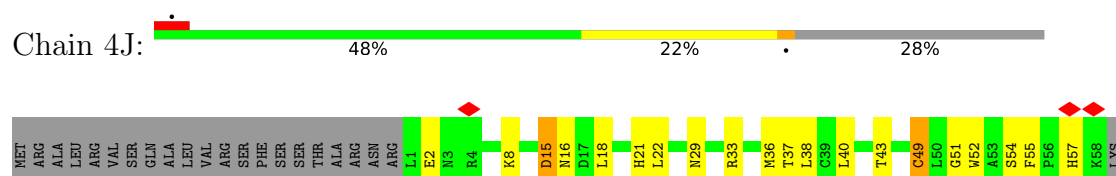
• Molecule 63: Cytochrome c oxidase subunit 6C



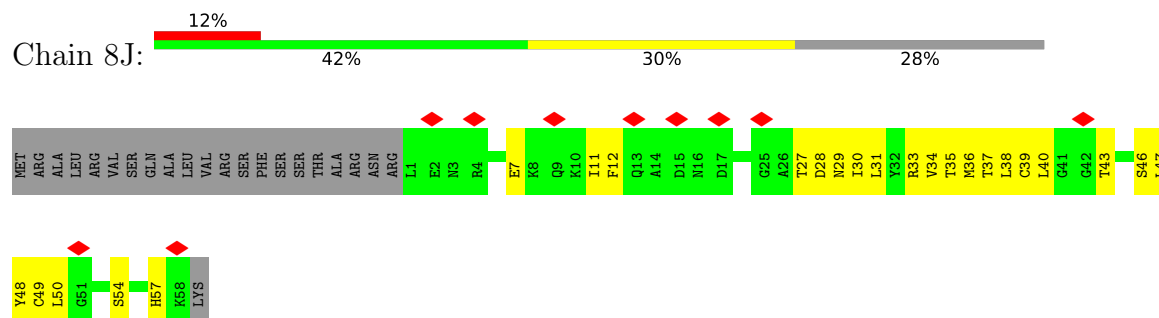
- Molecule 63: Cytochrome c oxidase subunit 6C



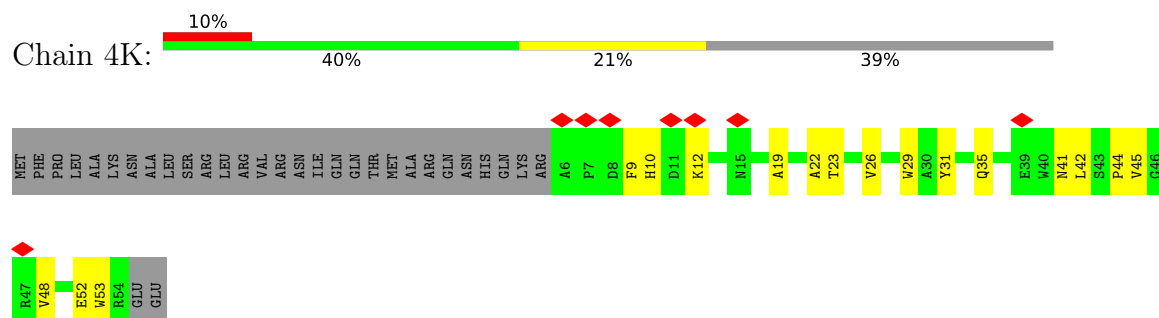
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



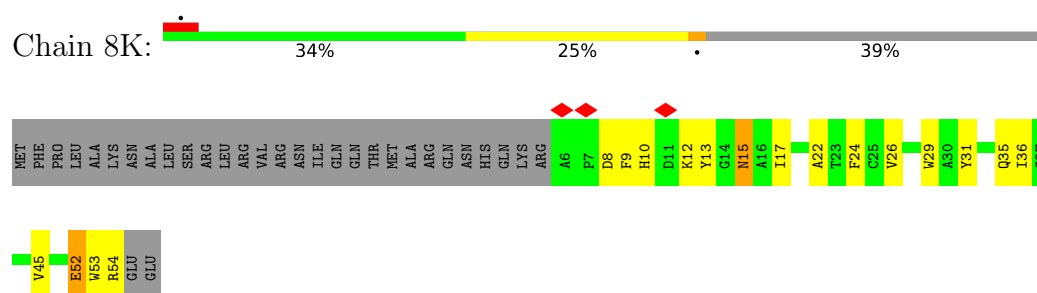
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



- Molecule 65: Cytochrome c oxidase subunit 7B



- Molecule 65: Cytochrome c oxidase subunit 7B



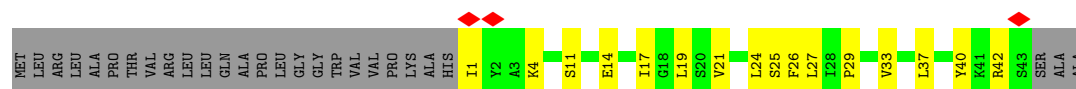
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



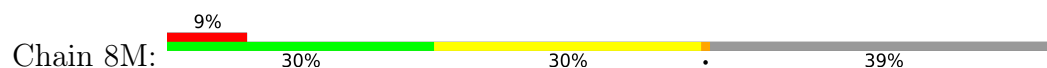
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



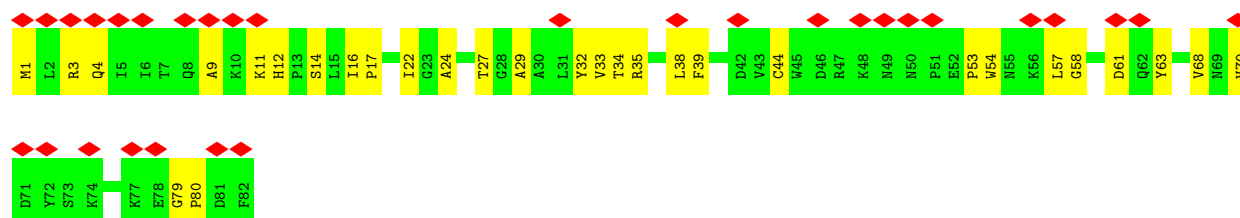
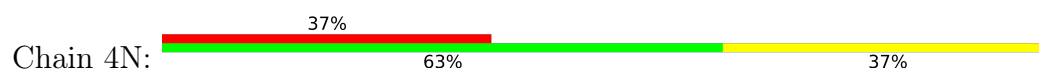
- Molecule 67: Cytochrome c oxidase subunit 8



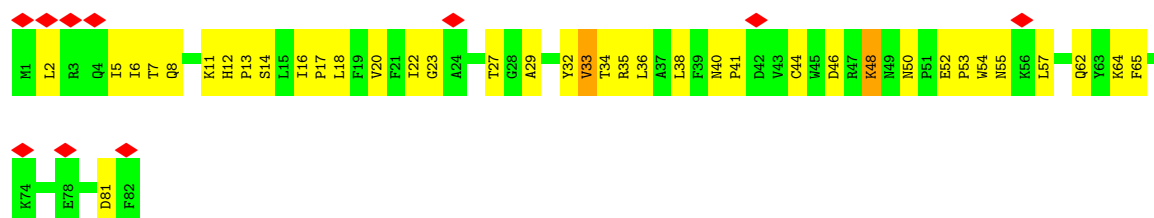
- Molecule 67: Cytochrome c oxidase subunit 8



- Molecule 68: Cytochrome c oxidase subunit NDUFA4



- Molecule 68: Cytochrome c oxidase subunit NDUFA4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	320000	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	1.149	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	572.0, 572.0, 572.0	wwPDB
Map dimensions	550, 550, 550	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.21	0/930	0.43	0/1271
2	1B	0.18	0/1273	0.39	0/1722
3	1C	0.12	0/1791	0.31	0/2439
4	1D	0.18	1/3545 (0.0%)	0.33	0/4806
5	1E	0.16	0/1698	0.37	0/2311
6	1F	0.16	0/3401	0.36	0/4595
7	1G	0.14	0/5451	0.35	0/7387
8	1H	0.24	0/2566	0.42	2/3509 (0.1%)
9	1I	0.12	0/1443	0.31	0/1952
10	1J	0.17	0/1364	0.44	0/1850
11	1K	0.16	0/751	0.38	0/1018
12	1L	0.16	0/4939	0.36	0/6718
13	1M	0.15	0/3713	0.34	0/5063
14	1N	0.29	1/2765 (0.0%)	0.41	1/3758 (0.0%)
15	1O	0.14	0/2650	0.34	0/3588
16	1P	0.15	0/2828	0.34	0/3834
17	1Q	0.15	0/1070	0.36	0/1446
18	1R	0.14	0/755	0.32	0/1018
19	1S	0.17	0/711	0.44	0/956
20	1T	0.18	0/701	0.43	0/946
20	1U	0.29	0/706	0.47	1/954 (0.1%)
21	1V	0.17	0/946	0.33	0/1281
22	1W	0.17	0/995	0.36	0/1340
23	1X	0.14	0/1436	0.39	0/1938
24	1Y	0.11	0/1037	0.25	0/1404
25	1Z	0.16	0/1199	0.31	0/1617
26	1a	0.14	0/577	0.38	0/777
27	1b	0.16	0/664	0.36	0/912
28	1c	0.14	0/430	0.32	0/581
29	1d	0.11	0/1016	0.27	0/1374
30	1e	0.15	0/836	0.37	0/1118

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	1f	0.17	0/499	0.44	0/673
32	1g	0.16	0/858	0.39	0/1165
33	1h	0.16	0/1184	0.37	0/1603
34	1i	0.16	0/1138	0.38	0/1551
35	1j	0.17	0/627	0.36	0/858
36	1k	0.16	0/668	0.35	0/903
37	1l	0.15	0/1365	0.36	0/1867
38	1m	0.23	0/1092	0.35	0/1481
39	1n	0.39	2/1549 (0.1%)	0.62	2/2098 (0.1%)
40	1o	0.16	0/1069	0.41	0/1430
41	1p	0.13	0/1481	0.35	0/1997
42	1q	0.13	0/1253	0.31	0/1704
43	1r	0.29	1/777 (0.1%)	0.40	0/1051
44	1s	0.16	0/394	0.40	0/533
45	3A	0.13	0/3481	0.35	0/4722
45	3N	0.13	0/3496	0.32	0/4723
46	3B	0.13	0/3190	0.33	0/4317
46	3O	0.17	0/3175	0.35	0/4292
47	3C	0.16	0/3123	0.36	0/4269
47	3P	0.15	0/3122	0.33	0/4269
48	3D	0.14	0/1946	0.36	0/2641
48	3Q	0.13	0/1962	0.34	0/2663
49	3E	0.18	0/1551	0.46	0/2098
49	3I	1.51	4/344 (1.2%)	2.00	12/468 (2.6%)
49	3R	0.56	2/1551 (0.1%)	0.76	2/2098 (0.1%)
49	3V	1.68	2/225 (0.9%)	3.23	5/303 (1.7%)
50	3F	0.12	0/888	0.29	0/1193
50	3S	0.09	0/888	0.24	0/1193
51	3G	0.14	0/649	0.39	0/878
51	3T	0.15	0/649	0.35	0/878
52	3H	0.21	0/539	0.80	2/724 (0.3%)
52	3U	0.18	0/539	0.44	0/724
53	3J	0.40	0/476	0.57	0/641
53	3W	0.37	0/476	0.50	0/641
54	3X	0.12	0/445	0.32	0/608
54	3Y	0.14	0/437	0.38	0/598
55	4A	0.18	0/4156	0.34	0/5679
55	8A	0.29	1/4156 (0.0%)	0.46	2/5679 (0.0%)
56	4B	0.25	0/1865	0.43	0/2544
56	8B	0.23	0/1865	0.51	0/2544
57	4C	0.26	1/2179 (0.0%)	0.35	0/2981
57	8C	0.22	0/2179	0.40	0/2981
58	4D	0.16	0/1197	0.39	0/1617

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
58	8D	0.31	0/1197	0.51	0/1617
59	4E	0.23	0/871	0.51	0/1182
59	8E	0.29	0/871	0.52	0/1182
60	4F	0.27	0/749	0.61	1/1016 (0.1%)
60	8F	0.14	0/749	0.38	0/1016
61	4G	0.19	0/644	0.47	1/881 (0.1%)
61	8G	0.13	0/644	0.37	0/881
62	4H	0.15	0/708	0.36	0/956
62	8H	0.29	1/708 (0.1%)	0.45	0/956
63	4I	0.19	0/563	0.46	0/748
63	8I	0.25	0/563	0.46	0/748
64	4J	0.17	0/466	0.44	0/631
64	8J	0.18	0/466	0.47	0/631
65	4K	0.15	0/396	0.40	0/543
65	8K	0.27	0/396	0.56	0/543
66	4L	0.18	0/394	0.37	0/528
66	8L	0.27	0/394	0.51	1/528 (0.2%)
67	4M	0.23	0/349	0.49	0/477
67	8M	0.39	0/349	0.51	0/477
68	4N	0.17	0/680	0.39	0/921
68	8N	0.33	0/680	0.62	0/921
All	All	0.22	16/131727 (0.0%)	0.43	32/178746 (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	1
49	3V	0	1
68	8N	0	1
All	All	0	3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	3V	49	VAL	C-N	22.83	1.70	1.33
49	3I	73	PRO	CG-CD	-19.98	0.82	1.50
49	3R	173	PRO	N-CD	16.16	1.70	1.47
49	3I	73	PRO	N-CD	13.25	1.66	1.47
14	1N	255	PRO	CA-C	-11.58	1.44	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	3V	49	VAL	O-C-N	-38.36	79.22	122.95
49	3R	173	PRO	CA-N-CD	-23.12	79.64	112.00
49	3I	73	PRO	CB-CG-CD	23.07	179.94	106.10
49	3V	49	VAL	CA-C-N	21.55	154.96	121.98
49	3V	49	VAL	C-N-CA	21.55	154.96	121.98

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
49	3V	48	SER	Mainchain
68	8N	48	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	916	0	950	79	0
2	1B	1242	0	1249	80	0
3	1C	1740	0	1691	40	0
4	1D	3452	0	3389	121	0
5	1E	1658	0	1662	67	0
6	1F	3325	0	3288	152	0
7	1G	5362	0	5388	173	0
8	1H	2504	0	2602	141	0
9	1I	1412	0	1366	62	0
10	1J	1329	0	1326	88	0
11	1K	750	0	798	57	0
12	1L	4818	0	4956	189	0
13	1M	3632	0	3836	146	0
14	1N	2712	0	2873	140	0
15	1O	2590	0	2556	92	0
16	1P	2751	0	2776	93	0
17	1Q	1047	0	1042	39	0
18	1R	741	0	704	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	1S	700	0	719	40	0
20	1T	689	0	687	42	0
20	1U	694	0	691	35	0
21	1V	927	0	972	25	0
22	1W	971	0	975	42	0
23	1X	1398	0	1378	45	0
24	1Y	1016	0	1020	31	0
25	1Z	1168	0	1161	58	0
26	1a	562	0	557	21	0
27	1b	643	0	645	23	0
28	1c	417	0	425	13	0
29	1d	985	0	978	29	0
30	1e	816	0	823	30	0
31	1f	487	0	498	20	0
32	1g	835	0	795	46	0
33	1h	1151	0	1164	32	0
34	1i	1100	0	1107	45	0
35	1j	601	0	546	36	0
36	1k	649	0	626	18	0
37	1l	1310	0	1204	43	0
38	1m	1062	0	1075	31	0
39	1n	1495	0	1434	53	0
40	1o	1045	0	1016	58	0
41	1p	1449	0	1416	62	0
42	1q	1212	0	1174	28	0
43	1r	759	0	783	29	0
44	1s	382	0	351	26	0
45	3A	3411	0	3308	72	0
45	3N	3424	0	3350	74	0
46	3B	3138	0	3116	68	0
46	3O	3124	0	3108	60	0
47	3C	3025	0	3090	73	0
47	3P	3024	0	3090	62	0
48	3D	1888	0	1834	49	0
48	3Q	1904	0	1849	50	0
49	3E	1518	0	1498	74	0
49	3I	340	0	359	18	0
49	3R	1518	0	1498	108	0
49	3V	224	0	241	19	0
50	3F	868	0	857	14	0
50	3S	868	0	857	9	0
51	3G	628	0	634	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	3T	628	0	634	23	0
52	3H	533	0	513	21	0
52	3U	533	0	513	18	0
53	3J	464	0	467	17	0
53	3W	464	0	467	15	0
54	3X	429	0	430	7	0
54	3Y	421	0	418	13	0
55	4A	4026	0	4005	196	0
55	8A	4026	0	4005	322	0
56	4B	1828	0	1836	123	0
56	8B	1828	0	1834	132	0
57	4C	2096	0	2027	100	0
57	8C	2096	0	2027	168	0
58	4D	1163	0	1143	79	0
58	8D	1163	0	1143	112	0
59	4E	852	0	845	73	0
59	8E	852	0	845	101	0
60	4F	734	0	718	34	0
60	8F	734	0	718	24	0
61	4G	617	0	585	17	0
61	8G	617	0	585	24	0
62	4H	687	0	645	23	0
62	8H	687	0	645	42	0
63	4I	550	0	560	32	0
63	8I	550	0	560	35	0
64	4J	456	0	459	35	0
64	8J	456	0	459	33	0
65	4K	383	0	366	22	0
65	8K	383	0	366	29	0
66	4L	381	0	380	27	0
66	8L	381	0	380	35	0
67	4M	338	0	345	30	0
67	8M	338	0	345	35	0
68	4N	660	0	664	29	0
68	8N	660	0	664	60	0
69	1A	47	0	71	3	0
69	1K	44	0	62	2	0
69	1L	91	0	136	8	0
69	1M	194	0	296	30	0
69	1N	49	0	75	5	0
69	1P	35	0	44	3	0
69	1Y	161	0	195	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	1d	49	0	75	5	0
69	1j	44	0	65	0	0
69	1m	41	0	59	0	0
69	3A	59	0	66	9	0
69	3C	69	0	86	9	0
69	3D	33	0	40	2	0
69	3G	29	0	32	1	0
69	3N	58	0	62	8	0
69	3P	33	0	40	0	0
69	3R	47	0	71	5	0
69	3Y	30	0	34	2	0
70	1A	70	0	88	7	0
70	1B	94	0	136	15	0
70	1H	102	0	161	12	0
70	1I	44	0	62	3	0
70	1M	79	0	109	10	0
70	1P	33	0	40	2	0
70	1Y	46	0	66	7	0
70	1d	39	0	52	8	0
70	1h	47	0	71	1	0
70	1q	49	0	75	4	0
70	3J	47	0	68	4	0
70	3R	45	0	64	4	0
70	3X	29	0	32	2	0
71	1B	8	0	0	2	0
71	1F	8	0	0	2	0
71	1G	16	0	0	3	0
71	1I	16	0	0	0	0
72	1E	4	0	0	0	0
72	1G	4	0	0	2	0
72	3E	4	0	0	2	0
72	3R	4	0	0	2	0
73	1F	31	0	19	4	0
74	1G	1	0	0	0	0
75	1H	51	0	46	1	0
75	1L	76	0	99	6	0
75	1N	62	0	68	3	0
75	1X	86	0	125	12	0
75	1d	65	0	77	6	0
75	1h	80	0	104	14	0
75	1q	61	0	66	2	0
75	3A	58	0	60	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	3G	108	0	104	8	0
75	3N	43	0	30	7	0
75	3P	56	0	56	9	0
75	3T	57	0	58	9	0
75	4B	100	0	156	14	0
75	4C	100	0	156	15	0
75	4D	100	0	156	17	0
75	8B	100	0	156	10	0
75	8C	100	0	156	16	0
75	8D	100	0	156	15	0
76	1O	32	0	12	3	0
77	1O	1	0	0	0	0
77	4A	1	0	0	0	0
77	8A	1	0	0	0	0
78	1P	48	0	26	2	0
79	1R	1	0	0	0	0
79	4F	1	0	0	0	0
79	8F	1	0	0	0	0
80	1T	37	0	0	0	0
80	1n	37	0	0	1	0
81	1Y	8	0	8	0	0
81	1q	8	0	8	2	0
82	1h	11	0	12	1	0
83	1i	29	0	39	0	0
84	1l	15	0	27	0	0
85	3C	86	0	60	2	0
85	3P	86	0	60	4	0
86	3D	42	0	32	2	0
86	3Q	43	0	32	3	0
87	4A	153	0	228	20	0
87	4B	102	0	151	8	0
87	4C	255	0	380	23	0
87	4G	51	0	76	5	0
87	4J	51	0	76	10	0
87	4K	51	0	76	2	0
87	4L	51	0	76	7	0
87	4M	51	0	76	3	0
87	8A	153	0	228	23	0
87	8B	102	0	151	11	0
87	8C	306	0	456	42	0
87	8G	51	0	76	8	0
87	8J	51	0	76	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	8K	51	0	76	3	0
87	8L	51	0	76	7	0
88	4A	120	0	108	10	0
88	8A	120	0	108	12	0
89	4A	1	0	0	0	0
89	8A	1	0	0	0	0
90	4A	1	0	0	0	0
90	8A	1	0	0	0	0
91	4B	2	0	0	2	0
91	8B	2	0	0	2	0
92	4B	52	0	80	8	0
92	8B	52	0	80	8	0
93	4C	52	0	72	5	0
93	4G	53	0	77	2	0
93	8C	52	0	72	5	0
93	8G	53	0	77	5	0
94	4H	5	0	0	0	0
94	8H	5	0	0	1	0
All	All	134346	0	135606	4916	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 4916 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:8B:52:HIS:CD2	56:8B:56:MET:HE1	1.45	1.51
49:3V:49:VAL:C	49:3V:50:LEU:N	1.69	1.49
57:4C:151:LEU:HD13	57:4C:159:MET:SD	1.50	1.48
59:8E:72:LYS:HB2	59:8E:82:TYR:CE2	1.47	1.47
68:8N:7:THR:C	68:8N:11:LYS:HZ3	1.23	1.43

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	113/115 (98%)	103 (91%)	8 (7%)	2 (2%)	6	6
2	1B	153/258 (59%)	145 (95%)	8 (5%)	0	100	100
3	1C	207/264 (78%)	199 (96%)	8 (4%)	0	100	100
4	1D	427/476 (90%)	412 (96%)	15 (4%)	0	100	100
5	1E	212/249 (85%)	200 (94%)	11 (5%)	1 (0%)	24	31
6	1F	430/464 (93%)	402 (94%)	25 (6%)	3 (1%)	18	23
7	1G	697/727 (96%)	668 (96%)	28 (4%)	1 (0%)	48	60
8	1H	316/318 (99%)	294 (93%)	20 (6%)	2 (1%)	21	27
9	1I	174/239 (73%)	167 (96%)	7 (4%)	0	100	100
10	1J	172/175 (98%)	161 (94%)	10 (6%)	1 (1%)	21	27
11	1K	96/98 (98%)	93 (97%)	2 (2%)	1 (1%)	12	15
12	1L	604/606 (100%)	563 (93%)	41 (7%)	0	100	100
13	1M	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
14	1N	345/347 (99%)	335 (97%)	9 (3%)	1 (0%)	36	46
15	1O	318/357 (89%)	305 (96%)	13 (4%)	0	100	100
16	1P	340/377 (90%)	326 (96%)	14 (4%)	0	100	100
17	1Q	127/175 (73%)	118 (93%)	9 (7%)	0	100	100
18	1R	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
19	1S	85/99 (86%)	80 (94%)	5 (6%)	0	100	100
20	1T	83/156 (53%)	82 (99%)	1 (1%)	0	100	100
20	1U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
21	1V	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
22	1W	113/128 (88%)	106 (94%)	7 (6%)	0	100	100
23	1X	169/172 (98%)	163 (96%)	5 (3%)	1 (1%)	21	27
24	1Y	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
25	1Z	139/144 (96%)	137 (99%)	2 (1%)	0	100	100
26	1a	68/70 (97%)	68 (100%)	0	0	100	100
27	1b	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
28	1c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	1d	117/122 (96%)	113 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	1e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
31	1f	55/135 (41%)	50 (91%)	5 (9%)	0	100	100
32	1g	98/154 (64%)	90 (92%)	8 (8%)	0	100	100
33	1h	136/189 (72%)	136 (100%)	0	0	100	100
34	1i	126/128 (98%)	118 (94%)	8 (6%)	0	100	100
35	1j	69/105 (66%)	67 (97%)	2 (3%)	0	100	100
36	1k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	146 (95%)	8 (5%)	0	100	100
38	1m	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
39	1n	170/179 (95%)	161 (95%)	9 (5%)	0	100	100
40	1o	120/137 (88%)	114 (95%)	6 (5%)	0	100	100
41	1p	171/176 (97%)	170 (99%)	1 (1%)	0	100	100
42	1q	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
43	1r	90/113 (80%)	87 (97%)	3 (3%)	0	100	100
44	1s	43/471 (9%)	42 (98%)	1 (2%)	0	100	100
45	3A	436/480 (91%)	428 (98%)	6 (1%)	2 (0%)	24	31
45	3N	444/480 (92%)	427 (96%)	16 (4%)	1 (0%)	43	55
46	3B	414/453 (91%)	403 (97%)	11 (3%)	0	100	100
46	3O	413/453 (91%)	404 (98%)	8 (2%)	1 (0%)	43	55
47	3C	377/379 (100%)	366 (97%)	11 (3%)	0	100	100
47	3P	377/379 (100%)	369 (98%)	8 (2%)	0	100	100
48	3D	235/326 (72%)	229 (97%)	6 (3%)	0	100	100
48	3Q	237/326 (73%)	231 (98%)	6 (2%)	0	100	100
49	3E	194/274 (71%)	177 (91%)	16 (8%)	1 (0%)	24	31
49	3I	45/274 (16%)	43 (96%)	2 (4%)	0	100	100
49	3R	194/274 (71%)	172 (89%)	18 (9%)	4 (2%)	5	4
49	3V	29/274 (11%)	29 (100%)	0	0	100	100
50	3F	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
50	3S	96/111 (86%)	96 (100%)	0	0	100	100
51	3G	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
51	3T	72/82 (88%)	71 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	3H	63/91 (69%)	62 (98%)	0	1 (2%)	7	7
52	3U	63/91 (69%)	62 (98%)	1 (2%)	0	100	100
53	3J	54/60 (90%)	52 (96%)	1 (2%)	1 (2%)	6	5
53	3W	54/60 (90%)	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%)	497 (97%)	14 (3%)	1 (0%)	43	55
55	8A	512/514 (100%)	497 (97%)	13 (2%)	2 (0%)	30	38
56	4B	225/229 (98%)	215 (96%)	10 (4%)	0	100	100
56	8B	225/229 (98%)	216 (96%)	9 (4%)	0	100	100
57	4C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
57	8C	257/261 (98%)	248 (96%)	9 (4%)	0	100	100
58	4D	137/169 (81%)	126 (92%)	11 (8%)	0	100	100
58	8D	137/169 (81%)	132 (96%)	5 (4%)	0	100	100
59	4E	103/152 (68%)	101 (98%)	2 (2%)	0	100	100
59	8E	103/152 (68%)	101 (98%)	2 (2%)	0	100	100
60	4F	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
60	8F	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
61	4G	73/97 (75%)	70 (96%)	3 (4%)	0	100	100
61	8G	73/97 (75%)	69 (94%)	4 (6%)	0	100	100
62	4H	80/86 (93%)	75 (94%)	5 (6%)	0	100	100
62	8H	80/86 (93%)	74 (92%)	6 (8%)	0	100	100
63	4I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
63	8I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
64	4J	56/80 (70%)	55 (98%)	1 (2%)	0	100	100
64	8J	56/80 (70%)	54 (96%)	2 (4%)	0	100	100
65	4K	47/80 (59%)	44 (94%)	3 (6%)	0	100	100
65	8K	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
66	4L	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
66	8L	44/63 (70%)	44 (100%)	0	0	100	100
67	4M	41/70 (59%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
67	8M	41/70 (59%)	41 (100%)	0	0	100	100
68	4N	80/82 (98%)	72 (90%)	7 (9%)	1 (1%)	9	10
68	8N	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	9	10
All	All	15889/19086 (83%)	15257 (96%)	603 (4%)	29 (0%)	44	55

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	1H	92	PRO
10	1J	66	VAL
23	1X	28	ALA
49	3E	271	VAL
53	3J	57	LYS

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%)	99 (100%)	0	100	100
2	1B	131/212 (62%)	130 (99%)	1 (1%)	73	86
3	1C	190/227 (84%)	190 (100%)	0	100	100
4	1D	371/405 (92%)	370 (100%)	1 (0%)	86	93
5	1E	183/207 (88%)	183 (100%)	0	100	100
6	1F	346/368 (94%)	344 (99%)	2 (1%)	78	89
7	1G	588/610 (96%)	587 (100%)	1 (0%)	87	94
8	1H	274/274 (100%)	273 (100%)	1 (0%)	84	92
9	1I	151/201 (75%)	151 (100%)	0	100	100
10	1J	140/141 (99%)	139 (99%)	1 (1%)	76	87
11	1K	84/84 (100%)	84 (100%)	0	100	100
12	1L	539/539 (100%)	539 (100%)	0	100	100
13	1M	408/408 (100%)	407 (100%)	1 (0%)	87	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	1N	310/310 (100%)	310 (100%)	0	100	100
15	1O	283/307 (92%)	283 (100%)	0	100	100
16	1P	296/323 (92%)	296 (100%)	0	100	100
17	1Q	117/152 (77%)	117 (100%)	0	100	100
18	1R	79/97 (81%)	78 (99%)	1 (1%)	61	77
19	1S	77/82 (94%)	77 (100%)	0	100	100
20	1T	79/133 (59%)	79 (100%)	0	100	100
20	1U	79/133 (59%)	79 (100%)	0	100	100
21	1V	100/101 (99%)	100 (100%)	0	100	100
22	1W	107/112 (96%)	107 (100%)	0	100	100
23	1X	153/154 (99%)	153 (100%)	0	100	100
24	1Y	101/102 (99%)	101 (100%)	0	100	100
25	1Z	123/124 (99%)	123 (100%)	0	100	100
26	1a	58/58 (100%)	58 (100%)	0	100	100
27	1b	69/70 (99%)	69 (100%)	0	100	100
28	1c	45/66 (68%)	45 (100%)	0	100	100
29	1d	106/109 (97%)	105 (99%)	1 (1%)	70	84
30	1e	87/94 (93%)	87 (100%)	0	100	100
31	1f	54/113 (48%)	54 (100%)	0	100	100
32	1g	92/129 (71%)	91 (99%)	1 (1%)	65	81
33	1h	121/158 (77%)	120 (99%)	1 (1%)	73	86
34	1i	120/120 (100%)	119 (99%)	1 (1%)	73	86
35	1j	62/84 (74%)	62 (100%)	0	100	100
36	1k	63/76 (83%)	63 (100%)	0	100	100
37	1l	141/161 (88%)	141 (100%)	0	100	100
38	1m	113/114 (99%)	112 (99%)	1 (1%)	70	84
39	1n	156/160 (98%)	156 (100%)	0	100	100
40	1o	110/119 (92%)	110 (100%)	0	100	100
41	1p	154/156 (99%)	153 (99%)	1 (1%)	78	89
42	1q	131/131 (100%)	131 (100%)	0	100	100
43	1r	85/98 (87%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	1s	44/351 (12%)	44 (100%)	0	100	100
45	3A	367/397 (92%)	366 (100%)	1 (0%)	86	93
45	3N	372/397 (94%)	370 (100%)	2 (0%)	81	90
46	3B	328/355 (92%)	327 (100%)	1 (0%)	86	93
46	3O	327/355 (92%)	327 (100%)	0	100	100
47	3C	332/332 (100%)	332 (100%)	0	100	100
47	3P	332/332 (100%)	330 (99%)	2 (1%)	78	89
48	3D	202/259 (78%)	202 (100%)	0	100	100
48	3Q	204/259 (79%)	203 (100%)	1 (0%)	81	90
49	3E	166/226 (74%)	165 (99%)	1 (1%)	78	89
49	3I	37/226 (16%)	37 (100%)	0	100	100
49	3R	166/226 (74%)	165 (99%)	1 (1%)	78	89
49	3V	24/226 (11%)	23 (96%)	1 (4%)	26	40
50	3F	90/99 (91%)	90 (100%)	0	100	100
50	3S	90/99 (91%)	90 (100%)	0	100	100
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	46/48 (96%)	46 (100%)	0	100	100
53	3W	46/48 (96%)	46 (100%)	0	100	100
54	3X	42/46 (91%)	42 (100%)	0	100	100
54	3Y	41/46 (89%)	41 (100%)	0	100	100
55	4A	424/424 (100%)	423 (100%)	1 (0%)	87	94
55	8A	424/424 (100%)	423 (100%)	1 (0%)	87	94
56	4B	210/211 (100%)	208 (99%)	2 (1%)	68	82
56	8B	210/211 (100%)	208 (99%)	2 (1%)	68	82
57	4C	223/225 (99%)	223 (100%)	0	100	100
57	8C	223/225 (99%)	222 (100%)	1 (0%)	84	92
58	4D	124/149 (83%)	124 (100%)	0	100	100
58	8D	124/149 (83%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	4E	92/124 (74%)	92 (100%)	0	100	100
59	8E	92/124 (74%)	91 (99%)	1 (1%)	65	81
60	4F	80/100 (80%)	79 (99%)	1 (1%)	61	77
60	8F	80/100 (80%)	80 (100%)	0	100	100
61	4G	65/80 (81%)	65 (100%)	0	100	100
61	8G	65/80 (81%)	65 (100%)	0	100	100
62	4H	73/76 (96%)	72 (99%)	1 (1%)	59	76
62	8H	73/76 (96%)	73 (100%)	0	100	100
63	4I	54/61 (88%)	54 (100%)	0	100	100
63	8I	54/61 (88%)	54 (100%)	0	100	100
64	4J	49/68 (72%)	47 (96%)	2 (4%)	27	41
64	8J	49/68 (72%)	48 (98%)	1 (2%)	48	67
65	4K	38/66 (58%)	38 (100%)	0	100	100
65	8K	38/66 (58%)	36 (95%)	2 (5%)	20	30
66	4L	39/55 (71%)	38 (97%)	1 (3%)	40	59
66	8L	39/55 (71%)	39 (100%)	0	100	100
67	4M	37/57 (65%)	36 (97%)	1 (3%)	39	58
67	8M	37/57 (65%)	36 (97%)	1 (3%)	39	58
68	4N	70/70 (100%)	70 (100%)	0	100	100
68	8N	70/70 (100%)	70 (100%)	0	100	100
All	All	13845/16096 (86%)	13802 (100%)	43 (0%)	84	93

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
60	4F	51	SER
56	8B	158	ASP
62	4H	31	GLN
66	4L	46	LYS
57	8C	92	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
66	4L	17	ASN
55	8A	328	HIS
59	8E	78	HIS
22	1W	51	GLN
21	1V	75	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	1N	1	14	8,9,10	0.56	0	8,9,11	1.02	1 (12%)
1	FME	1A	1	1	8,9,10	0.54	0	8,9,11	1.07	1 (12%)
56	FME	4B	1	56	8,9,10	0.56	0	8,9,11	0.99	1 (12%)
13	FME	1M	1	13	8,9,10	0.56	0	8,9,11	1.04	1 (12%)
55	FME	8A	1	55	8,9,10	0.55	0	8,9,11	1.16	1 (12%)
12	FME	1L	1	12	8,9,10	0.57	0	8,9,11	0.90	1 (12%)
11	FME	1K	1	11	8,9,10	0.55	0	8,9,11	0.98	1 (12%)
56	FME	8B	1	56	8,9,10	0.56	0	8,9,11	0.83	1 (12%)
8	FME	1H	1	8	8,9,10	0.56	0	8,9,11	1.01	1 (12%)
55	FME	4A	1	55	8,9,10	0.55	0	8,9,11	1.01	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
14	FME	1N	1	14	-	1/7/9/11	-
1	FME	1A	1	1	-	0/7/9/11	-
56	FME	4B	1	56	-	3/7/9/11	-
13	FME	1M	1	13	-	0/7/9/11	-
55	FME	8A	1	55	-	1/7/9/11	-
12	FME	1L	1	12	-	1/7/9/11	-
11	FME	1K	1	11	-	3/7/9/11	-
56	FME	8B	1	56	-	1/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
55	FME	4A	1	55	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1M	1	FME	O-C-CA	-2.63	118.01	124.77
11	1K	1	FME	O-C-CA	-2.61	118.07	124.77
1	1A	1	FME	O-C-CA	-2.60	118.08	124.77
8	1H	1	FME	O-C-CA	-2.57	118.17	124.77
55	8A	1	FME	O-C-CA	-2.48	118.38	124.77

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	1H	1	FME	O1-CN-N-CA
14	1N	1	FME	O1-CN-N-CA
56	4B	1	FME	O1-CN-N-CA
56	4B	1	FME	CB-CA-N-CN
56	8B	1	FME	O1-CN-N-CA

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1N	1	FME	2	0
1	1A	1	FME	3	0
56	4B	1	FME	2	0
13	1M	1	FME	1	0
55	8A	1	FME	1	0
11	1K	1	FME	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	8B	1	FME	1	0
55	4A	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 146 ligands modelled in this entry, 11 are monoatomic - leaving 135 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	$\# Z > 2$
87	PGV	4C	301	-	50,50,50	0.29	0	53,56,56	0.74	1 (1%)
73	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.67	1 (2%)
94	PO4	4H	101	-	4,4,4	0.97	0	6,6,6	0.47	0
75	CDL	1h	202	-	79,79,99	0.31	0	85,91,111	0.42	0
87	PGV	4A	603	-	50,50,50	0.28	0	53,56,56	0.35	0
70	PC1	1I	203	-	43,43,53	0.29	0	49,51,61	0.32	0
75	CDL	3G	103	-	55,55,99	0.34	0	61,67,111	0.48	0
92	PSC	8B	305	-	51,51,51	0.29	0	57,59,59	0.42	0
70	PC1	1A	202	-	34,34,53	0.37	0	40,42,61	0.44	0
69	3PE	3N	503	-	24,24,50	0.37	0	27,29,55	0.56	0
70	PC1	1B	203	-	47,47,53	0.29	0	53,55,61	0.42	0
70	PC1	1P	401	-	32,32,53	0.33	0	38,40,61	0.37	0
71	SF4	1F	502	6	0,12,12	-	-	-	-	-
75	CDL	3G	102	-	51,51,99	0.35	0	57,63,111	0.56	0
87	PGV	4J	101	-	50,50,50	0.30	0	53,56,56	0.38	0
69	3PE	1M	502	-	47,47,50	0.27	0	50,52,55	0.33	0
69	3PE	1Y	206	-	26,26,50	0.35	0	29,31,55	0.55	0
91	CUA	4B	304	56	0,1,1	-	-	-	-	-
94	PO4	8H	101	-	4,4,4	0.97	0	6,6,6	0.44	0
75	CDL	1N	902	-	61,61,99	0.31	0	67,73,111	0.69	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	PGV	4C	304	-	50,50,50	0.29	0	53,56,56	0.47	1 (1%)
87	PGV	8C	304	-	50,50,50	0.28	0	53,56,56	0.38	0
87	PGV	4A	601	-	50,50,50	0.28	0	53,56,56	0.40	0
87	PGV	4L	101	-	50,50,50	0.28	0	53,56,56	0.38	0
69	3PE	3C	503	-	34,34,50	0.32	0	37,39,55	0.45	0
69	3PE	1d	201	-	48,48,50	0.27	0	51,53,55	0.36	0
69	3PE	3A	503	-	31,31,50	0.41	0	34,36,55	0.48	0
75	CDL	1q	203	-	60,60,99	0.34	0	66,72,111	0.42	0
84	MYR	1l	201	-	13,14,15	0.31	0	12,13,15	0.29	0
70	PC1	1M	505	-	43,43,53	0.31	0	49,51,61	0.40	0
81	AYA	1Y	201	-	6,7,8	0.64	0	6,8,10	0.86	0
72	FES	1E	301	5	0,4,4	-	-	-	-	-
76	GTP	1O	401	77	33,34,34	0.56	0	50,54,54	0.57	0
87	PGV	4K	101	-	50,50,50	0.28	0	53,56,56	0.31	0
75	CDL	4C	305	-	99,99,99	0.27	0	105,111,111	0.39	0
70	PC1	1H	403	-	47,47,53	0.29	0	53,55,61	0.36	0
87	PGV	8C	301	-	50,50,50	0.27	0	53,56,56	0.35	0
85	HEM	3P	501	47	50,50,50	1.57	8 (16%)	67,82,82	1.61	11 (16%)
69	3PE	1j	101	-	43,43,50	0.29	0	46,48,55	0.44	0
92	PSC	4B	305	-	51,51,51	0.29	0	57,59,59	0.47	1 (1%)
86	HEC	3D	501	48	44,49,50	2.68	27 (61%)	56,80,82	2.03	16 (28%)
72	FES	3E	301	49	0,4,4	-	-	-	-	-
70	PC1	1d	202	-	38,38,53	0.31	0	44,46,61	0.47	0
70	PC1	1Y	207	-	45,45,53	0.29	0	51,53,61	0.34	0
87	PGV	4A	602	-	50,50,50	0.28	0	53,56,56	0.32	0
87	PGV	4C	303	-	50,50,50	0.28	0	53,56,56	0.39	0
69	3PE	3D	502	-	32,32,50	0.33	0	35,37,55	0.49	0
75	CDL	8D	201	-	99,99,99	0.27	0	105,111,111	0.41	0
69	3PE	3P	503	-	32,32,50	0.33	0	35,37,55	0.37	0
69	3PE	1M	501	-	44,44,50	0.29	0	47,49,55	0.34	0
69	3PE	3R	302	-	46,46,50	0.28	0	49,51,55	0.36	0
80	EHZ	1T	101	20	31,36,37	0.20	0	36,44,47	1.12	1 (2%)
70	PC1	1h	203	-	46,46,53	0.28	0	52,54,61	0.30	0
81	AYA	1q	202	-	6,7,8	0.62	0	6,8,10	0.89	0
93	PEK	8G	102	-	52,52,52	0.26	0	55,57,57	0.40	0
75	CDL	1X	201	-	85,85,99	0.29	0	91,97,111	0.39	0
86	HEC	3Q	501	48	46,50,50	2.62	27 (58%)	58,82,82	2.01	16 (27%)
82	AME	1h	201	-	9,10,11	0.51	0	9,11,13	0.99	1 (11%)
87	PGV	8B	302	-	50,50,50	0.28	0	53,56,56	0.37	0
71	SF4	1G	801	7	0,12,12	-	-	-	-	-
69	3PE	3A	502	-	26,26,50	0.36	0	29,31,55	0.64	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	CDL	1H	401	-	50,50,99	0.36	0	56,62,111	0.60	1 (1%)
69	3PE	1m	201	-	40,40,50	0.29	0	43,45,55	0.40	0
80	EHZ	1n	201	-	31,36,37	0.18	0	36,44,47	1.05	1 (2%)
70	PC1	1H	402	-	53,53,53	0.28	0	59,61,61	0.35	0
87	PGV	8K	101	-	50,50,50	0.29	0	53,56,56	0.32	0
87	PGV	8B	301	-	50,50,50	0.28	0	53,56,56	0.32	0
70	PC1	1A	203	-	34,34,53	0.33	0	40,42,61	0.39	0
69	3PE	3N	501	-	31,31,50	0.33	0	34,36,55	0.49	0
69	3PE	1L	703	-	44,44,50	0.29	0	47,49,55	0.34	0
69	3PE	3Y	101	-	29,29,50	0.34	0	32,34,55	0.42	0
87	PGV	8C	307	-	50,50,50	0.29	0	53,56,56	0.35	0
69	3PE	1L	701	-	45,45,50	0.28	0	48,50,55	0.33	0
75	CDL	3P	504	-	55,55,99	0.35	0	61,67,111	0.52	0
69	3PE	1M	506	-	49,49,50	0.28	0	52,54,55	0.33	0
69	3PE	3G	101	-	28,28,50	0.33	0	31,33,55	0.37	0
70	PC1	1M	503	-	34,34,53	0.32	0	40,42,61	0.52	0
93	PEK	4G	102	-	52,52,52	0.26	0	55,57,57	0.40	0
69	3PE	1P	403	-	34,34,50	0.31	0	37,39,55	0.43	0
69	3PE	1Y	204	-	29,29,50	0.34	0	32,34,55	0.80	1 (3%)
75	CDL	1d	203	-	64,64,99	0.32	0	70,76,111	0.41	0
75	CDL	8C	306	-	99,99,99	0.27	0	105,111,111	0.40	0
93	PEK	4C	307	-	51,51,52	0.26	0	54,56,57	0.42	0
87	PGV	8C	305	-	50,50,50	0.29	0	53,56,56	0.46	1 (1%)
75	CDL	4B	303	-	99,99,99	0.27	0	105,111,111	0.30	0
69	3PE	1M	504	-	50,50,50	0.28	0	53,55,55	0.46	0
69	3PE	1Y	203	-	39,39,50	0.31	0	42,44,55	0.50	0
71	SF4	1B	201	2	0,12,12	-	-	-	-	-
87	PGV	8A	601	-	50,50,50	0.29	0	53,56,56	0.41	0
87	PGV	4B	302	-	50,50,50	0.29	0	53,56,56	0.36	0
75	CDL	8B	303	-	99,99,99	0.27	0	105,111,111	0.30	0
87	PGV	4C	302	-	50,50,50	0.29	0	53,56,56	0.31	0
87	PGV	8L	101	-	50,50,50	0.28	0	53,56,56	0.41	0
75	CDL	3T	101	-	56,56,99	0.35	0	62,68,111	0.48	0
87	PGV	8J	101	-	50,50,50	0.28	0	53,56,56	0.40	0
93	PEK	8C	308	-	51,51,52	0.26	0	54,56,57	0.41	0
69	3PE	3C	504	-	33,33,50	0.33	0	36,38,55	0.41	0
72	FES	1G	803	7	0,4,4	-	-	-	-	-
88	HEA	8A	604	55	67,67,67	2.45	26 (38%)	81,103,103	2.54	33 (40%)
70	PC1	3J	101	-	46,46,53	0.28	0	52,54,61	0.32	0
75	CDL	1L	702	-	75,75,99	0.29	0	81,87,111	0.37	0
70	PC1	3X	101	-	28,28,53	0.36	0	34,36,61	0.48	0
87	PGV	4M	101	-	50,50,50	0.29	0	53,56,56	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	PGV	4G	101	-	50,50,50	0.28	0	53,56,56	0.45	1 (1%)
75	CDL	4D	201	-	99,99,99	0.27	0	105,111,111	0.43	0
87	PGV	8C	303	-	50,50,50	0.29	0	53,56,56	0.32	0
70	PC1	3R	303	-	44,44,53	0.29	0	50,52,61	0.36	0
71	SF4	1I	201	9	0,12,12	-	-	-	-	-
85	HEM	3C	501	47	50,50,50	1.56	8 (16%)	67,82,82	1.62	11 (16%)
75	CDL	3N	502	-	42,42,99	0.37	0	48,54,111	0.52	0
87	PGV	8C	302	-	50,50,50	0.29	0	53,56,56	0.72	1 (1%)
83	CHD	1i	201	-	32,32,32	0.51	0	51,51,51	0.57	0
72	FES	3R	301	49	0,4,4	-	-	-	-	-
87	PGV	4C	306	-	50,50,50	0.29	0	53,56,56	0.36	0
88	HEA	4A	605	55	67,67,67	2.45	26 (38%)	81,103,103	2.55	34 (41%)
70	PC1	1q	201	-	48,48,53	0.28	0	54,56,61	0.33	0
85	HEM	3P	502	47	50,50,50	1.56	8 (16%)	67,82,82	1.59	12 (17%)
70	PC1	1B	202	-	45,45,53	0.28	0	51,53,61	0.35	0
88	HEA	8A	605	55	67,67,67	2.45	26 (38%)	81,103,103	2.53	34 (41%)
69	3PE	1N	901	-	48,48,50	0.28	0	51,53,55	0.36	0
87	PGV	8A	603	-	50,50,50	0.28	0	53,56,56	0.33	0
69	3PE	1K	101	-	43,43,50	0.30	0	46,48,55	0.34	0
75	CDL	3A	501	-	57,57,99	0.33	0	63,69,111	0.42	0
87	PGV	4B	301	-	50,50,50	0.27	0	53,56,56	0.31	0
87	PGV	8G	101	-	50,50,50	0.29	0	53,56,56	0.45	1 (1%)
88	HEA	4A	604	55	67,67,67	2.45	25 (37%)	81,103,103	2.55	35 (43%)
87	PGV	8A	602	-	50,50,50	0.28	0	53,56,56	0.30	0
91	CUA	8B	304	56	0,1,1	-	-	-	-	-
69	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.36	0
69	3PE	1Y	202	-	30,30,50	0.32	0	33,35,55	0.53	0
69	3PE	1Y	205	-	32,32,50	0.32	0	35,37,55	0.52	0
71	SF4	1G	802	7	0,12,12	-	-	-	-	-
85	HEM	3C	502	-	50,50,50	1.56	9 (18%)	67,82,82	1.58	12 (17%)
71	SF4	1I	202	9	0,12,12	-	-	-	-	-
78	NDP	1P	402	-	51,52,52	0.50	0	71,80,80	0.83	2 (2%)

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
87	PGV	4C	301	-	-	11/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
73	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
75	CDL	1h	202	-	-	19/90/90/110	-
87	PGV	4A	603	-	-	3/55/55/55	-
70	PC1	1I	203	-	-	5/47/47/57	-
75	CDL	3G	103	-	-	8/66/66/110	-
92	PSC	8B	305	-	-	16/55/55/55	-
70	PC1	1A	202	-	-	4/38/38/57	-
69	3PE	3N	503	-	-	5/28/28/54	-
70	PC1	1B	203	-	-	10/51/51/57	-
70	PC1	1P	401	-	-	5/36/36/57	-
71	SF4	1F	502	6	-	-	0/6/5/5
75	CDL	3G	102	-	-	8/62/62/110	-
87	PGV	4J	101	-	-	7/55/55/55	-
69	3PE	1M	502	-	-	13/51/51/54	-
69	3PE	1Y	206	-	-	5/30/30/54	-
75	CDL	1N	902	-	-	15/71/71/110	-
87	PGV	4C	304	-	-	4/55/55/55	-
87	PGV	8C	304	-	-	13/55/55/55	-
87	PGV	4A	601	-	-	14/55/55/55	-
87	PGV	4L	101	-	-	5/55/55/55	-
69	3PE	3C	503	-	-	11/38/38/54	-
69	3PE	1d	201	-	-	7/52/52/54	-
69	3PE	3A	503	-	-	6/35/35/54	-
75	CDL	1q	203	-	-	6/71/71/110	-
84	MYR	1l	201	-	-	1/12/12/13	-
70	PC1	1M	505	-	-	13/47/47/57	-
81	AYA	1Y	201	-	-	0/5/6/8	-
72	FES	1E	301	5	-	-	0/1/1/1
76	GTP	1O	401	77	-	4/22/38/38	0/3/3/3
87	PGV	4K	101	-	-	14/55/55/55	-
75	CDL	4C	305	-	-	18/110/110/110	-
70	PC1	1H	403	-	-	4/51/51/57	-
87	PGV	8C	301	-	-	3/55/55/55	-
85	HEM	3P	501	47	-	9/14/54/54	-
69	3PE	1j	101	-	-	3/47/47/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
92	PSC	4B	305	-	-	14/55/55/55	-
86	HEC	3D	501	48	-	3/13/53/54	-
72	FES	3E	301	49	-	-	0/1/1/1
70	PC1	1d	202	-	-	7/42/42/57	-
70	PC1	1Y	207	-	-	8/49/49/57	-
87	PGV	4A	602	-	-	1/55/55/55	-
87	PGV	4C	303	-	-	9/55/55/55	-
69	3PE	3D	502	-	-	1/36/36/54	-
75	CDL	8D	201	-	-	14/110/110/110	-
69	3PE	3P	503	-	-	6/36/36/54	-
69	3PE	1M	501	-	-	6/48/48/54	-
69	3PE	3R	302	-	-	4/50/50/54	-
80	EHZ	1T	101	20	-	10/42/44/45	-
70	PC1	1h	203	-	-	12/50/50/57	-
81	AYA	1q	202	-	-	0/5/6/8	-
93	PEK	8G	102	-	-	6/56/56/56	-
75	CDL	1X	201	-	-	17/96/96/110	-
86	HEC	3Q	501	48	-	3/14/54/54	-
82	AME	1h	201	-	-	2/9/10/12	-
87	PGV	8B	302	-	-	5/55/55/55	-
71	SF4	1G	801	7	-	-	0/6/5/5
69	3PE	3A	502	-	-	7/30/30/54	-
75	CDL	1H	401	-	-	4/61/61/110	-
69	3PE	1m	201	-	-	9/44/44/54	-
80	EHZ	1n	201	-	-	4/42/44/45	-
70	PC1	1H	402	-	-	6/57/57/57	-
87	PGV	8K	101	-	-	13/55/55/55	-
87	PGV	8B	301	-	-	7/55/55/55	-
70	PC1	1A	203	-	-	2/38/38/57	-
69	3PE	3N	501	-	-	10/35/35/54	-
69	3PE	1L	703	-	-	6/48/48/54	-
69	3PE	3Y	101	-	-	5/33/33/54	-
87	PGV	8C	307	-	-	3/55/55/55	-
69	3PE	1L	701	-	-	4/49/49/54	-
75	CDL	3P	504	-	-	17/66/66/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	1M	506	-	-	7/53/53/54	-
69	3PE	3G	101	-	-	3/32/32/54	-
70	PC1	1M	503	-	-	6/38/38/57	-
93	PEK	4G	102	-	-	6/56/56/56	-
69	3PE	1P	403	-	-	5/38/38/54	-
69	3PE	1Y	204	-	-	9/33/33/54	-
75	CDL	1d	203	-	-	11/75/75/110	-
75	CDL	8C	306	-	-	18/110/110/110	-
93	PEK	4C	307	-	-	3/55/55/56	-
87	PGV	8C	305	-	-	6/55/55/55	-
75	CDL	4B	303	-	-	14/110/110/110	-
69	3PE	1M	504	-	-	10/54/54/54	-
69	3PE	1Y	203	-	-	14/43/43/54	-
71	SF4	1B	201	2	-	-	0/6/5/5
87	PGV	8A	601	-	-	11/55/55/55	-
87	PGV	4B	302	-	-	5/55/55/55	-
75	CDL	8B	303	-	-	15/110/110/110	-
87	PGV	4C	302	-	-	9/55/55/55	-
87	PGV	8L	101	-	-	5/55/55/55	-
75	CDL	3T	101	-	-	9/67/67/110	-
87	PGV	8J	101	-	-	9/55/55/55	-
93	PEK	8C	308	-	-	2/55/55/56	-
69	3PE	3C	504	-	-	8/37/37/54	-
72	FES	1G	803	7	-	-	0/1/1/1
88	HEA	8A	604	55	-	6/36/76/76	-
70	PC1	3J	101	-	-	1/50/50/57	-
75	CDL	1L	702	-	-	13/86/86/110	-
70	PC1	3X	101	-	-	2/32/32/57	-
87	PGV	4M	101	-	-	7/55/55/55	-
87	PGV	4G	101	-	-	10/55/55/55	-
75	CDL	4D	201	-	-	15/110/110/110	-
87	PGV	8C	303	-	-	10/55/55/55	-
70	PC1	3R	303	-	-	3/48/48/57	-
71	SF4	1I	201	9	-	-	0/6/5/5
85	HEM	3C	501	47	-	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	CDL	3N	502	-	-	8/53/53/110	-
87	PGV	8C	302	-	-	15/55/55/55	-
83	CHD	1i	201	-	-	2/9/74/74	0/4/4/4
87	PGV	4C	306	-	-	2/55/55/55	-
72	FES	3R	301	49	-	-	0/1/1/1
88	HEA	4A	605	55	-	5/36/76/76	-
70	PC1	1q	201	-	-	3/52/52/57	-
85	HEM	3P	502	47	-	8/14/54/54	-
70	PC1	1B	202	-	-	3/49/49/57	-
88	HEA	8A	605	55	-	6/36/76/76	-
69	3PE	1N	901	-	-	11/52/52/54	-
87	PGV	8A	603	-	-	4/55/55/55	-
69	3PE	1K	101	-	-	9/47/47/54	-
75	CDL	3A	501	-	-	1/68/68/110	-
87	PGV	4B	301	-	-	2/55/55/55	-
87	PGV	8G	101	-	-	8/55/55/55	-
88	HEA	4A	604	55	-	10/36/76/76	-
87	PGV	8A	602	-	-	8/55/55/55	-
69	3PE	1A	201	-	-	7/50/50/54	-
69	3PE	1Y	202	-	-	9/34/34/54	-
69	3PE	1Y	205	-	-	2/36/36/54	-
71	SF4	1G	802	7	-	-	0/6/5/5
85	HEM	3C	502	-	-	6/14/54/54	-
71	SF4	1I	202	9	-	-	0/6/5/5
78	NDP	1P	402	-	-	3/34/77/77	0/5/5/5

The worst 5 of 190 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	8A	604	HEA	FE-NB	5.66	2.12	1.94
88	4A	604	HEA	FE-ND	5.65	2.12	1.94
88	4A	604	HEA	FE-NB	5.64	2.12	1.94
88	8A	604	HEA	FE-ND	5.62	2.12	1.94
88	4A	605	HEA	FE-ND	5.61	2.12	1.94

The worst 5 of 231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	4A	605	HEA	C3D-C4D-ND	6.64	116.77	110.35
88	8A	605	HEA	C3D-C4D-ND	6.63	116.76	110.35
88	4A	604	HEA	C3D-C4D-ND	6.54	116.67	110.35
88	8A	604	HEA	C3D-C4D-ND	6.47	116.60	110.35
80	1T	101	EHZ	C10-S1-C9	6.20	120.16	101.84

There are no chirality outliers.

5 of 887 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1A	201	3PE	C11-O13-P-O12
69	1K	101	3PE	C1-O11-P-O13
69	1K	101	3PE	C1-O11-P-O14
69	1L	701	3PE	O32-C31-O31-C3
69	1L	701	3PE	C32-C31-O31-C3

There are no ring outliers.

121 monomers are involved in 594 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	4C	301	PGV	2	0
73	1F	501	FMN	4	0
75	1h	202	CDL	14	0
87	4A	603	PGV	10	0
70	1I	203	PC1	3	0
75	3G	103	CDL	6	0
92	8B	305	PSC	8	0
70	1A	202	PC1	7	0
69	3N	503	3PE	3	0
70	1B	203	PC1	9	0
70	1P	401	PC1	2	0
71	1F	502	SF4	2	0
75	3G	102	CDL	2	0
87	4J	101	PGV	10	0
69	1M	502	3PE	12	0
69	1Y	206	3PE	2	0
91	4B	304	CUA	2	0
94	8H	101	PO4	1	0
75	1N	902	CDL	3	0
87	4C	304	PGV	1	0
87	8C	304	PGV	7	0
87	4A	601	PGV	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	4L	101	PGV	7	0
69	3C	503	3PE	5	0
69	1d	201	3PE	5	0
69	3A	503	3PE	8	0
75	1q	203	CDL	2	0
70	1M	505	PC1	7	0
76	1O	401	GTP	3	0
87	4K	101	PGV	2	0
75	4C	305	CDL	15	0
70	1H	403	PC1	7	0
87	8C	301	PGV	5	0
85	3P	501	HEM	1	0
92	4B	305	PSC	8	0
86	3D	501	HEC	2	0
72	3E	301	FES	2	0
70	1d	202	PC1	8	0
70	1Y	207	PC1	7	0
87	4A	602	PGV	4	0
87	4C	303	PGV	7	0
69	3D	502	3PE	2	0
75	8D	201	CDL	15	0
69	1M	501	3PE	7	0
69	3R	302	3PE	5	0
70	1h	203	PC1	1	0
81	1q	202	AYA	2	0
93	8G	102	PEK	5	0
75	1X	201	CDL	12	0
86	3Q	501	HEC	3	0
82	1h	201	AME	1	0
87	8B	302	PGV	3	0
71	1G	801	SF4	3	0
69	3A	502	3PE	1	0
75	1H	401	CDL	1	0
80	1n	201	EHZ	1	0
70	1H	402	PC1	5	0
87	8K	101	PGV	3	0
87	8B	301	PGV	8	0
69	3N	501	3PE	5	0
69	1L	703	3PE	5	0
69	3Y	101	3PE	2	0
87	8C	307	PGV	8	0
69	1L	701	3PE	3	0

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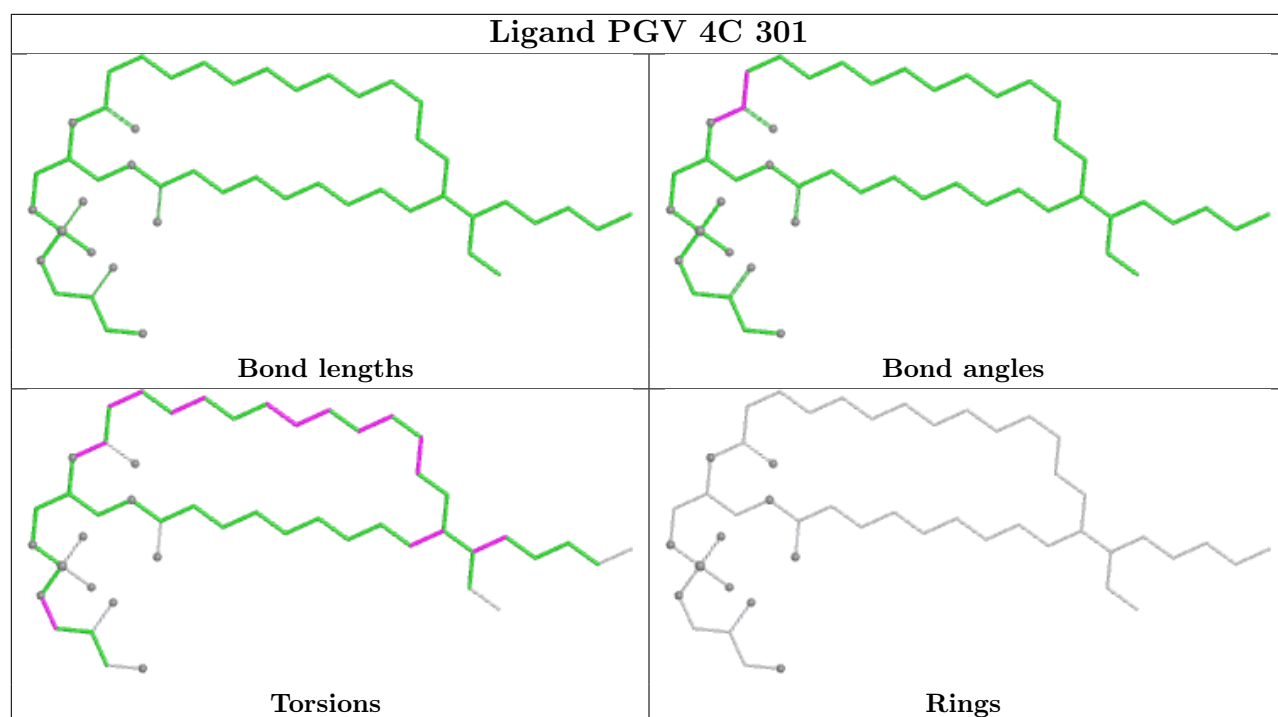
Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	3P	504	CDL	9	0
69	1M	506	3PE	3	0
69	3G	101	3PE	1	0
70	1M	503	PC1	3	0
93	4G	102	PEK	2	0
69	1P	403	3PE	3	0
69	1Y	204	3PE	5	0
75	1d	203	CDL	6	0
75	8C	306	CDL	16	0
93	4C	307	PEK	5	0
87	8C	305	PGV	10	0
75	4B	303	CDL	14	0
69	1M	504	3PE	11	0
69	1Y	203	3PE	9	0
71	1B	201	SF4	2	0
87	8A	601	PGV	10	0
87	4B	302	PGV	4	0
75	8B	303	CDL	10	0
87	4C	302	PGV	5	0
87	8L	101	PGV	7	0
75	3T	101	CDL	9	0
87	8J	101	PGV	4	0
93	8C	308	PEK	5	0
69	3C	504	3PE	4	0
72	1G	803	FES	2	0
88	8A	604	HEA	8	0
70	3J	101	PC1	4	0
75	1L	702	CDL	6	0
70	3X	101	PC1	2	0
87	4M	101	PGV	3	0
87	4G	101	PGV	5	0
75	4D	201	CDL	17	0
87	8C	303	PGV	8	0
70	3R	303	PC1	4	0
75	3N	502	CDL	7	0
87	8C	302	PGV	5	0
72	3R	301	FES	2	0
87	4C	306	PGV	8	0
88	4A	605	HEA	4	0
70	1q	201	PC1	4	0
85	3P	502	HEM	3	0
70	1B	202	PC1	7	0

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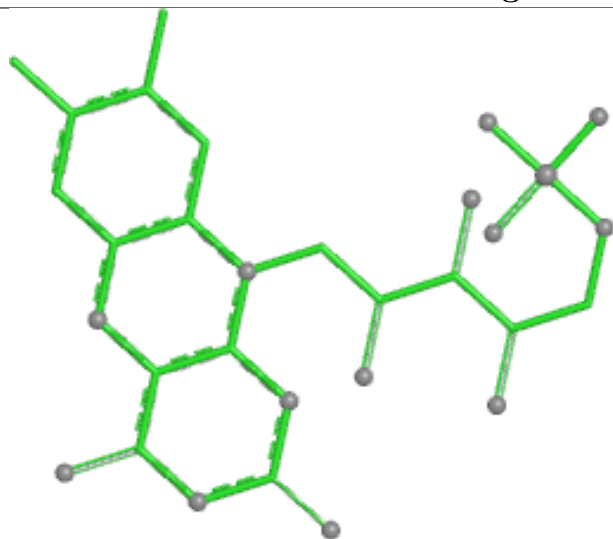
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	8A	605	HEA	4	0
69	1N	901	3PE	5	0
87	8A	603	PGV	5	0
69	1K	101	3PE	2	0
75	3A	501	CDL	3	0
87	4B	301	PGV	4	0
87	8G	101	PGV	8	0
88	4A	604	HEA	6	0
87	8A	602	PGV	8	0
91	8B	304	CUA	2	0
69	1A	201	3PE	3	0
69	1Y	202	3PE	7	0
69	1Y	205	3PE	3	0
85	3C	502	HEM	2	0
78	1P	402	NDP	2	0

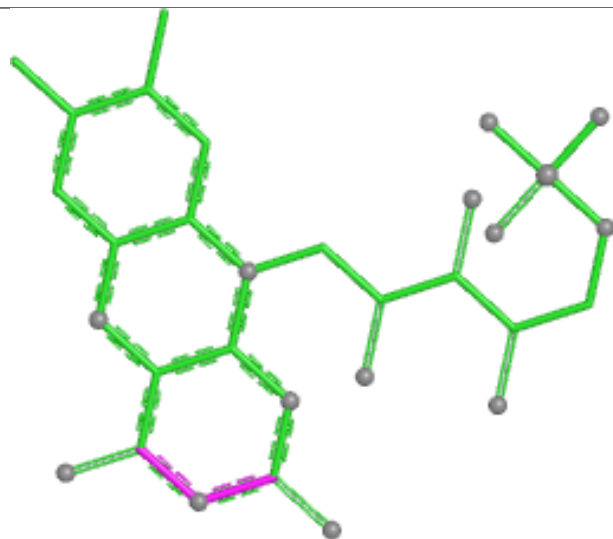
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



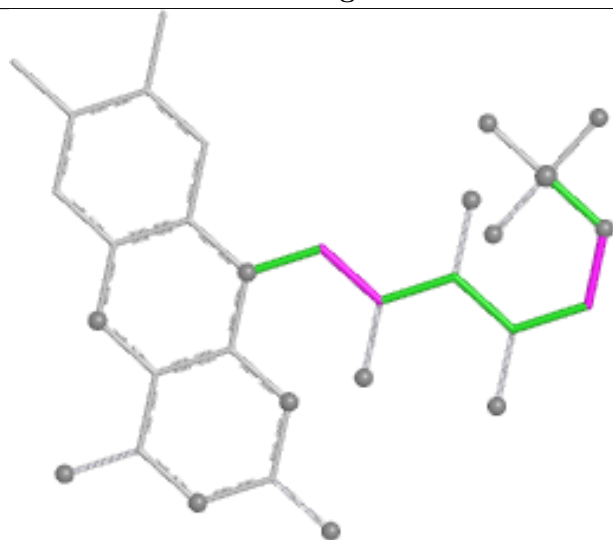
Ligand FMN 1F 501



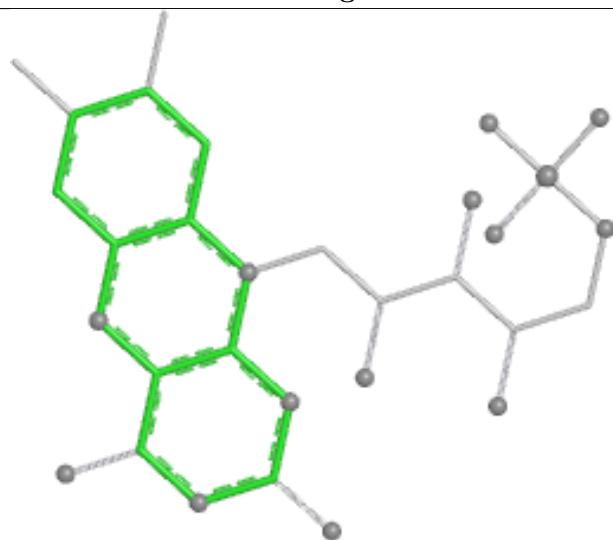
Bond lengths



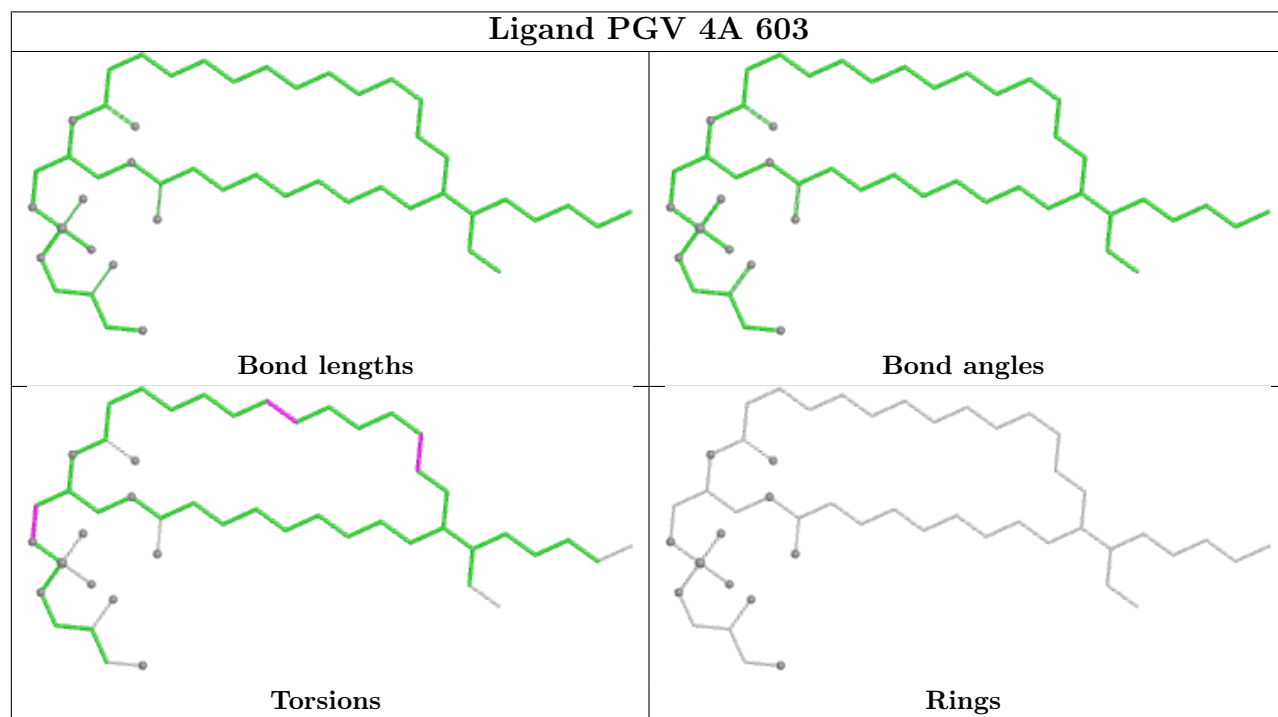
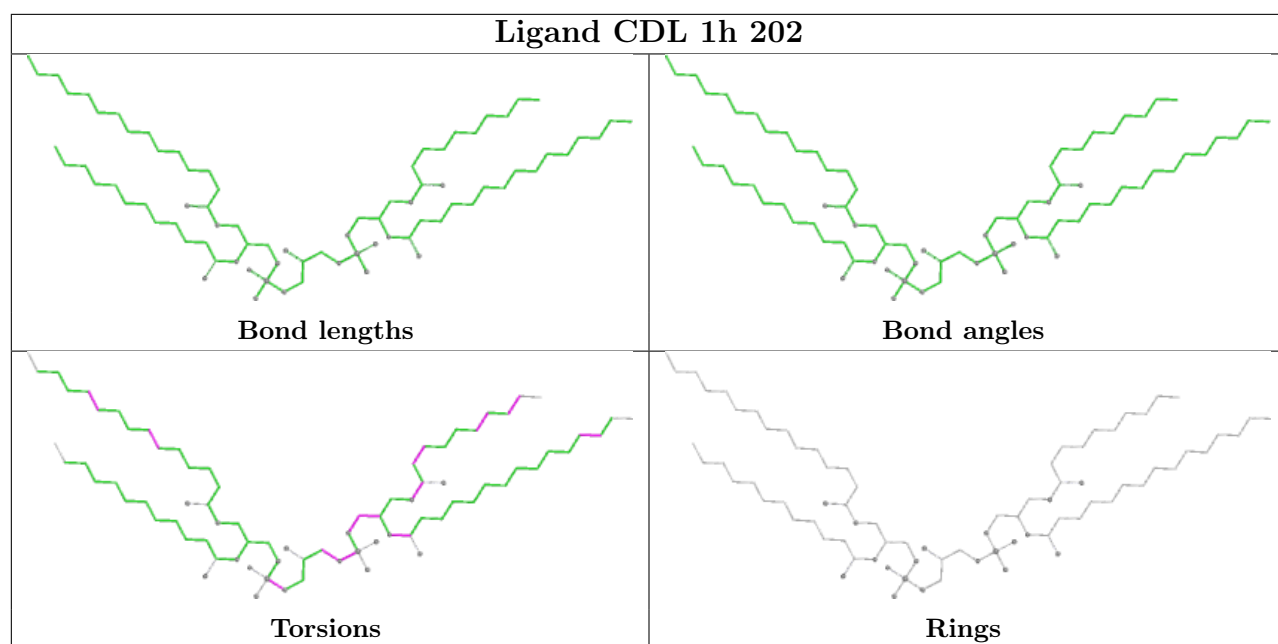
Bond angles

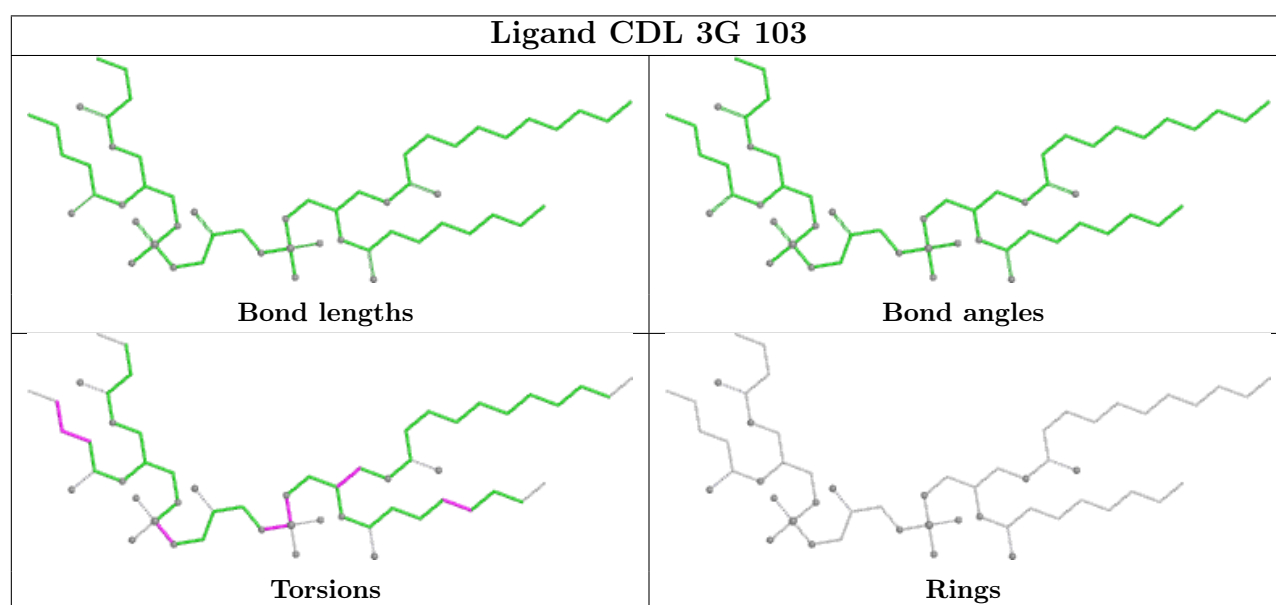
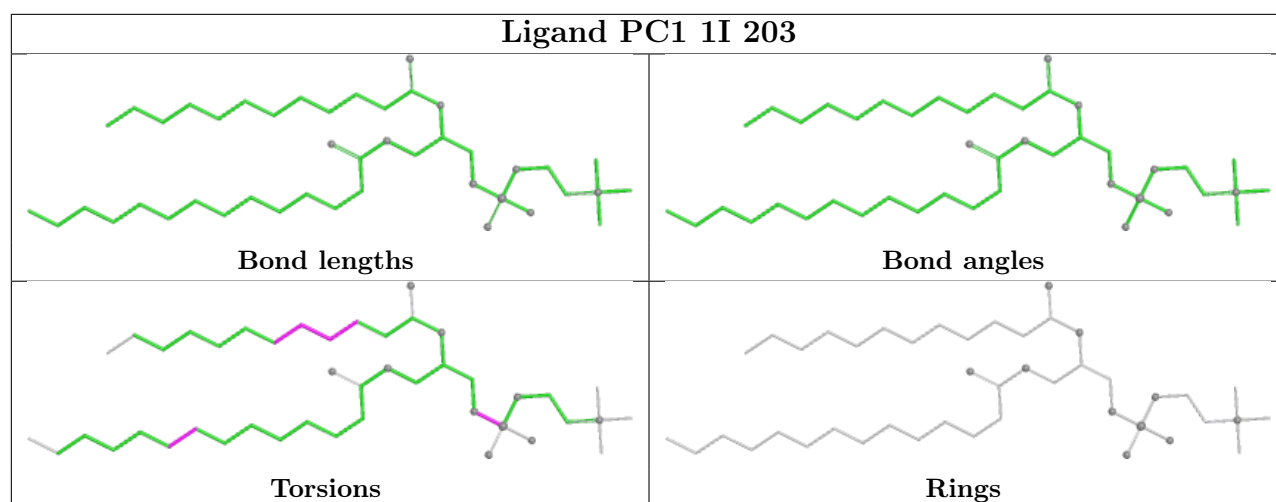


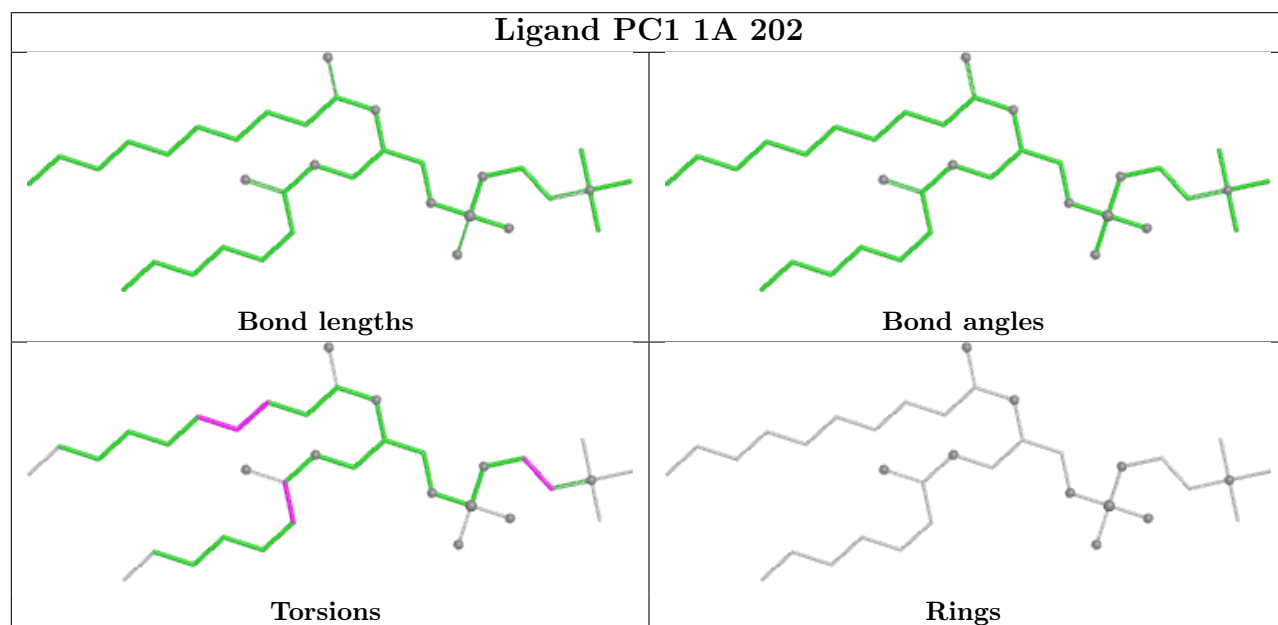
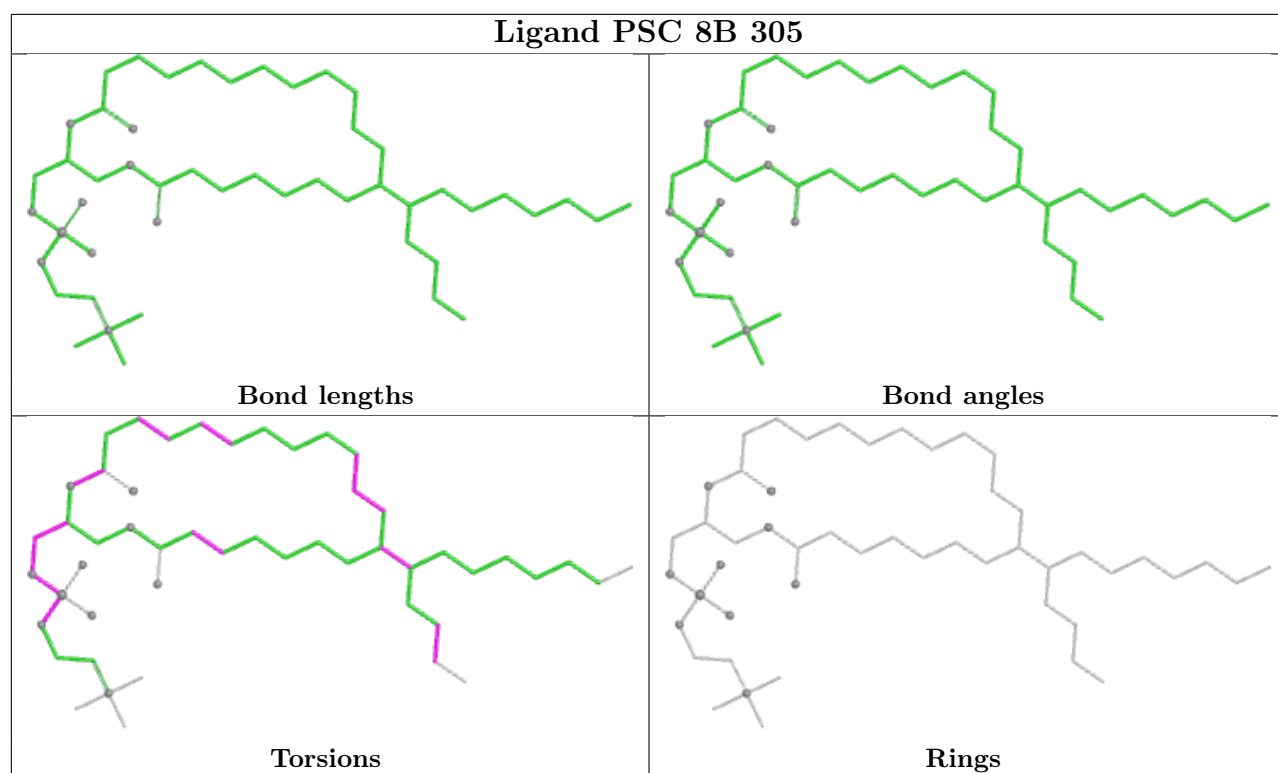
Torsions

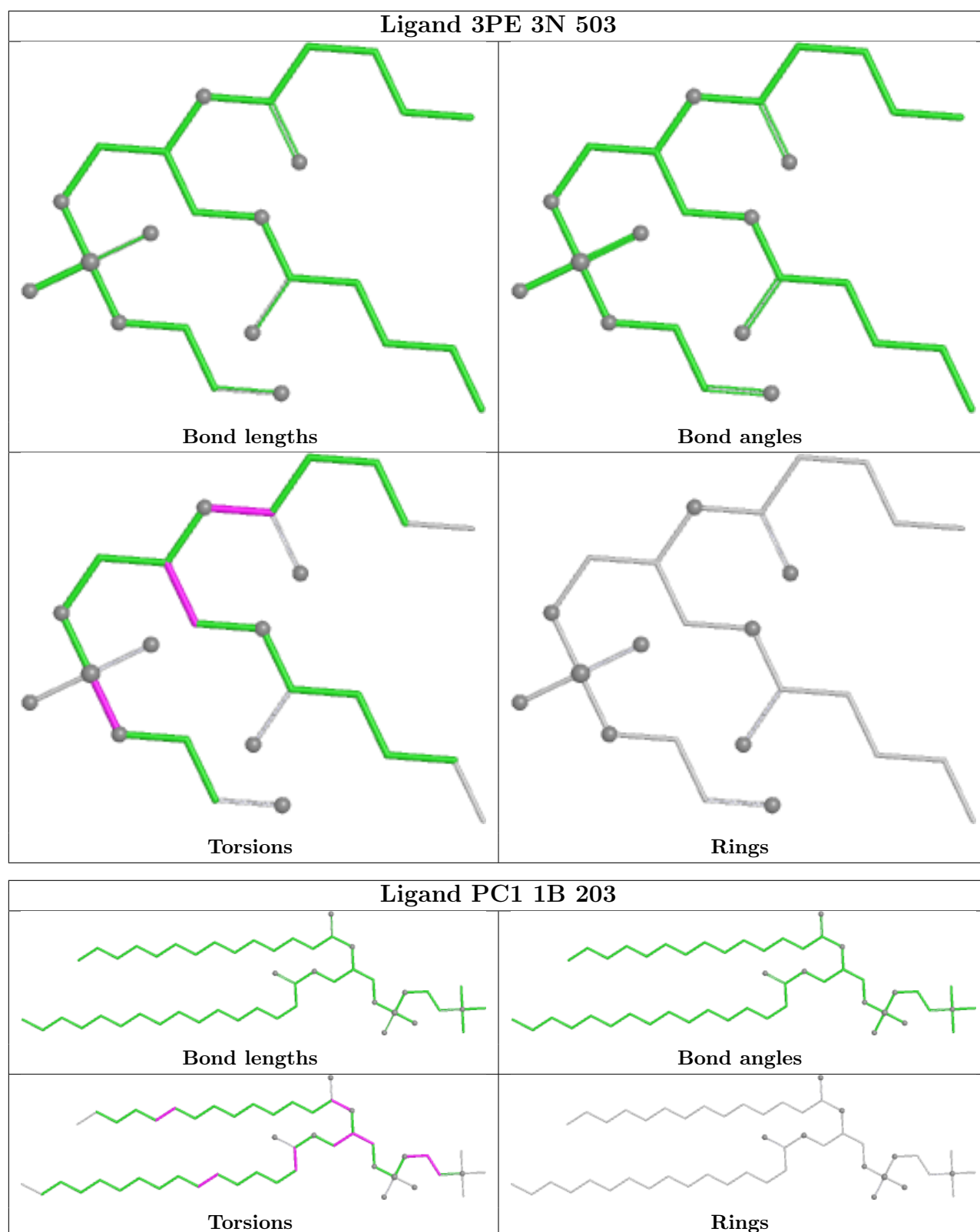


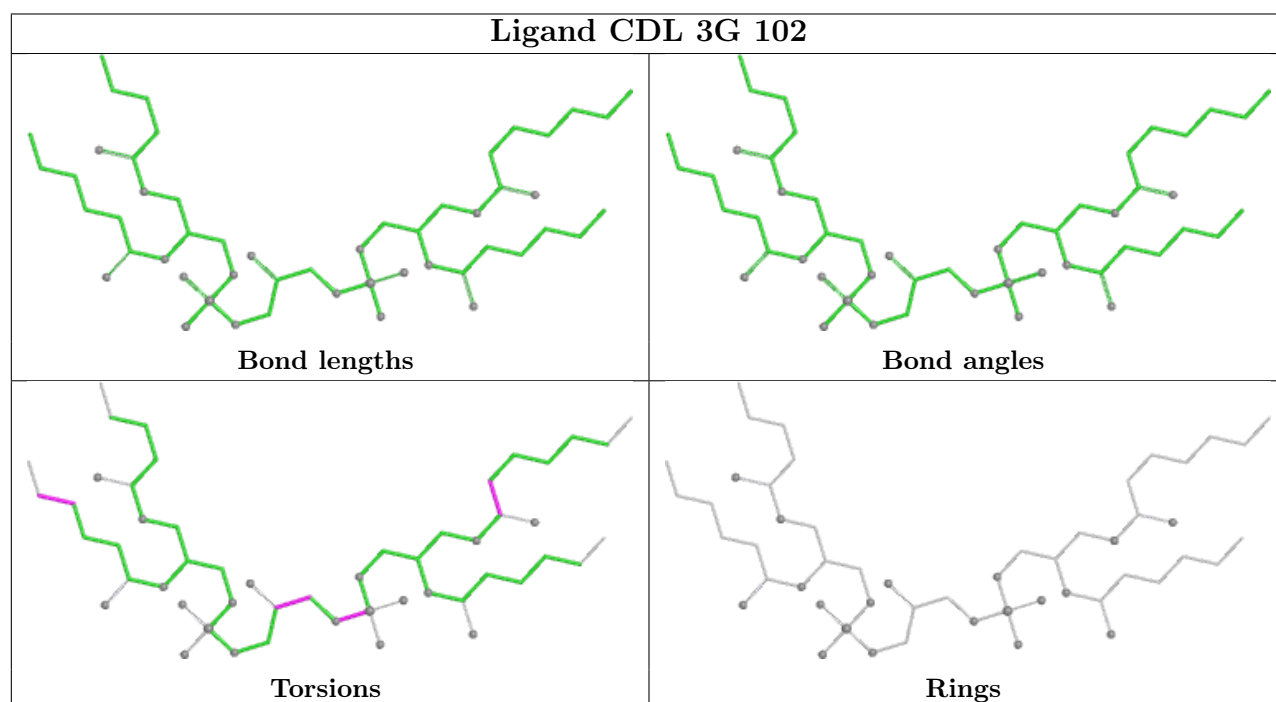
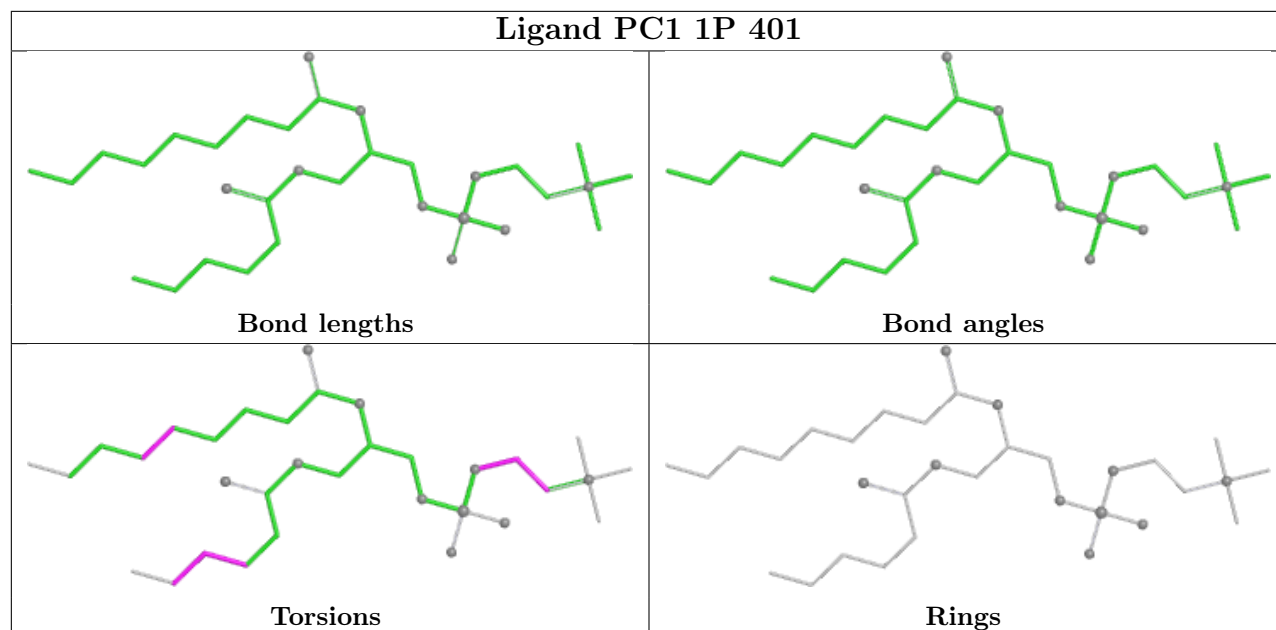
Rings

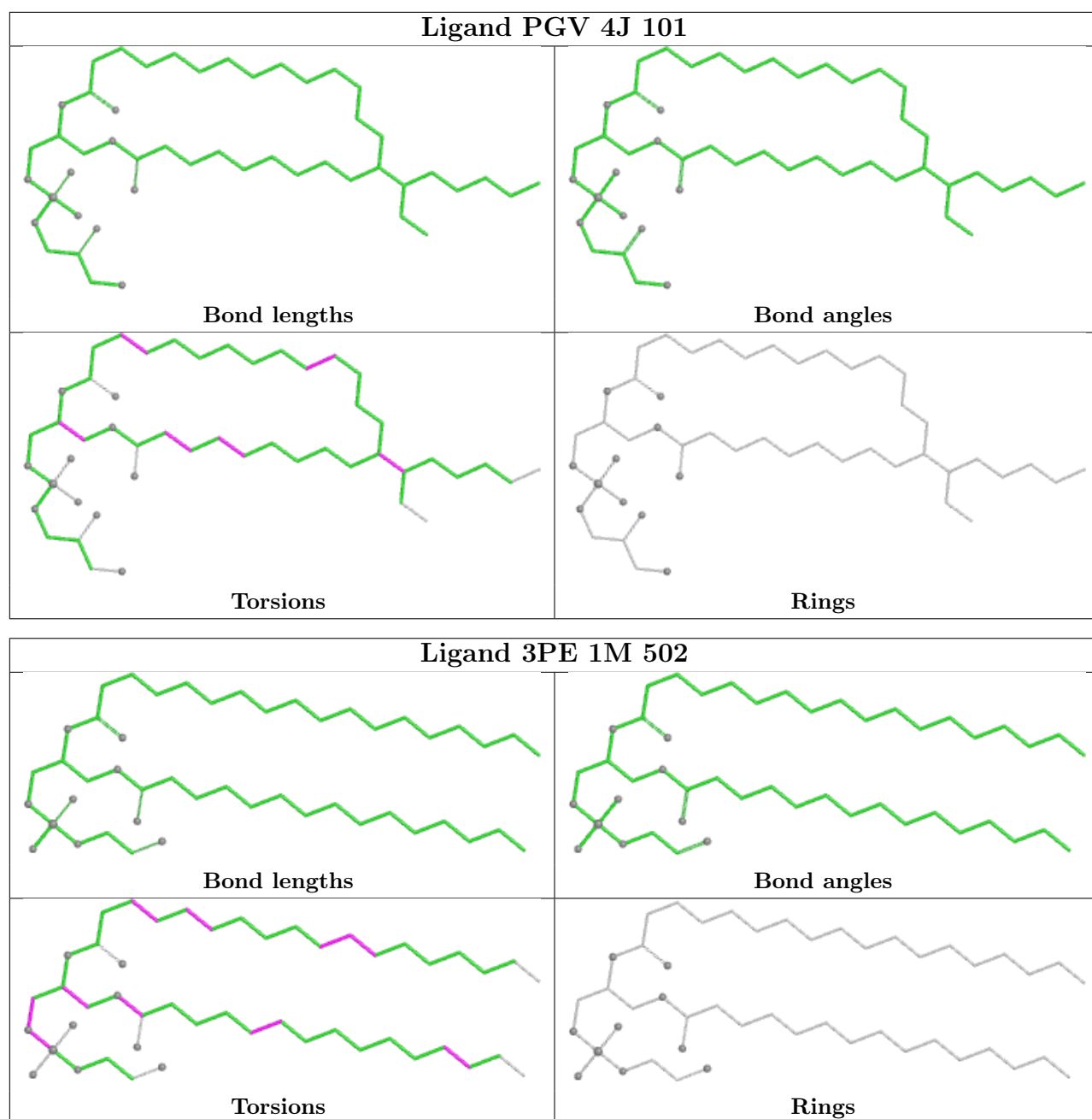


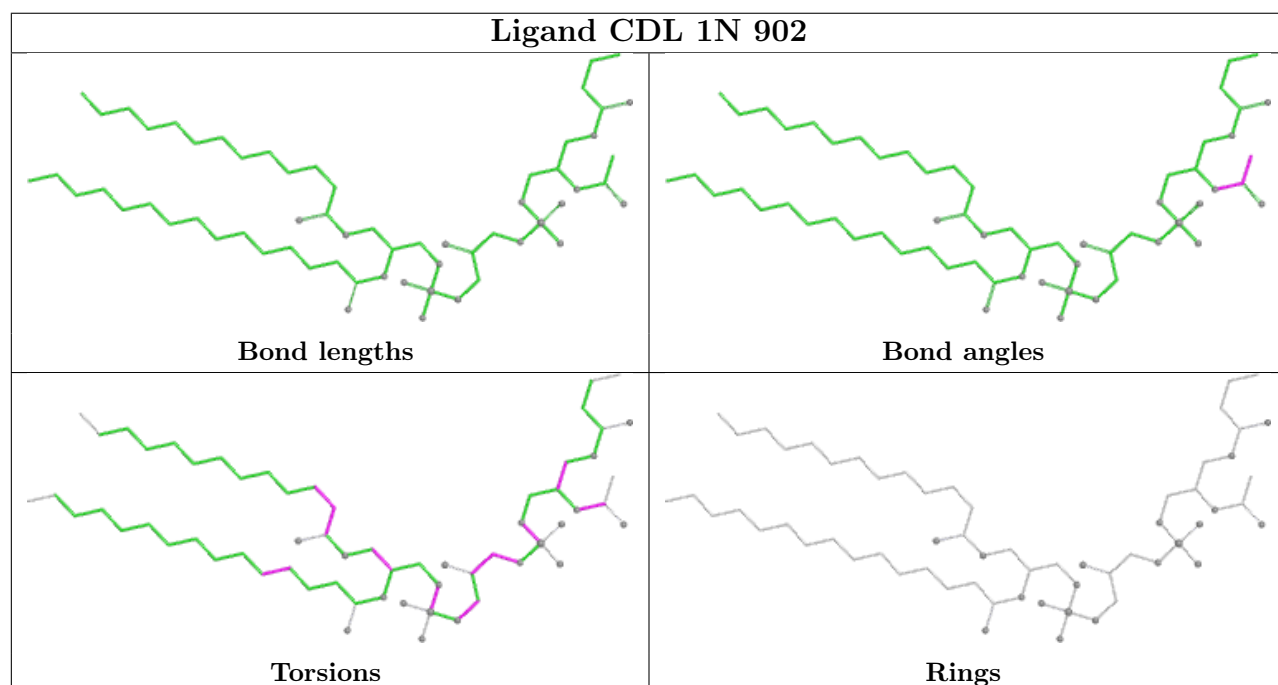
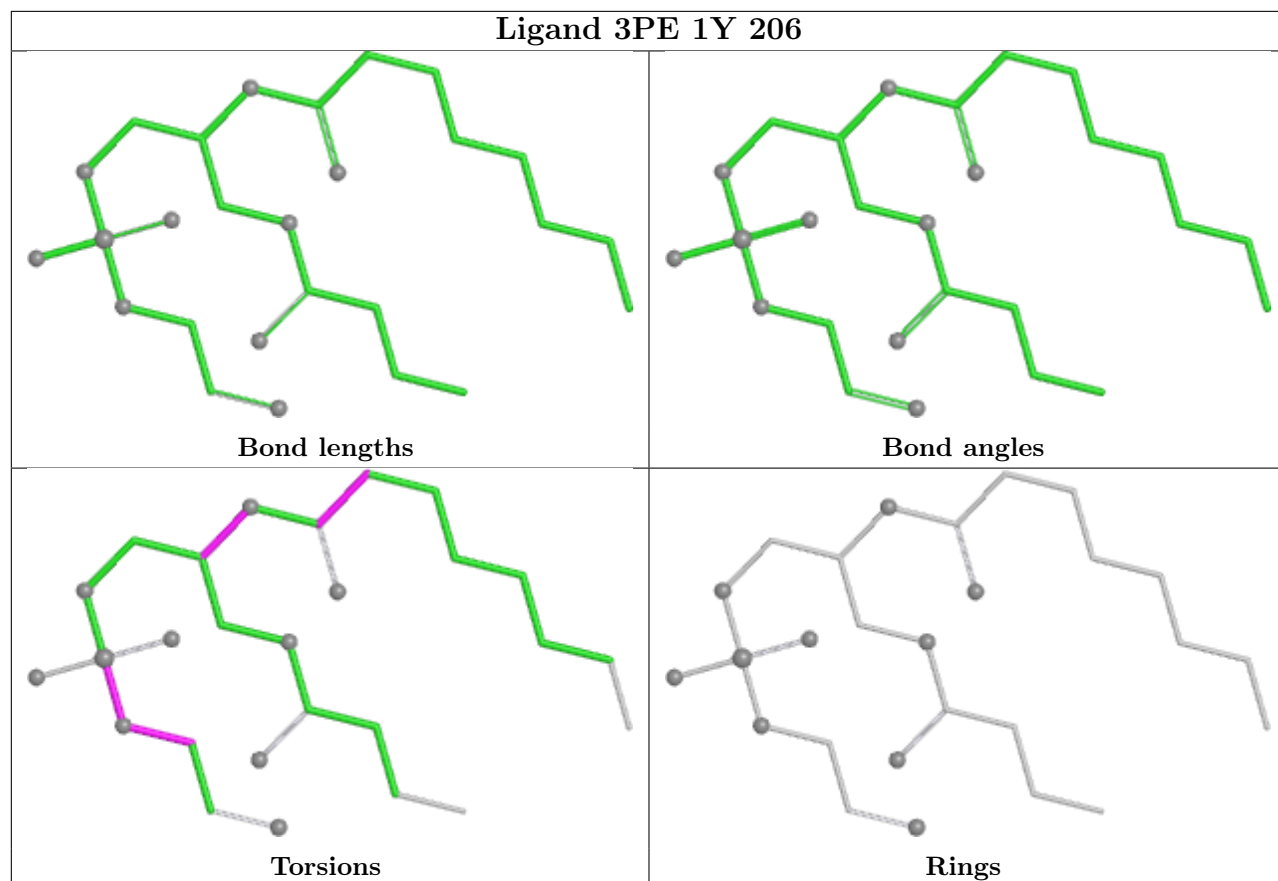


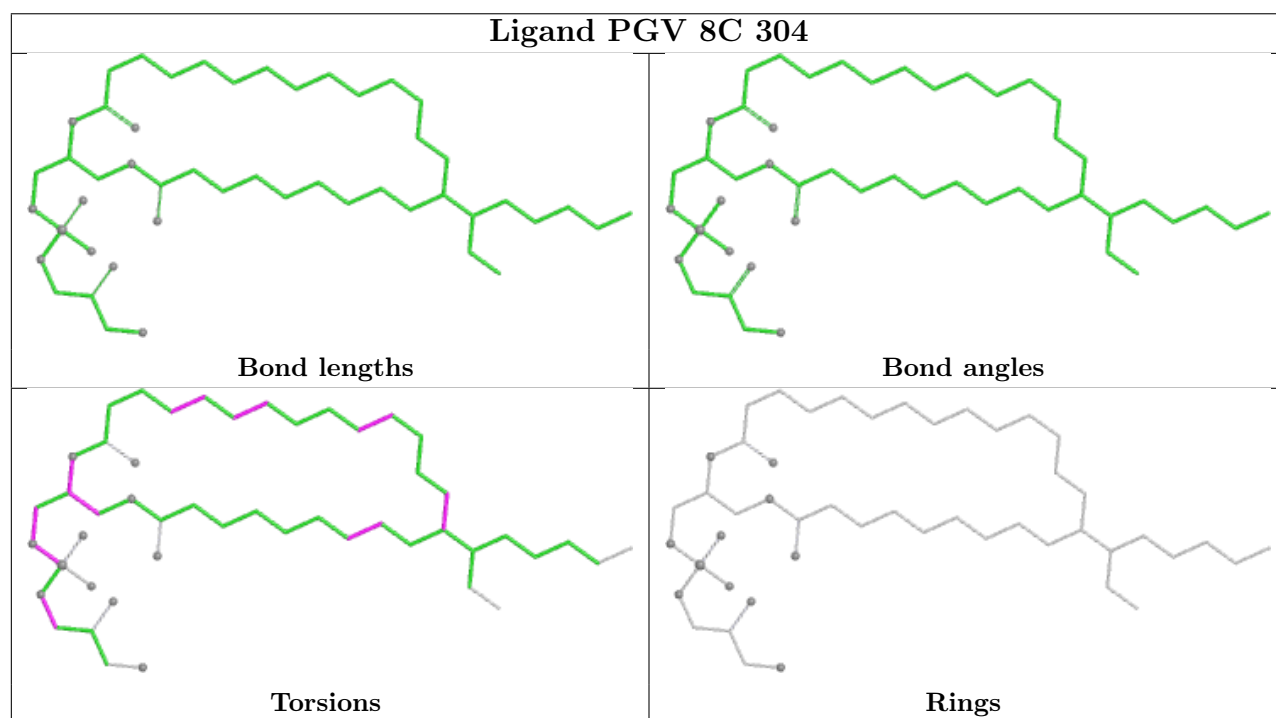
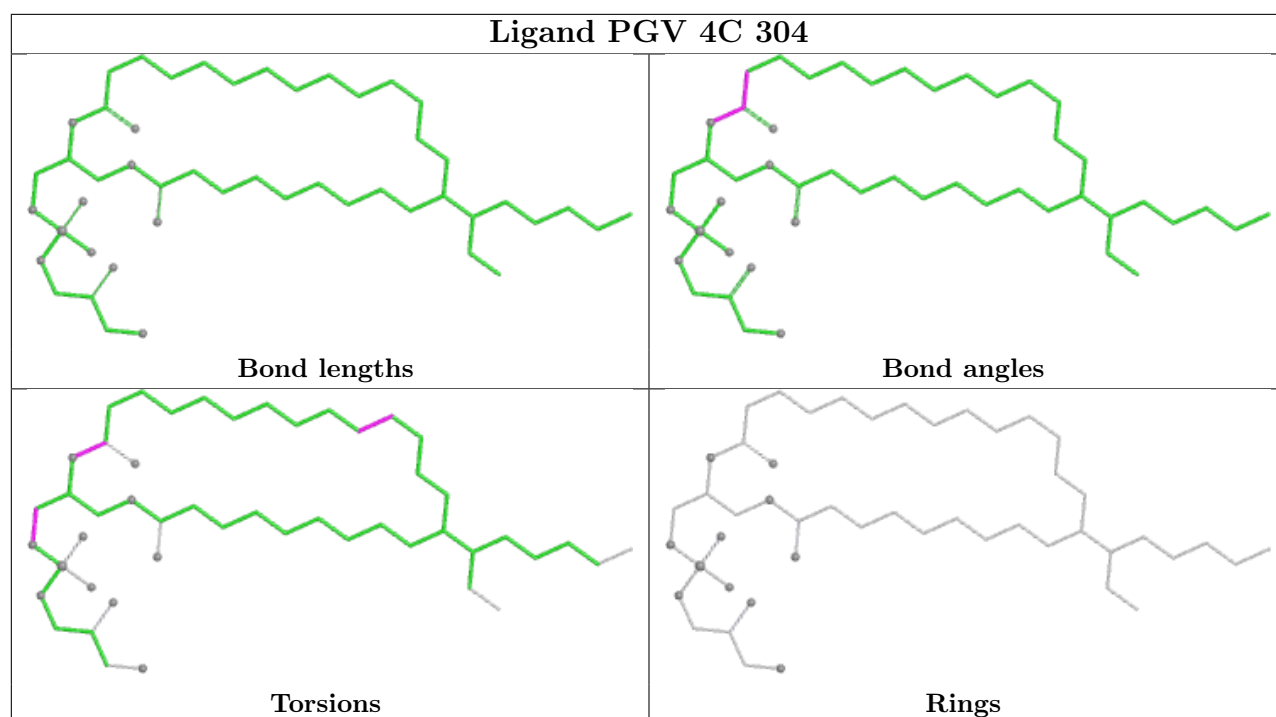


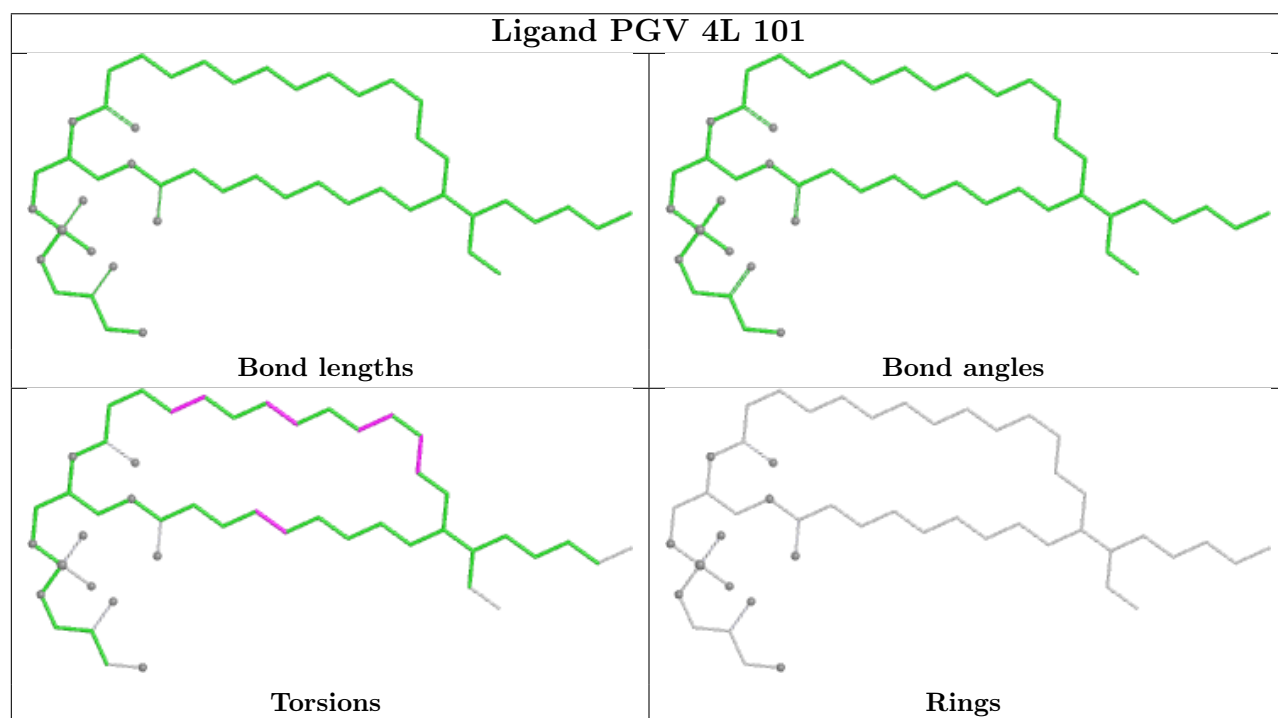
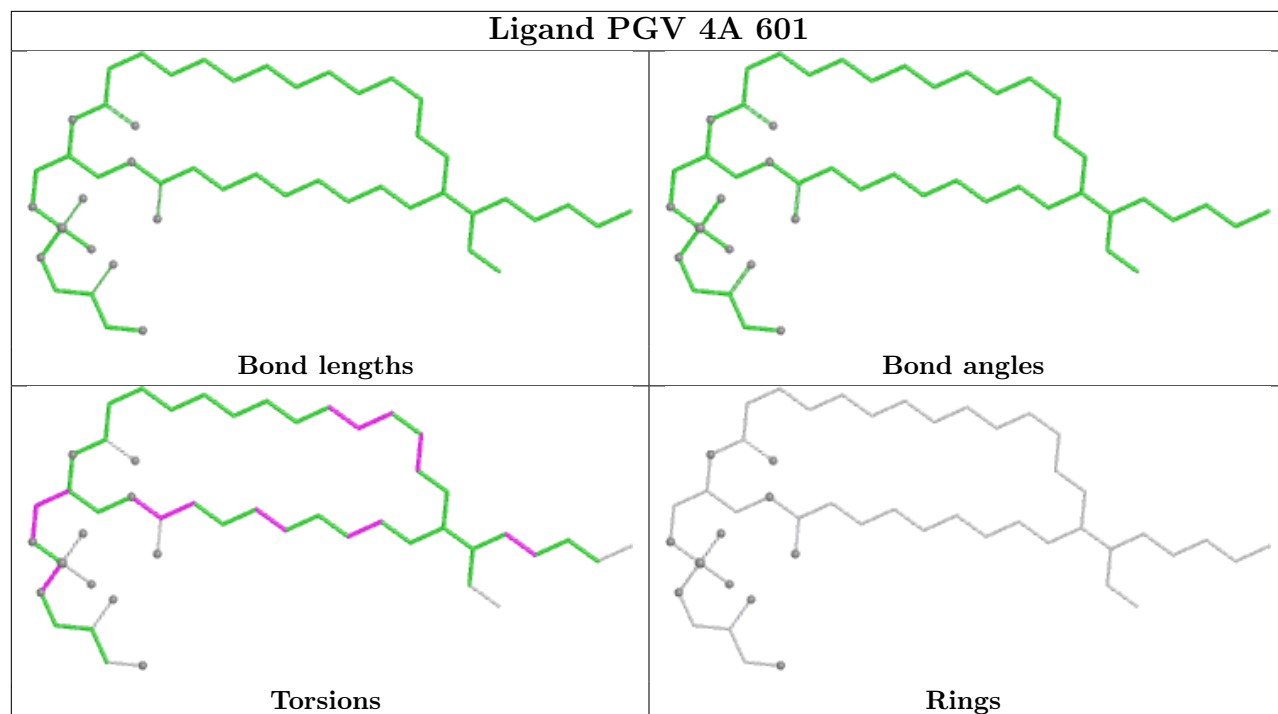


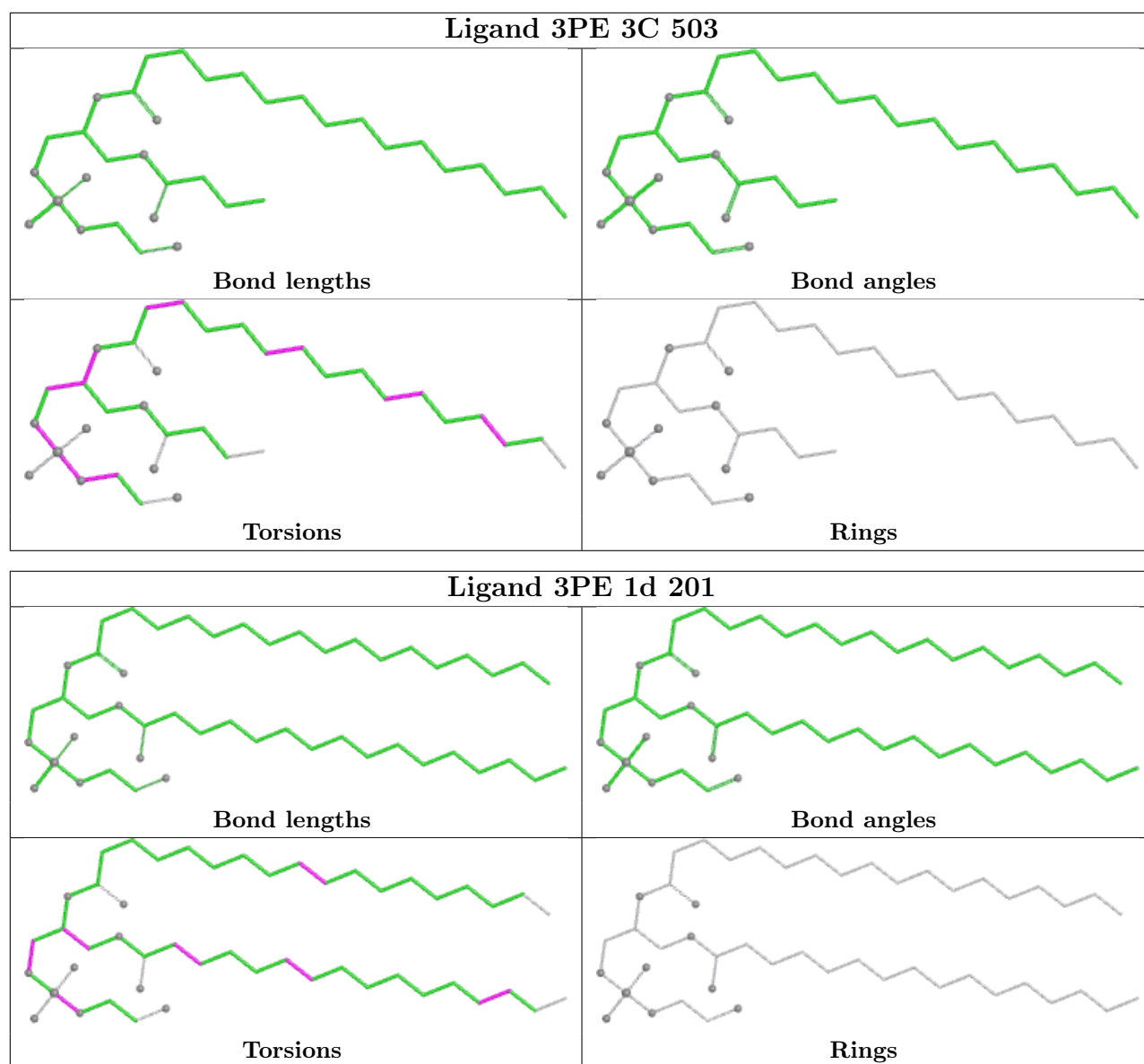


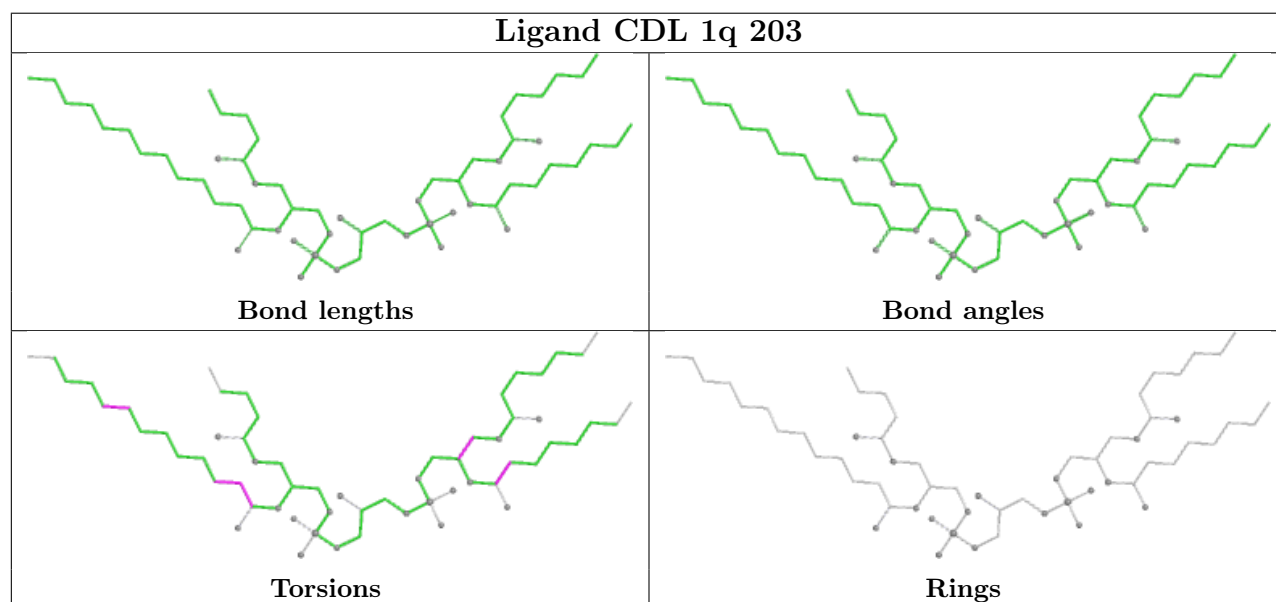
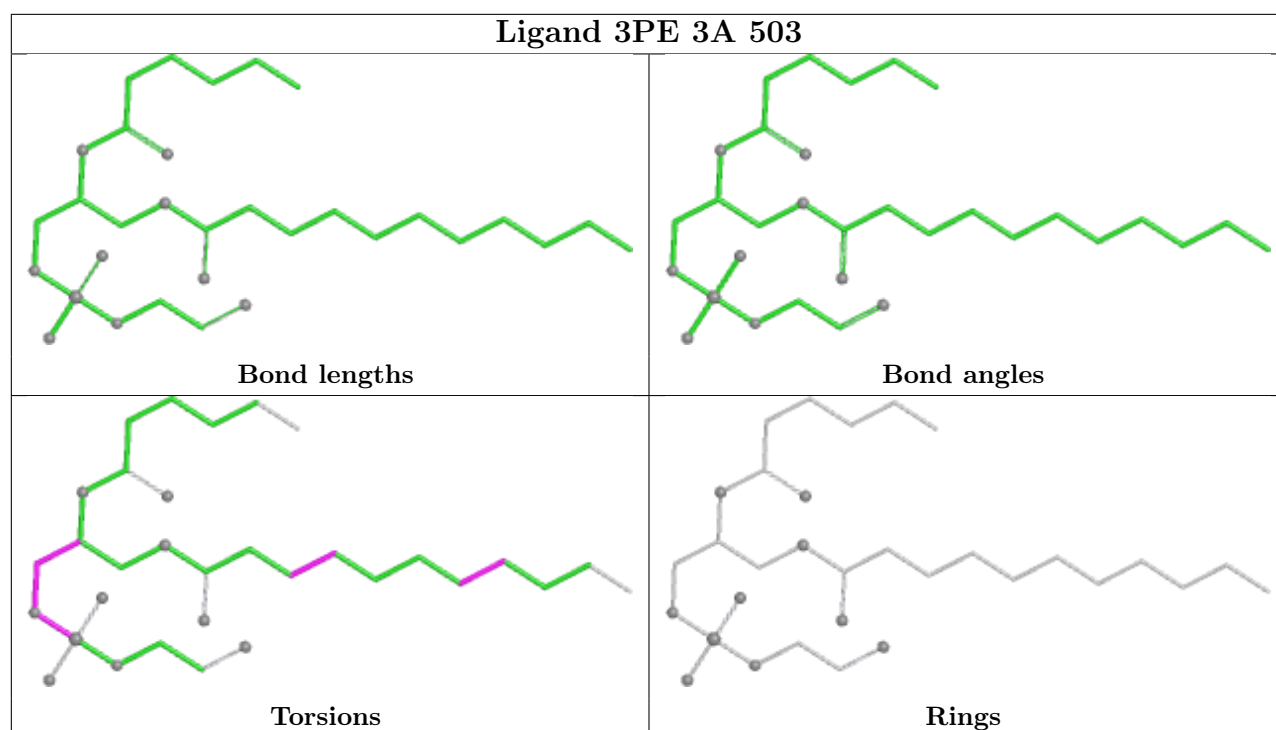


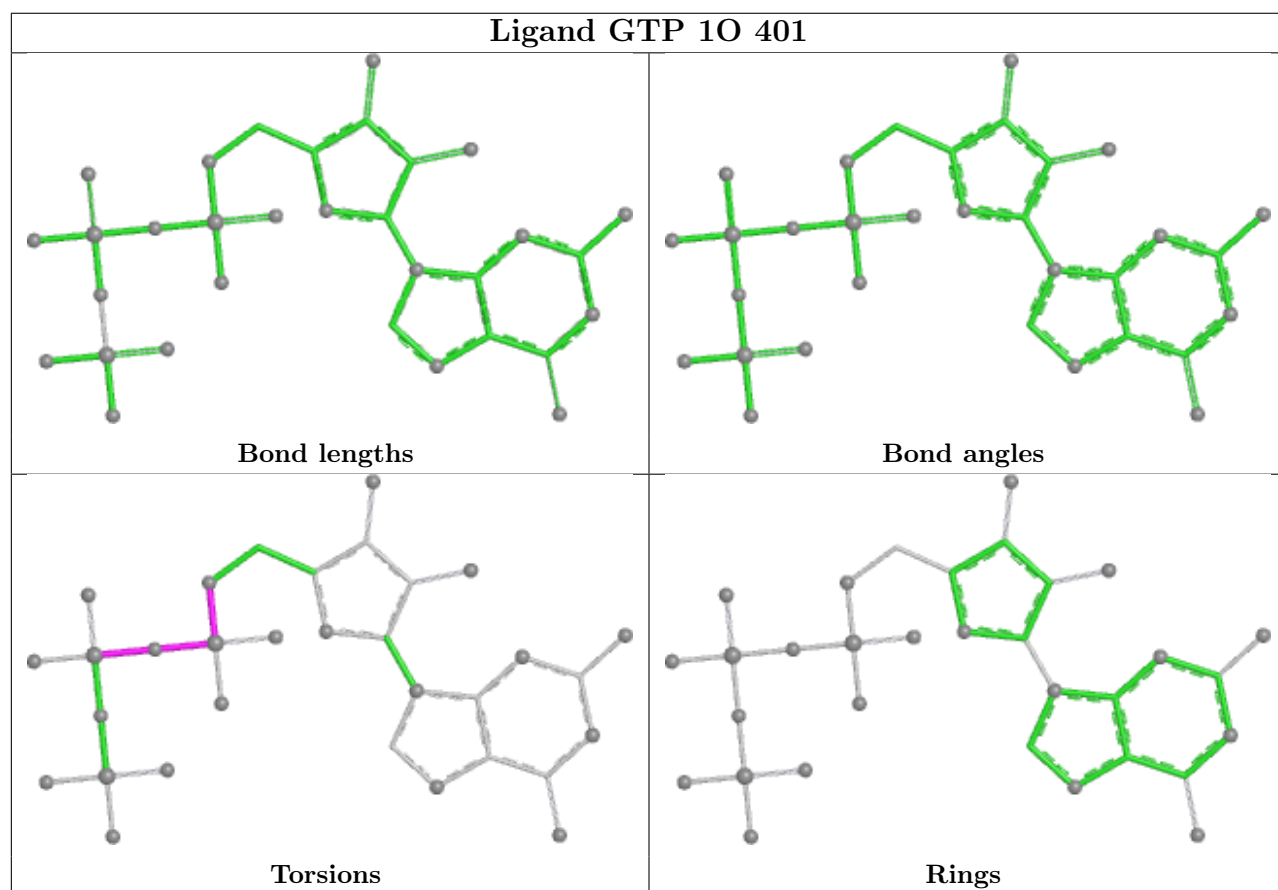
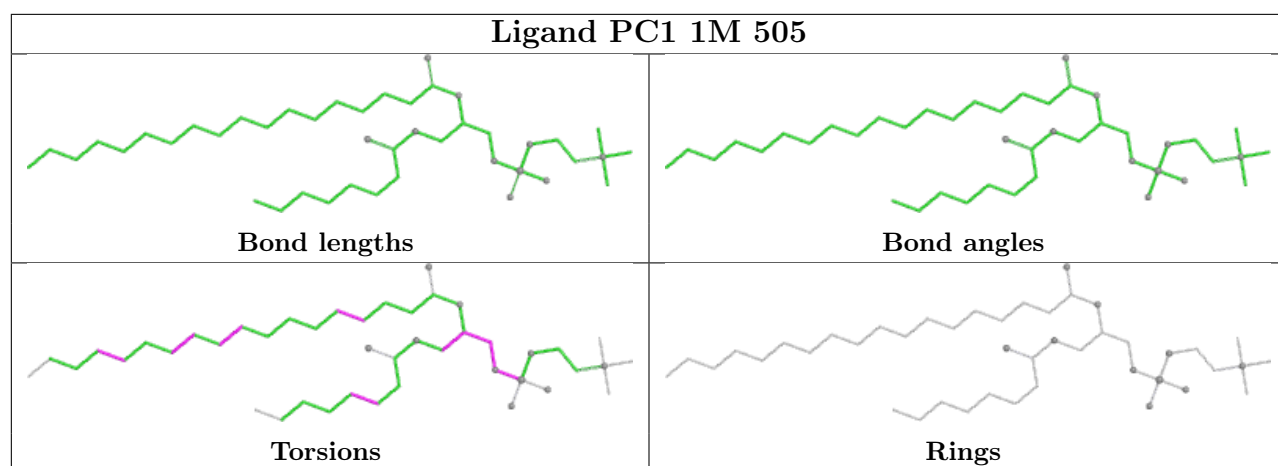


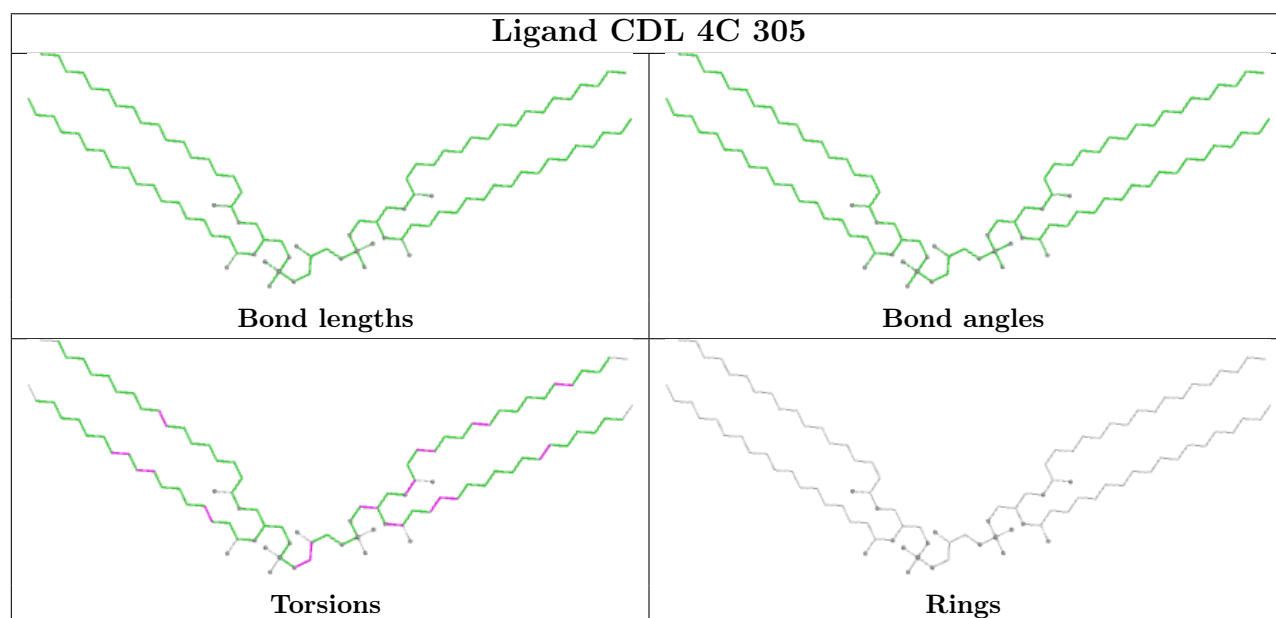
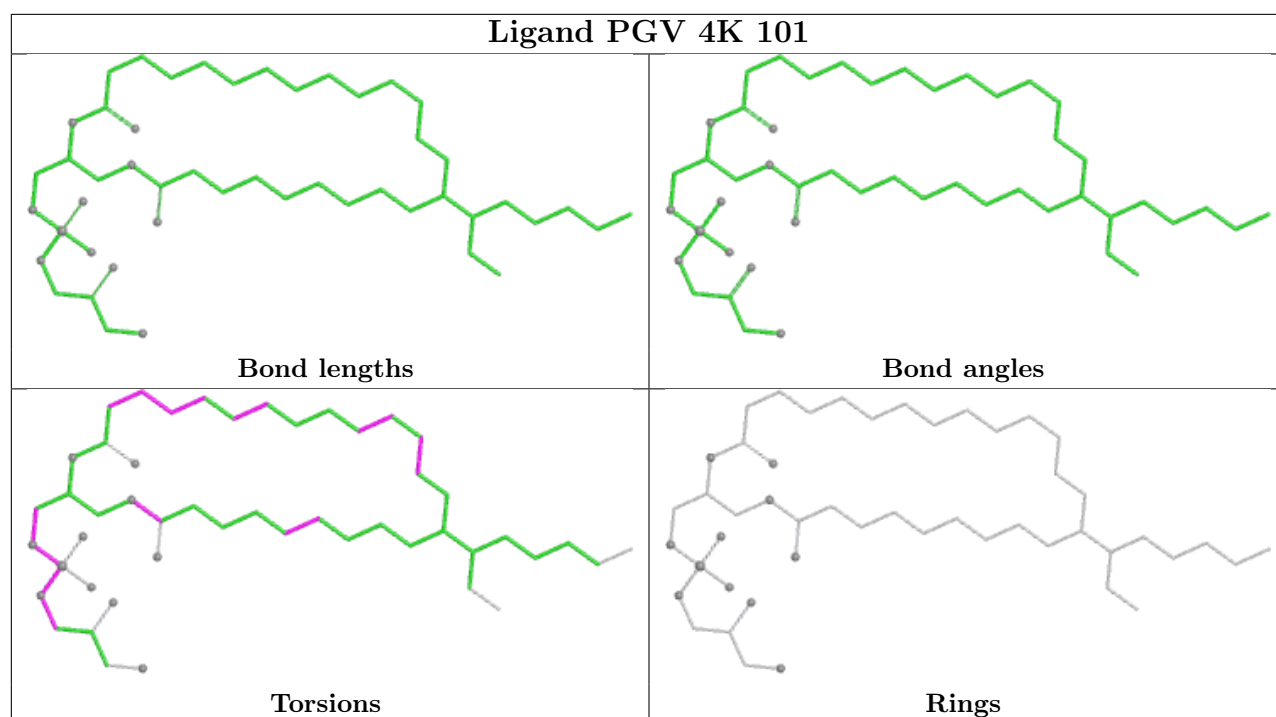


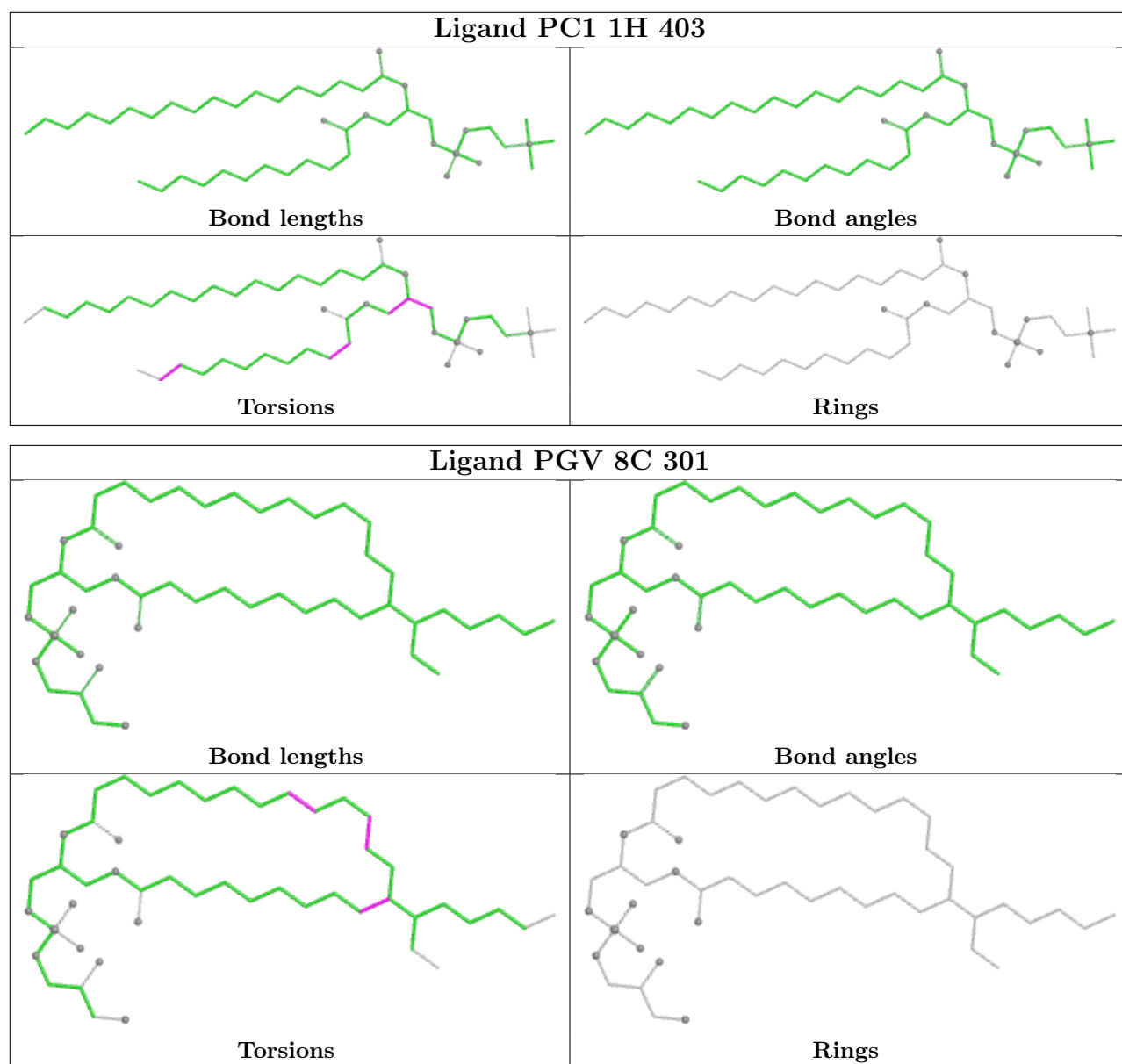




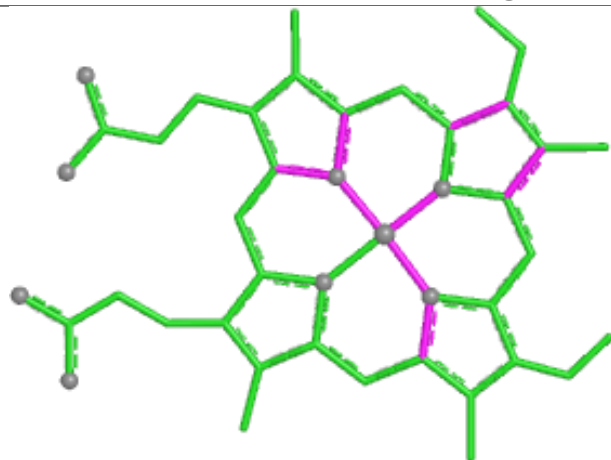




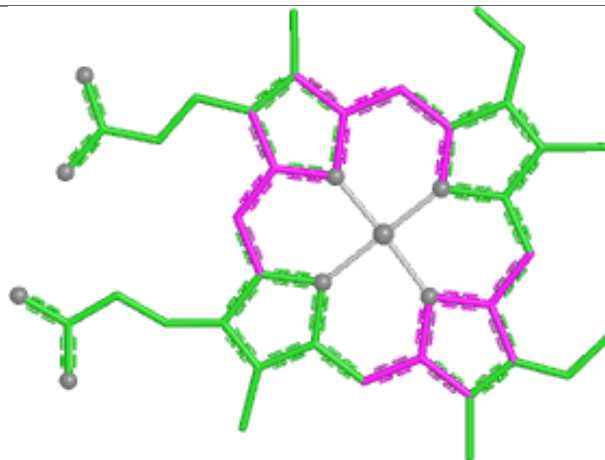




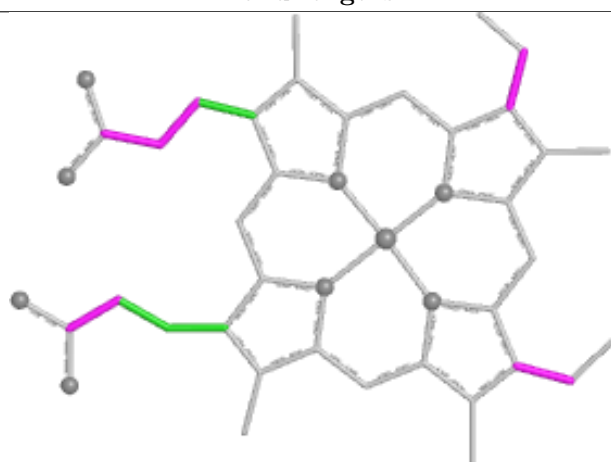
Ligand HEM 3P 501



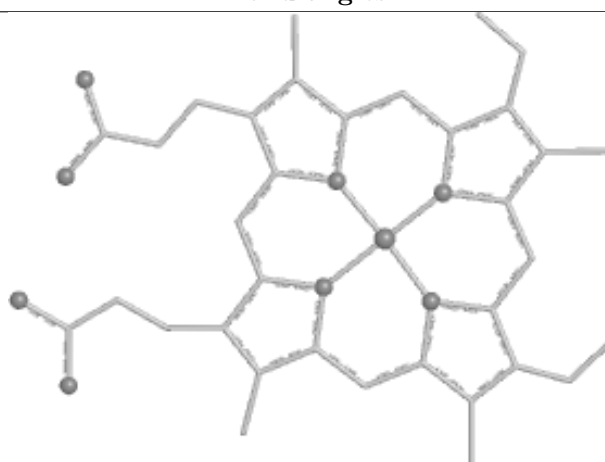
Bond lengths



Bond angles

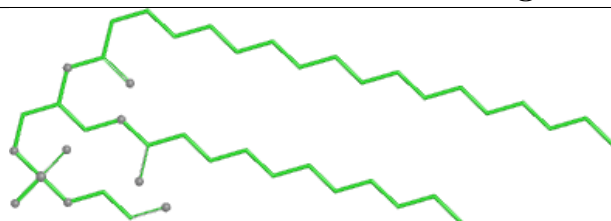


Torsions

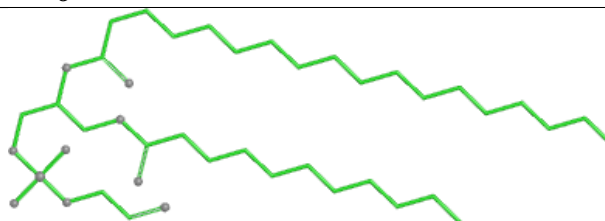


Rings

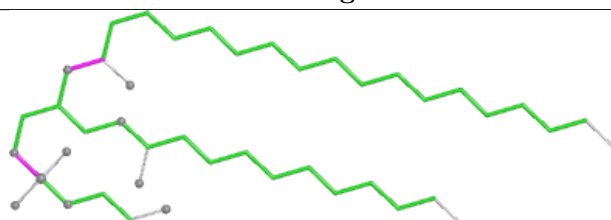
Ligand 3PE 1j 101



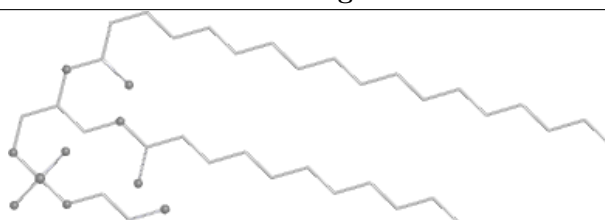
Bond lengths



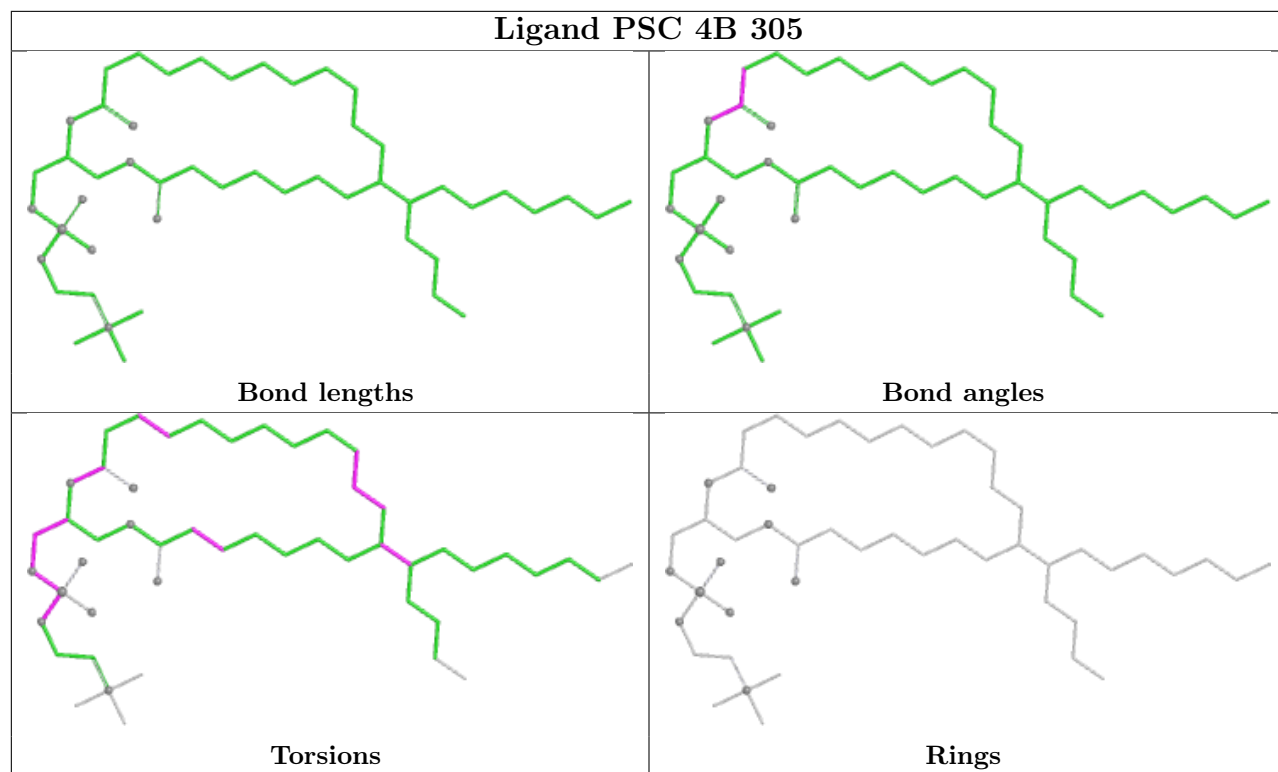
Bond angles



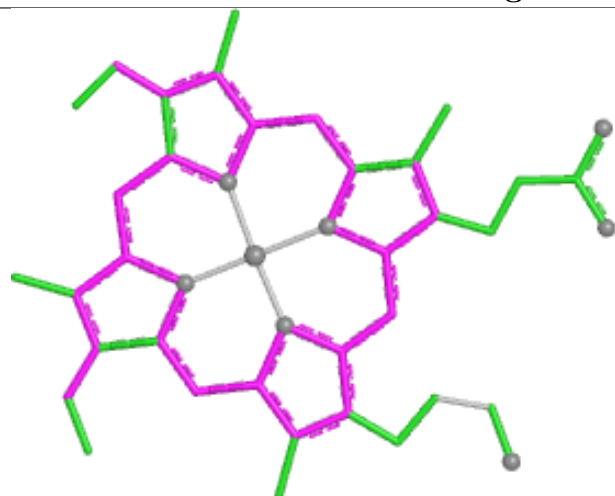
Torsions



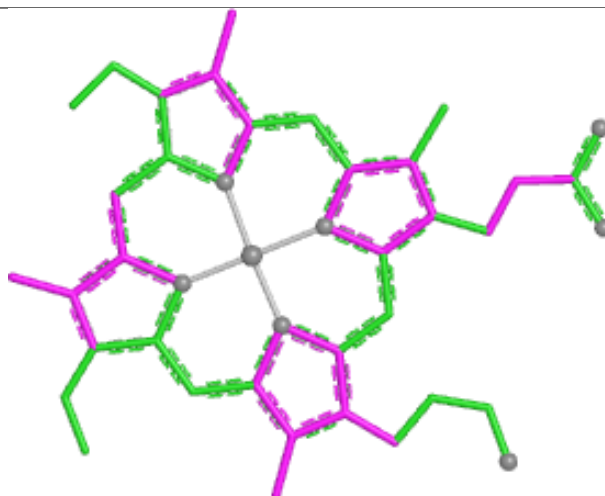
Rings



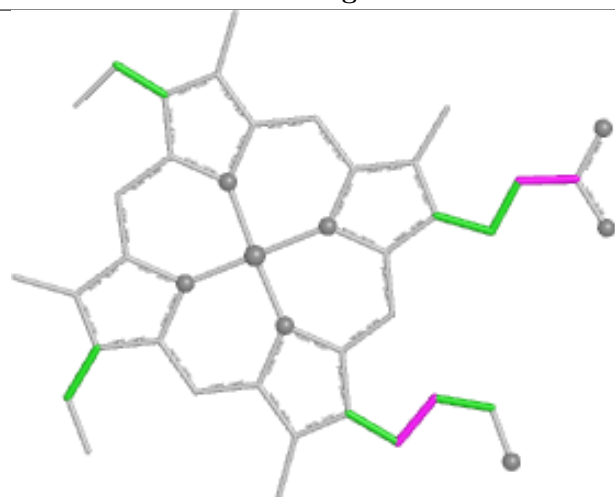
Ligand HEC 3D 501



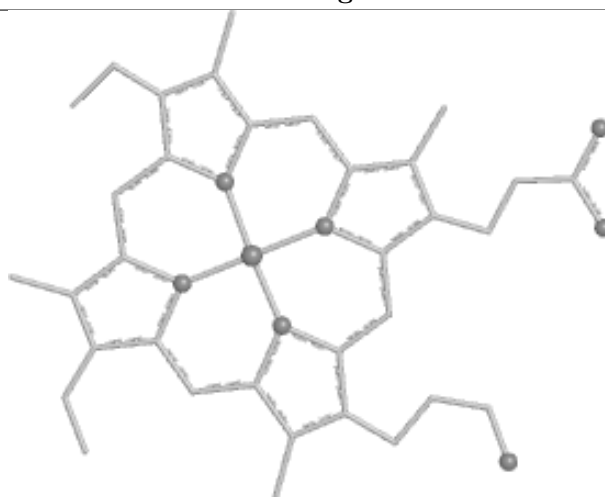
Bond lengths



Bond angles

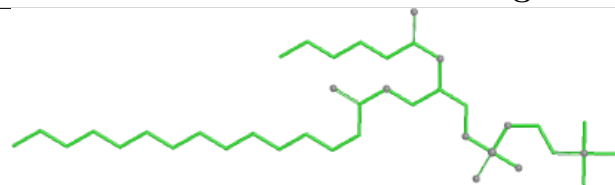


Torsions

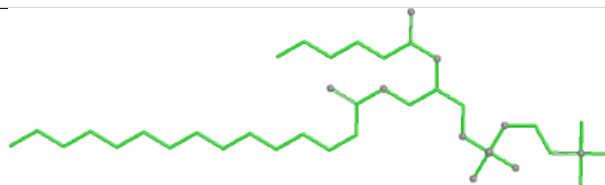


Rings

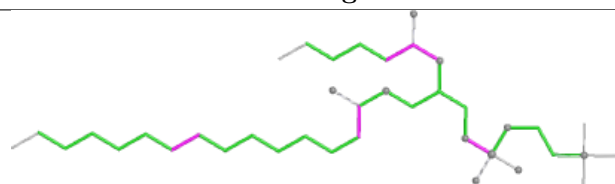
Ligand PC1 1d 202



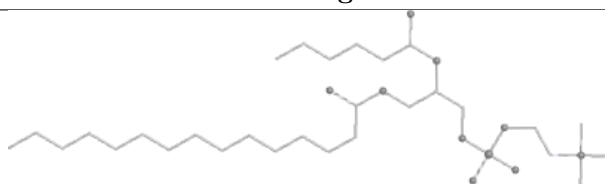
Bond lengths



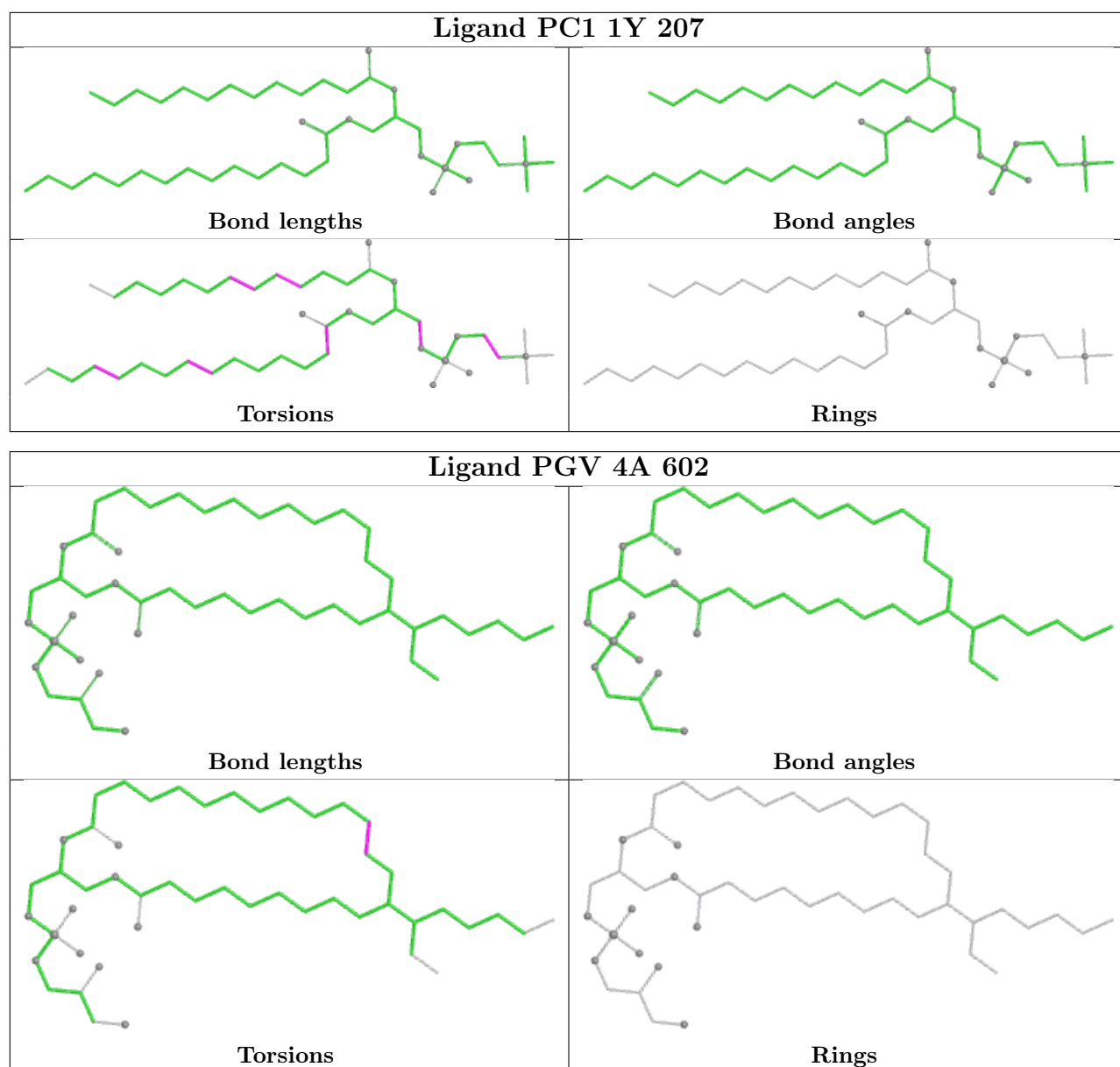
Bond angles

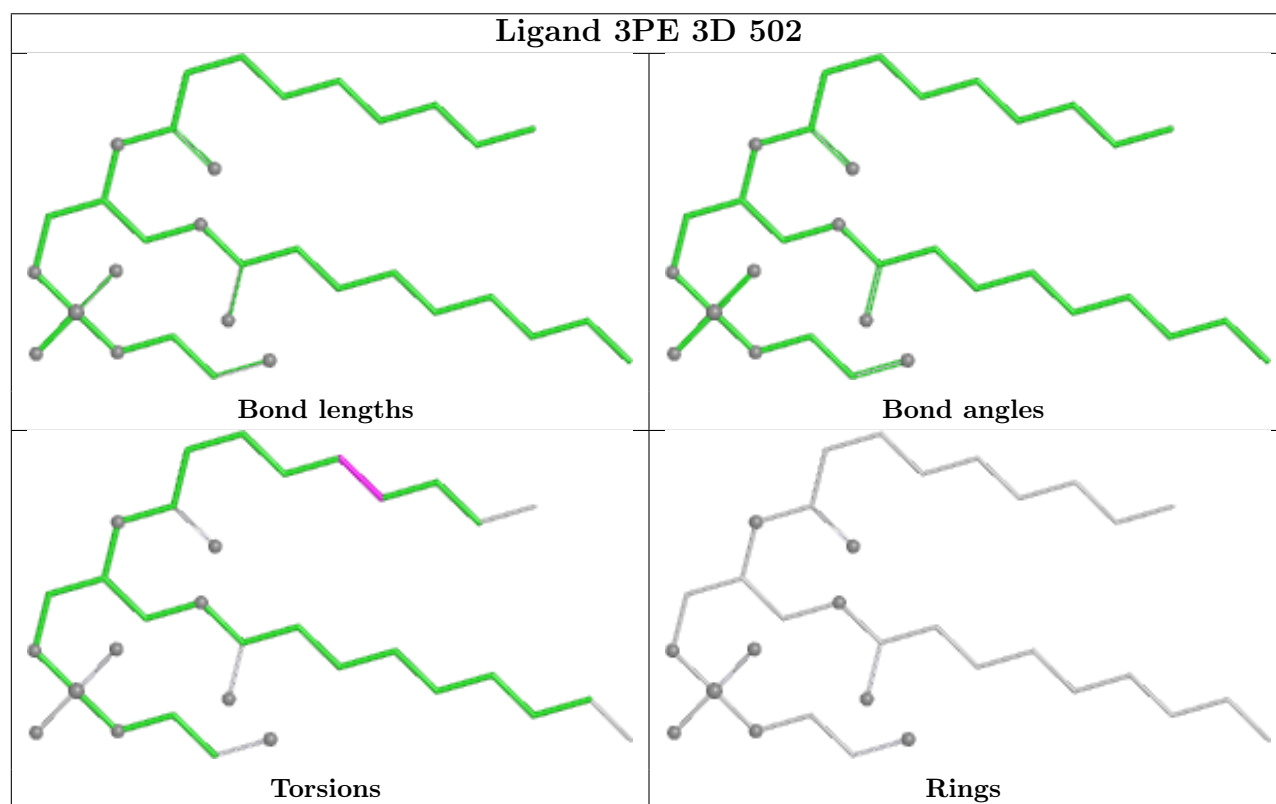
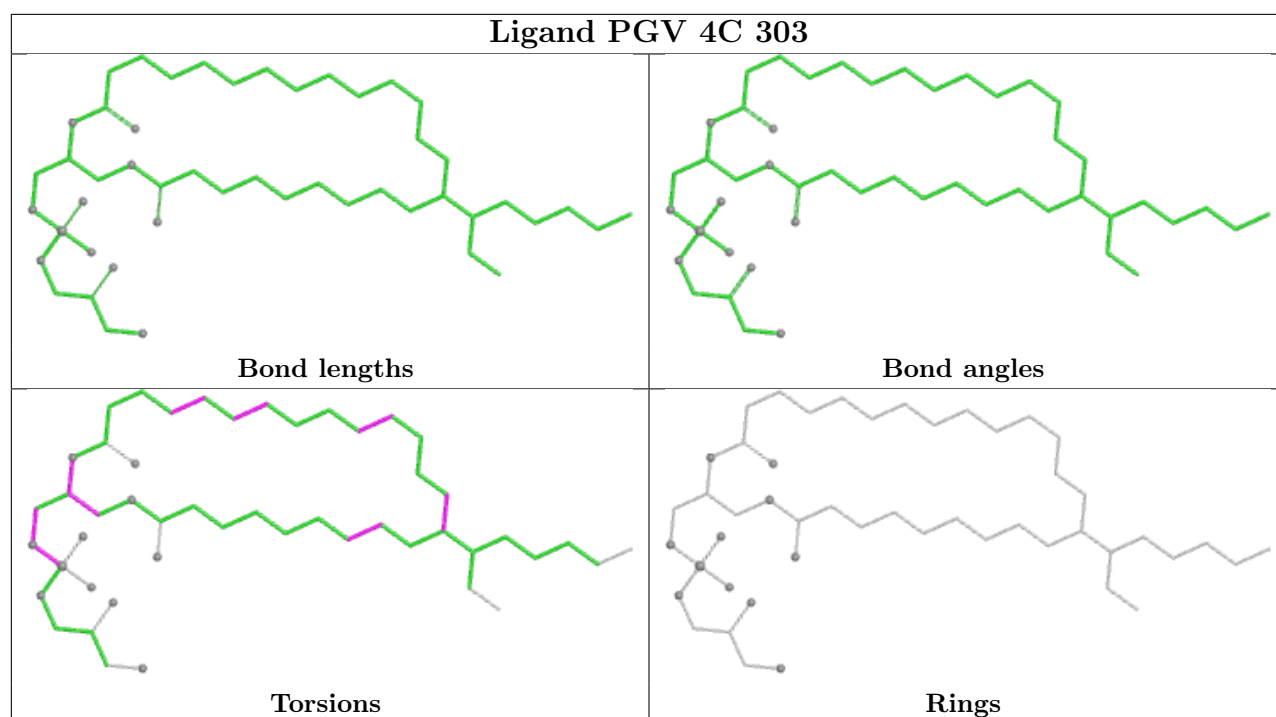


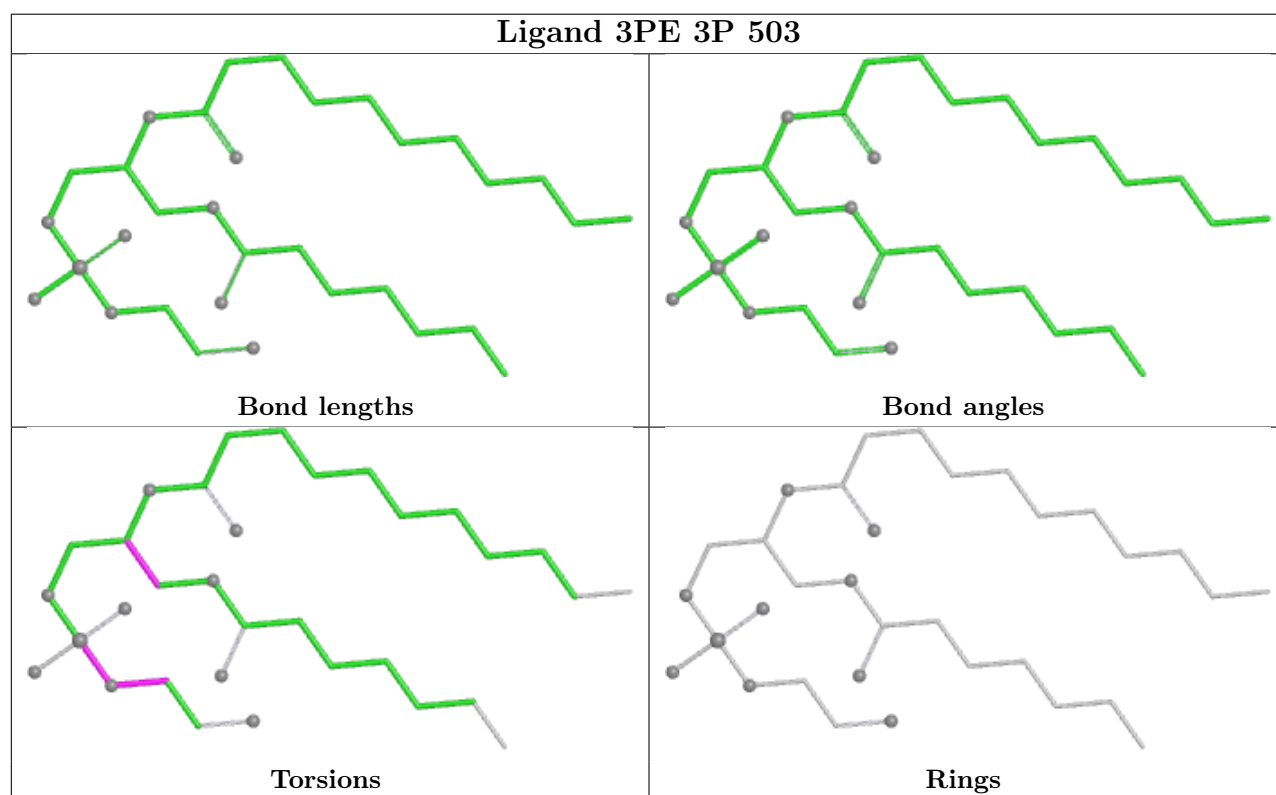
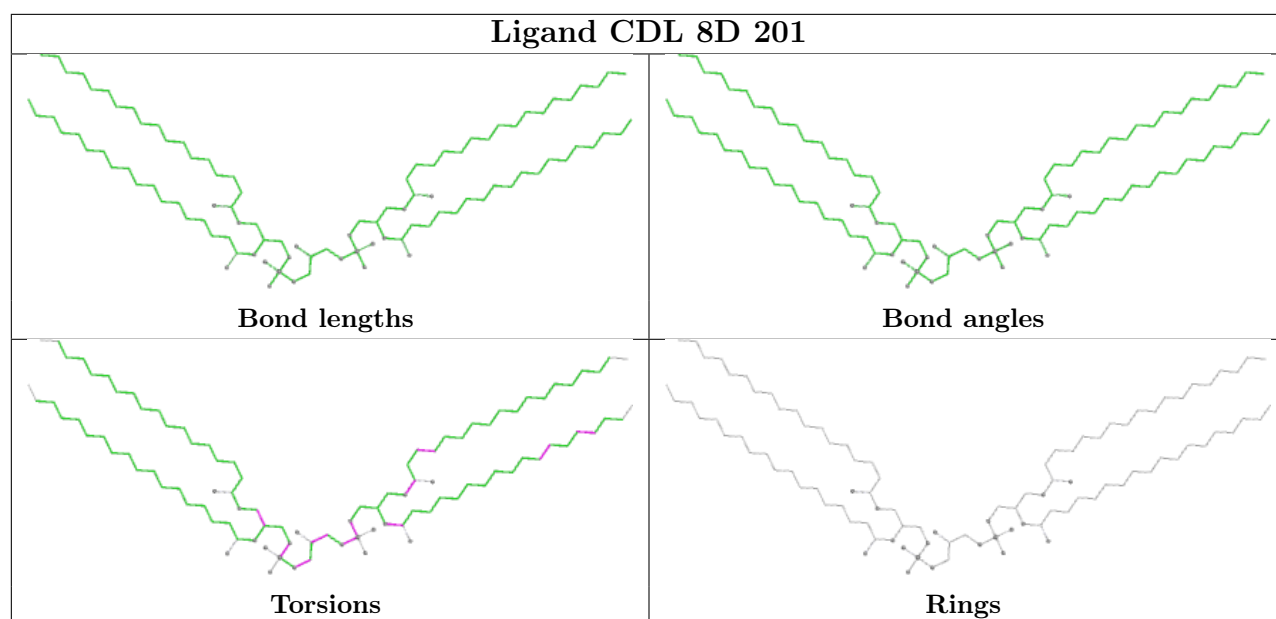
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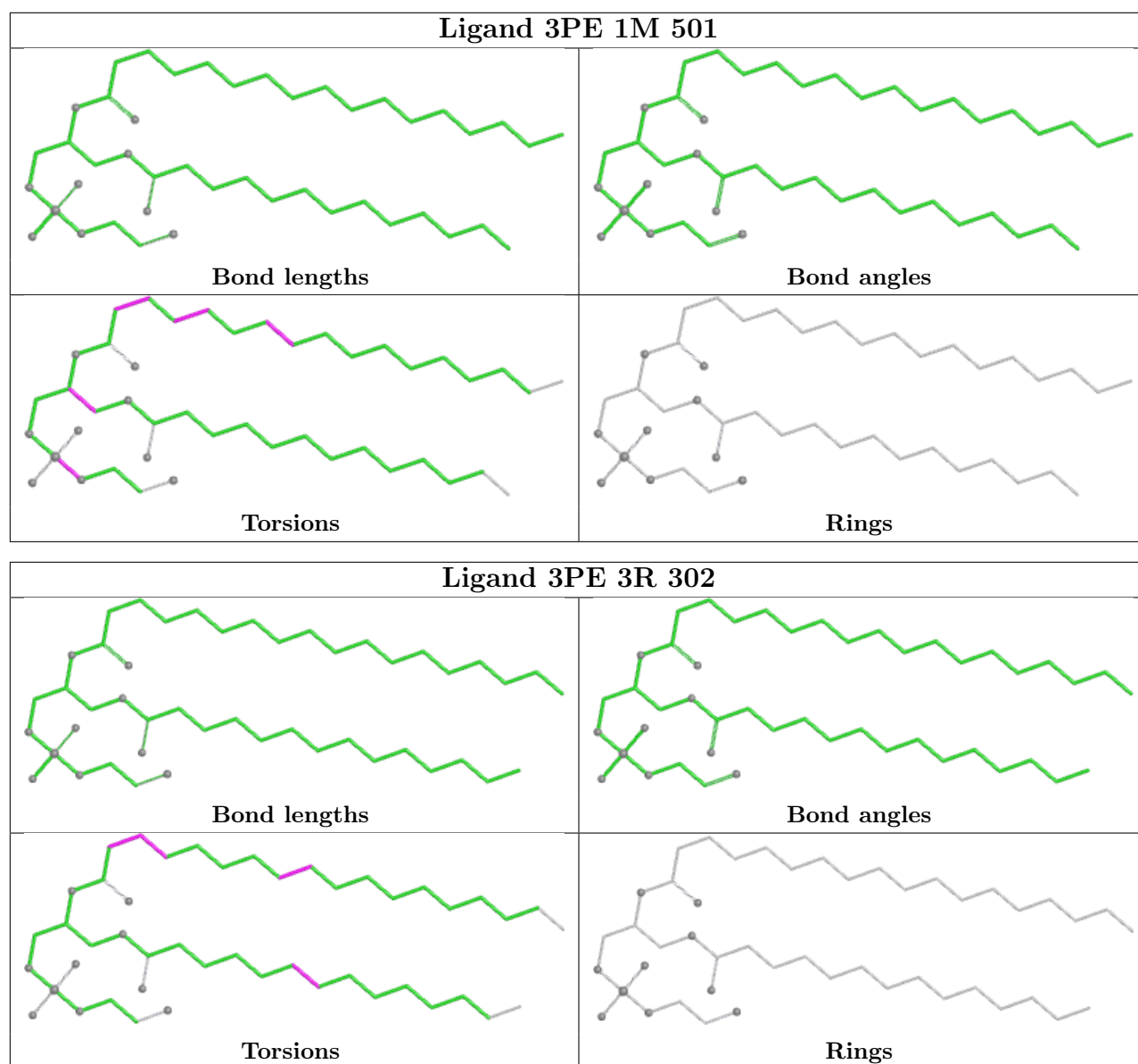


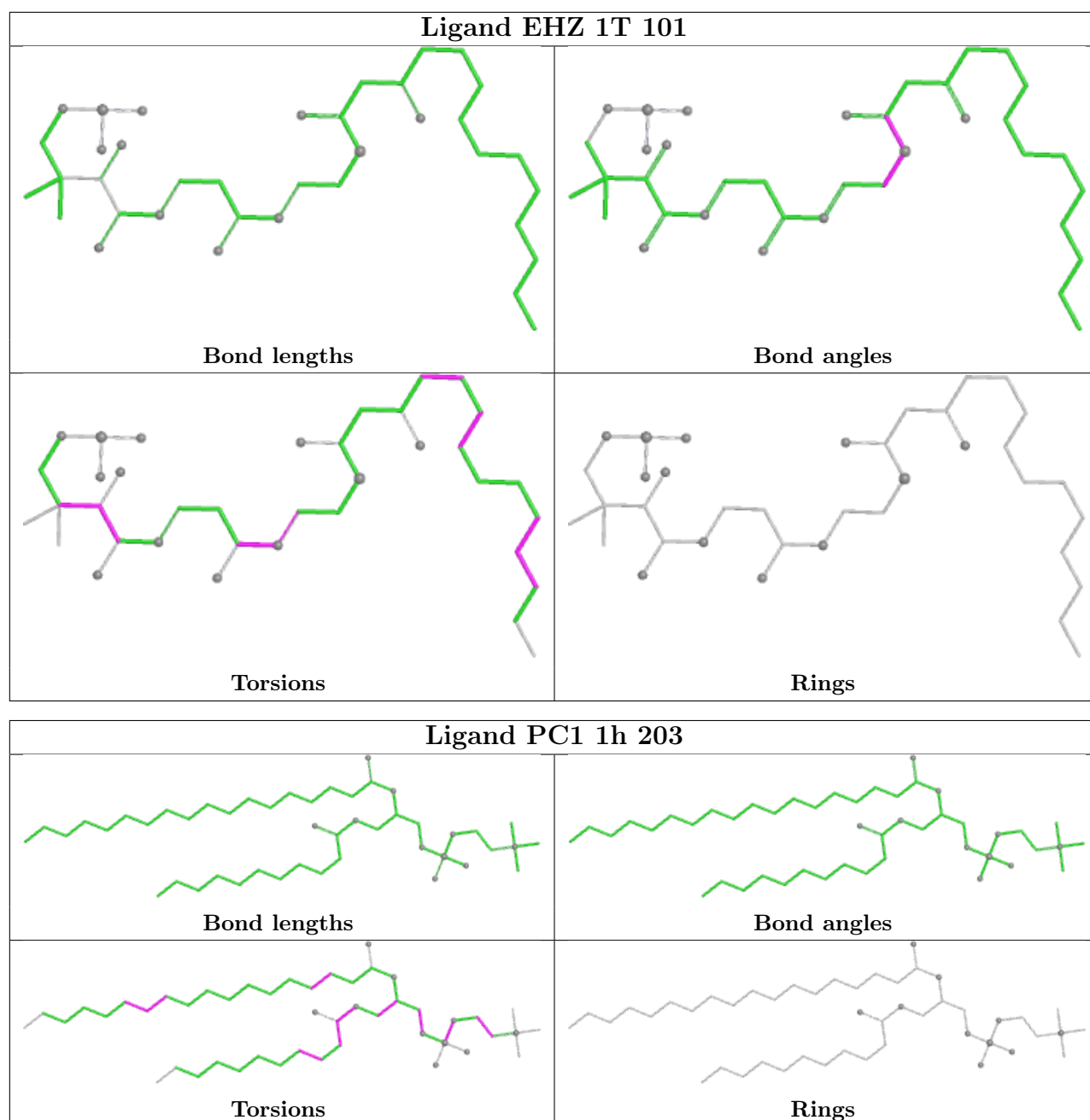
Rings

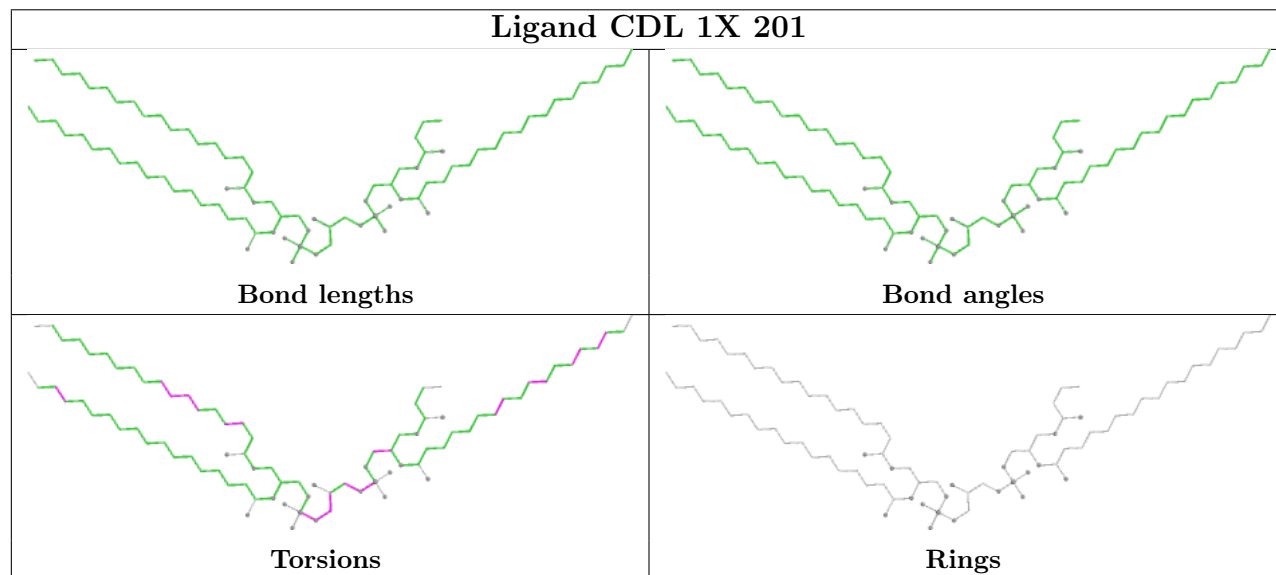
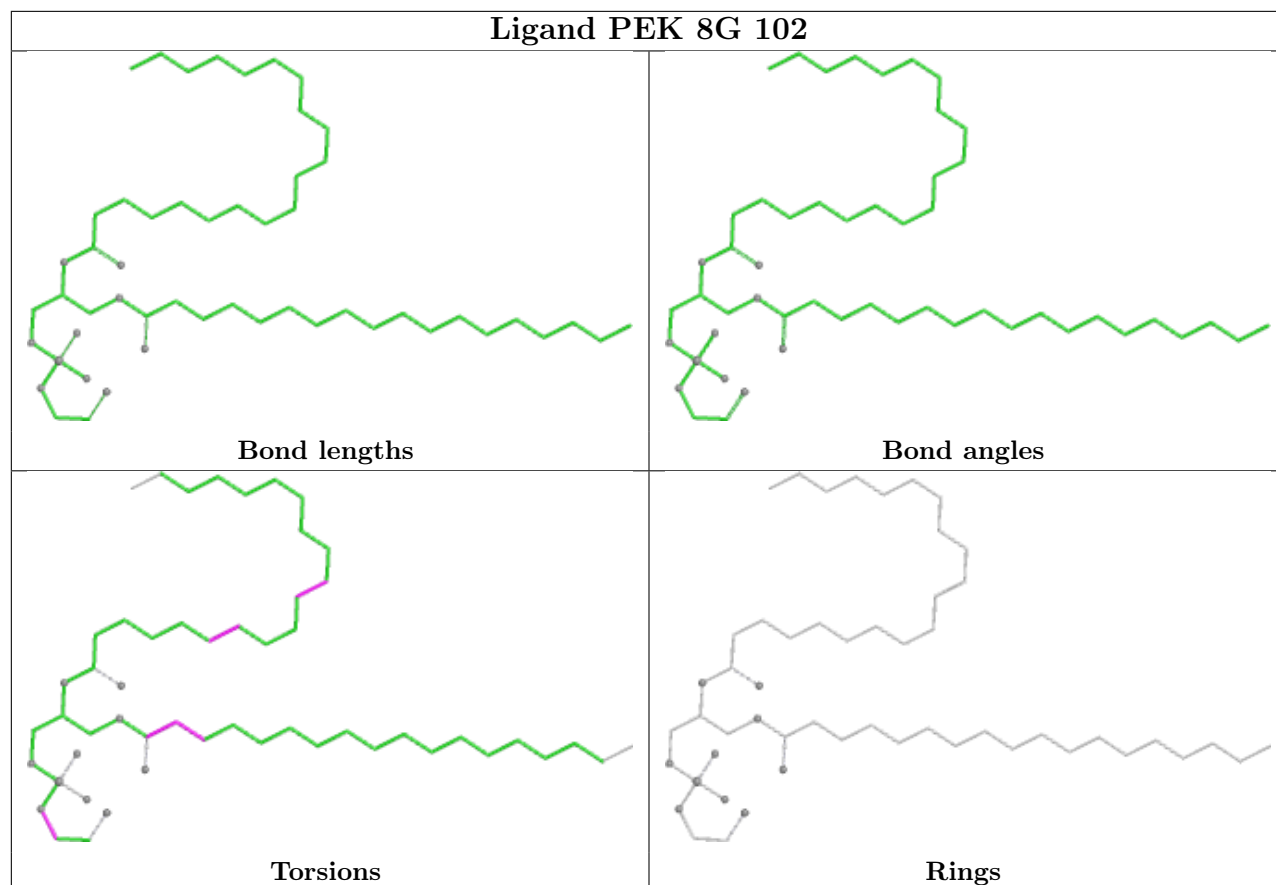




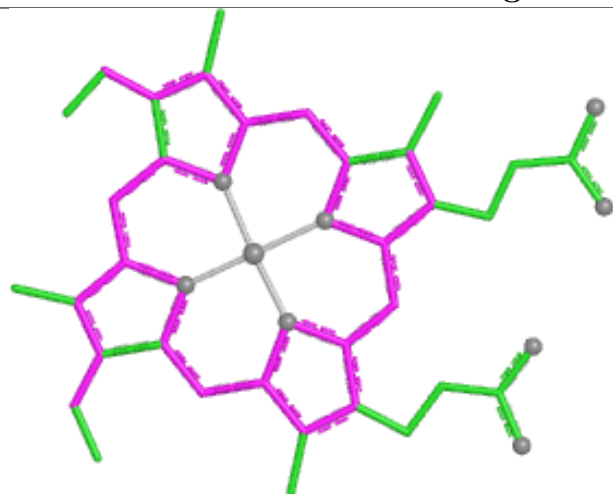




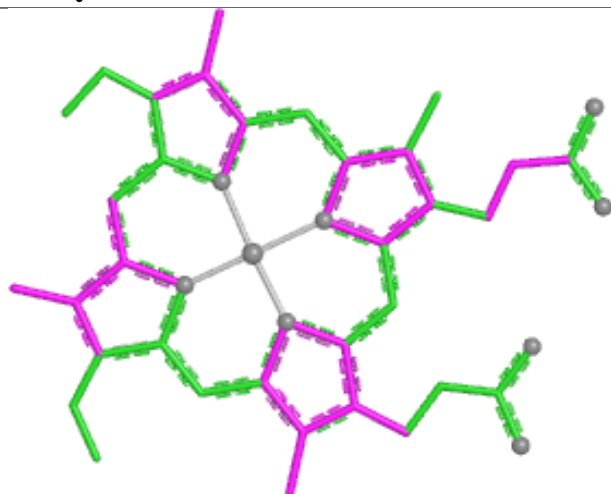




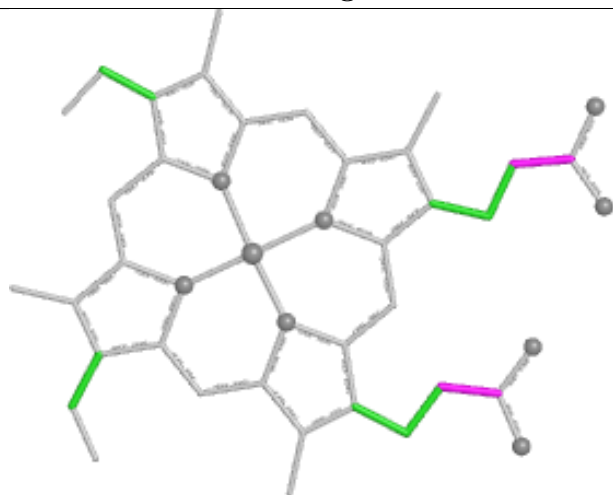
Ligand HEC 3Q 501



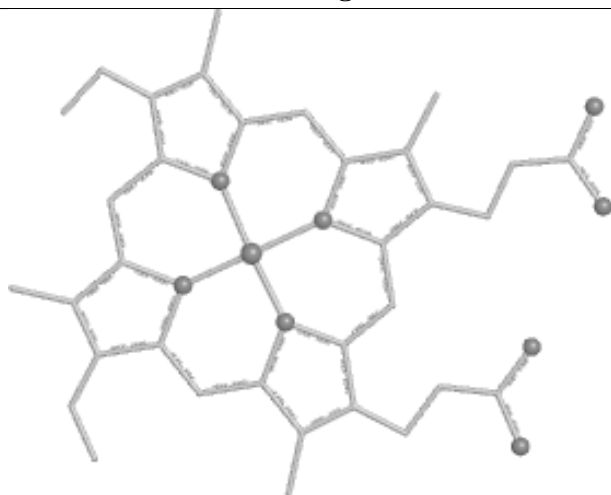
Bond lengths



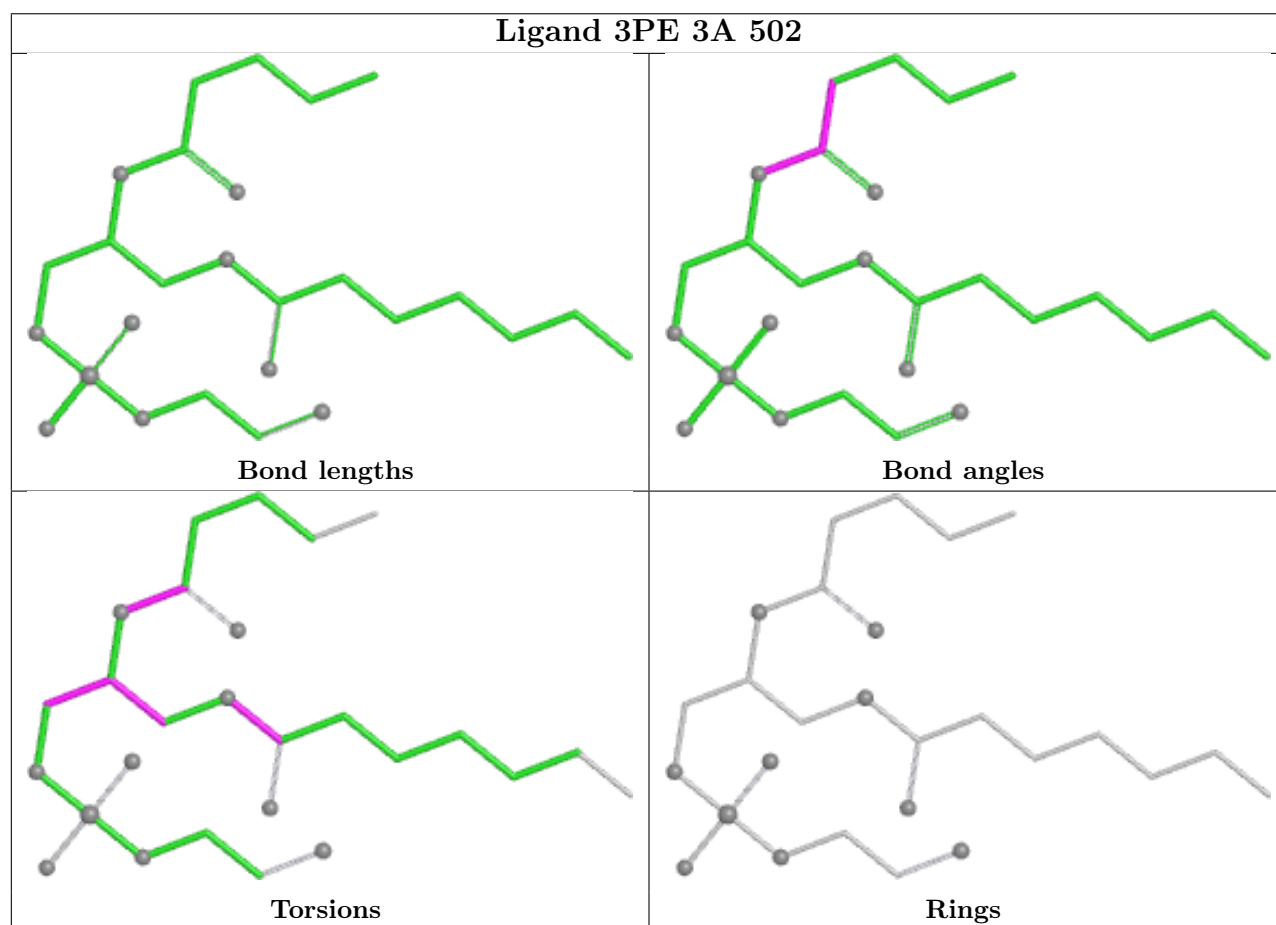
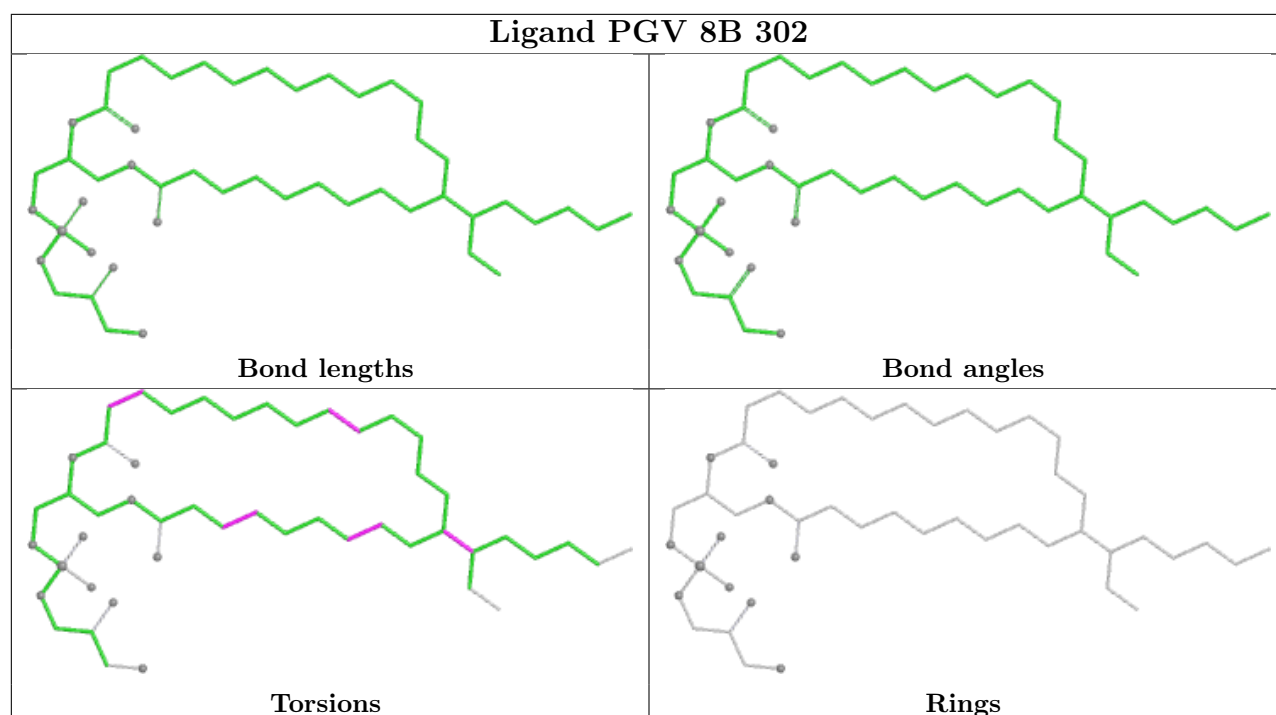
Bond angles

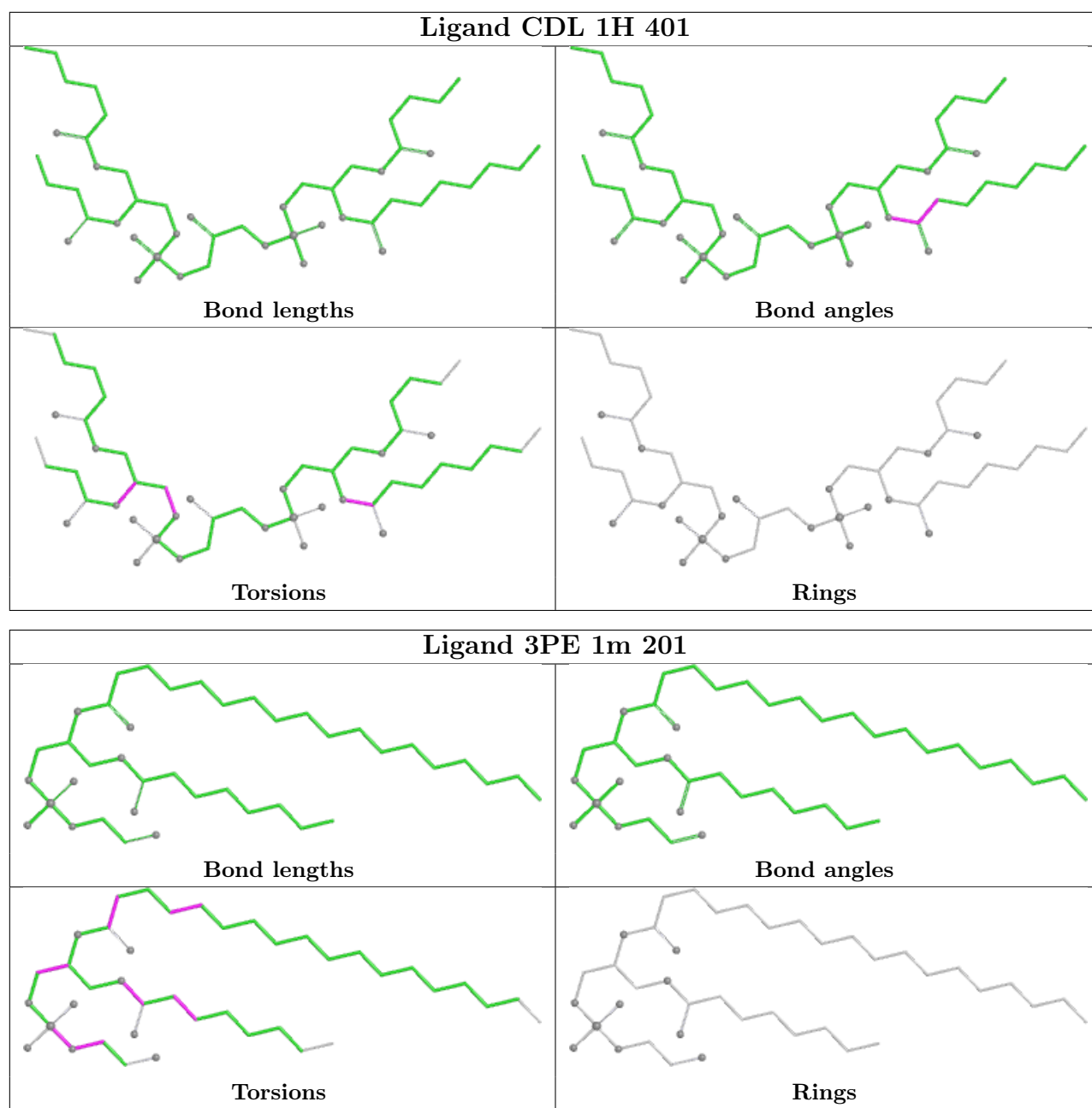


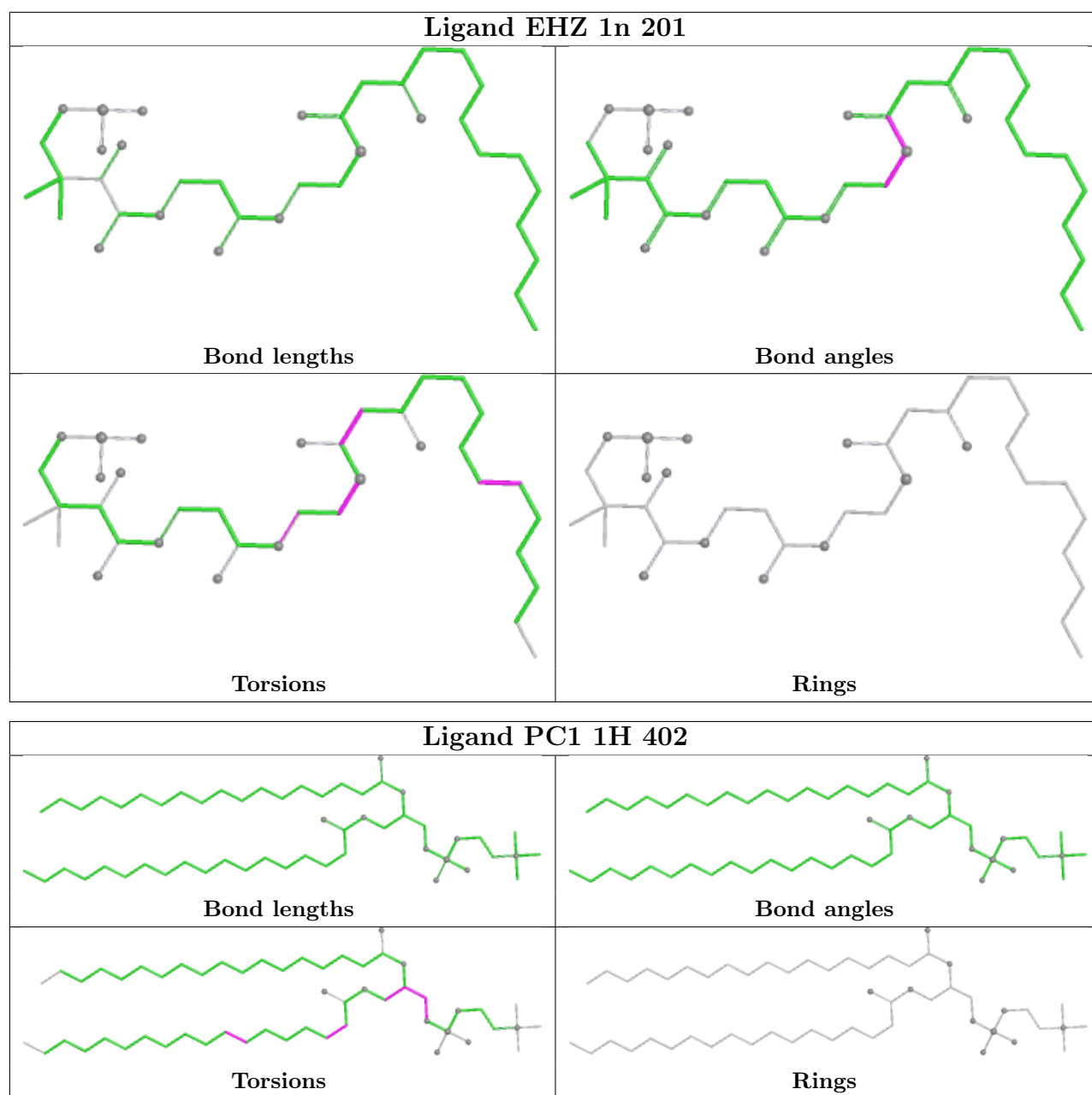
Torsions

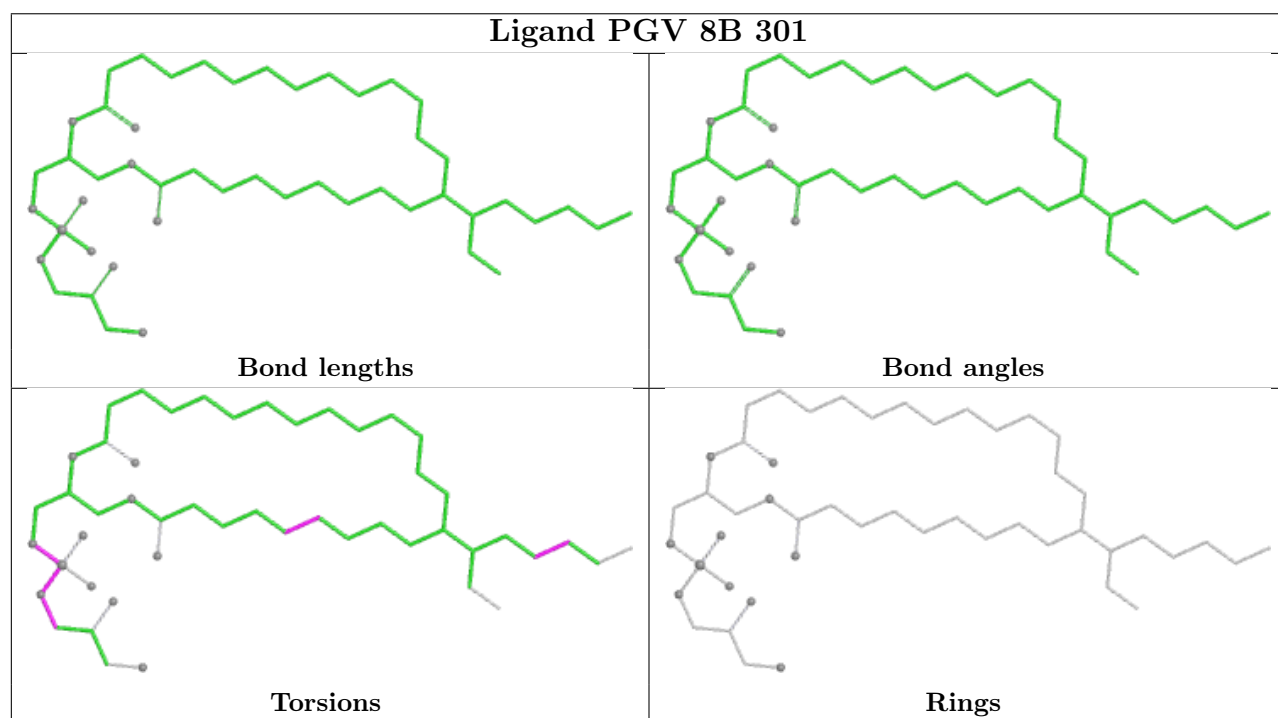
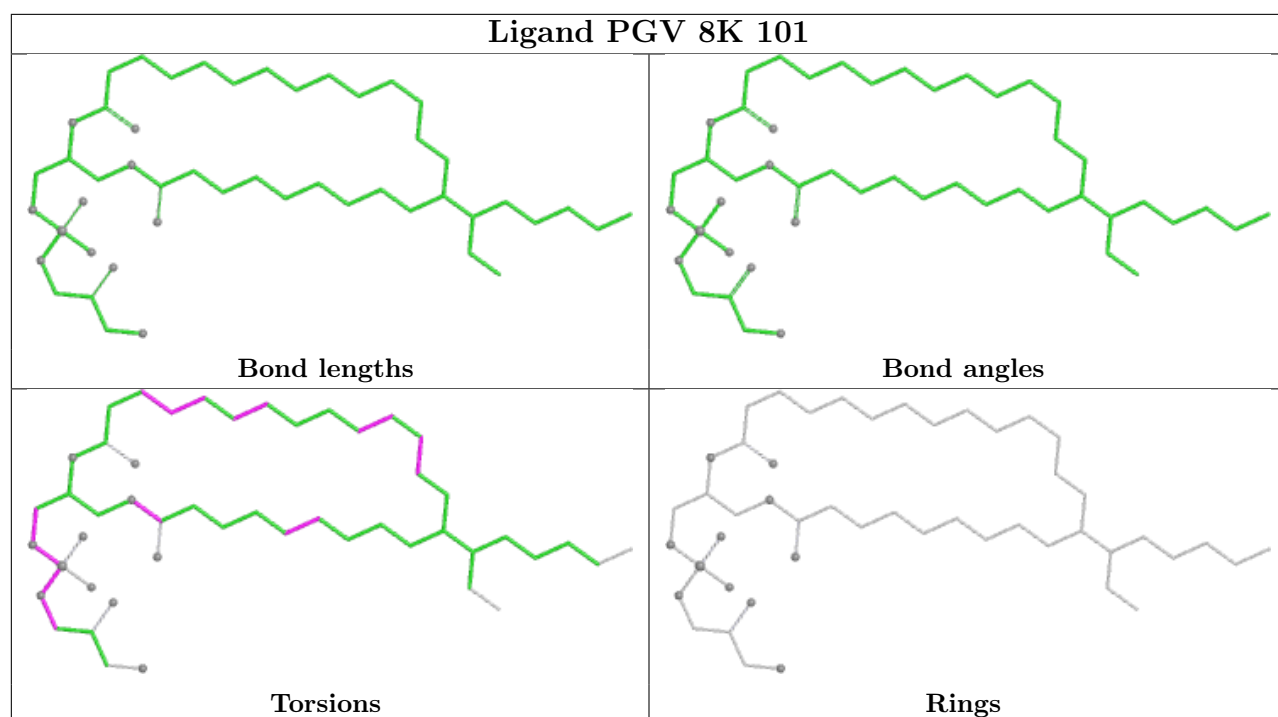


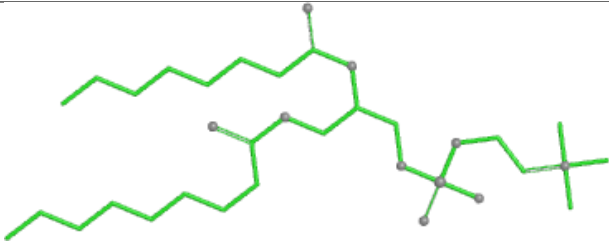
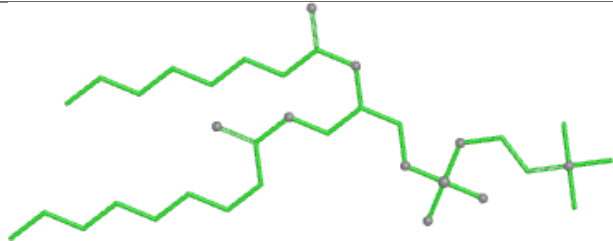
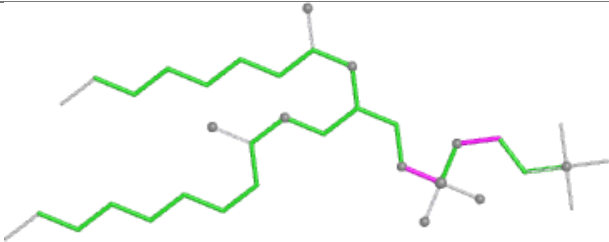
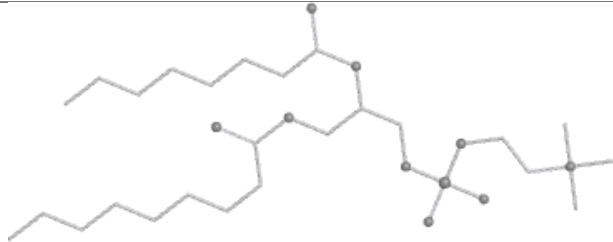
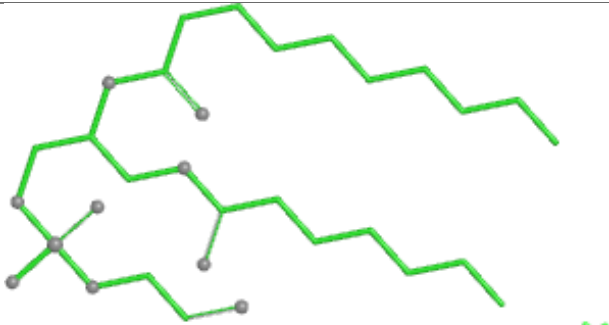
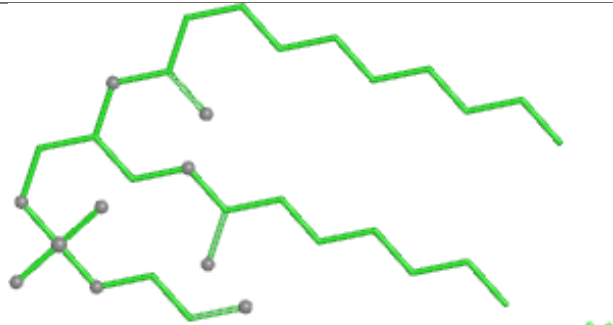
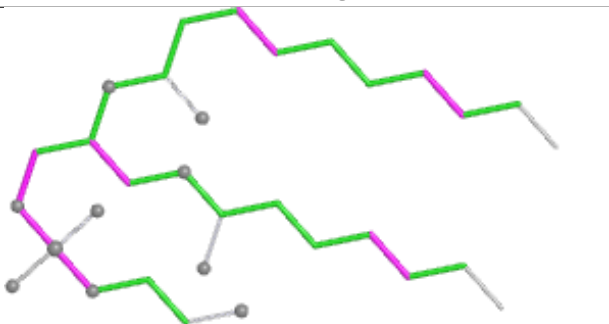
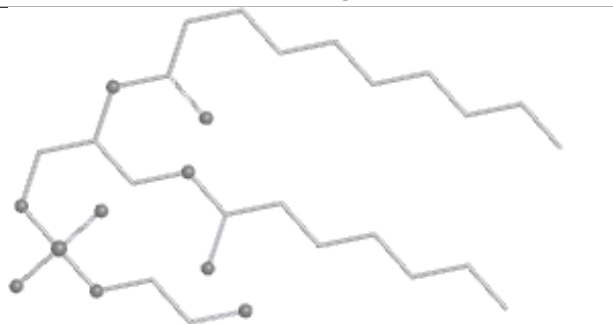
Rings

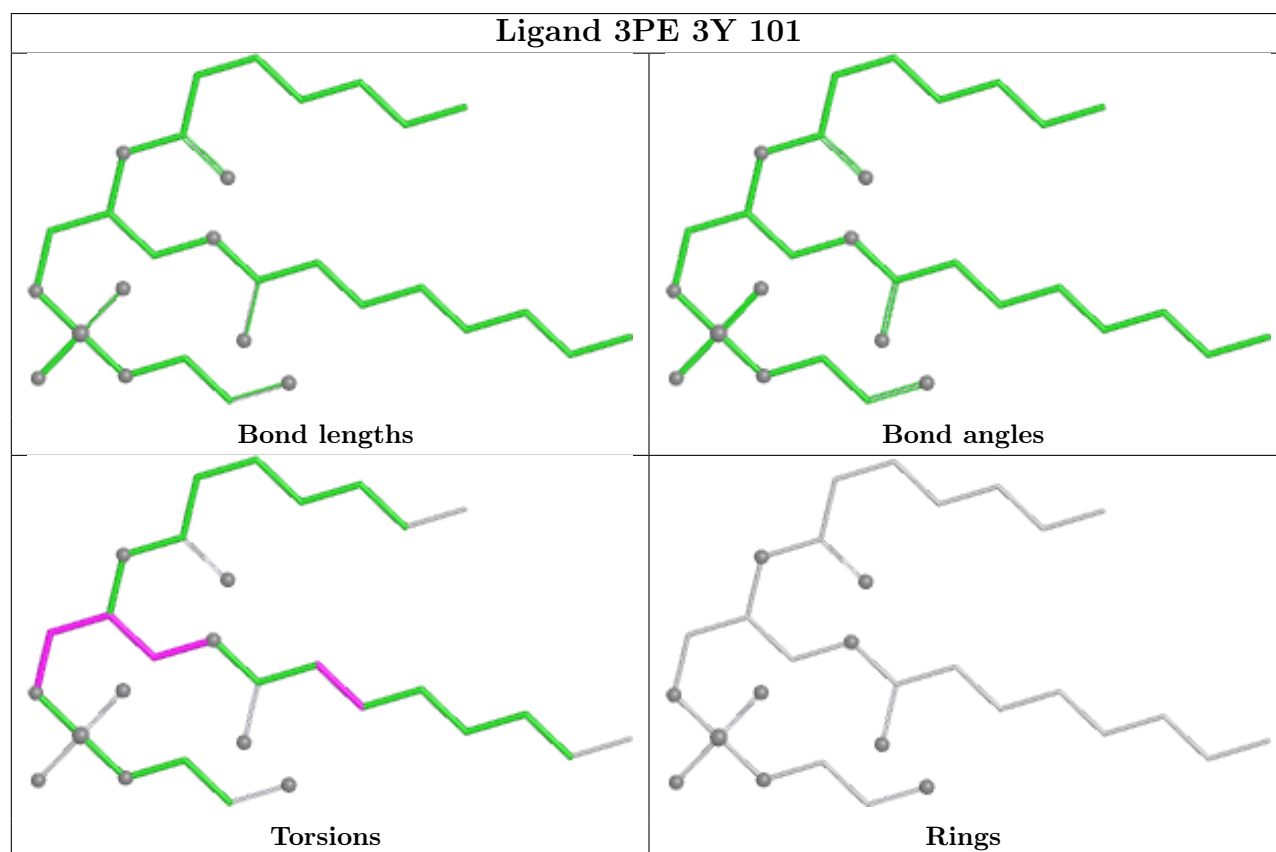
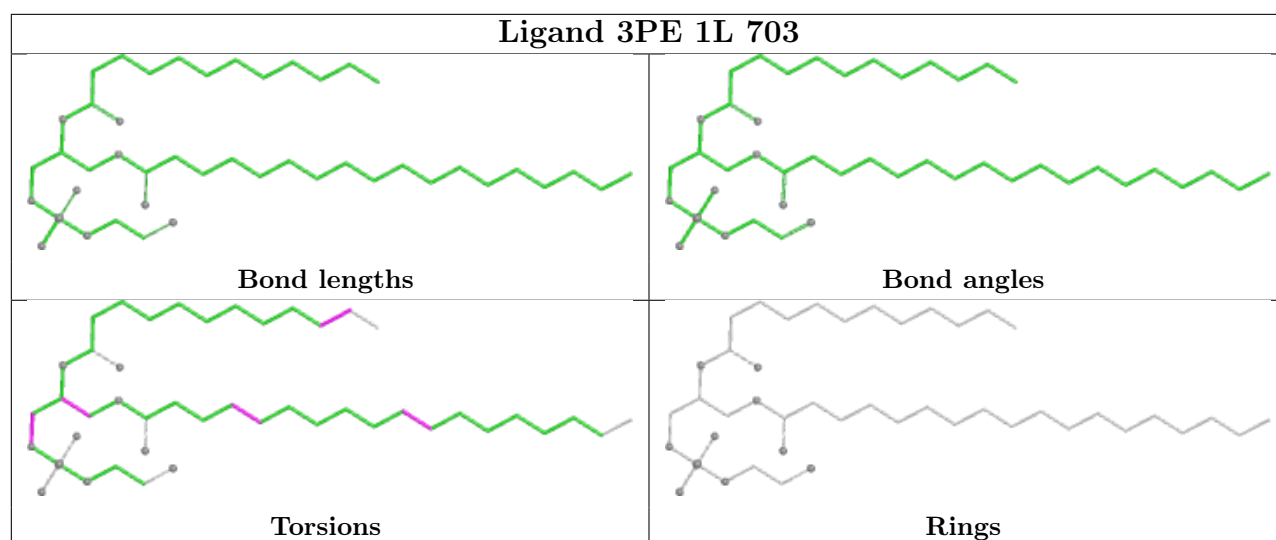


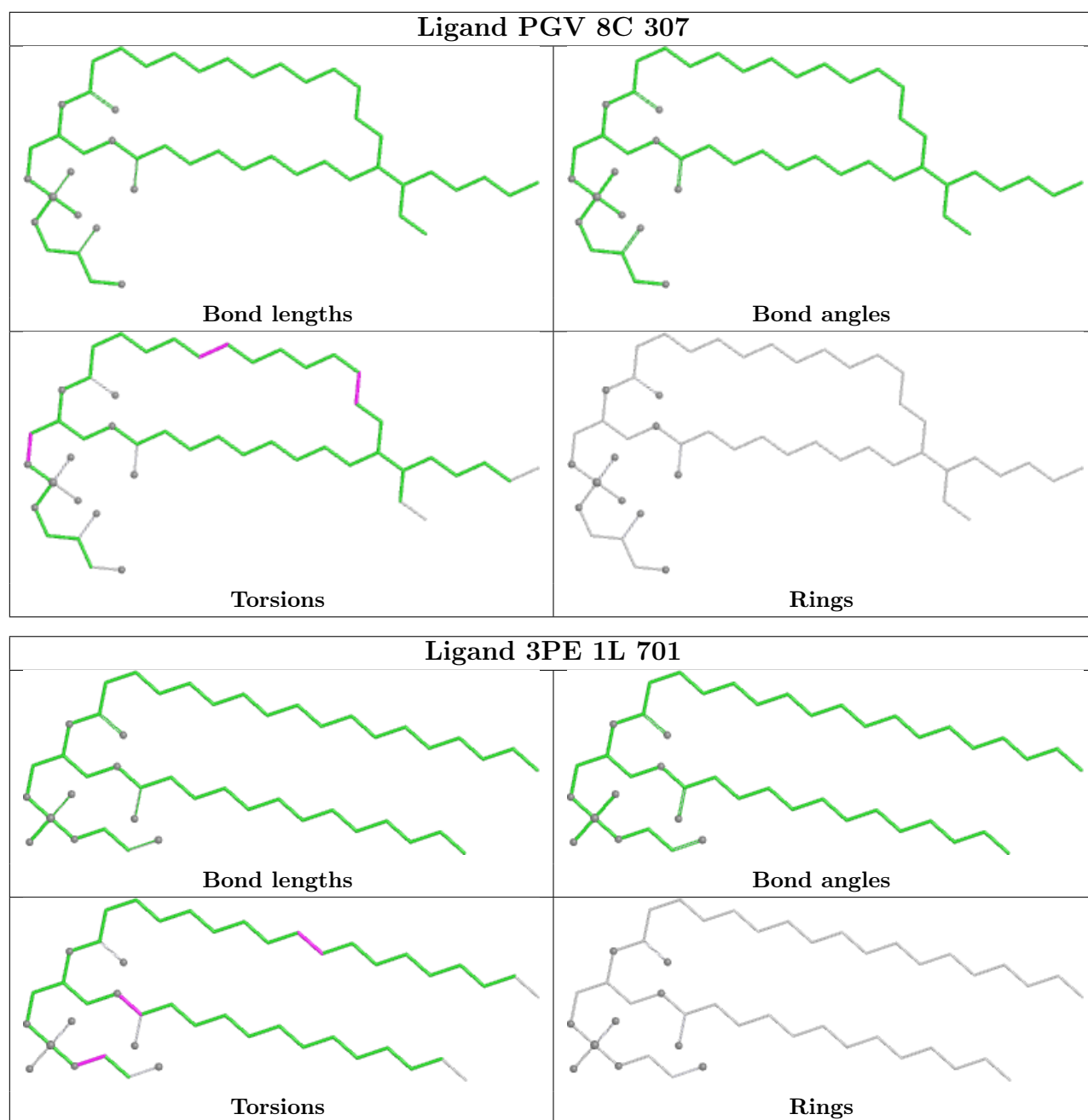


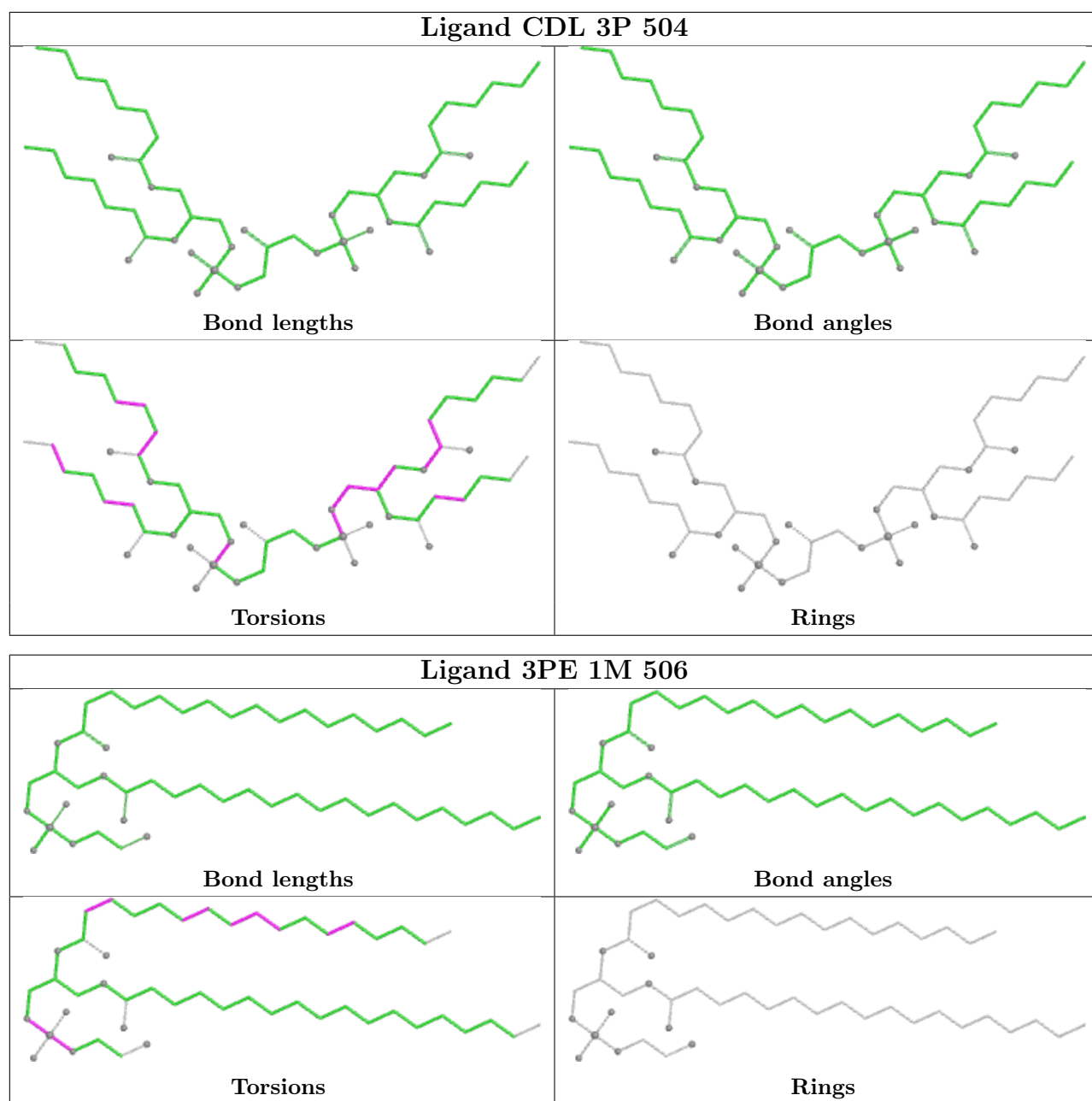


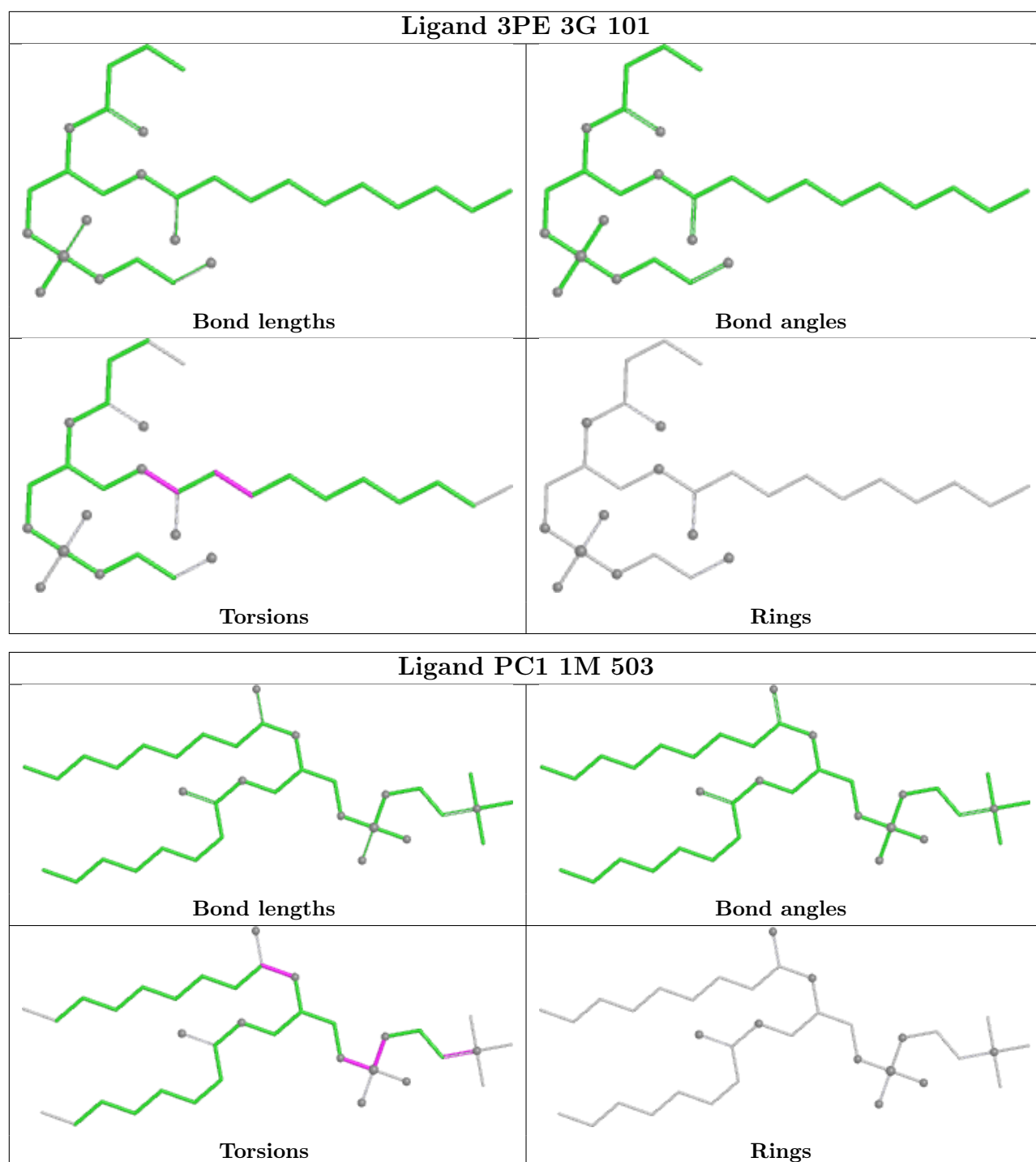


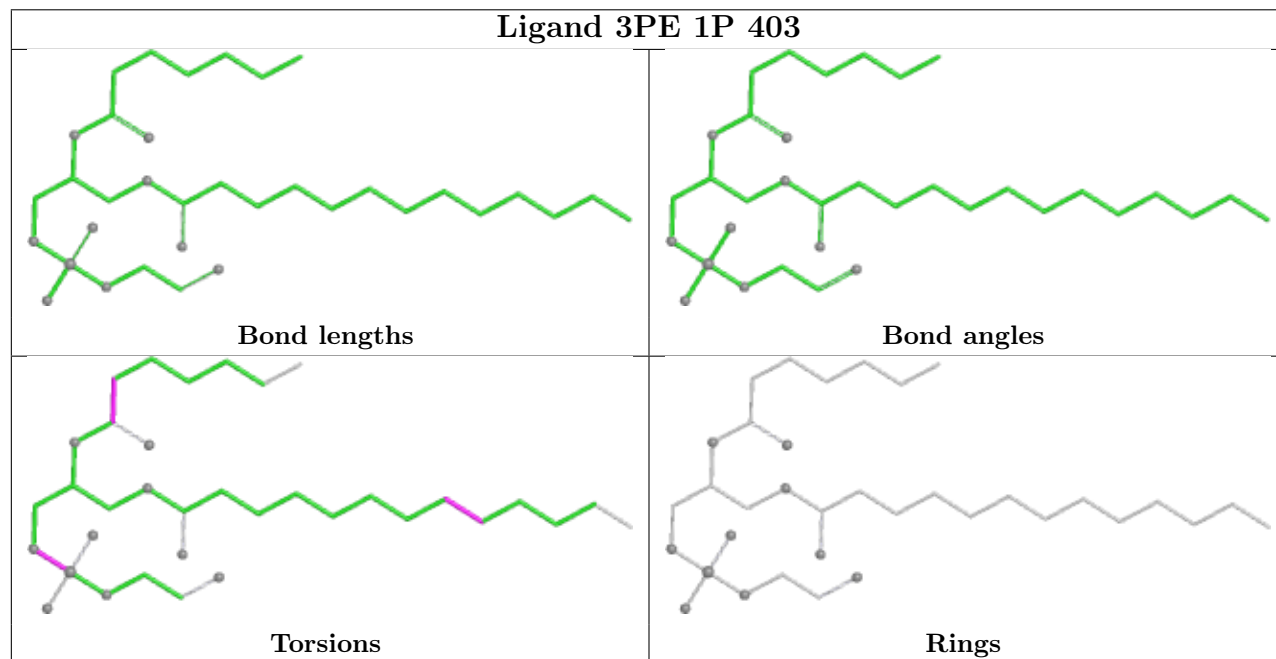
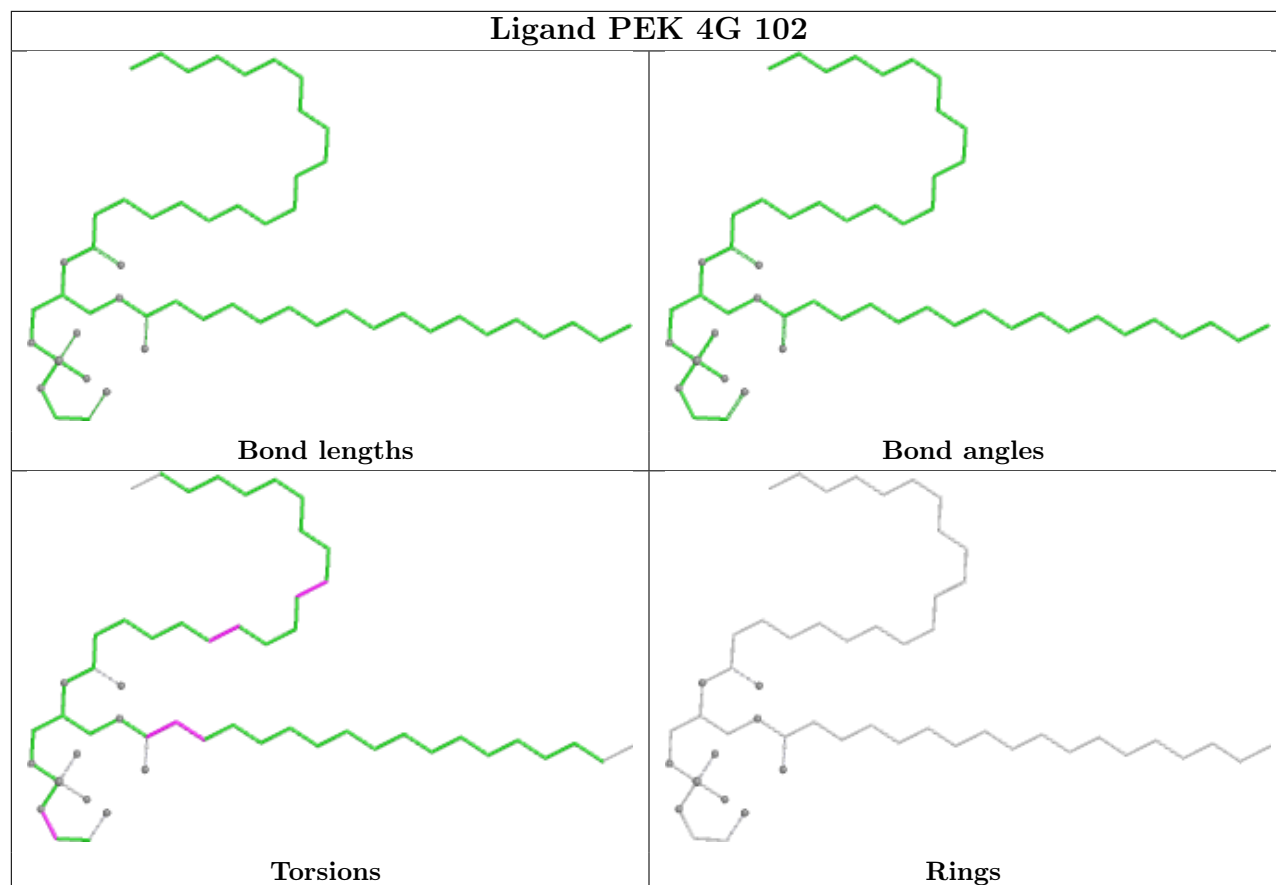
Ligand PC1 1A 203			
			
Bond lengths	Bond angles		
			
Torsions	Rings		
Ligand 3PE 3N 501			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

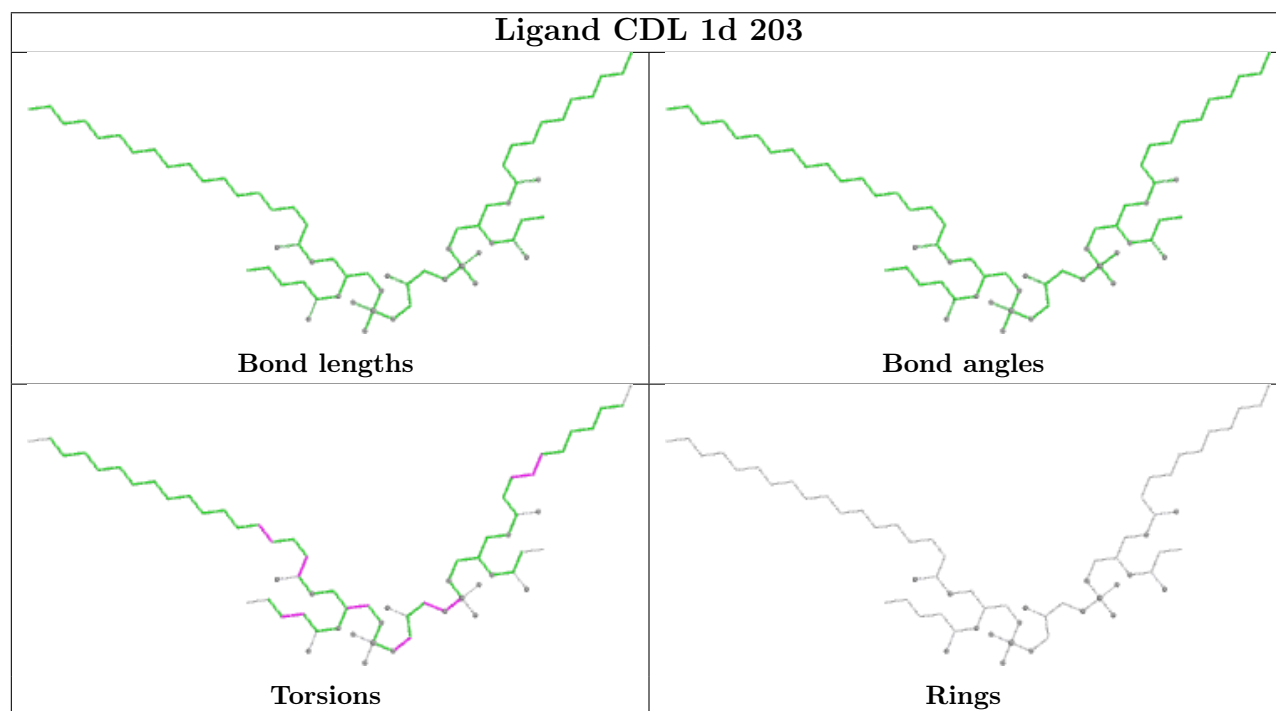
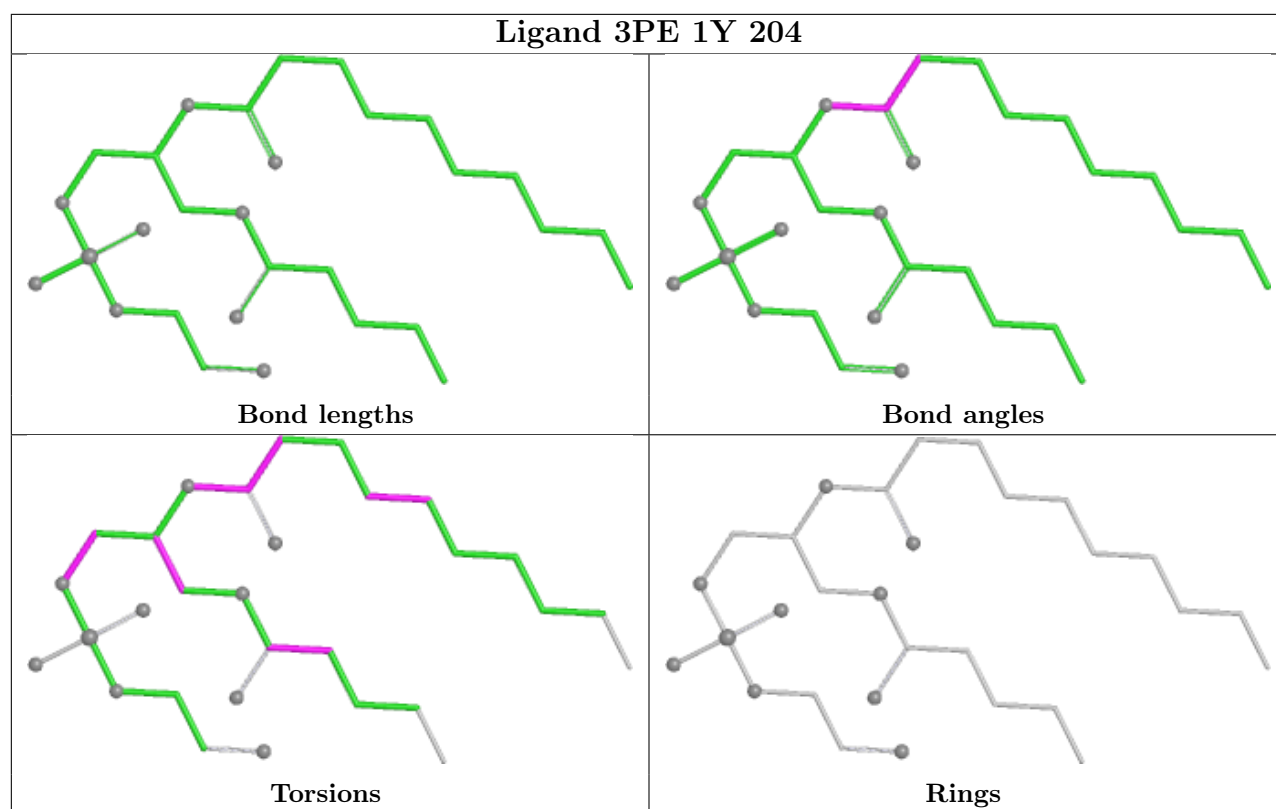


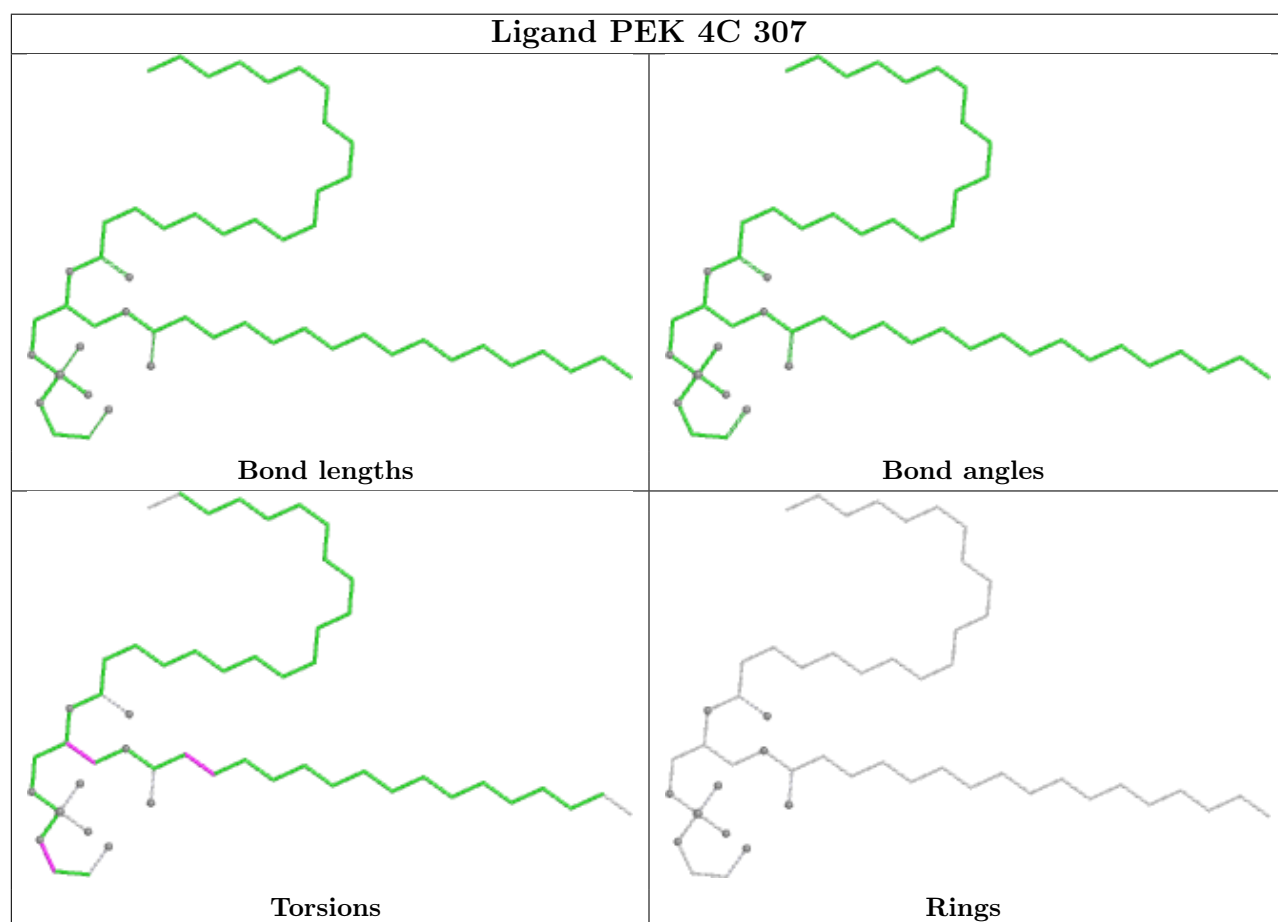
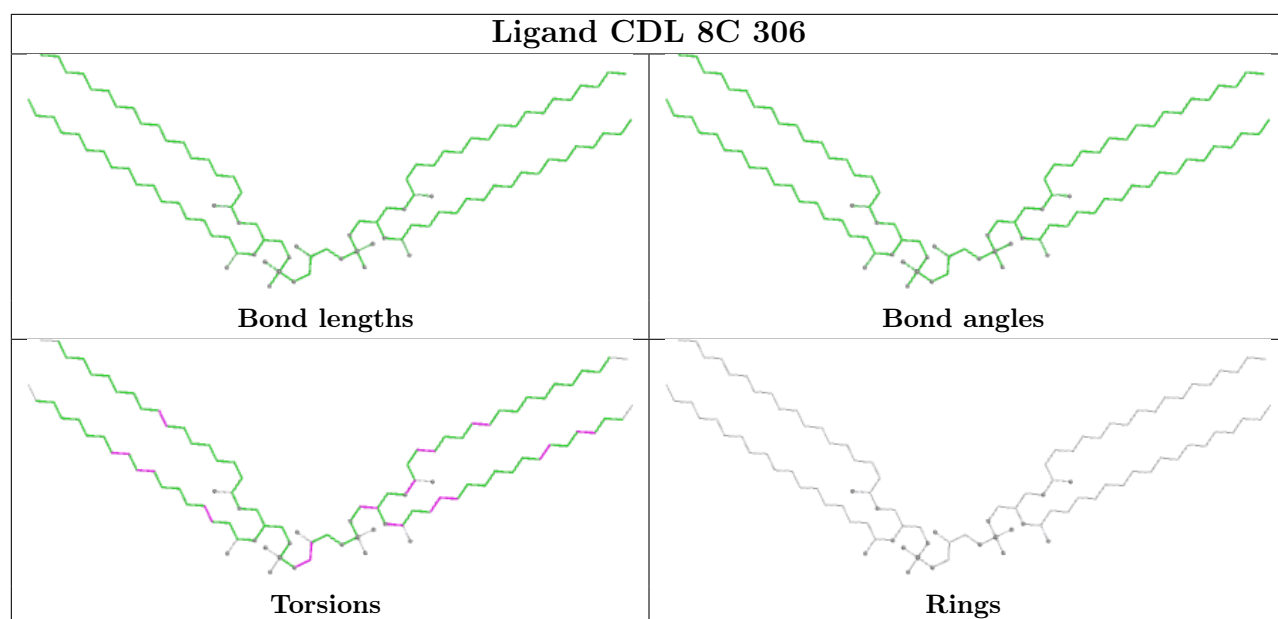


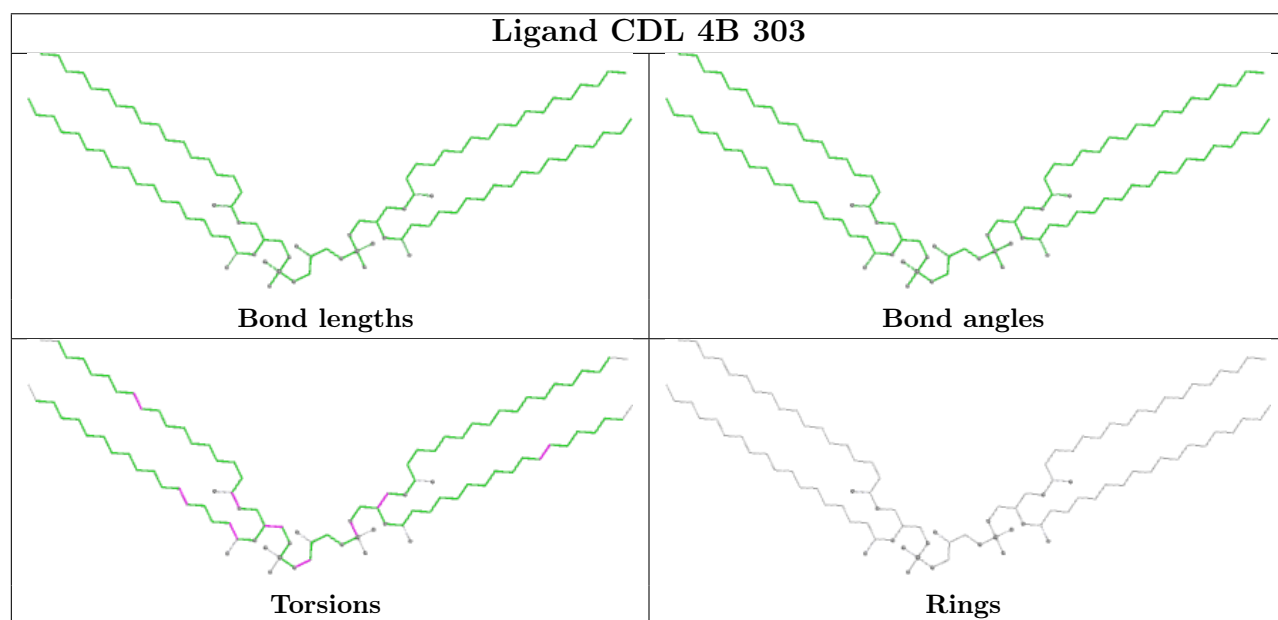
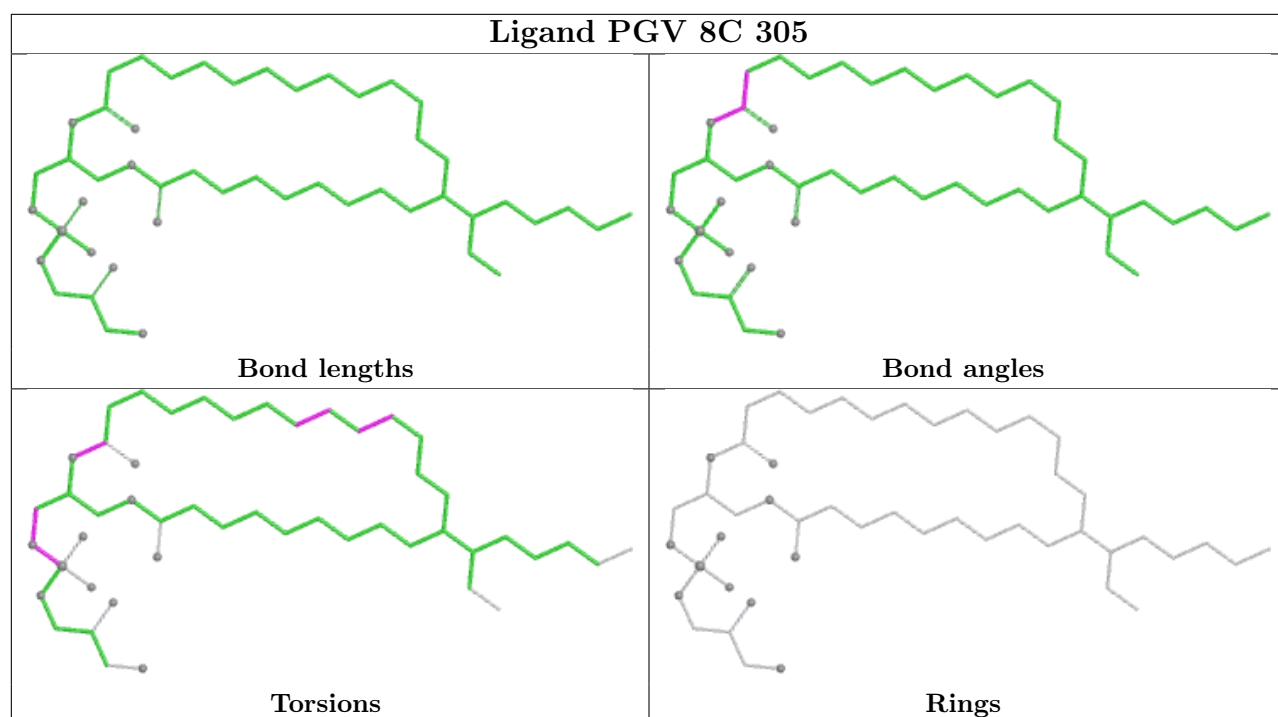


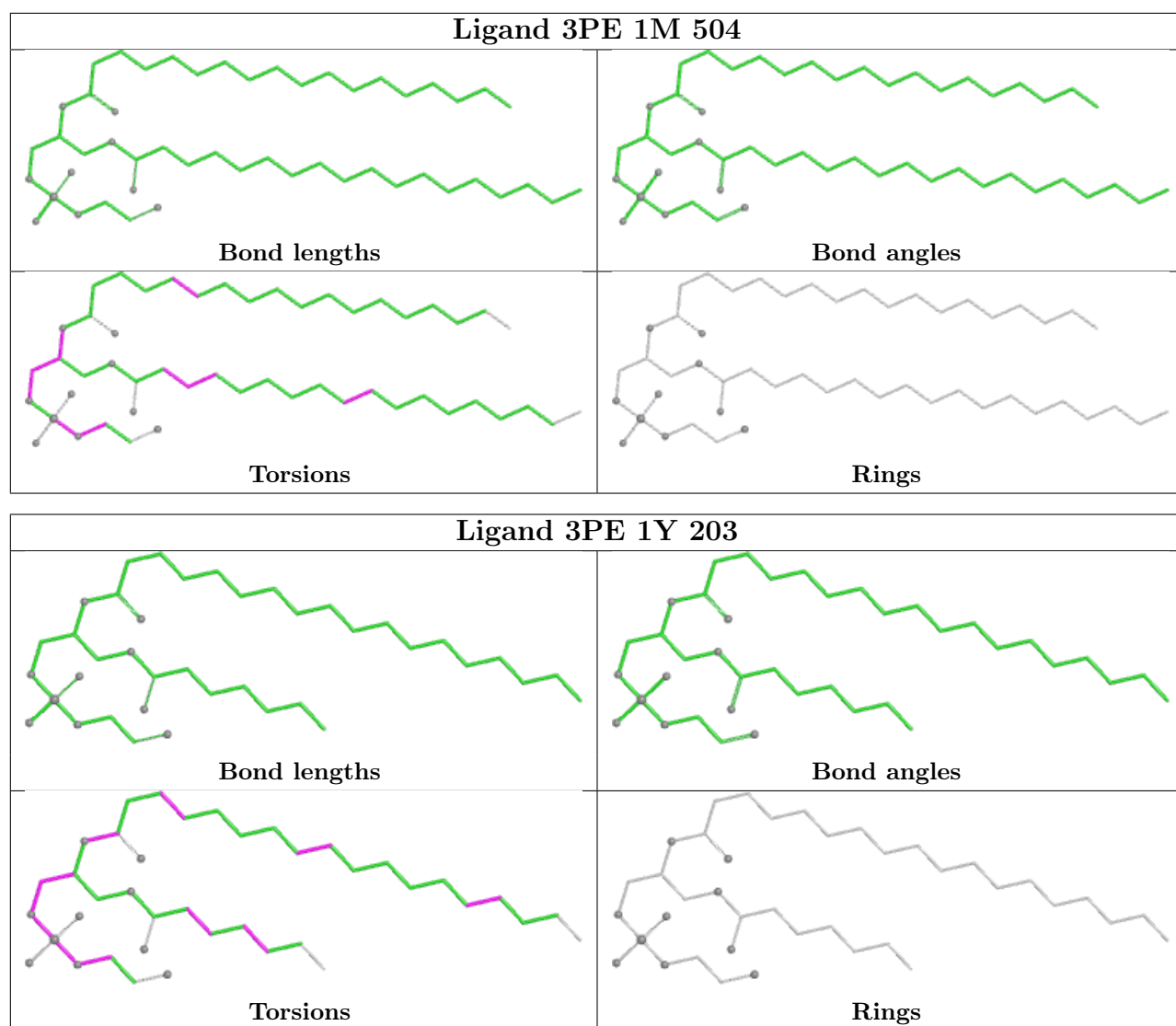


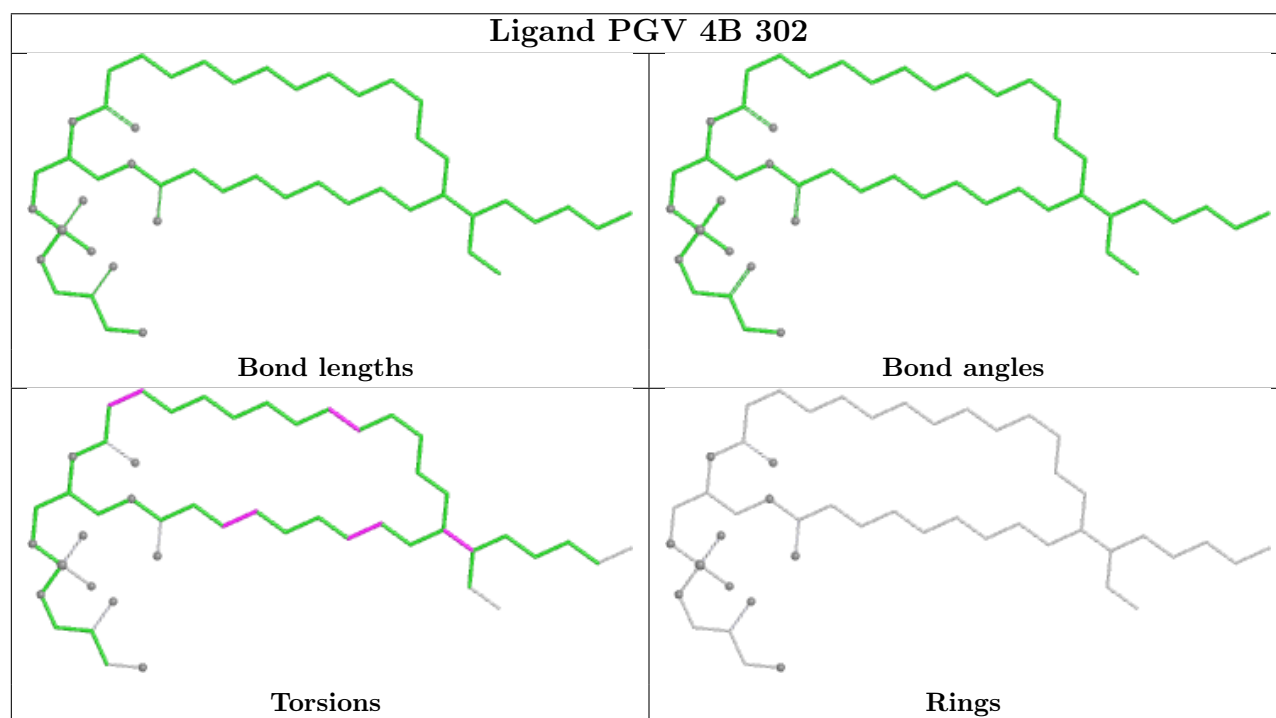
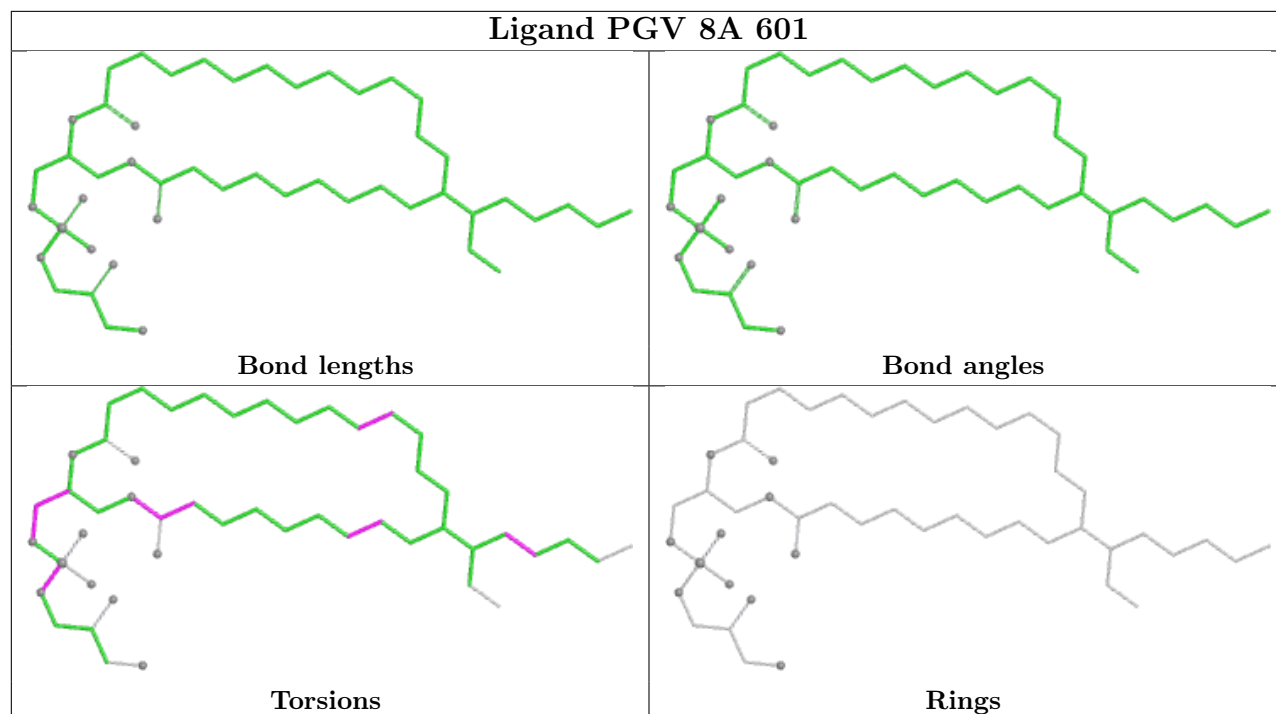


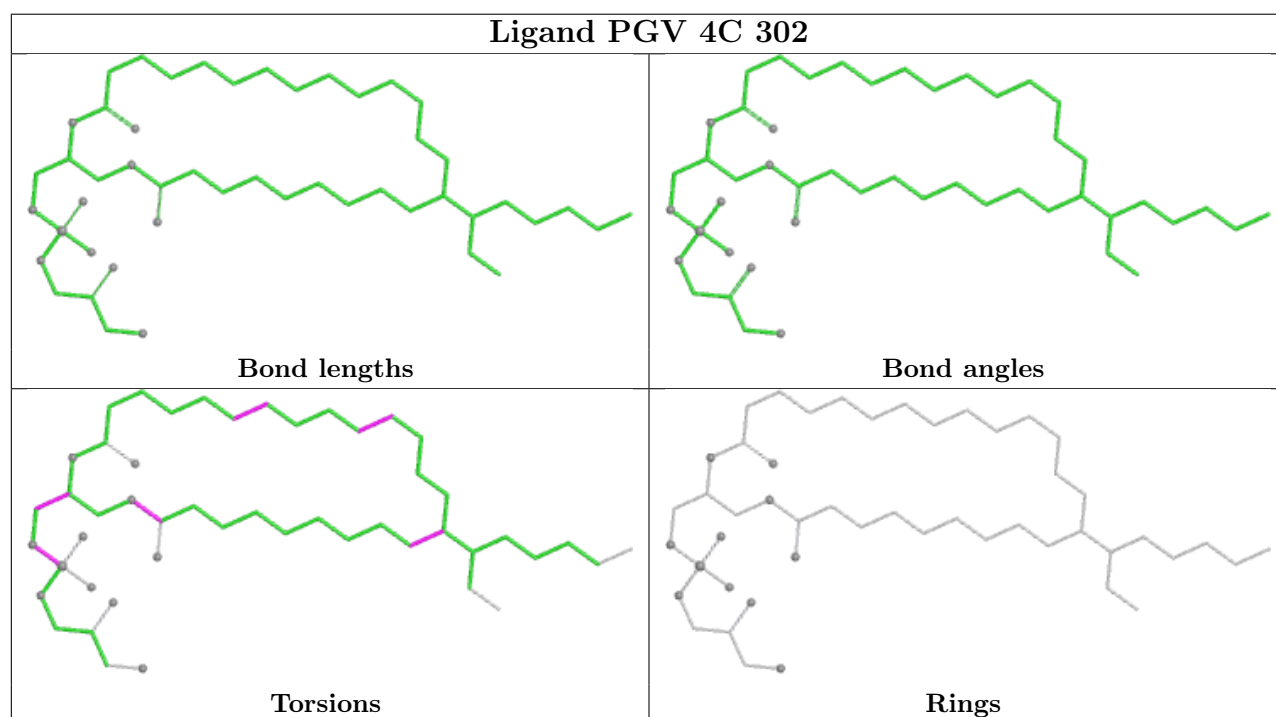
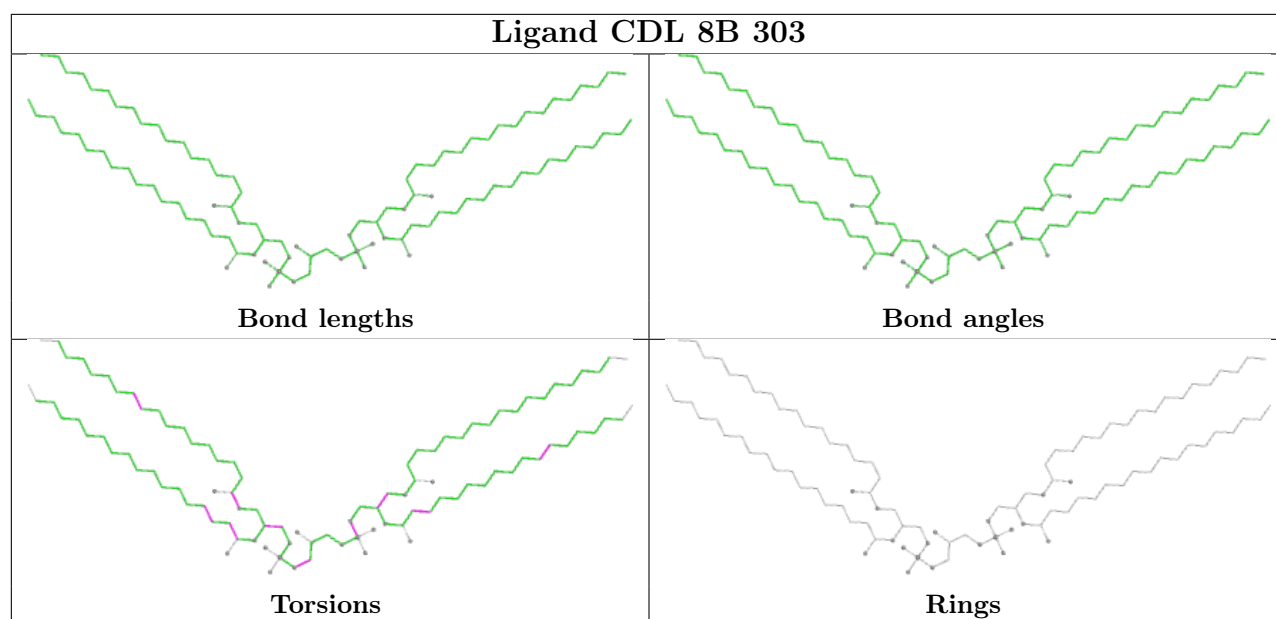


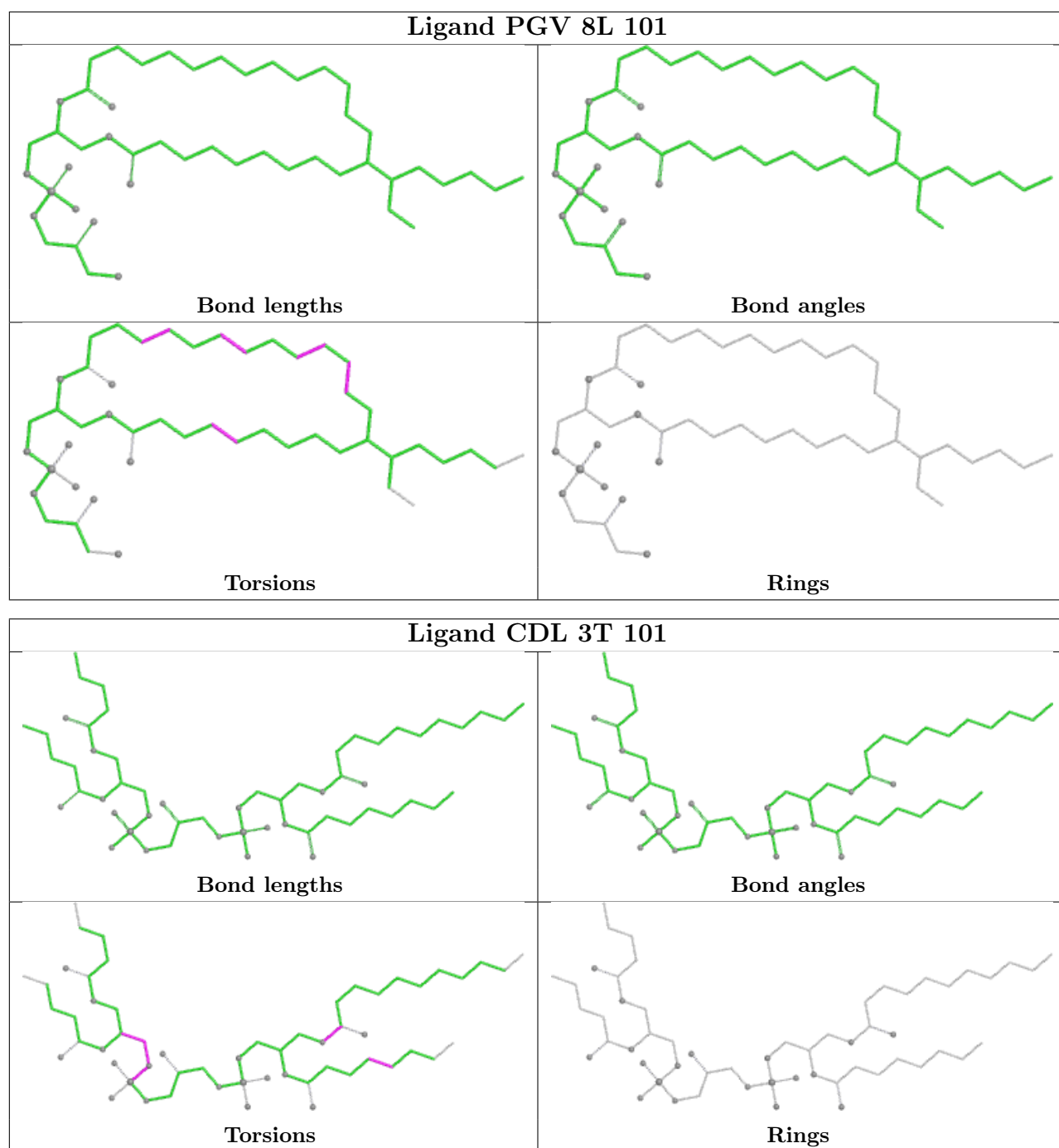


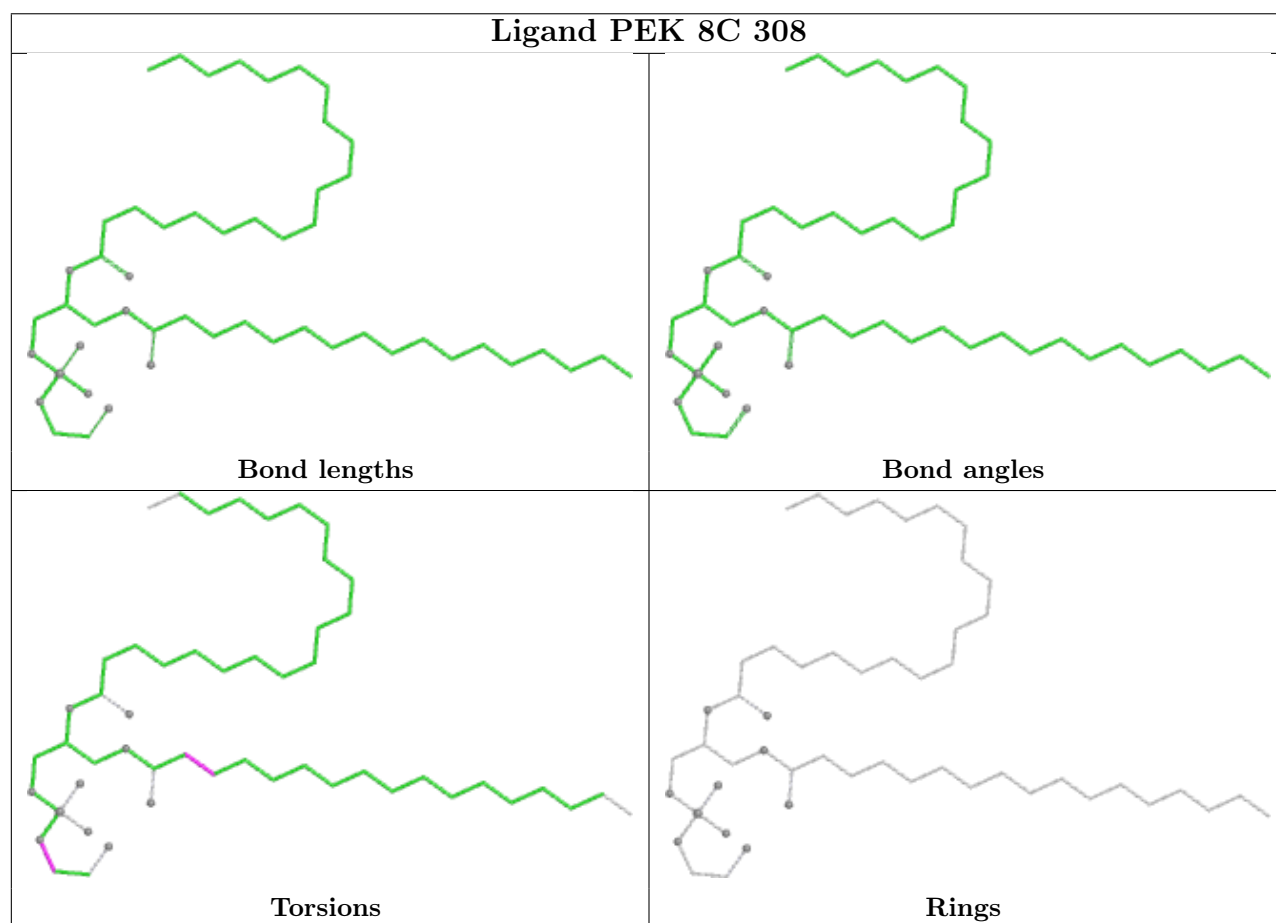
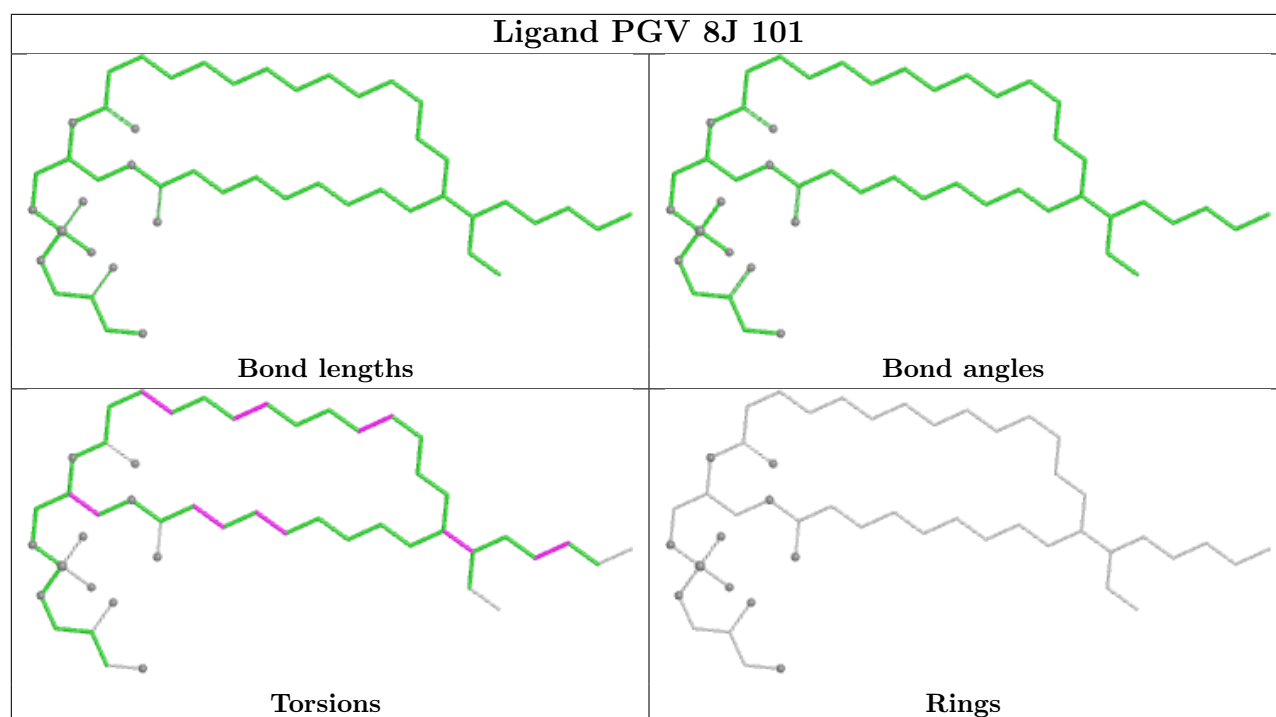


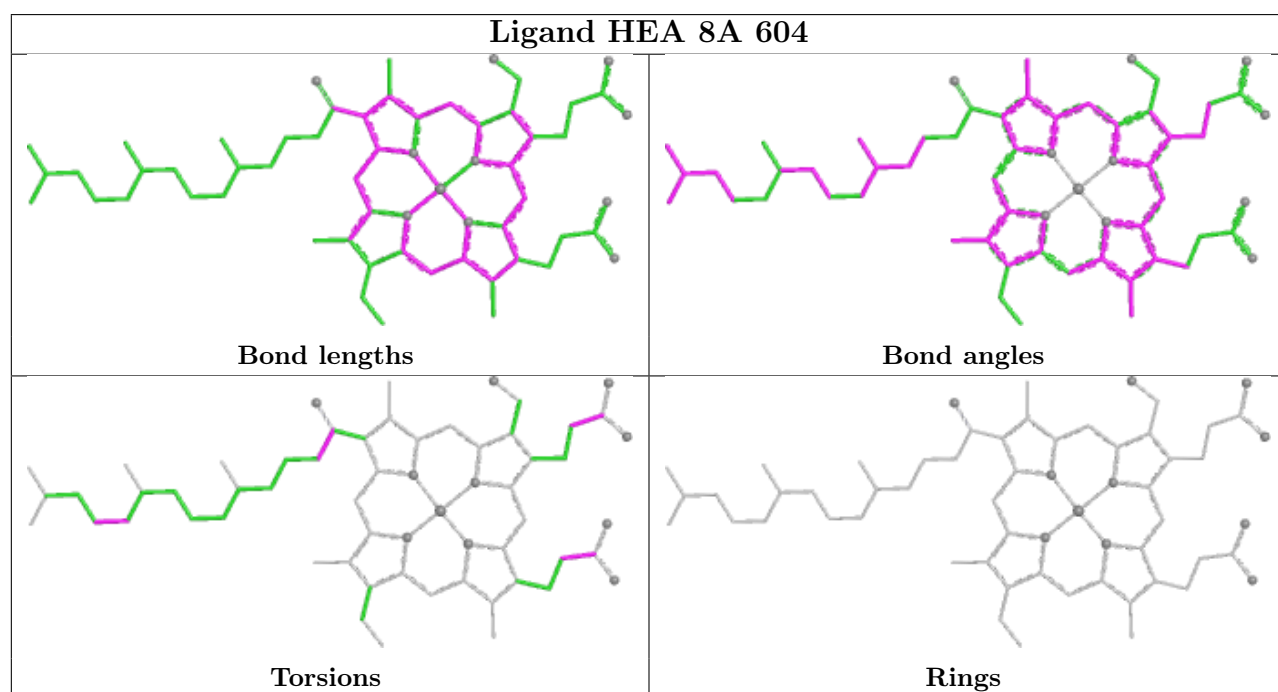
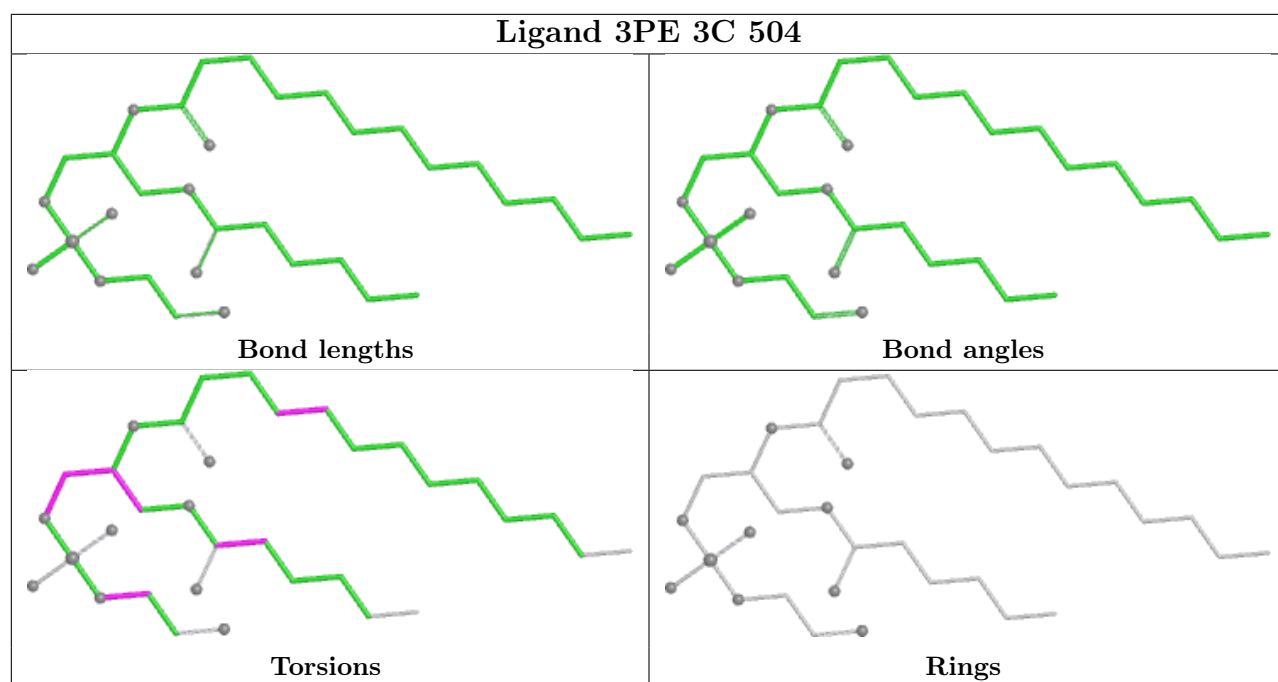


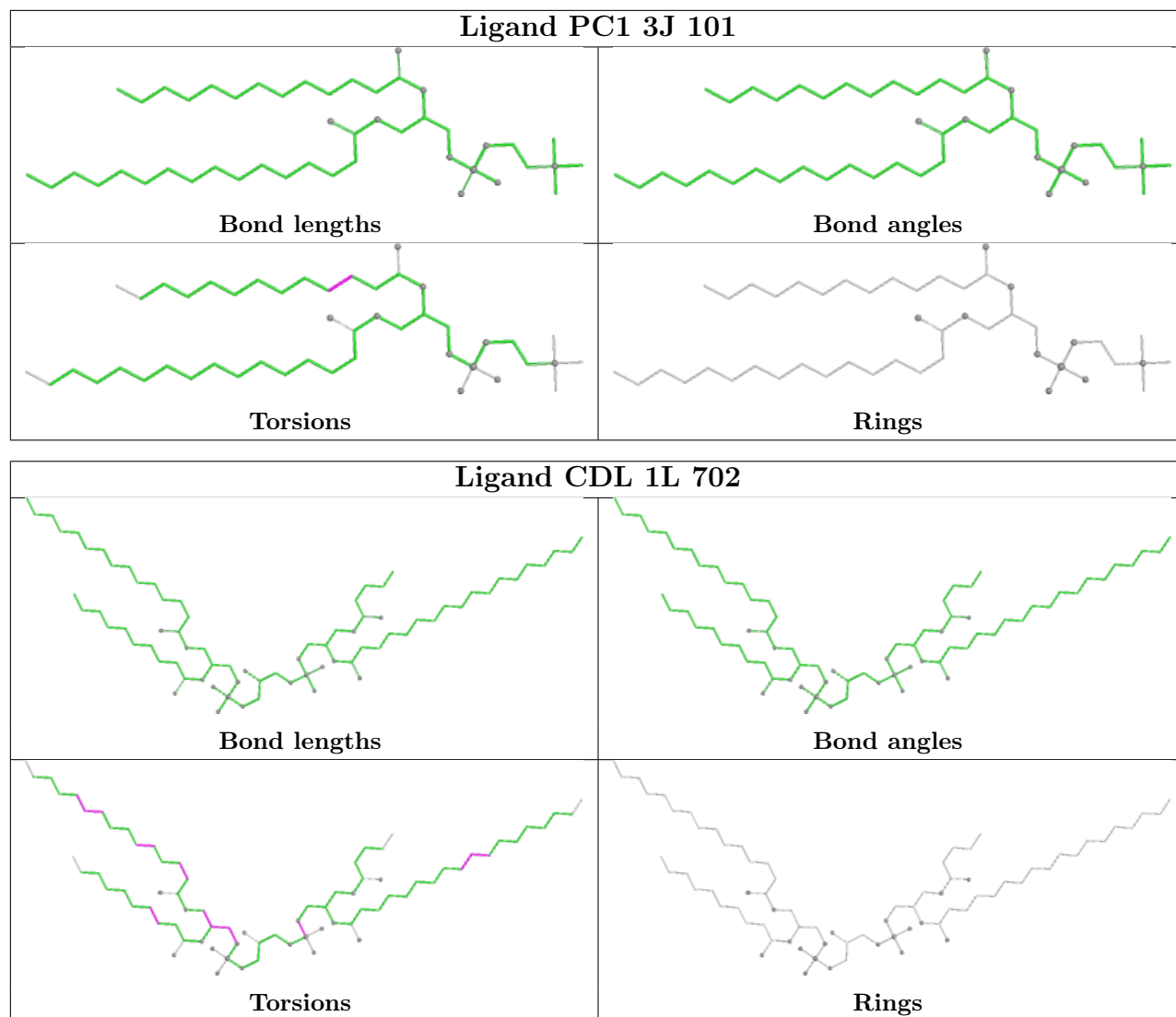


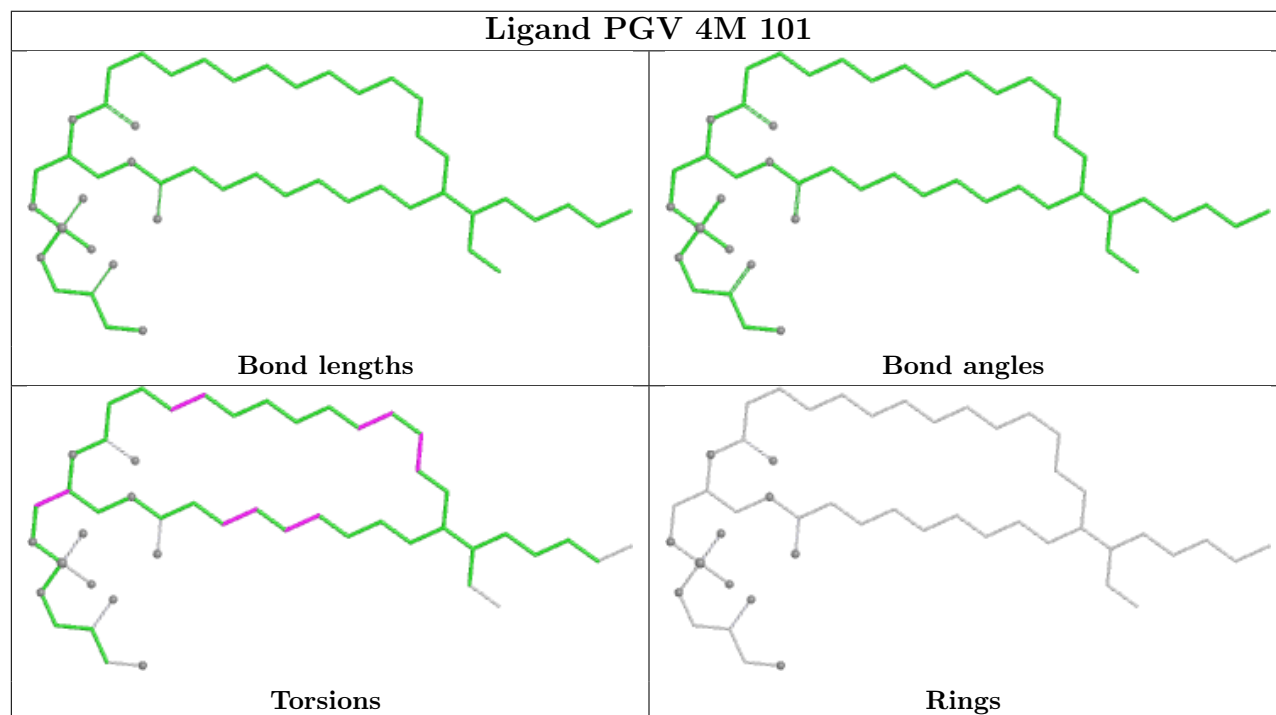
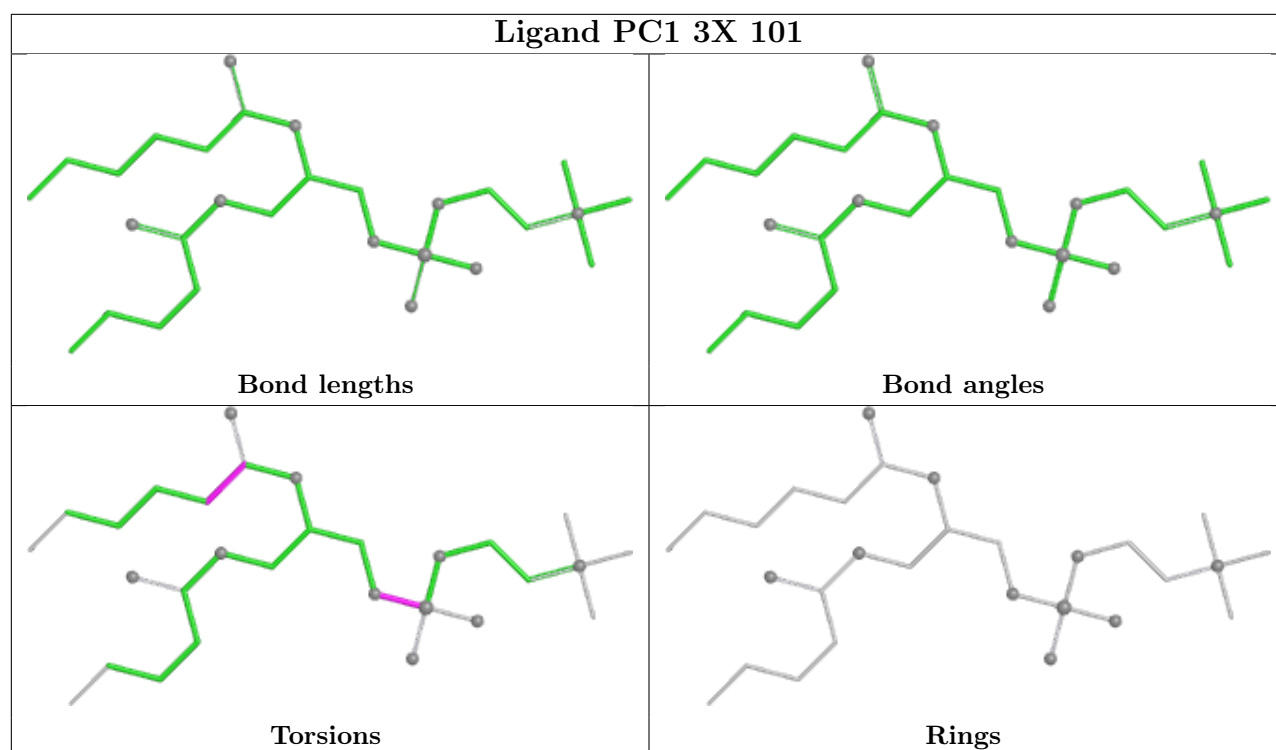


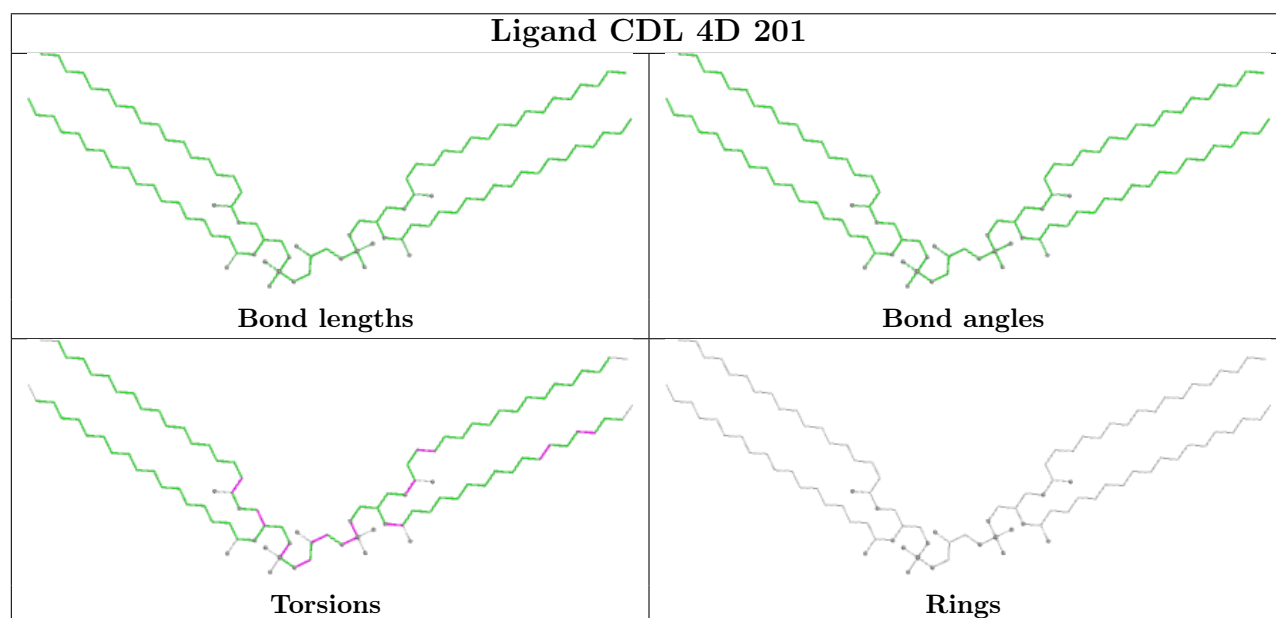
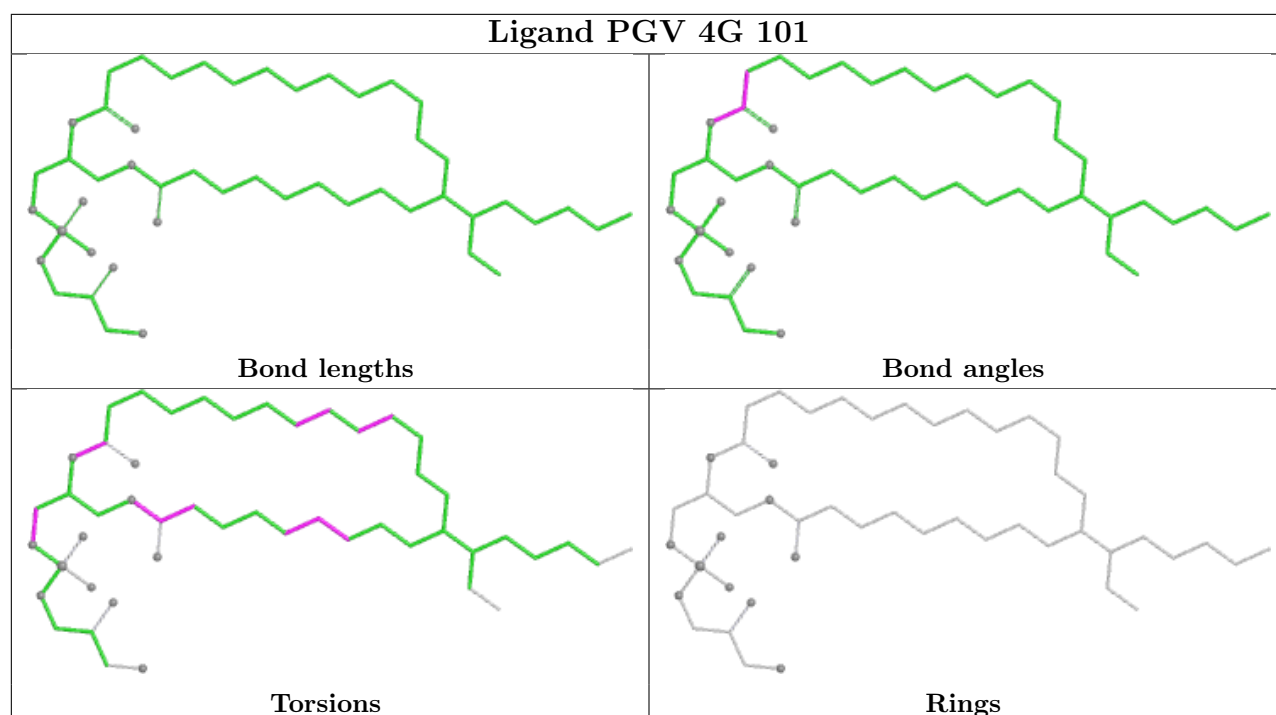


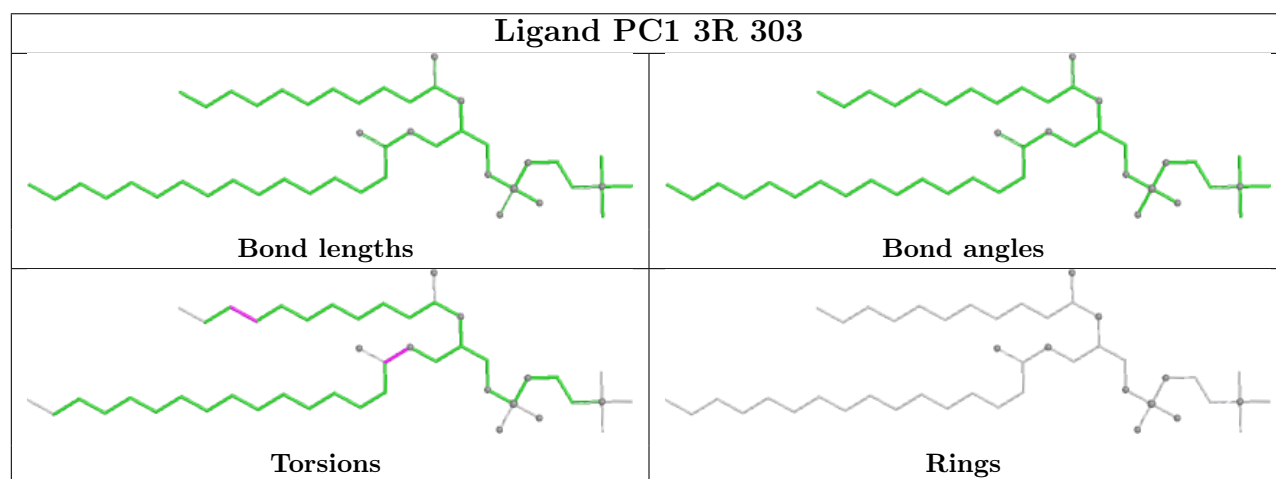
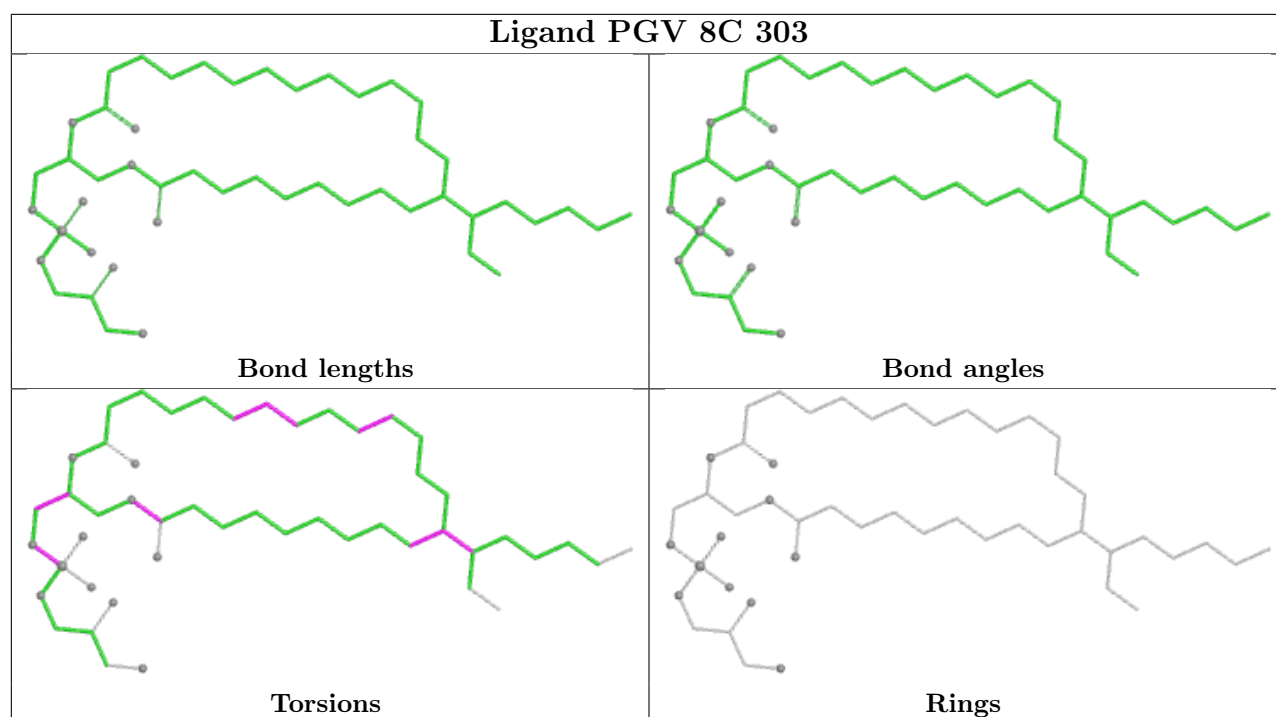




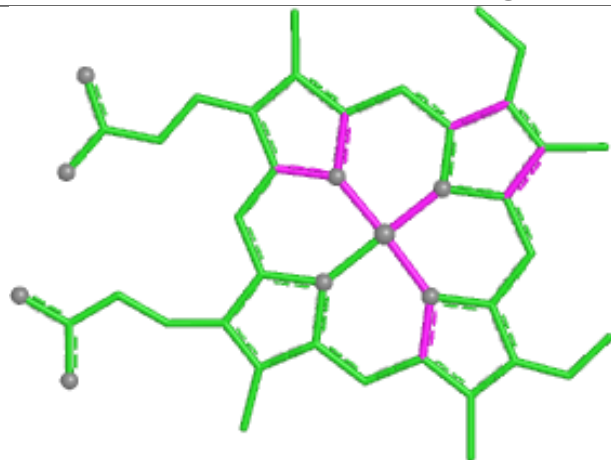




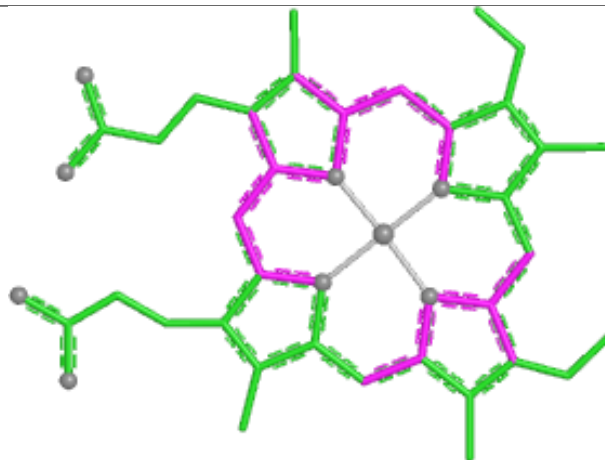




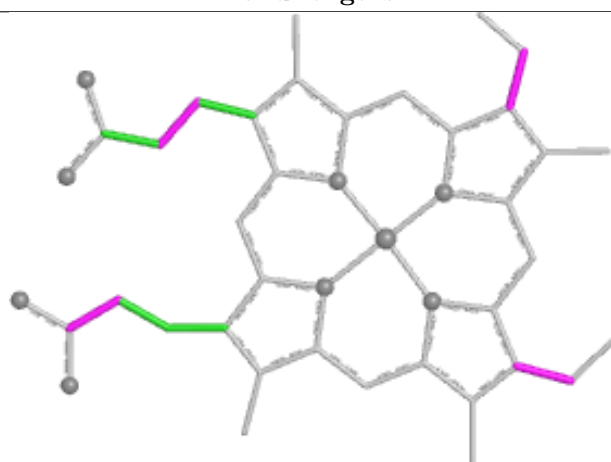
Ligand HEM 3C 501



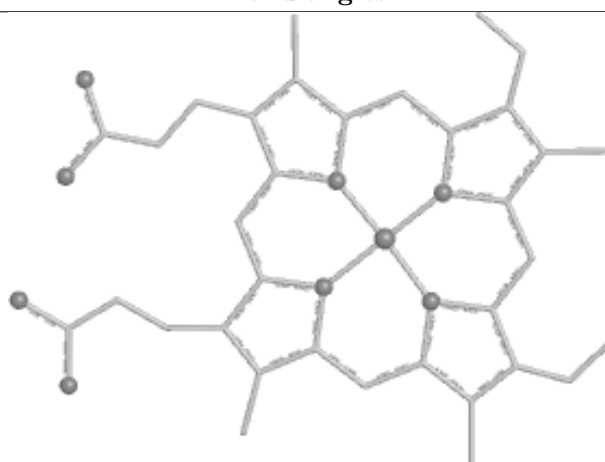
Bond lengths



Bond angles

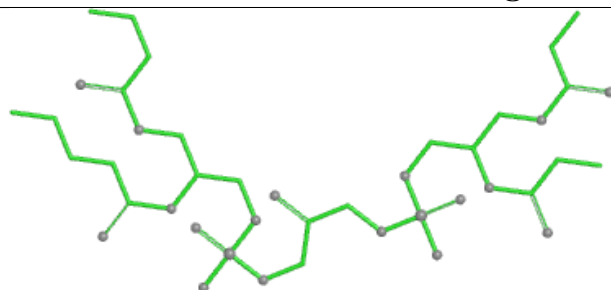


Torsions

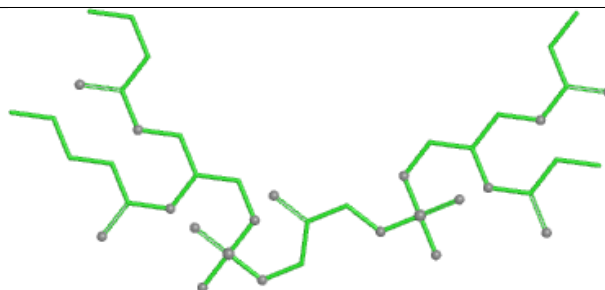


Rings

Ligand CDL 3N 502



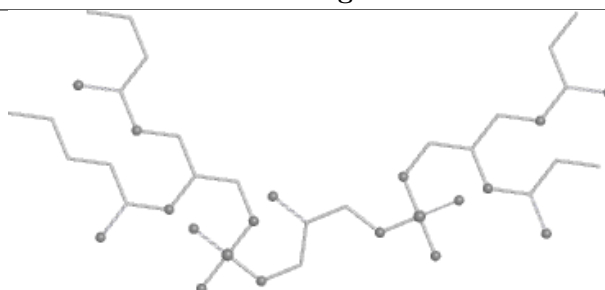
Bond lengths



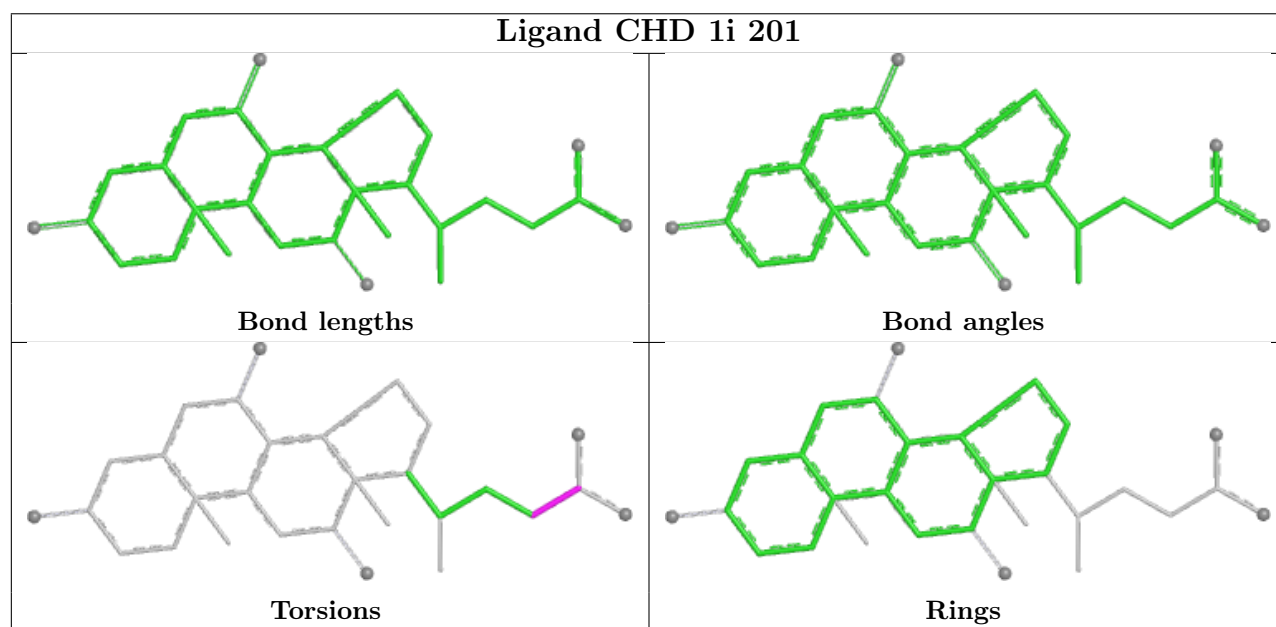
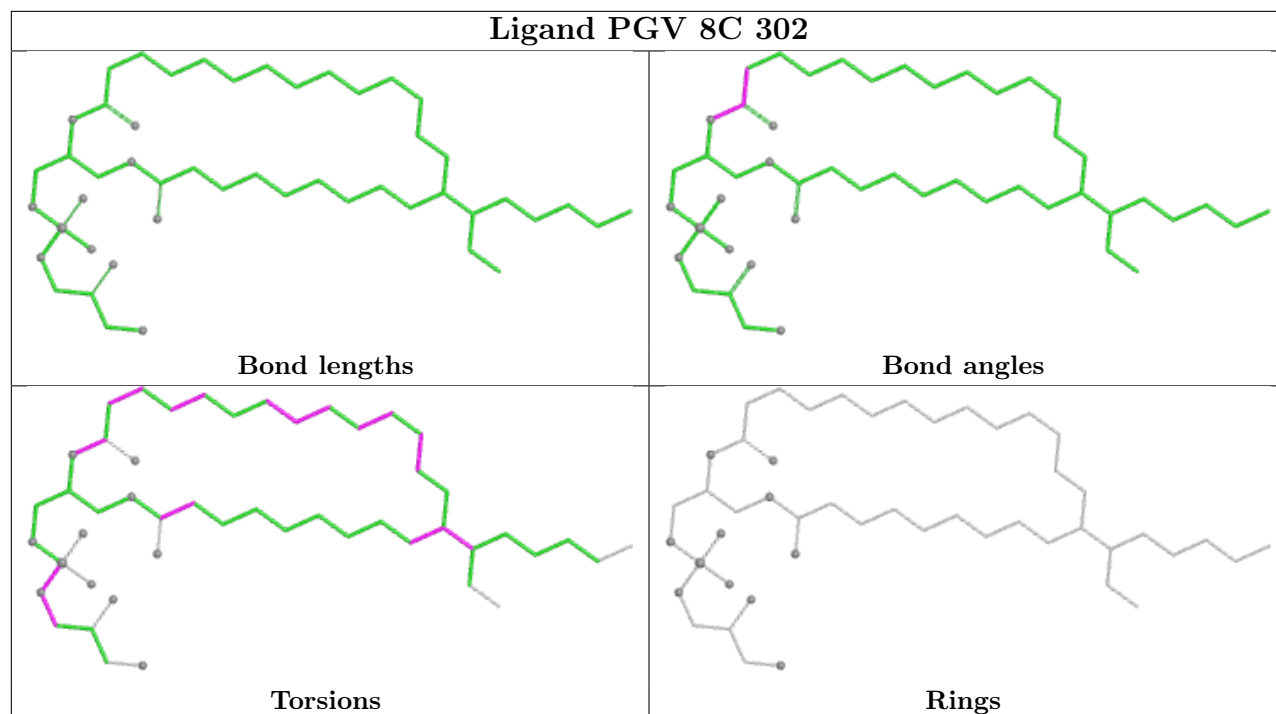
Bond angles

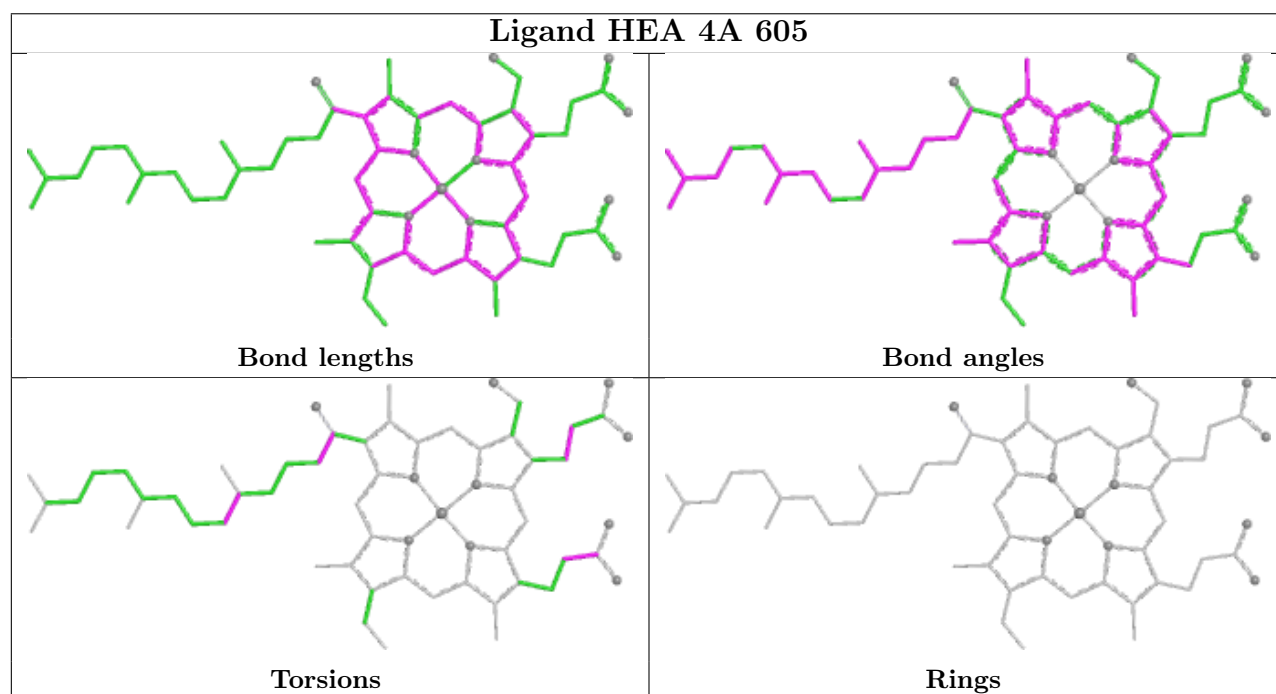
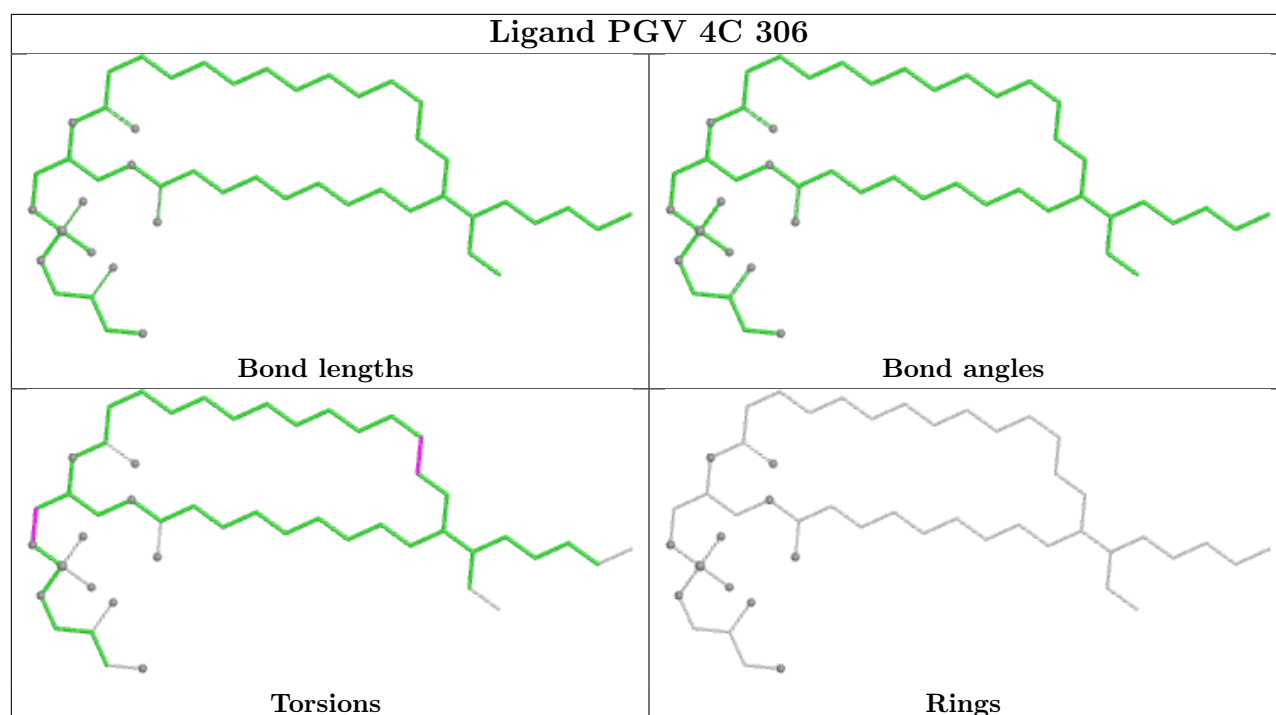


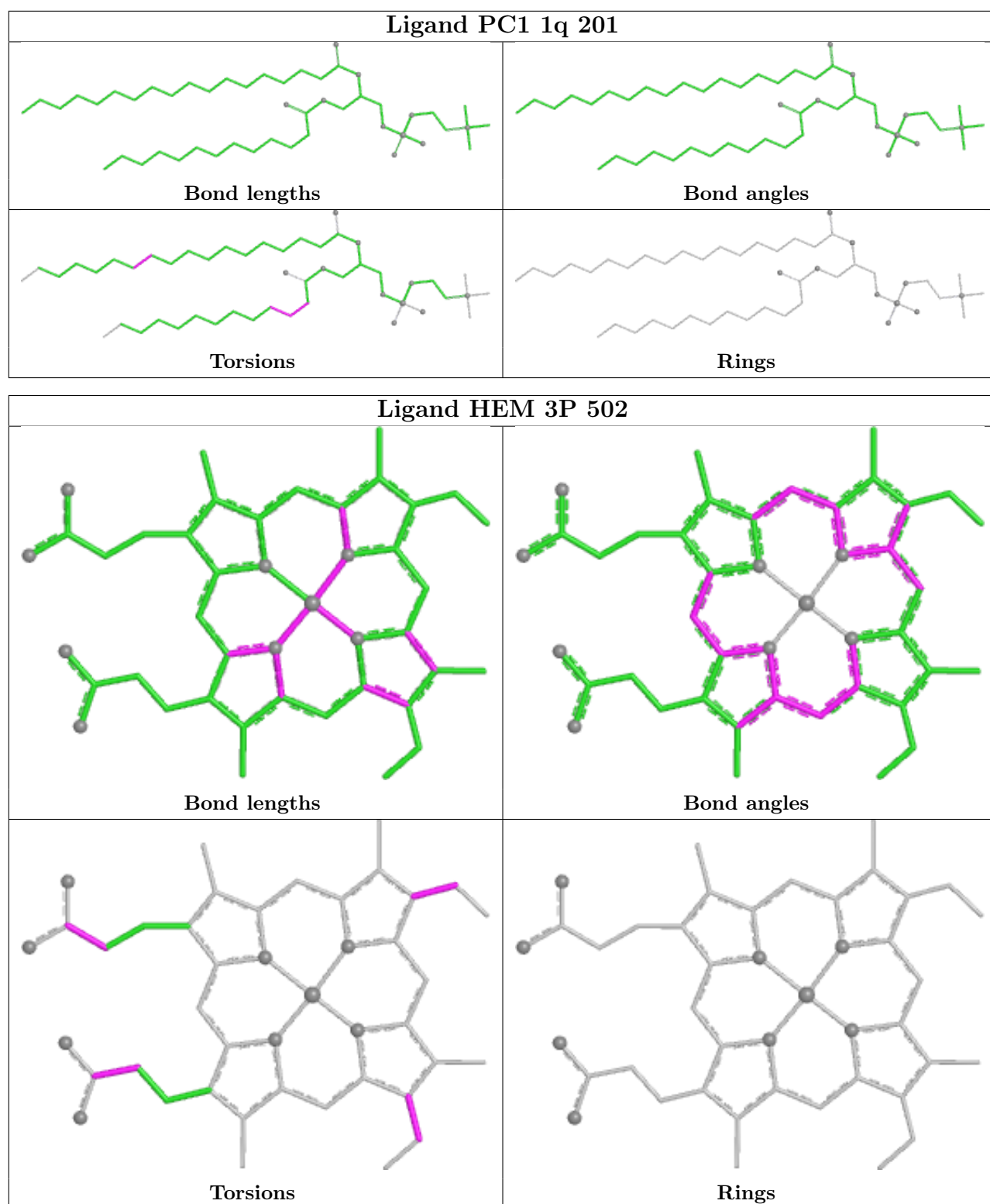
Torsions

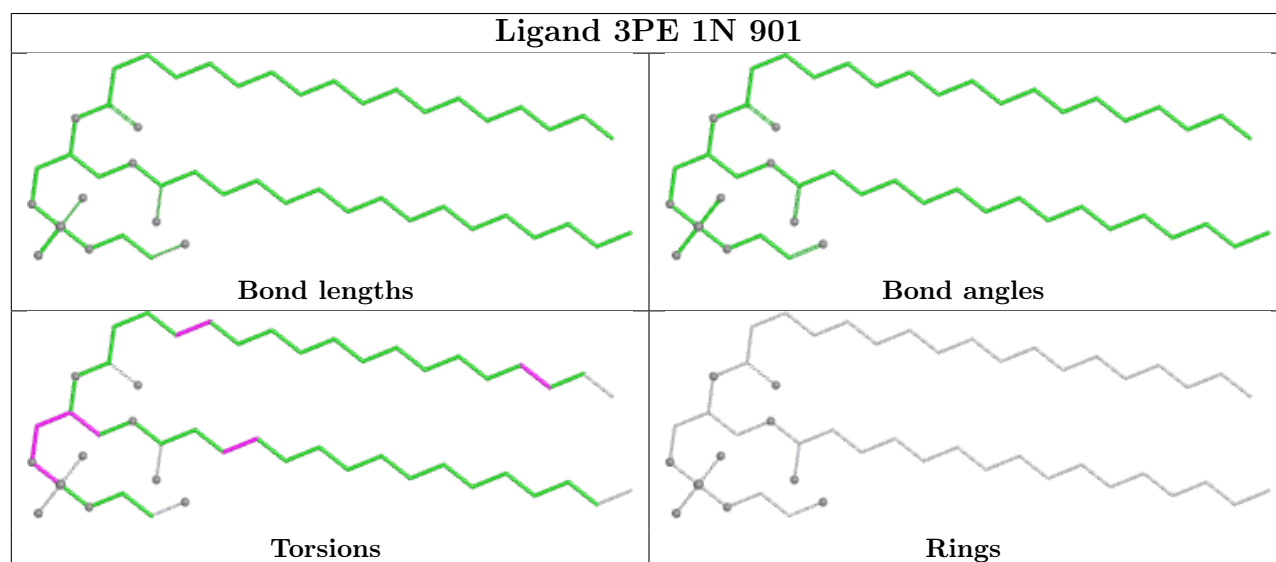
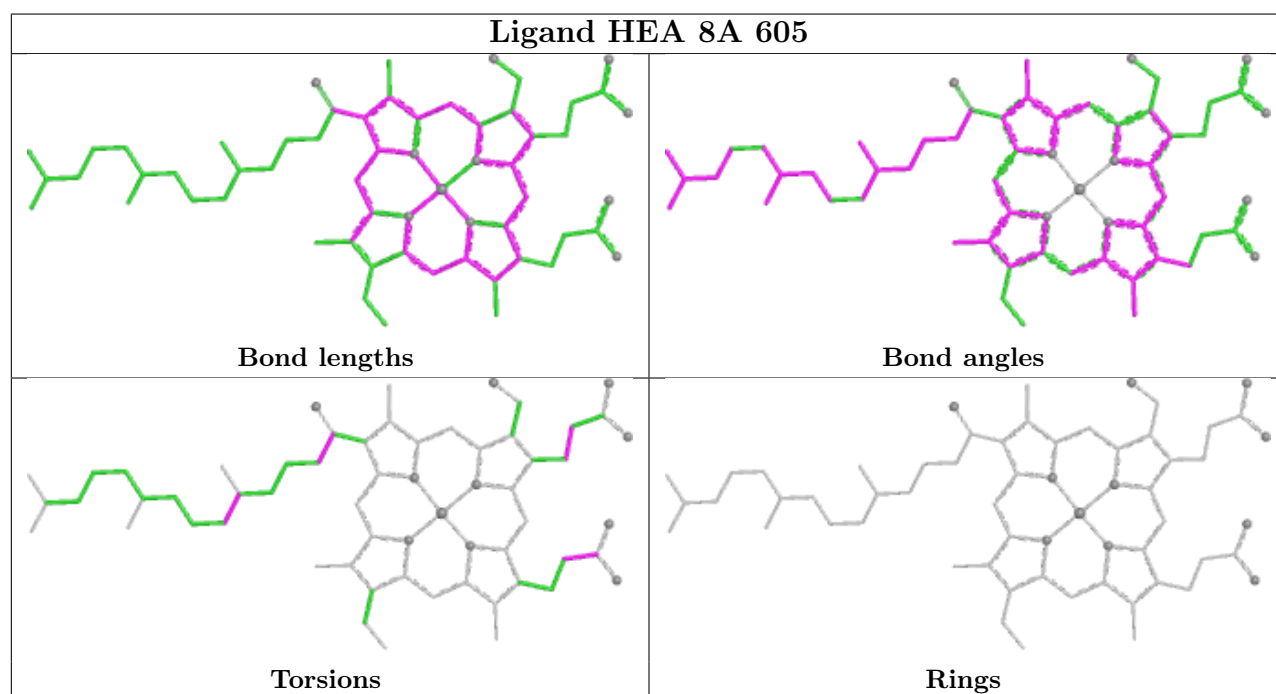
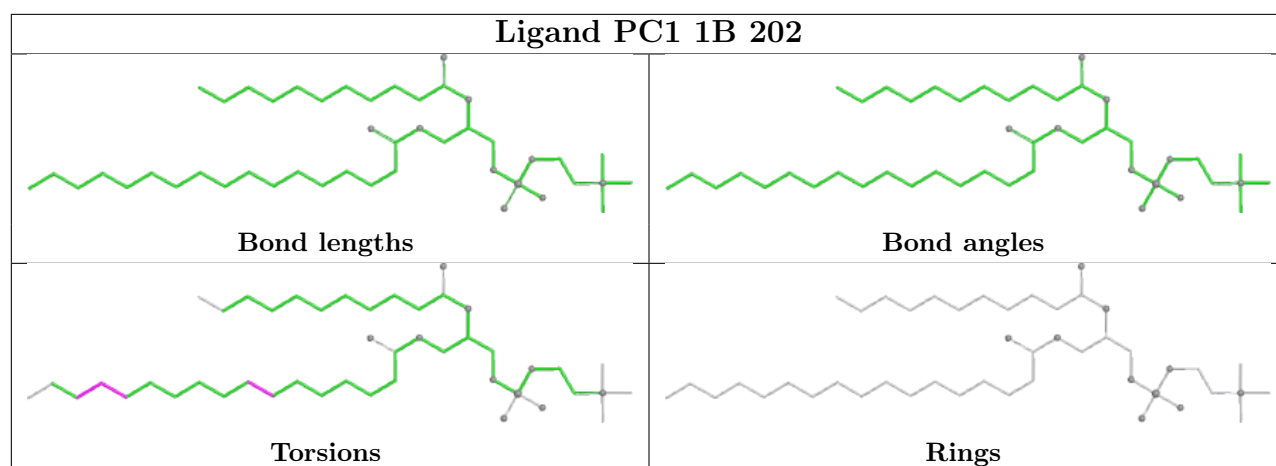


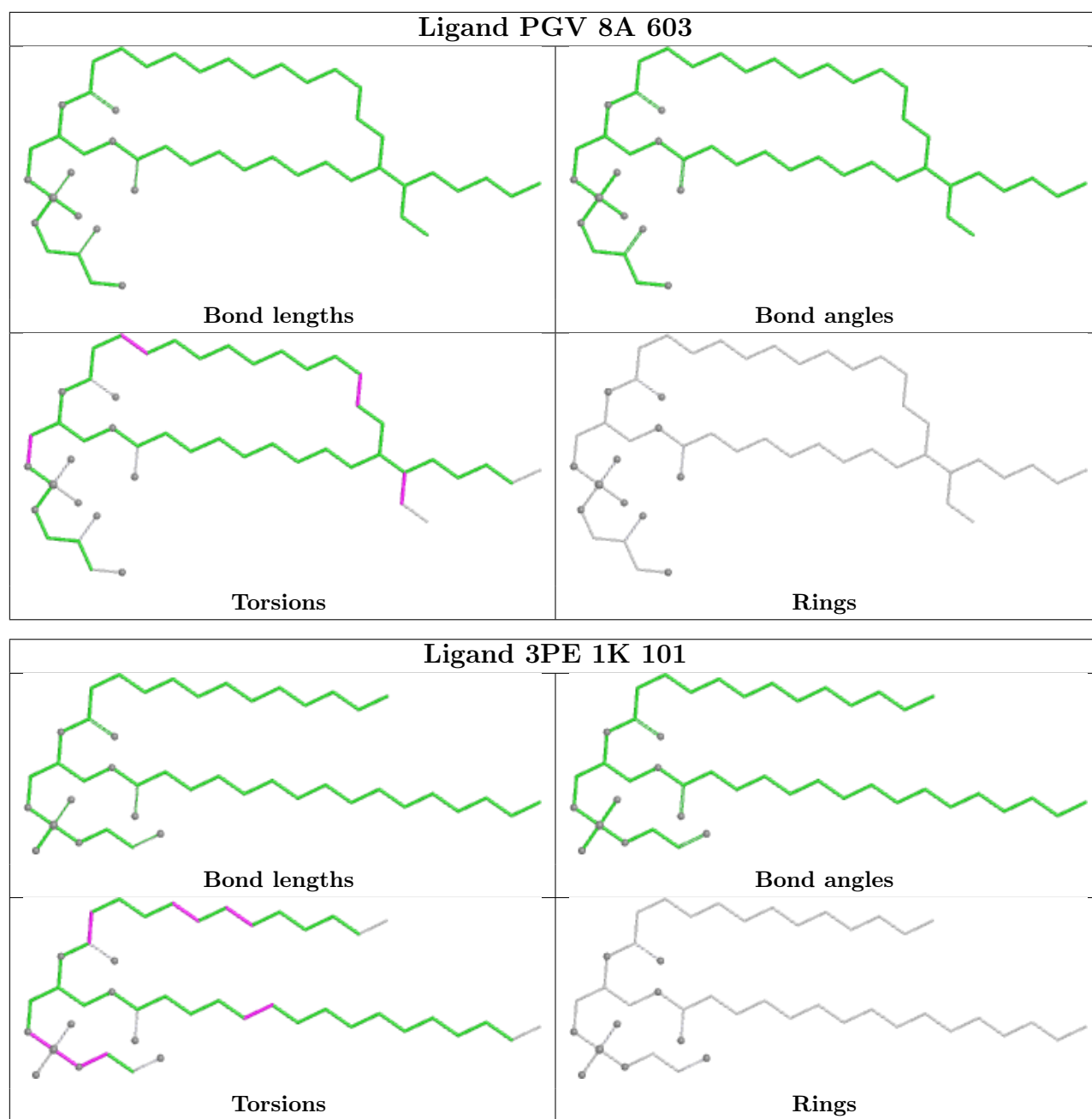
Rings

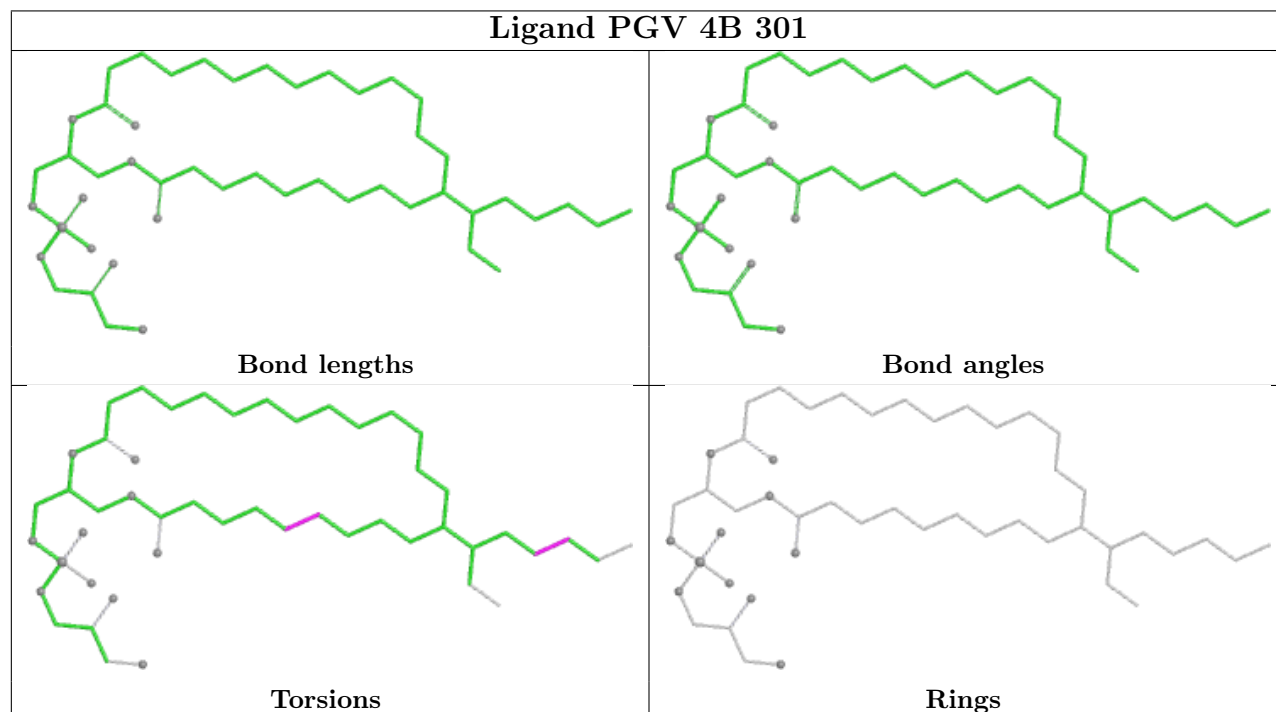
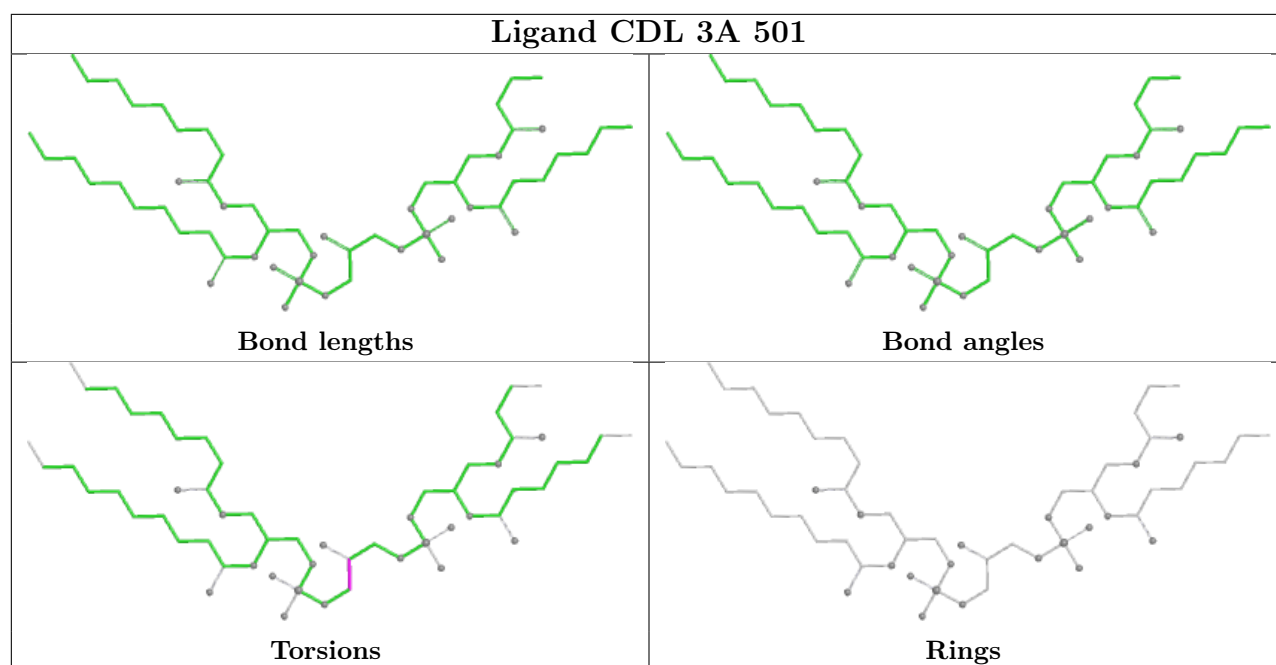


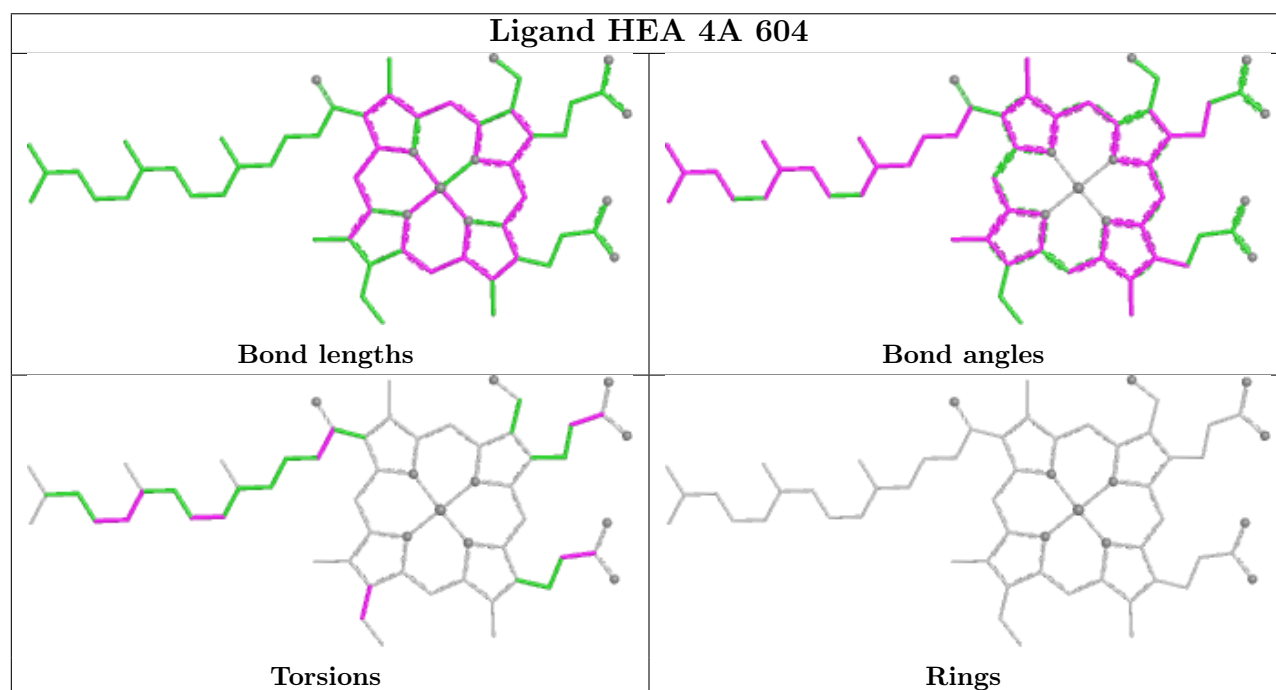
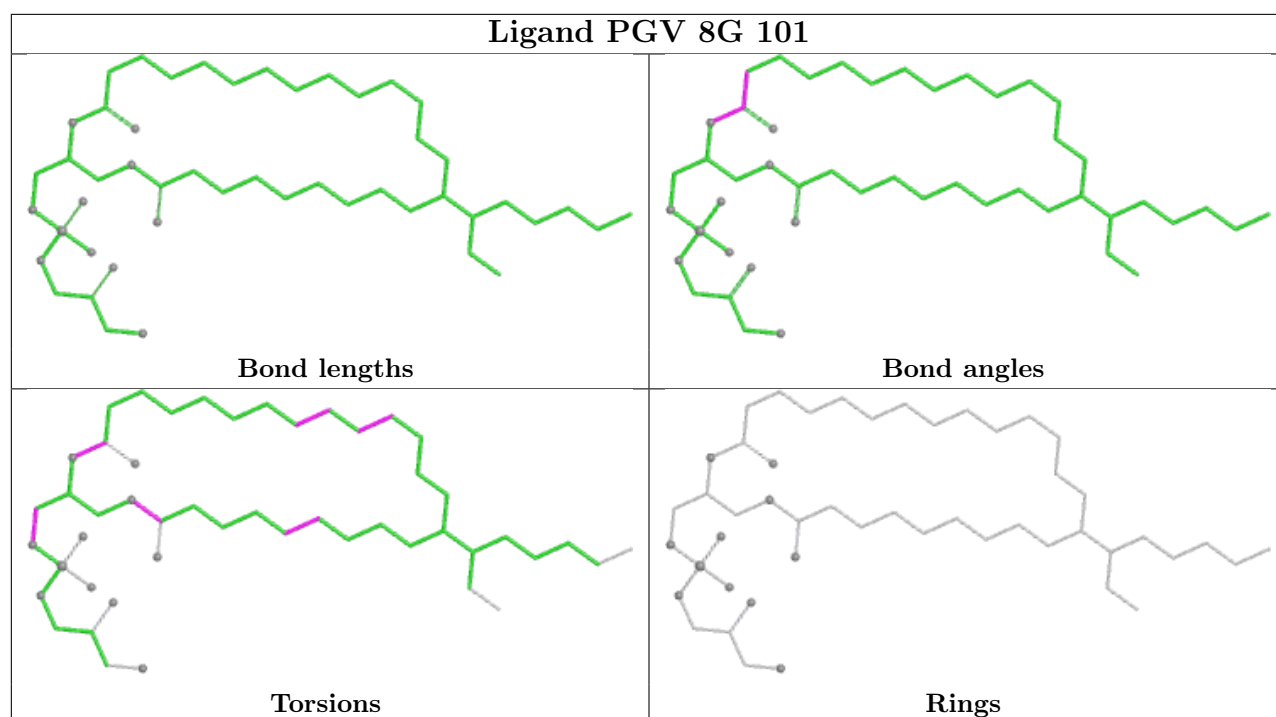


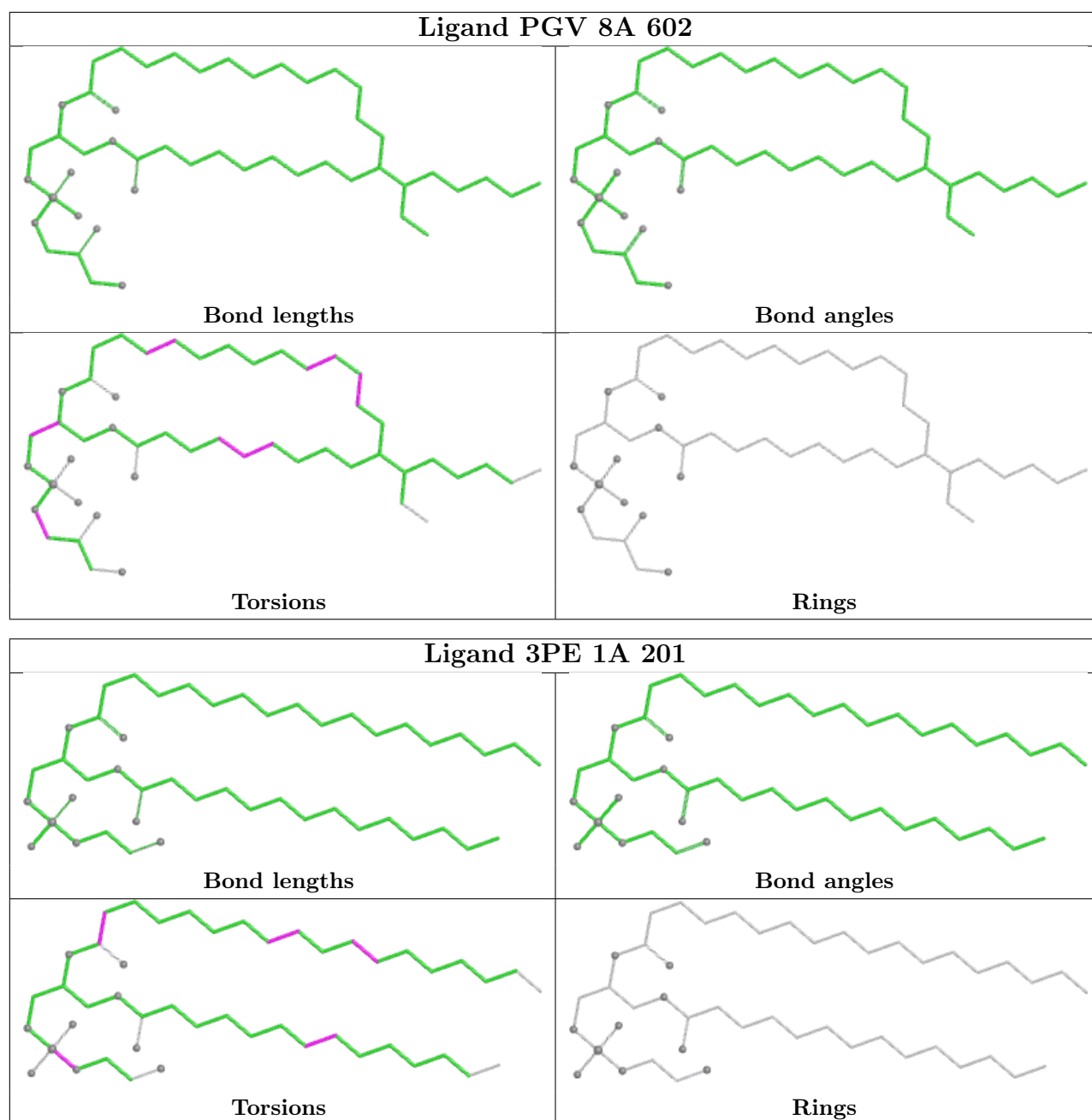


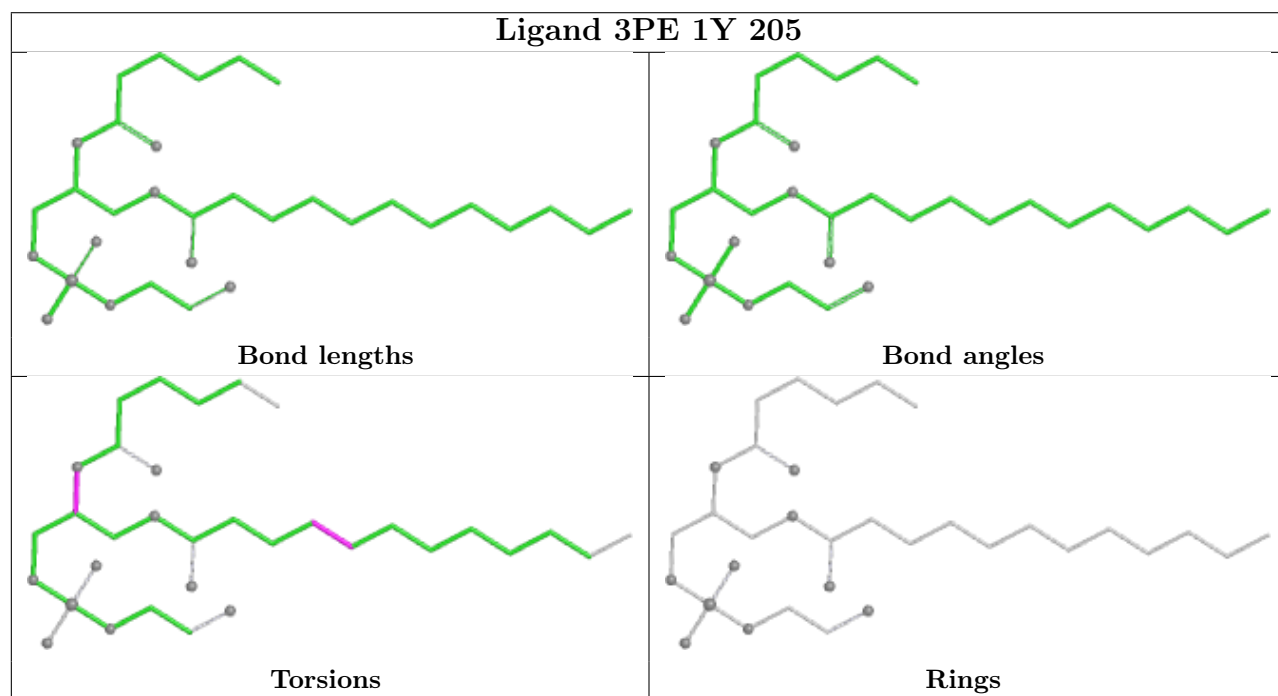
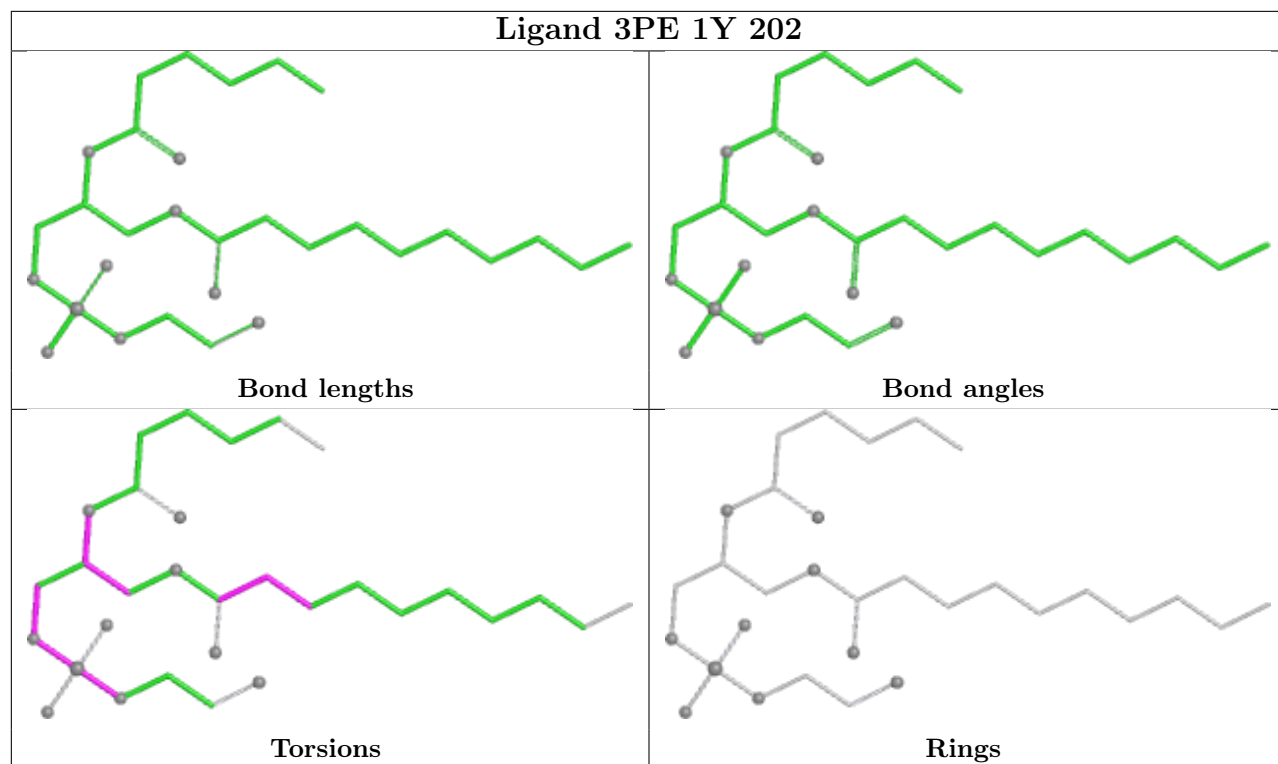




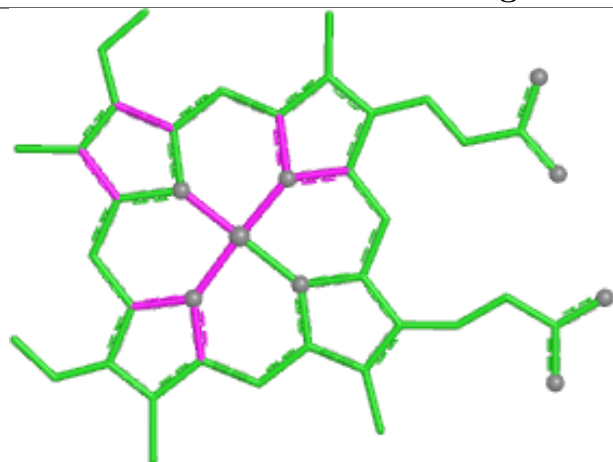




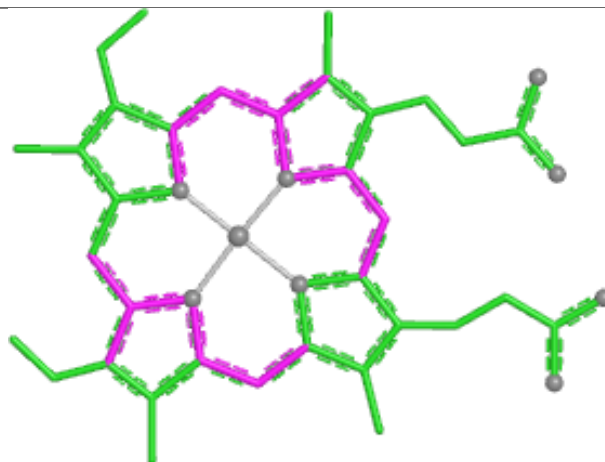




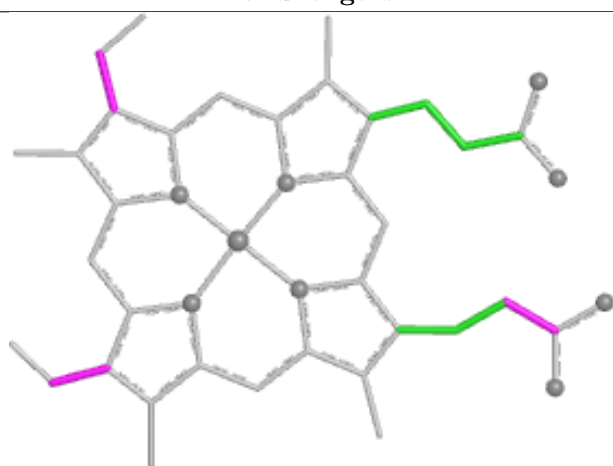
Ligand HEM 3C 502



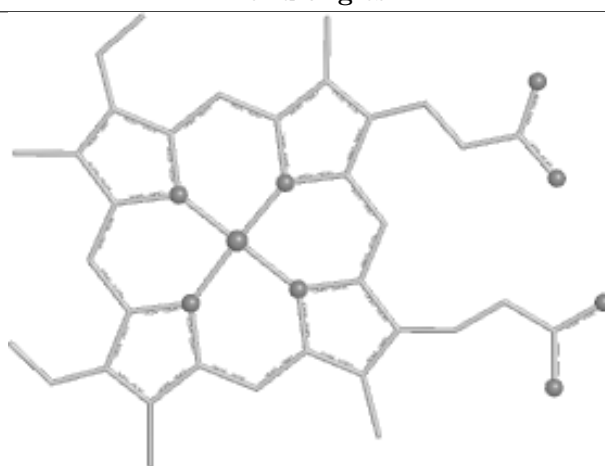
Bond lengths



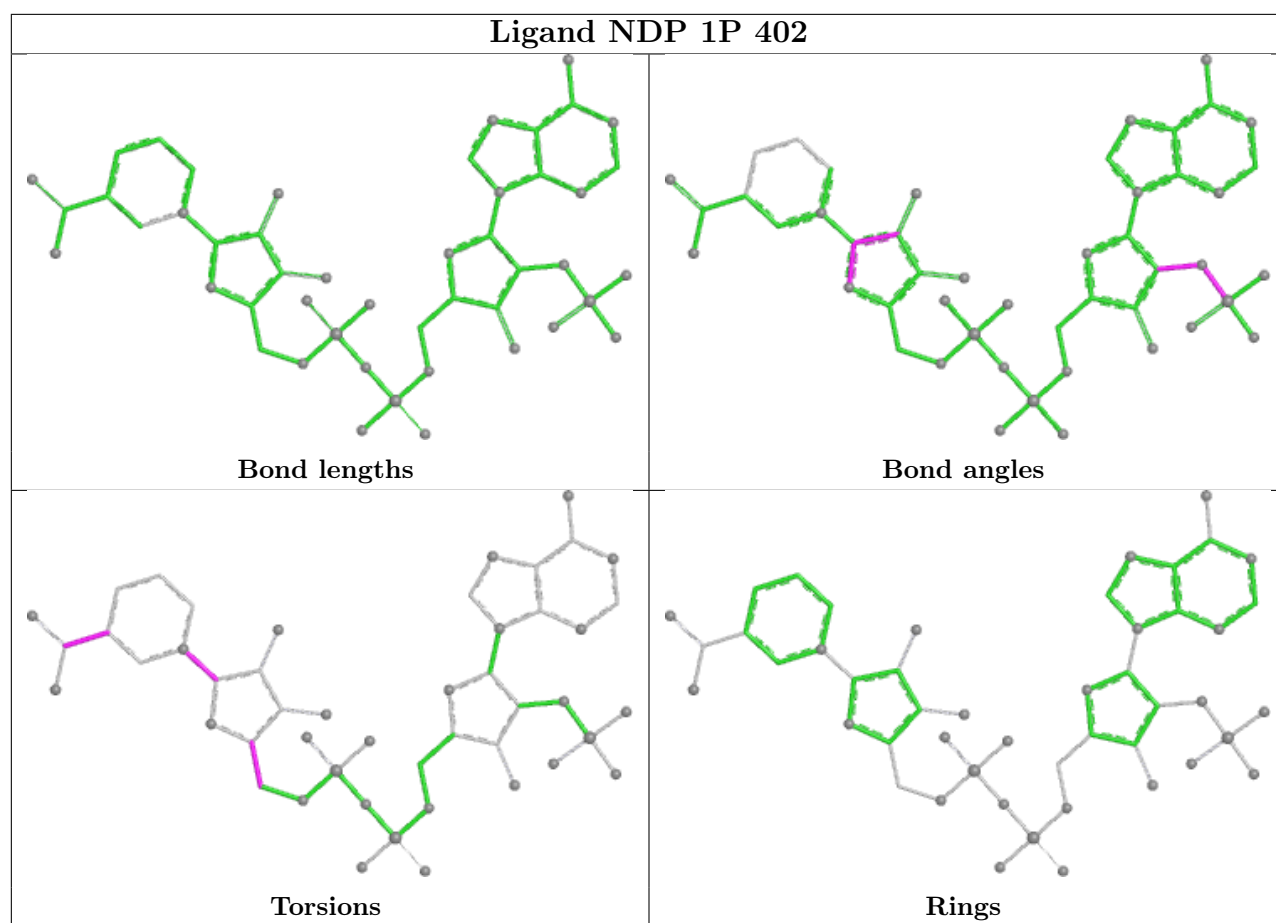
Bond angles



Torsions



Rings



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	3V	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3V	49:VAL	C	50:LEU	N	1.69
1	3V	48:SER	C	49:VAL	N	1.19

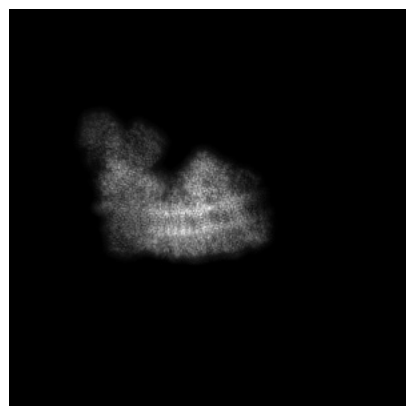
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42227. These allow visual inspection of the internal detail of the map and identification of artifacts.

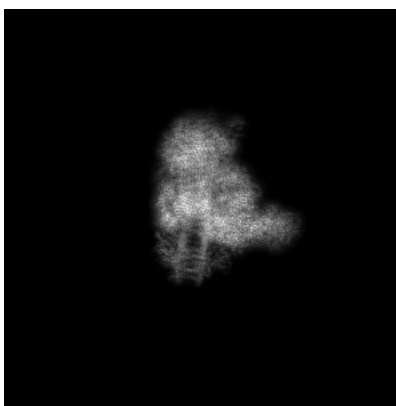
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

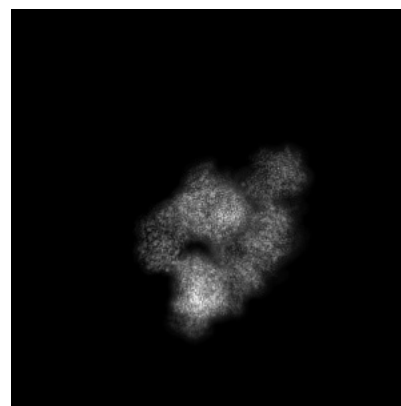
6.1.1 Primary map



X

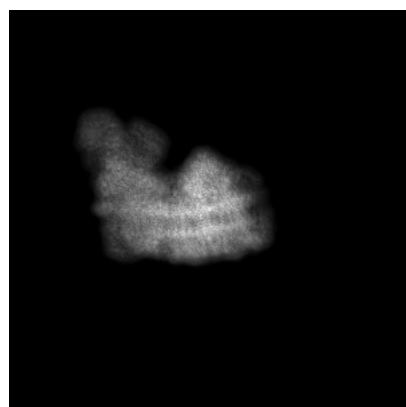


Y

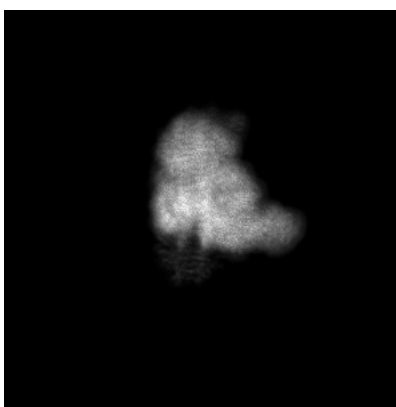


Z

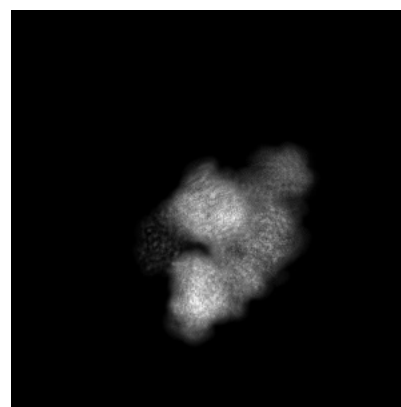
6.1.2 Raw map



X



Y

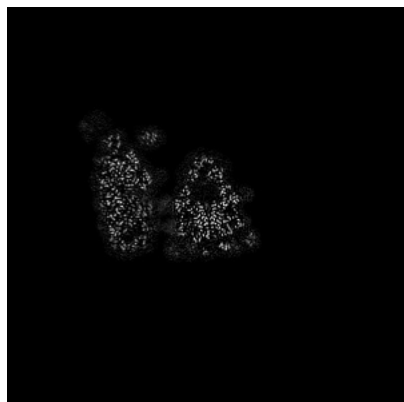


Z

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

6.2 Central slices [i](#)

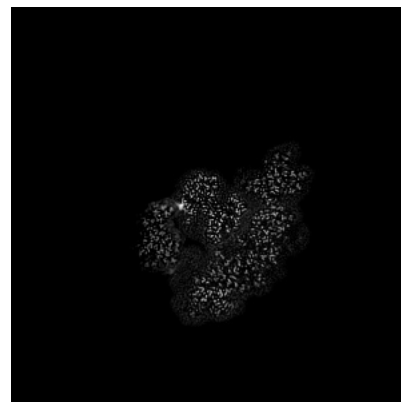
6.2.1 Primary map



X Index: 275

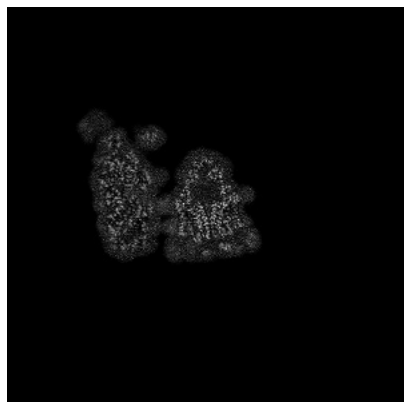


Y Index: 275

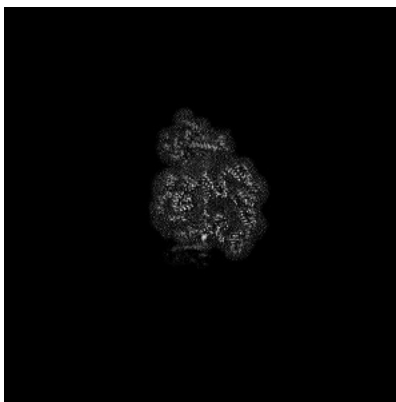


Z Index: 275

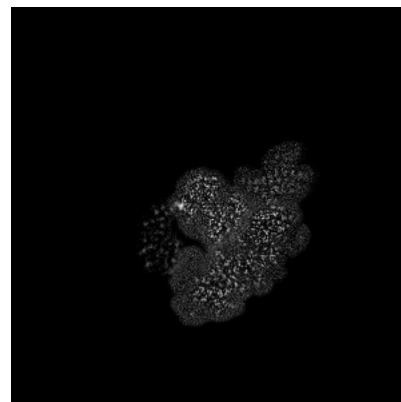
6.2.2 Raw map



X Index: 275



Y Index: 275

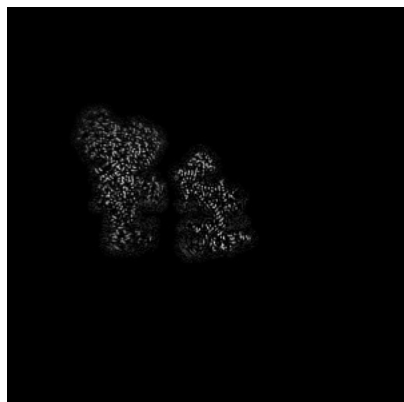


Z Index: 275

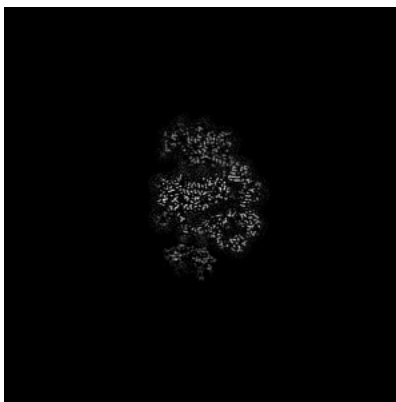
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

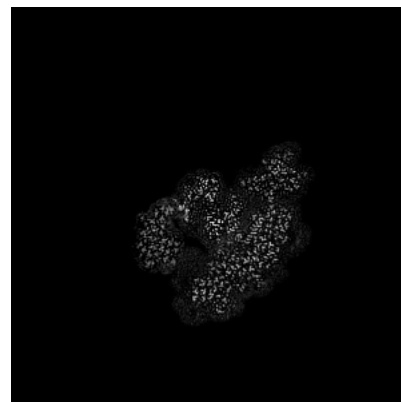
6.3.1 Primary map



X Index: 256

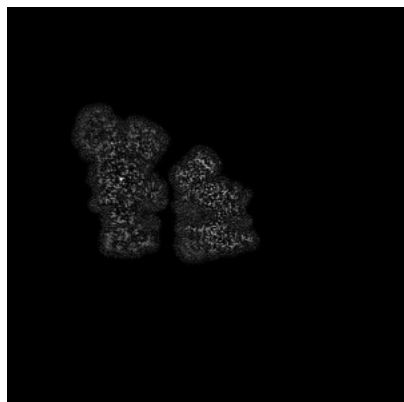


Y Index: 264

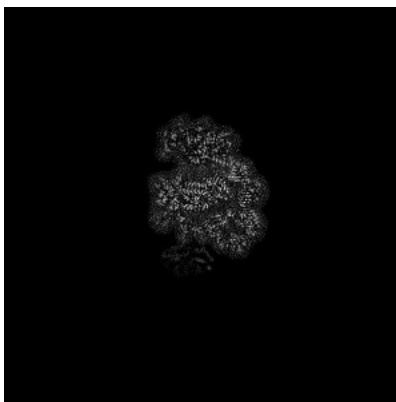


Z Index: 272

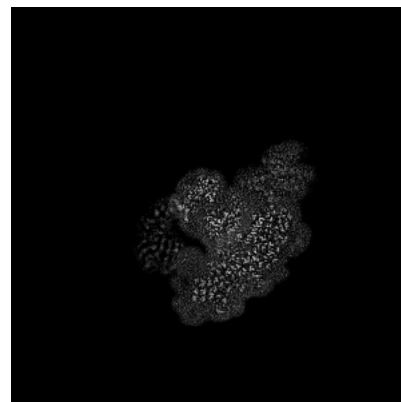
6.3.2 Raw map



X Index: 260



Y Index: 264

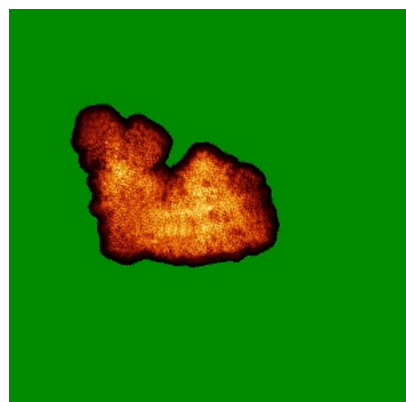


Z Index: 272

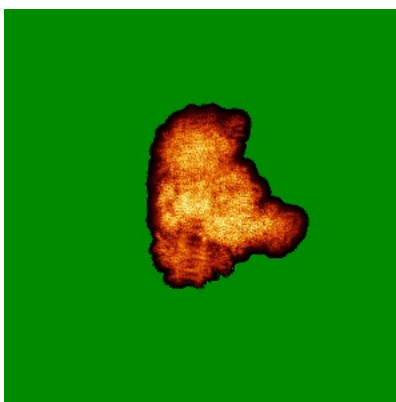
The images above show the largest variance slices of the map in three orthogonal directions.

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

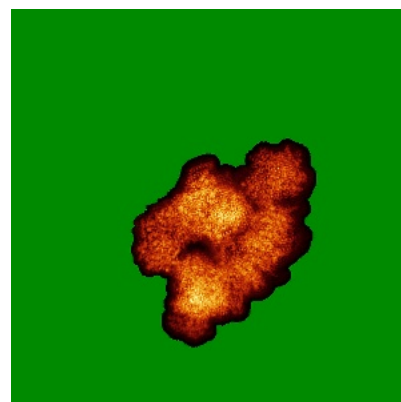
6.4.1 Primary map



X

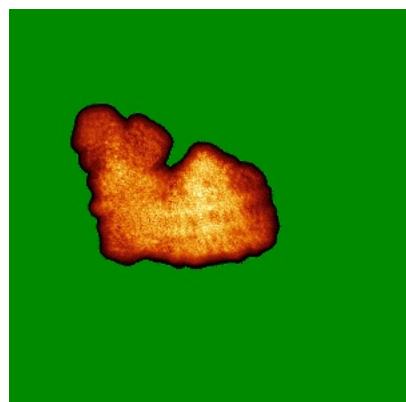


Y

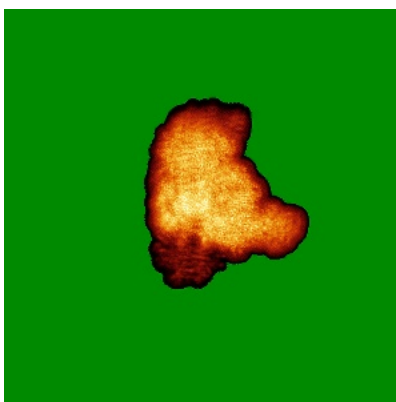


Z

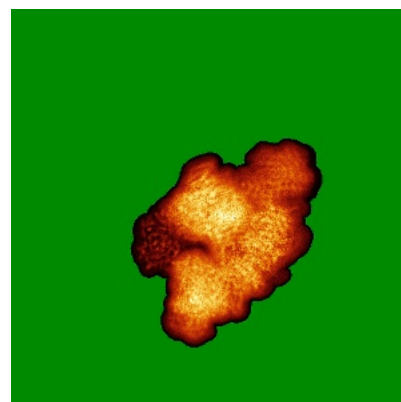
6.4.2 Raw map



X



Y

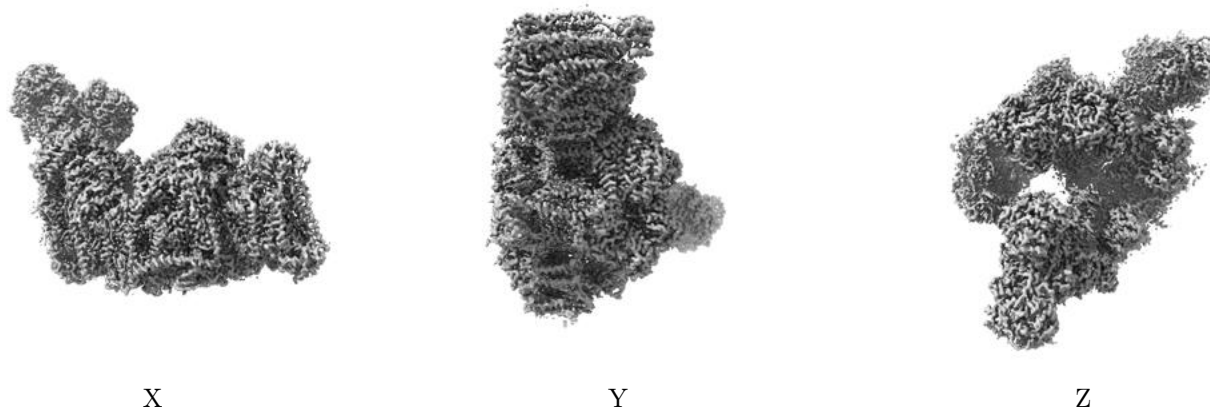


Z

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.

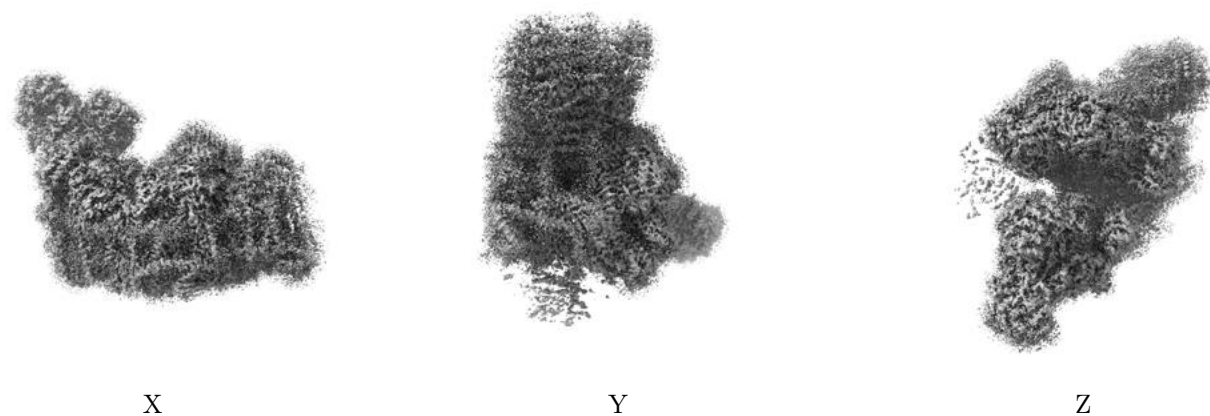
6.5 Orthogonal surface views [i](#)

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.

6.5.2 Raw map



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

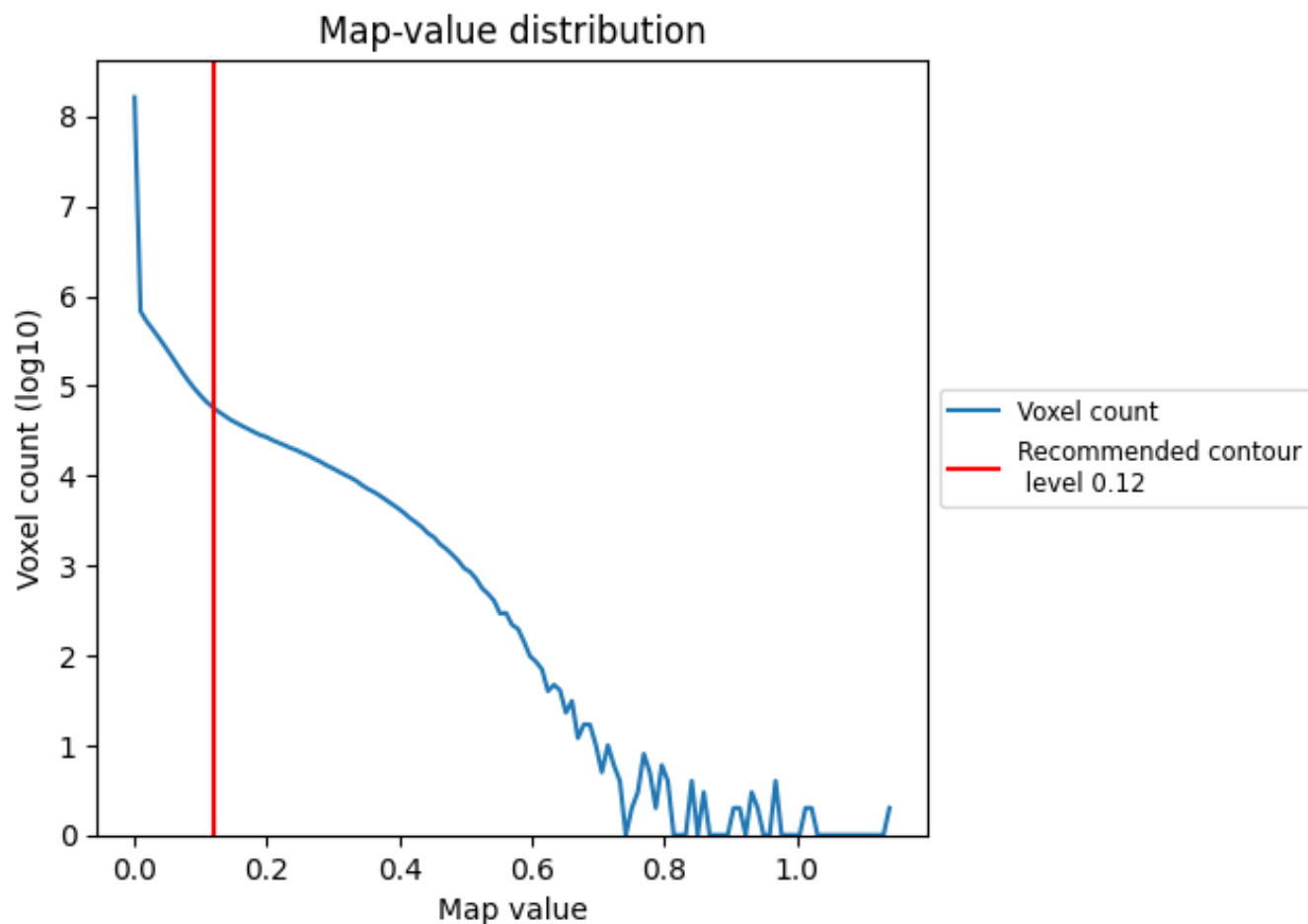
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

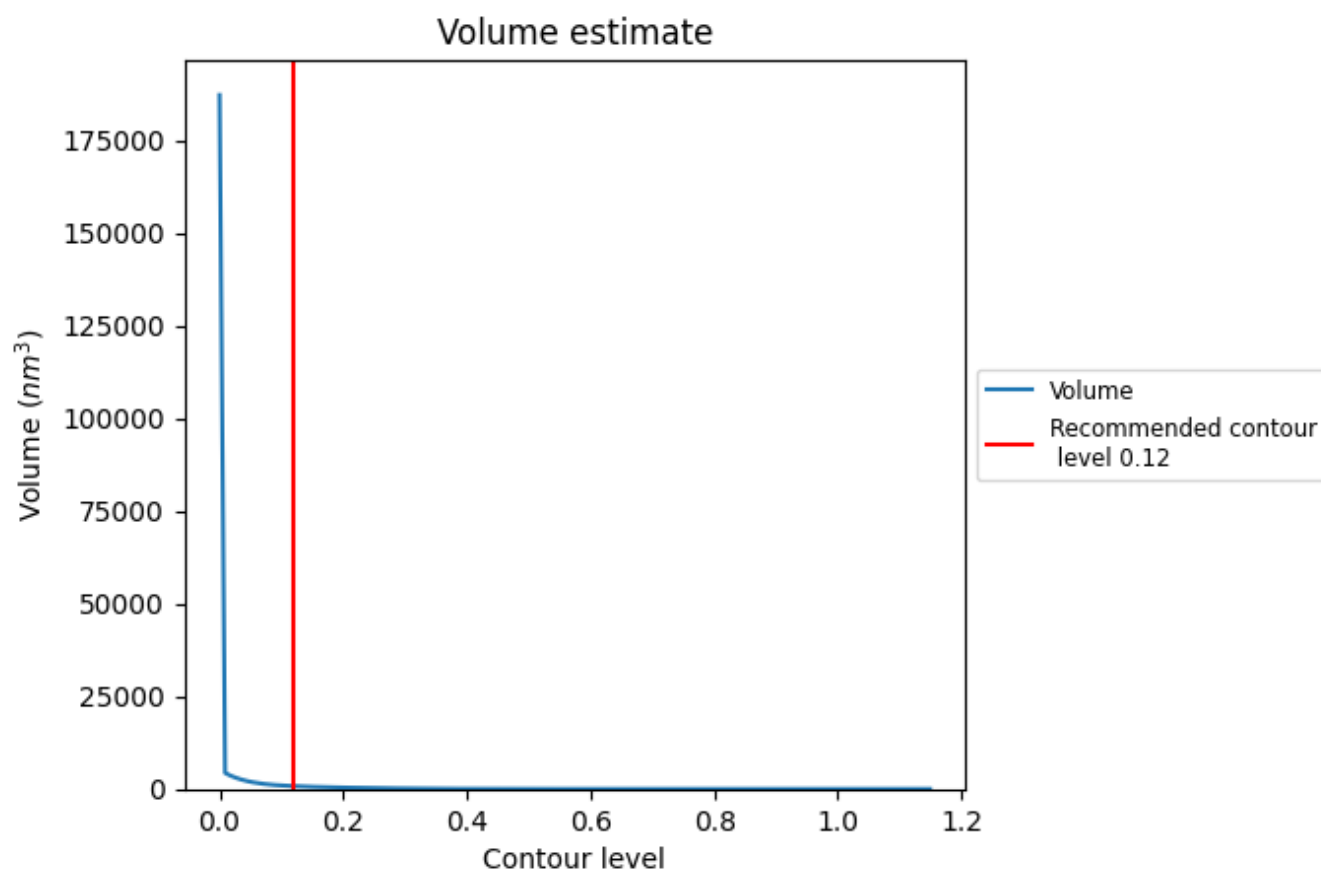
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

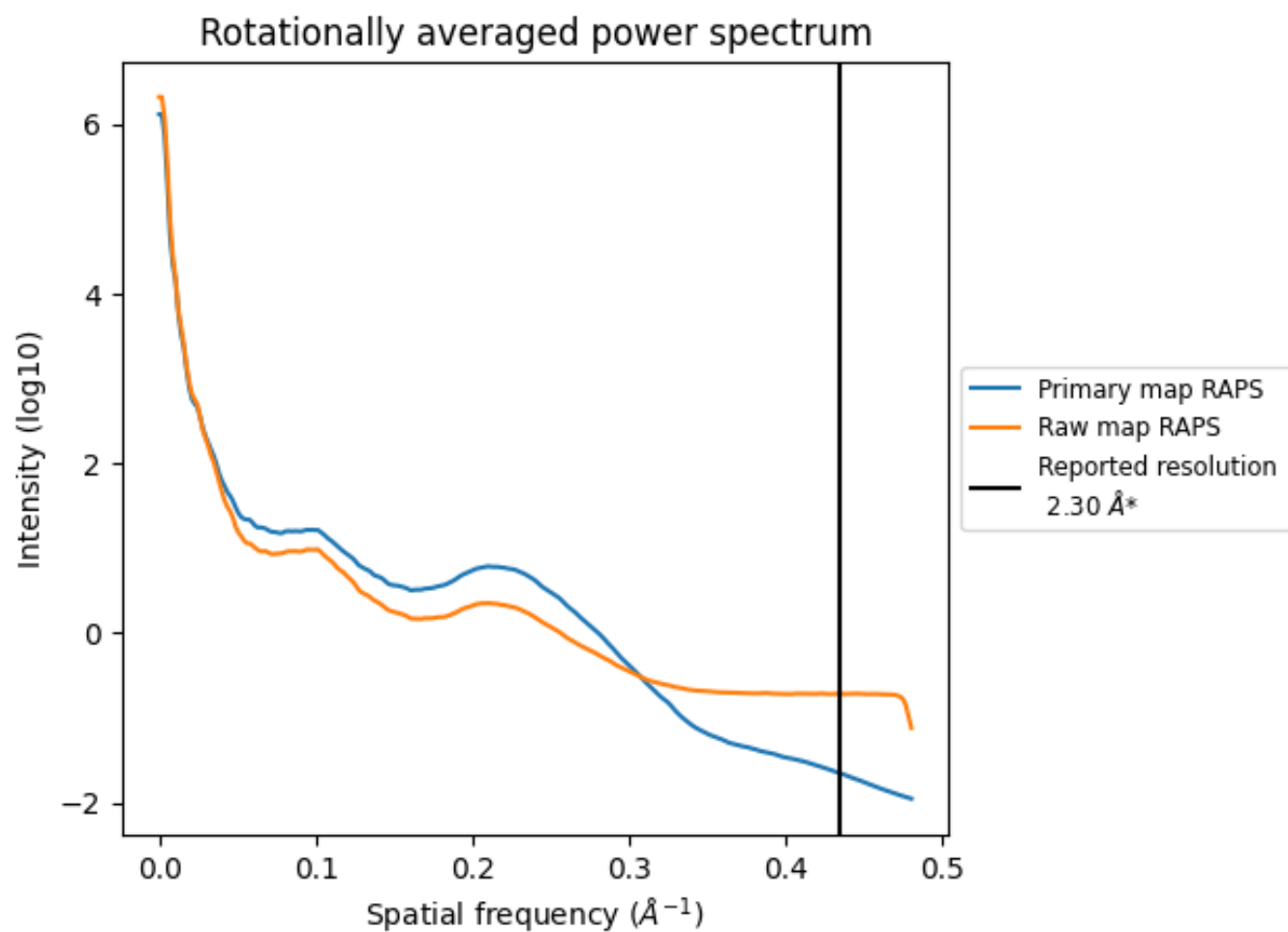
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 771 nm^3 ; this corresponds to an approximate mass of 696 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 ⓘ

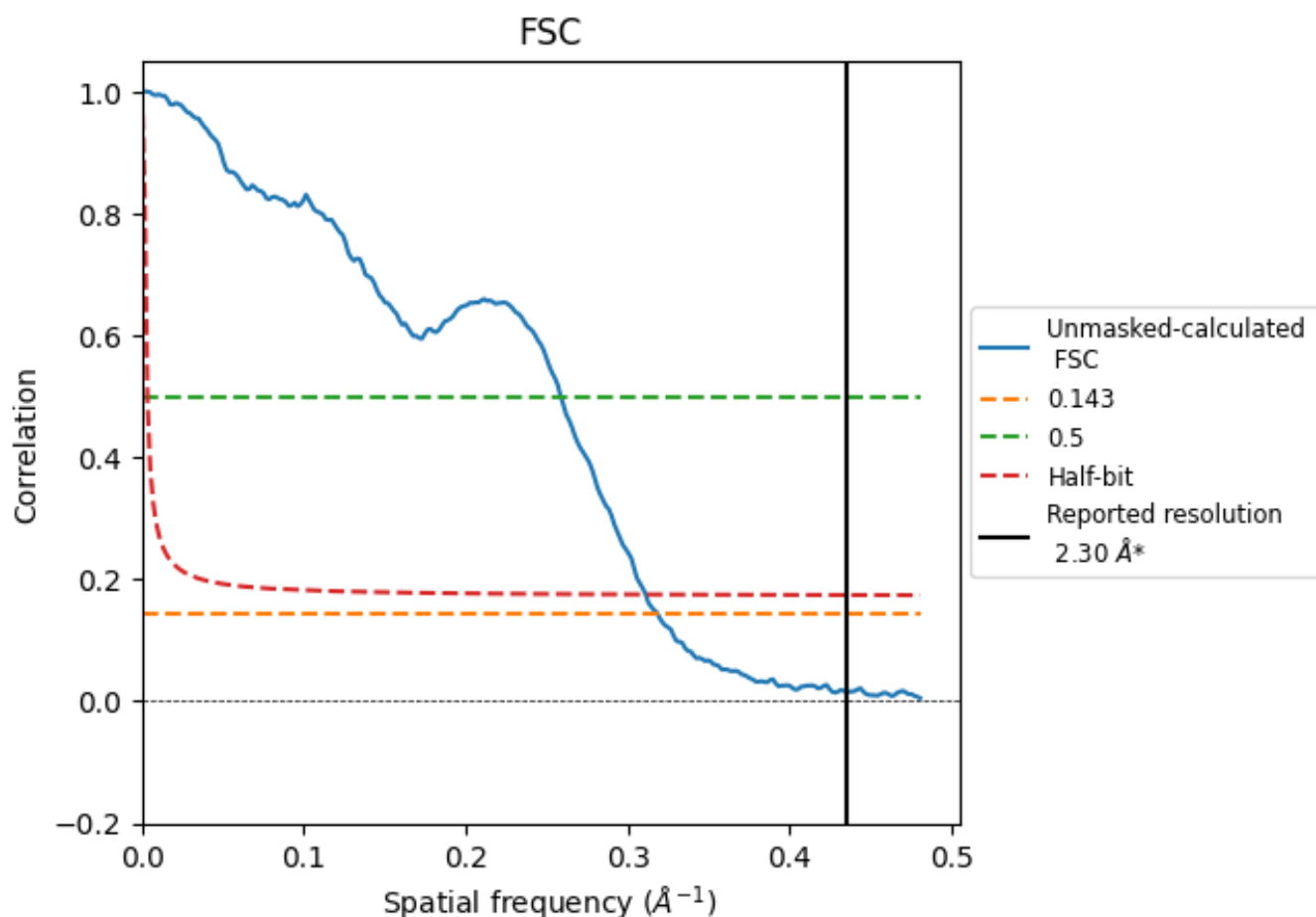


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.435 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

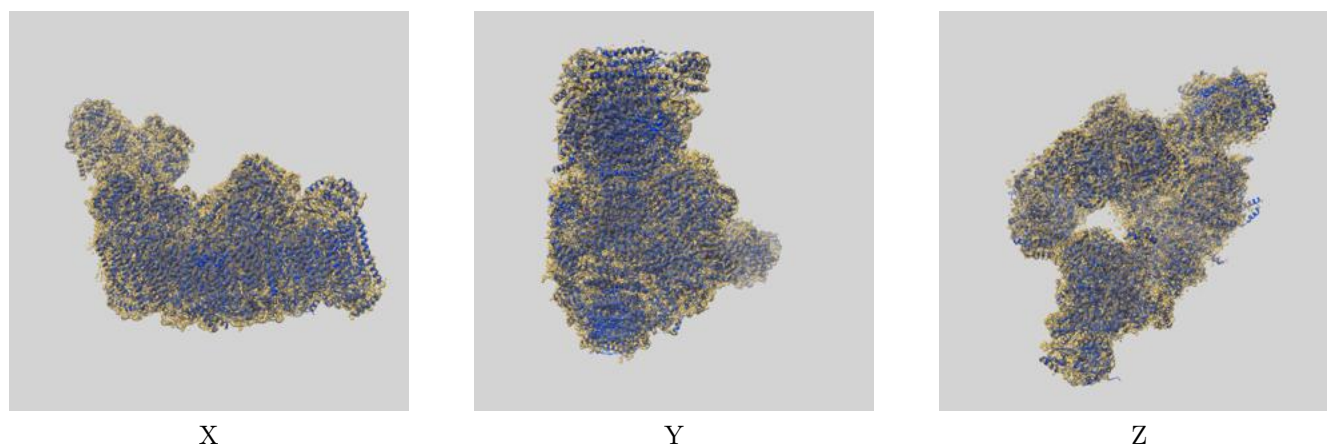
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	3.86	3.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.14 differs from the reported value 2.3 by more than 10 %

9 Map-model fit [i](#)

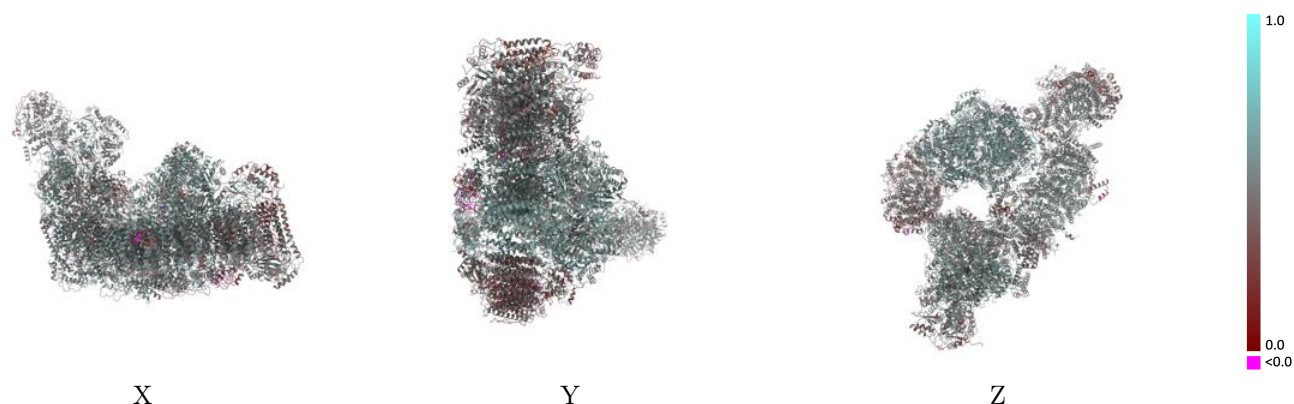
This section contains information regarding the fit between EMDB map EMD-42227 and PDB model 8UGJ. Per-residue inclusion information can be found in section 3 on page 38.

9.1 Map-model overlay [i](#)



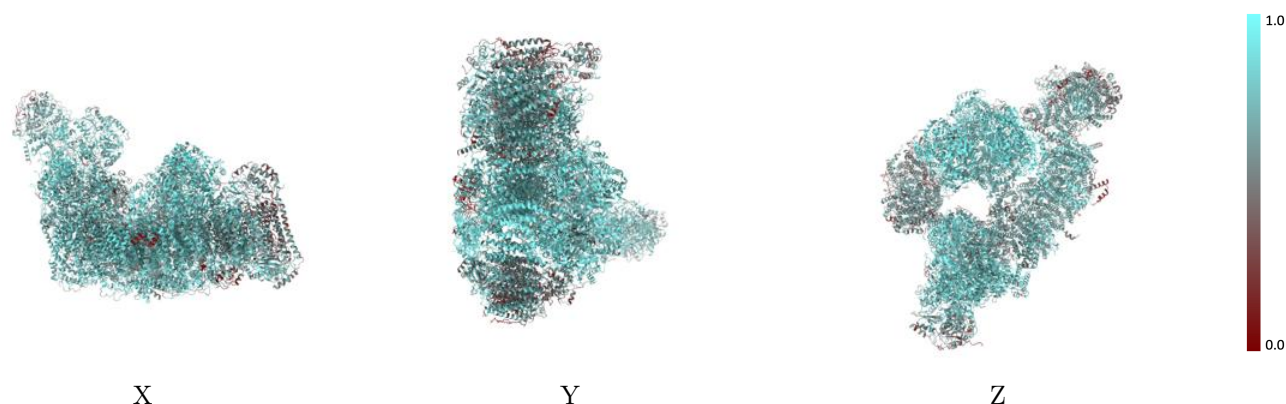
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



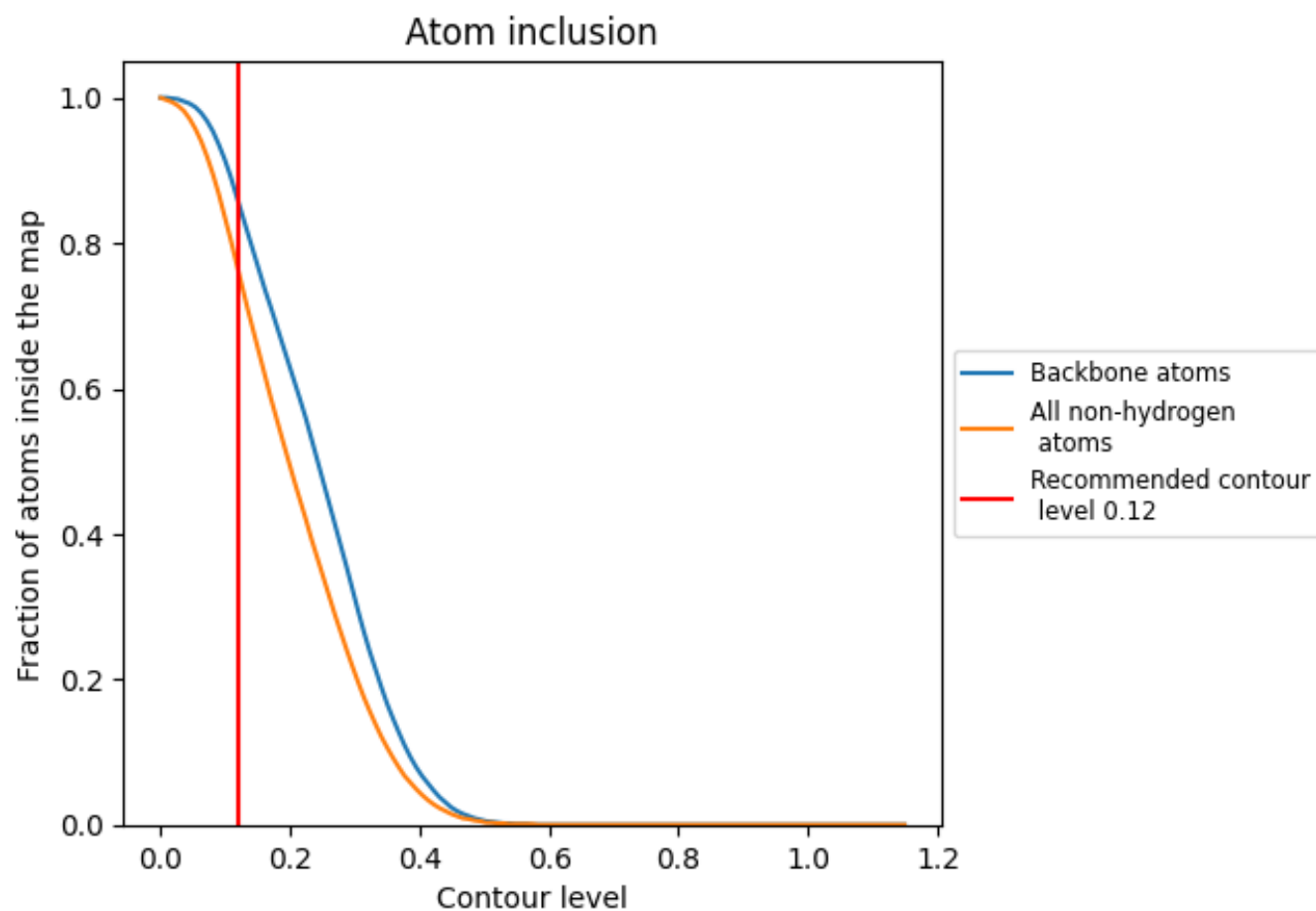
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 76% 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	 0.7620	 0.4950
1A	 0.6590	 0.4580
1B	 0.8660	 0.5350
1C	 0.8720	 0.5560
1D	 0.8450	 0.5410
1E	 0.6430	 0.4590
1F	 0.6550	 0.4660
1G	 0.8050	 0.5150
1H	 0.8060	 0.5140
1I	 0.8950	 0.5560
1J	 0.6710	 0.4620
1K	 0.7730	 0.5060
1L	 0.8300	 0.5200
1M	 0.8490	 0.5390
1N	 0.8340	 0.5390
1O	 0.7540	 0.4680
1P	 0.7610	 0.4890
1Q	 0.7830	 0.5130
1R	 0.8030	 0.5350
1S	 0.7300	 0.4740
1T	 0.5330	 0.3490
1U	 0.7690	 0.4940
1V	 0.7410	 0.4990
1W	 0.8070	 0.5110
1X	 0.7450	 0.5010
1Y	 0.7760	 0.4830
1Z	 0.7800	 0.5210
1a	 0.8400	 0.5270
1b	 0.7490	 0.4940
1c	 0.7170	 0.4900
1d	 0.7770	 0.5180
1e	 0.7480	 0.5190
1f	 0.6950	 0.4990
1g	 0.7700	 0.5060
1h	 0.7590	 0.5160



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Chain	Atom inclusion	Q-score
1i	 0.5600	 0.4240
1j	 0.6760	 0.4540
1k	 0.6750	 0.4500
1l	 0.8060	 0.5080
1m	 0.8060	 0.5160
1n	 0.8200	 0.5110
1o	 0.7010	 0.4450
1p	 0.7580	 0.5020
1q	 0.7880	 0.5240
1r	 0.8190	 0.5450
1s	 0.6280	 0.4670
3A	 0.8560	 0.5540
3B	 0.8650	 0.5550
3C	 0.9140	 0.5770
3D	 0.9080	 0.5710
3E	 0.5160	 0.3660
3F	 0.8710	 0.5680
3G	 0.8490	 0.5510
3H	 0.7930	 0.5240
3I	 0.4830	 0.4250
3J	 0.8800	 0.5130
3N	 0.9010	 0.5680
3O	 0.8710	 0.5560
3P	 0.9170	 0.5790
3Q	 0.9170	 0.5760
3R	 0.5040	 0.3410
3S	 0.8830	 0.5740
3T	 0.9110	 0.5600
3U	 0.8120	 0.5130
3V	 0.7290	 0.5270
3W	 0.9180	 0.5770
3X	 0.8590	 0.5500
3Y	 0.8180	 0.5350
4A	 0.7670	 0.4960
4B	 0.6290	 0.4440
4C	 0.6810	 0.4580
4D	 0.5470	 0.4050
4E	 0.5240	 0.3980
4F	 0.6500	 0.4690
4G	 0.5720	 0.4200
4H	 0.7020	 0.4510
4I	 0.5490	 0.4430

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Chain	Atom inclusion	Q-score
4J	 0.6570	 0.4500
4K	 0.4960	 0.4260
4L	 0.6710	 0.4540
4M	 0.5840	 0.4440
4N	 0.4840	 0.4220
8A	 0.7010	 0.4270
8B	 0.6480	 0.3960
8C	 0.6210	 0.3890
8D	 0.5890	 0.3680
8E	 0.5910	 0.3680
8F	 0.4800	 0.3690
8G	 0.5780	 0.3700
8H	 0.7180	 0.4000
8I	 0.7430	 0.4120
8J	 0.5710	 0.3790
8K	 0.6140	 0.3890
8L	 0.5740	 0.3870
8M	 0.6250	 0.3910
8N	 0.6560	 0.3990